

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID | Chemical_Name                     | CAS number | Therapeutic class      | Therapeutic<br>effect | Target type | Target names                                | Absorption<br>tissue | Protein<br>binding    | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail   |
|-----------------------------------|----------------|-----------|-----------------------------------|------------|------------------------|-----------------------|-------------|---|----------------------|-----------------------|-----------------|--|---|
| 3712 / 3716                       | A03            | Prestw-1  | Azaguanine-8                      | 134-58-7   | Oncology               | Antineoplastic        |             |   |                      |                       |                 | Pharmacological<br>tool                                  |   |
| 3712 / 3716                       | A05            | Prestw-2  | Allantoin                         | 97-59-6    | Dermatology            | Antipsoriatic         |             |   |                      |                       |                 |  |   |
| 3712 / 3716                       | A07            | Prestw-3  | Acetazolamide                     | 59-66-5    | Metabolism             | Anticonvulsant        | Enzyme      | Carbonic anhydrase                          | GI tract             | Carbonic<br>anhydrase | Yes             |  |   |
| 3712 / 3716                       | A09            | Prestw-4  | Metformin hydrochloride           | 1115-70-4  | Endocrinology          | Anorectic             |             |   | GI tract             | Plasmatic<br>proteins | Yes             | New therapeutic<br>use                                   | Potential<br>anticancer<br>agent  |
| 3712 / 3716                       | A11            | Prestw-5  | Atracurium besylate               | 64228-81-5 | Neuromuscular          | Curarizing            |             |   |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Quaternary<br>ammonium  |
| 3712 / 3716                       | A13            | Prestw-6  | Isoflupredone acetate             | 338-98-7   | Endocrinology          | Anti-inflammatory     |             |   |                      |                       |                 |  |   |
| 3712 / 3716                       | A15            | Prestw-7  | Amiloride hydrochloride dihydrate | 17440-83-4 | Metabolism             | Antihypertensive      | LGIC        | Amiloride-sensitive<br>sodium channel, ENaC | GI tract             |                       | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Potassium-<br>sparing agent   |
| 3712 / 3716                       | A17            | Prestw-8  | Amprolium hydrochloride           | 137-88-2   | Infectiology           | Anticoccidial         |             |   |                      |                       |                 | Veterinary use   | Poultry   |
| 3712 / 3716                       | A19            | Prestw-9  | Hydrochlorothiazide               | 58-93-5    | Metabolism             | Antihypertensive      | Carrier     | Solute carrier family 12<br>member 3        | GI tract             | Plasmatic<br>proteins | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Low-ceiling<br>diuretic   |
| 3712 / 3716                       | A21            | Prestw-10 | Sulfaguanidine                    | 57-67-0    | Infectiology           | Antibacterial         |             |   |                      |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Sulfonamide   |
| 3712 / 3716                       | C03            | Prestw-11 | Meticrane                         | 1084-65-7  | Metabolism             | Antihypertensive      |             |   |                      |                       |                 | Therapeutic<br>classification<br>(according ATC<br>code) | Low-ceiling<br>diuretic   |
| 3712 / 3716                       | C05            | Prestw-12 | Benzonatate                       | 104-31-4   | Neuromuscular          | Antitussive           |             |   |                      |                       | Yes             |  |   |
| 3712 / 3716                       | C07            | Prestw-13 | Hydroflumethiazide                | 135-09-1   | Metabolism             | Antihypertensive      |             |   | GI tract             |                       | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Low-ceiling<br>diuretic   |
| 3712 / 3716                       | C09            | Prestw-14 | Sulfacetamide sodic hydrate       | 6209-17-2  | Dermatology            | Antibacterial         |             |   | Eye                  |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Sulfonamide   |
| 3712 / 3716                       | C11            | Prestw-15 | Heptaminol hydrochloride          | 543-15-7   | Cardiovascular         | Analeptic             |             |   |                      |                       |                 |  |   |
| 3712 / 3716                       | C13            | Prestw-16 | Sulfathiazole                     | 72-14-0    | Infectiology           | Antibacterial         |             |   |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Short-acting<br>sulfonamide   |
| 3712 / 3716                       | C15            | Prestw-17 | Levodopa                          | 59-92-7    | Central Nervous System | Antiparkinsonian      |             |   | Jejunum              | Plasmatic<br>proteins | Yes             | Therapeutic use  | Association with<br>a peripheral<br>DOPA<br>decarboxylase<br>inhibitor (DDCI) |
| 3712 / 3716                       | C17            | Prestw-18 | Idoxuridine                       | 54-42-2    | Infectiology           | Antiviral             |             |   |                      |                       | Yes             |  |   |
| 3712 / 3716                       | C19            | Prestw-19 | Captopril                         | 62571-86-2 | Cardiovascular         | Antihypertensive      | Enzyme      | Angiotensin-converting<br>enzyme (ACE)      | GI tract             | Albumin               | Yes             |  |   |
| 3712 / 3716                       | C21            | Prestw-20 | Minoxidil                         | 38304-91-5 | Cardiovascular         | Anti-alopecia         |             |   | GI tract, Skin       | Plasmatic<br>proteins | Yes             | Administration route                                     | Topical use for<br>hair growth  |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID | Chemical_Name                     | CAS number | Therapeutic class      | Therapeutic<br>effect | Target type | Target names                                | Absorption<br>tissue | Protein<br>binding    | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail  |
|-----------------------------------|----------------|-----------|-----------------------------------|------------|------------------------|-----------------------|-------------|---|----------------------|-----------------------|-----------------|--|--|
| 3712 / 3716                       | E03            | Prestw-21 | Sulfaphenazole                    | 526-08-9   | Infectiology           | Antibacterial         |             |   |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Long-acting<br>sulfonamide   |
| 3712 / 3716                       | E05            | Prestw-22 | Panthenol (D)                     | 81-13-0    | Metabolism             | Anti-alopecia         |             |   | GI tract, Skin       |                       | Yes             | Chemical<br>classification                               | Vitamin B5<br>analog   |
| 3712 / 3716                       | E07            | Prestw-23 | Sulfadiazine                      | 68-35-9    | Infectiology           | Antibacterial         |             |   |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Intermediate-<br>acting<br>sulfonamide                               |
| 3712 / 3716                       | E09            | Prestw-24 | Norethynodrel                     | 68-23-5    | Endocrinology          | Contraceptive         |             |   |                      |                       | Yes             |  |  |
| 3712 / 3716                       | E11            | Prestw-25 | Thiamphenicol                     | 15318-45-3 | Infectiology           | Antibacterial         |             |   |                      | Plasmatic<br>proteins |                 | Chemical<br>classification<br>(according ATC<br>code)    | Amphenicol   |
| 3712 / 3716                       | E13            | Prestw-26 | Cimetidine                        | 51481-61-9 | Gastroenterology       | Antiulcer             | GPCR        | Histamine H2 receptor                       | GI tract             | Plasmatic<br>proteins | Yes             | New therapeutic<br>use                                   | Potential<br>anticancer<br>agent                                     |
| 3712 / 3716                       | E15            | Prestw-27 | Doxylamine succinate              | 562-10-7   | Allergology            | Anti-anorectic        | GPCR        | Histamine H1 receptor                       | GI tract             |                       | Yes             | Therapeutic use  | Antiemetic   |
| 3712 / 3716                       | E17            | Prestw-28 | Ethambutol dihydrochloride        | 1070-11-7  | Infectiology           | Antibacterial         |             |   | GI tract             |                       | Yes             |  |  |
| 3712 / 3716                       | E19            | Prestw-29 | Antipyrine                        | 60-80-0    | Central Nervous System | Analgesic             |             |   | GI tract             | Plasmatic<br>proteins |                 |  |  |
| 3712 / 3716                       | E21            | Prestw-30 | Antipyrine, 4-hydroxy             | 1672-63-5  | Metabolism             |                       |             |   |                      |                       |                 | Pharmacokinetics   | Active<br>metabolite of<br>Antipyrine (or<br>Phenazone)<br>Prestw-29 |
| 3712 / 3716                       | G03            | Prestw-31 | Chloramphenicol                   | 56-75-7    | Infectiology           | Antibacterial         |             |   |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Amphenicol   |
| 3712 / 3716                       | G05            | Prestw-32 | Epirizole                         | 18694-40-1 | Central Nervous System | Analgesic             |             |   |                      |                       |                 | Japan approved   |  |
| 3712 / 3716                       | G07            | Prestw-33 | Diprophylline                     | 479-18-5   | Cardiovascular         | Analeptic             |             |   |                      |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Xanthine   |
| 3712 / 3716                       | G09            | Prestw-34 | Triamterene                       | 396-01-0   | Metabolism             | Antihypertensive      | LGIC        | Amiloride-sensitive<br>sodium channel, ENaC | GI tract             | Plasmatic<br>proteins | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Potassium-<br>sparing agent  |
| 3712 / 3716                       | G11            | Prestw-35 | Dapsone                           | 80-08-0    | Infectiology           | Antibacterial         |             |   | GI tract             |                       | Yes             |  |  |
| 3712 / 3716                       | G13            | Prestw-36 | Troleandomycin                    | 2751-09-9  | Infectiology           | Antibacterial         |             |   |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Macrolide  |
| 3712 / 3716                       | G15            | Prestw-37 | Pyrimethamine                     | 58-14-0    | Infectiology           | Antimalarial          |             |   | GI tract             | Plasmatic<br>proteins | Yes             |  |  |
| 3712 / 3716                       | G17            | Prestw-38 | Hexamethonium dibromide dihydrate | 55-97-0    | Cardiovascular         | Antihypertensive      |             |   |                      |                       |                 |  |  |
| 3712 / 3716                       | G19            | Prestw-39 | Diflunisal                        | 22494-42-4 | Central Nervous System | Analgesic             | Enzyme      | Cyclooxygenase                              | GI tract             | Plasmatic<br>proteins | Yes             |  |  |
| 3712 / 3716                       | G21            | Prestw-40 | Niclosamide                       | 50-65-7    | Infectiology           | Anthelmintic          |             |   | GI tract             |                       | Yes             | New therapeutic<br>use                                   | Potential<br>anticancer<br>agent                                     |
| 3712 / 3716                       | I03            | Prestw-41 | Procaine hydrochloride            | 51-05-8    | Neuromuscular          | Local anesthetic      | Ion channel | Voltage-gated sodium<br>channel             |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Esters of<br>aminobenzoic<br>acid                                    |

| ICCB-L Plate (10 mM / 3.33 mM) | ICCB-L Well | Vendor_ID   | Chemical_Name                 | CAS number | Therapeutic class      | Therapeutic effect             | Target type            | Target names                          | Absorption tissue | Protein binding    | FDA approved | Additional info type                            | Additional info detail                                      |
|--------------------------------|-------------|-------------|-------------------------------|------------|------------------------|--------------------------------|------------------------|---------------------------------------|-------------------|--------------------|--------------|---|---|
| 3712 / 3716                    | I05         | Prestw-42   | Moxisylyte hydrochloride      | 964-52-3   | Cardiovascular         | Erectile dysfunction treatment |                        |                                       | GI tract          |                    |              |   |   |
| 3712 / 3716                    | I07         | Prestw-43   | Betazole hydrochloride        | 138-92-1   | Gastroenterology       | Diagnostic                     | GPCR                   | Histamine H2 receptor                 |                   |                    | Yes          |   |   |
| 3712 / 3716                    | I09         | Prestw-44   | Isoxicam                      | 34552-84-6 | Central Nervous System | Analgesic                      |                        |                                       |                   |                    |              |   |   |
| 3712 / 3716                    | I11         | Prestw-45   | Naproxen                      | 22204-53-1 | Central Nervous System | Analgesic                      | Enzyme                 | Cyclooxygenase                        | GI tract          | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | NSAID   |
| 3712 / 3716                    | I13         | Prestw-46   | Naphazoline hydrochloride     | 550-99-2   | Cardiovascular         | Nasal Decongestant             |                        |                                       | Nose, GI tract    |                    | Yes          | Therapeutic classification (according ATC code) | Sympathomimetic   |
| 3712 / 3716                    | I15         | Prestw-47   | Ticlopidine hydrochloride     | 53885-35-1 | Hematology             | Anticoagulant                  | GPCR                   | Purinergic receptor P2Y12             | GI tract          |                    | Yes          |   |   |
| 3712 / 3716                    | I17         | Prestw-48   | Dicyclomine hydrochloride     | 67-92-5    | Gastroenterology       | Antispastic                    |                        |                                       | GI tract          |                    | Yes          | Chemical classification (according ATC code)    | Synthetic anticholinergic, esters with tertiary amino group |
| 3712 / 3716                    | I19         | Prestw-49   | Amyleine hydrochloride        | 532-59-2   | Neuromuscular          | Local anesthetic               | Ion channel            | Voltage-gated sodium channel          |                   |                    |              | Chemical classification (according ATC code)    | Esters of benzoic acid                                      |
| 3712 / 3716                    | I21         | Prestw-50   | Lidocaine hydrochloride       | 73-78-9    | Cardiovascular         | Antiarrhythmic                 | Ion channel            | Voltage-gated sodium channel          | GI tract, Musc    | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | Antiarrhythmic, class Ib                                    |
| 3712 / 3716                    | K03         | Prestw-1795 | Mupirocin                     | 12650-69-0 | Infectiology           |                                |                        |                                       |                   |                    | Yes          |   |   |
| 3712 / 3716                    | K05         | Prestw-52   | Carbamazepine                 | 298-46-4   | Central Nervous System | Analgesic                      | Ion channel            | Voltage-gated sodium channel          |                   | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Carboxamide derivatives                                     |
| 3712 / 3716                    | K07         | Prestw-53   | Triflupromazine hydrochloride | 1098-60-8  | Central Nervous System | Antiemetic                     |                        |                                       |                   |                    | Yes          | New therapeutic use                             | Potential antibacterial                                     |
| 3712 / 3716                    | K09         | Prestw-54   | Mefenamic acid                | 61-68-7    | Central Nervous System | Analgesic                      | Enzyme                 | Cyclooxygenase                        | GI tract          | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | NSAID   |
| 3712 / 3716                    | K11         | Prestw-55   | Acetohexamide                 | 968-81-0   | Endocrinology          | Antidiabetic                   | Transmembrane receptor | Sulfonylurea receptors K-ATP channels |                   |                    | Yes          | Chemical classification (according ATC code)    | Sulfonamide urea derivative                                 |
| 3712 / 3716                    | K13         | Prestw-56   | Sulpiride                     | 15676-16-1 | Central Nervous System | Antidepressant                 |                        |                                       |                   | Plasmatic proteins |              | Chemical classification (according ATC code)    | Benzamide   |
| 3712 / 3716                    | K15         | Prestw-57   | Benoxinate hydrochloride      | 5987-82-6  | Neuromuscular          | Local anesthetic               |                        |                                       | Eye               |                    | Yes          |   |   |
| 3712 / 3716                    | K17         | Prestw-58   | Oxethazaine                   | 126-27-2   | Neuromuscular          | Local anesthetic               |                        |                                       | GI tract          |                    |              |   |   |
| 3712 / 3716                    | K19         | Prestw-59   | Pheniramine maleate           | 132-20-7   | Allergology            | Antihistaminic                 | GPCR                   | Histamine H1 receptor                 | GI tract          |                    | Yes          | Chemical classification (according ATC code)    | Substituted alkylamine                                      |
| 3712 / 3716                    | K21         | Prestw-60   | Tolazoline hydrochloride      | 59-97-2    | Cardiovascular         | Vasodilator                    |                        |                                       |                   |                    | Yes          | Chemical classification (according ATC code)    | Imidazoline derivative                                      |
| 3712 / 3716                    | M03         | Prestw-61   | Morantel tartrate             | 26155-31-7 | Infectiology           | Anthelmintic                   |                        |                                       |                   |                    |              | Veterinary use                                  |   |

| ICCB-L Plate (10 mM / 3.33 mM) | ICCB-L Well | Vendor_ID | Chemical_Name                   | CAS number | Therapeutic class      | Therapeutic effect | Target type      | Target names                         | Absorption tissue | Protein binding    | FDA approved | Additional info type                            | Additional info detail                                  |
|--------------------------------|-------------|-----------|---------------------------------|------------|------------------------|--------------------|------------------|--------------------------------------|-------------------|--------------------|--------------|---|---|
| 3712 / 3716                    | M05         | Prestw-62 | Homatropine hydrobromide (R,S)  | 51-56-9    | Diagnostic             | Antispastic        |                  |                                      | Eye               |                    | Yes          | Therapeutic classification (according ATC code) | Anticholinergic   |
| 3712 / 3716                    | M07         | Prestw-63 | Nifedipine                      | 21829-25-4 | Cardiovascular         | Antianginal        | Ion channel      | Voltage-gated L-type calcium channel | GI tract          | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Dihydropyridine derivatives                             |
| 3712 / 3716                    | M09         | Prestw-64 | Chlorpromazine hydrochloride    | 69-09-0    | Cardiovascular         | Antiemetic         | GPCR             | Dopamine D2 receptor                 |                   | Albumin            | Yes          | Chemical classification (according ATC code)    | Phenothiazine derivative                                |
| 3712 / 3716                    | M11         | Prestw-65 | Diphenhydramine hydrochloride   | 147-24-0   | Allergology            | Antiemetic         | GPCR             | Histamine H1 receptor                |                   |                    | Yes          | Chemical classification (according ATC code)    | Aminoalkyl ether  |
| 3712 / 3716                    | M13         | Prestw-66 | Minaprine dihydrochloride       | 25953-17-7 | Central Nervous System | Anti-Alzheimer     |                  |                                      |                   |                    |              |   |   |
| 3712 / 3716                    | M15         | Prestw-67 | Miconazole                      | 22916-47-8 | Infectiology           | Antifungal         |                  |                                      |                   |                    | Yes          | Chemical classification (according ATC code)    | Imidazole derivative                                    |
| 3712 / 3716                    | M17         | Prestw-68 | Isoxsuprine hydrochloride       | 579-56-6   | Cardiovascular         | Vasodilator        |                  |                                      | GI tract          |                    |              |   |   |
| 3712 / 3716                    | M19         | Prestw-69 | Acebutolol hydrochloride        | 34381-68-5 | Cardiovascular         | Antianginal        | GPCR             | Adrenergic receptor beta-1           | GI tract          | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | Selective beta-blocking agent                           |
| 3712 / 3716                    | M21         | Prestw-70 | Tolnaftate                      | 2398-96-1  | Infectiology           | Antifungal         |                  |                                      | Skin              |                    |              |   |   |
| 3712 / 3716                    | O03         | Prestw-71 | Todralazine hydrochloride       | 3778-76-5  | Cardiovascular         | Antihypertensive   |                  |                                      |                   |                    |              |   |   |
| 3712 / 3716                    | O05         | Prestw-72 | Imipramine hydrochloride        | 113-52-0   | Central Nervous System | Antidepressant     |                  |                                      |                   | Plasmatic proteins | Yes          |   |   |
| 3712 / 3716                    | O07         | Prestw-73 | Sulindac                        | 38194-50-2 | Central Nervous System | Analgesic          | Enzyme           | Cyclooxygenase                       | GI tract          | Plasmatic proteins | Yes          | Mechanism                                       | Apoptosis inducer                                       |
| 3712 / 3716                    | O09         | Prestw-74 | Amitriptyline hydrochloride     | 549-18-8   | Central Nervous System | Antidepressant     |                  |                                      |                   | Plasmatic proteins | Yes          |   |   |
| 3712 / 3716                    | O11         | Prestw-75 | Adiphenine hydrochloride        | 50-42-0    | Neuromuscular          | Antispastic        |                  |                                      |                   |                    |              |   |   |
| 3712 / 3716                    | O13         | Prestw-76 | Dibucaine                       | 85-79-0    | Neuromuscular          | Local anesthetic   | Ion channel      | Voltage-gated sodium channel         | Skin              |                    | Yes          | Chemical classification (according ATC code)    | Amides  |
| 3712 / 3716                    | O15         | Prestw-77 | Prednisone                      | 53-03-2    | Dermatology            | Anti-inflammatory  | Nuclear receptor | Glucocorticoid receptor              |                   |                    | Yes          | Chemical classification (according ATC code)    | Glucocorticoid  |
| 3712 / 3716                    | O17         | Prestw-78 | Thioridazine hydrochloride      | 130-61-0   | Central Nervous System | Antipsychotic      |                  |                                      |                   | Plasmatic proteins | Yes          | New therapeutic use                             | Potential antibacterial                                 |
| 3712 / 3716                    | O19         | Prestw-79 | Diphepanil methylsulfate        | 62-97-5    | Gastroenterology       | Antispastic        |                  |                                      |                   |                    | Yes          | Chemical classification (according ATC code)    | Synthetic anticholinergic, quaternary ammonium compound |
| 3712 / 3716                    | O21         | Prestw-80 | Trimethobenzamide hydrochloride | 554-92-7   | Central Nervous System | Antiemetic         |                  |                                      |                   |                    | Yes          |   |   |
| 3712 / 3716                    | A04         | Prestw-81 | Metronidazole                   | 443-48-1   | Infectiology           | Antiamoebic        |                  |                                      | GI tract          | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Nitroimidazole derivative                               |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                     | CAS number  | Therapeutic class      | Therapeutic effect | Target type      | Target names  | Absorption tissue | Protein binding  | FDA approved | Additional info type                            | Additional info detail            |
|-----------------------------------|----------------|-------------|-----------------------------------|-------------|------------------------|--------------------|------------------|---|-------------------|--|--------------|---|-----------------------------------|
| 3712 / 3716                       | A06            | Prestw-1424 | Fulvestrant                       | 129453-61-8 | Endocrinology          | Antineoplastic     | Nuclear receptor | Estrogen receptor                                       |                   | Very Low Density Lipoprotein (VLDL), Low Density Lipoprotein (LDL), High Density Lipoprotein (HDL) | Yes          |   |                                   |
| 3712 / 3716                       | A08            | Prestw-83   | Edrophonium chloride              | 116-38-1    | Diagnostic             | Anti-fatigue       |                  |   |                   |  | Yes          |   |                                   |
| 3712 / 3716                       | A10            | Prestw-84   | Moroxidine hydrochloride          | 3160-91-6   | Infectiology           | Antiviral          |                  |   |                   |  |              |   |                                   |
| 3712 / 3716                       | A12            | Prestw-85   | Baclofen (R,S)                    | 1134-47-0   | Central Nervous System | Antispastic        | GPCR             | GABA-B receptor   | GI tract          | Plasmatic proteins   | Yes          | New therapeutic use                             | Alcohol withdrawal                |
| 3712 / 3716                       | A14            | Prestw-86   | Acyclovir                         | 59277-89-3  | Metabolism             | Antiviral          |                  |   | GI tract          |  | Yes          |   |                                   |
| 3712 / 3716                       | A16            | Prestw-87   | Diazoxide                         | 364-98-7    | Cardiovascular         | Antidiuretic       |                  |   | GI tract          | Plasmatic proteins   | Yes          | Chemical classification (according ATC code)    | Thiazide derivative               |
| 3712 / 3716                       | A18            | Prestw-88   | Amidopyrine                       | 58-15-1     | Central Nervous System | Analgesic          |                  |   |                   |  |              |   |                                   |
| 3712 / 3716                       | A20            | Prestw-1179 | Busulfan                          | 55-98-1     | Oncology               | Antineoplastic     |                  |   |                   | Plasmatic proteins   | Yes          | Chemical classification (according ATC code)    | Alkylating agent                  |
| 3712 / 3716                       | A22            | Prestw-90   | Pindolol                          | 13523-86-9  | Cardiovascular         | Antianginal        | GPCR             | Adrenergic receptor beta                                | GI tract          | Plasmatic proteins   | Yes          | Therapeutic classification (according ATC code) | Non-selective beta-blocking agent |
| 3712 / 3716                       | C04            | Prestw-91   | Khellin                           | 82-02-0     | Cardiovascular         | Antispastic        |                  |   |                   |  |              |   |                                   |
| 3712 / 3716                       | C06            | Prestw-92   | Zimelidine dihydrochloride monohy | 61129-30-4  | Central Nervous System | Antidepressant     | Carrier          | Serotonin transporter                                   |                   |  |              |   |                                   |
| 3712 / 3716                       | C08            | Prestw-93   | Azacyclonol                       | 115-46-8    | Central Nervous System | Antipsychotic      |                  |   |                   |  |              |   |                                   |
| 3712 / 3716                       | C10            | Prestw-94   | Azathioprine                      | 446-86-6    | Oncology               | Antineoplastic     |                  |   |                   | Plasmatic proteins   | Yes          |   |                                   |
| 3712 / 3716                       | C12            | Prestw-95   | Lynestrenol                       | 52-76-6     | Endocrinology          | Contraceptive      | Nuclear receptor | Progesterone receptor                                   |                   |  |              |   |                                   |
| 3712 / 3716                       | C14            | Prestw-96   | Guanabenz acetate                 | 23256-50-0  | Central Nervous System | Antihypertensive   |                  |   | 75                |  | Yes          |   |                                   |
| 3712 / 3716                       | C16            | Prestw-97   | Disulfiram                        | 97-77-8     | Metabolism             | Antabuse effect    | Enzyme           | Alcohol dehydrogenase                                   |                   |  | Yes          | Therapeutic use                                 | First developed as antiparasitic  |
| 3712 / 3716                       | C18            | Prestw-98   | Acetylsalicylic acid              | 530-75-6    | Central Nervous System | Analgesic          |                  |   |                   |  |              |   |                                   |
| 3712 / 3716                       | C20            | Prestw-99   | Mianserine hydrochloride          | 21535-47-7  | Cardiovascular         | Antidepressant     |                  |   |                   | Plasmatic proteins   |              |   |                                   |
| 3712 / 3716                       | C22            | Prestw-100  | Nocodazole                        | 31430-18-9  | Oncology               | Antineoplastic     |                  |   |                   |  |              |   |                                   |
| 3712 / 3716                       | E04            | Prestw-101  | R(-) Apomorphine hydrochloride he | 41372-20-7  | Central Nervous System | Antiparkinsonian   |                  |   |                   |  | Yes          |   |                                   |
| 3712 / 3716                       | E06            | Prestw-102  | Amoxapine                         | 14028-44-5  | Central Nervous System | Antidepressant     |                  |   |                   |  | Yes          |   |                                   |
| 3712 / 3716                       | E08            | Prestw-103  | Cyproheptadine hydrochloride      | 969-33-5    | Allergology            | Antihistaminic     | GPCR             | Histamine H1 receptor                                   | GI tract          |  | Yes          |   |                                   |
| 3712 / 3716                       | E10            | Prestw-104  | Famotidine                        | 76824-35-6  | Gastroenterology       | Antiulcer          | GPCR             | Histamine H2 receptor                                   | GI tract          | Plasmatic proteins   | Yes          |   |                                   |
| 3712 / 3716                       | E12            | Prestw-105  | Danazol                           | 17230-88-5  | Endocrinology          | Anabolic           |                  |   |                   |  | Yes          |   |                                   |
| 3712 / 3716                       | E14            | Prestw-106  | Nicorandil                        | 65141-46-0  | Cardiovascular         | Antianginal        |                  |   | GI tract          | Plasmatic proteins   |              |   |                                   |
| 3712 / 3716                       | E16            | Prestw-1314 | Pioglitazone                      | 111025-46-8 | Endocrinology          |                    | Nuclear receptor | Peroxisome proliferator-activated receptor (PPAR) gamma | GI tract          | Plasmatic proteins   | Yes          | Chemical classification (according ATC code)    | Thiazolidinedione                 |
| 3712 / 3716                       | E18            | Prestw-108  | Nomifensine maleate               | 32795-47-4  | Central Nervous System | Antidepressant     |                  |   |                   |  |              |   |                                   |
| 3712 / 3716                       | E20            | Prestw-109  | Dizocipiline maleate              | 77086-22-7  | Central Nervous System | Anticonvulsant     |                  |   |                   |  |              |   |                                   |
| 3712 / 3716                       | E22            | Prestw-1192 | Oxandrolone                       | 53-39-4     | Endocrinology          |                    |                  |   |                   |  | Yes          | Chemical classification (according ATC code)    | Androstan derivative              |
| 3712 / 3716                       | G04            | Prestw-111  | Naloxone hydrochloride            | 357-08-4    | Central Nervous System | Opiate antidote    |                  |   |                   |  | Yes          |   |                                   |

| ICCB-L Plate (10 mM / 3.33 mM) | ICCB-L Well | Vendor_ID   | Chemical_Name                           | CAS number | Therapeutic class      | Therapeutic effect | Target type            | Target names                          | Absorption tissue | Protein binding    | FDA approved | Additional info type                            | Additional info detail            |
|--------------------------------|-------------|-------------|---|------------|------------------------|--------------------|------------------------|---------------------------------------|-------------------|--------------------|--------------|---|-----------------------------------|
| 3712 / 3716                    | G06         | Prestw-112  | Metolazone                              | 17560-51-9 | Cardiovascular         | Antihypertensive   |                        |                                       | GI tract          | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | Low-ceiling diuretic              |
| 3712 / 3716                    | G08         | Prestw-113  | Ciprofloxacin hydrochloride monohydrate | 93107-08-5 | Infectiology           | Antibacterial      |                        |                                       | Small intestine   | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Fluoroquinolone                   |
| 3712 / 3716                    | G10         | Prestw-114  | Ampicillin trihydrate                   | 7177-48-2  | Infectiology           | Antibacterial      |                        |                                       |                   | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Penicillin with extended spectrum |
| 3712 / 3716                    | G12         | Prestw-115  | Haloperidol                             | 52-86-8    | Central Nervous System | Antiemetic         |                        |                                       |                   | Plasmatic proteins | Yes          | Therapeutic use                                 | Antiemetic                        |
| 3712 / 3716                    | G14         | Prestw-116  | Naltrexone hydrochloride dihydrate      | 16676-29-2 | Central Nervous System | Analgesic          |                        |                                       |                   | Plasmatic proteins | Yes          |   |                                   |
| 3712 / 3716                    | G16         | Prestw-117  | Chlorpheniramine maleate                | 113-92-8   | Allergology            | Antihistaminic     | GPCR                   | Histamine H1 receptor                 | GI tract          | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Substituted alkylamine            |
| 3712 / 3716                    | G18         | Prestw-118  | Nalbuphine hydrochloride                | 23277-43-2 | Central Nervous System | Analgesic          | Nuclear receptor       | Opioid receptor delta                 |                   |                    | Yes          | Chemical classification (according ATC code)    | Opioid                            |
| 3712 / 3716                    | G20         | Prestw-119  | Picotamide monohydrate                  | 80530-63-8 | Hematology             | Anticoagulant      |                        |                                       | GI tract          |                    |              |   |                                   |
| 3712 / 3716                    | G22         | Prestw-120  | Triamcinolone                           | 124-94-7   | Endocrinology          | Anti-inflammatory  | Nuclear receptor       | Glucocorticoid receptor               |                   | albumin            | Yes          | Chemical classification (according ATC code)    | Glucocorticoid                    |
| 3712 / 3716                    | I04         | Prestw-121  | Bromocryptine mesylate                  | 22260-51-1 | Central Nervous System | Antiparkinsonian   |                        |                                       |                   |                    | Yes          | New therapeutic use                             | Antidiabetic                      |
| 3712 / 3716                    | I06         | Prestw-1471 | Amfepramone hydrochloride               | 90-84-6    | Central Nervous System |                    |                        |                                       | GI tract          |                    |              |   |                                   |
| 3712 / 3716                    | I08         | Prestw-123  | Dehydrocholic acid                      | 81-23-2    | Gastroenterology       | Choleretic         |                        |                                       |                   |                    |              |   |                                   |
| 3712 / 3716                    | I10         | Prestw-1184 | Tioconazole                             | 65899-73-2 | Infectiology           | Antifungal         |                        |                                       |                   |                    | Yes          | Chemical classification (according ATC code)    | Imidazole derivative              |
| 3712 / 3716                    | I12         | Prestw-125  | Perphenazine                            | 58-39-9    | Central Nervous System | Antiemetic         |                        |                                       |                   |                    | Yes          | Chemical classification (according ATC code)    | Phenothiazine derivative          |
| 3712 / 3716                    | I14         | Prestw-126  | Mefloquine hydrochloride                | 51773-92-3 | Infectiology           | Antimalarial       |                        |                                       | GI tract          | Plasmatic proteins | Yes          |   |                                   |
| 3712 / 3716                    | I16         | Prestw-127  | Isoconazole                             | 27523-40-6 | Infectiology           | Antibacterial      |                        |                                       |                   |                    |              | Chemical classification (according ATC code)    | Imidazole derivative              |
| 3712 / 3716                    | I18         | Prestw-128  | Spironolactone                          | 52-01-7    | Endocrinology          | Diuretic           | Nuclear receptor       | Mineralocorticoid receptor            | GI tract          |                    | Yes          | New therapeutic use                             | Antiandrogenic                    |
| 3712 / 3716                    | I20         | Prestw-129  | Pirenzepine dihydrochloride             | 29868-97-1 | Gastroenterology       | Antiulcer          |                        |                                       | GI tract          | Plasmatic proteins |              |   |                                   |
| 3712 / 3716                    | I22         | Prestw-130  | Dexamethasone acetate                   | 1177-87-3  | Endocrinology          | Anti-inflammatory  | Nuclear receptor       | Glucocorticoid receptor               |                   |                    | Yes          | Chemical classification (according ATC code)    | Glucocorticoid                    |
| 3712 / 3716                    | K04         | Prestw-131  | Glipizide                               | 29094-61-9 | Endocrinology          | Antidiabetic       | Transmembrane receptor | Sulfonylurea receptors K-ATP channels | GI tract          | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Sulfonamide urea derivative       |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID  | Chemical_Name                   | CAS number    | Therapeutic class      | Therapeutic<br>effect | Target type         | Target names                            | Absorption<br>tissue | Protein<br>binding                       | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail                   |
|-----------------------------------|----------------|------------|---------------------------------|---------------|------------------------|-----------------------|---------------------|---|----------------------|--|-----------------|--|---|
| 3712 / 3716                       | K06            | Prestw-132 | Loxapine succinate              | 27833-64-3    | Central Nervous System | Antipsychotic         |                     |   |                      |  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Oxazepine                                   |
| 3712 / 3716                       | K08            | Prestw-133 | Hydroxyzine dihydrochloride     | 2192-20-3     | Allergology            | Antiemetic            |                     |   |                      | Plasmatic<br>proteins                    | Yes             |  |   |
| 3712 / 3716                       | K10            | Prestw-134 | Diltiazem hydrochloride         | 33286-22-5    | Cardiovascular         | Antianginal           | Ion channel         | Voltage-gated L-type<br>calcium channel | GI tract             | Plasmatic<br>proteins                    | Yes             |  |   |
| 3712 / 3716                       | K12            | Prestw-135 | Methotrexate                    | 59-05-2       | Oncology               | Antineoplastic        | Enzyme              | Dihydrofolate reductase                 |                      | Plasmatic<br>proteins                    | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Folic acid<br>analogue                      |
| 3712 / 3716                       | K14            | Prestw-136 | Astemizole                      | 68844-77-9    | Allergology            | Antihistaminic        | GPCR                | Histamine H1 receptor                   | GI tract             | Plasmatic<br>proteins                    |                 | New therapeutic<br>use                                   | Anti-cancer                                 |
| 3712 / 3716                       | K16            | Prestw-137 | Clindamycin hydrochloride       | 21462-39-5    | Infectiology           | Antibacterial         |                     |   |                      | Plasmatic<br>proteins                    | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Lincosamide                                 |
| 3712 / 3716                       | K18            | Prestw-138 | Terfenadine                     | 50679-08-8    | Allergology            | Antihistaminic        | GPCR                | Histamine H1 receptor                   | GI tract             | Plasmatic<br>proteins                    |                 | Pharmacokinetics   | Prodrug of<br>Fexofenadine<br>(Prestw-1102) |
| 3712 / 3716                       | K20            | Prestw-139 | Cefotaxime sodium salt          | 64485-93-4    | Infectiology           | Antibacterial         |                     |   |                      | Plasmatic<br>proteins                    | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Third-generation<br>cephalosporin           |
| 3712 / 3716                       | K22            | Prestw-140 | Tetracycline hydrochloride      | 64-75-5       | Infectiology           | Antibacterial         |                     |   | Stomach              |  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Tetracycline                                |
| 3712 / 3716                       | M04            | Prestw-141 | Verapamil hydrochloride         | 152-11-4      | Cardiovascular         | Antihypertensive      | Ion channel         | Voltage-gated L-type<br>calcium channel | GI tract             | Plasmatic<br>proteins                    | Yes             |  |   |
| 3712 / 3716                       | M06            | Prestw-142 | Dipyridamole                    | 58-32-2       | Cardiovascular         | Anticoagulant         |                     |   | GI tract             | Albumin,<br>alpha-1-acid<br>glycoprotein | Yes             |  |   |
| 3712 / 3716                       | M08            | Prestw-143 | Chlorhexidine                   | 55-56-1       | Infectiology           | Antibacterial         |                     |   | Skin                 |  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Biguanide                                   |
| 3712 / 3716                       | M10            | Prestw-144 | Loperamide hydrochloride        | 34552-83-5    | Gastroenterology       | Antidiarrheal         |                     |   | GI tract             |  | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Antipropulsive                              |
| 3712 / 3716                       | M12            | Prestw-145 | Chlortetracycline hydrochloride | 64-72-2       | Infectiology           | Antiamebic            |                     |   |                      |  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Tetracycline                                |
| 3712 / 3716                       | M14            | Prestw-146 | Tamoxifen citrate               | 54965-24-1    | Endocrinology          | Antineoplastic        | Nuclear<br>receptor | Estrogen receptor                       |                      | Plasmatic<br>proteins                    | Yes             |  |   |
| 3712 / 3716                       | M16            | Prestw-147 | Nicergoline                     | not available | Cardiovascular         | Anti-ischemic         |                     |   | GI tract             |  |                 | Chemical<br>classification<br>(according ATC<br>code)    | Ergot alkaloids                             |
| 3712 / 3716                       | M18            | Prestw-148 | Canrenoic acid potassium salt   | 2181-04-6     | Endocrinology          | Antihypertensive      |                     |   |                      |  |                 | Therapeutic<br>classification<br>(according ATC<br>code) | Potassium-<br>sparing agent                 |
| 3712 / 3716                       | M20            | Prestw-149 | Thiopropazine dimesylate        | 2347-80-0     | Central Nervous System | Antiemetic            |                     |   |                      |  |                 | Chemical<br>classification<br>(according ATC<br>code)    | Phenothiazine<br>derivative                 |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name               | CAS number    | Therapeutic class      | Therapeutic<br>effect | Target type | Target names                      | Absorption<br>tissue | Protein<br>binding      | FDA<br>approved | Additional info<br>type                               | Additional info<br>detail                              |
|-----------------------------------|----------------|-------------|-----------------------------|---------------|------------------------|-----------------------|-------------|-----------------------------------|----------------------|-------------------------|-----------------|---|--|
| 3712 / 3716                       | M22            | Prestw-150  | Dihydroergotamine tartrate  | 5989-77-5     | Central Nervous System | Antimigraine          | GPCR        | Serotonin 1d (5-HT1d)<br>receptor |                      |                         | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Ergot alkaloid   |
| 3712 / 3716                       | O04            | Prestw-151  | Erythromycin                | 114-07-8      | Infectiology           | Antibacterial         |             |                                   |                      | Plasmatic<br>proteins   | Yes             | Reference   | J Antimicrob<br>Chemother.<br>2007 Mar<br>59(3):347-58 |
| 3712 / 3716                       | O06            | Prestw-1474 | Chloroxine                  | 773-76-2      | Dermatology            |                       |             |                                   |                      |                         | Yes             |   |  |
| 3712 / 3716                       | O08            | Prestw-153  | Didanosine                  | 69655-05-6    | Infectiology           | Antiviral             |             |                                   |                      | Plasmatic<br>proteins   | Yes             |   |  |
| 3712 / 3716                       | O10            | Prestw-154  | Josamycin                   | 16846-24-5    | Infectiology           | Antibacterial         |             |                                   | Small intestine      |                         |                 | Chemical<br>classification<br>(according ATC<br>code) | Macrolide  |
| 3712 / 3716                       | O12            | Prestw-155  | Paclitaxel                  | 33069-62-4    | Oncology               | Antineoplastic        |             |                                   |                      | Plasmatic<br>proteins   | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Taxane   |
| 3712 / 3716                       | O14            | Prestw-156  | Ivermectin                  | 70288-86-7    | Infectiology           | Anthelmintic          |             |                                   | GI tract             | Plasmatic<br>proteins   | Yes             |   |  |
| 3712 / 3716                       | O16            | Prestw-157  | Gallamine triethiodide      | 65-29-2       | Neuromuscular          | Muscle relaxant       |             |                                   |                      |                         | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Quaternary<br>ammonium                                 |
| 3712 / 3716                       | O18            | Prestw-158  | Neomycin sulfate            | 1405-10-3     | Infectiology           | Antibacterial         |             |                                   |                      |                         | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Aminoside  |
| 3712 / 3716                       | O20            | Prestw-159  | Dihydrostreptomycin sulfate | 5490-27-7     | Infectiology           | Antibacterial         |             |                                   |                      |                         | Yes             |   |  |
| 3712 / 3716                       | O22            | Prestw-160  | Gentamicine sulfate         | 1405-41-0     | Infectiology           | Antibacterial         |             |                                   |                      | Plasmatic<br>proteins   | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Aminoside  |
| 3712 / 3716                       | B03            | Prestw-161  | Isoniazid                   | 54-85-3       | Infectiology           | Antibacterial         |             |                                   |                      | Plasmatic<br>proteins   | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Hydrazide  |
| 3712 / 3716                       | B05            | Prestw-162  | Pentylenetetrazole          | 54-95-5       | Central Nervous System | Analeptic             |             |                                   |                      |                         |                 |   |  |
| 3712 / 3716                       | B07            | Prestw-163  | Chlorzoxazone               | 95-25-0       | Central Nervous System | Anticonvulsant        |             |                                   | GI tract             |                         | Yes             |   |  |
| 3712 / 3716                       | B09            | Prestw-164  | Ornidazole                  | 16773-42-5    | Infectiology           | Antibacterial         |             |                                   | GI tract             | Plasmatic<br>proteins   |                 | Chemical<br>classification<br>(according ATC<br>code) | Nitroimidazole<br>derivative                           |
| 3712 / 3716                       | B11            | Prestw-165  | Ethosuximide                | 77-67-8       | Central Nervous System | Anticonvulsant        |             |                                   |                      |                         | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Succinimide<br>derivatives                             |
| 3712 / 3716                       | B13            | Prestw-166  | Mafenide hydrochloride      | 138-37-4      | Infectiology           | Antibacterial         |             |                                   |                      |                         | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Sulfonamide  |
| 3712 / 3716                       | B15            | Prestw-167  | Riluzole hydrochloride      | not available | Central Nervous System | Antispastic           |             |                                   |                      | Albumin,<br>lipoprotein | Yes             |   |  |
| 3712 / 3716                       | B17            | Prestw-168  | Nitrofurantoin              | 67-20-9       | Infectiology           | Antibacterial         |             |                                   | Small intestine      | Plasmatic<br>proteins   | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Nitrofurantoin<br>derivative                           |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID  | Chemical_Name                 | CAS number | Therapeutic class      | Therapeutic<br>effect | Target type                | Target names                             | Absorption<br>tissue | Protein<br>binding    | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail                               |
|-----------------------------------|----------------|------------|-------------------------------|------------|------------------------|-----------------------|----------------------------|--|----------------------|-----------------------|-----------------|--|---|
| 3712 / 3716                       | B19            | Prestw-169 | Hydralazine hydrochloride     | 304-20-1   | Cardiovascular         | Antihypertensive      |                            |  | GI tract             | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Hydrazinophthal<br>azine derivative                     |
| 3712 / 3716                       | B21            | Prestw-170 | Phenelzine sulfate            | 156-51-4   | Central Nervous System | Antidepressant        | Enzyme                     | Monoamine oxidase                        | GI tract             |                       | Yes             |  |   |
| 3712 / 3716                       | D03            | Prestw-171 | Tranexamic acid               | 1197-18-8  | Hematology             | Hemostatic            |                            |  | GI tract             |                       | Yes             |  |   |
| 3712 / 3716                       | D05            | Prestw-172 | Etofyline                     | 519-37-9   | Cardiovascular         | Antispastic           |                            |  |                      |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Purine<br>derivative                                    |
| 3712 / 3716                       | D07            | Prestw-173 | Tranlycypromine hydrochloride | 1986-47-6  | Central Nervous System | Antidepressant        | Enzyme                     | Monoamine oxidase                        |                      |                       | Yes             |  |   |
| 3712 / 3716                       | D09            | Prestw-174 | Alverine citrate salt         | 5560-59-8  | Neuromuscular          | Antispastic           |                            |  | GI tract             |                       |                 |  |   |
| 3712 / 3716                       | D11            | Prestw-175 | Aceclofenac                   | 89796-99-6 | Central Nervous System | Analgesic             | Enzyme                     | Cyclooxygenase                           |                      | Plasmatic<br>proteins |                 | Therapeutic<br>classification<br>(according ATC<br>code) | NSAID   |
| 3712 / 3716                       | D13            | Prestw-176 | Iproniazide phosphate         | 305-33-9   | Cardiovascular         | Antidepressant        | Enzyme                     | Monoamine oxidase                        |                      |                       |                 |  |   |
| 3712 / 3716                       | D15            | Prestw-177 | Sulfamethoxazole              | 723-46-6   | Infectiology           | Antibacterial         |                            |  |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Intermediate-<br>acting<br>sulfonamide                  |
| 3712 / 3716                       | D17            | Prestw-178 | Mephesisin                    | 59-47-2    | Central Nervous System | Anticonvulsant        |                            |  | GI tract             |                       |                 | Side effect  | Drug abused   |
| 3712 / 3716                       | D19            | Prestw-179 | Phenformin hydrochloride      | 834-28-6   | Endocrinology          | Antidiabetic          |                            |  | GI tract             | Plasmatic<br>proteins |                 | Chemical<br>classification<br>(according ATC<br>code)    | Biguanide   |
| 3712 / 3716                       | D21            | Prestw-180 | Flutamide                     | 13311-84-7 | Oncology               | Antineoplastic        | Nuclear<br>receptor        | Androgen Receptor                        |                      | Plasmatic<br>proteins | Yes             |  |   |
| 3712 / 3716                       | F03            | Prestw-181 | Ampyrone                      | 83-07-8    | Central Nervous System | Analgesic             |                            |  |                      |                       |                 |  |   |
| 3712 / 3716                       | F05            | Prestw-182 | Levamisole hydrochloride      | 16595-80-5 | Immunology             | Anthelmintic          |                            |  | GI tract             |                       | Yes             |  |   |
| 3712 / 3716                       | F07            | Prestw-183 | Pargyline hydrochloride       | 306-07-0   | Cardiovascular         | Antidepressant        | Enzyme                     | Monoamine oxidase                        |                      |                       | Yes             |  |   |
| 3712 / 3716                       | F09            | Prestw-184 | Methocarbamol                 | 532-03-6   | Central Nervous System | Analgesic             |                            |  | GI tract             |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Carbamic acid<br>ester                                  |
| 3712 / 3716                       | F11            | Prestw-185 | Aztreonam                     | 78110-38-0 | Infectiology           | Antibacterial         |                            |  |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Monobactam  |
| 3712 / 3716                       | F13            | Prestw-186 | Cloxacillin sodium salt       | 642-78-4   | Infectiology           | Antibacterial         |                            |  |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Beta-lactamase<br>resistant<br>penicillin               |
| 3712 / 3716                       | F15            | Prestw-187 | Catharanthine                 | 2468-21-5  | Oncology               | Antineoplastic        |                            |  |                      |                       |                 | Pharmacological<br>tool                                  | Precursor to<br>vinblastine                             |
| 3712 / 3716                       | F17            | Prestw-188 | Pentolinium bitartrate        | 52-62-0    | Cardiovascular         | Antihypertensive      |                            |  |                      |                       | Yes             |  |   |
| 3712 / 3716                       | F19            | Prestw-189 | Aminopurine, 6-benzyl         | 1214-39-7  | Endocrinology          |                       |                            |  |                      |                       |                 | Pharmacological<br>tool                                  |   |
| 3712 / 3716                       | F21            | Prestw-190 | Tolbutamide                   | 64-77-7    | Endocrinology          | Antidiabetic          | Transmembr<br>ane receptor | Sulfonylurea receptors<br>K-ATP channels | GI tract             | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Sulfonamide<br>urea derivative                          |
| 3712 / 3716                       | H03            | Prestw-191 | Midodrine hydrochloride       | 3092-17-9  | Cardiovascular         | Antihypertensive      | GPCR                       | Adrenergic receptor<br>alpha-1           | GI tract             |                       | Yes             |  |   |
| 3712 / 3716                       | H05            | Prestw-192 | Thalidomide                   | 50-35-1    | Central Nervous System | Hypnotic              |                            |  |                      | Plasmatic<br>proteins | Yes             | Side effect  | Phocomelia<br>induced when<br>taken during<br>pregnancy |

| ICCB-L Plate (10 mM / 3.33 mM) | ICCB-L Well | Vendor_ID   | Chemical_Name                           | CAS number | Therapeutic class      | Therapeutic effect | Target type      | Target names                 | Absorption tissue | Protein binding                    | FDA approved | Additional info type                            | Additional info detail                      |
|--------------------------------|-------------|-------------|---|------------|------------------------|--------------------|------------------|------------------------------|-------------------|------------------------------------|--------------|---|---|
| 3712 / 3716                    | H07         | Prestw-193  | Oxolinic acid                           | 14698-29-4 | Metabolism             | Antibacterial      |                  |                              | GI tract          | Plasmatic proteins                 |              | Chemical classification (according ATC code)    | Quinolone                                   |
| 3712 / 3716                    | H09         | Prestw-194  | Nimesulide                              | 51803-78-2 | Metabolism             | Anti-inflammatory  | Enzyme           | Cyclooxygenase               | GI tract          | Plasmatic proteins                 |              | Therapeutic classification (according ATC code) | NSAID                                       |
| 3712 / 3716                    | H11         | Prestw-1231 | Asenapine maleate                       | 85650-56-2 | Central Nervous System | Antipsychotic      |                  |                              |                   | Albumin, alpha-1-acid glycoprotein | Yes          | Chemical classification (according ATC code)    | Oxepine                                     |
| 3712 / 3716                    | H13         | Prestw-196  | Pentoxifylline                          | 6493-05-6  | Cardiovascular         | Bronchodilator     |                  |                              | GI tract          | Plasmatic proteins                 | Yes          | Chemical classification (according ATC code)    | Purine derivative                           |
| 3712 / 3716                    | H15         | Prestw-197  | Metaraminol bitartrate                  | 33402-03-8 | Cardiovascular         | Antihypotensive    |                  |                              |                   |                                    | Yes          |   |   |
| 3712 / 3716                    | H17         | Prestw-198  | Salbutamol                              | 18559-94-9 | Neuromuscular          | Bronchodilator     | GPCR             | Adrenergic receptor beta-2   | Lung              |                                    |              |   |   |
| 3712 / 3716                    | H19         | Prestw-199  | Prilocaine hydrochloride                | 1786-81-8  | Neuromuscular          | Local anesthetic   | Ion channel      | Voltage-gated sodium channel | Skin              |                                    | Yes          | Chemical classification (according ATC code)    | Amides                                      |
| 3712 / 3716                    | H21         | Prestw-200  | Camptothecin (S,+)                      | 7689-03-4  | Oncology               | Antineoplastic     |                  |                              |                   |                                    |              |   |   |
| 3712 / 3716                    | J03         | Prestw-201  | Ranitidine hydrochloride                | 66357-59-3 | Gastroenterology       | Antilucer          | GPCR             | Histamine H2 receptor        | GI tract          |                                    | Yes          |   |   |
| 3712 / 3716                    | J05         | Prestw-202  | Tiratricol, 3,3',5-triiodothyroacetic a | 51-24-1    | Endocrinology          | Antihypothyroid    | Nuclear receptor | Thyroid hormone receptor     | GI tract          |                                    |              | Therapeutic use                                 | Previous uses as a fat-loss food supplement |
| 3712 / 3716                    | J07         | Prestw-203  | Flufenamic acid                         | 530-78-9   | Central Nervous System | Analgesic          |                  |                              |                   |                                    |              | Therapeutic classification (according ATC code) | NSAID                                       |
| 3712 / 3716                    | J09         | Prestw-204  | Flumequine                              | 42835-25-6 | Infectiology           | Antibacterial      |                  |                              |                   | Plasmatic proteins                 |              | Chemical classification (according ATC code)    | Quinolone                                   |
| 3712 / 3716                    | J11         | Prestw-205  | Tolfenamic acid                         | 13710-19-5 | Central Nervous System | Analgesic          | Enzyme           | Cyclooxygenase               | GI tract          | Plasmatic proteins                 |              | Therapeutic classification (according ATC code) | NSAID                                       |
| 3712 / 3716                    | J13         | Prestw-206  | Meclofenamic acid sodium salt mon       | 6385-02-0  | Central Nervous System | Anti-inflammatory  |                  |                              | GI tract          | Plasmatic proteins                 | Yes          | Therapeutic classification (according ATC code) | NSAID                                       |
| 3712 / 3716                    | J15         | Prestw-1181 | Tibolone                                | 5630-53-5  | Endocrinology          |                    |                  |                              |                   |                                    |              |   |   |
| 3712 / 3716                    | J17         | Prestw-208  | Trimethoprim                            | 738-70-5   | Infectiology           | Antibacterial      |                  |                              |                   | Plasmatic proteins                 | Yes          |   |   |
| 3712 / 3716                    | J19         | Prestw-209  | Metoclopramide monohydrochlorid         | 7232-21-5  | Central Nervous System | Antiemetic         | GPCR             | Dopamine receptor            | GI tract          | Plasmatic proteins                 | Yes          | Therapeutic classification (according ATC code) | Propulsive                                  |
| 3712 / 3716                    | J21         | Prestw-210  | Fenbendazole                            | 43210-67-9 | Infectiology           | Anthelmintic       |                  |                              |                   |                                    |              | Veterinary use                                  |   |
| 3712 / 3716                    | L03         | Prestw-211  | Piroxicam                               | 36322-90-4 | Central Nervous System | Analgesic          | Enzyme           | Cyclooxygenase               | GI tract          |                                    | Yes          | Therapeutic classification (according ATC code) | NSAID                                       |
| 3712 / 3716                    | L05         | Prestw-212  | Pyrantel tartrate                       | 33401-94-4 | Infectiology           | Anthelmintic       |                  |                              | GI tract          |                                    |              |   |   |
| 3712 / 3716                    | L07         | Prestw-213  | Fenspiride hydrochloride                | 5053-08-7  | Respiratory            | Antitussive        |                  |                              |                   |                                    |              |   |   |

| ICCB-L Plate (10 mM / 3.33 mM) | ICCB-L Well | Vendor_ID  | Chemical_Name                   | CAS number | Therapeutic class      | Therapeutic effect  | Target type      | Target names  | Absorption tissue | Protein binding    | FDA approved | Additional info type                            | Additional info detail              |
|--------------------------------|-------------|------------|---------------------------------|------------|------------------------|---------------------|------------------|---|-------------------|--------------------|--------------|---|-------------------------------------|
| 3712 / 3716                    | L09         | Prestw-214 | Gemfibrozil                     | 25812-30-0 | Metabolism             | Hypocholesterolemic | Nuclear receptor | Peroxisome proliferator-activated receptor (PPAR) alpha | GI tract          | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | Fibrate                             |
| 3712 / 3716                    | L11         | Prestw-215 | Mefexamide hydrochloride        | 3413-64-7  | Central Nervous System | CNS Stimulant       |                  |   |                   |                    |              |   |                                     |
| 3712 / 3716                    | L13         | Prestw-216 | Tiaprude hydrochloride          | 51012-33-0 | Central Nervous System | Antiemetic          |                  |   |                   |                    |              | Chemical classification (according ATC code)    | Benzamide                           |
| 3712 / 3716                    | L15         | Prestw-217 | Mebendazole                     | 31431-39-7 | Infectiology           | Anthelmintic        |                  |   | GI tract          |                    | Yes          |   |                                     |
| 3712 / 3716                    | L17         | Prestw-218 | Fenbufen                        | 36330-85-5 | Central Nervous System | Analgesic           | Enzyme           | Cyclooxygenase  | GI tract          |                    |              | Therapeutic classification (according ATC code) | NSAID                               |
| 3712 / 3716                    | L19         | Prestw-219 | Ketoprofen                      | 22071-15-4 | Central Nervous System | Analgesic           | Enzyme           | Cyclooxygenase  | GI tract          | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | NSAID                               |
| 3712 / 3716                    | L21         | Prestw-220 | Indapamide                      | 26807-65-8 | Metabolism             | Antihypertensive    | Carrier          | Solute carrier family 12 member 3                       | GI tract          | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | Low-ceiling diuretic                |
| 3712 / 3716                    | N03         | Prestw-221 | Norfloxacin                     | 70458-96-7 | Infectiology           | Antibacterial       |                  |   |                   |                    | Yes          | Chemical classification (according ATC code)    | Fluoroquinolone                     |
| 3712 / 3716                    | N05         | Prestw-222 | Antimycin A                     | 1397-94-0  | Infectiology           | Antibacterial       |                  |   |                   |                    |              |   |                                     |
| 3712 / 3716                    | N07         | Prestw-223 | Xylometazoline hydrochloride    | 1218-35-5  | Cardiovascular         | Nasal Decongestant  |                  |   |                   |                    |              | Therapeutic classification (according ATC code) | Sympathomimetic                     |
| 3712 / 3716                    | N09         | Prestw-224 | Oxymetazoline hydrochloride     | 2315-02-8  | Respiratory            | Nasal Decongestant  |                  |   | Nose, GI tract    |                    | Yes          | Therapeutic classification (according ATC code) | Sympathomimetic                     |
| 3712 / 3716                    | N11         | Prestw-225 | Nifenazone                      | 2139-47-1  | Central Nervous System | Analgesic           |                  |   |                   |                    |              | Therapeutic classification (according ATC code) | NSAID                               |
| 3712 / 3716                    | N13         | Prestw-226 | Griseofulvin                    | 126-07-8   | Infectiology           | Antifungal          |                  |   |                   | Plasmatic proteins | Yes          |   |                                     |
| 3712 / 3716                    | N15         | Prestw-227 | Clemizole hydrochloride         | 1163-36-6  | Allergology            | Antibacterial       |                  |   |                   |                    |              |   |                                     |
| 3712 / 3716                    | N17         | Prestw-228 | Tropicamide                     | 1508-75-4  | Neuromuscular          | Mydriatic           |                  |   | Eye               |                    | Yes          | Therapeutic classification (according ATC code) | Anticholinergic                     |
| 3712 / 3716                    | N19         | Prestw-229 | Nefopam hydrochloride           | 23327-57-3 | Central Nervous System | Analgesic           |                  |   |                   | Plasmatic proteins |              |   |                                     |
| 3712 / 3716                    | N21         | Prestw-230 | Phentolamine hydrochloride      | 73-05-2    | Cardiovascular         | Antihypertensive    |                  |   | GI tract          | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Imidazoline derivative              |
| 3712 / 3716                    | P03         | Prestw-231 | Etodolac                        | 41340-25-4 | Central Nervous System | Analgesic           | Enzyme           | Cyclooxygenase  |                   | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | NSAID                               |
| 3712 / 3716                    | P05         | Prestw-232 | Scopolamin-N-oxide hydrobromide | 6106-81-6  | Neuromuscular          | Antispastic         |                  |   |                   |                    | Yes          |   |                                     |
| 3712 / 3716                    | P07         | Prestw-233 | Hyoscyamine (L)                 | 101-31-5   | Central Nervous System | Antiemetic          |                  |   | GI tract          | Plasmatic proteins |              | Chemical classification (according ATC code)    | Belladonna alkaloid, tertiary amine |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name               | CAS number | Therapeutic class      | Therapeutic<br>effect | Target type         | Target names                         | Absorption<br>tissue | Protein<br>binding    | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail               |
|-----------------------------------|----------------|-------------|-----------------------------|------------|------------------------|-----------------------|---------------------|--------------------------------------|----------------------|-----------------------|-----------------|--|---|
| 3712 / 3716                       | P09            | Prestw-234  | Chlorphensin carbamate      | 886-74-8   | Central Nervous System | Muscle relaxant       |                     |                                      |                      |                       | Yes             |  |   |
| 3712 / 3716                       | P11            | Prestw-1771 | Carmofur                    | 61422-45-5 | Metabolism             | Antineoplastic        |                     |                                      |                      | Plasmatic<br>proteins |                 | Chemical<br>classification<br>(according ATC<br>code)    | Pyrimidine<br>analogue                  |
| 3712 / 3716                       | P13            | Prestw-236  | Dilazep dihydrochloride     | 20153-98-4 | Cardiovascular         | Antiplatelet          |                     |                                      |                      |                       |                 |  |   |
| 3712 / 3716                       | P15            | Prestw-237  | Ofloxacin                   | 82419-36-1 | Infectiology           | Antibacterial         |                     |                                      |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Fluoroquinolone                         |
| 3712 / 3716                       | P17            | Prestw-238  | Lomefloxacin hydrochloride  | 98079-52-8 | Infectiology           | Antibacterial         |                     |                                      |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Fluoroquinolone                         |
| 3712 / 3716                       | P19            | Prestw-239  | Orphenadrine hydrochloride  | 341-69-5   | Allergology            | Antihistaminic        |                     |                                      |                      |                       | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Anticholinergic<br>agent                |
| 3712 / 3716                       | P21            | Prestw-240  | Proglumide                  | 6620-60-6  | Gastroenterology       | Antiulcer             |                     |                                      |                      |                       |                 |  |   |
| 3712 / 3716                       | B04            | Prestw-241  | Mexiletine hydrochloride    | 5370-01-4  | Cardiovascular         | Antiarrhythmic        | LGIC                | Voltage-gated sodium<br>channel      | GI tract             | Plasmatic<br>proteins | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Antiarrhythmic,<br>class Ib             |
| 3712 / 3716                       | B06            | Prestw-242  | Flavoxate hydrochloride     | 3717-88-2  | Metabolism             | Antispastic           | Enzyme              | Phosphodiesterase 4                  |                      |                       | Yes             |  |   |
| 3712 / 3716                       | B08            | Prestw-243  | Bufexamac                   | 2438-72-4  | Central Nervous System | Analgesic             | Enzyme              | Cyclooxygenase                       |                      |                       |                 | Therapeutic<br>classification<br>(according ATC<br>code) | NSAID                                   |
| 3712 / 3716                       | B10            | Prestw-244  | Glutethimide, para-amino    | 125-84-8   | Oncology               | Antineoplastic        | Coenzyme            | Cytochrome P450<br>19A1              |                      |                       | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Aromatase<br>inhibitor                  |
| 3712 / 3716                       | B12            | Prestw-245  | Dropropizine (R,S)          | 17692-31-8 | Respiratory            | Antitussive           |                     |                                      | GI tract             | Plasmatic<br>proteins |                 |  |   |
| 3712 / 3716                       | B14            | Prestw-246  | Pinacidil                   | 85371-64-8 | Cardiovascular         | Antihypertensive      |                     |                                      | GI tract             | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Guanidine<br>derivative                 |
| 3712 / 3716                       | B16            | Prestw-247  | Albendazole                 | 54965-21-8 | Metabolism             | Anthelmintic          |                     |                                      | GI tract             |                       | Yes             |  |   |
| 3712 / 3716                       | B18            | Prestw-248  | Clonidine hydrochloride     | 4205-91-8  | Cardiovascular         | Analgesic             | GPCR                | Adrenergic receptor<br>alpha-2       | GI tract             | Plasmatic<br>proteins | Yes             |  |   |
| 3712 / 3716                       | B20            | Prestw-249  | Bupropion hydrochloride     | 31677-93-7 | Central Nervous System | Antidepressant        |                     |                                      |                      | Plasmatic<br>proteins | Yes             |  |   |
| 3712 / 3716                       | B22            | Prestw-250  | Alprenolol hydrochloride    | 13707-88-5 | Cardiovascular         | Antianginal           | GPCR                | Adrenergic receptor<br>beta          | GI tract             |                       |                 | Therapeutic<br>classification<br>(according ATC<br>code) | Non-selective<br>beta-blocking<br>agent |
| 3712 / 3716                       | D04            | Prestw-251  | Chlorothiazide              | 58-94-6    | Metabolism             | Antihypertensive      | Carrier             | Solute carrier family 12<br>member 3 | GI tract             |                       | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Low-ceiling<br>diuretic                 |
| 3712 / 3716                       | D06            | Prestw-252  | Diphenidol hydrochloride    | 3254-89-5  | Central Nervous System | Antiemetic            |                     |                                      |                      |                       | Yes             |  |   |
| 3712 / 3716                       | D08            | Prestw-253  | Norethindrone               | 68-22-4    | Endocrinology          | Contraceptive         | Nuclear<br>receptor | Progesterone receptor                |                      | Plasmatic<br>proteins | Yes             |  |   |
| 3712 / 3716                       | D10            | Prestw-254  | Nortriptyline hydrochloride | 894-71-3   | Central Nervous System | Antidepressant        |                     |                                      |                      |                       | Yes             |  |   |
| 3712 / 3716                       | D12            | Prestw-255  | Niflumic acid               | 4394-00-7  | Central Nervous System | Analgesic             | Enzyme              | Cyclooxygenase                       | GI tract             | Plasmatic<br>proteins |                 | Therapeutic<br>classification<br>(according ATC<br>code) | NSAID                                   |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID  | Chemical_Name              | CAS number | Therapeutic class      | Therapeutic<br>effect   | Target type         | Target names   | Absorption<br>tissue | Protein<br>binding                      | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail         |
|-----------------------------------|----------------|------------|----------------------------|------------|------------------------|-------------------------|---------------------|--|----------------------|---|-----------------|--|-----------------------------------|
| 3712 / 3716                       | D14            | Prestw-256 | Isotretinoin               | 4759-48-2  | Dermatology            | Keratolytic             |                     |  |                      | Albumin                                 | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Retinoid                          |
| 3712 / 3716                       | D16            | Prestw-257 | Retinoic acid              | 302-79-4   | Dermatology            | Keratolytic             |                     |  |                      |   |                 |  |                                   |
| 3712 / 3716                       | D18            | Prestw-258 | Antazoline hydrochloride   | 2508-72-7  | Allergology            | Antihistaminic          |                     |  |                      |   | Yes             |  |                                   |
| 3712 / 3716                       | D20            | Prestw-259 | Ethacrynic acid            | 58-54-8    | Metabolism             | Diuretic                | Carrier             | Solute carrier family 12<br>member 1                           | GI tract             |   | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | High-ceiling<br>diuretic          |
| 3712 / 3716                       | D22            | Prestw-260 | Praziquantel               | 55268-74-1 | Infectiology           | Anthelmintic            |                     |  | GI tract             |   | Yes             |  |                                   |
| 3712 / 3716                       | F04            | Prestw-261 | Ethisterone                | 434-03-7   | Endocrinology          | Contraceptive           |                     |  |                      |   |                 |  |                                   |
| 3712 / 3716                       | F06            | Prestw-262 | Triprolidine hydrochloride | 550-70-9   | Allergology            | Antihistaminic          | GPCR                | Histamine H1 receptor  |                      |   | Yes             |  |                                   |
| 3712 / 3716                       | F08            | Prestw-263 | Doxepin hydrochloride      | 1229-29-4  | Allergology            | Anticonvulsant          |                     |  |                      |   | Yes             |  |                                   |
| 3712 / 3716                       | F10            | Prestw-264 | Dyclonine hydrochloride    | 536-43-6   | Neuromuscular          | Local anesthetic        | Ion channel         | Voltage-gated sodium<br>channel                                |                      |   | Yes             |  |                                   |
| 3712 / 3716                       | F12            | Prestw-265 | Dimenhydrinate             | 523-87-5   | Allergology            | Antiemetic              | GPCR                | Histamine H1 receptor  | GI tract             |   | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Aminoalkyl ether                  |
| 3712 / 3716                       | F14            | Prestw-266 | Disopyramide               | 3737-09-5  | Cardiovascular         | Antiarrhythmic          | LGIC                | Voltage-gated sodium<br>channel                                | GI tract             | Alpha-1-acid<br>glycoprotein<br>(30-40) | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Antiarrhythmic,<br>class Ia       |
| 3712 / 3716                       | F16            | Prestw-267 | Clotrimazole               | 23593-75-1 | Infectiology           | Antibacterial           |                     |  |                      |   | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Imidazole<br>derivative           |
| 3712 / 3716                       | F18            | Prestw-268 | Vinpocetine                | 42971-09-5 | Cardiovascular         | CNS Stimulant           |                     |  |                      |   |                 |  |                                   |
| 3712 / 3716                       | F20            | Prestw-269 | Clomipramine hydrochloride | 17321-77-6 | Central Nervous System | Antidepressant          |                     |  |                      | Plasmatic<br>proteins                   | Yes             |  |                                   |
| 3712 / 3716                       | F22            | Prestw-270 | Fendiline hydrochloride    | 13636-18-5 | Cardiovascular         | Antianginal             |                     |  |                      |   |                 |  |                                   |
| 3712 / 3716                       | H04            | Prestw-271 | Vincamine                  | 1617-90-9  | Central Nervous System | CNS Stimulant           |                     |  |                      |   |                 |  |                                   |
| 3712 / 3716                       | H06            | Prestw-272 | Indomethacin               | 53-86-1    | Central Nervous System | Analgesic               | Enzyme              | Cyclooxygenase   | GI tract             | Plasmatic<br>proteins                   | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | NSAID                             |
| 3712 / 3716                       | H08            | Prestw-273 | Cortisone                  | 53-06-5    | Endocrinology          | Anti-inflammatory       | Nuclear<br>receptor | Glucocorticoid receptor  |                      |   | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Glucocorticoid                    |
| 3712 / 3716                       | H10            | Prestw-274 | Prednisolone               | 50-24-8    | Endocrinology          | Anti-inflammatory       | Nuclear<br>receptor | Glucocorticoid receptor  |                      |   | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Glucocorticoid                    |
| 3712 / 3716                       | H12            | Prestw-275 | Fenofibrate                | 49562-28-9 | Metabolism             | Hypocholesterole<br>mic | Nuclear<br>receptor | Peroxisome proliferator-<br>activated receptor<br>(PPAR) alpha | GI tract             | Albumin                                 | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Fibrate                           |
| 3712 / 3716                       | H14            | Prestw-276 | Bumetanide                 | 28395-03-1 | Metabolism             | Diuretic                | Carrier             | Solute carrier family 12<br>member 1                           | GI tract             | Plasmatic<br>proteins                   | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | High-ceiling<br>diuretic          |
| 3712 / 3716                       | H16            | Prestw-277 | Labetalol hydrochloride    | 32780-64-6 | Cardiovascular         | Antihypotensive         | GPCR                | Adrenergic receptor<br>alpha                                   | GI tract             | Plasmatic<br>proteins                   | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Alpha and beta<br>blocking agents |
| 3712 / 3716                       | H18            | Prestw-278 | Cinnarizine                | 298-57-7   | Allergology            | Antihistaminic          |                     |  | GI tract             |   |                 |  |                                   |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID  | Chemical_Name                       | CAS number  | Therapeutic class      | Therapeutic effect | Target type           | Target names  | Absorption tissue | Protein binding                    | FDA approved | Additional info type                            | Additional info detail         |
|-----------------------------------|----------------|------------|-------------------------------------|-------------|------------------------|--------------------|-----------------------|---|-------------------|------------------------------------|--------------|---|--------------------------------|
| 3712 / 3716                       | H20            | Prestw-279 | Methylprednisolone, 6-alpha         | 83-43-2     | Endocrinology          | Anti-inflammatory  | Nuclear receptor      | Glucocorticoid receptor                               |                   |                                    | Yes          | Chemical classification (according ATC code)    | Glucocorticoid                 |
| 3712 / 3716                       | H22            | Prestw-280 | Quinidine hydrochloride monohydrate | 6151-40-2   | Cardiovascular         | Antiarrhythmic     |                       |   | GI tract          | Plasmatic proteins                 | Yes          | Therapeutic classification (according ATC code) | Antiarrhythmic, class Ia       |
| 3712 / 3716                       | J04            | Prestw-281 | Fludrocortisone acetate             | 514-36-3    | Dermatology            | Anti-inflammatory  | Nuclear receptor      | Mineralocorticoid receptor                            |                   | Plasmatic proteins                 | Yes          | Chemical classification (according ATC code)    | Mineralocorticoid              |
| 3712 / 3716                       | J06            | Prestw-282 | Fenoterol hydrobromide              | 1944-12-3   | Neuromuscular          | Bronchodilator     | GPCR                  | Adrenergic receptor beta-2                            | Lung, GI tract    |                                    |              |   |                                |
| 3712 / 3716                       | J08            | Prestw-283 | Homochlorcyclizine dihydrochloride  | 1982-36-1   | Allergology            | Antihistaminic     |                       |   |                   |                                    |              |   |                                |
| 3712 / 3716                       | J10            | Prestw-284 | Diethylcarbamazine citrate          | 1642-54-2   | Infectiology           | Anthelmintic       |                       |   | GI tract          |                                    | Yes          |   |                                |
| 3712 / 3716                       | J12            | Prestw-285 | Chenodiol                           | 474-25-9    | Gastroenterology       | Cholagogue         |                       |   |                   |                                    | Yes          |   |                                |
| 3712 / 3716                       | J14            | Prestw-286 | Perhexiline maleate                 | 6724-53-4   | Cardiovascular         | Antianginal        |                       |   | GI tract          | Plasmatic proteins                 |              |   |                                |
| 3712 / 3716                       | J16            | Prestw-287 | Oxybutynin chloride                 | 1508-65-2   | Neuromuscular          | Antispastic        | GPCR                  | Muscarinic acetylcholine receptor M2                  |                   | Albumin                            | Yes          |   |                                |
| 3712 / 3716                       | J18            | Prestw-288 | Spiperone                           | 749-02-0    | Central Nervous System | Antipsychotic      |                       |   |                   |                                    |              | Japan approved                                  |                                |
| 3712 / 3716                       | J20            | Prestw-289 | Pyrilamine maleate                  | 59-33-6     | Allergology            | Antihistaminic     | GPCR                  | Histamine H1 receptor                                 | GI tract          |                                    | Yes          | Chemical classification (according ATC code)    | Substituted ethylene diamine   |
| 3712 / 3716                       | J22            | Prestw-290 | Sulfipyrazone                       | 57-96-5     | Hematology             | Antiplatelet       | Transmembrane protein | Canalicular multispecific organic anion transporter 1 | GI tract          | Plasmatic proteins                 | Yes          | Mechanism                                       | Increasing uric acid excretion |
| 3712 / 3716                       | L04            | Prestw-291 | Dantrolene sodium salt              | 14663-23-1  | Neuromuscular          | Muscle relaxant    | LGIC                  | Ryanodine receptor 1                                  | Intestine         | Plasmatic proteins                 | Yes          |   |                                |
| 3712 / 3716                       | L06            | Prestw-292 | Trazodone hydrochloride             | 25332-39-2  | Central Nervous System | Antidepressant     |                       |   |                   | Plasmatic proteins                 | Yes          |   |                                |
| 3712 / 3716                       | L08            | Prestw-293 | Glafenine hydrochloride             | 65513-72-6  | Metabolism             | Analgesic          |                       |   |                   |                                    |              |   |                                |
| 3712 / 3716                       | L10            | Prestw-294 | Pimethixene maleate                 | 13187-06-9  | Allergology            | Antihistaminic     |                       |   | GI tract          |                                    |              |   |                                |
| 3712 / 3716                       | L12            | Prestw-295 | Pergolide mesylate                  | 66104-23-2  | Central Nervous System | Antiparkinsonian   |                       |   |                   | Plasmatic proteins                 | Yes          |   |                                |
| 3712 / 3716                       | L14            | Prestw-296 | Acemetacin                          | 53164-05-9  | Metabolism             | Anti-inflammatory  | Enzyme                | Cyclooxygenase  | GI tract          |                                    |              | Therapeutic classification (according ATC code) | NSAID                          |
| 3712 / 3716                       | L16            | Prestw-297 | Benzydamine hydrochloride           | 132-69-4    | Central Nervous System | Analgesic          |                       |   |                   |                                    |              | Therapeutic classification (according ATC code) | NSAID                          |
| 3712 / 3716                       | L18            | Prestw-298 | Fipexide hydrochloride              | 34161-23-4  | Central Nervous System | Anti-fatigue       |                       |   |                   |                                    |              |   |                                |
| 3712 / 3716                       | L20            | Prestw-299 | Mifepristone                        | 84371-65-3  | Endocrinology          | Abortifacient      | Nuclear receptor      | Glucocorticoid receptor                               |                   | Albumin, alpha-1-acid glycoprotein | Yes          |   |                                |
| 3712 / 3716                       | L22            | Prestw-300 | Diperodon hydrochloride             | 537-12-2    | Neuromuscular          | Local anesthetic   |                       |   |                   |                                    |              |   |                                |
| 3712 / 3716                       | N04            | Prestw-301 | Lisinopril                          | 83915-83-7  | Cardiovascular         | Antihypertensive   | Enzyme                | Angiotensin-converting enzyme (ACE)                   | GI tract          | Angiotensin-converting enzyme      | Yes          |   |                                |
| 3712 / 3716                       | N06            | Prestw-302 | Lincomycin hydrochloride            | 859-18-7    | Infectiology           | Antibacterial      |                       |   |                   | Plasmatic proteins                 | Yes          | Chemical classification (according ATC code)    | Lincosamide                    |
| 3712 / 3716                       | N08            | Prestw-303 | Telenzepine dihydrochloride         | 147416-96-4 | Gastroenterology       | Antiulcer          |                       |   |                   |                                    |              |   |                                |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID  | Chemical_Name                        | CAS number | Therapeutic class      | Therapeutic<br>effect | Target type               | Target names                             | Absorption<br>tissue | Protein<br>binding          | FDA<br>approved | Additional info<br>type                               | Additional info<br>detail   |
|-----------------------------------|----------------|------------|--------------------------------------|------------|------------------------|-----------------------|---------------------------|--|----------------------|-----------------------------|-----------------|---|---|
| 3712 / 3716                       | N10            | Prestw-304 | Econazole nitrate                    | 24169-02-6 | Infectiology           | Antifungal            |                           |  |                      |                             | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Imidazole<br>derivative   |
| 3712 / 3716                       | N12            | Prestw-305 | Bupivacaine hydrochloride            | 18010-40-7 | Neuromuscular          | Local anesthetic      | Ion channel               | Voltage-gated sodium<br>channel          |                      | Alpha1-acid<br>glycoprotein | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Amides  |
| 3712 / 3716                       | N14            | Prestw-306 | Clemastine fumarate                  | 14976-57-9 | Allergology            | Antiemetic            | GPCR                      | Histamine H1 receptor                    | GI tract             |                             | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Aminoalkyl ether  |
| 3712 / 3716                       | N16            | Prestw-307 | Oxytetracycline dihydrate            | 6153-64-6  | Infectiology           | Antibacterial         |                           |  |                      | Plasmatic<br>proteins       | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Tetracycline  |
| 3712 / 3716                       | N18            | Prestw-308 | Pimozide                             | 2062-78-4  | Central Nervous System | Antipsychotic         |                           |  |                      |                             | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Diphenylbutylpiperidine<br>derivative                                   |
| 3712 / 3716                       | N20            | Prestw-309 | Amodiaquin dihydrochloride dihydrate | 6398-98-7  | Infectiology           | Anti-inflammatory     |                           |  | GI tract             |                             | Yes             |   |   |
| 3712 / 3716                       | N22            | Prestw-310 | Mebeverine hydrochloride             | 2753-45-9  | Neuromuscular          | Antispastic           |                           |  | GI tract             |                             |                 | Chemical<br>classification<br>(according ATC<br>code) | Synthetic<br>anticholinergic,<br>esters with<br>tertiary amino<br>group |
| 3712 / 3716                       | P04            | Prestw-311 | Ifenprodil tartrate                  | 23210-58-4 | Cardiovascular         | Vasodilator           |                           |  |                      |                             |                 |   |   |
| 3712 / 3716                       | P06            | Prestw-312 | Flunarizine dihydrochloride          | 30484-77-6 | Central Nervous System | Anticonvulsant        |                           |  |                      | Plasmatic<br>proteins       |                 |   |   |
| 3712 / 3716                       | P08            | Prestw-313 | Trifluoperazine dihydrochloride      | 440-17-5   | Central Nervous System | Antiemetic            |                           |  |                      |                             | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Phenothiazine<br>derivative   |
| 3712 / 3716                       | P10            | Prestw-314 | Enalapril maleate                    | 76095-16-4 | Cardiovascular         | Antihypertensive      | Enzyme                    | Angiotensin-converting<br>enzyme (ACE)   | GI tract             | Plasmatic<br>proteins       | Yes             |   |   |
| 3712 / 3716                       | P12            | Prestw-315 | Minocycline hydrochloride            | 13614-98-7 | Infectiology           | Antibacterial         |                           |  | GI tract             |                             | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Tetracycline  |
| 3712 / 3716                       | P14            | Prestw-316 | Glibenclamide                        | 10238-21-8 | Endocrinology          | Antidiabetic          | Transmembrane<br>receptor | Sulfonylurea receptors<br>K-ATP channels | GI tract             | Plasmatic<br>proteins       | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Sulfonamide<br>urea derivative  |
| 3712 / 3716                       | P16            | Prestw-317 | Guanethidine sulfate                 | 60-02-6    | Central Nervous System | Antihypertensive      |                           |  | GI tract             |                             | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Guanidine<br>derivative   |
| 3712 / 3716                       | P18            | Prestw-318 | Quinacrine dihydrochloride hydrate   | 69-05-6    | Infectiology           | Anthelmintic          |                           |  |                      |                             |                 | Therapeutic use                                       | Female<br>sterilization   |
| 3712 / 3716                       | P20            | Prestw-319 | Clofilium tosylate                   | 92953-10-1 | Cardiovascular         | Antiarrhythmic        |                           |  |                      |                             |                 |   |   |
| 3712 / 3716                       | P22            | Prestw-320 | Fluphenazine dihydrochloride         | 146-56-5   | Central Nervous System | Antipsychotic         |                           |  |                      | Plasmatic<br>proteins       | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Phenothiazine<br>derivative   |
| 3713 / 3717                       | A03            | Prestw-321 | Streptomycin sulfate                 | 3810-74-0  | Infectiology           | Antibacterial         |                           |  |                      | Plasmatic<br>proteins       | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Streptomycin  |
| 3713 / 3717                       | A05            | Prestw-322 | Alfuzosin hydrochloride              | 81403-68-1 | Cardiovascular         | Vasodilator           | GPCR                      | Adrenergic receptor<br>alpha-1           |                      | Plasmatic<br>proteins       | Yes             |   |   |

| ICCB-L Plate (10 mM / 3.33 mM) | ICCB-L Well | Vendor_ID  | Chemical_Name                    | CAS number    | Therapeutic class      | Therapeutic effect             | Target type            | Target names                             | Absorption tissue | Protein binding    | FDA approved | Additional info type                            | Additional info detail         |
|--------------------------------|-------------|------------|----------------------------------|---------------|------------------------|--------------------------------|------------------------|--|-------------------|--------------------|--------------|---|--------------------------------|
| 3713 / 3717                    | A07         | Prestw-323 | Chlorpropamide                   | 94-20-2       | Endocrinology          | Antidiabetic                   | Transmembrane receptor | Sulfonylurea receptors<br>K-ATP channels | GI tract          | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Sulfonamide urea derivative    |
| 3713 / 3717                    | A09         | Prestw-324 | Phenylpropanolamine hydrochlorid | 154-41-6      | Respiratory            | Antihypotensive                |                        |  |                   |                    | Yes          | Therapeutic classification (according ATC code) | Sympathomimetic                |
| 3713 / 3717                    | A11         | Prestw-325 | Ascorbic acid                    | 50-81-7       | Metabolism             | Anti-oxidant                   |                        |  | GI tract          |                    | Yes          |   |                                |
| 3713 / 3717                    | A13         | Prestw-326 | Methyldopa (L,-)                 | 555-30-6      | Cardiovascular         | Antihypertensive               |                        |  | GI tract          |                    | Yes          |   |                                |
| 3713 / 3717                    | A15         | Prestw-327 | Cefoperazone dihydrate           | not available | Infectiology           | Antibacterial                  |                        |  |                   | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Third-generation cephalosporin |
| 3713 / 3717                    | A17         | Prestw-328 | Zoxazolamine                     | 61-80-3       | Metabolism             | Antigout                       |                        |  |                   |                    |              |   |                                |
| 3713 / 3717                    | A19         | Prestw-329 | Tacrine hydrochloride            | 1684-40-8     | Central Nervous System | CNS Stimulant                  | Enzyme                 | Acetylcholinesterase                     |                   | Plasmatic proteins | Yes          |   |                                |
| 3713 / 3717                    | A21         | Prestw-330 | Bisoprolol fumarate              | 104344-23-2   | Cardiovascular         | Antianginal                    | GPCR                   | Adrenergic receptor beta-1               | GI tract          | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | Selective beta-blocking agent  |
| 3713 / 3717                    | C03         | Prestw-331 | Tremorine dihydrochloride        | 51-73-0       | Central Nervous System | CNS Stimulant                  |                        |  |                   |                    |              | Pharmacological tool                            | Parkinson-like effects         |
| 3713 / 3717                    | C05         | Prestw-332 | Practolol                        | 6673-35-4     | Cardiovascular         | Antianginal                    | GPCR                   | Adrenergic receptor beta-1               |                   |                    |              | Therapeutic classification (according ATC code) | Selective beta-blocking agent  |
| 3713 / 3717                    | C07         | Prestw-333 | Zidovudine, AZT                  | 30516-87-1    | Infectiology           | Antiviral                      |                        |  |                   | Plasmatic proteins | Yes          |   |                                |
| 3713 / 3717                    | C09         | Prestw-334 | Sulfisoxazole                    | 127-69-5      | Infectiology           | Antibacterial                  |                        |  |                   |                    | Yes          | Chemical classification (according ATC code)    | Short-acting sulfonamide       |
| 3713 / 3717                    | C11         | Prestw-335 | Zaprinast                        | 37762-06-4    | Cardiovascular         | Erectile dysfunction treatment |                        |  |                   |                    |              |   |                                |
| 3713 / 3717                    | C13         | Prestw-336 | Chlormezanone                    | 80-77-3       | Central Nervous System | Anxiolytic                     |                        |  |                   |                    | Yes          |   |                                |
| 3713 / 3717                    | C15         | Prestw-337 | Procainamide hydrochloride       | 614-39-1      | Cardiovascular         | Antiarrhythmic                 |                        |  | Intestine         | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | Antiarrhythmic, class Ia       |
| 3713 / 3717                    | C17         | Prestw-338 | N6-methyladenosine               | 1867-73-8     | Oncology               | Antineoplastic                 |                        |  |                   |                    |              | Pharmacological tool                            |                                |
| 3713 / 3717                    | C19         | Prestw-339 | Guanfacine hydrochloride         | 29110-48-3    | Cardiovascular         | Antihypertensive               |                        |  | GI tract          | Plasmatic proteins | Yes          |   |                                |
| 3713 / 3717                    | C21         | Prestw-340 | Domperidone                      | 57808-66-9    | Central Nervous System | Antiemetic                     | GPCR                   | Dopamine receptor                        | GI tract          | Plasmatic proteins |              | Side effect                                     | Risks of sudden death          |
| 3713 / 3717                    | E03         | Prestw-341 | Furosemide                       | 54-31-9       | Metabolism             | Antihypertensive               | Carrier                | Solute carrier family 12 member 1        | GI tract          | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | High-ceiling diuretic          |
| 3713 / 3717                    | E05         | Prestw-342 | Methapyrilene hydrochloride      | 135-23-9      | Allergology            | Antihistaminic                 | GPCR                   | Histamine H1 receptor                    |                   |                    |              | Chemical classification (according ATC code)    | Substituted ethylene diamine   |
| 3713 / 3717                    | E07         | Prestw-343 | Desipramine hydrochloride        | 58-28-6       | Central Nervous System | Antidepressant                 |                        |  |                   |                    | Yes          |   |                                |
| 3713 / 3717                    | E09         | Prestw-344 | Clorgyline hydrochloride         | 17780-75-5    | Central Nervous System | Antidepressant                 |                        |  |                   |                    |              |   |                                |
| 3713 / 3717                    | E11         | Prestw-345 | Clenbuterol hydrochloride        | 21898-19-1    | Neuromuscular          | Antiasthmatic                  | GPCR                   | Adrenergic receptor beta-2               |                   |                    |              | Side effect                                     | Anabolic effects               |
| 3713 / 3717                    | E13         | Prestw-346 | Maprotiline hydrochloride        | 10347-81-6    | Central Nervous System | Antidepressant                 |                        |  |                   | Plasmatic proteins | Yes          |   |                                |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                   | CAS number  | Therapeutic class      | Therapeutic effect | Target type      | Target names               | Absorption tissue | Protein binding    | FDA approved | Additional info type                            | Additional info detail              |
|-----------------------------------|----------------|-------------|---------------------------------|-------------|------------------------|--------------------|------------------|----------------------------|-------------------|--------------------|--------------|---|-------------------------------------|
| 3713 / 3717                       | E15            | Prestw-347  | Thioguanosine                   | 85-31-4     | Metabolism             | Antineoplastic     |                  |                            |                   |                    |              | Pharmacokinetics                                | Prodrug of Thioguanine(L01BB03)     |
| 3713 / 3717                       | E17            | Prestw-348  | Chlorprothixene hydrochloride   | 6469-93-8   | Central Nervous System | Antiemetic         |                  |                            |                   |                    | Yes          | Chemical classification (according ATC code)    | Thioxanthene derivative             |
| 3713 / 3717                       | E19            | Prestw-349  | Ritodrine hydrochloride         | 23239-51-2  | Neuromuscular          | Tocolytic          |                  |                            |                   |                    | Yes          | Therapeutic classification (according ATC code) | Sympathomimetics, labour repressant |
| 3713 / 3717                       | E21            | Prestw-350  | Clozapine                       | 5786-21-0   | Central Nervous System | Antiparkinsonian   |                  |                            |                   |                    | Yes          | Chemical classification (according ATC code)    | Diazepine                           |
| 3713 / 3717                       | G03            | Prestw-351  | Chlorthalidone                  | 77-36-1     | Metabolism             | Antihypertensive   |                  |                            | GI tract          | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | Low-ceiling diuretic                |
| 3713 / 3717                       | G05            | Prestw-352  | Dobutamine hydrochloride        | 49745-95-1  | Cardiovascular         | Analeptic          |                  |                            |                   |                    | Yes          |   |                                     |
| 3713 / 3717                       | G07            | Prestw-353  | Moclobemide                     | 71320-77-9  | Central Nervous System | Antidepressant     | Enzyme           | Monoamine oxidase A        |                   | Albumin            |              |   |                                     |
| 3713 / 3717                       | G09            | Prestw-354  | Clopamide                       | 636-54-4    | Metabolism             | Antihypertensive   |                  |                            | GI tract          | Plasmatic proteins |              | Therapeutic classification (according ATC code) | Low-ceiling diuretic                |
| 3713 / 3717                       | G11            | Prestw-355  | Hycanthone                      | 3105-97-3   | Infectiology           | Anthelmintic       |                  |                            |                   |                    |              |   |                                     |
| 3713 / 3717                       | G13            | Prestw-356  | Adenosine 5'-monophosphate mor  | 18422-05-4  | Cardiovascular         | Antiarrhythmic     |                  |                            | GI tract          |                    |              | Pharmacological tool                            | Endogenous nucleotide               |
| 3713 / 3717                       | G15            | Prestw-357  | Amoxicillin                     | 26787-78-0  | Metabolism             | Antibacterial      |                  |                            | GI tract          | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Penicillin with extended spectrum   |
| 3713 / 3717                       | G17            | Prestw-1603 | Pemirolast potassium            | 100299-08-9 | Ophthalmology          | Anti-inflammatory  |                  |                            |                   |                    | Yes          |   |                                     |
| 3713 / 3717                       | G19            | Prestw-359  | Dextromethorphan hydrobromide n | 6700-34-1   | Central Nervous System | Antitussive        |                  |                            | GI tract          |                    | Yes          | Chemical classification (according ATC code)    | Opium alkaloid derivative           |
| 3713 / 3717                       | G21            | Prestw-360  | Droperidol                      | 548-73-2    | Central Nervous System | Antipsychotic      |                  |                            |                   | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Butyrophenone derivative            |
| 3713 / 3717                       | I03            | Prestw-361  | Bambuterol hydrochloride        | 81732-46-9  | Neuromuscular          | Bronchodilator     | GPCR             | Adrenergic receptor beta-2 | GI tract          |                    | Yes          |   |                                     |
| 3713 / 3717                       | I05            | Prestw-362  | Betamethasone                   | 378-44-9    | Endocrinology          | Anti-inflammatory  | Nuclear receptor | Glucocorticoid receptor    |                   | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Glucocorticoid                      |
| 3713 / 3717                       | I07            | Prestw-363  | Colchicine                      | 64-86-8     | Metabolism             | Antigout           | Protein          | Tubulin beta chain         | GI tract          | Plasmatic proteins | Yes          |   |                                     |
| 3713 / 3717                       | I09            | Prestw-364  | Metergoline                     | 17692-51-2  | Central Nervous System | Antiprolactin      |                  |                            |                   |                    |              |   |                                     |
| 3713 / 3717                       | I11            | Prestw-365  | Brinzolamide                    | 138890-62-7 | Metabolism             | Antiglaucoma       | Enzyme           | Carbonic anhydrase         | Eye               | Plasmatic proteins | Yes          |   |                                     |
| 3713 / 3717                       | I13            | Prestw-366  | Ambroxol hydrochloride          | 23828-92-4  | Respiratory            | Expectorant        |                  |                            | GI tract          | Plasmatic proteins |              |   |                                     |
| 3713 / 3717                       | I15            | Prestw-367  | Benfluorex                      | 23602-78-0  | Central Nervous System | Anorectic          |                  |                            | GI tract          |                    |              |   |                                     |
| 3713 / 3717                       | I17            | Prestw-368  | Bepidil hydrochloride           | 74764-40-2  | Cardiovascular         | Antianginal        |                  |                            |                   |                    | Yes          |   |                                     |
| 3713 / 3717                       | I19            | Prestw-369  | Meloxicam                       | 71125-38-7  | Metabolism             | Anti-inflammatory  | Enzyme           | Cyclooxygenase-2           | GI tract          | Albumin            | Yes          | Therapeutic classification (according ATC code) | NSAID                               |

| ICCB-L Plate (10 mM / 3.33 mM) | ICCB-L Well | Vendor_ID   | Chemical_Name                | CAS number | Therapeutic class      | Therapeutic effect | Target type      | Target names  | Absorption tissue | Protein binding                      | FDA approved | Additional info type                            | Additional info detail         |
|--------------------------------|-------------|-------------|------------------------------|------------|------------------------|--------------------|------------------|---|-------------------|--------------------------------------|--------------|---|--------------------------------|
| 3713 / 3717                    | I21         | Prestw-370  | Benzbromarone                | 3562-84-3  | Cardiovascular         | Antianginal        |                  |   | GI tract          | Plasmatic proteins                   |              | Mechanism                                       | Increasing uric acid excretion |
| 3713 / 3717                    | K03         | Prestw-371  | Ketotifen fumarate           | 34580-14-8 | Allergology            | Antihistaminic     | GPCR             | Histamine H1 receptor                                   | GI tract          | Plasmatic proteins                   | Yes          |   |                                |
| 3713 / 3717                    | K05         | Prestw-372  | Debrisoquin sulfate          | 581-88-4   | Cardiovascular         | Antihypertensive   |                  |   | GI tract          |                                      |              | Chemical classification (according ATC code)    | Guanidine derivative           |
| 3713 / 3717                    | K07         | Prestw-373  | Amethopterin (R,S)           | 60388-53-6 | Immunology             | Anti-inflammatory  | Enzyme           | Dihydrofolate reductase                                 |                   | Plasmatic proteins                   |              | Chemical classification (according ATC code)    | Folic acid analogue            |
| 3713 / 3717                    | K09         | Prestw-374  | Methylergometrine maleate    | 57432-61-8 | Neuromuscular          | Hemostatic         |                  |   |                   |                                      |              | Chemical classification (according ATC code)    | Ergot alkaloid                 |
| 3713 / 3717                    | K11         | Prestw-375  | Methiothepin maleate         | 19728-88-2 | Central Nervous System | Antipsychotic      |                  |   |                   |                                      |              |   |                                |
| 3713 / 3717                    | K13         | Prestw-376  | Clofazimine                  | 2030-63-9  | Infectiology           | Antibacterial      |                  |   | GI tract          |                                      | Yes          |   |                                |
| 3713 / 3717                    | K15         | Prestw-377  | Nafronyl oxalate             | 3200-06-4  | Cardiovascular         | Anti-ischemic      |                  |   | GI tract          | Plasmatic proteins                   |              |   |                                |
| 3713 / 3717                    | K17         | Prestw-378  | Bezafibrate                  | 41859-67-0 | Metabolism             | Antilipemic        | Nuclear receptor | Peroxisome proliferator-activated receptor (PPAR) alpha | GI tract          | Plasmatic proteins                   |              | Therapeutic classification (according ATC code) | Fibrate                        |
| 3713 / 3717                    | K19         | Prestw-1152 | Nefazodone hydrochloride     | 82752-99-6 | Central Nervous System | Antidepressant     |                  |   |                   | Plasmatic proteins                   | Yes          |   |                                |
| 3713 / 3717                    | K21         | Prestw-380  | Clebopride maleate           | 84370-95-6 | Central Nervous System | Antiemetic         |                  |   |                   |                                      |              | Therapeutic classification (according ATC code) | Propulsive                     |
| 3713 / 3717                    | M03         | Prestw-381  | Lidoflazine                  | 3416-26-0  | Cardiovascular         | Antianginal        |                  |   |                   |                                      |              |   |                                |
| 3713 / 3717                    | M05         | Prestw-382  | Betaxolol hydrochloride      | 63659-19-8 | Cardiovascular         | Antiglaucoma       | GPCR             | Adrenergic receptor beta-1                              | GI tract          | Plasmatic proteins                   | Yes          | Therapeutic classification (according ATC code) | Selective beta-blocking agent  |
| 3713 / 3717                    | M07         | Prestw-383  | Nicardipine hydrochloride    | 54527-84-3 | Cardiovascular         | Antianginal        | Ion channel      | Voltage-gated L-type calcium channel                    | GI tract          | Alpha-acid glycoprotein, lipoprotein | Yes          | Chemical classification (according ATC code)    | Dihydropyridine derivatives    |
| 3713 / 3717                    | M09         | Prestw-384  | Probucol                     | 23288-49-5 | Metabolism             | Antilipemic        |                  |   | GI tract          |                                      | Yes          |   |                                |
| 3713 / 3717                    | M11         | Prestw-385  | Mitoxantrone dihydrochloride | 70476-82-3 | Oncology               | Antineoplastic     |                  |   |                   | Plasmatic proteins                   | Yes          | Chemical classification (according ATC code)    | Anthracycline derivative       |
| 3713 / 3717                    | M13         | Prestw-386  | GBR 12909 dihydrochloride    | 67469-78-7 | Central Nervous System | Antidepressant     |                  |   |                   |                                      |              |   |                                |
| 3713 / 3717                    | M15         | Prestw-387  | Carbetapentane citrate       | 23142-01-0 | Central Nervous System | Antispastic        |                  |   | GI tract          |                                      |              |   |                                |
| 3713 / 3717                    | M17         | Prestw-388  | Dequalinium dichloride       | 522-51-0   | Infectiology           | Antibacterial      |                  |   | Skin              |                                      |              | Chemical classification (according ATC code)    | Quinoline derivative           |
| 3713 / 3717                    | M19         | Prestw-389  | Ketoconazole                 | 65277-42-1 | Infectiology           | Antifungal         |                  |   |                   | albumin                              | Yes          | Chemical classification (according ATC code)    | Imidazole derivative           |
| 3713 / 3717                    | M21         | Prestw-390  | Fusidic acid sodium salt     | 751-94-0   | Infectiology           | Antibacterial      |                  |   |                   |                                      |              | Chemical classification (according ATC code)    | Steroid antibacterial          |
| 3713 / 3717                    | O03         | Prestw-391  | Terbutaline hemisulfate      | 23031-32-5 | Respiratory            | Antiasthmatic      | GPCR             | Adrenergic receptor beta-2                              | Lung              | Plasmatic proteins                   | Yes          |   |                                |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name               | CAS number  | Therapeutic class      | Therapeutic<br>effect | Target type         | Target names                            | Absorption<br>tissue | Protein<br>binding  | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail                   |
|-----------------------------------|----------------|-------------|-----------------------------|-------------|------------------------|-----------------------|---------------------|---|----------------------|---|-----------------|--|---|
| 3713 / 3717                       | O05            | Prestw-392  | Ketanserin tartrate hydrate | 83846-83-7  | Cardiovascular         | Antihypertensive      |                     |   | GI tract             | Plasmatic<br>proteins   |                 |  |   |
| 3713 / 3717                       | O07            | Prestw-393  | Hemicholinium bromide       | 312-45-8    | Neuromuscular          | Curarizing            |                     |   |                      |   |                 | Pharmacological<br>tool                                  |   |
| 3713 / 3717                       | O09            | Prestw-394  | Kanamycin A sulfate         | 25389-94-0  | Infectiology           | Antibacterial         |                     |   |                      |   | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Aminoside                                   |
| 3713 / 3717                       | O11            | Prestw-395  | Amikacin hydrate            | 37517-28-5  | Infectiology           | Antibacterial         |                     |   |                      | Plasmatic<br>proteins   | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Aminoside                                   |
| 3713 / 3717                       | O13            | Prestw-396  | Etoposide                   | 33419-42-0  | Oncology               | Antineoplastic        | Enzyme              | DNA topoisomerase II                    |                      | Plasmatic<br>proteins   | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Podophyllotoxin<br>derivative               |
| 3713 / 3717                       | O15            | Prestw-397  | Clomiphene citrate (Z,E)    | 50-41-9     | Endocrinology          |                       |                     |   | GI tract             |   | Yes             |  |   |
| 3713 / 3717                       | O17            | Prestw-398  | Oxantel pamoate             | 68813-55-8  | Infectiology           | Anthelmintic          |                     |   |                      |   |                 |  |   |
| 3713 / 3717                       | O19            | Prestw-399  | Prochlorperazine dimaleate  | 84-02-6     | Central Nervous System | Antiemetic            |                     |   |                      |   | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Phenothiazine<br>derivative                 |
| 3713 / 3717                       | O21            | Prestw-400  | Hesperidin                  | 520-26-3    | Oncology               | Anti-haemorrhoids     |                     |   |                      |   |                 |  |   |
| 3713 / 3717                       | A04            | Prestw-401  | Testosterone propionate     | 57-85-2     | Endocrinology          | Anabolic              |                     |   |                      |   | Yes             |  |   |
| 3713 / 3717                       | A06            | Prestw-1269 | Haloprogin                  | 777-11-7    | Infectiology           | Antifungal            |                     |   |                      |   | Yes             |  |   |
| 3713 / 3717                       | A08            | Prestw-403  | Thyroxine (L)               | 51-48-9     | Endocrinology          | Antihypothyroid       | Nuclear<br>receptor | Thyroid hormone<br>receptor             |                      | Thyroxine<br>Binding<br>Globuline<br>(TBG),<br>Thyroxine<br>Binding Pre-<br>Albumin<br>(TBPA),<br>Albumin | Yes             | Therapeutic use  | Lipid-lowering<br>due to<br>hyperthyroidism |
| 3713 / 3717                       | A10            | Prestw-1288 | Idebenone                   | 58186-27-9  | Oncology               | Antineoplastic        |                     |   |                      | Plasmatic<br>proteins   |                 |  |   |
| 3713 / 3717                       | A12            | Prestw-405  | Pepstatin A                 | 26305-03-3  | Infectiology           | Antiviral             |                     |   |                      |   |                 | Pharmacological<br>tool                                  |   |
| 3713 / 3717                       | A14            | Prestw-1796 | Delavirdine                 | 136817-59-9 | Infectiology           |                       |                     |   |                      |   | Yes             |  |   |
| 3713 / 3717                       | A16            | Prestw-407  | Adamantamine fumarate       | 80789-67-9  | Infectiology           | Antiviral             |                     |   |                      | Plasmatic<br>proteins   | Yes             |  |   |
| 3713 / 3717                       | A18            | Prestw-408  | Butoconazole nitrate        | 32872-77-1  | Infectiology           | Antibacterial         |                     |   |                      |   | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Imidazole<br>derivative                     |
| 3713 / 3717                       | A20            | Prestw-409  | Amiodarone hydrochloride    | 19774-82-4  | Cardiovascular         | Antianginal           |                     |   | GI tract             | Plasmatic<br>proteins   | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Antiarrhythmic,<br>class III                |
| 3713 / 3717                       | A22            | Prestw-410  | Amphotericin B              | 1397-89-3   | Infectiology           | Antibacterial         |                     |   |                      |   | Yes             |  |   |
| 3713 / 3717                       | C04            | Prestw-411  | Androsterone                | 53-41-8     | Endocrinology          | Anabolic              |                     |   |                      |   |                 |  |   |
| 3713 / 3717                       | C06            | Prestw-1489 | Amifostine                  | 20537-88-6  | Diagnostic             |                       |                     |   |                      |   | Yes             |  |   |
| 3713 / 3717                       | C08            | Prestw-413  | Carbarosone                 | 121-59-5    | Infectiology           | Antiamoebic           |                     |   |                      |   |                 | Veterinary use   | Poultry                                     |
| 3713 / 3717                       | C10            | Prestw-1219 | Amlodipine                  | 88150-42-9  | Cardiovascular         | Antihypertensive      | Ion channel         | Voltage-gated L-type<br>calcium channel | GI tract             | Plasmatic<br>proteins   | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Dihydropyridine<br>derivatives              |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                    | CAS number  | Therapeutic class      | Therapeutic<br>effect | Target type         | Target names                                | Absorption<br>tissue | Protein<br>binding                      | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail                        |
|-----------------------------------|----------------|-------------|----------------------------------|-------------|------------------------|-----------------------|---------------------|---|----------------------|---|-----------------|--|--|
| 3713 / 3717                       | C12            | Prestw-1147 | Modafinil                        | 68693-11-8  | Central Nervous System | CNS Stimulant         |                     |   |                      | Plasmatic<br>proteins                   | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Centrally acting<br>sympathomimetic              |
| 3713 / 3717                       | C14            | Prestw-416  | Bacampicillin hydrochloride      | 37661-08-8  | Infectiology           | Antibacterial         |                     |   |                      |   | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Penicillin with<br>extended<br>spectrum          |
| 3713 / 3717                       | C16            | Prestw-1298 | Lamivudine                       | 134678-17-4 | Infectiology           | Antiviral             |                     |   |                      | Plasmatic<br>proteins                   | Yes             |  |  |
| 3713 / 3717                       | C18            | Prestw-418  | Biotin                           | 58-85-5     | Metabolism             |                       |                     |   |                      |   | Yes             |  |  |
| 3713 / 3717                       | C20            | Prestw-419  | Bisacodyl                        | 603-50-9    | Gastroenterology       | Laxative              |                     |   |                      |   | Yes             |  |  |
| 3713 / 3717                       | C22            | Prestw-1242 | Erlotinib                        | 183321-74-6 | Oncology               | Antineoplastic        | Enzyme              | Receptor tyrosine-<br>protein kinase erbB-1 |                      | Albumin,<br>alpha1-acid<br>glycoprotein | Yes             |  |  |
| 3713 / 3717                       | E04            | Prestw-421  | Sulcotidil                       | 54063-56-8  | Neuromuscular          | Antiplatelet          |                     |   |                      |   |                 |  |  |
| 3713 / 3717                       | E06            | Prestw-1368 | Zotepine                         | 26615-21-4  | Central Nervous System | Antipsychotic         |                     |   |                      | Plasmatic<br>proteins                   |                 |  |  |
| 3713 / 3717                       | E08            | Prestw-423  | Carisoprodol                     | 78-44-4     | Central Nervous System | Analgesic             |                     |   | GI tract             |   | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Carbamic acid<br>ester                           |
| 3713 / 3717                       | E10            | Prestw-424  | Cephalosporanic acid, 7-amino    | 957-68-6    | Infectiology           | Antibacterial         |                     |   |                      |   |                 |  |  |
| 3713 / 3717                       | E12            | Prestw-425  | Chicago sky blue 6B              | 2610-05-1   | Central Nervous System |                       |                     |   |                      |   |                 | Pharmacological<br>tool                                  | Vital stain                                      |
| 3713 / 3717                       | E14            | Prestw-426  | Buflomedil hydrochloride         | 35543-24-9  | Cardiovascular         | Vasodilator           |                     |   | GI tract             |   |                 |  |  |
| 3713 / 3717                       | E16            | Prestw-1393 | Dibenzepine hydrochloride        | 315-80-0    | Central Nervous System | Antidepressant        |                     |   |                      |   |                 |  |  |
| 3713 / 3717                       | E18            | Prestw-428  | Roxatidine Acetate hydrochloride | 93793-83-0  | Gastroenterology       | Antiulcer             |                     |   | GI tract             |   |                 |  |  |
| 3713 / 3717                       | E20            | Prestw-1505 | Valacyclovir hydrochloride       | 124832-27-5 | Infectiology           | Antiviral             |                     |   |                      |   | Yes             |  |  |
| 3713 / 3717                       | E22            | Prestw-430  | Cisapride                        | 81098-60-4  | Gastroenterology       | Gastroprokinetic      | GPCR                | Serotonin 4 (5-HT4)<br>receptor             | GI tract             | Plasmatic<br>proteins                   | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Propulsive                                       |
| 3713 / 3717                       | G04            | Prestw-1303 | Pefloxacin                       | 70458-92-3  | Infectiology           | Antibacterial         |                     |   |                      | Plasmatic<br>proteins                   |                 | Chemical<br>classification<br>(according ATC<br>code)    | Fluoroquinolone                                  |
| 3713 / 3717                       | G06            | Prestw-432  | Corticosterone                   | 50-22-6     | Endocrinology          | Anti-inflammatory     |                     |   |                      |   |                 |  |  |
| 3713 / 3717                       | G08            | Prestw-433  | Cyanocobalamin                   | 68-19-9     | Metabolism             | Analgesic             |                     |   | Ileum                |   | Yes             | Therapeutic use  | Analgesic  |
| 3713 / 3717                       | G10            | Prestw-434  | Cefadroxil                       | 50370-12-2  | Infectiology           | Antibacterial         |                     |   | GI tract             |   | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | First-generation<br>cephalosporin                |
| 3713 / 3717                       | G12            | Prestw-435  | Cyclosporin A                    | 59865-13-3  | Immunology             | Immunosuppressant     |                     |   |                      | Lipoproteins                            | Yes             |  |  |
| 3713 / 3717                       | G14            | Prestw-436  | Digitoxigenin                    | 143-62-4    | Cardiovascular         | Cardiotonic           |                     |   |                      |   |                 |  |  |
| 3713 / 3717                       | G16            | Prestw-437  | Digoxin                          | 20830-75-5  | Cardiovascular         | Cardiotonic           |                     |   | GI tract             |   | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Digitalis<br>glycoside                           |
| 3713 / 3717                       | G18            | Prestw-438  | Doxorubicin hydrochloride        | 25316-40-9  | Infectiology           | Antibacterial         | DNA                 |   |                      |   | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Anthracycline                                    |
| 3713 / 3717                       | G20            | Prestw-439  | Carbimazole                      | 22232-54-8  | Metabolism             | Antihyperthyroid      | Enzyme              | Thyroid peroxidase                          |                      |   |                 | Chemical<br>classification<br>(according ATC<br>code)    | Sulfur-<br>containing<br>imidazole<br>derivative |
| 3713 / 3717                       | G22            | Prestw-440  | Epiandrosterone                  | 481-29-8    | Endocrinology          | Anabolic              |                     |   |                      |   |                 |  |  |
| 3713 / 3717                       | I04            | Prestw-441  | Estradiol-17 beta                | 50-28-2     | Endocrinology          | Antigonadotropin      | Nuclear<br>receptor | Estrogen receptor                           |                      |   | Yes             |  |  |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                     | CAS number  | Therapeutic class      | Therapeutic<br>effect | Target type         | Target names                    | Absorption<br>tissue      | Protein<br>binding   | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail                                 |
|-----------------------------------|----------------|-------------|-----------------------------------|-------------|------------------------|-----------------------|---------------------|---------------------------------|---------------------------|--|-----------------|--|---|
| 3713 / 3717                       | I06            | Prestw-1380 | Clobutinol hydrochloride          | 1215-83-4   | Central Nervous System | Antitussive           |                     |                                 |                           |  |                 |  |   |
| 3713 / 3717                       | I08            | Prestw-443  | Gabazine bromide                  | 105538-73-6 | Central Nervous System | CNS Stimulant         |                     |                                 |                           |  |                 | Pharmacological<br>tool                                  |   |
| 3713 / 3717                       | I10            | Prestw-1156 | Oxcarbazepine                     | 28721-07-5  | Central Nervous System | Anticonvulsant        | Ion channel         | Voltage-gated sodium<br>channel |                           | Albumin  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Carboxamide<br>derivatives                                |
| 3713 / 3717                       | I12            | Prestw-445  | Cyclobenzaprine hydrochloride     | 6202-23-9   | Neuromuscular          | Muscle relaxant       |                     |                                 | GI tract                  | Plasmatic<br>proteins  | Yes             |  |   |
| 3713 / 3717                       | I14            | Prestw-446  | Carteolol hydrochloride           | 51781-21-6  | Cardiovascular         | Antiglaucoma          | GPCR                | Adrenergic receptor<br>beta     | Eye, Systemic circulation |  | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Non-selective<br>beta-blocking<br>agent                   |
| 3713 / 3717                       | I16            | Prestw-447  | Hydrocortisone base               | 50-23-7     | Endocrinology          | Anti-inflammatory     | Nuclear<br>receptor | Glucocorticoid receptor         |                           |  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Glucocorticoid  |
| 3713 / 3717                       | I18            | Prestw-448  | Hydroxytacrine maleate (R,S)      | 118909-22-1 | Central Nervous System | Anti-Alzheimer        |                     |                                 |                           |  |                 | Pharmacokinetics   | Active<br>metabolite of<br>Tacrine<br>(withdrawn<br>drug) |
| 3713 / 3717                       | I20            | Prestw-449  | Pilocarpine nitrate               | 148-72-1    | Ophthalmology          | Antiglaucoma          |                     |                                 |                           |  | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Parasympathom<br>imetic                                   |
| 3713 / 3717                       | I22            | Prestw-450  | Dicloxacillin sodium salt hydrate | 13412-64-1  | Infectiology           | Antibacterial         |                     |                                 |                           |  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Beta-lactamase<br>resistant<br>penicillin                 |
| 3713 / 3717                       | K04            | Prestw-451  | Alizapride hydrochloride          | 59338-87-3  | Central Nervous System | Antiemetic            |                     |                                 | GI tract                  |  |                 | Therapeutic<br>classification<br>(according ATC<br>code) | Propulsive  |
| 3713 / 3717                       | K06            | Prestw-1161 | Stanozolol                        | 10418-03-8  | Endocrinology          |                       |                     |                                 | GI tract                  |  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Androstan<br>derivative                                   |
| 3713 / 3717                       | K08            | Prestw-1257 | Calcipotriene                     | 112965-21-6 | Dermatology            | Antipsoriatic         |                     |                                 | Skin                      |  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Vitamin D<br>analog                                       |
| 3713 / 3717                       | K10            | Prestw-1429 | Linezolid                         | 165800-03-3 | Infectiology           | Antibacterial         |                     |                                 |                           | Plasmatic<br>proteins  | Yes             |  |   |
| 3713 / 3717                       | K12            | Prestw-455  | Mebhydroline 1,5-naphtalenedisulf | 6153-33-9   | Allergology            | Antihistaminic        | GPCR                | Histamine H1 receptor           |                           |  |                 |  |   |
| 3713 / 3717                       | K14            | Prestw-456  | Meclocycline sulfosalicylate      | 73816-42-9  | Infectiology           | Antibacterial         |                     |                                 |                           |  | Yes             |  |   |
| 3713 / 3717                       | K16            | Prestw-457  | Meclozine dihydrochloride         | 1104-22-9   | Allergology            | Antiemetic            | GPCR                | Histamine H1 receptor           | GI tract                  |  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Piperazine<br>derivative                                  |
| 3713 / 3717                       | K18            | Prestw-458  | Melatonin                         | 73-31-4     | Central Nervous System | Anticonvulsant        | GPCR                | Melatonin receptor              |                           | Albumin,<br>alpha-1-acid<br>glycoprotein,<br>high density<br>lipoprotein |                 |  |   |
| 3713 / 3717                       | K20            | Prestw-1251 | Butalbital                        | 77-26-9     | Central Nervous System | Hypnotic              |                     |                                 |                           |  | Yes             |  |   |
| 3713 / 3717                       | K22            | Prestw-460  | Dinoprost trometamol              | 38362-01-5  | Endocrinology          | Oxytocic              |                     |                                 |                           | Albumin  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Prostaglandin   |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name              | CAS number  | Therapeutic class      | Therapeutic<br>effect | Target type         | Target names                            | Absorption<br>tissue | Protein<br>binding    | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail   |
|-----------------------------------|----------------|-------------|----------------------------|-------------|------------------------|-----------------------|---------------------|---|----------------------|-----------------------|-----------------|--|---|
| 3713 / 3717                       | M04            | Prestw-461  | Tropisetron hydrochloride  | 105826-92-4 | Central Nervous System | Antiemetic            | LGIC                | Serotonin 3 (5-HT3)<br>receptor         | GI tract             |                       |                 |  |   |
| 3713 / 3717                       | M06            | Prestw-462  | Cefixime                   | 79350-37-1  | Infectiology           | Antibacterial         |                     |   | GI tract             | Albumin               | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Third-generation<br>cephalosporin   |
| 3713 / 3717                       | M08            | Prestw-463  | Metrizamide                | 31112-62-6  | Diagnostic             | Contrastant           |                     |   |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Watersoluble,<br>nephrotropic,<br>low osmolar X-<br>ray contrast<br>media |
| 3713 / 3717                       | M10            | Prestw-1323 | Quetiapine hemifumarate    | 111974-72-2 | Central Nervous System | Antipsychotic         |                     |   |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Thiazepine  |
| 3713 / 3717                       | M12            | Prestw-1464 | Tosufloxacin hydrochloride | 100490-36-6 | Infectiology           | Antibacterial         |                     |   |                      |                       |                 |  |   |
| 3713 / 3717                       | M14            | Prestw-1400 | Efavirenz                  | 154598-52-4 | Infectiology           | Antiviral             |                     |   |                      | Albumin               | Yes             |  |   |
| 3713 / 3717                       | M16            | Prestw-1157 | Rifapentine                | 61379-65-5  | Infectiology           | Antibacterial         |                     |   |                      |                       | Yes             |  |   |
| 3713 / 3717                       | M18            | Prestw-468  | Neostigmine bromide        | 114-80-7    | Diagnostic             | Anti-fatigue          | Enzyme              | Acetylcholinesterase                    |                      |                       | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Parasympathom<br>imetic   |
| 3713 / 3717                       | M20            | Prestw-469  | Niridazole                 | 61-57-4     | Infectiology           | Anthelmintic          |                     |   |                      |                       |                 |  |   |
| 3713 / 3717                       | M22            | Prestw-470  | Ceforanide                 | 60925-61-3  | Infectiology           | Antibacterial         |                     |   |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Second-<br>generation<br>cephalosporin                                    |
| 3713 / 3717                       | O04            | Prestw-1358 | Vatalanib                  | 212141-54-3 | Oncology               | Antineoplastic        |                     |   |                      |                       |                 |  |   |
| 3713 / 3717                       | O06            | Prestw-1295 | Itopride                   | 122898-67-3 | Metabolism             |                       |                     |   |                      |                       |                 |  |   |
| 3713 / 3717                       | O08            | Prestw-473  | Cefotetan                  | 69712-56-7  | Infectiology           | Antibacterial         |                     |   |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Second-<br>generation<br>cephalosporin                                    |
| 3713 / 3717                       | O10            | Prestw-1254 | Fentiazac                  | 18046-21-4  | Metabolism             | Anti-inflammatory     | Enzyme              | Cyclooxygenase                          |                      |                       |                 | Therapeutic<br>classification<br>(according ATC<br>code) | NSAID   |
| 3713 / 3717                       | O12            | Prestw-475  | Brompheniramine maleate    | 980-71-2    | Allergology            | Antihistaminic        | GPCR                | Histamine H1 receptor                   | GI tract             | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Substituted<br>alkylamine   |
| 3713 / 3717                       | O14            | Prestw-476  | Primaquine diphosphate     | 63-45-6     | Infectiology           | Antimalarial          |                     |   | GI tract             | Plasmatic<br>proteins | Yes             |  |   |
| 3713 / 3717                       | O16            | Prestw-477  | Progesterone               | 57-83-0     | Endocrinology          | Progestogen           | Nuclear<br>receptor | Progesterone receptor                   |                      | Plasmatic<br>proteins | Yes             |  |   |
| 3713 / 3717                       | O18            | Prestw-478  | Felodipine                 | 72509-76-3  | Neuromuscular          | Antianginal           | Ion channel         | Voltage-gated L-type<br>calcium channel | GI tract             | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Dihydropyridine<br>derivatives  |
| 3713 / 3717                       | O20            | Prestw-1325 | Raclopride                 | 84225-95-6  | Central Nervous System |                       |                     |   |                      |                       |                 |  |   |
| 3713 / 3717                       | O22            | Prestw-1385 | Closantel                  | 57808-65-8  | Infectiology           | Anthelmintic          |                     |   |                      | Albumin               |                 | Veterinary use   | Cattle  |
| 3713 / 3717                       | B03            | Prestw-481  | Serotonin hydrochloride    | 153-98-0    | Central Nervous System | CNS Stimulant         |                     |   |                      |                       |                 | Pharmacological<br>tool                                  | Endogenous<br>monoamine<br>neurotransmitter                               |
| 3713 / 3717                       | B05            | Prestw-482  | Cefotiam hydrochloride     | 61622-34-2  | Infectiology           | Antibacterial         |                     |   |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Second-<br>generation<br>cephalosporin                                    |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name              | CAS number  | Therapeutic class      | Therapeutic<br>effect | Target type | Target names       | Absorption<br>tissue | Protein<br>binding    | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail                                      |
|-----------------------------------|----------------|-------------|----------------------------|-------------|------------------------|-----------------------|-------------|--------------------|----------------------|-----------------------|-----------------|--|--|
| 3713 / 3717                       | B07            | Prestw-1336 | Rofecoxib                  | 162011-90-7 | Metabolism             | Anti-inflammatory     | Enzyme      | Cyclooxygenase-2   | GI tract             | Plasmatic<br>proteins | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | NSAID  |
| 3713 / 3717                       | B09            | Prestw-484  | Benperidol                 | 2062-84-2   | Central Nervous System | Antipsychotic         |             |                    |                      |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Butyrophenone<br>derivative                                    |
| 3713 / 3717                       | B11            | Prestw-485  | Cefaclor hydrate           | 70356-03-5  | Infectiology           | Antibacterial         |             |                    | GI tract             |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Second-<br>generation<br>cephalosporin                         |
| 3713 / 3717                       | B13            | Prestw-486  | Colistin sulfate           | 1264-72-8   | Infectiology           | Antibacterial         |             |                    |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Polymyxin  |
| 3713 / 3717                       | B15            | Prestw-487  | Daunorubicin hydrochloride | 23541-50-6  | Infectiology           | Antibacterial         | DNA         |                    |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Anthracycline  |
| 3713 / 3717                       | B17            | Prestw-488  | Dosulepin hydrochloride    | 897-15-4    | Central Nervous System | Antidepressant        |             |                    |                      |                       |                 |  |  |
| 3713 / 3717                       | B19            | Prestw-489  | Ceftazidime pentahydrate   | 78439-06-2  | Infectiology           | Antibacterial         |             |                    |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Third-generation<br>cephalosporin                              |
| 3713 / 3717                       | B21            | Prestw-490  | Iobenguane sulfate         | 103346-16-3 | Oncology               | Antineoplastic        |             |                    | Liver, Lung          |                       | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Diagnostic<br>radiopharmaceu-<br>tical for tumour<br>detection |
| 3713 / 3717                       | D03            | Prestw-491  | Metixene hydrochloride     | 1553-34-0   | Central Nervous System | Antiparkinsonian      |             |                    |                      |                       |                 | Therapeutic<br>classification<br>(according ATC<br>code) | Anticholinergic<br>agent                                       |
| 3713 / 3717                       | D05            | Prestw-492  | Nitrofurantoin             | 59-87-0     | Infectiology           | Antibacterial         |             |                    | GI tract, Skin       |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Nitrofurantoin<br>derivative                                   |
| 3713 / 3717                       | D07            | Prestw-493  | Omeprazole                 | 73590-58-6  | Gastroenterology       | Antiulcer             | Enzyme      | H+/K+ ATPase       | Small intestine      | Plasmatic<br>proteins | Yes             |  |  |
| 3713 / 3717                       | D09            | Prestw-494  | Propylthiouracil           | 51-52-5     | Metabolism             | Antihyperthyroid      | Enzyme      | Thyroid peroxidase |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Thiouracil   |
| 3713 / 3717                       | D11            | Prestw-495  | Terconazole                | 67915-31-5  | Infectiology           | Antifungal            |             |                    |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Triazole<br>derivative   |
| 3713 / 3717                       | D13            | Prestw-496  | Tiaprofenic acid           | 33005-95-7  | Central Nervous System | Analgesic             | Enzyme      | Cyclooxygenase     | GI tract             | Plasmatic<br>proteins |                 | Therapeutic<br>classification<br>(according ATC<br>code) | NSAID  |
| 3713 / 3717                       | D15            | Prestw-497  | Vancomycin hydrochloride   | 1404-93-9   | Infectiology           | Antibacterial         |             |                    |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Glycopeptide   |
| 3713 / 3717                       | D17            | Prestw-498  | Artemisinin                | 63968-64-9  | Infectiology           | Antimalarial          |             |                    |                      |                       |                 |  |  |
| 3713 / 3717                       | D19            | Prestw-499  | Propafenone hydrochloride  | 34183-22-7  | Cardiovascular         | Antiarrhythmic        |             |                    | GI tract             |                       | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Antiarrhythmic,<br>class Ic                                    |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                        | CAS number   | Therapeutic class      | Therapeutic<br>effect | Target type | Target names                        | Absorption<br>tissue | Protein<br>binding | FDA<br>approved | Additional info<br>type                         | Additional info<br>detail                                    |
|-----------------------------------|----------------|-------------|--------------------------------------|--------------|------------------------|-----------------------|-------------|-------------------------------------|----------------------|--------------------|-----------------|---|--|
| 3713 / 3717                       | D21            | Prestw-500  | Ethamivan                            | 304-84-7     | Central Nervous System | Analeptic             |             |                                     |                      |                    |                 |   |  |
| 3713 / 3717                       | F03            | Prestw-501  | Vigabatrin hydrochloride             | 1391054-02-6 | Central Nervous System | Anticonvulsant        | Enzyme      | Gamma-amino-N-butyrate transaminase |                      | Plasmatic proteins | Yes             | Chemical classification (according ATC code)    | Fatty acid derivatives                                       |
| 3713 / 3717                       | F05            | Prestw-502  | Biperiden hydrochloride              | 1235-82-1    | Central Nervous System | Antiparkinsonian      |             |                                     |                      |                    | Yes             | Therapeutic classification (according ATC code) | Anticholinergic agent  |
| 3713 / 3717                       | F07            | Prestw-503  | Cetirizine dihydrochloride           | 83881-52-1   | Allergology            | Antihistaminic        | GPCR        | Histamine H1 receptor               | GI tract             | Plasmatic proteins | Yes             | Chemical classification (according ATC code)    | Piperazine derivative  |
| 3713 / 3717                       | F09            | Prestw-504  | Etifenin                             | 63245-28-3   | Diagnostic             | Chemosensitizer       |             |                                     |                      |                    |                 | Therapeutic use                                 | Association with radiopharmaceutical (technetium)            |
| 3713 / 3717                       | F11            | Prestw-505  | Metaproterenol sulfate, orciprenalin | 5874-97-5    | Respiratory            | Bronchodilator        | GPCR        | Adrenergic receptor beta-2          | GI tract             |                    | Yes             |   |  |
| 3713 / 3717                       | F13            | Prestw-506  | Sisomicin sulfate                    | 53179-09-2   | Infectiology           | Antibacterial         |             |                                     |                      |                    |                 | Chemical classification (according ATC code)    | Aminoside  |
| 3713 / 3717                       | F15            | Prestw-1159 | Sibutramine hydrochloride            | 125494-59-9  | Central Nervous System |                       |             |                                     | GI tract             | Plasmatic proteins | Yes             |   |  |
| 3713 / 3717                       | F17            | Prestw-110  | Acenocoumarol                        | 152-72-7     | Hematology             | Anticoagulant         |             |                                     | GI tract             |                    |                 | Therapeutic classification (according ATC code) | Vitamin K antagonist (VKA)                                   |
| 3713 / 3717                       | F19            | Prestw-509  | Bromperidol                          | 10457-90-6   | Central Nervous System | Antipsychotic         |             |                                     |                      |                    |                 | Chemical classification (according ATC code)    | Butyrophenone derivative                                     |
| 3713 / 3717                       | F21            | Prestw-510  | Cyclizine hydrochloride              | 303-25-3     | Allergology            | Antiemetic            | GPCR        | Histamine H1 receptor               |                      |                    | Yes             | Chemical classification (according ATC code)    | Piperazine derivative  |
| 3713 / 3717                       | H03            | Prestw-511  | Fluoxetine hydrochloride             | 59333-67-4   | Central Nervous System | Antidepressant        | Carrier     | Serotonin transporter               |                      | Plasmatic proteins | Yes             |   |  |
| 3713 / 3717                       | H05            | Prestw-512  | Iohexol                              | 66108-95-0   | Diagnostic             | Contrastant           |             |                                     |                      | Plasmatic proteins | Yes             | Chemical classification (according ATC code)    | Watersoluble, nephrotropic, low osmolar X-ray contrast media |
| 3713 / 3717                       | H07            | Prestw-513  | Norcyclobenzaprine                   | 303-50-4     | Gastroenterology       | Antiulcer             |             |                                     |                      |                    |                 | Pharmacokinetics                                | Active metabolite of Cyclobenzaprine (Prestw-445)            |
| 3713 / 3717                       | H09            | Prestw-514  | Pyrazinamide                         | 98-96-4      | Infectiology           | Antibacterial         |             |                                     |                      | Plasmatic proteins | Yes             |   |  |
| 3713 / 3717                       | H11            | Prestw-515  | Trimethadione                        | 127-48-0     | Central Nervous System | Anticonvulsant        |             |                                     |                      |                    | Yes             | Chemical classification (according ATC code)    | Oxazolidine derivatives                                      |
| 3713 / 3717                       | H13            | Prestw-516  | Lovastatin                           | 75330-75-5   | Metabolism             | Hypocholesterolemic   | Enzyme      | HMG-CoA reductase                   | GI tract             | Plasmatic proteins | Yes             |   |  |
| 3713 / 3717                       | H15            | Prestw-517  | Nystatine                            | 1400-61-9    | Infectiology           | Antifungal            |             |                                     |                      |                    | Yes             |   |  |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name             | CAS number  | Therapeutic class      | Therapeutic<br>effect | Target type | Target names                         | Absorption<br>tissue | Protein<br>binding    | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail               |
|-----------------------------------|----------------|-------------|---------------------------|-------------|------------------------|-----------------------|-------------|--------------------------------------|----------------------|-----------------------|-----------------|--|---|
| 3713 / 3717                       | H17            | Prestw-518  | Budesonide                | 51333-22-3  | Endocrinology          | Anti-inflammatory     |             |                                      | Ileum, Ascend        | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Glucocorticoid                          |
| 3713 / 3717                       | H19            | Prestw-519  | Imipenem                  | 74431-23-5  | Infectiology           | Antibacterial         |             |                                      |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Carbapenem                              |
| 3713 / 3717                       | H21            | Prestw-520  | Sulfasalazine             | 599-79-1    | Infectiology           | Antibacterial         |             |                                      | Intestine            |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Aminosalicic<br>acid derivative         |
| 3713 / 3717                       | J03            | Prestw-1430 | Lofexidine                | 31036-80-3  | Cardiovascular         | Antihypertensive      |             |                                      |                      |                       |                 |  |   |
| 3713 / 3717                       | J05            | Prestw-522  | Thioestrepton             | 1393-48-2   | Infectiology           | Antibacterial         |             |                                      |                      |                       |                 |  |   |
| 3713 / 3717                       | J07            | Prestw-1169 | Miglitol                  | 72432-03-2  | Endocrinology          | Antidiabetic          | Enzyme      | Alpha-glucosidase                    | GI tract             |                       | Yes             |  |   |
| 3713 / 3717                       | J09            | Prestw-524  | Tiabendazole              | 148-79-8    | Infectiology           | Antifungal            |             |                                      | GI tract             |                       |                 |  |   |
| 3713 / 3717                       | J11            | Prestw-525  | Rifampicin                | 13292-46-1  | Infectiology           | Antibacterial         |             |                                      | GI tract             | Plasmatic<br>proteins | Yes             |  |   |
| 3713 / 3717                       | J13            | Prestw-526  | Ethionamide               | 536-33-4    | Infectiology           | Antibacterial         |             |                                      | GI tract             | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Thiocarbamide<br>derivative             |
| 3713 / 3717                       | J15            | Prestw-527  | Tenoxicam                 | 59804-37-4  | Central Nervous System | Analgesic             | Enzyme      | Cyclooxygenase                       | GI tract             | Plasmatic<br>proteins |                 | Therapeutic<br>classification<br>(according ATC<br>code) | NSAID                                   |
| 3713 / 3717                       | J17            | Prestw-528  | Triflusal                 | 322-79-2    | Hematology             | Anticoagulant         |             |                                      | GI tract             | Plasmatic<br>proteins |                 |  |   |
| 3713 / 3717                       | J19            | Prestw-529  | Mesoridazine besylate     | 32672-69-8  | Central Nervous System | Antipsychotic         |             |                                      |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Phenothiazine<br>derivative             |
| 3713 / 3717                       | J21            | Prestw-530  | Trolox                    | 53188-07-1  | Metabolism             | Anti-oxidant          |             |                                      |                      |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Water-soluble<br>analog of<br>Vitamin E |
| 3713 / 3717                       | L03            | Prestw-531  | Pirenperone               | 75444-65-4  | Central Nervous System |                       |             |                                      |                      |                       |                 |  |   |
| 3713 / 3717                       | L05            | Prestw-1797 | Grepafloxacin             | 146863-02-7 | Infectiology           |                       |             |                                      |                      |                       | Yes             |  |   |
| 3713 / 3717                       | L07            | Prestw-533  | Phenacetin                | 62-44-2     | Central Nervous System | Analgesic             |             |                                      |                      |                       |                 |  |   |
| 3713 / 3717                       | L09            | Prestw-534  | Atovaquone                | 95233-18-4  | Infectiology           | Antimalarial          |             |                                      | GI tract             | Plasmatic<br>proteins | Yes             |  |   |
| 3713 / 3717                       | L11            | Prestw-535  | Methoxamine hydrochloride | 61-16-5     | Cardiovascular         | Antihypotensive       |             |                                      |                      | Plasmatic<br>proteins | Yes             |  |   |
| 3713 / 3717                       | L13            | Prestw-953  | (S)-(-)-Atenolol          | 93379-54-5  | Cardiovascular         | Antianginal           | GPCR        | Adrenergic receptor<br>beta-1        | GI tract             | Plasmatic<br>proteins | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Selective beta-<br>blocking agent       |
| 3713 / 3717                       | L15            | Prestw-537  | Piracetam                 | 7491-74-9   | Central Nervous System | CNS Stimulant         |             |                                      |                      |                       |                 |  |   |
| 3713 / 3717                       | L17            | Prestw-538  | Phenindione               | 83-12-5     | Hematology             | Anticoagulant         |             |                                      | GI tract             | Plasmatic<br>proteins | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Vitamin K<br>antagonist<br>(VKA)        |
| 3713 / 3717                       | L19            | Prestw-539  | Thiocolchicoside          | 602-41-5    | Central Nervous System | Antispastic           |             |                                      | GI tract             |                       |                 | New therapeutic<br>use                                   | Antioosteoporetic                       |
| 3713 / 3717                       | L21            | Prestw-540  | Clorsulon                 | 60200-06-8  | Infectiology           | Anthelmintic          |             |                                      |                      |                       |                 | Veterinary use   | Cattle                                  |
| 3713 / 3717                       | N03            | Prestw-541  | Ciclopirox ethanolamine   | 41621-49-2  | Infectiology           | Antibacterial         |             |                                      | Nail, Skin           |                       | Yes             |  |   |
| 3713 / 3717                       | N05            | Prestw-542  | Probenecid                | 57-66-9     | Metabolism             | Antigout              | Carrier     | Solute carrier family 22<br>member 6 | GI tract             | Plasmatic<br>proteins | Yes             | Mechanism  | Increasing uric<br>acid excretion       |
| 3713 / 3717                       | N07            | Prestw-543  | Bethahistine mesylate     | 54856-23-4  | Allergology            | Vasodilator           |             |                                      |                      |                       |                 |  |   |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                 | CAS number    | Therapeutic class      | Therapeutic effect  | Target type            | Target names                          | Absorption tissue   | Protein binding                                    | FDA approved | Additional info type                            | Additional info detail      |
|-----------------------------------|----------------|-------------|-------------------------------|---------------|------------------------|---------------------|------------------------|---------------------------------------|---------------------|--|--------------|---|-----------------------------|
| 3713 / 3717                       | N09            | Prestw-544  | Tobramycin                    | 32986-56-4    | Infectiology           | Antibacterial       |                        |                                       |                     | Plasmatic proteins                                 | Yes          | Chemical classification (according ATC code)    | Aminoside                   |
| 3713 / 3717                       | N11            | Prestw-545  | Tetramisole hydrochloride     | 5086-74-8     | Immunology             | Anthelmintic        |                        |                                       |                     |  |              | Veterinary use                                  | Pigeon                      |
| 3713 / 3717                       | N13            | Prestw-546  | Pregnenolone                  | 145-13-1      | Endocrinology          | Anabolic            |                        |                                       |                     |  |              |   |                             |
| 3713 / 3717                       | N15            | Prestw-547  | Molsidomine                   | 25717-80-0    | Cardiovascular         | Antianginal         |                        |                                       | GI tract            | Plasmatic proteins                                 |              |   |                             |
| 3713 / 3717                       | N17            | Prestw-548  | Chloroquine diphosphate       | 50-63-5       | Metabolism             | Anti-inflammatory   |                        |                                       | GI tract            | Albumin, Alpha-1-acid glycoprotein, gammaglobuline | Yes          | New therapeutic use                             | Anti-cancer                 |
| 3713 / 3717                       | N19            | Prestw-549  | Trimetazidine dihydrochloride | 13171-25-0    | Cardiovascular         | Antianginal         |                        |                                       | GI tract            | Plasmatic proteins                                 |              |   |                             |
| 3713 / 3717                       | N21            | Prestw-550  | Parthenolide                  | 20554-84-1    | Metabolism             | Anti-inflammatory   |                        |                                       |                     |  |              | New therapeutic use                             | Anti-cancer                 |
| 3713 / 3717                       | P03            | Prestw-551  | Hexetidine                    | 141-94-6      | Infectiology           | Antifungal          |                        |                                       |                     |  |              |   |                             |
| 3713 / 3717                       | P05            | Prestw-552  | Selegiline hydrochloride      | 14611-52-0    | Central Nervous System | Antiparkinsonian    | Enzyme                 | Monoamine oxidase B                   |                     | Plasmatic proteins                                 | Yes          |   |                             |
| 3713 / 3717                       | P07            | Prestw-553  | Pentamidine isethionate       | 140-64-7      | Infectiology           | Antifungal          |                        |                                       |                     |  | Yes          |   |                             |
| 3713 / 3717                       | P09            | Prestw-554  | Tolazamide                    | 1156-19-0     | Metabolism             | Antidiabetic        | Transmembrane receptor | Sulfonylurea receptors K-ATP channels | GI tract            |  | Yes          | Chemical classification (according ATC code)    | Sulfonamide urea derivative |
| 3713 / 3717                       | P11            | Prestw-555  | Nifuroxazide                  | 965-52-6      | Infectiology           | Antibacterial       |                        |                                       | GI tract            |  |              |   |                             |
| 3713 / 3717                       | P13            | Prestw-1144 | Mirtazapine                   | 61337-67-5    | Central Nervous System | Antidepressant      |                        |                                       |                     | Plasmatic proteins                                 | Yes          |   |                             |
| 3713 / 3717                       | P15            | Prestw-557  | Dirithromycin                 | 62013-04-1    | Infectiology           | Antibacterial       |                        |                                       |                     | Plasmatic proteins                                 | Yes          | Chemical classification (according ATC code)    | Macrolide                   |
| 3713 / 3717                       | P17            | Prestw-558  | Gliclazide                    | 21187-98-4    | Metabolism             | Anticoagulant       |                        |                                       | GI tract            | Plasmatic proteins                                 |              | Chemical classification (according ATC code)    | Sulfonamide urea derivative |
| 3713 / 3717                       | P19            | Prestw-559  | DO 897/99                     | not available | Central Nervous System | Antidepressant      |                        |                                       |                     |  |              | Pharmacological tool                            |                             |
| 3713 / 3717                       | P21            | Prestw-560  | Prenylamine lactate           | 69-43-2       | Cardiovascular         | Antianginal         |                        |                                       |                     |  |              |   |                             |
| 3713 / 3717                       | B04            | Prestw-1188 | Ziprasidone Hydrochloride     | 138982-67-9   | Central Nervous System | Antipsychotic       |                        |                                       |                     | Plasmatic proteins                                 | Yes          | Chemical classification (according ATC code)    | Indole derivative           |
| 3713 / 3717                       | B06            | Prestw-1441 | Mevastatin                    | 73573-88-3    | Cardiovascular         | Hypocholesterolemic |                        |                                       |                     |  |              |   |                             |
| 3713 / 3717                       | B08            | Prestw-1322 | Pyridostigmine iodide         | 4685-03-4     | Central Nervous System |                     | Enzyme                 | Acetylcholinesterase                  |                     |  | Yes          | Therapeutic classification (according ATC code) | Parasympathomimetic         |
| 3713 / 3717                       | B10            | Prestw-1491 | Pentobarbital                 | 76-74-4       | Central Nervous System | Anesthetic          |                        |                                       |                     | Plasmatic proteins                                 | Yes          | Chemical classification (according ATC code)    | Barbiturate                 |
| 3713 / 3717                       | B12            | Prestw-565  | Atropine sulfate monohydrate  | 5908-99-6     | Ophthalmology          | Antispastic         |                        |                                       | Eye, GI tract, Skin |  | Yes          | Therapeutic classification (according ATC code) | Anticholinergic             |
| 3713 / 3717                       | B14            | Prestw-566  | Eserine hemisulfate salt      | 64-47-1       | Central Nervous System | Antiglaucoma        |                        |                                       | GI tract            |  |              | Therapeutic classification (according ATC code) | Parasympathomimetic         |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name              | CAS number  | Therapeutic class      | Therapeutic<br>effect                | Target type         | Target names   | Absorption<br>tissue | Protein<br>binding                                    | FDA<br>approved | Additional info<br>type                               | Additional info<br>detail   |
|-----------------------------------|----------------|-------------|----------------------------|-------------|------------------------|--------------------------------------|---------------------|--|----------------------|---|-----------------|---|---|
| 3713 / 3717                       | B16            | Prestw-1139 | Itraconazole               | 84625-61-6  | Infectiology           | Antifungal                           |                     |  |                      | Albumin   | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Triazole<br>derivative  |
| 3713 / 3717                       | B18            | Prestw-1174 | Acarbose                   | 56180-94-0  | Endocrinology          | Antidiabetic                         | Enzyme              | Alpha-glucosidase  | Intestine            |   | Yes             |   |   |
| 3713 / 3717                       | B20            | Prestw-1403 | Entacapone                 | 130929-57-6 | Central Nervous System | Antiparkinsonian                     | Enzyme              | Catechol O-<br>methyltransferase                               |                      | Albumin   | Yes             |   |   |
| 3713 / 3717                       | B22            | Prestw-1449 | Nicotinamide               | 98-92-0     | Dermatology            |                                      |                     |  | GI tract             |   |                 |   |   |
| 3713 / 3717                       | D04            | Prestw-571  | Tetracaine hydrochloride   | 136-47-0    | Neuromuscular          |                                      | Ion channel         | Voltage-gated sodium<br>channel                                | Eye, Skin            |   | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Esters of<br>aminobenzoic<br>acid                                       |
| 3713 / 3717                       | D06            | Prestw-572  | Mometasone furoate         | 83919-23-7  | Endocrinology          | Anti-inflammatory                    |                     |  | Nose, Lung, G        | Plasmatic<br>proteins                                 | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Corticosteroid  |
| 3713 / 3717                       | D08            | Prestw-1467 | Troglitazone               | 97322-87-7  | Metabolism             | Antidiabetic                         | Nuclear<br>receptor | Peroxisome proliferator-<br>activated receptor<br>(PPAR) gamma |                      |   | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Thiazolidinedion<br>e   |
| 3713 / 3717                       | D10            | Prestw-574  | Dacarbazine                | 4342-03-4   | Oncology               | Antineoplastic                       |                     |  |                      | Plasmatic<br>proteins                                 | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Alkylating agent  |
| 3713 / 3717                       | D12            | Prestw-1351 | Tenatoprazole              | 113712-98-4 | Metabolism             | Antiulcer                            |                     |  |                      |   |                 |   |   |
| 3713 / 3717                       | D14            | Prestw-576  | Acetpromazine maleate salt | 3598-37-6   | Central Nervous System | Antiemetic                           |                     |  |                      |   |                 | Chemical<br>classification<br>(according ATC<br>code) | Phenothiazine<br>derivative   |
| 3713 / 3717                       | D16            | Prestw-1271 | Escitalopram oxalate       | 128196-01-0 | Central Nervous System | Antidepressant                       | Carrier             | Serotonin transporter  |                      | Plasmatic<br>proteins                                 | Yes             |   |   |
| 3713 / 3717                       | D18            | Prestw-1158 | Ropinirole hydrochloride   | 91374-20-8  | Central Nervous System | Antiparkinsonian                     |                     |  |                      | Plasmatic<br>proteins                                 | Yes             |   |   |
| 3713 / 3717                       | D20            | Prestw-1297 | Lacidipine                 | 103890-78-4 | Cardiovascular         | Antihypertensive                     | Ion channel         | Voltage-gated L-type<br>calcium channel                        | GI tract             | Albumin,<br>alpha-1-acid<br>glycoprotein              |                 | Chemical<br>classification<br>(according ATC<br>code) | Dihydropyridine<br>derivatives  |
| 3713 / 3717                       | D22            | Prestw-1228 | Argatroban                 | 74863-84-6  | Hematology             | Anticoagulant                        |                     |  |                      | Albumin (20),<br>alpha-1-acid<br>glycoprotein<br>(34) | Yes             |   |   |
| 3713 / 3717                       | F04            | Prestw-1328 | Reboxetine mesylate        | 98769-81-4  | Central Nervous System | Antidepressant                       |                     |  |                      | Plasmatic<br>proteins                                 |                 |   |   |
| 3713 / 3717                       | F06            | Prestw-1498 | Camylofine chlorhydrate    | 54-30-8     |                        |                                      |                     |  |                      |   |                 | Chemical<br>classification<br>(according ATC<br>code) | Synthetic<br>anticholinergic,<br>esters with<br>tertiary amino<br>group |
| 3713 / 3717                       | F08            | Prestw-583  | Papaverine hydrochloride   | 61-25-6     | Cardiovascular         | Antispastic                          |                     |  |                      | Plasmatic<br>proteins                                 |                 |   |   |
| 3713 / 3717                       | F10            | Prestw-584  | Yohimbine hydrochloride    | 65-19-0     | Cardiovascular         | Erectile<br>dysfunction<br>treatment |                     |  |                      |   |                 |   |   |
| 3713 / 3717                       | F12            | Prestw-1500 | Voriconazole               | 137234-62-9 | Infectiology           | Antifungal                           |                     |  |                      | Plasmatic<br>proteins                                 | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Triazole<br>derivative  |
| 3713 / 3717                       | F14            | Prestw-1211 | Alfacalcidol               | 41294-56-8  | Metabolism             | Antiosteoporetic                     |                     |  | GI tract             | Alpha-globulin  | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Vitamin D<br>analog   |

| ICCB-L Plate (10 mM / 3.33 mM) | ICCB-L Well | Vendor_ID   | Chemical_Name              | CAS number  | Therapeutic class      | Therapeutic effect | Target type | Target names                   | Absorption tissue | Protein binding    | FDA approved | Additional info type                            | Additional info detail               |
|--------------------------------|-------------|-------------|----------------------------|-------------|------------------------|--------------------|-------------|--------------------------------|-------------------|--------------------|--------------|---|--------------------------------------|
| 3713 / 3717                    | F16         | Prestw-587  | Cilostazol                 | 73963-72-1  | Hematology             | Anticoagulant      | Enzyme      | Phosphodiesterase 3            | GI tract          | Plasmatic proteins | Yes          |   |                                      |
| 3713 / 3717                    | F18         | Prestw-588  | Galanthamine hydrobromide  | 1953-04-4   | Central Nervous System | Analgesic          | Enzyme      | Acetylcholinesterase           |                   | Plasmatic proteins | Yes          |   |                                      |
| 3713 / 3717                    | F20         | Prestw-1130 | Azelastine hydrochloride   | 79307-93-0  | Immunology             | Antihistaminic     |             |                                | Nose, Eye, GI     | Plasmatic proteins | Yes          |   |                                      |
| 3713 / 3717                    | F22         | Prestw-1409 | Etretinate                 | 54350-48-0  | Dermatology            | Antipsoriatic      |             |                                | Small intestine   | Lipoproteins       | Yes          | Chemical classification (according ATC code)    | Retinoid                             |
| 3713 / 3717                    | H04         | Prestw-1274 | Emedastine                 | 87233-61-2  | Allergology            | Antihistaminic     |             |                                |                   |                    | Yes          |   |                                      |
| 3713 / 3717                    | H06         | Prestw-1407 | Etofenamate                | 30544-47-9  | Metabolism             | Anti-inflammatory  |             |                                |                   |                    |              | Therapeutic classification (according ATC code) | NSAID                                |
| 3713 / 3717                    | H08         | Prestw-1369 | Zaleplon                   | 151319-34-5 | Central Nervous System | Hypnotic           | LGIC        | GABA-A receptor                |                   |                    | Yes          | Chemical classification (according ATC code)    | Benzodiazepine related drug (Z-drug) |
| 3713 / 3717                    | H10         | Prestw-594  | Diclofenac sodium          | 15307-79-6  | Central Nervous System | Anti-inflammatory  | Enzyme      | Cyclooxygenase                 | GI tract, Skin    | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | NSAID                                |
| 3713 / 3717                    | H12         | Prestw-1410 | Exemestane                 | 107868-30-4 | Endocrinology          | Antineoplastic     | Coenzyme    | Cytochrome P450 19A1           |                   | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | Aromatase inhibitor                  |
| 3713 / 3717                    | H14         | Prestw-1499 | Fomepizole                 | 7554-65-6   | Metabolism             |                    |             |                                |                   |                    | Yes          |   |                                      |
| 3713 / 3717                    | H16         | Prestw-1183 | Temozolomide               | 85622-93-1  | Oncology               | Antineoplastic     |             |                                |                   | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Alkylating agent                     |
| 3713 / 3717                    | H18         | Prestw-598  | Xylazine                   | 7361-61-7   | Central Nervous System | Analgesic          |             |                                |                   |                    |              | Veterinary use                                  | Cat                                  |
| 3713 / 3717                    | H20         | Prestw-1132 | Celiprolol hydrochloride   | 57470-78-7  | Cardiovascular         | Antianginal        | GPCR        | Adrenergic receptor beta-1     | GI tract          | Plasmatic proteins |              | Therapeutic classification (according ATC code) | Selective beta-blocking agent        |
| 3713 / 3717                    | H22         | Prestw-1367 | Zopiclone                  | 43200-80-2  | Central Nervous System | Hypnotic           | LGIC        | GABA-A receptor                |                   | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Benzodiazepine related drug (Z-drug) |
| 3713 / 3717                    | J04         | Prestw-1198 | Tranilast                  | 53902-12-8  | Allergology            | Antiallergic       |             |                                |                   |                    |              | New therapeutic use                             | Anti-cancer                          |
| 3713 / 3717                    | J06         | Prestw-1182 | Tizanidine hydrochloride   | 51322-75-9  | Metabolism             | Muscle relaxant    |             |                                | GI tract          |                    | Yes          |   |                                      |
| 3713 / 3717                    | J08         | Prestw-1364 | Zafirlukast                | 107753-78-6 | Respiratory            | Antiasthmatic      | GPCR        | Cysteinyl leukotriene receptor |                   | Albumin            | Yes          |   |                                      |
| 3713 / 3717                    | J10         | Prestw-1252 | Butenafine Hydrochloride   | 101828-21-1 | Infectiology           | Antifungal         |             |                                | Skin              |                    | Yes          |   |                                      |
| 3713 / 3717                    | J12         | Prestw-1121 | Carbadox                   | 6804-07-5   | Infectiology           | Antibacterial      |             |                                |                   |                    |              |   |                                      |
| 3713 / 3717                    | J14         | Prestw-1331 | Rimantadine Hydrochloride  | 13392-28-4  | Infectiology           | Antiviral          |             |                                |                   | Albumin            | Yes          | Chemical classification (according ATC code)    | Cyclic amine                         |
| 3713 / 3717                    | J16         | Prestw-607  | Eburnamonine (-)           | 4880-88-0   | Central Nervous System | Vasodilator        |             |                                |                   |                    |              |   |                                      |
| 3713 / 3717                    | J18         | Prestw-1460 | Oxibendazol                | 20559-55-1  | Metabolism             |                    |             |                                |                   |                    |              | Veterinary use                                  | Cat                                  |
| 3713 / 3717                    | J20         | Prestw-1292 | Ipsapirone                 | 95847-70-4  | Central Nervous System |                    |             |                                |                   |                    |              |   |                                      |
| 3713 / 3717                    | J22         | Prestw-1284 | Hydroxychloroquine sulfate | 747-36-4    | Metabolism             | Antimalarial       |             |                                | GI tract          | Plasmatic proteins | Yes          | New therapeutic use                             | Immunomodulator                      |
| 3713 / 3717                    | L04         | Prestw-1431 | Loracarbef                 | 121961-22-6 | Infectiology           | Antibacterial      |             |                                | GI tract          |                    | Yes          | Chemical classification (according ATC code)    | Second-generation cephalosporin      |

| ICCB-L Plate (10 mM / 3.33 mM) | ICCB-L Well | Vendor_ID   | Chemical_Name               | CAS number  | Therapeutic class      | Therapeutic effect | Target type | Target names                                   | Absorption tissue | Protein binding    | FDA approved | Additional info type                            | Additional info detail                         |
|--------------------------------|-------------|-------------|-----------------------------|-------------|------------------------|--------------------|-------------|--|-------------------|--------------------|--------------|---|--|
| 3713 / 3717                    | L06         | Prestw-1501 | Fenipentol                  | 583-03-9    | Metabolism             | Choleretic         |             |  |                   |                    |              |   |  |
| 3713 / 3717                    | L08         | Prestw-1503 | Diosmin                     | 520-27-4    | Cardiovascular         |                    |             |  | GI tract          |                    |              | Chemical classification (according ATC code)    | Bioflavonoid                                   |
| 3713 / 3717                    | L10         | Prestw-1177 | Carbidopa                   | 28860-95-9  | Central Nervous System | Antiparkinsonian   |             |  |                   |                    | Yes          |   |  |
| 3713 / 3717                    | L12         | Prestw-1604 | (-)-Emtricitabine           | 143491-57-0 | Infectiology           | Antiviral          |             |  |                   | Plasmatic proteins | Yes          |   |  |
| 3713 / 3717                    | L14         | Prestw-616  | Demecarium bromide          | 56-94-0     | Ophthalmology          | Antiglaucoma       |             |  |                   |                    | Yes          | Therapeutic classification (according ATC code) | Parasympathomimetic                            |
| 3713 / 3717                    | L16         | Prestw-617  | Quipazine dimaleate salt    | 150323-78-7 | Central Nervous System | Antiemetic         |             |  |                   |                    |              | Pharmacological tool                            |  |
| 3713 / 3717                    | L18         | Prestw-1127 | Acipimox                    | 51037-30-0  | Metabolism             | Antilipemic        |             |  | GI tract          |                    |              | Chemical classification (according ATC code)    | Nicotinic acid derivative                      |
| 3713 / 3717                    | L20         | Prestw-619  | Diflorasone Diacetate       | 33564-31-7  | Endocrinology          | Anti-inflammatory  |             |  | Skin              |                    |              | Chemical classification (according ATC code)    | Corticosteroid, potent                         |
| 3713 / 3717                    | L22         | Prestw-1502 | Acamprosate calcium         | 77337-73-6  | Central Nervous System |                    |             |  |                   | Plasmatic proteins | Yes          |   |  |
| 3713 / 3717                    | N04         | Prestw-1506 | Mizolastine                 | 108612-45-9 | Allergology            |                    | GPCR        | Histamine H1 receptor                          | GI tract          | Plasmatic proteins |              |   |  |
| 3713 / 3717                    | N06         | Prestw-1217 | Amisulpride                 | 71675-85-9  | Central Nervous System | Antipsychotic      |             |  |                   | Plasmatic proteins |              | Chemical classification (according ATC code)    | Benzamide                                      |
| 3713 / 3717                    | N08         | Prestw-623  | Pyridoxine hydrochloride    | 58-56-0     | Metabolism             |                    |             |  | Small intestine   |                    | Yes          |   |  |
| 3713 / 3717                    | N10         | Prestw-1469 | Mercaptopurine              | 50-44-2     | Immunology             | Immunosuppressant  | Enzyme      | Hypoxanthine-guanine phosphoribosyltransferase |                   |                    | Yes          | Chemical classification (according ATC code)    | Purine analogue                                |
| 3713 / 3717                    | N12         | Prestw-1134 | Cytarabine                  | 147-94-4    | Oncology               | Antineoplastic     |             |  |                   | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Pyrimidine analogue                            |
| 3713 / 3717                    | N14         | Prestw-626  | Racecadotril                | 81110-73-8  | Gastroenterology       | Antidiarrheal      | Enzyme      | Enkephalinases                                 | GI tract          | Albumin            |              |   |  |
| 3713 / 3717                    | N16         | Prestw-627  | Folic acid                  | 59-30-3     | Metabolism             |                    |             |  | GI tract          |                    | Yes          |   |  |
| 3713 / 3717                    | N18         | Prestw-1129 | Benazepril hydrochloride    | 86541-74-4  | Cardiovascular         | Antihypertensive   | Enzyme      | Angiotensin-converting enzyme (ACE)            | GI tract          | Plasmatic proteins | Yes          |   |  |
| 3713 / 3717                    | N20         | Prestw-1178 | Aniracetam                  | 72432-10-1  | Central Nervous System | Anti-Alzheimer     |             |  |                   |                    |              |   |  |
| 3713 / 3717                    | N22         | Prestw-630  | Dimethisoquin hydrochloride | 2773-92-4   | Neuromuscular          | Antipruritic       |             |  |                   |                    |              |   |  |
| 3713 / 3717                    | P04         | Prestw-1210 | Alendronate sodium          | 121268-17-5 | Metabolism             | Antiestrogenic     |             |  | GI tract          | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Bisphosphonates                                |
| 3713 / 3717                    | P06         | Prestw-632  | Dipivefrin hydrochloride    | 64019-93-8  | Ophthalmology          | Antiglaucoma       |             |  |                   |                    | Yes          | Therapeutic classification (according ATC code) | Sympathomimetic                                |
| 3713 / 3717                    | P08         | Prestw-633  | Thiorphan                   | 76721-89-6  | Gastroenterology       | Antidiarrheal      |             |  |                   |                    |              | Pharmacokinetics                                | Active metabolite of Racecadotril (Prestw-626) |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                        | CAS number  | Therapeutic class      | Therapeutic effect | Target type            | Target names                           | Absorption tissue | Protein binding                   | FDA approved | Additional info type                            | Additional info detail                |
|-----------------------------------|----------------|-------------|--------------------------------------|-------------|------------------------|--------------------|------------------------|--|-------------------|-----------------------------------|--------------|---|---------------------------------------|
| 3713 / 3717                       | P10            | Prestw-1463 | Tomoxetine hydrochloride             | 82248-59-7  | Central Nervous System |                    |                        |  |                   | Albumin                           | Yes          | Therapeutic classification (according ATC code) | Centrally acting sympathomimetic      |
| 3713 / 3717                       | P12            | Prestw-1511 | Aceclidine Hydrochloride             | 6109-70-2   | Ophthalmology          | Antiglaucoma       |                        |  |                   |                                   |              | Therapeutic classification (according ATC code) | Parasympathomimetic                   |
| 3713 / 3717                       | P14            | Prestw-1488 | Penciclovir                          | 39809-25-1  | Infectiology           | Antiviral          |                        |  |                   |                                   | Yes          |   |                                       |
| 3713 / 3717                       | P16            | Prestw-1427 | Levetiracetam                        | 102767-28-2 | Central Nervous System | Anticonvulsant     |                        |  |                   | Plasmatic proteins                | Yes          |   |                                       |
| 3713 / 3717                       | P18            | Prestw-1392 | Dexfenfluramine hydrochloride        | 3239-45-0   | Central Nervous System | Anorectic          |                        |  | GI tract          | Plasmatic proteins                |              |   |                                       |
| 3713 / 3717                       | P20            | Prestw-1408 | Etoricoxib                           | 202409-33-4 | Central Nervous System | Analgesic          | Enzyme                 | Cyclooxygenase-2                       | GI tract          | Plasmatic proteins                |              | Therapeutic classification (according ATC code) | NSAID                                 |
| 3713 / 3717                       | P22            | Prestw-1341 | Sertindole                           | 106516-24-9 | Central Nervous System | Antipsychotic      |                        |  |                   |                                   |              | Chemical classification (according ATC code)    | Indole derivative                     |
| 3714 / 3718                       | A03            | Prestw-641  | Sulmazole                            | 73384-60-8  | Cardiovascular         | Cardiotonic        |                        |  |                   |                                   |              |   |                                       |
| 3714 / 3718                       | A05            | Prestw-1270 | Gefitinib                            | 184475-35-2 | Oncology               | Antineoplastic     | Enzyme                 | Epidermal growth factor receptor erbB1 |                   | Albumin, alpha1-acid glycoprotein | Yes          |   |                                       |
| 3714 / 3718                       | A07            | Prestw-643  | Flunisolide                          | 3385-03-3   | Endocrinology          | Anti-inflammatory  |                        |  |                   |                                   | Yes          | Chemical classification (according ATC code)    | Corticosteroid                        |
| 3714 / 3718                       | A09            | Prestw-644  | N-Acetyl-DL-homocysteine Thiolactone | 1195-16-0   | Respiratory            | Expectorant        |                        |  |                   |                                   |              |   |                                       |
| 3714 / 3718                       | A11            | Prestw-645  | Flurandrenolide                      | 1524-88-5   | Dermatology            | Anti-inflammatory  |                        |  | Skin              |                                   | Yes          | Chemical classification (according ATC code)    | Corticosteroid, potent                |
| 3714 / 3718                       | A13            | Prestw-1125 | Oxiconazole Nitrate                  | 64211-46-7  | Infectiology           | Antifungal         |                        |  | Skin              |                                   | Yes          | Chemical classification (according ATC code)    | Imidazole derivative                  |
| 3714 / 3718                       | A15            | Prestw-1166 | Rebamipide                           | 90098-04-7  | Metabolism             | Antiulcer          |                        |  |                   |                                   |              |   |                                       |
| 3714 / 3718                       | A17            | Prestw-1154 | Nilvadipine                          | 75530-68-6  | Cardiovascular         | Antianginal        | Ion channel            | Voltage-gated L-type calcium channel   |                   |                                   |              | Chemical classification (according ATC code)    | Dihydropyridine derivatives           |
| 3714 / 3718                       | A19            | Prestw-649  | Etanidazole                          | 22668-01-5  | Oncology               | Antineoplastic     |                        |  |                   |                                   |              |   |                                       |
| 3714 / 3718                       | A21            | Prestw-1601 | Pinaverium bromide                   | 53251-94-8  | Neuromuscular          | Antispastic        |                        |  | GI tract          | Plasmatic proteins                |              |   |                                       |
| 3714 / 3718                       | C03            | Prestw-651  | Glimepiride                          | 93479-97-1  | Endocrinology          | Antidiabetic       | Transmembrane receptor | Sulfonylurea receptors K-ATP channels  | GI tract          | Plasmatic proteins                | Yes          | Chemical classification (according ATC code)    | Sulfonamide urea derivative           |
| 3714 / 3718                       | C05            | Prestw-652  | Picrotoxinin                         | 17617-45-7  | Central Nervous System | Analeptic          |                        |  |                   |                                   |              |   |                                       |
| 3714 / 3718                       | C07            | Prestw-653  | Mepenzolate bromide                  | 76-90-4     | Neuromuscular          | Antispastic        |                        |  | GI tract          |                                   | Yes          | New therapeutic use                             | Chronic obstructive pulmonary disease |
| 3714 / 3718                       | C09            | Prestw-654  | Benfotiamine                         | 22457-89-2  | Metabolism             |                    |                        |  |                   |                                   |              | Chemical classification (according ATC code)    | Vitamin B1 derivative                 |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                             | CAS number  | Therapeutic class      | Therapeutic effect | Target type      | Target names                         | Absorption tissue | Protein binding      | FDA approved | Additional info type                            | Additional info detail              |
|-----------------------------------|----------------|-------------|---|-------------|------------------------|--------------------|------------------|--------------------------------------|-------------------|----------------------|--------------|---|-------------------------------------|
| 3714 / 3718                       | C11            | Prestw-655  | Halcinonide                               | 3093-35-4   | Dermatology            | Anti-inflammatory  |                  |                                      | Skin              |                      | Yes          | Chemical classification (according ATC code)    | Corticosteroid, very potent         |
| 3714 / 3718                       | C13            | Prestw-656  | Lanatoside C                              | 17575-22-3  | Cardiovascular         | Cardiotonic        |                  |                                      | GI tract          | Albumin              |              | Chemical classification (according ATC code)    | Digitalis glycoside                 |
| 3714 / 3718                       | C15            | Prestw-657  | Benzamil hydrochloride                    | 2898-76-2   | Metabolism             | Antihypertensive   |                  |                                      |                   |                      |              |   |                                     |
| 3714 / 3718                       | C17            | Prestw-658  | Suxibuzone                                | 27470-51-5  | Central Nervous System | Analgesic          |                  |                                      |                   |                      |              | Therapeutic classification (according ATC code) | NSAID                               |
| 3714 / 3718                       | C19            | Prestw-659  | 6-Furfurylaminopurine                     | 525-79-1    | Dermatology            |                    |                  |                                      |                   |                      |              |   |                                     |
| 3714 / 3718                       | C21            | Prestw-660  | Avermectin B1                             | 71751-41-2  | Infectiology           | Anthelmintic       |                  |                                      | Skin              |                      |              | Veterinary use                                  |                                     |
| 3714 / 3718                       | E03            | Prestw-1317 | Pranlukast                                | 103177-37-3 | Respiratory            | Antiasthmatic      | GPCR             | Cysteinyl leukotriene receptor 1     |                   |                      |              |   |                                     |
| 3714 / 3718                       | E05            | Prestw-1477 | D,L-Penicillamine                         | 52-66-4     | Central Nervous System | Analgesic          |                  |                                      | GI tract          | Collagen             | Yes          |   |                                     |
| 3714 / 3718                       | E07            | Prestw-1365 | Zileuton                                  | 111406-87-2 | Respiratory            | Antiasthmatic      |                  |                                      |                   |                      | Yes          |   |                                     |
| 3714 / 3718                       | E09            | Prestw-1432 | Loratadine                                | 79794-75-5  | Allergology            | Antihistaminic     | GPCR             | Histamine H1 receptor                | GI tract          | Plasmatic proteins   | Yes          |   |                                     |
| 3714 / 3718                       | E11            | Prestw-1387 | Tetraethylenepentamine pentahydrochloride | 4961-41-5   | Metabolism             | Antilipemic        |                  |                                      |                   |                      |              |   |                                     |
| 3714 / 3718                       | E13            | Prestw-666  | Nisoldipine                               | 63675-72-9  | Cardiovascular         | Antianginal        | Ion channel      | Voltage-gated L-type calcium channel | GI tract          | Plasmatic proteins   | Yes          | Chemical classification (according ATC code)    | Dihydropyridine derivatives         |
| 3714 / 3718                       | E15            | Prestw-1507 | Acefylline                                | 652-37-9    | Central Nervous System | CNS Stimulant      |                  |                                      |                   |                      |              | Chemical classification (according ATC code)    | Xanthine                            |
| 3714 / 3718                       | E17            | Prestw-1165 | Acitretin                                 | 55079-83-9  | Dermatology            | Antipsoriatic      |                  |                                      |                   | Albumin, lipoprotein | Yes          | Chemical classification (according ATC code)    | Retinoid                            |
| 3714 / 3718                       | E19            | Prestw-1162 | Zonisamide                                | 68291-97-4  | Central Nervous System | Anticonvulsant     |                  |                                      |                   | Plasmatic proteins   | Yes          |   |                                     |
| 3714 / 3718                       | E21            | Prestw-1173 | Irsogladine maleate                       | 84504-69-8  | Metabolism             | Antilucer          |                  |                                      |                   |                      |              |   |                                     |
| 3714 / 3718                       | G03            | Prestw-671  | Dydrogesterone                            | 152-62-5    | Endocrinology          | Progestogen        | Nuclear receptor | Progesterone receptor                |                   |                      | Yes          |   |                                     |
| 3714 / 3718                       | G05            | Prestw-1346 | Sumatriptan succinate                     | 103628-48-4 | Central Nervous System | Antimigraine       | GPCR             | Serotonin 1d (5-HT1d) receptor       |                   | Plasmatic proteins   | Yes          |   |                                     |
| 3714 / 3718                       | G07            | Prestw-1456 | Opipramol dihydrochloride                 | 909-39-7    | Central Nervous System | Antidepressant     |                  |                                      |                   |                      |              |   |                                     |
| 3714 / 3718                       | G09            | Prestw-1447 | Nalidixic acid sodium salt                | 3374-05-8   | Infectiology           | Antibacterial      |                  |                                      |                   | Plasmatic proteins   | Yes          | Chemical classification (according ATC code)    | Quinolone                           |
| 3714 / 3718                       | G11            | Prestw-1475 | Oxacillin sodium                          | 1173-88-2   | Infectiology           | Antibacterial      |                  |                                      |                   | Plasmatic proteins   | Yes          | Chemical classification (according ATC code)    | Beta-lactamase resistant penicillin |
| 3714 / 3718                       | G13            | Prestw-676  | Beta-Escin                                | 11072-93-8  | Metabolism             | Antineoplastic     |                  |                                      |                   |                      |              |   |                                     |
| 3714 / 3718                       | G15            | Prestw-631  | Thiamine hydrochloride                    | 67-03-8     | Immunology             | Immunostimulant    |                  |                                      | Small intestine   |                      | Yes          |   |                                     |
| 3714 / 3718                       | G17            | Prestw-1349 | Tazobactam                                | 89786-04-9  | Infectiology           | Antibacterial      |                  |                                      |                   | Plasmatic proteins   | Yes          | Chemical classification (according ATC code)    | Beta-lactamase inhibitor            |
| 3714 / 3718                       | G19            | Prestw-1285 | Ibandronate sodium                        | 114084-78-5 | Metabolism             | Antiosteoporetic   |                  |                                      | Upper GI tract    | Plasmatic proteins   | Yes          | Chemical classification (according ATC code)    | Bisphosphonates                     |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                       | CAS number  | Therapeutic class      | Therapeutic<br>effect | Target type      | Target names          | Absorption<br>tissue | Protein<br>binding                    | FDA<br>approved | Additional info<br>type                         | Additional info<br>detail  |
|-----------------------------------|----------------|-------------|-------------------------------------|-------------|------------------------|-----------------------|------------------|-----------------------|----------------------|---------------------------------------|-----------------|---|--|
| 3714 / 3718                       | G21            | Prestw-1363 | Warfarin                            | 81-81-2     | Hematology             | Anticoagulant         |                  |                       | GI tract             | Albumin                               | Yes             | Therapeutic classification (according ATC code) | Vitamin K antagonist (VKA)                                       |
| 3714 / 3718                       | I03            | Prestw-1318 | Pranoprofen                         | 52549-17-4  | Metabolism             | Anti-inflammatory     |                  |                       |                      |                                       |                 | Therapeutic classification (according ATC code) | NSAID  |
| 3714 / 3718                       | I05            | Prestw-1340 | Secnidazole                         | 3366-95-8   | Infectiology           | Antiamoebic           |                  |                       | GI tract             |                                       |                 | Chemical classification (according ATC code)    | Nitroimidazole derivative  |
| 3714 / 3718                       | I07            | Prestw-683  | Pempidine tartrate                  | 546-48-5    | Cardiovascular         | Antihypotensive       |                  |                       |                      |                                       |                 |   |  |
| 3714 / 3718                       | I09            | Prestw-1798 | Mirabegron                          | 223673-61-8 | Neuromuscular          |                       |                  |                       |                      |                                       | Yes             |   |  |
| 3714 / 3718                       | I11            | Prestw-1508 | Ibutilide fumarate                  | 122647-32-9 | Cardiovascular         | Antiarrhythmic        |                  |                       |                      | Plasmatic proteins                    | Yes             | Chemical classification (according ATC code)    | Antiarrhythmic, class III  |
| 3714 / 3718                       | I13            | Prestw-1799 | Tigecycline                         | 220620-09-7 | Infectiology           |                       |                  |                       |                      |                                       | Yes             |   |  |
| 3714 / 3718                       | I15            | Prestw-1465 | Tramadol hydrochloride              | 27203-92-5  | Central Nervous System | Analgesic             | Nuclear receptor | Opioid receptor mu    | GI tract             | Plasmatic proteins                    | Yes             | Chemical classification (according ATC code)    | Opioid   |
| 3714 / 3718                       | I17            | Prestw-688  | Estropiate                          | 7280-37-7   | Endocrinology          |                       |                  |                       |                      | Albumin, Sex hormone-binding globulin | Yes             |   |  |
| 3714 / 3718                       | I19            | Prestw-1253 | Butylscopolammonium (n-) bromide    | 149-64-4    | Central Nervous System | Antispastic           |                  |                       |                      |                                       |                 | Chemical classification (according ATC code)    | Belladonna alkaloid, semisynthetic, quaternary ammonium compound |
| 3714 / 3718                       | I21            | Prestw-1494 | Irinotecan hydrochloride trihydrate | 136572-09-3 | Oncology               | Antineoplastic        | Enzyme           | DNA topoisomerase I   |                      | Plasmatic proteins                    | Yes             |   |  |
| 3714 / 3718                       | K03            | Prestw-1353 | Tylosin                             | 1401-69-0   | Infectiology           | Antibacterial         |                  |                       |                      |                                       |                 | Veterinary use                                  | Cattle   |
| 3714 / 3718                       | K05            | Prestw-692  | Citalopram Hydrobromide             | 59729-32-7  | Central Nervous System | Antidepressant        | Carrier          | Serotonin transporter |                      | Plasmatic proteins                    | Yes             |   |  |
| 3714 / 3718                       | K07            | Prestw-693  | Promazine hydrochloride             | 53-60-1     | Central Nervous System | Antipsychotic         |                  |                       |                      |                                       | Yes             | Chemical classification (according ATC code)    | Phenothiazine derivative   |
| 3714 / 3718                       | K09            | Prestw-694  | Sulfamerazine                       | 127-79-7    | Infectiology           | Antibacterial         |                  |                       |                      |                                       | Yes             | Chemical classification (according ATC code)    | Long-acting sulfonamide  |
| 3714 / 3718                       | K11            | Prestw-1170 | Venlafaxine                         | 93413-69-5  | Central Nervous System | Antidepressant        |                  |                       |                      | Plasmatic proteins                    | Yes             |   |  |
| 3714 / 3718                       | K13            | Prestw-696  | Ethotoin                            | 86-35-1     | Central Nervous System | Anticonvulsant        |                  |                       |                      |                                       | Yes             | Chemical classification (according ATC code)    | Hydantoin derivatives  |
| 3714 / 3718                       | K15            | Prestw-697  | 3-alpha-Hydroxy-5-beta-androstan    | 53-42-9     | Endocrinology          |                       |                  |                       |                      |                                       |                 | Pharmacokinetics                                | Metabolite of testosterone                                       |
| 3714 / 3718                       | K17            | Prestw-698  | Tetrahydrozoline hydrochloride      | 522-48-5    | Cardiovascular         | Nasal Decongestant    |                  |                       |                      |                                       | Yes             | Therapeutic classification (according ATC code) | Sympathomimetic  |
| 3714 / 3718                       | K19            | Prestw-699  | Hexestrol                           | 84-16-2     | Endocrinology          | Antineoplastic        |                  |                       |                      |                                       |                 |   |  |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                     | CAS number | Therapeutic class      | Therapeutic<br>effect | Target type | Target names                    | Absorption<br>tissue | Protein<br>binding    | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail                                      |
|-----------------------------------|----------------|-------------|-----------------------------------|------------|------------------------|-----------------------|-------------|---------------------------------|----------------------|-----------------------|-----------------|--|--|
| 3714 / 3718                       | K21            | Prestw-700  | Cefmetazole sodium salt           | 56796-39-5 | Infectiology           | Antibacterial         |             |                                 |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Second-<br>generation<br>cephalosporin                         |
| 3714 / 3718                       | M03            | Prestw-701  | Trihexyphenidyl-D,L Hydrochloride | 58947-95-8 | Central Nervous System | Antiparkinsonian      |             |                                 |                      |                       | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Anticholinergic<br>agent                                       |
| 3714 / 3718                       | M05            | Prestw-702  | Succinylsulfathiazole             | 116-43-8   | Infectiology           | Antibacterial         |             |                                 | Intestine            |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Sulfonamide  |
| 3714 / 3718                       | M07            | Prestw-703  | Famprofazone                      | 22881-35-2 | Central Nervous System | Analgesic             |             |                                 |                      |                       |                 | Pharmacokinetics   | Source of<br>metamphetamin<br>e and<br>amphetamine in<br>urine |
| 3714 / 3718                       | M09            | Prestw-704  | Bromopride                        | 4093-35-0  | Central Nervous System | Antiemetic            |             |                                 |                      | Plasmatic<br>proteins |                 | Therapeutic<br>classification<br>(according ATC<br>code) | Propulsive   |
| 3714 / 3718                       | M11            | Prestw-705  | Methyl benzethonium chloride      | 25155-18-4 | Infectiology           | Antibacterial         |             |                                 |                      |                       |                 |  |  |
| 3714 / 3718                       | M13            | Prestw-706  | Chlorcyclizine hydrochloride      | 1620-21-9  | Allergology            | Antiemetic            | GPCR        | Histamine H1 receptor           |                      |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Piperazine<br>derivative                                       |
| 3714 / 3718                       | M15            | Prestw-707  | Diphenylpyraline hydrochloride    | 132-18-3   | Allergology            | Antihistaminic        | GPCR        | Histamine H1 receptor           | GI tract, Skin       |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Aminoalkyl ether   |
| 3714 / 3718                       | M17            | Prestw-708  | Benzethonium chloride             | 121-54-0   | Infectiology           | Antibacterial         |             |                                 | Skin                 |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Quaternary<br>ammonium   |
| 3714 / 3718                       | M19            | Prestw-709  | Trioxsalen                        | 3902-71-4  | Dermatology            |                       |             |                                 |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Psoralen   |
| 3714 / 3718                       | M21            | Prestw-1136 | Doxofylline                       | 69975-86-6 | Respiratory            | Bronchodilator        |             |                                 |                      | Plasmatic<br>proteins |                 | Chemical<br>classification<br>(according ATC<br>code)    | Xanthine   |
| 3714 / 3718                       | O03            | Prestw-711  | Sulfabenzamide                    | 127-71-9   | Infectiology           | Antibacterial         |             |                                 |                      |                       | Yes             |  |  |
| 3714 / 3718                       | O05            | Prestw-712  | Benzocaine                        | 94-09-7    | Neuromuscular          | Local anesthetic      | Ion channel | Voltage-gated sodium<br>channel |                      |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Esters of<br>aminobenzoic<br>acid                              |
| 3714 / 3718                       | O07            | Prestw-713  | Dipyron                           | 5907-38-0  | Central Nervous System | Analgesic             | Enzyme      | Lysosomal alpha-<br>glucosidase | GI tract             |                       |                 |  |  |
| 3714 / 3718                       | O09            | Prestw-714  | Isosorbide dinitrate              | 87-33-2    | Cardiovascular         | Antianginal           | Enzyme      | Soluble guanylate<br>cyclase    | GI tract             |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Organic nitrate  |
| 3714 / 3718                       | O11            | Prestw-715  | Sulfachloropyridazine             | 80-32-0    | Infectiology           | Antibacterial         |             |                                 |                      |                       |                 | Veterinary use   | Poultry  |
| 3714 / 3718                       | O13            | Prestw-716  | Pramoxine hydrochloride           | 637-58-1   | Neuromuscular          | Local anesthetic      |             |                                 | Skin                 |                       | Yes             |  |  |
| 3714 / 3718                       | O15            | Prestw-717  | Finasteride                       | 98319-26-7 | Endocrinology          | Anti-alopecia         | Enzyme      | Steroid 5-alpha-<br>reductase 2 |                      | Plasmatic<br>proteins | Yes             |  |  |
| 3714 / 3718                       | O17            | Prestw-718  | Fluorometholone                   | 426-13-1   | Endocrinology          | Anti-inflammatory     |             |                                 | Eye                  |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Corticosteroid   |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                      | CAS number | Therapeutic class      | Therapeutic<br>effect | Target type | Target names                    | Absorption<br>tissue | Protein<br>binding    | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail                        |
|-----------------------------------|----------------|-------------|------------------------------------|------------|------------------------|-----------------------|-------------|---------------------------------|----------------------|-----------------------|-----------------|--|--|
| 3714 / 3718                       | O19            | Prestw-719  | Cephalothin sodium salt            | 58-71-9    | Infectiology           | Antibacterial         |             |                                 |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | First-generation<br>cephalosporin                |
| 3714 / 3718                       | O21            | Prestw-720  | Cefuroxime sodium salt             | 56238-63-2 | Infectiology           | Antibacterial         |             |                                 |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Second-<br>generation<br>cephalosporin           |
| 3714 / 3718                       | A04            | Prestw-721  | Althiazide                         | 5588-16-9  | Metabolism             | Antihypertensive      |             |                                 | GI tract             |                       |                 | Therapeutic use  | Association with<br>potassium-<br>sparing agents |
| 3714 / 3718                       | A06            | Prestw-722  | Isopyrin hydrochloride             | 18342-39-7 | Central Nervous System | Analgesic             |             |                                 |                      |                       |                 |  |  |
| 3714 / 3718                       | A08            | Prestw-723  | Phenethicillin potassium salt      | 132-93-4   | Infectiology           | Antibacterial         |             |                                 |                      |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Beta-lactamase<br>sensitive<br>penicillin        |
| 3714 / 3718                       | A10            | Prestw-724  | Sulfamethoxy-pyridazine            | 80-35-3    | Infectiology           | Antibacterial         |             |                                 |                      |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Long-acting<br>sulfonamide                       |
| 3714 / 3718                       | A12            | Prestw-725  | Deferoxamine mesylate              | 138-14-7   | Diagnostic             | Chelating             |             |                                 |                      | Plasmatic<br>proteins | Yes             | New therapeutic<br>use                                   | Intracerebral<br>hemorrhage                      |
| 3714 / 3718                       | A14            | Prestw-726  | Mephentermine hemisulfate          | 1212-72-2  | Cardiovascular         | Antihypotensive       |             |                                 |                      |                       | Yes             | Side effect  | Drug abused                                      |
| 3714 / 3718                       | A16            | Prestw-1140 | Liranaftate                        | 88678-31-3 | Infectiology           | Antifungal            |             |                                 |                      |                       |                 |  |  |
| 3714 / 3718                       | A18            | Prestw-728  | Sulfadimethoxine                   | 122-11-2   | Infectiology           | Antibacterial         |             |                                 |                      | Plasmatic<br>proteins |                 | Chemical<br>classification<br>(according ATC<br>code)    | Long-acting<br>sulfonamide                       |
| 3714 / 3718                       | A20            | Prestw-729  | Sulfanilamide                      | 63-74-1    | Infectiology           | Antibacterial         |             |                                 |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Short-acting<br>sulfonamide                      |
| 3714 / 3718                       | A22            | Prestw-730  | Balsalazide Sodium                 | 80573-04-2 | Gastroenterology       | Anti-inflammatory     |             |                                 | Intestine            |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Aminosalicylic<br>acid derivative                |
| 3714 / 3718                       | C04            | Prestw-731  | Sulfaquinoxaline sodium salt       | 967-80-6   | Infectiology           | Antibacterial         |             |                                 |                      |                       |                 | Veterinary use   | Poultry  |
| 3714 / 3718                       | C06            | Prestw-732  | Streptozotocin                     | 18883-66-4 | Oncology               | Antineoplastic        |             |                                 |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Alkylating agent                                 |
| 3714 / 3718                       | C08            | Prestw-733  | Metoprolol-(+,-) (+)-tartrate salt | 56392-17-7 | Cardiovascular         | Antiarrhythmic        | GPCR        | Adrenergic receptor<br>beta-1   | GI tract             | Plasmatic<br>proteins | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Selective beta-<br>blocking agent                |
| 3714 / 3718                       | C10            | Prestw-734  | Flumethasone                       | 2135-17-3  | Metabolism             | Anti-inflammatory     |             |                                 |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Corticosteroid,<br>moderately<br>potent          |
| 3714 / 3718                       | C12            | Prestw-735  | Flecainide acetate                 | 54143-56-5 | Cardiovascular         | Antiarrhythmic        | LGIC        | Voltage-gated sodium<br>channel | GI tract             | Plasmatic<br>proteins | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Antiarrhythmic,<br>class Ic                      |
| 3714 / 3718                       | C14            | Prestw-736  | Cefazolin sodium salt              | 27164-46-1 | Metabolism             | Antibacterial         |             |                                 |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | First-generation<br>cephalosporin                |
| 3714 / 3718                       | C16            | Prestw-1702 | Trimetozine                        | 635-41-6   | Central Nervous System | Sedative              |             |                                 |                      |                       |                 |  |  |
| 3714 / 3718                       | C18            | Prestw-738  | Folinic acid calcium salt          | 6035-45-6  | Hematology             | Antianemic            |             |                                 | GI tract             |                       | Yes             |  |  |
| 3714 / 3718                       | C20            | Prestw-739  | Levonordefrin                      | 829-74-3   | Cardiovascular         | Vasoconstrictor       |             |                                 |                      |                       | Yes             |  |  |
| 3714 / 3718                       | C22            | Prestw-740  | Ebselen                            | 60940-34-3 | Metabolism             | Anti-inflammatory     |             |                                 |                      | Albumin               |                 |  |  |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                     | CAS number  | Therapeutic class      | Therapeutic effect | Target type      | Target names                | Absorption tissue | Protein binding    | FDA approved | Additional info type                            | Additional info detail                                  |
|-----------------------------------|----------------|-------------|-----------------------------------|-------------|------------------------|--------------------|------------------|-----------------------------|-------------------|--------------------|--------------|---|---|
| 3714 / 3718                       | E04            | Prestw-741  | Nadide                            | 53-84-9     | Metabolism             |                    |                  |                             |                   |                    |              | Side effect                                     | in case of eye contact                                  |
| 3714 / 3718                       | E06            | Prestw-742  | Sulfamethizole                    | 144-82-1    | Metabolism             | Antibacterial      |                  |                             |                   |                    | Yes          | Chemical classification (according ATC code)    | Short-acting sulfonamide                                |
| 3714 / 3718                       | E08            | Prestw-743  | Medrysone                         | 2668-66-8   | Metabolism             | Anti-inflammatory  |                  |                             |                   |                    | Yes          | Chemical classification (according ATC code)    | Corticosteroid  |
| 3714 / 3718                       | E10            | Prestw-744  | Flunixin meglumine                | 42461-84-7  | Central Nervous System | Analgesic          |                  |                             |                   | Plasmatic proteins |              | Veterinary use                                  | Cattle  |
| 3714 / 3718                       | E12            | Prestw-745  | Spiramycin                        | 8025-81-8   | Metabolism             | Antibacterial      |                  |                             |                   |                    |              | Chemical classification (according ATC code)    | Macrolide   |
| 3714 / 3718                       | E14            | Prestw-746  | Glycopyrrolate                    | 596-51-0    | Gastroenterology       | Antispastic        |                  |                             |                   |                    | Yes          | Therapeutic classification (according ATC code) | Anticholinergic   |
| 3714 / 3718                       | E16            | Prestw-1600 | Aprepitant                        | 170729-80-3 | Metabolism             | Antiemetic         | GPCR             | Neurokinin 1 receptor       | GI tract          | Plasmatic proteins | Yes          |   |   |
| 3714 / 3718                       | E18            | Prestw-748  | Monensin sodium salt              | 22373-78-0  | Infectiology           | Antibacterial      |                  |                             | GI tract          |                    |              | Veterinary use                                  | Cattle  |
| 3714 / 3718                       | E20            | Prestw-749  | Isoetharine mesylate salt         | 7279-75-6   | Respiratory            | Bronchodilator     | GPCR             | Adrenergic receptor beta-2  |                   |                    | Yes          |   |   |
| 3714 / 3718                       | E22            | Prestw-750  | Mevalonic-D, L acid lactone       | 674-26-0    | Cardiovascular         | Antilipemic        |                  |                             |                   |                    |              |   |   |
| 3714 / 3718                       | G04            | Prestw-751  | Terazosin hydrochloride           | 63590-64-7  | Cardiovascular         | Antihypertensive   | GPCR             | Adrenergic receptor alpha-1 |                   | Plasmatic proteins | Yes          |   |   |
| 3714 / 3718                       | G06            | Prestw-752  | Phenazopyridine hydrochloride     | 136-40-3    | Central Nervous System | Analgesic          |                  |                             |                   |                    | Yes          |   |   |
| 3714 / 3718                       | G08            | Prestw-753  | Demeclocycline hydrochloride      | 64-73-3     | Metabolism             | Antibacterial      |                  |                             |                   | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Tetracycline  |
| 3714 / 3718                       | G10            | Prestw-754  | Fenoprofen calcium salt dihydrate | 53746-45-5  | Metabolism             | Anti-inflammatory  | Enzyme           | Cyclooxygenase              | GI tract          | Albumin            | Yes          | Therapeutic classification (according ATC code) | NSAID   |
| 3714 / 3718                       | G12            | Prestw-755  | Piperacillin sodium salt          | 59703-84-3  | Metabolism             | Antibacterial      |                  |                             |                   | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Penicillin with extended spectrum                       |
| 3714 / 3718                       | G14            | Prestw-756  | Diethylstilbestrol                | 56-53-1     | Endocrinology          |                    | Nuclear receptor | Estrogen receptor           |                   |                    | Yes          | Chemical classification (according ATC code)    | Estrogen  |
| 3714 / 3718                       | G16            | Prestw-757  | Chlorotrianisene                  | 569-57-3    | Endocrinology          | Antineoplastic     | Nuclear receptor | Estrogen receptor beta      |                   |                    | Yes          |   |   |
| 3714 / 3718                       | G18            | Prestw-758  | Ribostamycin sulfate salt         | 53797-35-6  | Metabolism             | Antibacterial      |                  |                             |                   |                    |              | Chemical classification (according ATC code)    | Aminoside   |
| 3714 / 3718                       | G20            | Prestw-759  | Methacholine chloride             | 62-51-1     | Diagnostic             |                    |                  |                             |                   |                    | Yes          |   |   |
| 3714 / 3718                       | G22            | Prestw-760  | Pipenzolate bromide               | 125-51-9    | Gastroenterology       | Antispastic        |                  |                             |                   |                    |              | Chemical classification (according ATC code)    | Synthetic anticholinergic, quaternary ammonium compound |
| 3714 / 3718                       | I04            | Prestw-761  | Butamben                          | 94-25-7     | Central Nervous System | Anesthetic         |                  |                             |                   |                    |              |   |   |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID  | Chemical_Name               | CAS number | Therapeutic class      | Therapeutic<br>effect | Target type         | Target names                         | Absorption<br>tissue | Protein<br>binding    | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail   |
|-----------------------------------|----------------|------------|-----------------------------|------------|------------------------|-----------------------|---------------------|--------------------------------------|----------------------|-----------------------|-----------------|--|---|
| 3714 / 3718                       | I06            | Prestw-762 | Sulfapyridine               | 144-83-2   | Metabolism             | Antibacterial         |                     |                                      |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Short-acting<br>sulfonamide   |
| 3714 / 3718                       | I08            | Prestw-763 | Meclofenoxate hydrochloride | 3685-84-5  | Central Nervous System | CNS Stimulant         |                     |                                      |                      |                       | Yes             |  |   |
| 3714 / 3718                       | I10            | Prestw-764 | Furaltadone hydrochloride   | 3759-92-0  | Infectiology           | Antibacterial         |                     |                                      |                      |                       | Yes             | Veterinary use   |   |
| 3714 / 3718                       | I12            | Prestw-765 | Ethoxyquin                  | 91-53-2    | Metabolism             | Antifungal            |                     |                                      |                      |                       |                 |  |   |
| 3714 / 3718                       | I14            | Prestw-766 | Tinidazole                  | 19387-91-8 | Infectiology           | Antiamoebic           |                     |                                      | GI tract             | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Nitroimidazole<br>derivative  |
| 3714 / 3718                       | I16            | Prestw-767 | Guanadrel sulfate           | 22195-34-2 | Cardiovascular         | Antihypertensive      |                     |                                      |                      |                       | Yes             |  |   |
| 3714 / 3718                       | I18            | Prestw-768 | Vidarabine                  | 5536-17-4  | Metabolism             | Antiviral             |                     |                                      |                      |                       | Yes             |  |   |
| 3714 / 3718                       | I20            | Prestw-769 | Sulfamerter                 | 651-06-9   | Metabolism             | Antibacterial         |                     |                                      |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Long-acting<br>sulfonamide  |
| 3714 / 3718                       | I22            | Prestw-770 | Isopropamide iodide         | 71-81-8    | Metabolism             | Antiulcer             |                     |                                      |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Synthetic<br>anticholinergic,<br>quaternary<br>ammonium<br>compound |
| 3714 / 3718                       | K04            | Prestw-771 | Alclometasone dipropionate  | 66734-13-2 | Metabolism             | Anti-inflammatory     |                     |                                      | Skin                 |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Corticosteroid,<br>moderately<br>potent                             |
| 3714 / 3718                       | K06            | Prestw-772 | Leflunomide                 | 75706-12-6 | Immunology             | Immunosuppressant     | Enzyme              | Dihydroorotate<br>dehydrogenase      |                      | Albumin               | Yes             |  |   |
| 3714 / 3718                       | K08            | Prestw-773 | Norgestrel(-)-D             | 797-63-7   | Endocrinology          | Contraceptive         | Nuclear<br>receptor | Estrogen receptor                    |                      |                       | Yes             | Therapeutic use  | High dose for<br>emergency<br>contraception                         |
| 3714 / 3718                       | K10            | Prestw-774 | Fluocinonide                | 356-12-7   | Metabolism             | Anti-inflammatory     |                     |                                      | Skin                 |                       | Yes             | Pharmacokinetics   | Prodrug of<br>Fluocinolone<br>acetonide<br>(Prestw-1419)            |
| 3714 / 3718                       | K12            | Prestw-775 | Sulfamethazine sodium salt  | 1981-58-4  | Metabolism             | Antibacterial         |                     |                                      |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Short-acting<br>sulfonamide   |
| 3714 / 3718                       | K14            | Prestw-776 | Guaifenesin                 | 93-14-1    | Respiratory            | Bronchodilator        |                     |                                      | GI tract             |                       | Yes             |  |   |
| 3714 / 3718                       | K16            | Prestw-777 | Alexidine dihydrochloride   | 22573-93-9 | Infectiology           | Antibacterial         |                     |                                      |                      |                       |                 | New therapeutic<br>use                                   | Anti-cancer   |
| 3714 / 3718                       | K18            | Prestw-778 | Proadifen hydrochloride     | 62-68-0    | Neuromuscular          | Local anesthetic      |                     |                                      |                      |                       |                 |  |   |
| 3714 / 3718                       | K20            | Prestw-779 | Zomepirac sodium salt       | 64092-48-4 | Metabolism             | Anti-inflammatory     | Enzyme              | Cyclooxygenase                       |                      |                       |                 | Therapeutic<br>classification<br>(according ATC<br>code) | NSAID   |
| 3714 / 3718                       | K22            | Prestw-780 | Cinoxacin                   | 28657-80-9 | Metabolism             | Antibacterial         |                     |                                      |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Quinolone   |
| 3714 / 3718                       | M04            | Prestw-781 | Clobetasol propionate       | 25122-46-7 | Metabolism             | Anti-inflammatory     |                     |                                      | Skin                 |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Corticosteroid,<br>very potent                                      |
| 3714 / 3718                       | M06            | Prestw-782 | Podophyllotoxin             | 518-28-5   | Metabolism             | Antiviral             |                     |                                      | Skin                 |                       |                 |  |   |
| 3714 / 3718                       | M08            | Prestw-783 | Clofibric acid              | 882-09-7   | Metabolism             | Antilipemic           |                     |                                      |                      |                       | Yes             |  |   |
| 3714 / 3718                       | M10            | Prestw-784 | Bendroflumethiazide         | 73-48-3    | Cardiovascular         | Antihypertensive      | Carrier             | Solute carrier family 12<br>member 3 | GI tract             | Plasmatic<br>proteins | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Low-ceiling<br>diuretic   |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID  | Chemical_Name                  | CAS number | Therapeutic class      | Therapeutic<br>effect | Target type         | Target names                    | Absorption<br>tissue | Protein<br>binding    | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail                              |
|-----------------------------------|----------------|------------|--------------------------------|------------|------------------------|-----------------------|---------------------|---------------------------------|----------------------|-----------------------|-----------------|--|--|
| 3714 / 3718                       | M12            | Prestw-785 | Dicumarol                      | 66-76-2    | Hematology             | Anticoagulant         |                     |                                 |                      |                       | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Vitamin K<br>antagonist<br>(VKA)                       |
| 3714 / 3718                       | M14            | Prestw-786 | Methimazole                    | 60-56-0    | Endocrinology          |                       | Enzyme              | Thyroid peroxidase              |                      | Plasmatic<br>proteins | Yes             | Pharmacokinetics   | Active<br>metabolite of<br>Carbimazole<br>(Prestw-439) |
| 3714 / 3718                       | M16            | Prestw-787 | Merbromin                      | 129-16-8   | Infectiology           | Antibacterial         |                     |                                 | Skin                 |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Mercurial<br>product                                   |
| 3714 / 3718                       | M18            | Prestw-788 | Hexylcaine hydrochloride       | 532-76-3   | Dermatology            | Anesthetic            | Ion channel         | Voltage-gated sodium<br>channel |                      |                       | Yes             |  |  |
| 3714 / 3718                       | M20            | Prestw-789 | Drofenine hydrochloride        | 548-66-3   | Neuromuscular          | Antispastic           |                     |                                 |                      |                       |                 |  |  |
| 3714 / 3718                       | M22            | Prestw-790 | Cycloheximide                  | 66-81-9    | Infectiology           | Antibacterial         |                     |                                 |                      |                       |                 |  |  |
| 3714 / 3718                       | O04            | Prestw-791 | (R) -Naproxen sodium salt      | 23979-41-1 | Metabolism             | Anti-inflammatory     | Enzyme              | Cyclooxygenase                  | GI tract             | Plasmatic<br>proteins | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | NSAID  |
| 3714 / 3718                       | O06            | Prestw-792 | Propidium iodide               | 25535-16-4 | Infectiology           | Antibacterial         |                     |                                 |                      |                       |                 |  |  |
| 3714 / 3718                       | O08            | Prestw-793 | Cloperastine hydrochloride     | 14984-68-0 | Respiratory            | Antitussive           |                     |                                 | GI tract             |                       |                 |  |  |
| 3714 / 3718                       | O10            | Prestw-794 | Eucatropine hydrochloride      | 536-93-6   | Neuromuscular          | Antiglaucoma          |                     |                                 |                      |                       |                 |  |  |
| 3714 / 3718                       | O12            | Prestw-795 | Isocarboxazid                  | 59-63-2    | Central Nervous System | Antidepressant        | Enzyme              | Monoamine oxidase               |                      |                       | Yes             |  |  |
| 3714 / 3718                       | O14            | Prestw-796 | Lithocholic acid               | 434-13-9   | Metabolism             | Cholagogue            |                     |                                 |                      |                       |                 |  |  |
| 3714 / 3718                       | O16            | Prestw-797 | Methotrimeprazine maleat salt  | 7104-38-3  | Central Nervous System | Analgesic             | GPCR                | Dopamine D2 receptor            |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Phenothiazine<br>derivative                            |
| 3714 / 3718                       | O18            | Prestw-798 | Dienestrol                     | 84-17-3    | Endocrinology          |                       | Nuclear<br>receptor | Estrogen receptor               |                      |                       | Yes             |  |  |
| 3714 / 3718                       | O20            | Prestw-799 | Pridinol methanesulfonate salt | 6856-31-1  | Central Nervous System | Antiparkinsonian      |                     |                                 |                      |                       |                 |  |  |
| 3714 / 3718                       | O22            | Prestw-800 | Amrnone                        | 60719-84-8 | Cardiovascular         |                       | Enzyme              | Phosphodiesterases              |                      | Plasmatic<br>proteins | Yes             |  |  |
| 3714 / 3718                       | B03            | Prestw-801 | Carbinoxamine maleate salt     | 3505-38-2  | Allergology            | Antihistaminic        | GPCR                | Histamine H1 receptor           |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Aminoalkyl ether                                       |
| 3714 / 3718                       | B05            | Prestw-802 | Methazolamide                  | 554-57-4   | Metabolism             | Antiglaucoma          | Enzyme              | Carbonic anhydrase              | GI tract             | Plasmatic<br>proteins | Yes             |  |  |
| 3714 / 3718                       | B07            | Prestw-803 | Pyrrithidione                  | 77-04-3    | Central Nervous System | Hypnotic              |                     |                                 |                      |                       |                 |  |  |
| 3714 / 3718                       | B09            | Prestw-804 | Spectinomycin dihydrochloride  | 21736-83-4 | Metabolism             | Antibacterial         |                     |                                 |                      | Plasmatic<br>proteins | Yes             |  |  |
| 3714 / 3718                       | B11            | Prestw-805 | Piromidic acid                 | 19562-30-2 | Metabolism             | Antibacterial         |                     |                                 |                      |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Quinolone  |
| 3714 / 3718                       | B13            | Prestw-806 | Trimipramine maleate salt      | 521-78-8   | Central Nervous System | Antidepressant        |                     |                                 |                      | Plasmatic<br>proteins | Yes             |  |  |
| 3714 / 3718                       | B15            | Prestw-807 | Chloropyramine hydrochloride   | 6170-42-9  | Allergology            | Antihistaminic        | GPCR                | Histamine H1 receptor           |                      |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Substituted<br>ethylene<br>diamine                     |
| 3714 / 3718                       | B17            | Prestw-808 | Furazolidone                   | 67-45-8    | Metabolism             |                       |                     |                                 |                      |                       | Yes             |  |  |
| 3714 / 3718                       | B19            | Prestw-809 | Dichlorphenamide               | 120-97-8   | Ophthalmology          | Antiglaucoma          | Enzyme              | Carbonic anhydrase              |                      |                       | Yes             |  |  |
| 3714 / 3718                       | B21            | Prestw-810 | Sulconazole nitrate            | 61318-91-0 | Metabolism             | Antifungal            |                     |                                 | Skin                 |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Imidazole<br>derivative                                |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name            | CAS number | Therapeutic class      | Therapeutic<br>effect | Target type         | Target names                         | Absorption<br>tissue | Protein<br>binding    | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail   |
|-----------------------------------|----------------|-------------|--------------------------|------------|------------------------|-----------------------|---------------------|--------------------------------------|----------------------|-----------------------|-----------------|--|---|
| 3714 / 3718                       | D03            | Prestw-1233 | Auranofin                | 34031-32-8 | Metabolism             | Analgesic             |                     |                                      | GI tract             |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Gold<br>preparation   |
| 3714 / 3718                       | D05            | Prestw-812  | Cromolyn disodium salt   | 15826-37-6 | Allergology            | Antiasthmatic         |                     |                                      |                      |                       | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Anticholinergic   |
| 3714 / 3718                       | D07            | Prestw-813  | Bucladesine sodium salt  | 16980-89-5 | Cardiovascular         |                       | Enzyme              | Phosphodiesterases                   |                      |                       |                 |  |   |
| 3714 / 3718                       | D09            | Prestw-814  | Cefsulodin sodium salt   | 52152-93-9 | Metabolism             | Antibacterial         |                     |                                      |                      | Plasmatic<br>proteins |                 | Chemical<br>classification<br>(according ATC<br>code)    | Third-generation<br>cephalosporin                                   |
| 3714 / 3718                       | D11            | Prestw-815  | Fosfosal                 | 6064-83-1  | Central Nervous System | Analgesic             |                     |                                      |                      |                       |                 |  |   |
| 3714 / 3718                       | D13            | Prestw-816  | Suprofen                 | 40828-46-4 | Central Nervous System | Analgesic             | Enzyme              | Cyclooxygenase                       | Eye                  |                       | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | NSAID   |
| 3714 / 3718                       | D15            | Prestw-1509 | Deflazacort              | 14484-47-0 | Immunology             | Anti-inflammatory     | Nuclear<br>receptor | Glucocorticoid receptor              |                      |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Glucocorticoid  |
| 3714 / 3718                       | D17            | Prestw-818  | Nadolol                  | 42200-33-9 | Cardiovascular         | Antianginal           | GPCR                | Adrenergic receptor<br>beta          | GI tract             | Plasmatic<br>proteins | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Non-selective<br>beta-blocking<br>agent                             |
| 3714 / 3718                       | D19            | Prestw-819  | Moxalactam disodium salt | 64953-12-4 | Metabolism             | Antibacterial         |                     |                                      |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Third-generation<br>cephalosporin                                   |
| 3714 / 3718                       | D21            | Prestw-820  | Aminophylline            | 317-34-0   | Cardiovascular         | Bronchodilator        |                     |                                      |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Xanthine  |
| 3714 / 3718                       | F03            | Prestw-821  | Azlocillin sodium salt   | 37091-65-9 | Metabolism             | Antibacterial         |                     |                                      |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Penicillin with<br>extended<br>spectrum                             |
| 3714 / 3718                       | F05            | Prestw-822  | Clidinium bromide        | 3485-62-9  | Neuromuscular          | Antispastic           |                     |                                      | GI tract             |                       | Yes             | Therapeutic use  | Association with<br>psycholeptics                                   |
| 3714 / 3718                       | F07            | Prestw-823  | Sulfamonomethoxine       | 1220-83-3  | Metabolism             | Antibacterial         |                     |                                      |                      |                       |                 |  | Veterinary use  |
| 3714 / 3718                       | F09            | Prestw-824  | Benzthiazide             | 91-33-8    | Cardiovascular         | Antihypertensive      |                     |                                      |                      |                       | Yes             |  |   |
| 3714 / 3718                       | F11            | Prestw-825  | Trichlormethiazide       | 133-67-5   | Cardiovascular         | Antihypertensive      | Carrier             | Solute carrier family 12<br>member 3 |                      |                       | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Low-ceiling<br>diuretic   |
| 3714 / 3718                       | F13            | Prestw-826  | Oxalamine citrate salt   | 1949-20-8  | Central Nervous System | Anti-inflammatory     |                     |                                      |                      |                       |                 |  |   |
| 3714 / 3718                       | F15            | Prestw-827  | Propantheline bromide    | 50-34-0    | Neuromuscular          | Antispastic           |                     |                                      | GI tract             |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Synthetic<br>anticholinergic,<br>quaternary<br>ammonium<br>compound |
| 3714 / 3718                       | F17            | Prestw-1361 | Viloxazine hydrochloride | 35604-67-2 | Central Nervous System | Antidepressant        |                     |                                      |                      |                       |                 |  |   |
| 3714 / 3718                       | F19            | Prestw-829  | Dimethadione             | 695-53-4   | Central Nervous System | Anticonvulsant        |                     |                                      |                      |                       |                 | New therapeutic<br>use                                   | Pancreatic<br>stones  |
| 3714 / 3718                       | F21            | Prestw-830  | Ethaverine hydrochloride | 985-13-7   | Central Nervous System | Antispastic           |                     |                                      |                      |                       |                 |  |   |
| 3714 / 3718                       | H03            | Prestw-831  | Butacaine                | 149-16-6   | Dermatology            | Anesthetic            | Ion channel         | Voltage-gated sodium<br>channel      |                      |                       |                 |  |   |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                     | CAS number  | Therapeutic class      | Therapeutic<br>effect | Target type         | Target names                | Absorption<br>tissue | Protein<br>binding                       | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail   |
|-----------------------------------|----------------|-------------|-----------------------------------|-------------|------------------------|-----------------------|---------------------|-----------------------------|----------------------|--|-----------------|--|---|
| 3714 / 3718                       | H05            | Prestw-832  | Cefoxitin sodium salt             | 33564-30-6  | Metabolism             | Antibacterial         |                     |                             |                      | Plasmatic<br>proteins                    | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Second-<br>generation<br>cephalosporin                                    |
| 3714 / 3718                       | H07            | Prestw-833  | Ifosfamide                        | 3778-73-2   | Oncology               | Antineoplastic        |                     |                             |                      |  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Alkylating agent  |
| 3714 / 3718                       | H09            | Prestw-834  | Novobiocin sodium salt            | 1476-53-5   | Metabolism             | Antibacterial         |                     |                             |                      |  | Yes             | Veterinary use   | Cattle  |
| 3714 / 3718                       | H11            | Prestw-1800 | Zolmitriptan                      | 139264-17-8 | Central Nervous System |                       |                     |                             |                      |  | Yes             |  |   |
| 3714 / 3718                       | H13            | Prestw-836  | Indoprofen                        | 31842-01-0  | Central Nervous System | Analgesic             | Enzyme              | Cyclooxygenase              |                      |  |                 | Therapeutic<br>classification<br>(according ATC<br>code) | NSAID   |
| 3714 / 3718                       | H15            | Prestw-837  | Carbenoxolone disodium salt       | 7421-40-1   | Metabolism             | Antiulcer             |                     |                             | Stomach              | Plasmatic<br>proteins                    |                 |  |   |
| 3714 / 3718                       | H17            | Prestw-838  | Iocetamic acid                    | 16034-77-8  | Diagnostic             | Contrastant           |                     |                             |                      |  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Watersoluble,<br>hepatotropic X-<br>ray contrast<br>media                 |
| 3714 / 3718                       | H19            | Prestw-839  | Ganciclovir                       | 82410-32-0  | Metabolism             | Antiviral             |                     |                             |                      |  | Yes             |  |   |
| 3714 / 3718                       | H21            | Prestw-840  | Ethopropazine hydrochloride       | 1094-08-2   | Central Nervous System | Antiparkinsonian      |                     |                             |                      |  | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Anticholinergic<br>agent  |
| 3714 / 3718                       | J03            | Prestw-1455 | Olanzapine                        | 132539-06-1 | Central Nervous System | Antipsychotic         |                     |                             |                      | Albumin,<br>alpha-1-acid<br>glycoprotein | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Diazepine   |
| 3714 / 3718                       | J05            | Prestw-842  | Trimeprazine tartrate             | 4330-99-8   | Allergology            | Antihistaminic        | GPCR                | Histamine H1 receptor       |                      |  | Yes             | New therapeutic<br>use                                   | Antibacterial   |
| 3714 / 3718                       | J07            | Prestw-843  | Nafcillin sodium salt monohydrate | 7177-50-6   | Metabolism             | Antibacterial         |                     |                             |                      |  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Beta-lactamase<br>resistant<br>penicillin                                 |
| 3714 / 3718                       | J09            | Prestw-844  | Procyclidine hydrochloride        | 1508-76-5   | Central Nervous System | Antiparkinsonian      |                     |                             |                      |  | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Anticholinergic<br>agent  |
| 3714 / 3718                       | J11            | Prestw-845  | Amiprilose hydrochloride          | 60414-06-4  | Immunology             | Immunomodulator       |                     |                             |                      |  |                 |  |   |
| 3714 / 3718                       | J13            | Prestw-846  | Ethinylestradiol 3-methyl ether   | 72-33-3     | Endocrinology          |                       |                     |                             |                      |  | Yes             |  |   |
| 3714 / 3718                       | J15            | Prestw-847  | (-) -Levobunolol hydrochloride    | 27912-14-7  | Ophthalmology          | Antiglaucoma          |                     |                             | Eye                  |  | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Beta-blocking<br>agent  |
| 3714 / 3718                       | J17            | Prestw-848  | Iodixanol                         | 92339-11-2  | Diagnostic             | Contrastant           |                     |                             |                      | Plasmatic<br>proteins                    | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Watersoluble,<br>nephrotropic,<br>low osmolar X-<br>ray contrast<br>media |
| 3714 / 3718                       | J19            | Prestw-1379 | Clinafloxacin                     | 105956-97-6 | Infectiology           | Antibacterial         |                     |                             |                      |  |                 |  |   |
| 3714 / 3718                       | J21            | Prestw-850  | Equilin                           | 474-86-2    | Endocrinology          |                       |                     |                             |                      |  |                 | New therapeutic<br>use                                   | Antialzheimer   |
| 3714 / 3718                       | L03            | Prestw-851  | Paroxetine Hydrochloride          | 110429-35-1 | Central Nervous System | Antidepressant        | Carrier             | Serotonin transporter       |                      | Plasmatic<br>proteins                    | Yes             |  |   |
| 3714 / 3718                       | L05            | Prestw-1454 | Nylidrin                          | 447-41-6    | Cardiovascular         | Vasodilator           |                     |                             |                      |  |                 |  |   |
| 3714 / 3718                       | L07            | Prestw-853  | Liothyronine                      | 6893-02-3   | Endocrinology          |                       | Nuclear<br>receptor | Thyroid hormone<br>receptor | GI tract             | Plasmatic<br>proteins                    | Yes             |  |   |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                  | CAS number  | Therapeutic class      | Therapeutic effect | Target type      | Target names                | Absorption tissue | Protein binding    | FDA approved | Additional info type                            | Additional info detail                                       |
|-----------------------------------|----------------|-------------|--------------------------------|-------------|------------------------|--------------------|------------------|-----------------------------|-------------------|--------------------|--------------|---|--|
| 3714 / 3718                       | L09            | Prestw-854  | Roxithromycin                  | 80214-83-1  | Metabolism             | Antibacterial      |                  |                             |                   |                    |              | Chemical classification (according ATC code)    | Macrolide  |
| 3714 / 3718                       | L11            | Prestw-855  | Beclomethasone dipropionate    | 5534-09-8   | Metabolism             | Anti-inflammatory  |                  |                             | Lung, GI tract    |                    | Yes          | Chemical classification (according ATC code)    | Glucocorticoid   |
| 3714 / 3718                       | L13            | Prestw-856  | Tolmetin sodium salt dihydrate | 64490-92-2  | Metabolism             | Anti-inflammatory  | Enzyme           | Cyclooxygenase              | GI tract          | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | NSAID  |
| 3714 / 3718                       | L15            | Prestw-857  | (+) -Levobunolol hydrochloride | 47141-41-3  | Ophthalmology          | Antiglaucoma       |                  |                             | Eye               |                    | Yes          | Therapeutic classification (according ATC code) | Beta blocking agent  |
| 3714 / 3718                       | L17            | Prestw-858  | Doxazosin mesylate             | 77883-43-3  | Cardiovascular         | Antihypertensive   | GPCR             | Adrenergic receptor alpha-1 | GI tract          | Plasmatic proteins | Yes          |   |  |
| 3714 / 3718                       | L19            | Prestw-859  | Fluvastatin sodium salt        | 93957-55-2  | Cardiovascular         | Antilipemic        | Enzyme           | HMG-CoA reductase           | GI tract          | Plasmatic proteins | Yes          |   |  |
| 3714 / 3718                       | L21            | Prestw-860  | Methylhydantoin-5-(L)          | 40856-73-3  | Central Nervous System | Anticonvulsant     |                  |                             |                   |                    |              |   |  |
| 3714 / 3718                       | N03            | Prestw-861  | Gabapentin                     | 60142-96-3  | Central Nervous System | Anticonvulsant     |                  |                             | GI tract          | Plasmatic proteins | Yes          |   |  |
| 3714 / 3718                       | N05            | Prestw-862  | Raloxifene hydrochloride       | 82640-04-8  | Endocrinology          |                    | Nuclear receptor | Estrogen receptor           |                   | Plasmatic proteins | Yes          |   |  |
| 3714 / 3718                       | N07            | Prestw-1801 | Ciclesonide                    | 126544-47-6 | Respiratory            |                    |                  |                             |                   |                    | Yes          |   |  |
| 3714 / 3718                       | N09            | Prestw-864  | Methylhydantoin-5-(D)          | 55147-68-7  |                        |                    |                  |                             |                   |                    |              |   |  |
| 3714 / 3718                       | N11            | Prestw-865  | Simvastatin                    | 79902-63-9  | Cardiovascular         | Antilipemic        | Enzyme           | HMG-CoA reductase           | GI tract          | Plasmatic proteins | Yes          |   |  |
| 3714 / 3718                       | N13            | Prestw-866  | Azacytidine-5                  | 320-67-2    | Oncology               | Antineoplastic     |                  |                             |                   |                    |              | Chemical classification (according ATC code)    | Pyrimidine analogue  |
| 3714 / 3718                       | N15            | Prestw-867  | Paromomycin sulfate            | 1263-89-4   | Metabolism             | Antiamoebic        |                  |                             | GI tract          |                    | Yes          |   |  |
| 3714 / 3718                       | N17            | Prestw-868  | Acetaminophen                  | 103-90-2    | Central Nervous System | Analgesic          |                  |                             | GI tract          | Plasmatic proteins | Yes          |   |  |
| 3714 / 3718                       | N19            | Prestw-869  | Phthalylsulfathiazole          | 85-73-4     | Metabolism             | Antibacterial      |                  |                             | Intestine         |                    |              | Chemical classification (according ATC code)    | Sulfonamide  |
| 3714 / 3718                       | N21            | Prestw-870  | Luteolin                       | 491-70-3    | Respiratory            | Expectorant        |                  |                             |                   |                    |              |   |  |
| 3714 / 3718                       | P03            | Prestw-871  | Iopamidol                      | 60166-93-0  | Diagnostic             | Contrastant        |                  |                             |                   |                    | Yes          | Chemical classification (according ATC code)    | Watersoluble, nephrotropic, low osmolar X-ray contrast media |
| 3714 / 3718                       | P05            | Prestw-872  | Iopromide                      | 73334-07-3  | Diagnostic             | Contrastant        |                  |                             |                   |                    | Yes          | Chemical classification (according ATC code)    | Watersoluble, nephrotropic, low osmolar X-ray contrast media |
| 3714 / 3718                       | P07            | Prestw-873  | Theophylline monohydrate       | 5967-84-0   | Cardiovascular         | Bronchodilator     |                  |                             |                   | Plasmatic proteins | Yes          | Chemical classification (according ATC code)    | Xanthine   |
| 3714 / 3718                       | P09            | Prestw-874  | Theobromine                    | 83-67-0     | Cardiovascular         | Bronchodilator     |                  |                             |                   |                    |              | Chemical classification (according ATC code)    | Xanthine   |



| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                         | CAS number  | Therapeutic class      | Therapeutic effect | Target type             | Target names                         | Absorption tissue | Protein binding    | FDA approved | Additional info type                            | Additional info detail   |
|-----------------------------------|----------------|-------------|---------------------------------------|-------------|------------------------|--------------------|-------------------------|--------------------------------------|-------------------|--------------------|--------------|---|--|
| 3714 / 3718                       | D22            | Prestw-900  | Methylatropine nitrate                | 52-88-0     | Neuromuscular          | Antispastic        |                         |                                      |                   |                    |              | Chemical classification (according ATC code)    | Belladonna alkaloid, semisynthetic, quaternary ammonium compound |
| 3714 / 3718                       | F04            | Prestw-901  | Hymecromone                           | 90-33-5     | Metabolism             | Muscle relaxant    |                         |                                      | GI tract          |                    |              |   |  |
| 3714 / 3718                       | F06            | Prestw-1512 | Abacavir Sulfate                      | 188062-50-2 | Infectiology           | Antiviral          |                         |                                      |                   | Plasmatic proteins | Yes          |   |  |
| 3714 / 3718                       | F08            | Prestw-903  | Diloxanide furoate                    | 3736-81-0   | Metabolism             | Antiamoebic        |                         |                                      | GI tract          |                    |              |   |  |
| 3714 / 3718                       | F10            | Prestw-904  | Metyrapone                            | 54-36-4     | Endocrinology          |                    |                         |                                      | GI tract          |                    | Yes          |   |  |
| 3714 / 3718                       | F12            | Prestw-905  | Urapidil hydrochloride                | 64887-14-5  | Cardiovascular         | Antihypertensive   | GPCR                    | Adrenergic receptor alpha-1          | GI tract          |                    |              |   |  |
| 3714 / 3718                       | F14            | Prestw-906  | Fluspirilen                           | 1841-19-6   | Central Nervous System | Antipsychotic      |                         |                                      |                   |                    |              | Chemical classification (according ATC code)    | Diphenylbutylpiperidine derivative                               |
| 3714 / 3718                       | F16            | Prestw-907  | S-(+)-ibuprofen                       | 51146-56-6  | Central Nervous System | Analgesic          | Enzyme                  | Cyclooxygenase                       | GI tract          | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | NSAID  |
| 3714 / 3718                       | F18            | Prestw-908  | Ethinodiol diacetate                  | 297-76-7    | Endocrinology          | Contraceptive      |                         |                                      |                   |                    | Yes          |   |  |
| 3714 / 3718                       | F20            | Prestw-909  | Nabumetone                            | 42924-53-8  | Central Nervous System | Analgesic          | Enzyme                  | Cyclooxygenase                       | GI tract          | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | NSAID  |
| 3714 / 3718                       | F22            | Prestw-910  | Nisoxetine hydrochloride              | 57754-86-6  | Central Nervous System | Antidepressant     |                         |                                      |                   |                    |              | Pharmacological tool                            |  |
| 3714 / 3718                       | H04            | Prestw-911  | (+)-Isoproterenol (+)-bitartrate salt | 14638-70-1  | Respiratory            | Antiasthmatic      |                         |                                      |                   |                    | Yes          |   |  |
| 3714 / 3718                       | H06            | Prestw-912  | Monobenzone                           | 103-16-2    | Dermatology            |                    |                         |                                      | Skin              |                    | Yes          |   |  |
| 3714 / 3718                       | H08            | Prestw-913  | 2-Aminobenzenesulfonamide             | 3306-62-5   | Metabolism             | Diuretic           |                         |                                      |                   |                    |              | Pharmacological tool                            |  |
| 3714 / 3718                       | H10            | Prestw-914  | Estrone                               | 53-16-7     | Endocrinology          |                    | Nuclear receptor        | Estrogen receptor beta               |                   |                    | Yes          |   |  |
| 3714 / 3718                       | H12            | Prestw-915  | Lorglumide sodium salt                | 97964-56-2  | Metabolism             | Antiulcer          | Trans-membrane receptor | Cholecystokinin receptor antagonist  |                   |                    |              |   |  |
| 3714 / 3718                       | H14            | Prestw-916  | Nitrendipine                          | 39562-70-4  | Cardiovascular         | Antihypertensive   | Ion channel             | Voltage-gated L-type calcium channel | GI tract          | Plasmatic proteins |              | Chemical classification (according ATC code)    | Dihydropyridine derivatives                                      |
| 3714 / 3718                       | H16            | Prestw-917  | Flurbiprofen                          | 5104-49-4   | Central Nervous System | Analgesic          | Enzyme                  | Cyclooxygenase                       | GI tract          | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | NSAID  |
| 3714 / 3718                       | H18            | Prestw-918  | Nimodipine                            | 66085-59-4  | Cardiovascular         | Vasodilator        | Ion channel             | Voltage-gated L-type calcium channel | GI tract          |                    | Yes          | Chemical classification (according ATC code)    | Dihydropyridine derivatives                                      |
| 3714 / 3718                       | H20            | Prestw-919  | Bacitracin                            | 1405-87-4   | Metabolism             | Antibacterial      |                         |                                      |                   |                    | Yes          |   |  |
| 3714 / 3718                       | H22            | Prestw-920  | L(-)-vesamicol hydrochloride          | 112709-59-8 | Neuromuscular          |                    |                         |                                      |                   |                    |              |   |  |
| 3714 / 3718                       | J04            | Prestw-921  | Nizatidine                            | 76963-41-2  | Metabolism             | Antiulcer          | GPCR                    | Histamine H2 receptor                | GI tract          |                    | Yes          |   |  |
| 3714 / 3718                       | J06            | Prestw-922  | Thioperamide maleate                  | 106243-16-7 | Central Nervous System | Antiemetic         | GPCR                    | Histamine H3 receptor                |                   |                    |              |   |  |
| 3714 / 3718                       | J08            | Prestw-923  | Xamoterol hemifumarate                | 73210-73-8  | Cardiovascular         |                    |                         |                                      |                   | Plasmatic proteins |              |   |  |
| 3714 / 3718                       | J10            | Prestw-924  | Rolipram                              | 61413-54-5  | Central Nervous System | Antidepressant     |                         |                                      |                   |                    |              |   |  |
| 3714 / 3718                       | J12            | Prestw-925  | Thonzonium bromide                    | 553-08-2    | Dermatology            | Antiseptic         |                         |                                      |                   |                    | Yes          |   |  |
| 3714 / 3718                       | J14            | Prestw-926  | Idazoxan hydrochloride                | 79944-56-2  | Central Nervous System | Antiparkinsonian   | Trans-membrane receptor | kappa receptor                       |                   |                    |              | New therapeutic use                             | Anti-cancer  |



| ICCB-L Plate (10 mM / 3.33 mM) | ICCB-L Well | Vendor_ID   | Chemical_Name              | CAS number  | Therapeutic class      | Therapeutic effect | Target type      | Target names                 | Absorption tissue | Protein binding           | FDA approved | Additional info type                            | Additional info detail            |
|--------------------------------|-------------|-------------|----------------------------|-------------|------------------------|--------------------|------------------|------------------------------|-------------------|---------------------------|--------------|---|-----------------------------------|
| 3714 / 3718                    | N22         | Prestw-1279 | Stavudine                  | 3056-17-5   | Infectiology           | Antiviral          |                  |                              |                   | Plasmatic proteins        | Yes          |   |                                   |
| 3714 / 3718                    | P04         | Prestw-951  | Crotamiton                 | 483-63-6    | Dermatology            | Antipruritic       |                  |                              |                   |                           | Yes          | Veterinary use                                  | Human use also                    |
| 3714 / 3718                    | P06         | Prestw-1197 | Toremifene                 | 89778-26-7  | Endocrinology          | Antineoplastic     | Nuclear receptor | Estrogen receptor            |                   | Albumin                   | Yes          |   |                                   |
| 3714 / 3718                    | P08         | Prestw-536  | (R)-(+)-Atenolol           | 56715-13-0  | Cardiovascular         | Antianginal        | GPCR             | Adrenergic receptor beta-1   | GI tract          | Plasmatic proteins        | Yes          | Therapeutic classification (according ATC code) | Selective beta-blocking agent     |
| 3714 / 3718                    | P10         | Prestw-954  | Tyloxapol                  | 25301-02-4  | Respiratory            | Mucolytic          |                  |                              |                   |                           | Yes          |   |                                   |
| 3714 / 3718                    | P12         | Prestw-955  | Florfenicol                | 73231-34-2  | Metabolism             | Antibacterial      |                  |                              |                   |                           |              | Veterinary use                                  | Cattle                            |
| 3714 / 3718                    | P14         | Prestw-956  | Megestrol acetate          | 595-33-5    | Endocrinology          | Antineoplastic     | Nuclear receptor | Progesterone receptor        |                   | Plasmatic proteins        | Yes          | Chemical classification (according ATC code)    | Progestogen                       |
| 3714 / 3718                    | P16         | Prestw-957  | Deoxycorticosterone        | 64-85-7     | Endocrinology          | Anti-inflammatory  | Nuclear receptor | Mineralocorticoid receptor   |                   |                           |              | Chemical classification (according ATC code)    | Mineralocorticoid                 |
| 3714 / 3718                    | P18         | Prestw-958  | Urosiol                    | 128-13-2    | Metabolism             |                    |                  |                              | Small intestine   |                           |              |   |                                   |
| 3714 / 3718                    | P20         | Prestw-959  | Proparacaine hydrochloride | 5875-06-9   | Central Nervous System | Anesthetic         | Ion channel      | Voltage-gated sodium channel |                   |                           | Yes          |   |                                   |
| 3714 / 3718                    | P22         | Prestw-960  | Aminocaproic acid          | 60-32-2     | Allergology            | Antifibrinolytic   |                  |                              | GI tract          |                           | Yes          |   |                                   |
| 3715 / 3719                    | A03         | Prestw-961  | Denatonium benzoate        | 3734-33-6   | Neuromuscular          |                    |                  |                              |                   |                           |              | Pharmaceutical use                              | Nail lacquer                      |
| 3715 / 3719                    | A05         | Prestw-1259 | Canrenone                  | 976-71-6    | Endocrinology          | Diuretic           |                  |                              |                   |                           |              | Therapeutic classification (according ATC code) | Potassium-sparing agent           |
| 3715 / 3719                    | A07         | Prestw-963  | Enilconazole               | 35554-44-0  | Metabolism             | Antifungal         |                  |                              |                   |                           | Yes          | Veterinary use                                  |                                   |
| 3715 / 3719                    | A09         | Prestw-964  | Methacycline hydrochloride | 3963-95-9   | Metabolism             | Antibacterial      |                  |                              |                   | Plasmatic proteins        | Yes          | Chemical classification (according ATC code)    | Tetracycline                      |
| 3715 / 3719                    | A11         | Prestw-1415 | Floxuridine                | 50-91-9     | Oncology               | Antineoplastic     |                  |                              |                   |                           | Yes          |   |                                   |
| 3715 / 3719                    | A13         | Prestw-966  | Sotalol hydrochloride      | 959-24-0    | Cardiovascular         | Antianginal        | GPCR             | Adrenergic receptor beta     | GI tract          | Plasmatic proteins        | Yes          | Therapeutic classification (according ATC code) | Non-selective beta-blocking agent |
| 3715 / 3719                    | A15         | Prestw-1267 | Gestrinone                 | 16320-04-0  | Endocrinology          | Contraceptive      |                  |                              |                   |                           |              |   |                                   |
| 3715 / 3719                    | A17         | Prestw-968  | Decamethonium bromide      | 541-22-0    | Neuromuscular          | Muscle relaxant    |                  |                              |                   |                           | Yes          |   |                                   |
| 3715 / 3719                    | A19         | Prestw-1514 | Darifenacin hydrobromide   | 133099-07-7 | Neuromuscular          |                    |                  |                              |                   | Alpha-1-acid glycoprotein | Yes          |   |                                   |
| 3715 / 3719                    | A21         | Prestw-1602 | Indatraline hydrochloride  | 86939-10-8  | Central Nervous System | Antidepressant     |                  |                              |                   |                           |              |   |                                   |
| 3715 / 3719                    | C03         | Prestw-971  | Remoxipride Hydrochloride  | 73220-03-8  | Central Nervous System | Antipsychotic      |                  |                              |                   | Plasmatic proteins        |              | Chemical classification (according ATC code)    | Benzamide                         |
| 3715 / 3719                    | C05         | Prestw-972  | THIP Hydrochloride         | 85118-33-8  | Central Nervous System | Sedative           |                  |                              |                   |                           |              |   |                                   |
| 3715 / 3719                    | C07         | Prestw-973  | Pirlindole mesylate        | 60762-57-4  | Central Nervous System | Antidepressant     |                  |                              |                   |                           |              |   |                                   |
| 3715 / 3719                    | C09         | Prestw-974  | Pronethalol hydrochloride  | 51-02-5     | Cardiovascular         | Antianginal        |                  |                              |                   |                           |              | Pharmaceutical use                              | Beta-blocking agent               |
| 3715 / 3719                    | C11         | Prestw-975  | Naftopidil dihydrochloride | 57149-08-3  | Cardiovascular         | Antihypertensive   |                  |                              |                   |                           |              |   |                                   |
| 3715 / 3719                    | C13         | Prestw-976  | Tracazolate hydrochloride  | 41094-88-6  | Central Nervous System | Anticonvulsant     |                  |                              |                   |                           |              | Pharmacological tool                            |                                   |
| 3715 / 3719                    | C15         | Prestw-977  | Zardaverine                | 101975-10-4 | Respiratory            | Bronchodilator     |                  |                              |                   |                           |              |   |                                   |
| 3715 / 3719                    | C17         | Prestw-978  | Memantine Hydrochloride    | 41100-52-1  | Central Nervous System | Anti-Alzheimer     | LGIC             | Glutamate [NMDA] receptor    |                   | Plasmatic proteins        | Yes          |   |                                   |
| 3715 / 3719                    | C19         | Prestw-979  | Ozagrel hydrochloride      | 78712-43-3  | Cardiovascular         | Antianginal        |                  |                              |                   |                           |              |   |                                   |
| 3715 / 3719                    | C21         | Prestw-980  | Piribedil hydrochloride    | 78213-63-5  | Cardiovascular         | Antiparkinsonian   |                  |                              |                   |                           |              |   |                                   |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                 | CAS number  | Therapeutic class      | Therapeutic<br>effect | Target type         | Target names                         | Absorption<br>tissue        | Protein<br>binding    | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail      |
|-----------------------------------|----------------|-------------|-------------------------------|-------------|------------------------|-----------------------|---------------------|--------------------------------------|-----------------------------|-----------------------|-----------------|--|--------------------------------|
| 3715 / 3719                       | E03            | Prestw-981  | Nitrocaramiphen hydrochloride | 98636-73-8  | Central Nervous System |                       |                     |                                      |                             |                       |                 |  |                                |
| 3715 / 3719                       | E05            | Prestw-982  | Nandrolone                    | 434-22-0    | Endocrinology          | Antianemic            |                     |                                      |                             |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Estren<br>derivative           |
| 3715 / 3719                       | E07            | Prestw-983  | Dimaprit dihydrochloride      | 23256-33-9  | Metabolism             |                       |                     |                                      |                             |                       |                 |  |                                |
| 3715 / 3719                       | E09            | Prestw-1459 | Oxfendazol                    | 53716-50-0  | Metabolism             |                       |                     |                                      |                             | Plasmatic<br>proteins |                 | Veterinary use   | Cattle                         |
| 3715 / 3719                       | E11            | Prestw-1268 | Guaiacol                      | 90-05-1     | Respiratory            | Expectorant           |                     |                                      |                             |                       |                 |  |                                |
| 3715 / 3719                       | E13            | Prestw-986  | Proscillaridin A              | 466-06-8    | Cardiovascular         |                       |                     |                                      |                             |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Scilla glycoside               |
| 3715 / 3719                       | E15            | Prestw-1316 | Pramipexole dihydrochloride   | 104632-25-9 | Central Nervous System | Antiparkinsonian      |                     |                                      |                             | Plasmatic<br>proteins | Yes             |  |                                |
| 3715 / 3719                       | E17            | Prestw-1452 | Norgestimate                  | 35189-28-7  | Endocrinology          |                       | Nuclear<br>receptor | Progesterone receptor                |                             |                       | Yes             |  |                                |
| 3715 / 3719                       | E19            | Prestw-1374 | Chlormadinone acetate         | 302-22-7    | Endocrinology          | Antineoplastic        | Nuclear<br>receptor | Progesterone receptor                |                             |                       |                 |  |                                |
| 3715 / 3719                       | E21            | Prestw-1310 | Phenylbutazone                | 50-33-9     | Metabolism             | Anti-inflammatory     | Enzyme              | Cyclooxygenase                       | Skin                        |                       | Yes             | Veterinary use   | No more human<br>use           |
| 3715 / 3719                       | G03            | Prestw-991  | Gliqidone                     | 33342-05-1  | Endocrinology          | Antidiabetic          |                     |                                      |                             |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Sulfonamide<br>urea derivative |
| 3715 / 3719                       | G05            | Prestw-992  | Pizotifen malate              | 5189-11-7   | Allergology            | Antihistaminic        |                     |                                      |                             | Plasmatic<br>proteins |                 |  |                                |
| 3715 / 3719                       | G07            | Prestw-993  | Ribavirin                     | 36791-04-5  | Metabolism             | Antiviral             |                     |                                      | GI tract, Respiratory tract |                       | Yes             | New therapeutic<br>use                                   | Anti-cancer                    |
| 3715 / 3719                       | G09            | Prestw-994  | Cyclopentiazide               | 742-20-1    | Cardiovascular         | Antihypertensive      | Carrier             | Solute carrier family 12<br>member 3 |                             |                       |                 | Therapeutic<br>classification<br>(according ATC<br>code) | Low-ceiling<br>diuretic        |
| 3715 / 3719                       | G11            | Prestw-995  | Fluvoxamine maleate           | 61718-82-9  | Central Nervous System | Antidepressant        | Carrier             | Serotonin transporter                |                             | Plasmatic<br>proteins | Yes             | New therapeutic<br>use                                   | Antipsychotic                  |
| 3715 / 3719                       | G13            | Prestw-1321 | Prothionamide                 | 14222-60-7  | Infectiology           | Antibacterial         |                     |                                      |                             |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Thiocarbamide<br>derivative    |
| 3715 / 3719                       | G15            | Prestw-997  | Fluticasone propionate        | 80474-14-2  | Cardiovascular         | Anti-inflammatory     |                     |                                      | Nose, Lung, S               | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Glucocorticoid                 |
| 3715 / 3719                       | G17            | Prestw-998  | Zuclopentixol dihydrochloride | 633-59-0    | Central Nervous System | Antipsychotic         | GPCR                | Dopamine D1 receptor                 |                             | Plasmatic<br>proteins |                 | Chemical<br>classification<br>(according ATC<br>code)    | Thioxanthene<br>derivative     |
| 3715 / 3719                       | G19            | Prestw-999  | Proguanil hydrochloride       | 637-32-1    | Metabolism             | Antimalarial          |                     |                                      | GI tract                    | Plasmatic<br>proteins | Yes             |  |                                |
| 3715 / 3719                       | G21            | Prestw-1000 | Lymecycline                   | 992-21-2    | Metabolism             | Antibacterial         |                     |                                      |                             |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Tetracycline                   |
| 3715 / 3719                       | I03            | Prestw-1001 | Alfadolone acetate            | 23930-37-2  | Central Nervous System | Anesthetic            |                     |                                      |                             |                       |                 |  |                                |
| 3715 / 3719                       | I05            | Prestw-1002 | Alfaxalone                    | 23930-19-0  | Central Nervous System | Anesthetic            |                     |                                      |                             |                       |                 | Therapeutic<br>classification<br>(according ATC<br>code) | General<br>anesthetic          |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name               | CAS number  | Therapeutic class      | Therapeutic<br>effect          | Target type      | Target names                         | Absorption<br>tissue | Protein<br>binding | FDA<br>approved | Additional info<br>type                         | Additional info<br>detail           |
|-----------------------------------|----------------|-------------|-----------------------------|-------------|------------------------|--------------------------------|------------------|--------------------------------------|----------------------|--------------------|-----------------|---|-------------------------------------|
| 3715 / 3719                       | I07            | Prestw-1003 | Azapropazone                | 13539-59-8  | Central Nervous System | Analgesic                      |                  |                                      | GI tract             |                    |                 | Therapeutic classification (according ATC code) | NSAID                               |
| 3715 / 3719                       | I09            | Prestw-1004 | Meptazinol hydrochloride    | 59263-76-2  | Central Nervous System | Analgesic                      |                  |                                      |                      |                    |                 | Chemical classification (according ATC code)    | Opioid                              |
| 3715 / 3719                       | I11            | Prestw-1005 | Apramycin                   | 37321-09-8  | Metabolism             | Antibacterial                  |                  |                                      | GI tract             |                    |                 | Veterinary use                                  | Cattle                              |
| 3715 / 3719                       | I13            | Prestw-1802 | Darunavir                   | 635728-49-3 | Infectiology           |                                |                  |                                      |                      |                    | Yes             |   |                                     |
| 3715 / 3719                       | I15            | Prestw-1007 | Fursultiamine Hydrochloride | 2105-43-3   | Metabolism             | Anti-Alzheimer                 |                  |                                      |                      |                    |                 |   |                                     |
| 3715 / 3719                       | I17            | Prestw-1008 | Gabexate mesilate           | 56974-61-9  | Hematology             | Anticoagulant                  |                  |                                      |                      |                    |                 |   |                                     |
| 3715 / 3719                       | I19            | Prestw-1009 | Pivampicillin               | 33817-20-8  | Metabolism             | Antibacterial                  |                  |                                      |                      |                    |                 | Chemical classification (according ATC code)    | Penicillin with extended spectrum   |
| 3715 / 3719                       | I21            | Prestw-1746 | Lodoxamide                  | 53882-12-5  | Allergology            | Antihistaminic                 |                  |                                      |                      |                    | Yes             |   |                                     |
| 3715 / 3719                       | K03            | Prestw-1011 | Flucloxacillin sodium       | 1847-24-1   | Metabolism             | Antibacterial                  |                  |                                      |                      |                    |                 | Chemical classification (according ATC code)    | Beta-lactamase resistant penicillin |
| 3715 / 3719                       | K05            | Prestw-1012 | Trapidil                    | 15421-84-8  | Cardiovascular         | Vasodilator                    |                  |                                      |                      |                    |                 |   |                                     |
| 3715 / 3719                       | K07            | Prestw-1013 | Deptropine citrate          | 2169-75-7   | Allergology            | Antihistaminic                 |                  |                                      |                      |                    |                 |   |                                     |
| 3715 / 3719                       | K09            | Prestw-1014 | Sertraline                  | 79617-96-2  | Central Nervous System | Antidepressant                 | Carrier          | Serotonin transporter                |                      | Plasmatic proteins | Yes             |   |                                     |
| 3715 / 3719                       | K11            | Prestw-1015 | Ethamsylate                 | 2624-44-4   | Cardiovascular         | Antiplatelet                   |                  |                                      | GI tract             | Plasmatic proteins |                 |   |                                     |
| 3715 / 3719                       | K13            | Prestw-1016 | Moxonidine                  | 75438-57-2  | Cardiovascular         | Antihypertensive               | Protein          | Imidazoline i1 receptor              | GI tract             | Plasmatic proteins |                 |   |                                     |
| 3715 / 3719                       | K15            | Prestw-1017 | Etilefrine hydrochloride    | 534-87-2    | Cardiovascular         | Vasoconstrictor                |                  |                                      |                      | Albumin (8)        |                 |   |                                     |
| 3715 / 3719                       | K17            | Prestw-1018 | Alprostadil                 | 745-65-3    | Cardiovascular         | Erectile dysfunction treatment |                  |                                      |                      | Plasmatic proteins | Yes             |   |                                     |
| 3715 / 3719                       | K19            | Prestw-1019 | Tribenoside                 | 10310-32-4  | Cardiovascular         |                                |                  |                                      |                      |                    |                 |   |                                     |
| 3715 / 3719                       | K21            | Prestw-1020 | Rimexolone                  | 49697-38-3  | Metabolism             | Anti-inflammatory              | Nuclear receptor | Glucocorticoid receptor              |                      |                    | Yes             | Chemical classification (according ATC code)    | Glucocorticoid                      |
| 3715 / 3719                       | M03            | Prestw-1021 | Isradipine                  | 75695-93-1  | Cardiovascular         | Antianginal                    | Ion channel      | Voltage-gated L-type calcium channel | GI tract             |                    | Yes             | Chemical classification (according ATC code)    | Dihydropyridine derivatives         |
| 3715 / 3719                       | M05            | Prestw-1774 | Nifekalant                  | 130636-43-0 | Cardiovascular         | Antiarrhythmic                 |                  |                                      |                      |                    |                 |   |                                     |
| 3715 / 3719                       | M07            | Prestw-1023 | Isometheptene mucate        | 7492-31-1   | Cardiovascular         | Antimigraine                   |                  |                                      |                      |                    |                 |   |                                     |
| 3715 / 3719                       | M09            | Prestw-1024 | Nifurtimox                  | 23256-30-6  | Metabolism             |                                |                  |                                      |                      |                    |                 | Chemical classification (according ATC code)    | Nitrofuran derivative               |
| 3715 / 3719                       | M11            | Prestw-1025 | Letrozole                   | 112809-51-5 | Oncology               | Antineoplastic                 | Coenzyme         | Cytochrome P450 19A1                 |                      | Albumin (55%)      | Yes             | Therapeutic classification (according ATC code) | Aromatase inhibitor                 |
| 3715 / 3719                       | M13            | Prestw-1026 | Arbutin                     | 497-76-7    | Metabolism             | Antibacterial                  |                  |                                      |                      |                    |                 | New therapeutic use                             | Depigmentation treatment            |
| 3715 / 3719                       | M15            | Prestw-1027 | Tocainide hydrochloride     | 71395-14-7  | Cardiovascular         | Anesthetic                     | LGIC             | Voltage-gated sodium channel         | GI tract             | Plasmatic proteins | Yes             | Therapeutic classification (according ATC code) | Antiarrhythmic, class Ib            |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name               | CAS number  | Therapeutic class      | Therapeutic effect | Target type            | Target names                          | Absorption tissue | Protein binding                    | FDA approved | Additional info type                            | Additional info detail                                  |
|-----------------------------------|----------------|-------------|-----------------------------|-------------|------------------------|--------------------|------------------------|---------------------------------------|-------------------|------------------------------------|--------------|---|---|
| 3715 / 3719                       | M17            | Prestw-1028 | Benzathine benzylpenicillin | 5928-84-7   | Metabolism             | Antibacterial      |                        |                                       |                   | Plasmatic proteins                 | Yes          | Chemical classification (according ATC code)    | Beta-lactamase sensitive penicillin                     |
| 3715 / 3719                       | M19            | Prestw-1029 | Risperidone                 | 106266-06-2 | Central Nervous System | Antipsychotic      |                        |                                       |                   | Albumin, alpha-1-acid glycoprotein | Yes          |   |   |
| 3715 / 3719                       | M21            | Prestw-1030 | Torsemide                   | 56211-40-6  | Cardiovascular         | Antihypertensive   | Carrier                | Solute carrier family 12 member 1     |                   |                                    | Yes          | Therapeutic classification (according ATC code) | High-ceiling diuretic                                   |
| 3715 / 3719                       | O03            | Prestw-1031 | Halofantrine hydrochloride  | 36167-63-2  | Metabolism             | Antimalarial       |                        |                                       | GI tract          |                                    | Yes          |   |   |
| 3715 / 3719                       | O05            | Prestw-1032 | Articaine hydrochloride     | 23964-57-0  | Central Nervous System | Anesthetic         | Ion channel            | Voltage-gated sodium channel          |                   |                                    | Yes          | Chemical classification (according ATC code)    | Amides  |
| 3715 / 3719                       | O07            | Prestw-1033 | Nomegestrol acetate         | 58652-20-3  | Endocrinology          | Contraceptive      | Nuclear receptor       | Progesterone receptor                 |                   | Plasmatic proteins                 |              |   |   |
| 3715 / 3719                       | O09            | Prestw-1034 | Pancuronium bromide         | 15500-66-0  | Neuromuscular          | Muscle relaxant    |                        |                                       |                   | Plasmatic proteins                 | Yes          | Chemical classification (according ATC code)    | Quaternary ammonium                                     |
| 3715 / 3719                       | O11            | Prestw-1035 | Molindone hydrochloride     | 15622-65-8  | Central Nervous System | Antipsychotic      |                        |                                       |                   |                                    | Yes          | Chemical classification (according ATC code)    | Indole derivative                                       |
| 3715 / 3719                       | O13            | Prestw-1036 | Alcuronium chloride         | 15180-03-7  | Neuromuscular          | Muscle relaxant    |                        |                                       |                   |                                    |              | Chemical classification (according ATC code)    | Curare alkaloid   |
| 3715 / 3719                       | O15            | Prestw-1037 | Zalcitabine                 | 7481-89-2   | Metabolism             | Antiviral          |                        |                                       |                   | Plasmatic proteins                 | Yes          |   |   |
| 3715 / 3719                       | O17            | Prestw-1038 | Methyldopate hydrochloride  | 2508-79-4   | Cardiovascular         | Antihypertensive   |                        |                                       |                   |                                    | Yes          |   |   |
| 3715 / 3719                       | O19            | Prestw-1039 | Levocabastine hydrochloride | 79547-78-7  | Allergology            | Antihistaminic     |                        |                                       |                   |                                    | Yes          |   |   |
| 3715 / 3719                       | O21            | Prestw-1040 | Pyrvinium pamoate           | 3546-41-6   | Metabolism             |                    |                        |                                       | GI tract          |                                    | Yes          | New therapeutic use                             | Anti-cancer   |
| 3715 / 3719                       | A04            | Prestw-1041 | Etomidate                   | 33125-97-2  | Central Nervous System | Anesthetic         |                        |                                       |                   | Plasmatic proteins                 | Yes          | Therapeutic classification (according ATC code) | General anesthetic                                      |
| 3715 / 3719                       | A06            | Prestw-1042 | Tridihexethyl chloride      | 4310-35-4   | Neuromuscular          | Antispastic        |                        |                                       |                   |                                    | Yes          | Chemical classification (according ATC code)    | Synthetic anticholinergic, quaternary ammonium compound |
| 3715 / 3719                       | A08            | Prestw-1043 | Penbutolol sulfate          | 38363-32-5  | Cardiovascular         | Antianginal        | GPCR                   | Adrenergic receptor beta              | GI tract          | Plasmatic proteins                 | Yes          | Therapeutic classification (according ATC code) | Non-selective beta-blocking agent                       |
| 3715 / 3719                       | A10            | Prestw-1044 | Prednicarbate               | 73771-04-7  | Metabolism             | Anti-Inflammatory  |                        |                                       | Skin              |                                    | Yes          | Chemical classification (according ATC code)    | Corticosteroid, potent                                  |
| 3715 / 3719                       | A12            | Prestw-1045 | Sertaconazole nitrate       | 99592-39-9  | Metabolism             | Antibacterial      |                        |                                       | Skin, Vagina      |                                    | Yes          | Chemical classification (according ATC code)    | Imidazole derivative                                    |
| 3715 / 3719                       | A14            | Prestw-1046 | Repaglinide                 | 135062-02-1 | Endocrinology          | Antidiabetic       | Transmembrane receptor | Sulfonylurea receptors K-ATP channels | GI tract          | Plasmatic proteins                 | Yes          |   |   |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name               | CAS number  | Therapeutic class      | Therapeutic effect | Target type | Target names                 | Absorption tissue | Protein binding    | FDA approved | Additional info type                            | Additional info detail                                       |
|-----------------------------------|----------------|-------------|-----------------------------|-------------|------------------------|--------------------|-------------|------------------------------|-------------------|--------------------|--------------|---|--|
| 3715 / 3719                       | A16            | Prestw-1047 | Piretanide                  | 55837-27-9  | Cardiovascular         | Antihypertensive   |             |                              | GI tract          | Albumin            |              | Therapeutic classification (according ATC code) | High-ceiling diuretic  |
| 3715 / 3719                       | A18            | Prestw-1048 | Piperacetazine              | 3819-00-9   | Central Nervous System | Antipsychotic      |             |                              |                   |                    | Yes          |   |  |
| 3715 / 3719                       | A20            | Prestw-1049 | Oxyphenbutazone             | 129-20-4    | Metabolism             | Anti-inflammatory  | Enzyme      | Cyclooxygenase               |                   |                    | Yes          | Therapeutic classification (according ATC code) | NSAID  |
| 3715 / 3719                       | A22            | Prestw-1050 | Quinethazone                | 73-49-4     | Cardiovascular         | Antihypertensive   |             |                              |                   |                    | Yes          | Therapeutic classification (according ATC code) | Low-ceiling diuretic   |
| 3715 / 3719                       | C04            | Prestw-1051 | Moricizine hydrochloride    | 31883-05-3  | Cardiovascular         | Antiarrhythmic     |             |                              |                   | Plasmatic proteins | Yes          |   |  |
| 3715 / 3719                       | C06            | Prestw-1052 | Iopanoic acid               | 96-83-3     | Diagnostic             | Contrastant        |             |                              |                   | Albumin            | Yes          | Chemical classification (according ATC code)    | Watersoluble, hepatotropic X-ray contrast media              |
| 3715 / 3719                       | C08            | Prestw-1053 | Pivmecillinam hydrochloride | 32887-03-9  | Metabolism             | Antibacterial      |             |                              | GI tract          | Plasmatic proteins |              | Chemical classification (according ATC code)    | Penicillin with extended spectrum                            |
| 3715 / 3719                       | C10            | Prestw-1054 | Levopropoxyphene napsylate  | 5714-90-9   | Central Nervous System | Analgesic          |             |                              |                   |                    | Yes          |   |  |
| 3715 / 3719                       | C12            | Prestw-1055 | Piperidolate hydrochloride  | 129-77-1    | Neuromuscular          | Antispastic        |             |                              |                   |                    |              | Chemical classification (according ATC code)    | Synthetic anticholinergic, esters with tertiary amino group  |
| 3715 / 3719                       | C14            | Prestw-1056 | Trifluridine                | 70-00-8     | Metabolism             | Antiviral          |             |                              | Eye               |                    | Yes          |   |  |
| 3715 / 3719                       | C16            | Prestw-1057 | Oxprenolol hydrochloride    | 6452-73-9   | Cardiovascular         | Antianginal        | GPCR        | Adrenergic receptor beta     | GI tract          | Plasmatic proteins | Yes          | Therapeutic classification (according ATC code) | Non-selective beta-blocking agent                            |
| 3715 / 3719                       | C18            | Prestw-1058 | Ondansetron Hydrochloride   | 103639-04-9 | Central Nervous System | Antianemic         | LGIC        | Serotonin 3 (5-HT3) receptor | GI tract          | Plasmatic proteins | Yes          |   |  |
| 3715 / 3719                       | C20            | Prestw-1059 | Propoxycaïne hydrochloride  | 550-83-4    | Central Nervous System | Anesthetic         | Ion channel | Voltage-gated sodium channel |                   |                    | Yes          |   |  |
| 3715 / 3719                       | C22            | Prestw-1060 | Oxaprozin                   | 21256-18-8  | Central Nervous System | Analgesic          | Enzyme      | Cyclooxygenase               | GI tract          |                    | Yes          | Therapeutic classification (according ATC code) | NSAID  |
| 3715 / 3719                       | E04            | Prestw-1061 | Phensuximide                | 86-34-0     | Central Nervous System | Anticonvulsant     |             |                              |                   |                    | Yes          | Chemical classification (according ATC code)    | Succinimide derivatives                                      |
| 3715 / 3719                       | E06            | Prestw-1062 | Ioxaglic acid               | 59017-64-0  | Diagnostic             | Contrastant        |             |                              |                   |                    | Yes          | Chemical classification (according ATC code)    | Watersoluble, nephrotropic, low osmolar X-ray contrast media |
| 3715 / 3719                       | E08            | Prestw-1063 | Naftifine hydrochloride     | 65473-14-5  | Infectiology           | Antifungal         |             |                              | Skin              |                    | Yes          |   |  |
| 3715 / 3719                       | E10            | Prestw-1064 | Mepylcaine hydrochloride    | 956-03-6    | Neuromuscular          | Local anesthetic   | Ion channel | Voltage-gated sodium channel |                   |                    |              |   |  |
| 3715 / 3719                       | E12            | Prestw-1065 | Milrinone                   | 78415-72-2  | Cardiovascular         | Vasodilator        | Enzyme      | Phosphodiesterases           |                   | Plasmatic proteins | Yes          |   |  |
| 3715 / 3719                       | E14            | Prestw-1066 | Methanetheline bromide      | 53-46-3     | Neuromuscular          | Antispastic        |             |                              |                   |                    | Yes          | Chemical classification (according ATC code)    | Synthetic anticholinergic, quaternary ammonium compound      |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                 | CAS number  | Therapeutic class      | Therapeutic<br>effect   | Target type         | Target names   | Absorption<br>tissue   | Protein<br>binding           | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail                 |
|-----------------------------------|----------------|-------------|-------------------------------|-------------|------------------------|-------------------------|---------------------|--|------------------------|------------------------------|-----------------|--|---|
| 3715 / 3719                       | E16            | Prestw-1067 | Ticarcillin sodium            | 74682-62-5  | Infectiology           | Antibacterial           |                     |  |                        | Plasmatic<br>proteins        | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Penicillin with<br>extended<br>spectrum   |
| 3715 / 3719                       | E18            | Prestw-1068 | Thiethylperazine dimalate     | 52239-63-1  | Central Nervous System | Antiemetic              | GPCR                | Dopamine D2 receptor   |                        |                              | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Phenothiazine<br>derivative               |
| 3715 / 3719                       | E20            | Prestw-1069 | Mesalamine                    | 89-57-6     | Metabolism             | Anti-inflammatory       |                     |  | Small intestine, Colon |                              | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Aminosalicic<br>acid derivative           |
| 3715 / 3719                       | E22            | Prestw-1362 | Vorinostat                    | 149647-78-9 | Oncology               | Antineoplastic          |                     |  |                        | Plasmatic<br>proteins        | Yes             |  |   |
| 3715 / 3719                       | G04            | Prestw-1071 | Imidurea                      | 39236-46-9  | Infectiology           | Antifungal              |                     |  |                        |                              |                 |  |   |
| 3715 / 3719                       | G06            | Prestw-1072 | Lansoprazole                  | 103577-45-3 | Metabolism             | Antiulcer               | Enzyme              | H+/K+ ATPase   | Small intestine        | Plasmatic<br>proteins        | Yes             |  |   |
| 3715 / 3719                       | G08            | Prestw-1073 | Bethanechol chloride          | 590-63-6    | Metabolism             |                         |                     |  |                        |                              | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Parasympathom<br>imetic                   |
| 3715 / 3719                       | G10            | Prestw-1074 | Cyproterone acetate           | 427-51-0    | Endocrinology          | Antineoplastic          |                     |  |                        |                              |                 |  |   |
| 3715 / 3719                       | G12            | Prestw-1075 | (R)-Propranolol hydrochloride | 13071-11-9  | Cardiovascular         | Antianginal             | GPCR                | Adrenergic receptor<br>beta                                    | GI tract               | Albumin                      | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Non-selective<br>beta-blocking<br>agent   |
| 3715 / 3719                       | G14            | Prestw-1076 | Ciprofibrate                  | 52214-84-3  | Metabolism             | Hypocholesterole<br>mic | Nuclear<br>receptor | Peroxisome proliferator-<br>activated receptor<br>(PPAR) alpha | GI tract               | Plasmatic<br>proteins        |                 | Therapeutic<br>classification<br>(according ATC<br>code) | Fibrate                                   |
| 3715 / 3719                       | G16            | Prestw-1420 | Formestane                    | 566-48-3    | Endocrinology          | Antineoplastic          | Coenzyme            | Cytochrome P450<br>19A1  |                        | Plasmatic<br>proteins        |                 | Therapeutic<br>classification<br>(according ATC<br>code) | Aromatase<br>inhibitor                    |
| 3715 / 3719                       | G18            | Prestw-1078 | Benzylpenicillin sodium       | 69-57-8     | Infectiology           | Antibacterial           |                     |  |                        |                              | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Beta-lactamase<br>sensitive<br>penicillin |
| 3715 / 3719                       | G20            | Prestw-1803 | Methicillin sodium            | 7246-14-2   | Oncology               |                         |                     |  |                        |                              | Yes             |  |   |
| 3715 / 3719                       | G22            | Prestw-1080 | Methiazole                    | 108579-67-5 | Infectiology           | Anthelmintic            |                     |  |                        |                              |                 |  |   |
| 3715 / 3719                       | I04            | Prestw-1081 | (S)-propranolol hydrochloride | 4199-10-4   | Cardiovascular         | Antianginal             | GPCR                | Adrenergic receptor<br>beta                                    | GI tract               | Alpha-1-acid<br>glycoprotein | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Non-selective<br>beta-blocking<br>agent   |
| 3715 / 3719                       | I06            | Prestw-1082 | (-)-Eseroline fumarate salt   | 104015-29-4 | Central Nervous System | Analgesic               |                     |  |                        |                              |                 |  |   |
| 3715 / 3719                       | I08            | Prestw-1294 | Isosorbide mononitrate        | 16051-77-7  | Cardiovascular         | Antianginal             | Enzyme              | Soluble guanylate<br>cyclase                                   | GI tract               |                              | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Organic nitrate                           |
| 3715 / 3719                       | I10            | Prestw-1516 | Levalbuterol hydrochloride    | 50293-90-8  | Respiratory            | Antiasthmatic           | GPCR                | Adrenergic receptor<br>beta-2                                  |                        |                              | Yes             |  |   |
| 3715 / 3719                       | I12            | Prestw-1493 | Topiramate                    | 97240-79-4  | Central Nervous System | Anticonvulsant          | Ion channel         | Voltage-gated sodium<br>channel                                | GI tract               | Plasmatic<br>proteins        | Yes             | New therapeutic<br>use                                   | Anorectic                                 |
| 3715 / 3719                       | I14            | Prestw-1086 | D-cycloserine                 | 68-41-7     | Infectiology           | Antibacterial           |                     |  | GI tract               |                              | Yes             |  |   |
| 3715 / 3719                       | I16            | Prestw-1804 | Nelarabine                    | 121032-29-9 | Infectiology           |                         |                     |  |                        |                              | Yes             |  |   |
| 3715 / 3719                       | I18            | Prestw-1088 | (+,-)-Synephrine              | 94-07-5     | Cardiovascular         | Vasoconstrictor         |                     |  |                        |                              |                 |  |   |
| 3715 / 3719                       | I20            | Prestw-1089 | (S)-(-)-Cycloserine           | 339-72-0    | Infectiology           | Antibacterial           |                     |  | GI tract               |                              | Yes             |  |   |
| 3715 / 3719                       | I22            | Prestw-1090 | Homosalate                    | 118-56-9    | Dermatology            | Radioprotectant         |                     |  |                        |                              |                 |  |   |
| 3715 / 3719                       | K04            | Prestw-1091 | Spaglumic acid                | 4910-46-7   | Allergology            | Antiallergic            |                     |  |                        |                              |                 |  |   |
| 3715 / 3719                       | K06            | Prestw-1092 | Ranolazine                    | 95635-55-5  | Cardiovascular         | Antianginal             |                     |  |                        |                              | Yes             |  |   |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                   | CAS number  | Therapeutic class      | Therapeutic<br>effect | Target type         | Target names                           | Absorption<br>tissue | Protein<br>binding                    | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail                        |
|-----------------------------------|----------------|-------------|---------------------------------|-------------|------------------------|-----------------------|---------------------|--|----------------------|---------------------------------------|-----------------|--|--|
| 3715 / 3719                       | K08            | Prestw-1443 | Misoprostol                     | 59122-46-2  | Metabolism             | Antiulcer             |                     |  | GI tract             |                                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Prostaglandin                                    |
| 3715 / 3719                       | K10            | Prestw-1094 | Sulfadoxine                     | 2447-57-6   | Infectiology           | Antibacterial         |                     |  |                      |                                       | Yes             | Human use  | Association with<br>Pyrimethamine<br>(Prestw-37) |
| 3715 / 3719                       | K12            | Prestw-1095 | Cyclopentolate hydrochloride    | 5870-29-1   | Metabolism             |                       |                     |  | Eye                  |                                       | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Anticholinergic                                  |
| 3715 / 3719                       | K14            | Prestw-1096 | Estriol                         | 50-27-1     | Endocrinology          |                       | Nuclear<br>receptor | Estrogen receptor                      |                      |                                       |                 |  |  |
| 3715 / 3719                       | K16            | Prestw-1097 | (-)-Isoproterenol hydrochloride | 5984-95-2   | Cardiovascular         | Bronchodilator        |                     |  |                      |                                       | Yes             |  |  |
| 3715 / 3719                       | K18            | Prestw-1339 | Sarafloxacin                    | 98105-99-8  | Infectiology           | Antibacterial         |                     |  |                      |                                       |                 |  |  |
| 3715 / 3719                       | K20            | Prestw-1099 | Nialamide                       | 51-12-7     | Central Nervous System | Antidepressant        | Enzyme              | Monoamine oxidase                      |                      |                                       |                 |  |  |
| 3715 / 3719                       | K22            | Prestw-1195 | Toltrazuril                     | 69004-03-1  | Infectiology           | Anticoccidial         |                     |  |                      |                                       |                 | Veterinary use   | Cattle   |
| 3715 / 3719                       | M04            | Prestw-1101 | Perindopril                     | 82834-16-0  | Cardiovascular         | Antihypertensive      | Enzyme              | Angiotensin-converting<br>enzyme (ACE) | GI tract             |                                       | Yes             |  |  |
| 3715 / 3719                       | M06            | Prestw-1102 | Fexofenadine hydrochloride      | 153439-40-8 | Allergology            | Antihistaminic        | GPCR                | Histamine H1 receptor                  | GI tract             | Plasmatic<br>proteins                 | Yes             |  |  |
| 3715 / 3719                       | M08            | Prestw-1202 | 4-aminosalicylic acid           | 65-49-6     | Infectiology           | Antibacterial         |                     |  |                      | Plasmatic<br>proteins                 | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Aminosalicic<br>acid derivative                  |
| 3715 / 3719                       | M10            | Prestw-1104 | Clonixin Lysinate               | 55837-30-4  | Central Nervous System | Analgesic             |                     |  |                      |                                       | Yes             |  |  |
| 3715 / 3719                       | M12            | Prestw-1105 | Verteporfin                     | 129497-78-5 | Ophthalmology          |                       |                     |  |                      | Albumin (81),<br>lipoproteines<br>(6) | Yes             |  |  |
| 3715 / 3719                       | M14            | Prestw-1106 | Meropenem                       | 96036-03-2  | Infectiology           | Antibacterial         |                     |  |                      |                                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Carbapenem                                       |
| 3715 / 3719                       | M16            | Prestw-1107 | Ramipril                        | 87333-19-5  | Cardiovascular         | Antihypertensive      | Enzyme              | Angiotensin-converting<br>enzyme (ACE) | GI tract             | Plasmatic<br>proteins                 | Yes             |  |  |
| 3715 / 3719                       | M18            | Prestw-1108 | Mephentoin                      | 50-12-4     | Central Nervous System | Anticonvulsant        |                     |  |                      |                                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Hydantoin<br>derivatives                         |
| 3715 / 3719                       | M20            | Prestw-1109 | Rifabutin                       | 72559-06-9  | Infectiology           | Antibacterial         |                     |  |                      | Plasmatic<br>proteins                 | Yes             |  |  |
| 3715 / 3719                       | M22            | Prestw-1110 | Parbendazole                    | 14255-87-9  | Infectiology           |                       |                     |  |                      |                                       |                 | Veterinary use   |  |
| 3715 / 3719                       | O04            | Prestw-1111 | Mecamylamine hydrochloride      | 826-39-1    | Cardiovascular         | Antihypertensive      |                     |  |                      |                                       | Yes             |  |  |
| 3715 / 3719                       | O06            | Prestw-1112 | Procarbazine hydrochloride      | 366-70-1    | Oncology               | Antineoplastic        | DNA                 |  | GI tract             |                                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Methylhydrazine<br>derivative                    |
| 3715 / 3719                       | O08            | Prestw-1113 | Viomycin sulfate                | 37883-00-4  | Infectiology           | Antibacterial         |                     |  |                      |                                       | Yes             |  |  |
| 3715 / 3719                       | O10            | Prestw-1114 | Saquinavir mesylate             | 149845-06-7 | Immunology             | Antiviral             |                     |  |                      | Plasmatic<br>proteins                 | Yes             |  |  |
| 3715 / 3719                       | O12            | Prestw-1115 | Ronidazole                      | 7681-76-7   | Infectiology           | Antibacterial         |                     |  |                      |                                       |                 | Veterinary use   | Pigeon   |
| 3715 / 3719                       | O14            | Prestw-1116 | Dorzolamide hydrochloride       | 130693-82-2 | Cardiovascular         | Antiglaucoma          | Enzyme              | Carbonic anhydrase                     | Eye                  | Plasmatic<br>proteins                 | Yes             |  |  |
| 3715 / 3719                       | O16            | Prestw-1117 | Azaperone                       | 1649-18-9   | Central Nervous System | Antipsychotic         |                     |  |                      |                                       |                 | Veterinary use   | Swine  |
| 3715 / 3719                       | O18            | Prestw-1118 | Cefepime hydrochloride          | 123171-59-5 | Infectiology           | Antibacterial         |                     |  |                      |                                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Fourth-<br>generation<br>cephalosporin           |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name              | CAS number  | Therapeutic class      | Therapeutic<br>effect | Target type | Target names                 | Absorption<br>tissue | Protein<br>binding       | FDA<br>approved | Additional info<br>type                         | Additional info<br>detail         |
|-----------------------------------|----------------|-------------|----------------------------|-------------|------------------------|-----------------------|-------------|------------------------------|----------------------|--------------------------|-----------------|---|-----------------------------------|
| 3715 / 3719                       | O20            | Prestw-1119 | Clocortolone pivalate      | 34097-16-0  | Endocrinology          | Anti-inflammatory     |             |                              |                      |                          | Yes             | Chemical classification (according ATC code)    | Corticosteroid, moderately potent |
| 3715 / 3719                       | O22            | Prestw-1120 | Nadifloxacin               | 124858-35-1 | Infectiology           | Antibacterial         |             |                              |                      |                          |                 |   |                                   |
| 3715 / 3719                       | B03            | Prestw-1283 | Buspirone hydrochloride    | 33386-08-2  | Central Nervous System |                       |             |                              |                      | Plasmatic proteins       | Yes             |   |                                   |
| 3715 / 3719                       | B05            | Prestw-1222 | Anastrozole                | 120511-73-1 | Oncology               | Antineoplastic        | Coenzyme    | Cytochrome P450 19A1         |                      | Plasmatic proteins       | Yes             | Therapeutic classification (according ATC code) | Aromatase inhibitor               |
| 3715 / 3719                       | B07            | Prestw-1399 | Doxycycline hydrochloride  | 10592-13-9  | Metabolism             | Antibacterial         |             |                              | Upper GI tract       | Plasmatic proteins       | Yes             | Chemical classification (according ATC code)    | Tetracycline                      |
| 3715 / 3719                       | B09            | Prestw-1345 | Sulbactam                  | 68373-14-8  | Infectiology           | Antibacterial         |             |                              |                      | Plasmatic proteins       | Yes             | Chemical classification (according ATC code)    | Beta-lactamase inhibitor          |
| 3715 / 3719                       | B11            | Prestw-1414 | Fleroxacin                 | 79660-72-3  | Infectiology           | Antibacterial         |             |                              |                      | Plasmatic proteins       |                 | Chemical classification (according ATC code)    | Fluoroquinolone                   |
| 3715 / 3719                       | B13            | Prestw-1315 | Clavulanate potassium salt | 58001-44-8  | Infectiology           | Antibacterial         |             |                              |                      | Plasmatic proteins       | Yes             | Therapeutic use                                 | Association with penicillin       |
| 3715 / 3719                       | B15            | Prestw-1482 | Valproic acid              | 99-66-1     | Central Nervous System | Anticonvulsant        |             |                              |                      | Plasmatic proteins       | Yes             | Chemical classification (according ATC code)    | Fatty acid derivatives            |
| 3715 / 3719                       | B17            | Prestw-1280 | Mepivacaine hydrochloride  | 1722-62-9   | Neuromuscular          | Local anesthetic      | Ion channel | Voltage-gated sodium channel |                      | Alpha1-acid glycoprotein | Yes             | Chemical classification (according ATC code)    | Amides                            |
| 3715 / 3719                       | B19            | Prestw-1478 | Rifaximin                  | 80621-81-4  | Infectiology           | Antibacterial         |             |                              |                      | Plasma proteins          | Yes             |   |                                   |
| 3715 / 3719                       | B21            | Prestw-1473 | Estradiol Valerate         | 979-32-8    | Endocrinology          | Contraceptive         |             |                              |                      |                          | Yes             |   |                                   |
| 3715 / 3719                       | D03            | Prestw-1206 | Acetylcysteine             | 616-91-1    | Metabolism             | Mucolytic             |             |                              | GI tract, Lung       |                          | Yes             |   |                                   |
| 3715 / 3719                       | D05            | Prestw-1435 | Melengestrol acetate       | 2919-66-6   | Endocrinology          |                       |             |                              |                      |                          |                 |   | Veterinary use                    |
| 3715 / 3719                       | D07            | Prestw-1246 | Bromhexine hydrochloride   | 611-75-6    | Respiratory            | Expectorant           |             |                              | GI tract, Lung       | Plasmatic proteins       |                 |   |                                   |
| 3715 / 3719                       | D09            | Prestw-1223 | Anethole-trithione         | 532-11-6    | Metabolism             | Choleretic            |             |                              | GI tract             |                          |                 |   |                                   |
| 3715 / 3719                       | D11            | Prestw-1476 | Amcinonide                 | 51022-69-6  | Metabolism             | Anti-inflammatory     |             |                              | Skin                 |                          | Yes             | Chemical classification (according ATC code)    | Corticosteroid, potent            |
| 3715 / 3719                       | D13            | Prestw-1256 | Caffeine                   | 58-08-2     | Central Nervous System | CNS Stimulant         |             |                              |                      | Plasmatic proteins       | Yes             | New therapeutic use                             | Antialzheimer                     |
| 3715 / 3719                       | D15            | Prestw-1262 | Carvedilol                 | 72956-09-3  | Cardiovascular         | Antihypertensive      | GPCR        | Adrenergic receptor alpha    | GI tract             | Plasmatic proteins       | Yes             | Therapeutic classification (according ATC code) | Alpha and beta blocking agents    |
| 3715 / 3719                       | D17            | Prestw-1282 | Methenamine                | 100-97-0    | Infectiology           | Antibacterial         |             |                              | GI tract             |                          | Yes             |   |                                   |
| 3715 / 3719                       | D19            | Prestw-1308 | Phentermine hydrochloride  | 1197-21-3   | Central Nervous System |                       |             |                              | GI tract             |                          | Yes             |   |                                   |
| 3715 / 3719                       | D21            | Prestw-1394 | Diclazuril                 | 101831-37-2 | Metabolism             |                       |             |                              |                      |                          |                 | Veterinary use                                  | Cattle                            |
| 3715 / 3719                       | F03            | Prestw-1249 | Famciclovir                | 104227-87-4 | Infectiology           | Antiviral             |             |                              |                      |                          | Yes             |   |                                   |
| 3715 / 3719                       | F05            | Prestw-1398 | Dopamine hydrochloride     | 62-31-7     | Cardiovascular         | Antihypertensive      |             |                              |                      |                          | Yes             |   |                                   |
| 3715 / 3719                       | F07            | Prestw-1263 | Cefdinir                   | 91832-40-5  | Infectiology           | Antibacterial         |             |                              |                      |                          | Yes             | Chemical classification (according ATC code)    | Third-generation cephalosporin    |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name             | CAS number  | Therapeutic class      | Therapeutic<br>effect                | Target type         | Target names   | Absorption<br>tissue | Protein<br>binding                       | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail |
|-----------------------------------|----------------|-------------|---------------------------|-------------|------------------------|--------------------------------------|---------------------|--|----------------------|--|-----------------|--|---------------------------|
| 3715 / 3719                       | F09            | Prestw-1261 | Carprofen                 | 53716-49-7  | Metabolism             | Anti-inflammatory                    |                     |  | GI tract             | Plasmatic<br>proteins                    | Yes             | Veterinary use   | Cat                       |
| 3715 / 3719                       | F11            | Prestw-1371 | Celecoxib                 | 169590-42-5 | Metabolism             | Anti-inflammatory                    | Enzyme              | Cyclooxygenase-2   | GI tract             | Plasmatic<br>proteins                    | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | NSAID                     |
| 3715 / 3719                       | F13            | Prestw-1258 | Candesartan               | 139481-59-7 | Cardiovascular         | Antihypertensive                     | GPCR                | Angiotensin II receptor<br>type 1 (AT-1)                       | GI tract             | Plasmatic<br>proteins                    | Yes             |  |                           |
| 3715 / 3719                       | F15            | Prestw-1483 | Fludarabine               | 21679-14-1  | Oncology               | Antineoplastic                       |                     |  |                      |  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Purine analogue           |
| 3715 / 3719                       | F17            | Prestw-1484 | Cladribine                | 4291-63-8   | Oncology               | Antineoplastic                       |                     |  |                      | Plasmatic<br>proteins                    | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Purine analogue           |
| 3715 / 3719                       | F19            | Prestw-1356 | Vardenafil                | 224785-90-4 | Cardiovascular         | Erectile<br>dysfunction<br>treatment | Enzyme              | Phosphodiesterase 5  |                      | Plasmatic<br>proteins                    | Yes             |  |                           |
| 3715 / 3719                       | F21            | Prestw-1417 | Fluconazole               | 86386-73-4  | Metabolism             | Antifungal                           |                     |  |                      | Plasmatic<br>proteins                    | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Triazole<br>derivative    |
| 3715 / 3719                       | H03            | Prestw-1203 | 5-fluorouracil            | 51-21-8     | Oncology               | Antineoplastic                       | DNA                 |  |                      |  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Pyrimidine<br>analogue    |
| 3715 / 3719                       | H05            | Prestw-1487 | Mesna                     | 19767-45-4  | Oncology               | Chemoprotectant                      |                     |  | Small intestine      |  | Yes             | Mechanism  | Acrolein<br>antidote      |
| 3715 / 3719                       | H07            | Prestw-1444 | Mitotane                  | 53-19-0     | Endocrinology          | Antineoplastic                       |                     |  | GI tract             |  | Yes             |  |                           |
| 3715 / 3719                       | H09            | Prestw-1497 | Ambrisentan               | 177036-94-1 | Cardiovascular         | Antihypertensive                     | GPCR                | Endothelin receptor ET-<br>A                                   | GI tract             | Albumin,<br>alpha-1-acid<br>glycoprotein | Yes             |  |                           |
| 3715 / 3719                       | H11            | Prestw-1479 | Triclosan                 | 3380-34-5   | Infectiology           | Antibacterial                        |                     |  | Skin                 |  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Phenol and<br>derivative  |
| 3715 / 3719                       | H13            | Prestw-1401 | Enoxacin                  | 84294-96-2  | Infectiology           | Antibacterial                        |                     |  |                      | Plasmatic<br>proteins                    | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Fluoroquinolone           |
| 3715 / 3719                       | H15            | Prestw-1307 | Olopatadine hydrochloride | 140462-76-6 | Allergology            | Antihistaminic                       |                     |  | Nose, Eye, GI tract  |  | Yes             |  |                           |
| 3715 / 3719                       | H17            | Prestw-1187 | Granisetron               | 109889-09-0 | Endocrinology          | Antiemetic                           | LGIC                | Serotonin 3 (5-HT3)<br>receptor                                | GI tract             | Plasmatic<br>proteins                    | Yes             |  |                           |
| 3715 / 3719                       | H19            | Prestw-1224 | Anthralin                 | 1143-38-0   | Dermatology            | Antipsoriatic                        |                     |  | Skin                 |  |                 | Chemical<br>classification<br>(according ATC<br>code)    | Antracen<br>derivative    |
| 3715 / 3719                       | H21            | Prestw-1492 | Lamotrigine               | 84057-84-1  | Central Nervous System | Anticonvulsant                       | Ion channel         | Voltage-gated sodium<br>channel                                |                      | Plasmatic<br>proteins                    | Yes             | New therapeutic<br>use                                   | Antidepressant            |
| 3715 / 3719                       | J03            | Prestw-1383 | Clofibrate                | 637-07-0    | Metabolism             | Antilipemic                          | Nuclear<br>receptor | Peroxisome proliferator-<br>activated receptor<br>(PPAR) alpha | GI tract             |  | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Fibrate                   |
| 3715 / 3719                       | J05            | Prestw-1481 | Cyclophosphamide          | 50-18-0     | Immunology             | Antineoplastic                       |                     |  |                      |  | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Alkylating agent          |
| 3715 / 3719                       | J07            | Prestw-1229 | Aripiprazole              | 129722-12-9 | Central Nervous System | Antipsychotic                        |                     |  |                      | Albumin                                  | Yes             | New therapeutic<br>use                                   | Antialzheimer             |

| ICCB-L Plate (10 mM / 3.33 mM) | ICCB-L Well | Vendor_ID   | Chemical_Name                | CAS number  | Therapeutic class      | Therapeutic effect | Target type      | Target names                          | Absorption tissue | Protein binding                    | FDA approved | Additional info type                            | Additional info detail       |
|--------------------------------|-------------|-------------|------------------------------|-------------|------------------------|--------------------|------------------|---------------------------------------|-------------------|------------------------------------|--------------|---|------------------------------|
| 3715 / 3719                    | J09         | Prestw-1405 | Ethinylestradiol             | 57-63-6     | Endocrinology          | Contraceptive      | Nuclear receptor | Estrogen receptor                     |                   | Albumin                            | Yes          |   |                              |
| 3715 / 3719                    | J11         | Prestw-1419 | Fluocinolone acetonide       | 67-73-2     | Metabolism             | Anti-inflammatory  |                  |                                       | Ocular            |                                    | Yes          | Chemical classification (according ATC code)    | Corticosteroid, potent       |
| 3715 / 3719                    | J13         | Prestw-1343 | Sparfloxacin                 | 110871-86-8 | Infectiology           | Antibacterial      |                  |                                       |                   |                                    | Yes          | Chemical classification (according ATC code)    | Fluoroquinolone              |
| 3715 / 3719                    | J15         | Prestw-1390 | Desloratadine                | 100643-71-8 | Allergology            | Antihistaminic     | GPCR             | Histamine H1 receptor                 | GI tract          | Plasmatic proteins                 | Yes          |   |                              |
| 3715 / 3719                    | J17         | Prestw-1378 | Clarithromycin               | 81103-11-9  | Infectiology           | Antibacterial      |                  |                                       |                   | Plasmatic proteins                 | Yes          | Chemical classification (according ATC code)    | Macrolide                    |
| 3715 / 3719                    | J19         | Prestw-1199 | Tripelennamine hydrochloride | 154-69-8    | Allergology            | Antihistaminic     | GPCR             | Histamine H1 receptor                 |                   |                                    | Yes          | Chemical classification (according ATC code)    | Substituted ethylene diamine |
| 3715 / 3719                    | J21         | Prestw-1352 | Tulobuterol                  | 41570-61-0  | Respiratory            | Bronchodilator     | GPCR             | Adrenergic receptor beta-2            |                   |                                    |              |   |                              |
| 3715 / 3719                    | L03         | Prestw-1196 | Topotecan                    | 123948-87-8 | Oncology               | Antineoplastic     | Enzyme           | DNA topoisomerase I                   |                   | Plasmatic proteins                 | Yes          |   |                              |
| 3715 / 3719                    | L05         | Prestw-1232 | Atorvastatin                 | 134523-00-5 | Metabolism             |                    | Enzyme           | HMG-CoA reductase                     | GI tract          | Plasmatic proteins                 | Yes          |   |                              |
| 3715 / 3719                    | L07         | Prestw-1234 | Azithromycin                 | 83905-01-5  | Infectiology           | Antibacterial      |                  |                                       |                   | Plasmatic proteins                 | Yes          | Chemical classification (according ATC code)    | Macrolide                    |
| 3715 / 3719                    | L09         | Prestw-1286 | Ibutilast                    | 50847-11-5  | Metabolism             | Anti-inflammatory  | Enzyme           | Phosphodiesterase 4                   |                   |                                    | Japan appro  | New therapeutic use                             | Methamphetamine withdrawal   |
| 3715 / 3719                    | L11         | Prestw-1433 | Losartan                     | 114798-26-4 | Cardiovascular         | Antihypertensive   | GPCR             | Angiotensin II receptor type 1 (AT-1) | GI tract          | Albumin                            | Yes          |   |                              |
| 3715 / 3719                    | L13         | Prestw-1236 | Benzotropine mesylate        | 132-17-2    | Central Nervous System | Antiparkinsonian   |                  |                                       |                   | Plasmatic proteins                 | Yes          | Therapeutic classification (according ATC code) | Anticholinergic agent        |
| 3715 / 3719                    | L15         | Prestw-1359 | Vecuronium bromide           | 50700-72-6  | Metabolism             | Muscle relaxant    |                  |                                       |                   |                                    | Yes          | Chemical classification (according ATC code)    | Quaternary ammonium          |
| 3715 / 3719                    | L17         | Prestw-1350 | Telmisartan                  | 144701-48-4 | Cardiovascular         | Antihypertensive   | GPCR             | Angiotensin II receptor type 1 (AT-1) | GI tract          | Albumin, alpha-1-acid glycoprotein | Yes          |   |                              |
| 3715 / 3719                    | L19         | Prestw-1490 | Nalmefene hydrochloride      | 58895-64-0  | Central Nervous System |                    |                  |                                       |                   | Plasmatic proteins                 | Yes          | New therapeutic use                             | Alcohol withdrawal           |
| 3715 / 3719                    | L21         | Prestw-1241 | Bifonazole                   | 60628-96-8  | Infectiology           | Antifungal         |                  |                                       | Skin              |                                    |              | Chemical classification (according ATC code)    | Imidazole derivative         |
| 3715 / 3719                    | N03         | Prestw-1265 | Gatifloxacin                 | 112811-59-3 | Infectiology           | Antibacterial      |                  |                                       |                   | Plasmatic proteins                 | Yes          | Chemical classification (according ATC code)    | Fluoroquinolone              |
| 3715 / 3719                    | N05         | Prestw-1244 | Bosentan                     | 147536-97-8 | Cardiovascular         | Vasodilator        | GPCR             | Endothelin receptor ET-A              | GI tract          | Albumin                            | Yes          |   |                              |
| 3715 / 3719                    | N07         | Prestw-1266 | Gemcitabine                  | 95058-81-4  | Oncology               | Antineoplastic     |                  |                                       |                   | Plasmatic proteins                 | Yes          | Chemical classification (according ATC code)    | Pyrimidine analogue          |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name               | CAS number  | Therapeutic class      | Therapeutic<br>effect | Target type         | Target names   | Absorption<br>tissue | Protein<br>binding                                  | FDA<br>approved | Additional info<br>type                               | Additional info<br>detail   |
|-----------------------------------|----------------|-------------|-----------------------------|-------------|------------------------|-----------------------|---------------------|--|----------------------|---|-----------------|---|---|
| 3715 / 3719                       | N09            | Prestw-1190 | Olmesartan                  | 144689-63-4 | Cardiovascular         | Antihypertensive      | GPCR                | Angiotensin II receptor<br>type 1 (AT-1)                       | GI tract             | Plasmatic<br>proteins                               | Yes             | Pharmacokinetics                                      | Prodrug of<br>Olmesartan acid   |
| 3715 / 3719                       | N11            | Prestw-1480 | Racemephrine hydrochloride  | 329-63-5    | Cardiovascular         | Bronchodilator        |                     |  |                      |   | Yes             |   |   |
| 3715 / 3719                       | N13            | Prestw-1189 | Montelukast                 | 158966-92-8 | Respiratory            | Antiasthmatic         | GPCR                | Cysteinyl leukotriene<br>receptor 1                            |                      | Plasmatic<br>proteins                               | Yes             |   |   |
| 3715 / 3719                       | N15            | Prestw-1180 | Docetaxel                   | 114977-28-5 | Oncology               | Antineoplastic        |                     |  |                      | Plasmatic<br>proteins                               | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Taxane  |
| 3715 / 3719                       | N17            | Prestw-1376 | Cilnidipine                 | 132203-70-4 | Cardiovascular         | Antihypertensive      | Ion channel         | Voltage-gated L-type<br>calcium channel                        |                      |   |                 | Chemical<br>classification<br>(according ATC<br>code) | Dihydropyridine<br>derivatives  |
| 3715 / 3719                       | N19            | Prestw-1291 | Imiquimod                   | 99011-02-6  | Dermatology            | Antiviral             |                     |  | Skin                 |   | Yes             |   |   |
| 3715 / 3719                       | N21            | Prestw-1423 | Fosinopril                  | 98048-97-6  | Cardiovascular         | Antihypertensive      | Enzyme              | Angiotensin-converting<br>enzyme (ACE)                         | GI tract             | Plasmatic<br>proteins                               | Yes             |   |   |
| 3715 / 3719                       | P03            | Prestw-1290 | Imatinib                    | 152459-95-5 | Oncology               | Antineoplastic        | Enzyme              | Bcr/Abl fusion protein   |                      | Albumin,<br>alphaglycoprot<br>eins,<br>lipoproteins | Yes             | New therapeutic<br>use                                | Pulmonary<br>antihypertensive   |
| 3715 / 3719                       | P05            | Prestw-1446 | Moxifloxacin                | 151096-09-2 | Infectiology           | Antibacterial         |                     |  |                      | Plasmatic<br>proteins                               | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Fluoroquinolone   |
| 3715 / 3719                       | P07            | Prestw-1421 | Formoterol fumarate         | 43229-80-7  | Respiratory            | Antiasthmatic         | GPCR                | Adrenergic receptor<br>beta-2                                  | Lung, GI tract       | Albumin<br>(34%)                                    | Yes             |   |   |
| 3715 / 3719                       | P09            | Prestw-1338 | Rufloxacin                  | 101363-10-4 | Infectiology           | Antibacterial         |                     |  |                      |   |                 | Chemical<br>classification<br>(according ATC<br>code) | Fluoroquinolone   |
| 3715 / 3719                       | P11            | Prestw-1319 | Pravastatin                 | 81093-37-0  | Metabolism             | Antilipemic           | Enzyme              | HMG-CoA reductase  | GI tract             | Plasmatic<br>proteins                               | Yes             |   |   |
| 3715 / 3719                       | P13            | Prestw-1337 | Rosiglitazone Hydrochloride | 122320-73-4 | Metabolism             | Antidiabetic          | Nuclear<br>receptor | Peroxisome proliferator-<br>activated receptor<br>(PPAR) gamma | GI tract             | Plasmatic<br>proteins                               | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Thiazolidinedion<br>e   |
| 3715 / 3719                       | P15            | Prestw-1334 | Rivastigmine                | 123441-03-2 | Central Nervous System |                       | Enzyme              | Acetylcholinesterase   |                      | Plasmatic<br>proteins                               | Yes             |   |   |
| 3715 / 3719                       | P17            | Prestw-1342 | Sildenafil                  | 139755-83-2 | Cardiovascular         | Antihypertensive      | Enzyme              | Phosphodiesterase 5  |                      | Plasmatic<br>proteins                               | Yes             | New therapeutic<br>use                                | Wound healing   |
| 3715 / 3719                       | P19            | Prestw-1207 | Acetylsalicylic acid        | 50-78-2     | Central Nervous System | Analgesic             | Enzyme              | Cyclooxygenase   | GI tract             | Plasmatic<br>proteins                               | Yes             |   |   |
| 3715 / 3719                       | P21            | Prestw-1472 | Hexachlorophene             | 70-30-4     | Infectiology           | Antiseptic            |                     |  | Skin                 |   | Yes             | Chemical<br>classification<br>(according ATC<br>code) | Phenol and<br>derivative  |
| 3715 / 3719                       | B04            | Prestw-1764 | Nelfinavir mesylate         | 159989-65-8 | Infectiology           | Antiviral             |                     |  |                      | Plasmatic<br>proteins                               | Yes             |   |   |
| 3715 / 3719                       | B06            | Prestw-1749 | Sildenafil                  | 160970-54-7 | Cardiovascular         | Antihypertensive      | GPCR                | Adrenergic receptor<br>alpha-1                                 |                      | Plasmatic<br>proteins                               | Yes             |   |   |
| 3715 / 3719                       | B08            | Prestw-1777 | Trimebutine                 | 39133-31-8  | Neuromuscular          | Antispastic           |                     |  | GI tract             |   |                 | Chemical<br>classification<br>(according ATC<br>code) | Synthetic<br>anticholinergic,<br>esters with<br>tertiary amino<br>group |
| 3715 / 3719                       | B10            | Prestw-1739 | Nevirapine                  | 129618-40-2 | Infectiology           | Antiviral             |                     |  |                      | Plasmatic<br>proteins                               | Yes             |   |   |
| 3715 / 3719                       | B12            | Prestw-1707 | Doxapram hydrochloride      | 7081-53-0   | Respiratory            | Analeptic             |                     |  |                      |   | Yes             |   |   |
| 3715 / 3719                       | B14            | Prestw-1718 | Amlexanox                   | 68302-57-8  | Allergology            | Anti-inflammatory     |                     |  | GI tract             |   | Yes             |   |   |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name                | CAS number  | Therapeutic class      | Therapeutic<br>effect | Target type           | Target names                          | Absorption<br>tissue | Protein<br>binding                 | FDA<br>approved | Additional info<br>type                      | Additional info<br>detail      |
|-----------------------------------|----------------|-------------|------------------------------|-------------|------------------------|-----------------------|-----------------------|---------------------------------------|----------------------|------------------------------------|-----------------|--|--------------------------------|
| 3715 / 3719                       | B16            | Prestw-1719 | Amorolfine hydrochloride     | 78613-38-4  | Infectiology           | Antifungal            |                       |                                       | Nail, Skin           |                                    | Yes             |  |                                |
| 3715 / 3719                       | B18            | Prestw-1786 | Enrofloxacin                 | 93106-60-6  | Infectiology           | Antibacterial         |                       |                                       |                      |                                    |                 | Veterinary use                               | Cat                            |
| 3715 / 3719                       | B20            | Prestw-1784 | Ubenimex                     | 58970-76-6  | Oncology               | Antineoplastic        |                       |                                       |                      |                                    |                 |  |                                |
| 3715 / 3719                       | B22            | Prestw-1778 | Troxipide                    | 99777-81-8  | Metabolism             | Antiulcer             |                       |                                       |                      |                                    |                 |  |                                |
| 3715 / 3719                       | D04            | Prestw-1773 | Ipriflavone                  | 35212-22-7  | Metabolism             | Antiosteoporetic      |                       |                                       |                      |                                    |                 |  |                                |
| 3715 / 3719                       | D06            | Prestw-1762 | Ezetimibe                    | 163222-33-1 | Metabolism             | Hypocholesterolemic   | Protein               | Niemann-Pick C1-like protein 1        | GI tract             | Plasmatic proteins                 | Yes             |  |                                |
| 3715 / 3719                       | D08            | Prestw-1761 | Rizatriptan benzoate         | 145202-66-0 | Central Nervous System | Antimigraine          | GPCR                  | Serotonin 1d (5-HT1d) receptor        |                      | Plasmatic proteins                 | Yes             |  |                                |
| 3715 / 3719                       | D10            | Prestw-1760 | Tegaserod maleate            | 189188-57-6 | Gastroenterology       | Gastroprokinetic      |                       |                                       | GI tract             | Alpha-acid glycoprotein            | Yes             |  |                                |
| 3715 / 3719                       | D12            | Prestw-1758 | Pantoprazole sodium          | 138786-67-1 | Metabolism             | Antiulcer             | Enzyme                | H+/K+ ATPase                          | Small intestine      | Plasmatic proteins                 | Yes             |  |                                |
| 3715 / 3719                       | D14            | Prestw-1753 | Tegafur                      | 17902-23-7  | Oncology               | Antineoplastic        |                       |                                       | GI tract             |                                    |                 | Chemical classification (according ATC code) | Pyrimidine analogue            |
| 3715 / 3719                       | D16            | Prestw-1732 | Tolcapone                    | 134308-13-7 | Central Nervous System | Antiparkinsonian      | Enzyme                | Catechol O-methyltransferase          |                      | Albumin                            | Yes             |  |                                |
| 3715 / 3719                       | D18            | Prestw-1716 | Altrenogest                  | 850-52-2    | Endocrinology          | Progestogen           |                       |                                       |                      |                                    |                 | Veterinary use                               | Horse                          |
| 3715 / 3719                       | D20            | Prestw-1711 | Felbamate                    | 25451-15-4  | Central Nervous System | Antiepileptic         |                       |                                       |                      | Albumin                            | Yes             |  |                                |
| 3715 / 3719                       | D22            | Prestw-1709 | Estramustine                 | 2998-57-4   | Oncology               | Antineoplastic        |                       |                                       | GI tract             |                                    | Yes             |  |                                |
| 3715 / 3719                       | F04            | Prestw-1708 | (R)-Duloxetine hydrochloride | 116539-60-7 |                        |                       |                       |                                       |                      | Albumin, alpha-1-acid glycoprotein | Yes             |  |                                |
| 3715 / 3719                       | F06            | Prestw-1706 | Donepezil hydrochloride      | 120011-70-3 | Central Nervous System | Anti-Alzheimer        | Enzyme                | Acetylcholinesterase                  |                      | Plasmatic proteins                 | Yes             |  |                                |
| 3715 / 3719                       | F08            | Prestw-1703 | 1,8-Dihydroxyanthraquinone   | 117-10-2    | Gastroenterology       | Laxative              |                       |                                       |                      |                                    |                 |  |                                |
| 3715 / 3719                       | F10            | Prestw-1733 | Nitazoxanide                 | 55981-09-4  | Infectiology           | Antiprotozoal         |                       |                                       |                      |                                    | Yes             |  |                                |
| 3715 / 3719                       | F12            | Prestw-1748 | Nateginide                   | 105816-04-4 | Endocrinology          | Antidiabetic          | Transmembrane protein | Sulfonylurea receptors K-ATP channels | GI tract             | Albumin                            | Yes             |  |                                |
| 3715 / 3719                       | F14            | Prestw-1721 | Avobenzone                   | 70356-09-1  | Dermatology            | Cytoprotectant        |                       |                                       |                      |                                    | Yes             |  |                                |
| 3715 / 3719                       | F16            | Prestw-1715 | Algestone acetophenide       | 24356-94-3  | Endocrinology          | Contraceptive         |                       |                                       |                      |                                    |                 |  |                                |
| 3715 / 3719                       | F18            | Prestw-1763 | Actarit                      | 18699-02-0  | Immunology             | Anti-inflammatory     |                       |                                       |                      |                                    |                 |  |                                |
| 3715 / 3719                       | F20            | Prestw-1710 | Ethoxzolamide                | 452-35-7    | Ophthalmology          | Antiglaucoma          |                       |                                       |                      |                                    | Yes             |  |                                |
| 3715 / 3719                       | F22            | Prestw-1722 | Azatadine maleate            | 3978-86-7   | Allergology            | Antihistaminic        | GPCR                  | Histamine H1 receptor                 | GI tract             |                                    | Yes             |  |                                |
| 3715 / 3719                       | H04            | Prestw-1717 | Aminacrine                   | 90-45-9     | Infectiology           | Antiseptic            |                       |                                       | Skin                 |                                    |                 | Chemical classification (according ATC code) | Acridine derivative            |
| 3715 / 3719                       | H06            | Prestw-1792 | Pidotimod                    | 121808-62-6 | Immunology             | Immunostimulant       |                       |                                       |                      |                                    |                 |  |                                |
| 3715 / 3719                       | H08            | Prestw-1766 | Benidipine hydrochloride     | 91599-74-5  | Cardiovascular         | Antihypertensive      | Ion channel           | Voltage-gated L-type calcium channel  |                      |                                    |                 | Chemical classification (according ATC code) | Dihydropyridine derivatives    |
| 3715 / 3719                       | H10            | Prestw-1770 | Perospirone                  | 150915-41-6 | Central Nervous System | Antipsychotic         |                       |                                       |                      |                                    |                 |  |                                |
| 3715 / 3719                       | H12            | Prestw-1726 | Cefpiramide                  | 70797-11-4  | Infectiology           | Antibacterial         |                       |                                       |                      |                                    | Yes             | Chemical classification (according ATC code) | Third-generation cephalosporin |
| 3715 / 3719                       | H14            | Prestw-1713 | Fenoldopam                   | 67227-56-9  | Cardiovascular         | Antihypertensive      |                       |                                       |                      |                                    | Yes             | New therapeutic use                          | Chemoprotectant                |
| 3715 / 3719                       | H16            | Prestw-1714 | Adapalene                    | 106685-40-9 | Dermatology            | Keratolytic           |                       |                                       | Skin                 |                                    | Yes             | Chemical classification (according ATC code) | Retinoid                       |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name              | CAS number  | Therapeutic class      | Therapeutic<br>effect | Target type | Target names                             | Absorption<br>tissue | Protein<br>binding    | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail  |
|-----------------------------------|----------------|-------------|----------------------------|-------------|------------------------|-----------------------|-------------|--|----------------------|-----------------------|-----------------|--|--|
| 3715 / 3719                       | H18            | Prestw-1705 | Diatrizoic acid dihydrate  | 50978-11-5  | Diagnostic             | Contrastant           |             |  |                      |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Watersoluble,<br>nephrotropic,<br>high osmolar X-<br>ray contrast<br>media |
| 3715 / 3719                       | H20            | Prestw-1743 | Dofetilide                 | 115256-11-6 | Cardiovascular         | Antiarrhythmic        |             |  | GI tract             | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Antiarrhythmic,<br>class III   |
| 3715 / 3719                       | H22            | Prestw-1776 | Phenprobamate              | 673-31-4    | Central Nervous System | Muscle relaxant       |             |  |                      |                       |                 | Chemical<br>classification<br>(according ATC<br>code)    | Carbamic acid<br>ester   |
| 3715 / 3719                       | J04            | Prestw-1730 | Cefuroxime axetil          | 64544-07-6  | Infectiology           | Antibacterial         |             |  |                      | Plasmatic<br>proteins | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Second-<br>generation<br>cephalosporin                                     |
| 3715 / 3719                       | J06            | Prestw-1720 | Anagrelide                 | 68475-42-3  | Hematology             | Thrombolytic          |             |  | GI tract             |                       | Yes             |  |  |
| 3715 / 3719                       | J08            | Prestw-1701 | Clopidogrel                | 113665-84-2 | Cardiovascular         | Antiplatelet          | GPCR        | Purinergic receptor<br>P2Y12             | GI tract             | Plasmatic<br>proteins | Yes             |  |  |
| 3715 / 3719                       | J10            | Prestw-1723 | Benzoxiquine               | 86-75-9     | Infectiology           | Antiseptic            |             |  |                      |                       |                 |  |  |
| 3715 / 3719                       | J12            | Prestw-1785 | Phenothiazine              | 92-84-2     | Central Nervous System | Antipsychotic         |             |  |                      |                       |                 |  |  |
| 3715 / 3719                       | J14            | Prestw-1769 | Enalaprilat dihydrate      | 84680-54-6  | Cardiovascular         | Antihypertensive      | Enzyme      | Angiotensin-converting<br>enzyme (ACE)   | GI tract             |                       | Yes             | Pharmacokinetics   | Active<br>metabolite of<br>Enalapril<br>(Prestw-314)                       |
| 3715 / 3719                       | J16            | Prestw-1791 | Pregabalin                 | 148553-50-8 | Central Nervous System | Anticonvulsant        |             |  |                      | Plasmatic<br>proteins | Yes             | New therapeutic<br>use                                   | Neuropathic<br>pain killer   |
| 3715 / 3719                       | J18            | Prestw-1787 | Homoveratrylamine          | 120-20-7    | Cardiovascular         | Antihypertensive      |             |  |                      |                       |                 |  |  |
| 3715 / 3719                       | J20            | Prestw-1731 | Zoledronic acid hydrate    | 165800-06-6 | Oncology               | Antiosteoporetic      |             |  |                      |                       | Yes             | New therapeutic<br>use                                   | Anti-cancer  |
| 3715 / 3719                       | J22            | Prestw-1727 | Cefpodoxime proxetil       | 87239-81-4  | Infectiology           | Antibacterial         |             |  |                      | Albumin               | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Third-generation<br>cephalosporin  |
| 3715 / 3719                       | L04            | Prestw-1736 | Irbesartan                 | 138402-11-6 | Cardiovascular         | Antihypertensive      | GPCR        | Angiotensin II receptor<br>type 1 (AT-1) | GI tract             |                       | Yes             |  |  |
| 3715 / 3719                       | L06            | Prestw-1737 | Indinavir sulfate          | 157810-81-6 | Infectiology           | Antiviral             |             |  |                      | Plasmatic<br>proteins | Yes             |  |  |
| 3715 / 3719                       | L08            | Prestw-1750 | Terbinafine                | 91161-71-6  | Infectiology           | Antifungal            |             |  | GI tract, Skin       | Plasmatic<br>proteins | Yes             |  |  |
| 3715 / 3719                       | L10            | Prestw-1700 | Histamine dihydrochloride  | 56-92-8     | Oncology               | Antineoplastic        |             |  |                      |                       | Yes             |  |  |
| 3715 / 3719                       | L12            | Prestw-1734 | Rasagiline                 | 136236-51-6 | Central Nervous System | Antiparkinsonian      | Enzyme      | Monoamine oxidase B                      |                      | Plasmatic<br>proteins | Yes             |  |  |
| 3715 / 3719                       | L14            | Prestw-1712 | Flumethasone pivalate      | 2002-29-1   | Dermatology            | Anti-inflammatory     |             |  |                      |                       | Yes             | Pharmacokinetics   | Prodrug of<br>Flumethasone<br>(Prestw-1712)                                |
| 3715 / 3719                       | L16            | Prestw-1756 | Lofepamine                 | 23047-25-8  | Central Nervous System | Antidepressant        |             |  |                      |                       |                 |  |  |
| 3715 / 3719                       | L18            | Prestw-1759 | Valdecoxib                 | 181695-72-7 | Metabolism             | Antiarthritic         | Enzyme      | Cyclooxygenase-2                         | GI tract             | Plasmatic<br>proteins | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | NSAID  |
| 3715 / 3719                       | L20            | Prestw-1740 | Besifloxacin hydrochloride | 141388-76-3 | Ophthalmology          | Antibacterial         |             |  | Eye                  |                       | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Fluoroquinolone  |
| 3715 / 3719                       | L22            | Prestw-1782 | Ritonavir                  | 155213-67-5 | Infectiology           | Antiviral             |             |  |                      | Plasmatic<br>proteins | Yes             |  |  |

| ICCB-L Plate<br>(10 mM / 3.33 mM) | ICCB-L<br>Well | Vendor_ID   | Chemical_Name               | CAS number  | Therapeutic class      | Therapeutic<br>effect | Target type | Target names                             | Absorption<br>tissue | Protein<br>binding           | FDA<br>approved | Additional info<br>type                                  | Additional info<br>detail               |
|-----------------------------------|----------------|-------------|-----------------------------|-------------|------------------------|-----------------------|-------------|--|----------------------|------------------------------|-----------------|--|---|
| 3715 / 3719                       | N04            | Prestw-1752 | Epirubicin hydrochloride    | 56390-09-1  | Oncology               | Antineoplastic        |             |  |                      |                              | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Anthracycline                           |
| 3715 / 3719                       | N06            | Prestw-1741 | Loteprednol etabonate       | 82034-46-6  | Ophthalmology          | Anti-inflammatory     |             |  | Eye                  |                              | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Corticosteroid                          |
| 3715 / 3719                       | N08            | Prestw-1744 | Tolterodine tartrate        | 209747-05-7 | Neuromuscular          | Muscle relaxant       |             |  |                      | Alpha-1-acid<br>glycoprotein | Yes             |  |   |
| 3715 / 3719                       | N10            | Prestw-1775 | Lomerizine hydrochloride    | 101477-54-7 | Central Nervous System | Antimigraine          |             |  |                      |                              |                 |  |   |
| 3715 / 3719                       | N12            | Prestw-1772 | Ampiroxicam                 | 99464-64-9  | Immunology             | Anti-inflammatory     |             |  |                      |                              |                 |  |   |
| 3715 / 3719                       | N14            | Prestw-1781 | Alosetron hydrochloride     | 122852-69-1 | Central Nervous System | Antidiarrheal         |             |  | GI tract             | Plasmatic<br>proteins        | Yes             |  |   |
| 3715 / 3719                       | N16            | Prestw-1738 | Risedronic acid monohydrate | 105462-24-6 | Metabolism             | Antiestrogenic        |             |  | GI tract             | Plasmatic<br>proteins        | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Bisphosphonate<br>s                     |
| 3715 / 3719                       | N18            | Prestw-1783 | Palonosetron hydrochloride  | 135729-62-3 | Central Nervous System | Antiemetic            | LGIC        | Serotonin 3 (5-HT3)<br>receptor          |                      | Plasmatic<br>proteins        | Yes             |  |   |
| 3715 / 3719                       | N20            | Prestw-1780 | Oxymetholone                | 434-07-1    | Endocrinology          | Anabolic              |             |  |                      |                              | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Androstan<br>derivative                 |
| 3715 / 3719                       | N22            | Prestw-1765 | Latanoprost                 | 145773-22-4 | Ophthalmology          | Antiglaucoma          |             |  | Eye                  |                              | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Prostaglandin<br>analogue               |
| 3715 / 3719                       | P04            | Prestw-1745 | Cisatracurium besylate      | 64228-79-1  | Neuromuscular          | Muscle relaxant       |             |  |                      |                              | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Quaternary<br>ammonium                  |
| 3715 / 3719                       | P06            | Prestw-1794 | Pemetrexed disodium         | 357166-30-4 | Oncology               | Antineoplastic        | Enzyme      | Thymidylate synthase                     |                      | Plasmatic<br>proteins        | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Folic acid<br>analogue                  |
| 3715 / 3719                       | P08            | Prestw-1793 | Raltitrexed                 | 112887-68-0 | Oncology               | Antineoplastic        | Enzyme      | Thymidylate synthase                     |                      | Plasmatic<br>proteins        |                 | Chemical<br>classification<br>(according ATC<br>code)    | Folic acid<br>analogue                  |
| 3715 / 3719                       | P10            | Prestw-1729 | Ceftibuten                  | 97519-39-6  | Infectiology           | Antibacterial         |             |  |                      |                              | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Third-generation<br>cephalosporin       |
| 3715 / 3719                       | P12            | Prestw-1735 | Valsartan                   | 137862-53-4 | Cardiovascular         | Vasodilator           | GPCR        | Angiotensin II receptor<br>type 1 (AT-1) | GI tract             | Albumin                      | Yes             |  |   |
| 3715 / 3719                       | P14            | Prestw-1788 | Milnacipran hydrochloride   | 101152-94-7 | Central Nervous System | Antidepressant        |             |  |                      | Plasmatic<br>proteins        | Yes             | New therapeutic<br>use                                   | Neuropathic<br>pain killer              |
| 3715 / 3719                       | P16            | Prestw-1768 | Triclabendazole             | 68786-66-3  | Infectiology           | Anthelmintic          |             |  | GI tract             | Albumin                      |                 |  |   |
| 3715 / 3719                       | P18            | Prestw-1751 | Brimonidine L-Tartrate      | 70359-46-5  | Ophthalmology          | Antiglaucoma          |             |  | Eye                  | Plasmatic<br>proteins        | Yes             | Therapeutic<br>classification<br>(according ATC<br>code) | Sympathomimet<br>ic                     |
| 3715 / 3719                       | P20            | Prestw-1704 | Desonide                    | 638-94-8    | Dermatology            | Antipsoriatic         |             |  | Skin                 |                              | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Corticosteroid,<br>moderately<br>potent |
| 3715 / 3719                       | P22            | Prestw-1728 | Cefprozil                   | 121123-17-9 | Infectiology           | Antibacterial         |             |  | GI tract             |                              | Yes             | Chemical<br>classification<br>(according ATC<br>code)    | Second-<br>generation<br>cephalosporin  |