

SUPPORTING INFORMATION

Drug effect prediction by polypharmacology-based interaction profiling

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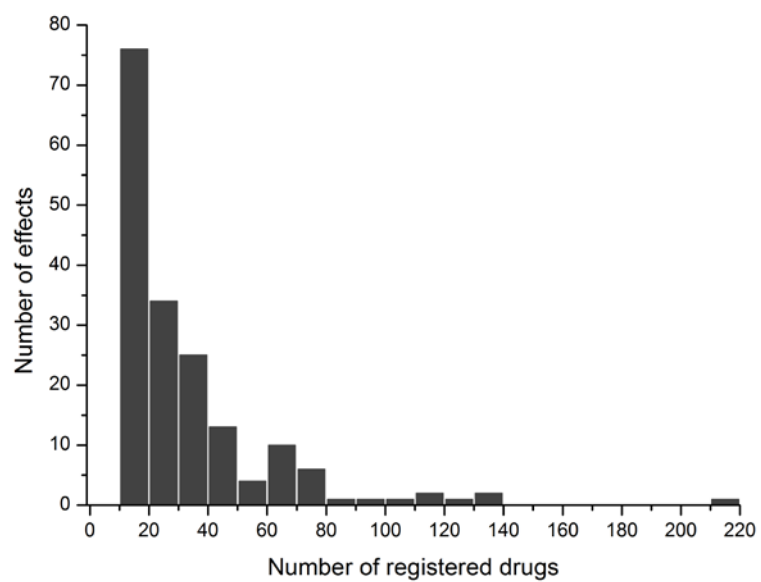


Figure S1. Distribution of the number of registered drugs to the studied 177 effects.

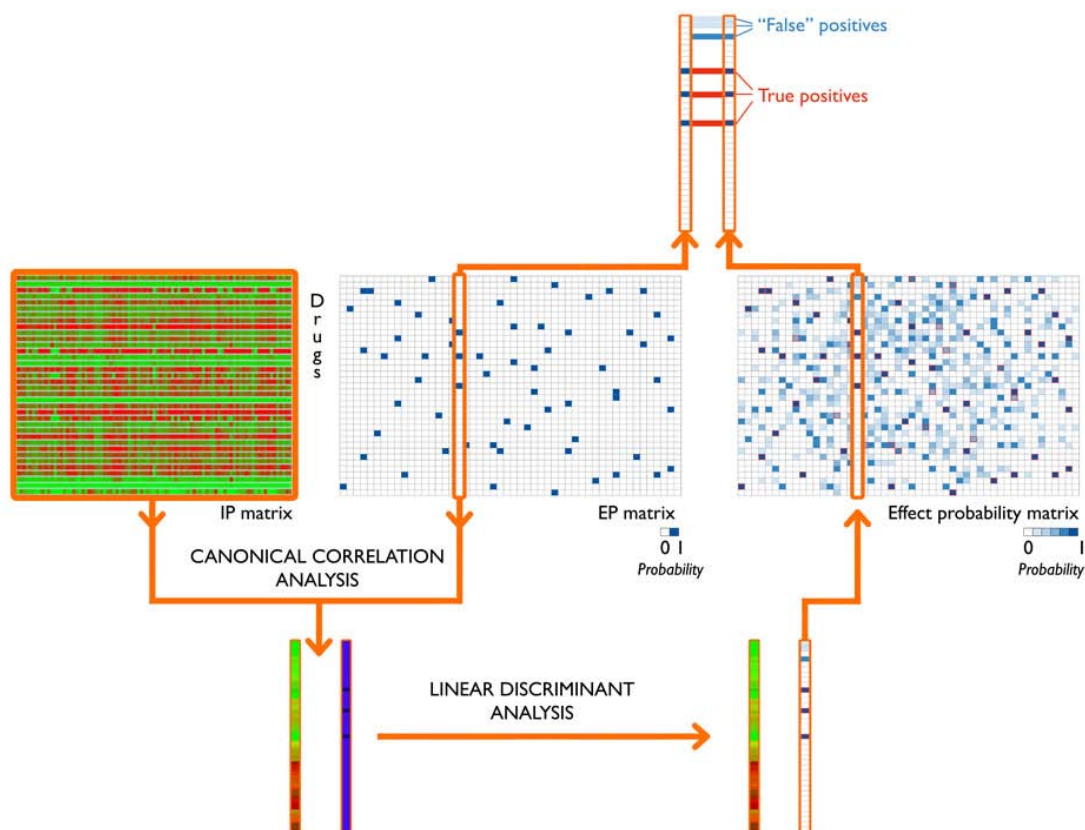


Figure S2. Mechanism of the effect prediction. First, canonical correlation analysis is performed on the IP matrix and a selected effect category, resulting in a vector pair that are the linear combinations of the original interaction matrix and effect vector, respectively. Then, linear discriminant analysis is conducted in order to generate a classification function that calculates the probability that a given drug will possess the studied effect. This analysis is repeated for the studied 177 effect, producing a recalculated EP matrix. (Note that probability values in this matrix are continuous.) Comparison of the original and the recalculated vector of an effect category reveals the true positive hits (i.e., the matches; highlighted with red) and the “false” positives (differences; highlighted with light blue).

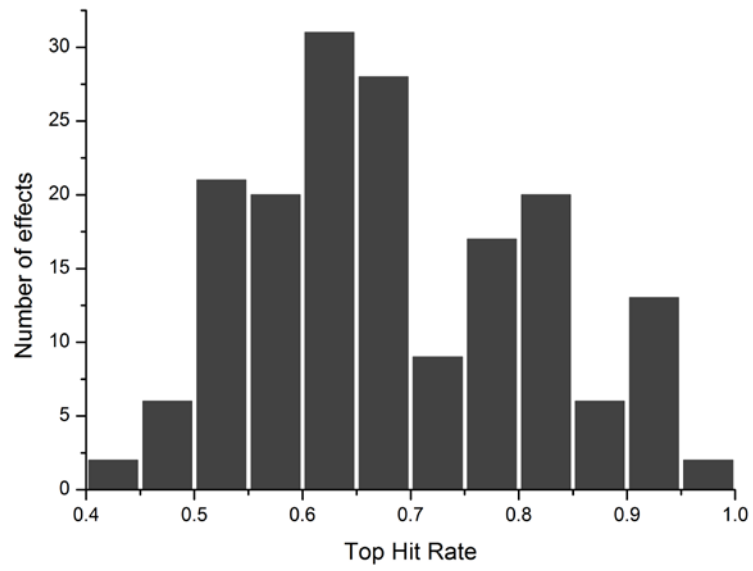


Figure S3. Distribution of the top hit rate values among the 177 studied effects.

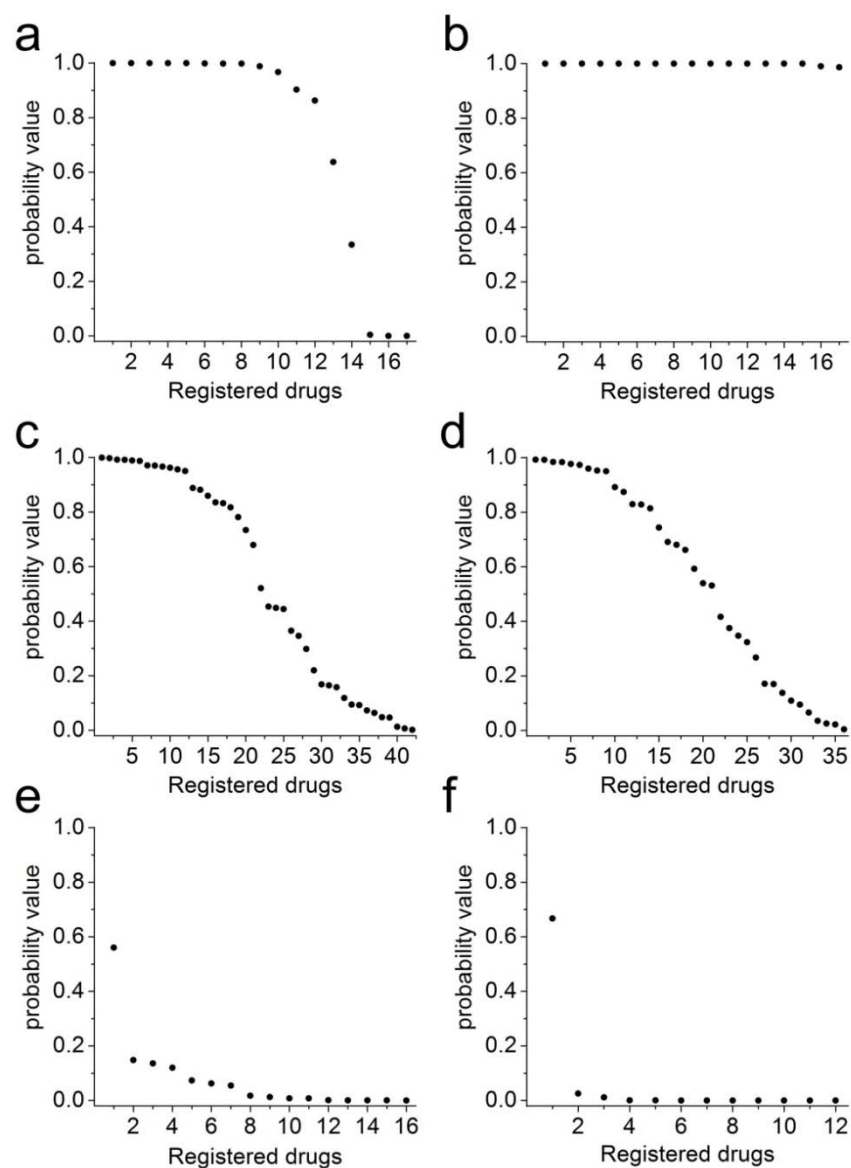


Figure S4. Probability values for six effect categories: a – Adrenergic beta agonist, b – Barbiturate, c – Cholinergic agent, d – Muscarinic agent, e – Platelet aggregation inhibitor, f – Gastrointestinal agent. The individual probability values of each drug of the studied effect categories are plotted in decreasing order. Note the different shapes of the probability value curves: parts a and b refer to cohesive groups, c and d show groups that need reclassification, e and f represent effect categories with low predictive power.

Table S1. List of the names and DrugBank codes of the used 1,177 drugs.

DB code	Drug name	DB code	Drug name
DB00114	Pyridoxal Phosphate	DB00780	Phenelzine
DB00116	Tetrahydrofolic acid	DB00782	Propantheline
DB00117	L-Histidine	DB00783	Estradiol
DB00118	S-Adenosylmethionine	DB00784	Mefenamic acid
DB00119	Pyruvic acid	DB00786	Marimastat
DB00120	L-Phenylalanine	DB00787	Aciclovir
DB00121	Biotin	DB00788	Naproxen
DB00122	Choline	DB00790	Perindopril
DB00123	L-Lysine	DB00791	Uracil mustard
DB00125	L-Arginine	DB00792	Tripelennamine
DB00126	Vitamin C	DB00793	Haloprogin
DB00127	Spermine	DB00794	Primidone
DB00128	L-Aspartic Acid	DB00795	Sulfasalazine
DB00129	L-Ornithine	DB00796	Candesartan
DB00130	L-Glutamine	DB00797	Tolazoline
DB00131	Adenosine monophosphate	DB00798	Gentamicin
DB00132	Alpha-Linolenic Acid	DB00800	Fenoldopam
DB00133	L-Serine	DB00801	Halazepam
DB00134	L-Methionine	DB00802	Alfentanil
DB00135	L-Tyrosine	DB00804	Dicyclomine
DB00136	Calcitriol	DB00805	Minaprine
DB00137	Xanthophyll	DB00806	Pentoxifylline
DB00138	L-Cystine	DB00807	Proparacaine
DB00139	Succinic acid	DB00808	Indapamide
DB00140	Riboflavin	DB00809	Tropicamide
DB00141	N-Acetyl-D-glucosamine	DB00810	Biperiden
DB00142	L-Glutamic Acid	DB00811	Ribavirin
DB00143	Glutathione	DB00812	Phenylbutazone
DB00144	Phosphatidylserine	DB00813	Fentanyl
DB00145	Glycine	DB00814	Meloxicam
DB00146	Calcidiol	DB00816	Orciprenaline
DB00147	Pyridoxal	DB00817	Rosoxacin
DB00148	Creatine	DB00818	Propofol
DB00149	L-Leucine	DB00819	Acetazolamide
DB00150	L-Tryptophan	DB00820	Tadalafil
DB00151	L-Cysteine	DB00821	Carprofen
DB00152	Thiamine	DB00822	Disulfiram
DB00153	Ergocalciferol	DB00823	Ethynodiol Diacetate

DB00154	gamma-Homolinolenic acid	DB00824	Enprofylline
DB00155	L-Citrulline	DB00825	Menthol
DB00156	L-Threonine	DB00826	Natamycin
DB00158	Folic Acid	DB00827	Cinoxacin
DB00159	Icosapent	DB00828	Fosfomycin
DB00160	L-Alanine	DB00829	Diazepam
DB00161	L-Valine	DB00830	Phenmetrazine
DB00162	Vitamin A	DB00831	Trifluoperazine
DB00163	Vitamin E	DB00832	Phensuximide
DB00165	Pyridoxine	DB00833	Cefaclor
DB00166	Lipoic Acid	DB00834	Mifepristone
DB00167	L-Isoleucine	DB00835	Brompheniramine
DB00168	Aspartame	DB00836	Loperamide
DB00169	Cholecalciferol	DB00837	Progabide
DB00170	Menadione	DB00838	Clocortolone
DB00171	Adenosine triphosphate	DB00839	Tolazamide
DB00172	L-Proline	DB00841	Dobutamine
DB00173	Adenine	DB00842	Oxazepam
DB00174	L-Asparagine	DB00843	Donepezil
DB00175	Pravastatin	DB00844	Nalbuphine
DB00176	Fluvoxamine	DB00845	Clofazimine
DB00177	Valsartan	DB00846	Flurandrenolide
DB00178	Ramipril	DB00847	Cysteamine
DB00179	Masoprocol	DB00848	Levamisole
DB00180	Flunisolide	DB00849	Methylphenobarbital
DB00181	Baclofen	DB00850	Perphenazine
DB00183	Pentagastrin	DB00851	Dacarbazine
DB00184	Nicotine	DB00852	Pseudoephedrine
DB00185	Cevimeline	DB00853	Temozolomide
DB00186	Lorazepam	DB00854	Levorphanol
DB00187	Esmolol	DB00855	Aminolevulinic acid
DB00188	Bortezomib	DB00856	Chlorphenesin
DB00189	Ethchlorvynol	DB00857	Terbinafine
DB00190	Carbidopa	DB00858	Dromostanolone
DB00191	Phentermine	DB00859	Penicillamine
DB00192	Indecainide	DB00860	Prednisolone
DB00193	Tramadol	DB00861	Diflunisal
DB00194	Vidarabine	DB00862	Vardenafil
DB00195	Betaxolol	DB00863	Ranitidine
DB00196	Fluconazole	DB00864	Tacrolimus
DB00198	Oseltamivir	DB00865	Benzphetamine
DB00199	Erythromycin	DB00866	Alprenolol

DB00201	Caffeine	DB00867	Ritodrine
DB00202	Succinylcholine	DB00869	Dorzolamide
DB00203	Sildenafil	DB00870	Suprofen
DB00204	Dofetilide	DB00871	Terbutaline
DB00205	Pyrimethamine	DB00872	Conivaptan
DB00206	Reserpine	DB00873	Loteprednol Etabonate
DB00207	Azithromycin	DB00874	Guaifenesin
DB00208	Ticlopidine	DB00875	Flupenthixol
DB00209	Trospium	DB00876	Eprosartan
DB00210	Adapalene	DB00878	Chlorhexidine
DB00211	Midodrine	DB00879	Emtricitabine
DB00212	Remikiren	DB00880	Chlorothiazide
DB00213	Pantoprazole	DB00881	Quinapril
DB00214	Torasemide	DB00882	Clomifene
DB00215	Citalopram	DB00883	Isosorbide Dinitrate
DB00216	Eletriptan	DB00884	Risedronate
DB00217	Bethanidine	DB00885	Pemirolast
DB00218	Moxifloxacin	DB00887	Bumetanide
DB00219	Oxyphenonium	DB00888	Mechlorethamine
DB00220	Nelfinavir	DB00889	Granisetron
DB00221	Isoetharine	DB00890	Dienestrol
DB00222	Glimepiride	DB00891	Sulfapyridine
DB00223	Diflorasone	DB00892	Oxybuprocaine
DB00224	Indinavir	DB00894	Testolactone
DB00226	Guanadrel Sulfate	DB00896	Rimexolone
DB00227	Lovastatin	DB00897	Triazolam
DB00229	Cefotiam	DB00899	Remifentanyl
DB00230	Pregabalin	DB00900	Didanosine
DB00231	Temazepam	DB00902	Methdilazine
DB00232	Methyclothiazide	DB00903	Ethacrynic acid
DB00233	Aminosalicylic Acid	DB00904	Ondansetron
DB00234	Reboxetine	DB00905	Bimatoprost
DB00235	Milrinone	DB00906	Tiagabine
DB00236	Pipobroman	DB00907	Cocaine
DB00237	Butabarbital	DB00908	Quinidine
DB00238	Nevirapine	DB00909	Zonisamide
DB00239	Oxiconazole	DB00910	Paricalcitol
DB00240	Alclometasone	DB00911	Tinidazole
DB00241	Butalbital	DB00912	Repaglinide
DB00242	Cladribine	DB00913	Anileridine
DB00243	Ranolazine	DB00914	Phenformin
DB00244	Mesalazine	DB00915	Amantadine

DB00245	Benztropine	DB00916	Metronidazole
DB00246	Ziprasidone	DB00917	Dinoprostone
DB00247	Methysergide	DB00918	Almotriptan
DB00248	Cabergoline	DB00919	Spectinomycin
DB00249	Idoxuridine	DB00920	Ketotifen
DB00250	Dapsone	DB00921	Buprenorphine
DB00251	Terconazole	DB00922	Levosimendan
DB00252	Phenytoin	DB00923	Ceforanide
DB00253	Medrysone	DB00924	Cyclobenzaprine
DB00254	Doxycycline	DB00925	Phenoxybenzamine
DB00255	Diethylstilbestrol	DB00927	Famotidine
DB00256	Lymecycline	DB00928	Azacitidine
DB00257	Clotrimazole	DB00929	Misoprostol
DB00259	Sulfanilamide	DB00931	Methacycline
DB00260	Cycloserine	DB00932	Tipranavir
DB00261	Anagrelide	DB00933	Mesoridazine
DB00262	Carmustine	DB00934	Maprotiline
DB00263	Sulfisoxazole	DB00935	Oxymetazoline
DB00264	Metoprolol	DB00936	Salicylic acid
DB00265	Crotamiton	DB00937	Diethylpropion
DB00266	Dicumarol	DB00938	Salmeterol
DB00267	Cefmenoxime	DB00939	Meclofenamic acid
DB00268	Ropinirole	DB00940	Methantheline
DB00269	Chlorotrianisene	DB00942	Cycrimine
DB00270	Isradipine	DB00943	Zalcitabine
DB00271	Diatrizoate	DB00944	Demecarium bromide
DB00272	Betazole	DB00945	Aspirin
DB00273	Topiramate	DB00946	Phenprocoumon
DB00274	Cefmetazole	DB00947	Fulvestrant
DB00275	Olmesartan	DB00948	Mezlocillin
DB00276	Amsacrine	DB00949	Felbamate
DB00277	Theophylline	DB00950	Fexofenadine
DB00278	Argatroban	DB00951	Isoniazid
DB00279	Liothyronine	DB00952	Naratriptan
DB00280	Disopyramide	DB00953	Rizatriptan
DB00281	Lidocaine	DB00954	Dirithromycin
DB00282	Pamidronate	DB00955	Netilmicin
DB00283	Clemastine	DB00956	Hydrocodone
DB00284	Acarbose	DB00957	Norgestimate
DB00285	Venlafaxine	DB00959	Methylprednisolone
DB00286	Conjugated Estrogens	DB00960	Pindolol
DB00287	Travoprost	DB00961	Mepivacaine

DB00288	Amcinonide	DB00962	Zaleplon
DB00289	Atomoxetine	DB00963	Bromfenac
DB00291	Chlorambucil	DB00964	Apraclonidine
DB00292	Etomidate	DB00966	Telmisartan
DB00293	Raltitrexed	DB00967	Desloratadine
DB00294	Etonogestrel	DB00968	Methyldopa
DB00295	Morphine	DB00969	Alosetron
DB00296	Ropivacaine	DB00972	Azelastine
DB00298	Dapiprazole	DB00973	Ezetimibe
DB00299	Penciclovir	DB00974	Edetic Acid
DB00300	Tenofovir	DB00975	Dipyridamole
DB00301	Flucloxacillin	DB00976	Telithromycin
DB00302	Tranexamic Acid	DB00977	Ethinyl Estradiol
DB00303	Ertapenem	DB00978	Lomefloxacin
DB00304	Desogestrel	DB00979	Cyclopentolate
DB00305	Mitomycin	DB00980	Ramelteon
DB00306	Talbutal	DB00981	Physostigmine
DB00307	Bexarotene	DB00983	Formoterol
DB00308	Ibutilide	DB00984	Nandrolone
DB00309	Vindesine	DB00986	Glycopyrrolate
DB00310	Chlorthalidone	DB00987	Cytarabine
DB00311	Ethoxzolamide	DB00988	Dopamine
DB00312	Pentobarbital	DB00989	Rivastigmine
DB00313	Valproic Acid	DB00990	Exemestane
DB00315	Zolmitriptan	DB00991	Oxaprozin
DB00316	Acetaminophen	DB00992	Methyl aminolevulinate
DB00317	Gefitinib	DB00993	Azathioprine
DB00318	Codeine	DB00996	Gabapentin
DB00319	Piperacillin	DB00997	Doxorubicin
DB00320	Dihydroergotamine	DB00998	Frovatriptan
DB00321	Amitriptyline	DB00999	Hydrochlorothiazide
DB00322	Floxuridine	DB01000	Cyclacillin
DB00323	Tolcapone	DB01001	Salbutamol
DB00324	Fluorometholone	DB01002	Levobupivacaine
DB00327	Hydromorphone	DB01003	Cromoglicate
DB00328	Indomethacin	DB01004	Ganciclovir
DB00330	Ethambutol	DB01005	Hydroxyurea
DB00331	Metformin	DB01006	Letrozole
DB00332	Ipratropium	DB01007	Tioconazole
DB00333	Methadone	DB01008	Busulfan
DB00334	Olanzapine	DB01009	Ketoprofen
DB00335	Atenolol	DB01010	Edrophonium

DB00336	Nitrofurazone	DB01011	Metirapone
DB00337	Pimecrolimus	DB01012	Cinacalcet
DB00339	Pyrazinamide	DB01013	Clobetasol
DB00340	Metixene	DB01014	Balsalazide
DB00341	Cetirizine	DB01015	Sulfamethoxazole
DB00342	Terfenadine	DB01016	Glibenclamide
DB00343	Diltiazem	DB01017	Minocycline
DB00344	Protriptyline	DB01018	Guanfacine
DB00345	Aminohippurate	DB01019	Bethanechol
DB00346	Alfuzosin	DB01020	Isosorbide Mononitrate
DB00347	Trimethadione	DB01021	Trichlormethiazide
DB00348	Nitisinone	DB01022	Phytonadione
DB00349	Clobazam	DB01023	Felodipine
DB00350	Minoxidil	DB01024	Mycophenolic acid
DB00351	Megestrol	DB01025	Amlexanox
DB00352	Thioguanine	DB01026	Ketoconazole
DB00353	Methylergonovine	DB01028	Methoxyflurane
DB00354	Bucizine	DB01029	Irbesartan
DB00355	Aztreonam	DB01030	Topotecan
DB00356	Chlorzoxazone	DB01031	Ethinamate
DB00357	Aminogluthethimide	DB01032	Probenecid
DB00358	Mefloquine	DB01033	Mercaptopurine
DB00359	Sulfadiazine	DB01034	Cerulein
DB00360	Tetrahydrobiopterin	DB01035	Procainamide
DB00361	Vinorelbine	DB01036	Tolterodine
DB00363	Clozapine	DB01037	Selegiline
DB00365	Grepafloxacin	DB01038	Carphenazine
DB00366	Doxylamine	DB01039	Fenofibrate
DB00367	Levonorgestrel	DB01041	Thalidomide
DB00368	Norepinephrine	DB01042	Melphalan
DB00369	Cidofovir	DB01043	Memantine
DB00370	Mirtazapine	DB01044	Gatifloxacin
DB00371	Meprobamate	DB01046	Lubiprostone
DB00372	Thiethylperazine	DB01047	Fluocinonide
DB00373	Timolol	DB01048	Abacavir
DB00374	Treprostinil	DB01050	Ibuprofen
DB00376	Trihexyphenidyl	DB01051	Novobiocin
DB00377	Palonosetron	DB01053	Penicillin G
DB00378	Dydrogesterone	DB01054	Nitrendipine
DB00379	Mexiletine	DB01055	Mimosine
DB00380	Dexrazoxane	DB01056	Tocainide
DB00381	Amlodipine	DB01057	Echothiophate Iodide

DB00382	Tacrine	DB01058	Praziquantel
DB00383	Oxyphencyclimine	DB01059	Norfloxacin
DB00384	Triamterene	DB01060	Amoxicillin
DB00385	Valrubicin	DB01061	Azlocillin
DB00387	Procyclidine	DB01062	Oxybutynin
DB00388	Phenylephrine	DB01063	Acetophenazine
DB00389	Carbimazole	DB01064	Isoproterenol
DB00390	Digoxin	DB01065	Melatonin
DB00391	Sulpiride	DB01066	Cefditoren
DB00392	Ethopropazine	DB01067	Glipizide
DB00393	Nimodipine	DB01068	Clonazepam
DB00394	Beclomethasone	DB01069	Promethazine
DB00395	Carisoprodol	DB01070	Dihydrotachysterol
DB00396	Progesterone	DB01071	Mequitazine
DB00397	Phenylpropanolamine	DB01072	Atazanavir
DB00398	Sorafenib	DB01073	Fludarabine
DB00399	Zoledronate	DB01074	Perhexiline
DB00400	Griseofulvin	DB01075	Diphenhydramine
DB00401	Nisoldipine	DB01076	Atorvastatin
DB00402	Eszopiclone	DB01077	Etidronic acid
DB00404	Alprazolam	DB01080	Vigabatrin
DB00405	Dexbrompheniramine	DB01081	Diphenoxylate
DB00406	Gentian Violet	DB01082	Streptomycin
DB00408	Loxapine	DB01083	Orlistat
DB00409	Remoxipride	DB01084	Emedastine
DB00410	Mupirocin	DB01085	Pilocarpine
DB00411	Carbachol	DB01086	Benzocaine
DB00412	Rosiglitazone	DB01087	Primaquine
DB00413	Pramipexole	DB01088	Iloprost
DB00414	Acetohexamide	DB01089	Deserpidine
DB00415	Ampicillin	DB01090	Pentolinium
DB00417	Penicillin V	DB01091	Butenafine
DB00418	Secobarbital	DB01092	Ouabain
DB00419	Miglustat	DB01094	Hesperetin
DB00420	Promazine	DB01095	Fluvastatin
DB00421	Spironolactone	DB01096	Oxamniquine
DB00422	Methylphenidate	DB01097	Leflunomide
DB00423	Methocarbamol	DB01098	Rosuvastatin
DB00424	Hyoscyamine	DB01099	Flucytosine
DB00425	Zolpidem	DB01100	Pimozide
DB00427	Triprolidine	DB01102	Arbutamine
DB00428	Streptozocin	DB01103	Quinacrine

DB00429	Carboprost Tromethamine	DB01104	Sertraline
DB00430	Cefpiramide	DB01105	Sibutramine
DB00431	Lindane	DB01106	Levocabastine
DB00432	Trifluridine	DB01107	Methypylon
DB00433	Prochlorperazine	DB01108	Trilostane
DB00434	Cyproheptadine	DB01110	Miconazole
DB00436	Bendroflumethiazide	DB01112	Cefuroxime
DB00437	Allopurinol	DB01113	Papaverine
DB00438	Ceftazidime	DB01114	Chlorpheniramine
DB00440	Trimethoprim	DB01115	Nifedipine
DB00441	Gemcitabine	DB01116	Trimethaphan
DB00442	Entecavir	DB01117	Atovaquone
DB00443	Betamethasone	DB01118	Amiodarone
DB00444	Teniposide	DB01119	Diazoxide
DB00445	Epirubicin	DB01120	Gliclazide
DB00446	Chloramphenicol	DB01121	Phenacemide
DB00447	Loracarbef	DB01122	Amibenonium
DB00448	Lansoprazole	DB01123	Proflavine
DB00449	Dipivefrin	DB01124	Tolbutamide
DB00450	Droperidol	DB01125	Anisindione
DB00451	Levothyroxine	DB01126	Dutasteride
DB00452	Framycetin	DB01127	Econazole
DB00453	Clomocycline	DB01128	Bicalutamide
DB00454	Meperidine	DB01129	Rabeprazole
DB00455	Loratadine	DB01130	Prednicarbate
DB00456	Cefalotin	DB01131	Proguanil
DB00457	Prazosin	DB01132	Pioglitazone
DB00458	Imipramine	DB01133	Tiludronate
DB00459	Acitretin	DB01134	Desoxycorticosterone Pivalate
DB00460	Verteporfin	DB01136	Carvedilol
DB00461	Nabumetone	DB01137	Levofloxacin
DB00462	Methylscopolamine	DB01138	Sulfinpyrazone
DB00463	Metharbital	DB01139	Cephapirin
DB00465	Ketorolac	DB01140	Cefadroxil
DB00467	Enoxacin	DB01142	Doxepin
DB00468	Quinine	DB01143	Amifostine
DB00469	Tenoxicam	DB01144	Dichlorphenamide
DB00470	Marinol	DB01145	Sulfoxone
DB00471	Montelukast	DB01146	Diphenylpyraline
DB00472	Fluoxetine	DB01147	Cloxacillin
DB00473	Hexylcaine	DB01148	Flavoxate
DB00474	Methohexital	DB01149	Nefazodone

DB00475	Chlordiazepoxide	DB01150	Cefprozil
DB00476	Duloxetine	DB01151	Desipramine
DB00477	Chlorpromazine	DB01153	Sertaconazole
DB00478	Rimantadine	DB01154	Thiamylal
DB00479	Amikacin	DB01155	Gemifloxacin
DB00480	Lenalidomide	DB01156	Bupropion
DB00481	Raloxifene	DB01157	Trimetrexate
DB00482	Celecoxib	DB01158	Bretylium
DB00483	Gallamine Triethiodide	DB01161	Chloroprocaine
DB00484	Brimonidine	DB01162	Terazosin
DB00485	Dicloxacillin	DB01166	Cilostazol
DB00486	Nabilone	DB01167	Itraconazole
DB00487	Pefloxacin	DB01168	Procarbazine
DB00488	Altretamine	DB01170	Guanethidine
DB00489	Sotalol	DB01171	Moclobemide
DB00490	Buspirone	DB01172	Kanamycin
DB00491	Miglitol	DB01173	Orphenadrine
DB00492	Fosinopril	DB01174	Phenobarbital
DB00493	Cefotaxime	DB01175	Escitalopram
DB00494	Entacapone	DB01176	Cyclizine
DB00495	Zidovudine	DB01177	Idarubicin
DB00496	Darifenacin	DB01178	Chlormezanone
DB00497	Oxycodone	DB01179	Podofilox
DB00498	Phenindione	DB01180	Rescinnamine
DB00499	Flutamide	DB01181	Ifosfamide
DB00500	Tolmetin	DB01182	Propafenone
DB00501	Cimetidine	DB01183	Naloxone
DB00502	Haloperidol	DB01184	Domperidone
DB00503	Ritonavir	DB01185	Fluoxymesterone
DB00504	Levallorphan	DB01186	Pergolide
DB00505	Tridihexethyl	DB01188	Ciclopirox
DB00507	Nitazoxanide	DB01189	Desflurane
DB00508	Triflupromazine	DB01190	Clindamycin
DB00513	Aminocaproic Acid	DB01191	Dexfenfluramine
DB00514	Dextromethorphan	DB01192	Oxymorphone
DB00518	Albendazole	DB01193	Acebutolol
DB00519	Trandolapril	DB01194	Brinzolamide
DB00521	Carteolol	DB01195	Flecainide
DB00522	Bentiromide	DB01196	Estramustine
DB00524	Metolazone	DB01197	Captopril
DB00525	Tolnaftate	DB01199	Tubocurarine
DB00527	Dibucaine	DB01200	Bromocriptine

DB00528	Lercanidipine	DB01202	Levetiracetam
DB00529	Foscarnet	DB01203	Nadolol
DB00530	Erlotinib	DB01204	Mitoxantrone
DB00531	Cyclophosphamide	DB01205	Flumazenil
DB00532	Mephenytoin	DB01206	Lomustine
DB00535	Cefdinir	DB01207	Ridogrel
DB00537	Ciprofloxacin	DB01208	Sparfloxacin
DB00539	Toremifene	DB01209	Dezocine
DB00540	Nortriptyline	DB01210	Levobunolol
DB00541	Vincristine	DB01212	Ceftriaxone
DB00542	Benazepril	DB01213	Fomepizole
DB00543	Amoxapine	DB01214	Metipranolol
DB00544	Fluorouracil	DB01215	Estazolam
DB00545	Pyridostigmine	DB01216	Finasteride
DB00546	Adinazolam	DB01217	Anastrozole
DB00547	Desoximetasone	DB01218	Halofantrine
DB00548	Azelaic Acid	DB01219	Dantrolene
DB00549	Zafirlukast	DB01220	Rifaximin
DB00550	Propylthiouracil	DB01221	Ketamine
DB00551	Acetohydroxamic Acid	DB01222	Budesonide
DB00552	Pentostatin	DB01224	Quetiapine
DB00553	Methoxsalen	DB01227	Levomethadyl Acetate
DB00554	Piroxicam	DB01228	Encainide
DB00555	Lamotrigine	DB01229	Paclitaxel
DB00557	Hydroxyzine	DB01231	Diphenidol
DB00558	Zanamivir	DB01232	Saquinavir
DB00559	Bosentan	DB01233	Metoclopramide
DB00560	Tigecycline	DB01234	Dexamethasone
DB00561	Doxapram	DB01235	Levodopa
DB00562	Benzthiazide	DB01237	Bromodiphenhydramine
DB00563	Methotrexate	DB01238	Aripiprazole
DB00564	Carbamazepine	DB01239	Chlorprothixene
DB00566	Succimer	DB01240	Epoprostenol
DB00567	Cephalexin	DB01241	Gemfibrozil
DB00568	Cinnarizine	DB01242	Clomipramine
DB00570	Vinblastine	DB01243	Chloroxine
DB00571	Propranolol	DB01244	Bepridil
DB00572	Atropine	DB01245	Decamethonium
DB00573	Fenoprofen	DB01246	Trimeprazine
DB00575	Clonidine	DB01247	Isocarboxazid
DB00576	Sulfamethizole	DB01248	Docetaxel
DB00578	Carbenicillin	DB01250	Olsalazine

DB00579	Mazindol	DB01251	Gliquidone
DB00581	Lactulose	DB01252	Mitiglinide
DB00582	Voriconazole	DB01253	Ergonovine
DB00583	L-Carnitine	DB01254	Dasatinib
DB00584	Enalapril	DB01256	Retapamulin
DB00585	Nizatidine	DB01258	Aliskiren
DB00586	Diclofenac	DB01259	Lapatinib
DB00587	Cinalukast	DB01260	Desonide
DB00588	Fluticasone Propionate	DB01261	Sitagliptin
DB00589	Lisuride	DB01262	Decitabine
DB00590	Doxazosin	DB01264	Darunavir
DB00591	Fluocinolone Acetonide	DB01265	Telbivudine
DB00592	Piperazine	DB01267	Paliperidone
DB00593	Ethosuximide	DB01268	Sunitinib
DB00594	Amiloride	DB01273	Varenicline
DB00595	Oxytetracycline	DB01274	Arformoterol
DB00596	Halobetasol Propionate	DB01275	Hydralazine
DB00598	Labetalol	DB01280	Nelarabine
DB00599	Thiopental	DB01283	Lumiracoxib
DB00600	Monobenzene	DB01288	Fenoterol
DB00601	Linezolid	DB01289	Glisoxepide
DB00603	Medroxyprogesterone	DB01291	Pirbuterol
DB00604	Cisapride	DB01295	Bevantolol
DB00605	Sulindac	DB01296	Glucosamine
DB00606	Cyclothiazide	DB01297	Practolol
DB00607	Nafcillin	DB01298	Sulfacytine
DB00608	Chloroquine	DB01299	Sulfadoxine
DB00609	Ethionamide	DB01301	Rolitetraacycline
DB00610	Metaraminol	DB01320	Fosphenytoin
DB00611	Butorphanol	DB01324	Polythiazide
DB00612	Bisoprolol	DB01325	Quinethazone
DB00613	Amodiaquine	DB01326	Cefamandole
DB00614	Furazolidone	DB01327	Cefazolin
DB00617	Paramethadione	DB01328	Cefonicid
DB00618	Demeclocycline	DB01330	Cefotetan
DB00619	Imatinib	DB01331	Cefoxitin
DB00620	Triamcinolone	DB01332	Ceftizoxime
DB00621	Oxandrolone	DB01333	Cefradine
DB00622	Nicardipine	DB01340	Cilazapril
DB00623	Fluphenazine	DB01342	Forasartan
DB00624	Testosterone	DB01348	Spirapril
DB00625	Efavirenz	DB01349	Tasosartan

DB00627	Niacin	DB01351	Amobarbital
DB00628	Clorazepate	DB01352	Aprobarbital
DB00629	Guanabenz	DB01353	Butethal
DB00630	Alendronate	DB01354	Heptabarbital
DB00631	Clofarabine	DB01355	Hexobarbital
DB00632	Docosanol	DB01357	Mestranol
DB00633	Dexmedetomidine	DB01359	Penbutolol
DB00634	Sulfacetamide	DB01364	Ephedrine
DB00635	Prednisone	DB01365	Mephentermine
DB00636	Clofibrate	DB01366	Procaterol
DB00637	Astemizole	DB01367	Rasagiline
DB00639	Butoconazole	DB01380	Cortisone acetate
DB00640	Adenosine	DB01382	Glycodiazine
DB00641	Simvastatin	DB01384	Paramethasone
DB00642	Pemetrexed	DB01392	Yohimbine
DB00643	Mebendazole	DB01393	Bezafibrate
DB00645	Dyclonine	DB01394	Colchicine
DB00647	Propoxyphene	DB01395	Drospirenone
DB00648	Mitotane	DB01399	Salsalate
DB00649	Stavudine	DB01400	Neostigmine
DB00650	Leucovorin	DB01403	Methotrimeprazine
DB00651	Dyphylline	DB01406	Danazol
DB00652	Pentazocine	DB01407	Clenbuterol
DB00654	Latanoprost	DB01408	Bambuterol
DB00655	Estrone	DB01409	Tiotropium
DB00656	Trazodone	DB01410	Ciclesonide
DB00657	Mecamylamine	DB01411	Pranlukast
DB00659	Acamprosate	DB01412	Theobromine
DB00660	Metaxalone	DB01413	Cefepime
DB00661	Verapamil	DB01414	Cefacetrile
DB00662	Trimethobenzamide	DB01415	Ceftibuten
DB00663	Flumethasone Pivalate	DB01416	Cefpodoxime
DB00664	Sulfametopyrazine	DB01418	Acenocoumarol
DB00665	Nilutamide	DB01419	Antrafenine
DB00668	Epinephrine	DB01420	Testosterone Propionate
DB00669	Sumatriptan	DB01422	Nitroxoline
DB00670	Pirenzepine	DB01423	Stepronin
DB00671	Cefixime	DB01424	Aminophenazone
DB00672	Chlorpropamide	DB01425	Alizapride
DB00673	Aprepitant	DB01426	Ajmaline
DB00674	Galantamine	DB01427	Amrinone
DB00675	Tamoxifen	DB01429	Aprindine

DB00676	Benzyl Benzoate	DB01430	Almitrine
DB00677	Isoflurophate	DB01431	Allylestrenol
DB00678	Losartan	DB01435	Antipyrine
DB00679	Thioridazine	DB01436	Alfacalcidol
DB00680	Moricizine	DB01437	Glutethimide
DB00682	Warfarin	DB01438	Phenazopyridine
DB00683	Midazolam	DB01440	Gamma Hydroxybutyric Acid
DB00684	Tobramycin	DB01463	Fencamfamine
DB00685	Trovafloxacin	DB01544	Flunitrazepam
DB00687	Fludrocortisone	DB01558	Bromazepam
DB00689	Cephaloglycin	DB01559	Clotiazepam
DB00690	Flurazepam	DB01567	Fludiazepam
DB00691	Moexipril	DB01576	Dextroamphetamine
DB00692	Phentolamine	DB01577	Methamphetamine
DB00694	Daunorubicin	DB01579	Phendimetrazine
DB00695	Furosemide	DB01580	Oxprenolol
DB00696	Ergotamine	DB01581	Sulfamerazine
DB00697	Tizanidine	DB01582	Sulfamethazine
DB00698	Nitrofurantoin	DB01586	Ursodeoxycholic acid
DB00699	Nicergoline	DB01587	Ketazolam
DB00700	Eplerenone	DB01588	Prazepam
DB00701	Amprenavir	DB01589	Quazepam
DB00703	Methazolamide	DB01594	Cinolazepam
DB00704	Naltrexone	DB01595	Nitrazepam
DB00705	Delavirdine	DB01597	Cilastatin
DB00706	Tamsulosin	DB01598	Imipenem
DB00708	Sufentanil	DB01599	Probuco
DB00709	Lamivudine	DB01600	Tiaprofenic acid
DB00710	Ibandronate	DB01602	Bacampicillin
DB00711	Diethylcarbamazine	DB01603	Meticillin
DB00712	Flurbiprofen	DB01604	Pivampicillin
DB00714	Apomorphine	DB01605	Pivmecillinam
DB00715	Paroxetine	DB01606	Tazobactam
DB00716	Nedocromil	DB01607	Ticarcillin
DB00717	Norethindrone	DB01608	Propericiazine
DB00718	Adefovir Dipivoxil	DB01609	Deferasirox
DB00719	Azatadine	DB01610	Valganciclovir
DB00721	Procaine	DB01611	Hydroxychloroquine
DB00722	Lisinopril	DB01612	Amyl Nitrite
DB00723	Methoxamine	DB01613	Erythrityl Tetranitrate
DB00724	Imiquimod	DB01614	Acepromazine
DB00726	Trimipramine	DB01615	Aceprometazine

DB00727	Nitroglycerin	DB01616	Alverine
DB00728	Rocuronium	DB01618	Molindone
DB00730	Thiabendazole	DB01619	Phenindamine
DB00731	Nateglinide	DB01620	Pheniramine
DB00733	Pralidoxime	DB01621	Pipotiazine
DB00734	Risperidone	DB01622	Thiopropazine
DB00735	Naftifine	DB01623	Thiothixene
DB00736	Esomeprazole	DB01624	Zuclopenthixol
DB00737	Meclizine	DB01625	Isopropamide
DB00738	Pentamidine	DB01626	Pargyline
DB00739	Hetacillin	DB01627	Lincomycin
DB00740	Riluzole	DB01628	Etoricoxib
DB00741	Hydrocortisone	DB02300	Calcipotriol
DB00742	Mannitol	DB02546	Vorinostat
DB00744	Zileuton	DB02703	Fusidic Acid
DB00745	Modafinil	DB04552	Niflumic Acid
DB00746	Deferoxamine	DB04570	Latamoxef
DB00747	Scopolamine	DB04573	Estriol
DB00748	Carbinoxamine	DB04575	Quinestrol
DB00749	Etodolac	DB04794	Bifonazole
DB00750	Prilocaine	DB04835	Maraviroc
DB00751	Epinastine	DB04837	Chlophedianol
DB00752	Tranylcypromine	DB04838	Cyclandelate
DB00754	Ethotoin	DB04840	Debrisoquin
DB00755	Tretinoin	DB04841	Flunarizine
DB00756	Hexachlorophene	DB04842	Fluspirilene
DB00757	Dolasetron	DB04843	Mepenzolate
DB00758	Clopidogrel	DB04844	Tetrabenazine
DB00759	Tetracycline	DB04861	Nebivolol
DB00760	Meropenem	DB04878	Voglibose
DB00763	Methimazole	DB04880	Enoximone
DB00764	Mometasone	DB04890	Bepotastine
DB00765	Metyrosine	DB04896	Milnacipran
DB00766	Clavulanate	DB04930	Permethrin
DB00767	Benzquinamide	DB04942	Tamibarotene
DB00768	Olopatadine	DB04948	Lofexidine
DB00769	Hydrocortamate	DB04967	Lucanthone
DB00770	Alprostadiol	DB05246	Methsuximide
DB00771	Clidinium	DB06144	Sertindole
DB00772	Malathion	DB06148	Mianserin
DB00773	Etoposide	DB06151	Acetylcysteine
DB00774	Hydroflumethiazide	DB06155	Rimonabant

DB00775 Tirofiban
DB00776 Oxcarbazepine
DB00777 Propiomazine
DB00778 Roxithromycin
DB00779 Nalidixic Acid

DB06262 Droxidopa
DB06267 Udenafil
DB06274 Alvimopan
DB06288 Amisulpride

Table S2. List of the names and the Protein Data Bank entries of the used 149 proteins.

PDB code	Protein name
13gs	Glutathione S-transferase pi
1a3b	Prothrombin
1aj0	Dihydropteroate synthase
1aj6	DNA topoisomerase II
1apy	Human aspartylglucosaminidase
1aq1	Human cyclin dependent kinase 2
1auk	Human arylsulfatase A
1b2y	Pancreatic alpha-amylase precursor
1b3d	Stromelysin-1
1bj4	Serine hydroxymethyltransferase, cytosolic
1bj5	Human serum albumin
1blc	Beta-lactamase
1bwc	Glutathione reductase (mitochondrial)
1bzm	Carbonic anhydrase I
1c5o	Urokinase type plasminogen activator
1cjf	Profilin
1c jy	Enoyl-[acyl-carrier-protein] reductase
1d3g	Human dihydroorotate dehydrogenase
1dfv	Human neutrophil gelatinase
1dkf	Retinoic acid receptor alpha
1dug	Glutathione S-transferase from <i>Schistosoma japonicum</i>
1e51	Delta-aminolevulinic acid dehydratase
1ewf	Bactericidal permeability-increasing protein
1exa	Retinoic acid receptor gamma-2
1ezf	Human squalene synthase
1f0x	D-lactate dehydrogenase
1f5f	Sex hormone-binding globulin precursor
1fcy	Retinoic acid receptor gamma-1
1fj4	3-oxoacyl-[acyl-carrier-protein] synthase I
1fkd	FK506-binding protein 1A
1g3m	Human estrogen sulfotransferase
1g9v	Hemoglobin
1gkc	Matrix metalloprotease 9
1hcn	Human chorionic gonadotropin
1hrn	Renin
1hso	Alcohol dehydrogenase alpha chain
1hsz	Alcohol dehydrogenase beta chain

1ht0	Alcohol dehydrogenase gamma chain
1hur	Human ADP-ribosylation factor 1
1hvr	HIV-1 protease
1ig3	Thiamine pyrophosphokinase
1j3j	Bifunctional dihydrofolate reductase-thymidylate synthase
1j8u	Phenylalanine-4-hydroxylase
1k0e	Para-aminobenzoate synthase component I
1kfy	Fumarate reductase flavoprotein subunit
1ki0	Human angiotensin
1kpg	Cyclopropane-fatty-acyl-phospholipid synthase 1
1ksp	DNA polymerase I
1kvo	Human phospholipase A2
1l7z	Calmodulin
1lo6	Human kallikrein 6
1lpb	Pancreatic triacylglycerol lipase precursor
1lpg	Coagulation factor X
1lxi	Bone morphogenic protein 7
1mf8	Calcineurin B subunit isoform 1
1mp8	Focal adhesion kinase
1mzs	3-oxoacyl-[acyl-carrier-protein] synthase III
1n52	Cap binding complex
1n5u	Serum albumin precursor
1nhz	Glucocorticoid receptor
1nrg	Pyridoxine-5'-phosphate oxidase
1of1	Thymidine kinase
1okc	ADP/ATP carrier protein heart isoform T1
1opb	Retinol-binding protein II
1oq5	Carbonic anhydrase II
1oth	Human ornithine transcarbamoylase
1p0p	Cholinesterase
1p60	Deoxycytidine kinase
1ph0	Tyrosine-protein phosphatase, non-receptor type 1
1qh5	Human glyoxalase II
1qkm	Human oestrogen receptor beta
1qon	Acetylcholinesterase precursor
1r1h	Enkephalinase
1r5l	Human alpha-tocopherol transfer protein
1r9o	Cytochrome P450C9
1rbp	Plasma retinol-binding protein
1ro9	cAMP phosphodiesterase
1rsz	Purine nucleoside phosphorylase
1rwx	Caspase-1 precursor

1s1d	Human apyrase
1s2c	Prostaglandin D2 11-ketoreductase
1sr7	Progesterone receptor hormone
1sz7	Human BET3
1t46	Mast/stem cell growth factor receptor precursor
1t65	Androgen receptor
1uae	UDP-N-acetylglucosamine 1-carboxyvinyltransferase
1uhl	Retinoic acid receptor RXR-beta
1uze	Angiotensin-converting enzyme
1v97	Xanthine oxidase
1w6k	Human oxidosqualene cyclase
1x9d	Human class I alpha-1,2-mannosidase
1x9n	DNA ligase I
1xap	Retinoic acid receptor beta
1xkk	Epidermal growth factor receptor precursor
1xpc	Estrogen receptor
1xzx	Thyroid hormone receptor beta-1
1y6a	Vascular endothelial growth factor receptor 2 precursor
1yb5	Human zeta-crystallin
1ytv	Vasopressin V1a receptor
1z57	Human CLK1
1zcm	Human calpain protease
1zd3	Human soluble epoxide hydrolase
1zid	Enoyl-[acyl-carrier-protein] reductase
1zx0	Human guanidinoacetate N-methyltransferase
1zxm	Human topo IIa ATPase/AMP-PNP
1zy7	Human adenosine deaminase that acts on RNA
1zsq	Miotubularin-related protein 2
1zsx	Human potassium channel Kv beta subunit
2a1h	Human mitochondrial branched chain aminotransferase
2a5d	Human ADP-ribosylation factor 6
2aax	Mineralocorticoid receptor
2aeb	Human arginase I
2afw	Human glutaminyl cyclase
2ag4	GM2-activator protein
2aid	HIV-1 reverse transcriptase
2avd	Human catechol-O-methyltransferase
2axm	Heparin-binding growth factor 1 precursor
2az5	Tumor necrosis factor alpha
2b2u	Human CDH1
2bat	Neuraminidase
2bka	CC3

2bm2	Human beta-II tryptase
2bxs	Monoamine oxidase A
2c67	Monoamine oxidase B
2cbz	Human multidrug resistance protein 1
2cca	Peroxidase/catalase T
2cjz	Human protein tyrosine phosphatase PTPN5
2cmd	<i>E. coli</i> malate dehydrogenase
2cmw	Human casein kinase 1 gamma-1
2d0t	Human indoleamine 2,3-dioxygenase
2f4j	Proto-oncogene tyrosine-protein kinase ABL1
2f6q	Human peroxisomal delta3, delta2 enoyl CoA isomerase
2fbr	Transthyretin precursor
2fvv	Human diphosphoinositol polyphosphate phosphohydrolase 1
2fy3	Human choline acetyltransferase
2g5r	Siglec-7
2g72	Human phenylethanolamine N-methyltransferase
2gwh	Human sulfotransferase SULT1C2
2h7j	Cathepsin S
2ipx	Human fibrillarin
2iwz	Human mitochondrial beta-ketoacyl ACP synthase
2jis	Human cysteine sulfinic acid decarboxylase
2oaz	Human methionine aminopeptidase-2
2ozu	Human MYST histone acetyltransferase 3
2p0a	Human synapsin III
2p54	PPAR alpha
2pk4	Human plasminogen kringle
3fap	FKBP12-rapamycin complex-associated protein
3nos	Nitric-oxide synthase, endothelial

Table S3. Detailed results of the protein set evaluation: mean and standard deviation of AUC values for different protein sets.

Effect	10 proteins		40 proteins		70 proteins		100 proteins		130 proteins	
	mean	std	mean	std	mean	std	mean	std	mean	std
Adrenergic Agent	0.7096	0.05	0.8082	0.0072	0.8512	0.0096	0.892	0.002	0.9089	0.0059
Adrenergic Agonist	0.7958	0.0478	0.8868	0.0252	0.9167	0.0104	0.9446	0.0108	0.9582	0.0076
Adrenergic Alpha Agonist	0.8634	0.0337	0.956	0.0104	0.9678	0.0117	0.9788	0.0045	0.9874	0.0018
Adrenergic Alpha Antagonist	0.7299	0.0818	0.8794	0.0073	0.9316	0.0198	0.9521	0.0127	0.9698	0.0009
Adrenergic Antagonist	0.7135	0.0561	0.8471	0.0064	0.9036	0.0118	0.933	0.0041	0.9415	0.0057
Adrenergic Beta Agonist	0.8225	0.0544	0.954	0.0245	0.9793	0.0133	0.9821	0.0034	0.9918	0.0021
Adrenergic Beta Antagonist	0.8401	0.0235	0.9304	0.0198	0.9806	0.0032	0.9836	0.0017	0.9856	0.0018
Adrenergic Uptake Inhibitor	0.8202	0.0259	0.9245	0.023	0.9495	0.0179	0.9762	0.004	0.9832	0.003
Alkylating Agent	0.7874	0.0384	0.8857	0.0352	0.9475	0.0203	0.9725	0.0077	0.9733	0.0067
Amphetamine	0.8883	0.0203	0.9433	0.0072	0.9786	0.0028	0.9862	0.0038	0.9911	0.0013
Analgesic Agent	0.6921	0.01	0.7796	0.0192	0.8447	0.0061	0.8696	0.0092	0.8837	0.0055
Analgesic Agent, Non Narcotic	0.7687	0.0326	0.8933	0.009	0.9263	0.0165	0.9638	0.0156	0.9736	0.0041
Analgesic Agent, Opioid	0.8562	0.0286	0.9534	0.0173	0.973	0.0091	0.9868	0.0009	0.9881	0.0027
Anesthetic Agent	0.7133	0.0413	0.8266	0.0288	0.901	0.0195	0.9161	0.0057	0.9517	0.0043
Anesthetic Agent, Intravenous	0.6647	0.0688	0.9389	0.0082	0.9789	0.0045	0.9863	0.0076	0.9932	0.0044
Anesthetic Agent, Local	0.7902	0.0641	0.8809	0.0252	0.9456	0.0113	0.9608	0.0128	0.9747	0.0028
Angiotensin Converting Enzy	0.8318	0.0198	0.9668	0.0036	0.9833	0.0011	0.9932	0.0032	0.9976	0.0005
Anthelmintic Agent	0.868	0.0174	0.9416	0.0197	0.9853	0.0013	0.9906	0.0008	0.9945	0.0017
Anti Allergic Agent	0.7622	0.0014	0.8434	0.0101	0.8983	0.0055	0.9149	0.0034	0.9341	0.0027
Anti Anxiety Agent	0.7346	0.045	0.8449	0.0274	0.8949	0.0141	0.9078	0.012	0.918	0.0053
Anti Dyskinesia Agent	0.7202	0.0656	0.83	0.027	0.9115	0.0155	0.9426	0.0111	0.9628	0.0081
Anti Emetic Agent	0.7702	0.0336	0.839	0.0206	0.8894	0.0065	0.9094	0.0047	0.9317	0.0011
Anti HIV Agent	0.814	0.0342	0.8922	0.0051	0.943	0.0084	0.9345	0.0071	0.9638	0.0111
Anti Infective Agent	0.7084	0.0246	0.7696	0.0013	0.8017	0.0101	0.8269	0.0039	0.8382	0.0016
Anti Infective Agent, Local	0.7698	0.0497	0.8283	0.028	0.9271	0.0119	0.9575	0.0058	0.9818	0.0058
Anti Infective Agent, Urinal	0.8336	0.0133	0.905	0.0191	0.9453	0.0199	0.9631	0.003	0.9806	0.0046
Anti Inflammatory Agent	0.7286	0.0111	0.7945	0.0106	0.8593	0.0059	0.8841	0.0045	0.9008	0.0058
Anti Migraine Agent	0.7178	0.0271	0.876	0.0288	0.9222	0.009	0.9286	0.0121	0.9329	0.0015
Anti Obesity Agent	0.8123	0.0135	0.9087	0.0258	0.9692	0.0123	0.9797	0.0042	0.9898	0.0014
Anti Ulcer Agent	0.7484	0.0214	0.8777	0.0016	0.9326	0.0124	0.9506	0.0078	0.9715	0.0078
Antianginal Agent	0.7499	0.0522	0.8509	0.0205	0.9005	0.0142	0.9343	0.006	0.964	0.002
Antiarrhythmic Agent	0.6885	0.0311	0.7944	0.0109	0.8468	0.0188	0.886	0.0081	0.911	0.0039
Antiasthmatic Agent	0.7114	0.0303	0.812	0.0246	0.8936	0.0282	0.9275	0.0124	0.9494	0.0068
Antibacterial Agent	0.7931	0.0259	0.8758	0.0091	0.9133	0.0055	0.9427	0.0059	0.9489	0.0011
Antibiotic	0.7858	0.0301	0.8675	0.0039	0.8958	0.01	0.9286	0.0103	0.9337	0.0036

Anticholesteremic Agent	0.7502	0.0124	0.8877	0.0142	0.9598	0.0121	0.9846	0.0065	0.9929	0.0011
Anticoagulant	0.7316	0.0546	0.9109	0.0332	0.9588	0.0048	0.9739	0.0148	0.9833	0.0026
Anticonvulsant	0.7338	0.0655	0.8719	0.0122	0.9153	0.0134	0.939	0.0055	0.955	0.0033
Antidepressant	0.7753	0.0176	0.8854	0.0142	0.9047	0.02	0.9303	0.0028	0.9487	0.0027
Antidepressant, Second Generation	0.7412	0.0266	0.8813	0.0448	0.9302	0.0143	0.9539	0.0178	0.9736	0.012
Antifungal Agent	0.706	0.0315	0.8587	0.0269	0.9277	0.0166	0.9547	0.0093	0.9688	0.0038
Antiglaucoma Agent	0.739	0.0659	0.8328	0.0304	0.9234	0.0288	0.942	0.0064	0.9596	0.0042
Antihypertensive Agent	0.648	0.0119	0.7468	0.0168	0.7981	0.0103	0.8503	0.0103	0.8857	0.0028
Antihypocalcemic Agent	0.7995	0.0657	0.9255	0.0278	0.9652	0.0066	0.9827	0.0086	0.9884	0.002
Antimalarial Agent	0.7459	0.0475	0.8821	0.0093	0.929	0.0167	0.9695	0.0055	0.9843	0.0025
Antimanic Agent	0.7676	0.0548	0.9322	0.0137	0.9727	0.0077	0.9814	0.0033	0.9909	0.0028
Antimetabolite	0.8578	0.0238	0.907	0.0215	0.9326	0.0145	0.9499	0.0052	0.9681	0.0038
Antimuscarinic Agent	0.7864	0.0084	0.9084	0.0231	0.9393	0.0047	0.9582	0.006	0.9705	0.0022
Antineoplastic Agent	0.6336	0.0105	0.7437	0.0141	0.7838	0.0138	0.8199	0.0109	0.8473	0.003
Antineoplastic Agent, Alkylating	0.8017	0.075	0.897	0.0533	0.9528	0.0228	0.9781	0.005	0.9736	0.005
Antineoplastic Agent, Antimetabolite	0.824	0.0284	0.9415	0.0335	0.973	0.0066	0.9775	0.0066	0.988	0.0021
Antineoplastic Agent, Hormonal	0.8303	0.0258	0.9327	0.0152	0.9534	0.0143	0.9738	0.0043	0.9823	0.0016
Antioxidant	0.7475	0.0274	0.9187	0.0301	0.95	0.0319	0.9723	0.0109	0.9857	0.0051
Antiparkinson Agent	0.7195	0.0277	0.8618	0.0134	0.9117	0.0139	0.9424	0.014	0.9589	0.0055
Antiprotozoal Agent	0.7304	0.0692	0.8457	0.0062	0.9027	0.0179	0.9326	0.0125	0.9424	0.0197
Antipruritic Agent	0.7888	0.0262	0.882	0.0164	0.9252	0.0121	0.9228	0.0126	0.9466	0.0047
Antipsychotic	0.785	0.0065	0.8706	0.0031	0.9112	0.0184	0.9292	0.0093	0.9454	0.002
Antipyretic	0.8288	0.0496	0.8992	0.0025	0.9562	0.0097	0.9721	0.0085	0.9831	0.0032
Antirheumatic Agent	0.7172	0.095	0.8496	0.0271	0.9428	0.0168	0.9548	0.0103	0.9724	0.0048
Antispasmodic Agent	0.7641	0.017	0.9044	0.0199	0.9411	0.004	0.9523	0.0028	0.9622	0.0005
Antitussive	0.8348	0.0748	0.9721	0.0137	0.9827	0.0086	0.9916	0.0024	0.993	0.0012
Antiviral Agent	0.7814	0.0271	0.8448	0.0242	0.9049	0.005	0.9288	0.0077	0.9528	0.0073
Barbiturate	0.8793	0.0833	0.9971	0.0022	0.9992	0.0003	0.9997	0.0002	0.9996	0.0003
Benzimidazole	0.8151	0.0462	0.9396	0.0259	0.9658	0.0236	0.9731	0.0072	0.9786	0.0107
Benzodiazepine	0.886	0.0823	0.9846	0.0089	0.9971	0.0004	0.9984	0.0004	0.9983	0.0014
Beta Lactame Antibiotic	0.8846	0.0119	0.9688	0.0148	0.9789	0.0052	0.9873	0.0047	0.9917	0.0011
Bone Density Conservation Agent	0.7668	0.0489	0.8857	0.0178	0.928	0.0077	0.9707	0.0085	0.9801	0.0075
Bronchodilator Agent	0.6902	0.0315	0.8244	0.0134	0.8929	0.0152	0.8992	0.011	0.9268	0.0069
Calcium Channel Agent	0.685	0.0423	0.8311	0.0169	0.9047	0.0141	0.9407	0.0142	0.9523	0.0053
Calcium Channel Blocker	0.6987	0.0516	0.8441	0.0257	0.9199	0.011	0.9441	0.0162	0.9629	0.0016
Carbohydrate Derivative	0.9334	0.0322	0.9791	0.0033	0.9905	0.0021	0.9942	0.0014	0.9951	0.0002
Cardiotonic Agent	0.7543	0.0233	0.9161	0.0185	0.9512	0.0155	0.9821	0.0063	0.9882	0.0023
Cardiovascular Agent	0.6856	0.0146	0.8813	0.0147	0.9097	0.0135	0.9653	0.0059	0.9799	0.0034
Catecholamine	0.9018	0.0474	0.9729	0.0142	0.9949	0.0028	0.9965	0.0014	0.9994	0.0003
Cell Wall Synthesis Inhibitor	0.8636	0.0056	0.9461	0.0096	0.96	0.0073	0.9816	0.0044	0.9861	0.0017
Central Nervous System Agent	0.7653	0.0579	0.8326	0.016	0.9231	0.0187	0.9219	0.0113	0.9598	0.006
Central Nervous System Stimulant	0.778	0.0181	0.8578	0.0421	0.9608	0.0128	0.9668	0.0102	0.9875	0.0011

Cephalosporin	0.9236	0.0056	0.9799	0.0032	0.9878	0.0021	0.9952	0.0019	0.9971	0.0002
Cholinergic Agent	0.7272	0.0399	0.8461	0.0287	0.9059	0.02	0.9427	0.0071	0.9586	0.0055
Cholinergic Antagonist	0.7611	0.0333	0.884	0.0272	0.9322	0.0088	0.9458	0.0061	0.9665	0.0041
Cholinesterase Inhibitor	0.7718	0.0552	0.9346	0.0151	0.9638	0.0125	0.9775	0.0106	0.9917	0.002
Contraceptive Agent	0.9452	0.01	0.9731	0.0177	0.9911	0.0047	0.9969	0.0011	0.9984	0.0008
Corticosteroid	0.9693	0.0105	0.9865	0.0049	0.9926	0.0027	0.996	0.0003	0.9967	0.0003
Corticosteroid, Topical	0.9842	0.0004	0.9914	0.0024	0.9956	0.0008	0.9965	0.0004	0.9969	0.0005
Cyclooxygenase Inhibitor	0.8121	0.0627	0.8949	0.01	0.9638	0.0069	0.9711	0.0089	0.9862	0.0033
Depressant	0.7246	0.0254	0.8265	0.0082	0.8821	0.0153	0.9158	0.0104	0.9269	0.0053
Dermatologic Agent	0.7703	0.0106	0.897	0.0125	0.9468	0.0138	0.9636	0.0051	0.9752	0.0059
Dihydropyridine	0.9281	0.0063	0.9773	0.0085	0.9852	0.0058	0.9921	0.0019	0.9978	0.0007
Diuretic	0.7795	0.0097	0.8622	0.023	0.9015	0.0108	0.9363	0.0208	0.9483	0.0032
Dopamine Agent	0.7059	0.0349	0.8133	0.0382	0.8634	0.0008	0.8834	0.009	0.9113	0.0025
Dopamine Agonist	0.7798	0.024	0.9299	0.0272	0.9813	0.0075	0.9951	0.0021	0.9976	0.0007
Dopamine Antagonist	0.782	0.0304	0.8987	0.0099	0.9329	0.0044	0.9352	0.0141	0.957	0.0032
Dopamine Uptake Inhibitor	0.7998	0.0257	0.9309	0.0211	0.9654	0.0068	0.9777	0.0053	0.9872	0.0017
Ergoline Derivative	0.8182	0.0754	0.9589	0.0292	0.984	0.0041	0.9895	0.0145	0.9988	0.0012
Ergosterol Synthesis Inhibitor	0.8057	0.0061	0.9399	0.0209	0.9789	0.0081	0.9912	0.0033	0.9937	0.0015
Estrogen	0.9319	0.0293	0.9884	0.0085	0.9955	0.0007	0.9983	0.0005	0.9993	0.0004
Ethanolamine Derivative	0.7072	0.0293	0.813	0.031	0.8666	0.0074	0.9078	0.0128	0.9223	0.0025
Fluoroquinolone	0.9555	0.0264	0.9975	0.0022	0.9992	0.0005	0.9998	0.0002	1	0.0001
Folic Acid Antagonist	0.8173	0.0515	0.9531	0.0012	0.9605	0.0046	0.976	0.015	0.9838	0.0036
GABA Agent	0.7311	0.0457	0.8753	0.0104	0.922	0.0031	0.9461	0.0103	0.9648	0.0051
Gastrointestinal Agent	0.662	0.0399	0.9039	0.0534	0.9091	0.0162	0.9537	0.0077	0.9655	0.0051
Glucocorticoid	0.9691	0.0112	0.9858	0.006	0.9931	0.0019	0.9966	0.0017	0.9973	0.0002
Glutamate Receptor Antagonist	0.7758	0.0312	0.9081	0.006	0.9221	0.0126	0.9435	0.0037	0.962	0.0064
Guanidine Derivative	0.8156	0.0184	0.9145	0.0073	0.9521	0.02	0.9729	0.0053	0.9832	0.0022
Histamine Agent	0.7542	0.0301	0.8486	0.0174	0.8869	0.005	0.8999	0.0197	0.9258	0.0053
Histamine Antagonist	0.7699	0.0417	0.851	0.0204	0.8928	0.0075	0.9052	0.0161	0.9268	0.0032
Histamine H1 Antagonist	0.7862	0.0501	0.8904	0.0243	0.9313	0.007	0.9409	0.0143	0.9628	0.0038
Histamine H1 Antagonist, Non-sedating	0.8179	0.0561	0.9351	0.0076	0.9893	0.0078	0.9943	0.0044	0.9984	0.0007
Hormone Replacement Agent	0.9257	0.0107	0.9619	0.016	0.9868	0.0052	0.9939	0.0014	0.9972	0.0014
Hypnotic and or Sedative	0.7322	0.0348	0.887	0.026	0.9137	0.0015	0.9285	0.0066	0.9399	0.0055
Hypoglycemic Agent	0.7877	0.047	0.9292	0.0136	0.9632	0.0063	0.9762	0.0053	0.9863	0.0004
Imidazole Derivative	0.6655	0.0421	0.8503	0.0171	0.8894	0.0143	0.904	0.0019	0.9323	0.0071
Immunosuppressive Agent	0.733	0.0093	0.8502	0.0224	0.8931	0.0099	0.9203	0.0105	0.9401	0.011
Indole Derivative	0.7496	0.0103	0.9011	0.0128	0.9344	0.0051	0.9591	0.0011	0.9691	0.0084
Muscarinic Agent	0.7521	0.0137	0.8969	0.0246	0.9311	0.0051	0.9571	0.0047	0.9664	0.0025
Muscle Relaxant	0.6776	0.0328	0.8131	0.0027	0.8507	0.0137	0.8772	0.015	0.9019	0.0174
Muscle Relaxant, Central	0.7857	0.0461	0.9149	0.0376	0.955	0.0043	0.9784	0.0093	0.9874	0.0055
Muscle Relaxant, Skeletal	0.7245	0.0603	0.8483	0.0308	0.8782	0.0261	0.9154	0.0123	0.9413	0.0131
Narcotic	0.8498	0.0187	0.9481	0.0145	0.9687	0.0108	0.9825	0.0042	0.987	0.0022

Neuroprotective Agent	0.7167	0.0176	0.8265	0.0451	0.9004	0.0437	0.9404	0.0023	0.9479	0.0121
Neurotransmitter Uptake Inhibitor	0.7728	0.0341	0.8833	0.0108	0.9051	0.0046	0.9231	0.0065	0.943	0.0049
Nitro Compound	0.796	0.1248	0.9249	0.0296	0.9635	0.0061	0.9818	0.0025	0.9915	0.0018
Nonsteroidal Anti Inflammatory Agent	0.7292	0.0195	0.8078	0.0217	0.8778	0.0182	0.8923	0.0103	0.925	0.0041
Norepinephrine Reuptake Inhibitor	0.8388	0.0134	0.952	0.0279	0.9742	0.0159	0.9887	0.0028	0.9944	0.0004
Nucleic Acid Synthesis Inhibitor	0.7404	0.0137	0.8244	0.0024	0.8595	0.0073	0.8764	0.0105	0.9023	0.0017
Nucleoside or Nucleotide	0.9418	0.03	0.9881	0.0011	0.9898	0.0035	0.995	0.0004	0.998	0.0005
Nucleoside or Nucleotide Analogue	0.9139	0.0305	0.976	0.0074	0.9852	0.0059	0.9941	0.0014	0.9973	0.0002
Opiate Agent	0.8595	0.0282	0.9536	0.0087	0.9578	0.0065	0.9772	0.0025	0.9835	0.0035
Opiate Agonist	0.8538	0.0367	0.9575	0.0144	0.9669	0.0043	0.9814	0.0029	0.9874	0.0023
Opioid	0.8947	0.0244	0.9646	0.0065	0.9776	0.0053	0.984	0.0058	0.9873	0.003
Parasympatholytic	0.7792	0.0293	0.9189	0.0116	0.9501	0.0094	0.9585	0.0149	0.9793	0.0022
Parasympathomimetic	0.8014	0.0263	0.9683	0.0038	0.985	0.0044	0.989	0.0031	0.9953	0.002
Penicillin	0.8916	0.0505	0.9785	0.0126	0.9901	0.0077	0.9984	0.0001	0.9994	0.0005
Phenothiazine	0.8748	0.0281	0.9709	0.0122	0.9879	0.0044	0.9927	0.0027	0.9952	0.0013
Phosphodiesterase Inhibitor	0.8303	0.0249	0.9208	0.0272	0.9653	0.0139	0.9738	0.0079	0.985	0.0046
Piperazine Derivative	0.7838	0.0211	0.8964	0.0182	0.9264	0.0091	0.9619	0.0036	0.9713	0.0012
Piperidine Derivative	0.73	0.0278	0.8322	0.0124	0.8746	0.005	0.9186	0.0051	0.944	0.0068
Platelet Aggregation Inhibitor	0.7223	0.0453	0.8296	0.0194	0.9015	0.0129	0.9487	0.0124	0.9544	0.0031
Potassium Channel Agent	0.8047	0.0789	0.9172	0.0173	0.943	0.0234	0.9741	0.0159	0.9819	0.0112
Potassium Channel Blocker	0.8085	0.0822	0.9345	0.0121	0.9587	0.0215	0.9728	0.0151	0.9796	0.0101
Progestin	0.962	0.0129	0.9845	0.0048	0.995	0.0017	0.9986	0.0002	0.9988	0.0006
Prostaglandin Derivative	0.8766	0.0431	0.9758	0.0079	0.9908	0.0022	0.9951	0.0019	0.9982	0.0013
Protein Synthesis Inhibitor	0.8444	0.0262	0.8977	0.0036	0.9342	0.0279	0.9455	0.0114	0.9556	0.0096
Purine Derivative	0.9577	0.02	0.9834	0.005	0.9896	0.005	0.9938	0.0031	0.9976	0.0003
Pyridine Derivative	0.6593	0.007	0.7767	0.0191	0.8259	0.0163	0.883	0.0122	0.9144	0.0021
Pyrimidine Derivative	0.7812	0.0352	0.8975	0.0373	0.9275	0.0229	0.9488	0.0083	0.9725	0.0077
Quaternary Amine	0.7066	0.0251	0.8167	0.0132	0.8701	0.0031	0.9083	0.0058	0.9332	0.0029
Quinoline Derivative	0.7573	0.0308	0.9097	0.0249	0.9642	0.0163	0.9919	0.0031	0.9959	0.0005
Quinolone	0.9102	0.0352	0.994	0.0038	0.9971	0.0012	0.9988	0.0003	0.9991	0.0003
Respiratory Smooth Muscle Relaxant	0.7552	0.0094	0.8981	0.0107	0.9347	0.0236	0.9333	0.0164	0.9614	0.012
Respiratory System Agent	0.6633	0.0279	0.7909	0.0194	0.8456	0.0061	0.8821	0.0155	0.8938	0.0078
Reverse Transcriptase Inhibitor	0.828	0.0213	0.9295	0.0051	0.9463	0.0077	0.9553	0.0028	0.9764	0.0085
Serotonin Agent	0.7449	0.05	0.8625	0.007	0.8882	0.0137	0.9169	0.0128	0.9406	0.0034
Serotonin Agonist	0.8469	0.0182	0.9359	0.0086	0.9663	0.0118	0.9787	0.0117	0.9902	0.0025
Serotonin Antagonist	0.7635	0.0565	0.8849	0.014	0.9292	0.0077	0.9487	0.0112	0.9643	0.0041
Serotonin Reuptake Inhibitor	0.8005	0.0386	0.9176	0.022	0.9495	0.013	0.9622	0.0092	0.9721	0.0075
Sodium Channel Blocker	0.7341	0.0473	0.8145	0.0267	0.8744	0.0103	0.8958	0.0094	0.9137	0.0045
Sodium Chloride Symporter Inhibitor	0.8458	0.0444	0.955	0.0049	0.9844	0.0031	0.9982	0.001	0.9993	0.0004
Steroidal	0.9282	0.0037	0.9738	0.0097	0.9849	0.0057	0.9898	0.0034	0.9949	0.0026
Steroidal Anti Inflammatory Agent	0.9829	0.0022	0.9946	0.0014	0.9967	0.0012	0.9981	0.0007	0.9988	0.0002
Stimulant	0.7605	0.0043	0.8689	0.0263	0.9408	0.0144	0.9549	0.0167	0.9728	0.0084

Sulfonamide	0.749	0.0335	0.8592	0.0135	0.8951	0.0088	0.9291	0.0064	0.9356	0.0031
Sulfone	0.7604	0.0065	0.8717	0.0131	0.9355	0.0066	0.9533	0.0015	0.9671	0.0007
Sulfonylurea	0.8356	0.0666	0.9697	0.0218	0.9938	0.0018	0.9972	0.0034	0.9991	0.0008
Sympatholytic	0.7316	0.0295	0.8475	0.0494	0.9078	0.0243	0.9442	0.0169	0.9567	0.0054
Sympathomimetic	0.8196	0.0531	0.8913	0.0112	0.92	0.0134	0.944	0.0087	0.9654	0.0055
Tetracycline	0.9456	0.039	0.9932	0.0079	0.9995	0.0005	1	0.0001	1	0.0001
Tetrazole Derivative	0.8327	0.0229	0.9304	0.0106	0.9734	0.0081	0.9749	0.0093	0.9876	0.0016
Thiazide	0.8681	0.0394	0.9628	0.0055	0.9897	0.0064	0.9981	0.0014	0.9991	0.0006
Thiazole	0.8672	0.0114	0.9262	0.0055	0.9745	0.0064	0.9742	0.0058	0.988	0.0032
Tocolytic Agent	0.781	0.0079	0.9347	0.0211	0.9588	0.011	0.9745	0.0045	0.9801	0.0083
Triazole Derivative	0.7901	0.02	0.8762	0.0063	0.9258	0.0242	0.9333	0.0085	0.9563	0.0073
Tricyclic Antidepressant	0.8659	0.07	0.9828	0.0007	0.9899	0.0017	0.9953	0.0005	0.9964	0.0012
Trifluormethyl Derivative	0.688	0.0161	0.8019	0.0191	0.8648	0.0257	0.9121	0.0217	0.9311	0.0111
Vasoconstrictor	0.7698	0.0306	0.854	0.0284	0.8938	0.0347	0.9305	0.0091	0.9442	0.0021
Vasodilator	0.6323	0.0205	0.7665	0.0101	0.7989	0.0135	0.8395	0.0061	0.8654	0.0071
2 Hydroxy 3 aminopropoxy Derivative	0.8368	0.0339	0.9271	0.0067	0.9813	0.0025	0.9833	0.0049	0.9914	0.0013

Random protein sets of 10, 40, 70, 100 and 130 proteins were used to reproduce the IPs, then DPM method was performed and AUC values were extracted for each effect. The means of 3 independent runs and the standard deviations are displayed in the table. The low values of the standard deviations show that the composition of the sets does not affect the AUC values. On the other hand the increasing number of the applied proteins saturates the AUC values i.e. the prediction accuracy.

Table S4. Maximal obtainable AUC values for the 177 studied effects and the calculated protein set sizes required for 90% accuracy.

Effect	Maximal obtainable AUC	Number of proteins required for 90% saturation
Adrenergic Agent	0.933	41
Adrenergic Agonist	0.986	37
Adrenergic Alpha Agonist	1.000	15
Adrenergic Alpha Antagonist	1.000	48
Adrenergic Antagonist	0.981	51
Adrenergic Beta Agonist	1.000	19
Adrenergic Beta Antagonist	1.000	16
Adrenergic Uptake Inhibitor	0.996	20
Alkylating Agent	0.997	26
Amphetamine	0.997	12
Analgesic Agent	0.910	44
Analgesic Agent, Non Narcotic	1.000	40
Analgesic Agent, Opioid	0.991	7
Anesthetic Agent	0.972	44
Anesthetic Agent, Local	0.980	28
Anesthetic Agent. Intravenous	1.000	22
Angiotensin-Converting Enzyme Inhibitor	1.000	16
Anthelmintic Agent	1.000	31
Anti-Allergic Agent	0.936	22
Antianginal Agent	1.000	65
Anti-Anxiety Agent	0.920	21
Antiarrhythmic Agent	1.000	121
Antiasthmatic Agent	1.000	62
Antibacterial Agent	0.958	22
Antibiotic	0.942	21
Anticholesteremic Agent	1.000	28
Anticoagulant	1.000	38
Anticonvulsant	0.987	40
Antidepressant	0.960	23
Antidepressant, Second Generation	1.000	44
Anti-Dyskinesia Agent	1.000	58
Anti-Emetic Agent	0.943	33

Antifungal Agent	1.000	57
Antiglaucoma Agent	0.983	40
Antihypertensive Agent	1.000	170
Antihypocalcemic Agent	1.000	38
Anti-Infective Agent	0.844	20
Anti-Infective Agent, Local	1.000	48
Anti-Infective Agent, Urinary	0.991	27
Anti-Inflammatory Agent	0.921	46
Antimalarial Agent	1.000	43
Antimanic Agent	1.000	26
Antimetabolite	0.954	7
Anti-Migraine Agent	0.988	64
Antimuscarinic Agent	0.970	14
Antineoplastic Agent	0.942	137
Antineoplastic Agent, Alkylating	1.000	26
Antineoplastic Agent, Antimetabolite	0.993	11
Antineoplastic Agent, Hormonal	0.984	15
Anti-Obesity Agent	1.000	26
Antioxidant	1.000	31
Antiparkinson Agent	0.994	45
Antiprotozoal Agent	1.000	60
Antipruritic Agent	0.955	19
Antipsychotic	0.983	40
Antipyretic	1.000	25
Antirheumatic Agent	1.000	53
Antispasmodic Agent	0.983	30
Antitussive	0.997	7
Anti-Ulcer Agent	1.000	53
Antiviral Agent	0.973	34
Barbiturate	1.000	5
Benzimidazole	1.000	27
Benzodiazepine	1.000	10
Beta Lactame Antibiotic	0.997	13
Bone Density Conservation Agent	1.000	46
Bronchodilator Agent	0.948	35
Calcium Channel Agent	0.987	49
Calcium Channel Blocker	1.000	51
Carbohydrate Derivative	1.000	11
Cardiotonic Agent	1.000	27
Cardiovascular Agent	1.000	46
Catecholamine	1.000	6
Cell Wall Synthesis Inhibitor	0.989	14

Central Nervous System Agent	0.975	34
Central Nervous System Stimulant	1.000	25
Cephalosporin	0.999	9
Cholinergic Agent	0.992	50
Cholinergic Antagonist	0.976	26
Cholinesterase Inhibitor	1.000	30
Contraceptive Agent	1.000	6
Corticosteroid	1.000	6
Corticosteroid, Topical	1.000	5
Cyclooxygenase Inhibitor	1.000	31
Depressant	0.926	22
Dermatologic Agent	1.000	36
Dihydropyridine	1.000	10
Diuretic	0.957	25
Dopamine Agent	0.941	47
Dopamine Agonist	1.000	27
Dopamine Antagonist	0.984	32
Dopamine Uptake Inhibitor	0.994	15
Ergoline Derivative	1.000	15
Ergosterol Synthesis Inhibitor	1.000	18
Estrogen	1.000	7
Ethanolamine Derivative	0.994	81
Fluoroquinolone	1.000	5
Folic Acid Antagonist	1.000	23
GABA Agent	0.996	40
Gastrointestinal Agent	1.000	52
Glucocorticoid	1.000	6
Glutamate Receptor Antagonist	0.985	29
Guanidine Derivative	1.000	29
Histamine Agent	0.952	34
Histamine Antagonist	0.944	25
Histamine H1 Antagonist	0.970	19
Histamine H1 Antagonist, Non-sedating	1.000	11
Hormone Replacement Agent	1.000	12
Hypnotic and/or Sedative	0.959	27
Hypoglycemic Agent	1.000	31
Imidazole Derivative	1.000	88
Immunosuppressive Agent	1.000	68
Indole Derivative	1.000	42
Muscarinic Agent	0.977	22
Muscle Relaxant	0.942	51
Muscle Relaxant, Central	1.000	27

Muscle Relaxant, Skeletal	0.953	24
Narcotic	0.989	8
Neuroprotective Agent	0.984	45
Neurotransmitter Uptake Inhibitor	0.953	22
Nitro Compound	1.000	23
Nonsteroidal Anti-Inflammatory Agent	1.000	100
Norepinephrine Reuptake Inhibitor	1.000	15
Nucleic Acid Synthesis Inhibitor	0.912	22
Nucleoside or Nucleotide	1.000	3
Nucleoside or Nucleotide Analogue	0.997	6
Opiate Agent	0.982	7
Opiate Agonist	0.989	8
Opioid	0.988	5
Parasympatholytic	0.983	20
Parasympathomimetic	1.000	19
Penicillin	1.000	10
Phenothiazine	1.000	9
Phosphodiesterase Inhibitor	1.000	25
Piperazine Derivative	1.000	38
Piperidine Derivative	1.000	74
Platelet Aggregation Inhibitor	1.000	78
Potassium Channel Agent	1.000	32
Potassium Channel Blocker	1.000	28
Progestin	1.000	5
Prostaglandin Derivative	1.000	10
Protein Synthesis Inhibitor	0.961	17
Purine Derivative	1.000	7
Pyridine Derivative	1.000	124
Pyrimidine Derivative	0.989	32
Quaternary Amine	1.000	101
Quinoline Derivative	1.000	32
Quinolone	1.000	7
Respiratory Smooth Muscle Relaxant	0.973	25
Respiratory System Agent	0.952	69
Reverse Transcriptase Inhibitor	0.985	14
Serotonin Agent	0.970	43
Serotonin Agonist	1.000	28
Serotonin Antagonist	0.999	38
Serotonin Reuptake Inhibitor	1.000	29
Sodium Channel Blocker	0.925	28
Sodium Chloride Symporter Inhibitor	1.000	16
Steroidal	1.000	7

Steroidal Anti-Inflammatory Agent	1.000	6
Stimulant	0.975	20
Sulfonamide	0.975	46
Sulfone	1.000	44
Sulfonylurea	1.000	15
Sympatholytic	0.977	37
Sympathomimetic	0.966	16
Tetracycline	1.000	5
Tetrazole Derivative	1.000	18
Thiazide	1.000	15
Thiazole	0.988	11
Tocolytic Agent	1.000	36
Triazole Derivative	0.966	35
Tricyclic Antidepressant	1.000	6
Trifluormethyl Derivative	1.000	85
Vasoconstrictor	1.000	68
Vasodilator	0.959	123
2-Hydroxy-3-aminopropoxy Derivative	1.000	15