

Supplementary Material I. The benchmark dataset consisted of 876 drugs, which were classified into 4 target groups.

1. Drugs in target group “G Protein-coupled Receptors”

D00059	D00076	D00079	D00089	D00095	D00101
D00113	D00116	D00136	D00138	D00146	D00147
D00176	D00180	D00232	D00234	D00235	D00241
D00255	D00270	D00274	D00281	D00283	D00284
D00291	D00295	D00300	D00308	D00318	D00320
D00356	D00373	D00378	D00390	D00400	D00411
D00415	D00419	D00422	D00426	D00432	D00451
D00454	D00458	D00465	D00479	D00480	D00482
D00483	D00485	D00493	D00494	D00502	D00503
D00511	D00513	D00514	D00520	D00522	D00523
D00524	D00559	D00560	D00561	D00563	D00597
D00598	D00599	D00603	D00608	D00609	D00610
D00627	D00632	D00634	D00644	D00646	D00659
D00662	D00663	D00666	D00669	D00672	D00674
D00676	D00682	D00684	D00702	D00715	D00717
D00722	D00723	D00726	D00769	D00774	D00778
D00779	D00780	D00782	D00789	D00794	D00797
D00798	D00799	D00800	D00819	D00836	D00837
D00838	D00839	D00842	D00843	D00847	D00987
D00989	D00996	D01000	D01002	D01008	D01017
D01019	D01024	D01025	D01028	D01044	D01051
D01096	D01118	D01148	D01163	D01164	D01172
D01177	D01182	D01205	D01226	D01227	D01236
D01295	D01297	D01307	D01321	D01336	D01358
D01360	D01369	D01373	D01399	D01428	D01448
D01452	D01462	D01468	D01471	D01485	D01685
D01692	D01699	D01745	D01871	D01939	D01964
D01973	D02004	D02022	D02037	D02070	D02071
D02076	D02081	D02082	D02100	D02116	D02147
D02211	D02212	D02213	D02234	D02235	D02249
D02271	D02338	D02340	D02342	D02343	D02349
D02357	D02358	D02363	D02369	D02374	D02419
D02599	D02613	D02721	D02724	D02730	D02738
D02824	D02825	D02829	D02846	D02968	D02976
D02983	D03165	D03197	D03503	D03504	D03505
D03535	D03556	D03621	D03622	D03654	D03693
D03704	D03713	D03729	D03879	D04006	D04040
D04057	D04157	D04187	D04716	D04883	D04970
D05008	D05113	D05127	D05312	D05523	D05575

D05632	D05738	D05792	D05938	D06056	D06213
D06247	D06330	D07122	D07124	D07129	D07132
D07156	D07218	D07229	D07312	D07377	D07398
D07431	D07461	D07463	D07482	D07483	D07489
D07511	D07526	D07534	D07538	D07543	D07593
D07617	D07620	D07624	D07662	D07665	D07667
D07713	D07748	D07759	D07765	D07803	D07805
D07809	D07820	D07837	D07838	D07862	D07868
D07870	D07874	D07878	D07887	D07890	D07900
D07905	D07906	D07916	D07977	D07990	D08090
D08113	D08146	D08305	D08339	D08397	D08426
D08473	D08585	D08600	D08611	D08636	D08685
D08687					

2. Drugs in target group “Nuclear Receptors”

D00066	D00067	D00075	D00088	D00129	D00165
D00182	D00185	D00187	D00244	D00246	D00279
D00289	D00292	D00299	D00312	D00316	D00327
D00334	D00395	D00407	D00408	D00443	D00462
D00565	D00577	D00585	D00586	D00596	D00689
D00898	D00950	D00951	D00952	D00954	D00956
D00957	D00958	D00961	D00962	D00965	D00966
D00972	D00975	D00977	D01011	D01112	D01115
D01161	D01217	D01272	D01294	D01327	D01357
D01366	D01368	D01387	D01402	D01442	D01464
D01510	D01619	D01637	D01639	D01689	D01708
D01820	D02217	D02287	D02367	D02815	D03106
D03493	D03521	D03595	D03696	D03697	D03917
D04104	D04208	D05209	D06171	D06551	D07116
D07495	D07536	D07715	D07719	D07726	D07827
D07939	D08052	D08166	D08167	D08610	

3. Drugs in target group “Ion Channels”

D00011	D00110	D00225	D00228	D00250	D00252
D00267	D00271	D00280	D00293	D00294	D00303
D00311	D00319	D00326	D00331	D00336	D00354
D00358	D00380	D00387	D00394	D00418	D00430
D00437	D00438	D00477	D00492	D00506	D00512
D00533	D00537	D00538	D00539	D00549	D00551
D00552	D00553	D00615	D00616	D00619	D00631
D00639	D00640	D00647	D00649	D00693	D00694
D00701	D00706	D00711	D00714	D00732	D00733
D00735	D00738	D00758	D00759	D00760	D00765
D00766	D00767	D00811	D00812	D00815	D00821

D00822	D00825	D01173	D01179	D01253	D01285
D01287	D01310	D01354	D01372	D01450	D01546
D01599	D01657	D02074	D02078	D02086	D02087
D02182	D02220	D02356	D02360	D02362	D02408
D02537	D02574	D02624	D02716	D03562	D03740
D03991	D04048	D04905	D05077	D06172	D07283
D07445	D07447	D07450	D07473	D07791	D07845
D07894	D08098	D08127	D08174	D08215	D08283
D08435	D08458	D08490	D08690		

4. Drugs in target group “Enzymes”

D00107	D00109	D00112	D00118	D00120	D00125
D00126	D00130	D00131	D00132	D00141	D00142
D00145	D00153	D00160	D00183	D00184	D00186
D00196	D00204	D00210	D00211	D00212	D00216
D00217	D00218	D00220	D00222	D00224	D00240
D00251	D00256	D00257	D00258	D00259	D00260
D00262	D00263	D00264	D00273	D00296	D00297
D00298	D00302	D00310	D00315	D00317	D00321
D00322	D00330	D00333	D00350	D00351	D00353
D00355	D00359	D00362	D00401	D00410	D00412
D00413	D00414	D00416	D00417	D00421	D00423
D00424	D00429	D00434	D00435	D00445	D00447
D00448	D00450	D00453	D00455	D00459	D00466
D00469	D00488	D00497	D00510	D00518	D00535
D00558	D00562	D00564	D00567	D00574	D00578
D00579	D00580	D00582	D00587	D00592	D00621
D00622	D00624	D00652	D00653	D00667	D00670
D00707	D00718	D00724	D00749	D00753	D00762
D00781	D00785	D00786	D00870	D00871	D00872
D00873	D00874	D00878	D00879	D00880	D00887
D00889	D00893	D00894	D00895	D00896	D00900
D00902	D00903	D00904	D00905	D00906	D00907
D00908	D00909	D00910	D00911	D00912	D00917
D00919	D00920	D00921	D00922	D00923	D00927
D00929	D00939	D00960	D00963	D00964	D00968
D00970	D00994	D00995	D01001	D01049	D01053
D01055	D01070	D01074	D01075	D01093	D01133
D01136	D01142	D01147	D01155	D01157	D01178
D01180	D01196	D01199	D01223	D01240	D01251
D01276	D01280	D01283	D01325	D01334	D01415
D01489	D01526	D01560	D01572	D01581	D01601
D01628	D01653	D01687	D01720	D01739	D01811
D01819	D01844	D01896	D01904	D01949	D01982

D02085	D02119	D02121	D02137	D02166	D02190
D02193	D02194	D02196	D02199	D02201	D02203
D02216	D02221	D02222	D02228	D02229	D02241
D02258	D02267	D02299	D02301	D02306	D02307
D02318	D02323	D02336	D02339	D02344	D02345
D02348	D02350	D02353	D02365	D02368	D02376
D02405	D02415	D02418	D02441	D02471	D02481
D02482	D02483	D02495	D02501	D02555	D02558
D02709	D02922	D02923	D03034	D03082	D03150
D03208	D03211	D03349	D03410	D03428	D03432
D03546	D03656	D03710	D03715	D03731	D03752
D03753	D03769	D03771	D03795	D03798	D03820
D03822	D03828	D03882	D04008	D04112	D04196
D04197	D04515	D04720	D05021	D05022	D05032
D05177	D05353	D05407	D05411	D05529	D05590
D05947	D06074	D06412	D06503	D06637	D06675
D06881	D07057	D07064	D07452	D07471	D07472
D07474	D07487	D07596	D07598	D07614	D07621
D07626	D07635	D07636	D07639	D07643	D07644
D07645	D07647	D07648	D07650	D07651	D07653
D07654	D07658	D07659	D07661	D07698	D07712
D07733	D07751	D07782	D07869	D07871	D07892
D07896	D07901	D07925	D07961	D07965	D07992
D08011	D08012	D08109	D08120	D08143	D08218
D08237	D08261	D08306	D08380	D08401	D08410
D08469	D08514	D08534	D08556	D08557	D08605
D08618	D08668				