

Fig. S1

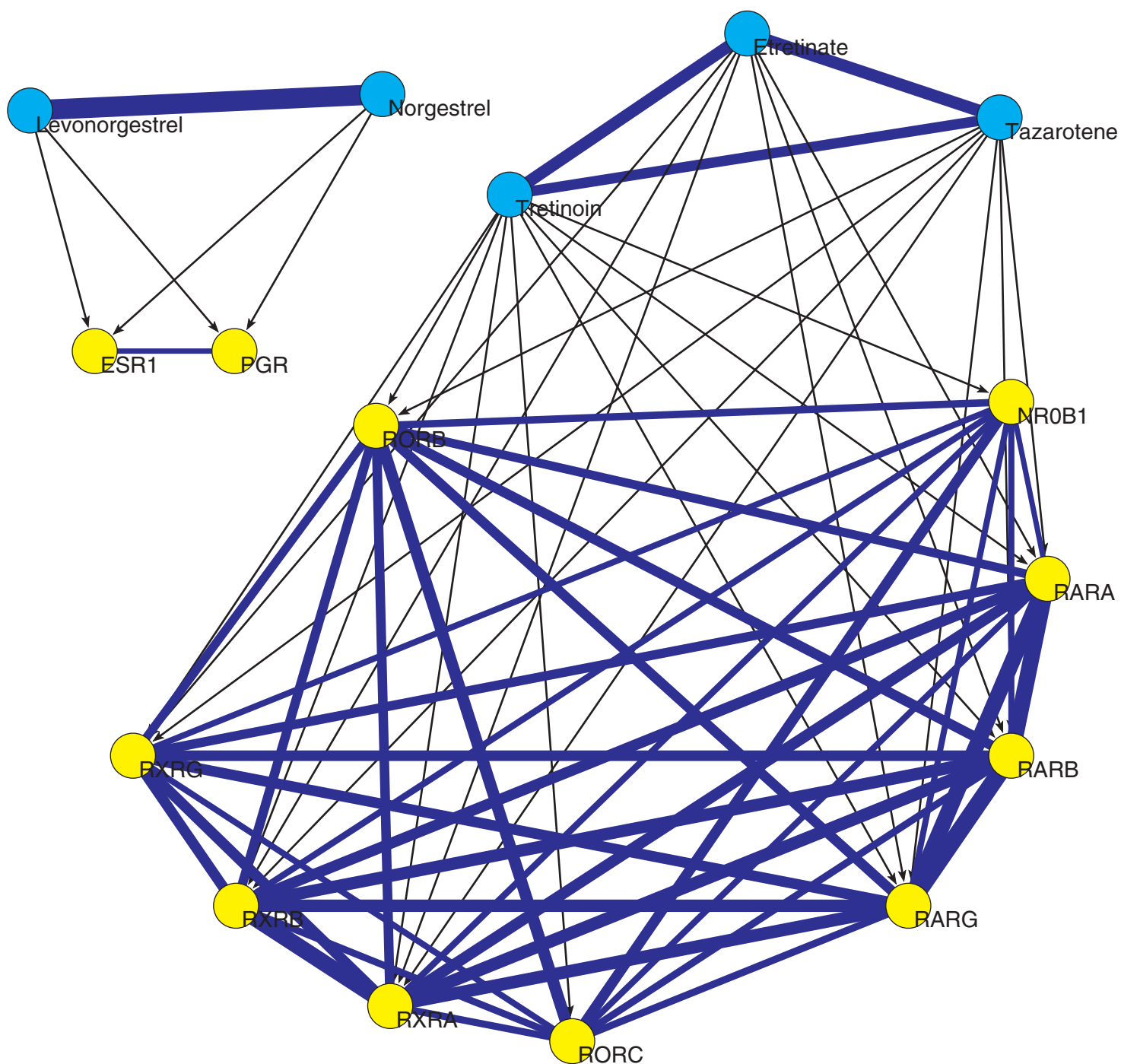


Fig. S2

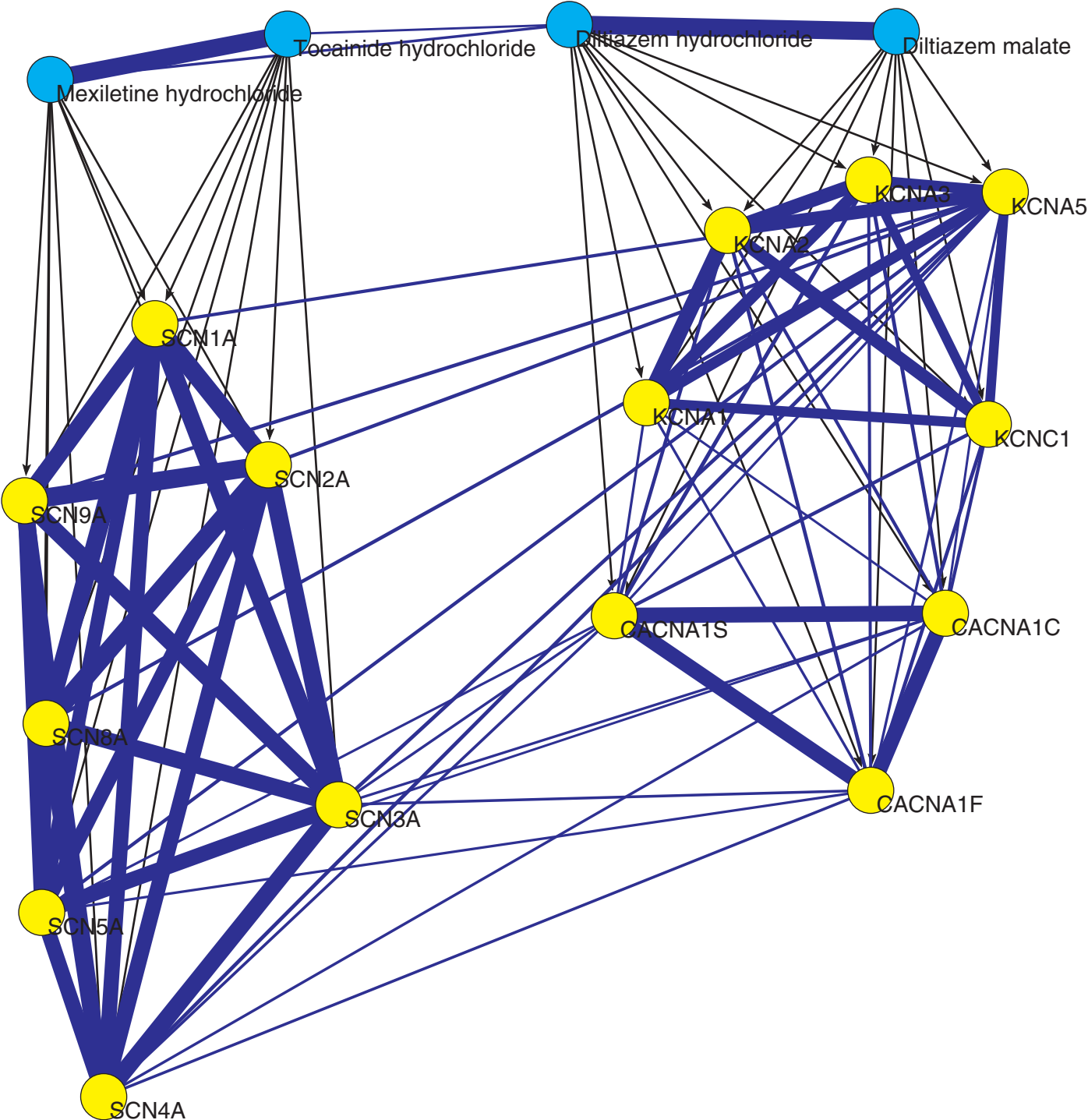
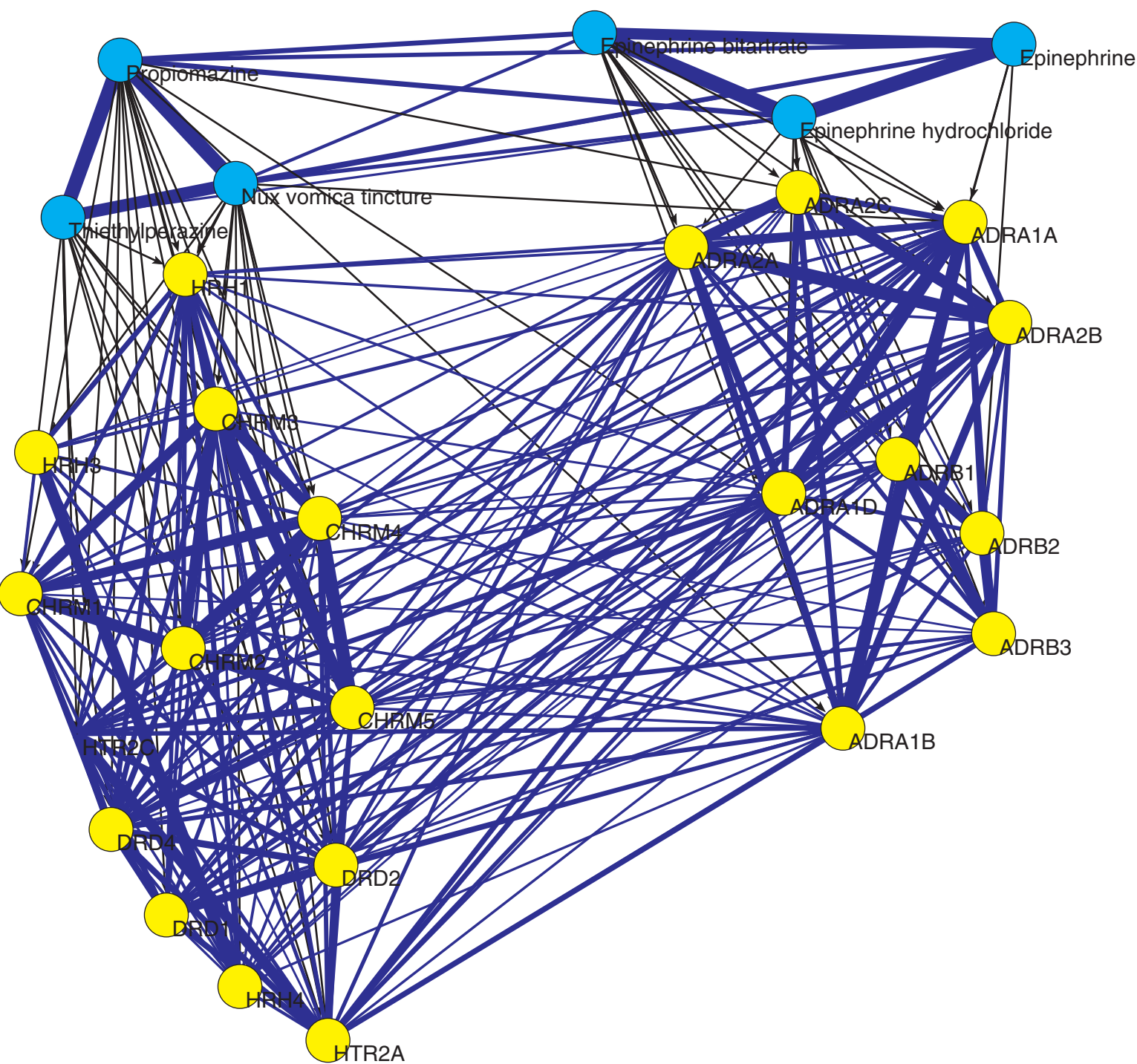


Fig. S3



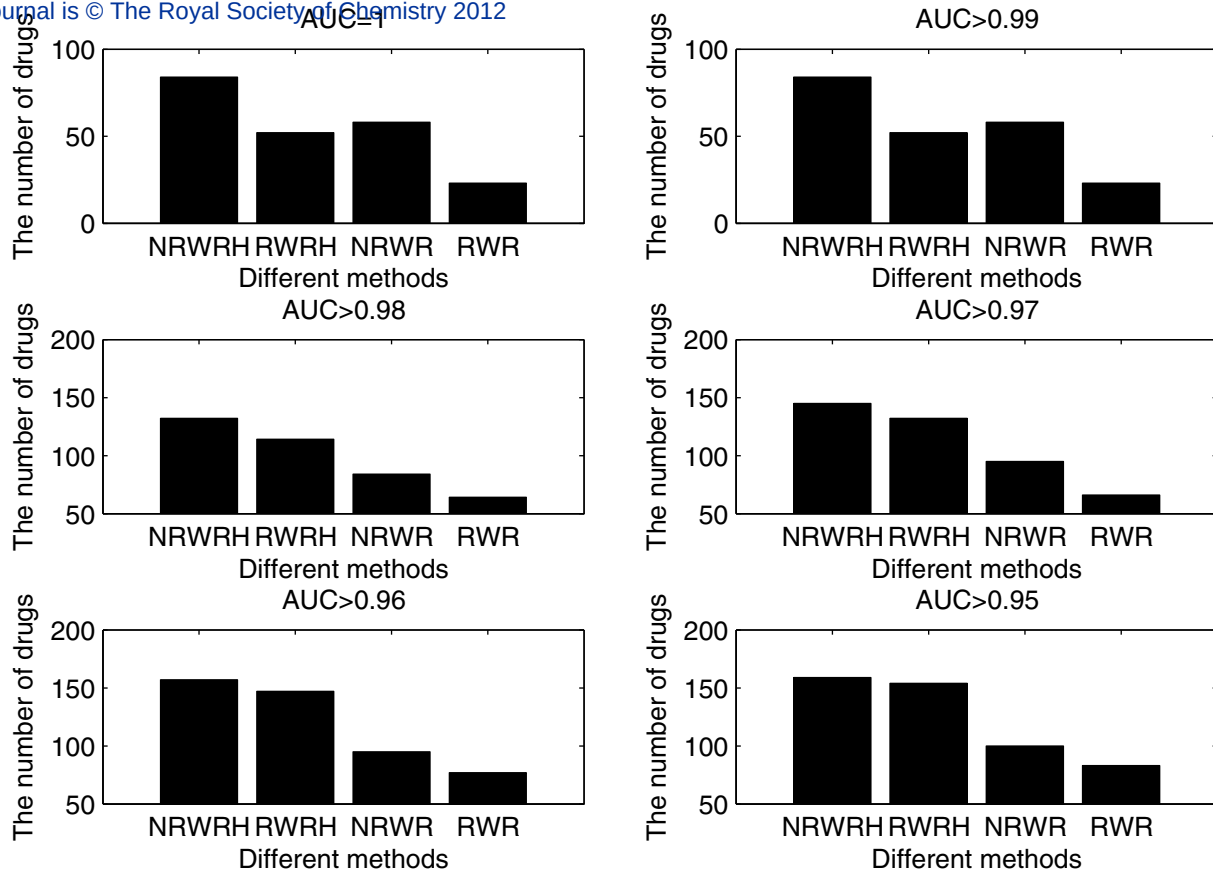


Fig. S4

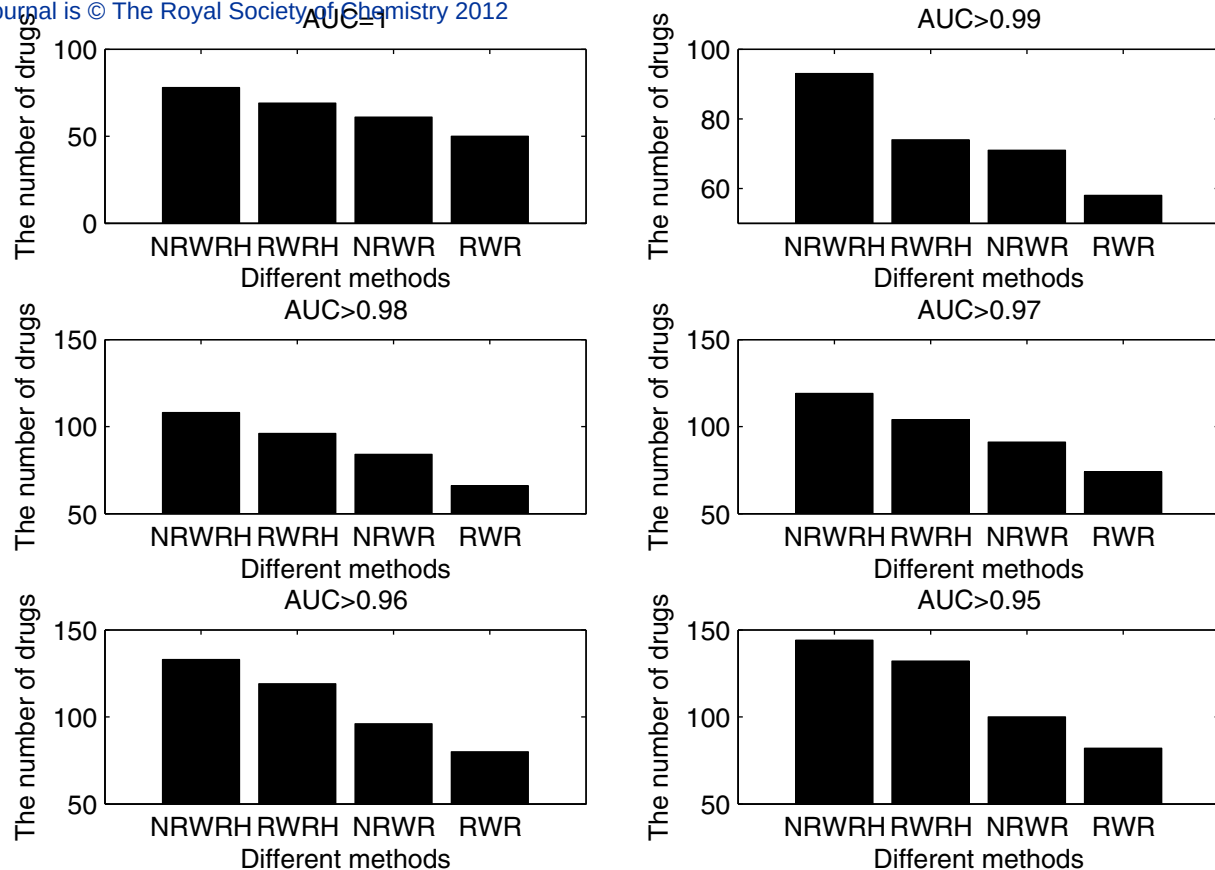


Fig. S5

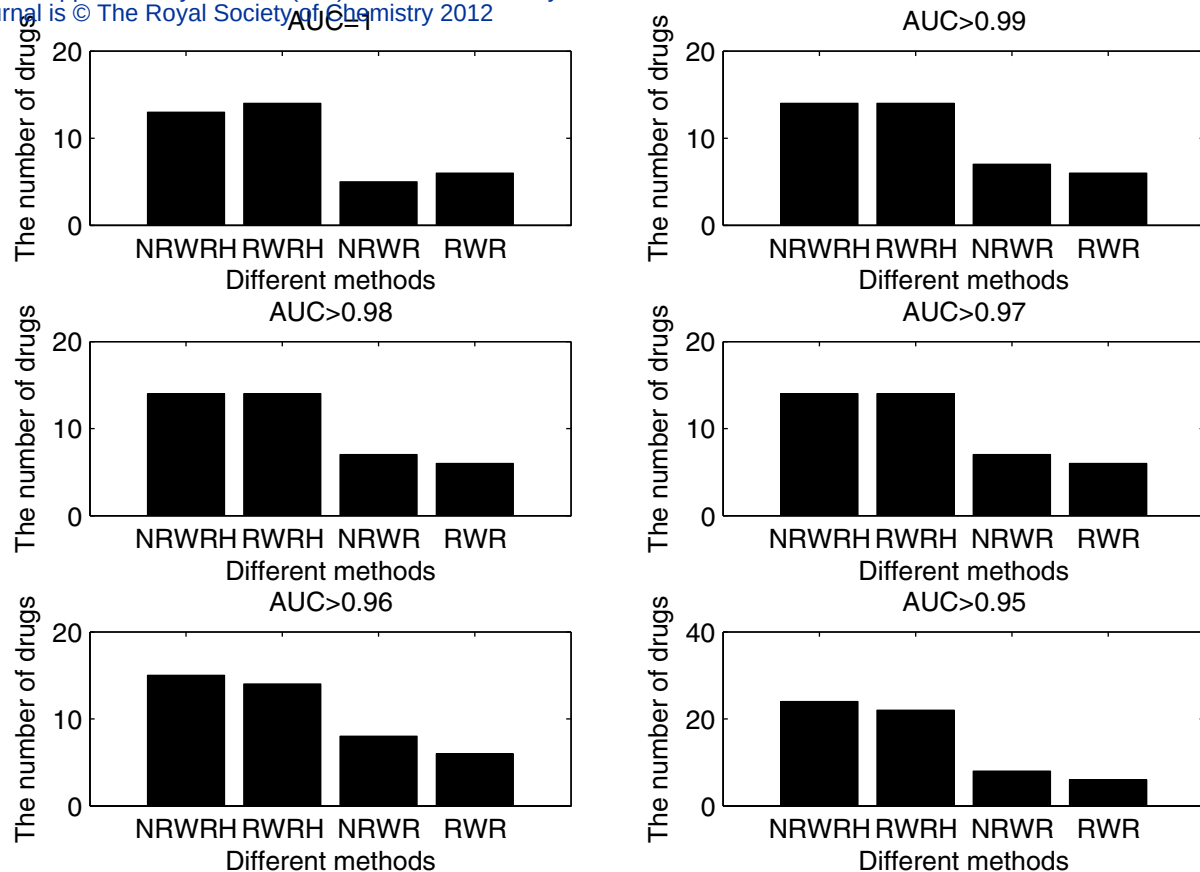


Fig. S6

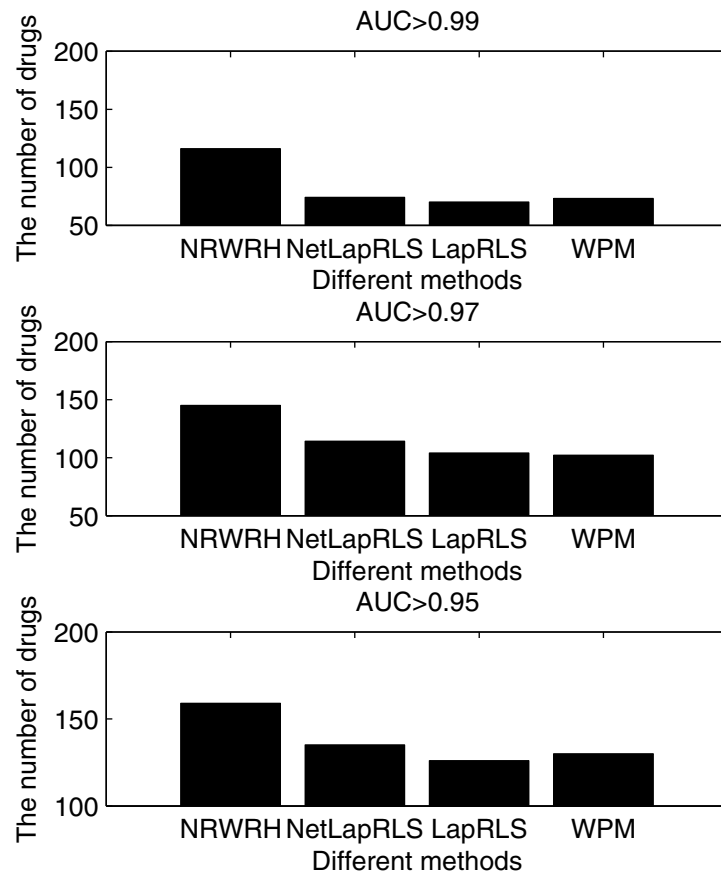
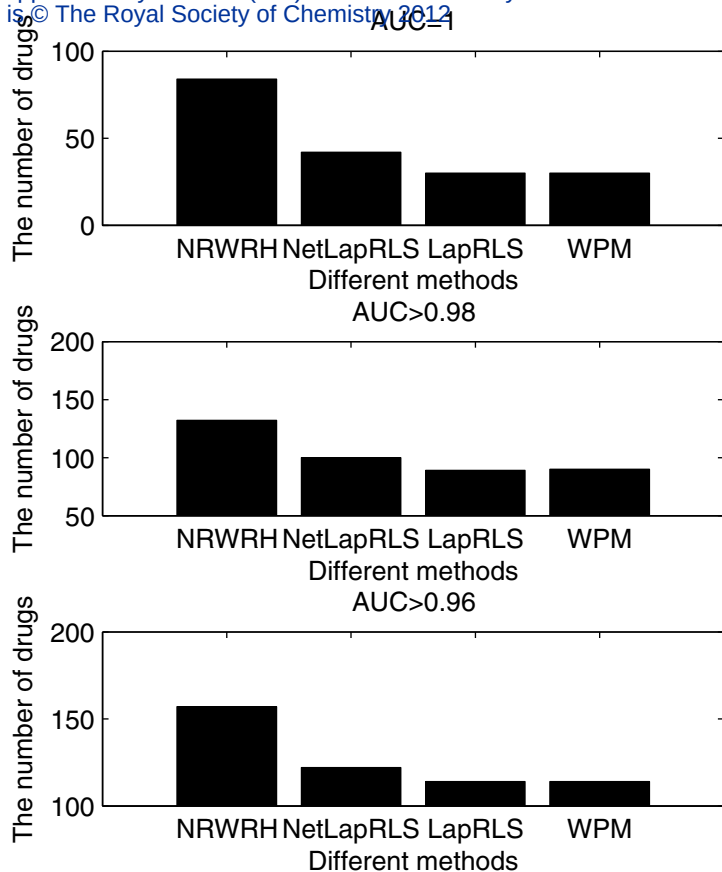


Fig. S7

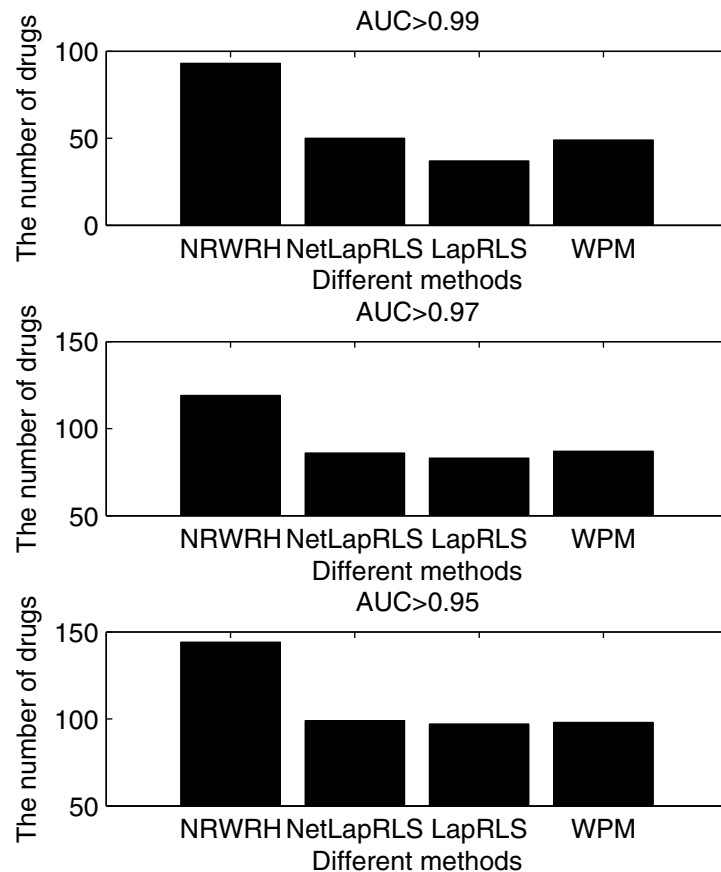
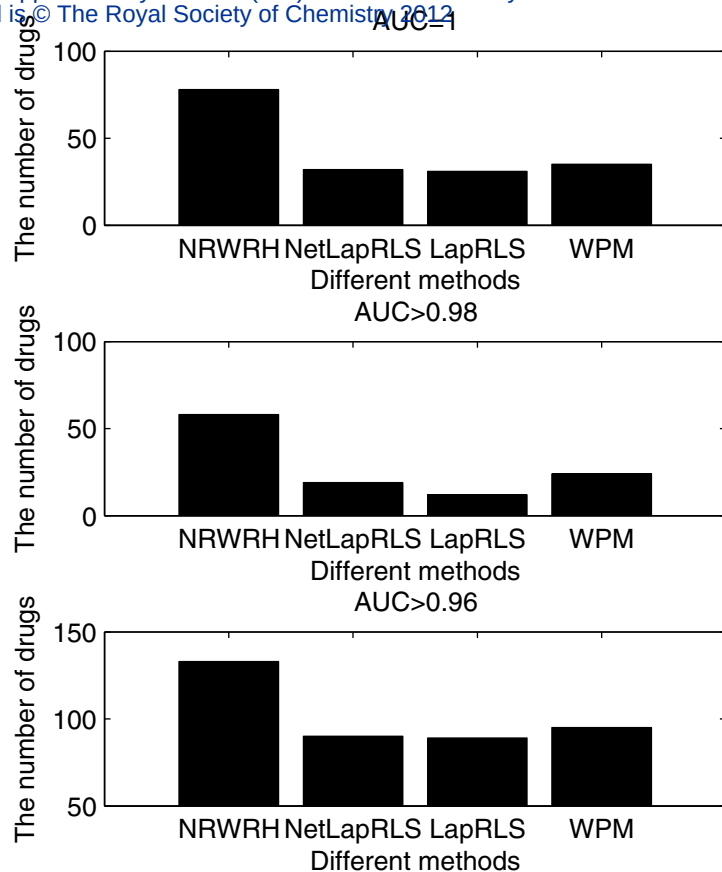


Fig. S8

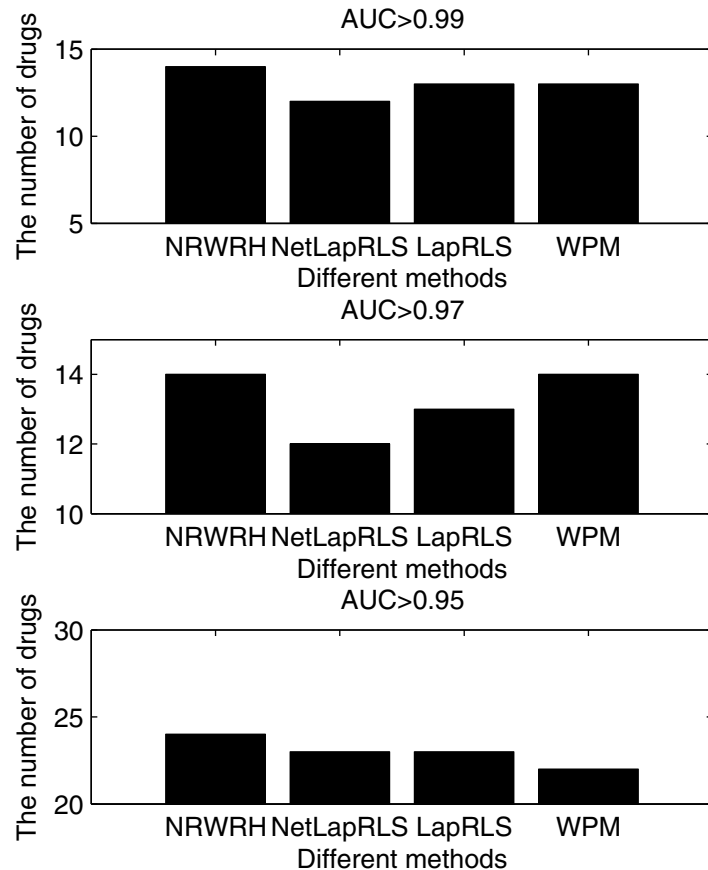
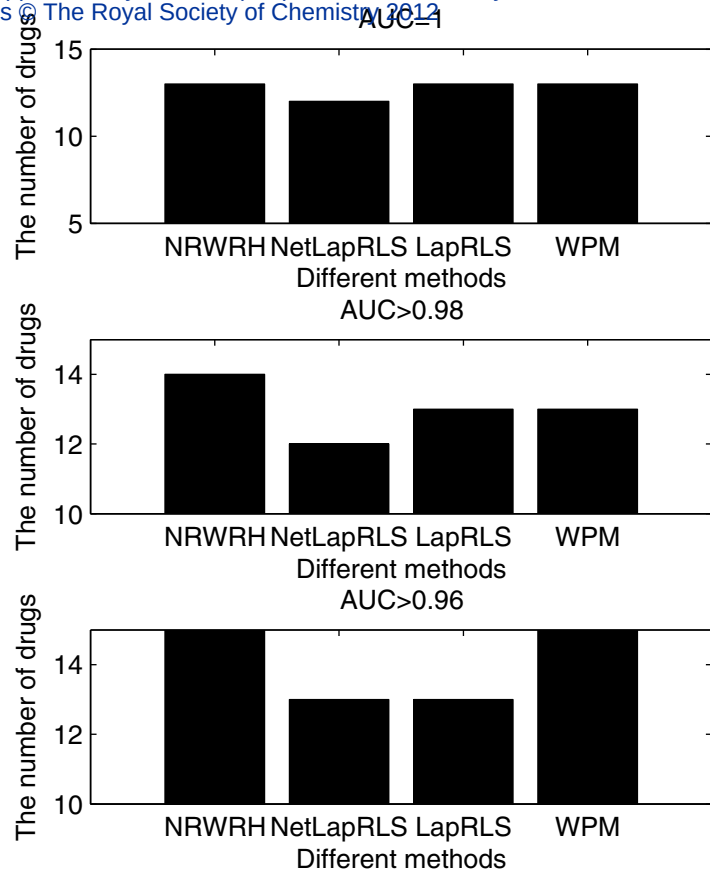


Fig. S9

Suppl. Table S1: Performance evaluation in terms of sensitivity and specificity in the dataset of Ion channel.

Ion channel	Sensitivity (Top 1%)	Specificity (Top 1%)	Sensitivity (Top 1)	Specificity (Top 1)
NRWRH	0.7927	0.9939	0.7331	0.9985
NRWR	0.7561	0.9937	0.7107	0.9983
RWRH	0.5799	0.9927	0.4885	0.9971
RWR	0.5549	0.9925	0.4580	0.9969

Suppl. Table S2: Performance evaluation in terms of sensitivity and specificity in the dataset of GPCR.

GPCR	Sensitivity (Top 1%)	Specificity (Top 1%)	Sensitivity (Top 1)	Specificity (Top 1)
NRWRH	0.6315	0.9958	0.6315	0.9958
NRWR	0.5795	0.9952	0.5795	0.9952
RWRH	0.5197	0.9945	0.5197	0.9945
RWR	0.4441	0.9936	0.4441	0.9936

Suppl. Table S3: Performance evaluation in terms of sensitivity and specificity in the dataset of nuclear receptor

Nuclear receptor	Sensitivity (Top 1%)	Specificity (Top 1%)	Sensitivity (Top 1)	Specificity (Top 1)
NRWRH	0.5000	0.9771	0.5000	0.9771
NRWR	0.4111	0.9730	0.4111	0.9730
RWRH	0.4333	0.9740	0.4333	0.9740
RWR	0.3444	0.9700	0.3444	0.9700

Suppl. Table S4: The effect of parameter η value on the cross validation result of NRWRH.

η	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
Enzyme	0.9520	0.9533	0.9543	0.9550	0.9553	0.9554	0.9553	0.9550	0.9541
GPCR	0.9441	0.9447	0.9457	0.9463	0.9469	0.9474	0.9474	0.9458	0.9394
Ion channel	0.9702	0.9707	0.9716	0.9722	0.9731	0.9737	0.9740	0.9736	0.9694
Nuclear receptor	0.8680	0.8665	0.8670	0.8680	0.8738	0.8743	0.8738	0.8728	0.8689

Suppl. Table S5: The effect of parameter w_d value on the cross validation result of NRWRH.

w_d	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
Enzyme	0.9534	0.9534	0.9534	0.9533	0.9533	0.9533	0.9533	0.9534	0.9533
GPCR	0.9445	0.9446	0.9447	0.9447	0.9447	0.9448	0.9449	0.9449	0.9449
Ion channel	0.9706	0.9706	0.9706	0.9706	0.9707	0.9707	0.9708	0.9708	0.9709
Nuclear receptor	0.8666	0.8680	0.8675	0.8665	0.8665	0.8665	0.8665	0.8670	0.8670

Suppl. Table S6: The effect of parameter w_t value on the cross validation result of NRWRH.

w_t	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
Enzyme	0.9505	0.9510	0.9516	0.9525	0.9533	0.9542	0.9552	0.9563	0.9575
GPCR	0.9438	0.9449	0.9448	0.9449	0.9447	0.9445	0.9438	0.9421	0.9392
Ion channel	0.9623	0.9644	0.9673	0.9695	0.9707	0.9719	0.9728	0.9729	0.9716
Nuclear receptor	0.8713	0.8728	0.8733	0.8670	0.8665	0.8676	0.8616	0.8611	0.8396

Suppl. Table S7: Performance improvement over previous methods in terms of sensitivity and specificity in the dataset of Ion channel.

Ion channel	Sensitivity (Top 1%)	Specificity (Top 1%)	Sensitivity (Top 1)	Specificity (Top 1)
NRWRH	0.7927	0.9939	0.7331	0.9985
NetLapRLS	0.6443	0.9930	0.6016	0.9977
LapRLS	0.5562	0.9925	0.4864	0.9971
WPM	0.5108	0.9923	0.4512	0.9969

Suppl. Table S8: Performance improvement over previous methods in terms of sensitivity and specificity in the dataset of GPCR.

GPCR	Sensitivity (Top 1%)	Specificity (Top 1%)	Sensitivity (Top 1)	Specificity (Top 1)
NRWRH	0.6315	0.9958	0.6315	0.9958
NetLapRLS	0.3654	0.9927	0.3654	0.9927
LapRLS	0.3118	0.9921	0.3118	0.9921
WPM	0.3402	0.9924	0.3402	0.9924

Suppl. Table S9: Performance improvement over previous methods in terms of sensitivity and specificity in the dataset of nuclear receptor.

Nuclear receptor	Sensitivity (Top 1%)	Specificity (Top 1%)	Sensitivity (Top 1)	Specificity (Top 1)
NRWRH	0.5000	0.9771	0.5000	0.9771
NetLapRLS	0.3889	0.9720	0.3889	0.9720
LapRLS	0.3667	0.9710	0.3667	0.9710
WPM	0.4000	0.9725	0.4000	0.9725

Table S10

Drug ID	Target Protein ID	Evidence
D00002	hsa: 219	DrugBank
D00005	hsa: 4128	
D00007	hsa: 32	
D00014	hsa: 124	
D00018	hsa: 1636	
D00021	hsa: 84706	
D00027	hsa: 32	
D00029	hsa: 10295	
D00032	hsa: 5743	
D00035	hsa: 1636	
D00036	hsa: 5743	
D00037	hsa: 57016	
D00038	hsa: 2639	
D00039	hsa: 36	
D00041	hsa: 10295	
D00043	hsa: 1990	
D00045	hsa: 112	
D00049	hsa: 5743	
D00050	hsa: 5743	
D00052	hsa: 1636	
D00054	hsa: 28972	Supertarget
D00055	hsa: 1806	
D00065	hsa: 57176	
D00070	hsa: 5742	
D00086	hsa: 1636	
D00094	hsa: 217	
D00097	hsa: 5743	
D00103	hsa: 1636	
D00107	hsa: 1636	
D00109	hsa: 246	
D00118	hsa: 3906	
D00120	hsa: 2326	
D00125	hsa: 7150	
D00126	hsa: 246	
D00127	hsa: 246	
D00129	hsa: 1593	
D00130	hsa: 246	
D00131	hsa: 8854	DrugBank
D00132	hsa: 3551	
D00136	hsa: 1551	
D00139	hsa: 1543	
D00141	hsa: 3906	
D00142	hsa: 5743	
D00145	hsa: 5743	
D00148	hsa: 10901	
D00151	hsa: 246	

D00153	hsa: 64816	DrugBank
D00155	hsa: 4282	
D00158	hsa: 246	
D00160	hsa: 5445	
D00168	hsa: 5148	
D00169	hsa: 246	
D00183	hsa: 7150	
D00184	hsa: 5478	
D00185	hsa: 64902	
D00186	hsa: 7150	
D00187	hsa: 1593	
D00188	hsa: 1594	
D00196	hsa: 2098	
D00198	hsa: 5742	
D00203	hsa: 30	
D00208	hsa: 4835	
D00216	hsa: 1504	
D00217	hsa: 2878	
D00218	hsa: 476	
D00219	hsa: 3290	
D00222	hsa: 38	
D00224	hsa: 35	
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D00231	hsa: 5145	
D00234	hsa: 1551	
D00251	hsa: 5742	
D00252	hsa: 1551	
D00270	hsa: 5624	
D00274	hsa: 1551	
D00279	hsa: 9388	
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D00285	hsa: 5743	
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D00298	hsa: 495	
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D00325	hsa: 5049	
D00328	hsa: 5049	
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D00332	hsa: 36	
D00333	hsa: 28	
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D00387	hsa: 1551
D00391	hsa: 28
D00394	hsa: 472
D00398	hsa: 28
D00401	hsa: 8288
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D00416	hsa: 1562
D00417	hsa: 30833
D00418	hsa: 10935
D00421	hsa: 5742
D00423	hsa: 3615
D00425	hsa: 246
D00434	hsa: 1551
D00437	hsa: 1559
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D00451	hsa: 4593
D00452	hsa: 246
D00454	hsa: 1543
D00455	hsa: 476
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D00463	hsa: 246
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D00488	hsa: 5743
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D00503	hsa: 1551
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D00516	hsa: 3055
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D00519	hsa: 476

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D00535	hsa: 64850
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D00537	hsa: 759
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D00569	hsa: 1545
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D00596	hsa: 1562
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D00733	hsa: 43
D00749	hsa: 1806
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D00762	hsa: 5053
D00771	hsa: 1548
D00781	hsa: 5742
D00785	hsa: 84171
D00786	hsa: 5742
D00805	hsa: 2098
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D00813	hsa: 246
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D00964	hsa: 1586
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D00969	hsa: 246
D00970	hsa: 246
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D00998	hsa: 590
D01001	hsa: 590
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D01061	hsa: 7155
D01064	hsa: 5049
D01069	hsa: 5742
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D01097	hsa: 84171

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D01119	hsa: 5743
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D01136	hsa: 5327
D01164	hsa: 1573
D01180	hsa: 2582
D01183	hsa: 246
D01196	hsa: 476
D01198	hsa: 5145
D01211	hsa: 5049
D01223	hsa: 3988
D01228	hsa: 590
D01240	hsa: 495
D01256	hsa: 377677
D01264	hsa: 7150
D01275	hsa: 7150
D01276	hsa: 1636
D01325	hsa: 246
D01332	hsa: 3906
D01346	hsa: 1990
D01364	hsa: 239
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D01370	hsa: 28972
D01397	hsa: 246
D01425	hsa: 1586
D01432	hsa: 7155
D01441	hsa: 5743
D01475	hsa: 246
D01513	hsa: 246
D01547	hsa: 246
D01549	hsa: 5742
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D01811	hsa: 246
D01825	hsa: 5049
D01828	hsa: 5743
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D01911	hsa: 5149
D01915	hsa: 1576
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D01977	hsa: 1445
D01981	hsa: 5624
D01984	hsa: 476
D02008	hsa: 5145
D02017	hsa: 5145
D02042	hsa: 5145
D02068	hsa: 590
D02110	hsa: 246
D02115	hsa: 5743
D02166	hsa: 7150
D02168	hsa: 7155
D02173	hsa: 590
D02176	hsa: 1636
D02193	hsa: 2098
D02194	hsa: 1636
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D02258	hsa: 1576
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D02304	hsa: 1636
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D02355	hsa: 246
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D02441	hsa: 760
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D03775	hsa: 5742
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D03784	hsa: 8529
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D03798	hsa: 2639
D03803	hsa: 57016
D03805	hsa: 57016
D03806	hsa: 57016
D03807	hsa: 57016
D03816	hsa: 1576
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D03823	hsa: 590	
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D03828	hsa: 5049	
D03829	hsa: 1636	
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D04966	hsa: 3480	
D04983	hsa: 326625	
D05341	hsa: 1562	
D05353	hsa: 1562	
D05407	hsa: 28	
D05458	hsa: 4128	DrugBank
D06238	hsa: 5743	

Table S11

Drug ID	Target Protein ID	Evidence
D00035	hsa: 6530	
D00110	hsa: 6534	
D00136	hsa: 116443	
D00195	hsa: 1141	
D00219	hsa: 3766	
D00225	hsa: 2570	
D00227	hsa: 10369	
D00228	hsa: 6531	
D00234	hsa: 90134	
D00252	hsa: 6323	KEGG
D00274	hsa: 90134	
D00283	hsa: 170572	
D00293	hsa: 8001	
D00294	hsa: 10060	
D00303	hsa: 6323	KEGG
D00319	hsa: 774	
D00326	hsa: 3762	
D00329	hsa: 2570	
D00331	hsa: 2566	
D00332	hsa: 10060	
D00335	hsa: 3764	
D00336	hsa: 3783	
D00338	hsa: 2555	
D00340	hsa: 56659	
D00345	hsa: 3785	
D00349	hsa: 774	
D00351	hsa: 90134	
D00354	hsa: 6336	
D00358	hsa: 6332	
D00364	hsa: 3737	
D00367	hsa: 6529	
D00373	hsa: 3762	
D00379	hsa: 3764	
D00380	hsa: 3766	
D00392	hsa: 8912	
D00394	hsa: 6531	
D00418	hsa: 3766	
D00437	hsa: 6332	
D00438	hsa: 779	KEGG
D00451	hsa: 170572	
D00456	hsa: 9177	KEGG
D00464	hsa: 2555	
D00474	hsa: 2555	
D00477	hsa: 6336	
D00480	hsa: 3781	
D00495	hsa: 8912	

D00499	hsa: 2570	
D00504	hsa: 6326	
D00512	hsa: 10060	
D00513	hsa: 170572	
D00519	hsa: 56659	
D00521	hsa: 90134	
D00524	hsa: 1134	
D00528	hsa: 10369	
D00530	hsa: 2742	
D00533	hsa: 6328	KEGG
D00536	hsa: 8001	
D00537	hsa: 2899	KEGG
D00538	hsa: 6331	
D00539	hsa: 777	
D00542	hsa: 6262	
D00543	hsa: 2555	
D00544	hsa: 2555	
D00545	hsa: 2570	
D00546	hsa: 2555	
D00547	hsa: 2570	
D00548	hsa: 2570	
D00549	hsa: 8001	
D00550	hsa: 2570	
D00552	hsa: 6331	KEGG
D00553	hsa: 6328	KEGG
D00560	hsa: 6332	
D00563	hsa: 9177	KEGG
D00574	hsa: 1145	
D00593	hsa: 3766	
D00594	hsa: 3766	
D00607	hsa: 6531	
D00611	hsa: 1141	KEGG
D00615	hsa: 774	
D00616	hsa: 776	KEGG
D00617	hsa: 774	
D00618	hsa: 6332	
D00619	hsa: 3742	
D00629	hsa: 6332	
D00631	hsa: 56479	
D00633	hsa: 8001	
D00636	hsa: 3739	
D00638	hsa: 6336	
D00639	hsa: 6336	
D00640	hsa: 6336	
D00642	hsa: 6336	
D00647	hsa: 54207	
D00648	hsa: 3764	

D00649	hsa: 6330	
D00650	hsa: 56659	
D00651	hsa: 56659	
D00654	hsa: 56659	
D00656	hsa: 56659	
D00658	hsa: 56659	
D00677	hsa: 8001	
D00678	hsa: 8001	
D00694	hsa: 2555	KEGG
D00697	hsa: 2555	
D00704	hsa: 2555	
D00708	hsa: 6328	
D00709	hsa: 6326	
D00711	hsa: 2566	
D00726	hsa: 1138	
D00732	hsa: 6332	
D00733	hsa: 6328	KEGG
D00735	hsa: 6332	
D00738	hsa: 6332	
D00739	hsa: 6332	
D00740	hsa: 6332	
D00741	hsa: 6332	
D00759	hsa: 1136	
D00760	hsa: 1136	
D00761	hsa: 1136	
D00765	hsa: 1136	
D00771	hsa: 56659	
D00775	hsa: 2898	
D00779	hsa: 1136	
D00791	hsa: 3781	
D00798	hsa: 3762	
D00799	hsa: 3782	
D00809	hsa: 3780	
D00812	hsa: 3781	
D00816	hsa: 3781	
D00823	hsa: 3762	
D00831	hsa: 3785	
D00960	hsa: 1145	
D00963	hsa: 1145	
D00964	hsa: 1145	
D01071	hsa: 2555	KEGG
D01108	hsa: 776	
D01111	hsa: 3766	
D01118	hsa: 116444	
D01242	hsa: 3781	
D01243	hsa: 6332	
D01253	hsa: 2555	KEGG

D01256	hsa: 2893	
D01275	hsa: 3710	
D01287	hsa: 6332	
D01295	hsa: 6332	
D01350	hsa: 3710	
D01448	hsa: 3782	
D01450	hsa: 6332	
D01453	hsa: 10369	
D01575	hsa: 3781	
D01599	hsa: 3758	DrugBank
D01603	hsa: 6531	
D01712	hsa: 10369	
D01768	hsa: 6331	
D01799	hsa: 3758	
D01828	hsa: 10060	
D01854	hsa: 3758	
D01969	hsa: 778	KEGG
D02041	hsa: 2743	
D02086	hsa: 6332	
D02087	hsa: 6336	
D02088	hsa: 6336	
D02092	hsa: 90134	
D02098	hsa: 8645	
D02101	hsa: 1141	
D02163	hsa: 3781	
D02173	hsa: 1141	
D02204	hsa: 1141	KEGG
D02207	hsa: 2566	
D02234	hsa: 3782	
D02237	hsa: 6531	
D02253	hsa: 2566	KEGG
D02261	hsa: 3742	
D02262	hsa: 3742	
D02272	hsa: 6336	
D02347	hsa: 6263	
D02356	hsa: 2893	
D02360	hsa: 6530	
D02362	hsa: 6530	DrugBank
D02409	hsa: 10369	
D02461	hsa: 2566	
D02485	hsa: 90134	
D02546	hsa: 2895	
D02566	hsa: 6531	
D02630	hsa: 777	
D02914	hsa: 774	
D03037	hsa: 3785	
D03180	hsa: 2555	

D03274	hsa: 3780	
D03365	hsa: 1137	DrugBank
D03450	hsa: 56659	
D03580	hsa: 1141	
D03742	hsa: 6530	
D03826	hsa: 1141	
D03830	hsa: 776	KEGG
D03878	hsa: 2559	
D03991	hsa: 6336	
D04034	hsa: 3780	
D04048	hsa: 6332	
D04370	hsa: 9177	KEGG
D04790	hsa: 9992	
D04985	hsa: 2555	
D04999	hsa: 6529	
D05024	hsa: 774	
D05077	hsa: 6328	KEGG
D05156	hsa: 1141	
D05453	hsa: 1141	
D05458	hsa: 6529	
D05461	hsa: 2566	
D06106	hsa: 2555	KEGG
D06172	hsa: 6328	KEGG

Table S12

Drug ID	Target Protein ID	Evidence
D00049	hsa: 8843	DrugBank
D00059	hsa: 1816	KEGG
D00079	hsa: 5731	DrugBank
D00094	hsa: 2912	
D00095	hsa: 155	KEGG, SuperTarget
D00106	hsa: 9934	
D00110	hsa: 1813	
D00113	hsa: 1815	
D00136	hsa: 152	
D00139	hsa: 10161	
D00180	hsa: 5733	
D00225	hsa: 10161	
D00227	hsa: 136	
D00232	hsa: 1132	KEGG
D00234	hsa: 1128	
D00235	hsa: 155	
D00241	hsa: 2914	
D00255	hsa: 152	
D00270	hsa: 3358	KEGG
D00274	hsa: 1132	
D00281	hsa: 155	
D00283	hsa: 1814	
D00295	hsa: 148	
D00300	hsa: 1128	
D00301	hsa: 4986	
D00306	hsa: 148	
D00318	hsa: 3269	
D00332	hsa: 135	
D00336	hsa: 5737	
D00356	hsa: 5739	
D00364	hsa: 1815	
D00371	hsa: 135	KEGG, DrugBank
D00380	hsa: 10161	
D00394	hsa: 10161	
D00397	hsa: 1133	KEGG
D00400	hsa: 3577	
D00410	hsa: 10161	
D00411	hsa: 5729	
D00415	hsa: 3355	SuperTarget, DrugBank
D00419	hsa: 5731	KEGG
D00422	hsa: 148	
D00426	hsa: 151	
D00432	hsa: 148	
D00437	hsa: 152	
D00440	hsa: 148	
D00442	hsa: 6755	KEGG, DrugBank

D00443	hsa: 3577	
D00451	hsa: 3363	
D00454	hsa: 3350	
D00465	hsa: 1132	
D00480	hsa: 1815	
D00483	hsa: 148	
D00493	hsa: 1815	
D00494	hsa: 1815	
D00498	hsa: 4986	KEGG, DrugBank
D00499	hsa: 338442	
D00503	hsa: 1816	
D00509	hsa: 155	
D00513	hsa: 3363	
D00514	hsa: 151	KEGG
D00520	hsa: 1815	
D00521	hsa: 1815	
D00522	hsa: 3577	
D00523	hsa: 3577	
D00524	hsa: 1132	KEGG
D00525	hsa: 1129	KEGG
D00528	hsa: 57105	
D00540	hsa: 1132	KEGG
D00542	hsa: 10161	
D00559	hsa: 1813	KEGG
D00560	hsa: 3356	
D00563	hsa: 152	KEGG
D00574	hsa: 10161	
D00598	hsa: 155	
D00601	hsa: 155	
D00604	hsa: 147	
D00606	hsa: 146	
D00607	hsa: 155	
D00609	hsa: 155	
D00613	hsa: 146	
D00627	hsa: 3577	
D00632	hsa: 155	
D00635	hsa: 155	
D00645	hsa: 155	
D00646	hsa: 1132	
D00665	hsa: 1815	
D00666	hsa: 1815	
D00673	hsa: 148	
D00674	hsa: 3354	
D00675	hsa: 3355	
D00676	hsa: 3354	
D00682	hsa: 5739	
D00683	hsa: 153	

D00684	hsa: 153	
D00687	hsa: 153	
D00688	hsa: 153	
D00715	hsa: 1129	KEGG
D00726	hsa: 3363	
D00760	hsa: 1128	
D00765	hsa: 1128	
D00769	hsa: 9934	
D00775	hsa: 222545	
D00779	hsa: 1132	KEGG
D00780	hsa: 1814	
D00790	hsa: 1816	
D00837	hsa: 4985	DrugBank
D00838	hsa: 4985	
D00845	hsa: 4986	
D00954	hsa: 147	
D00965	hsa: 147	
D00987	hsa: 1814	
D00996	hsa: 3362	
D01020	hsa: 151	
D01022	hsa: 155	
D01024	hsa: 151	
D01051	hsa: 3354	
D01071	hsa: 10161	
D01103	hsa: 1129	KEGG
D01118	hsa: 1129	KEGG
D01126	hsa: 2913	
D01164	hsa: 3354	
D01227	hsa: 4988	
D01236	hsa: 6755	
D01242	hsa: 1815	
D01269	hsa: 1129	
D01295	hsa: 3356	
D01297	hsa: 1129	
D01324	hsa: 1815	
D01332	hsa: 1815	
D01346	hsa: 2916	
D01352	hsa: 5731	
D01358	hsa: 151	KEGG
D01386	hsa: 153	KEGG
D01390	hsa: 148	
D01441	hsa: 1909	
D01454	hsa: 148	
D01462	hsa: 1814	
D01603	hsa: 155	
D01652	hsa: 10161	
D01692	hsa: 147	DrugBank

D01699	hsa: 1133	
D01712	hsa: 140	
D01713	hsa: 152	
D01717	hsa: 59340	
D01745	hsa: 1814	
D01782	hsa: 1815	
D01828	hsa: 57105	
D01871	hsa: 1815	
D01891	hsa: 5732	KEGG
D01925	hsa: 4988	
D01964	hsa: 5739	
D01965	hsa: 151	
D01973	hsa: 3361	
D01994	hsa: 3361	
D02007	hsa: 4988	
D02066	hsa: 148	
D02070	hsa: 1815	
D02076	hsa: 146	
D02082	hsa: 3577	
D02147	hsa: 153	
D02149	hsa: 3362	
D02150	hsa: 148	
D02234	hsa: 151	
D02237	hsa: 155	
D02250	hsa: 6751	KEGG
D02278	hsa: 2913	
D02279	hsa: 2913	
D02327	hsa: 1129	
D02338	hsa: 148	
D02340	hsa: 1812	DrugBank
D02342	hsa: 155	
D02349	hsa: 151	KEGG
D02354	hsa: 1816	
D02356	hsa: 152	
D02357	hsa: 3358	KEGG, DrugBank
D02358	hsa: 154	
D02359	hsa: 153	
D02361	hsa: 3362	
D02374	hsa: 148	
D02566	hsa: 147	
D02578	hsa: 3356	
D02588	hsa: 4988	
D02614	hsa: 154	
D02671	hsa: 3358	
D02721	hsa: 5732	
D02725	hsa: 5732	KEGG
D02826	hsa: 3355	

D02884	hsa: 140	
D02910	hsa: 154	
D03165	hsa: 1814	
D03187	hsa: 5739	
D03210	hsa: 3577	
D03274	hsa: 146	
D03365	hsa: 338442	
D03415	hsa: 148	KEGG
D03442	hsa: 153	
D03490	hsa: 155	KEGG
D03503	hsa: 148	
D03621	hsa: 1132	
D03642	hsa: 5737	
D03654	hsa: 1133	
D03858	hsa: 1132	
D03879	hsa: 148	
D03880	hsa: 155	
D03881	hsa: 155	
D03966	hsa: 2914	
D04006	hsa: 135	
D04034	hsa: 146	
D04040	hsa: 3577	
D04375	hsa: 151	KEGG
D04625	hsa: 154	KEGG
D04716	hsa: 4986	
D04979	hsa: 1815	
D05113	hsa: 4986	DrugBank
D05129	hsa: 1241	
D05246	hsa: 3577	
D05312	hsa: 6751	
D05341	hsa: 6755	
D05740	hsa: 3355	
D05792	hsa: 153	
D05938	hsa: 4986	
D06056	hsa: 3361	
D06396	hsa: 3361	

Table S13

Drug ID	Target Protein ID	Evidence
D00040	hsa: 6096	KEGG
D00066	hsa: 2100	
D00067	hsa: 2100	
D00075	hsa: 4306	
D00088	hsa: 4306	
D00094	hsa: 6095	
D00105	hsa: 2104	
D00129	hsa: 8856	
D00143	hsa: 7421	
D00163	hsa: 7421	
D00182	hsa: 2099	
D00187	hsa: 8856	
D00188	hsa: 8856	
D00211	hsa: 7421	
D00246	hsa: 4306	
D00279	hsa: 5468	
D00299	hsa: 8856	
D00312	hsa: 2100	KEGG
D00316	hsa: 6096	
D00327	hsa: 2100	Supertarget
D00348	hsa: 5915	
D00443	hsa: 2908	Supertarget
D00462	hsa: 4306	
D00506	hsa: 8856	Supertarget
D00554	hsa: 2100	
D00565	hsa: 5468	
D00577	hsa: 5241	
D00585	hsa: 2099	
D00586	hsa: 4306	
D00596	hsa: 5465	
D00627	hsa: 5465	
D00690	hsa: 2099	
D00730	hsa: 7421	KEGG
D00898	hsa: 2100	
D00930	hsa: 8856	
D00950	hsa: 2100	KEGG
D00951	hsa: 2099	
D00954	hsa: 2100	
D00956	hsa: 4306	
D00961	hsa: 4306	
D00962	hsa: 2100	
D00965	hsa: 4306	
D01115	hsa: 2908	
D01132	hsa: 6097	
D01161	hsa: 2104	
D01217	hsa: 2099	

D01294	hsa: 2100
D01387	hsa: 4306
D01441	hsa: 6096
D01689	hsa: 4306
D02217	hsa: 2104
D02367	hsa: 2100
D04066	hsa: 2104
D05341	hsa: 6256