PDB code_Chain	Nuclear Receptor	Phylogenetic Class	Signaling Group	Resolution (Ang.)	SiteScore	size	Dscore	volume	exposure	enclosure
1NAV_A	TR_alpha	NR1A1	M/E	2.50	1.185	165	1.209	241.472	0.324	0.930
1BSX_A	TR_beta	NR1A2	M/E	3.70	1.214	196	1.239	232.211	0.213	0.965
1N46_A	TR_beta	NR1A2	M/E	2.20	1.197	150	1.204	165.669	0.206	0.979
1NAX_A	TR_beta	NR1A2	M/E	2.70	1.208	153	1.225	197.568	0.261	0.974
1NQ0_A	TR_beta	NR1A2	M/E	2.40	1.214	183	1.247	223.636	0.250	0.951
1NQ1_A	TR_beta	NR1A2	M/E	2.90	1.205	162	1.229	195.510	0.253	0.956
1NQ2_A	TR_beta	NR1A2	M/E	2.40	1.219	168	1.245	219.520	0.253	0.970
1NUO_A	TR_beta	NR1A2	M/E	3.10	1.160	173	1.171	279.202	0.373	0.922
1Q4X_A	TR_beta	NR1A2	M/E	2.80	1.214	225	1.258	343.000	0.288	0.930
1R6G_A	TR_beta	NR1A2	M/E	3.00	1.238	196	1.279	246.960	0.180	0.967
1XZX_X	TR_beta	NR1A2	M/E	2.50	1.248	170	1.292	185.906	0.217	0.975
1Y0X_X	TR_beta	NR1A2	M/E	3.10	1.245	169	1.288	201.684	0.207	0.973
2J4A_A	TR_beta	NR1A2	M/E	2.20	1.257	155	1.308	175.959	0.217	0.973
2PIN_A	TR_beta	NR1A2	M/E	2.30	1.236	169	1.275	219.863	0.249	0.969
3D57_A	TR_beta	NR1A2	M/E	2.20	1.249	166	1.296	208.887	0.228	0.971
3GWS_X	TR_beta	NR1A2	M/E	2.20	1.230	170	1.263	203.399	0.238	0.973
3HZF_A	TR_beta	NR1A2	M/E	2.50	1.200	143	1.211	189.336	0.278	0.974
3IMY_A	TR_beta	NR1A2	M/E	2.55	1.255	163	1.306	211.631	0.256	0.972
1DKF_B	RAR_alpha	NR1B1	M/E	2.50	1.178	242	1.230	468.195	0.355	0.868
1XAP_A	RAR_beta	NR1B2	M/E	2.10	1.309	184	1.401	237.699	0.233	0.963
1EXA_A	RAR_gamma	NR1B3	M/E	1.59	1.288	173	1.384	232.211	0.311	0.931
1EXX_A	RAR_gamma	NR1B3	M/E	1.67	1.322	163	1.422	205.114	0.285	0.968
1FCX_A	RAR_gamma	NR1B3	M/E	1.47	1.278	198	1.376	253.820	0.298	0.915
1FCY_A	RAR_gamma	NR1B3	M/E	1.30	1.265	188	1.353	255.535	0.314	0.916
1FCZ_A	RAR_gamma	NR1B3	M/E	1.38	1.312	164	1.409	199.969	0.251	0.959
1FD0_A	RAR_gamma	NR1B3	M/E	1.38	1.279	185	1.376	253.134	0.305	0.918
2LBD_A	RAR_gamma	NR1B3	M/E	2.06	1.250	171	1.336	245.245	0.342	0.898
3LBD_A	RAR_gamma	NR1B3	M/E	2.40	1.315	150	1.410	196.196	0.235	0.966
4LBD_A	RAR_gamma	NR1B3	M/E	2.50	1.282	173	1.370	254.849	0.319	0.935
1I7G_A	PPAR_alpha	NR1C1	Metabolic	2.20	1.153	274	1.189	474.026	0.430	0.867
1K7L_A	PPAR_alpha	NR1C1	Metabolic	2.50	1.155	410	1.200	689.087	0.362	0.853
1KKQ_A	PPAR_alpha	NR1C1	Metabolic	3.00	1.150	515	1.203	1534.582	0.441	0.831
2NPA_A	PPAR_alpha	NR1C1	Metabolic	2.30	1.155	405	1.177	675.710	0.364	0.893
2P54_A	PPAR_alpha	NR1C1	Metabolic	1.79	1.186	304	1.235	526.162	0.414	0.885
2REW_A	PPAR_alpha	NR1C1	Metabolic	2.35	1.134	438	1.182	680.512	0.415	0.820
2ZNN_A	PPAR_alpha	NR1C1	Metabolic	2.01	1.188	367	1.244	621.859	0.357	0.874
3ET1_A	PPAR_alpha	NR1C1	Metabolic	2.50	1.181	358	1.220	723.044	0.358	0.898
3G8I_A	PPAR_alpha	NR1C1	Metabolic	2.20	1.164	369	1.187	541.597	0.285	0.903
1GWX_A	PPAR_beta/delta	NR1C2	Metabolic	2.50	1.148	358	1.189	628.719	0.346	0.850
1Y0S_A	PPAR_beta/delta	NR1C2	Metabolic	2.65	1.151	341	1.181	563.892	0.317	0.875

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	Nuclear Receptor	Phylogenetic Class	Signaling Group	Resolution (Ang.)	SiteScore	size	Dscore	volume	exposure	enclosure
2AWH_A	PPAR_beta/delta	NR1C2	Metabolic	2.00	1.251	221	1.328	375.242	0.354	0.919
2B50_A	PPAR_beta/delta	NR1C2	Metabolic	2.00	1.193	244	1.240	440.069	0.416	0.898
2BAW_A	PPAR_beta/delta	NR1C2	Metabolic	2.30	1.237	253	1.303	441.441	0.374	0.917
2J14_A	PPAR_beta/delta	NR1C2	Metabolic	2.80	1.212	223	1.282	379.015	0.389	0.879
2ZNP_A	PPAR_beta/delta	NR1C2	Metabolic	3.00	1.169	292	1.214	556.689	0.417	0.871
2ZNQ_A	PPAR_beta/delta	NR1C2	Metabolic	2.65	1.198	251	1.252	512.785	0.386	0.890
3D5F_A	PPAR_beta/delta	NR1C2	Metabolic	2.20	1.245	236	1.314	419.489	0.387	0.924
3DY6_A	PPAR_beta/delta	NR1C2	Metabolic	2.90	1.159	273	1.188	484.316	0.424	0.888
3ET2_A	PPAR_beta/delta	NR1C2	Metabolic	2.24	1.160	277	1.178	512.785	0.407	0.909
3GZ9_A	PPAR_beta/delta	NR1C2	Metabolic	2.00	1.205	258	1.252	509.012	0.443	0.911
1FM6_D	PPAR_gamma	NR1C3	Metabolic	2.10	1.141	267	1.149	593.390	0.431	0.901
1FM9_D	PPAR_gamma	NR1C3	Metabolic	2.10	1.165	404	1.197	755.972	0.370	0.889
1I7I_A	PPAR_gamma	NR1C3	Metabolic	2.35	1.172	257	1.215	539.539	0.411	0.877
1KNU_A	PPAR_gamma	NR1C3	Metabolic	2.50	1.136	417	1.159	620.830	0.326	0.868
1NYX_A	PPAR_gamma	NR1C3	Metabolic	2.65	1.127	328	1.145	513.128	0.329	0.866
1RDT_D	PPAR_gamma	NR1C3	Metabolic	2.40	1.151	308	1.193	490.833	0.388	0.851
1WM0_X	PPAR_gamma	NR1C3	Metabolic	2.90	1.181	315	1.199	476.770	0.346	0.935
1ZEO_A	PPAR_gamma	NR1C3	Metabolic	2.50	1.172	332	1.192	539.882	0.337	0.921
1ZGY_A	PPAR_gamma	NR1C3	Metabolic	1.80	1.150	295	1.178	757.344	0.491	0.875
2ATH_A	PPAR_gamma	NR1C3	Metabolic	2.28	1.159	330	1.182	720.643	0.429	0.898
2F4B_A	PPAR_gamma	NR1C3	Metabolic	2.07	1.146	399	1.175	932.274	0.412	0.870
2FVJ_A	PPAR_gamma	NR1C3	Metabolic	1.99	1.131	342	1.166	682.570	0.393	0.838
2G0G_A	PPAR_gamma	NR1C3	Metabolic	2.54	1.165	290	1.184	617.400	0.429	0.916
2G0H_A	PPAR_gamma	NR1C3	Metabolic	2.30	1.134	331	1.137	787.185	0.482	0.898
2GTK_A	PPAR_gamma	NR1C3	Metabolic	2.10	1.173	199	1.231	377.300	0.370	0.851
2HWQ_A	PPAR_gamma	NR1C3	Metabolic	1.97	1.141	300	1.184	700.406	0.444	0.839
2HWR_A	PPAR_gamma	NR1C3	Metabolic	2.34	1.144	305	1.188	694.918	0.440	0.842
2I4J_A	PPAR_gamma	NR1C3	Metabolic	2.10	1.137	404	1.154	680.512	0.355	0.880
2I4P_A	PPAR_gamma	NR1C3	Metabolic	2.10	1.133	422	1.150	762.146	0.365	0.874
2I4Z_A	PPAR_gamma	NR1C3	Metabolic	2.25	1.149	394	1.173	676.053	0.342	0.884
2OM9_A	PPAR_gamma	NR1C3	Metabolic	2.80	1.120	401	1.115	815.997	0.386	0.877
2P4Y_A	PPAR_gamma	NR1C3	Metabolic	2.25	1.118	278	1.137	492.548	0.335	0.851
2POB_A	PPAR_gamma	NR1C3	Metabolic	2.30	1.162	344	1.193	623.231	0.373	0.887
2PRG_A	PPAR_gamma	NR1C3	Metabolic	2.3	1.144	347	1.185	841.379	0.476	0.845
2Q59_A	PPAR_gamma	NR1C3	Metabolic	2.20	1.182	304	1.235	506.611	0.304	0.872
2Q6R_A	PPAR_gamma	NR1C3	Metabolic	2.4	1.115	322	1.143	619.800	0.389	0.830
2Q6S_B	PPAR_gamma	NR1C3	Metabolic	2.4	1.144	279	1.121	479.510	0.391	0.913
2VST_A	PPAR_gamma	NR1C3	Metabolic	2.35	1.132	325	1.158	742.938	0.403	0.856
2VV0_A	PPAR_gamma	NR1C3	Metabolic	2.55	1.168	292	1.206	572.124	0.405	0.883
2VV1_A	PPAR_gamma	NR1C3	Metabolic	2.20	1.138	283	1.161	591.675	0.456	0.872

PDB code_Chain	Nuclear Receptor	Phylogenetic Class	Signaling Group	Resolution (Ang.)	SiteScore	size	Dscore	volume	exposure	enclosure
2VV2_A	PPAR_gamma	NR1C3	Metabolic	2.75	1.155	282	1.190	574.525	0.434	0.870
2VV3_A	PPAR_gamma	NR1C3	Metabolic	2.85	1.094	278	1.090	597.506	0.401	0.838
2VV4_A	PPAR_gamma	NR1C3	Metabolic	2.35	1.126	287	1.141	561.148	0.425	0.870
2ZK1_A	PPAR_gamma	NR1C3	Metabolic	2.61	1.167	373	1.189	584.815	0.327	0.909
2ZK2_A	PPAR_gamma	NR1C3	Metabolic	2.26	1.163	384	1.187	717.213	0.334	0.900
2ZK3_A	PPAR_gamma	NR1C3	Metabolic	2.58	1.176	300	1.190	486.374	0.326	0.937
2ZK4_A	PPAR_gamma	NR1C3	Metabolic	2.57	1.133	431	1.132	710.696	0.377	0.897
2ZK5_A	PPAR_gamma	NR1C3	Metabolic	2.45	1.200	200	1.224	330.995	0.361	0.951
2ZNO_A	PPAR_gamma	NR1C3	Metabolic	2.40	1.136	352	1.185	662.676	0.453	0.821
2ZVT_A	PPAR_gamma	NR1C3	Metabolic	1.90	1.147	305	1.157	527.191	0.397	0.905
3B3K_A	PPAR_gamma	NR1C3	Metabolic	2.60	1.191	328	1.233	591.675	0.459	0.904
3BC5_A	PPAR_gamma	NR1C3	Metabolic	2.27	1.116	266	1.129	425.320	0.340	0.862
3CDP_A	PPAR_gamma	NR1C3	Metabolic	2.80	1.194	271	1.245	572.810	0.490	0.893
3CDS_A	PPAR_gamma	NR1C3	Metabolic	2.65	1.169	323	1.207	693.203	0.476	0.882
3CS8_A	PPAR_gamma	NR1C3	Metabolic	2.30	1.148	337	1.169	655.816	0.414	0.887
3CWD_A	PPAR_gamma	NR1C3	Metabolic	2.40	1.139	297	1.151	557.375	0.390	0.891
3DZU_D	PPAR_gamma	NR1C3	Metabolic	3.20	1.145	363	1.177	671.594	0.422	0.862
3DZY_D	PPAR_gamma	NR1C3	Metabolic	3.10	1.143	284	1.177	546.399	0.438	0.856
3E00_D	PPAR_gamma	NR1C3	Metabolic	3.10	1.161	263	1.186	751.513	0.461	0.897
3ET3_A	PPAR_gamma	NR1C3	Metabolic	1.95	1.157	264	1.189	509.355	0.415	0.879
3FEI_A	PPAR_gamma	NR1C3	Metabolic	2.40	1.154	314	1.191	479.171	0.357	0.866
3FEJ_A	PPAR_gamma	NR1C3	Metabolic	2.01	1.094	270	1.111	568.694	0.518	0.825
3FUR_A	PPAR_gamma	NR1C3	Metabolic	2.30	1.124	243	1.144	456.190	0.448	0.857
3G9E_A	PPAR_gamma	NR1C3	Metabolic	2.30	1.103	324	1.131	575.554	0.459	0.816
3H0A_D	PPAR_gamma	NR1C3	Metabolic	2.10	1.107	420	1.096	732.991	0.349	0.858
3HO0_A	PPAR_gamma	NR1C3	Metabolic	2.60	1.222	280	1.287	552.230	0.452	0.903
3HOD_A	PPAR_gamma	NR1C3	Metabolic	2.10	1.208	269	1.257	541.597	0.458	0.913
3IA6_B	PPAR_gamma	NR1C3	Metabolic	2.31	1.146	334	1.181	778.953	0.426	0.857
4PRG_A	PPAR_gamma	NR1C3	Metabolic	2.90	1.079	457	1.089	779.639	0.344	0.816
1N83_A	ROR_alpha	NR1F1	Metabolic	1.63	1.198	243	1.251	502.152	0.349	0.895
1S0X_A	ROR_alpha	NR1F1	Metabolic	2.20	1.177	249	1.207	434.924	0.301	0.910
1P8D_A	LXR_beta	NR1H2	Metabolic	2.80	1.232	261	1.287	427.721	0.320	0.932
1PQ6_A	LXR_beta	NR1H2	Metabolic	2.40	1.161	227	1.196	416.402	0.370	0.878
1PQ9_A	LXR_beta	NR1H2	Metabolic	2.10	1.298	115	1.374	129.997	0.230	0.982
1PQC_A	LXR_beta	NR1H2	Metabolic	2.80	1.256	161	1.313	261.023	0.310	0.961
1UPV_A	LXR_beta	NR1H2	Metabolic	2.10	1.237	172	1.300	346.087	0.430	0.923
1UPW_A	LXR_beta	NR1H2	Metabolic	2.40	1.238	171	1.303	346.773	0.370	0.925
3KFC_A	LXR_beta	NR1H2	Metabolic	2.40	1.220	248	1.251	331.681	0.255	0.962
1UHL_B	LXR_alpha	NR1H3	Metabolic	2.90	1.215	219	1.273	566.979	0.350	0.905
2ACL_B	LXR_alpha	NR1H3	Metabolic	2.80	1.253	235	1.315	340.942	0.300	0.948

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PDB code_Chain	Nuclear Receptor	Phylogenetic Class	Signaling Group	Resolution (Ang.)	SiteScore	size	Dscore	volume	exposure	enclosure
3FAL_B	LXR_alpha	NR1H3	Metabolic	2.36	1.173	224	1.181	376.614	0.370	0.946
3FC6_B	LXR_alpha	NR1H3	Metabolic	2.06	1.199	268	1.252	445.900	0.380	0.892
1OSH_A	FXR	NR1H4	Metabolic	1.80	1.212	194	1.284	364.952	0.368	0.877
3BEJ_A	FXR	NR1H4	Metabolic	1.90	1.150	219	1.168	401.653	0.385	0.896
3DCT_A	FXR	NR1H4	Metabolic	2.50	1.218	295	1.276	536.109	0.363	0.909
3FLI_A	FXR	NR1H4	Metabolic	2.00	1.256	222	1.320	327.220	0.240	0.946
3GD2_A	FXR	NR1H4	Metabolic	3.20	1.207	261	1.258	441.100	0.319	0.910
3L1B_A	FXR	NR1H4	Metabolic	1.90	1.171	181	1.264	396.850	0.436	0.782
3OKH_A	FXR	NR1H4	Metabolic	2.50	1.204	236	1.276	468.540	0.306	0.866
3OKI_A	FXR	NR1H4	Metabolic	2.00	1.165	242	1.222	414.340	0.414	0.841
3OLF_A	FXR	NR1H4	Metabolic	1.90	1.198	240	1.238	406.110	0.330	0.919
3OMK_A	FXR	NR1H4	Metabolic	1.90	1.168	249	1.210	407.140	0.393	0.873
3OMM_A	FXR	NR1H4	Metabolic	2.10	1.251	193	1.315	352.260	0.263	0.943
3OOF_A	FXR	NR1H4	Metabolic	2.29	1.197	230	1.229	390.330	0.341	0.932
3OOK_A	FXR	NR1H4	Metabolic	2.29	1.164	220	1.207	382.440	0.415	0.867
1DB1_A	VDR	NR1I1	M/E	1.80	1.241	202	1.295	360.150	0.299	0.946
1IE8_A	VDR	NR1I1	M/E	1.52	1.234	199	1.282	332.367	0.279	0.950
1IE9_A	VDR	NR1I1	M/E	1.40	1.236	200	1.285	327.908	0.267	0.950
1S0Z_A	VDR	NR1I1	M/E	2.50	1.231	210	1.279	368.039	0.281	0.944
1S19_A	VDR	NR1I1	M/E	2.10	1.222	203	1.264	359.121	0.319	0.945
1TXI_A	VDR	NR1I1	M/E	1.90	1.236	213	1.288	359.464	0.263	0.943
2HAM_A	VDR	NR1I1	M/E	1.90	1.237	211	1.287	342.314	0.262	0.947
2HAR_A	VDR	NR1I1	M/E	1.90	1.234	210	1.283	342.657	0.281	0.947
2HAS_A	VDR	NR1I1	M/E	1.96	1.223	234	1.266	350.203	0.207	0.946
2HB7_A	VDR	NR1I1	M/E	1.80	1.231	208	1.278	347.459	0.304	0.947
2HB8_A	VDR	NR1I1	M/E	2.00	1.233	211	1.281	347.802	0.287	0.948
3CS4_A	VDR	NR1I1	M/E	2.00	1.237	204	1.288	349.860	0.284	0.948
3CS6_A	VDR	NR1I1	M/E	1.80	1.237	203	1.287	343.343	0.280	0.948
1ILH_A	PXR	NR1I2	Metabolic	2.76	1.232	184	1.307	634.207	0.496	0.896
1M13_A	PXR	NR1I2	Metabolic	2.15	1.205	240	1.261	655.473	0.412	0.896
1NRL_A	PXR	NR1I2	Metabolic	2.00	1.233	221	1.293	533.365	0.379	0.926
1SKX_A	PXR	NR1I2	Metabolic	2.80	1.148	135	1.226	548.800	0.611	0.782
2O9I_A	PXR	NR1I2	Metabolic	2.80	1.225	233	1.277	490.147	0.372	0.931
2QNV_A	PXR	NR1I2	Metabolic	2.80	1.165	163	1.224	559.090	0.438	0.840
3HLV_B	PXR	NR1I2	Metabolic	2.10	1.227	245	1.281	529.249	0.359	0.927
1XV9_B	CAR	NR1I3	Metabolic	2.70	1.292	176	1.376	280.231	0.276	0.958
1XVP_B	CAR	NR1I3	Metabolic	2.60	1.316	171	1.414	282.975	0.299	0.963
1PZL_A	HNF4_alpha	NR2A1	Metabolic	2.10	1.312	150	1.404	185.906	0.194	0.970
3FS1_A	HNF4_alpha	NR2A1	Metabolic	2.20	1.338	149	1.443	176.988	0.195	0.977
1LV2_A	HNF4_gamma	NR2A2	Metabolic	2.70	1.272	185	1.347	245.588	0.312	0.949

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	Nuclear Receptor	Phylogenetic Class	Signaling Group	Resolution (Ang.)	SiteScore	size	Dscore	volume	exposure	enclosure
1FBY_A	RXR_alpha	NR2B1	Metabolic	2.25	1.289	165	1.367	234.612	0.276	0.965
1FM6_A	RXR_alpha	NR2B1	Metabolic	2.10	1.254	192	1.314	252.791	0.336	0.953
1FM9_A	RXR_alpha	NR2B1	Metabolic	2.10	1.285	179	1.360	229.810	0.263	0.964
1G5Y_A	RXR_alpha	NR2B1	Metabolic	2.00	1.123	198	1.164	774.494	0.564	0.818
1K74_A	RXR_alpha	NR2B1	Metabolic	2.30	1.281	178	1.356	249.361	0.313	0.962
1MV9_A	RXR_alpha	NR2B1	Metabolic	1.90	1.283	203	1.358	252.791	0.270	0.962
1MVC_A	RXR_alpha	NR2B1	Metabolic	1.90	1.192	201	1.208	294.637	0.356	0.955
1MZN_A	RXR_alpha	NR2B1	Metabolic	1.90	1.215	191	1.243	258.279	0.341	0.964
1RDT_A	RXR_alpha	NR2B1	Metabolic	2.40	1.251	172	1.308	262.052	0.301	0.955
1XLS_A	RXR_alpha	NR2B1	Metabolic	2.96	1.240	190	1.284	270.284	0.329	0.966
1XV9_A	RXR_alpha	NR2B1	Metabolic	2.70	1.305	195	1.397	272.685	0.247	0.959
1XVP_A	RXR_alpha	NR2B1	Metabolic	2.60	1.320	205	1.421	250.047	0.273	0.962
2ACL_A	RXR_alpha	NR2B1	Metabolic	2.80	1.212	199	1.248	330.652	0.343	0.943
2P1T_A	RXR_alpha	NR2B1	Metabolic	1.80	1.202	191	1.230	310.758	0.341	0.946
2P1U_A	RXR_alpha	NR2B1	Metabolic	2.20	1.285	169	1.361	234.955	0.275	0.962
2P1V_A	RXR_alpha	NR2B1	Metabolic	2.20	1.202	222	1.232	311.101	0.347	0.941
2ZXZ_A	RXR_alpha	NR2B1	Metabolic	3.00	1.292	148	1.370	216.433	0.305	0.969
2ZY0_A	RXR_alpha	NR2B1	Metabolic	2.90	1.281	151	1.352	221.921	0.263	0.966
3DZU_A	RXR_alpha	NR2B1	Metabolic	3.20	1.309	197	1.406	272.342	0.284	0.956
3DZY_A	RXR_alpha	NR2B1	Metabolic	3.10	1.253	196	1.327	347.116	0.310	0.926
3E00_A	RXR_alpha	NR2B1	Metabolic	3.10	1.293	158	1.375	223.979	0.298	0.960
3FAL_A	RXR_alpha	NR2B1	Metabolic	2.36	1.136	126	1.173	297.724	0.440	0.844
3FC6_A	RXR_alpha	NR2B1	Metabolic	2.06	1.145	120	1.188	368.725	0.508	0.842
3H0A_A	RXR_alpha	NR2B1	Metabolic	2.10	1.266	183	1.332	281.603	0.304	0.956
1H9U_A	RXR_beta	NR2B2	Metabolic	2.70	1.279	173	1.370	240.786	0.276	0.926
1UHL_A	RXR_beta	NR2B2	Metabolic	2.90	1.210	184	1.240	295.323	0.405	0.953
1A52_A	ER_alpha	NR3A1	Endocrine	2.80	1.239	149	1.303	249.361	0.280	0.926
1ERE_A	ER_alpha	NR3A1	Endocrine	3.10	1.306	134	1.389	191.051	0.202	0.977
1ERR_A	ER_alpha	NR3A1	Endocrine	2.60	1.184	137	1.266	303.212	0.450	0.821
1G50_A	ER_alpha	NR3A1	Endocrine	2.90	1.338	137	1.442	191.737	0.203	0.979
1GWQ_A	ER_alpha	NR3A1	Endocrine	2.45	1.286	127	1.355	156.408	0.216	0.976
1GWR_A	ER_alpha	NR3A1	Endocrine	2.40	1.287	121	1.358	197.225	0.275	0.974
1L2I_A	ER_alpha	NR3A1	Endocrine	1.95	1.287	140	1.360	207.172	0.235	0.972
1PCG_A	ER_alpha	NR3A1	Endocrine	2.70	1.288	129	1.360	198.597	0.237	0.974
1QKT_A	ER_alpha	NR3A1	Endocrine	2.20	1.183	158	1.240	341.285	0.365	0.865
1QKU_A	ER_alpha	NR3A1	Endocrine	3.20	1.318	135	1.410	196.882	0.229	0.975
1R5K_A	ER_alpha	NR3A1	Endocrine	2.70	1.226	193	1.270	313.845	0.283	0.948
1SJ0_A	ER_alpha	NR3A1	Endocrine	1.90	1.164	178	1.231	364.609	0.449	0.824
1UOM_A	ER_alpha	NR3A1	Endocrine	2.28	1.231	136	1.320	223.979	0.333	0.869
1X7E_A	ER_alpha	NR3A1	Endocrine	2.80	1.295	143	1.372	185.906	0.201	0.975

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	Nuclear Receptor	Phylogenetic Class	Signaling Group	Resolution (Ang.)	SiteScore	size	Dscore	volume	exposure	enclosure
1X7R_A	ER_alpha	NR3A1	Endocrine	2.00	1.305	136	1.388	163.954	0.195	0.977
1XP1_A	ER_alpha	NR3A1	Endocrine	1.80	1.113	265	1.151	503.867	0.425	0.810
1XP6_A	ER_alpha	NR3A1	Endocrine	1.70	1.128	251	1.166	411.257	0.383	0.829
1XP9_A	ER_alpha	NR3A1	Endocrine	1.80	1.125	252	1.149	396.165	0.311	0.852
1XPC_A	ER_alpha	NR3A1	Endocrine	1.60	1.103	276	1.140	465.794	0.426	0.798
1XQC_A	ER_alpha	NR3A1	Endocrine	2.05	1.224	146	1.302	281.946	0.336	0.882
1YIM_A	ER_alpha	NR3A1	Endocrine	1.90	1.102	265	1.126	445.557	0.400	0.822
1YIN_A	ER_alpha	NR3A1	Endocrine	2.20	1.199	146	1.272	295.323	0.368	0.857
1ZKY_A	ER_alpha	NR3A1	Endocrine	2.25	1.275	140	1.336	185.563	0.200	0.980
2AYR_A	ER_alpha	NR3A1	Endocrine	1.90	1.107	287	1.161	534.737	0.423	0.773
2B1V_A	ER_alpha	NR3A1	Endocrine	1.80	1.285	134	1.351	173.558	0.212	0.982
2B1Z_A	ER_alpha	NR3A1	Endocrine	1.78	1.306	133	1.390	183.505	0.194	0.976
2BJ4_A	ER_alpha	NR3A1	Endocrine	2.00	1.212	139	1.298	215.404	0.368	0.850
2FAI_A	ER_alpha	NR3A1	Endocrine	2.10	1.295	140	1.372	188.650	0.213	0.977
2G44_A	ER_alpha	NR3A1	Endocrine	2.65	1.305	126	1.390	206.829	0.232	0.972
2I0G_A	ER_alpha	NR3A1	Endocrine	1.60	1.162	269	1.221	433.552	0.393	0.836
2I0J_A	ER_alpha	NR3A1	Endocrine	2.90	1.236	143	1.316	235.641	0.296	0.892
2IOK_A	ER_alpha	NR3A1	Endocrine	2.40	1.236	152	1.338	311.101	0.374	0.850
2JF9_A	ER_alpha	NR3A1	Endocrine	2.10	1.224	139	1.316	193.109	0.294	0.854
2JFA_A	ER_alpha	NR3A1	Endocrine	2.55	1.192	126	1.260	206.829	0.330	0.857
2OCF_A	ER_alpha	NR3A1	Endocrine	2.95	1.287	143	1.359	185.220	0.239	0.973
2OUZ_A	ER_alpha	NR3A1	Endocrine	2.00	1.124	226	1.171	540.911	0.446	0.809
2P15_A	ER_alpha	NR3A1	Endocrine	1.94	1.230	191	1.280	321.734	0.327	0.939
2POG_A	ER_alpha	NR3A1	Endocrine	1.84	1.235	150	1.316	272.342	0.353	0.888
2Q70_A	ER_alpha	NR3A1	Endocrine	1.95	1.181	151	1.240	268.569	0.398	0.861
2QA6_A	ER_alpha	NR3A1	Endocrine	2.60	1.283	113	1.350	139.258	0.175	0.976
2QA8_A	ER_alpha	NR3A1	Endocrine	1.85	1.302	140	1.385	163.954	0.222	0.974
2QAB_A	ER_alpha	NR3A1	Endocrine	1.89	1.312	121	1.398	157.780	0.154	0.980
2QE4_A	ER_alpha	NR3A1	Endocrine	2.40	1.261	142	1.353	225.694	0.272	0.902
2QGT_A	ER_alpha	NR3A1	Endocrine	2.15	1.303	137	1.383	183.505	0.208	0.979
2QGW_A	ER_alpha	NR3A1	Endocrine	2.39	1.298	130	1.374	159.495	0.177	0.978
2QH6_A	ER_alpha	NR3A1	Endocrine	2.70	1.225	206	1.268	382.102	0.405	0.947
2QR9_A	ER_alpha	NR3A1	Endocrine	2.00	1.321	136	1.420	215.404	0.236	0.965
2QSE_A	ER_alpha	NR3A1	Endocrine	1.85	1.286	132	1.356	181.447	0.228	0.975
2QXM_A	ER_alpha	NR3A1	Endocrine	2.30	1.289	132	1.363	192.080	0.224	0.971
2QXS_A	ER_alpha	NR3A1	Endocrine	1.70	1.148	212	1.183	349.174	0.335	0.860
2R6W_A	ER_alpha	NR3A1	Endocrine	2.00	1.171	154	1.254	276.115	0.412	0.802
2R6Y_A	ER_alpha	NR3A1	Endocrine	2.00	1.173	143	1.231	294.980	0.426	0.852
3DT3_A	ER_alpha	NR3A1	Endocrine	2.40	1.223	158	1.297	328.594	0.360	0.886
3ERD_A	ER_alpha	NR3A1	Endocrine	2.03	1.309	136	1.395	175.959	0.218	0.978

PDB code_Chain	Nuclear Receptor	Phylogenetic Class	Signaling Group	Resolution (Ang.)	SiteScore	size	Dscore	volume	exposure	enclosure
3ERT_A	ER_alpha	NR3A1	Endocrine	1.90	1.200	161	1.282	415.373	0.449	0.840
1L2J_B	ER_beta	NR3A2	Endocrine	2.95	1.173	141	1.232	337.169	0.376	0.849
1NDE_A	ER_beta	NR3A2	Endocrine	3.00	1.197	184	1.267	343.343	0.361	0.858
1QKM_A	ER_beta	NR3A2	Endocrine	1.80	1.318	116	1.408	134.799	0.165	0.980
1QKN_A	ER_beta	NR3A2	Endocrine	2.25	1.223	132	1.303	219.863	0.327	0.876
1U3Q_A	ER_beta	NR3A2	Endocrine	2.40	1.318	131	1.407	139.944	0.225	0.983
1U3R_A	ER_beta	NR3A2	Endocrine	2.21	1.317	137	1.407	169.442	0.235	0.978
1U3S_A	ER_beta	NR3A2	Endocrine	2.50	1.321	142	1.417	179.732	0.215	0.974
1U9E_A	ER_beta	NR3A2	Endocrine	2.40	1.335	125	1.436	156.065	0.194	0.983
1X76_A	ER_beta	NR3A2	Endocrine	2.20	1.322	123	1.413	161.896	0.217	0.983
1X78_A	ER_beta	NR3A2	Endocrine	2.30	1.333	125	1.432	155.379	0.199	0.983
1X7B_A	ER_beta	NR3A2	Endocrine	2.30	1.344	123	1.450	139.601	0.169	0.985
1X7J_A	ER_beta	NR3A2	Endocrine	2.30	1.318	129	1.407	158.809	0.213	0.981
1YY4_A	ER_beta	NR3A2	Endocrine	2.70	1.326	120	1.421	173.215	0.231	0.979
1YYE_A	ER_beta	NR3A2	Endocrine	2.03	1.325	135	1.420	152.978	0.196	0.980
1ZAF_A	ER_beta	NR3A2	Endocrine	2.20	1.329	134	1.427	162.925	0.202	0.978
2GIU_A	ER_beta	NR3A2	Endocrine	2.20	1.287	147	1.360	199.283	0.250	0.973
2JJ3_A	ER_beta	NR3A2	Endocrine	2.28	1.331	127	1.430	170.128	0.206	0.979
2NV7_A	ER_beta	NR3A2	Endocrine	2.10	1.335	139	1.436	151.606	0.201	0.982
2QTU_A	ER_beta	NR3A2	Endocrine	2.53	1.316	126	1.422	186.935	0.254	0.946
2Z4B_A	ER_beta	NR3A2	Endocrine	2.34	1.309	134	1.407	171.500	0.230	0.952
2PJL_A	ERR_alpha	NR3B1	Metabolic	2.30	1.195	160	1.240	216.776	0.234	0.905
2E2R_A	ERR_gamma	NR3B3	Metabolic	1.60	1.275	108	1.333	126.910	0.206	0.984
2EWP_A	ERR_gamma	NR3B3	Metabolic	2.30	1.178	163	1.244	271.313	0.366	0.841
2GPP_A	ERR_gamma	NR3B3	Metabolic	2.60	1.195	144	1.215	217.805	0.276	0.950
2GPU_A	ERR_gamma	NR3B3	Metabolic	1.70	1.174	195	1.242	341.628	0.405	0.835
2GPV_A	ERR_gamma	NR3B3	Metabolic	2.85	1.217	135	1.299	233.240	0.360	0.864
2P7G_A	ERR_gamma	NR3B3	Metabolic	2.10	1.272	93	1.339	124.166	0.250	0.984
2P7Z_A	ERR_gamma	NR3B3	Metabolic	2.50	1.163	170	1.225	269.255	0.339	0.832
2ZAS_A	ERR_gamma	NR3B3	Metabolic	2.00	1.218	88	1.253	109.760	0.254	0.988
2ZKC_A	ERR_gamma	NR3B3	Metabolic	1.70	1.287	110	1.354	132.741	0.247	0.985
1M2Z_A	GR	NR3C1	Endocrine	2.50	1.211	161	1.236	240.100	0.265	0.963
1NHZ_A	GR	NR3C1	Endocrine	2.30	1.102	156	1.146	487.060	0.532	0.786
1P93_A	GR	NR3C1	Endocrine	2.70	1.238	171	1.289	276.458	0.250	0.951
3BQD_A	GR	NR3C1	Endocrine	2.50	1.208	244	1.244	411.943	0.333	0.936
3CLD_A	GR	NR3C1	Endocrine	2.84	1.253	167	1.310	273.028	0.209	0.956
3E7C_A	GR	NR3C1	Endocrine	2.15	1.169	238	1.191	414.001	0.298	0.915
3GN8_A	GR	NR3C1	Endocrine	2.50	1.246	146	1.293	209.230	0.189	0.969
3H52_A	GR	NR3C1	Endocrine	2.80	1.264	178	1.344	344.715	0.323	0.929
3K23_B	GR	NR3C1	Endocrine	3.00	1.207	270	1.250	455.161	0.289	0.925

PDB code_Chain	Nuclear Receptor	Phylogenetic Class	Signaling Group	Resolution (Ang.)	SiteScore	size	Dscore	volume	exposure	enclosure
1Y9R_A	MR	NR3C2	Endocrine	1.96	1.287	143	1.357	177.674	0.210	0.977
1YA3_A	MR	NR3C2	Endocrine	2.34	1.275	138	1.340	203.056	0.242	0.972
2A3I_A	MR	NR3C2	Endocrine	1.95	1.238	140	1.275	191.394	0.231	0.974
2AA2_A	MR	NR3C2	Endocrine	1.95	1.248	142	1.291	191.051	0.193	0.978
2AA5_A	MR	NR3C2	Endocrine	2.20	1.250	141	1.295	186.935	0.242	0.975
2AA6_A	MR	NR3C2	Endocrine	1.95	1.266	143	1.319	183.162	0.178	0.980
2AA7_A	MR	NR3C2	Endocrine	2.20	1.255	128	1.302	182.476	0.251	0.979
2AAX_A	MR	NR3C2	Endocrine	1.75	1.252	151	1.297	189.679	0.209	0.979
2AB2_A	MR	NR3C2	Endocrine	1.85	1.265	142	1.320	194.481	0.237	0.977
2ABI_A	MR	NR3C2	Endocrine	2.33	1.247	137	1.290	186.249	0.217	0.976
2OAX_A	MR	NR3C2	Endocrine	2.29	1.282	146	1.353	230.496	0.223	0.968
1A28_A	PR	NR3C3	Endocrine	1.80	1.296	147	1.374	208.201	0.265	0.974
1E3K_A	PR	NR3C3	Endocrine	2.80	1.260	141	1.311	173.558	0.194	0.977
1SQN_A	PR	NR3C3	Endocrine	1.45	1.291	146	1.366	202.370	0.211	0.974
1SR7_A	PR	NR3C3	Endocrine	1.46	1.282	166	1.360	282.975	0.284	0.955
1ZUC_A	PR	NR3C3	Endocrine	2.00	1.273	138	1.332	173.558	0.220	0.980
2W8Y_A	PR	NR3C3	Endocrine	1.80	1.279	165	1.350	252.791	0.260	0.966
3KBA_A	PR	NR3C3	Endocrine	2.00	1.278	140	1.347	215.404	0.296	0.968
1E3G_A	AR	NR3C4	Endocrine	2.40	1.279	129	1.341	158.123	0.168	0.980
1GS4_A	AR	NR3C4	Endocrine	1.95	1.241	153	1.281	206.486	0.215	0.974
1T5Z_A	AR	NR3C4	Endocrine	2.30	1.294	134	1.368	187.278	0.207	0.977
1T63_A	AR	NR3C4	Endocrine	2.07	1.292	131	1.366	192.766	0.243	0.976
1T65_A	AR	NR3C4	Endocrine	1.66	1.290	136	1.363	187.278	0.218	0.976
1XJ7_A	AR	NR3C4	Endocrine	2.70	1.262	127	1.320	207.515	0.274	0.966
1XOW_A	AR	NR3C4	Endocrine	1.80	1.298	133	1.374	158.123	0.174	0.983
1XQ3_A	AR	NR3C4	Endocrine	2.25	1.305	133	1.385	163.611	0.208	0.981
1Z95_A	AR	NR3C4	Endocrine	1.80	1.296	162	1.377	215.404	0.210	0.970
2AM9_A	AR	NR3C4	Endocrine	1.64	1.284	133	1.355	190.022	0.244	0.970
2AMA_A	AR	NR3C4	Endocrine	1.90	1.264	133	1.321	188.650	0.249	0.972
2AMB_A	AR	NR3C4	Endocrine	1.75	1.261	144	1.315	187.278	0.200	0.973
2AO6_A	AR	NR3C4	Endocrine	1.89	1.301	129	1.379	159.838	0.199	0.982
2AX6_A	AR	NR3C4	Endocrine	1.50	1.275	111	1.335	131.026	0.218	0.981
2AX7_A	AR	NR3C4	Endocrine	1.90	1.274	147	1.338	188.650	0.272	0.973
2AX8_A	AR	NR3C4	Endocrine	1.70	1.265	148	1.322	202.027	0.285	0.972
2AX9_A	AR	NR3C4	Endocrine	1.65	1.275	119	1.335	148.176	0.207	0.979
2AXA_A	AR	NR3C4	Endocrine	1.80	1.281	144	1.350	197.568	0.273	0.973
2HVC_A	AR	NR3C4	Endocrine	2.10	1.243	131	1.284	164.983	0.234	0.976
2OZ7_A	AR	NR3C4	Endocrine	1.80	1.259	157	1.316	238.042	0.259	0.964
2PIO_A	AR	NR3C4	Endocrine	2.03	1.264	138	1.323	197.568	0.254	0.967
2PIP_A	AR	NR3C4	Endocrine	1.80	1.270	146	1.334	195.510	0.215	0.967

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	Nuclear Receptor	Phylogenetic Class	Signaling Group	Resolution (Ang.)	SiteScore	size	Dscore	volume	exposure	enclosure
2PIQ_A	AR	NR3C4	Endocrine	2.40	1.279	140	1.349	194.824	0.251	0.967
2PIR_A	AR	NR3C4	Endocrine	2.10	1.281	142	1.354	213.689	0.245	0.965
2PIT_A	AR	NR3C4	Endocrine	1.76	1.283	141	1.354	193.795	0.221	0.970
2PIU_A	AR	NR3C4	Endocrine	2.12	1.270	139	1.327	174.587	0.201	0.980
2PIV_A	AR	NR3C4	Endocrine	1.95	1.276	149	1.343	190.365	0.199	0.969
2PIW_A	AR	NR3C4	Endocrine	2.58	1.273	135	1.334	184.877	0.211	0.976
2PIX_A	AR	NR3C4	Endocrine	2.40	1.295	141	1.372	199.283	0.199	0.974
2PKL_A	AR	NR3C4	Endocrine	2.49	1.317	130	1.406	162.582	0.161	0.979
2PNU_A	AR	NR3C4	Endocrine	1.65	1.256	200	1.314	282.289	0.225	0.959
2Q7I_A	AR	NR3C4	Endocrine	1.87	1.325	132	1.419	166.355	0.195	0.983
2Q7J_A	AR	NR3C4	Endocrine	1.90	1.319	125	1.408	163.954	0.204	0.983
2Q7K_A	AR	NR3C4	Endocrine	1.80	1.323	131	1.414	165.326	0.155	0.984
2Q7L_A	AR	NR3C4	Endocrine	1.92	1.296	130	1.372	181.447	0.198	0.979
2Z4J_A	AR	NR3C4	Endocrine	2.60	1.301	127	1.380	189.336	0.253	0.978
3B5R_A	AR	NR3C4	Endocrine	1.80	1.277	159	1.344	207.858	0.264	0.972
3B65_A	AR	NR3C4	Endocrine	1.80	1.299	153	1.378	194.824	0.257	0.974
3B66_A	AR	NR3C4	Endocrine	1.65	1.294	147	1.373	207.515	0.279	0.972
3B67_A	AR	NR3C4	Endocrine	1.90	1.219	156	1.248	234.955	0.307	0.965
3B68_A	AR	NR3C4	Endocrine	1.90	1.287	157	1.361	201.341	0.249	0.971

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	contact	phobic	philic	balance	don/acc	refdist	refmin	refavg	sitemin
1NAV_A	1.325	3.047	0.887	3.436	0.819	2.911	0.085	0.572	0.953
1BSX_A	1.274	2.967	0.858	3.459	0.285	0.287	0.213	0.589	1.004
1N46_A	1.298	3.603	0.991	3.635	0.223	0.348	0.169	0.561	0.901
1NAX_A	1.333	3.629	0.917	3.959	0.275	1.725	0.165	0.620	0.693
1NQ0_A	1.268	3.507	0.810	4.331	0.344	0.732	0.081	0.608	1.055
1NQ1_A	1.248	2.766	0.872	3.171	0.385	0.646	0.137	0.601	1.052
1NQ2_A	1.302	3.436	0.849	4.046	0.219	0.740	0.157	0.638	0.803
1NUO_A	1.246	2.421	0.991	2.444	0.492	0.720	0.216	0.673	1.259
1Q4X_A	1.237	3.421	0.735	4.652	0.220	0.537	0.166	0.600	1.268
1R6G_A	1.230	3.346	0.741	4.515	0.345	0.702	0.082	0.621	1.338
1XZX_X	1.303	4.146	0.715	5.798	0.236	0.837	0.195	0.559	0.706
1Y0X_X	1.309	3.939	0.722	5.453	0.192	0.848	0.219	0.609	0.775
2J4A_A	1.314	4.675	0.662	7.067	0.248	0.549	0.067	0.617	0.960
2PIN_A	1.253	3.383	0.757	4.468	0.288	0.132	0.241	0.554	0.964
3D57_A	1.286	3.974	0.695	5.718	0.324	0.463	0.132	0.631	0.777
3GWS_X	1.265	3.740	0.801	4.669	0.308	0.952	0.179	0.587	0.798
3HZF_A	1.360	3.662	0.963	3.804	0.541	1.853	0.136	0.584	0.991
3IMY_A	1.262	3.945	0.667	5.911	0.259	0.688	0.180	0.622	1.117
1DKF_B	1.158	2.791	0.709	3.935	0.462	0.955	0.210	0.670	1.225
1XAP_A	1.264	4.699	0.358	13.135	0.254	0.389	0.098	0.581	0.549
1EXA_A	1.260	4.272	0.353	12.103	0.520	0.380	0.129	0.587	0.924
1EXX_A	1.250	4.506	0.303	14.864	0.366	0.344	0.161	0.641	1.185
1FCX_A	1.222	4.222	0.347	12.151	0.343	1.303	0.148	0.609	1.368
1FCY_A	1.226	4.225	0.421	10.039	0.246	1.432	0.062	0.582	1.416
1FCZ_A	1.280	4.856	0.326	14.896	0.327	0.227	0.113	0.570	1.047
1FD0_A	1.239	4.355	0.353	12.331	0.254	1.112	0.076	0.610	1.380
2LBD_A	1.181	4.046	0.436	9.271	0.195	0.845	0.111	0.595	0.587
3LBD_A	1.302	4.775	0.337	14.183	0.214	0.020	0.156	0.591	0.533
4LBD_A	1.250	3.858	0.402	9.587	0.364	0.717	0.124	0.571	1.176
1I7G_A	1.127	1.960	0.833	2.353	0.623	2.149	0.098	0.623	1.726
1K7L_A	1.109	2.047	0.772	2.653	0.714	3.037	0.123	0.603	1.473
1KKQ_A	1.102	1.816	0.723	2.511	0.900	3.221	0.353	1.202	3.556
2NPA_A	1.166	2.017	0.915	2.203	0.635	3.034	0.217	0.591	2.077
2P54_A	1.120	2.177	0.726	2.999	0.680	2.118	0.146	0.572	1.351
2REW_A	1.074	2.241	0.767	2.921	0.798	1.965	0.221	0.561	2.835
2ZNN_A	1.120	2.360	0.678	3.483	0.628	2.606	0.150	0.624	0.517
3ET1_A	1.150	2.191	0.795	2.756	0.760	3.727	0.133	0.575	1.132
3G8I_A	1.212	2.216	0.905	2.449	0.874	3.792	0.188	0.623	1.561
1GWX_A	1.118	2.017	0.799	2.524	0.768	2.995	0.241	0.684	1.534
1Y0S_A	1.142	2.176	0.869	2.504	0.582	2.996	0.149	0.692	1.663

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	contact	phobic	philic	balance	don/acc	refdist	refmin	refavg	sitemin
2AWH_A	1.181	3.589	0.503	7.138	0.775	1.467	0.153	0.672	1.418
2B50_A	1.132	2.811	0.731	3.845	0.661	1.601	0.088	0.631	1.629
2BAW_A	1.171	3.553	0.573	6.198	0.533	1.055	0.212	0.693	1.124
2J14_A	1.211	3.152	0.568	5.550	0.681	1.767	0.071	0.598	1.390
2ZNP_A	1.158	2.579	0.762	3.384	0.667	2.406	0.116	0.626	0.607
2ZNQ_A	1.166	2.696	0.683	3.946	0.743	1.911	0.147	0.639	0.382
3D5F_A	1.209	3.374	0.554	6.092	0.731	0.883	0.124	0.586	0.857
3DY6_A	1.151	2.411	0.873	2.763	1.066	1.423	0.087	0.602	1.717
3ET2_A	1.210	2.024	0.942	2.149	0.680	1.929	0.231	0.568	1.934
3GZ9_A	1.208	2.613	0.720	3.630	0.720	1.199	0.071	0.585	1.134
1FM6_D	1.195	1.836	1.016	1.806	0.863	1.695	0.059	0.648	1.542
1FM9_D	1.161	1.987	0.848	2.342	0.750	2.979	0.186	0.625	2.561
1I7I_A	1.146	2.228	0.771	2.891	0.600	1.628	0.076	0.650	2.043
1KNU_A	1.165	1.647	0.927	1.778	0.809	2.256	0.128	0.676	1.601
1NYX_A	1.195	1.657	0.964	1.719	0.455	1.735	0.098	0.585	0.674
1RDT_D	1.109	2.137	0.791	2.701	0.542	1.216	0.172	0.608	2.068
1WM0_X	1.248	2.083	0.925	2.252	0.837	2.618	0.234	0.578	0.790
1ZEO_A	1.223	2.030	0.922	2.201	0.532	3.178	0.165	0.682	1.788
1ZGY_A	1.161	1.669	0.880	1.896	0.970	2.518	0.137	0.595	2.292
2ATH_A	1.184	1.843	0.911	2.023	0.821	2.340	0.227	0.612	1.105
2F4B_A	1.157	1.678	0.882	1.902	0.713	3.136	0.151	0.700	0.362
2FVJ_A	1.106	1.846	0.848	2.177	0.976	2.661	0.073	0.695	0.384
2G0G_A	1.204	1.540	0.938	1.641	0.514	3.326	0.262	0.593	1.615
2G0H_A	1.157	1.473	1.048	1.406	0.757	2.934	0.078	0.601	2.435
2GTK_A	1.062	2.263	0.673	3.363	0.937	1.142	0.316	0.666	2.398
2HWQ_A	1.102	1.581	0.797	1.983	0.666	3.057	0.098	0.861	1.160
2HWR_A	1.098	1.628	0.789	2.063	0.811	2.603	0.094	0.784	0.690
2I4J_A	1.176	1.952	0.962	2.029	0.652	3.301	0.151	0.755	1.441
2I4P_A	1.170	1.847	0.966	1.913	0.638	2.985	0.160	0.772	0.856
2I4Z_A	1.215	2.108	0.912	2.310	0.550	3.154	0.155	0.753	1.587
2OM9_A	1.153	1.411	1.077	1.310	0.460	1.948	0.218	0.750	1.102
2P4Y_A	1.151	1.696	0.961	1.765	0.621	2.100	0.132	0.867	1.214
2POB_A	1.158	1.933	0.856	2.259	0.427	1.199	0.176	0.664	2.491
2PRG_A	1.135	1.807	0.802	2.253	0.631	2.053	0.105	0.635	2.762
2Q59_A	1.147	2.556	0.701	3.649	0.583	1.690	0.165	0.695	0.846
2Q6R_A	1.112	1.558	0.905	1.720	0.963	1.718	0.217	0.758	0.667
2Q6S_B	1.263	1.710	1.124	1.522	0.829	2.813	0.165	0.608	0.831
2VST_A	1.117	1.686	0.908	1.856	0.831	1.866	0.240	0.887	1.271
2VV0_A	1.157	2.216	0.809	2.739	0.621	2.083	0.115	0.731	1.255
2VV1_A	1.154	1.814	0.926	1.958	0.578	1.744	0.075	0.795	0.357

PDB code_Chain	contact	phobic	philic	balance	don/acc	refdist	refmin	refavg	sitemin
2VV2_A	1.123	1.973	0.835	2.363	0.746	2.027	0.105	0.806	1.395
2VV3_A	1.129	1.130	1.082	1.045	0.707	1.918	0.322	0.845	1.710
2VV4_A	1.162	1.601	0.984	1.627	0.602	1.308	0.318	0.995	0.849
2ZK1_A	1.189	1.956	0.907	2.156	0.899	2.481	0.130	0.769	1.291
2ZK2_A	1.194	2.167	0.900	2.409	0.853	1.653	0.074	0.838	1.491
2ZK3_A	1.239	1.953	0.958	2.038	0.889	1.907	0.229	0.828	2.297
2ZK4_A	1.238	2.060	1.062	1.939	0.702	1.146	0.079	0.782	2.472
2ZK5_A	1.240	2.759	0.881	3.133	0.931	0.203	0.156	0.649	1.083
2ZNO_A	1.079	2.052	0.761	2.696	0.591	2.989	0.162	0.875	1.692
2ZVT_A	1.199	1.970	0.999	1.972	0.704	2.352	0.238	0.651	1.192
3B3K_A	1.187	2.501	0.765	3.271	0.887	1.046	0.311	0.717	1.791
3BC5_A	1.113	1.585	1.007	1.574	0.551	2.457	0.090	0.573	2.812
3CDP_A	1.180	2.472	0.708	3.492	1.759	1.048	0.134	0.602	1.203
3CDS_A	1.174	2.479	0.805	3.080	0.886	2.360	0.134	0.637	3.079
3CS8_A	1.179	1.943	0.929	2.093	0.635	2.082	0.222	0.690	1.819
3CWD_A	1.172	1.830	0.993	1.844	0.358	0.705	0.124	0.720	1.185
3DZU_D	1.131	1.972	0.859	2.297	0.861	3.067	0.054	0.577	1.058
3DZY_D	1.095	1.838	0.848	2.167	0.610	2.876	0.141	0.588	0.443
3E00_D	1.154	1.637	0.897	1.823	0.516	0.754	0.162	1.004	0.804
3ET3_A	1.190	1.788	0.853	2.097	0.456	2.537	0.305	0.637	2.104
3FEI_A	1.156	1.896	0.824	2.300	0.962	4.296	0.071	0.693	1.383
3FEJ_A	1.052	1.531	0.995	1.539	1.321	2.377	0.266	0.640	1.961
3FUR_A	1.147	1.729	0.951	1.819	0.572	1.910	0.071	0.624	0.988
3G9E_A	1.072	1.546	0.916	1.687	1.084	1.675	0.224	0.656	1.618
3H0A_D	1.147	1.735	1.100	1.578	0.561	1.764	0.205	0.609	1.237
3HO0_A	1.177	2.651	0.598	4.435	0.670	0.819	0.179	0.745	1.198
3HOD_A	1.170	2.496	0.707	3.529	0.741	1.397	0.079	0.748	1.756
3IA6_B	1.113	1.955	0.838	2.334	0.730	1.844	0.228	0.631	2.060
4PRG_A	1.084	1.347	1.046	1.289	0.802	2.789	0.191	0.745	1.601
1N83_A	1.120	2.367	0.694	3.408	0.422	2.613	0.105	0.736	0.915
1S0X_A	1.154	2.068	0.857	2.414	0.687	1.406	0.089	0.693	0.685
1P8D_A	1.208	2.766	0.650	4.259	2.284	0.823	0.319	0.641	1.409
1PQ6_A	1.167	2.569	0.830	3.095	1.075	1.576	0.164	0.715	1.425
1PQ9_A	1.256	3.602	0.476	7.572	1.905	0.455	0.143	0.618	0.797
1PQC_A	1.183	2.995	0.624	4.798	0.971	0.174	0.212	0.652	0.767
1UPV_A	1.168	2.624	0.593	4.424	2.142	1.092	0.229	0.753	1.439
1UPW_A	1.186	2.749	0.590	4.658	1.348	1.028	0.219	0.776	1.450
3KFC_A	1.249	2.778	0.816	3.403	1.155	2.021	0.290	0.619	0.661
1UHL_B	1.161	2.265	0.645	3.510	1.375	1.020	0.148	0.828	1.653
2ACL_B	1.211	2.917	0.595	4.904	1.842	1.842	0.075	0.650	1.231

PDB code_Chain	contact	phobic	philic	balance	don/acc	refdist	refmin	refavg	sitemin
3FAL_B	1.247	2.256	1.001	2.254	1.057	1.777	0.334	0.762	0.621
3FC6_B	1.187	2.937	0.684	4.296	0.659	1.657	0.082	0.622	0.408
1OSH_A	1.159	2.888	0.560	5.158	0.985	0.828	0.131	0.723	1.548
3BEJ_A	1.191	1.764	0.949	1.859	0.391	1.415	0.135	0.644	0.561
3DCT_A	1.217	3.152	0.644	4.896	0.928	1.077	0.088	0.650	1.287
3FLI_A	1.215	3.424	0.574	5.963	0.864	1.138	0.063	0.612	1.031
3GD2_A	1.147	2.679	0.699	3.832	0.468	1.520	0.131	0.590	1.024
3L1B_A	1.038	2.983	0.446	6.682	0.347	2.854	0.149	1.336	1.346
3OKH_A	1.118	2.758	0.564	4.891	0.364	1.142	0.157	0.697	1.230
3OKI_A	1.138	2.368	0.682	3.472	1.131	1.355	0.170	0.741	0.316
3OLF_A	1.219	2.790	0.777	3.590	0.821	0.467	0.109	0.731	0.684
3OMK_A	1.156	2.499	0.779	3.208	0.901	0.902	0.217	0.716	0.513
3OMM_A	1.235	3.011	0.586	5.138	1.404	1.266	0.158	0.747	0.519
3OOF_A	1.223	2.397	0.828	2.893	0.814	0.962	0.176	0.648	0.452
3OOK_A	1.138	2.106	0.778	2.708	1.228	1.079	0.204	0.676	0.476
1DB1_A	1.172	2.495	0.651	3.831	0.983	0.653	0.117	0.658	0.610
1IE8_A	1.195	2.553	0.699	3.652	0.837	0.544	0.186	0.696	0.739
1IE9_A	1.198	2.644	0.690	3.833	1.093	0.630	0.195	0.705	0.686
1S0Z_A	1.185	2.572	0.696	3.695	1.148	1.220	0.145	0.694	1.332
1S19_A	1.169	2.598	0.745	3.487	0.955	0.907	0.080	0.689	1.142
1TXI_A	1.173	2.668	0.668	3.996	0.860	0.874	0.115	0.661	1.502
2HAM_A	1.197	2.823	0.678	4.165	0.908	0.295	0.147	0.662	1.123
2HAR_A	1.194	2.680	0.689	3.889	1.054	0.665	0.057	0.655	1.041
2HAS_A	1.185	2.593	0.742	3.494	0.910	0.441	0.159	0.637	1.303
2HB7_A	1.163	2.612	0.705	3.704	0.841	0.695	0.091	0.681	0.957
2HB8_A	1.154	2.490	0.698	3.568	0.788	0.813	0.154	0.667	1.161
3CS4_A	1.158	2.809	0.675	4.159	0.847	0.691	0.082	0.689	0.879
3CS6_A	1.187	2.656	0.680	3.907	1.106	0.704	0.141	0.734	0.742
1ILH_A	1.024	2.139	0.523	4.086	1.031	0.419	0.173	1.174	1.233
1M13_A	1.128	2.163	0.662	3.266	0.639	3.343	0.209	1.127	0.436
1NRL_A	1.190	2.563	0.622	4.118	1.041	1.905	0.230	0.902	1.407
1SKX_A	0.890	1.689	0.560	3.014	0.778	1.223	0.137	1.591	1.020
2O9I_A	1.194	2.272	0.680	3.342	1.519	1.997	0.225	0.835	1.460
2QNV_A	1.110	1.878	0.673	2.789	0.776	1.636	0.250	1.181	0.988
3HLV_B	1.200	2.622	0.660	3.971	0.977	2.422	0.045	0.863	1.822
1XV9_B	1.144	3.562	0.425	8.378	0.526	0.411	0.108	0.711	0.892
1XVP_B	1.204	4.087	0.320	12.755	1.393	0.760	0.205	0.599	1.590
1PZL_A	1.233	4.926	0.362	13.621	0.248	0.943	0.091	0.586	1.529
3FS1_A	1.239	4.929	0.256	19.284	0.524	0.863	0.037	0.541	1.425
1LV2_A	1.182	3.930	0.497	7.914	0.289	0.475	0.181	0.581	1.579

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	contact	phobic	philic	balance	don/acc	refdist	refmin	refavg	sitemin
1FBY_A	1.212	4.339	0.466	9.302	0.160	0.314	0.171	0.652	0.726
1FM6_A	1.213	3.639	0.608	5.987	0.444	0.109	0.218	0.562	0.865
1FM9_A	1.221	4.087	0.485	8.425	0.264	0.069	0.134	0.563	0.893
1G5Y_A	1.049	1.901	0.818	2.325	0.429	1.981	0.139	1.119	0.604
1K74_A	1.216	4.142	0.494	8.379	0.482	0.192	0.249	0.747	0.616
1MV9_A	1.212	4.338	0.487	8.913	0.130	0.268	0.138	0.641	1.137
1MVC_A	1.235	2.941	0.936	3.142	0.223	1.390	0.085	0.612	1.340
1MZN_A	1.244	3.249	0.846	3.842	0.306	0.264	0.198	0.570	0.725
1RDT_A	1.192	3.233	0.630	5.135	0.298	0.174	0.090	0.684	0.709
1XLS_A	1.239	3.095	0.723	4.283	0.411	0.877	0.084	0.635	0.425
1XV9_A	1.204	4.410	0.362	12.168	0.371	0.737	0.305	0.662	1.192
1XVP_A	1.184	4.619	0.295	15.684	0.355	1.024	0.171	0.590	1.502
2ACL_A	1.240	3.459	0.791	4.374	0.422	0.451	0.166	0.670	0.423
2P1T_A	1.243	3.080	0.852	3.615	0.383	1.236	0.184	0.640	0.562
2P1U_A	1.221	3.940	0.480	8.216	0.549	0.505	0.205	0.604	0.479
2P1V_A	1.235	3.250	0.835	3.894	0.548	0.844	0.138	0.632	0.433
2ZXZ_A	1.207	3.971	0.464	8.553	0.495	0.346	0.208	0.634	0.751
2ZY0_A	1.213	3.804	0.513	7.422	0.147	0.276	0.126	0.619	0.908
3DZU_A	1.201	4.710	0.330	14.287	0.878	0.864	0.247	0.675	1.080
3DZY_A	1.195	3.398	0.518	6.557	0.637	0.720	0.041	0.708	0.599
3E00_A	1.208	3.918	0.432	9.069	0.262	0.565	0.245	0.599	1.111
3FAL_A	1.138	2.348	0.838	2.801	0.372	2.186	0.110	1.030	1.170
3FC6_A	1.104	2.224	0.791	2.813	1.020	0.701	0.237	0.909	1.449
3H0A_A	1.230	3.256	0.558	5.838	0.585	1.024	0.090	0.681	1.445
1H9U_A	1.187	3.848	0.383	10.037	0.459	0.290	0.216	0.591	1.068
1UHL_A	1.216	3.230	0.835	3.868	0.387	0.760	0.191	0.591	1.070
1A52_A	1.222	3.259	0.589	5.534	1.001	0.722	0.106	0.667	1.198
1ERE_A	1.201	3.910	0.420	9.307	0.758	0.365	0.089	0.630	0.830
1ERR_A	1.038	2.434	0.511	4.767	2.376	2.425	0.049	0.886	1.395
1G50_A	1.260	4.683	0.261	17.936	0.659	0.523	0.131	0.691	0.900
1GWQ_A	1.253	3.848	0.523	7.359	0.770	0.453	0.176	0.732	0.769
1GWR_A	1.215	3.538	0.512	6.909	0.676	0.183	0.173	0.661	0.613
1L2I_A	1.199	3.836	0.501	7.658	0.755	0.368	0.164	0.729	0.478
1PCG_A	1.254	3.666	0.503	7.284	1.215	0.304	0.039	0.671	0.984
1QKT_A	1.115	2.427	0.672	3.611	1.580	1.624	0.311	0.709	1.166
1QKU_A	1.241	4.404	0.354	12.433	1.578	0.555	0.106	0.671	0.787
1R5K_A	1.228	2.628	0.734	3.580	0.897	0.578	0.155	0.645	0.330
1SJ0_A	1.044	2.446	0.623	3.926	1.451	1.191	0.280	0.808	0.505
1UOM_A	1.075	3.593	0.435	8.267	1.781	3.261	0.158	1.109	0.784
1X7E_A	1.240	4.446	0.471	9.448	0.824	0.591	0.206	0.726	0.837

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	contact	phobic	philic	balance	don/acc	refdist	refmin	refavg	sitemin
1X7R_A	1.219	4.496	0.423	10.628	1.043	0.571	0.204	0.694	0.944
1XP1_A	1.056	1.619	0.845	1.916	1.101	1.574	0.115	0.632	1.327
1XP6_A	1.084	1.799	0.834	2.156	1.254	1.508	0.277	0.658	1.388
1XP9_A	1.097	1.926	0.927	2.078	0.848	1.712	0.178	0.678	1.188
1XPC_A	1.067	1.588	0.855	1.857	1.195	2.146	0.214	0.663	1.040
1XQC_A	1.135	3.204	0.512	6.254	2.238	2.114	0.132	0.836	0.710
1YIM_A	1.093	1.545	0.943	1.639	0.977	2.202	0.107	0.641	1.332
1YIN_A	1.075	2.426	0.560	4.328	1.695	2.257	0.177	0.884	1.344
1ZKY_A	1.201	3.503	0.590	5.940	0.513	0.238	0.123	0.661	0.534
2AYR_A	1.030	2.208	0.745	2.961	0.555	1.366	0.121	0.736	1.065
2B1V_A	1.269	3.985	0.546	7.297	0.924	0.204	0.114	0.582	0.990
2B1Z_A	1.201	3.850	0.416	9.259	1.851	0.326	0.136	0.679	0.916
2BJ4_A	1.042	2.697	0.466	5.791	2.400	1.977	0.134	0.916	0.605
2FAI_A	1.199	4.056	0.473	8.573	0.572	0.419	0.270	0.686	0.596
2G44_A	1.233	4.367	0.408	10.702	1.087	0.099	0.210	0.704	0.576
2I0G_A	1.095	2.292	0.676	3.388	1.664	0.956	0.250	0.694	0.786
2I0J_A	1.133	3.099	0.490	6.329	1.267	1.148	0.281	0.756	1.018
2IOK_A	1.052	3.166	0.344	9.203	1.807	0.553	0.138	0.735	1.444
2JF9_A	1.084	3.325	0.420	7.921	2.136	1.677	0.257	0.938	0.902
2JFA_A	1.062	2.929	0.596	4.917	1.365	3.214	0.351	1.817	0.802
2OCF_A	1.200	3.616	0.507	7.133	0.634	0.480	0.107	0.645	0.811
2OUZ_A	1.059	1.730	0.781	2.215	1.278	2.027	0.125	0.836	1.495
2P15_A	1.213	3.349	0.685	4.887	0.987	0.585	0.117	0.634	1.279
2POG_A	1.059	3.385	0.479	7.060	1.443	0.594	0.196	0.652	0.999
2Q70_A	1.036	2.455	0.666	3.687	1.093	0.917	0.150	0.698	1.034
2QA6_A	1.220	3.671	0.538	6.824	0.739	0.236	0.313	0.657	0.914
2QA8_A	1.247	4.617	0.428	10.794	0.516	0.407	0.322	0.671	0.728
2QAB_A	1.263	4.351	0.398	10.936	0.554	0.647	0.088	0.592	0.805
2QE4_A	1.163	3.809	0.394	9.662	1.510	0.410	0.142	0.655	0.394
2QGT_A	1.238	4.053	0.442	9.169	0.655	0.605	0.110	0.613	0.625
2QGW_A	1.238	4.223	0.468	9.021	0.889	0.311	0.229	0.623	0.553
2QH6_A	1.256	2.941	0.738	3.987	1.410	1.429	0.085	0.648	0.617
2QR9_A	1.215	4.415	0.303	14.593	1.337	0.713	0.236	0.842	0.631
2QSE_A	1.224	3.829	0.518	7.392	0.694	0.310	0.310	0.726	0.595
2QXM_A	1.232	3.737	0.491	7.611	0.758	0.600	0.255	0.708	0.453
2QXS_A	1.130	1.972	0.836	2.359	1.095	0.649	0.157	0.611	0.904
2R6W_A	1.003	2.283	0.512	4.460	2.328	2.928	0.135	1.082	1.409
2R6Y_A	1.059	2.245	0.674	3.329	1.459	1.927	0.152	0.946	0.913
3DT3_A	1.096	2.771	0.536	5.167	1.345	0.280	0.192	0.673	1.053
3ERD_A	1.224	4.411	0.406	10.863	0.935	0.144	0.279	0.586	0.661

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	contact	phobic	philic	balance	don/acc	refdist	refmin	refavg	sitemin
3ERT_A	1.024	2.490	0.496	5.025	1.776	0.735	0.195	1.025	0.537
1L2J_B	1.084	2.366	0.667	3.548	0.996	1.154	0.189	0.726	1.154
1NDE_A	1.081	3.021	0.577	5.240	1.040	0.844	0.074	0.787	1.185
1QKM_A	1.252	4.684	0.368	12.724	0.852	0.309	0.197	0.587	0.708
1QKN_A	1.118	3.233	0.500	6.469	1.278	3.258	0.134	1.709	0.864
1U3Q_A	1.267	4.937	0.376	13.136	0.709	0.184	0.156	0.557	0.857
1U3R_A	1.228	4.844	0.368	13.148	0.900	0.830	0.178	0.615	1.085
1U3S_A	1.227	4.837	0.331	14.598	1.130	0.562	0.171	0.568	1.034
1U9E_A	1.230	5.114	0.289	17.688	1.000	0.856	0.090	0.603	0.766
1X76_A	1.231	4.556	0.360	12.672	1.182	0.437	0.180	0.613	0.574
1X78_A	1.238	5.179	0.299	17.298	1.873	0.218	0.127	0.641	0.589
1X7B_A	1.266	5.513	0.249	22.178	0.839	0.281	0.156	0.586	0.613
1X7J_A	1.213	4.432	0.372	11.921	1.760	0.417	0.154	0.683	0.790
1YY4_A	1.238	4.530	0.325	13.922	2.195	0.468	0.259	0.759	0.759
1YYE_A	1.231	4.626	0.330	14.030	1.397	0.674	0.236	0.657	0.937
1ZAF_A	1.255	4.696	0.305	15.396	1.487	0.570	0.139	0.642	0.775
2GIU_A	1.213	3.839	0.502	7.652	1.019	1.127	0.182	0.684	0.856
2JJ3_A	1.213	4.850	0.298	16.277	0.769	0.560	0.184	0.707	0.574
2NV7_A	1.253	4.860	0.287	16.942	0.751	0.192	0.092	0.594	0.654
2QTU_A	1.202	4.503	0.262	17.154	1.208	0.478	0.114	0.750	0.829
2Z4B_A	1.236	4.223	0.319	13.246	1.300	0.276	0.064	0.620	0.832
2PJL_A	1.143	2.597	0.746	3.480	5.779	0.548	0.084	0.705	1.835
2E2R_A	1.285	3.367	0.605	5.566	1.354	0.056	0.159	0.595	1.148
2EWP_A	1.050	2.624	0.614	4.270	7.645	0.412	0.174	0.692	0.262
2GPP_A	1.351	3.247	0.905	3.588	1.459	0.950	0.109	0.621	1.284
2GPU_A	1.126	2.737	0.611	4.478	4.328	0.746	0.127	0.616	1.126
2GPV_A	1.083	3.239	0.489	6.620	2.899	1.452	0.236	0.875	0.681
2P7G_A	1.270	4.154	0.484	8.578	3.425	0.125	0.135	0.625	1.209
2P7Z_A	1.040	2.304	0.658	3.504	2.999	1.139	0.305	0.808	0.649
2ZAS_A	1.272	3.397	0.680	4.993	0.918	0.198	0.172	0.632	1.025
2ZKC_A	1.237	3.654	0.543	6.734	1.342	0.384	0.290	0.693	0.832
1M2Z_A	1.209	1.852	0.864	2.144	1.273	0.261	0.201	0.693	1.251
1NHZ_A	1.005	1.335	0.814	1.641	1.242	1.622	0.152	0.936	1.276
1P93_A	1.209	2.569	0.681	3.775	1.808	0.444	0.073	0.712	1.068
3BQD_A	1.227	2.423	0.789	3.071	0.866	1.340	0.198	0.719	0.481
3CLD_A	1.204	2.817	0.625	4.510	1.453	0.289	0.134	0.687	1.185
3E7C_A	1.257	2.002	0.915	2.187	0.876	1.322	0.184	0.637	0.507
3GN8_A	1.241	2.476	0.701	3.531	1.273	0.213	0.202	0.672	1.122
3H52_A	1.177	3.238	0.469	6.902	2.081	1.058	0.069	0.699	0.879
3K23_B	1.252	2.550	0.752	3.391	0.945	0.650	0.137	0.636	1.168

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	contact	phobic	philic	balance	don/acc	refdist	refmin	refavg	sitemin
1Y9R_A	1.245	3.901	0.521	7.492	0.839	0.140	0.205	0.671	1.056
1YA3_A	1.228	3.307	0.561	5.892	0.922	0.213	0.310	0.676	1.177
2A3I_A	1.215	2.572	0.764	3.366	0.993	0.214	0.142	0.642	1.122
2AA2_A	1.225	3.014	0.723	4.169	0.701	0.141	0.157	0.640	0.922
2AA5_A	1.225	2.746	0.705	3.897	1.227	0.416	0.131	0.664	1.351
2AA6_A	1.218	3.147	0.642	4.905	0.833	0.094	0.211	0.630	1.020
2AA7_A	1.216	2.849	0.691	4.126	0.469	0.345	0.192	0.680	0.920
2AAX_A	1.234	3.151	0.705	4.470	0.998	0.135	0.231	0.615	1.078
2AB2_A	1.216	3.156	0.630	5.006	1.345	0.383	0.117	0.768	1.045
2ABI_A	1.224	2.787	0.721	3.867	1.130	0.137	0.242	0.702	0.994
2OAX_A	1.220	3.177	0.514	6.184	1.870	0.149	0.214	0.708	0.904
1A28_A	1.207	3.438	0.463	7.429	1.841	0.230	0.049	0.667	0.979
1E3K_A	1.251	2.847	0.662	4.302	3.147	0.822	0.068	0.584	0.649
1SQN_A	1.231	3.495	0.486	7.189	2.534	0.729	0.115	0.631	1.382
1SR7_A	1.179	3.049	0.470	6.485	1.525	0.222	0.094	0.668	0.611
1ZUC_A	1.264	3.142	0.602	5.221	1.695	0.337	0.197	0.578	0.688
2W8Y_A	1.203	3.443	0.520	6.625	2.146	0.420	0.236	0.706	0.995
3KBA_A	1.218	3.291	0.532	6.182	3.055	0.372	0.069	0.673	0.776
1E3G_A	1.295	3.701	0.572	6.467	1.485	0.268	0.195	0.630	0.670
1GS4_A	1.240	3.007	0.747	4.024	0.797	0.538	0.116	0.714	0.787
1T5Z_A	1.231	3.650	0.484	7.546	1.273	0.247	0.129	0.654	0.769
1T63_A	1.203	3.413	0.488	6.990	1.435	0.183	0.258	0.631	0.762
1T65_A	1.166	3.563	0.498	7.149	1.561	0.408	0.066	0.624	0.780
1XJ7_A	1.223	3.149	0.612	5.145	1.152	0.397	0.163	0.716	0.722
1XOW_A	1.257	4.001	0.478	8.365	1.746	0.317	0.098	0.609	0.856
1XQ3_A	1.266	3.922	0.440	8.916	1.342	0.229	0.104	0.653	0.730
1Z95_A	1.291	3.766	0.446	8.452	3.315	0.404	0.168	0.588	1.478
2AM9_A	1.205	3.562	0.512	6.956	0.632	0.745	0.085	0.630	0.728
2AMA_A	1.222	3.295	0.619	5.321	0.709	0.673	0.115	0.604	0.746
2AMB_A	1.242	3.595	0.642	5.601	1.534	0.536	0.151	0.619	0.937
2AO6_A	1.264	3.996	0.460	8.696	1.636	0.341	0.104	0.622	0.835
2AX6_A	1.319	3.602	0.595	6.055	1.745	0.554	0.249	0.616	1.204
2AX7_A	1.299	3.950	0.570	6.929	2.901	0.491	0.203	0.546	1.396
2AX8_A	1.281	2.720	0.617	4.411	1.420	0.388	0.129	0.569	1.734
2AX9_A	1.282	3.482	0.590	5.900	2.337	0.452	0.054	0.568	1.076
2AXA_A	1.337	3.617	0.534	6.780	1.318	0.420	0.128	0.593	1.664
2HVC_A	1.209	3.052	0.742	4.114	1.283	0.435	0.194	0.609	0.703
2OZ7_A	1.188	2.912	0.621	4.689	0.248	0.522	0.236	0.661	0.898
2PIO_A	1.201	3.122	0.606	5.150	0.873	0.462	0.183	0.631	0.664
2PIP_A	1.195	3.226	0.570	5.657	0.841	0.290	0.140	0.618	0.782

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	contact	phobic	philic	balance	don/acc	refdist	refmin	refavg	sitemin
2PIQ_A	1.218	3.575	0.525	6.812	1.230	0.197	0.130	0.642	0.786
2PIR_A	1.180	3.315	0.507	6.542	0.145	0.382	0.105	0.635	0.741
2PIT_A	1.221	3.317	0.517	6.419	0.863	0.464	0.079	0.626	0.599
2PIU_A	1.248	3.270	0.617	5.304	1.218	0.361	0.110	0.621	0.814
2PIV_A	1.219	3.221	0.547	5.893	0.836	0.422	0.197	0.627	0.595
2PIW_A	1.202	3.309	0.588	5.629	0.579	0.468	0.113	0.634	0.610
2PIX_A	1.206	3.439	0.467	7.361	1.556	0.391	0.204	0.631	0.692
2PKL_A	1.225	3.849	0.371	10.376	0.367	0.300	0.139	0.582	0.767
2PNU_A	1.241	3.247	0.618	5.251	0.883	0.502	0.169	0.583	1.282
2Q7I_A	1.227	4.153	0.340	12.224	1.416	0.501	0.064	0.595	0.752
2Q7J_A	1.238	4.413	0.374	11.805	1.654	0.696	0.151	0.649	0.780
2Q7K_A	1.271	4.290	0.356	12.037	1.576	0.708	0.107	0.596	0.815
2Q7L_A	1.243	3.563	0.475	7.501	2.239	0.260	0.159	0.657	0.768
2Z4J_A	1.212	3.623	0.451	8.027	1.298	0.235	0.214	0.656	0.815
3B5R_A	1.315	3.642	0.550	6.623	2.136	0.423	0.188	0.649	1.874
3B65_A	1.356	4.160	0.448	9.276	1.749	0.958	0.100	0.603	1.201
3B66_A	1.338	3.844	0.462	8.318	2.357	0.707	0.191	0.627	1.858
3B67_A	1.288	2.551	0.831	3.071	0.928	0.334	0.136	0.565	1.542
3B68_A	1.329	3.624	0.495	7.315	1.492	0.911	0.176	0.591	1.779

Cognate Ligand (SMILE)	PDB code_Chain
O=C(O)Cc1cc(Cl)c(c(Cl)c1)Oc(c2)ccc(O)c2C(C)C	1NAV_A
O=C(O)[C@@H]([NH4])Cc(cc1I)cc(I)c1Oc(cc2)cc(I)c2O	1BSX_A
CC(C)c1c(O)ccc(c1)Oc(c2C)c(C)cc(c2)-n(c(=O)[nH]3)ncc3=O	1N46_A
O=C(O)Cc1cc(Cl)c(c(Cl)c1)Oc(c2)ccc(O)c2C(C)C	1NAX_A
O=C(O)Cc(cc1I)cc(I)c1Oc(cc2)cc(I)c2O	1NQ0_A
O=C(O)Cc(cc1I)cc(I)c1Oc(cc2)cc(I)c2O	1NQ1_A
O=C(O)Cc(cc1I)cc(I)c1Oc(cc2)cc(I)c2O	1NQ2_A
O=C(O)Cc(cc1I)cc(I)c1Oc(cc2)cc(I)c2O	1NUO_A
O=C(O)COc(cc1C)cc(C)c1Cc(c2)ccc(O)c2Cc3ccccc3	1Q4X_A
c1ccccc1CCNC(=O)c2c(O)ccc(c2)Oc(c(Br)c3)c(Br)cc3CC(O)O	1R6G_A
O=C(O)[C@@H]([NH4])Cc(cc1I)cc(I)c1Oc(cc2)cc(I)c2O	1XZX_X
O=C(O)[C@@H]([NH4])Cc(cc1I)cc(I)c1Oc(cc2I)cc(I)c2O	1Y0X_X
O=C(O)CCc1cc(Br)c(c(Br)c1)Oc(c2)ccc(O)c2C(C)C	2J4A_A
O=C(O)Cc(cc1I)cc(I)c1Oc(cc2)cc(I)c2O	2PIN_A
O=C(O)Cc(cc1I)cc(I)c1Oc(cc2)cc(I)c2O	3D57_A
O=C(O)[C@@H]([NH4])Cc(cc1I)cc(I)c1Oc(cc2)cc(I)c2O	3GWS_X
O=C(O)COc(cc1C)cc(C)c1Cc(c2)ccc(O)c2C(C)C	3HZF_A
O=C(O)COc(cc1C)cc(C)c1Cc(c2)ccc(O)c2C(C)C	3IMY_A
O=C(O)c1ccc(cc1)NC(=O)c(cc2)cc(c23)C(CCC3(C)C)c(c4)cnc(c45)cccc5	1DKF_B
O=C(O)c1ccc(cc1)/C=C(\C)c(c2)ccc(c23)C(C)(C)CCC3(C)C	1XAP_A
O=C(O)c1cc(F)c(cc1)NC(=O)[C@H](O)c(c2)ccc(c23)C(C)(C)CCC3(C)C	1EXA_A
O=C(O)c1cc(F)c(cc1)NC(=O)[C@@H](O)c(c2)ccc(c23)C(C)(C)CCC3(C)C	1EXX_A
O=C(O)c(c1)ccc(c12)cc(cc2)[C@H](O)c(c3)ccc(c34)C(C)(C)CCC4(C)C	1FCX_A
c1cc(C(=O)O)cc(c12)ccc(c2)C(=O)c(c3)ccc(c34)C(C)(C)CCC4(C)C	1FCY_A
O=C(O)c1ccc(cc1)\C=C\C(=O)c(c2)ccc(c23)C(C)(C)CCC3(C)C	1FCZ_A
c1cc(C(=O)O)cc(c12)ccc(c2)C(=N/O)\c(c3)ccc(c34)C(C)(C)CCC4(C)C	1FD0_A
O=C(O)\C=C(C)\C=C\C=C(C)\C=C\C(C1(C)C)=C(C)CCC1	2LBD_A
O=C(O)\C=C(C)\C=C\C=C(C)/C=C/C(C1(C)C)=C(C)CCC1	3LBD_A
O=C(O)c1cc(F)c(cc1)NC(=O)[C@@H](O)c(c2)ccc(c23)C(C)(C)CCC3(C)C	4LBD_A
CCO[C@H](C(=O)O)Cc1ccc(cc1)OCCc2ccc(cc2)OS(=O)(=O)C	1I7G_A
c1ccccc1C(=O)\C=C(\C)N[C@H](C(=O)O)Cc2ccc(cc2)OCCC3=NC(OC3C)c4ccccc4	1K7L_A
c1cc(C(F)(F)F)ccc1C(=O)\C=C(\C)N[C@H](CNC(=O)CC)Cc2ccc(cc2)OCCc3c(C)oc(n3)-c4ccccc4	1KKQ_A
CCCO\N=C(C)\[C@H](C(=O)O)Cc1ccc(cc1)OCc2c(C)oc(n2)-c3ccccc3	2NPA_A
O=C(O)C(C)(C)Oc(cc1)ccc1CNC(=O)c2c(C)nc(s2)-c(cc3)ccc3C(F)(F)F	2P54_A
COc(cc1)ccc1N2[C@H](C(=O)O)[C@@H](C2=O)Cc3cc(ccc3)OCCc4c(C)oc(n4)-c5ccccc5	2REW_A
CC[C@H](C(=O)O)Cc(c1)ccc(OCCC)c1CNC(=O)c2ccc(cc2)C34C[C@@H]5C[C@H](C3)C[C@H](C4)C5	2ZNN_A
COc(c1)ccc(c12)n(cc2CCC(=O)O)S(=O)(=O)c(cc3)ccc3OC	3ET1_A
CO[C@H](C(=O)O)Cc(c(c12)scc1)ccc2OCCC3=NC(OC3C)c4ccccc4	3G8I_A
O=C(O)C(C)(C)Oc(cc1)ccc1CCCN(C(=O)Nc(c2Cl)cccc2Cl)CCc3c(F)cccc3Cl	1GWX_A
CC[C@@](C)(C(=O)O)Oc(cc1)ccc1CCN(CCCCCCC)C(=O)Nc2c(F)cc(F)cc2	1Y0S_A

Cognate Ligand (SMILE)	PDB code_Chain
O=C(O)CCCCCCCCC/C=C\CCCCCC	2AWH_A
O=C(O)CCCCCCCCC/C=C\CCCCCC	2B50_A
O=C(O)CCCCCCCCC/C=C\CCCCCC	2BAW_A
c1ccccc1-c2onc(-c(ccc3)cc3CC(=O)O)c2C(=O)NCCOc4c(Cl)cc(Cl)cc4	2J14_A
CC[C@H](C(=O)O)Cc(c1)ccc(OCCCC)c1CNC(=O)c2c(F)cc(C(F)(F)F)cc2	2ZNP_A
CC[C@H](C(=O)O)Cc(c1)ccc(OC)c1CNC(=O)c2c(F)cc(C(F)(F)F)cc2	2ZNQ_A
O=C(O)COc1ccc(cc1)OCCCOc(cc2)c(CCC)c(O)c2C(=O)C	3D5F_A
c1cccc(c1C(=O)O)NC(=O)c2cc(ccc2)S(=O)(=O)N(CC3)Cc(c34)cccc4	3DY6_A
COc(c1)ccc(c12)n(cc2CCC(=O)O)S(=O)(=O)c(cc3)ccc3OC	3ET2_A
FC(F)(F)c1ccc(cc1)OCc2cc(OCC#C)c(cc2)Sc(c(C)c3C)ccc3OCC(=O)O	3GZ9_A
N1C=CCC=C1N(C)CCOc(cc2)ccc2C[C@@H](C3=O)SC(=O)N3	1FM6_D
c1ccccc1C(=O)c2c(cccc2)N[C@H](C(=O)O)Cc3ccc(cc3)OCCc4c(C)oc(n4)-c5ccccc5	1FM9_D
CCO[C@H](C(=O)O)Cc1ccc(cc1)OCCc2ccc(cc2)OS(=O)(=O)C	1I7I_A
CCO[C@H](C(=O)O)Cc1ccc(cc1)OCCn(c2cccc3)c(c4c23)cccc4	1KNU_A
CCO[C@H](C(=O)O)Cc1ccc(cc1)OCCN2c(cccc3)c3Oc(c24)cccc4	1NYX_A
c1ccccc1C(=O)c2c(cccc2)N[C@H](C(=O)O)Cc3ccc(cc3)OCCc4c(C)oc(n4)-c5ccccc5	1RDT_D
c1cc(Cl)cc(Cl)c1C(=O)Nc(c2C(=O)O)ccc(c2)Oc3ncccn3	1WM0_X
CC(C)c(cc1)ccc1[C@@H](C(=O)O)Oc(c(c2)CCC)c(CCC)c(c23)on(C)c3=O	1ZEO_A
N1C=CCC=C1N(C)CCOc(cc2)ccc2C[C@@H](C3=O)SC(=O)N3	1ZGY_A
O=C(O)Cn(cc1)c(c12)ccc(c2)OCCCOc(cc3)c(CCC)c(c34)onc4C(F)(F)F	2ATH_A
O=C(O)Cn(cc1)c(c12)ccc(c2)OCCCOc(c3CCC)ccc(c34)cc(cc4)C(=O)c5ccccc5	2F4B_A
COc(cc1)c(OC)cc1Cc(c(c23)cc(OC)c(c3)OC)ncc2C[NH2](CC4)CC[C@@H]4c5c(OC)cccc5	2FVJ_A
s1cccc1-c2cc(NS(=O)(=O)c(cc3F)ccc3)n(n2)-c4ccc(F)cc4	2G0G_A
FC(F)(F)c1cc(C(F)(F)F)cc(c1)S(=O)(=O)Nc(cc2-c3cccs3)n(n2)-c4ccc(F)cc4	2G0H_A
CCO[C@H](C(=O)O)Cc(c1)ccc(c12)n(cc2)Cc3c(C)oc(n3)-c4c(Cl)cccc4	2GTK_A
O=C(O)COc(c1)ccc(c12)n(cc2)CCCOc(c3CCC)ccc(c34)cc(cc4)C(=O)c5ccccc5	2HWQ_A
O=C(O)C(C)(C)Oc1cccc(c12)n(cc2)CCCOc(c3CCC)ccc(c34)cc(cc4)C(=O)c5ccccc5	2HWR_A
CC[C@](C)(C(=O)O)Oc(cc1)ccc1CCN(CCCCCCC)c(n2)oc(c23)cccc3	2I4J_A
CC[C@@](C)(C(=O)O)Oc(cc1)ccc1CCN(CCCCCCC)c(n2)oc(c23)cccc3	2I4P_A
CC[C@@](C)(C(=O)O)Oc(cc1)ccc1CCN(CCCCCCC)c(n2)oc(c23)cccc3	2I4Z_A
CCCCCCC(C)(C)c(cc1O)cc(c12)OC(C)(C)[C@H]3[C@H]2CC(C(=O)O)=CC3	2OM9_A
O=C(O)[C@@H](C)Oc(c1)ccc(Cl)c1Cn(c(c23)cc(cc3)OC(F)(F)F)c(C)c2-c4noc(c45)cc(cc5)OC	2P4Y_A
c1ccccc1C(=O)c2c(cccc2)N[C@H](CNC(=O)C)Cc3ccc(cc3)OCCc4c(C)oc(n4)-c5ccccc5	2POB_A
N1C=CCC=C1N(C)CCOc(cc2)ccc2C[C@@H](C3=O)SC(=O)N3	2PRG_A
c1cccc(O[C@@H](C)C(=O)O)c1Cc2c(C)n(c(c23)ccc(c3)OC(F)(F)F)C(=O)c4ccc(cc4)OC	2Q59_A
c1ccccc1Sc2c(C(=O)O)n(c(c23)ccc(Cl)c3)Cc4cc(OC)ccc4	2Q6R_A
c1cc(Cl)cc(Cl)c1C(=O)Nc(c2C(=O)O)ccc(c2)Oc3ncccn3	2Q6S_B
O=C(O)CCCCCCC\C=C/C=C/[C@@H](O)CCCCC	2VST_A
O=C(O)CC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CC	2VV0_A
O=C(O)CC[C@H](O)\C=C\C=C/C/C=C\C/C=C\C/C=C\C/C=C\CC	2VV1_A

Cognate Ligand (SMILE)	PDB code_Chain
O=C(O)CCC[C@@H](O)\C=C\C=C/C/C=C\C/C=C\C/C=C\CC	2VV2_A
O=C(O)CCC(=O)C/C=C/CC/C=C\C/C=C\C/C=C\C/C=C\CC	2VV3_A
O=C(O)CCCCC(=O)C[C@@H](O)/C=C\C/C=C\CCCCC	2VV4_A
O=C(O)CCC/C=C\C[C@H]1C=CC(=O)/C1=C/C=C\CCCCC	2ZK1_A
O=C(O)CCC/C=C\C[C@H]1C=CC(=O)\C1=C/C=C\CCCCC	2ZK2_A
O=C(O)CCC/C=C\CC(=O)/C=C/C=C\C/C=C\CCCCC	2ZK3_A
CCCCCC(=O)/C=C/C=C\C/C=C\C/C=C\CCCC(=O)O	2ZK4_A
CCC/C([N+]([O-])=O)=C/c1ccc(o1)-c(ccc2)cc2C(=O)O	2ZK5_A
CC[C@H](C(=O)O)Cc1cc(ccc1)CNC(=O)c2ccc(cc2)C34C[C@@H]5C[C@H](C3)C[C@H](C4)C5	2ZNO_A
O=C(O)CCC/C=C\C[C@H]1C=CC(=O)/C1=C/C=C\CCCCC	2ZVT_A
c1ccccc1C[C@@H](C(=O)O)Oc(cc2)ccc2-c3ccccc3	3B3K_A
c1ccccc1-n(n2)nc(c2CC(=O)O)Cc3cc(ccc3)OCCc4c(C)oc(n4)-c5ccccc5	3BC5_A
c1ccccc1C[C@@H](C(=O)O)Oc2ccc(Cl)cc2	3CDP_A
c1ccccc1C[C@@H](C(=O)O)Oc(cc2)ccc2CC	3CDS_A
N1C=CCC=C1N(C)CCOc(cc2)ccc2C[C@@H](C3=O)SC(=O)N3	3CS8_A
CCCCC/C=C\C/C([N+]([O-])=O)=C\CCCCCCCC(=O)O	3CWD_A
c1cc(Cl)cc(Cl)c1C(=O)Nc(c2C(=O)O)ccc(c2)Oc3ncccn3	3DZU_D
N1C=CCC=C1N(C)CCOc(cc2)ccc2C[C@@H](C3=O)SC(=O)N3	3DZY_D
[O-][N+](=O)c(c1)ccc(Cl)c1C(=O)Nc2ccccc2	3E00_D
COc(c1)ccc(c12)n(cc2CCC(=O)O)S(=O)(=O)c(cc3)ccc3OC	3ET3_A
CCO[C@H](C(=O)O)Cc1c(C)cc(cc1)OCc2csc(n2)-c3ccc(Cl)cc3	3FEI_A
CCO[C@H](C(=O)O)Cc1c(C)cc(cc1)OCc2csc(n2)-c3ccc(Cl)cc3	3FEJ_A
c1cccc(c12)ncc(c2)Oc3c(Cl)cc(cc3Cl)NS(=O)(=O)c4c(Cl)cc(Cl)cc4	3FUR_A
CO[C@H](C(=O)O)Cc(c(c12)scc1)ccc2OCCc3c(C)oc(n3)-c4ccccc4	3G9E_A
FC(F)(F)c1ccc(cc1)OCc2cc(OCC#CCC)c(cc2)Sc(c(c34)CCCC4)ccc3OCC(=O)O	3H0A_D
c1ccccc1C[C@@H](C(=O)O)Oc(cc2)ccc2Cc3ccccc3	3HO0_A
CCOP(=O)(OCC)/C(P(=O)(OCC)OCC)=C/c(c1)cc(C(C)(C)C)c(O)c1C(C)(C)C	3HOD_A
n1ccnn1[C@H](C(=O)O)Cc2ccc(cc2)CCCc3c(C)oc(n3)-c4ccccc4	3IA6_B
C1C=CCC=C1CN(C[C@@H]2C=CC=CC2)C(=O)C[C@@H](C3=O)S[C@@H](CCCCCCC)N3CCCCc(cc4)ccc4C(=O)O	4PRG_A
CC(C)CCC[C@@H](C)[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)C(=CC3)C[C@@H](O)CC4	1N83_A
CC(C)CCC[C@@H](C)[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)C(=CC3)C[C@H](CC4)OS(=O)(=O)O	1S0X_A
CC1(C)[C@@H](O1)CC[C@@H](C)[C@H]2CC[C@H]([C@@]23C)[C@H]4[C@H](CC3)[C@]5(C)C(=CC4)C[C@@H](O)CC5	1P8D_A
O=C(O)Cc1cc(ccc1)OCCCN(Cc(c(Cl)c2C(F)(F)F)ccc2)CC(c3ccccc3)c4ccccc4	1PQ6_A
FC(F)(F)C(C(F)(F)F)(O)c1ccc(cc1)NCC(F)(F)F	1PQ9_A
FC(F)(F)C(C(F)(F)F)(O)c1ccc(cc1)N(CC(F)(F)F)S(=O)(=O)c2ccccc2	1PQC_A
FC(F)(F)C(C(F)(F)F)(O)c1ccc(cc1)N(CC(F)(F)F)S(=O)(=O)c2ccccc2	1UPV_A
FC(F)(F)C(C(F)(F)F)(O)c1ccc(cc1)N(CC(F)(F)F)S(=O)(=O)c2ccccc2	1UPW_A
c1ccc(C(F)(F)F)c(c12)nccc2-c3cc(ccc3)Oc4cc(S(=O)(=O)C)ccc4	3KFC_A
FC(F)(F)C(C(F)(F)F)(O)c1ccc(cc1)N(CC(F)(F)F)S(=O)(=O)c2ccccc2	1UHL_B
c1ccccc1CN(C2=O)C(=O)C(=C2c3ccccc3)Nc4ccc(cc4)OC	2ACL_B

Cognate Ligand (SMILE)	PDB code_Chain
FC(F)(F)C(C(F)(F)F)(O)c1ccc(cc1)N(CCCC)Cc2cc(OC)c(c(Cl)c2)OC	3FAL_B
O=C(O)Cn(cc1)c(c12)cccc2OCCCN(Cc(c(Cl)c3C(F)(F)F)ccc3)CC(c4ccccc4)c5ccccc5	3FC6_B
COC(=O)CCc1cc(ccc1)N(C(=O)C2CCCCC2)Cc3ccc(cc3)-c4ccc(cc4)N(C)C	1OSH_A
c1cc(O)ccc1C(=O)[C@H]2CC[C@H]([C@@]23C)[C@H]4[C@H](CC3)[C@]5(C)C(=CC4)C=C(C(=O)O)CC5	3BEJ_A
O=C(O)c1cc(ccc1)\C=C\c2c(Cl)cc(cc2)OCc3c(C(C)C)onc3-c4c(Cl)cccc4Cl	3DCT_A
c1cc(F)c(F)cc1C(=O)N(C=C2C(=O)OC(C)C)CC(C)(C)[C@H]3[C@H]2Nc(c34)cccc4	3FLI_A
O=C(O)c1cc(ccc1)\C=C\c2c(Cl)cc(cc2)OCc3c(C(C)C)onc3C[S@@](=O)c4c(Cl)cccc4Cl	3GD2_A
c1cc(F)cc2[nH]c(c3c12)C(C(=O)OC(C)C)=CN(CC3(C)C)C(=O)c4ccc(cc4)OCCCN5CCOCC5	3L1B_A
C1CCCCC1NC(=O)[C@H](C2CCCCC2)n3c(-c4ccc(Cl)cc4)nc(c35)ccc(c5)C(=O)O	3OKH_A
C1CCCCC1NC(=O)[C@H](C2CCCCC2)n(c(c34)cccc3)c(n4)-c5ccc(Cl)cc5	3OKI_A
O=C(O)c1cc(C)c(cc1)NC(=O)[C@H](C2CCCCC2)n(c(c34)cc(F)c(F)c3)c(n4)-c5ccc(Cl)cc5	3OLF_A
c1cccc(c1C)NC(=O)[C@H](C2CCCCC2)n(c(c34)cc(F)c(F)c3)c(n4)-c5ccc(Cl)cc5	3OMK_A
O=C(O)c1cc(F)c(cc1)NC(=O)[C@H](C2CCCCC2)n(c(c34)cc(F)c(F)c3)c(n4)-c5ccc(Cl)cc5	3OMM_A
O=C(O)c1ccc(cc1)NC(=O)[C@H](C2CCCCC2)n(c(c34)cc(F)c(F)c3)c(n4)-c5ccc(Cl)cc5	3OOF_A
O=C(O)c1cc(F)c(c(F)c1)NC(=O)[C@H](C2CCCCC2)n(c(c34)cc(F)c(F)c3)c(n4)-c5ccc(Cl)cc5	3OOK_A
CC(C)(O)CCC[C@@H](C)[C@H]1CC[C@H]([C@@]12C)\C(CCC2)=C\C=C3/C(=C)[C@@H](O)C[C@@H](C3)O	1DB1_A
CCC(O)(CC)CCCO[C@H](C)[C@H]1CC[C@H]([C@@]12C)\C(CCC2)=C\C=C3/C(=C)[C@@H](O)C[C@@H](C3)O	1IE8_A
CC(C)(O)CCC[C@H](C)[C@H]1CC[C@H]([C@@]12C)\C(CCC2)=C\C=C3/C(=C)[C@@H](O)C[C@@H](C3)O	1IE9_A
CCC(O)(CC)/C=C/C=C/[C@@H](C)[C@H]1CC[C@H]([C@@]12C)\C(CCC2)=C\C=C3/C(=C)[C@@H](O)C[C@@H](C3)O	1S0Z_A
C1CC1[C@H](O)\C=C\[C@@H](C)[C@H]2CC[C@H]([C@@]23C)\C(CCC3)=C\C=C4/C(=C)[C@@H](O)C[C@@H](C4)O	1S19_A
CC(C)(O)C#CC[C@@H](C)[C@H]1CCC([C@@]12C)\C(CCC2)=C\C[C@H]3C[C@@H](O)C[C@@H](C3)O	1TXI_A
CC(C)(O)CCC[C@@H](C)[C@H]1CC[C@H]([C@@]12C)\C(CCC2)=C\C=C3/C(=C)[C@@H](O)[C@H]([C@@H](C3)O)CCC	2HAM_A
CC(C)(O)CCC[C@@H](C)[C@H]1CC[C@H]([C@@]12C)\C(CCC2)=C\C=C3/C(=C)[C@@H](O)[C@H]([C@@H](C3)O)OCCCO	2HAR_A
CC(C)(O)CCC[C@@H](C)[C@H]1CC[C@H]([C@@]12C)\C(CCC2)=C\C=C3/C(=C)[C@@H](O)[C@H]([C@@H](C3)O)OCCC	2HAS_A
CC(C)(O)CCC[C@@H](C)[C@H]1CC[C@H]([C@@]12C)\C(CCC2)=C\C=C3/C(=C)[C@@H](O)[C@H]([C@@H](C3)O)CCCO	2HB7_A
CC(C)(O)CCC[C@@H](C)[C@H]1CC[C@H]([C@@]12C)\C(CCC2)=C\C=C3/C(=C)[C@@H](O)[C@@H](C)[C@@H](C3)O	2HB8_A
CC(C)(O)C[C@H](CO1)C[C@@]1(C)[C@H]2CC[C@H]([C@@]23C)\C(CCC3)=C\C=C4/C(=C)[C@@H](O)C[C@@H](C4)O	3CS4_A
CC(C)(O)C[C@@H](CO1)C[C@@]1(C)[C@H]2CC[C@H]([C@@]23C)\C(CCC3)=C\C=C4/C(=C)[C@@H](O)C[C@@H](C4)O	3CS6_A
CCOP(=O)(OCC)/C(P(=O)(OCC)OCC)=C/c(c1)cc(C(C)(C)C)c(O)c1C(C)(C)C	1ILH_A
C/C(C)=C/CC[C@]1(C)[C@H](C\C=C(\C)C)C[C@@](C\C=C(\C)C)(C(=O)[C@@]12C(=O)C(C)C)C(=O)C(=C2O)C\C=C(\C)C	1M13_A
CCOP(=O)(OCC)/C(P(=O)(OCC)OCC)=C/c(c1)cc(C(C)(C)C)c(O)c1C(C)(C)C	1NRL_A
O1\C=C\[C@H](OC)[C@@H](C)[C@@H](OC(=O)C)[C@H](C)[C@H](O)[C@H](C)[C@@H](O)[C@@H](C)\C=C\C=C(\C)C(=O)Nc(c2O)c(/C=N/N(CC3)CCN3C)c(O)c4c2c(O)c(C)c(O5)c4C(=O)[C@@]15C	1SKX_A
FC(F)(F)C(C(F)(F)F)(O)c1ccc(cc1)N(CC(F)(F)F)S(=O)(=O)c2ccccc2	2O9I_A
C/C(C)=C/CC1(C\C=C(\C)C)C(=O)C(C(=O)C(C)C)C(=O)C(C1=O)C\C=C(\C)C	2QNV_A
c1ccccc1C[C@@H](C(=O)O)Oc(cc2)ccc2CCc3ccccc3	3HLV_B
CC(=O)[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)[C@H](CC3)CC(=O)CC4	1XV9_B
c1cc(Cl)ccc1-c(n2)c(n(c23)ccs3)/C=N/OCc4cc(Cl)c(Cl)cc4	1XVP_B
O=C(O)CCCCCCCCCCCCC	1PZL_A
O=C(O)CCCCCCCCCCCCC	3FS1_A
O=C(O)CCCCCCCCCCCCCC	1LV2_A

Cognate Ligand (SMILE)	PDB code_Chain
O=C(O)\C=C(C)\C=C\C=C(C)/C=C/C(C1(C)C)=C(C)CCC1	1FBY_A
O=C(O)\C=C(C)\C=C\C=C(C)/C=C/C(C1(C)C)=C(C)CCC1	1FM6_A
O=C(O)\C=C(C)\C=C\C=C(C)/C=C/C(C1(C)C)=C(C)CCC1	1FM9_A
O=C(O)\C=C(C)\C=C\C=C(C)\C=C\C(C1(C)C)=C(C)CCC1	1G5Y_A
O=C(O)\C=C(C)\C=C\C=C(C)/C=C/C(C1(C)C)=C(C)CCC1	1K74_A
O=C(O)CCCCCCCCCCC/C=C/CCCCCCCC	1MV9_A
O=C(O)c1ccc(cc1)C2(OCCO2)c(c3)ccc(c34)C(C)(C)CCC4(C)C	1MVC_A
O=C(O)c1ccc(cc1)C2(OCCO2)c(c3)ccc(c34)C(C)(C)CCC4(C)C	1MZN_A
O=C(O)/C=C/c(c1)oc(c12)cccc2-c(c3)ccc(c34)C(C)(C)CCC4(C)C	1RDT_A
O=C(O)\C=C(C)\C=C\C/C(C)=C/CC(C1(C)C)=C(C)CCC1	1XLS_A
O=C(O)CCCCCCCCCCCCCC	1XV9_A
O=C(O)CCCCCCCCCCCCCC	1XVP_A
O=C(O)\C=C(C)\C=C\C=C(C)/C=C/C(C1(C)C)=C(C)CCC1	2ACL_A
O=C(O)/C=C/c1cc(c(O)cc1)-c(c2)c(OC)cc(c23)C(C)(C)CCC3(C)C	2P1T_A
O=C(O)/C=C/c1cc(c(O)cc1)-c(c2)c(OCC)cc(c23)C(C)(C)CCC3(C)C	2P1U_A
O=C(O)/C=C/c1cc(c(O)cc1)-c(c2)c(OCCC)cc(c23)C(C)(C)CCC3(C)C	2P1V_A
O=C(O)c1ccc(cc1)C2(OCCO2)c(c3)ccc(c34)C(C)(C)CC4(C)C	2ZXZ_A
O=C(O)c1ccc(cc1)C2(OCCO2)c(c3)ccc(c34)[Si](C)(C)C[Si]4(C)C	2ZY0_A
O=C(O)\C=C(C)\C=C\C=C(C)/CCC(C1(C)C)=C(C)CCC1	3DZU_A
O=C(O)\C=C(C)\C=C\C=C(C)/CCC(C1(C)C)=C(C)CCC1	3DZY_A
O=C(O)\C=C(C)\C=C\C=C(C)/CCC(C1(C)C)=C(C)CCC1	3E00_A
O=C(O)\C=C(C)\C=C\C=C(C)/C=C/C(C1(C)C)=C(C)CCC1	3FAL_A
O=C(O)\C=C(C)\C=C\C=C(C)/C=C/C(C1(C)C)=C(C)CCC1	3FC6_A
c1cc(C(=O)O)ccc1C(=C)c(c2)c(C)cc(c23)C(C)(C)CCC3(C)C	3H0A_A
O=C(O)c1ccc(nc1)C2(CC2)c(c(C)c3)cc(c34)C(C)(C)CCC4(C)C	1H9U_A
O=C(O)\C=C(C)\C=C\C[C@@H](C)CCCC(C)(C)OC	1UHL_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)c4c(CC3)cc(O)cc4	1A52_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)c4c(CC3)cc(O)cc4	1ERE_A
c1cc(O)cc(c12)sc(-c3ccc(O)cc3)c2C(=O)c4ccc(cc4)OCC[NH2]5CCCCC5	1ERR_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)c4c(CC3)cc(O)cc4	1G50_A
c1cc(O)cc(c12)sc(c2)-c3ccc(O)cc3	1GWQ_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)c4c(CC3)cc(O)cc4	1GWR_A
c1c(O)ccc2c1C[C@@H](CC)C3=C2[C@H](CC)Cc(c34)cc(O)cc4	1L2I_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)c4c(CC3)cc(O)cc4	1PCG_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)c4c(CC3)cc(O)cc4	1QKT_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)c4c(CC3)cc(O)cc4	1QKU_A
c1ccccc1C(\CC)=C(c2ccccc2)/c3ccc(cc3)\C=C\C(=O)O	1R5K_A
C1CCCC[NH2]1CCOc(cc2)ccc2[C@H](O3)[C@@H](c4ccc(O)cc4)Sc(c35)cc(O)cc5	1SJ0_A
C1CCCC[NH2]1CCOc(cc2)ccc2[C@H]3N(c4ccccc4)CCc(c35)cc(O)cc5	1UOM_A
c1c(O)cc(CC#N)c(c12)OC(C2)c3ccc(O)cc3	1X7E_A

Cognate Ligand (SMILE)	PDB code_Chain
Oc1cc(O)cc(c12)occ(c2=O)-c3ccc(O)cc3	1X7R_A
C[C@@H]1[C@@H](C)C[NH2](C1)CCOc(cc2)ccc2[C@H](O3)[C@@H](c4ccc(O)cc4)Sc(c35)cc(O)cc5	1XP1_A
C[C@H]1[C@H](C)C[NH2](C1)CCOc(cc2)ccc2[C@H](O3)[C@@H](c4ccc(O)cc4)Sc(c35)cc(O)cc5	1XP6_A
C1CCC[NH2]1[C@@H](C)COc(cc2)ccc2[C@H](O3)[C@@H](c4ccc(O)cc4)Sc(c35)cc(O)cc5	1XP9_A
C1CCC[NH2]1[C@H](C)COc(cc2)ccc2[C@H](O3)[C@@H](c4ccc(O)cc4)Sc(c35)cc(O)cc5	1XPC_A
c1cc(O)cc(c12)CCN(c3ccccc3)[C@@H]2c4ccc(cc4)N(C5)CC[NH2]([C@H]56)CCCC6	1XQC_A
C1CCC[NH2]1CCOc(cc2)ccc2[C@H](Oc(c34)ccc(c3)O)[C@H]([C@@H]4C)c5ccc(O)cc5	1YIM_A
C1CCCC[NH2]1CCOc(cc2)ccc2[C@H](Oc(c34)ccc(c3F)O)[C@H]([C@@H]4C)c5ccc(O)cc5	1YIN_A
OC[C@]12[C@H](C)C=C(C)[C@H]([C@H]1C)[C@@H](OC2)c3ccc(O)cc3	1ZKY_A
C1CCCC[NH2]1CCOc2ccc(cc2)Oc3c(-c4ccc(cc4)S(=O)(=O)C)ccc(c35)cc(O)cc5	2AYR_A
OC[C@]12CC=C(C)[C@H](C1)[C@H](OC2)c3ccc(O)cc3	2B1V_A
C[C@@]1(O)CC[C@H]([C@@]12C)c3c(CC2)c4c(cc3)cc(O)cc4	2B1Z_A
c1ccccc1C(\CC)=C(c2ccc(O)cc2)/c3ccc(cc3)OCC[NH2](C)C	2BJ4_A
OC[C@@]12[C@H](C)[C@@H]([C@@H](C)CC1)[C@H](OC2)c3ccc(O)cc3	2FAI_A
CC([C@@H]12)=CC[C@@H](C2)C(C)(C)O[C@H]1c3ccc(O)cc3	2G44_A
c1cc(O)ccc1[C@@H]([C@H]([C@@H]23)CCC2)Oc4c3cc(O)cc4	2I0G_A
c1cc(O)ccc1[C@@H]([C@H]([C@@H]23)CCC2)Oc4c3cc(O)cc4	2I0J_A
c1cccc(c12)[nH]c(-c3ccccc3)c2CC(=O)N[C@H](C)CCc4ccc(O)cc4	2IOK_A
c1ccccc1C(\CC)=C(c2ccc(O)cc2)/c3ccc(cc3)OCC[NH2](C)C	2JF9_A
c1cc(O)cc(c12)sc(-c3ccc(O)cc3)c2C(=O)c4ccc(cc4)OCC[NH2]5CCCCC5	2JFA_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)c4c(CC3)cc(O)cc4	2OCF_A
C1CCC[NH2]1CCOc(cc2)ccc2[C@H]3[C@@H](c4ccccc4)CCc(c35)cc(O)cc5	2OUZ_A
c1cccc(c1C(F)(F)F)\C=C\[C@]2(O)CC[C@H]([C@@]23C)[C@H]4[C@H](CC3)c5c(CC4)cc(O)cc5	2P15_A
c1cc(O)ccc1[C@@H]([C@H]([C@@H]23)CCC2)Oc4c3c(O)ccc4	2POG_A
c1cc(O)ccc1[C@@H]([C@H]([C@@H]23)CC(F)(F)C2)Oc4c3cc(O)cc4	2Q70_A
c1cc(O)cc(c12)n[nH]c2-c3c(O)cc(O)cc3	2QA6_A
Oc1cc(O)cc(c12)occ(c2=O)-c3ccc(O)cc3	2QA8_A
c1cc(O)ccc1-n(c2CC)nc(c23)ccc(c3)O	2QAB_A
COCc1cc(O)cc2c1O[C@H]([C@H]([C@H]23)CCC3)c4ccc(O)cc4	2QE4_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H]([C@H](C2)COC)c4c(CC3)cc(O)cc4	2QGT_A
c1c(O)ccc(c12)nn(c2Cl)-c3ccc(O)cc3	2QGW_A
CCOC(=O)[C@@H]1[C@H](C(=O)OCC)[C@@H](O2)C(c3ccc(O)cc3)=C([C@H]12)c4ccc(O)cc4	2QH6_A
COC(=O)C([C@H]12)=C(C(=O)OC)[C@H](O2)C(c3ccc(O)cc3)=C1c4ccc(O)cc4	2QR9_A
Cn1c(N)nc(c12)ncc(c2)-c3ccc(O)cc3	2QSE_A
Cn1c(N)nc(c12)ncc(c2)-c3ccccc3	2QXM_A
c1cc(O)cc(c12)sc(-c3ccc(O)cc3)c2C(=O)c4ccc(cc4)OCC[NH2]5CCCCC5	2QXS_A
c1cc(O)cc(c12)sc(-c3ccc(O)cc3)c2C(=O)c4ccc(cc4)OCC[NH2](CC5)CC[C@@H]5C	2R6W_A
c1cc(O)cc(c12)sc(-c3ccc(O)cc3)c2C(=O)c4ccc(cc4)OCC[NH2]5CCCC5	2R6Y_A
c1cc(O)cc(c12)cc(C)c(-c3cc(O)ccc3)c2Oc4ccc(O)cc4	3DT3_A
c1cc(O)ccc1C(\CC)=C(/CC)c2ccc(O)cc2	3ERD_A

Cognate Ligand (SMILE)	PDB code_Chain
c1ccccc1C(\CC)=C(c2ccc(O)cc2)/c3ccc(cc3)OCC[NH2](C)C	3ERT_A
c1c(O)ccc2c1C[C@@H](CC)C3=C2[C@H](CC)Cc(c34)cc(O)cc4	1L2J_B
c1cc(Cl)ccc1CCCSc(n2)nc(N3CC[NH3]CC3)nc2NCCc4ccc(O)cc4	1NDE_A
Oc1cc(O)cc(c12)occ(c2=O)-c3ccc(O)cc3	1QKM_A
c1cc(O)cc(c12)sc(-c3ccc(O)cc3)c2C(=O)c4ccc(cc4)OCC[NH2]5CCCCC5	1QKN_A
c1cc(O)cc(c12)onc2-c3c(O)cc(O)cc3	1U3Q_A
c1cc(O)cc(c12)OC(N2)c3cccc(c34)c(O)ccc4	1U3R_A
c1cc(O)cc(c12)onc2-c(c3)ccc(c34)cc(O)cc4	1U3S_A
c1c(O)ccc(c12)OC(C2)c3ccc(O)cc3	1U9E_A
c1c(O)cc(C#N)c(c12)oc(c2)-c3ccc(O)cc3	1X76_A
c1c(O)cc(CC#N)c(c12)oc(c2)-c3ccc(O)cc3	1X78_A
C=Cc1cc(O)cc(c12)nc(o2)-c3cc(F)c(O)cc3	1X7B_A
Oc1cc(O)cc(c12)occ(c2=O)-c3ccc(O)cc3	1X7J_A
Clc1c(O)ccc(c12)cc(cc2)-c3ccc(O)cc3	1YY4_A
c1cc(O)c(F)cc1-c(cc2C#N)cc(c23)ccc(c3)O	1YYE_A
c1c(O)ccc(c12)C(Br)=C(C2=O)c3ccc(O)cc3	1ZAF_A
CCCC[C@@]12C(=C(Br)C(=O)CC2)c3c(C1)cc(O)cc3	2GIU_A
COCc1cc(O)cc2c1O[C@H]([C@H]([C@H]23)CCC3)c4ccc(O)cc4	2JJ3_A
O\N=C\c1ccc(c(c12)cccc2)-c3ccc(O)cc3	2NV7_A
COCc1cc(O)cc2c1O[C@H]([C@H]([C@H]23)CC(F)(F)C3)c4ccc(O)cc4	2QTU_A
c1cc(O)ccc1[C@@H]([C@H]([C@@H]23)CC(F)(F)C2)Oc4c3cc(O)cc4	2Z4B_A
C1CCCCC1C[NH3]Cc2cn(c(c23)cccc3)-c(cc4)ccc4C	2PJL_A
c1cc(O)ccc1C(C)(C)c2ccc(O)cc2	2E2R_A
c1ccccc1C(\CCCO)=C(c2ccc(O)cc2)/c3ccc(cc3)OCC[NH2](C)C	2EWP_A
c1cc(O)ccc1C(=O)NNCc(cc2)ccc2C(C)C	2GPP_A
c1ccccc1C(\CC)=C(c2ccc(O)cc2)/c3ccc(cc3)OCC[NH2](C)C	2GPU_A
c1ccccc1C(\CC)=C(c2ccc(O)cc2)/c3ccc(cc3)OCC[NH2](C)C	2GPV_A
c1cc(O)ccc1C(C)(C)c2ccc(O)cc2	2P7G_A
c1ccccc1C(\CC)=C(c2ccc(O)cc2)/c3ccc(cc3)OCC[NH2](C)C	2P7Z_A
c1ccccc1C(C)(C)c2ccc(O)cc2	2ZAS_A
c1cc(O)ccc1C2(CCCCC2)c3ccc(O)cc3	2ZKC_A
OCC(=O)[C@@]1(O)[C@H](C)C[C@H]([C@@]12C)[C@H]3[C@](F)([C@H](C2)O)[C@]4(C)C(CC3)=CC(=O)C=C4	1M2Z_A
CC#C[C@]1(O)CC[C@H]([C@@]12C)[C@H]3C(=C4C(CC3)=CC(=O)CC4)[C@H](C2)c5ccc(cc5)N(C)C	1NHZ_A
OCC(=O)[C@@]1(O)[C@H](C)C[C@H]([C@@]12C)[C@H]3[C@](F)([C@H](C2)O)[C@]4(C)C(CC3)=CC(=O)C=C4	1P93_A
OCC(=O)[C@@]1(O)[C@H](C)C[C@H]([C@@]12C)[C@H]3[C@H]([C@H](C2)O)[C@]4(C)C(C(C)=C3)=Cc5c(C4)cnn5C6=CCCC=C6	3BQD_A
o1cccc1C(=O)O[C@]2(C(=O)SCF)[C@H](C)C[C@H]([C@@]23C)[C@H]4[C@](F)([C@H](C3)O)[C@]5(C)C([C@@H](F)C4)=CC(=O)C=C5	3CLD_A
Clc1cccc(Cl)c1C(=O)N(CC)C[C@@](C(F)(F)F)(O)CNC(=O)c2c(N)n(nc2)-c3ccc(F)cc3	3E7C_A
OCC(=O)[C@@]1(O)[C@H](C)C[C@H]([C@@]12C)[C@H]3[C@](F)([C@H](C2)O)[C@]4(C)C(CC3)=CC(=O)C=C4	3GN8_A
CC#C[C@]1(O)CC[C@H]([C@@]12C)[C@H]3C(=C4C(CC3)=CC(=O)CC4)[C@H](C2)c5ccc(cc5)N(C)C	3H52_A
c1c(F)ccc(OC)c1C(C)(C)C[C@@](C(F)(F)F)(O)CNc2cc(C)cc(c23)n(nc3)-c(ccc4)cc4C(=O)N5CCC[C@@H]5C(=O)N	3K23_B

Cognate Ligand (SMILE)	PDB code_Chain
OCC(=O)[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)C(CC3)=CC(=O)CC4	1Y9R_A
CC(=O)[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)C(CC3)=CC(=O)CC4	1YA3_A
OCC(=O)[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H]([C@H](C2)O)[C@]4(C)C(CC3)=CC(=O)CC4	2A3I_A
OCC(=O)[C@H]1CC[C@H]([C@@]12C=O)[C@H]3[C@H]([C@H](C2)O)[C@]4(C)C(CC3)=CC(=O)CC4	2AA2_A
CC(=O)[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)C(CC3)=CC(=O)CC4	2AA5_A
CC(=O)[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)C(CC3)=CC(=O)CC4	2AA6_A
OCC(=O)[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)C(CC3)=CC(=O)CC4	2AA7_A
O\C=C(O)\[C@@]1(O)CC[C@H]([C@@]12C)[C@H]3[C@H](C(=O)C2)[C@]4(C)C(CC3)=CC(=O)C=C4	2AAX_A
CC(=O)S[C@@H]1CC(=CC(=O)CC2)[C@@]2(C)[C@@H](CC3)[C@@H]1[C@H](CC4)[C@@]3(C)[C@]45CCC(=O)O5	2AB2_A
OCC(=O)[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)C(CC3)CC(=O)CC4	2ABI_A
CC(=O)S[C@@H]1CC(=CC(=O)CC2)[C@@]2(C)[C@@H](CC3)[C@@H]1[C@H](CC4)[C@@]3(C)[C@]45CCC(=O)O5	2OAX_A
CC(=O)[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)C(CC3)=CC(=O)CC4	1A28_A
C[C@]1(O)CC[C@H]([C@@]12C)[C@H]3C(C=C2)=C4C(CC3)=CC(=O)CC4	1E3K_A
C#C[C@]1(O)CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@@H]4C(CC3)=CC(=O)CC4	1SQN_A
o1cccc1C(=O)O[C@]2(C(=O)CCl)[C@H](C)C[C@H]([C@@]23C)[C@H]4[C@](Cl)([C@H](C3)O)[C@]5(C)C(CC4)=CC(=O)C=C5	1SR7_A
N#Cc1ccc(n1C)-c(c2)ccc(c23)NC(=S)OC3(C)C	1ZUC_A
CC#C[C@]1(O)CC[C@H]([C@@]12C)[C@H]3C(=C4C(CC3)=CC(=O)CC4)[C@H](C2)c5ccc(cc5)N(C)C	2W8Y_A
CS(=O)(=O)N(C1)CC[C@@H]1N(c(cc2)cc(Cl)c2C#N)Cc3c(C)cccc3	3KBA_A
C[C@]1(O)CC[C@H]([C@@]12C)[C@H]3C(C=C2)=C4C(CC3)=CC(=O)CC4	1E3G_A
OCC(=O)[C@@]1(O)CC[C@H]([C@@]12C)[C@H]3[C@](F)([C@H](C2)O)[C@]4(C)C(CC3)=CC(=O)CC4	1GS4_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)[C@@H](CC3)CC(=O)CC4	1T5Z_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)[C@@H](CC3)CC(=O)CC4	1T63_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)[C@@H](CC3)CC(=O)CC4	1T65_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)[C@@H](CC3)CC(=O)CC4	1XJ7_A
C[C@]1(O)CC[C@H]([C@@]12C)[C@H]3C(C=C2)=C4C(CC3)=CC(=O)CC4	1XOW_A
C[C@]1(O)CC[C@H]([C@@]12C)[C@H]3C(C=C2)=C4C(CC3)=CC(=O)CC4	1XQ3_A
N#Cc1c(C(F)(F)F)cc(cc1)NC(=O)[C@@](C)(O)CS(=O)(=O)c(cc2)ccc2F	1Z95_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)C(CC3)=CC(=O)CC4	2AM9_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)[C@@H](CC3)CC(=O)CC4	2AMA_A
CC[C@]1(O)CC[C@H]([C@@]12CC)[C@H]3C(C=C2)=C4C(CC3)=CC(=O)CC4	2AMB_A
C[C@]1(O)CC[C@H]([C@@]12C)[C@H]3C(C=C2)=C4C(CC3)=CC(=O)CC4	2AO6_A
CC(C)(O)C(=O)Nc(c1)ccc([N+]([O-])=O)c1C(F)(F)F	2AX6_A
FC(F)(F)c1c([N+]([O-])=O)ccc(c1)NC(=O)[C@@](C)(O)COc2ccc(F)cc2	2AX7_A
FC(F)(F)c1c([N+]([O-])=O)ccc(c1)NC(=O)[C@@](C)(O)COc2ccc(F)cc2	2AX8_A
BrC[C@](C)(O)C(=O)Nc(c1)ccc([N+]([O-])=O)c1C(F)(F)F	2AX9_A
FC(F)(F)c1c([N+]([O-])=O)ccc(c1)NC(=O)[C@@](C)(O)COc2ccc(F)cc2	2AXA_A
FC(F)(F)CN(CC(F)(F)F)c(c1)ccc(c12)[nH]c(=O)cc2C(F)(F)F	2HVC_A
CC(=O)O[C@]1(C(=O)C)CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@@]4(C)[C@@H]5[C@@H](C5)C(=O)CC4=C(Cl)C3	2OZ7_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)[C@@H](CC3)CC(=O)CC4	2PIO_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)[C@@H](CC3)CC(=O)CC4	2PIP_A

Cognate Ligand (SMILE)	PDB code_Chain
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)[C@@H](CC3)CC(=O)CC4	2PIQ_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)[C@@H](CC3)CC(=O)CC4	2PIR_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)[C@@H](CC3)CC(=O)CC4	2PIT_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)[C@@H](CC3)CC(=O)CC4	2PIU_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)[C@@H](CC3)CC(=O)CC4	2PIV_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)[C@@H](CC3)CC(=O)CC4	2PIW_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)[C@@H](CC3)CC(=O)CC4	2PIX_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)[C@@H](CC3)CC(=O)CC4	2PKL_A
c1c(F)cc(F)cc1COCC[C@]23[C@@H](CC[C@@H]2O)[C@H]4[C@H](CC3)[C@]5(C)[C@@H](CC4)CC(=O)CC5	2PNU_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)C(CC3)=CC(=O)CC4	2Q7I_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)C(CC3)=CC(=O)CC4	2Q7J_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)C(CC3)=CC(=O)CC4	2Q7K_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)C(CC3)=CC(=O)CC4	2Q7L_A
O[C@H]1CC[C@H]([C@@]12C)[C@H]3[C@H](CC2)[C@]4(C)[C@@H](CC3)CC(=O)CC4	2Z4J_A
N#Cc1c(C(F)(F)F)cc(cc1)NC(=O)[C@@](C)(O)COc(c2)ccc(Cl)c2F	3B5R_A
N#Cc1c(I)cc(cc1)NC(=O)[C@@](C)(O)COc(cc2)ccc2C#N	3B65_A
N#Cc1c(C(F)(F)F)cc(cc1)NC(=O)[C@@](C)(O)COc(cc2)ccc2[N+]([O-])=O	3B66_A
FC(F)(F)c1c([N+]([O-])=O)ccc(c1)NC(=O)[C@@](C)(O)COc2c(F)c(F)c(F)c2F	3B67_A
FC(F)(F)c1c([N+]([O-])=O)ccc(c1)NC(=O)[C@@](C)(O)COc(cc2)ccc2NC(=O)C	3B68_A

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	Ligand Profile	volume	donorHB	accptHB	QPlogPo/w	MW	SASA	FOSA	FISA	PISA	WPSA	PSA
1NAV_A	Agonist	1047.201	2	3.25	4.361	355.217	594.987	195.012	148.283	142.016	109.676	79.236
1BSX_A	Agonist	1051.276	4	4.25	1.299	650.978	596.642	48.339	190.36	143.694	214.249	103.009
1N46_A	Agonist	1144.652	2	4.75	3.324	367.404	620.6	274.317	174.444	171.839	0	112.657
1NAX_A	Agonist	1042.086	2	3.25	4.325	355.217	590.911	190.563	148.263	144.644	107.441	79.235
1NQ0_A	Agonist	973.989	2	3.25	4.305	621.936	562.513	41.193	150.421	156.416	214.483	80.765
1NQ1_A	Agonist	973.019	2	3.25	4.303	621.936	563.601	43.179	149.685	156.378	214.359	80.272
1NQ2_A	Agonist	973.754	2	3.25	4.306	621.936	564.184	43.26	149.895	156.717	214.312	80.24
1NUO_A	Agonist	974.025	2	3.25	4.31	621.936	565.214	43.179	149.685	157.991	214.359	80.272
1Q4X_A	Agonist	1246.063	2	3.5	5.256	376.451	696.794	226.738	153.898	316.158	0	80.256
1R6G_A	Agonist	1366.795	3	6.15	4.568	551.231	761.196	122.979	177.121	341.689	119.407	107.944
1XZX_X	Agonist	1051.266	4	4.25	1.304	650.978	597.407	48.346	189.76	145.089	214.212	103.013
1Y0X_X	Agonist	1111.483	4	4.25	1.97	776.874	628.604	48.351	182.652	103.795	293.807	101.475
2J4A_A	Antagonist	1113.859	2	3.25	4.857	458.146	631.08	222.301	142.108	149.485	117.186	76.96
2PIN_A	Agonist	973.988	2	3.25	4.305	621.936	562.513	41.193	150.421	156.416	214.483	80.765
3D57_A	Agonist	974.743	2	3.25	4.302	621.936	565.293	41.251	151.547	158.176	214.32	80.76
3GWS_X	Agonist	1051.275	4	4.25	1.299	650.978	596.64	48.338	190.359	143.693	214.25	103.009
3HZF_A	Agonist	1119.302	2	3.5	4.282	328.407	635.496	342.871	150.113	142.512	0	78.469
3IMY_A	Agonist	1119.274	2	3.5	4.282	328.407	635.458	342.843	150.113	142.502	0	78.469
1DKF_B	Antagonist	1424.995	2	5.5	5.55	450.536	786.72	195.594	174.221	416.905	0	97.986
1XAP_A	Agonist	1206.094	1	2	6.022	348.484	671.625	374.072	106.807	190.746	0	50.362
1EXA_A	Agonist	1238.988	3	6.2	3.611	399.461	679.993	308.918	190.205	165.485	15.385	104.67
1EXX_A	Agonist	1263.249	3	6.2	3.855	399.461	704.12	323.91	184.924	158.811	36.475	104.718
1FCX_A	Agonist	1267.988	2	3.7	5.252	388.505	691.794	319.201	148.403	224.19	0	70.748
1FCY_A	Agonist	1259.377	1	4	5.282	386.49	698.443	309.232	149.201	240.011	0	76.931
1FCZ_A	Agonist	1228.352	1	4	5.037	362.468	691.696	324.793	151.531	215.372	0	77.381
1FD0_A	Agonist	1295.473	2	4.7	4.848	401.504	716.296	308.801	174.815	232.68	0	85.84
2LBD_A	Agonist	1141.819	1	2	5.472	300.44	649.007	487.027	103.845	58.135	0	49.649
3LBD_A	Agonist	1140.578	1	2	5.466	300.44	647.466	483.938	103.826	59.702	0	49.642
4LBD_A	Agonist	1263.255	3	6.2	3.855	399.461	704.127	323.909	184.92	158.818	36.48	104.718
1I7G_A	Agonist	1314.856	1	8.95	3.306	408.465	759.095	321.847	180.603	255.912	0.733	110.952
1K7L_A	Agonist	1666.412	1	7.95	6.597	512.604	918.575	271.143	130.514	516.918	0	111.51
1KKQ_A	Antagonist	1888.659	1	7.25	7.806	619.682	1010.805	329.324	96.268	468.418	116.796	97.917
2NPA_A	Agonist	1502.263	1	7.45	5.607	436.507	865.8	393.237	125.003	347.56	0	99.354
2P54_A	Agonist	1378.032	2	6.75	5.368	478.485	768.975	233.562	137.647	250.146	147.621	98.269
2REW_A	Agonist	1619.152	1	7.5	6.488	512.561	906.436	298.471	125.191	482.774	0	111.274
2ZNN_A	Agonist	1682.338	2	5.25	7.312	503.68	911.87	618.035	126.435	167.4	0	90.213
3ET1_A	Agonist	1152.33	1	8	2.722	389.422	647.178	247.109	176.971	221.283	1.814	105.316
3G8I_A	Agonist	1348.897	1	7.65	4.853	439.525	741.934	270.148	103.165	333.766	34.855	83.591
1GWX_A	Agonist	1652.66	2	4.75	7.696	581.898	889.709	239.667	110.419	373.335	166.289	84.679
1Y0S_A	Agonist	1642.798	2	4.75	7.109	490.589	914.924	477.225	114.459	244.78	78.46	85.054

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	Ligand Profile	volume	donorHB	accptHB	QPlogPo/w	MW	SASA	FOSA	FISA	PISA	WPSA	PSA
2AWH_A	Agonist	1233.447	1	2	5.967	282.465	732.521	604.517	109.68	18.325	0	51.746
2B50_A	Agonist	1233.438	1	2	5.967	282.465	732.513	604.509	109.68	18.324	0	51.746
2BAW_A	Agonist	1233.452	1	2	5.967	282.465	732.535	604.531	109.68	18.323	0	51.745
2J14_A	Agonist	1459.378	2	6.75	5.892	511.36	801.552	95.756	157.57	409.372	138.854	114.735
2ZNP_A	Agonist	1424.784	2	5.25	6.185	469.475	779.215	346.796	135.899	142.904	153.616	90.329
2ZNQ_A	Agonist	1262.944	2	5.25	5.158	427.395	712.594	247.225	141.928	169.935	153.506	91.509
3D5F_A	Agonist	1346.563	1	6	4.657	402.443	778.053	359.849	191.425	226.779	0	119.828
3DY6_A	Partial agonist	1186.704	1	8	3.012	436.481	596.915	98.497	188.582	308.595	1.24	119.564
3ET2_A	Agonist	1152.334	1	8	2.722	389.422	647.183	247.111	176.968	221.29	1.814	105.315
3GZ9_A	Agonist	1502.314	1.5	4.25	7.497	516.531	810.881	272.785	111.532	278.118	148.445	71.349
1FM6_D	Agonist	1124.132	2	4.75	3.774	359.442	644.877	235.552	123.159	243.471	42.696	92.512
1FM9_D	Agonist	1736.54	1	6.75	7.753	546.621	959.796	171.934	127.824	660.038	0	107.947
1I7I_A	Agonist	1314.818	1	8.95	3.306	408.465	759.06	321.821	180.614	255.893	0.733	110.957
1KNU_A	Agonist	1306.517	1	4.45	5.969	403.477	725.251	219.504	94.314	411.433	0	64.755
1NYX_A	Agonist	1318.876	1	5.45	5.689	419.476	736.066	190.883	91.3	453.883	0	74.757
1RDT_D	Agonist	1738.097	1	6.75	7.785	546.621	961.574	175.699	124.814	661.06	0	108.384
1WM0_X	Agonist	1108.199	1	6	4.051	404.209	634.878	0	154.459	359.611	120.808	108.806
1ZEO_A	Agonist	1351.911	1	5.75	5.123	425.524	717.834	463.916	131.014	122.903	0	95.957
1ZGY_A	Agonist	1124.13	2	4.75	3.774	359.442	644.875	235.551	123.159	243.469	42.696	92.512
2ATH_A	Agonist	1413.879	1	5	6.32	476.451	800.17	277.18	145.364	261.614	116.012	95.333
2F4B_A	Agonist	1685.416	1	5.5	7.693	521.612	930.065	274.899	143.955	511.21	0	93.821
2FVJ_A	Partial agonist	1736.205	0	6.75	7.138	542.674	937.707	615.667	5.859	316.182	0	50.058
2G0G_A	Partial agonist	1123.758	1	5.5	4.437	417.447	607.881	0	85.249	384.345	138.287	61.275
2G0H_A	Partial agonist	1239.837	1	5.5	5.561	535.454	633.801	1.429	83.6	281.618	267.154	61.644
2GTK_A	Agonist	1365.991	1	5.7	5.897	438.91	766.113	281.364	98.53	329.638	56.581	77.142
2HWQ_A	Agonist	1699.472	1	5.5	7.664	521.612	942.45	261.049	162.166	519.235	0	94.977
2HWR_A	Agonist	1774.771	1	5.5	8.28	549.665	962.829	331.501	138.824	492.504	0	89.554
2I4J_A	Agonist	1586.21	1	5.25	7.259	452.592	889.989	493.862	95.065	301.062	0	72.878
2I4P_A	Partial agonist	1560.393	1	5.25	7.149	452.592	867.434	481.228	87.229	298.977	0	71.808
2I4Z_A	Partial agonist	1570.237	1	5.25	7.207	452.592	877.567	489.085	88.004	300.479	0	71.95
2OM9_A	Partial agonist	1370.293	2	3.5	5.843	400.557	755.486	542.692	141.229	71.565	0	76.328
2P4Y_A	Partial agonist	1498.259	1	5	6.87	574.94	784.428	230.585	153.497	275.423	124.923	101.581
2POB_A	Antagonist	1880.832	1	7.25	7.607	573.69	1034.027	292.135	84.326	657.565	0	100.893
2PRG_A	Agonist	1124.139	2	4.75	3.774	359.442	644.883	235.556	123.16	243.471	42.696	92.512
2Q59_A	Agonist	1465.015	1	6.5	6.416	527.496	784.264	253.298	98.868	309.89	122.209	96.673
2Q6R_A	Partial agonist	1220.63	1	2.75	6.602	423.913	662.985	122.793	74.827	368.601	96.765	55.232
2Q6S_B	Partial agonist	1105.108	1	6	4.126	404.209	634.743	0	141.768	375.148	117.827	108.642
2VST_A	Agonist	1233.278	2	3.7	4.815	296.449	733.38	545.756	145.412	42.212	0	71.612
2VV0_A	Agonist	1259.27	1	2	6.225	328.494	658.77	466.394	109.598	82.778	0	51.758
2VV1_A	Agonist	1247.056	2	3.7	5.268	344.493	649.667	425.518	110.8	113.35	0	69.498

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	Ligand Profile	volume	donorHB	accptHB	QPlogPo/w	MW	SASA	FOSA	FISA	PISA	WPSA	PSA
2VV2_A	Agonist	1190.941	2	3.7	4.648	318.455	642.18	412.051	143.605	86.525	0	72.969
2VV3_A	Agonist	1218.063	1	4	5.096	344.493	627.812	442.917	112.751	72.144	0	75.483
2VV4_A	Agonist	1178.482	1	4.7	4.233	310.433	673.228	487.828	148.822	36.578	0	99.133
2ZK1_A	Agonist	1194.186	1	4	4.661	316.439	677.794	407.352	157.072	113.37	0	79.535
2ZK2_A	Agonist	1193.985	1	4	4.66	316.439	677.535	407.095	157.071	113.37	0	79.534
2ZK3_A	Agonist	1190.96	1	4	4.817	318.455	654.573	462.878	125.027	66.668	0	76.681
2ZK4_A	Agonist	1224.577	1	4	5.106	318.455	680.769	490.75	114.881	75.138	0	78.844
2ZK5_A	Agonist	980.013	1	4.5	3.224	301.298	565.931	173.068	159.938	232.924	0	98.022
2ZNO_A	Agonist	1478.588	2	4.5	6.326	445.6	807.131	457.722	135.752	213.657	0	83.149
2ZVT_A	Agonist	1188.98	1	4	4.575	316.439	678.81	407.719	163.613	107.478	0	81.317
3B3K_A	Agonist	1023.114	1	2.75	4.843	318.371	559.146	31.61	103.752	423.784	0	57.542
3BC5_A	Agonist	1491.815	1	6.75	5.983	494.549	764.208	205.348	125.97	432.889	0	106.776
3CDP_A	Partial agonist	855.878	1	2.75	4.108	276.719	490.57	24.134	92.75	302.011	71.675	54.423
3CDS_A	Agonist	929.657	1	2.75	4.175	270.327	528.344	154.471	92.762	281.111	0	54.426
3CS8_A	Agonist	1124.129	2	4.75	3.774	359.442	644.873	235.551	123.156	243.47	42.696	92.511
3CWD_A	Agonist	1192.883	1	4	4.267	325.447	657.592	429.498	199.652	28.442	0	95.988
3DZU_D	Agonist	1108.238	1	6	4.05	404.209	634.75	0	154.557	359.391	120.801	108.825
3DZY_D	Agonist	1124.132	2	4.75	3.774	359.442	644.875	235.557	123.154	243.468	42.696	92.509
3E00_D	Antagonist	836.242	1	3.5	2.772	276.679	505.015	0	135.151	310.002	59.862	78.657
3ET3_A	Partial agonist	1151.337	1	8	2.716	389.422	647.219	247.125	176.946	221.334	1.815	105.309
3FEI_A	Agonist	1319.72	1	5.95	5.633	431.933	734.694	257.348	99.936	263.972	113.439	72.026
3FEJ_A	Agonist	1292.576	1	5.95	5.378	431.933	691.682	227.362	106.342	256.963	101.015	74.795
3FUR_A	Antagonist	1275.294	1	6	5.327	514.209	692.844	0	105.327	364.266	223.251	66.681
3G9E_A	Agonist	1296.641	1	6.45	5.037	437.509	681.834	170.18	111.266	366.384	34.004	87.402
3H0A_D	Partial agonist	1719.143	1	4.25	9.003	570.622	940.148	377.406	112.157	301.518	149.067	70.748
3HO0_A	Agonist	1090.224	1	2.75	5.276	332.398	601.625	67.093	103.376	431.156	0	57.382
3HOD_A	Agonist	1561.358	1	10.75	4.195	504.539	789.894	717.773	54.332	17.712	0.076	64.858
3IA6_B	Agonist	1379.565	1	6.5	5.287	416.479	775.64	210.334	134.965	430.341	0	98.637
4PRG_A	Partial agonist	2015.621	1	8.5	7.161	618.873	1031.838	530.185	139.236	337.974	24.443	96.07
1N83_A	Agonist	1386.841	1	1.7	7.013	386.66	728.429	651.091	48.894	28.444	0	22.273
1S0X_A	Agonist	1515.277	1	4	6.684	466.718	805.008	625.379	148.171	29.945	1.513	72.713
1P8D_A	Agonist	1362.425	1	3.7	6.01	400.643	704.072	626.734	48.893	28.445	0	35.142
1PQ6_A	Agonist	1548.746	1	4.75	5.918	582.061	742.77	143.098	29.871	466.591	103.211	59.207
1PQ9_A	Agonist	819.065	2	1	4.663	341.176	485.851	44.537	41.13	98.474	301.711	29.632
1PQC_A	Agonist	1114.19	1	4.5	5.088	481.332	612.074	34.239	88.446	214.07	275.319	52.674
1UPV_A	Agonist	1121.106	1	4.5	5.081	481.332	619.275	22.266	95.871	229.813	271.325	54.149
1UPW_A	Agonist	1121.099	1	4.5	5.081	481.332	619.269	22.267	95.868	229.81	271.324	54.149
3KFC_A	Agonist	1249.727	0	5.5	5.108	443.44	692.678	79.504	83.606	417.318	112.25	55.391
1UHL_B	Agonist	1121.098	1	4.5	5.081	481.332	619.267	22.265	95.868	229.811	271.324	54.149
2ACL_B	Agonist	1220.336	1	4.25	5.287	384.434	677.563	129.992	64.236	483.336	0	70.549

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	Ligand Profile	volume	donorHB	accptHB	QPlogPo/w	MW	SASA	FOSA	FISA	PISA	WPSA	PSA
3FAL_B	Agonist	1371.513	1	2.5	7.761	499.88	757.053	373.83	27.312	105.801	250.111	34.077
3FC6_B	Agonist	1739.456	1	4.75	6.849	621.098	878.544	107.358	101.018	527.007	143.162	64.203
1OSH_A	Agonist	1639.506	0	6	6.963	498.664	853.569	520.009	61.453	272.108	0	63.931
3BEJ_A	Agonist	1292.245	2	4.75	4.668	420.547	685.48	311.445	189.47	184.565	0	95.295
3DCT_A	Agonist	1557.099	1	4.25	7.876	542.845	859.041	169.056	145.666	382.581	161.739	82.86
3FLI_A	Agonist	1323.341	0	5	5.053	440.489	693.12	285.72	77.256	241.307	88.836	68.76
3GD2_A	Agonist	1604.831	1	8.25	6.04	604.931	828.63	199.701	184.258	297.151	147.52	100.611
3L1B_A	Agonist	1758.046	0	8.45	5.98	563.668	950.028	561.702	89.137	252.092	47.097	92.47
3OKH_A	Agonist	1470.428	2	6	5.388	494.032	766.18	367.804	125.5	201.241	71.636	93.379
3OKI_A	Agonist	1418.929	1	4	6.263	450.022	750.682	394.565	31.992	252.491	71.634	43.381
3OLF_A	Agonist	1515.1	2	6	6.573	537.992	798.8	225.16	144.307	268.96	160.373	93.422
3OMK_A	Agonist	1432.336	1	4	7.369	493.983	756.104	225.136	37.514	333.08	160.373	43.054
3OMM_A	Agonist	1491.049	2	6	6.507	541.956	797.946	180.941	144.715	295.662	176.628	94.149
3OOF_A	Agonist	1482.081	2	6	6.4	523.966	793.042	181.004	144.987	306.689	160.362	94.447
3OOK_A	Agonist	1501.326	2	6	6.656	559.947	797.414	176.485	145.233	268.19	207.505	94.312
1DB1_A	Agonist	1462.379	3	4.15	5.514	416.643	766.42	618.12	122.441	25.859	0	63.46
1IE8_A	Agonist	1622.52	3	5.85	5.902	460.696	862.493	723.787	112.842	25.864	0	69.244
1IE9_A	Agonist	1466.167	3	4.15	5.528	416.643	772.088	622.71	123.515	25.863	0	63.429
1S0Z_A	Agonist	1601.786	3	4.15	6.483	454.692	849.788	695.424	110.873	43.491	0	60.604
1S19_A	Agonist	1417.466	3	5.1	4.851	412.611	746.069	586.393	126.101	33.575	0	64.04
1TXI_A	Agonist	1439.696	3	4.15	5.301	402.616	785.558	644.652	128.084	12.821	0	64.557
2HAM_A	Agonist	1637.154	3	4.15	6.746	458.723	867.442	736.489	102.577	28.376	0	59.726
2HAR_A	Agonist	1703.947	4	7.55	5.137	490.722	908.468	710.875	168.88	28.712	0	92.887
2HAS_A	Agonist	1680.657	3	5.85	6.263	474.723	894.755	754.434	113.046	27.275	0	69.871
2HB7_A	Agonist	1660.069	4	5.85	5.599	474.723	880.115	692.647	159.09	28.379	0	82.858
2HB8_A	Agonist	1519.486	3	4.15	5.955	430.67	801.685	666.059	109.9	25.726	0	61.095
3CS4_A	Agonist	1481.019	3	4.9	5.334	444.653	771.164	621.665	123.661	25.837	0	69.73
3CS6_A	Agonist	1484.504	3	4.9	5.402	444.653	778.436	634.318	116.751	27.366	0	69.152
1ILH_A	Agonist	1529.918	1	10.75	4.066	504.539	754.779	694.655	46.871	12.34	0.914	67.592
1M13_A	Agonist	1796.887	0	5.75	8.006	536.793	885.678	810.369	37.003	38.306	0	67.85
1NRL_A	Agonist	1528.841	1	10.75	4.002	504.539	764.575	686.538	56.013	19.806	2.218	67.234
1SKX_A	Agonist	2248.58	6	20.35	2.867	822.951	1032.045	783.951	199.452	48.642	0	210.679
2O9I_A	Antagonist	1114.194	1	4.5	5.088	481.332	612.081	34.239	88.446	214.075	275.322	52.674
2QNV_A	Agonist	1341.181	0	8	3.677	400.557	676.874	582.679	71.933	22.262	0	82.124
3HLV_B	Agonist	1127.485	1	2.75	5.522	346.425	613.069	67.161	104.255	441.653	0	57.621
1XV9_B	Agonist	1051.419	0	4	3.733	316.483	561.349	466.691	94.658	0	0	55.693
1XVP_B	Agonist	1124.775	0	4.7	5.188	436.742	596.526	65.023	36.585	299.202	195.715	32.889
1PZL_A	Agonist	1010.699	1	2	4.517	228.374	612.125	502.446	109.68	0	0	51.745
3FS1_A	Agonist	1010.699	1	2	4.517	228.374	612.126	502.446	109.68	0	0	51.745
1LV2_A	Agonist	1131.925	1	2	5.293	256.428	678.166	568.486	109.68	0	0	51.745

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	Ligand Profile	volume	donorHB	accptHB	QPlogPo/w	MW	SASA	FOSA	FISA	PISA	WPSA	PSA
1FBY_A	Agonist	1140.65	1	2	5.467	300.44	647.641	484.065	103.828	59.749	0	49.652
1FM6_A	Agonist	1139.934	1	2	5.462	300.44	646.777	483.827	103.826	59.124	0	49.652
1FM9_A	Agonist	1139.939	1	2	5.462	300.44	646.781	483.831	103.827	59.123	0	49.652
1G5Y_A	Agonist	1142.689	1	2	5.478	300.44	648.094	486.247	103.845	58.002	0	49.649
1K74_A	Agonist	1140.015	1	2	5.462	300.44	646.587	483.759	103.829	59	0	49.652
1MV9_A	Agonist	1482.331	1	2	7.569	338.573	871.015	745.729	109.68	15.607	0	51.746
1MVC_A	Agonist	1231.19	1	3.5	5.507	380.483	670.099	412.884	106.808	150.406	0	62.917
1MZN_A	Agonist	1231.377	1	3.5	5.508	380.483	672.565	414.79	106.808	150.966	0	62.915
1RDT_A	Agonist	1239.172	1	2.5	6.024	374.479	692.201	337.336	114.813	240.052	0	59.791
1XLS_A	Agonist	1144.194	1	2	5.466	302.456	643.665	500.773	103.895	38.997	0	49.642
1XV9_A	Agonist	1071.308	1	2	4.905	242.401	645.144	535.463	109.68	0	0	51.745
1XVP_A	Agonist	1071.313	1	2	4.905	242.401	645.147	535.467	109.68	0	0	51.745
2ACL_A	Agonist	1140.648	1	2	5.467	300.44	647.644	484.064	103.827	59.753	0	49.652
2P1T_A	Partial agonist	1262.042	2	3.5	5.159	380.483	701.42	411.467	152.494	137.46	0	78.291
2P1U_A	Partial agonist	1324.255	2	3.5	5.575	394.51	731.406	449.411	148.438	133.557	0	77.553
2P1V_A	Partial agonist	1379.251	2	3.5	5.913	408.536	753.494	478.104	148.983	126.406	0	76.889
2ZXZ_A	Agonist	1196.223	1	3.5	5.298	366.456	657.375	387.782	106.809	162.785	0	62.906
2ZY0_A	Agonist	1296.018	1	3.5	5.935	398.605	711.537	438.948	106.809	165.78	0	62.925
3DZU_A	Agonist	1121.15	1	2	5.341	302.456	618.263	459.626	103.807	54.83	0	49.643
3DZY_A	Agonist	1121.152	1	2	5.341	302.456	618.252	459.614	103.807	54.831	0	49.643
3E00_A	Agonist	1121.15	1	2	5.341	302.456	618.255	459.617	103.807	54.83	0	49.643
3FAL_A	Agonist	1140.147	1	2	5.463	300.44	646.768	483.733	103.828	59.207	0	49.652
3FC6_A	Agonist	1139.936	1	2	5.462	300.44	646.78	483.827	103.827	59.125	0	49.652
3H0A_A	Agonist	1195.817	1	2	5.907	348.484	655.268	400.807	106.823	147.637	0	50.366
1H9U_A	Agonist	1219.382	1	3	5.563	363.499	660.982	447.213	110.464	103.305	0	59.978
1UHL_A	Agonist	1063.427	1	2.75	4.615	268.395	622.004	494.768	103.733	23.503	0	57.525
1A52_A	Agonist	910.352	2	2.45	4.004	272.386	511.15	303.648	95.839	111.663	0	43.692
1ERE_A	Agonist	910.353	2	2.45	4.004	272.386	511.15	303.649	95.839	111.663	0	43.693
1ERR_A	Antagonist	1477.819	2	6.25	4.832	473.586	824.811	282.161	141.116	364.579	36.955	81.174
1G50_A	Agonist	910.352	2	2.45	4.004	272.386	511.15	303.648	95.839	111.663	0	43.692
1GWQ_A	Agonist	771.332	2	1.5	2.956	242.292	467.813	0	109.441	322.364	36.008	45.104
1GWR_A	Agonist	910.352	2	2.45	4.004	272.386	511.15	303.648	95.839	111.663	0	43.692
1L2I_A	Antagonist	1063.068	2	1.5	4.53	320.43	591.904	287.748	109.437	194.719	0	45.114
1PCG_A	Agonist	910.352	2	2.45	4.004	272.386	511.15	303.648	95.839	111.663	0	43.692
1QKT_A	Agonist	910.352	2	2.45	4.004	272.386	511.15	303.648	95.839	111.663	0	43.692
1QKU_A	Agonist	910.352	2	2.45	4.004	272.386	511.15	303.648	95.839	111.663	0	43.692
1R5K_A	Antagonist	1208.625	1	2	6.272	354.448	669.921	118.22	114.69	437.011	0	51.618
1SJ0_A	Partial agonist	1431.659	2	5.5	5.002	463.59	789.296	307.868	110.713	345.52	25.194	65.694
1UOM_A	Antagonist	1435.102	1	4.5	5.946	428.573	789.851	354.558	56.298	378.995	0	37.199
1X7E_A	Agonist	886.084	2	3.75	2.161	267.284	525.443	101.819	177.001	246.623	0	78.6

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	Ligand Profile	volume	donorHB	accptHB	QPlogPo/w	MW	SASA	FOSA	FISA	PISA	WPSA	PSA
1X7R_A	Agonist	806.688	2	3.75	1.67	270.241	480.232	0	187.061	293.171	0	98.585
1XP1_A	Antagonist	1493.671	2	5.5	5.371	477.617	818.883	334.601	113.529	345.559	25.194	66.199
1XP6_A	Antagonist	1493.292	2	5.5	5.367	477.617	818.284	334.166	113.692	345.232	25.195	66.287
1XP9_A	Antagonist	1429.755	2	5.5	4.976	463.59	781.807	302.254	112.585	341.772	25.196	65.462
1XPC_A	Agonist	1431.757	2	5.5	4.986	463.59	784.174	305.26	112.684	341.036	25.194	65.043
1XQC_A	Partial agonist	1427.666	1	4.75	5.756	439.599	768.968	361.334	57.366	350.268	0	32.24
1YIM_A	Antagonist	1423.252	2	5	5.012	445.557	779.876	344.225	113.599	322.051	0	66.397
1YIN_A	Antagonist	1499.046	2	5	5.626	477.574	818.418	369.034	107.669	313.365	28.349	63.697
1ZKY_A	Agonist	936.272	2	4.15	2.81	288.386	515.135	272.574	94.122	148.44	0	50.976
2AYR_A	Antagonist	1589.996	1	8	4.854	517.639	862.541	359.296	135.009	368.181	0.055	78.727
2B1V_A	Agonist	867.183	2	4.15	2.369	260.332	496.665	226.739	99.249	170.677	0	51.218
2B1Z_A	Agonist	923.43	2	1.5	3.825	282.382	515.875	252.191	84.675	179.009	0	40.733
2BJ4_A	Antagonist	1336.517	1	3.5	5.71	387.521	723.845	300.593	59.763	363.49	0	36.094
2FAI_A	Agonist	919.313	2	4.15	2.655	276.375	521.731	279.666	98.754	143.311	0	49.054
2G44_A	Agonist	888.98	1	1.5	4.004	258.36	496.853	285.061	54.7	157.091	0	29.171
2I0G_A	Agonist	922.152	2	2.25	3.428	282.338	530.43	162.366	109.321	258.743	0	51.617
2I0J_A	Agonist	922.41	2	2.25	3.43	282.338	530.423	162.363	109.32	258.74	0	51.616
2IOK_A	Antagonist	1251.89	3	3.25	4.493	398.504	660.97	144.878	104.184	411.909	0	67.566
2JF9_A	Antagonist	1356.674	1	3.5	5.85	387.521	752.944	314.016	59.861	379.067	0	35.831
2JFA_A	Antagonist	1480.695	2	6.25	4.88	473.586	825.543	282.169	137.781	368.055	37.538	81.621
2OCF_A	Agonist	910.352	2	2.45	4.004	272.386	511.15	303.648	95.839	111.663	0	43.692
2OUZ_A	Antagonist	1389.545	1	3.5	6.047	413.558	767.271	346.336	58.98	361.955	0	35.739
2P15_A	Agonist	1305.953	2	1.5	6.702	442.52	699.197	264.156	80.167	270.828	84.046	40.331
2POG_A	Agonist	919.083	2	2.25	3.541	282.338	525.986	155.008	93.639	277.339	0	49.888
2Q70_A	Agonist	948.191	2	2.25	3.884	318.319	544.712	97.697	109.327	261.808	75.88	51.859
2QA6_A	Partial agonist	751.392	4	3.25	0.901	242.234	455.836	0	207.676	248.159	0	95.967
2QA8_A	Agonist	806.621	2	3.75	1.67	270.241	480.176	0	187.051	293.125	0	98.578
2QAB_A	Partial agonist	837.901	2	2.5	2.687	254.288	494.603	106.54	127.117	260.946	0	61.621
2QE4_A	Agonist	1029.539	2	3.95	3.394	326.391	569.357	266.525	109.294	193.537	0	58.725
2QGT_A	Agonist	1029.167	2	4.15	3.309	316.439	562.651	362.731	95.928	103.992	0	51.497
2QGW_A	Partial agonist	782.758	2	2.5	2.584	260.679	473.218	0	127.326	291.419	54.473	61.694
2QH6_A	Partial agonist	1287.23	2	7.2	3.427	424.449	698.586	322.021	154.097	222.468	0	112.216
2QR9_A	Partial agonist	1170.216	2	7.2	2.501	394.38	644.494	217.73	188.203	238.561	0	123.565
2QSE_A	Partial agonist	788.718	3	3.75	1.435	240.264	476.526	78.192	166.932	231.402	0	77.342
2QXM_A	Agonist	766.589	2	3	2.185	224.265	464.81	78.192	112.207	274.411	0	54.789
2QXS_A	Antagonist	1480.669	2	6.25	4.88	473.586	825.489	282.13	137.775	368.038	37.545	81.615
2R6W_A	Agonist	1513.724	2	6.25	5.046	487.612	821.948	306.203	139.889	339.17	36.686	81.705
2R6Y_A	Partial agonist	1408.074	2	6.25	4.348	459.559	768.98	253.981	144.874	333.506	36.619	82.143
3DT3_A	Antagonist	1090.671	3	2.75	3.872	358.393	599.685	67.901	157.5	374.283	0	73.767
3ERD_A	Agonist	951.228	2	1.5	5.056	268.355	540.511	184.925	109.37	246.215	0	45.09

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	Ligand Profile	volume	donorHB	accptHB	QPlogPo/w	MW	SASA	FOSA	FISA	PISA	WPSA	PSA
3ERT_A	Antagonist	1354.507	1	3.5	5.835	387.521	749.952	313.064	59.867	377.02	0	35.832
1L2J_B	Antagonist	1059.05	2	1.5	4.498	320.43	583.851	286.816	109.425	187.609	0	45.111
1NDE_A	Antagonist	1553.319	3	6.25	5.491	485.046	884.433	324.445	117.961	332.842	109.186	80.906
1QKM_A	Antagonist	806.688	2	3.75	1.67	270.241	480.232	0	187.061	293.171	0	98.585
1QKN_A	Antagonist	1480.655	2	6.25	4.88	473.586	825.488	282.133	137.776	368.035	37.544	81.619
1U3Q_A	Agonist	747.317	3	3.75	0.963	243.218	454.022	0	203.6	250.422	0	92.546
1U3R_A	Agonist	854.726	3	3.25	1.975	279.295	500.287	17.454	117.607	365.225	0	65.213
1U3S_A	Agonist	863.99	2	3	2.532	277.279	512.274	0	161.408	350.866	0	71.804
1U9E_A	Agonist	757.576	2	2.25	2.434	228.247	457.424	58.244	109.304	289.876	0	53.269
1X76_A	Agonist	810.96	2	3.5	1.861	251.241	492.397	0	178.375	314.022	0	78.462
1X78_A	Agonist	868.565	2	3.5	2.228	265.268	516.565	47.525	173.45	295.589	0	78.041
1X7B_A	Agonist	850.65	2	3.5	2.6	271.247	513.434	63.95	124.64	281.539	43.304	63.639
1X7J_A	Agonist	806.687	2	3.75	1.67	270.241	480.231	0	187.062	293.17	0	98.585
1YY4_A	Agonist	835.257	2	1.5	3.51	270.715	498.16	0	102.727	336.685	58.747	44.119
1YYE_A	Agonist	873.808	2	3	2.621	279.27	521.528	0	172.988	305.159	43.381	70.62
1ZAF_A	Agonist	825.798	2	3.5	2.298	317.138	493.206	0	155.892	277.347	59.967	77.33
2GIU_A	Agonist	934.183	1	2.75	3.607	335.24	528.893	268.51	103.416	97.397	59.57	51.092
2JJ3_A	Agonist	1067.001	2	3.95	3.63	326.391	601.8	285.877	109.249	206.674	0	58.306
2NV7_A	Partial agonist	874.582	2	3.95	2.447	263.295	517.696	16.347	135.448	365.9	0	59.645
2QTU_A	Agonist	1091.47	2	3.95	4.071	362.372	610.757	221.178	109.247	204.447	75.885	58.335
2Z4B_A	Agonist	947.828	2	2.25	3.846	318.319	543.331	108.011	109.322	258.713	67.285	51.792
2PJL_A	Antagonist	1223.443	1	1.5	6.151	332.488	701.591	382.134	4.625	314.832	0	14.691
2E2R_A	Agonist	806.872	2	1.5	3.317	228.29	471.911	114.139	109.419	248.352	0	45.102
2EWP_A	Antagonist	1440.787	2	5.2	5.082	417.547	791.335	299.889	116.293	375.153	0	58.941
2GPP_A	Agonist	1023.812	3	4.25	2.996	284.357	607.232	199.726	126.49	281.016	0	75.208
2GPU_A	Antagonist	1354.41	1	3.5	5.833	387.521	748.849	313.058	59.866	375.925	0	35.831
2GPV_A	Antagonist	1352.704	1	3.5	5.816	387.521	744.04	314.175	59.928	369.938	0	34.039
2P7G_A	Agonist	806.745	2	1.5	3.318	228.29	471.911	114.139	109.419	248.352	0	45.102
2P7Z_A	Antagonist	1339.736	1	3.5	5.735	387.521	730.664	306.153	59.118	365.392	0	36.072
2ZAS_A	Agonist	783.886	1	0.75	3.934	212.291	459.374	114.134	54.71	290.53	0	22.551
2ZKC_A	Agonist	907.216	2	1.5	3.582	268.355	519.465	175.182	109.47	234.813	0	45.112
1M2Z_A	Agonist	1139.082	3	8.15	1.83	392.466	605.073	331.868	178.913	79.831	14.461	106.26
1NHZ_A	Antagonist	1414.901	1	3.75	6.107	429.601	754.019	539.255	94.523	120.24	0	53.001
1P93_A	Agonist	1139.081	3	8.15	1.83	392.466	605.072	331.868	178.912	79.831	14.461	106.26
3BQD_A	Agonist	1494.958	3	7.15	4.577	490.641	778.881	472.663	142.521	163.697	0	93.249
3CLD_A	Agonist	1436.093	1	8.2	4.757	538.578	748.026	291.535	114.939	229.947	111.605	100.472
3E7C_A	Agonist	1432.138	3	6	5.683	562.35	766.919	139.781	117.427	327.718	181.993	106.37
3GN8_A	Agonist	1139.081	3	8.15	1.83	392.466	605.072	331.868	178.912	79.831	14.461	106.26
3H52_A	Antagonist	1415.624	1	3.75	6.113	429.601	755.826	539.552	94.46	121.814	0	52.987
3K23_B	Agonist	1832.911	4	8.25	5.826	655.691	921.336	406.089	157.333	247.83	110.084	125.164

PDB code_Chain	Ligand Profile	volume	donorHB	accptHB	QPlogPo/w	MW	SASA	FOSA	FISA	PISA	WPSA	PSA
1Y9R_A	Agonist	1075.643	1	5.7	2.728	330.466	579.428	408.42	141.562	29.447	0	76.221
1YA3_A	Agonist	1053.224	0	4	3.87	314.467	567.111	447.07	90.595	29.447	0	54.492
2A3I_A	Agonist	1084.292	2	7.4	1.939	346.466	579.497	388.638	162.24	28.619	0	92.066
2AA2_A	Agonist	1083.417	2	9.4	1.074	360.449	577.381	345.252	203.524	28.605	0	120.044
2AA5_A	Agonist	1053.224	0	4	3.87	314.467	567.111	447.07	90.595	29.446	0	54.492
2AA6_A	Agonist	1053.224	0	4	3.87	314.467	567.111	447.07	90.595	29.446	0	54.492
2AA7_A	Agonist	1075.642	1	5.7	2.728	330.466	579.428	408.419	141.562	29.447	0	76.221
2AAX_A	Agonist	1057.652	3	7.2	1.573	358.433	561.094	272.421	192.581	96.093	0	106.329
2AB2_A	Antagonist	1239.767	0	7	3.139	416.574	648.836	476.611	133.456	22.525	16.244	92.425
2ABI_A	Agonist	1080.247	1	5.7	2.7	332.482	577.787	432.639	145.149	0	0	76.35
2OAX_A	Antagonist	1259.44	0	7	3.086	416.574	663.946	471.246	157.385	23.424	11.891	97.222
1A28_A	Agonist	1053.224	0	4	3.87	314.467	567.111	447.07	90.594	29.446	0	54.492
1E3K_A	Agonist	948.286	1	2.75	3.385	284.397	527.449	363.478	90.683	73.288	0	49.206
1SQN_A	Agonist	998.826	1.5	2.75	3.358	298.424	554.932	391.105	92.852	70.975	0	49.518
1SR7_A	Agonist	1396.721	1	8.2	4.389	521.436	699.503	283.835	116.268	220.495	78.906	99.107
1ZUC_A	Agonist	961.606	1	4.5	3.3	297.374	561.654	204.83	89.108	185.104	82.611	59.092
2W8Y_A	Antagonist	1411.668	1	3.75	6.086	429.601	750.608	536.161	94.588	119.859	0	52.921
3KBA_A	Partial agonist	1214.05	0	7	3.262	403.926	661.79	233.098	150.804	212.166	65.722	71.288
1E3G_A	Agonist	948.286	1	2.75	3.385	284.397	527.449	363.478	90.683	73.288	0	49.206
1GS4_A	Agonist	1098.961	3	8.15	1.584	380.455	581.372	359.301	185.781	28.206	8.083	108.51
1T5Z_A	Agonist	968.983	1	3.7	3.659	290.445	525.144	430.003	95.141	0	0	50.506
1T63_A	Agonist	968.984	1	3.7	3.659	290.445	525.144	430.003	95.141	0	0	50.506
1T65_A	Agonist	968.984	1	3.7	3.659	290.445	525.144	430.003	95.141	0	0	50.506
1XJ7_A	Agonist	968.983	1	3.7	3.659	290.445	525.144	430.003	95.141	0	0	50.506
1XOW_A	Agonist	948.286	1	2.75	3.385	284.397	527.449	363.478	90.683	73.288	0	49.206
1XQ3_A	Agonist	948.286	1	2.75	3.385	284.397	527.449	363.478	90.683	73.288	0	49.206
1Z95_A	Agonist	1166.582	1	7.75	3.015	430.373	658.333	80.983	175.787	247.498	154.065	109.954
2AM9_A	Agonist	962.433	1	3.7	3.32	288.429	524.41	395.378	99.588	29.444	0	50.852
2AMA_A	Agonist	968.984	1	3.7	3.659	290.445	525.144	430.003	95.141	0	0	50.506
2AMB_A	Agonist	1038.519	1	2.75	4.157	312.451	564.911	416.211	82.137	66.562	0	47.958
2AO6_A	Agonist	948.286	1	2.75	3.385	284.397	527.449	363.478	90.683	73.288	0	49.206
2AX6_A	Agonist	839.503	2	4.25	2.252	292.214	500.839	149.533	147.462	101.071	102.772	95.361
2AX7_A	Agonist	1123.96	2	5	3.928	402.302	648.465	91.447	146.046	266.895	144.078	101.505
2AX8_A	Agonist	1123.946	2	5	3.928	402.302	648.448	91.442	146.043	266.885	144.078	101.503
2AX9_A	Agonist	885.832	2	4.25	2.658	371.11	524.528	111.371	145.693	100.859	166.605	94.473
2AXA_A	Agonist	1123.947	2	5	3.928	402.302	648.452	91.443	146.044	266.887	144.078	101.502
2HVC_A	Agonist	935.657	1	3.5	4.353	392.224	539.95	49.956	85.118	107.68	297.195	44.797
2OZ7_A	Agonist	1243.354	0	6	3.923	418.959	652.746	477.905	113.842	2.404	58.596	79.633
2PIO_A	Agonist	968.984	1	3.7	3.659	290.445	525.144	430.003	95.141	0	0	50.506
2PIP_A	Agonist	968.984	1	3.7	3.659	290.445	525.144	430.003	95.141	0	0	50.506

Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

PDB code_Chain	Ligand Profile	volume	donorHB	accptHB	QPlogPo/w	MW	SASA	FOSA	FISA	PISA	WPSA	PSA
2PIQ_A	Agonist	968.984	1	3.7	3.659	290.445	525.144	430.003	95.141	0	0	50.506
2PIR_A	Agonist	968.984	1	3.7	3.659	290.445	525.144	430.003	95.141	0	0	50.506
2PIT_A	Agonist	968.984	1	3.7	3.659	290.445	525.144	430.003	95.141	0	0	50.506
2PIU_A	Agonist	968.983	1	3.7	3.659	290.445	525.143	430.003	95.141	0	0	50.506
2PIV_A	Agonist	968.984	1	3.7	3.659	290.445	525.144	430.003	95.141	0	0	50.506
2PIW_A	Agonist	968.984	1	3.7	3.659	290.445	525.144	430.003	95.141	0	0	50.506
2PIX_A	Agonist	968.983	1	3.7	3.659	290.445	525.144	430.003	95.141	0	0	50.506
2PKL_A	Agonist	968.984	1	3.7	3.659	290.445	525.144	430.003	95.141	0	0	50.506
2PNU_A	Agonist	1382.16	1	5.4	5.578	446.576	737.257	422.818	92.264	128.216	93.959	57.057
2Q7I_A	Agonist	962.433	1	3.7	3.32	288.429	524.41	395.378	99.588	29.444	0	50.852
2Q7J_A	Agonist	962.433	1	3.7	3.32	288.429	524.41	395.378	99.588	29.444	0	50.852
2Q7K_A	Agonist	962.433	1	3.7	3.32	288.429	524.41	395.378	99.588	29.444	0	50.852
2Q7L_A	Agonist	962.433	1	3.7	3.32	288.429	524.41	395.378	99.588	29.444	0	50.852
2Z4J_A	Agonist	968.983	1	3.7	3.659	290.445	525.144	430.003	95.141	0	0	50.506
3B5R_A	Agonist	1163.979	2	5.5	4.336	416.759	680.236	91.492	129.16	242.595	216.989	85.101
3B65_A	Agonist	1115.304	2	7	2.554	447.231	647.283	95.616	189.621	285.871	76.175	108.417
3B66_A	Agonist	1177.746	2	6.5	2.957	409.321	686.714	91.246	226.223	262.164	107.082	130.024
3B67_A	Agonist	1157.927	2	5	4.625	474.264	656.376	86.52	134.455	150.356	285.046	100.18
3B68_A	Agonist	1276.328	3	7.5	3.101	441.363	734.936	185.746	204.232	247.918	97.041	140.188