

Table S1. Two hundred fifty-six complexes with the highest absolute affinities from docking with AutoDock Vina (kcal/mol).

PDB ID	PATHWAY	COMPOUND	AF AVERAGE	SD
1FCX	Nuclear Receptor	BAP	-11,00	0,26
1FCX	Nuclear Receptor	APAP	-6,9	0,00
1FCX	Nuclear Receptor	NAPQI	-7,30	0,17
1G1U	Nuclear Receptor	BAP	-10,90	0,00
1G1U	Nuclear Receptor	APAP	-6,667	0,23
1G1U	Nuclear Receptor	NAPQI	-6,633	0,06
1G1U	Nuclear Receptor	AM404	-8,73	0,25
1G5Y	Nuclear Receptor	BAP	-10,83	0,06
1G5Y	Nuclear Receptor	NAPQI	-6,633	0,25
1G5Y	Nuclear Receptor	AM404	-8,43	0,40
1GIH	Cell Proliferation	BAP	-10,80	0,00
1GIH	Cell Proliferation	APAP-GLUTATHIONE	-8,433	0,32
1HK4	Thyroid	BAP	-12,70	0,10
1HK4	Thyroid	APAP	-6,7	0,00
1HK4	Thyroid	NAPQI	-6,97	0,06
1HK4	Thyroid	APAP-GLUTATHIONE	-9,03	0,72
1HK4	Thyroid	AM404	-8,80	0,35
1J1A	Neuroprotection	BAP	-10,60	0,00
1J1A	Neuroprotection	AM404	-7,97	0,64
1NSI	Inflammation	BAP	-10,80	0,35
1NSI	Inflammation	APAP	-6,867	0,12
1NSI	Inflammation	APAP-GLUCURONIDE	-9,83	0,38
1NSI	Inflammation	APAP-GLUTATHIONE	-8,467	0,32
1OJC	Neuroprotection	APAP-GLUCURONIDE	-9,47	0,15
1OJC	Neuroprotection	AM404	-8,47	1,88
1OL5	Cell Proliferation	BAP	-11,67	0,06
1OL5	Cell Proliferation	AM404	-8,37	0,38
1P8D	Nuclear Receptor	BAP	-12,20	0,10
1P8D	Nuclear Receptor	NAPQI	-6,90	0,00
1P8D	Nuclear Receptor	APAP-GLUCURONIDE	-9,60	0,26
1P8D	Nuclear Receptor	AM404	-8,63	1,77
1RY8	Cytochrome P450	BAP	-11,27	0,06
1RY8	Cytochrome P450	NAPQI	-6,467	0,06
1RY8	Cytochrome P450	APAP-GLUCURONIDE	-9,20	0,00
1TQN	Cytochrome P450	BAP	-11,00	0,00
1TQN	Cytochrome P450	NAPQI	-6,8	0,10
1TQN	Cytochrome P450	APAP-GLUTATHIONE	-8,733	0,35
1TQN	Cytochrome P450	AM404	-8,50	0,17
1UY6	Heat Shock	BAP	-11,80	0,00

1UY6	Heat Shock	NAPQI	-6,5	0,00
1UY6	Heat Shock	APAP-GLUTATHIONE	-8,567	0,21
1UY6	Heat Shock	AM404	-8,10	0,61
1UY7	Heat Shock	BAP	-12,10	0,00
1UY7	Heat Shock	APAP	-6,867	0,06
1UY7	Heat Shock	NAPQI	-6,733	0,06
1UY7	Heat Shock	APAP-GLUTATHIONE	-8,6	0,30
1UY8	Heat Shock	BAP	-12,00	0,00
1UY8	Heat Shock	APAP	-6,7	0,00
1UY8	Heat Shock	NAPQI	-6,8	0,00
1UY8	Heat Shock	APAP-GLUTATHIONE	-8,433	0,15
1UY8	Heat Shock	AM404	-8,13	0,64
1UY9	Heat Shock	BAP	-12,00	0,00
1UY9	Heat Shock	APAP	-6,9	0,00
1UY9	Heat Shock	NAPQI	-6,667	0,06
1UY9	Heat Shock	AM404	-8,27	0,23
1UYC	Heat Shock	BAP	-11,90	0,00
1UYC	Heat Shock	APAP	-6,667	0,06
1UYC	Heat Shock	NAPQI	-6,733	0,12
1UYC	Heat Shock	APAP-GLUTATHIONE	-8,933	0,06
1UYC	Heat Shock	AM404	-8,23	0,21
1UYD	Heat Shock	BAP	-12,10	0,00
1UYD	Heat Shock	NAPQI	-6,6	0,00
1UYD	Heat Shock	APAP-GLUTATHIONE	-8,733	0,06
1UYD	Heat Shock	AM404	-8,33	0,49
1UYE	Heat Shock	BAP	-12,03	0,06
1UYE	Heat Shock	APAP	-6,767	0,06
1UYE	Heat Shock	NAPQI	-6,7	0,00
1UYE	Heat Shock	APAP-GLUTATHIONE	-8,7	0,40
1UYE	Heat Shock	AM404	-8,30	0,00
1UYF	Heat Shock	BAP	-12,10	0,00
1UYF	Heat Shock	NAPQI	-6,567	0,06
1UYF	Heat Shock	AM404	-8,37	0,40
1UYG	Heat Shock	BAP	-12,00	0,00
1UYG	Heat Shock	APAP	-6,8	0,10
1UYG	Heat Shock	NAPQI	-6,8	0,20
1UYG	Heat Shock	AM404	-8,30	0,17
1UYH	Heat Shock	BAP	-11,70	0,00
1UYH	Heat Shock	APAP	-6,9	0,00
1UYH	Heat Shock	NAPQI	-6,867	0,06
1UYH	Heat Shock	AM404	-8,50	0,36
1UYI	Heat Shock	BAP	-11,13	0,25
1UYI	Heat Shock	NAPQI	-6,6	0,17

1UYK	Heat Shock	BAP	-11,93	0,06
1UYK	Heat Shock	NAPQI	-6,8	0,17
1UYK	Heat Shock	AM404	-8,10	0,53
1UYM	Heat Shock	BAP	-12,20	0,00
1UYM	Heat Shock	NAPQI	-6,7	0,00
1UYM	Heat Shock	AM404	-7,90	0,20
1X78	Apoptosis	BAP	-11,80	0,26
1X78	Apoptosis	APAP	-6,6	0,00
1X78	Apoptosis	NAPQI	-6,533	0,12
1XAP	Nuclear Receptor	BAP	-12,00	0,00
1XAP	Nuclear Receptor	APAP	-7	0,00
1XAP	Nuclear Receptor	NAPQI	-7,40	0,00
1XAP	Nuclear Receptor	APAP-GLUCURONIDE	-9,30	0,00
1YRP	Skin Fibrosis	BAP	-11,40	0,00
1YRP	Skin Fibrosis	APAP-GLUTATHIONE	-8,667	0,06
1Z57	Cell Proliferation	BAP	-12,40	0,00
1Z57	Cell Proliferation	APAP	-6,8	0,00
1Z57	Cell Proliferation	NAPQI	-6,90	0,00
1Z57	Cell Proliferation	APAP-GLUTATHIONE	-9,43	0,12
1Z57	Cell Proliferation	AM404	-8,20	0,10
2BYB	Neuroprotection	BAP	-10,70	0,00
2BYB	Neuroprotection	APAP-GLUCURONIDE	-9,40	0,44
2FWY	Heat Shock	BAP	-11,70	0,00
2FWY	Heat Shock	APAP	-6,8	0,00
2FWY	Heat Shock	NAPQI	-6,567	0,06
2FWY	Heat Shock	APAP-GLUTATHIONE	-8,8	0,30
2FWY	Heat Shock	AM404	-8,30	0,26
2FWZ	Heat Shock	BAP	-11,80	0,00
2FWZ	Heat Shock	NAPQI	-6,467	0,06
2FWZ	Heat Shock	APAP-GLUTATHIONE	-8,467	0,21
2FWZ	Heat Shock	AM404	-8,13	0,29
2H55	Heat Shock	BAP	-11,70	0,00
2H55	Heat Shock	APAP	-6,8	0,00
2H55	Heat Shock	NAPQI	-6,733	0,15
2H55	Heat Shock	APAP-GLUTATHIONE	-8,8	0,26
2H55	Heat Shock	AM404	-8,30	0,10
2HI4	Cytochrome P450	BAP	-13,97	0,25
2HI4	Cytochrome P450	APAP	-7,1	0,00
2HI4	Cytochrome P450	NAPQI	-6,8	1,04
2PVR	Cell Proliferation	BAP	-12,00	0,00
2PVR	Cell Proliferation	APAP	-6,633	0,06
2PVR	Cell Proliferation	AM404	-8,67	0,76
2XSI	Insuline signaling	BAP	-13,00	0,00

2XSI	Insuline signaling	APAP	-6,667	0,06
2XSI	Insuline signaling	NAPQI	-6,7	0,26
2XSI	Insuline signaling	APAP-GLUCURONIDE	-8,87	0,57
2XSI	Insuline signaling	APAP-GLUTATHIONE	-9	0,10
2XSI	Insuline signaling	AM404	-8,43	0,21
2XVT	Insuline signaling	BAP	-10,67	0,23
2XVT	Insuline signaling	APAP-GLUTATHIONE	-8,7	0,20
2ZJW	Apoptosis	BAP	-12,60	0,00
2ZJW	Apoptosis	APAP	-6,7	0,00
2ZJW	Apoptosis	NAPQI	-6,5	0,00
2ZJW	Apoptosis	APAP-GLUCURONIDE	-9,07	0,06
2ZJW	Apoptosis	APAP-GLUTATHIONE	-8,5	0,26
2ZJW	Apoptosis	AM404	-8,10	0,36
3D90	Coagulation	BAP	-10,60	0,69
3D90	Coagulation	NAPQI	-6,467	0,06
3D90	Coagulation	APAP-GLUCURONIDE	-9,17	0,06
3EAH	Cancer Cell Proliferation	BAP	-11,03	0,15
3EAH	Cancer Cell Proliferation	APAP	-7	0,00
3EAH	Cancer Cell Proliferation	NAPQI	-6,7	0,30
3EAH	Cancer Cell Proliferation	APAP-GLUCURONIDE	-9,50	0,00
3EAH	Cancer Cell Proliferation	AM404	-8,00	0,30
3FT8	Heat Shock	BAP	-12,10	0,00
3FT8	Heat Shock	APAP	-6,9	0,00
3FT8	Heat Shock	NAPQI	-6,467	0,06
3FT8	Heat Shock	APAP-GLUCURONIDE	-9,07	0,06
3FT8	Heat Shock	APAP-GLUTATHIONE	-8,667	0,12
3FT8	Heat Shock	AM404	-7,97	0,40
3H1V	Insuline signaling	BAP	-10,90	0,00
3H1V	Insuline signaling	APAP-GLUCURONIDE	-9,20	0,00
3H1V	Insuline signaling	AM404	-7,93	0,21
3KVV	Apoptosis	BAP	-12,37	0,06
3KVV	Apoptosis	APAP	-6,633	0,06
3KVV	Apoptosis	NAPQI	-6,8	0,17
3KVV	Apoptosis	AM404	-8,57	0,35
3LKJ	Apoptosis	BAP	-12,20	0,00
3LKJ	Apoptosis	APAP-GLUCURONIDE	-9,37	0,06
3LKJ	Apoptosis	APAP-GLUTATHIONE	-9,73	0,29
3LKJ	Apoptosis	AM404	-9,07	0,23
3mdy	Neuroprotection	BAP	-11,93	0,12
3mdy	Neuroprotection	NAPQI	-6,7	0,00
3mdy	Neuroprotection	APAP-GLUCURONIDE	-9,70	0,00
3MWD	Insuline signaling	BAP	-11,07	0,12
3MWD	Insuline signaling	AM404	-7,97	0,67

3NMQ	Cancer Cell Proliferation	BAP	-11,80	0,00
3NMQ	Cancer Cell Proliferation	APAP	-6,7	0,00
3NMQ	Cancer Cell Proliferation	NAPQI	-6,767	0,06
3O0I	Cancer Cell Proliferation	BAP	-12,20	0,00
3O0I	Cancer Cell Proliferation	APAP	-7	0,00
3O0I	Cancer Cell Proliferation	NAPQI	-6,8	0,00
3O0I	Cancer Cell Proliferation	APAP-GLUTATHIONE	-8,767	0,32
3O0I	Cancer Cell Proliferation	AM404	-8,63	0,64
3O96	Coagulation	BAP	-11,83	0,06
3O96	Coagulation	APAP-GLUTATHIONE	-8,967	0,35
3O96	Coagulation	AM404	-8,80	0,10
3PM0	Cytochrome P450	BAP	-12,10	3,16
3PM0	Cytochrome P450	APAP	-7,7	0,00
3PM0	Cytochrome P450	NAPQI	-7,80	0,69
3PM0	Cytochrome P450	APAP-GLUCURONIDE	-9,07	0,15
3PM0	Cytochrome P450	APAP-GLUTATHIONE	-8,867	0,51
3PM0	Cytochrome P450	AM404	-7,90	1,44
3UA1	Neuroprotection	BAP	-11,60	0,00
3UA1	Neuroprotection	NAPQI	-6,667	0,06
3UA1	Neuroprotection	AM404	-8,53	0,21
3UNJ	Cancer Cell Proliferation	BAP	-11,47	0,06
3UNJ	Cancer Cell Proliferation	APAP	-6,7	0,00
3UNJ	Cancer Cell Proliferation	NAPQI	-6,833	0,23
3UNJ	Cancer Cell Proliferation	AM404	-8,10	0,17
3VHE	Angiogenesis	BAP	-11,57	0,46
3VHE	Angiogenesis	APAP	-7,2	0,00
3VHE	Angiogenesis	NAPQI	-6,8	0,00
3VHE	Angiogenesis	AM404	-8,27	0,15
3ZGV	Neuroprotection	BAP	-10,60	0,60
3ZGV	Neuroprotection	APAP	-6,667	0,06
3ZGV	Neuroprotection	NAPQI	-6,7	0,10
3ZGV	Neuroprotection	AM404	-8,43	1,27
4A7A	Neuroprotection	APAP-GLUCURONIDE	-9,27	0,93
4A7A	Neuroprotection	AM404	-7,87	1,53
4ACG	Cancer Cell Proliferation	BAP	-10,60	0,00
4ACG	Cancer Cell Proliferation	APAP	-6,9	0,00
4AOJ	Apoptosis	BAP	-12,47	0,06
4AOJ	Apoptosis	APAP	-6,6	0,00
4C9X	Oxidative Stress	BAP	-10,90	0,00
4C9X	Oxidative Stress	NAPQI	-6,633	0,06
4DM8	Nuclear Receptor	BAP	-10,67	2,27
4DM8	Nuclear Receptor	APAP	-6,933	0,23
4DM8	Nuclear Receptor	APAP-GLUTATHIONE	-8,567	0,25

4drj	Neuroprotection	BAP	-12,10	0,00
4drj	Neuroprotection	APAP-GLUCURONIDE	-9,47	0,06
4drj	Neuroprotection	AM404	-8,60	0,00
4EY4	Neuroprotection	BAP	-11,73	0,06
4EY4	Neuroprotection	APAP	-6,9	0,00
4EY4	Neuroprotection	APAP-GLUCURONIDE	-8,90	0,00
4EY6	Neuroprotection	BAP	-11,20	0,26
4EY6	Neuroprotection	APAP	-6,8	0,17
4EY6	Neuroprotection	APAP-GLUCURONIDE	-9,00	0,00
4EY7	Neuroprotection	BAP	-11,87	0,06
4EY7	Neuroprotection	APAP	-6,767	0,06
4EY7	Neuroprotection	NAPQI	-6,633	0,57
4EY7	Neuroprotection	APAP-GLUCURONIDE	-9,70	0,17
4EY7	Neuroprotection	AM404	-8,27	1,27
4FYR	Coagulation	BAP	-11,20	0,00
4FYR	Coagulation	NAPQI	-6,833	0,06
4FYR	Coagulation	APAP-GLUCURONIDE	-9,37	0,29
4FYR	Coagulation	APAP-GLUTATHIONE	-8,5	0,36
4FYR	Coagulation	AM404	-8,10	0,30
4QVX	Apoptosis	BAP	-10,83	0,12
4QVX	Apoptosis	APAP	-7,0	0,00
4QVX	Apoptosis	NAPQI	-6,5	0,10
4QVX	Apoptosis	AM404	-8,83	0,74
4RG2	Cell Proliferation	BAP	-14,10	0,00
4RG2	Cell Proliferation	APAP	-7,5	0,10
4RG2	Cell Proliferation	NAPQI	-7,30	0,46
4XRY	Cytochrome P450	BAP	-11,03	0,47
4XRY	Cytochrome P450	APAP-GLUCURONIDE	-9,07	0,57
4XRY	Cytochrome P450	AM404	-7,97	0,64
5ANS	Oxidative Stress	BAP	-11,03	0,06
5ANS	Oxidative Stress	NAPQI	-6,7	0,00
5ANV	Oxidative Stress	BAP	-11,10	0,00
5ANV	Oxidative Stress	APAP	-6,7	0,00
5ANV	Oxidative Stress	NAPQI	-6,6	0,00
5FNC	Cell Proliferation	BAP	-11,90	0,00
5FNC	Cell Proliferation	NAPQI	-6,767	0,06
5FNC	Cell Proliferation	APAP-GLUTATHIONE	-8,5	0,40
5FNC	Cell Proliferation	AM404	-8,17	0,25
5gpg	Neuroprotection	BAP	-11,40	0,00
5gpg	Neuroprotection	APAP-GLUCURONIDE	-8,90	0,00
5gpg	Neuroprotection	AM404	-8,23	0,12
5j20	Heat Shock	BAP	-11,40	0,00
5j20	Heat Shock	NAPQI	-6,467	0,23

5j20	Heat Shock	APAP-GLUCURONIDE	-9,27	0,06
5j20	Heat Shock	AM404	-8,10	0,00

PDB ID: Protein Data Bank Identification Code. The runs were performed in triplicate.