Supporting Information

Discovery of Novel Antimalarial Compounds Enabled by QSAR-Based Virtual Screening

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Supplementary Table 1. Features of 10 sets of DBS models and their external accuracy.

Model Set ID	M0	M1	M2	M3	M4	M5	M6	M7	M8	M9
# of Compounds	423	421	423	423	422	422	422	423	423	422
# of Accepted models used for prediction	63	71	68	124	27	55	44	58	58	48
# of Descriptors	344	342	346	340	342	340	351	352	345	333
CCR	0.67	0.61	0.61	0.67	0.66	0.60	0.66	0.65	0.62	0.60

Supplementary Table 2. Counts of molecules in external evaluation set (70 compounds) that were marked as “inconclusive” at different CPTs for SBS and DBS models, respectively.

CPT	0.55/0.45	0.6/0.4	0.65/0.35	0.7/0.3	0.8/0.2	0.9/0.1
SBS Models	3	5	7	10	18	24
DBS Models	9	18	24	34	56	62

Supplementary Table 3. Structures, antimalarial activity and drug susceptibility of 176 virtual screening hits.

Chemicals with confirmed antimalarial activity are shown in bold.

REGNUM	Smiles	Antimalarial Activity (EC50, μM)		Drug Susceptibility (EC50, μM)	
		3D7	K1	BJ	HEPG2
SJ000565000	N12CCC(CC1C(c3ccnc(cccc4)c34)OC(=O)C5CC5)C(C=C)C2.Cl	**0.0956**	**0.3178**	**>*19.2663**	**-†**
SJ000565062	c12c(cccc1)cccc2OCC(O)CN(CCCC)CCCC.Cl	**1.5466**	**0.1457**	**>28.6957**	**11.4906**
SJ000565033	c1(cc(C)nc(ccc(OC)c2)c12)Nc(cc3)ccc3OCC	**1.7216**	**6.0942**	**>27.3641**	**>27.3641**
SJ000173328	c1(cc(C)nc(ccc(OCC)c2)c12)Nc(ccc(c34)OCCO3)c4.Cl	**1.9858**	**>17.9429**	**>32.4728**	**>32.4728**
SJ000565039	c1(ccccc1OCC(O)CNC(C)c2ccccc2)C(C)(C)C.Cl	**3.0999**	**0.7109**	**21.7739**	**>27.2826**
SJ000565002	c12c(cccc1)ccc(OCC(O)CN(CCCC)CCCC)c2.Cl	**3.4873**	**0.7575**	**>32.3370**	**-**
SJ000565115	N(Cc(cc1)ccc1OCc2ccccc2)C(C)C(O)c3ccccc3.Cl	**3.8999**	**0.6032**	**>30.7609**	**>30.7609**
SJ000565043	c1(nc(C)cc2Nc3ccc(c(OC)c3)OC)c2ccc(cccc4)c14	**3.9945**	**>10.3904**	**>18.8043**	**6.4956**
SJ000205073	N(Cc(cc1)ccc1OCC=C)C(C)C(O)c2ccccc2.Cl	**4.9445**	**>12.0420**	**>21.7935**	**>21.7935**
SJ000565072	n(ccn1CCCOc(cc2)ccc2C(C)(C)c3ccccc3)c1.C(O)(=O)C(O)=O	**5.3775**	**>12.5225**	**>22.6630**	**>22.6630**
SJ000188975	N(CCc(c12)cccc1)(CC(O)COc3ccc(cc3C(C)(C)C)C)C2.Cl	**6.0279**	**1.6561**	**>29.5652**	**>29.5652**
SJ000565117	n(ccn1CCCCOc2ccccc2Cc3ccccc3)c1.Cl	**8.151**	**>20.4805**	**>37.0652**	**>37.0652**
SJ000565031	S(N)(=O)(=O)c1ccc(cc1)Nc(c(cc2)c3cc2[N+](=O)[O-])c(cccc4C)c4n3	**>13.6787**	**0.5332**	**>24.7554**	**>24.7554**
SJ000150414	c1(ccccc1OCCN(CC)CC)C(CCc2ccccc2)=O.Cl	**>18.7688**	**1.0081**	**>33.9674**	**>33.9674**
SJ000565025	c12c(cccc1)ccc(OCCCCCNCCCC)c2	**>13.0931**	**1.3621**	**>23.6957**	**12.8188**
SJ000564998	[n+]1(C)ccc(c2c1Cc(ccc(c3OC)OC)c3)cc(c(OC)c2)OC.[I-]	**>17.1471**	**2.0551**	**>31.0326**	**>31.0326**
SJ000565010	N1(CCCCC1)CCCCCOc(ccc(c23)cccc2)c3	**>12.6426**	**2.4118**	**11.1753**	**8.4292**

* "Greater than" means that there was a change in effect (i.e., some growth inhibition), but the isotherm did not saturate. Therefore, it doesn't indicate inactive, but no assignable numeric value for potency.

† No dose-response curve was derived from experiments.

SJ000202592	C(O)(=O)C(O)=O.c1(cc(Cl)ccc1OCCCCNCC(C)O)Cc2ccccc2	**>7.0571**	**2.5655**	**>12.7717**	**>12.7717**
SJ000565067	C(O)(=O)C(O)=O.c1(ccccc1OCCCCN2CCCCC2)c3ccccc3	**>13.5135**	**3.1098**	**>24.4565**	**>24.4565**
SJ000183110	C(O)(=O)C(O)=O.N(C)(CCCCOc(cc1)ccc1CC)Cc2ccccc2	**>12.4024**	**4.7387**	**>22.4457**	**>22.4457**
SJ000565003	c1(c(ccc2C(CC3)(CCO3)CNCCC(c4ccccc4)c5ccccc5)OCCO1)c2.Cl	**>13.7538**	**5.2169**	**18.1739**	**>24.8913**
SJ000565071	C(O)(=O)C(O)=O.C(c1ccccc1)(=O)c2ccc(cc2)OCCCCN3CCC(CC3)C	**>14.8348**	**6.1013**	**>26.8478**	**>26.8478**
SJ000565094	N1(CCCCC1)CC(O)COc(cc2)ccc2OCc3ccccc3	**>14.9550**	**6.1575**	**>27.0652**	**>27.0652**
SJ000565077	C(O)(=O)C(O)=O.N(C)(CCCCOc1ccccc(CC)c1)Cc2ccccc2	**>16.8168**	**6.2246**	**>30.4348**	**>30.4348**
SJ000565064	C(CCCC)(CC(OCC)=O)(C1=O)C(=O)N(N1c2ccccc2)c3ccccc3	**>16.5616**	**7.9107**	**>29.9728**	**26.6172**
SJ000565100	C(O)(=O)C(O)=O.N(CCOc1ccc(cc1OC)CC=C)(CCc(c23)cccc2)C3	>2.8228	<0.0001	>5.1087	>5.1087
SJ000126082	C(/CC(O)=O)(\C(O)=O)=C\C(O)=O	>15.0150	<0.0008	>27.1739	-
SJ000039232	S(N)(=O)(=O)c1ccc(cc1)NC(=O)c(c2c(cccc2)nc3c4ccccc4C)c3	>10.0150	>10.0150	>18.1250	>18.1250
SJ000565120	c1(OC)cc(CNCc2ccccn2)ccc1OCc(cc3)ccc3F.Cl	<0.0005	>10.0300	>18.1522	>18.1522
SJ000565058	c12c(cccn1)cccc2OCCOCCOc(ccc(c3C)C)c3	>10.4805	>10.4805	>18.9674	>18.9674
SJ000565036	c1(C(C)C)ccc(cc1C)OCC(O)CNC(C)c2ccccc2.Cl	>10.7207	>10.7207	>19.4022	>19.4022
SJ000565080	C(O)(=O)C(O)=O.c1c(cccc1Oc2ccccc2)OCCCCNC(C)CC	>10.7808	>10.7808	>19.5109	7.7858
SJ000565012	c1(OCCCCCN2CCCCC2)cc(C)cc(C)c1C	>10.8408	>10.8408	>19.6196	>19.6196
SJ000565023	n1c(ccc(c23)cccc2)c3c4c(CCC4)c1c(cc5OC)cc(c5OC)OC	>10.8408	>10.8408	>19.6196	>19.6196
SJ000338146	c1(c(cccc1CNCc(cc2)ccn2)OC)OCc(cc3)ccc3Cl.Cl	>10.9610	>10.9610	>19.8370	>19.8370
SJ000565005	N(CCc(c12)cc(c(OC)c1)OC)(Cc(cc3)ccc3c4ccccc4)C2	>11.0210	>11.0210	>19.9457	>19.9457
SJ000565087	C(O)(=O)C(O)=O.c1(CC)cc(OCCCCNCc2ccccc2)ccc1Cl	>11.1111	>11.1111	>20.1087	13.6906
SJ000565020	C1(CCC(CC1)NCCc(cc2)ccc2OC)c3ccccc3	>11.2012	>11.2012	>20.2717	>20.2717
SJ000203427	C(COc1ccccc1CNCC(C)C)(NCCc2ccccc2)=O.Cl	>11.2162	>11.2162	>20.2989	>20.2989
SJ000565028	n(ccn1CCCCCCOc2c(C)cc(cc2C)C)	>11.2312	>11.2312	>20.3261	>20.3261

	c1				
SJ000565007	c1(C)c(C)c(OC)ccc1CN2CCC(CC2)Cc3ccccc3	>11.2613	>11.2613	>20.3804	-
SJ000506625	n1(c2ccccc2)c(ccc(c3)NCc(cc4)ccc4OCC)c3nc1	>11.3063	>11.3063	>20.4620	>20.4620
SJ000565124	c1(OC)cc(CNCc2ccccn2)ccc1OCc3cccc(C)c3.Cl	>11.4865	>11.4865	>20.7880	>20.7880
SJ000338434	c1(OC)cc(CNCc(cc2)ccn2)ccc1OCc(cc3)ccc3F.Cl	>11.5015	>11.5015	>20.8152	>20.8152
SJ000565024	c12c(cccc1)CCCC2NCc(ccc(c3OCC)OC)c3	>11.5015	>11.5015	>20.8152	>20.8152
SJ000565083	N1(CCOCCOc2cccc(cccc3)c23)CC(C)CC(C)C1.C(O)(=O)C(O)=O	>11.5616	>11.5616	>20.9239	>20.9239
SJ000299062	c12c(cccc1)cccc2OCCCCCN(CC)CC	>11.5916	>11.5916	>20.9783	>20.9783
SJ000565097	N(CCc(c12)cccc1)(CC(O)COc(ccc(c3C)Cl)c3)C2.Cl	>11.6216	>11.6216	>21.0326	>21.0326
SJ000331443	N1(CCC(CC1)Cc2ccccc2)Cc(ccc(c3C)OC)c3	>11.7417	>11.7417	>21.2500	>21.2500
SJ000565121	c1(OC)cc(CNCc2ccccn2)ccc1OCc3cccc(Cl)c3.Cl	>11.7568	>11.7568	>21.2772	>21.2772
SJ000565112	c1(ccc(cc1OCC)CNCc2ccccc2)OC3CCCC3.Cl	>11.7718	>11.7718	>21.3043	>21.3043
SJ000565061	N(Cc1ccccc1)(Cc2ccccc2)CC(O)COc3ccccc3C.Cl	>11.8018	>11.8018	>21.3587	>21.3587
SJ000565017	c(c(OC)ccc1c2ccccc2)(NCC(CC3)=CCC3C(C)=C)c1	>11.8318	>11.8318	>21.4130	>21.4130
SJ000203158	c1(cc(C)ccc1OCCCNCC(C)O)Cc2ccccc2.Cl	>11.8919	>11.8919	>21.5217	8.6902
SJ000565085	c1(C)c(Cl)ccc(OCCCCN(C)Cc2ccccc2)c1C.C(O)(=O)C(O)=O	>11.9520	>11.9520	>21.6304	>21.6304
SJ000565104	n1cn(c2c1cccc2)CCCCOc(c(c(c3Cl)C)C)cc3.C(C(=O)O)(=O)O	>11.9520	>11.9520	>21.6304	>21.6304
SJ000565092	N(CCCCOc1ccccc1c2ccccc2)(CC3C)CC(O3)C.C(O)(=O)C(O)=O	>12.0721	>12.0721	>21.8478	>21.8478
SJ000565096	c1(OCCCN(CCc(c23)cccc2)C3)cc(C)ccc1C(C)C.Cl	>12.1321	>12.1321	>21.9565	>21.9565
SJ000565084	C(O)(=O)C(O)=O.c1(OC)cc(ccc1OCCCCN(C)Cc2ccccc2)\C=C\C	>12.1622	>12.1622	>22.0109	>22.0109
SJ000565090	C(O)(=O)C(O)=O.c1(OCCCNCCc2ccccc2)cc(C)ccc1C(C)C	>12.1622	>12.1622	>22.0109	10.0292
SJ000565018	N(CC1)(CCN1C2CCc(c3C2)cccc3)c4ccccc4OC	>12.1772	>12.1772	>22.0380	>22.0380
SJ000331940	c1(C)cc(ccc1OC)CN(CCCC)Cc2ccccc2	>12.2222	>12.2222	>22.1196	-

SJ000565059	N(Cc1ccccc1)(Cc2ccccc2)CC(O)COc(cc3)ccc3C.Cl	>12.2222	>12.2222	>22.1196	>22.1196
SJ000112434	C(O)(=O)C(O)=O.c1(cc(ccc1OC)CN(C)CCc2ccccn2)OCc3ccccc3	>12.3123	>12.3123	>22.2826	>22.2826
SJ000334205	c12c(cccn1)cccc2OCCOCCOc(cc3)ccc3CC	>12.3123	>12.3123	>22.2826	>22.2826
SJ000197026	c1(OCC)cc(ccc1OCC(C)C)CNC(C)c2ccccc2.Cl	>12.4625	>12.4625	>22.5543	>22.5543
SJ000565078	C(O)(=O)C(O)=O.c1(OCCCCN(C)Cc2ccccc2)c(C)cc(cc1C)C	>12.5526	>12.5526	>22.7174	>22.7174
SJ000565081	C(O)(=O)C(O)=O.c1(OCCCN(C)Cc2ccccc2)cc(C)ccc1C(C)C	>12.6426	>12.6426	>22.8804	>22.8804
SJ000565065	C(CCCC)(CC(OC)=O)(C1=O)C(=O)N(N1c2ccccc2)c3ccccc3	>12.6577	>12.6577	>22.9076	>22.9076
SJ000565022	n1c(ccc(c23)cccc2)c3c4c(CCC4)c1c(cc5OC)cc(c5O)OC	>12.7027	>12.7027	>22.9891	>22.9891
SJ000565106	n1cn(c2c1cccc2)CCOc3ccc(c4c3cccc4)Cl.C(C(=O)O)(=O)O	>12.8679	>12.8679	>23.2880	>23.2880
SJ000166650	c12c(cccn1)cccc2OCCOc3ccc(cc3OC)C	>12.8829	>12.8829	>23.3152	>23.3152
SJ000565129	c1(nccc(cc(c(OC)c2)OC)c12)C(N)c3ccc(c(OC)c3)OC	>12.8829	>12.8829	>23.3152	>23.3152
SJ000334212	c12c(cccn1)cccc2OCCOCCOc3ccc(cc3OC)CC=C	>12.9429	>12.9429	>23.4239	22.5869
SJ000565032	n1c(ccc(c23)cccc2)c3c4c(CCC4)c1c5ccc(c(OC)c5)OC	>12.9730	>12.9730	>23.4783	>23.4783
SJ000565014	N1(CCC(CC1)C)Cc(ccc(c2OCc3ccccc3)OC)c2	>13.0030	>13.0030	>23.5326	-
SJ000565019	c12c(CCC1)ccc(c2)NCc(cc3)ccc3OCCCC	>13.0631	>13.0631	>23.6413	>23.6413
SJ000565095	N(CCCCOc1ccc(cc1C)C)(CCc(c23)cccc2)C3.Cl	>13.2733	>13.2733	>24.0217	>24.0217
SJ000565027	C(O)(=O)C(O)=O.c1(OCC)cc(ccc1OC)CNC(c2ccccc2)Cc3ccccc3	>13.3033	>13.3033	>24.0761	>24.0761
SJ000565076	c1(C)cc(C)ccc1OCCCCNCCc2ccccc2	>13.3934	>13.3934	>24.2391	>24.2391
SJ000565114	C(COc1ccccc1CNC2CCCC2)(=O)NCc3ccccc3.Cl	>13.4084	>13.4084	>24.2663	>24.2663
SJ000565107	c1(OCc2ccccc2)c(OC)cc(cc1Cl)CNCc(cc3)ccn3.Cl	>13.6336	>13.6336	>24.6739	>24.6739
SJ000565016	c1(OC)cc(CCNC(CCc(c23)cccc2)C3)ccc1OC	>13.6637	>13.6637	>24.7283	>24.7283
SJ000565044	N1(CCC(CC1)Cc2ccccc2)CC(O)COc3cccc(OC)c3.Cl	>13.6637	>13.6637	>24.7283	>24.7283
SJ000565021	N(CCc(c12)cc(c(OC)c1)OC)(C(CC3	>13.6937	>13.6937	>24.7826	>24.7826

	)CCC3c4ccccc4)C2				
SJ000196267	c1(OC)cc(ccc1OCC(C)C)CNC(C)c2ccccc2.Cl	>13.8739	>13.8739	>25.1087	>25.1087
SJ000565119	c1(OC)cc(CNCc(cccn2)c2)ccc1OCc(ccc3Cl)cc3.Cl	>13.9339	>13.9339	>25.2174	>25.2174
SJ000565079	C(O)(=O)C(O)=O.c1(OCCCCN(C)Cc2ccccc2)cc(C)cc(C)c1C	>13.9640	>13.9640	>25.2717	>25.2717
SJ000565128	c1(OC)cc(CNCc2ccccn2)ccc1OCc3ccccc3C.Cl	>13.9940	>13.9940	>25.3261	>25.3261
SJ000204946	c(c(OCCC)c(OCC)cc1CNCCc2ccccc2)c1Cl.Cl	>14.0841	>14.0841	>25.4891	>25.4891
SJ000158312	N(CCc(c12)cccc1)(CC(O)COc3ccc(cc3OC)CC=C)C2.Cl	>14.2643	>14.2643	>25.8152	>25.8152
SJ000565130	c1(OCC)cc(CNCC(C)O)ccc1OCc(ccc2C)cc2.Cl	>14.3544	>14.3544	>25.9783	19.2475
SJ000565109	n1cn(c2c1cc(C)c(c2)C)CCCCOc3ccccc3C.Cl	>14.3844	>14.3844	>26.0326	>26.0326
SJ000565073	C(=N/O)(/c1ccc(c(OC)c1)OC)\c2nccc(cc(c(OC)c3)OC)c23	>14.3994	>14.3994	>26.0598	8.1823
SJ000197009	c1(OCc2ccccc2)c(OCC)cc(cc1Cl)CNCC(C)C	>14.4745	>14.4745	>26.1957	>26.1957
SJ000565029	n1(c(cc2)ccc2c3ccccc3)c4c(nc1)cccc4	>14.5345	>14.5345	>26.3043	17.5032
SJ000338135	c1(OC)cc(CNCc(cc2)ccn2)ccc1OCc3ccccc3C.Cl	>14.5946	>14.5946	>26.4130	>26.4130
SJ000565015	N1(C\C=C\c2ccccc2OC)CCC(CC1)Cc3ccccc3	>14.6547	>14.6547	>26.5217	>26.5217
SJ000565063	N(C)(C1CCCCC1)CC(O)COc(ccc(c23)cccc2)c3.Cl	>14.6547	>14.6547	>26.5217	>26.5217
SJ000565037	N(CCc(c12)cccc1)(CC(O)COc(cc3)cc(c3C(C)C)C)C2.Cl	>14.8048	>14.8048	>26.7935	>26.7935
SJ000113011	c1(c(cccc1CN([H])Cc(cccn2)c2)OC)OCc(cc3)ccc3F.Cl	>14.8649	>14.8649	>26.9022	>26.9022
SJ000565013	c12c(cccc1)cccc2OCCCCCCN(CC)CC.Cl	>14.9249	>14.9249	>27.0109	-
SJ000333948	c1(C(C)C)ccc(cc1)OCCOCCOc2ccccc2OC	>15.0150	>15.0150	>27.1739	>27.1739
SJ000334022	c1(OC)cc(C)ccc1OCCCCOc2ccc(cc2C)Cl	>15.0150	>15.0150	>27.1739	>27.1739
SJ000334045	c1(OC)cc(CC=C)ccc1OCCOCCOc2ccc(cc2C)C	>15.0150	>15.0150	>27.1739	>27.1739
SJ000334145	c1(OC)cc(ccc1OCCCCOc2ccccc2Cl)\C=C\C	>15.0150	>15.0150	>27.1739	>27.1739
SJ000334362	c1(OC)cc(C)ccc1OCCCCOc(cccc2C(C)C)c2	>15.0150	>15.0150	>27.1739	>27.1739

SJ000565001	c1(O)c(cc(cc1C(C)(C)C)CCC#N)C(C)(C)C	>15.0150	>15.0150	>27.1739	-
SJ000565006	C1(=O)C(CCC(\C=C\c(cc2)ccc2OCC)=C1)CCc3ccccc3	>15.0150	>15.0150	>27.1739	-
SJ000565008	c1c(C)cccc1OCCCCCOc2cccc(C)c2	>15.0150	>15.0150	>27.1739	-
SJ000565009	c1(C)cc(OCCCCOc(ccc(c2C)C)c2)ccc1C	>15.0150	>15.0150	>27.1739	-
SJ000565011	c(OCCCCCOc(cc1)ccc1C)(cc2)ccc2C	>15.0150	>15.0150	>27.1739	>27.1739
SJ000565035	N(CCc(c12)cccc1)(CC(O)COc3cc(C)ccc3C(C)C)C2.Cl	>15.0150	>15.0150	>27.1739	>27.1739
SJ000565046	c1(OCCOCCOc2ccc(cc2OC)CC=C)cc(C)cc(C)c1C	>15.0150	>15.0150	>27.1739	23.9473
SJ000565047	c1(OCCCCOc2cccc(cccn3)c23)c(ccccc1OC)OC	>15.0150	>15.0150	>27.1739	>27.1739
SJ000565048	c1(OC)cc(CC=C)ccc1OCCOCCOc(cc2)ccc2C(C)(C)C	>15.0150	>15.0150	>27.1739	3.5123
SJ000565049	c1(OC)cc(CC=C)ccc1OCCCOc2ccc(cc2C)Cl	>15.0150	>15.0150	>27.1739	10.7284
SJ000565050	c1(OC)cc(C)ccc1OCCCCOc(ccc(c2C)Cl)c2	>15.0150	>15.0150	>27.1739	>27.1739
SJ000565052	c1(OCCCCOc2ccccc2OC)cc(C)ccc1C(C)C	>15.0150	>15.0150	>27.1739	>27.1739
SJ000565053	c1(C)c(C)cccc1OCCCCOc2ccc(cc2OC)CC=C	>15.0150	>15.0150	>27.1739	8.1025
SJ000565054	c1(OCCCCOc2ccc(cc2OC)C)cc(C)ccc1Cl	>15.0150	>15.0150	>27.1739	11.1228
SJ000565055	c1(C)c(C)cccc1OCCCCOc2ccc(cc2OC)\C=C\C	>15.0150	>15.0150	>27.1739	>27.1739
SJ000565056	c1(OCCCCOc2ccc(cc2OC)C)c(C)ccc(C)c1C	>15.0150	>15.0150	>27.1739	>27.1739
SJ000565057	c1(C)c(Cl)ccc(OCCCCOc2cccc(OC)c2)c1C	>15.0150	>15.0150	>27.1739	>27.1739
SJ000551062	N(C1CCCCC1)CC(O)COc(cc2)ccc2OCc3ccccc3	>15.0450	>15.0450	>27.2283	>27.2283
SJ000565030	N12C(=NCC1)SC=C2c3ccccc3.Br	>15.0751	>15.0751	>27.2826	>27.2826
SJ000565110	n1cn(c2c1cc(C)c(c2)C)CCOc3cccc(Cl)c3Cl	>15.0901	>15.0901	>27.3098	>27.3098
SJ000565038	N(CCc(c12)cccc1)(CC(O)COc3cc(C)ccc3C)C2.Cl	>15.2553	>15.2553	>27.6087	>27.6087
SJ000565127	c1(OCC)cc(CNCc(cc2)ccn2)ccc1OCc3ccccc3.Cl	>15.3303	>15.3303	>27.7446	>27.7446
SJ000146936	N1(CCC(CC1)C)Cc(ccc(c2OC)OCc3ccccc3)c2	>15.6156	>15.6156	>28.2609	-

SJ000565069	c1(C)cc(C)ccc1OCCCCN(C)Cc2ccccc2	>15.6156	>15.6156	>28.2609	>28.2609
SJ000565088	C(O)(=O)C(O)=O.c1(OC)cc(CC=C)ccc1OCCCNCc2ccccc2	>15.6156	>15.6156	>28.2609	>28.2609
SJ000334298	c12c(cccn1)cccc2OCCOCCOc3ccccc3CC	>15.7958	>15.7958	>28.5870	>28.5870
SJ000208200	c12c(cccn1)cccc2OCCOc(cc3)ccc3CCC(C)=O	>15.9159	>15.9159	>28.8043	>28.8043
SJ000565004	C(=C/c1ccccc1)(/NC(C)=O)\C(=O)NC(CCSC)C(O)=O	>16.0511	>16.0511	>29.0489	>29.0489
SJ000565126	c1(OC)cc(CNCc(cccn2)c2)ccc1OCc3ccccc3C.Cl	>16.2162	>16.2162	>29.3478	>29.3478
SJ000158276	N(CCc(c12)cccc1)(CC(O)COc3ccc(cc3C)C)C2.Cl	>16.3964	>16.3964	>29.6739	>29.6739
SJ000204340	c1(OCC)cc(CNCCc2ccccc2)ccc1OCC(C)C.Cl	>16.6366	>16.6366	>30.1087	>30.1087
SJ000565042	n1(c2ccc(cc2)OC)c(ccc(c3)NCc(ccc(c4OC)OC)c4)c3nc1	>16.8018	>16.8018	>30.4076	>30.4076
SJ000564999	[n+]1(CC)ccc(c2c1Cc(ccc(c3OC)OC)c3)cc(c(OC)c2)OC.[I-]	>16.9369	>16.9369	>30.6522	10.8472
SJ000565066	C(O)(=O)C(O)=O.C(c1ccccc1)(=O)c2ccc(cc2)OCCCCN3CCCCC3	>17.0270	>17.0270	>30.8152	>30.8152
SJ000565125	c1(OC)cc(CNCc(cccn2)c2)ccc1OCc3cccc(C)c3.Cl	>17.0270	>17.0270	>30.8152	>30.8152
SJ000565113	c1(ccc(cc1OCC)CNCCc2ccccc2)OC3CCCC3.Cl	>17.6577	>17.6577	25.3217	13.0954
SJ000565099	N(CCc(c12)cccc1)(CC(O)COc3c(C)cccc3C)C2.Cl	>18.1682	>18.1682	>32.8804	>32.8804
SJ000565102	c1(ccc(cc1OCC)CNC(C)c2ccccc2)OC3CCCC3.Cl	>18.5285	>18.5285	>33.5326	14.8248
SJ000565070	C(O)(=O)C(O)=O.C(c1ccccc1)(=O)c2ccc(cc2)OCCN3CCC(CC3)C	>18.7087	>18.7087	>33.8587	>33.8587
SJ000565101	C(COc1ccccc1CNC2CCCCC2)(=O)Nc(cc3)ccc3C.Cl	>19.0240	>19.0240	>34.4293	>34.4293
SJ000565122	c1(OCC)cc(CNCc(cccn2)c2)ccc1OCc3ccccc3.Cl	>19.5345	>19.5345	>35.3533	>35.3533
SJ000565051	c12c(cccn1)cccc2OCCOCCOc(c3)cc(cc3C)C	>19.8799	>19.8799	>35.9783	>35.9783
SJ000034041	n1(Cc(cc2)ccc2C)c3c(nc1COc(cc4)ccc4OC)cccc3	>19.9550	>19.9550	>36.1141	25.5324
SJ000565118	n(ccn1CCOc2ccc(cc2Cc3ccccc3)C)c1.Cl	>19.9550	>19.9550	>36.1141	>36.1141
SJ000565111	N(CCc(c12)cccc1)(CC(COCCOc3c(C)cccc3C)O)C2.Cl	>20.2402	>20.2402	>36.6304	>36.6304
SJ000565108	N1(CCCOc2ccccc2F)CCC(CC1)Cc3	>20.3303	>20.3303	>36.7935	14.1835

	ccccc3.Cl				
SJ000198578	n(c(cccc1)c1n2CCOc3ccccc3C(C)CC)c2.Cl	>20.3604	>20.3604	>36.8478	>36.8478
SJ000565105	n(c(cccc1)c1n2CCOc(cc3)ccc3c4ccccc4)c2	>5.8258	>5.8258	>10.5435	>10.5435
SJ000565034	n(\N=C\c(cc1)ccc1OCCOc2cc(C)ccc2C(C)C)(c3)cnn3	>6.4565	>6.4565	>11.6848	>11.6848
SJ000565103	N(c1ccccc1C)C(COc2ccccc2CNC3CCCCC3)=O	>6.6366	>6.6366	>12.0109	11.4974
SJ000565075	C(O)(=O)C(O)=O.c1c(cccc1Oc2ccccc2)OCCOCCN(C)Cc3ccccc3	>7.0270	>7.0270	>12.7174	>12.7174
SJ000565098	N1(CCC(CC1)Cc2ccccc2)CC(O)COc3ccccc3F.Cl	>7.6877	>7.6877	>13.9130	>13.9130
SJ000334048	c1(cc(C)ccc1OCCOCCOc2cccc(cccn3)c23)C(C)(C)C	>7.7477	>7.7477	>14.0217	>14.0217
SJ000177447	C(O)(=O)C(O)=O.C(c1ccccc1)(=O)c2ccc(cc2)OCCCCN(CC)CC	>7.8679	>7.8679	>14.2391	>14.2391
SJ000156724	c1(cc(ccc1OC)CNC(CC)CC)OCc2ccccc2	>8.0480	>8.0480	>14.5652	>14.5652
SJ000565068	C(O)(=O)C(O)=O.c1(OCCCNCc2ccccc2)cc(C)ccc1C(C)C	>8.0480	>8.0480	>14.5652	>14.5652
SJ000565040	N1(CCCCCOc2c(C)cccc2C)CCC(CC1)C	>8.3483	>8.3483	>15.1087	>15.1087
SJ000565116	c1(OC)cc(ccc1OCC(O)c2ccccc2)CNC3CCCC3.Cl	>8.5586	>8.5586	>15.4891	>15.4891
SJ000565045	n(\N=C\c1cccc(OCCOc2ccc(cc2OC)CC=C)c1)(cnn3)c3	>8.6486	>8.6486	>15.6522	>15.6522
SJ000565089	N(CCCCOc(ccc(c12)cccc1)c2)(CC3C)CC(O3)C	>8.7988	>8.7988	>15.9239	-
SJ000565091	c1(ccccc1OCCCN(C)Cc2ccccc2)C(C)CC	>8.8589	>8.8589	>16.0326	>16.0326
SJ000565060	c12c(cccc1)cccc2OCC(O)CN(CCC)CCC.Cl	>9.0090	>9.0090	>16.3043	>16.3043
SJ000565074	C(O)(=O)C(O)=O.c1(Cl)cc(C)cc(C)c1OCCCCNCc2ccccc2	>9.2192	>9.2192	>16.6848	>16.6848
SJ000565123	c1(OC)cc(CNCc2ccccn2)ccc1OCc(cc3)ccc3C.Cl	>9.2192	>9.2192	>16.6848	>16.6848
SJ000565082	n1c(C)ccc(cccc2OCCOCCOc3c(C)cccc3CC=C)c12	>9.6396	>9.6396	>17.4457	>17.4457
SJ000565093	n(CC(O)COc(cc1)ccc1OCc2ccccc2)(c3c(n4)cccc3)c4	>9.7147	>9.7147	>17.5815	>17.5815
SJ000565026	c12c(cccc1)cccc2OCCCCCNCCCC	>9.7598	>9.7598	>17.6630	>17.6630
SJ000565041	C(O)(=O)C(O)=O.N1(CCCCOc(ccc(c23)cccc2)c3)CCC(CC1)C	>9.7898	>9.7898	>17.7174	>17.7174
SJ000565086	c1(C)cc(C)ccc1OCCCCNC(C)c2ccc	>9.9399	>9.9399	>17.9891	>17.9891

	cc2				

Supplementary Table 4. Structures, antimalarial activity and drug susceptibility of 42 putative inactives selected by QSAR models.

REGNUM	Smiles	Antimalarial Activity (EC50, µM)		Drug Susceptibility (EC50, µM)
		3D7	K1	BJ
SJ000016645	C(Oc1ccccc1)(=C(C)O2)C(=O)c(c23)ccc(O)c3O	>15.0150	>15.0150	>27.1739
SJ000016649	C(Oc1ccccc1)(=C(C)O2)C(=O)c(c23)ccc(O)c3C	>15.0150	>15.0150	>27.1739
SJ000043189	C1(Oc2cccc(OC)c2)=C(C)Oc3c(ccc(O)c3)C1=O	>15.0150	>15.0150	>27.1739
SJ000169987	c(ccc(c1C)OC(C)=O)(C2=O)c1OC=C2Oc3ccccc3	>15.0150	>15.0150	>27.1739
SJ000170212	c(ccc(c1C)O)(C2=O)c1OC=C2Oc3ccccc3	>15.0150	>15.0150	>27.1739
SJ000170220	C(Oc1ccccc1F)(=C(C)O2)C(=O)c(c23)ccc(O)c3C	>15.0150	>15.0150	>27.1739
SJ000170354	C(Oc1ccccc1F)(=COc2c3ccc(OC)c2C)C3=O	>15.0150	>15.0150	>27.1739
SJ000170391	C(Oc1ccccc1F)(=C(C)O2)C(=O)c(c23)ccc(O)c3CN(C)C	>10.0000	>10.0000	>18.0978
SJ000170503	c1(c(cc(O)c(CC)c1)OC=C2Oc(cc3)ccc3F)C2=O	>15.0150	>15.0150	>27.1739
SJ000170703	C1(Oc2ccccc2)=C(C)Oc(c3C1=O)cc(cc3C)O	>15.0150	>15.0150	>27.1739
SJ000170877	C(Oc1ccccc1F)(=COc2c3ccc(OC(C)=O)c2C)C3=O	>15.0150	>15.0150	>27.1739
SJ000174499	c(ccc(c1C)O)(C2=O)c1OC=C2Oc(cc3)ccc3F	>15.0150	>15.0150	>27.1739
SJ000175490	C1(Oc(ccc(c23)cccc2)c3)=COc(c4C1=O)cc(cc4)O	>15.0150	>15.0150	>27.1739
SJ000176490	C1(=O)c(ccc(c2C)O)c2OC(C)=C1c3ccc(cc3)OC	>15.0150	>15.0150	>27.1739
SJ000206080	C1(C2c3cccc(O)c3)=C(Oc(cccc4)c4C1=O)C(N2C)=O	>19.0390	>19.0390	>34.4565
SJ000290740	C1(Oc(cc2)ccc2OC)=COc(c3C1=O)cc(cc3)O	>15.0150	>15.0150	>27.1739
SJ000565131	C1(Oc(cc2)ccc2C(OC)=O)=C(C)Oc3c(ccc(O)c3)C1=O	>15.0150	>15.0150	>27.1739
SJ000565132	C1(Oc(cc2)ccc2C(O)=O)=COc(c3C1=O)cc(cc3)OC	>15.0150	>15.0150	>27.1739
SJ000565133	C1(C(=O)CC(CC1=O)(C)C)(C2c3ccc(cc3)OC)OC(=C24)CC(CC4=O)(C)C	>15.0150	>15.0150	>27.1739
SJ000565134	c12c(cc(OC(C)C(OC)=O)cc1O)OC(=CC2=O)c3ccccc3	>15.0150	>15.0150	>27.1739
SJ000565135	C1(Oc(cc(C)cc2C)c2)=COc(c3C1=O)cc(cc3)O	>15.0150	>15.0150	>27.1739
SJ000565136	C1(Oc2cccc(C)c2)=COc(c3C1=O)cc(cc3)O	>15.0150	>15.0150	>27.1739
SJ000565137	C1(c2ccccc2Cl)=C(C)Oc3c(ccc(O)c3O)C1=O	>15.0150	>15.0150	>27.1739
SJ000565138	C1(Oc2ccccc2F)=COc(c3C1=O)cc(cc3)OC	>15.0150	>15.0150	>27.1739
SJ000565139	C(Oc(cc1)ccc1F)(=C(C)O2)C(=O)c(c23)ccc(O)c	>15.0150	>15.0150	>27.1739

	3O			
SJ000565140	C1(=O)c(ccc(c2C)O)c2OC(C)=C1c3ccccc3	>15.0150	>15.0150	>27.1739
SJ000565141	C1(Oc(cc2)ccc2C)=COc(c3C1=O)cc(cc3)O	>15.0150	>15.0150	>27.1739
SJ000565142	C(Oc1ccccc1F)(=COc(c23)cc(c(CC)c2)O)C3=O	>15.0150	>15.0150	>27.1739
SJ000565143	C(Oc(cc1)ccc1F)(=C(C)O2)C(=O)c(c23)ccc(O)c3C	>15.0150	>15.0150	>27.1739
SJ000565144	C1(=COc(c2C1=O)cc(cc2)O)Oc3cc(C)ccc3C	>15.0150	>15.0150	>27.1739
SJ000565145	C1(Oc(cc2)ccc2C(C)C)=COc(c3C1=O)cc(cc3)O	>15.0150	>15.0150	>27.1739
SJ000565146	C(c1ccc(cc1)OCC)(Oc(ccc(c2)O)c2C3=O)=C3	>15.0150	>15.0150	>27.1739
SJ000565147	C1(c2ccc(c(OCC)c2)O)=CC(c3c(cccc3)O1)=O	>15.0150	>15.0150	>27.1739
SJ000565148	C1(c2ccccc2OC)=C(CC)Oc3c(ccc(O)c3)C1=O	>15.0150	>15.0150	>27.1739
SJ000565149	C1(c2ccc(c(OC)c2)OC)=C(C)Oc3c(ccc(O)c3)C1=O	>15.0150	>15.0150	>27.1739
SJ000565150	C1(Oc2cccc(OC)c2)=COc(c3C1=O)cc(cc3)OC	>15.0150	>15.0150	>27.1739
SJ000565151	C1(Oc(cc2)ccc2OCC)=C(C)Oc3c(ccc(O)c3)C1=O	>15.0150	>15.0150	>27.1739
SJ000565152	C1(Oc2ccccc2CC)=COc(c3C1=O)cc(cc3)O	>15.0150	>15.0150	>27.1739
SJ000565153	C1(c(ccc(c23)OCO2)c3)=C(O)C(c(ccc(Cl)c4)c4O1)=O	>15.0150	>15.0150	>27.1739
SJ000565154	C1(c2ccccc2OC)=C(O)C(c(ccc(Cl)c3)c3O1)=O	>15.0150	>15.0150	>27.1739
SJ000565155	C1(C2c3ccc(cc3)O)=C(Oc(ccc(Cl)c4)c4C1=O)C(N2C)=O	>15.3754	>15.3754	>27.8261
SJ000565156	C1(C2c3cccc(O)c3)=C(Oc(ccc(Cl)c4)c4C1=O)C(N2C)=O	>12.2823	>12.2823	>22.2283

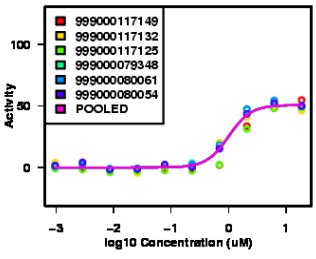
Supplementary Table 5. Novel scaffolds found in confirmed 25 virtual screening hits.

Parent Chemical REGNUM	Core Structure
SJ000565000	C(OC(C1CCNC2CCCCC12)C3CC4CCN3CC4)C5CC5
SJ000565062	C1CCC2CCCCC2C1
SJ000565033	C1CCC(CC1)NC2CCNC3CCCCC23
SJ000173328	C1CCC2C(CCNC2C1)NC3CCC4OCCOC4C3
SJ000565039	C(CNCC1CCCCC1)COC2CCCCC2
SJ000565115	C(CC1CCCCC1)NCC2CCC(CC2)OCC3CCCCC3
SJ000565043	C1CCC(CC1)NC2CCNC3C4CCCCC4CCC23
SJ000205073	C(CC1CCCCC1)NCC2CCCCC2
SJ000565072	C(COC1CCC(CC2CCCCC2)CC1)CN3CCNC3
SJ000188975	C(COC1CCCCC1)CN2CCC3CCCCC3C2
SJ000565117	C(CCN1CCNC1)COC2CCCCC2CC3CCCCC3
SJ000565031	C1CCC(CC1)NC2C3CCCCC3NC4CCCCC24
SJ000150414	C(CC1CCCCC1)CC2CCCCC2
SJ000564998	C(C1CCCCC1)C2NCCC3CCCCC23
SJ000565010	C(CCOC1CCC2CCCCC2C1)CCN3CCCCC3
SJ000202592	C(C1CCCCC1)C2CCCCC2
SJ000565067	C(CCN1CCCCC1)COC2CCCCC2C3CCCCC3
SJ000183110	C(CCOC1CCCCC1)CNCC2CCCCC2
SJ000565003	C(CC(C1CCCCC1)C2CCCCC2)NCC3(CCOCC3)C4CCC5OCCOC5C4
SJ000565071	C(CCN1CCCCC1)COC2CCC(CC3CCCCC3)CC2
SJ000565094	C(COC1CCC(CC1)OCC2CCCCC2)CN3CCCCC3
SJ000565064	C1CCC(CC1)N2CCCN2C3CCCCC3

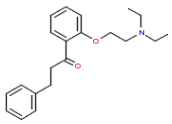
Supplementary Table 6. Dose response behavior of confirmed 25 virtual screening hits.

SJ000150414

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
A1	POOLED	1.0081 (0.8789 - 1.1563)	-2.3 (-2.8 - -1.7)	0 - 51	0.0081

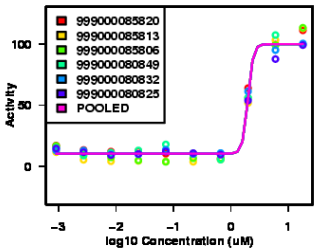


SJ000150414-2

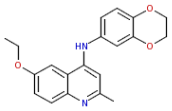
Consensus EC50 (uM):	1.0081
Consensus EC10 (uM):	0.3827
Consensus EC90 (uM):	2.6557

SJ000173328

3D7



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
A1	POOLED	1.9858 (1.8936 - 2.0825)	-9.6 (-83.8 - 64.7)	10 - 100	0.0000

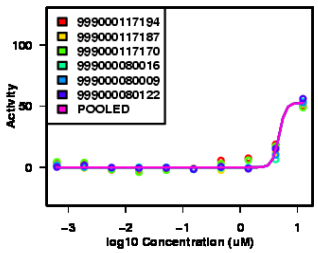


S_J000173328-2

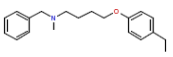
Consensus EC50 (uM):	1.9858
Consensus EC10 (uM):	1.5785
Consensus EC90 (uM):	2.4981

SJ000183110

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
A1	POOLED	4.7387 (1.9685 - 11.4070)	-7.6 (-56.3 - 41.1)	0 - 53	0.0210

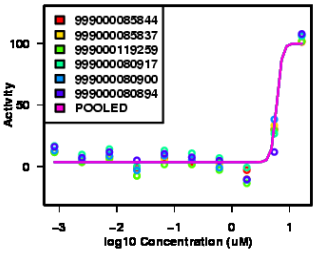


S_J000183110-2

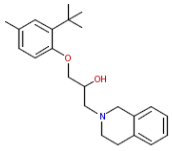
Consensus EC50 (uM):	4.7387
Consensus EC10 (uM):	3.5526
Consensus EC90 (uM):	6.3207

SJ000188975

3D7



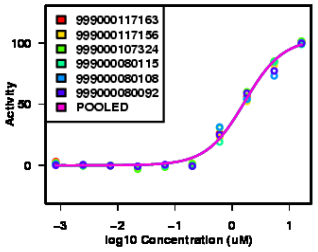
CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
A1	POOLED	6.0279 (2.5452 - 14.2762)	-9.7 (-91.6 - 72.2)	4 - 100	0.0036



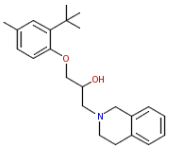
S_J000188975-2

Consensus EC50 (uM):	6.0279
Consensus EC10 (uM):	4.8064
Consensus EC90 (uM):	7.5598

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
B1	POOLED	1.6561 (1.2402 - 2.2115)	-1.3 (-1.6 - -1.0)	0 - 104	0.3786

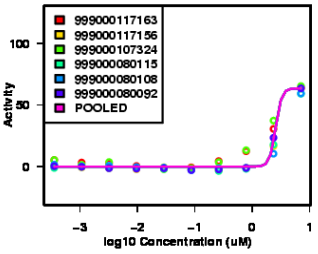


S_J000188975-2

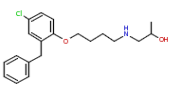
Consensus EC50 (uM):	1.6561
Consensus EC10 (uM):	0.3080
Consensus EC90 (uM):	8.9039

SJ000202592

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
A1	POOLED	2.5655 (1.4744 - 4.4640)	-8.4 (-62.0 - 45.2)	0 - 64	0.0149

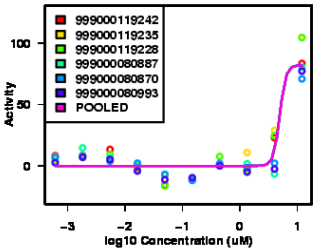


S_J000202592-2

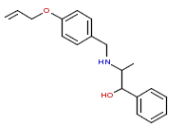
Consensus EC50 (uM):	2.5655
Consensus EC10 (uM):	1.9773
Consensus EC90 (uM):	3.3287

SJ000205073

3D7



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
B1	POOLED	4.9445 (0.0111 - 1204.2042)	-8.2 (-247.3 - 230.9)	0 - 82	0.0374

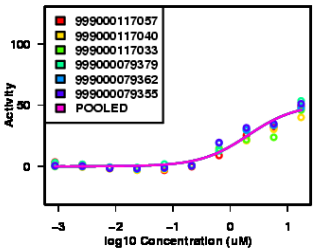


SJ000205073-2

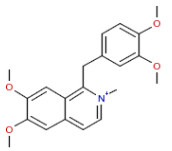
Consensus EC50 (uM):	4.9445
Consensus EC10 (uM):	3.7836
Consensus EC90 (uM):	6.4616

SJ000564998

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
B1	POOLED	2.0551 (0.6502 - 6.4952)	-1.0 (-1.7 - -0.4)	0 - 51	0.2758

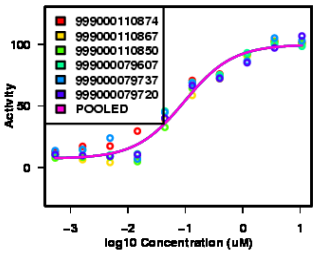


SJ000564998-1

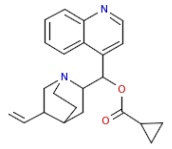
Consensus EC50 (uM):	2.0551
Consensus EC10 (uM):	0.2510
Consensus EC90 (uM):	16.8253

SJ000565000

3D7



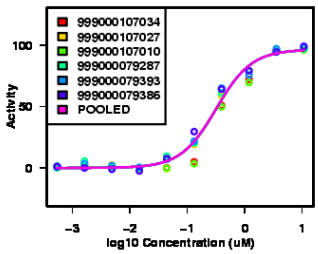
CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
A1	POOLED	0.0956 (0.0582 - 0.1572)	-1.0 (-1.5 - -0.6)	7 - 100	0.0677



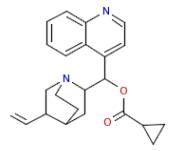
SJ000565000-1

Consensus EC50 (uM):	0.0956
Consensus EC10 (uM):	0.0114
Consensus EC90 (uM):	0.7994

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
A1	POOLED	0.3178 (0.2477 - 0.4079)	-1.4 (-1.8 - -1.0)	0 - 97	0.0886

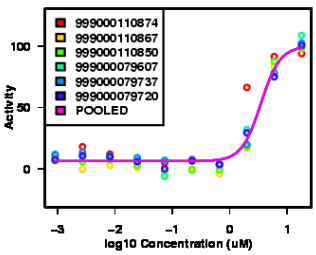


SJ000565000-1

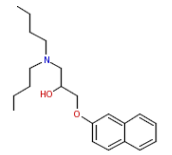
Consensus EC50 (uM):	0.3178
Consensus EC10 (uM):	0.0671
Consensus EC90 (uM):	1.5057

SJ000565002

3D7



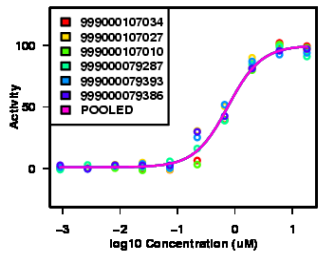
CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
A1	POOLED	3.4873 (2.9123 - 4.1759)	-2.6 (-3.4 - -1.8)	6 - 100	0.1857



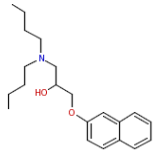
SJ000565002-1

Consensus EC50 (uM):	3.4873
Consensus EC10 (uM):	1.5056
Consensus EC90 (uM):	8.0775

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
A1	POOLED	0.7575 (0.6156 - 0.9323)	-1.5 (-1.9 - -1.1)	1 - 100	0.0707

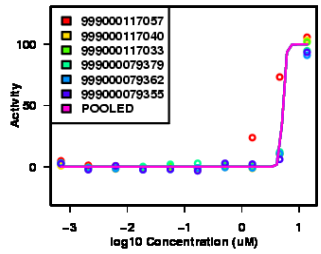


SJ000565002-1

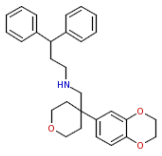
Consensus EC50 (uM): 0.7575
Consensus EC10 (uM): 0.1756
Consensus EC90 (uM): 3.2675

SJ000565003

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
A1	POOLED	5.2169 (1.4102 - 19.2989)	-16.5 (-183.6 - 150.6)	0 - 100	0.0000

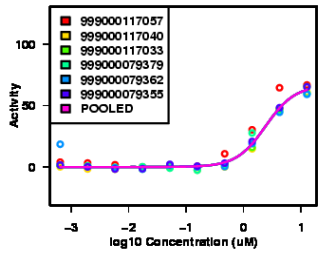


SJ000565003-1

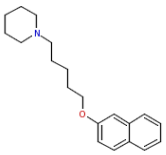
Consensus EC50 (uM): 5.2169
Consensus EC10 (uM): 4.5665
Consensus EC90 (uM): 5.9599

SJ000565010

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
B1	POOLED	2.4118 (2.0609 - 2.8224)	-1.7 (-2.0 - -1.4)	0 - 67	0.4705

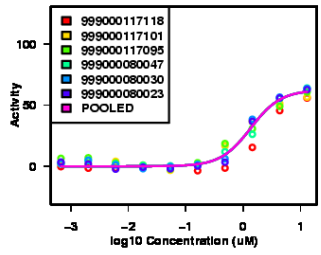


SJ000565010-1

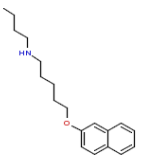
Consensus EC50 (uM): 2.4118
Consensus EC10 (uM): 0.6695
Consensus EC90 (uM): 8.6884

SJ000565025

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
A1	POOLED	1.3621 (1.1067 - 1.6764)	-1.7 (-2.1 - -1.2)	0 - 62	0.1751

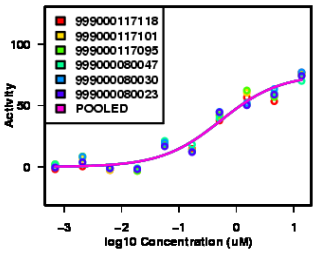


SJ000565025-1

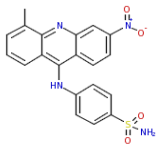
Consensus EC50 (uM): 1.3621
Consensus EC10 (uM): 0.3642
Consensus EC90 (uM): 5.0950

SJ000565031

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
B1	POOLED	0.5332 (0.1464 - 1.9414)	-0.8 (-1.5 - -0.2)	0 - 76	0.2677

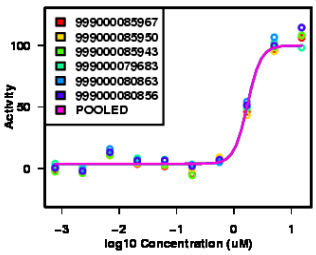


SJ000565031-1

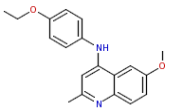
Consensus EC50 (uM):	0.5332
Consensus EC10 (uM):	0.0391
Consensus EC90 (uM):	7.2625

SJ000565033

3D7



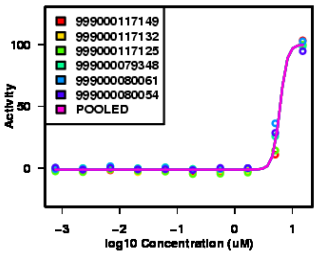
CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
A1	POOLED	1.7216 (1.4875 - 1.9925)	-3.7 (-8.9 - 1.5)	4 - 100	0.0070



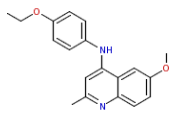
SJ000565033-1

Consensus EC50 (uM):	1.7216
Consensus EC10 (uM):	0.9566
Consensus EC90 (uM):	3.0981

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
A1	POOLED	6.0942 (5.0955 - 7.2888)	-7.0 (-13.6 - -0.4)	-1 - 100	0.0816

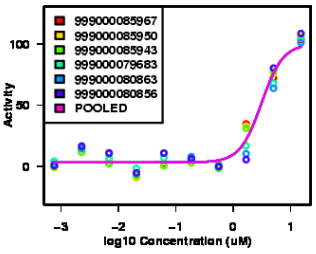


SJ000565033-1

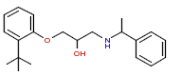
Consensus EC50 (uM):	6.0942
Consensus EC10 (uM):	4.4495
Consensus EC90 (uM):	8.3470

SJ000565039

3D7



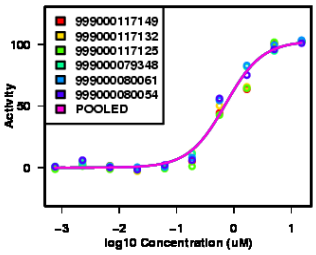
CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
B1	POOLED	3.0999 (2.2839 - 4.2074)	-2.3 (-3.4 - -1.3)	3 - 100	0.3516



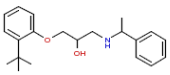
SJ000565039-1

Consensus EC50 (uM):	3.0999
Consensus EC10 (uM):	1.2140
Consensus EC90 (uM):	7.9155

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
A1	POOLED	0.7109 (0.4441 - 1.1382)	-1.4 (-2.0 - -0.8)	0 - 103	0.1414

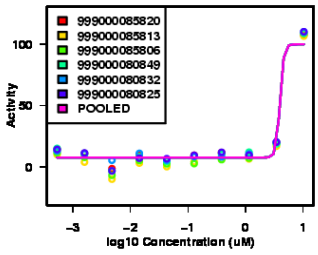


SJ000565039-1

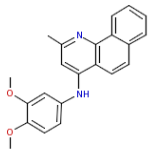
Consensus EC50 (uM):	0.7109
Consensus EC10 (uM):	0.1414
Consensus EC90 (uM):	3.5754

SJ000565043

3D7



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
B1	POOLED	3.9945 (0.2789 - 57.2061)	-13.4 (-262.7 - 236.0)	8 - 100	0.0003

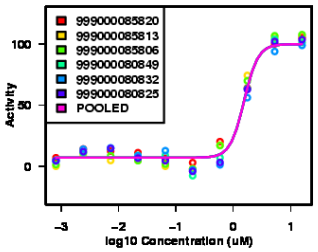


SJ000565043-1

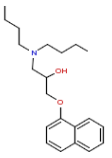
Consensus EC50 (uM):	3.9945
Consensus EC10 (uM):	3.3892
Consensus EC90 (uM):	4.7080

SJ000565062

3D7



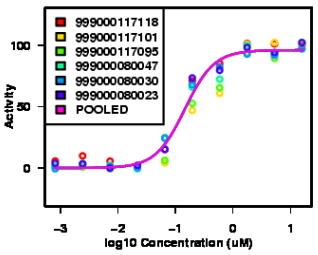
CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
A1	POOLED	1.5466 (1.2257 - 1.9514)	-3.6 (-7.5 - 0.4)	7 - 100	0.0050



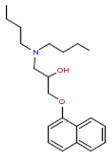
SJ000565062-1

Consensus EC50 (uM):	1.5466
Consensus EC10 (uM):	0.8385
Consensus EC90 (uM):	2.8526

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
A1	POOLED	0.1457 (0.0992 - 0.2139)	-1.7 (-2.8 - -0.6)	0 - 96	0.0033

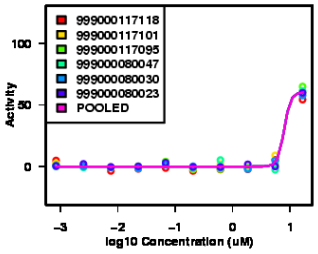


SJ000565062-1

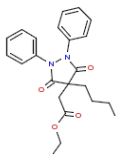
Consensus EC50 (uM):	0.1457
Consensus EC10 (uM):	0.0405
Consensus EC90 (uM):	0.5246

SJ000565064

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
B1	POOLED	7.9107 (0.0603 - 1038.0750)	-7.8 (-112.0 - 96.5)	0 - 60	0.0900

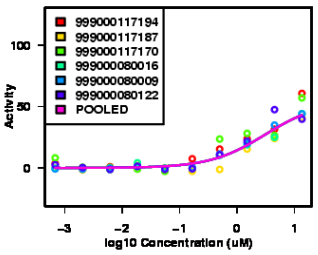


SJ000565064-1

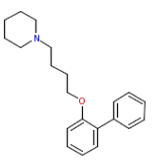
Consensus EC50 (uM):	7.9107
Consensus EC10 (uM):	5.9634
Consensus EC90 (uM):	10.4941

SJ000565067

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
B1	POOLED	3.1098 (0.8048 - 12.0166)	-0.9 (-1.4 - -0.4)	0 - 54	0.6041

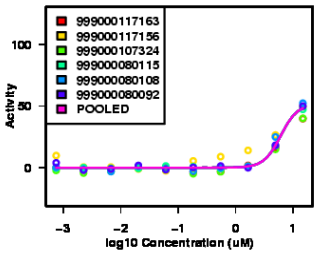


SJ000565067-1

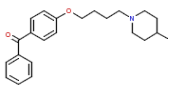
Consensus EC50 (uM):	3.1098
Consensus EC10 (uM):	0.2767
Consensus EC90 (uM):	34.9557

SJ000565071

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
B1	POOLED	6.1013 (4.6441 - 8.0156)	-3.0 (-5.3 - -0.7)	0 - 52	0.6379

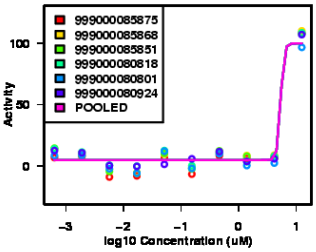


S J000565071-1

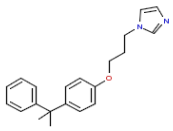
Consensus EC50 (uM):	6.1013
Consensus EC10 (uM):	2.9305
Consensus EC90 (uM):	12.7027

SJ000565072

3D7



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
B1	POOLED	5.3775 (0.0215 - 1252.2523)	-14.9 (-338.4 - 308.6)	5 - 100	0.0004

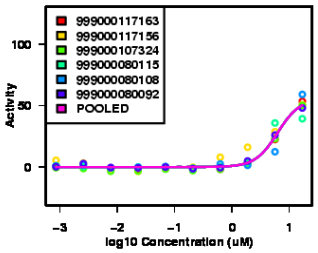


S J000565072-1

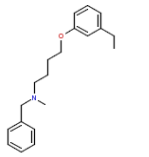
Consensus EC50 (uM):	5.3775
Consensus EC10 (uM):	4.6396
Consensus EC90 (uM):	6.2327

SJ000565077

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
B1	POOLED	6.2246 (5.2155 - 7.4289)	-2.3 (-3.0 - -1.5)	0 - 56	0.6473

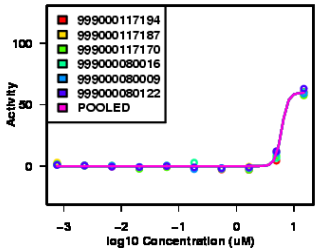


S J000565077-1

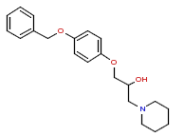
Consensus EC50 (uM):	6.2246
Consensus EC10 (uM):	2.3553
Consensus EC90 (uM):	16.4501

SJ000565094

K1



CurveClass	AssayPlate	EC50 (uM)	Hill	Range	Endslope
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
Replicates are not independent. Only POOLED curve was fit.					
A1	POOLED	6.1575 (1.7385 - 21.8094)	-7.8 (-54.3 - 38.6)	0 - 60	0.0304

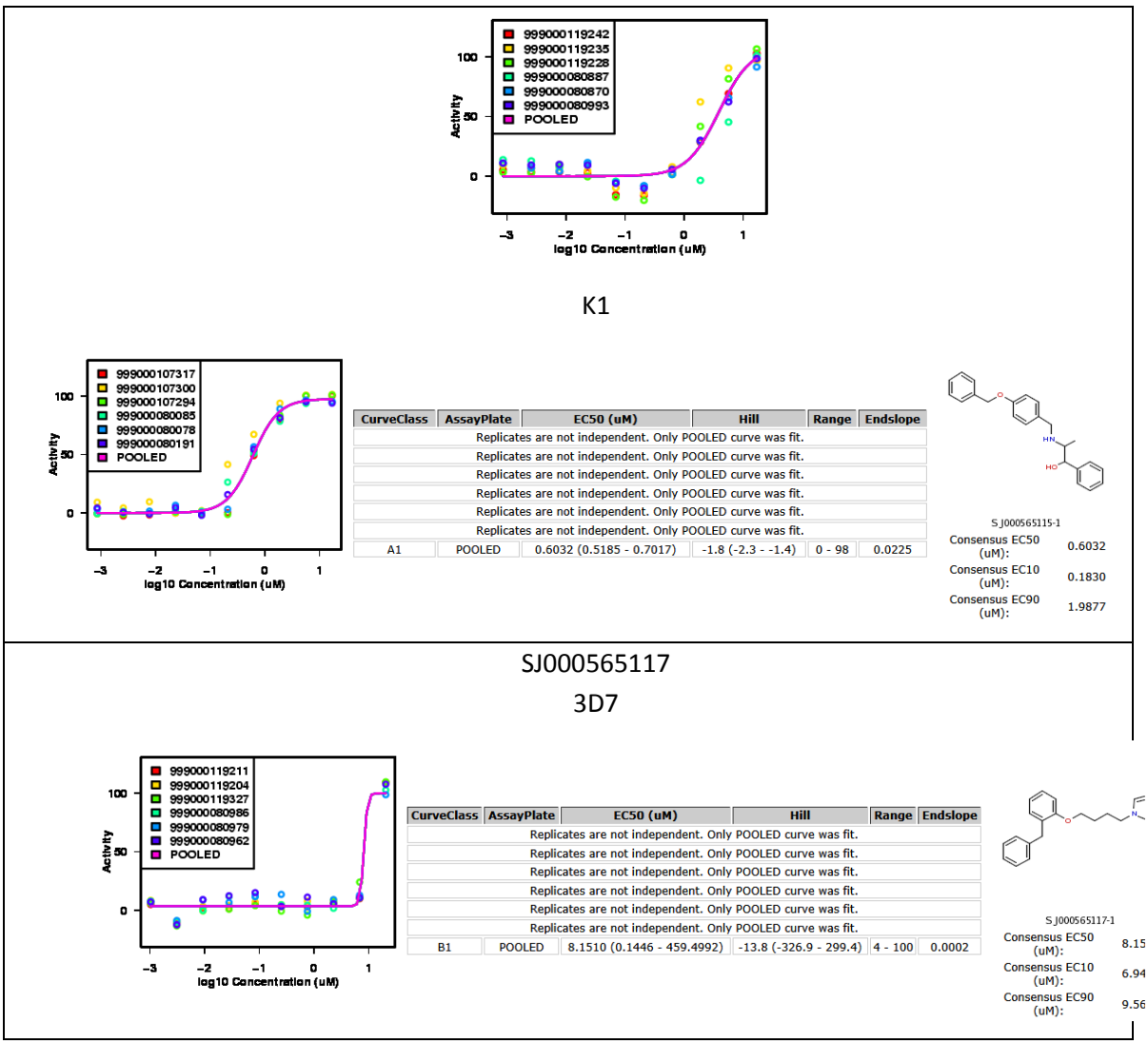


S J000565094-1

Consensus EC50 (uM):	6.1575
Consensus EC10 (uM):	4.6479
Consensus EC90 (uM):	8.1574

SJ000565115

3D7



Supplementary Table 7. Purity information of 176 virtual screening hits[‡].

REGNUM	Purity	Purity Method
SJ000034041	>95%	UVTWC_ELSD
SJ000039232	>95%	UVTWC_ELSD
SJ000112434	>95%	UVTWC_ELSD
SJ000113011	>95%	UVTWC_ELSD
SJ000126082	>95%	UVTWC_ELSD
SJ000146936	>95%	UVTWC_ELSD
SJ000150414	>95%	UVTWC_ELSD
SJ000156724	>95%	UVTWC_ELSD

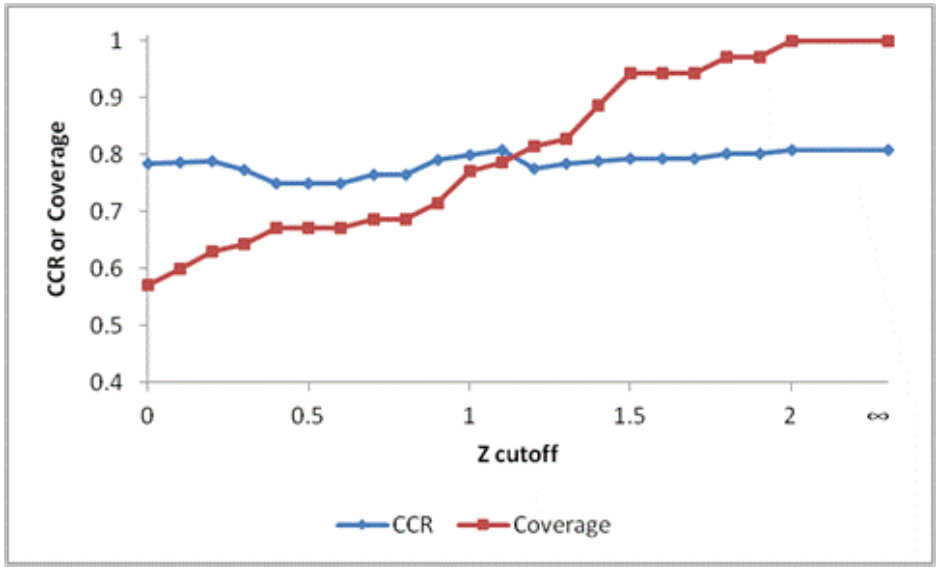
[‡] Purity and identity of the compounds was confirmed at SJCRH by LC/UV/ELSD/MS with purity being measured as the average of that seen by UV and ELSD and identity being confirmed by MS. The details of purity assessment could be found in this paper: Dual Detection Approach to a More Accurate Measure of Relative Purity in High-Throughput Characterization of Compound Collections. Andrew Lemoff and Bing Yan. Journal of Combinatorial Chemistry. 2008, 10, (5), 746-751.

SJ000158276	>95%	UVTWC_ELSD
SJ000158312	>95%	UVTWC_ELSD
SJ000166650	>95%	UVTWC_ELSD
SJ000173328	>95%	UVTWC_ELSD
SJ000177447	>95%	UVTWC_ELSD
SJ000183110	>95%	UVTWC_ELSD
SJ000188975	>95%	UVTWC_ELSD
SJ000196267	>95%	UVTWC_ELSD
SJ000197009	>95%	UVTWC_ELSD
SJ000197026	90-95%	UVTWC_ELSD
SJ000198578	>95%	UVTWC_ELSD
SJ000202592	90-95%	UVTWC_ELSD
SJ000203158	90-95%	UVTWC_ELSD
SJ000203427	>95%	UVTWC_ELSD
SJ000204340	90-95%	UVTWC_ELSD
SJ000204946	>95%	UVTWC_ELSD
SJ000205073	>95%	UVTWC_ELSD
SJ000208200	>95%	UVTWC_ELSD
SJ000299062	50-60%	UVTWC_ELSD
SJ000331443	>95%	UVTWC_ELSD
SJ000331940	85-90%	UVTWC_ELSD
SJ000333948	90-95%	UVTWC_ELSD
SJ000334022	>95%	UVTWC_ELSD
SJ000334045	85-90%	UVTWC_ELSD
SJ000334048	>95%	UVTWC_ELSD
SJ000334145	>95%	UVTWC_ELSD
SJ000334205	>95%	UVTWC_ELSD
SJ000334212	90-95%	UVTWC_ELSD
SJ000334298	>95%	UVTWC_ELSD
SJ000334362	>95%	UVTWC_ELSD
SJ000338135	>95%	UVTWC_ELSD
SJ000338146	>95%	UVTWC_ELSD
SJ000338434	>95%	UVTWC_ELSD
SJ000506625	>95%	UVTWC_ELSD
SJ000551062	>95%	UVTWC_ELSD
SJ000564998	>95%	UVTWC_ELSD
SJ000564999	>95%	UVTWC_ELSD
SJ000565000	80-85%	UVTWC_ELSD
SJ000565001	>95%	UVTWC_ELSD
SJ000565002	>95%	UVTWC_ELSD
SJ000565003	>95%	UVTWC_ELSD
SJ000565004	>95%	UVTWC_ELSD
SJ000565005	>95%	UVTWC_ELSD
SJ000565006	>95%	UVTWC_ELSD
SJ000565007	>95%	UVTWC_ELSD

SJ000565008	>95%	UVTWC_ELSD
SJ000565009	>95%	UVTWC_ELSD
SJ000565010	>95%	UVTWC_ELSD
SJ000565011	>95%	UVTWC_ELSD
SJ000565012	90-95%	UVTWC_ELSD
SJ000565013	>95%	UVTWC_ELSD
SJ000565014	>95%	UVTWC_ELSD
SJ000565015	>95%	UVTWC_ELSD
SJ000565016	>95%	UVTWC_ELSD
SJ000565017	85-90%	UVTWC_ELSD
SJ000565018	>95%	UVTWC_ELSD
SJ000565019	>95%	UVTWC_ELSD
SJ000565020	>95%	UVTWC_ELSD
SJ000565021	>95%	UVTWC_ELSD
SJ000565022	>95%	UVTWC_ELSD
SJ000565023	>95%	UVTWC_ELSD
SJ000565024	>95%	UVTWC_ELSD
SJ000565025	>95%	UVTWC_ELSD
SJ000565026	>95%	UVTWC_ELSD
SJ000565027	>95%	UVTWC_ELSD
SJ000565028	90-95%	UVTWC_ELSD
SJ000565029	>95%	UVTWC_ELSD
SJ000565030	>95%	UVTWC_ELSD
SJ000565031	90-95%	UVTWC_ELSD
SJ000565032	>95%	UVTWC_ELSD
SJ000565033	>95%	UVTWC_ELSD
SJ000565034	>95%	UVTWC_ELSD
SJ000565035	60-70%	UVTWC_ELSD
SJ000565036	>95%	UVTWC_ELSD
SJ000565037	>95%	UVTWC_ELSD
SJ000565038	90-95%	UVTWC_ELSD
SJ000565039	>95%	UVTWC_ELSD
SJ000565040	50-60%	UVTWC_ELSD
SJ000565041	>95%	UVTWC_ELSD
SJ000565042	>95%	UVTWC_ELSD
SJ000565043	>95%	UVTWC_ELSD
SJ000565044	>95%	UVTWC_ELSD
SJ000565045	>95%	UVTWC_ELSD
SJ000565046	>95%	UVTWC_ELSD
SJ000565047	>95%	UVTWC_ELSD
SJ000565048	90-95%	UVTWC_ELSD
SJ000565049	>95%	UVTWC_ELSD
SJ000565050	>95%	UVTWC_ELSD
SJ000565051	>95%	UVTWC_ELSD
SJ000565052	>95%	UVTWC_ELSD

SJ000565053	90-95%	UVTWC_ELSD
SJ000565054	>95%	UVTWC_ELSD
SJ000565055	>95%	UVTWC_ELSD
SJ000565056	90-95%	UVTWC_ELSD
SJ000565057	>95%	UVTWC_ELSD
SJ000565058	>95%	UVTWC_ELSD
SJ000565059	>95%	UVTWC_ELSD
SJ000565060	>95%	UVTWC_ELSD
SJ000565061	85-90%	UVTWC_ELSD
SJ000565062	>95%	UVTWC_ELSD
SJ000565063	>95%	UVTWC_ELSD
SJ000565064	>95%	UVTWC_ELSD
SJ000565065	>95%	UVTWC_ELSD
SJ000565066	50-60%	UVTWC_ELSD
SJ000565067	>95%	UVTWC_ELSD
SJ000565068	>95%	UVTWC_ELSD
SJ000565069	90-95%	UVTWC_ELSD
SJ000565070	>95%	UVTWC_ELSD
SJ000565071	>95%	UVTWC_ELSD
SJ000565072	>95%	UVTWC_ELSD
SJ000565073	>95%	UVTWC_ELSD
SJ000565074	90-95%	UVTWC_ELSD
SJ000565075	90-95%	UVTWC_ELSD
SJ000565076	70-80%	UVTWC_ELSD
SJ000565077	>95%	UVTWC_ELSD
SJ000565078	>95%	UVTWC_ELSD
SJ000565079	>95%	UVTWC_ELSD
SJ000565080	>95%	UVTWC_ELSD
SJ000565081	90-95%	UVTWC_ELSD
SJ000565082	90-95%	UVTWC_ELSD
SJ000565083	>95%	UVTWC_ELSD
SJ000565084	>95%	UVTWC_ELSD
SJ000565085	>95%	UVTWC_ELSD
SJ000565086	>95%	UVTWC_ELSD
SJ000565087	>95%	UVTWC_ELSD
SJ000565088	>95%	UVTWC_ELSD
SJ000565089	>95%	UVTWC_ELSD
SJ000565090	>95%	UVTWC_ELSD
SJ000565091	>95%	UVTWC_ELSD
SJ000565092	>95%	UVTWC_ELSD
SJ000565093	>95%	UVTWC_ELSD
SJ000565094	>95%	UVTWC_ELSD
SJ000565095	90-95%	UVTWC_ELSD
SJ000565096	>95%	UVTWC_ELSD
SJ000565097	>95%	UVTWC_ELSD

SJ000565098	>95%	UVTWC_ELSD
SJ000565099	>95%	UVTWC_ELSD
SJ000565100	>95%	UVTWC_ELSD
SJ000565101	>95%	UVTWC_ELSD
SJ000565102	>95%	UVTWC_ELSD
SJ000565103	90-95%	UVTWC_ELSD
SJ000565104	>95%	UVTWC_ELSD
SJ000565105	90-95%	UVTWC_ELSD
SJ000565106	>95%	UVTWC_ELSD
SJ000565107	>95%	UVTWC_ELSD
SJ000565108	85-90%	UVTWC_ELSD
SJ000565109	>95%	UVTWC_ELSD
SJ000565110	>95%	UVTWC_ELSD
SJ000565111	>95%	UVTWC_ELSD
SJ000565112	>95%	UVTWC_ELSD
SJ000565113	>95%	UVTWC_ELSD
SJ000565114	>95%	UVTWC_ELSD
SJ000565115	>95%	UVTWC_ELSD
SJ000565116	>95%	UVTWC_ELSD
SJ000565117	90-95%	UVTWC_ELSD
SJ000565118	>95%	UVTWC_ELSD
SJ000565119	>95%	UVTWC_ELSD
SJ000565120	>95%	UVTWC_ELSD
SJ000565121	>95%	UVTWC_ELSD
SJ000565122	>95%	UVTWC_ELSD
SJ000565123	>95%	UVTWC_ELSD
SJ000565124	>95%	UVTWC_ELSD
SJ000565125	>95%	UVTWC_ELSD
SJ000565126	>95%	UVTWC_ELSD
SJ000565127	>95%	UVTWC_ELSD
SJ000565128	>95%	UVTWC_ELSD
SJ000565129	>95%	UVTWC_ELSD
SJ000565130	>95%	UVTWC_ELSD



Supplementary Figure 1. Variability of CCR and coverage as a function of the applicability domain.