Additional file 4:

Supplemental Data - VLS hitlists and Compound Structures and Properties

>300,000 compounds were screened against 3 models of the *Plasmodium* aldolase-TRAP complex. The following tables list the final sets of compounds obtained for each receptor:

The table headings are defined as follows:

- Compound #: a unique number (1-60) assigned to each compound
- VLS score: the lowest energy score obtained for each compound after 3 rounds of screening against the receptor model
- Docking score: the energy score obtained for each compound when it was re-docking to its receptor using a slower, more robust docking algorithm
- Score difference: (Docking score) – (VLS score)
- RMSD: root-mean-squared deviation of the docked position and conformation of the compound between the VLS and re-docking runs

VLS hits for "2pc4 model"

Compound #	VLS Score	Docking Score	Score Difference	RMSD (Å)
4	-37.50	-36.92	0.58	0.08
40	-34.07	-37.10	-3.03	0.00
44	-43.32	-43.28	0.05	0.00
45	-46.36	-36.59	9.77	1.98
47	-36.64	-37.11	-0.47	2.14
56	-32.92	-32.18	0.75	1.73

VLS hits for "falciparum model"

Compound #	VLS Score	Docking Score	Score Difference	RMSD (Å)
3	-36.51	-36.50	0.01	0.00
5	-33.66	-33.42	0.24	0.75
15	-36.22	-33.04	3.18	0.21
22	-33.63	-35.83	-2.20	0.05
32	-37.62	-34.41	3.21	0.48
37	-34.12	-33.16	0.96	0.09
40	-33.30	-36.58	-3.28	0.08
43	-32.39	-32.34	0.06	0.02
46	-32.55	-32.56	-0.01	0.00
53	-32.21	-32.23	-0.03	0.01
55	-37.23	-37.01	0.22	0.10

VLS hits for "gapped-pocket model"

Compound #	VLS Score	Docking Score	Score Difference	RMSD (Å)
1	-32.43	-33.19	-0.76	0.03
2	-36.41	-42.87	-6.47	0.07
5	-36.46	-36.53	-0.06	0.75
6	-37.08	-36.52	0.56	0.03
7	-35.10	-35.59	-0.49	0.05
8	-33.05	-33.11	-0.06	0.03
9	-36.10	-33.41	2.69	0.17
10	-35.37	-35.32	0.05	1.87
11	-32.71	-32.41	0.30	1.70
12	-35.11	-32.30	2.81	2.72
13	-33.02	-34.97	-1.95	2.12
14	-35.00	-34.46	0.54	0.01
16	-35.12	-34.91	0.21	0.00
17	-34.25	-34.32	-0.07	0.02
18	-35.05	-34.92	0.13	0.00
19	-34.49	-34.12	0.37	0.00
20	-34.78	-32.09	2.69	2.22
21	-35.30	-35.28	0.02	0.03
23	-37.96	-43.33	-5.37	0.09
24	-32.67	-32.79	-0.11	0.03
25	-32.61	-32.44	0.17	0.01
26	-37.45	-37.65	-0.20	0.00
27	-35.54	-41.36	-5.83	0.05
28	-34.21	-33.17	1.03	2.21
29	-35.18	-42.15	-6.97	2.27
30	-33.65	-33.36	0.30	1.81
31	-34.27	-33.76	0.51	0.02
33	-39.25	-38.68	0.57	0.03
34	-36.53	-36.82	-0.29	0.00
35	-32.47	-33.42	-0.95	1.81
36	-33.16	-32.87	0.29	0.01
38	-35.19	-35.18	0.01	0.00
39	-38.55	-37.22	1.34	0.04
41	-38.86	-38.45	0.41	0.00
42	-34.08	-34.01	0.08	0.00
48	-32.34	-33.15	-0.81	4.14
49	-37.85	-37.39	0.46	0.03
50	-32.98	-36.85	-3.87	0.68
51	-37.08	-37.01	0.08	0.03
52	-38.58	-37.99	0.60	6.84
54	-35.14	-41.21	-6.06	0.09
57	-35.55	-35.89	-0.34	0.00
58	-33.41	-33.16	0.25	1.66

Compound #	VLS Score	Docking Score	Score Difference	RMSD (Å)
59	-32.74	-32.69	0.05	2.26
60	-34.63	-32.09	2.53	0.02

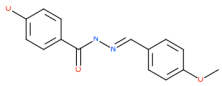
Compound Structures & Properties

The compounds in the ChemBridge (San Diego, CA) screening library are generally uncharacterized. However, several physical and chemical features including solubility, hydrophobicity, flexibility, polarity, etc., can be predicted based on the compounds' formula and molecular structure. These features are listed below for each of the final 60 VLS hits.

Compound # 1

Chembridge ID 5112957

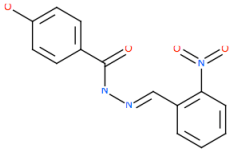
MW	270.3
Formula	C15 H14 N2 O3
Name	4-hydroxy-N'-(4-methoxybenzylidene) benzohydrazide
LogSW	-2.453
RB	3
tPSA	70.92
hDon	2
hAcc	4
cLogP	2.18
molLogP	3.01264
SMILES	C(C=C(O)C=C1)=C1C(=O)N/N=C/C (C=CC(=C1)OC)=C1



Compound # 2

Chembridge ID 5112979

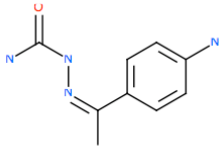
MW	285.3
Formula	C14 H11 N3 O4
Name	4-hydroxy-N'-(2-nitrobenzylidene) benzohydrazide
LogSW	-2.799
RB	3
tPSA	104.83
hDon	2
hAcc	5
cLogP	2
molLogP	2.47206
SMILES	O=N(=O)C(C=CC=C1)=C1/C=N/NC(=O) C(C=CC(O)=C1)=C1



Compound # 3

Chembridge ID 5121901

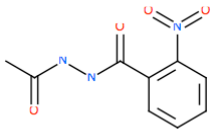
MW	192.2
Formula	C9 H12 N4 O
Name	1-(4-aminophenyl)-1-ethanone semicarbazone
LogSW	-1.833
RB	2
tPSA	93.5
hDon	3
hAcc	2
cLogP	1.44
molLogP	.889302
SMILES	C(C=C(N)C=C1)=C1/C(=N\NC(=O)N)C



Compound # 4

Chembridge ID 5153389

MW	223.2
Formula	C9 H9 N3 O4
Name	N'-acetyl-2-nitrobenzohydrazide
LogSW	-2.179
RB	2
tPSA	101.34
hDon	2
hAcc	4
cLogP	-.41
molLogP	.041457
SMILES	O=N(=O)C(C=CC=C1)=C1C(=O)NNC (=O)C

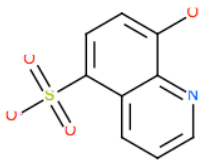


MW: molecular weight, g/mol	hDon: # of hydrogen-bond donors
LogSW: predicted aqueous solubility	hAcc: # of hydrogen-bond acceptors
RB: # of rotatable bonds	cLogP: predicted octanol-water partition coefficient (Chembridge algorithm)
tPSA: total polar surface area (Angstroms^2)	molLogP: predicted octanol-water partition coefficient (Molsoft algorithm)
	SMILES: Simplified Molecular Input Line Entry Specification

Compound # 5

Chembridge ID 5153799

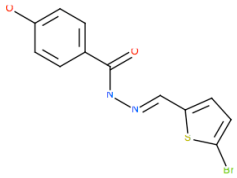
MW	225.2
Formula	C9 H7 N O4 S
Name	8-hydroxy-5-quinolinesulfonic acid
LogSW	.343
RB	1
tPSA	87.49
hDon	2
hAcc	5
cLogP	-.71
molLogP	.616233
SMILES	C(C1)=C(C2C(C=1O)=NC=CC=2)S(=O)(=O)[O-]



Compound # 6

Chembridge ID 5227275

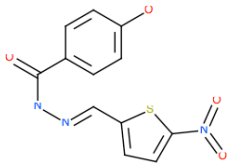
MW	325.2
Formula	C12 H9 Br N2 O2 S
Name	N'-[(5-bromo-2-thienyl)methylene]-4-hydroxybenzohydrazide
LogSW	-3.391
RB	3
tPSA	61.69
hDon	2
hAcc	3
cLogP	2.81
molLogP	3.62692
SMILES	C(C=C(S1)/C=N/NC(=O)C(C=CC(=C2)O)=C2)=C1[Br]



Compound # 7

Chembridge ID 5227278

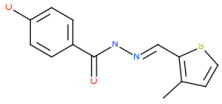
MW	291.3
Formula	C12 H9 N3 O4 S
Name	4-hydroxy-N'-[(5-nitro-2-thienyl) methylene]benzohydrazide
LogSW	-2.62
RB	3
tPSA	104.83
hDon	2
hAcc	5
cLogP	1.74
molLogP	2.75402
SMILES	C(C=C(S1)/C=N/NC(=O)C(C=CC(=C2)O)=C2)=C1N(=O)=O



Compound # 8

Chembridge ID 5227280

MW	260.3
Formula	C13 H12 N2 O2 S
Name	4-hydroxy-N'-[(3-methyl-2-thienyl) methylene]benzohydrazide
LogSW	-2.569
RB	3
tPSA	61.69
hDon	2
hAcc	3
cLogP	2.4
molLogP	3.07727
SMILES	C(=N/NC(=O)C(C=CC(O)=C1)=C1)/C(SC=C1)=C1C

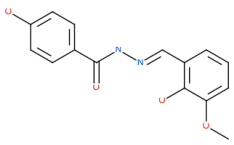


MW: molecular weight, g/mol	hDon: # of hydrogen-bond donors
LogSW: predicted aqueous solubility	hAcc: # of hydrogen-bond acceptors
RB: # of rotatable bonds	cLogP: predicted octanol-water partition coefficient (Chembridge algorithm)
tPSA: total polar surface area (Angstroms^2)	molLogP: predicted octanol-water partition coefficient (Molsoft algorithm)
	SMILES: Simplified Molecular Input Line Entry Specification

Compound # 9

Chembridge ID 5227289

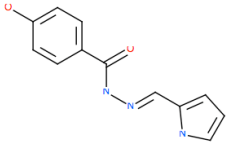
MW	286.3
Formula	C15 H14 N2 O4
Name	4-hydroxy-N'-(2-hydroxy-3-methoxybenzylidene)benzohydrazide
LogSW	-1.938
RB	3
tPSA	91.15
hDon	3
hAcc	5
cLogP	1.44
molLogP	2.51318
SMILES	C(=N/NC(=O)C(C=CC(O)=C1)=C1)/C(C=CC1)=C(C=1OC)O



Compound # 10

Chembridge ID 5227292

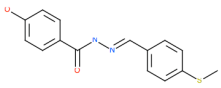
MW	229.2
Formula	C12 H11 N3 O2
Name	4-hydroxy-N'-(1H-pyrrol-2-ylmethylene) benzohydrazide
LogSW	-1.027
RB	3
tPSA	77.48
hDon	3
hAcc	3
cLogP	.86
molLogP	1.87264
SMILES	N(C=CC1)C=1/C=N/NC(=O)C(C=CC(=C1)O)=C1



Compound # 11

Chembridge ID 5227298

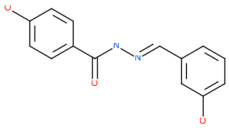
MW	286.4
Formula	C15 H14 N2 O2 S
Name	4-hydroxy-N'-[4-(methylthio) benzylidene]benzohydrazide
LogSW	-3.117
RB	3
tPSA	61.69
hDon	2
hAcc	3
cLogP	2.82
molLogP	3.60632
SMILES	C(C=C(O)C=C1)=C1C(=O)N/N=C/C(C=CC(=C1)SC)=C1



Compound # 12

Chembridge ID 5227303

MW	256.3
Formula	C14 H12 N2 O3
Name	4-hydroxy-N'-(3-hydroxybenzylidene) benzohydrazide
LogSW	-1.847
RB	3
tPSA	81.92
hDon	3
hAcc	4
cLogP	1.59
molLogP	2.66317
SMILES	C(C=C(O)C=C1)=C1C(=O)N/N=C/C(C=CC=C1O)=C1

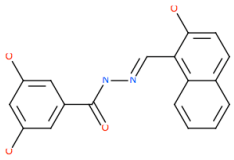


MW: molecular weight, g/mol	hDon: # of hydrogen-bond donors
LogSW: predicted aqueous solubility	hAcc: # of hydrogen-bond acceptors
RB: # of rotatable bonds	cLogP: predicted octanol-water partition coefficient (Chembridge algorithm)
tPSA: total polar surface area (Angstroms^2)	molLogP: predicted octanol-water partition coefficient (Molsoft algorithm)
	SMILES: Simplified Molecular Input Line Entry Specification

Compound # 13

Chembridge ID 5227326

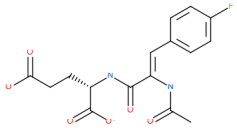
MW	322.3
Formula	C18 H14 N2 O4
Name	3,5-dihydroxy-N'-[(2-hydroxy-1-naphthyl)methylene]benzohydrazide
LogSW	-2.849
RB	3
tPSA	102.15
hDon	4
hAcc	5
cLogP	2.2
molLogP	3.61119
SMILES	C(C(O)=CC(O)=C1)=C1C(=O)N/N=C/C(C(O)=CC1)=C2C=1C=CC=C2



Compound # 14

Chembridge ID 5252622

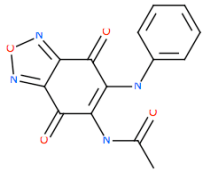
MW	352.3
Formula	C16 H17 F N2 O6
Name	N-[2-(acetylamino)-3-(4-fluorophenyl) acryloyl]glutamic acid
LogSW	-3.028
RB	8
tPSA	132.8
hDon	4
hAcc	6
cLogP	-.06
molLogP	.451621
SMILES	C(/C(C=CC(F)=C1)=C1)=C(/C(=O)N[C@H](C(=O)[O-])CCC(=O)[O-])NC(=O)C



Compound # 15

Chembridge ID 5256251

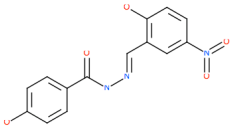
MW	298.3
Formula	C14 H10 N4 O4
Name	N-(6-anilino-4,7-dioxo-4,7-dihydro -2,1,3-benzoxadiazol-5-yl)acetamide
LogSW	-2.17
RB	3
tPSA	114.19
hDon	2
hAcc	6
cLogP	.93
molLogP	.926853
SMILES	O=C(C(=NON1)C=1C(=O)C1NC(C=CC=C2)=C2)C=1NC(=O)C



Compound # 16

Chembridge ID 5256921

MW	301.3
Formula	C14 H11 N3 O5
Name	4-hydroxy-N'-(2-hydroxy-5-nitrobenzylidene)benzohydrazide
LogSW	-2.5
RB	3
tPSA	125.06
hDon	3
hAcc	6
cLogP	1.97
molLogP	2.21263
SMILES	C(C(=C(O)C=C1)/C=N/NC(=O)C(C=CC(=C2)O)=C2)=C1N(=O)=O

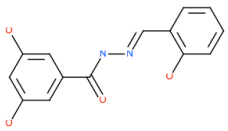


MW: molecular weight, g/mol	hDon: # of hydrogen-bond donors
LogSW: predicted aqueous solubility	hAcc: # of hydrogen-bond acceptors
RB: # of rotatable bonds	cLogP: predicted octanol-water partition coefficient (Chembridge algorithm)
tPSA: total polar surface area (Angstroms^2)	molLogP: predicted octanol-water partition coefficient (Molsoft algorithm)
	SMILES: Simplified Molecular Input Line Entry Specification

Compound # 17

Chembridge ID 5264148

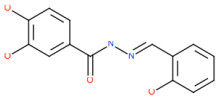
MW	272.3
Formula	C14 H12 N2 O4
Name	3,5-dihydroxy-N'-(2-hydroxybenzylidene)benzohydrazide
LogSW	-1.486
RB	3
tPSA	102.15
hDon	4
hAcc	5
cLogP	1.03
molLogP	2.28373
SMILES	C(C(O)=CC(O)=C1)=C1C(=O)N/N=C/C(C=CC=C1)=C1O



Compound # 18

Chembridge ID 5266986

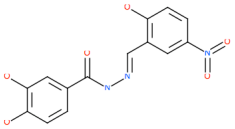
MW	272.3
Formula	C14 H12 N2 O4
Name	3,4-dihydroxy-N'-(2-hydroxybenzylidene)benzohydrazide
LogSW	-1.545
RB	3
tPSA	102.15
hDon	4
hAcc	5
cLogP	1.1
molLogP	2.16371
SMILES	C(C(O)=C(O)C=C1)=C1C(=O)N/N=C/C(C=CC=C1)=C1O



Compound # 19

Chembridge ID 5267209

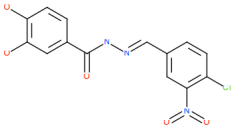
MW	317.3
Formula	C14 H11 N3 O6
Name	3,4-dihydroxy-N'-(2-hydroxy-5-nitrobenzylidene)benzohydrazide
LogSW	-2.189
RB	3
tPSA	145.29
hDon	4
hAcc	7
cLogP	1.47
molLogP	1.83319
SMILES	C(C(=C(O)C=C1)/C=N/NC(=O)C(C=CC(=C2O)O)=C2)=C1N(=O)=O



Compound # 20

Chembridge ID 5267603

MW	335.7
Formula	C14 H10 Cl N3 O5
Name	N'-(4-chloro-3-nitrobenzylidene)-3,4-dihydroxybenzohydrazide
LogSW	-3.183
RB	3
tPSA	125.06
hDon	3
hAcc	6
cLogP	2.02
molLogP	2.80693
SMILES	C(C(O)=C(C=C1)O)=C1C(=O)N/N=C/C(C=CC([Cl])=C1N(=O)=O)=C1

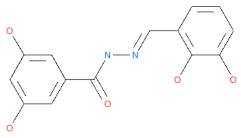


MW: molecular weight, g/mol	hDon: # of hydrogen-bond donors
LogSW: predicted aqueous solubility	hAcc: # of hydrogen-bond acceptors
RB: # of rotatable bonds	cLogP: predicted octanol-water partition coefficient (Chembridge algorithm)
tPSA: total polar surface area (Angstroms^2)	molLogP: predicted octanol-water partition coefficient (Molsoft algorithm)
	SMILES: Simplified Molecular Input Line Entry Specification

Compound # 21

Chembridge ID 5280090

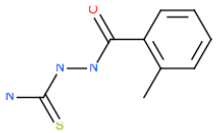
MW	288.3
Formula	C14 H12 N2 O5
Name	N'-(2,3-dihydroxybenzylidene)-3,5-dihydroxybenzohydrazide
LogSW	-1.09
RB	3
tPSA	122.38
hDon	5
hAcc	6
cLogP	0.43
molLogP	1.90429
SMILES	C(C(O)=CC(O)=C1)=C1C(=O)N/N=C/C(C=CC1)=C(C=1O)O



Compound # 22

Chembridge ID 5302171

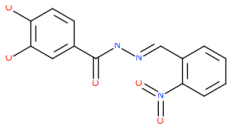
MW	209.3
Formula	C9 H11 N3 O S
Name	2-(2-methylbenzoyl) hydrazinecarbothioamide
LogSW	-2.786
RB	2
tPSA	67.15
hDon	3
hAcc	1
cLogP	2.41
molLogP	.739915
SMILES	S=C(N)NNC(=O)C(C=CC=C1)=C1C



Compound # 23

Chembridge ID 5312165

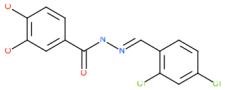
MW	301.3
Formula	C14 H11 N3 O5
Name	3,4-dihydroxy-N'-(2-nitrobenzylidene) benzohydrazide
LogSW	-2.497
RB	3
tPSA	125.06
hDon	3
hAcc	6
cLogP	1.51
molLogP	2.09262
SMILES	C(C(O)=C(O)C=C1)=C1C(=O)N/N=C/C(C=CC=C1)=C1N(=O)=O



Compound # 24

Chembridge ID 5315106

MW	325.2
Formula	C14 H10 Cl2 N2 O3
Name	N'-(2,4-dichlorobenzylidene)-3,4-dihydroxybenzohydrazide
LogSW	-3.715
RB	3
tPSA	81.92
hDon	3
hAcc	4
cLogP	3.19
molLogP	3.85176
SMILES	C(C(O)=C(C=C1)O)=C1C(=O)N/N=C/C(C=CC([Cl])=C1)=C1[Cl]

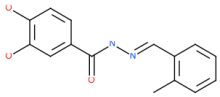


MW: molecular weight, g/mol	hDon: # of hydrogen-bond donors
LogSW: predicted aqueous solubility	hAcc: # of hydrogen-bond acceptors
RB: # of rotatable bonds	cLogP: predicted octanol-water partition coefficient (Chembridge algorithm)
tPSA: total polar surface area (Angstroms^2)	molLogP: predicted octanol-water partition coefficient (Molsoft algorithm)
	SMILES: Simplified Molecular Input Line Entry Specification

Compound # 25

Chembridge ID 5316181

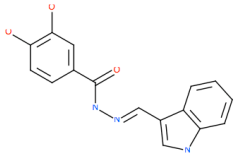
MW	270.3
Formula	C15 H14 N2 O3
Name	3,4-dihydroxy-N'-(2-methylbenzylidene) benzohydrazide
LogSW	-2.522
RB	3
tPSA	81.92
hDon	3
hAcc	4
cLogP	2.26
molLogP	2.82429
SMILES	C(C(O)=C(O)C=C1)=C1C(=O)N/N=C/C (C=CC=C1)=C1C



Compound # 26

Chembridge ID 5318411

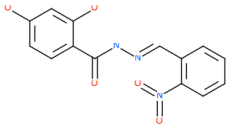
MW	295.3
Formula	C16 H13 N3 O3
Name	3,4-dihydroxy-N'-(1H-indol-3-ylmethylene)benzohydrazide
LogSW	-2.268
RB	3
tPSA	97.71
hDon	4
hAcc	4
cLogP	1.75
molLogP	2.76061
SMILES	N(C(C=CC=C1)=C1C1/C=N/NC(=O)C (C=CC(O)=C2O)=C2)C=1



Compound # 27

Chembridge ID 5320663

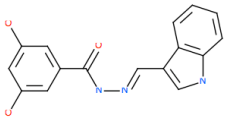
MW	301.3
Formula	C14 H11 N3 O5
Name	2,4-dihydroxy-N'-(2-nitrobenzylidene) benzohydrazide
LogSW	-3.248
RB	3
tPSA	125.06
hDon	3
hAcc	6
cLogP	2.39
molLogP	2.09262
SMILES	C(C=C(O)C1)=C(C=1O)C(=O)N/N=C/C (C=CC=C1)=C1N(=O)=O



Compound # 28

Chembridge ID 5321784

MW	295.3
Formula	C16 H13 N3 O3
Name	3,5-dihydroxy-N'-(1H-indol-3-ylmethylene)benzohydrazide
LogSW	-2.209
RB	3
tPSA	97.71
hDon	4
hAcc	4
cLogP	1.68
molLogP	2.88063
SMILES	N(C(C=CC=C1)=C1C1/C=N/NC(=O)C (C=C(O)C=C2O)=C2)C=1

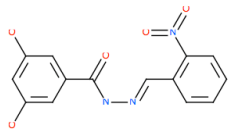


MW: molecular weight, g/mol	hDon: # of hydrogen-bond donors
LogSW: predicted aqueous solubility	hAcc: # of hydrogen-bond acceptors
RB: # of rotatable bonds	cLogP: predicted octanol-water partition coefficient (Chembridge algorithm)
tPSA: total polar surface area (Angstroms^2)	molLogP: predicted octanol-water partition coefficient (Molsoft algorithm)
	SMILES: Simplified Molecular Input Line Entry Specification

Compound # 29

Chembridge ID 5322358

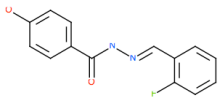
MW	301.3
Formula	C14 H11 N3 O5
Name	3,5-dihydroxy-N'-(2-nitrobenzylidene) benzohydrazide
LogSW	-2.437
RB	3
tPSA	125.06
hDon	3
hAcc	6
cLogP	1.44
molLogP	2.21263
SMILES	O=N(=O)C(C=CC=C1)=C1/C=N/NC(=O) C(C=C(O)C=C1O)=C1



Compound # 30

Chembridge ID 5331708

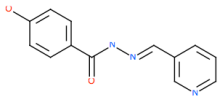
MW	258.3
Formula	C14 H11 F N2 O2
Name	N'-(2-fluorobenzylidene)-4-hydroxybenzohydrazide
LogSW	-2.554
RB	3
tPSA	61.69
hDon	2
hAcc	3
cLogP	2.4
molLogP	3.07193
SMILES	C(=N/NC(=O)C(C=CC(O)=C1)=C1)/C (C=CC=C1)=C1F



Compound # 31

Chembridge ID 5336667

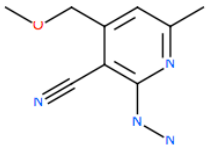
MW	241.2
Formula	C13 H11 N3 O2
Name	4-hydroxy-N'-(3-pyridinylmethylene) benzohydrazide
LogSW	.271
RB	3
tPSA	74.58
hDon	2
hAcc	4
cLogP	.76
molLogP	1.87335
SMILES	C(=N/NC(=O)C(C=CC(O)=C1)=C1)/C (C=CC=N1)=C1



Compound # 32

Chembridge ID 5377378

MW	192.2
Formula	C9 H12 N4 O
Name	2-hydrazino-4-(methoxymethyl)-6-methylnicotinonitrile
LogSW	-1.594
RB	2
tPSA	83.96
hDon	2
hAcc	3
cLogP	.85
molLogP	-.071091
SMILES	N#CC(C(=CC(C)=N1)COC)=C1NN

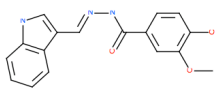


MW: molecular weight, g/mol	hDon: # of hydrogen-bond donors
LogSW: predicted aqueous solubility	hAcc: # of hydrogen-bond acceptors
RB: # of rotatable bonds	cLogP: predicted octanol-water partition coefficient (Chembridge algorithm)
tPSA: total polar surface area (Angstroms^2)	molLogP: predicted octanol-water partition coefficient (Molsoft algorithm)
	SMILES: Simplified Molecular Input Line Entry Specification

Compound # 33

Chembridge ID 5466567

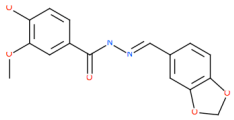
MW	309.3
Formula	C17 H15 N3 O3
Name	4-hydroxy-N'-(1H-indol-3-ylmethylene) -3-methoxybenzohydrazide
LogSW	-3.215
RB	3
tPSA	86.71
hDon	3
hAcc	4
cLogP	2.06
molLogP	3.11008
SMILES	N(C(C=CC=C1)=C1C1/C=N/NC(=O)C (C=CC(O)=C2OC)=C2)C=1



Compound # 34

Chembridge ID 5466778

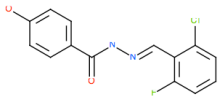
MW	314.3
Formula	C16 H14 N2 O5
Name	N'-(1,3-benzodioxol-5-ylmethylene)-4- hydroxy-3-methoxybenzohydrazide
LogSW	-2.884
RB	3
tPSA	89.38
hDon	2
hAcc	6
cLogP	1.63
molLogP	3.04285
SMILES	C(C(=C(O)C=C1)OC)=C1C(=O)N/N=C/C (C=CC(OCO1)=C12)=C2



Compound # 35

Chembridge ID 5475747

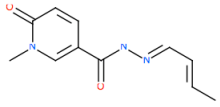
MW	292.7
Formula	C14 H10 Cl F N2 O2
Name	N'-(2-chloro-6-fluorobenzylidene)-4- hydroxybenzohydrazide
LogSW	-3.411
RB	3
tPSA	61.69
hDon	2
hAcc	3
cLogP	3.11
molLogP	3.66622
SMILES	C(=N/NC(=O)C(C=CC(O)=C1)=C1)/C(C ([Cl])=CC=C1)=C1F



Compound # 36

Chembridge ID 5493440

MW	219.2
Formula	C11 H13 N3 O2
Name	N'-2-buten-1-ylidene-1-methyl-6-oxo -1,6-dihydro-3-pyridinecarbohydrazide
LogSW	-2.081
RB	3
tPSA	63.46
hDon	1
hAcc	3
cLogP	1.5
molLogP	.792339
SMILES	C(N(C)C(=O)C=C1)=C1C(=O) N/N=C/C=C/C

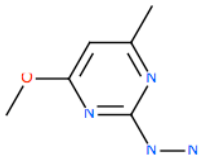


MW: molecular weight, g/mol	hDon: # of hydrogen-bond donors
LogSW: predicted aqueous solubility	hAcc: # of hydrogen-bond acceptors
RB: # of rotatable bonds	cLogP: predicted octanol-water partition coefficient (Chembridge algorithm)
tPSA: total polar surface area (Angstroms^2)	molLogP: predicted octanol-water partition coefficient (Molsoft algorithm)
	SMILES: Simplified Molecular Input Line Entry Specification

Compound # 37

Chembridge ID 5511358

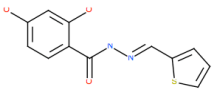
MW	154.2
Formula	C6 H10 N4 O
Name	2-hydrazino-4-methoxy-6-methylpyrimidine
LogSW	-1.266
RB	1
tPSA	73.06
hDon	2
hAcc	3
cLogP	1.1
molLogP	.043357
SMILES	C(C(C)=NC(NN)=N1)=C1OC



Compound # 38

Chembridge ID 5521698

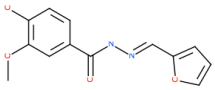
MW	262.3
Formula	C12 H10 N2 O3 S
Name	2,4-dihydroxy-N'-(2-thienylmethylene) benzohydrazide
LogSW	-2.489
RB	3
tPSA	81.92
hDon	3
hAcc	4
cLogP	2.29
molLogP	2.4167
SMILES	C(C=C(C1)O)=C(C=1O)C(=O)N/N=C/C (=CC=C1)S1



Compound # 39

Chembridge ID 5532286

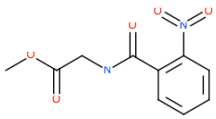
MW	260.2
Formula	C13 H12 N2 O4
Name	N'-(2-furylmethylene)-4-hydroxy-3-methoxybenzohydrazide
LogSW	-2.158
RB	3
tPSA	84.06
hDon	2
hAcc	5
cLogP	1.24
molLogP	2.11852
SMILES	C(C(=C(O)C=C1)OC)=C1C(=O)N/N=C/C (=CC=C1)O1



Compound # 40

Chembridge ID 5562286

MW	238.2
Formula	C10 H10 N2 O5
Name	methyl N-(2-nitrobenzoyl)glycinate
LogSW	-2.749
RB	3
tPSA	98.54
hDon	1
hAcc	5
cLogP	.13
molLogP	.333642
SMILES	O=N(=O)C(C=CC=C1)=C1C(=O)NCC (=O)OC

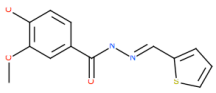


MW: molecular weight, g/mol	hDon: # of hydrogen-bond donors
LogSW: predicted aqueous solubility	hAcc: # of hydrogen-bond acceptors
RB: # of rotatable bonds	cLogP: predicted octanol-water partition coefficient (Chembridge algorithm)
tPSA: total polar surface area (Angstroms^2)	molLogP: predicted octanol-water partition coefficient (Molsoft algorithm)
	SMILES: Simplified Molecular Input Line Entry Specification

Compound # 41

Chembridge ID 5567417

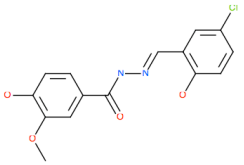
MW	276.3
Formula	C13 H12 N2 O3 S
Name	4-hydroxy-3-methoxy-N'-(2-thienylmethylene)benzohydrazide
LogSW	-2.676
RB	3
tPSA	70.92
hDon	2
hAcc	4
cLogP	1.71
molLogP	2.76616
SMILES	C(C(=C(O)C=C1)OC)=C1C(=O)N/N=C/C(=CC=C1)S1



Compound # 42

Chembridge ID 5630714

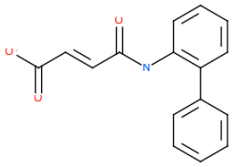
MW	320.7
Formula	C15 H13 Cl N2 O4
Name	N'-(5-chloro-2-hydroxybenzylidene)-4-hydroxy-3-methoxybenzohydrazide
LogSW	-3.017
RB	3
tPSA	91.15
hDon	3
hAcc	5
cLogP	2.41
molLogP	3.2275
SMILES	C(C(=C(O)C=C1)OC)=C1C(=O)N/N=C/C(C=C([Cl])C=C1)=C1O



Compound # 43

Chembridge ID 5774457

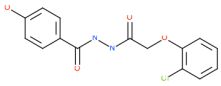
MW	267.3
Formula	C16 H13 N O3
Name	4-(2-biphenylylamino)-4-oxo-2-butenoic acid
LogSW	-2.73
RB	4
tPSA	66.4
hDon	2
hAcc	3
cLogP	1.85
molLogP	3.25109
SMILES	C(=C/C(=O)[O-])/C(=O)NC(C=CC=C1)=C1C(C=CC=C1)=C1



Compound # 44

Chembridge ID 5798683

MW	320.7
Formula	C15 H13 Cl N2 O4
Name	N'-[(2-chlorophenoxy)acetyl]-4-hydroxybenzohydrazide
LogSW	-3
RB	5
tPSA	87.66
hDon	3
hAcc	4
cLogP	2.39
molLogP	2.13078
SMILES	C(C(=O)NNC(=O)C(C=CC(O)=C1)=C1)OC(C=CC=C1)=C1[Cl]

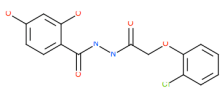


MW: molecular weight, g/mol	hDon: # of hydrogen-bond donors
LogSW: predicted aqueous solubility	hAcc: # of hydrogen-bond acceptors
RB: # of rotatable bonds	cLogP: predicted octanol-water partition coefficient (Chembridge algorithm)
tPSA: total polar surface area (Angstroms^2)	molLogP: predicted octanol-water partition coefficient (Molsoft algorithm)
	SMILES: Simplified Molecular Input Line Entry Specification

Compound # 45

Chembridge ID 5799663

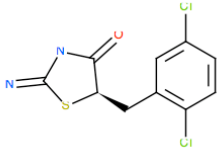
MW	336.7
Formula	C15 H13 Cl N2 O5
Name	N'-[(2-chlorophenoxy)acetyl]-2,4-dihydroxybenzohydrazide
LogSW	-3.441
RB	5
tPSA	107.89
hDon	4
hAcc	5
cLogP	2.77
molLogP	1.75134
SMILES	C(C=C(O)C1)=C(C=1O)C(=O)NNC(=O)COC(C=CC=C1)=C1[Cl]



Compound # 46

Chembridge ID 5851839

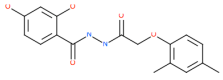
MW	275.2
Formula	C10 H8 Cl2 N2 O S
Name	5-(2,5-dichlorobenzyl)-2-imino-1,3-thiazolidin-4-one
LogSW	-4.478
RB	2
tPSA	52.95
hDon	2
hAcc	2
cLogP	3.83
molLogP	2.44747
SMILES	C([C@@H](SC(=N)N1)C1=O)C(C=C(C=C1)[Cl])=C1[Cl]



Compound # 47

Chembridge ID 5853551

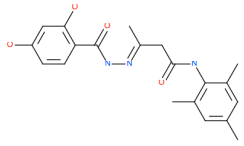
MW	330.3
Formula	C17 H18 N2 O5
Name	N'-[(2,4-dimethylphenoxy)acetyl]-2,4-dihydroxybenzohydrazide
LogSW	-3.719
RB	5
tPSA	107.89
hDon	4
hAcc	5
cLogP	3.15
molLogP	1.83934
SMILES	C(C=C(O)C1)=C(C=1O)C(=O)NNC(=O)COC(C=CC(=C1)C)=C1C



Compound # 48

Chembridge ID 6213095

MW	369.4
Formula	C20 H23 N3 O4
Name	3-[(2,4-dihydroxybenzoyl)hydrazono]-N-mesitylbutanamide
LogSW	-2.526
RB	5
tPSA	111.02
hDon	4
hAcc	5
cLogP	1.42
molLogP	3.0898
SMILES	C(C(=O)NC(C(C)=CC(C)=C1)=C1C)/C(=N/NC(=O)C(C=CC(O)=C1)=C1O)C

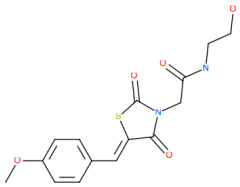


MW: molecular weight, g/mol	hDon: # of hydrogen-bond donors
LogSW: predicted aqueous solubility	hAcc: # of hydrogen-bond acceptors
RB: # of rotatable bonds	cLogP: predicted octanol-water partition coefficient (Chembridge algorithm)
tPSA: total polar surface area (Angstroms^2)	molLogP: predicted octanol-water partition coefficient (Molsoft algorithm)
	SMILES: Simplified Molecular Input Line Entry Specification

Compound # 49

Chembridge ID 6326744

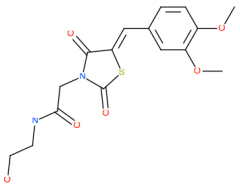
MW	336.4
Formula	C15 H16 N2 O5 S
Name	N-(2-hydroxyethyl)-2-[5-(4-methoxybenzylidene)-2,4-dioxo-1,3-thiazolidin-3-yl]acetamide
LogSW	-2.549
RB	5
tPSA	95.94
hDon	2
hAcc	5
cLogP	1.05
molLogP	.945202
SMILES	C(=C(S1)/C(N(C1=O)CC(=O)NCCO)=O)/C(C=CC(=C1)OC)=C1



Compound # 50

Chembridge ID 6348549

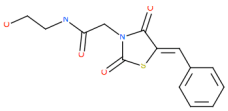
MW	366.4
Formula	C16 H18 N2 O6 S
Name	2-[5-(3,4-dimethoxybenzylidene)-2,4-dioxo-1,3-thiazolidin-3-yl]-N-(2-hydroxyethyl)acetamide
LogSW	-2.546
RB	5
tPSA	105.17
hDon	2
hAcc	6
cLogP	.79
molLogP	.915229
SMILES	C(=C(S1)/C(N(C1=O)CC(=O)NCCO)=O)/C(C=CC(=C1OC)OC)=C1



Compound # 51

Chembridge ID 6356536

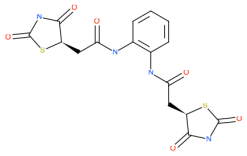
MW	306.3
Formula	C14 H14 N2 O4 S
Name	2-(5-benzylidene-2,4-dioxo-1,3-thiazolidin-3-yl)-N-(2-hydroxyethyl) acetamide
LogSW	-2.399
RB	5
tPSA	86.71
hDon	2
hAcc	4
cLogP	1.13
molLogP	.855157
SMILES	C(=C(S1)/C(N(C1=O)CC(=O)NCCO)=O)/C(C=CC=C1)=C1



Compound # 52

Chembridge ID 6631742

MW	422.4
Formula	C16 H14 N4 O6 S2
Name	N,N'-1,2-phenylenebis[2-(2,4-dioxo-1,3-thiazolidin-5-yl)acetamide]
LogSW	-3.205
RB	6
tPSA	150.54
hDon	4
hAcc	6
cLogP	-.45
molLogP	-.696903
SMILES	C([C@@H](SC(=O)N1)C1=O)C(=O)NC(C=CC=C1)=C1NC(=O)C[C@@H](SC(=O)N1)C1=O

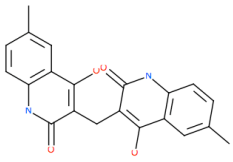


MW: molecular weight, g/mol	hDon: # of hydrogen-bond donors
LogSW: predicted aqueous solubility	hAcc: # of hydrogen-bond acceptors
RB: # of rotatable bonds	cLogP: predicted octanol-water partition coefficient (Chembridge algorithm)
tPSA: total polar surface area (Angstroms^2)	molLogP: predicted octanol-water partition coefficient (Molsoft algorithm)
	SMILES: Simplified Molecular Input Line Entry Specification

Compound # 53

Chembridge ID 6946462

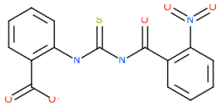
MW	362.4
Formula	C21 H18 N2 O4
Name	3,3'-methylenebis(4-hydroxy-6-methyl-2 (1H)-quinolinone)
LogSW	-3.695
RB	2
tPSA	106.18
hDon	4
hAcc	4
cLogP	2.17
molLogP	3.08223
SMILES	C(C(C(=O)N1)=C(C2=C1C=CC(C)=C2) O)C(C(=O)N1)=C(C2=C1C=CC(=C2)C)O



Compound # 54

Chembridge ID 6949907

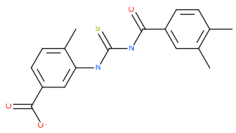
MW	345.3
Formula	C15 H11 N3 O5 S
Name	2-({[(2-nitrobenzoyl)amino] carbonothioyl}amino)benzoic acid
LogSW	-4.089
RB	3
tPSA	121.57
hDon	3
hAcc	5
cLogP	2.32
molLogP	1.98676
SMILES	O=N(=O)C(C=CC=C1)=C1C(=O)NC(=S) NC(C=CC=C1)=C1C(=O)[O-]



Compound # 55

Chembridge ID 6988892

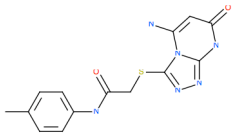
MW	342.4
Formula	C18 H18 N2 O3 S
Name	3-({[(3,4-dimethylbenzoyl)amino] carbonothioyl}amino)-4-methylbenzoic acid
LogSW	-4.711
RB	3
tPSA	78.43
hDon	3
hAcc	3
cLogP	3.53
molLogP	3.52074
SMILES	C(C(C(=O)[O-])=CC1)=C(C=1C)NC(=S) NC(=O)C(C=CC(=C1C)C)=C1



Compound # 56

Chembridge ID 7446357

MW	330.4
Formula	C14 H14 N6 O2 S
Name	2-[(5-amino-7-oxo-7,8-dihydro[1,2,4] triazolo[4,3-a]pyrimidin-3-yl)thio]-N-(4-methylphenyl)acetamide
LogSW	-3.189
RB	4
tPSA	118.17
hDon	3
hAcc	4
cLogP	-.222
molLogP	1.3939
SMILES	C(C(=O)N1)=C(N(C1=NN1)C=1SCC(=O) NC(C=CC(=C1)C)=C1)N

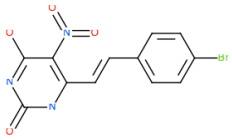


MW: molecular weight, g/mol	hDon: # of hydrogen-bond donors
LogSW: predicted aqueous solubility	hAcc: # of hydrogen-bond acceptors
RB: # of rotatable bonds	cLogP: predicted octanol-water partition coefficient (Chembridge algorithm)
tPSA: total polar surface area (Angstroms^2)	molLogP: predicted octanol-water partition coefficient (Molsoft algorithm)
	SMILES: Simplified Molecular Input Line Entry Specification

Compound # 57

Chembridge ID 7507803

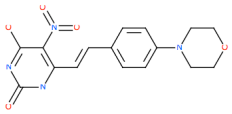
MW	338.1
Formula	C12 H8 Br N3 O4
Name	6-[2-(4-bromophenyl)vinyl]-4-hydroxy-5-nitro-2(1H)-pyrimidinone
LogSW	-3.035
RB	2
tPSA	109.12
hDon	2
hAcc	5
cLogP	2.003
molLogP	1.969
SMILES	C(/C(NC(=O)N1)=C(C=1O)N(=O)=O)=C/C(C=CC([Br])=C1)=C1



Compound # 58

Chembridge ID 7530375

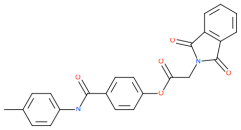
MW	344.3
Formula	C16 H16 N4 O5
Name	4-hydroxy-6-{2-[4-(4-morpholinyl) phenyl]vinyl}-5-nitro-2(1H)-pyrimidinone
LogSW	-3.452
RB	3
tPSA	121.59
hDon	2
hAcc	6
cLogP	.96
molLogP	.975792
SMILES	C(/C(NC(=O)N1)=C(C=1O)N(=O)=O)=C/C(C=CC(=C1)N(CCOC2)C2)=C1



Compound # 59

Chembridge ID 7608933

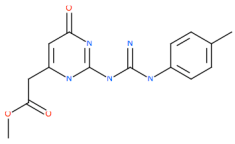
MW	414.4
Formula	C24 H18 N2 O5
Name	4-{[(4-methylphenyl)amino]carbonyl} phenyl (1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)acetate
LogSW	-5.227
RB	6
tPSA	92.78
hDon	1
hAcc	5
cLogP	3.785
molLogP	3.94171
SMILES	C(C(=O)OC(C=CC(=C1)C(=O)NC(C=CC(C)=C2)=C2)=C1)N(C(=O)C(C=CC=C1)=C12)C2=O



Compound # 60

Chembridge ID 7666888

MW	315.3
Formula	C15 H17 N5 O3
Name	methyl [2-({imino[(4-methylphenyl) amino]methyl}amino)-6-oxo-3,6-dihydro-4-pyrimidinyl]acetate
LogSW	-2.315
RB	6
tPSA	119.96
hDon	4
hAcc	5
cLogP	-.724
molLogP	.491161
SMILES	C(C(=O)N=C(NC(=N)NC(C=CC(C)=C1)=C1)N1)=C1CC(=O)OC



MW: molecular weight, g/mol	hDon: # of hydrogen-bond donors
LogSW: predicted aqueous solubility	hAcc: # of hydrogen-bond acceptors
RB: # of rotatable bonds	cLogP: predicted octanol-water partition coefficient (Chembridge algorithm)
tPSA: total polar surface area (Angstroms^2)	molLogP: predicted octanol-water partition coefficient (Molsoft algorithm)
	SMILES: Simplified Molecular Input Line Entry Specification