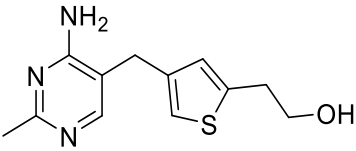
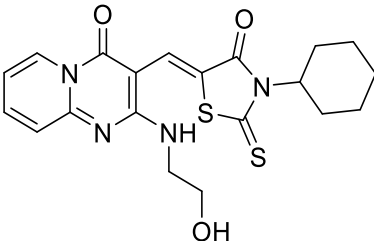
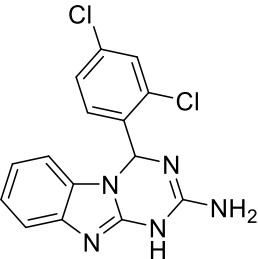
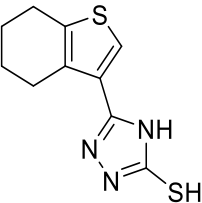
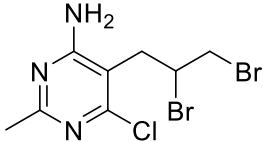
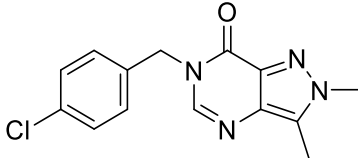
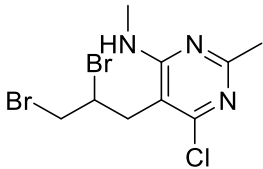
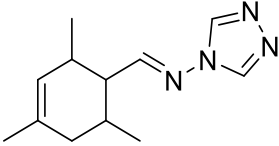
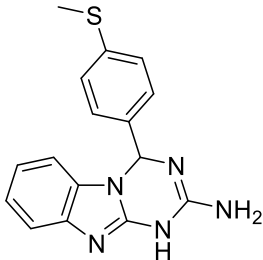


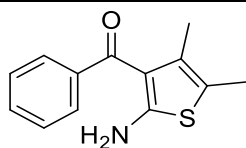
Supplementary Tables

Table S1: Structures, SMILES codes and supplier ID of hits from the first round of LBVS.

Cmpd. No.	Structure, SMILES and supplier ID	MW	cLogP	IC ₅₀ (μM)
	 <p>DZT</p>			
11	 <p>OCCNC1=C(\C=C2/SC(=S)N(C3CCCCC3)C2=O)C(=O)N2C=CC=CC2=N1</p> <p>OSSK_026083</p>	430.54	2.37	60 ± 5
12	 <p>NC1=NC(C2=CC=C(C=C2Cl)Cl)N3C(N1)=NC4=CC=CC=C34</p> <p>OSSK_676817</p>	332.19	4.45	145 ± 17
32	 <p>SC1=NN=C(C2=CSC3=C2CCCC3)N1</p> <p>OSSK_626533</p>	237.34	3.06	528 ± 118

33	 <chem>CC1=NC(N)=C(C(Cl)=N1)CC(CBr)Br</chem> OSSL_119803	343.45	3.09	748 ± 131
34	 <chem>CN1N=C2C(N=CN(C2=O)CC3=CC=C(C=C3)Cl)=C1C</chem> OSSL_160939	288.74	2.29	~ 1000
35	 <chem>CNC1=C(C(Cl)=NC(C)=N1)CC(CBr)Br</chem> OSSK_356137	357.47	3.43	~ 40% inhibition at 1000 µM
36	 <chem>CC1CC(C)=CC(C1/C=N/N2C=NN=C2)C</chem> OSSK_356851	218.30	0.87	~ 30 % inhibition at 1000 µM
37	 <chem>CSC1=CC=C(C2N=C(NC3=NC4=C(N23)C=CC=C4)N)C=C1</chem>	309.39	3.87	>60

OSSK_676806



38

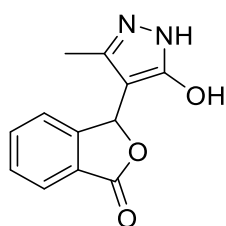
231.31

4.36

> 120

CC1=C(C(C(C2=CC=CC=C2)=O)=C(S1)
N)C

OSSK_998770



39

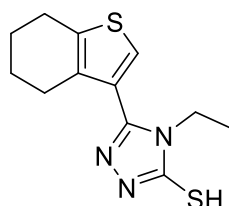
230.22

1.53

> 1000

CC1=NNC(O)=C1C2OC(C3=CC=CC=C2
3)=O

OSSK_734675



40

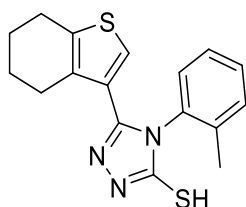
265.39

3.64

> 240

CCN1C(S)=NN=C1C2=CSC3=C2CCCC3

OSSK_040776



41

327.46

5.46

> 8

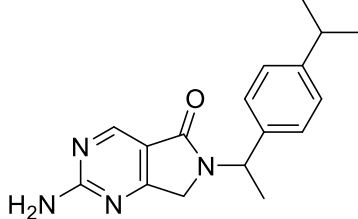
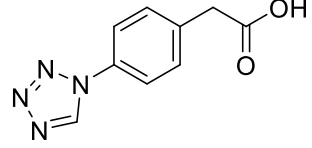
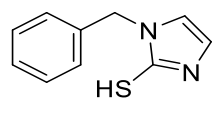
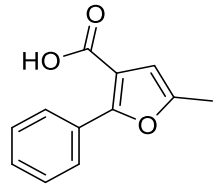
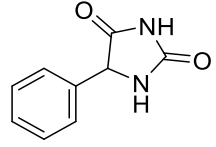
CC1=CC=CC=C1N2C(S)=NN=C2C3=CS
C4=C3CCCC4

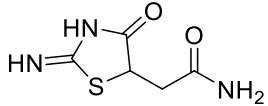
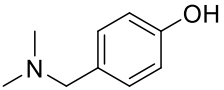
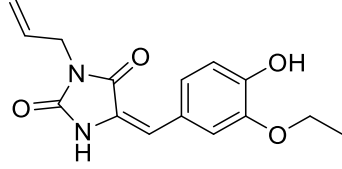
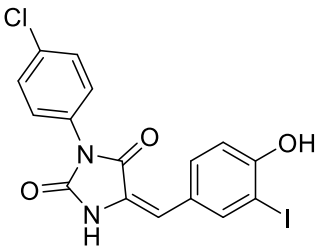
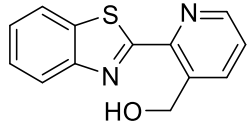
OSSK_041451

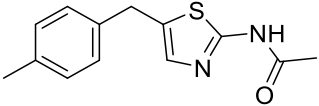
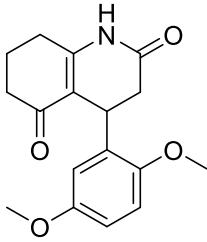
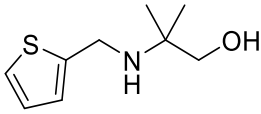
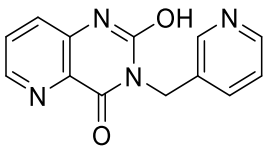
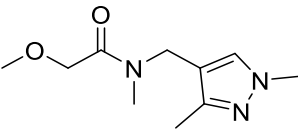
42		392.32	3.18	> 30
	<chem>CC1=NN(C(C)=C1Br)CCC2=NN=C(N2C C3=CC=CC=C3)S</chem>			
	OSSK_041558			
43		318.31	2.72	> 500
	<chem>OC1=NC=NC(O)=C1C(C2=C(N=CN=C2 O)O)C3=CC=CS3</chem>			
	OSSK_373400			
44		246.31	1.05	> 1000
	<chem>CC1=CC=CC(C(N2CCC(C(N)=O)CC2)=O)=C1</chem>			
	OSSK_389140			
45		351.45	6.60	> 15
	<chem>CC1=C(C(NC2=CC=CC=C2)=NC(C3=CC =CC=C3)=N1)CC4=CC=CC=C4</chem>			
	OSSK_468268			

46		332.37	2.74	> 500
	<chem>COC1=CC=C2NC=C(C2=C1)C3NC(N)=N C4=NC5=C(N34)C=CC=C5</chem> OSSK_531783			
47		360.46	4.94	>30
	<chem>CC(C1=CC=C(C=C1)CN(C2=CC=CC=N2))C(COC3=CC=CC=C3)=O</chem> OSSK_771297			
48		313.33	3.62	> 500
	<chem>OC(CCC1=CC=C(C2=CC=C(C=C2)F)N1 CC3=CC=CO3)=O</chem> OSSK_995312			
49		267.29	2.06	> 1000
	<chem>CC1=CC=C(C2NC(N)=NC3=NC4=C(N23) C=CC=C4)O1</chem> OSSL_009157			

50		373.82	2.73	> 240
	<chem>COC1=CC(OC)=C(C(Cl)=C1)/C=C2SC(N(C\2=O)CC(O)=O)=S</chem>			
	OSSL_122234			
51		246.29	1.22	> 1000
	<chem>NN1C(S)=NN=C1CN2C=NC3=CC=CC=C23</chem>			
	OSSL_259003			
52		271.38	3.22	> 240
	<chem>CCNC(NC1=CC=C(C=C1)CC2=CC=NC=C2)=S</chem>			
	OSSL_301953			
	1			
Cmpd No.	Structure, SMILES and supplier ID	MW	cLogP	IC ₅₀ (μM)
3		294.40	4.00	317 ± 29
	<chem>CC(C)C1=CC=C(C=C1)CN2C(CCO)=NC3=CC=CC=C23</chem>			
	OSSK_927261			

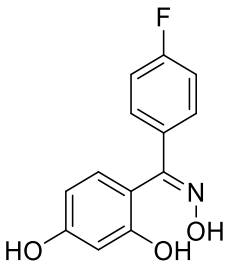
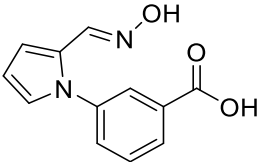
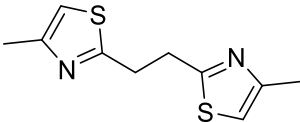
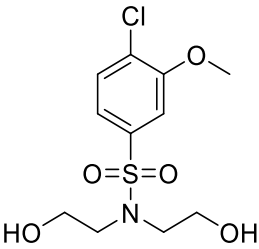
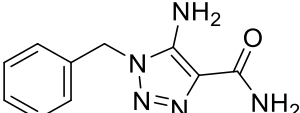
<p>4</p>	 <p><chem>CC(C1=CC=C(C(N2CC3=C(C2=O)C=NC(N)=N3)C=C1)C</chem></p> <p>OSSL_332078</p>	296.37	2.42	935 ± 117
<p>53</p>	 <p><chem>OC(CC1=CC=C(N2C=NN=N2)C=C1)=O</chem></p> <p>OSSL_014662</p>	204.19	0.65	~ 25 % inhibition at 1000 µM
<p>54</p>	 <p><chem>SC1=NC=CN1CC2=CC=CC=C2</chem></p> <p>OSSL_312724</p>	190.26	2.47	> 500
<p>55</p>	 <p><chem>CC1=CC(C(O)=O)=C(C2=CC=CC=C2)O1</chem></p> <p>OSSL_295114</p>	202.21	2.54	> 1000
<p>56</p>	 <p><chem>O=C1NC(C2=CC=CC=C2)C(N1)=O</chem></p> <p>OSSL_299665</p>	176.18	0.49	> 1000

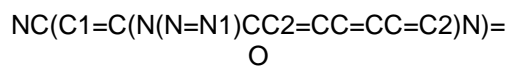
57	 <chem>NC(CC1SC(NC1=O)=N)=O</chem> OSSK_303386	173.19	-1.15	> 1000
58	 <chem>CN(CC1=CC=C(C=C1)O)C</chem> OSSK_366315	151.21	1.61	> 1000
59	 <chem>CCOC1=CC(/C=C2NC(N(C/2=O)CC=C)=O)=CC=C1O</chem> OSSK_441886	288.30	1.53	> 30
60	 <chem>OC1=CC=C(C=C1I)/C=C2NC(N(C3=CC=C(C=C3)Cl)C/2=O)=O</chem> OSSK_441901	440.62	3.79	> 120
61	 <chem>OCC1=C(C2=NC3=CC=CC=C3S2)N=CC=C1</chem> OSSK_470489	242.30	2.54	> 60

<p>62</p>	 <p><chem>CC(=O)NC1=NC=C(S1)CC2=CC=C(C=C2)C</chem></p> <p>OSSK_475789</p>	246.33	3.29	> 30
<p>63</p>	 <p><chem>COC1=CC=C(C(C2CC(=O)NCC2)C(=O)O)=C1OC</chem></p> <p>OSSK_614781</p>	301.34	1.13	> 500
<p>64</p>	 <p><chem>CC(C)(O)CNCC1=CC=CS1</chem></p> <p>OSSK_616553</p>	185.29	1.45	> 1000
<p>65</p>	 <p><chem>OC1=NC2=C(C(N1CC3=CN=CC=C3)=O)N=CC=C2</chem></p> <p>OSSK_840158</p>	254.25	1.30	>240
<p>66</p>	 <p><chem>COCC(=O)N(C)CC1=CN(N=C1C)C</chem></p> <p>OSSK_891366</p>	211.27	-0.47	>1000

67		221.30	1.07	>1000
	<chem>CCN1N=CC=C1CN(C(C2CCCC2)=O)C</chem> OSSK_891525			
68		233.27	1.25	> 1000
	<chem>CN1C(C2=CC=CC=C2)C(C(O)=O)CCC1=O</chem> OSSL_107834			
69		266.39	1.47	> 1000
	<chem>CCCCNC(N(CC1=C(N(N=C1C)CC)C)C)=O</chem> OSSL_161624			
70		203.25	0.82	> 1000
	<chem>COC1=CC=C(C=C1N)CN2C=CN=C2</chem> OSSL_303243			
71		354.45	3.77	> 60
	<chem>CCC1CCC2(N=C(N(C2=O)CC(C3=CC=C4CCCC4=C3)=O)O)CC1</chem> OSSL_309452			

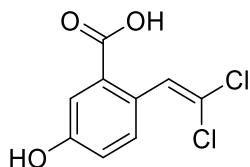
72		378.29	3.65	> 120
	<chem>CC1=CC(C)=NN1CCC2=NN=C(N2C3=C C=C(C=C3)Br)S</chem> OSSL_311660			
73		313.42	3.40	> 500
	<chem>CC1=CC(C)=NN1CCC2=NN=C(N2C3=C C=C(C=C3)C)S</chem> OSSL_311662			
74		192.22	-0.25	> 1000
	<chem>CC1=CC(C)=NN1CCC2=NN=CO2</chem> OSSL_311751			
75		253.31	2.38	> 1000
	<chem>NC(C1=NC2=CC=CC=C2N1)CC3=CC=C (C=C3)O</chem> OSSL_317110			
	2			

Cmpd. No.	Structure, SMILES and supplier ID	MW	cLogP	IC ₅₀ (μM)
5	 <chem>O/N=C(C1=CC=C(C=C1O)O)/C2=CC=C(C=C2)F</chem> OSSL_151911	247.23	2.98	528 ± 43
6	 <chem>O/N=C/C1=CC=CN1C2=CC=CC(C(=O)O)=C2</chem> OSSK_600760	230.22	2.23	455 ± 81
76	 <chem>CC1=CSC(CCC2=NC(C)=CS2)=N1</chem> OSSK_269157	224.34	1.82	~ 25 % inhibition at 1000 μM
77	 <chem>COC1=CC(S(=O)(N(CCO)CCO)=O)=CC=C1Cl</chem> OSSL_292991	309.76	0.09	~ 25 % inhibition at 2000 μM
78	 <chem>Nc1nnn(CNc2ccccc2)c1C(=O)N</chem>	217.23	0.89	> 240



OSSL_296278

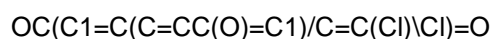
79



233.04

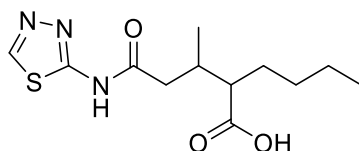
2.82

> 1000



OSSL_304940

80



285.36

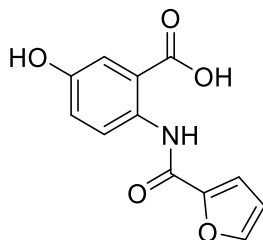
2.10

> 1000



OSSK_308957

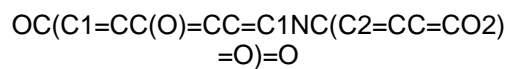
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247.21

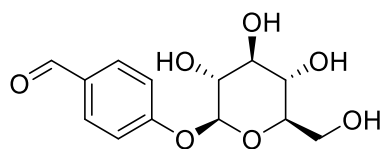
2.13

>60



OSSK_403603

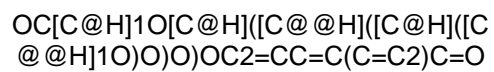
82



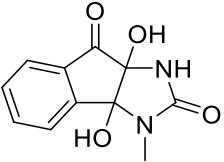
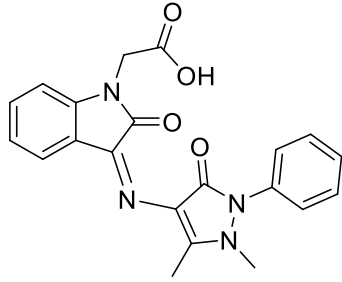
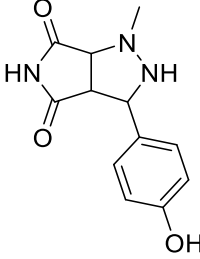
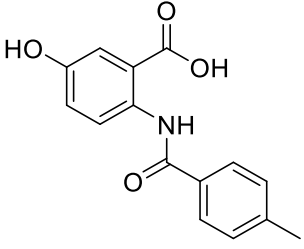
284.26

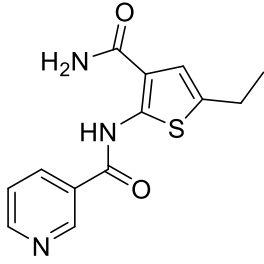
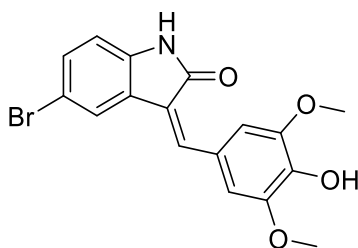
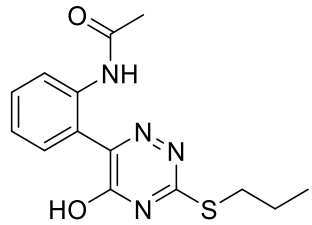
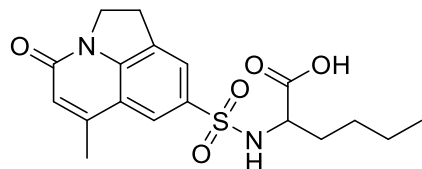
-0.89

> 1000



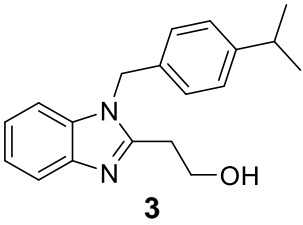
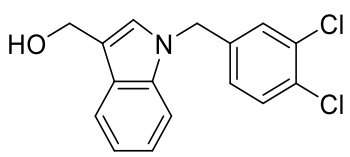
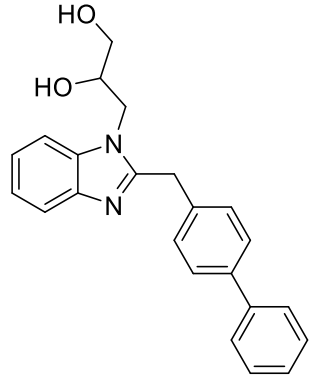
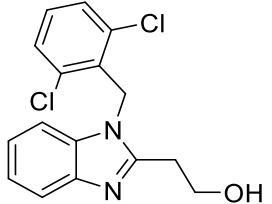
OSSK_404842

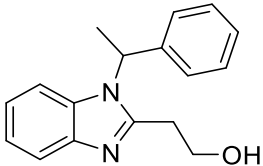
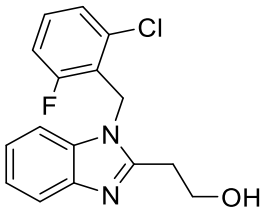
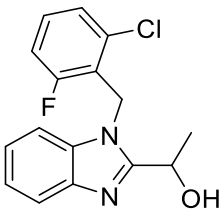
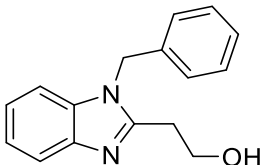
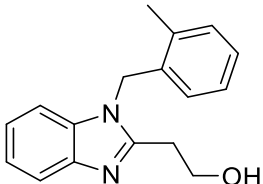
<p>83</p>	 <p><chem>CN1C(NC2(C(C3=CC=CC=C3C12O)=O)O)=O</chem></p> <p>OSSK_451422</p>	<p>234.21</p>	<p>0.16</p>	<p>> 1000</p>
<p>84</p>	 <p><chem>CN1N(C2=CC=CC=C2)C(C(N=C3C(N(C4=CC=CC=C4)CC(O)=O)=O)=C1C)=O</chem></p> <p>OSSK_488329</p>	<p>390.40</p>	<p>1.49</p>	<p>> 120</p>
<p>85</p>	 <p><chem>CN1NC(C2=CC=C(C=C2)O)C3C1C(NC3=O)=O</chem></p> <p>OSSK_645367</p>	<p>247.25</p>	<p>-0.57</p>	<p>> 120</p>
<p>86</p>	 <p><chem>CC1=CC=C(C(NC2=CC=C(C=C2C(O)=O)O)=O)C=C1</chem></p> <p>OSSK_706039</p>	<p>271.27</p>	<p>3.58</p>	<p>> 120</p>

<p>87</p>	 <p> <chem>CCC1=CC(C(N)=O)=C(S1)NC(C2=CC=CN=C2)=O</chem> OSSK_807467 </p>	<p>275.33</p>	<p>2.38</p>	<p>> 60</p>
<p>88</p>	 <p> <chem>COC1=CC(/C=C2C(=O)Nc3ccc(Br)cc32)=CC(OC)=C1O</chem> OSSL_267571 </p>	<p>376.21</p>	<p>3.42</p>	<p>> 120</p>
<p>89</p>	 <p> <chem>CCCSC1=NC(O)=C(C2=CC=CC=C2NC(=O)N=N1)</chem> OSSL_268532 </p>	<p>304.37</p>	<p>2.13</p>	<p>> 120</p>
<p>90</p>	 <p> <chem>CCCCC(C(O)=O)NS(=O)(=O)(C1=CC2=C3N(C(C=C(C3=C1)C)=O)CC2)=O</chem> OSSL_304616 </p>	<p>378.44</p>	<p>2.09</p>	<p>> 60</p>

91		213.34	2.45	> 1000
	<chem>NC1=CC=C(C2=CC=CC=C2C(O)=O)C=C</chem>			
	OSSL_312689			
92		250.28	1.96	> 60
	<chem>COC1=CC(/C=N/N2C=NN=C2S)=CC=C1</chem>			
	OSSK_001945			

Table S2: Structures, SMILES codes and supplier ID of hits from the second round of LBVS.

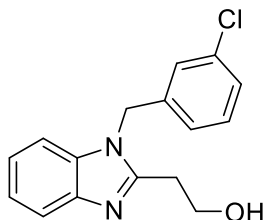
Cmpd. No.	Structure, SMILES and supplier ID	MW	cLogP	IC ₅₀ (μM)
	 <p style="text-align: center;">3</p>			
7	 <p style="text-align: center;"> <chem>OCC1=CN(CC2=CC=C(Cl)C(Cl)=C2)C3=C1C=CC=C3</chem> OSSL_652383 </p>	306.19	4.46	34 ± 4
93	 <p style="text-align: center;"> <chem>OC(CO)CN1C(CC2=CC=C(C3=CC=CC=C3)C=C2)=NC4=CC=CC=C41</chem> OSSK_769093 </p>	358.44	3.77	381 ± 122
94	 <p style="text-align: center;"> <chem>OCCC1=NC2=CC=CC=C2N1CC3=C(Cl)C=CC=C3Cl</chem> OSSK_932460 </p>	321.20	3.96	465 ± 167

<p>95</p>	 <p>OCCC1=NC2=CC=CC=C2N1C(C)C3=CC=CC=C3</p> <p>OSSK_286476</p>	<p>266.34</p>	<p>3.17</p>	<p>720 ± 252</p>
<p>96</p>	 <p>OCCC1=NC2=CC=CC=C2N1CC3=C(F)C=CC=C3Cl</p> <p>OSSK_932461</p>	<p>304.75</p>	<p>3.50</p>	<p>900 ± 390</p>
<p>97</p>	 <p>OC(C)C1=NC2=CC=CC=C2N1CC3=C(F)C=CC=C3Cl</p> <p>OSSK_464452</p>	<p>304.75</p>	<p>3.83</p>	<p>1100 ± 300</p>
<p>98</p>	 <p>OCCC1=NC2=CC=CC=C2N1CC3=CC=CC=C3</p> <p>OSSK_932458</p>	<p>252.32</p>	<p>2.75</p>	<p>2900 ± 600</p>
<p>99</p>		<p>266.34</p>	<p>3.26</p>	<p>> 500</p>

OCCC1=NC2=CC=CC=C2N1CC3=CC=C
C=C3C

OSSK_927258

100



286.76

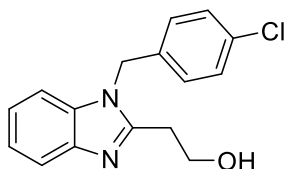
3.35

> 236

OCCC1=NC2=CC=CC=C2N1CC3=CC=C
C(Cl)=C3

OSSK_927259

101



286.76

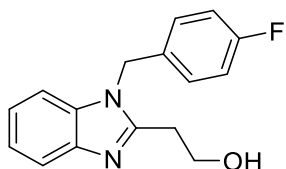
3.35

> 440

OCCC1=NC2=CC=CC=C2N1CC3=CC=C
(Cl)C=C3

OSSK_932459

102



270.31

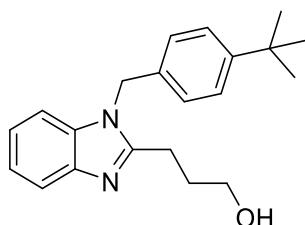
2.89

> 540

OCCC1=NC2=CC=CC=C2N1CC3=CC=C
(F)C=C3

OSSK_932462

103



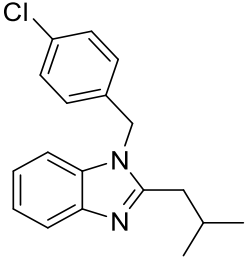
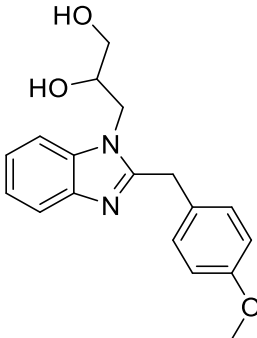
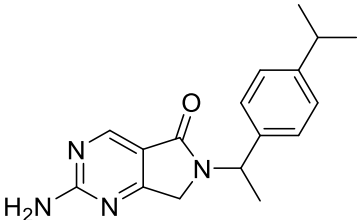
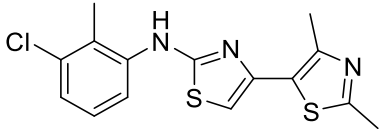
322.45

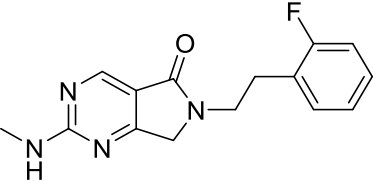
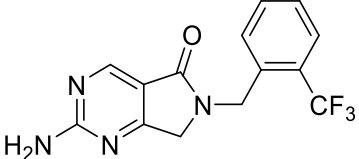
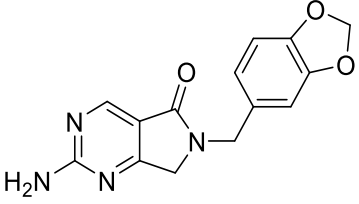
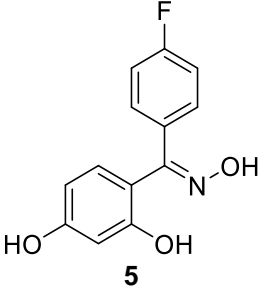
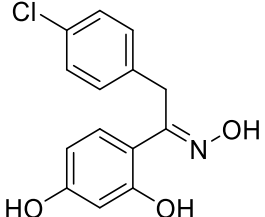
4.58

> 90

OCCCC1=NC2=CC=CC=C2N1CC3=CC=C
C(C(C)(C)C)C=C3

OSSK_286458

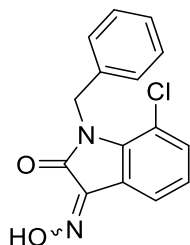
<p>104</p>	 <p>CC(C)CC1=NC2=CC=CC=C2N1CC3=CC=C(C)C=C3</p> <p>OSSK_286117</p>	<p>298.81</p>	<p>5.37</p>	<p>> 63</p>
<p>105</p>	 <p>COC(C=C1)=CC=C1CC2=NC3=CC=CC=C3N2CC(O)CO</p> <p>OSSK_356610</p>	<p>312.37</p>	<p>1.96</p>	<p>> 2000</p>
	 <p>4</p>			
Cmpd. No.	Structure, SMILES and supplier ID	MW	cLogP	IC ₅₀ (μM)
<p>8</p>	 <p>CC1=C(NC2=NC(C3=C(C)N=C(C)S3)=CS2)C=CC=C1Cl</p> <p>OSSK_523229</p>	<p>335.87</p>	<p>4.82</p>	<p>92 ± 17</p>

<p>106</p>	 <p><chem>O=C1N(CCC2=CC=CC=C2F)CC3=NC(NC)=NC=C31</chem></p> <p>OSSL_317963</p>	<p>286.31</p>	<p>1.49</p>	<p>> 340</p>
<p>107</p>	 <p><chem>NC1=NC=C2C(CN(CC3=C(C(F)(F)F)C=C3)C2=O)=N1</chem></p> <p>OSSL_317988</p>	<p>308.26</p>	<p>1.63</p>	<p>> 380</p>
<p>108</p>	 <p><chem>NC1=NC=C2C(CN(CC3=CC(OCO4)=C4C=C3)C2=O)=N1</chem></p> <p>OSSL_318222</p>	<p>284.28</p>	<p>0.38</p>	<p>> 260</p>
	 <p>5</p>			
Cmpd. No.	Structure, SMILES and supplier ID	MW	cLogP	IC ₅₀ (μM)
<p>9</p>		<p>277.70</p>	<p>3.37</p>	<p>44 ± 8</p>

OC1=CC=C(/C(CC2=CC=C(Cl)C=C2)=N/
O)C(O)=C1

OSSK_862931

109



286.72

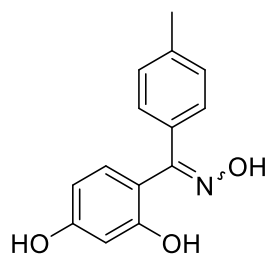
3.15

165 ± 21

O=C(/C1=NO)N(CC2=CC=CC=C2)C3=C
1C=CC=C3Cl

OSSL_327325

110



243.26

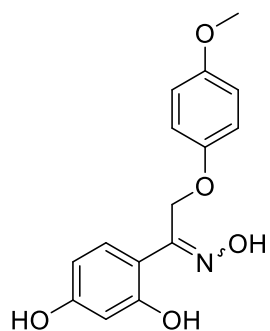
3.35

> 1000

O/N=C(C1=CC=C(C)C=C1)/C2=CC=C(O)
C=C2O

OSSL_151910

111



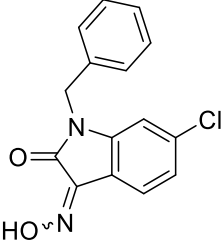
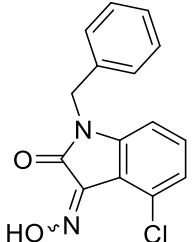
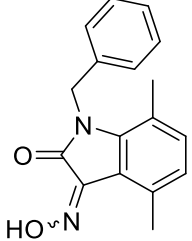
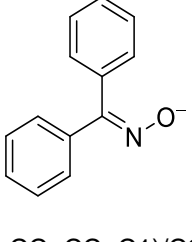
289.29

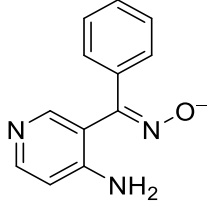
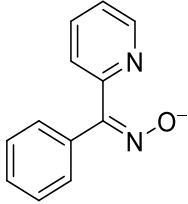
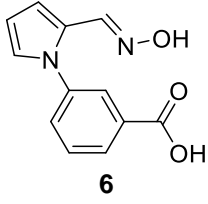
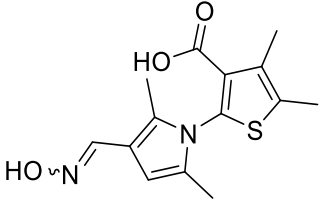
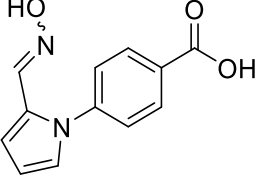
2.29

> 300

O/N=C(COC1=CC=C(OC)C=C1)/C2=CC
=C(O)C=C2O

OSSL_151915

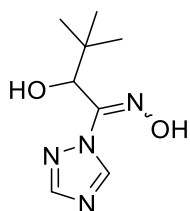
<p>112</p>	 <p><chem>ClC1=CC(N(CC2=CC=CC=C2)C(=O)N)C=C1</chem></p> <p>OSSL_327230</p>	<p>286.72</p>	<p>3.15</p>	<p>> 900</p>
<p>113</p>	 <p><chem>O=C(/C1=NO)N(CC2=CC=CC=C2)C3=C1C(Cl)=CC=C3</chem></p> <p>OSSL_327325</p>	<p>286.72</p>	<p>3.15</p>	<p>> 30</p>
<p>114</p>	 <p><chem>O=C(/C1=NO)N(CC2=CC=CC=C2)C3=C1C(C)=CC=C3</chem></p> <p>OSSL_328145</p>	<p>280.33</p>	<p>3.58</p>	<p>> 60</p>
<p>115</p>	 <p><chem>[O-]N=C(C1=CC=CC=C1)/C2=CC=CC=C2</chem></p> <p>OSSL_379701</p>	<p>196.23</p>	<p>3.44</p>	<p>> 500</p>

<p>116</p>	 <p>[O-]/N=C(C1=CC=CC=C1)/C2=CN=CC=C 2N OSSL_302816</p>	<p>212.23</p>	<p>1.40</p>	<p>> 2000</p>
<p>117</p>	 <p>[O-]/N=C(C1=NC=CC=C1)/C2=CC=CC=C 2 OSSL_750176</p>	<p>197.22</p>	<p>2.61</p>	<p>> 500</p>
 <p>6</p>				
Cmpd. No.	Structure, SMILES and supplier ID	MW	cLogP	IC ₅₀ (μM)
<p>118</p>	 <p>CC1=C(/C=N/O)C=C(C)N1C2=C(C(O)=O))C(C)=C(C)S2 OSSK_632565</p>	<p>292.35</p>	<p>3.82</p>	<p>> 800</p>
<p>119</p>		<p>230.22</p>	<p>2.23</p>	<p>> 500</p>

OC(C1=CC=C(N2C(/C=N/O)=CC=C2)C=C1)=O

OSSK_632073

120



198.23

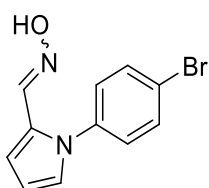
0.82

> 200

OC(C(C)(C)C)/C(N1C=NC=N1)=N/O

OSSL_128671

121



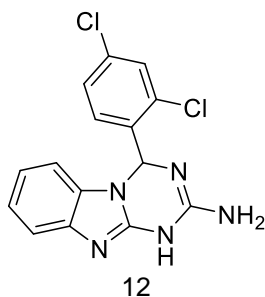
265.11

3.35

> 200

BrC1=CC=C(N2C(/C=N/O)=CC=C2)C=C1

OSSK_777326



Cmpd. No.

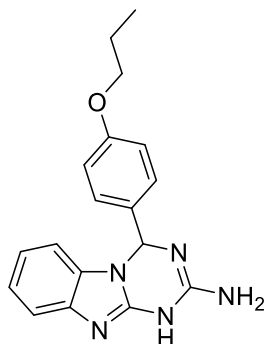
Structure, SMILES and supplier ID

MW

cLogP

IC₅₀ (μM)

122



321.38

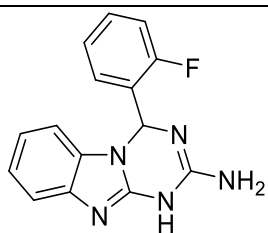
3.97

> 50

NC1=NC(C2=CC=C(OCCC)C=C2)N3C(N1)=NC4=CC=CC=C34

OSSK_784042

123



281.29

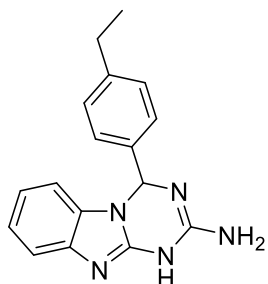
2.94

> 120

NC1=NC(C2=CC=CC=C2F)N3C(N1)=NC4=CC=CC=C34

OSSK_676133

124



291.36

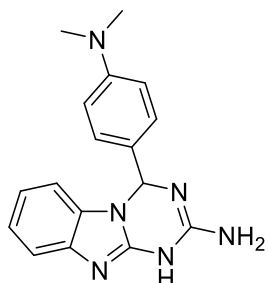
4.20

> 30

NC1=NC(C2=CC=C(CC)C=C2)N3C(N1)=NC4=CC=CC=C34

OSSK_676805

125



306.37

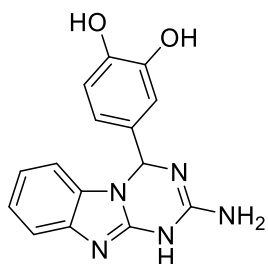
2.90

> 200

NC1=NC(C2=CC=C(N(C)C)C=C2)N3C(N1)=NC4=CC=CC=C34

OSSK_676809

126



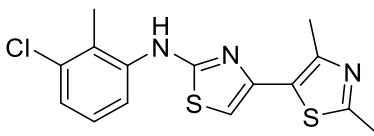
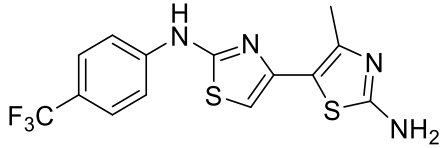
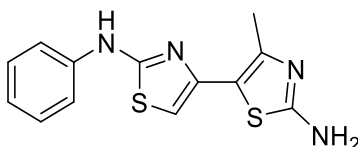
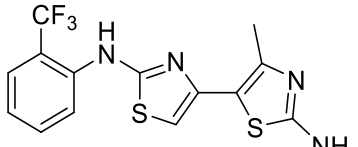
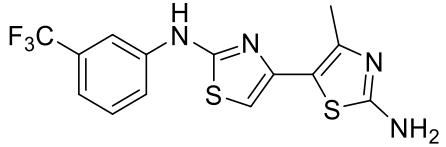
295.30

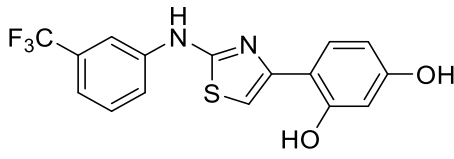
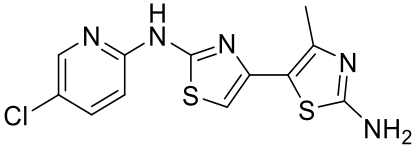
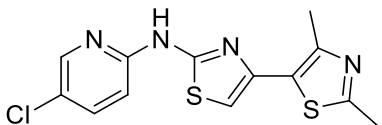
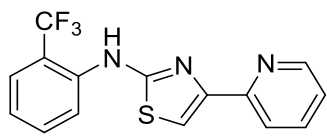
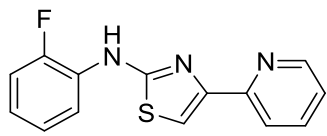
2.19

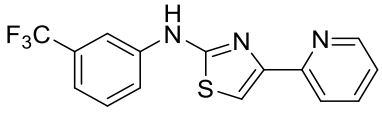
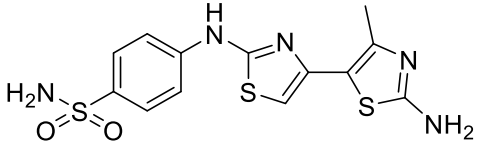
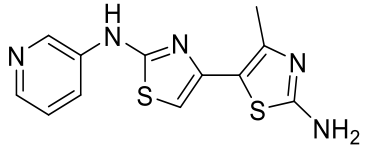
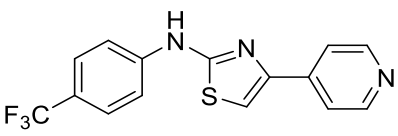
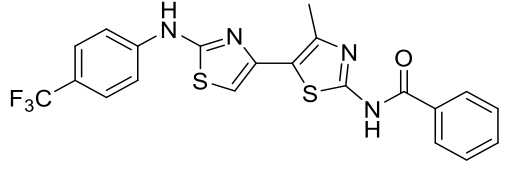
> 160

NC1=NC(C2=CC=C(O)C(O)=C2)N3C(N1)=NC4=CC=CC=C34

Table S3: Structures, SMILES codes and supplier ID of hits from the third round of LBVS.

Cmpd. No.	Structure, SMILES and supplier ID	MW	cLogP	IC ₅₀ (μM)
	 <p style="text-align: center;">8</p>			
10	 <p style="text-align: center;"> <chem>CC1=C(SC(N)=N1)C2=CSC(NC3=CC=C(C(F)(F)F)C=C3)=N2</chem> OSSL_650294 </p>	356.39	4.31	32 ± 3
26	 <p style="text-align: center;"> <chem>CC1=C(SC(N)=N1)C2=CSC(NC3=CC=C(C=C3)=N2</chem> OSSK_672441 </p>	288.39	3.43	> 120
27	 <p style="text-align: center;"> <chem>CC1=C(SC(N)=N1)C2=CSC(NC3=C(C(F)(F)F)C=CC3)=N2</chem> OSSL_648433 </p>	356.39	4.31	45 ± 4
28		356.39	4.31	56 ± 9

	<chem>CC1=C(SC(N)=N1)C2=CSC(NC3=CC(C(F)(F)F)=CC=C3)=N2</chem> OSSK_523240			
29	 <chem>OC(C=C(O)C=C1)=C1C2=CSC(NC3=CC(C(F)(F)F)=CC=C3)=N2</chem> OSSK_137545	352.33	5.06	48 ± 9
30	 <chem>CC1=C(SC(N)=N1)C2=CSC(NC3=NC=C(Cl)C=C3)=N2</chem> OSSL_648436	323.82	3.41	54 ± 7
31	 <chem>CC1=C(SC(C)=N1)C2=CSC(NC3=NC=C(Cl)C=C3)=N2</chem> OSSL_631964	322.83	3.68	> 500
127	 <chem>FC1=C(NC2=NC(C3=CC=CC=N3)=CS2)C=CC=C1(F)F</chem> OSSL_648411	321.32	4.84	86 ± 5
128	 <chem>FC1=C(NC2=NC(C3=CC=CC=N3)=CS2)C=CC=C1</chem>	271.31	4.10	100 ± 27

OSSL_648413				
129		321.32	4.84	168 ± 18
	<chem>FC(C1=CC=CC(NC2=NC(C3=CC=CC=N3)=CS2)=C1)(F)F</chem>			
OSSL_648412				
130		367.46	2.04	315 ± 47
	<chem>CC1=C(SC(N)=N1)C2=CSC(NC3=CC=C(S(N)(=O)=O)C=C3)=N2</chem>			
OSSK_320567				
131		289.38	2.21	377 ± 102
	<chem>CC1=C(SC(N)=N1)C2=CSC(NC3=CN=C(C=C3)=N2</chem>			
OSSL_648437				
132		321.32	4.45	> 60
	<chem>FC(C1=CC=C(NC2=NC(C3=CC=NC=C3)=CS2)C=C1)(F)F</chem>			
OSSL_648422				
133		460.49	6.23	> 120
	<chem>CC1=C(SC(NC(C2=CC=CC=C2)=O)=N1)C3=CSC(NC4=CC=C(C(F)(F)F)C=C4)=N3</chem>			
OSSK_630272				

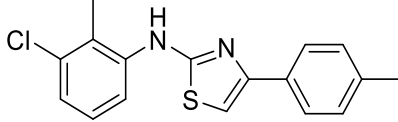
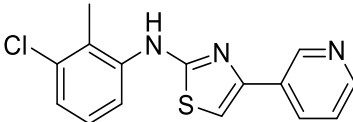
	134	<chem>CC1=C(NC2=NC(C3=CC=C(C)C=C3)=CS2)C=CC=C1Cl</chem>	314.83	6.42	> 16
OSSL_960616					
	135	<chem>CC1=C(NC2=NC(C3=CC=CN=C3)=CS2)C=CC=C1Cl</chem>	301.79	4.69	> 200
OSSK_523203					

Table S4: Toxicity of **9** and **10** on zebrafish larvae.

Cmpd. No.	Conc. [μM]	24 h (2 dpf)	48 h (3 dpf)	72 h (4 dpf)	96 h (5 dpf)
9	100	5	2	0	0
	30	10	10	10	10
	10	10	10	10	10
	2	10	10	10	10
10	100	0	0	0	0
	30	2	0	0	0
	10	10	10	10	10
	2	10	10	10	10
DMSO	1 %	10	10	10	10
Danieau's	-	10	10	10	10

Fish line: TLF. Incubation with compounds started at 1 dpf. Visual screening (microscopy) daily until 5 dpf. 10 larvae per condition. The number of living zebrafish larvae is given. Dpf, days post fertilization.

Table S5: MIC values for final hits against *E. coli* TolC strain.

Cmpd. No.	7	9	10
MIC [μM]	22.0 ± 1.0	21.9 ± 1.3	22.2 ± 3.1

Table S6: Frequency-of-resistance development of **10** and selected antibiotics (rifampicin, chloramphenicol and ciprofloxacin) at 4x and 2x MIC.

Cmpd.	4x MIC	2x MIC
10	$< 8.7 * 10^{-10}$	$3.3 * 10^{-9}$
Rif	$1.7 * 10^{-9}$	$3.8 * 10^{-9}$
Cam	$< 8.7 * 10^{-10}$	$2.9 * 10^{-10}$
Cip	$1.7 * 10^{-9}$	$7.5 * 10^{-9}$

Rif, Rifampicin; Cam, Chloramphenicol; Cip, Ciprofloxacin.