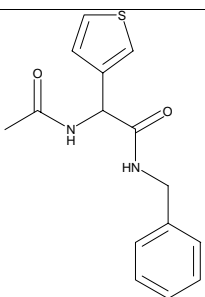
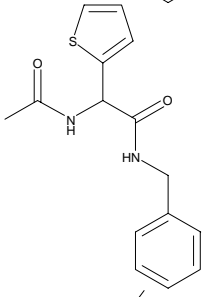
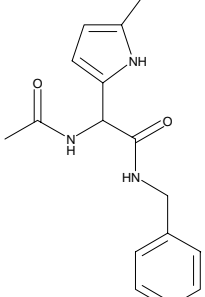
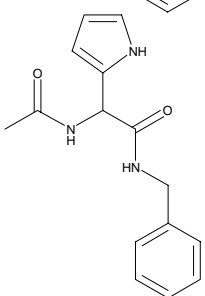
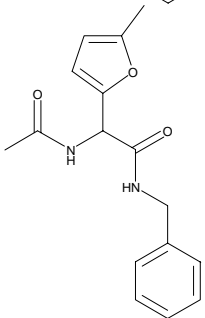
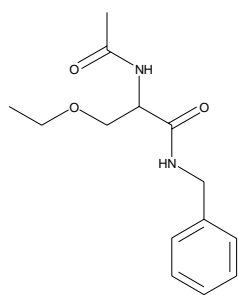


Supporting Information.

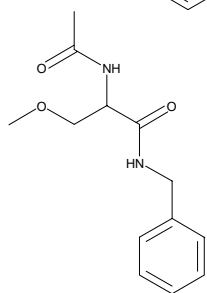
I. 48 anticonvulsant structure and their ED₅₀ used in ALL-QSAR modeling¹²

Structure	Compound Name	Activity log(umol/kg)
	93	2.48
	92	2.19
	90	2.11
	89	1.77
	88	1.83



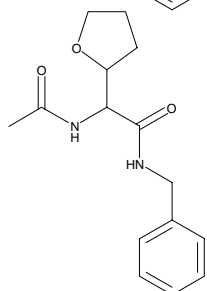
74

1.81



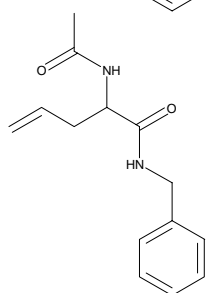
73

1.52



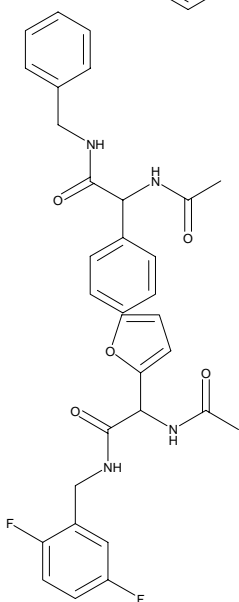
68

2.27



67

2.16

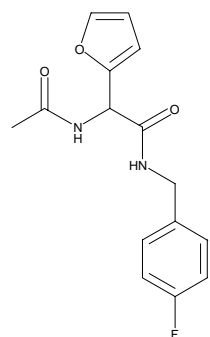


37

2.06

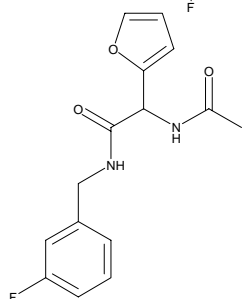
31

1.89



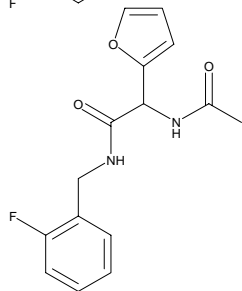
30

1.64



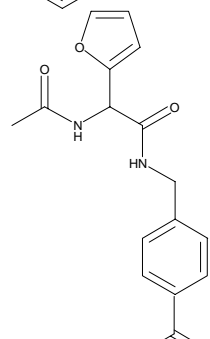
29

1.66



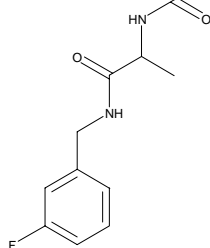
28

2.14



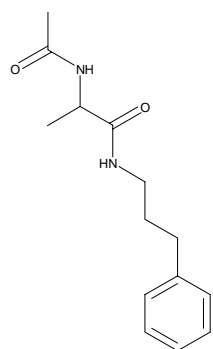
27

1.58



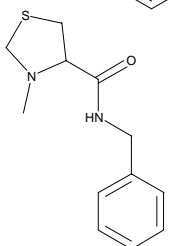
24

2.51



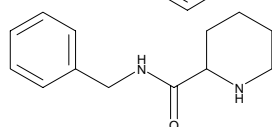
21

2.55



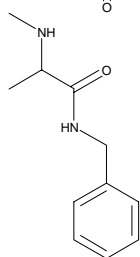
192

2.09



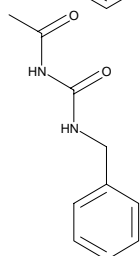
191

2.39



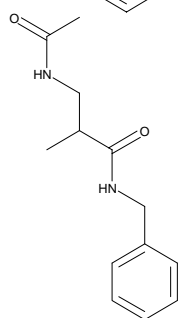
189

2.21



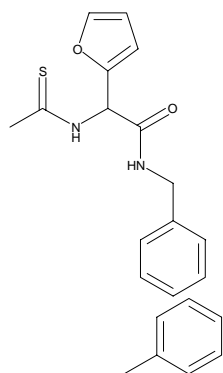
188

2.50



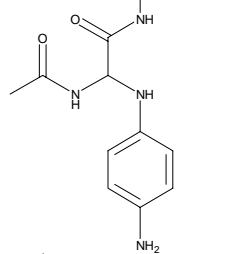
183

3.06



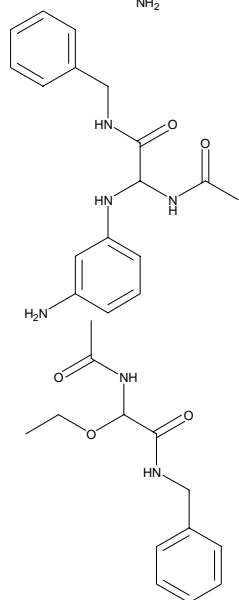
172

1.80



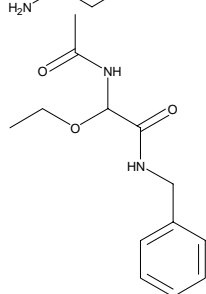
170

2.75



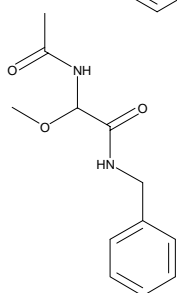
169

2.50



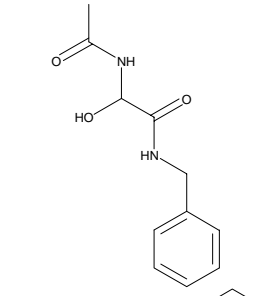
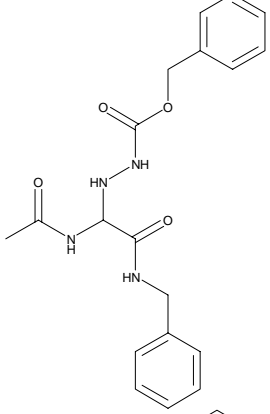
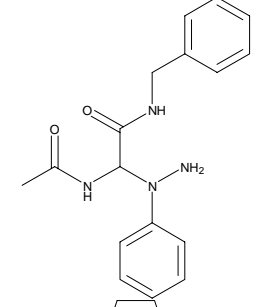
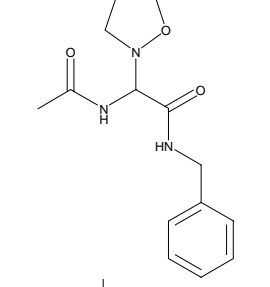
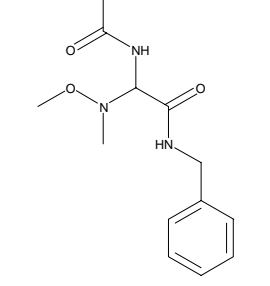
159

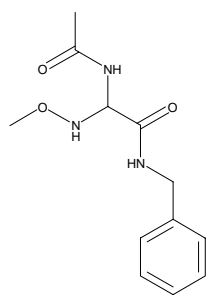
2.39



158

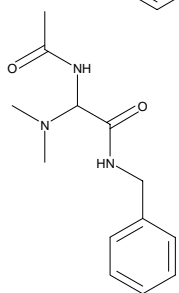
2.62

	157	2.56
	145	2.18
	144	2.14
	142	2.05
	141	1.40



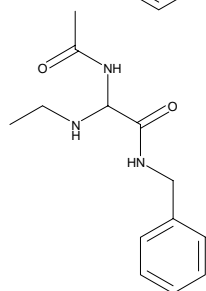
139

1.39



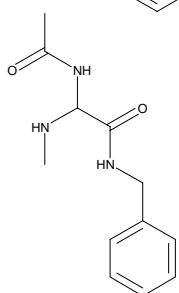
125

2.26



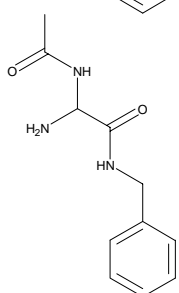
124

2.23



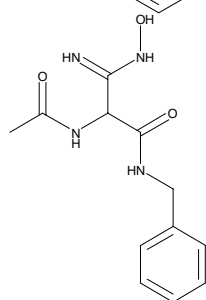
123

2.28



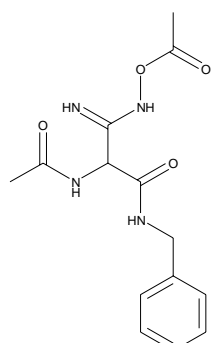
122

2.47



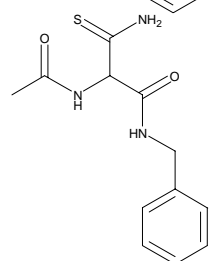
120

2.63



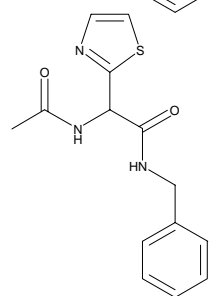
119

2.66



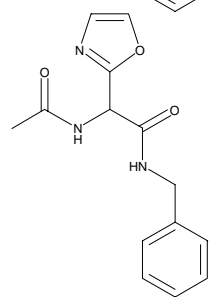
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2.51



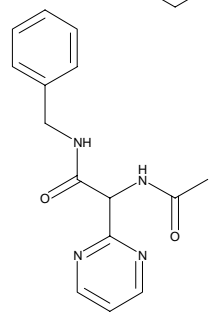
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1.62



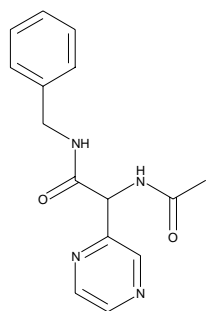
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1.58



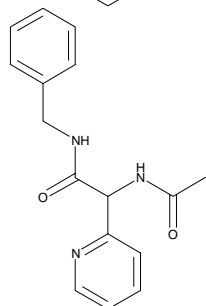
111

1.45



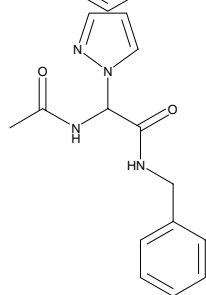
110

1.72



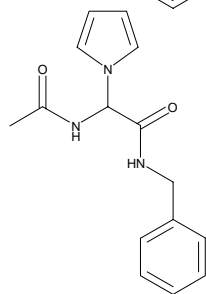
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1.58



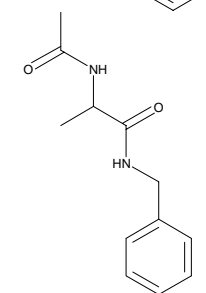
104

1.78



103

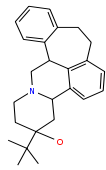
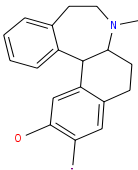
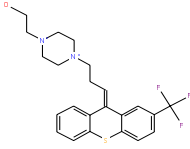
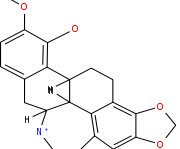
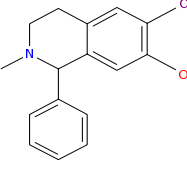
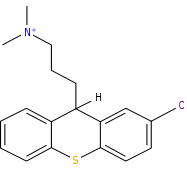
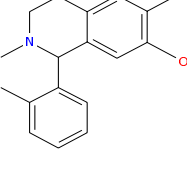
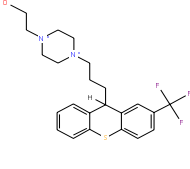
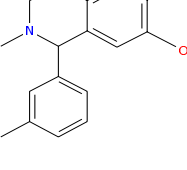
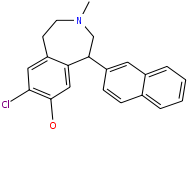
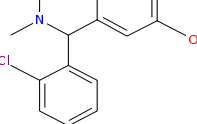
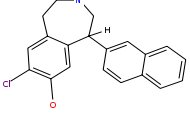
2.47



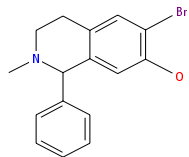
1

2.54

II. 48 D1 antagonist chemical structure and their competitive binding affinities used in ALL-QSAR modeling¹¹

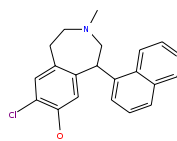
ANT01	Structure	-Log(K _i)	ANT29	Structure	-Log(K _i)
		9			5.96
ANT02		7.97	BUIBOCAPNINE		5.36
ANT03		8.28	CHLORPROMAZINE		4.1
ANT04		8.43	FLUPHELAZINE		4.95
ANT05		8.38	NNC01-0004		5.85
ANT07		8.43	NNC01-0012		4.69

ANT08



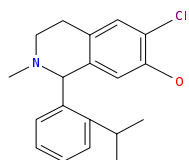
7.97

NIC01-6035



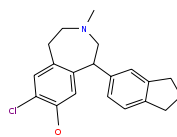
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ANT09



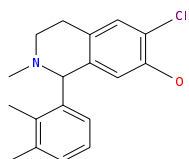
8.56

NIC01-6059



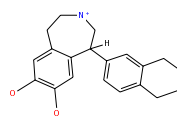
6.52

ANT10



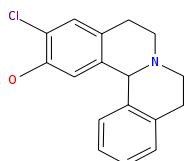
8

NIC01-6127



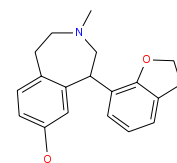
3.88

ANT12



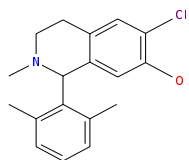
5.68

NIC01-6534



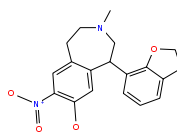
5.69

ANT14



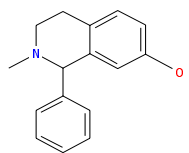
8.43

NIC01-6687



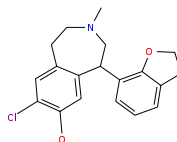
5

ANT15



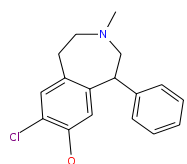
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NIC01-6756



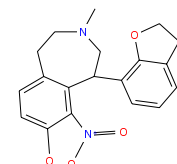
6.69

ANT16



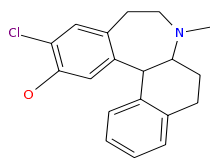
9.4

NIC01-6787



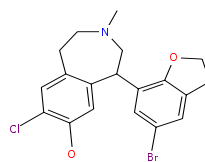
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ANT17



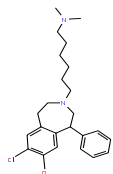
8.3

NNC02-0010



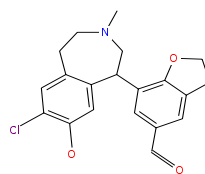
6

ANT18



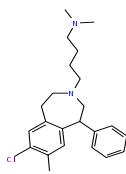
6.94

NNC22-0004



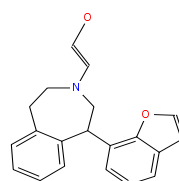
4.76

ANT19



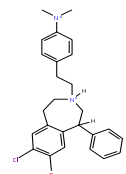
6.86

NNC22-0101



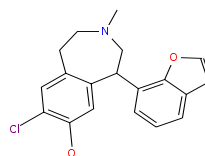
4.46

ANT20



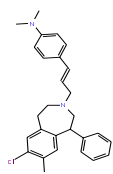
7.43

NNC22-0112



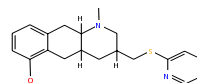
6.74

ANT21



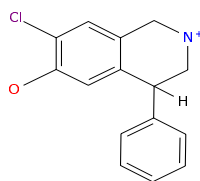
7.54

S02_G1C_756



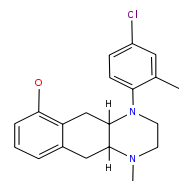
5.95

ANT22



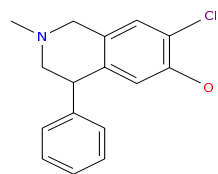
6.55

S02_P5D_958



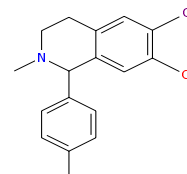
9.8

ANT23



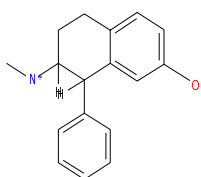
7.06

ANT06



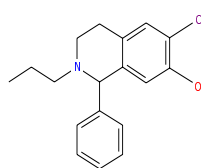
8.28

ANT24



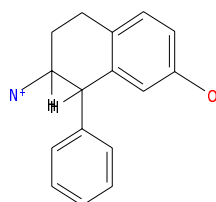
5.46

ANT11



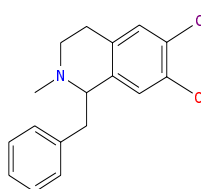
7.05

ANT25



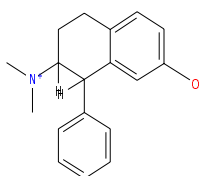
5.53

ANT13



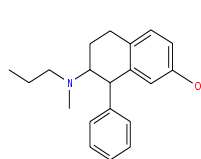
7.24

ANT26



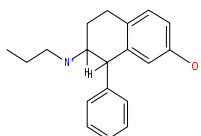
5.85

ANT28



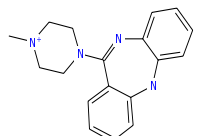
5.82

ANT27



6.02

CLOZAPINE



4.8

III. Predicted and actual ED₅₀ for 9 anticonvulsant agents in the test set (for Figure 6).

Compound Name	Actual ED ₅₀ (log(umol/kg))	Predicted ED ₅₀ (log(umol/kg))
108	1.58	1.78
92	2.19	2.27
104	1.78	1.65
21	2.55	2.67
112	1.58	1.47
110	1.72	1.53
90	2.11	1.93
172	1.80	1.73
122	2.47	2.43

IV. Predicted and actual ED₅₀ for 14 anticonvulsant agents in the test set (for Figure 7).

Compound Name	Actual ED ₅₀ (log(umol/kg))	Predicted ED ₅₀ (log(umol/kg))
24	2.51	2.48
108	1.58	1.76
123	2.28	2.29
68	2.27	1.99
89	1.77	1.59
67	2.16	2.37
112	1.58	1.30
125	2.26	2.49
111	1.45	1.35
169	2.50	2.51
90	2.11	1.97
29	1.66	1.93
103	2.47	2.18
31	1.89	2.02

V. Predicted and actual pK_i for 11 D₁ antagonists in the test set (for Figure 9).

Compound Name	Actual pK_i (-logM)	Predicted pK_i (-logM)
ant20	7.43	7.41
ant07	8.43	9.22
ant26	5.85	6.20
ant05	8.38	8.97
NNC01-0035	4.48	4.57
ant14	8.43	8.46
ant06	8.28	8.76
NNC02-0010	6	6.23
ant28	5.82	5.96
NNC01-0756	6.69	6.32
ant12	5.68	5.66

VI. Predicted and actual pK_i for 14 D₁ antagonists in the test set (for Figure 10).

Compound Name	Actual pK_i (-logM)	Predicted pK_i (-logM)
ant20	7.43	7.15
ant26	5.85	5.77
ant08	7.97	Not predicted
ant13	7.24	6.86
ant05	8.38	8.90
NNC01-0035	4.48	5.03
ant14	8.43	8.68
ant21	7.54	7.41
NNC01-0127	3.88	Not predicted
ant06	8.28	8.52
NNC02-0010	6	5.62
ant10	8	9.08
ant03	8.28	8.01
NNC01-0012	4.69	5.32
ant15	6.37	5.33
ant24	5.46	5.56

VII. Predicted and actual IGC₅₀ for 45 phenols in the external set (for Figure 11).

CAS Number	Actual -logIGC₅₀	Predicted -logIGC₅₀	CAS Number	Actual -logIGC₅₀	Predicted -logIGC₅₀	CAS Number	Actual -logIGC₅₀	Predicted -logIGC₅₀
620-24-6	-1.043	-0.642	6627-55-0	0.599	0.468	488-17-5	0.28	0.259
498-00-0	-0.7	-1.030	367-27-1	0.604	0.629	615-67-8	1.262	1.332
106-44-5	-0.184	-0.314	122-94-1	0.701	1.082	608-43-5	1.413	1.849
498-02-2	-0.12	0.038	35421-08-0	0.796	1.023	573-56-8	0.539	0.886
371-41-5	0.017	0.567	527-54-8	0.932	0.423	609-89-2	1.745	1.865
105-67-9	0.07	-0.046	99-71-8	0.979	0.484	935-95-5	2.222	2.348
99-76-3	0.084	-0.488	90-43-7	1.094	1.533	119-33-5	0.571	0.809
108-68-9	0.113	0.098	583-78-8	1.125	1.172	446-36-6	1.125	1.013
95-65-8	0.122	0.130	591-20-8	1.145	1.044	100-02-7	1.42	1.402
123-07-9	0.205	0.041	7463-51-6	1.268	1.176	150-19-6	-0.326	-0.233
2416-94-6	0.277	0.220	7530-27-0	1.276	1.510	70-70-2	0.053	-0.256
1450-72-2	0.31	0.209	95-77-2	1.745	1.459	95-88-5	0.125	0.294
615-74-7	0.393	0.328	128-37-0	1.796	2.062	645-56-7	0.643	0.512
106-48-9	0.545	0.683	13037-86-0	2.033	2.079	576-24-9	1.276	0.860
120-47-8	0.573	0.487	933-78-8	2.373	2.343	95-71-6	1.858	1.624

VIII. Predicted and actual $-\log(\text{IGC}_{50})$ for 50 phenols in the external set (for Figure 12).

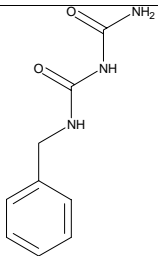
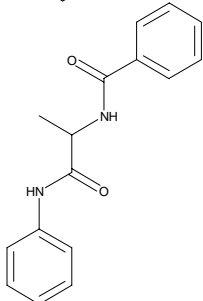
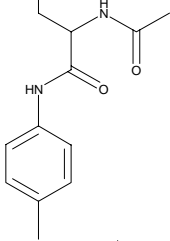
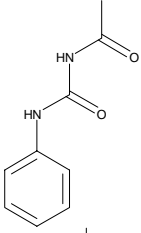
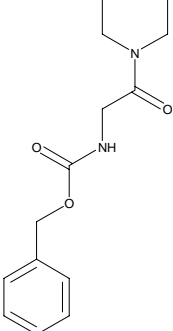
CAS Number	Actual $-\log\text{IGC}_{50}$	Predicted $-\log\text{IGC}_{50}$	CAS Number	Actual $-\log\text{IGC}_{50}$	Predicted $-\log\text{IGC}_{50}$
4383-06--6	-0.99	-0.699	1138-52-9	1.638	1.876
619-57-8	-0.78	-1.138	2631-77-8	2.34	1.569
95-48-7	-0.295	-0.203	591-27-5	-0.524	-0.516
106-44-5	-0.184	-0.212	123-30-8	-0.076	NP
498-02-2	-0.12	0.056	87-66-1	0.85	NP
19438-10-9	-0.046	0.413	608-43-5	1.413	1.459
121-33-5	-0.03	-0.167	1198-55-6	1.697	2.432
4421-08--3	-0.03	0.120	87-87-6	2.109	2.275
371-41-5	0.017	0.205	329-71-5	0.95	0.779
582-24-1	0.078	-0.294	42454-06-8	0.33	0.321
99-76-3	0.084	-0.144	119-33-5	0.571	0.872
526-75-0	0.122	0.113	104-91-6	0.654	0.694
936-02-7	0.181	0.007	601-89-8	0.658	0.321
875-59-2	0.19	-0.551	3316-09--4	1.17	0.917
123-07-9	0.205	0.314	394-33-2	1.3838	1.388
7781-98-8	0.478	0.187	89-64-5	2.053	2.286
367-27-1	0.604	0.862	5471-51-2	-0.4974	-0.699
618-45-1	0.612	0.532	103-16-2	1.038	1.498
97-54-1	0.75	0.280	95-86-3	0.127	NP
1137-42-4	1.024	1.219	700-13-0	1.342	1.443
2491-32-9	1.0691	1.569	95-71-6	1.858	1.423
88-04-0	1.201	1.090	769-39-1	1.167	1.460
7530-27-0	1.276	1.627	88-75-5	0.67	1.058
28994-41-4	1.311	1.370	394-41-2	0.935	0.891
90-60-8	1.55	1.157	88-30-2	1.652	NP

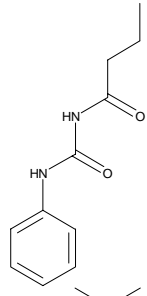
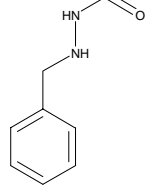
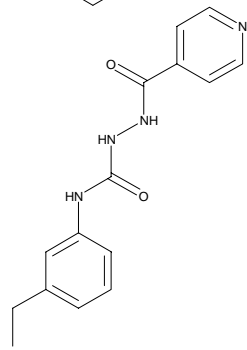
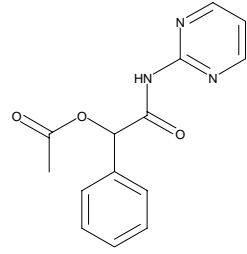
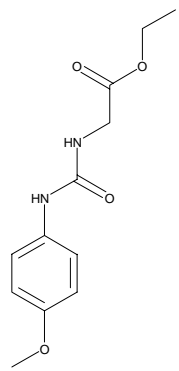
NP: not predicted

IX. Some Structures Obtained from ALL-QSAR Screening of NCI.

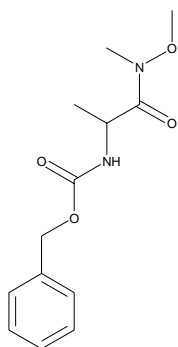
Black: Structures overlapped with previous mining using *k*NN

Blue: Missed from previous mining using *k*NN¹²

ID	Structure	Cmpd Name	Mol Weight	ALL-QSAR prediction log(umol/kg)	ALL-QSAR Prediction (mg/kg)	<i>k</i> NN prediction (mg/kg)
13		28653	193.21	1.18	2.90	45.4
20		43159	268.32	1.97	25.01	28.3
21		43160	296.37	2.27	54.55	31.8
27		60262	178.19	2.33	38.26	38
39		125635	264.32	2.09	32.23	17

40		131980	206.24	2.22	34.11	55.8
42		137956	193.25	2.39	47.68	24.7
60		241640	284.32	1.36	6.53	20
71		527069	271.27	1.41	6.94	16.9
Missed		216931	252.27			18.4

Missed



655432 266.30

12.1
