

QSAR modeling of toxicity of chemical mixtures

Supplementary repository of the thesis

Submitted by-

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Table 1. Training-Test division for mixtures-out cross-validation mentioned in “3.2.6. *Cross-validation*” section in the thesis

Mixture No.	Components in Mixture	Mass Ratio	Log 1/EC50 (mol/l)
51	Chlorobenzene (#1) + Bromobenzene(#3)	2:1	3.73
52	Chlorobenzene (#1) + Bromobenzene(#3)	1:1	3.67
53	Chlorobenzene (#1) + Bromobenzene(#3)	1:2	3.76
54*	Chlorobenzene (#1) + 1,2,3-Trichlorobenzene (#2)	2:1	3.89
55*	Chlorobenzene (#1) + 1,2,3-Trichlorobenzene (#2)	1:1	3.85
56*	Chlorobenzene (#1) + 1,2,3-Trichlorobenzene (#2)	1:2	4.21
57	Chlorobenzene (#1) + 1-Bromo-2,3-dichlorobenzene (#4)	2:1	3.9
58	Chlorobenzene (#1) + 1-Bromo-2,3-dichlorobenzene (#4)	1:1	3.74
59	Chlorobenzene (#1) + 1-Bromo-2,3-dichlorobenzene (#4)	1:2	4.07
60*	Bromobenzene (#3) + 1,2,3-Trichlorobenzene (#2)	2:1	4.06
61*	Bromobenzene (#3) + 1,2,3-Trichlorobenzene (#2)	1:1	3.98
62*	Bromobenzene (#3) + 1,2,3-Trichlorobenzene (#2)	1:2	4.19
63	Bromobenzene (#3) + 1-Bromo-2,3-dichlorobenzene (#4)	2:1	4.04
64	Bromobenzene (#3) + 1-Bromo-2,3-dichlorobenzene (#4)	1:1	3.95
65	Bromobenzene (#3) + 1-Bromo-2,3-dichlorobenzene (#4)	1:2	4.18
66	1,2,3-Trichlorobenzene (#2) + 1-Bromo-2,3-dichlorobenzene (#4)	2:1	4.7
67	1,2,3-Trichlorobenzene (#2) + 1-Bromo-2,3-dichlorobenzene (#4)	1:1	4.76
68	1,2,3-Trichlorobenzene (#2) + 1-Bromo-2,3-dichlorobenzene (#4)	1:2	4.7
69	Chlorobenzene (#1) + Phenol (#5)	2:1	3.2

70	Chlorobenzene (#1) + Phenol (#5)	1:1	3.03
71	Chlorobenzene (#1) + Phenol (#5)	1:2	2.91
72	Chlorobenzene (#1) + 2,4-Dichlorophenol (#6)	2:1	3.57
73	Chlorobenzene (#1) + 2,4-Dichlorophenol (#6)	1:1	3.42
74	Chlorobenzene (#1) + 2,4-Dichlorophenol (#6)	1:2	3.68
75*	Chlorobenzene (#1) + Aniline (#7)	2:1	2.45
76*	Chlorobenzene (#1) + Aniline (#7)	1:1	2.45
77*	Chlorobenzene (#1) + Aniline (#7)	1:2	2.22
78	Chlorobenzene (#1) + 3,4-Dichloroaniline (#8)	2:1	3.52
79	Chlorobenzene (#1) + 3,4-Dichloroaniline (#8)	1:1	3.67
80	Chlorobenzene (#1) + 3,4-Dichloroaniline (#8)	1:2	3.81
81	Bromobenzene (#3) + Phenol (#5)	2:1	3.17
82	Bromobenzene (#3) + Phenol (#5)	1:1	3.28
83	Bromobenzene (#3) + Phenol (#5)	1:2	3.07
84*	Bromobenzene (#3) + 2,4-Dichlorophenol (#6)	2:1	3.8
85*	Bromobenzene (#3) + 2,4-Dichlorophenol (#6)	1:1	3.77
86*	Bromobenzene (#3) + 2,4-Dichlorophenol (#6)	1:2	3.82
87	Bromobenzene (#3) + Aniline (#7)	2:1	2.63
88	Bromobenzene (#3) + Aniline (#7)	1:1	2.68
89	Bromobenzene (#3) + Aniline (#7)	1:2	2.38
90	Bromobenzene (#3) + 3,4-Dichloroaniline (#8)	2:1	2.91
91	Bromobenzene (#3) + 3,4-Dichloroaniline (#8)	1:1	3.87
92	Bromobenzene (#3) + 3,4-Dichloroaniline (#8)	1:2	4.04
93*	1,2,3-Trichlorobenzene (#2) + Phenol (#5)	2:1	3.05
94*	1,2,3-Trichlorobenzene (#2) + Phenol (#5)	1:1	3.39
95*	1,2,3-Trichlorobenzene (#2) + Phenol (#5)	1:2	2.98
96	1,2,3-Trichlorobenzene (#2) + 2,4-Dichlorophenol (#6)	2:1	4.41
97	1,2,3-Trichlorobenzene (#2) + 2,4-Dichlorophenol (#6)	1:1	4.27

98	1,2,3-Trichlorobenzene (#2) + 2,4-Dichlorophenol (#6)	1:2	4.21
99	1,2,3-Trichlorobenzene (#2) + Aniline (#7)	2:1	2.39
100	1,2,3-Trichlorobenzene (#2) + Aniline (#7)	1:1	2.63
101	1,2,3-Trichlorobenzene (#2) + Aniline (#7)	1:2	2.45
102	1,2,3-Trichlorobenzene (#2) + 3,4-Dichloroaniline (#8)	2:1	4.1
103	1,2,3-Trichlorobenzene (#2) + 3,4-Dichloroaniline (#8)	1:1	4.29
104	1,2,3-Trichlorobenzene (#2) + 3,4-Dichloroaniline (#8)	1:2	4.15
105	1-Bromo-2,3-dichlorobenzene (#4) + Phenol (#5)	2:1	3.32
106	1-Bromo-2,3-dichlorobenzene (#4) + Phenol (#5)	1:1	3.42
107	1-Bromo-2,3-dichlorobenzene (#4) + Phenol (#5)	1:2	3.12
108	1-Bromo-2,3-dichlorobenzene (#4) + 2,4-Dichlorophenol (#6)	2:1	4.61
109	1-Bromo-2,3-dichlorobenzene (#4) + 2,4-Dichlorophenol (#6)	1:1	4.66
110	1-Bromo-2,3-dichlorobenzene (#4) + 2,4-Dichlorophenol (#6)	1:2	4.53
111	1-Bromo-2,3-dichlorobenzene (#4) + Aniline (#7)	2:1	2.56
112	1-Bromo-2,3-dichlorobenzene (#4) + Aniline (#7)	1:1	2.91
113	1-Bromo-2,3-dichlorobenzene (#4) + Aniline (#7)	1:2	2.57
114*	1-Bromo-2,3-dichlorobenzene (#4) + 3,4-Dichloroaniline (#8)	2:1	4.29
115*	1-Bromo-2,3-dichlorobenzene (#4) + 3,4-Dichloroaniline (#8)	1:1	4.52
116*	1-Bromo-2,3-dichlorobenzene (#4) + 3,4-Dichloroaniline (#8)	1:2	4.32
117*	Phenol (#5) + 2,4-Dichlorophenol (#6)	2:1	3.22
118*	Phenol (#5) + 2,4-Dichlorophenol (#6)	1:1	3.11

119*	Phenol (#5) + 2,4-Dichlorophenol (#6)	1:2	3.29
120	Phenol (#5) + Aniline (#7)	2:1	2.18
121	Phenol (#5) + Aniline (#7)	1:1	2.5
122	Phenol (#5) + Aniline (#7)	1:2	2.33
123	Phenol (#5) + 3,4-Dichloroaniline (#8)	2:1	3.37
124	Phenol (#5) + 3,4-Dichloroaniline (#8)	1:1	3.16
125	Phenol (#5) + 3,4-Dichloroaniline (#8)	1:2	3.54
126	2,4-Dichlorophenol (#6) + Aniline (#7)	2:1	2.43
127	2,4-Dichlorophenol (#6) + Aniline (#7)	1:1	2.6
128	2,4-Dichlorophenol (#6) + Aniline (#7)	1:2	2.61
129*	2,4-Dichlorophenol (#6) + 3,4-Dichloroaniline (#8)	2:1	4.17
130*	2,4-Dichlorophenol (#6) + 3,4-Dichloroaniline (#8)	1:1	4.44
131*	2,4-Dichlorophenol (#6) + 3,4-Dichloroaniline (#8)	1:2	4.23
132	Aniline (#7) + 3,4-Dichloroaniline (#8)	2:1	2.55
133	Aniline (#7) + 3,4-Dichloroaniline (#8)	1:1	2.5
134	Aniline (#7) + 3,4-Dichloroaniline (#8)	1:2	2.71

*Test set mixtures; #Serial number of component

Table 2. Training-Test division for compounds-out cross-validation mentioned in “3.2.6. *Cross-validation*” section in the thesis

Mixture No.	Components in Mixture	Mass ratio	Log 1/EC50 (mol/l)
51	Chlorobenzene (#1) + Bromobenzene(#3)	2:1	3.73
52	Chlorobenzene (#1) + Bromobenzene(#3)	1:1	3.67
53	Chlorobenzene (#1) + Bromobenzene(#3)	1:2	3.76
54	Chlorobenzene (#1) + 1,2,3-Trichlorobenzene (#2)	2:1	3.89
55	Chlorobenzene (#1) + 1,2,3-Trichlorobenzene (#2)	1:1	3.85
56	Chlorobenzene (#1) + 1,2,3-Trichlorobenzene (#2)	1:2	4.21
57	Chlorobenzene (#1) + 1-Bromo-2,3-dichlorobenzene (#4)	2:1	3.9
58	Chlorobenzene (#1) + 1-Bromo-2,3-dichlorobenzene (#4)	1:1	3.74

59	Chlorobenzene (#1) + 1-Bromo-2,3-dichlorobenzene (#4)	1:2	4.07
60	Bromobenzene (#3) + 1,2,3-Trichlorobenzene (#2)	2:1	4.06
61	Bromobenzene (#3) + 1,2,3-Trichlorobenzene (#2)	1:1	3.98
62	Bromobenzene (#3) + 1,2,3-Trichlorobenzene (#2)	1:2	4.19
63	Bromobenzene (#3) + 1-Bromo-2,3-dichlorobenzene (#4)	2:1	4.04
64	Bromobenzene (#3) + 1-Bromo-2,3-dichlorobenzene (#4)	1:1	3.95
65	Bromobenzene (#3) + 1-Bromo-2,3-dichlorobenzene (#4)	1:2	4.18
66	1,2,3-Trichlorobenzene (#2) + 1-Bromo-2,3-dichlorobenzene (#4)	2:1	4.7
67	1,2,3-Trichlorobenzene (#2) + 1-Bromo-2,3-dichlorobenzene (#4)	1:1	4.76
68	1,2,3-Trichlorobenzene (#2) + 1-Bromo-2,3-dichlorobenzene (#4)	1:2	4.7
69*	Chlorobenzene (#1) + Phenol (#5)	2:1	3.2
70*	Chlorobenzene (#1) + Phenol (#5)	1:1	3.03
71*	Chlorobenzene (#1) + Phenol (#5)	1:2	2.91
72	Chlorobenzene (#1) + 2,4-Dichlorophenol (#6)	2:1	3.57
73	Chlorobenzene (#1) + 2,4-Dichlorophenol (#6)	1:1	3.42
74	Chlorobenzene (#1) + 2,4-Dichlorophenol (#6)	1:2	3.68
75	Chlorobenzene (#1) + Aniline (#7)	2:1	2.45
76	Chlorobenzene (#1) + Aniline (#7)	1:1	2.45
77	Chlorobenzene (#1) + Aniline (#7)	1:2	2.22
78	Chlorobenzene (#1) + 3,4-Dichloroaniline (#8)	2:1	3.52
79	Chlorobenzene (#1) + 3,4-Dichloroaniline (#8)	1:1	3.67
80	Chlorobenzene (#1) + 3,4-Dichloroaniline (#8)	1:2	3.81
81*	Bromobenzene (#3) + Phenol (#5)	2:1	3.17
82*	Bromobenzene (#3) + Phenol (#5)	1:1	3.28
83*	Bromobenzene (#3) + Phenol (#5)	1:2	3.07
84	Bromobenzene (#3) + 2,4-Dichlorophenol (#6)	2:1	3.8
85	Bromobenzene (#3) + 2,4-Dichlorophenol (#6)	1:1	3.77
86	Bromobenzene (#3) + 2,4-Dichlorophenol (#6)	1:2	3.82
87	Bromobenzene (#3) + Aniline (#7)	2:1	2.63
88	Bromobenzene (#3) + Aniline (#7)	1:1	2.68

89	Bromobenzene (#3) + Aniline (#7)	1:2	2.38
90	Bromobenzene (#3) + 3,4-Dichloroaniline (#8)	2:1	2.91
91	Bromobenzene (#3) + 3,4-Dichloroaniline (#8)	1:1	3.87
92	Bromobenzene (#3) + 3,4-Dichloroaniline (#8)	1:2	4.04
93*	1,2,3-Trichlorobenzene (#2) + Phenol (#5)	2:1	3.05
94*	1,2,3-Trichlorobenzene (#2) + Phenol (#5)	1:1	3.39
95*	1,2,3-Trichlorobenzene (#2) + Phenol (#5)	1:2	2.98
96	1,2,3-Trichlorobenzene (#2) + 2,4-Dichlorophenol (#6)	2:1	4.41
97	1,2,3-Trichlorobenzene (#2) + 2,4-Dichlorophenol (#6)	1:1	4.27
98	1,2,3-Trichlorobenzene (#2) + 2,4-Dichlorophenol (#6)	1:2	4.21
99	1,2,3-Trichlorobenzene (#2) + Aniline (#7)	2:1	2.39
100	1,2,3-Trichlorobenzene (#2) + Aniline (#7)	1:1	2.63
101	1,2,3-Trichlorobenzene (#2) + Aniline (#7)	1:2	2.45
102	1,2,3-Trichlorobenzene (#2) + 3,4-Dichloroaniline (#8)	2:1	4.1
103	1,2,3-Trichlorobenzene (#2) + 3,4-Dichloroaniline (#8)	1:1	4.29
104	1,2,3-Trichlorobenzene (#2) + 3,4-Dichloroaniline (#8)	1:2	4.15
105*	1-Bromo-2,3-dichlorobenzene (#4) + Phenol (#5)	2:1	3.32
106*	1-Bromo-2,3-dichlorobenzene (#4) + Phenol (#5)	1:1	3.42
107*	1-Bromo-2,3-dichlorobenzene (#4) + Phenol (#5)	1:2	3.12
108	1-Bromo-2,3-dichlorobenzene (#4) + 2,4-Dichlorophenol (#6)	2:1	4.61
109	1-Bromo-2,3-dichlorobenzene (#4) + 2,4-Dichlorophenol (#6)	1:1	4.66
110	1-Bromo-2,3-dichlorobenzene (#4) + 2,4-Dichlorophenol (#6)	1:2	4.53
111	1-Bromo-2,3-dichlorobenzene (#4) + Aniline (#7)	2:1	2.56
112	1-Bromo-2,3-dichlorobenzene (#4) + Aniline (#7)	1:1	2.91
113	1-Bromo-2,3-dichlorobenzene (#4) + Aniline (#7)	1:2	2.57
114	1-Bromo-2,3-dichlorobenzene (#4) + 3,4-Dichloroaniline (#8)	2:1	4.29
115	1-Bromo-2,3-dichlorobenzene (#4) + 3,4-Dichloroaniline (#8)	1:1	4.52
116	1-Bromo-2,3-dichlorobenzene (#4) + 3,4-Dichloroaniline (#8)	1:2	4.32
117*	Phenol (#5) + 2,4-Dichlorophenol (#6)	2:1	3.22
118*	Phenol (#5) + 2,4-Dichlorophenol (#6)	1:1	3.11

119*	Phenol (#5) + 2,4-Dichlorophenol (#6)	1:2	3.29
120*	Phenol (#5) + Aniline (#7)	2:1	2.18
121*	Phenol (#5) + Aniline (#7)	1:1	2.5
122*	Phenol (#5) + Aniline (#7)	1:2	2.33
123*	Phenol (#5) + 3,4-Dichloroaniline (#8)	2:1	3.37
124*	Phenol (#5) + 3,4-Dichloroaniline (#8)	1:1	3.16
125*	Phenol (#5) + 3,4-Dichloroaniline (#8)	1:2	3.54
126	2,4-Dichlorophenol (#6) + Aniline (#7)	2:1	2.43
127	2,4-Dichlorophenol (#6) + Aniline (#7)	1:1	2.6
128	2,4-Dichlorophenol (#6) + Aniline (#7)	1:2	2.61
129	2,4-Dichlorophenol (#6) + 3,4-Dichloroaniline (#8)	2:1	4.17
130	2,4-Dichlorophenol (#6) + 3,4-Dichloroaniline (#8)	1:1	4.44
131	2,4-Dichlorophenol (#6) + 3,4-Dichloroaniline (#8)	1:2	4.23
132	Aniline (#7) + 3,4-Dichloroaniline (#8)	2:1	2.55
133	Aniline (#7) + 3,4-Dichloroaniline (#8)	1:1	2.5
134	Aniline (#7) + 3,4-Dichloroaniline (#8)	1:2	2.71

*Test set mixtures; #Serial number of component; **Phenol (#5)** is absent in training set

Table 3. Training-test division of mixtures out cross-validation mentioned in “3.3.4. *Feature selection and model development*” section in the thesis

Sl. No.	Composition	Molar concentration ratio	pEC50
21	Diclofenac (#6) + Oxytetracycline (#4)	0.75:0.25	1.55
22	Diclofenac (#6) + Oxytetracycline (#4)	0.5:0.5	1.44
23	Diclofenac (#6) + Oxytetracycline (#4)	0.25:0.75	1.32
24*	Diclofenac (#6) + Carbamazepine (#3)	0.75:0.25	1.4
25*	Diclofenac (#6) + Carbamazepine (#3)	0.5:0.5	1.27
26*	Diclofenac (#6) + Carbamazepine (#3)	0.25:0.75	1.13
27	Diclofenac (#6) + Dexamethasone (#5)	0.75:0.25	1.35
28	Diclofenac (#6) + Dexamethasone (#5)	0.5:0.5	1.24

29	Diclofenac (#6) + Dexamethasone (#5)	0.25:0.75	1.17
30	Diclofenac (#6) + Azithromycin (#1)	0.75:0.25	1.23
31	Diclofenac (#6) + Azithromycin (#1)	0.5:0.5	1.08
32	Diclofenac (#6) + Azithromycin (#1)	0.25:0.75	0.87
33*	Diclofenac (#6) + Erythromycin (#2)	0.75:0.25	1.26
34*	Diclofenac (#6) + Erythromycin (#2)	0.5:0.5	1.06
35*	Diclofenac (#6) + Erythromycin (#2)	0.25:0.75	0.9
36	Oxytetracycline (#4) + Carbamazepine (#3)	0.75:0.25	1.06
37	Oxytetracycline (#4) + Carbamazepine (#3)	0.5:0.5	1.06
38	Oxytetracycline (#4) + Carbamazepine (#3)	0.25:0.75	0.89
39	Oxytetracycline (#4) + Dexamethasone (#5)	0.75:0.25	0.96
40	Oxytetracycline (#4) + Dexamethasone (#5)	0.5:0.5	0.99
41	Oxytetracycline (#4) + Dexamethasone (#5)	0.25:0.75	0.97
42*	Oxytetracycline (#4) + Azithromycin (#1)	0.75:0.25	0.95
43*	Oxytetracycline (#4) + Azithromycin (#1)	0.5:0.5	0.86
44*	Oxytetracycline (#4) + Azithromycin (#1)	0.25:0.75	0.79
45	Oxytetracycline (#4) + Erythromycin (#2)	0.75:0.25	0.94
46	Oxytetracycline (#4) + Erythromycin (#2)	0.5:0.5	0.84
47	Oxytetracycline (#4) + Erythromycin (#2)	0.25:0.75	0.76
48*	Carbamazepine (#3) + Dexamethasone (#5)	0.75:0.25	0.8
49*	Carbamazepine (#3) + Dexamethasone (#5)	0.5:0.5	0.87
50*	Carbamazepine (#3) + Dexamethasone (#5)	0.25:0.75	0.95
51	Carbamazepine (#3) + Azithromycin (#1)	0.75:0.25	0.82
52	Carbamazepine (#3) + Azithromycin (#1)	0.5:0.5	0.8
53	Carbamazepine (#3) + Azithromycin (#1)	0.25:0.75	0.83
54	Carbamazepine (#3) + Erythromycin (#2)	0.75:0.25	0.75
55	Carbamazepine (#3) + Erythromycin (#2)	0.5:0.5	0.79
56	Carbamazepine (#3) + Erythromycin (#2)	0.25:0.75	0.74

57	Dexamethasone (#5) + Azithromycin (#1)	0.75:0.25	0.89
58	Dexamethasone (#5) + Azithromycin (#1)	0.5:0.5	0.83
59	Dexamethasone (#5) + Azithromycin (#1)	0.25:0.75	0.8
60	Dexamethasone (#5) + Erythromycin (#2)	0.75:0.25	0.82
61	Dexamethasone (#5) + Erythromycin (#2)	0.5:0.5	0.84
62	Dexamethasone (#5) + Erythromycin (#2)	0.25:0.75	0.76
63*	Azithromycin (#1) + Erythromycin (#2)	0.75:0.25	0.8
64*	Azithromycin (#1) + Erythromycin (#2)	0.5:0.5	0.76
65*	Azithromycin (#1) + Erythromycin (#2)	0.25:0.75	0.73
66	Isoproturon (#12) + Alachlor (#11)	0.75:0.25	0.9
67	Isoproturon (#12) + Alachlor (#11)	0.5:0.5	0.88
68	Isoproturon (#12) + Alachlor (#11)	0.25:0.75	0.74
69*	Isoproturon (#12) + Diuron (#13)	0.75:0.25	0.86
70*	Isoproturon (#12) + Diuron (#13)	0.5:0.5	0.8
71*	Isoproturon (#12) + Diuron (#13)	0.25:0.75	0.64
72	Isoproturon (#12) + Chlorfenvinphos (#14)	0.75:0.25	0.93
73	Isoproturon (#12) + Chlorfenvinphos (#14)	0.5:0.5	0.98
74	Isoproturon (#12) + Chlorfenvinphos (#14)	0.25:0.75	1
75	Alachlor (#11) + Diuron (#13)	0.75:0.25	0.69
76	Alachlor (#11) + Diuron (#13)	0.5:0.5	0.61
77	Alachlor (#11) + Diuron (#13)	0.25:0.75	0.64
78	Alachlor (#11) + Chlorfenvinphos (#14)	0.75:0.25	0.75
79	Alachlor (#11) + Chlorfenvinphos (#14)	0.5:0.5	0.88
80	Alachlor (#11) + Chlorfenvinphos (#14)	0.25:0.75	1.03
81	Diuron (#13) + Chlorfenvinphos (#14)	0.75:0.25	0.74
82	Diuron (#13) + Chlorfenvinphos (#14)	0.5:0.5	0.9
83	Diuron (#13) + Chlorfenvinphos (#14)	0.25:0.75	0.97
84*	Diclofenac (#6) + Isoproturon (#12)	0.75:0.25	1.39

85*	Diclofenac (#6) + Isoproturon (#12)	0.5:0.5	1.41
86*	Diclofenac (#6) + Isoproturon (#12)	0.25:0.75	1.55
87	Diclofenac (#6) + Alachlor (#11)	0.75:0.25	1.51
88	Diclofenac (#6) + Alachlor (#11)	0.5:0.5	1.01
89	Diclofenac (#6) + Alachlor (#11)	0.25:0.75	0.82
90	Diclofenac (#6) + Diuron (#13)	0.75:0.25	1.44
91	Diclofenac (#6) + Diuron (#13)	0.5:0.5	1.26
92	Diclofenac (#6) + Diuron (#13)	0.25:0.75	1.03
93	Diclofenac (#6) + Chlorfenvinphos (#14)	0.75:0.25	1.85
94	Diclofenac (#6) + Chlorfenvinphos (#14)	0.5:0.5	1.8
95	Diclofenac (#6) + Chlorfenvinphos (#14)	0.25:0.75	1.8
96*	Oxytetracycline (#4) + Isoproturon (#12)	0.75:0.25	0.87
97*	Oxytetracycline (#4) + Isoproturon (#12)	0.5:0.5	0.86
98*	Oxytetracycline (#4) + Isoproturon (#12)	0.25:0.75	0.86
99	Oxytetracycline (#4) + Alachlor (#11)	0.75:0.25	1.29
100	Oxytetracycline (#4) + Alachlor (#11)	0.5:0.5	1.18
101	Oxytetracycline (#4) + Alachlor (#11)	0.25:0.75	1
102	Oxytetracycline (#4) + Diuron (#13)	0.75:0.25	1.1
103	Oxytetracycline (#4) + Diuron (#13)	0.5:0.5	1.04
104	Oxytetracycline (#4) + Diuron (#13)	0.25:0.75	0.94
105	Oxytetracycline (#4) + Chlorfenvinphos (#14)	0.75:0.25	1.33
106	Oxytetracycline (#4) + Chlorfenvinphos (#14)	0.5:0.5	1.36
107	Oxytetracycline (#4) + Chlorfenvinphos (#14)	0.25:0.75	1.45
108*	Carbamazepine (#3) + Isoproturon (#12)	0.75:0.25	0.84
109*	Carbamazepine (#3) + Isoproturon (#12)	0.5:0.5	0.7
110*	Carbamazepine (#3) + Isoproturon (#12)	0.25:0.75	0.71
111	Carbamazepine (#3) + Alachlor (#11)	0.75:0.25	0.85
112	Carbamazepine (#3) + Alachlor (#11)	0.5:0.5	0.78

113	Carbamazepine (#3) + Alachlor (#11)	0.25:0.75	0.66
114*	Carbamazepine (#3) + Diuron (#13)	0.75:0.25	0.66
115*	Carbamazepine (#3) + Diuron (#13)	0.5:0.5	0.76
116*	Carbamazepine (#3) + Diuron (#13)	0.25:0.75	0.61
117	Carbamazepine (#3) + Chlorfenvinphos (#14)	0.75:0.25	0.85
118	Carbamazepine (#3) + Chlorfenvinphos (#14)	0.5:0.5	1.02
119	Carbamazepine (#3) + Chlorfenvinphos (#14)	0.25:0.75	1.16
120	Dexamethasone (#5) + Isoproturon (#12)	0.75:0.25	0.91
121	Dexamethasone (#5) + Isoproturon (#12)	0.5:0.5	0.75
122	Dexamethasone (#5) + Isoproturon (#12)	0.25:0.75	0.63
123*	Dexamethasone (#5) + Alachlor (#11)	0.75:0.25	1.14
124*	Dexamethasone (#5) + Alachlor (#11)	0.5:0.5	1.04
125*	Dexamethasone (#5) + Alachlor (#11)	0.25:0.75	0.87
126	Dexamethasone (#5) + Diuron (#13)	0.75:0.25	0.96
127	Dexamethasone (#5) + Diuron (#13)	0.5:0.5	0.91
128	Dexamethasone (#5) + Diuron (#13)	0.25:0.75	0.82
129	Dexamethasone (#5) + Chlorfenvinphos (#14)	0.75:0.25	1.1
130	Dexamethasone (#5) + Chlorfenvinphos (#14)	0.5:0.5	1.25
131	Dexamethasone (#5) + Chlorfenvinphos (#14)	0.25:0.75	1.36
132	Erythromycin (#2) + Isoproturon (#12)	0.75:0.25	0.66
133	Erythromycin (#2) + Isoproturon (#12)	0.5:0.5	0.63
134	Erythromycin (#2) + Isoproturon (#12)	0.25:0.75	0.74
135*	Erythromycin (#2) + Alachlor (#11)	0.75:0.25	1.55
136*	Erythromycin (#2) + Alachlor (#11)	0.5:0.5	0.97
137*	Erythromycin (#2) + Alachlor (#11)	0.25:0.75	0.75
138	Erythromycin (#2) + Diuron (#13)	0.75:0.25	0.87
139	Erythromycin (#2) + Diuron (#13)	0.5:0.5	0.81
140	Erythromycin (#2) + Diuron (#13)	0.25:0.75	0.75

141	Erythromycin (#2) + Chlorfenvinphos (#14)	0.75:0.25	0.98
142	Erythromycin (#2) + Chlorfenvinphos (#14)	0.5:0.5	1.45
143	Erythromycin (#2) + Chlorfenvinphos (#14)	0.25:0.75	1.55
144	Azithromycin (#1) + Isoproturon (#12)	0.75:0.25	0.76
145	Azithromycin (#1) + Isoproturon (#12)	0.5:0.5	0.81
146	Azithromycin (#1) + Isoproturon (#12)	0.25:0.75	0.85
147	Azithromycin (#1) + Alachlor (#11)	0.75:0.25	0.88
148	Azithromycin (#1) + Alachlor (#11)	0.5:0.5	1.06
149	Azithromycin (#1) + Alachlor (#11)	0.25:0.75	0.82
150*	Azithromycin (#1) + Diuron (#13)	0.75:0.25	1.02
151*	Azithromycin (#1) + Diuron (#13)	0.5:0.5	0.96
152*	Azithromycin (#1) + Diuron (#13)	0.25:0.75	1.02
153	Azithromycin (#1) + Chlorfenvinphos (#14)	0.75:0.25	1.08
154	Azithromycin (#1) + Chlorfenvinphos (#14)	0.5:0.5	1.39
155	Azithromycin (#1) + Chlorfenvinphos (#14)	0.25:0.75	1.65
156	Omeprazole (#10) + Imatinib (#8)	0.75:0.25	2.98
157	Omeprazole (#10) + Imatinib (#8)	0.5:0.5	2.7
158	Omeprazole (#10) + Imatinib (#8)	0.25:0.75	2.28
159	Omeprazole (#10) + Tobramycin (#9)	0.75:0.25	2.73
160	Omeprazole (#10) + Tobramycin (#9)	0.5:0.5	2.33
161	Omeprazole (#10) + Tobramycin (#9)	0.25:0.75	1.8
162*	Omeprazole (#10) + Desloratadine (#7)	0.75:0.25	2.98
163*	Omeprazole (#10) + Desloratadine (#7)	0.5:0.5	2.55
164*	Omeprazole (#10) + Desloratadine (#7)	0.25:0.75	1.93
165	Imatinib (#8) + Tobramycin (#9)	0.75:0.25	0.39
166	Imatinib (#8) + Tobramycin (#9)	0.5:0.5	0.26
167	Imatinib (#8) + Tobramycin (#9)	0.25:0.75	0.13
168	Imatinib (#8) + Desloratadine (#7)	0.75:0.25	0.65

169	Imatinib (#8) + Desloratadine (#7)	0.5:0.5	0.49
170	Imatinib (#8) + Desloratadine (#7)	0.25:0.75	0.29
171*	Tobramycin (#9) + Desloratadine (#7)	0.75:0.25	0.09
172*	Tobramycin (#9) + Desloratadine (#7)	0.5:0.5	0.04
173*	Tobramycin (#9) + Desloratadine (#7)	0.25:0.75	0.02
174*	Tetracycline hydrochloride (#15) + Dichlorvos (#19)	0.078:0.922	2.94
175*	Tetracycline hydrochloride (#15) + Dichlorvos (#19)	0.033:0.967	2.58
176*	Tetracycline hydrochloride (#15) + Dichlorvos (#19)	0.017:0.983	2.37
177*	Tetracycline hydrochloride (#15) + Dichlorvos (#19)	0.008:0.992	2.04
178*	Tetracycline hydrochloride (#15) + Dichlorvos (#19)	0.003:0.997	1.86
179	Tetracycline hydrochloride (#15) + Trichlorfon (#18)	0.054:0.946	3.47
180	Tetracycline hydrochloride (#15) + Trichlorfon (#18)	0.022:0.978	3.35
181	Tetracycline hydrochloride (#15) + Trichlorfon (#18)	0.011:0.989	3.3
182	Tetracycline hydrochloride (#15) + Trichlorfon (#18)	0.006:0.994	3.26
183	Tetracycline hydrochloride (#15) + Trichlorfon (#18)	0.002:0.998	3.24
184	Tetracycline hydrochloride (#15) + Linuron (#20)	0.814:0.186	4.16
185	Tetracycline hydrochloride (#15) + Linuron (#20)	0.636:0.364	4.26
186	Tetracycline hydrochloride (#15) + Linuron (#20)	0.467:0.533	4.25
187	Tetracycline hydrochloride (#15) + Linuron (#20)	0.304:0.696	4.24
188	Tetracycline hydrochloride (#15) + Linuron (#20)	0.149:0.851	4.23
189	Chloramphenicol (#16) + Dichlorvos (#19)	0.549:0.451	3.15
190	Chloramphenicol (#16) + Dichlorvos (#19)	0.328:0.672	3.21
191	Chloramphenicol (#16) + Dichlorvos (#19)	0.196:0.804	3.25
192	Chloramphenicol (#16) + Dichlorvos (#19)	0.109:0.891	3.28
193	Chloramphenicol (#16) + Dichlorvos (#19)	0.046:0.954	3.28
194	Chloramphenicol (#16) + Linuron (#20)	0.984:0.016	3.01
195	Chloramphenicol (#16) + Linuron (#20)	0.962:0.038	3.11
196	Chloramphenicol (#16) + Linuron (#20)	0.927:0.073	3.22

197	Chloramphenicol (#16) + Linuron (#20)	0.861:0.136	3.37
198	Chloramphenicol (#16) + Linuron (#20)	0.717:0.283	3.61
199*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17)	0.033:0.483:0.484	3.34
200*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17)	0.037:0.367:0.596	3.35
201*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17)	0.038:0.277:0.684	3.06
202*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17)	0.041:0.166:0.793	3.12
203*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17)	0.12:0.279:0.601	3.08
204	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Linuron (#20)	0.06:0.871:0.069	3.62
205	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Linuron (#20)	0.083:0.833:0.084	3.32
206	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Linuron (#20)	0.11:0.795:0.095	3.5
207	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Linuron (#20)	0.173:0.71:0.117	3.21
208	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Linuron (#20)	0.253:0.589:0.158	3.77
209	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Trichlorfon (#18)	0.01:0.141:0.849	2.95
210	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Trichlorfon (#18)	0.013:0.133:0.854	2.57
211	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Trichlorfon (#18)	0.017:0.124:0.858	2.59
212	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Trichlorfon (#18)	0.027:0.112:0.861	2.78
213	Tetracycline hydrochloride (#15) + Chloramphenicol	0.043:0.1:0.857	2.89

	(#16) + Trichlorfon (#18)		
214*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17) + Linuron (#20)	0.032:0.465:0.466:0.037	3.3
215*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17) + Linuron (#20)	0.035:0.354:0.575:0.036	3.28
216*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17) + Linuron (#20)	0.037:0.268:0.663:0.032	3.19
217*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17) + Linuron (#20)	0.039:0.162:0.772:0.027	3.2
218*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17) + Linuron (#20)	0.039:0.091:0.846:0.024	3.32

*Test set mixtures

Table 4. Training-test division of compounds-out cross-validation mentioned in “3.3.4. *Feature selection and model development*” section in the thesis

Sl. No.	Composition	Molar concentration ratio	pEC50
21*	Diclofenac (#6) + Oxytetracycline (#4)	0.75:0.25	1.55
22*	Diclofenac (#6) + Oxytetracycline (#4)	0.5:0.5	1.44
23*	Diclofenac (#6) + Oxytetracycline (#4)	0.25:0.75	1.32
24*	Diclofenac (#6) + Carbamazepine (#3)	0.75:0.25	1.4
25*	Diclofenac (#6) + Carbamazepine (#3)	0.5:0.5	1.27
26*	Diclofenac (#6) + Carbamazepine (#3)	0.25:0.75	1.13
27*	Diclofenac (#6) + Dexamethasone (#5)	0.75:0.25	1.35
28*	Diclofenac (#6) + Dexamethasone (#5)	0.5:0.5	1.24
29*	Diclofenac (#6) + Dexamethasone (#5)	0.25:0.75	1.17

30*	Diclofenac (#6) + Azithromycin (#1)	0.75:0.25	1.23
31*	Diclofenac (#6) + Azithromycin (#1)	0.5:0.5	1.08
32*	Diclofenac (#6) + Azithromycin (#1)	0.25:0.75	0.87
33*	Diclofenac (#6) + Erythromycin (#2)	0.75:0.25	1.26
34*	Diclofenac (#6) + Erythromycin (#2)	0.5:0.5	1.06
35*	Diclofenac (#6) + Erythromycin (#2)	0.25:0.75	0.9
36	Oxytetracycline (#4) + Carbamazepine (#3)	0.75:0.25	1.06
37	Oxytetracycline (#4) + Carbamazepine (#3)	0.5:0.5	1.06
38	Oxytetracycline (#4) + Carbamazepine (#3)	0.25:0.75	0.89
39	Oxytetracycline (#4) + Dexamethasone (#5)	0.75:0.25	0.96
40	Oxytetracycline (#4) + Dexamethasone (#5)	0.5:0.5	0.99
41	Oxytetracycline (#4) + Dexamethasone (#5)	0.25:0.75	0.97
42	Oxytetracycline (#4) + Azithromycin (#1)	0.75:0.25	0.95
43	Oxytetracycline (#4) + Azithromycin (#1)	0.5:0.5	0.86
44	Oxytetracycline (#4) + Azithromycin (#1)	0.25:0.75	0.79
45	Oxytetracycline (#4) + Erythromycin (#2)	0.75:0.25	0.94
46	Oxytetracycline (#4) + Erythromycin (#2)	0.5:0.5	0.84
47	Oxytetracycline (#4) + Erythromycin (#2)	0.25:0.75	0.76
48	Carbamazepine (#3) + Dexamethasone (#5)	0.75:0.25	0.8
49	Carbamazepine (#3) + Dexamethasone (#5)	0.5:0.5	0.87
50	Carbamazepine (#3) + Dexamethasone (#5)	0.25:0.75	0.95
51	Carbamazepine (#3) + Azithromycin (#1)	0.75:0.25	0.82

52	Carbamazepine (#3) + Azithromycin (#1)	0.5:0.5	0.8
53	Carbamazepine (#3) + Azithromycin (#1)	0.25:0.75	0.83
54	Carbamazepine (#3) + Erythromycin (#2)	0.75:0.25	0.75
55	Carbamazepine (#3) + Erythromycin (#2)	0.5:0.5	0.79
56	Carbamazepine (#3) + Erythromycin (#2)	0.25:0.75	0.74
57	Dexamethasone (#5) + Azithromycin (#1)	0.75:0.25	0.89
58	Dexamethasone (#5) + Azithromycin (#1)	0.5:0.5	0.83
59	Dexamethasone (#5) + Azithromycin (#1)	0.25:0.75	0.8
60	Dexamethasone (#5) + Erythromycin (#2)	0.75:0.25	0.82
61	Dexamethasone (#5) + Erythromycin (#2)	0.5:0.5	0.84
62	Dexamethasone (#5) + Erythromycin (#2)	0.25:0.75	0.76
63	Azithromycin (#1) + Erythromycin (#2)	0.75:0.25	0.8
64	Azithromycin (#1) + Erythromycin (#2)	0.5:0.5	0.76
65	Azithromycin (#1) + Erythromycin (#2)	0.25:0.75	0.73
66	Isoproturon (#12) + Alachlor (#11)	0.75:0.25	0.9
67	Isoproturon (#12) + Alachlor (#11)	0.5:0.5	0.88
68	Isoproturon (#12) + Alachlor (#11)	0.25:0.75	0.74
69	Isoproturon (#12) + Diuron (#13)	0.75:0.25	0.86
70	Isoproturon (#12) + Diuron (#13)	0.5:0.5	0.8
71	Isoproturon (#12) + Diuron (#13)	0.25:0.75	0.64
72	Isoproturon (#12) + Chlorfenvinphos (#14)	0.75:0.25	0.93
73	Isoproturon (#12) + Chlorfenvinphos (#14)	0.5:0.5	0.98

74	Isoproturon (#12) + Chlorfenvinphos (#14)	0.25:0.75	1
75	Alachlor (#11) + Diuron (#13)	0.75:0.25	0.69
76	Alachlor (#11) + Diuron (#13)	0.5:0.5	0.61
77	Alachlor (#11) + Diuron (#13)	0.25:0.75	0.64
78	Alachlor (#11) + Chlorfenvinphos (#14)	0.75:0.25	0.75
79	Alachlor (#11) + Chlorfenvinphos (#14)	0.5:0.5	0.88
80	Alachlor (#11) + Chlorfenvinphos (#14)	0.25:0.75	1.03
81	Diuron (#13) + Chlorfenvinphos (#14)	0.75:0.25	0.74
82	Diuron (#13) + Chlorfenvinphos (#14)	0.5:0.5	0.9
83	Diuron (#13) + Chlorfenvinphos (#14)	0.25:0.75	0.97
84*	Diclofenac (#6) + Isoproturon (#12)	0.75:0.25	1.39
85*	Diclofenac (#6) + Isoproturon (#12)	0.5:0.5	1.41
86*	Diclofenac (#6) + Isoproturon (#12)	0.25:0.75	1.55
87*	Diclofenac (#6) + Alachlor (#11)	0.75:0.25	1.51
88*	Diclofenac (#6) + Alachlor (#11)	0.5:0.5	1.01
89*	Diclofenac (#6) + Alachlor (#11)	0.25:0.75	0.82
90*	Diclofenac (#6) + Diuron (#13)	0.75:0.25	1.44
91*	Diclofenac (#6) + Diuron (#13)	0.5:0.5	1.26
92*	Diclofenac (#6) + Diuron (#13)	0.25:0.75	1.03
93*	Diclofenac (#6) + Chlorfenvinphos (#14)	0.75:0.25	1.85
94*	Diclofenac (#6) + Chlorfenvinphos (#14)	0.5:0.5	1.8
95*	Diclofenac (#6) + Chlorfenvinphos (#14)	0.25:0.75	1.8

96	Oxytetracycline (#4) + Isoproturon (#12)	0.75:0.25	0.87
97	Oxytetracycline (#4) + Isoproturon (#12)	0.5:0.5	0.86
98	Oxytetracycline (#4) + Isoproturon (#12)	0.25:0.75	0.86
99	Oxytetracycline (#4) + Alachlor (#11)	0.75:0.25	1.29
100	Oxytetracycline (#4) + Alachlor (#11)	0.5:0.5	1.18
101	Oxytetracycline (#4) + Alachlor (#11)	0.25:0.75	1
102	Oxytetracycline (#4) + Diuron (#13)	0.75:0.25	1.1
103	Oxytetracycline (#4) + Diuron (#13)	0.5:0.5	1.04
104	Oxytetracycline (#4) + Diuron (#13)	0.25:0.75	0.94
105	Oxytetracycline (#4) + Chlorfenvinphos (#14)	0.75:0.25	1.33
106	Oxytetracycline (#4) + Chlorfenvinphos (#14)	0.5:0.5	1.36
107	Oxytetracycline (#4) + Chlorfenvinphos (#14)	0.25:0.75	1.45
108	Carbamazepine (#3) + Isoproturon (#12)	0.75:0.25	0.84
109	Carbamazepine (#3) + Isoproturon (#12)	0.5:0.5	0.7
110	Carbamazepine (#3) + Isoproturon (#12)	0.25:0.75	0.71
111	Carbamazepine (#3) + Alachlor (#11)	0.75:0.25	0.85
112	Carbamazepine (#3) + Alachlor (#11)	0.5:0.5	0.78
113	Carbamazepine (#3) + Alachlor (#11)	0.25:0.75	0.66
114	Carbamazepine (#3) + Diuron (#13)	0.75:0.25	0.66
115	Carbamazepine (#3) + Diuron (#13)	0.5:0.5	0.76
116	Carbamazepine (#3) + Diuron (#13)	0.25:0.75	0.61
117	Carbamazepine (#3) + Chlorfenvinphos (#14)	0.75:0.25	0.85

118	Carbamazepine (#3) + Chlorfenvinphos (#14)	0.5:0.5	1.02
119	Carbamazepine (#3) + Chlorfenvinphos (#14)	0.25:0.75	1.16
120	Dexamethasone (#5) + Isoproturon (#12)	0.75:0.25	0.91
121	Dexamethasone (#5) + Isoproturon (#12)	0.5:0.5	0.75
122	Dexamethasone (#5) + Isoproturon (#12)	0.25:0.75	0.63
123	Dexamethasone (#5) + Alachlor (#11)	0.75:0.25	1.14
124	Dexamethasone (#5) + Alachlor (#11)	0.5:0.5	1.04
125	Dexamethasone (#5) + Alachlor (#11)	0.25:0.75	0.87
126	Dexamethasone (#5) + Diuron (#13)	0.75:0.25	0.96
127	Dexamethasone (#5) + Diuron (#13)	0.5:0.5	0.91
128	Dexamethasone (#5) + Diuron (#13)	0.25:0.75	0.82
129	Dexamethasone (#5) + Chlorfenvinphos (#14)	0.75:0.25	1.1
130	Dexamethasone (#5) + Chlorfenvinphos (#14)	0.5:0.5	1.25
131	Dexamethasone (#5) + Chlorfenvinphos (#14)	0.25:0.75	1.36
132	Erythromycin (#2) + Isoproturon (#12)	0.75:0.25	0.66
133	Erythromycin (#2) + Isoproturon (#12)	0.5:0.5	0.63
134	Erythromycin (#2) + Isoproturon (#12)	0.25:0.75	0.74
135	Erythromycin (#2) + Alachlor (#11)	0.75:0.25	1.55
136	Erythromycin (#2) + Alachlor (#11)	0.5:0.5	0.97
137	Erythromycin (#2) + Alachlor (#11)	0.25:0.75	0.75
138	Erythromycin (#2) + Diuron (#13)	0.75:0.25	0.87
139	Erythromycin (#2) + Diuron (#13)	0.5:0.5	0.81

140	Erythromycin (#2) + Diuron (#13)	0.25:0.75	0.75
141	Erythromycin (#2) + Chlorfenvinphos (#14)	0.75:0.25	0.98
142	Erythromycin (#2) + Chlorfenvinphos (#14)	0.5:0.5	1.45
143	Erythromycin (#2) + Chlorfenvinphos (#14)	0.25:0.75	1.55
144	Azithromycin (#1) + Isoproturon (#12)	0.75:0.25	0.76
145	Azithromycin (#1) + Isoproturon (#12)	0.5:0.5	0.81
146	Azithromycin (#1) + Isoproturon (#12)	0.25:0.75	0.85
147	Azithromycin (#1) + Alachlor (#11)	0.75:0.25	0.88
148	Azithromycin (#1) + Alachlor (#11)	0.5:0.5	1.06
149	Azithromycin (#1) + Alachlor (#11)	0.25:0.75	0.82
150	Azithromycin (#1) + Diuron (#13)	0.75:0.25	1.02
151	Azithromycin (#1) + Diuron (#13)	0.5:0.5	0.96
152	Azithromycin (#1) + Diuron (#13)	0.25:0.75	1.02
153	Azithromycin (#1) + Chlorfenvinphos (#14)	0.75:0.25	1.08
154	Azithromycin (#1) + Chlorfenvinphos (#14)	0.5:0.5	1.39
155	Azithromycin (#1) + Chlorfenvinphos (#14)	0.25:0.75	1.65
156	Omeprazole (#10) + Imatinib (#8)	0.75:0.25	2.98
157	Omeprazole (#10) + Imatinib (#8)	0.5:0.5	2.7
158	Omeprazole (#10) + Imatinib (#8)	0.25:0.75	2.28
159	Omeprazole (#10) + Tobramycin (#9)	0.75:0.25	2.73
160	Omeprazole (#10) + Tobramycin (#9)	0.5:0.5	2.33
161	Omeprazole (#10) + Tobramycin (#9)	0.25:0.75	1.8

162	Omeprazole (#10) + Desloratadine (#7)	0.75:0.25	2.98
163	Omeprazole (#10) + Desloratadine (#7)	0.5:0.5	2.55
164	Omeprazole (#10) + Desloratadine (#7)	0.25:0.75	1.93
165	Imatinib (#8) + Tobramycin (#9)	0.75:0.25	0.39
166	Imatinib (#8) + Tobramycin (#9)	0.5:0.5	0.26
167	Imatinib (#8) + Tobramycin (#9)	0.25:0.75	0.13
168	Imatinib (#8) + Desloratadine (#7)	0.75:0.25	0.65
169	Imatinib (#8) + Desloratadine (#7)	0.5:0.5	0.49
170	Imatinib (#8) + Desloratadine (#7)	0.25:0.75	0.29
171	Tobramycin (#9) + Desloratadine (#7)	0.75:0.25	0.09
172	Tobramycin (#9) + Desloratadine (#7)	0.5:0.5	0.04
173	Tobramycin (#9) + Desloratadine (#7)	0.25:0.75	0.02
174*	Tetracycline hydrochloride (#15) + Dichlorvos (#19)	0.078:0.922	2.94
175*	Tetracycline hydrochloride (#15) + Dichlorvos (#19)	0.033:0.967	2.58
176*	Tetracycline hydrochloride (#15) + Dichlorvos (#19)	0.017:0.983	2.37
177*	Tetracycline hydrochloride (#15) + Dichlorvos (#19)	0.008:0.992	2.04
178*	Tetracycline hydrochloride (#15) + Dichlorvos (#19)	0.003:0.997	1.86
179*	Tetracycline hydrochloride (#15) + Trichlorfon (#18)	0.054:0.946	3.47
180*	Tetracycline hydrochloride (#15) + Trichlorfon (#18)	0.022:0.978	3.35
181*	Tetracycline hydrochloride (#15) + Trichlorfon (#18)	0.011:0.989	3.3
182*	Tetracycline hydrochloride (#15) + Trichlorfon (#18)	0.006:0.994	3.26
183*	Tetracycline hydrochloride (#15) + Trichlorfon (#18)	0.002:0.998	3.24

184*	Tetracycline hydrochloride (#15) + Linuron (#20)	0.814:0.186	4.16
185*	Tetracycline hydrochloride (#15) + Linuron (#20)	0.636:0.364	4.26
186*	Tetracycline hydrochloride (#15) + Linuron (#20)	0.467:0.533	4.25
187*	Tetracycline hydrochloride (#15) + Linuron (#20)	0.304:0.696	4.24
188	Tetracycline hydrochloride (#15) + Linuron (#20)	0.149:0.851	4.23
189	Chloramphenicol (#16) + Dichlorvos (#19)	0.549:0.451	3.15
190	Chloramphenicol (#16) + Dichlorvos (#19)	0.328:0.672	3.21
191	Chloramphenicol (#16) + Dichlorvos (#19)	0.196:0.804	3.25
192	Chloramphenicol (#16) + Dichlorvos (#19)	0.109:0.891	3.28
193	Chloramphenicol (#16) + Dichlorvos (#19)	0.046:0.954	3.28
194	Chloramphenicol (#16) + Linuron (#20)	0.984:0.016	3.01
195	Chloramphenicol (#16) + Linuron (#20)	0.962:0.038	3.11
196	Chloramphenicol (#16) + Linuron (#20)	0.927:0.073	3.22
197	Chloramphenicol (#16) + Linuron (#20)	0.861:0.136	3.37
198	Chloramphenicol (#16) + Linuron (#20)	0.717:0.283	3.61
199*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17)	0.033:0.483:0.484	3.34
200*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17)	0.037:0.367:0.596	3.35
201*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17)	0.038:0.277:0.684	3.06
202*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17)	0.041:0.166:0.793	3.12
203*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17)	0.12:0.279:0.601	3.08

204*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Linuron (#20)	0.06:0.871:0.069	3.62
205*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Linuron (#20)	0.083:0.833:0.084	3.32
206*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Linuron (#20)	0.11:0.795:0.095	3.5
207*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Linuron (#20)	0.173:0.71:0.117	3.21
208*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Linuron (#20)	0.253:0.589:0.158	3.77
209*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Trichlorfon (#18)	0.01:0.141:0.849	2.95
210*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Trichlorfon (#18)	0.013:0.133:0.854	2.57
211*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Trichlorfon (#18)	0.017:0.124:0.858	2.59
212*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Trichlorfon (#18)	0.027:0.112:0.861	2.78
213*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Trichlorfon (#18)	0.043:0.1:0.857	2.89
214*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17) + Linuron (#20)	0.032:0.465:0.466:0.037	3.3
215*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17) + Linuron (#20)	0.035:0.354:0.575:0.036	3.28
216*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17) + Linuron (#20)	0.037:0.268:0.663:0.032	3.19
217*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17) + Linuron (#20)	0.039:0.162:0.772:0.027	3.2
218*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17) + Linuron (#20)	0.039:0.091:0.846:0.024	3.32

*Test set mixtures; each data point of the test set contains either Diclofenac (#6) or Tetracycline hydrochloride (#15) which are not present in the training set.

Table 5. Training-test division of everything-out cross-validation mentioned in “*3.3.4. Feature selection and model development*” section in the thesis

Sl. No.	Composition	Molar concentration ratio	pEC50
21	Diclofenac (#6) + Oxytetracycline (#4)	0.75:0.25	1.55
22	Diclofenac (#6) + Oxytetracycline (#4)	0.5:0.5	1.44
23	Diclofenac (#6) + Oxytetracycline (#4)	0.25:0.75	1.32
24	Diclofenac (#6) + Carbamazepine (#3)	0.75:0.25	1.4
25	Diclofenac (#6) + Carbamazepine (#3)	0.5:0.5	1.27
26	Diclofenac (#6) + Carbamazepine (#3)	0.25:0.75	1.13
27	Diclofenac (#6) + Dexamethasone (#5)	0.75:0.25	1.35
28	Diclofenac (#6) + Dexamethasone (#5)	0.5:0.5	1.24
29	Diclofenac (#6) + Dexamethasone (#5)	0.25:0.75	1.17
30	Diclofenac (#6) + Azithromycin (#1)	0.75:0.25	1.23
31	Diclofenac (#6) + Azithromycin (#1)	0.5:0.5	1.08
32	Diclofenac (#6) + Azithromycin (#1)	0.25:0.75	0.87
33	Diclofenac (#6) + Erythromycin (#2)	0.75:0.25	1.26
34	Diclofenac (#6) + Erythromycin (#2)	0.5:0.5	1.06
35	Diclofenac (#6) + Erythromycin (#2)	0.25:0.75	0.9
36	Oxytetracycline (#4) + Carbamazepine (#3)	0.75:0.25	1.06
37	Oxytetracycline (#4) + Carbamazepine (#3)	0.5:0.5	1.06
38	Oxytetracycline (#4) + Carbamazepine (#3)	0.25:0.75	0.89

39	Oxytetracycline (#4) + Dexamethasone (#5)	0.75:0.25	0.96
40	Oxytetracycline (#4) + Dexamethasone (#5)	0.5:0.5	0.99
41	Oxytetracycline (#4) + Dexamethasone (#5)	0.25:0.75	0.97
42	Oxytetracycline (#4) + Azithromycin (#1)	0.75:0.25	0.95
43	Oxytetracycline (#4) + Azithromycin (#1)	0.5:0.5	0.86
44	Oxytetracycline (#4) + Azithromycin (#1)	0.25:0.75	0.79
45	Oxytetracycline (#4) + Erythromycin (#2)	0.75:0.25	0.94
46	Oxytetracycline (#4) + Erythromycin (#2)	0.5:0.5	0.84
47	Oxytetracycline (#4) + Erythromycin (#2)	0.25:0.75	0.76
48	Carbamazepine (#3) + Dexamethasone (#5)	0.75:0.25	0.8
49	Carbamazepine (#3) + Dexamethasone (#5)	0.5:0.5	0.87
50	Carbamazepine (#3) + Dexamethasone (#5)	0.25:0.75	0.95
51	Carbamazepine (#3) + Azithromycin (#1)	0.75:0.25	0.82
52	Carbamazepine (#3) + Azithromycin (#1)	0.5:0.5	0.8
53	Carbamazepine (#3) + Azithromycin (#1)	0.25:0.75	0.83
54	Carbamazepine (#3) + Erythromycin (#2)	0.75:0.25	0.75
55	Carbamazepine (#3) + Erythromycin (#2)	0.5:0.5	0.79
56	Carbamazepine (#3) + Erythromycin (#2)	0.25:0.75	0.74
57	Dexamethasone (#5) + Azithromycin (#1)	0.75:0.25	0.89
58	Dexamethasone (#5) + Azithromycin (#1)	0.5:0.5	0.83
59	Dexamethasone (#5) + Azithromycin (#1)	0.25:0.75	0.8
60	Dexamethasone (#5) + Erythromycin (#2)	0.75:0.25	0.82

61	Dexamethasone (#5) + Erythromycin (#2)	0.5:0.5	0.84
62	Dexamethasone (#5) + Erythromycin (#2)	0.25:0.75	0.76
63	Azithromycin (#1) + Erythromycin (#2)	0.75:0.25	0.8
64	Azithromycin (#1) + Erythromycin (#2)	0.5:0.5	0.76
65	Azithromycin (#1) + Erythromycin (#2)	0.25:0.75	0.73
66	Isoproturon (#12) + Alachlor (#11)	0.75:0.25	0.9
67	Isoproturon (#12) + Alachlor (#11)	0.5:0.5	0.88
68	Isoproturon (#12) + Alachlor (#11)	0.25:0.75	0.74
69	Isoproturon (#12) + Diuron (#13)	0.75:0.25	0.86
70	Isoproturon (#12) + Diuron (#13)	0.5:0.5	0.8
71	Isoproturon (#12) + Diuron (#13)	0.25:0.75	0.64
72	Isoproturon (#12) + Chlorfenvinphos (#14)	0.75:0.25	0.93
73	Isoproturon (#12) + Chlorfenvinphos (#14)	0.5:0.5	0.98
74	Isoproturon (#12) + Chlorfenvinphos (#14)	0.25:0.75	1
75	Alachlor (#11) + Diuron (#13)	0.75:0.25	0.69
76	Alachlor (#11) + Diuron (#13)	0.5:0.5	0.61
77	Alachlor (#11) + Diuron (#13)	0.25:0.75	0.64
78	Alachlor (#11) + Chlorfenvinphos (#14)	0.75:0.25	0.75
79	Alachlor (#11) + Chlorfenvinphos (#14)	0.5:0.5	0.88
80	Alachlor (#11) + Chlorfenvinphos (#14)	0.25:0.75	1.03
81	Diuron (#13) + Chlorfenvinphos (#14)	0.75:0.25	0.74
82	Diuron (#13) + Chlorfenvinphos (#14)	0.5:0.5	0.9

83	Diuron (#13) + Chlorfenvinphos (#14)	0.25:0.75	0.97
84	Diclofenac (#6) + Isoproturon (#12)	0.75:0.25	1.39
85	Diclofenac (#6) + Isoproturon (#12)	0.5:0.5	1.41
86	Diclofenac (#6) + Isoproturon (#12)	0.25:0.75	1.55
87	Diclofenac (#6) + Alachlor (#11)	0.75:0.25	1.51
88	Diclofenac (#6) + Alachlor (#11)	0.5:0.5	1.01
89	Diclofenac (#6) + Alachlor (#11)	0.25:0.75	0.82
90	Diclofenac (#6) + Diuron (#13)	0.75:0.25	1.44
91	Diclofenac (#6) + Diuron (#13)	0.5:0.5	1.26
92	Diclofenac (#6) + Diuron (#13)	0.25:0.75	1.03
93	Diclofenac (#6) + Chlorfenvinphos (#14)	0.75:0.25	1.85
94	Diclofenac (#6) + Chlorfenvinphos (#14)	0.5:0.5	1.8
95	Diclofenac (#6) + Chlorfenvinphos (#14)	0.25:0.75	1.8
96	Oxytetracycline (#4) + Isoproturon (#12)	0.75:0.25	0.87
97	Oxytetracycline (#4) + Isoproturon (#12)	0.5:0.5	0.86
98	Oxytetracycline (#4) + Isoproturon (#12)	0.25:0.75	0.86
99	Oxytetracycline (#4) + Alachlor (#11)	0.75:0.25	1.29
100	Oxytetracycline (#4) + Alachlor (#11)	0.5:0.5	1.18
101	Oxytetracycline (#4) + Alachlor (#11)	0.25:0.75	1
102	Oxytetracycline (#4) + Diuron (#13)	0.75:0.25	1.1
103	Oxytetracycline (#4) + Diuron (#13)	0.5:0.5	1.04
104	Oxytetracycline (#4) + Diuron (#13)	0.25:0.75	0.94

105	Oxytetracycline (#4) + Chlorfenvinphos (#14)	0.75:0.25	1.33
106	Oxytetracycline (#4) + Chlorfenvinphos (#14)	0.5:0.5	1.36
107	Oxytetracycline (#4) + Chlorfenvinphos (#14)	0.25:0.75	1.45
108	Carbamazepine (#3) + Isoproturon (#12)	0.75:0.25	0.84
109	Carbamazepine (#3) + Isoproturon (#12)	0.5:0.5	0.7
110	Carbamazepine (#3) + Isoproturon (#12)	0.25:0.75	0.71
111	Carbamazepine (#3) + Alachlor (#11)	0.75:0.25	0.85
112	Carbamazepine (#3) + Alachlor (#11)	0.5:0.5	0.78
113	Carbamazepine (#3) + Alachlor (#11)	0.25:0.75	0.66
114	Carbamazepine (#3) + Diuron (#13)	0.75:0.25	0.66
115	Carbamazepine (#3) + Diuron (#13)	0.5:0.5	0.76
116	Carbamazepine (#3) + Diuron (#13)	0.25:0.75	0.61
117	Carbamazepine (#3) + Chlorfenvinphos (#14)	0.75:0.25	0.85
118	Carbamazepine (#3) + Chlorfenvinphos (#14)	0.5:0.5	1.02
119	Carbamazepine (#3) + Chlorfenvinphos (#14)	0.25:0.75	1.16
120	Dexamethasone (#5) + Isoproturon (#12)	0.75:0.25	0.91
121	Dexamethasone (#5) + Isoproturon (#12)	0.5:0.5	0.75
122	Dexamethasone (#5) + Isoproturon (#12)	0.25:0.75	0.63
123	Dexamethasone (#5) + Alachlor (#11)	0.75:0.25	1.14
124	Dexamethasone (#5) + Alachlor (#11)	0.5:0.5	1.04
125	Dexamethasone (#5) + Alachlor (#11)	0.25:0.75	0.87
126	Dexamethasone (#5) + Diuron (#13)	0.75:0.25	0.96

127	Dexamethasone (#5) + Diuron (#13)	0.5:0.5	0.91
128	Dexamethasone (#5) + Diuron (#13)	0.25:0.75	0.82
129	Dexamethasone (#5) + Chlorfenvinphos (#14)	0.75:0.25	1.1
130	Dexamethasone (#5) + Chlorfenvinphos (#14)	0.5:0.5	1.25
131	Dexamethasone (#5) + Chlorfenvinphos (#14)	0.25:0.75	1.36
132	Erythromycin (#2) + Isoproturon (#12)	0.75:0.25	0.66
133	Erythromycin (#2) + Isoproturon (#12)	0.5:0.5	0.63
134	Erythromycin (#2) + Isoproturon (#12)	0.25:0.75	0.74
135	Erythromycin (#2) + Alachlor (#11)	0.75:0.25	1.55
136	Erythromycin (#2) + Alachlor (#11)	0.5:0.5	0.97
137	Erythromycin (#2) + Alachlor (#11)	0.25:0.75	0.75
138	Erythromycin (#2) + Diuron (#13)	0.75:0.25	0.87
139	Erythromycin (#2) + Diuron (#13)	0.5:0.5	0.81
140	Erythromycin (#2) + Diuron (#13)	0.25:0.75	0.75
141	Erythromycin (#2) + Chlorfenvinphos (#14)	0.75:0.25	0.98
142	Erythromycin (#2) + Chlorfenvinphos (#14)	0.5:0.5	1.45
143	Erythromycin (#2) + Chlorfenvinphos (#14)	0.25:0.75	1.55
144	Azithromycin (#1) + Isoproturon (#12)	0.75:0.25	0.76
145	Azithromycin (#1) + Isoproturon (#12)	0.5:0.5	0.81
146	Azithromycin (#1) + Isoproturon (#12)	0.25:0.75	0.85
147	Azithromycin (#1) + Alachlor (#11)	0.75:0.25	0.88
148	Azithromycin (#1) + Alachlor (#11)	0.5:0.5	1.06

149	Azithromycin (#1) + Alachlor (#11)	0.25:0.75	0.82
150	Azithromycin (#1) + Diuron (#13)	0.75:0.25	1.02
151	Azithromycin (#1) + Diuron (#13)	0.5:0.5	0.96
152	Azithromycin (#1) + Diuron (#13)	0.25:0.75	1.02
153	Azithromycin (#1) + Chlorfenvinphos (#14)	0.75:0.25	1.08
154	Azithromycin (#1) + Chlorfenvinphos (#14)	0.5:0.5	1.39
155	Azithromycin (#1) + Chlorfenvinphos (#14)	0.25:0.75	1.65
156	Omeprazole (#10) + Imatinib (#8)	0.75:0.25	2.98
157	Omeprazole (#10) + Imatinib (#8)	0.5:0.5	2.7
158	Omeprazole (#10) + Imatinib (#8)	0.25:0.75	2.28
159	Omeprazole (#10) + Tobramycin (#9)	0.75:0.25	2.73
160	Omeprazole (#10) + Tobramycin (#9)	0.5:0.5	2.33
161	Omeprazole (#10) + Tobramycin (#9)	0.25:0.75	1.8
162	Omeprazole (#10) + Desloratadine (#7)	0.75:0.25	2.98
163	Omeprazole (#10) + Desloratadine (#7)	0.5:0.5	2.55
164	Omeprazole (#10) + Desloratadine (#7)	0.25:0.75	1.93
165	Imatinib (#8) + Tobramycin (#9)	0.75:0.25	0.39
166	Imatinib (#8) + Tobramycin (#9)	0.5:0.5	0.26
167	Imatinib (#8) + Tobramycin (#9)	0.25:0.75	0.13
168	Imatinib (#8) + Desloratadine (#7)	0.75:0.25	0.65
169	Imatinib (#8) + Desloratadine (#7)	0.5:0.5	0.49
170	Imatinib (#8) + Desloratadine (#7)	0.25:0.75	0.29

171	Tobramycin (#9) + Desloratadine (#7)	0.75:0.25	0.09
172	Tobramycin (#9) + Desloratadine (#7)	0.5:0.5	0.04
173	Tobramycin (#9) + Desloratadine (#7)	0.25:0.75	0.02
174*	Tetracycline hydrochloride (#15) + Dichlorvos (#19)	0.078:0.922	2.94
175*	Tetracycline hydrochloride (#15) + Dichlorvos (#19)	0.033:0.967	2.58
176*	Tetracycline hydrochloride (#15) + Dichlorvos (#19)	0.017:0.983	2.37
177*	Tetracycline hydrochloride (#15) + Dichlorvos (#19)	0.008:0.992	2.04
178*	Tetracycline hydrochloride (#15) + Dichlorvos (#19)	0.003:0.997	1.86
179*	Tetracycline hydrochloride (#15) + Trichlorfon (#18)	0.054:0.946	3.47
180*	Tetracycline hydrochloride (#15) + Trichlorfon (#18)	0.022:0.978	3.35
181*	Tetracycline hydrochloride (#15) + Trichlorfon (#18)	0.011:0.989	3.3
182*	Tetracycline hydrochloride (#15) + Trichlorfon (#18)	0.006:0.994	3.26
183*	Tetracycline hydrochloride (#15) + Trichlorfon (#18)	0.002:0.998	3.24
184*	Tetracycline hydrochloride (#15) + Linuron (#20)	0.814:0.186	4.16
185*	Tetracycline hydrochloride (#15) + Linuron (#20)	0.636:0.364	4.26
186*	Tetracycline hydrochloride (#15) + Linuron (#20)	0.467:0.533	4.25
187*	Tetracycline hydrochloride (#15) + Linuron (#20)	0.304:0.696	4.24
188*	Tetracycline hydrochloride (#15) + Linuron (#20)	0.149:0.851	4.23
189*	Chloramphenicol (#16) + Dichlorvos (#19)	0.549:0.451	3.15
190*	Chloramphenicol (#16) + Dichlorvos (#19)	0.328:0.672	3.21
191*	Chloramphenicol (#16) + Dichlorvos (#19)	0.196:0.804	3.25
192*	Chloramphenicol (#16) + Dichlorvos (#19)	0.109:0.891	3.28

193*	Chloramphenicol (#16) + Dichlorvos (#19)	0.046:0.954	3.28
194*	Chloramphenicol (#16) + Linuron (#20)	0.984:0.016	3.01
195*	Chloramphenicol (#16) + Linuron (#20)	0.962:0.038	3.11
196*	Chloramphenicol (#16) + Linuron (#20)	0.927:0.073	3.22
197*	Chloramphenicol (#16) + Linuron (#20)	0.861:0.136	3.37
198*	Chloramphenicol (#16) + Linuron (#20)	0.717:0.283	3.61
199*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17)	0.033:0.483:0.484	3.34
200*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17)	0.037:0.367:0.596	3.35
201*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17)	0.038:0.277:0.684	3.06
202*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17)	0.041:0.166:0.793	3.12
203*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17)	0.12:0.279:0.601	3.08
204*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Linuron (#20)	0.06:0.871:0.069	3.62
205*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Linuron (#20)	0.083:0.833:0.084	3.32
206*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Linuron (#20)	0.11:0.795:0.095	3.5
207*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Linuron (#20)	0.173:0.71:0.117	3.21
208*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Linuron (#20)	0.253:0.589:0.158	3.77
209*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Trichlorfon (#18)	0.01:0.141:0.849	2.95
210*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Trichlorfon (#18)	0.013:0.133:0.854	2.57

211*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Trichlorfon (#18)	0.017:0.124:0.858	2.59
212*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Trichlorfon (#18)	0.027:0.112:0.861	2.78
213*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Trichlorfon (#18)	0.043:0.1:0.857	2.89
214*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17) + Linuron (#20)	0.032:0.465:0.466:0.037	3.3
215*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17) + Linuron (#20)	0.035:0.354:0.575:0.036	3.28
216*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17) + Linuron (#20)	0.037:0.268:0.663:0.032	3.19
217*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17) + Linuron (#20)	0.039:0.162:0.772:0.027	3.2
218*	Tetracycline hydrochloride (#15) + Chloramphenicol (#16) + Metribuzine (#17) + Linuron (#20)	0.039:0.091:0.846:0.024	3.32

*Test set mixtures; all components of the test set are unique to the training set

Table 6. Source Dataset mentioned in “**3.4.1. Toxicity data**” section in the thesis (Carnesecchi et al., 2020)

Sl. No.	Component A	Component B	Observed toxicity
SM1	Acetamiprid	Piperonyl butoxide	-0.068
SM2	Acetamiprid	Tribufos/Butifos	-0.378
SM3	Acetamiprid	diethyl but-2-enedioate	-0.841
SM4	Acetamiprid	Triflumizole	1.523
SM5	Acetamiprid	Propiconazole	1.155

SM6	Acetamiprid	Triadimefon	1.097
SM7	Acetamiprid	Epoxiconazole	0.301
SM8	Acetamiprid	Uniconazole	-0.049
SM9	Imidacloprid	Piperonyl butoxide	1.979
SM10	Imidacloprid	Triflumizole	2.013
SM11	Imidacloprid	Propiconazole	1.921
SM12	Thiacloprid	Acetamiprid	1.046
SM13	Thiacloprid	Triflumizole	2.000
SM14	Thiacloprid	Propiconazole	1.523
SM15	Acetamiprid	Fenbuconazole	-1.155
SM16	Imidacloprid	Fenbuconazole	0.523
SM17	Coumaphos	diethyl but-2-enedioate	-1.299
SM18	Coumaphos	Tribufos/Butifos	-0.863
SM19	Coumaphos	Piperonyl butoxide	-0.702
SM20	Coumaphos	Fluvalinate	-1.322

SM21	Coumaphos	Fluvalinate	-1.106
SM22	Coumaphos	Fluvalinate	-0.782
SM23	Coumaphos	Fluvalinate	-0.782
SM24	Fluvalinate	Coumaphos	-0.788
SM25	Fluvalinate	Coumaphos	-0.517
SM26	Fluvalinate	Coumaphos	-0.428
SM27	Fluvalinate	Coumaphos	-0.185
SM28	Fluvalinate	Coumaphos	0.678
SM29	Fluvalinate	Coumaphos	0.108
SM30	Fluvalinate	Fenpyroximate	-0.380
SM31	Fluvalinate	Amitraz	-0.573
SM32	Fluvalinate	Thymol	-1.009
SM33	Fluvalinate	Oxalic acid	-0.848
SM34	Fluvalinate	Pyraclostrobin	-0.646
SM35	Fluvalinate	Boscalid	-1.064

SM36	Fluvalinate	Chlorothalonil	-0.860
SM37	Fluvalinate	Prochloraz	2.000
SM38	Fluvalinate	Diethyl 2-betenedioate	-0.917
SM39	Fluvalinate	Tribufos/Butifos	-0.292
SM40	Fluvalinate	Piperonyl butoxide	2.000
SM41	Coumaphos	Fluvalinate	-0.813
SM42	Coumaphos	Fenpyroximate	-0.615
SM43	Coumaphos	Amitraz	-0.964
SM44	Coumaphos	Thymol	-1.364
SM45	Coumaphos	Oxalic acid	-1.167
SM46	Coumaphos	Boscalid	-1.354
SM47	Coumaphos	Chlorothalonil	-1.220
SM48	Coumaphos	Prochloraz	0.357
SM49	Coumaphos	Diethyl 2-betenedioate	-1.299
SM50	Coumaphos	Tribufos/Butifos	-0.863

SM51	Coumaphos	Piperonyl butoxide	-0.702
SM52	Fenpyroximate	Fluvalinate	-0.744
SM53	Fenpyroximate	Coumaphos	-0.307
SM54	Fenpyroximate	Amitraz	-0.255
SM55	Fenpyroximate	Thymol	-0.567
SM56	Fenpyroximate	Oxalic acid	-0.176
SM57	Fenpyroximate	Pyrachlostrobin	-0.320
SM58	Fenpyroximate	Boscalid	-0.751
SM59	Fenpyroximate	Chlorothalonil	-0.807
SM60	Fenpyroximate	Prochloraz	0.602
SM61	Fenpyroximate	Diethyl 2-betenedioate	-0.641
SM62	Fenpyroximate	Tribufos/Butifos	-0.100
SM63	Fenpyroximate	Piperonyl butoxide	0.569
SM64	Amitraz	Fluvalinate	-0.688
SM65	Amitraz	Coumaphos	-0.436

SM66	Amitraz	Fenpyroximate	-0.660
SM67	Amitraz	Thymol	-0.592
SM68	Amitraz	Oxalic acid	-1.164
SM69	Amitraz	Pyrachlostrobin	-0.215
SM70	Amitraz	Boscalid	-0.683
SM71	Amitraz	Chlorothalonil	-0.524
SM72	Amitraz	Prochloraz	-0.394
SM73	Amitraz	Diethyl 2-betenedioate	-0.362
SM74	Amitraz	Tribufos/Butifos	-0.336
SM75	Amitraz	Piperonyl butoxide	-0.382
SM76	Thymol	Fluvalinate	-1.207
SM77	Thymol	Coumaphos	-1.310
SM78	Thymol	Fenpyroximate	-1.543
SM79	Thymol	Amitraz	-1.635
SM80	Thymol	Oxalic acid	-1.487

SM81	Thymol	Pyrachlostrobin	-1.450
SM82	Thymol	Boscalid	-1.673
SM83	Thymol	Chlorothalonil	-1.474
SM84	Thymol	Prochloraz	-1.591
SM85	Thymol	Diethyl 2-betenedioate	-1.806
SM86	Thymol	Tribufos/Butifos	-1.545
SM87	Thymol	Piperonyl butoxide	-1.511
SM88	Fluvalinate	Piperonyl butoxide	-1.041
SM89	Fluvalinate	Prochloraz	-1.045
SM90	Fluvalinate	Propiconazole	-1.143
SM91	Fluvalinate	Fenbuconazole	-1.021
SM92	Fluvalinate	Metconazole	-1.104
SM93	Fluvalinate	Myclobutanil	-1.111
SM94	Fluvalinate	Piperonyl butoxide	-0.928
SM95	Fluvalinate	Prochloraz	-0.667

SM96	Fluvalinate	Propiconazole	-0.776
SM97	Fluvalinate	Fenbuconazole	-0.793
SM98	Fluvalinate	Metconazole	-0.717
SM99	Fluvalinate	Myclobutanil	-0.574
SM100	Fluvalinate	Piperonyl butoxide	-0.188
SM101	Fluvalinate	Prochloraz	0.658
SM102	Fluvalinate	Propiconazole	0.131
SM103	Fluvalinate	Fenbuconazole	0.260
SM104	Fluvalinate	Metconazole	0.347
SM105	Fluvalinate	Myclobutanil	0.921
SM106	Cyfluthrin	Diethyl 2-betenedioate	1.222
SM107	Cyfluthrin	Tribufos/Butifos	1.523
SM108	Cyfluthrin	Piperonyl butoxide	2.699
SM109	Cyhalothrin	Diethyl 2-betenedioate	1.398
SM110	Cyhalothrin	Tribufos/Butifos	1.523

SM111	Cyhalothrin	Piperonyl butoxide	2.886
SM112	Fluvalinate	Diethyl 2-betenedioate	-0.917
SM113	Fluvalinate	Tribufos/Butifos	-0.292
SM114	Fluvalinate	Piperonyl butoxide	2.000
SM115	Phenothrin	Amitraz	0.444
SM116	Phenothrin	Coumaphos*2	0.854
SM117	Phenothrin	Piperonyl butoxide	0.620
SM118	Phenothrin	Amitraz	0.252
SM119	Phenothrin	Coumaphos*2	0.796
SM120	Phenothrin	Piperonyl butoxide	0.495
SM121	Phenothrin	Amitraz	0.444
SM122	Phenothrin	Coumaphos*2	0.824
SM123	Phenothrin	Piperonyl butoxide	0.620

*SM: Source mixture