



SUPPLEMENTARY MATERIAL TO  
**Use of GA-ANN and GA-SVM for a QSPR study on the aqueous  
solubility of pesticides**

AMEL BOUAKKADIA<sup>1,2\*</sup>, NOUREDDINE KERTIOU<sup>1,2</sup>, RANA AMIRI<sup>1</sup>,  
YOUSOUF DRIUCHE<sup>1</sup> and DJELLOUL MESSADI<sup>1</sup>

<sup>1</sup>Environmental and Food Safety Laboratory, Department of Chemistry, Badji Mokhtar  
University – Annaba, BP. 12, 23000 Annaba, Algeria and <sup>2</sup>Abbes Laghrour University,  
Faculty of Sciences and Technology – Khenchela, BP 1252 Route de Batna,  
40004 Khenchela, Algeria

J. Serb. Chem. Soc. 86 (7–8) (2021) 673–684

TABLE S-I. Pesticides compounds used in this study and their solubility

No	Name	log (S / mg L <sup>-1</sup> )
1	2-ethylamino-4-(isopropylamino)-6-(methylthio)-s triazine	2.27
2	methyl $\alpha$ -[(4,6-dimethoxypyrimidin-2-ylcarbamoylethyl)sulfamoyl]- <i>o</i> -toluate	2.08
3	S-Ethyl diisobutyl carbamothioate	1.64
4	ethyl 2-(4-chloro-6-methoxypyrimidin-2-ylcarbamoylethyl)sulfamoyl benzoate	3.08
5	3-[4-(4-chlorophenoxy)phenyl]-1,1-dimethyl-urea	0.4
6	1-(2-chlorophenylsulfonyl)-3-(4-methoxy-6-methyl-1,3,5-triazin-2-yl)urea	4.45
7	3,6-dichloropyridine-2-carboxylic acid	5.16
8	(2-hydroxyethyl)ammonium 3,6-dichloropyridine-2-carboxylate	5.75
9	2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methylpropanenitrile	2.23
10	S-ethyl N-cyclohexyl-N-ethyl carbamothioate	1.98
11	2,4-Dichlorophenoxyacetic acid	2.95
12	diethylammonium (2,4-dichlorophenoxy) acetate	5.9
13	methyl 2-(2,4-dichlorophenoxy)acetate	2
14	2,3,6-trichlorobenzoic acid	3.89
15	ethyl 3-phenyl carbamoyloxycarbanilate	0.95
16	(2R)-2-(2,4-dichlorophenoxy)propionic acid	2.77
17	3-[4-(4-methoxyphenoxy)phenyl]-1,1-dimethylurea	1.3
18	6-ethylthio-N <sup>2</sup> ,N <sup>4</sup> -diisopropyl-1,3,5-triazine-2,4-diamine	1.2
19	3-(3,4-dichlorophenyl)-1,1-dimethylurea	1.62
20	S-ethyl dipropyl(thiocarbamate)	2.54
21	methyl 2-[(4-ethoxy-6-methylamino-1,3,5-triazin-2-yl)carbamoylethyl]benzoate	1.7
22	ethyl (RS)-2-[4-(6-chloro-1,3-benzoxazol-2-yloxy)phenoxy] propionate	-0.1

\* Corresponding author. E-mail: amelbouakkadia@yahoo.fr

TABLE S-I. Continued

23	butyl (RS)-2-{4-[5-(trifluoromethyl)-2-pyridyloxy]phenoxy}propionate	0
24	butyl (R)-2-{4-[5-(trifluoromethyl)-2-pyridyloxy]phenoxy}propionate	0.3
25	(RS)-1-methylheptyl 4-amino-3,5-dichloro-6-fluoro-2-pyridyloxyacetate	-1.05
26	<i>N</i> -(phosphonomethyl) glycine	4.08
27	(RS)-2-{4-[3-chloro-5-(trifluoromethyl)-2-pyridyloxy]phenoxy}propionic acid	1.64
28	3-(4-isopropylphenyl)-1,1-dimethylurea	1.81
29	3-cyclohexyl-1,5,6,7-tetrahydrocyclopentapyrimidine-2,4(3 <i>H</i> )-dione	0.78
30	3-(3,4-dichlorophenyl)-1-methoxy-1-methylurea	1.88
31	4-(4-chloro- <i>o</i> -tolylloxy)butyric acid	1.64
32	(RS)-2-(4-chloro- <i>o</i> -tolylloxy)propionic acid	2.87
33	4-amino-4,5-dihydro-3-methyl-6-phenyl-1,2,4-triazin-5-on	3.23
34	2-(3,4-dichlorophenyl)-4-methyl-1,2,4-oxadiazolidine-3,5-dion	0.18
35	3-(3-chloro-4-methoxyphenyl)-1,1-dimethylurea	2.83
36	methyl 2-(4-methoxy-6-methyl-1,3,5-triazin-2-ylcarbamoylsulfamoyl)benzoate	3.98
37	(RS)- <i>N,N</i> -diethyl-2-(1-naphthylloxy)propionamide	1.87
38	<i>S</i> -propyl butyl(ethyl) thiocarbamate	2
39	4-amino-3,5,6-trichloropyridine-2-carboxylic acid	2.63
40	<i>N</i> <sup>2</sup> , <i>N</i> <sup>4</sup> -diisopropyl-6-methoxy-1,3,5-triazine-2,4-diamine	2.86
41	<i>N</i> <sup>2</sup> , <i>N</i> <sup>4</sup> -diisopropyl-6-methylthio-1,3,5-triazine-2,4-diamine	1.52
42	6-chloro- <i>N</i> <sup>2</sup> , <i>N</i> <sup>4</sup> -diisopropyl-1,3,5-triazine-2,4-diamine	0.93
43	<i>S</i> -benzyl dipropyl (thiocarbamate)	1.12
44	ethyl (2RS)-2-[4-(6-chloroquinoxalin-2-yloxy)phenoxy] propionate	-0.51
45	1-(4,6-dimethoxypyrimidin-2-yl)-3-(3-ethylsulfonyl-2-pyridylsulfonyl)urea	3.86
46	6-chloro- <i>N</i> <sup>2</sup> , <i>N</i> <sup>4</sup> -diethyl-1,3,5-triazine-2,4-diamine	0.79
47	1-(5- <i>tert</i> -butyl-1,3,4-thiadiazol-2-yl)-1,3-dimethylurea	3.4
48	3- <i>tert</i> -butyl-5-chloro-6-methyluracil	2.85
49	<i>N</i> <sup>2</sup> - <i>tert</i> -butyl- <i>N</i> <sup>4</sup> -ethyl-6-methylthio-1,3,5-triazine-2,4-diamine	1.34
50	methyl 3-(4-methoxy-6-methyl-1,3,5-triazin-2-ylcarbamoylsulfamoyl)thiophene-2-carboxylate	3.8
51	<i>S</i> -4-chlorobenzyl diethyl(thiocarbamate)	1.45
52	<i>S</i> -2,3,3-trichloroallyl diisopropyl(thiocarbamate)	0.6
53	methyl 2-[4-methoxy-6-methyl-1,3,5-triazin-2-yl(methyl)carbamoylsulfamoyl] benzoate	3.18
54	3,5,6-trichloro-2-pyridyloxyacetic acid	3.91
55	2-butoxyethyl 3,5,6-trichloro-2-pyridyloxyacetate	1.36
56	methyl 2-[4-dimethylamino-6-(2,2,2-trifluoroethoxy)-1,3,5-triazin-2-ylcarbamoylsulfamoyl] tototoluate	2.04
57	1,1-dimethyl-3-( $\alpha,\alpha,\alpha$ -trifluoro- <i>m</i> -tolyl)urea	2.04
58	<i>iso</i> -octyl 4-chloro- <i>o</i> -tolylloxyacetate	0.7
59*	methyl 2-[4,6-bis(difluoromethoxy)pyrimidin-2-ylcarbamoylsulfamoyl] benzoate	2.39
60*	1-(2-methylcyclohexyl)-3-phenylurea	1.26
61*	6-chloro- <i>N</i> -ethyl- <i>N'</i> -isopropyl-1,3,5-triazin-2,4-diamine	1.52

TABLE S-I. Continued

62*	5-bromo-3-(butan-2-yl)-6-methylpyrimidine-2,4(1 <i>H</i> ,3 <i>H</i> )-dione	2.85
63*	(R)-1-(Ethylcarbamoyl)ethylcarbanilate	3.54
64*	isopropyl (3-chlorophenyl)carbamate	1.95
65*	4-(2,4-dichlorophenoxy)butanoic acid	1.66
66*	(2,4,5-trichlorophenoxy)acetic acid	2.18
67*	<i>N</i> <sup>2</sup> -isopropyl- <i>N</i> <sup>4</sup> -methyl-6-methylthio-1,3,5-triazine-2,4-diamine	2.76
68*	(2 <i>RS</i> )-2-(2,4-dichlorophenoxy)propionic acid	2.54
69*	Haloxypopethoxyethyl	0.11
70*	4-chloro- <i>o</i> -tolylxyacetic acid	2.87
71*	(R)-2-(4-chloro- <i>o</i> -tolylxy)propionic acid	2.93
72*	1-(1,3-benzothiazol-2-yl)-1,3-dimethylurea	1.77
73*	4-amino-6- <i>tert</i> -butyl-4,5-dihydro-3-methylthio-1,2,4-triazin-5-one	3.09
74*	methyl 3-(3-methylcarbaniloxy)carbanilate	0.67
75*	1-(4-methoxy-6-methyl-1,3,5-triazin-2-yl)-3-[2-(3,3,3-trifluoropropyl)phenylsulfonyl] urea	3.6
76*	<i>N</i> <sup>2</sup> - <i>tert</i> -butyl-6-chloro- <i>N</i> <sup>4</sup> -ethyl-1,3,5-triazine-2,4-diamine	0.93
77*	1-[2-(2-chloroethoxy)phenylsulfonyl]-3-(4-methoxy-6-methyl-1,3,5-triazin-2-yl) urea	2.91
78*	<i>S</i> -propyl dipropyl(thiocarbamate)	2.03
79*	( <i>RS</i> )-3-(3,5-dichlorophenyl)-5-methyl-5-vinylloxazolidine-2,4-dione	0.53
80*	2-isopropylideneaminoxyethyl (R)-2-[4-(6-chloroquinoxalin-2-yloxy)phenoxy] propionate	-0.2

\*Validation set

TABLE S-II. Experimental, predicted values of log *S*, and descriptors values for the training and validation sets

N°	log ( <i>S</i> <sub>exp</sub> / mg l <sup>-1</sup> )	log ( <i>S</i> <sub>pred</sub> / mg l <sup>-1</sup> )		MAT8m	RNCG	ALOGP2	MAXDN	Mor26u
		ANN	SVM					
1	2.27	1.97007	2.04153	0.166	0.141	7.524	1.042	0.495
2	2.07918	2.80591	2.84972	-0.1	0.136	3.054	5.054	-0.081
3	1.64345	1.93482	2.03343	0	0.161	12.345	1.435	0.635
4	3.07918	2.98359	2.8582	-0.004	0.143	5.956	5.299	0.103
5	0.39794	0.800011	0.700217	-0.277	0.153	11.403	1.837	-0.136
6	4.4456	3.18637	3.12269	-0.042	0.162	3.456	5.049	-0.053
7	5.15534	4.23823	4.63397	0	0.333	5.064	2.85	-0.088
8	5.74819	4.72705	6.22588	0	0.422	1.409	1.403	0.05
9	2.23	1.72042	1.45922	0.123	0.134	5.456	2.006	-0.003
10	1.97772	1.85824	1.78546	0.13	0.167	11.136	1.387	0.349
11	2.94939	3.18143	2.97726	-0.15	0.262	7.907	2.717	-0.17
12	5.90091	4.34909	5.12943	0	0.349	0.232	0.406	0.139
13	2	3.03824	2.78796	0.049	0.251	9.381	2.129	-0.011
14	3.88649	3.71569	3.90686	0	0.33	11.748	2.854	-0.213
15	0.95424	1.27221	1.30116	0.685	0.115	10.775	2.278	-0.057
16	2.77085	2.2878	1.99897	-0.064	0.208	10.172	2.712	-0.126
17	1.30103	1.0429	0.869131	-0.452	0.14	7.268	1.834	-0.041

TABLE S-II. Continued

18	1.2	1.08567	1.57748	0.144	0.109	12.036	1.033	0.615
19	1.62325	1.83547	1.67145	-1.18	0.222	6.155	1.872	-0.088
20	2.53656	2.3036	2.1091	0	0.187	8.265	1.429	0.263
21	1.69897	2.91823	2.91128	-0.157	0.133	3.143	5.299	0.02
22	-0.09691	-0.127375	-0.117151	-0.107	0.132	22.584	2.076	-0.05
23	0	0.116869	0.503699	-0.135	0.099	28.423	5.696	0.176
24	0.30103	0.116869	0.503699	-0.135	0.099	28.423	5.696	0.176
25	-1.04576	-0.252303	-0.273216	-0.017	0.114	28.798	2.679	0.285
26	4.07918	3.90895	3.96613	0	0.242	4.273	4.902	-0.112
27	1.63749	0.900297	1.70448	-0.002	0.118	19.501	5.797	-0.174
28	1.81291	1.94637	1.76373	-0.595	0.168	5.506	1.771	0.243
29	0.77815	1.93203	1.64045	0.269	0.133	4.686	1.859	0.05
30	1.87506	2.29495	1.96685	-0.564	0.2	5.414	2.059	0.029
31	1.64345	2.04425	1.72174	-0.246	0.184	8.938	2.466	0.036
32	2.8657	2.68557	2.29279	0.842	0.183	9.067	2.653	-0.131
33	3.23	3.26032	2.69202	0.429	0.188	0.284	2.006	-0.032
34	0.17609	1.40374	1.18311	-0.665	0.188	8.466	2.406	-0.249
35	2.83123	2.84747	2.42529	-0.079	0.198	3.241	1.865	0.067
36	3.97772	3.53736	3.24333	-0.069	0.142	1.103	5.273	0.269
37	1.86923	1.0971	1.00116	0.023	0.137	10.733	1.805	0.059
38	2	1.93799	1.82598	0.141	0.173	11.096	1.419	0.319
39	2.63347	3.51021	3.27951	0	0.256	4.701	2.977	-0.203
40	2.86	2.23532	2.0885	0.516	0.13	6.565	1.36	0.449
41	1.52	1.67701	1.93075	0.154	0.131	9.738	1.044	0.593
42	0.934	1.54919	1.47091	0.151	0.134	8.487	1.476	0.25
43	1.12057	0.544881	0.618408	0.104	0.152	16.889	1.461	-0.001
44	-0.50864	-0.298238	-0.16316	0.023	0.12	21.98	2.07	-0.285
45	3.86332	2.64188	2.9698	-0.125	0.103	1.32	5.522	-0.083
46	0.792	2.3567	2.01921	0.178	0.164	4.658	1.47	0.153
47	3.39794	3.40434	3.06829	0.187	0.159	2.054	1.855	0.748
48	2.85126	2.54508	2.07957	0	0.151	1.016	2.111	0.074
49	1.34	1.40891	1.43875	0.154	0.126	8.691	1.305	0.301
50	3.79727	3.38015	3.17407	-0.06	0.136	1.007	5.219	0.183
51	1.44716	1.28912	1.2225	0.13	0.182	13.888	1.528	-0.038
52	0.60206	0.645302	0.943595	-1.126	0.186	15.682	1.683	0.242
53	3.17609	3.08267	3.19066	-0.075	0.143	1.578	5.285	-0.122
54	3.90849	3.10932	2.99134	-0.415	0.274	9.449	2.797	-0.114
55	1.36173	0.609083	0.590257	-0.068	0.159	20.456	2.21	0.174
56	2.04139	2.43526	2.38896	-1.27	0.167	4.387	5.654	-0.093
57	0.69897	-0.319298	-0.0707111	0.337	0.129	34.033	1.992	0.418
58	2.04139	2.14982	2.2675	-0.34	0.122	10.701	5.922	0.123
59*	1.52	2.10053	1.9355	0.163	0.143	6.43	1.473	0.362
60*	2.8451	2.35458	1.93893	0	0.146	1.99	2.009	0.096
61*	3.54407	3.14343	2.65957	0.368	0.135	0.899	2.281	0.475
62*	1.94939	1.15193	1.07316	-0.042	0.148	10.255	2.59	-0.233

TABLE S-II. Continued

63*	1.66276	2.2624	1.95081	-0.122	0.205	10.036	2.499	-0.034
64*	2.17609	2.79982	2.72653	-0.383	0.275	12.085	2.757	-0.172
65*	2.76	2.32061	2.35449	0	0.152	5.732	1.076	0.557
66*	2.54407	2.2878	1.99897	-0.064	0.208	10.172	2.712	-0.126
67*	0.11394	0.558332	1.07797	0.028	0.101	23.862	5.797	0.082
68*	2.8657	3.45844	2.9976	0.681	0.228	6.936	2.658	-0.058
69*	2.92942	2.68557	2.29279	0.842	0.183	9.067	2.653	-0.131
70*	1.77085	2.57556	2.12201	0.163	0.171	3.16	1.825	0.029
71*	3.09	3.46152	3.13894	0	0.177	2.15	1.947	0.688
72*	0.6721	1.15908	1.27212	0.767	0.116	11.696	2.277	-0.122
73*	3.60206	2.56352	2.75728	-0.086	0.137	8.116	5.697	-0.039
74*	0.929	2.03968	1.98117	0.151	0.136	7.511	1.479	0.494
75*	2.91116	3.07567	3.00836	-0.063	0.148	3.395	5.116	-0.003
76*	2.03342	1.90878	1.81662	0.141	0.173	11.55	1.412	0.338
77*	0.53148	0.304822	0.214497	-0.789	0.14	13.412	2.605	-0.164
78*	-0.20066	0.0957958	0.142756	-0.006	0.102	17.699	2.16	0.077
79*	2.38561	2.2525	2.3682	0.047	0.129	11.456	5.561	0.053
80*	1.25527	1.04243	0.975408	0.186	0.141	9.759	1.755	-0.189

\*Validation set