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PREDICTION OF BIOACCUMULATION FACTORS OF SOME COMMON HERBICIDES THROUGH QSAR BASED BIOINFORMATICS

SHASHI PRABHA AGRAWAL

Department of Zoology,
D.A.V. (PG) College,
Civil Lines, KANPUR (INDIA)
shashiagarwal29@gmail.com

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ABSTRACT

In present study I used QSAR (Quantitative structural activity relationship) model to predict bioaccumulation factor of herbicides. Here I have taken 40 herbicides and predicted with the help of T.E.S.T.software. I analysed that experimental log 10 value of one herbicides was greater than 3.50 (value recorded 3.51). It means it was potent to BAF. I also observed that out of 40 herbicides , experimental log10 value for BAF of 14 herbicides and predicted log10 value of 31 herbicides were below 3.50. It means that these herbicides were not potent to BAF.

Figure : 00 References : 02 Table : 01

KEY WORDS : Bioaccumulation factor, Herbicides, QSAR

Introduction

Herbicides are chemicals used to manipulate or control undesirable vegetation. The most frequent application of herbicides occurs in row-crop farming, where they are applied before or during planting to maximize crop productivity by minimizing other vegetation.

Bioaccumulation is a function of the bioavailability of contaminants in combination with species-specific uptake and elimination processes. Toxicity is determined by the exposure of an animal to bioavailable contaminants in concert with the animal's sensitivity to the contaminant. These processes have been shown to be a function of the organism's lipid content, size, growth rate, gender, diet, and ability to metabolize or transform a given contaminant, as well as the chemical conditions of the surrounding medium (US EPA2000).

Bioaccumulation of toxic persistent organic contaminants by aquatic organisms is an ongoing concern for several federal agencies, including the U.S. Environmental Protection Agency (EPA), U.S. Army Corps of Engineers (USACE), National Oceanic and Atmospheric Administration (NOAA), U.S. Fish and Wildlife Service (FWS), and US EPA (2000).

Bioaccumulation assessment is important in the scientific evaluation of risks that chemicals may pose to humans and the environment and is a current focus of regulatory effort. The status of bioaccumulation evaluations for organic chemicals in aquatic systems is reviewed to reduce uncertainty in bioaccumulation measurement to provide quality data for assessment and to assist in model development[1].

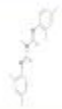
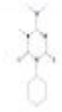
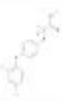
When considering computational models for prediction, QSAR methods are more reliable. T.E.S.T. provides multiple prediction methodologies. In present study we have used consensus approach of T.E.S.T. because it was shown to achieve the best prediction results during external validation.

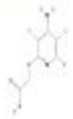
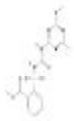
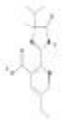
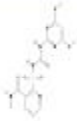
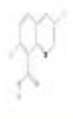
Methodology

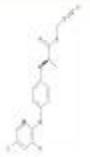
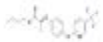
In this study toxicity estimation tool was used for the prediction of bioaccumulation factor (T.E.S.T. 4.1). T.E.S.T. allowed a user to estimate without requiring any external programs. Users could input a chemical to be evaluated by drawing it in an included chemical sketcher window, entering a structure test file. Once a chemical had been entered , its toxicity was estimated using QSAR methodology.

TABLE -1 : Herbicide Bioaccumulation Factor Prediction

S. No.	Name	ID	Cid	Experimental Value Log10	Predicted Value Log10	Experimental Value	Predicted Value	Structure
1	2,4-Dichlorophenoxy	2-(2,4-dichlorophenoxy)acetic acid	1486	-0.50	0.71	0.32	5.12	
2	Atrazine	6-chloro-N4-ethyl-N2-propan-2-yl-1,3,5-triazine-2,4-diamine	2256	0.56	0.96	3.61	9.18	
3	Bentazone	2,2-dioxo-3-propan-2-yl-1H-2$l^{6},1,3-benzothiadiazin-4-one	2328	N/A	N/A	N/A	N/A	
4	Dicamba	3,6-dichloro-2-methoxybenzoic acid	3030	N/A	0.50	N/A	3.17	
5	Dichlobenil	2,6-dichlorobenzonitrile	3031	N/A	1.36	N/A	22.68	
6	Diuron	3-(3,4-dichlorophenyl)-1,1-dimethylurea	3120	0.74	1.31	5.46	20.56	
7	Glyphosate	2-amino-4-[hydroxy(methyl)phosphoryl]butanoic acid	4794	N/A	-1.14	N/A	7.21E-02	
8	Simazine	6-chloro-N2,N4-diethyl-1,3,5-triazine-2,4-diamine	5216	1.11	0.63	12.83	4.30	
9	Trifluralin	2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)aniline	5569	3.51	2.17	3261.00	147.54	
10	Mecoprop	2-(4-chloro-2-methylphenoxy)propanoic acid	7153	0.48	0.54	3.00	3.47	
11	Naptalam	2-[(1-naphthalenylamino)-oxomethyl]benzoic acid	8594	N/A	0.95	N/A	8.96	
12	Linuron	3-(3,4-dichlorophenyl)-1-methoxy-1-methylurea	9502	1.29	N/A	19.49	N/A	
13	Bensulide	N-[2-[di(propan-2-yloxy)phosphinothioylthio]ethyl]benzenesulfonamide	12932	N/A	1.06	N/A	11.61	
14	EPTC	N,N-dipropylcarbamothioic acid S-ethyl ester	12968	N/A	1.01	N/A	10.19	

15	Bromoxynil	C1_1371279871797	15531	0.84	1.36	6.84	22.73	
16	Clopyralid	3,6-dichloro-2-pyridinecarboxylic acid	15553	0.00	0.43	1.00	2.72	
17	Napropamide	N,N-diethyl-2-(1-naphthalenyloxy)propanamide	27189	N/A	1.87	N/A	74.79	
18	Metribuzine	4-amino-6-tert-butyl-3-(methylthio)-1,2,4-triazin-5-one	30479	N/A	N/A	N/A	N/A	
19	Propyzamide	3,5-dichloro-N-(2-methylbut-3-yn-2-yl)benzamide	32154	N/A	N/A	N/A	N/A	
20	Amitraz	N'-(2,4-dimethylphenyl)-N-[(2,4-dimethylphenyl)iminomethyl]-N-methylmethanimidamide	36324	3.26	2.26	1838.00	183.65	
21	Oxyfluorfen	2-chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene	39327	N/A	2.34	N/A	217.77	
22	Difenzoquate	1,2-dimethyl-3,5-diphenylpyrazol-1-ium	39425	N/A	N/A	N/A	N/A	
23	Hexazinone	3-cyclohexyl-6-(dimethylamino)-1-methyl-1,3,5-triazine-2,4-dione	39965	0.85	0.78	7.00	5.99	
24	Diclofop-methyl	2-[4-(2,4-dichlorophenoxy)phenoxy]propanoic acid methyl ester	39985	N/A	2.67	N/A	465.38	
25	Ethalfluralin	N-ethyl-N-(2-methylprop-2-enyl)-2,6-dinitro-4-(trifluoromethyl)aniline	41381	N/A	2.52	N/A	334.39	
26	Fluroxypyr	2-[(4-amino-3,5-dichloro-6-fluoro-2-pyridinyl)oxy]acetic acid	50465	1.79	0.56	62.10	3.63	

27	Sethoxydim	2-[1-(ethoxyamino)butylidene]-5-[2-(ethylthio)propyl]cyclohexane-1,3-dione	52923	N/A	N/A	N/A	N/A	
28	Metsulfuron	2-[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]-oxomethyl]sulfamoyl]benzoic acid methyl ester	52999	N/A	-0.20	N/A	0.63	
29	Imazethapyr	5-ethyl-2-(4-methyl-5-oxo-4-propan-2-yl-1H-imidazol-2-yl)-3-pyridinecarboxylic acid	54740	0.20	0.95	1.60	8.96	
30	Nicosulfuron	2-[[[(4,6-dimethoxy-2-pyrimidinyl)amino]-oxomethyl]sulfamoyl]-N,N-dimethyl-3-pyridinecarboxamide	73281	N/A	-0.40	N/A	0.40	
31	Isoxaben	2,6-dimethoxy-N-[3-(3-methylpentan-3-yl)-5-isoxazolyl]benzamide	73672	N/A	1.55	N/A	35.57	
32	Thifensulfuron	3-[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]-oxomethyl]sulfamoyl]-2-thiophenecarboxylic acid methyl ester	73674	-0.10	-0.13	0.80	0.74	
33	Ethametsulfuron	2-[[[[4-ethoxy-6-(methylamino)-1,3,5-triazin-2-yl]amino]-oxomethyl]sulfamoyl]benzoic acid	86304	N/A	-0.69	N/A	0.20	
34	Quinclorac	3,7-dichloro-8-quinolinecarboxylic acid	91731	-0.10	0.79	0.80	6.15	
35	Tralkoxydim	2-[1-(ethoxyamino)propylidene]-5-(2,4,6-trimethylphenyl)cyclohexane-1,3-dione	91746	N/A	N/A	N/A	N/A	

36	Rimsulfuron	1-(4,6-dimethoxy-2-pyrimidinyl)-3-[(3-ethylsulfonyl-2-pyridinyl)sulfonyl]urea	91779	N/A	-0.21	N/A	0.61	
37	Clodinafop-propargyl	(2R)-2-[4-[(5-chloro-3-fluoro-2-pyridinyl)oxy]phenoxy]propanoic acid prop-2-ynyl ester	92431	N/A	N/A	N/A	N/A	
38	Fluazifop-p-butyl	C1_13757139466860	3033674	N/A	2.09	N/A	124.23	
39	Imazamethabenz	4-methyl-2-(4-methyl-5-oxo-4-propan-2-yl-1H-imidazol-2-yl)benzoic acid	303482	N/A	0.65	N/A	4.50	
40	Glufosinate ammonium	-	11564649	No data available	--	--	--	

Results and Discussion

Prediction of 40 Herbicides was done for bioaccumulation factor with the help of T.E.S.T. (4.1) software. It was observed that out of 40 insecticides experimental log 10 value for bioaccumulation factor of 24 herbicides and predicted log 10 values of 8 herbicides were not available. Experimental log 10 value of one herbicides was greater than 3.50 (value recorded 3.51). It means it was potent to BAF. Out of 40 herbicides , experimental log10 value for BAF of 14 herbicides and log10 value of 31 herbicides are below 3.50. It means that these herbicides were not potent to BAF.

Conclusion

The study was untaken to determine the bioaccumulation factor of 40 Herbicides. In present analysis it was found that out of 40herbicides one is potent and others are safe to use. Now I conclude that the herbicides which are showing potent values, should be tested *in vivo or in vitro*.

References

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2. U.S. Environmental Protection Agency Bioaccumulation Analysis Workgroup Washington, DC 20460February 2000