IJPSR (2014), Vol. 5, Issue 12 **(Research Article)**

INTERNATIONAL JOURNAL OF PHARMACEUTICAL SCIENCES AND RESEARCH

Received on 10 May, 2014; received in revised form, 07 July, 2014; accepted, 18 August, 2014; published 01 December, 2014

PREDICTION OF LD_{50} OF SOME COMMON PESTICIDES THROUGH QSAR (AN ALTERNATIVE METHOD TO SAVE EXPERIMENTAL ANIMALS)

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Keywords:

Toxicity, QSAR, Pesticides, LD $_{50}$

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ABSTRACT: The most common test of acute toxicity is the LD_{50} test. LD_{50} means, the lethal dose of a substance that will kills 50% of animals. But this requires large number of animals. To reduce the sacrifice of animals. In present study we are using QSAR based software T.E.S.T. (toxicity estimation search tool 4.1 version) for predicting oral LD_{50}. For prediction of oral LD_{50} we have taken 100 insecticides, 40 fungicides and 40 herbicides. During our analysis we find that for experimental oral LD $_{50}$, 27 insecticides are highly (value between 5-50) and 36 are moderate potent (value between 50-500). For predicted oral LD $_{50}$ value, 24 insecticides are highly and 34 are moderate potent. For fungicides 3 experimental and 3 predicted are moderate potent. For herbicides 6 experimental and 7 predicted herbicides are moderate LD $_{50}$ potent.

INTRODUCTION: Acute toxicity of a drug can be determined by the calculation of LD_{50}, i.e., the dose that will kill 50% of animals of a particular species. Many different substances are tested in this way, including all drugs, agricultural chemicals, cleaners, some cosmetics and their ingredients[1]. The smaller the LD_{50} value, the more toxic is chemical. The opposite is also true: the larger the LD_{50} value, the lower the toxicity. It was developed in 1920's and called "classical LD50" involved 100 animals for 5 dose-groups, later in 1981 it was modified by the Organization for Economic Cooperation and Development (OECD) and reduced number upto 30 for 3 dose-groups. In 1987 further reduced to 20 animals [2].

QUICK RESPONSE CODE

DOI: 10.13040/IJPSR.0975-8232.5(12).5356-73

Article can be accessed online on: www.ijpsr.com

DOI link: http://dx.doi.org/10.13040/IJPSR.0975-8232.5(12).5356-73

Mice, rats, rabbits, guinea pigs, cats, dogs, fish, monkeys and birds are used for LD_{50} study[3]. The LD_{50} values of a new drug are determined by various route of administration (intravenous, intraperitoneal, subcutaneous and oral) [4]. Results of LD_{50} study may affected by some factors which are - Species, Age, Sex, Amount of food, Social environment, Route of exposure (oral, dermal, inhalation) and Physical environment such as temperature and humidity.

FRAME (Fund for the Replacement of Animals in Medical Experiment) believes that the lethal dose test is unnecessarily cruel and scientifically invalid. The test involves giving groups of animal doses of a test substance until it kills half of them. Several countries, including the UK, have taken steps to ban the oral LD_{50} and the OECD; the International government's advisory body abolished the requirement for the oral test in 2001[5]. Patricia *et.al.* predicted acute mammalian toxicity for sulphur mustard and its breakdown products with the help of QSAR.[6]

Quantitative Structure Activity Relationships (QSARs) are mathematical models that are used to predict measures of toxicity from physical characteristics of the structure of chemicals (known as molecular descriptors). Acute toxicities (such as the concentration which causes half of fish to die) are one example of toxicity measures which may be predicted from QSARs (http://www.epa.gov/nrmrl/std/cppb/war/sim_war.htm).[7]

The QSAR models used for regulatory purposes should be associated with the following purposes.

- To defined end points
- An unambiguous algorithm
- Appropriate measures of goodness-of-fit robustness and predictability
- A mechanistic interpretation if possible.

Generally, the prime aim in developing QSAR is so that it can be used for predicting purposes. It is therefore important that the statistics given with the QSAR give an indication of its predictability.

MATERIALS AND METHODS:

Materials: Tools and Databases

Tools: Toxicity Estimation Software Tool (T.E.S.T. Version 4.1) is used.8

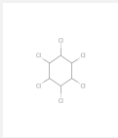
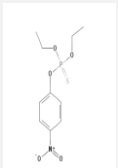
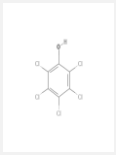
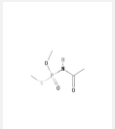
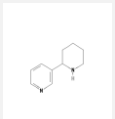
Databases: Pubchem is used as a detabase

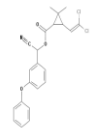
Methodology: A list of common pesticides is prepared and there structure files are derived from the database. QSAR methodology is used to determine the LD_{50} of 180 pesticides. LD_{50} potent insecticides, fungicides and herbicides are selected and studied further and results are discussed.

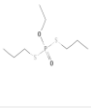
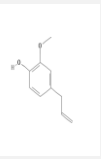
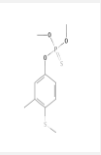
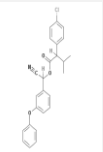
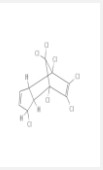
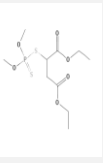
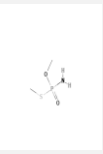
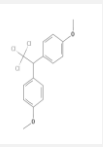
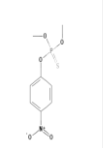
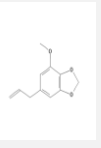
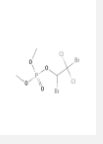
RESULTS AND DISCUSSIONS:

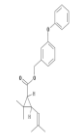
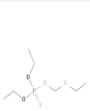
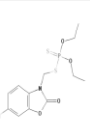
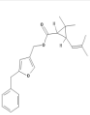
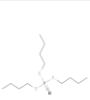
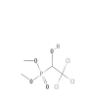
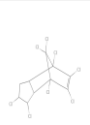
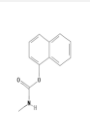
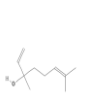
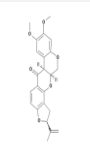
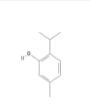
Prediction of LD_{50} of 100 Insecticides 40 fungicides and 40 Herbicides was done with the help of T.E.S.T. **(4.1 software)**.

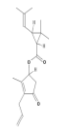
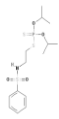
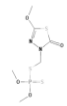
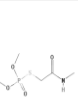
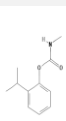
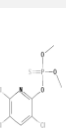
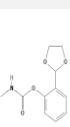
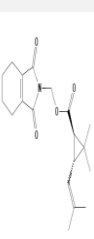
TABLE 1: INSECTICIDE ORAL LD_{50} PREDICTION

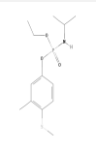
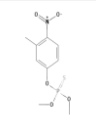
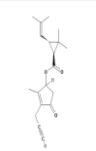
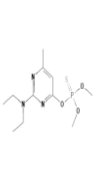
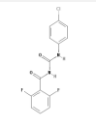
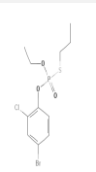
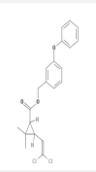
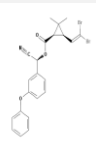
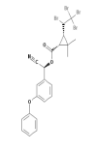
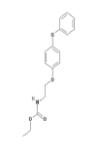
S. No.	Name	Experimental Value -Log10(mol/kg)	Predicted Value -Log10(mol/kg)	Experimental Value mg/kg	Predicted Value mg/kg	Structure
1	Clordecone	3.73	3.34	91.35	225.08	
2	Lindane	3.58	2.70	75.97	586.32	
3	Parathion	5.16	4.78	2.00	4.79	
4	Pentachlorophenol	3.99	3.07	27.00	226.83	
5	Acephate	2.42	2.72	699.68	345.72	
6	Anabasine	N/A	2.61	N/A	398.24	

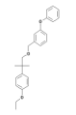
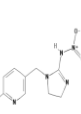
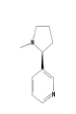
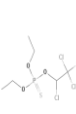
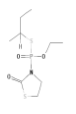
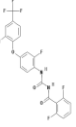
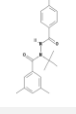
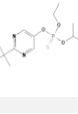
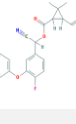
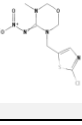
7	Azinphos-methyl	4.66	3.88	7.01	42.30	
8	Bendiocarb	3.75	3.92	39.98	26.63	
9	Caffeine	3.00	2.84	192.00	278.14	
10	Carbofuran	4.65	3.81	5.00	34.50	
11	Chlorpyrifos	3.63	3.51	82.00	107.95	
12	Cypermethrin	3.86	2.99	57.47	430.22	
13	Diazinon	3.66	3.37	65.98	130.65	
14	Dichlorvos	4.11	4.22	17.00	13.45	
15	Dimethoate	3.58	3.34	60.03	104.69	
16	Disulfoton	5.02	4.61	2.60	6.79	
17	Endosulfal	3.73	3.61	75.95	98.84	

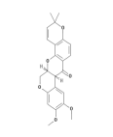
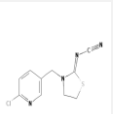
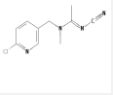
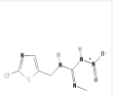
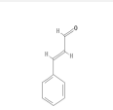
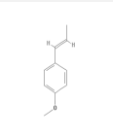
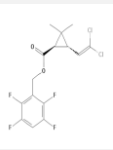
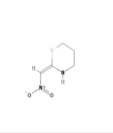
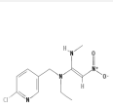
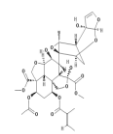
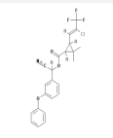
18	Ethoprop	3.85	3.96	34.00	26.31	
19	Eugenol	1.93	1.87	1929.42	2210.59	
20	Fenthion	3.19	3.74	180.14	50.71	
21	Fenvalerate	3.78	3.09	70.17	343.99	
22	Heptachlor	3.97	2.83	40.00	549.37	
23	Melathion	3.06	2.86	289.76	459.13	
24	Methamidophos	4.28	3.51	7.49	43.60	
25	Methoxychlor	2.27	2.60	1856.30	862.81	
26	Parathion-methyl	4.64	3.88	6.02	34.62	
27	Myristicin	1.65	1.91	4264.04	2380.80	
28	Naled	3.62	3.63	91.98	89.10	

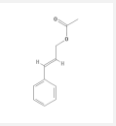
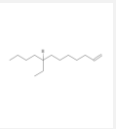
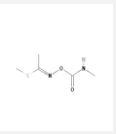
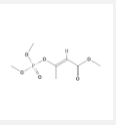
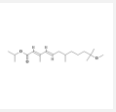
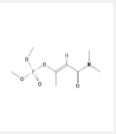
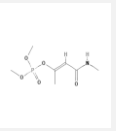
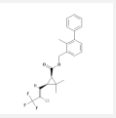
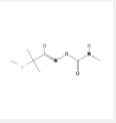
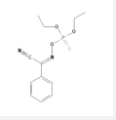
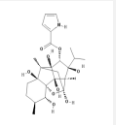
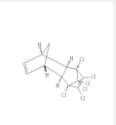
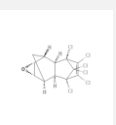
29	Oxydemeton-methyl	3.91	4.18	30.03	16.40	
30	Phenothrin	N/A	3.00	N/A	350.25	
31	Phorate	5.42	5.34	1.00	1.20	
32	Phosalone	3.64	3.15	85.05	259.48	
33	Resmethrin	2.44	2.77	1243.18	573.59	
34	Tribufos	3.32	3.12	149.87	239.71	
35	Trichlorfon	2.76	2.56	450.48	701.87	
36	Chlordane	3.31	2.76	199.77	714.47	
37	Carbaryl	2.94	2.72	229.99	383.64	
38	Linalool	1.74	1.88	2788.11	2054.27	
39	Derris	3.82	2.85	59.98	554.73	
40	Thymol	2.18	2.32	981.26	714.92	

41	Hexacloro benzene	1.46	2.59	9988.01	728.40	
42	Allethrin	2.64	2.91	684.94	374.43	
43	Phosmet	3.54	3.91	92.58	38.90	
44	Bensulide	3.17	3.69	271.28	81.59	
45	Methidathion	4.18	4.06	20.02	26.50	
46	Omethoate	3.85	3.42	29.98	81.12	
47	Myrex	3.37	3.78	234.85	90.73	
48	Isoprocarb	2.63	2.85	449.95	272.96	
49	Chlorpyriphos-methyl	2.25	2.73	1826.35	602.78	
50	Dioxacarb	3.95	3.12	24.99	168.86	
51	TEtramethrin	1.85	2.02	4638.93	3165.69	

52	Terbufos	5.26	5.06	1.60	2.53	
53	Fenamiphos	4.58	4.35	8.00	13.40	
54	Fenitrothion	3.04	3.81	249.97	43.33	
55	Prallethrin	2.82	2.14	459.98	2176.13	
56	Primiphos-methyl	2.39	2.82	1249.80	464.79	
57	Diflubenzuron	1.83	2.21	4638.11	1902.10	
58	Profefenofos	3.02	3.34	357.66	171.10	
59	Permethrin	3.01	2.59	383.28	1009.55	
60	Deltamethrin	3.80	3.77	80.07	85.76	
61	Tralomethrin	3.83	3.08	99.05	549.68	
62	Fenoxycarb	1.25	2.37	16791.91	1279.74	

63	Dieldrin	4.00	4.55	38.27	10.83	
64	Benzoylureas	N/A	1.97	N/A	1764.15	
65	Etofenprox	N/A	2.53	N/A	1111.77	
66	Imidacloprid	N/A	3.05	N/A	227.18	
67	Nicotianarustia	3.51	2.20	50.03	1018.97	
68	Chlorithoxyfos	5.22	2.99	2.00	340.53	
69	Fosthizate	3.70	3.85	57.07	40.43	
70	Flufenoxuron	N/A	2.94	N/A	560.01	
71	Tebufenozide	N/A	2.24	N/A	2024.28	
72	Phostebupirim	N/A	3.58	N/A	83.94	
73	Cyfluthrin	2.68	3.02	899.08	411.46	
74	Thiamethoxam	N/A	2.32	N/A	1393.74	

75	Deguelin	N/A	2.60	N/A	982.26	
76	Thiacloprid	2.76	2.31	444.32	1232.67	
77	Aletamiprid	N/A	2.52	N/A	678.93	
78	Clothianidin	N/A	2.44	N/A	898.84	
79	Cinnamaldehyde	N/A	1.75	N/A	2375.46	
80	Anethole	1.85	1.85	2088.85	2096.99	
81	Citral	2.48	1.70	499.56	3022.51	
82	Transfluthrin	N/A	3.56	N/A	103.38	
83	Nithiazine	N/A	2.15	N/A	1146.15	
84	Nitenpyram	2.24	2.45	1576.04	954.59	
85	Cyhazothrin	N/A	4.42	N/A	27.18	
86	Azadirachtin	3.90	3.01	55.99	442.40	

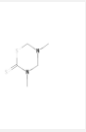
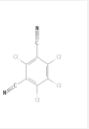
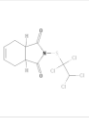
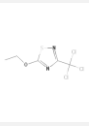
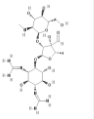
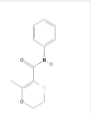
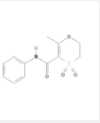
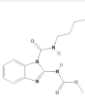
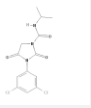
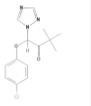
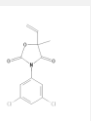
87	Cinnamyl acetate	1.73	1.78	3296.70	2937.49	
88	Tetrachlorvinphos	1.96	2.76	4003.44	633.60	
89	Methomyl	4.04	3.47	14.69	54.94	
90	Mevinphos	4.87	4.48	3.00	7.51	
91	Methoprene	1.09	1.86	25009.42	4263.43	
92	Dicrotophos	4.26	4.52	13.01	7.21	
93	Monocrotophos	4.45	4.42	7.99	8.40	
94	Bifenthrin	3.89	3.68	54.48	88.78	
95	Aldicarb	5.58	4.37	0.50	8.16	
96	Phoxim	3.00	2.82	299.71	452.50	
97	Ryanodine	2.82	3.65	750.56	109.34	
98	Aldrin	3.97	3.31	39.01	178.57	
99	Eldrin	4.00	4.55	38.27	10.83	
100	Polyketide	3.10	2.89	260.33	423.14	-

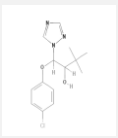
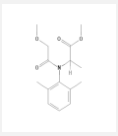
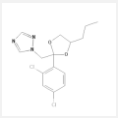
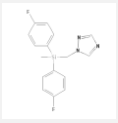
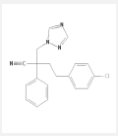
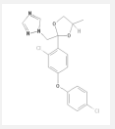
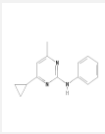
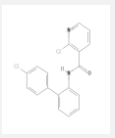
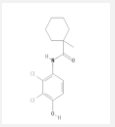
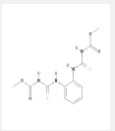
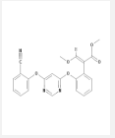
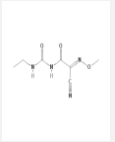
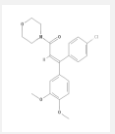
Prediction of oral LD 50 of 100 Insecticides were done with the help of T.E.S.T. (4.1) software. We analysed that out of 100 insecticides, experimental value of 16 insecticides were not available. 63 Insecticides were found to be LD50 potent. Out of 63 insecticides, experimental oral LD 50 value of 27 insecticides were highly potent (Value from 5-50 mg/kg) and experimental LD 50 value of 36 insecticides were moderate potent (value between 50-500) and predicted oral LD 50 value of 24 insecticides were highly and 34 were moderate potent (value between 50-500 mg/kg).

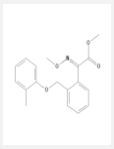
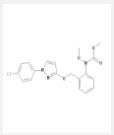
Further we observed that out of 100 insecticides oral LD 50 value of 33 predicted and 18 experimental insecticides were non toxic because their values were greater than 500 mg/kg. It means that the possibility of being lethal of these insecticides were very less.

TABLE 2: FUNGICIDE ORAL LD50 PREDICTION

S.No.	Name	Experimental Value -Log10(mol/kg)	Predicted Value -Log10(mol/kg)	Experimental Value mg/kg	Predicted Value mg/kg	Structure
1	Formaldehyde	N/A	N/A	N/A	N/A	
2	Thiabendazole	1.99	2.63	2078.64	472.52	
3	Thiram	2.63	2.20	559.86	1525.03	
4	Myclobutanil	2.26	2.17	1601.81	1966.01	
5	Dicloro	1.76	1.84	1945.54	1615.62	
6	Quintozene	2.43	2.03	1099.75	2777.18	
7	Dicloran	1.94	1.89	2398.90	2689.48	
8	Anilazine	2.01	2.25	2698.79	1564.98	
9	Captan	1.52	2.23	8994.75	1769.19	
10	Folpet	2.05	2.18	2637.01	1953.15	

11	Dazomet	2.70	2.92	320.14	195.88	
12	Chlorothalonil	1.42	2.26	9993.52	1452.63	
13	Difolatan	1.42	2.26	9993.52	1452.63	
14	Etridiazole	N/A	3.00	N/A	285.53	
15	Chloroneb	1.28	1.66	10992.49	4542.46	
16	Streptomycin sulphate	N/A	2.65	N/A	1303.38	
17	Carbathilin	2.74	2.47	430.21	801.79	
18	Oxycarboxin	2.13	2.20	2000.08	1679.38	
19	Carbendazim	1.48	2.10	6404.87	1523.79	
20	Benomyl	1.46	2.10	9998.54	2294.36	
21	Triforine	1.86	2.56	6004.40	1194.78	
22	Iprodione	1.98	2.08	3497.55	2776.64	
23	Triadiamefon	2.91	2.54	363.10	847.06	
24	Vinclozoline	1.46	2.21	9989.60	1776.31	

25	Triadimenol	1.89	2.40	3801.88	1179.80	
26	Metalaxyl	2.69	2.16	566.47	1941.47	
27	Propiconazole	2.35	2.52	1518.25	1026.26	
28	Flusilazole	2.67	2.30	674.38	1588.08	
29	Fenbuconazole	N/A	2.54	N/A	976.38	
30	Difenoconazole	N/A	2.54	N/A	976.38	
31	Cyprodinil	N/A	2.39	N/A	909.20	
32	Boscalid	N/A	1.97	N/A	3707.00	
33	Fenhexamid	N/A	2.64	N/A	686.15	
34	Thiophanate-methyl	1.71	2.29	6646.37	1764.70	
35	Azoxystrobin	N/A	2.77	N/A	688.92	
36	Cymoxanil	2.00	2.56	3896.80	1069.41	
37	Dimethomorph	N/A	2.20	N/A	1968.83	

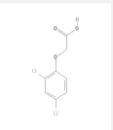
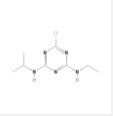
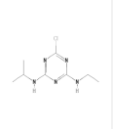
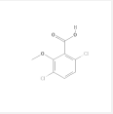
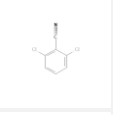
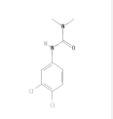
38	Kresoxim-methyl	N/A	N/A	N/A	N/A	
39	Pyrachlostobin	N/A	N/A	N/A	N/A	
40	Sulphur	N/A	2.81	N/A	655.39	

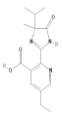
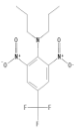
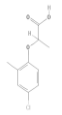
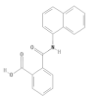
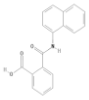
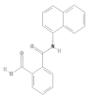
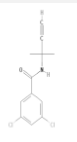
Prediction of oral L.D_{50} of 40 fungicides were done with the help of T.E.S.T. (Toxicity Estimation Software Tool 4.1 version).We analysed that out of 40 fungicides predicted oral LD 50 value of 34 fungicides and experimental oral LD_{50} value of 29 fungicides were greater than 500 mg/kg (50-500 mg/kg – Moderate toxicity). It means that the possibility of being lethal of these fungicides were very less or not toxic.

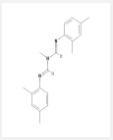
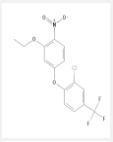
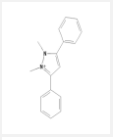
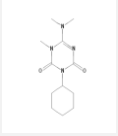
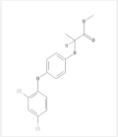
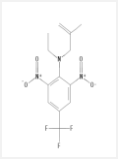
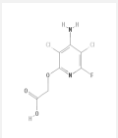
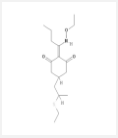
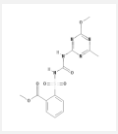
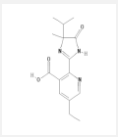
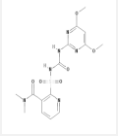
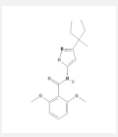
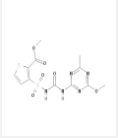
Further we observed that out of 40 fungicides predicted oral LD_{50} value of 3 fungicides (472.52, 195.88 and 285.83) and experimental oral LD_{50} value of 3 fungicides (320.14, 430.21 and 363.10) were below 500 mg/kg (value between 50-500 mg/kg moderate) it means that these fungicides had moderate toxicity.

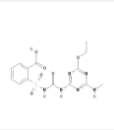
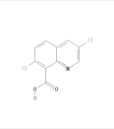
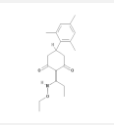
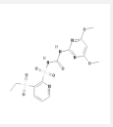
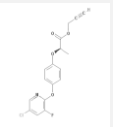
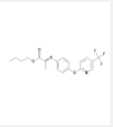
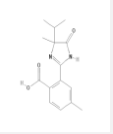
According to our T.E.S.T. analysis Predicted oral LD_{50} value of 3 fungicides and experimental oral LD_{50} value of 12 fungicides were not available.

TABLE 3: HERBICIDE ORAL LD_{50} PREDICTION

S No.	Name	Experi mental Value -Log10(mol/kg)	Predicted Value -Log10(mol/kg)	Experi mental Value mg/kg	Predicted Value mg/kg	Structure
1	2,4-Dichlorophenoxy	2.77	2.58	375.38	586.33	
2	Atrazine	2.51	2.15	672.81	1541.40	
3	Bentazone	2.34	2.18	1100.96	1587.99	
4	Dicamba	2.33	2.46	1038.65	762.69	
5	Dichlobenil	1.80	2.56	2707.41	472.73	
6	Diuron	2.36	2.48	1017.56	763.84	

7	Glyphosate	N/A	1.42	N/A	6933.86	
8	Simazine	2.32	2.21	972.04	1247.55	
9	Trifluralin	2.24	1.71	1929.57	6533.64	
10	Mecoprop	2.52	2.50	649.76	675.61	
11	Naptalam	1.55	1.70	8191.63	5852.01	
12	Linuron	2.34	2.38	1146.55	1026.80	
13	Bensulide	3.17	3.69	271.28	81.59	
14	EPTC	2.32	2.31	916.83	921.93	
15	Bromoxynil	3.16	3.30	189.82	139.81	
16	Clopyralid	1.65	1.96	4298.34	2096.18	
17	Napropamide	1.65	1.96	4298.34	2096.18	
18	Metribuzine	1.74	2.05	4995.67	2391.93	
19	Propyzamide	1.88	2.33	3353.34	1209.02	
20	Amitraz	2.86	3.27	400.44	156.96	

21	Oxyfluorfen	1.86	2.23	5004.64	2140.35	
22	Difenzoquate	2.72	2.64	469.71	577.60	
23	Hexazinone	2.17	1.98	1690.52	2670.13	
24	Diclofop-methyl	2.82	2.69	511.69	699.46	
25	Ethafluralin	1.52	2.24	9996.21	1935.70	
26	Fluroxypyr	2.02	2.85	2407.73	360.16	
27	Sethoxydim	N/A	2.25	N/A	1859.81	
28	Metsulfuron	N/A	1.89	N/A	4882.04	
29	Imazethapyr	N/A	2.72	N/A	547.47	
30	Nicosulfuron	N/A	2.21	N/A	2549.11	
31	Isoxaben	N/A	3.31	N/A	164.08	
32	Thifensulfuron	N/A	2.19	N/A	2486.60	
33	Ethametsulfuron	N/A	2.12	N/A	2984.84	

34	Quinclorac	2.04	1.97	2192.42	2575.35	
35	Tralkoxydim	N/A	2.38	N/A	1382.46	
36	Rimsulfuron	N/A	1.98	N/A	4508.78	
37	Clodnafop-propargyl	N/A	2.30	N/A	1750.95	
38	Fluazifop-p-butyl	2.12	2.42	2908.39	1447.95	
39	Imazamethabenz	N/A	2.78	N/A	458.33	
40	Glufosinate ammonium	No valid structure found	--	--	--	

Prediction of oral LD $_{50}$ of 40 Herbicides was done with the help of T.E.S.T 4.1 software. We analysed that out of 40 herbicides predicted LD $_{50}$ value of 7 herbicides (472.7, 81, 59, 139.81, 156.9, 360.16, 164.08 and 458.3) and experimental LD $_{50}$ Value of 6 herbicides (357.3, 271.2, 189.92, 400.4, 469.7 and 511) were moderate LD $_{50}$ potent (Value between 50-500 mg/kg).

Further we observed that out of 40 herbicides predicted LD $_{50}$ of 31 herbicides and experimental LD_{50} value of 22 herbicides were greater than 500 mg/kg body weight. It means that the possibility of being lethal of these herbicides were very less. The experimental value of 12 herbicides was not available. No valid structure and data was available for Imazamethabenz herbicide.

DISCUSSIONS: Out of 100 insecticides, 51insecticides (experimental+ predicted) are LD_{50}

potent. Out of 51 insecticides, 24 predicted highly LD $_{50}$ potent insecticides are Parathion,

Azinphosmethyl, Carbofuran, Diclorvos, Disulphoton, Ethoprop, Mathamidophos, Parathion

–methyl, Nailed, Oxydemeton- methyl, Phorate, Phosmet, Methidathion, Turbufos, Phenomiphos, Fenitrothion, Dieldrin, Fosthizale, Cyhazothrin, Mevinphos,Dicrotophos, Monocrotophos, Aldicarb, Eldrin **(Table 1)**.

Out of 51 insecticides, 27 insecticides with highly potent experimental LD_{50} values are Parathion, Pentachlorophenol, Azinphosmethyl, Bendiocarb, Carbofuran, Dichlorvos, Disulphoton, Ethoprop, Heptachlor, Methamidophos, Parathion- methyl,

Oxydemeton-methyl, Phorate, Methidathion, Omethoate, Dioxacarb, Terbufos, Fenaniphos, Dieldrin, Chlorithoxyfos, Methomyl, Mevinphos, Dicrotophos, Monocrotophos, Aldicarb, Aldrin, Eldrin **(Table 1).**

The insecticides whose both experimental and predicted LD_{50} values are highly potent – Parathion, Azinphosmethyl, Bendiocarb,

Carbofuran, Dichlorvos, Disulphoton, Ethoprop, Methamidophos, Parathion- methyl, Oxydemeton-methyl, Phorate, Methidathion, Terbufos, Fenaniphos, Dieldrin, Mevinphos, Dicrotophos, Monocrotophos, Eldicarb, Eldrin **(Table 1).**

These 20 insecticides are highly potent both in experimental and predicted value. So it is strongly recommended to check its mutagenicity and LD_{50} *in -vivo* and *in - vitro.*

Out of 40 fungicides 6 moderate LD_{50} potent fungicides are Thiabendazole, Etridiazale, Diazomet (3 predicted fungicides) and Carbathilin, Triadiamet, Diazomet (3 experimental fungicides). One fungicide with both experimental and predicted LD_{50} potent is Diazomet **(Table 2)**.

In herbicides 13 are moderate LD_{50} potent. 7 Predicted LD_{50} potent herbicides are Dichlobenil, Bensulide, Bromoxynil, Amitraz, Fluroxypyr, Isoxaben, Imazamethabenz and 6 experimental LD_{50} potent herbicides are 2,4-Dichlorophenoxy, Bensulide, Bromoxynil Amitraz, Difenzoquate, Diclofop-methyl .Both experimental and predicted moderate LD_{50} potent herbicides are Bensulide, Bromoxinil and Amitraz **(Table 3)**.

CONCLUSIONS: QSAR have long been used for predicting wide range of endpoints. In present analysis 180 pesticides were taken. We found that out of 180 pesticides (100 insecticides, 40 fungicides and 40 herbicides), value of experimental oral LD 50 for 27 insecticides are highly (value between 5-50) and 36 are moderate potent (value between 50-500). For predicted oral LD_{50} value, 24 insecticides are highly and 34 are moderate potent. For 40 fungicides, 3 experimental and 3 predicted fungicides are moderate LD_{50} potent. For 40 herbicides, 6 experimental and 7 predicted herbicides are moderate LD_{50} potent. Now we conclude that pesticides which have potent potential value should analyze with more than two predictor (Topkat, Admet) also for more reliability.

ACKNOWLEDGEMENT: We are thankful to BIFC DG (PG) College Kanpur, for providing laboratory facilities & encouragement during the study.

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How to cite this article:
Agrawal SP and Saxena VL: Prediction of LD_{50} of Some Common Pesticides through QSAR (An Alternative Method to Save Experimental Animals). Int J Pharm Sci Res 2014; 5(12): 5356-73. doi: 10.13040/IJPSR.0975-8232.5 (12).5356-73.