

## In Silico Toxicity Prediction of Some Common Insecticides

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**Abstract :** Insecticides are agents of chemical or biological origin that control insects. Control may result from killing the insects or otherwise preventing it from engaging in behaviors deemed destructive. Insecticides may be natural or manmade. In prediction of toxicity, the use of *in silico* prediction methods such as QSAR (Qantitative Stuructural Activity Relationship) model is required or encouraged in order to increase efficiency and minimize the reliance on animal testing. In the present study prediction of 100 insecticides for mutagenicity are done with the help of T.E.S.T.(Toxicity Estimation software Tool, 4.1 version). In our study we have analyzed that out of 100 insecticides experimental value of mutagenicity is not available for 60 insecticides which are predicted by T.E.S.T. Out of 100 insecticides 27 showed positive mutagenicity and 40 negative mutagenicity. There are 4 insecticides whose mutagenicity is experimentally positive but predicted value is negative. further in our analysis we have observed that there are 3 insecticides whose mutagenicity is experimentally negative but predicted value is positive.

Key words: Insecticides, Mutagenicity and QSAR.

#### **INTRODUCTION**

We live in a world of chemicals. More than 60 million chemical compounds were known to exist as of 26 May 2011 . Fortunately we are exposed to only a fraction of these during our lifetime (Front Pharmecol 2011). Insecticides are agents of chemical or biological origin that control insects. Insecticides may be natural or manmade and are applied to target pests in a myriad of formulations and delivery systems (sprays, baits, slowrelease diffusion, etc.). Some insecticides harm water quality or affect organisms in other ways; for example, the insecticide carbaryl (a carbamate insecticide) is listed as a carcinogen by the state of California and as a possible hormone disruptor by the state of Illinois' EPA (Katarina L 2011). The newer insecticides are designed to be more

\*Correspondent author : Phone : 09335014995 E-mail : agrawals111@yahoo.in specific and less persistent in the environment. Many studies worldwide have reported the presence of DDT and its metabolites in samples of breast milk. In Dehli, a breast feeding infant receives 12 times the acceptable limit of DDT and in Brazil 4 times that limit. In Zimbabwe, studies in some regions have found all the samples of breast milk contaminated with DDT. Mohamed.H. (2003) investigated 15 different types of canned and frozen fruits and vegitables samples and found residue of pyrithroids, herbicides, fungicides and carbamates in different food samples. HCH, DDT, aldrin, dieldrin, endrin, chlordane, heptachlor, toxaphene, HCB are organochlorin which are environmentally persistent semi-volatile, highbioaccumulative and high toxic (Yu et al., 2005). According to a report of WHO and UNEP, worldwide there are more than 26 million human pesticide poisonings with about 220,000 deaths per year (Richter, 2002).

In Present study we have analysed 100 insecticides

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An International Biannual Refereed Journal of Life Sciences

for their mutagenicity.

### **MATERIALS & METHODS**

The analysis of mutagenicity of insecticides are done with the help of T.E.S.T.(toxicity estimation tool test ) software 4.1version.The structure of a chemical simply entered through importing it from a database of structures. After entering the structure , insecticides toxicity are estimated using its advanced methodologies.

### RESULTS

Prediction of Mutagenicity of 100 Insecticides were done with the help of T.E.S.T. (4.1 software). During

this analysis we observed that out of 100 insecticides, experimental value of 27 insecticides were found to be positive mutagenic agent. So there is a strong need to check their genotoxic levels *in vitro* or *in vivo*. Other 40 insecticides are negative mutagenic agent.

We also observed that there are 4 insecticides whose experimental mutagenicity are positive and predicted mutagenicity negative. And other 3 insecticides are showing experimental value negative and predicted value positive.

We also observed that out of 100 insecticides mutagenicity of 60 insecticides are not available.

ID	INSECTISIDE	EXPERIMENTAL	PREDICTED	STRUCTU RE
1-cid991	Parathion	Negative	Positive	X
2-cid2566	Carbofuran	Negative	Positive	ž
3 - cid 3039	Dichlorvos	Positive	Negative	Ser.
4-cid3082	Dimethoate	Positive	Negative	44
5-cid4420	Naled	N/A	Positive	44
6-cid4618	Oxydemeton- methyl	N/A	Positive	
7-cid4767	Phenothrin	Positive	Negative	0.04 M

 Table I :Result of Insecticides Mutaginicity

# Agrawal et al. : In Silico Toxicity Prediction of Some Common Insecticides

### Table I continued....

8-cid 11442	Allethrin	N/A	Positive	JAN AN
9-cid 12932	Bensulide	N/A	Positive	the the
10-cid 13709	Methidathion	N/A	Positive	4
11-cid 17517	Isoprocarb	N/A	Positive	45
12-cid 21803	Chlorpyriphos- methyl	Negative	Positive	xf.
13-cid 23421	Dioxacarb	N/A	Positive	*\$
14-cid 24365	Tetramethrin	N/A	Positive	det x
15-cid 51605	Fenoxycarb	N/A	Positive	Por x
16- cid 86418	Imidacloprid	N/A	Positive	
17-107646	Thiamethoxam	N/A	Positive	τά <sup>δ</sup>
18-cid 107935	Deguelin	N/A	Positive	×09265.

Table I continued....

## Biospectra : Vol. 8(2), September, 2013, Special issue.

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19-cid 115224	Thiacloprid	N/A	Positive	.005
20-cid 213021	Aletamiprid	N/A	Positive	.00
21-cid 213027	Clothianidin	N/A	Positive	sy's
22- cid656612	Transfluthrin	N/A	Positive	, XI. XI.
23-cid3034287	Nitenpyram	N/A	Positive	itro.
24-cid 5353758	Methomyl	N/A	Positive	
25-cid 5371560	Dicrotophos	N/A	Positive	-\$+ <del>1</del> 4
26-cid 5371562	Monocrotophos	Positive	Negative	
27-cid 56660531	Polyketide	N/A	Positive	Julie

#### **DISCUSSION**

The environmental pollution caused by pesticides in Asia, Africa, Latin America, the Middle East and Eastern Europe are now serious. Even in earlier years the residuals of DDT, lindane and dieldrin in fish, eggs and vegetables have been much beyond the safe range in India (Wu, 1986). In India the DDT content in human body was ever the highest in the world (IAEES 2011). As early as in 1972, the uses of DDT and related organochlorinated insecticides were banned in the United States (SDNX, 2005). Chen (2004) found that the incidence of breast cancer was linearly correlated with the frequency of pesticide uses, and organochlorined pesticide, DDT, and its derivative, DDE, is likely responsible for breast cancer. Women who are pregnant or breast-feeding should check with their doctors before working with pesticides (insecticides, herbicides or fungicides) as some pesticides may be harmful to the fetus (unborn baby) or to breastfed infants.( CCHS 2010). In present study, like other studies we have also analysed mutagenicity of different insecticides .

### **CONCLUSION:**

QSAR have long been used for predicting wide range of endpoints. In present analysis, using QSAR methodology we have predicted mutagenicity of 100 insecticides.Out of 100 insecticides experimental value of 60 insecticides are not available in our T.E.S.T. analysis. So we have to check its mutagenicity experimentally. 27 insecticides are showing positive mutagenicity. Now we conclude that the insecticides which were showing potent values, have strong need to test in *vivo*.

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#### REFERENCES

- 1. Canadian Centre for Occupational Health & Safety, 2010: Copyright ©1997-2013.
- Chen JP, Lin G, Zhou BS. 2004. Correlation between pesticides exposure and mortality of breast cancer. China Public Health, 20: 289-290.
- 3. **Frontiers in Pharmacology, 2011.** In Silico Toxicologynon testing methods.
- 4. Katarina Lah, 2011. Biological Properties of Insecticides.
- 5. Mohamed H. EL-Saeid, 2003. Pesticide Residues in Canned Foods, Fruits, and Vegetables: The Application of Supercritical Fluid Extraction and Chromatographic Techniques in the Analysis, Research Article The Scientific World Journal (3), 1314–1326.
- Richter ED. 2002. Acute human poisonings. In: Encyclopedia of Pest Management (Ed D Pimentel). Dekker,New York, 3–6.
- 7. **SDNX. 2005**. Reduction situation of pesticide applications of some countries. Shandong Pesticide News, 11:34.
- 8. Yu G, Niu JF, Huang J, POPs, 2005. A New Global Environmental Problem. Science and Technology Press, Beijing, China.
- 9. Wen J, Zhang Fu, Bin J, Jian FO. 2011. Global pesticide consumption and pollution: with China as a focus. Proceedings of the International Academy of Ecology and Environmental Sciences, 2011, 1(2):125-144.
- Wu SP, Cao J, Li BG. 2003. Residues and distribution of organochlorine pesticides in airborne particles of different sizes from urban areas. Research of Environmental Sciences, 16(4): 36-39

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