

## Supplementary Material

### Predicting aquatic toxicities of benzene derivatives in multiple test species using local, global and interspecies QSTR modeling approaches

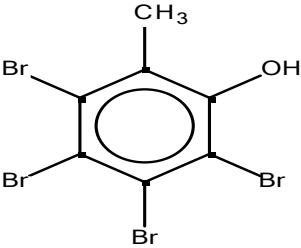
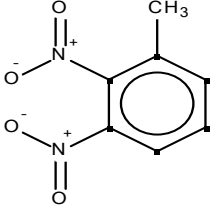
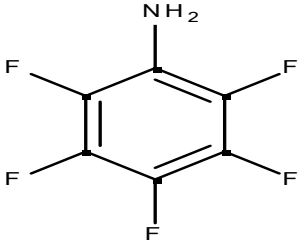
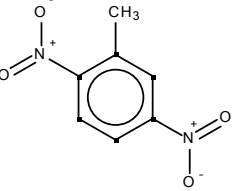
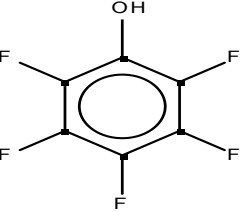
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CSIR-Indian Institute of Toxicology Research,  
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**\*Author for all correspondence**

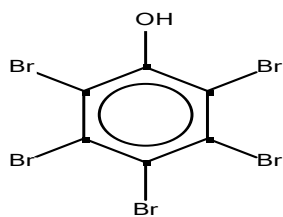
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**Table SI 1:** Structure influential chemicals and response outliers in L-QSTR models

Structure Influential chemicals		Response outliers	
Chemical name	Chemical structure	Chemical name	Chemical structure
<b>DTB L-QSTR model</b>			
3,4,5,6-Tetrabromo-o-cresol		2,3-dinitrotoluene	
Pentafluoroaniline		2,5-dinitrotoluene	
Pentafluorophenol			

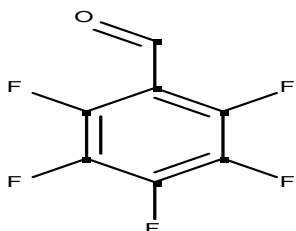
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Pentabromophenol



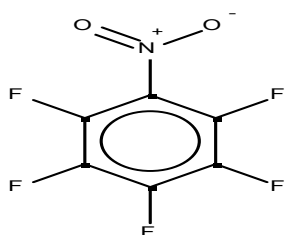
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Pentafluorobenzaldehyde



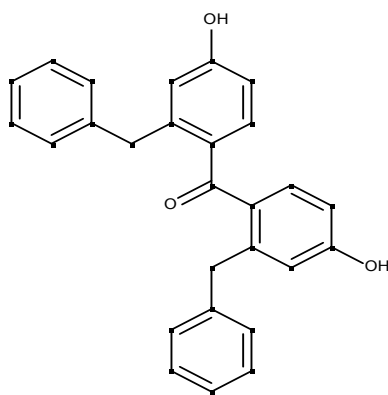
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Pentafluoronitrobenzene



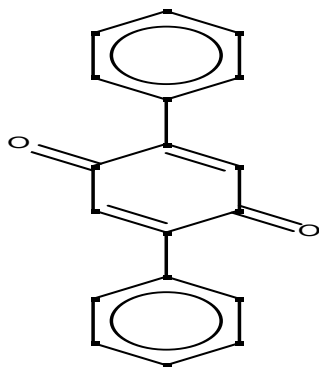
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Benzyl-4-hydroxyphenyl ketone

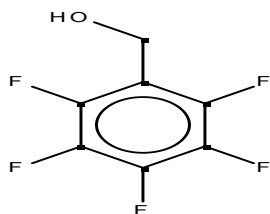


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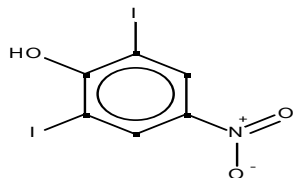
2,5-Diphenyl-1,4-benzoquinone



Pentafluorobenzyl alcohol

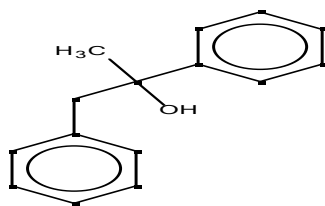


2,6-Iodo-4-nitrophenol

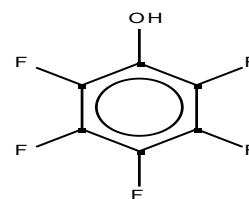


### SVM L-QSTR model

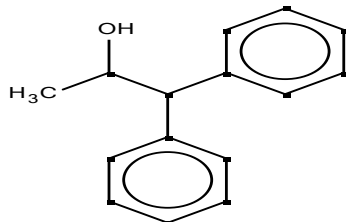
(±)-1,2-Diphenyl-2-propanol



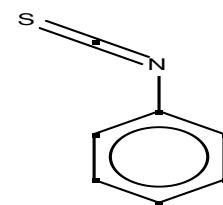
Pentafluorophenol



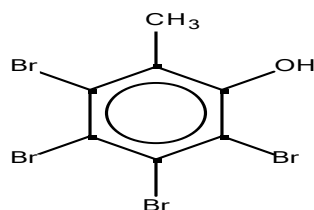
1,1-Diphenyl-2-propanol



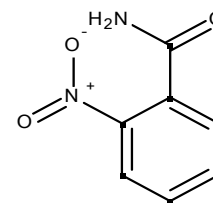
Phenyl isothiocyanate



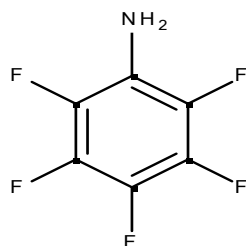
3,4,5,6-Tetrabromo-o-cresol



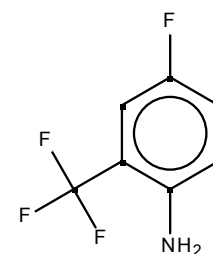
2-Nitrobenzamide



Pentafluoroaniline

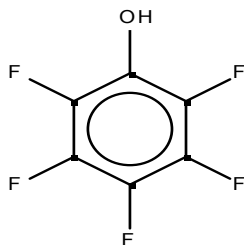


$\alpha,\alpha,\alpha,4$ -Tetrafluoro-o-toluidine



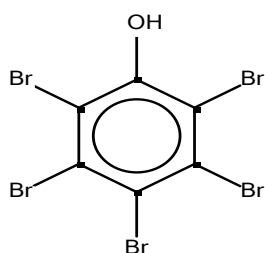
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Pentafluorophenol



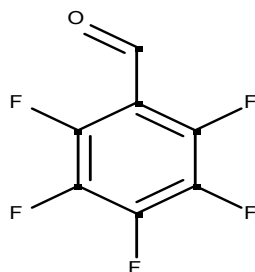
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Pentabromophenol



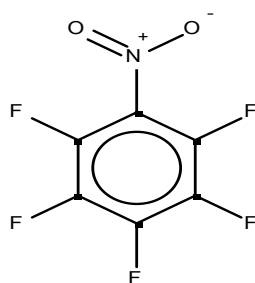
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Pentafluoro  
benzaldehyde



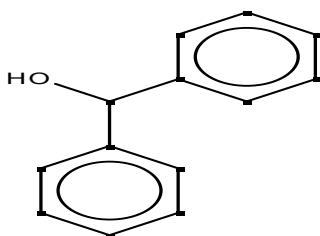
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Pentafluoro  
nitrobenzene



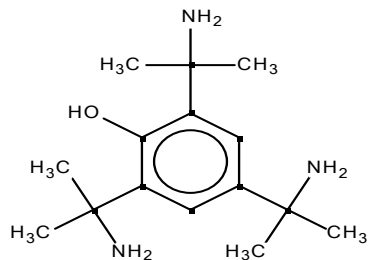
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Benzhydrol



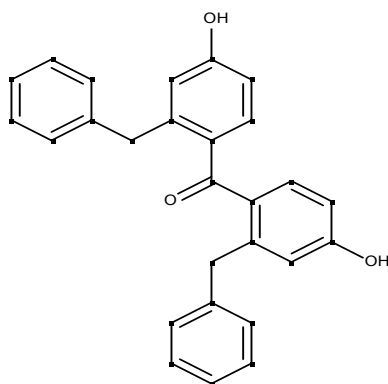
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2,4,6-tris-  
(Dimethylaminomethyl)  
phenol



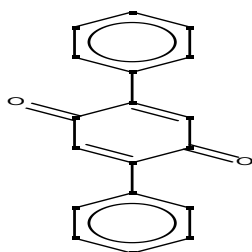
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Benzyl-4-  
hydroxyphenyl ketone



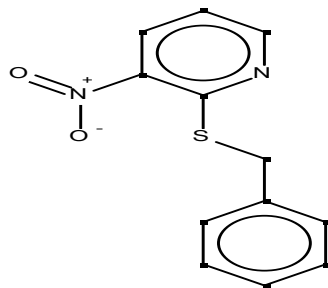
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2,5-Diphenyl-1,4-  
benzoquinone



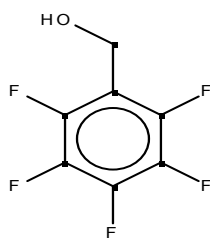
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2-(Benzylthio)-3-  
nitropyridine

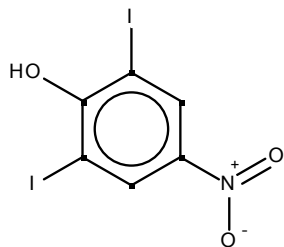


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Pentafluorobenzyl  
alcohol

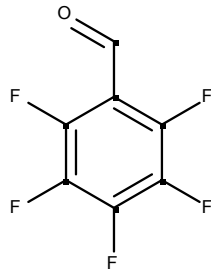


2,6-Iodo-4-nitrophenol

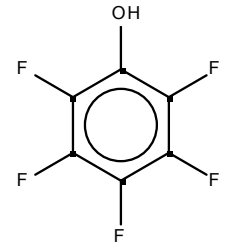
**Table SI 2:** structure influential chemicals and response outliers in G-QSTR models

Structure Influential chemicals		Response outliers	
Chemical name	Chemical structure	Chemical name	Chemical structure
		<b>S.no.</b>	
3,4,5,6-Tetrabromo-o-cresol		<b>1</b>	1,3-dichlorobenzene 
Pentauroaniline		<b>2</b>	2,5-dinitrotoluene 
Pentafluorophenol		<b>3</b>	2,6-dinitrotoluene 
2,6-Iodo-4-nitrophenol		<b>4</b>	2-methyl-3,6-dinitroaniline 

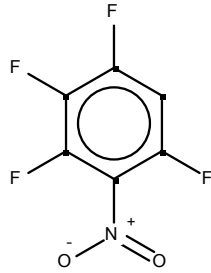
Pentafluorobenzaldehyde



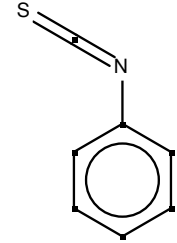
5 Pentafluorophenol



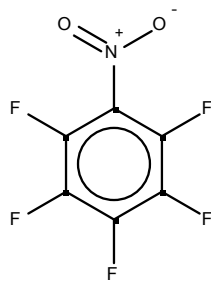
2,3,4,6-Tetrafluoronitrobenzene



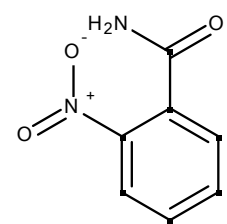
6 Phenyl isothiocyanate



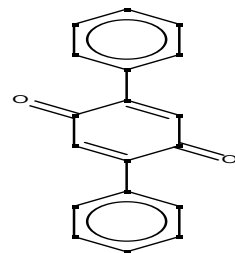
Pentafluoronitrobenzene



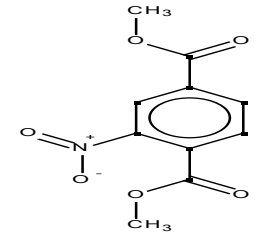
7 2-Nitrobenzamide



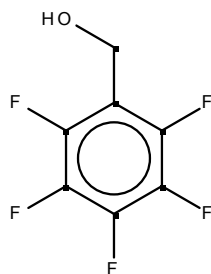
2,5-Diphenyl-1,4-benzoquinone



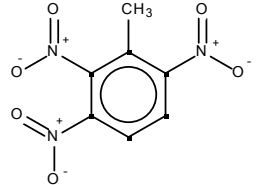
8 Dimethylnitroterephthalate



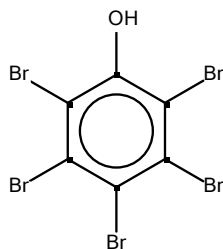
Pentafluorobenzyl alcohol



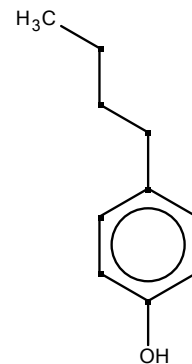
9 2,3,6-trinitrotoluene



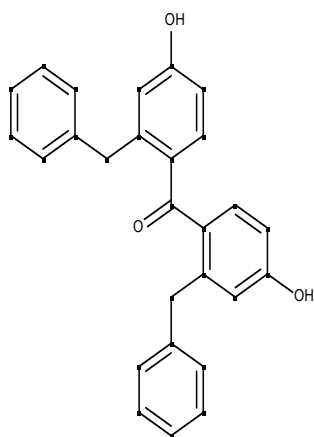
Pentabromophenol



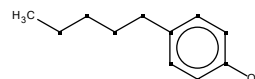
10 4-butylphenol



Benzyl-4-hydroxyphenyl ketone



11 4-pentylphenol



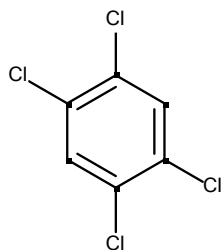
Response outlier no. 1-4 are present in DTB G-QSTR model; Response outlier no. 5-11 are present in SVM G-QSTR model

**Table SI 3:** structure influential chemicals in QAAR model for *P. reticulata*

**Chemical name**

**Chemical structure**

1,2,4,5-Tetrachlorobenzene





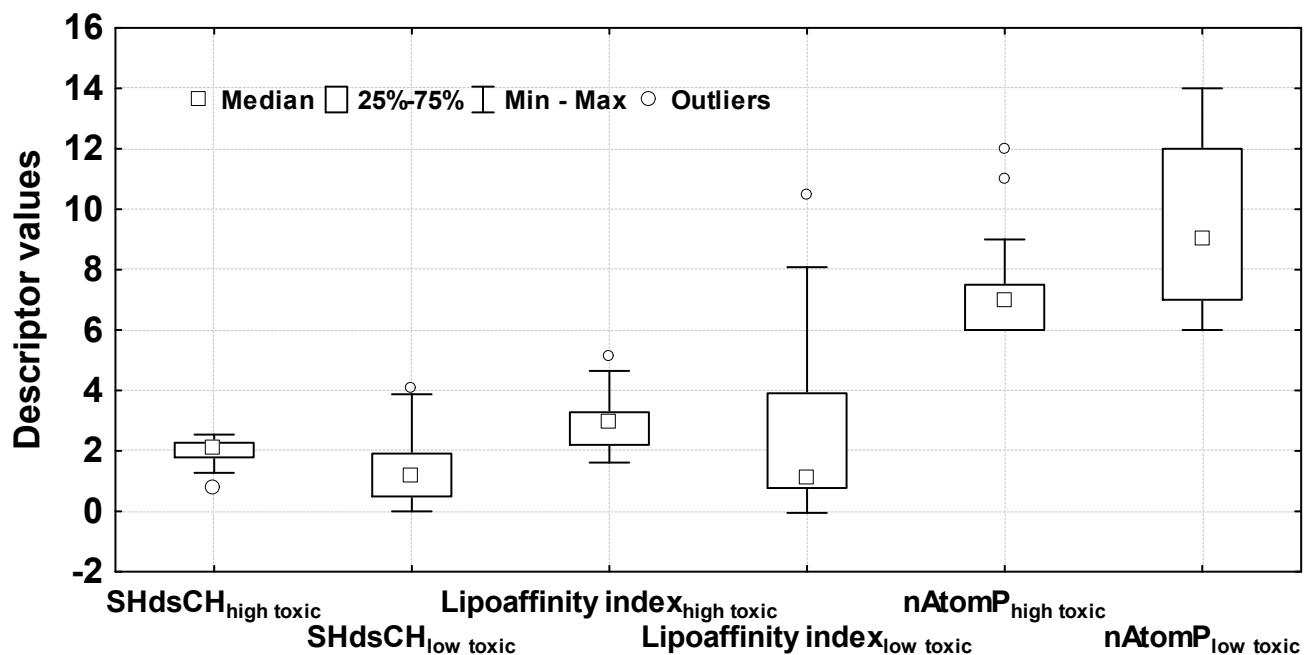
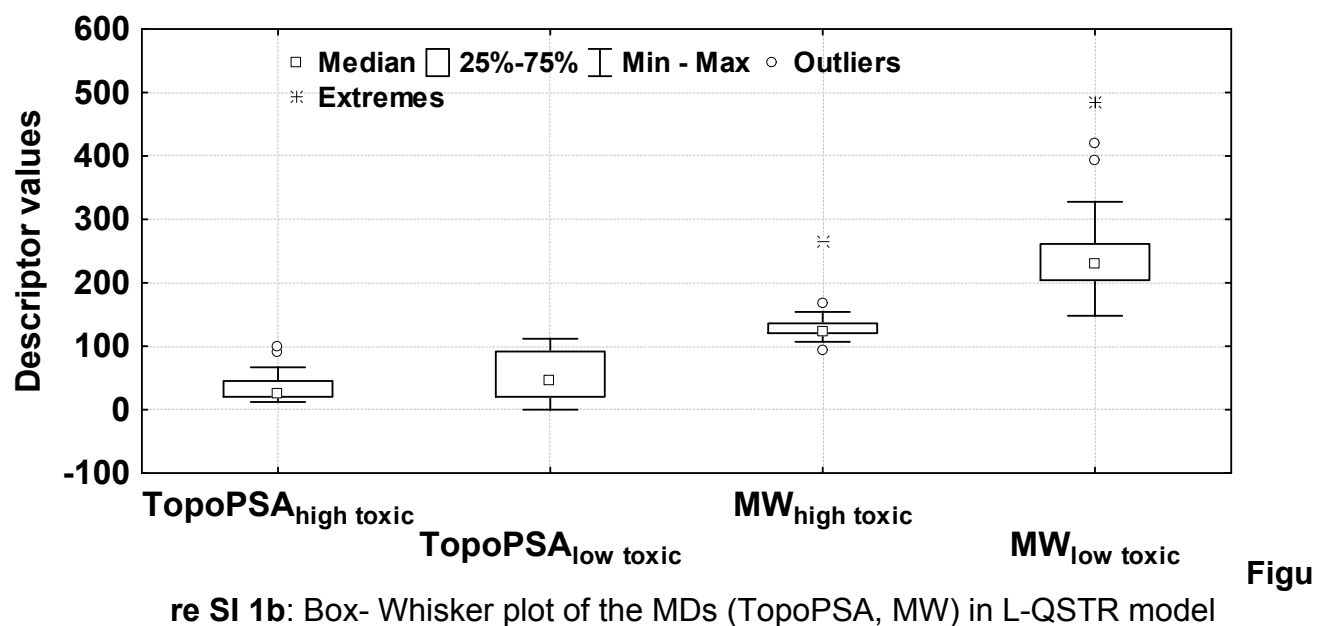


Figure SI 1a: Box- Whisker plot of the MDs (SHdsCH, Lipoaffinity index and nAtomP) in L-QSTR models



re SI 1b: Box- Whisker plot of the MDs (TopoPSA, MW) in L-QSTR model