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Accessory Information

Sorption of a Xenobiotic Contaminant in Clean and Petroleum-Contaminated Soil: Roles of Water and Xenobiotic Size

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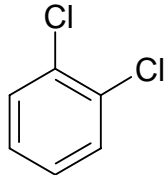
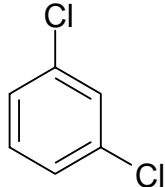
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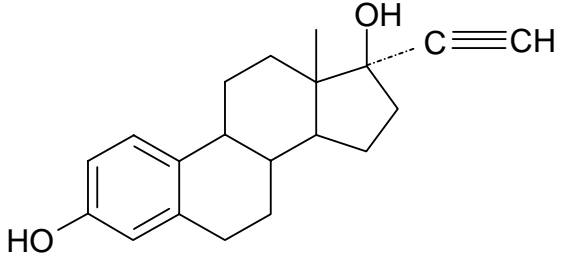
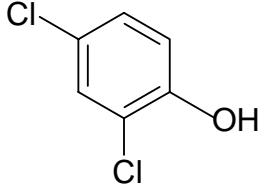
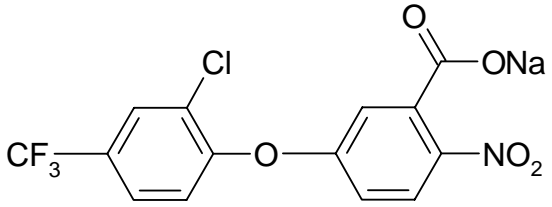
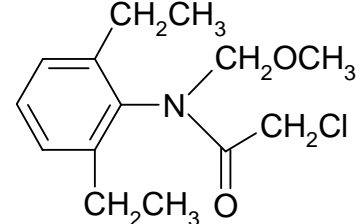
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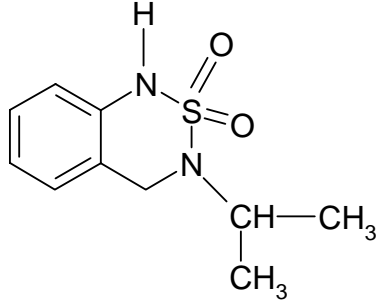
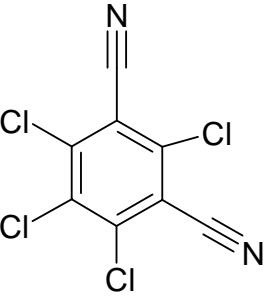
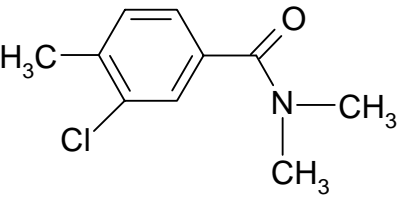
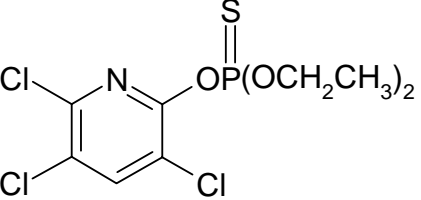
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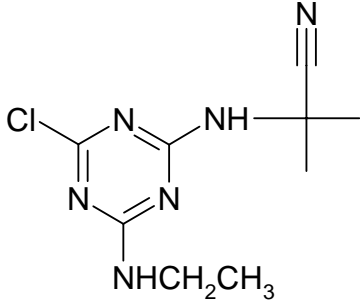
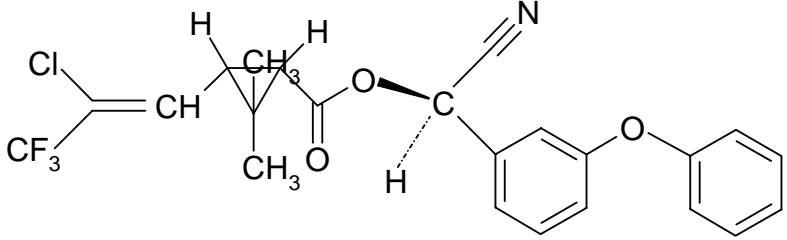
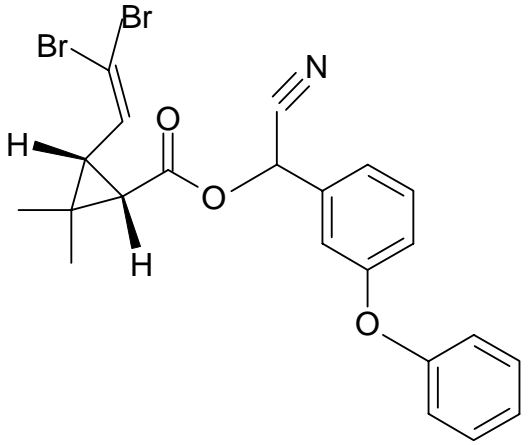
Supplementary material supporting Figure 4

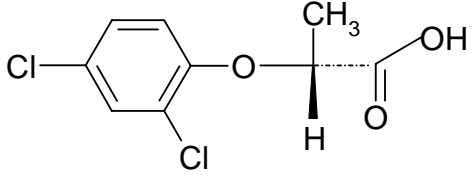
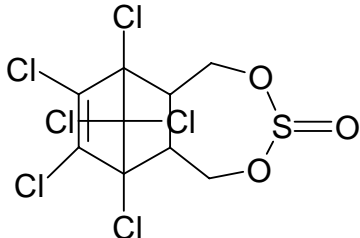
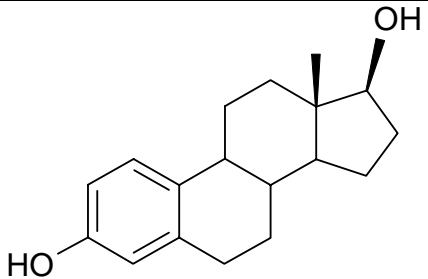
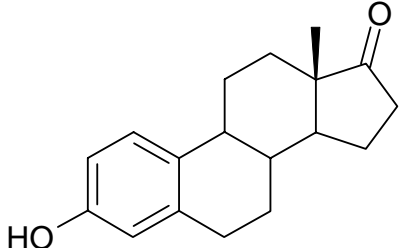
The following table identifies the studies found dealing with slow uptake. The structure of each pesticide (as used in the computer model) is shown with accompanying chemical and common names, longest axis ('size'), length of the uptake time in the study(s) reported (in days), and the references.

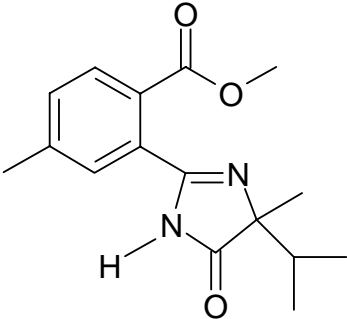
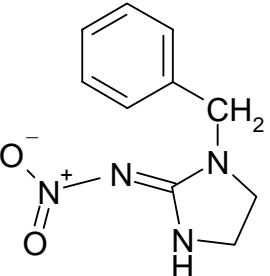
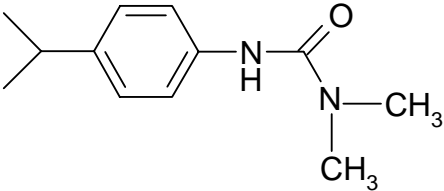
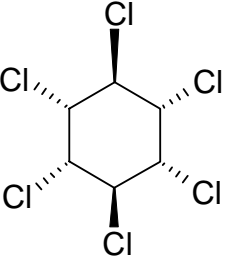
Structure	Name: 1. Common 2. Chemical	Size (Å)	Sorption study Time (d)	Reference
	1,2-dichlorobenzene	5.611	38	Deitsch et al, 1998. Deitsch et al, 2000. Culver et al, 2000.
	1,3-dichlorobenzene	5.592	30	Xia and Pignatello, 2001.

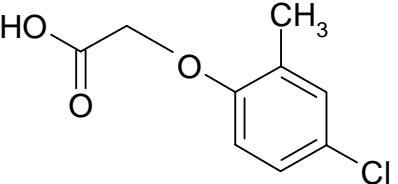
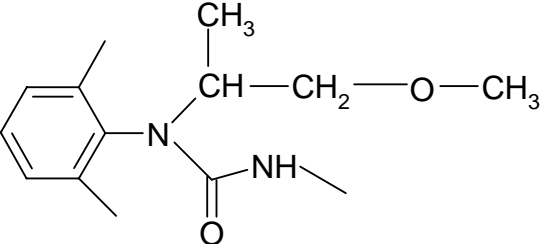
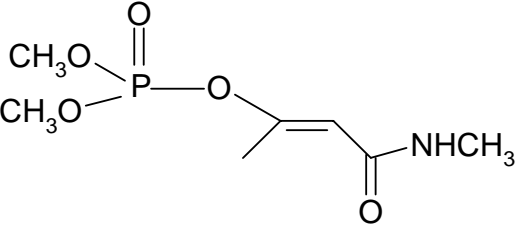
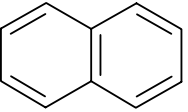
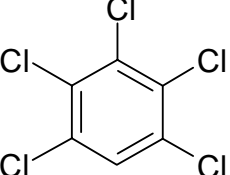
	17 α -ethinyl estradiol	13.865	0.37	Colucci and Topp, 2001.
	2,4-dichlorophenol	6.251	20	Xia and Pignatello, 2001. Zuloaga et al, 1999.
	Acifluoren 5-(2-chloro-4-(trifluoromethyl)phenoxy)-2-nitrobenzoic acid	12.235	1	Locke et al, 1997.
	Alachlor 2-chloro-2',6'-diethyl-N-(methoxy methyl)-acetanilide	8.653	14	Laabs et al, 2002.

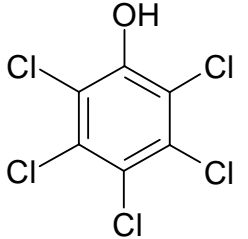
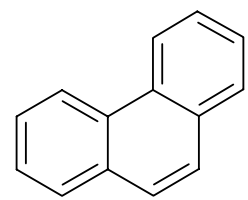
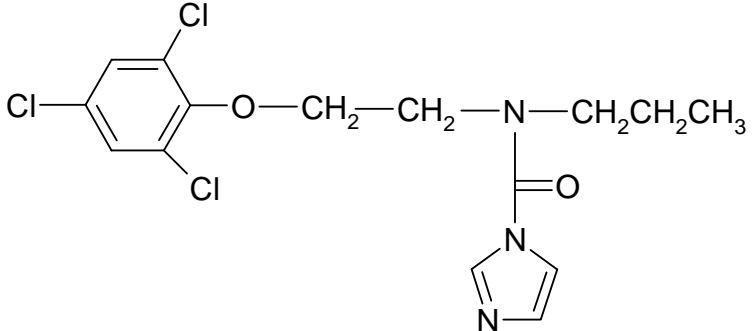
	<p>Bentazone</p> <p>3-isopropyl-1H-2,1,3-benzothiadiazin-4-(3H)-one-2,2-dioxide</p>	9.337	2.083	Thorstensen et al, 2001
	<p>Chlorothalonil</p> <p>Tetrachloroisophthalonitrile</p>	7.156	18	Gamble et al, 2000.
	<p>Chlortoluron</p> <p>1,1-dimethyl-3-(3-chloro-4-methylbenzene) urea</p>	9.587	10	Altfelder et al, 1999.
	<p>Chlorpyrifos</p> <p>O,O-diethyl-O-(3,5,6-trichloro-2-pyridinyl)phosphorothiolate</p>	11.527	2.5	Agdi et al, 2000.

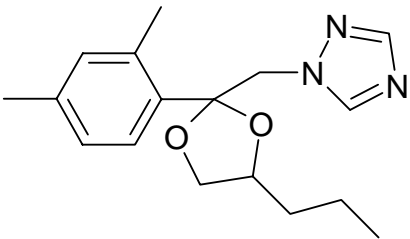
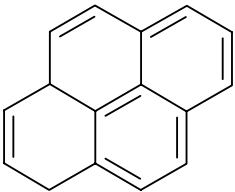
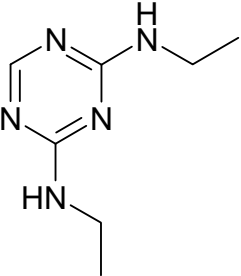
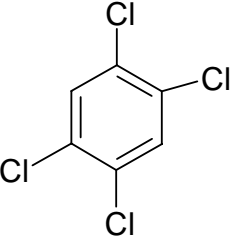
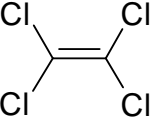
	<p>Cyanazine</p> <p>2-[[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl] amino]-2-methyl propane nitrile</p>	11.298	2	Reddy et al, 1998.
	<p>λ-cyhalothrin</p> <p>(RS)-α-cyano-3-phenoxybenzyl-3-(2-chloro-3,3,3-trifluoropropenyl)-2,2-dimethylcyclopropane carboxylate</p>	12.191	1.8	Reddy et al, 1998.
	<p>Deltamethrin</p> <p>(S)-α-cyano-3-phenoxybenzyl-(1R,3S)-3-(2,2-dibromo-vinyl)-2,2-dimethylcyclopropane carboxylate</p>	11.931	2.029	Zhu, 2002.

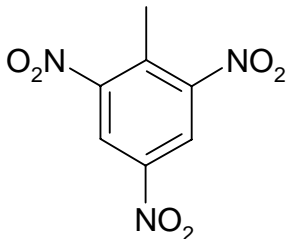
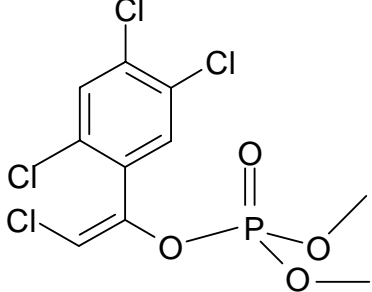
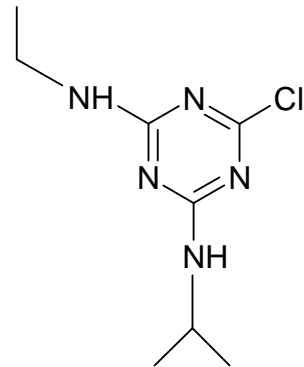
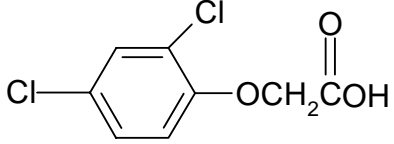
	<p>Dichloroprop</p> <p>2-(2,4-dichlorophenoxy)propanoic acid</p>	8.448	2.24	Thorstensen et al, 2001.
	<p>Endosulfan a</p> <p>6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-6,9-methano-2,4,3-benzodioxathiopin-3-oxide</p>	6.389	26.05	Colucci et al, 2001.
	17β-estradiol	12.053	0.477	Colucci et al, 2001.
	Estrone	11.068	1.55	Colucci et al, 2001.

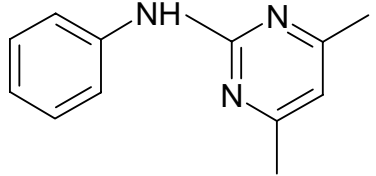
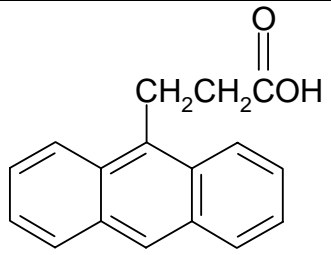
	<p>Imazamethabenz</p> <p>2-[4,5-dihydro-4-methyl-4-(1-methylethyl)-5-oxo-1H-imidazol-2-yl]-4-methylbenzoic acid</p>	11.393	2.083	Carton et al, 1997.
	<p>Imidachloprid</p> <p>2-(4,5-dihydro-4-methyl-4-(1-[(chloro-3-pyridinyl)methyl]-4,5-dihydro-N-nitro-1H-imidazol-2-amine</p>	9.24	14	Benoit et al, 1999. Piatt and Brusseau, 1998.
	<p>Isoproturon</p> <p>N,N-dimethyl-N'-[4-(1-methylethyl) phenyl] urea</p>	11.926	1.25	Worrall et al, 1997.
	<p>Lindane</p> <p>1,2,3,4,5,6-hexachlorocyclohexane</p>	6.316	67	Headly et al, 1998.

	<p>MCPA (4-chloro-2-methyl phenoxy) acetic acid</p>	8.297	8.233	Thorstensen et al, 2001.
	<p>Metolachlor 2-chloro-N-(2-ethyl-6-methyl phenyl)-N-(2- methoxy[1,2,4]triazolo[1,5-a] pyrimidine-2-sulfonamide</p>	8.636	3.45	Laabs et al, 2002. Zhu, 2002.
	<p>Monocrotophos Dimethyl-(E)-(1-methyl-3- methyl carbonyl) vinyl phosphate</p>	8.127	4.7	Laabs et al, 2002.
	<p>Naphthalene</p>	7.191	0.625	Bayard et al, 1998.
	<p>Pentachlorobenzene</p>	6.273	42	Schlebaum et al, 1998.

	Pentachlorophenol	6.308	18	Divincenzo and Sparks, 1997.
	Phenanthrene	9.306	3.5	Karapanagioti and Sabatini, 2000, Braida et al, 2001, Johnson and Weber, 2001, Rugner et al, 1999, Hundal et al, 2001.
	Prochloraz N-propyl-N-[2-(2,4,1-trichlorophenoxy) ethyl-1H-imidazole-1-carboxamide	10.73	1	Thorstensen et al, 2001.

	<p>Propiconazole</p> <p>1-[[2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxolan-2-yl]methyl]-1H-1,2,4-triazole</p>	11.077	2.08	Thorstensen et al, 2001.
	Pyrene	9.918	2.5	White and Pignatello, 1999, Kogel-Knabner et al, 2000.
	<p>Simazine</p> <p>6-chloro-N,N'-diethyl-1,3,5-triazine-2,4-diamine</p>	9.552	3.07	Laabs et al, 2002.
	Tetrachlorobenzene	4.365	55	Ball and Roberts, 1991.
	Tetrachloroethylene	6.251	40	Ball and Roberts, 1991.

	2,4,6-trinitrotoluene	6.947	15	Eriksson and Skyllberg, 2001.
	Trifluralin 2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl) benzenamine	10.641	1.81	Laabs et al, 2002.
	Atrazine 6-chloro-N ² -ethyl-N ⁴ -isopropyl-1,3,5-triazine-2,4-diamine	8.076	17	Agdi et al, 2000, Zhu, 2002.
	2,4-D (2,4-dichlorophenoxy) acetic acid	9.418	11	Belliveau et al, 2000.

 <p>The structure shows a benzene ring attached to the nitrogen atom of a pyrimidine ring. The pyrimidine ring has methyl groups at the 4 and 6 positions.</p>	Pyrimethanil N-(4,6-dimethyl pyrimidin-2-yl) aniline	10.623	14	Capri et al, 2001.
 <p>The structure shows an anthracene ring system with a propanoic acid chain (-CH₂CH₂COOH) attached to the 9-position.</p>	9-A 9-anthracene propanoic acid	9.695	3	Todoruk, this work.

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