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SUPPLEMENTARY MATERIAL TO

Density functional theory calculation of lipophilicity for organophosphate type pesticides

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TABLE S-I. IUPAC names of all 22 OPs pesticides investigated in present study

Pesticide	Systematic name
Acephate	*N*-[Methoxy(methylsulfanyl)phosphoryl]acetamide
Aspon	*O,O,O′,O′*–Tetrapropyl dithiopyrophosphate
Carbophenothion	*S*-[[(4-Chlorophenyl)thio]methyl] *O,O*-diethyl phosphorodithioate
Chlorpyrifos	*O,O*-Diethyl *O*-3,5,6-trichloropyridin-2-yl phosphorothioate
Coumaphos	*O*-(3-Chloro-4-methyl-2-oxo-2H-chromen-7-yl) *O,O*-diethyl phosphorothioate
Crufomate	*N*-[(4-*tert*-Butyl-2-chlorophenoxy)methoxyphosphoryl]methanamine
Diazinon	*O,O*-Diethyl *O*-[2-isopropyl-6-methylpyrimidin-4-yl] phosphorothioate
Dichlorvos	2,2-Dichloroethenyl dimethyl phosphate
Dimethoate	*O,O*-Dimethyl *S*-[2-(methylamino)-2-oxoethyl] phosphorodithioate
Dioxathion	*S,S′*-1,4-Dioxane-2,3-diyl *O,O,O′,O′*-tetraethyl bis(dithiophosphate)
Disulfoton	*O,O*-Diethyl *S*-[2-(ethylsulfanyl)ethyl] phosphorodithioate
Ethion	*O,O,O′,O′*-Tetraethyl *S,S′*-methylene bis(phosphorodithioate)
Fenitrothion	*O,O*-Dimethyl *O*-(3-methyl-4-nitrophenyl)phosphorothioate
Fenthion	*O,O*-Dimethyl *O*-[3-methyl-4-(methylsulfanyl)phenyl] phosphorothioate
Fonofos	*O*-Ethyl S-phenyl ethylphosphonodithioate
Malathion	Diethyl 2-[(dimethoxyphosphorothioyl)sulfanyl]butanedioate
Methyl parathion	*O,O*-Dimethyl-*O*-4-nitrophenylphosphorothioate
Monocrotophos	Dimethyl (E)-1-methyl-2-(methylcarbamoyl)vinyl phosphate
Parathion	*O,O*-Diethyl *O*-4-nitrophenyl phosphorothioate

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TABLE S-I. Continued

Pesticide	Systematic name
Phorate	*O,O*-Diethyl *S*-[(ethylsulfanyl)methyl] phosphorodithioate
Phosalone	6-Chloro-3-{[(diethoxyphosphinothioyl)sulfanyl]methyl}-1,3-benzoxazol-2-one
Temephos	*O,O,O′,O′*-Tetramethyl *O,O′*-sulfanediylbis(1,4-phenylene) diphosphorothioate

TABLE S-II. Calculated solvation free energy change of transfer from the gas phase to water phase ($\Delta G_{solv(water)}$ / kcal mol^{-1}) and octanol phase ($\Delta G_{solv(octanol)}$ / kcal mol^{-1}) under standard state conditions, and corresponding log K_{OW} values of examined OPs pesticide set at M062X/6-31+G(d,p) level of theory, with experimentally determined log *P*

Organophosphate	$\Delta G_{solv(water)}$	$\Delta G_{solv(octanol)}$	log K_{ow}	log *P* (exp.)	Ref.
Acephate	–17.7	–17.1	–0.4	–0.8	1
Aspon	–10.3	–19.3	5.8	6.0	1
Carbophenothion	–9.9	–17.0	5.2	5.3	1
Chlorpyrifos	–5.7	–13.0	5.4	5.0	2
Coumaphos	–12.2	–17.7	4.1	4.5	3
Crufomate	–11.9	–15.6	2.7	3.4	1
Diazinon	–8.8	–14.3	4.0	3.8	1
Dichlorvos	–7.3	–10.3	2.2	1.4	1
Dimethoate	–15.2	–16.1	0.7	0.8	1
Dioxathion	–15.2	–22.3	5.2	4.3	1
Disulfoton	–9.3	–16.2	5.1	4.0	1
Ethion	–10.9	–18.3	5.5	5.1	1
Fenitrothion	–7.9	–11.8	2.8	3.3	1
Fenthion	–7.7	–13.2	4.0	4.1	4
Fonofos	–11.3	–16.3	3.7	3.9	1
Malathion	–13.8	–17.4	2.7	2.4	1
Methyl parathion	–7.9	–11.3	2.5	2.9	1
Monocrotophos	–16.8	–15.7	–0.8	–0.2	1
Parathion	–8.4	–13.4	3.7	3.8	1
Phorate	–8.1	–14.0	4.3	3.6	1
Phosalone	–12.7	–17.8	3.8	4.4	1
Temephos	–11.1	–19.0	6.6	6.0	1

TABLE S-III. Calculated solvation free energy change of transfer from the gas phase to water phase ($\Delta G_{solv(water)}$/kcal mol^{-1}) and octanol phase ($\Delta G_{solv(octanol)}$/kcal mol^{-1}) under standard state conditions, and corresponding log K_{OW} values of examined OPs pesticide set at PBE/6--31+G(d,p) level of theory, with experimentally determined log *P*

Organophosphate	$\Delta G_{solv(water)}$	$\Delta G_{solv(octanol)}$	log K_{ow}	log *P* (exp.)	Ref.
Acephate	–15.5	–15.5	0.0	–0.8	1
Aspon	–8.7	–19.1	6.3	6.0	1
Carbophenothion	–9.3	–16.8	5.5	5.3	1
Chlorpyrifos	–5.2	–12.5	5.3	5.0	2
Coumaphos	–11.2	–16.9	4.1	4.5	3
Crufomate	–9.3	–14.8	4.0	3.4	1
Diazinon	–8.8	–14.6	3.8	3.8	1

TABLE S-III. Continued

Organophosphate	$\Delta G_{solv(water)}$	$\Delta G_{solv(octanol)}$	log K_{ow}	log P (exp.)	Ref.
Dichlorvos	–5.9	–9.3	2.5	1.4	1
Dimethoate	–15.0	–16.2	0.9	0.8	1
Dioxathion	–14.4	–22.5	5.9	4.3	1
Disulfoton	–8.9	–16.1	5.3	4.0	1
Ethion	–10.4	–18.7	6.0	5.1	1
Fenitrothion	–6.9	–11.1	3.1	3.3	1
Fenthion	–7.1	–12.7	4.2	4.1	4
Fonofos	–9.9	–15.5	4.1	3.9	1
Malathion	–12.8	–16.7	2.9	2.4	1
Methyl parathion	–7.0	–10.6	2.6	2.9	1
Monocrotophos	–14.7	–15.2	0.4	–0.2	1
Parathion	–7.5	–12.7	4.2	3.8	1
Phorate	–7.8	–14.3	4.8	3.6	1
Phosalone	–11.9	–17.3	4.0	4.4	1
Temephos	–9.7	–18.3	7.6	6.0	1

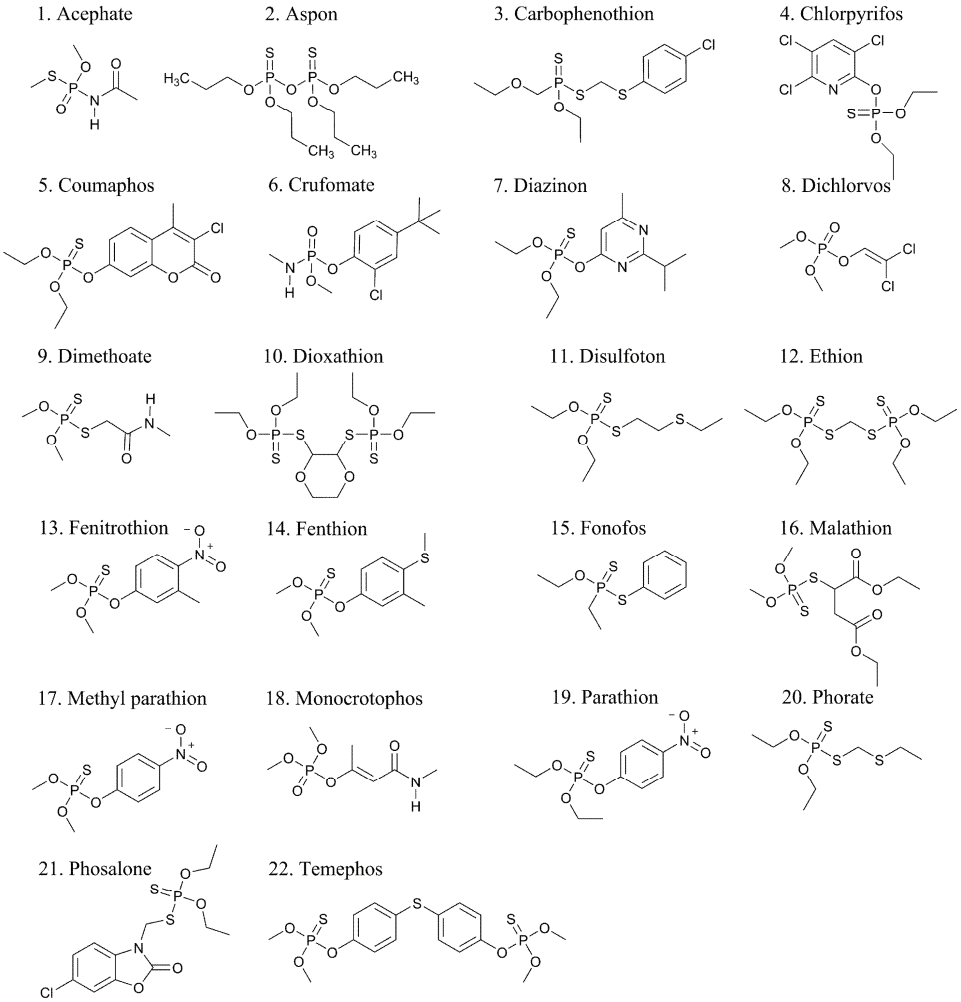

Fig. S-1. The structures of 22 OPs pesticides presented in this work.

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