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基于概念密度泛函理论磷酸酯类反应性物质毒性预测

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Toxicity Prediction of Organophosphorus Chemical Reactivity Compounds Based on conceptual DFT

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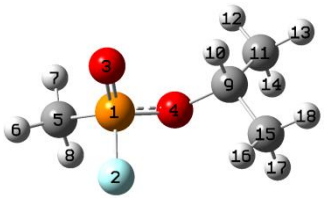
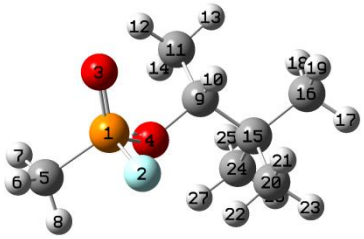
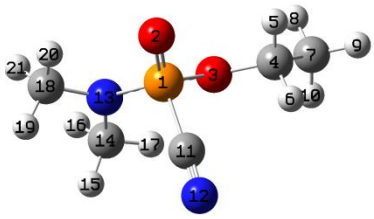
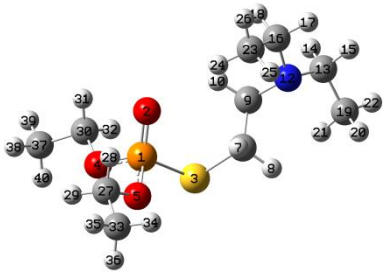
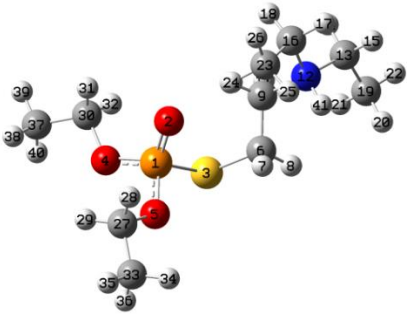
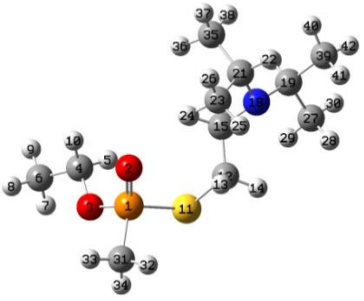
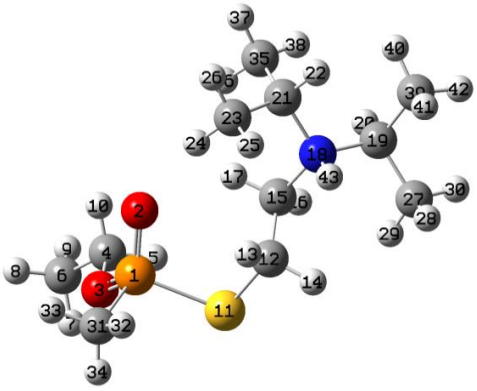
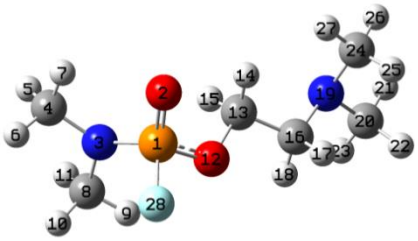
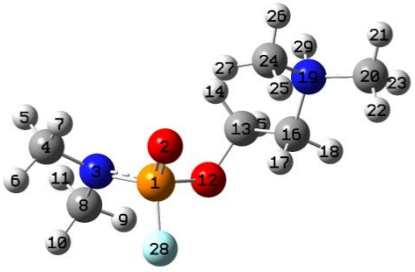
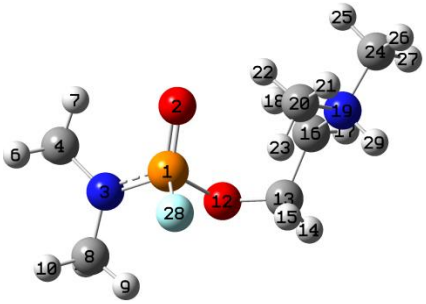
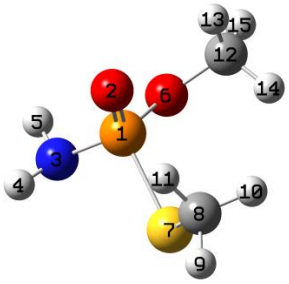
表 S1　训练集及测试集化合物名称、结构及优化后的最低能量构象

Table S1　The name, structure and the lowest energy conformation of the training set and the test set.

No	Name	Structure and the lowest energy conformation
1	sarin	
2	soman	
3	tabun	
4	amiton	
5	amiton+NH[a]	
6	VX	

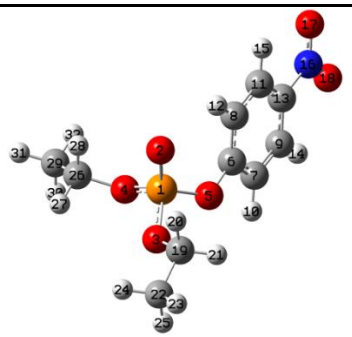
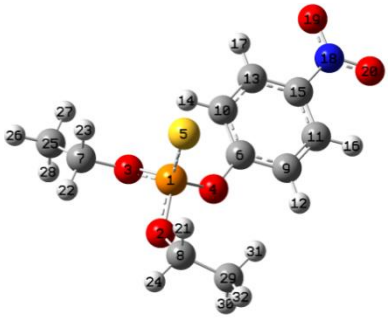
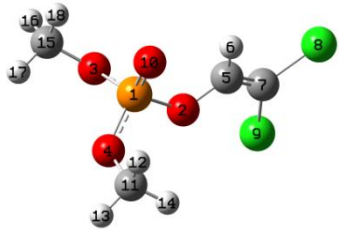
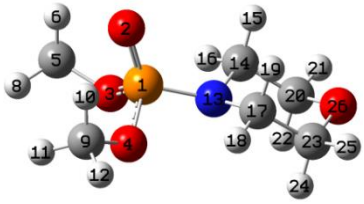
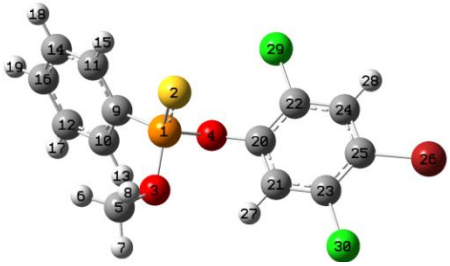
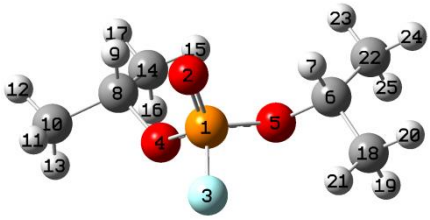
to be continued

continued Table S1

No	Name	Structure and the lowest energy comformation
7	VX+NH[a]	
8	GV	
9	GV+NH[a]	
10	GV+NH-Ninvert[b]	
11	methamidophos	

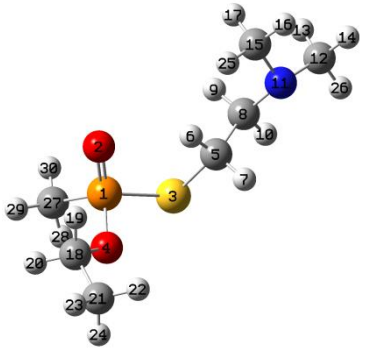
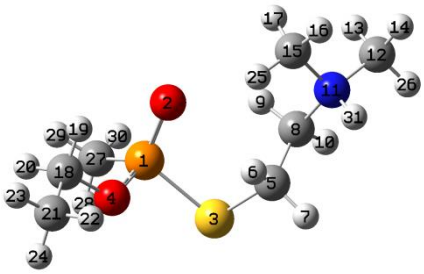
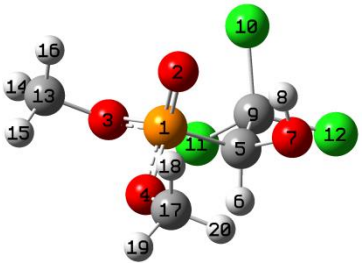
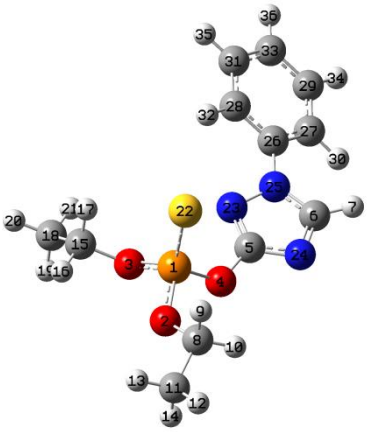
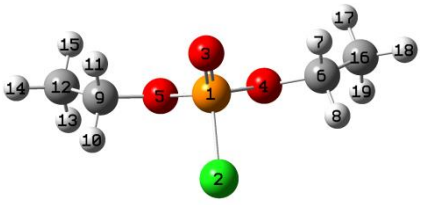
to be continued

continued Table S1

No	Name	Structure and the lowest energy comformation
12	paraoxon	
13	parathion	
14	dichlorvos	
15	DMMPA	
16	leptophos	
17	diisopropylphosphorofluoridate	

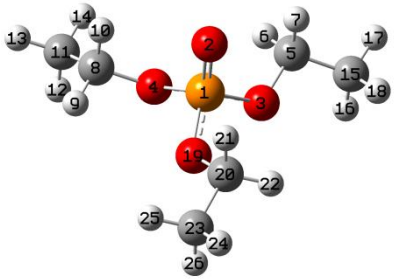
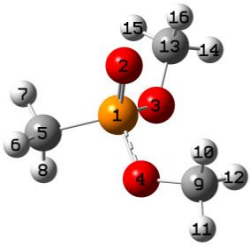
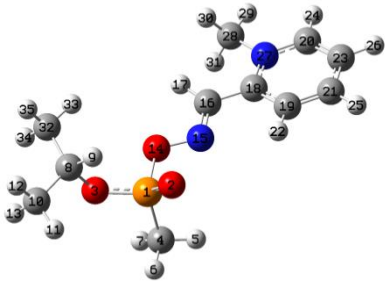
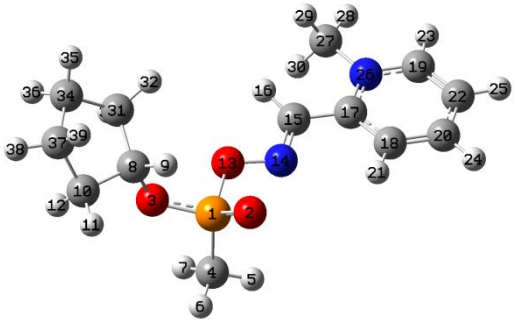
to be continued

continued Table S1

No	Name	Structure and the lowest energy comformation
18	EDMM	
19	EDMM+NH[a]	
20	trichlorfon	
21	triazophos	
22	DCP	

to be continued

continued Table S1

No	Name	Structure and the lowest energy comformation
23	TEP	
24	DMMP	
25	24-optfreq	
26	27-optfreq	

Note: a) “+NH” in the molecular name column indicated that the calculated value is protonated form for substituted tertiaryamine, b) “+NH-Ninvert” indicated the inverted conformation for substituted tertiaryamine in protonated form.

表 S2-1　B3LYP/6-311++G(2*d*,3*p*)/gas 条件的单点计算结果

Table S2-1　Results of single point calculation at B3LYP/6-311++G(2*d*,3*p*)/gas level.

B3LYP-gas	pLD_{50}(rat)/(μg kg^{-1})	ACD(LogP)	HC_LogP	Volume	Surface_area1	Surface area2	N^+
sarin	3.66	0.55	0.88	449.36	313.55	177.62	0
soman	4.01	1.78	2.26	573.37	361.66	231.22	0
tabun	3.31	−1.16	0.21	528.94	350.66	239.15	0
amiton	3.22	2.51	2.25	865.12	533.1	314.04	1
amiton+NH	3.22	2.51	1.53	863.08	528.81	315.02	1
VX	4.43	2.02	2.15	857.50	512.95	287.99	1
VX+NH	4.43	2.02	1.43	857.09	509.12	291.09	1
GV	3.72	−0.63	0.28	621.04	400.01	288.37	1
GV+NH	3.72	−0.63	−0.44	615.32	392.09	280.51	1
GV+NH-Ninvert	3.72	−0.63	−0.44	632.70	406.37	296.36	1
methamidophos	1.82	−0.82	0.37	422.7	293.59	209.81	0
paraoxon	3.15	2.31	2.87	776.34	496.58	446.65	0
parathion	2.70	3.84	3.52	792.79	489.21	457.8	0
dichlorvos	1.82	0.71	1.38	571.31	381.58	402.51	0
DMMPA	−0.38	−1.85	−0.19	578.21	371.72	276.96	0
leptophos	0.87	6.25	5.72	912.58	545.36	742.26	0
diisopropyl	2.89	1.17	2.22	573.47	372.45	202.56	0
EDMM	4.27	0.26	0.64	697.59	442.92	292.88	1
EDMM+NH	4.27	0.26	−0.08	687.01	427.23	286.58	1
trichlorfon	0.80	0.48	1.4	596.87	377.46	376.31	0
triazophos	0.97	3.99	3.74	893.33	546.56	442.58	0
DCP	1.60	1.21	1.68	514.26	354.79	226.77	0
TEP	0.10	1.08	1.58	608.61	405.52	200.43	0
DMMP	−0.30	−0.78	−0.02	411.94	289.96	174.7	0
24-optfreq		−3.71	2.39	808.88	506.56	361.33	1
27-optfreq		−3.08	2.82	875.20	542.89	361.43	1

B3LYP-gas	pK_a	HOMO	LUMO	LUMO−HOMON	LUMO−HOMON+1	LUMO-HOMON-1	P-charge	$f_P(-)$	$f_C(-)$
sarin	3.15	−0.30853	−0.01552	7.973270916	0.599471548	10.23128948	2.39323	0.04233	−0.00455
soman	3.15	−0.30182	−0.01629	7.769728148	0.537701216	9.456031	2.39693	0.03169	−0.02751
tabun	9.21	−0.27529	−0.02279	6.870929	0.475114536	7.6736712	2.30801	0.04865	0.00334
amiton	9.99	−0.21574	−0.01174	5.5511664	0.322729576	7.037736108	2.22079	-0.0028	0.0008
amiton+NH	9.99	−0.37238	−0.14426	6.207510192	0.893628944	6.55527444	2.25657	0.03566	0.00537
VX	9.99	−0.20997	−0.01374	5.339732268	0.369533528	6.8913377	2.00131	-0.00064	−0.00016
VX+NH	9.99	−0.37102	−0.1384	6.329962392	0.816075884	6.580309112	2.02916	0.04545	0.00511
GV	3.15	−0.23216	−0.01579	5.887773892	0.4217798	7.7417002	2.55768	0.01366	0.00695
GV+NH	3.15	−0.37391	−0.16792	5.605317484	1.124927544	9.330585524	2.56211	0.03655	0.00741
GV+NH-Ninvert	3.15	−0.37658	−0.16635	5.720694668	1.034312916	9.208677556	2.55776	0.03711	0.00138
methamidophos	10.24	−0.25407	−0.0186	6.407515452	0.566273396	7.379241688	2.10542	0.04128	0.01306
paraoxon	7.11	−0.27701	−0.1003	4.808561836	0.314021864	4.612910432	2.59854	0.01961	0.00387
parathion	7.11	−0.26027	−0.10055	4.346236752	0.456610648	5.130475064	2.06917	0.01876	0.00472
dichlorvos	25.01	−0.25291	−0.02184	6.287784412	0.567089744	5.333745716	2.58576	0.0217	0.00106
DMMPA	15.36	−0.24616	−0.01311	6.34166338	0.54695316	8.522128888	2.53048	0.02865	0.00424
leptophos	9.95	−0.2502	−0.06096	5.149523184	0.7075016	5.074147052	1.83612	0.01947	0.0044
diisopropyl	16.01	−0.30782	−0.01442	7.98388344	0.456066416	9.62882466	2.61035	0.0246	-0.00767
EDMM	9.99	−0.22366	−0.01408	5.703007128	0.338512304	7.040457268	1.9968	0.00515	0.00111
EDMM+NH	9.99	−0.37686	−0.16074	5.880970992	1.11023328	6.262477624	2.01884	0.04085	0.00445
trichlorfon	15.36	−0.30221	−0.05833	6.636365008	0.477291464	7.008619696	2.38787	0.03141	0.0073
triazophos	8.09	−0.24322	−0.05039	5.247212828	0.316198792	5.571302984	2.07714	0.0131	0.01191
DCP	1.01	−0.30256	−0.01735	7.761020436	0.420147104	7.990958456	2.32076	0.03758	0.01196
TEP	15.81	−0.29188	−0.00926	7.690542392	0.459059692	9.445690592	2.59677	0.03292	0.0189
DMMP	15.36	−0.29271	−0.0123	7.630404756	0.61634274	9.817128932	2.37509	0.05541	0.01058
24-optfreq	6.79	−0.39618	−0.24429	4.133169924	2.127130772	4.401204184	2.35055	0.02566	-0.00532
27-optfreq	6.79	-0.39265	-0.24378	4.050990892	2.126042308	4.401204184	2.34991	0.02378	-0.01052

continued Table S2-1

B3LYP-gas	$f_C(-)$_largest	*I*	*A*	*I-A*	*μ*	*η*	*ω*
sarin	−0.00455	10.62338	0.400016	10.22336	−5.5117	5.11168	2.971508
soman	−0.02751	10.12265	0.347828	9.774822	−5.23524	4.887411	2.80391
tabun	0.05643	9.538905	0.326101	9.212804	−4.9325	4.606402	2.640845
amiton	0.05273	7.727014	0.387114	7.339901	−4.05706	3.66995	2.242506
amiton+NH	0.02298	12.12186	−2.72825	14.85011	−4.69681	7.425055	1.485509
VX	0.04808	7.47529	0.36253	7.11276	−3.91891	3.55638	2.15919
VX+NH	0.02603	12.1114	−2.63416	14.7455	−4.73861	7.37277	1.52279
GV	0.0427	8.280127	0.321656	7.958472	−4.30089	3.979236	2.324274
GV+NH	0.04963	12.30365	−3.16866	15.47231	−4.56749	7.736156	1.348344
GV+NH-Ninvert	0.04919	12.37832	−3.14093	15.51924	−4.6187	7.759622	1.374574
methamidophos	0.03081	9.112435	0.430038	8.682398	−4.77124	4.341199	2.621937
paraoxon	0.00387	9.326928	−0.82099	10.14792	−4.25297	5.073959	1.782409
parathion	0.00472	8.77754	−0.86911	9.64666	−3.95422	4.82333	1.62085
dichlorvos	0.00441	8.952195	0.368766	8.583429	−4.66048	4.291714	2.530466
DMMPA	0.02748	8.573088	0.409889	8.163199	−4.49149	4.081599	2.47127
leptophos	0.0044	8.235885	−0.33412	8.570002	−3.95088	4.285001	1.82141
diisopropyl	−0.00767	10.45402	0.384872	10.06914	−5.41944	5.034572	2.916869
EDMM	0.02676	8.091356	0.364121	7.727235	−4.22774	3.863618	2.313088
EDMM+NH	0.02473	12.32954	−3.06068	15.39022	−4.63443	7.695111	1.395557
trichlorfon	0.03867	10.10123	0.063453	10.03778	−5.08234	5.018888	2.573298
triazophos	0.00446	8.111586	0.079881	8.031705	−4.09573	4.015852	2.088602
DCP	0.01196	10.36616	0.386323	9.97984	−5.37624	4.98992	2.896237
TEP	0.0189	9.994019	0.446124	9.547895	−5.22007	4.773947	2.853943
DMMP	0.01058	10.24669	0.48364	9.763048	−5.36516	4.881524	2.948361
24-optfreq	0.02571	12.40689	−4.95841	17.3653	−3.72424	8.682649	0.798716
27-optfreq	−0.00871	12.1823	−4.95024	17.13254	−3.61603	8.56627	0.763205

B3LYP-gas	bond order						
	bo1_X	**bo2_O-C**	**bo3_N**	**bo4_N+1**	**bo5_N-1**	**bo6_P-X**	**bo7_O-C**
sarin	0.6085	0.8214	0.6085	0.6021	0.6579	0.0006	-0.002
soman	0.6082	0.8166	0.6082	0.6037	0.6505	0.0189	-0.0294
tabun	0.7699	0.8402	0.7206	0.7302	0.685	0.129	0.0376
amiton	0.9321	0.7019	0.7019	0.7081	0.7338	0.0454	0.017
amiton+NH	0.8793	0.822	0.7432	0.7191	0.786	0.0825	0.036
VX	0.8870	0.8554	0.6996	0.7073	0.7289	0.0403	0.0089
VX+NH	0.8384	0.8345	0.7417	0.7213	0.7213	0.1171	0.0259
GV	0.7210	0.8567	0.623	0.6173	0.647	0.0404	0.0141
GV+NH	0.6735	0.9076	0.6486	0.6341	0.6968	0.152	0.03
GV+NH-Ninvert	0.6849	0.9041	0.6169	0.6144	0.6639	0.1609	0.038
methamidophos	0.9137	0.8821	0.6958	0.6971	0.7437	0.091	0.0233
paraoxon	0.6623	0.8439	0.6623	0.7123	0.5891	0.0732	0.0168
parathion	0.6471	0.8432	0.6471	0.7005	0.6544	0.025	0.0181
dichlorvos	0.6652	0.8686	0.6652	0.6572	0.5746	0.0906	0.0257
DMMPA	0.7097	0.8797	0.7097	0.7171	0.6922	0.0897	0.0272
leptophos	0.6379	0.8736	0.6379	0.6178	0.6304	-0.0412	0.0144
diisopropyl	0.6351	0.8212	0.6351	0.6282	0.6744	0.0034	0.0128
EDMM	0.9166	0.8564	0.6878	0.6955	0.7202	0.0714	0.0197
EDMM+NH	0.8734	0.83	0.7321	0.7115	0.7758	0.0976	0.0395
trichlorfon	0.7195	0.8686	0.7195	0.7036	0.7569	0.0212	0.0194
triazophos	0.6378	0.8454	0.6378	0.6614	0.6326	0.0052	0.0192

to be continued

continued Table S2-1

B3LYP-gas	bond order						
	bo1_X	bo2_O-C	bo3_N	bo4_N+1	bo5_N-1	bo6_P-X	bo7_O-C
DCP	0.8157	0.8413	0.7498	0.7518	0.7954	0.0208	0.0208
TEP	0.7218	0.8539	0.7218	0.7239	0.7498	0.0294	0.0294
DMMP	0.6887	0.8825	0.6887	0.6978	0.7395	−0.0508	0.0223
24-optfreq	0.5448	0.7962	0.5448	0.6099	0.5309	0.0139	0.0132
27-optfreq	0.5457	0.8184	0.5457	0.6113	0.5414	0.0043	-0.0103

表 S2-2　B3LYP/6-311++G*(2d,3p)*/water/CPCM 条件的单点计算结果

Table S2-2　Results of single point calculation at B3LYP/6-311++G(2*d*,3*p*)/water/CPCM level.

B3LYP-water	pLD_{50}(rat)/(μg·kg^{-1})	ACD(LogP)	HC_LogP	Volume	Surface_area1	Surface area2	N^+
sarin	3.66	0.55	0.88	449.36	313.55	177.62	0
soman	4.01	1.78	2.26	573.37	361.66	231.22	0
tabun	3.31	−1.16	0.21	528.94	350.66	239.15	0
amiton	3.22	2.51	2.25	865.12	533.1	314.04	1
amiton+NH	3.22	2.51	1.53	863.08	528.81	315.02	1
VX	4.43	2.02	2.15	857.5	512.95	287.99	1
VX+NH	4.43	2.02	1.43	857.09	509.12	291.09	1
GV	3.72	−0.63	0.28	621.04	400.01	288.37	1
GV+NH	3.72	−0.63	−0.44	615.32	392.09	280.51	1
GV+NH-Ninvert	3.72	−0.63	−0.44	632.7	406.37	296.36	1
methamidophos	1.82	−0.82	0.37	422.7	293.59	209.81	0
paraoxon	3.15	2.31	2.87	776.34	496.58	446.65	0
parathion	2.70	3.84	3.52	792.79	489.21	457.8	0
dichlorvos	1.82	0.71	1.38	571.31	381.58	402.51	0
DMMPA	-0.38	−1.85	−0.19	578.21	371.72	276.96	0
leptophos	0.87	6.25	5.72	912.58	545.36	742.26	0
diisopropyl	2.89	1.17	2.22	573.47	372.45	202.56	0
EDMM	4.27	0.26	0.64	697.59	442.92	292.88	1
EDMM+NH	4.27	0.26	−0.08	687.01	427.23	286.58	1
trichlorfon	0.80	0.48	1.4	596.87	377.46	376.31	0

B3LYP-water	pK_a	HOMO	LUMO	LUMO-HOMO*N*	LUMO-HOMO*N*+1	LUMO-HOMO*N*-1	P-charge	f_P(-)	f_C(-)
sarin	3.15	−0.31703	−0.01172	8.307973596	1.279217316	9.975500444	2.40603	0.03574	−0.00519
soman	3.15	−0.30784	−0.0123	8.042116264	0.940977128	9.287863312	2.4093	0.02659	−0.02881
tabun	9.21	−0.27304	−0.02992	6.615684192	0.989685892	7.768095452	2.32376	0.03282	−0.00112
amiton	9.99	−0.2224	−0.0154	5.6328012	1.326837616	6.906031964	2.22975	−0.00124	0.00053
amiton+NH	9.99	−0.27586	−0.02512	6.823036584	1.435684016	7.0818189	2.24157	0.03475	0.00396
VX	9.99	−0.21564	−0.01505	5.458374844	1.27758462	6.823036584	2.00954	−0.00053	0.00042
VX+NH	9.99	−0.27091	−0.02376	6.72534694	1.408744532	7.1838624	2.0209	0.04231	0.00195
GV	3.15	−0.23139	−0.01021	6.018661688	0.937983852	6.967258064	2.56763	0.00129	0.00368
GV+NH	3.15	−0.27113	−0.0192	6.855418388	1.873790776	9.229630488	2.56611	0.02531	0.00525
GV+NH-Ninver	3.15	−0.2707	−0.01888	6.852425112	1.835694536	9.11316484	2.56528	0.02309	−0.00383
methamidophos	10.24	−0.25963	−0.01863	6.5579956	1.212548896	7.131071896	2.11672	0.03405	0.00706
paraoxon	7.11	−0.27518	−0.11153	4.45317834	2.6871455	4.871420632	2.60784	0.01539	0.00159
parathion	7.11	−0.26254	−0.11248	4.083372696	2.669730076	4.908700524	2.10006	0.02836	0.00412
dichlorvos	25.01	−0.25755	−0.02467	6.337037408	1.113770788	6.171046648	2.6005	0.00961	−0.00282
DMMPA	15.36	−0.25119	−0.01075	6.542757104	1.345069388	8.493012476	2.54636	0.02041	−0.00092
leptophos	9.95	−0.25648	−0.06099	5.319595684	0.830498032	5.269254224	1.8694	0.02354	0.00138
diisopropyl	16.01	−0.31809	−0.01244	8.31722554	1.316769324	9.50501188	2.62587	0.02079	−0.01016
EDMM	9.99	−0.22995	−0.01605	5.82056124	1.060436052	6.703033428	2.00504	-0.00214	−0.0003
EDMM+NH	9.99	−0.27069	−0.02848	6.590921636	1.608477676	7.057872692	2.01169	0.0338	−0.00095
trichlorfon	15.36	−0.30921	−0.05851	6.82194812	1.618273852	7.063315012	2.39892	0.02972	0.00372

to be continued

continued Table S2-2

B3LYP-water	$f_C(-)$_largest	*I*	*A*	*I–A*	*μ*	*η*	*ω*
sarin	−0.00519	8.672897	−0.83017	9.503071	−3.92136	4.751536	1.618117
soman	−0.02881	8.374152	−0.75836	9.132514	−3.80789	4.566257	1.587741
tabun	0.04751	7.434341	−0.92715	8.361495	−3.25359	4.180748	1.266026
amiton	0.05766	6.027883	−0.90731	6.935191	−2.56029	3.467596	0.94519
Amiton + NH	0.03266	7.55903	−1.17963	8.738664	−3.1897	4.369332	1.164272
VX	0.05144	5.84726	−0.86718	6.714439	−2.49004	3.35722	0.923428
VX + NH	0.03531	7.416303	−1.1332	8.549506	−3.14155	4.274753	1.154375
GV	0.05745	6.31162	−0.70216	7.013784	−2.80473	3.506892	1.121577
GV + NH	0.04476	7.432396	−1.35771	8.79011	−3.03734	4.395055	1.049525
GV + NH-Ninvert	0.04552	7.416246	−1.34646	8.76271	−3.03489	4.381355	1.051109
methamidophos	0.03765	7.071972	−0.96585	8.037817	−3.05306	4.018909	1.159667
paraoxon	0.00159	7.420318	−3.08319	10.50351	−2.16856	5.251755	0.447723
parathion	0.00412	7.079835	−3.10962	10.18945	−1.98511	5.094727	0.386738
dichlorvos	0.00166	7.012185	−0.95708	7.969268	−3.02755	3.984634	1.150177
DMMPA	0.02416	6.789834	−0.82791	7.617742	−2.98096	3.808871	1.166506
leptophos	0.00138	6.834373	−1.84031	8.674678	−2.49703	4.337339	0.718779
diisopropyl	−0.01016	8.72193	−0.81998	9.541907	−3.95098	4.770954	1.635964
EDMM	0.01346	6.25001	−0.8283	7.078313	−2.71085	3.539156	1.038203
EDMM + NH	0.02925	7.385697	−1.33915	8.724843	−3.02328	4.362422	1.047606
trichlorfon	0.0341	8.376858	−1.75174	10.1286	−3.31256	5.064299	1.083373

B3LYP-water	bond order						
	bo1_X	**bo2_O-C**	**bo3_N**	**bo4_N + 1**	**bo5_N-1**	**bo6_P-X**	**bo7_O-C**
sarin	0.6016	0.8072	0.6016	0.5929	0.6466	0.0069	-0.0058
soman	0.6018	0.8063	0.6018	0.5892	0.6382	0.0307	-0.0371
tabun	0.7571	0.8249	0.745	0.6788	0.7019	0.1411	0.022
amiton	0.9345	0.7137	0.7137	0.701	0.7221	0.0144	0.0028
Amiton + NH	0.9093	0.829	0.7266	0.7214	0.7714	0.1057	0.0231
VX	0.8906	0.8453	0.7104	0.6989	0.7193	0.0153	0.0024
VX + NH	0.8658	0.8392	0.7238	0.7188	0.75	0.1158	0.0142
GV	0.7346	0.847	0.61	0.6102	0.6145	0.0183	-0.0059
GV + NH	0.7053	0.8732	0.6184	0.6161	0.6653	0.1499	0.0168
GV + NH-Ninvert	0.713	0.8722	0.6063	0.6046	0.648	0.1499	0.0217
methamidophos	0.9184	0.8716	0.7051	0.693	0.7459	0.1094	0.0134
paraoxon	0.6548	0.8293	0.6548	0.6786	0.6005	0.0543	0.0075
parathion	0.6494	0.8284	0.6494	0.6748	0.6816	0.0167	0.0119
dichlorvos	0.6601	0.8548	0.6601	0.6867	0.5952	0.0649	0.0104
DMMPA	0.7202	0.8683	0.7202	0.7236	0.6984	0.0929	0.0153
leptophos	0.6401	0.8595	0.6401	0.6017	0.6324	-0.046	0.0081
diisopropyl	0.6268	0.8018	0.6268	0.6196	0.6645	0.0191	0.0122
EDMM	0.922	0.8429	0.7013	0.6886	0.7069	0.0189	0.0027
EDMM + NH	0.8984	0.8372	0.7102	0.7057	0.7506	0.103	0.0222
trichlorfon	0.7289	0.8574	0.7289	0.7146	0.7396	0.0245	0.0164

表 S2-3　MP2/6-311++G(2*d*,3*p*)/gas 条件的单点计算结果

Table S2-3　Results of single point calculation at MP2/6-311++G(2*d*,3*p*)/gas level.

MP2-gas	pLD_{50}(rat)/(μg ㎏$^{-1}$)	ACD(LogP)	HC_LogP	Volume	Surface_area1	Surface area2	N^+
sarin	3.66	0.55	0.88	449.36	313.55	177.62	0
soman	4.01	1.78	2.26	573.37	361.66	231.22	0
tabun	3.31	−1.16	0.21	528.94	350.66	239.15	0
amiton	3.22	2.51	2.25	865.12	533.10	314.04	1
Amiton + NH	3.22	2.51	1.53	863.08	528.81	315.02	1
VX	4.43	2.02	2.15	857.50	512.95	287.99	1
VX + NH	4.43	2.02	1.43	857.09	509.12	291.09	1
GV	3.72	−0.63	0.28	621.04	400.01	288.37	1
GV + NH	3.72	−0.63	−0.44	615.32	392.09	280.51	1
GV + NH-Ninvert	3.72	−0.63	−0.44	632.7	406.37	296.36	1
methamidophos	1.82	−0.82	0.37	422.7	293.59	209.81	0
paraoxon	3.15	2.31	2.87	776.34	496.58	446.65	0
parathion	2.70	3.84	3.52	792.79	489.21	457.8	0
dichlorvos	1.82	0.71	1.38	571.31	381.58	402.51	0
DMMPA	−0.38	−1.85	−0.19	578.21	371.72	276.96	0
leptophos	0.87	6.25	5.72	912.58	545.36	742.26	0
diisopropyl	2.89	1.17	2.22	573.47	372.45	202.56	0
EDMM	4.27	0.26	0.64	697.59	442.92	292.88	1
EDMM + NH	4.27	0.26	−0.08	687.01	427.23	286.58	1
trichlorfon	0.80	0.48	1.4	596.87	377.46	376.31	0

MP2-gas	pK_a	HOMO	LUMO	LUMO−HOMON	LUMO−HOMON	LUMO−HOMON	P-charge	f_P(-)	f_C(-)
				N	$N+1$	$N-1$			
sarin	3.15	−0.46242	0.03596	13.56171721	2.165771244	15.73701251	2.59194	0.10936	0.07159
soman	3.15	−0.44746	0.03498	13.1279643	2.003590108	14.80800849	2.59556	0.10397	0.06827
tabun	9.21	−0.40767	0.03387	12.01500986	2.046584436	14.70161113	2.51022	0.0612	0.00141
amiton	9.99	−0.34467	0.03898	10.43973034	1.562490072	10.94341706	2.42253	0.02944	0.00237
Amiton + NH	9.99	−0.48891	−0.06718	11.47594807	2.93749222	13.7690696	2.45836	0.02635	0.00246
VX	9.99	−0.33763	0.03787	10.2179558	1.68847978	10.61524516	2.18018	0.04663	0.00099
VX + NH	9.99	−0.48651	−0.0628	11.52982704	2.788372652	14.09207129	2.20815	0.04293	0.00181
GV	3.15	−0.36639	0.0345	10.90885832	1.92930244	10.15754605	2.7721	0.06001	0.00749
GV + NH	3.15	−0.5092	−0.08495	11.5445213	3.592203316	16.04695264	2.77594	0.05204	0.00646
GV + NH-Ninvert	3.15	−0.50964	−0.08425	11.57554252	3.446621256	16.03008144	2.77396	0.04696	0.00026
methamidophos	10.24	−0.37065	0.04026	11.18151856	2.163050084	13.96553735	2.30827	0.03646	0.009
paraoxon	7.11	−0.36415	0.03184	10.77552148	4.544065084	12.08086194	2.81188	0.01479	0.00177
parathion	7.11	−0.35973	0.03157	10.64789908	4.626788348	11.06450868	2.28068	0.01281	0.00443
dichlorvos	25.01	−0.35808	0.03579	10.71783289	2.162505852	13.17095863	2.79955	0.0158	0.00183
DMMPA	15.36	−0.38042	0.03788	11.38261228	1.95787462	14.36337094	2.73999	0.05811	0.00329
leptophos	9.95	−0.33869	0.03095	10.05849582	3.346482568	10.16543741	2.03007	0.02875	0.01118
diisopropyl	16.01	−0.46857	0.03743	13.7690696	1.92794186	14.76583051	2.83067	0.09101	0.06992
EDMM	9.99	−0.35676	0.03759	10.73089446	1.641131596	11.19131473	2.17528	0.03722	0.00053
EDMM + NH	9.99	−0.49165	−0.07836	11.24628216	3.270017972	13.64416836	2.1955	0.029	−0.0005
trichlorfon	15.36	−0.44149	0.03797	13.04687374	2.941846076	13.91002569	2.58075	0.11019	0.01389

to be continued

continued Table S2-3

MP2-gas	f_C(-)_largest	*I*	*A*	*I*−*A*	*μ*	*η*	*ω*
sarin	0.07159	11.8142	0.717637	11.09656	−6.26592	5.548281	3.538188
soman	0.06827	11.53237	0.662133	10.87024	−6.09725	5.435119	3.420024
tabun	0.10162	9.916936	0.642972	9.273964	−5.27995	4.636982	3.006041
amiton	0.03902	9.042413	0.773043	8.26937	−4.90773	4.134685	2.912651
amiton+NH	0.03119	12.32985	−2.44588	14.77573	−4.94198	7.387867	1.652926
VX	0.03999	8.962028	0.722512	8.239516	−4.84227	4.119758	2.845747
VX + NH	0.03185	12.2505	−2.33318	14.58368	−4.95866	7.291842	1.686013
GV	0.10291	9.675158	0.656346	9.018812	−5.16575	4.509406	2.958815
GV + NH	0.09916	12.68719	−2.93093	15.61812	−4.87813	7.80906	1.523625
GV + NH-Ninvert	0.10028	12.76029	−2.91539	15.67568	−4.92245	7.837839	1.545742
methamidophos	0.0514	9.318057	0.799007	8.51905	−5.05853	4.259525	3.003709
paraoxon	0.02131	10.21218	0.855546	9.356638	−5.53386	4.678319	3.272934
parathion	0.06461	9.313572	0.832478	8.481094	−5.07303	4.240547	3.034465
dichlorvos	0.00516	9.255365	0.726471	8.528895	−4.99092	4.264447	2.920573
DMMPA	0.08929	9.224413	0.75585	8.468563	−4.99013	4.234281	2.940453
leptophos	0.06006	9.043533	0.652246	8.391287	−4.84789	4.195644	2.800766
diisopropyl	0.06992	11.70288	0.739306	10.96358	−6.22109	5.481788	3.530054
EDMM	0.03649	9.049645	0.718729	8.330916	−4.88419	4.165458	2.863464
EDMM + NH	0.03033	12.47829	−2.77577	15.25406	−4.85126	7.627029	1.54285
trichlorfon	0.03473	11.08653	0.62822	10.45831	−5.85737	5.229153	3.280534

MP2-gas	bond order						
	bo1_X	**bo2_O − C**	**bo3_N**	**bo4_N + 1**	**bo5_N − 1**	**bo6_P − X**	**bo7_O − C**
sarin	0.5735	0.7987	0.5735	0.5665	0.554	0.1525	0.0598
soman	0.5733	0.7938	0.5733	0.5677	0.559	0.1466	0.0552
tabun	0.756	0.8171	0.6925	0.6971	0.6438	0.1523	0.045
amiton	0.9408	0.8276	0.6698	0.686	0.7234	0.1388	0.0425
amiton+NH	0.8947	0.8002	0.705	0.6873	0.7579	0.1368	0.0458
VX	0.9026	0.834	0.666	0.6875	0.7219	0.1368	0.0236
VX + NH	0.8596	0.8118	0.7013	0.6851	0.7189	0.1407	0.0258
GV	0.6895	0.8328	0.5872	0.5817	0.6248	0.1564	0.0339
GV + NH	0.647	0.8857	0.6091	0.5991	0.6567	0.1753	0.034
GV+NH-Ninvert	0.6536	0.8833	0.5814	0.5828	0.6299	0.1829	0.0463
methamidophos	0.9267	0.8564	0.6669	0.6798	0.7343	0.1513	0.025
paraoxon	0.633	0.8212	0.633	0.6733	0.5552	0.0778	0.0181
parathion	0.6204	0.8205	0.6204	0.665	0.7236	0.0332	0.0253
dichlorvos	0.6378	0.8429	0.6378	0.6214	0.5504	0.0874	0.0267
DMMPA	0.6789	0.8535	0.6789	0.6898	0.6265	0.1304	0.0374
leptophos	0.612	0.8464	0.612	0.555	0.6965	0.0249	0.0191
diisopropyl	0.5985	0.7992	0.5985	0.5905	0.5648	0.1478	0.0615
EDMM	0.9288	0.8361	0.6579	0.6726	0.7127	0.1462	0.0419
EDMM + NH	0.8902	0.8091	0.695	0.682	0.7471	0.1425	0.0454
trichlorfon	0.6856	0.8417	0.6856	0.5699	0.7853	0.0295	0.0268
triazophos	0.609	0.8219	0.609	0.6453	0.6916	-0.0826	0.0257
DCP	0.8216	0.8177	0.713	0.7232	0.7817	0.036	0.036
TEP	0.6886	0.8325	0.6886	0.6913	0.6061	0.0481	0.0825
DMMP	0.6591	0.8566	0.6591	0.6716	0.522	0.1371	0.0266
24-optfreq	0.5314	0.7742	0.5314	0.5793	0.4166	0.0025	0.0309
27-optfreq	0.5322	0.796	0.5322	0.5804	0.4169	0.1153	0.03

表 S2-4　MP2/6-311++G(2*d*,3*p*)/water/CPCM 条件的单点计算结果

Table S2-4　Results of single point calculation at MP2/6-311++G(2*d*,3*p*)/water/CPCM level.

MP2-water	pLD_{50}(rat)/(μg ⋅kg^{-1})	ACD(LogP)	HC_LogP	Volume	Surface_area1	Surface area2	N^+
sarin	3.66	0.55	0.88	449.36	313.55	177.62	0
soman	4.01	1.78	2.26	573.37	361.66	231.22	0
tabun	3.31	−1.16	0.21	528.94	350.66	239.15	0
amiton	3.22	2.51	2.25	865.12	533.1	314.04	1
amiton+NH	3.22	2.51	1.53	863.08	528.81	315.02	1
VX	4.43	2.02	2.15	857.5	512.95	287.99	1
VX+NH	4.43	2.02	1.43	857.09	509.12	291.09	1
GV	3.72	−0.63	0.28	621.04	400.01	288.37	1
GV+NH	3.72	−0.63	-0.44	615.32	392.09	280.51	1
GV+NH-Ninvert	3.72	−0.63	-0.44	632.7	406.37	296.36	1
methamidophos	1.82	−0.82	0.37	422.7	293.59	209.81	0
paraoxon	3.15	2.31	2.87	776.34	496.58	446.65	0
parathion	2.70	3.84	3.52	792.79	489.21	457.8	0
dichlorvos	1.82	0.71	1.38	571.31	381.58	402.51	0
DMMPA	−0.38	−1.85	-0.19	578.21	371.72	276.96	0
leptophos	0.87	6.25	5.72	912.58	545.36	742.26	0
diisopropyl	2.89	1.17	2.22	573.47	372.45	202.56	0
EDMM	4.27	0.26	0.64	697.59	442.92	292.88	1
EDMM+NH	4.27	0.26	−0.08	687.01	427.23	286.58	1
trichlorfon	0.80	0.48	1.4	596.87	377.46	376.31	0

MP2-water	pK_a	HOMO	LUMO	LUMO−HOMON	LUMO−HOMON	LUMO−HOMON	P-charge	f_P(-)	f_C(-)
				N	*N*+1	*N*-1			
sarin	3.15	−0.47351	0.04164	14.01805574	2.490405632	15.2725105	2.60397	0.08602	0.06525
soman	3.15	−0.44782	0.0402	13.27980503	2.223731952	14.25479666	2.60705	0.0866	0.06897
tabun	9.21	−0.40475	0.04203	12.15759865	4.869787936	14.77644303	2.52664	0.04248	−0.00239
amiton	9.99	−0.35233	0.04063	10.69307034	3.786222024	11.09063181	2.43184	0.03013	0.00275
amiton+NH	9.99	−0.39228	0.03812	11.71187264	4.585970948	14.41425664	2.44305	0.02904	0.00296
VX	9.99	−0.34398	0.03964	10.43891399	3.71846514	10.83103315	2.18708	0.04278	0.00134
VX+NH	9.99	−0.38596	0.0373	11.51758182	4.482294752	14.08662897	2.19825	0.04075	0.00123
GV	3.15	−0.36573	0.04126	11.07484908	3.280630496	11.10695877	2.78349	0.03816	0.00702
GV+NH	3.15	−0.40692	0.03739	12.090386	4.949245808	15.26461914	2.78232	0.0371	0.00556
GV+NH-Ninvert	3.15	−0.40552	0.03763	12.05882054	4.857542716	15.14896984	2.78388	0.03173	−0.00495
methamidophos	10.24	−0.37661	0.04329	11.42615084	3.602271608	13.7622667	2.31815	0.03067	0.00404
paraoxon	7.11	−0.36283	0.02967	10.680553	8.131098196	11.86371337	2.82207	0.00748	0.00118
parathion	7.11	−0.36244	0.02853	10.63891925	8.164024232	10.84599953	2.31227	0.02818	0.00382
dichlorvos	25.01	−0.36321	0.04204	11.0275009	4.822167636	13.56579895	2.81469	0.00463	−0.00214
DMMPA	15.36	−0.38598	0.0415	11.63241477	3.019943368	13.62566447	2.75578	0.04564	−0.00204
leptophos	9.95	−0.34522	0.03918	10.46013904	4.9389054	10.60789803	2.06378	0.04262	0.00708
diisopropyl	16.01	−0.47438	0.0419	14.04880485	3.91983098	14.65018121	2.84698	0.07436	0.06209
EDMM	9.99	−0.36339	0.04062	10.99375852	3.843094268	11.19131473	2.18198	0.04392	0.00262
EDMM+NH	9.99	−0.38697	0.03775	11.55731075	4.784071396	14.0191442	2.18864	0.02918	−0.00344
trichlorfon	15.36	−0.4488	0.04233	13.36443311	5.32803128	13.91437954	2.59128	−0.00149	−0.00048

to be continued

continued Table S2-4

MP2-water	f_C(-)_largest	I	A	$I-A$	μ	η	ω
sarin	0.06525	9.826432	−0.43952	10.26595	−4.69346	5.132973	2.145788
soman	0.06897	9.765036	−0.41191	10.17694	−4.67656	5.088472	2.149
tabun	0.09103	7.78297	−0.26842	8.051393	−3.75727	4.025697	1.753374
amiton	0.03978	7.317263	−0.64121	7.958472	−3.33803	3.979236	1.40007
amiton+NH	0.03597	7.674541	−1.03345	8.70799	−3.32055	4.353995	1.266196
VX	0.04098	7.135899	−0.61826	7.75416	−3.25882	3.87708	1.369575
VX+NH	0.03738	7.50956	−1.00017	8.509726	−3.2547	4.254863	1.244817
GV	0.09171	7.66387	−0.4546	8.118466	−3.60464	4.059233	1.600476
GV+NH	0.0912	7.803375	−1.20035	9.003722	−3.30151	4.501861	1.21061
GV+NH-Ninvert	0.0921	7.784235	−1.18596	8.970193	−3.29914	4.485097	1.213387
methamidophos	0.04743	7.175283	−0.64062	7.815902	−3.26733	3.907951	1.365864
paraoxon	0.02901	8.376291	−1.475	9.851291	−3.45065	4.925645	1.208669
parathion	0.02401	7.286746	−1.47965	8.766399	−2.90355	4.383199	0.961693
dichlorvos	0.00155	7.330465	−0.43742	7.76788	−3.44652	3.88394	1.529186
DMMPA	0.08494	7.413183	−0.38347	7.796649	−3.51486	3.898324	1.584557
leptophos	0.03001	7.235325	−1.09839	8.333714	−3.06847	4.166857	1.129808
diisopropyl	0.06209	9.899553	−0.60705	10.5066	−4.64625	5.2533	2.054677
EDMM	0.04077	9.380112	−0.63649	10.0166	−4.37181	5.008299	1.908108
EDMM+NH	0.03354	7.514835	−1.16443	8.679267	−3.1752	4.339633	1.161608
trichlorfon	0.04154	8.998394	−1.29725	10.29564	−3.85057	5.147821	1.440116

MP2-water	bond order						
	bo1_X	bo2_O-C	bo3_N	bo4_N+1	bo5_N-1	bo6_P-X	bo7_O-C
sarin	0.5669	0.7835	0.5669	0.5645	0.5738	0.1515	0.0577
soman	0.5672	0.7826	0.5672	0.5652	0.5721	0.1522	0.0527
tabun	0.7448	0.7999	0.7144	0.6566	0.6712	0.1514	0.0271
amiton	0.9429	0.8132	0.6807	0.6807	0.7214	0.1155	0.0244
amiton+NH	0.9217	0.8071	0.6912	0.6892	0.7332	0.1133	0.025
VX	0.906	0.8228	0.6757	0.676	0.718	0.1123	0.0138
VX+NH	0.8847	0.8162	0.6865	0.6846	0.7294	0.1129	0.0143
GV	0.7018	0.8219	0.5753	0.5751	0.6287	0.1619	0.0193
GV+NH	0.6756	0.8507	0.5829	0.5826	0.6363	0.1647	0.0184
GV+NH-Ninvert	0.68	0.85	0.5717	0.572	0.6202	0.1631	0.0275
methamidophos	0.9307	0.8448	0.6752	0.6746	0.7253	0.1219	0.0147
paraoxon	0.6273	0.805	0.6273	0.6452	0.5719	0.0554	0.0074
parathion	0.6233	0.804	0.6233	0.6424	0.6784	0.0172	0.0191
dichlorvos	0.6326	0.8272	0.6326	0.6768	0.5732	0.0594	0.0103
dmmpa	0.6881	0.8407	0.6881	0.6964	0.6401	0.1252	0.0239
leptophos	0.6142	0.8304	0.6142	0.5689	0.667	0.0132	0.0154
diisopropyl	0.5908	0.7779	0.5908	0.5879	0.5842	0.1474	0.06
EDMM	0.9317	0.8215	0.6704	0.6788	0.7127	0.1491	0.0273
EDMM+NH	0.9115	0.8152	0.6777	0.6766	0.716	0.1205	0.0243
trichlorfon	0.696	0.8304	0.696	0.5653	0.7058	0.0165	0.0064

表 S3-1　概念密度泛函方法(CDFT)选择的 11 个方程组预测结果及平均值

Table S3-1　Prediction results and average value with selected 11 established equations based on CDFT method.

Name	pLD_{50}_rat	STEPWISE Predicted pLD_{50}_rat	linear+ spline_ L7-C5	linear+ spline_ L5-C4	linear+ spline_ L7-C6	linear+ spline_ L8-C3	spline_ L5-C6	spline_ L5-C4	spline_ L9-C4
Training sets									
sarin	3.66	3.87	3.75	3.60	3.73	3.52	3.62	3.94	3.68
soman	4.01	3.57	4.04	3.95	4.05	3.93	3.93	3.94	3.94
tabun	3.31	2.33	3.51	3.32	3.39	3.19	2.91	3.21	3.26
amiton+NH	3.22	3.91	3.38	3.90	3.33	3.64	4.04	3.51	3.20
VX+NH	4.43	4.28	4.28	4.21	4.27	4.22	4.24	4.23	4.52
GV+NH-Ninvert	3.72	3.42	3.69	3.84	3.69	3.88	3.74	3.91	3.70
methamidophos	1.82	0.66	1.74	1.64	1.72	1.59	1.04	1.63	1.79
paraoxon	3.15	3.02	3.01	3.10	3.13	3.26	2.88	2.75	3.11
parathion	2.70	2.09	2.64	2.39	2.69	2.75	2.25	2.75	2.70
dichlorvos	1.82	2.23	1.93	2.05	1.92	1.98	2.04	1.63	1.88
DMMPA	−0.38	0.68	−0.42	−0.38	−0.40	-0.40	0.67	−0.27	−0.39
leptophos	0.87	1.16	0.95	1.00	0.90	0.82	0.91	0.98	0.86
diisopropyl	2.89	3.65	2.70	3.03	2.68	3.02	3.11	2.78	2.94
EDMM+NH	4.27	3.93	4.25	3.85	4.34	4.04	4.23	4.32	4.27
trichlorfon	0.80	1.48	0.83	0.79	0.86	0.84	0.68	0.98	0.83
Testing sets									
triazophos	0.97	1.51	−0.06	1.99	0.00	0.24	1.87	2.16	−0.55
DCP	1.60	2.02	1.59	2.01	1.64	1.84	0.91	-0.24	1.00
TEP	0.10	1.93	1.48	1.78	1.54	1.59	1.00	0.26	1.63
DMMP	−0.30	1.54	−0.44	0.03	-0.51	-0.10	−1.21	−0.18	−0.04
24-optfreq		6.82	9.30	0.23	9.06	5.84	6.17	5.12	9.81
27-optfreq		6.10	8.80	0.28	8.56	5.52	5.17	3.94	9.43

Name	logki	pLD_{50}_rat	spline_L8-C3	linear_L5-C4	linear_L8-C8	Average value of 11 pred.	Residue
Training sets							
sarin	4.95	3.66	3.57	3.62	3.50	**3.67**	0.01
soman	5.45	4.01	3.87	3.93	4.17	**3.94**	−0.07
tabun	4.49	3.31	3.57	2.91	3.32	**3.17**	−0.14
amiton+NH	4.2	3.22	3.79	4.04	3.43	**3.65**	0.43
VX+NH	5.51	4.43	4.20	4.24	4.28	**4.27**	−0.16
GV+NH-Ninvert		3.72	3.65	3.74	3.73	**3.73**	0.01
methamidophos		1.82	1.72	1.04	1.89	**1.50**	−0.32
paraoxon		3.15	3.13	2.88	3.05	**3.03**	−0.12
parathion		2.70	2.53	2.25	2.67	**2.52**	−0.18
dichlorvos		1.82	2.03	2.04	1.80	**1.96**	0.14
DMMPA		−0.38	-0.43	0.67	-0.41	**-0.10**	0.28
leptophos		0.87	0.90	0.91	0.88	**0.93**	0.06
diisopropyl		2.89	3.10	3.11	2.89	**3.00**	0.11
EDMM+NH		4.27	3.90	4.23	4.27	**4.15**	−0.12
trichlorfon		0.80	0.75	0.68	0.82	**0.87**	0.07
Testing sets							
triazophos		0.97	−0.46	1.87	0.51	**0.83**	−0.14
DCP		1.60	2.27	0.91	1.66	**1.42**	−0.18
TEP		0.10	1.96	1.00	0.47	**1.33**	1.23
DMMP		−0.30	0.54	−1.21	-1.48	**-0.28**	0.02
24-optfreq	7.11		5.17	6.17	6.60	**6.39**	
27-optfreq	7.11		4.52	5.17	5.11	**5.69**	

表 S3-2　常规 2D-QSAR 优选的 9 个方程组预测结果及平均值

Table S3-2　Prediction results and average value with selected 9 established equations based on conventional 2D-QSAR method.

Name	pLD_{50}	linear _L9-C6	Linear _L9-C5	Linear _L8-C5	Linea _L4-C5	Linear _L6-C4	Linear _L8-C2	Linear _L5-C3	linear_ L5-C2	STEPWISE Predicted pLD_{50}	Average value of 9 pred.	Residue
Training Sets												
sarin	3.66	3.71	3.57	3.77	3.01	3.48	3.89	3.70	4.00	3.65	**3.64**	−0.02
soman	4.01	3.99	4.25	4.18	4.21	4.27	4.00	3.87	4.04	4.01	**4.09**	0.08
tabun	3.31	3.30	3.15	3.17	3.51	3.18	2.68	3.65	3.31	3.30	**3.25**	−0.06
amiton+NH	3.22	3.26	3.34	3.32	3.29	3.31	3.22	3.11	2.53	3.22	**3.18**	−0.04
VX+NH	4.43	4.44	4.35	4.51	4.87	4.28	4.78	4.69	4.40	4.43	**4.53**	0.10
GV+NH-Ninvert	3.72	3.78	3.58	3.70	3.47	3.69	3.89	3.73	3.70	3.71	**3.69**	−0.03
methamidophos	1.82	1.80	1.88	1.88	2.36	1.97	1.69	1.66	2.07	1.83	**1.91**	0.09
paraoxon	−0.38	−0.41	−0.33	−0.28	−0.23	−0.21	0.14	0.07	0.29	-0.36	**-0.15**	0.23
parathion	4.27	4.11	4.30	4.10	3.87	4.34	4.12	4.08	4.15	4.27	**4.15**	−0.12
dichlorvos	0.87	0.85	0.87	0.90	1.30	0.79	1.06	0.67	0.42	0.87	**0.86**	−0.01
DMMPA	1.82	1.86	1.91	1.75	1.79	1.90	2.08	1.90	2.84	1.84	**1.99**	0.17
leptophos	3.15	3.16	3.13	3.32	3.37	3.42	3.08	2.87	3.07	3.15	**3.17**	0.02
diisopropyl	2.70	2.72	2.70	2.41	2.46	2.39	2.67	3.16	2.36	2.70	**2.62**	−0.08
EDMM+NH	2.89	2.89	2.84	2.70	2.21	2.69	2.49	2.19	2.29	2.89	**2.58**	−0.31
trichlorfon	0.80	0.82	0.74	0.87	0.80	0.78	0.52	0.96	0.85	0.80	**0.79**	−0.01
Testing Sets												
triazophos	0.97	−0.15	−0.19	0.22	−0.48	-0.56	0.14	−1.19	0.02	1.51	**-0.08**	−1.05
DCP	1.60	1.76	1.58	1.91	1.27	1.39	1.53	0.96	2.04	2.22	**1.63**	0.03
TEP	0.10	2.12	3.53	3.00	3.34	3.48	2.02	1.25	2.38	3.57	**2.74**	2.64
DMMP	−0.30	1.00	1.10	1.20	1.04	1.00	1.59	2.37	2.06	2.99	**1.59**	2.01
24-optfreq		1.23	0.57	0.52	0.67	0.91	1.58	0.54	1.75	2.54	**1.15**	
27-optfreq		0.38	0.01	−0.18	0.26	0.58	1.37	−0.35	1.56	2.41	**0.67**	