Supplementary Information

MANUSCRIPT TITLE: Acetonitrile-driven interface force field reconstruction of HLB-SPME: Insight into pesticide adsorption mechanism based on energy lattice point models

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Table S1. Instrument parameters for the 125 analytes

Compound	Retention time (t/min)	Q1/Q3（m/z）	DP	CE
acetochlor	9.02	270.1/224.1/148.1	50	15/22
alachlor	9.21	270.1/238.1/162.1	50	13/28
albendazole	4.96	266.1/234.1/192	60	28/38
azinphos-methyl	6.06	318/132/125	58	22/33
chlorpyrifos	19.02	349.9/197.9/97	75	28/45
Coumaphos	12.46	363/307/227	100	23/35
disulfoton	13.44	275/89/61	50	17/46
diuron	5.51	233/72/46	50	37/34
ethoprophos	9.08	243.1/130.9/97	67	26/43
malathion	7.9	331/127/99	70	16/32
phosalone	13.57	368/322/182	76	13/20
propanil	6.75	218/162/127	71	21/37
thiabendazole	3.04	202/175/131.1	100	34/43
myclobutanil	8.47	289.1/125/70	80	46/35
pyridaphenthion	8.62	341.1/205/189.1	94	30/30
fonofos	11.49	247/137/109	50	14/25
malaoxon	4.21	315.1/127/99	70	16/31
demeton-S-sulfone	3.45	291/263/235	70	16/31
disulfoton sulfone	11.84	307/153/125	70	15/22
disulfoton sulfoxide	4.88	291/213/185	60	12/17
formothion	4.99	258/199/125	50	12/32
phorate sulfoxide	4.88	277/199/153	25	13/19
phorate sulfone	5.1	293/115/97	65	35/50

phenthoate	11.21	321/163.1/79.1	51	17/51
sulfotep	11.59	323/171.1/115	70	19/40
chlorpyrifos-methyl	13.83	323.9/125.1	65	28
terbuthylazine	6.86	230.1/174.1/104	40	23/41
phenmedipham	6.34	301.1/168.1/136	70	11/29
terbufos sulfoxide	6.53	305/187/130.9	57	20/38
quinalphos	10.65	299.1/163/147.1	77	31/29
cyanazine	3.91	241.1/214.1/104	60	24/40
fenamiphos	10.77	304.1/217/202	90	31/47
propyzamide	7.53	256/190/173	67	19/31
triazophos	8.83	314.1/162.1/119.1	80	24/50
iprobenfos	11.02	289.1/205/91.1	40	13/30
ethofumesate	6.8	287.1/259.1/121.1	80	12/20
diflubenzuron	10.72	311/158/141	45	20/49
etrimfos	11.2	293.1/265/125	80	26/34
pendimethalin	19.04	282.1/212.1/194.1	40	15/28
isazofos	8.4	316/164/122	70	23/35
triadimefon	8.08	294.1/225.1/119.1	70	17/21
isoprothiolane	7.73	291.1/231/198	65	16/30
mepronil	7.88	270.1/228.1/119	60	20/32
terbufos sulfone	6.56	321/115/97	75	39/57
metalaxyl	5.34	280.2/220.1/192.1	75	18/24
fenarimol	9.25	331/268.1/259	90	31/34
fenoxaprop-ethyl	16.98	362.1/228/244.1	60	24/32
fluazifop-butyl	18.17	384.1/328.1/282	105	24/29
oxadixyl	3.8	279.1/219.1/132.1	68	17/41

bensulfuron-methyl	6.42	411.1/182.1/149.1	40	26
chlorimuron-ethyl	8.06	415/186/121	40	25/24
lactofen	19.19	479.1/344/223	40	21/48
heptenophos	5.57	251/127/125	65	20/18
lufenuron	20.22	511/158/141	100	20/60
prochloraz	10.51	376.2/308/266	50	15/22
flusilazole	10.89	316.1/247.1/165.1	50	26/37
tebuconazole	11.93	308.2/125/70	95	47/49
fenbuconazole	10.75	337.1/125/70	95	42/43
metconazole	13.2	320.2/125/70	75	56/62
ipconazole	16.04	334.2/125/70	40	59/57
carfentrazone-ethyl	11.49	412/366/346.1	95	24/32
dimethomorph	8.02	388.1/301.1/165.1	105	29/43
cyprodinil	6.66	226.1/108.1/93.1	96	35/50
sulfentrazone	4.43	387/307/146	100	29/57
thifluzamide	10.5	528.8/488.8/148	100	38/60
flufenacet	9.45	364.1/194.1/152.1	70	16/27
pyrimethanil	5.5	200.1/183.1/168.1	60	33/40
pencycuron	14.26	329.1/218.1/125	100	21/35
fenpropidin	6.01	274.3/147.1/117.1	40	39/69
chlorfluazuron	21.07	540/384.9/382.9/158	100	30/20
diflufenican	16	395.1/266/246	60	34/46
dimethenamid	6.78	276.1/244.1/168.1	60	20/33
cadusafos	14.11	271.1/159/131	40	19/31
flurtamone	7.05	334.1/303.1/247.1	50	20/30
halosulfuron-methyl	9.03	435/182.1/139.1	40	24/62

flufenoxuron	20.98	489/158/141	71	27/65
tebufenozide	10.99	353.2/297.2/133.1	65	11/24
triflusulfuron-methyl	8.25	493.1/461.1/264.1	40	18/30
imibenconazole	19.01	411/171/125	50	25/50
novaluron	18.5	493/158.1/141	91	27/69
fluthiacet-methyl	7.05	404/344/274	40	31/39
zoxamide	12.08	336/204/187	90	23/31
isofenphos-methyl	8.44	332.1/231/121	50	19/43
pyribenzoxim	19.08	610.2/413.1/180.1	50	17/48
dinotefuran	2.66	203.1/157.1/129.1	65	11/16
boscalid	7.5	343/307.1/140	100	28/27
famoxadone	13.77	392.2/331.1/238.1	65	12/24
prochloraz metabolite	12.72	325/282/129.1	90.000	21/25
thiophanate-methyl	4.14	343.1/311/151	60.000	15/26
nitenpyram	2.79	271.1/225.1/99	70.000	16/22
benazolin-ethyl	6.39	272/198/170	65.000	20/33
methacrifos	5.87	241/209/125	58.000	11/25
pyrethrin I	20.75	329.2/161.2/133.1	75.000	13/22
methoprene	21.84	279/237/191	60.000	9/11
monocrotophos	3.04	224.1/127/98.1	60.000	21/17
thiamethoxam	2.98	292/211.1/181.1	60.000	16/30
pyraclostrobin	13.62	388.1/194.1/163.1	50.000	18/36
metrafenone	13.84	409.1/227/209.1	71.000	27/21
triticonazole	9.42	318.1/125/70	80.000	51/46
cyazofamid	10.1	325.1/261.1/108	70.000	15/20
silthiofam	10.75	268.1/252.1/139	60.000	12/24

tolfenpyrad	18.87	384.1/197.1/171	40.000	35/33
amisulbrom	16.71	466/227/148.1	90.000	27/64
proquinazid	20.36	373/331/288.9	80.000	31/21
fluopyram	9.07	397.1/208/173	60.000	30/40
flubendiamide	12.81	705/571/531	150.000	45/55
fenoxanil	10.55	329.1/302.1/86.1	78.000	16/25
picoxystrobin	11.2	368.1/205.1/145.1	54.000	13/27
pyrisoxazole	4.23	289.1/151.1/120	50.000	20/30
cyantraniliprole	4.71	474/444/285.9	60.000	27/18
metaflumizone	20.15	507.1/287.1/178	80.000	33/32
trifloxystrobin	16.06	409.1/186.1/145	40.000	23/63
penflufen	11.32	318.2/234.1/141	100.000	22/37
sedaxane	8.71	332.2/292.1/159	40.000	20/25
triflumizole metabolite	3.95	295/215/195	90.000	31/38
ametoctradin	14.2	276.2/176.1/149	40.000	51/50
fluxapyroxad	8.24	382.1/362.1/342.1	90.000	20/28
propaquizafop	18.13	444.1/371.1/100.1	100.000	19/21
coumoxystrobin	19.26	437.2/205.1/145.1	65.000	12/34
spirotetramat-enol	4.83	302.2/270.1/216.1	60.000	27/38
prochloraz metabolite	12.72	325/282/129.1	90.000	21/25
enestroburin	18.19	400.1/178/137	45.000	20/38
spirotetramat-keto-hydroxy	5.86	318.2/300.2/214.1	70.000	18/37
spirotetramat-enol-glucoside	3.18	464.2/302.2/216.1	60.000	24/61
clethodim sulfone	5.96	392.1/300.1/164.1	60.000	20/37

Table S2. the Log P, K values of the compounds used for the correlation study

Number	Compound	Log P	K_w	K_{w-s}
1	acetochlor	3.32	2.200	5.560
2	alachlor	3.43	1.1497	9.780
3	albendazole	3.07	1.118	13.745
4	azinphos-methyl	2.93	1.893	10.873
5	chlorpyrifos	4.60	1.755	7.440
6	Coumaphos	3.89	1.653	8.267
7	disulfoton	2.95	1.102	5.148
8	diuron	2.48	0.946	11.644
9	ethoprophos	3.23	1.821	9.791
10	malathion	1.79	2.976	5.602
11	phosalone	4.00	1.953	8.173
12	propanil	2.95	1.005	6.443
13	thiabendazole	2.15	0.998	12.549
14	myclobutanil	3.72	1.125	5.705
15	pyridaphenthion	2.69	1.167	6.173
16	fonofos	3.41	1.471	15.509
17	malaoxon	0.89	1.821	10.576
18	demeton-S-sulfone	1.04	1.882	9.459
19	disulfoton sulfone	1.94	1.342	12.544
20	disulfoton sulfoxide	1.84	1.601	9.592
21	formothion	0.26	2.032	10.306
22	phorate sulfoxide	1.82	1.005	9.259
23	phorate sulfone	1.92	1.102	16.681
24	phenthoate	3.07	1.195	5.280
25	sulfotep	2.59	0.973	7.383
26	chlorpyrifos-methyl	3.90	1.101	5.727
27	terbuthylazine	2.74	1.086	9.699
28	phenmedipham	3.42	1.793	12.464

29	terbufos sulfoxide	2.41	1.113	5.958
30	quinalphos	3.01	1.617	7.030
31	cyanazine	2.34	0.803	16.997
32	fenamiphos	3.05	0.975	9.889
33	propyzamide	4.14	1.487	13.616
34	triazophos	3.07	0.817	14.771
35	iprobenfos	3.43	1.215	11.481
36	ethofumesate	2.46	0.611	8.881
37	diflubenzuron	3.47	1.905	5.309
38	etrimfos	2.57	1.344	17.115
39	pendimethalin	4.17	1.350	5.524
40	isazofos	3.10	1.244	9.218
41	triadimefon	3.64	1.692	4.845
42	isoprothiolane	2.96	1.095	9.112
43	mepronil	3.81	1.116	8.910
44	terbufos sulfone	2.50	0.978	6.517
45	metalaxyl	2.06	1.200	15.131
46	fenarimol	3.83	1.578	6.222
47	fenoxaprop-ethyl	4.65	1.091	8.050
48	fluazifop-butyl	5.22	1.440	6.421
49	oxadixyl	1.70	1.171	12.313
50	bensulfuron-methyl	1.85	1.443	8.872
51	chlorimuron-ethyl	2.54	2.777	5.025
52	lactofen	5.29	1.985	8.117
53	heptenophos	0.86	1.109	15.211
54	lufenuron	6.54	2.188	7.040
55	prochloraz	4.41	2.265	8.030
56	flusilazole	5.09	1.011	9.413
57	tebuconazole	3.63	1.519	16.450

58	fenbuconazole	4.30	1.482	5.373
59	metconazole	3.58	2.177	5.539
60	ipconazole	4.01	1.486	6.079
61	carfentrazone-ethyl	4.00	2.190	4.565
62	dimethomorph	3.51	1.117	9.336
63	cyprodinil	3.45	1.392	11.797
64	sulfentrazone	2.26	1.216	8.501
65	thifluzamide	6.61	1.640	10.619
66	flufenacet	3.41	1.227	12.761
67	pyrimethanil	2.69	1.052	12.337
68	pencycuron	4.80	2.084	10.440
69	fenpropidin	3.76	1.863	8.264
70	chlorfluazuron	6.69	2.088	5.096
71	diflufenican	4.92	1.305	7.633
72	dimethenamid	2.23	1.081	15.374
73	cadusafos	3.99	1.087	6.156
74	flurtamone	4.01	0.823	13.258
75	halosulfuron-methyl	1.49	2.910	10.614
76	flufenoxuron	6.18	1.583	10.288
77	tebufenozide	4.92	1.234	6.148
78	triflusulfuron-methyl	2.81	2.835	8.526
79	imibenconazole	5.48	0.858	15.008
80	novaluron	6.80	1.964	5.119
81	fluthiacet-methyl	3.98	1.088	9.025
82	zoxamide	4.29	2.819	15.548
83	isofenphos-methyl	3.16	1.243	7.128
84	pyribenzoxim	7.48	1.694	7.639
85	dinotefuran	1.70	1.957	17.308
86	boscalid	4.52	1.421	7.947

87	famoxadone	4.88	1.911	10.566
88	prochloraz metabolite	3.87	1.405	5.151
89	thiophanate-methyl	3.21	2.659	10.654
90	nitenpyram	-1.09	1.953	18.577
91	benazolin-ethyl	2.82	0.932	15.913
92	methacrifos	0.85	0.903	16.367
93	pyrethrin I	4.51	1.155	13.772
94	methoprene	5.06	1.103	13.144
95	monocrotophos	-0.63	2.153	17.094
96	thiamethoxam	2.69	1.198	14.882
97	pyraclostrobin	4.64	2.323	5.068
98	metrafenone	4.89	2.477	11.140
99	triticonazole	3.40	1.382	6.720
100	cyazofamid	2.54	1.158	16.261
101	silthiofam	3.63	0.891	6.110
102	tolfenpyrad	5.22	1.403	4.540
103	amisulbrom	2.23	1.033	7.594
104	proquinazid	4.00	2.123	7.856
105	fluopyram	4.48	1.019	6.530
106	flubendiamide	5.30	1.616	7.167
107	fenoxanil	4.06	0.949	17.868
108	picoxystrobin	3.90	1.780	5.011
109	pyrisoxazole	2.59	1.297	15.167
110	cyantraniliprole	3.74	1.906	14.972
111	metaflumizone	7.21	2.816	6.803
112	trifloxystrobin	4.05	1.486	5.418
113	penflufen	4.08	1.171	7.653
114	sedaxane	3.56	1.260	6.157
115	triflumizole metabolite	3.12	1.311	15.215

116	ametoctradin	4.66	1.106	14.642
117	fluxapyroxad	4.28	2.052	6.229
118	propaquizafop	4.05	1.095	14.747
119	coumoxystrobin	5.47	2.017	6.765
120	spirotetramat-enol	1.84	1.563	14.107
121	prochloraz metabolite	3.78	1.048	14.546
122	enestroburin	4.12	2.330	9.162
123	spirotetramat-keto-hydroxy	1.94	1.621	6.933
124	spirotetramat-enol-glucoside	0.61	1.802	14.882
125	clethodim sulfone	1.40	1.539	8.787

K_w: Adsorption coefficient of pesticides in pure water
$K_{w\text{-}s}$: Adsorption coefficient of pesticides in aqueous solutions containing 1 μg/mL acetonitrile
DP and CE values presented are the mean values.

Table S3 The coefficients and associated variables for the equation of Kw 2D QSPR.

Coefficient	Variable	Coefficient	Variable	Coefficient	Variable	Coefficient	Variable
ALogP	1.02E-05	Count<ECFP_6:-1100000244>	1.11E-05	Count<ECFP_6:864518973>	-5.8E-06	Count<ECFP_6:6865857320>	-1.6E-06
Molecular_Weight	0.002307	Count<ECFP_6:226796801>	5.04E-06	Count<ECFP_6:-1764455838>	1.73E-06	Count<ECFP_6:-1072294614>	4.57E-07
Num_H_Donors	1.36E-05	Count<ECFP_6:220735655>	1.45E-06	Count<ECFP_6:-175507738>	1.32E-06	Count<ECFP_6:1337040050>	3.49E-06
Num_H_Acceptors	3.06E-05	Count<ECFP_6:-1236483485>	8.49E-06	Count<ECFP_6:-992506539>	-3.7E-07	Count<ECFP_6:-176494269>	-4.6E-07
Num_RotatableBonds	3.86E-05	Count<ECFP_6:-177077903>	3.02E-06	Count<ECFP_6:-167460056>	-4.4E-07	Count<ECFP_6:1564392544>	-1.6E-06
Num_Rings	6.85E-06	Count<ECFP_6:1335691903>	7.69E-08	Count<ECFP_6:2106656448>	2.29E-06	Count<ECFP_6:1854732111>	-8.5E-07
Num_AromaticRings	6.22E-06	Count<ECFP_6:1996767644>	1.5E-07	Count<ECFP_6:864909220>	8.08E-06	Count<ECFP_6:1841329970>	4.54E-07
Molecular_Fractional	1.66E-07	Count<ECFP_6:-	4.35E-06	Count<ECFP_6:-	-1E-06	Count<ECFP_6:67	-1.6E-06

PolarSurfaceArea		786013480>		845108448>		6555381>	
Count<ECFP_6:-817402818>	3.16E-07	Count<ECFP_6:1430169877>	2.43E-06	Count<ECFP_6:-826638028>	-1.8E-06	Count<ECFP_6:-677055651>	3.55E-08
Count<ECFP_6:-1046436026>	4.34E-06	Count<ECFP_6:1997021792>	3.48E-06	Count<ECFP_6:672362763>	-9E-07	Count<ECFP_6:-708878603>	-1.5E-06
Count<ECFP_6:-1059365320>	6.35E-06	Count<ECFP_6:2007300961>	5.12E-06	Count<ECFP_6:1310520534>	-3.1E-06	Count<ECFP_6:-1925046727>	9.11E-07
Count<ECFP_6:-1074141656>	7.59E-06	Count<ECFP_6:1559650422>	-7.1E-07	Count<ECFP_6:-1250439909>	-3.9E-06	Count<ECFP_6:-797085356>	1.22E-06
Count<ECFP_6:-1897341097>	4.05E-06	Count<ECFP_6:734603939>	-3E-06	Count<ECFP_6:834876373>	-1.1E-06	Count<ECFP_6:-2024255407>	3.39E-06
Count<ECFP_6:642810091>	-9.48E-07	Count<ECFP_6:863188371>	-2.6E-06	Count<ECFP_6:-949601813>	-3.2E-06	Count<ECFP_6:683445015>	-1.1E-06
Count<ECFP_6:-1085223908>	2.80E-06	Count<ECFP_6:859796174>	2.73E-06	Count<ECFP_6:-830332112>	-1.3E-06	Count<ECFP_6:670515721>	3.64E-07
Count<ECFP_6:-182236392>	2.56E-06	Count<ECFP_6:655739385>	-1.7E-06	Count<ECFP_6:1433087471>	-1.5E-07	Count<ECFP_6:1571214559>	-1.8E-06

Count<ECFP_6:-1910270391>	-9.19E-07	Count<ECFP_6:-677309799>	-4E-06	Count<ECFP_6:898418220>	1.47E-06		

Note: Kw [PLSTempModel] = 0.7097 + 1.017e-05 * [ALogP] + 0.002307 * [Molecular_Weight] + 1.362e-05 * [Num_H_Donors] + 3.06e-05 * [Num_H_Acceptors] + 3.862e-05 * [Num_RotatableBonds] + 6.851e-06 * [Num_Rings] + 6.222e-06 * [Num_AromaticRings] + 1.656e-07 * [Molecular_FractionalPolarSurfaceArea] + 3.162e-07 * [Count<ECFP_6:817402818>] + 4.344e-06 * [Count<ECFP_6:-1046436026>] + 6.349e-06 * [Count<ECFP_6:-1059365320>] + 7.593e-06 * [Count<ECFP_6:-1074414165>] + 4.048e-06 * [Count<ECFP_6:-1897341097>] + 9.476e-007 * [Count<ECFP_6:642810091>] + 2.801e-06 * [Count<ECFP_6:-1085223908>] + 2.561e-06 * [Count<ECFP_6:-182236392>] - 9.191e-007 * [Count<ECFP_6:-1910270391>] + 1.112e-05 * [Count<ECFP_6:1100000244>]+5.041e06*[Count<ECFP_6:226796801>]+1.446e06*[Count<ECFP_6:220735655>] + 8.492e-06 * [Count<ECFP_6:-1236483485>] + 3.018e-06 * [Count<ECFP_6:-177077903>] + 7.686e-08 * [Count<ECFP_6:1335691903>] + 1.497e-07 * [Count<ECFP_6:1996767644>] + 4.345e-06 * [Count<ECFP_6:-786013480>] + 2.432e-06 * [Count<ECFP_6:1430169877>] + 3.484e-06 * [Count<ECFP_6:1997021792>] + 5.115e-06 * [Count<ECFP_6:2007300961>] - 7.087e-007 * [Count<ECFP_6:1559650422>] - 2.954e-006 * [Count<ECFP_6:734603939>]2.644e006*[Count<ECFP_6:863188371>]+2.726e006*[Count<ECFP_6:859796174>] - 1.687e-06 * [Count<ECFP_6:655739385>] - 4.032e-006 * [Count<ECFP_6:-677309799>] - 5.776e-006 * [Count<ECFP_6:864518973>] + 1.735e-06 * [Count<ECFP_6:-1764455838>] + 1.32e-006 * [Count<ECFP_6:-175507738>] - 3.7e-007 * [Count<ECFP_6:-992506539>] - 4.352e-007 * [Count<ECFP_6:-167460056>] + 2.288e-06*[Count<ECFP_6:2106656448>]+8.083e06*[Count<ECFP_6:864909220>]1.007e006*[Count<ECFP_6:845108448>] - 1.769e-006 *

[Count<ECFP_6:826638028>] - 9.03e-007 * [Count<ECFP_6:672362763>] - 3.051e-006 * [Count<ECFP_6:1310520534>]3.868e006*[Count<ECFP_6:1250439909>]1.145e006*[Count<ECFP_6:834876373>]3.225e006*[Count<ECFP_6:949601813>]1.279e006*[Count<ECFP_6:830332112>]1.511e007*[Count<ECFP_6:1433087471>]+1.474e06*[Count<ECFP_6:898418220>]1.625e006*[Count<ECFP_6:6895587320>]+4.572e-07* [Count<ECFP_6:1072294614>]+3.494e-06*[Count<ECFP_6:1337040050>] - 4.637e-007 * [Count<ECFP_6:-176494269>]1.595e006*[Count<ECFP_6:1564392544>]8.504e007*[Count<ECFP_6:1854732111>]+4.536e07*[Count<ECFP_6:1841329970>]1.568e006*[Count<ECFP_6:676555381>]+3.548e08*[Count<ECFP_6:677055651>] - 1.516e-006 * [Count<ECFP_6:-708878603>] + 9.115e-07 * [Count<ECFP_6:-1925046727>] + 1.223e-06 * [Count<ECFP_6:797085356>]+3.393e06*[Count<ECFP_6:2024255407>]1.112e006*[Count<ECFP_6:683445015>]+3.639e07*[Count<ECFP_6:670515721>]1.83e006*[Count<ECFP_6:1571214559>]。

Table S4 the coefficients and associated variables for the equation of Kw 3D QSAR.

Variable	Coefficient	Variable	Coefficient	Variable	Coefficient	Variable	Coefficient	Variable	Coefficient
VdW_7_6_1	-0.00292	VdW_4_11_4	-0.0001	VdW_7_3_10	-0.0174	VdW_12_8_13	0.00665	VdW_15_8_6	0.006747
Ele_7_6_1	0.003745	VdW_5_12_8	0.029165	VdW_11_14_6	-0.01183	VdW_11_13_12	0.00243	VdW_8_16_7	0.006252
VdW_13_9_5	0.02725	VdW_8_13_5	-0.01049	VdW_9_1_6	0.01476	VdW_12_15_5	-0.01144	Ele_6_8_8	-0.03177
VdW_5_8_3	-0.0001	Ele_10_7_9	-0.01432	VdW_13_6_8	-0.01076	VdW_5_8_6	0.007471	VdW_13_5_9	0.030983
VdW_7_3_6	0.005902	VdW_10_9_10	0.007587	VdW_4_7_11	-0.01481	VdW_11_11_13	-0.00728	VdW_9_12_9	-0.04179
VdW_13_10_5	-0.0023	VdW_15_13_9	0.010079	VdW_7_7_12	-0.03553	VdW_7_4_5	0.007444	VdW_12_4_10	-0.00177
VdW_10_2_4	-0.00573	VdW_14_11_5	0.021005	Ele_7_9_9	-0.04703	VdW_7_10_10	-0.00721	VdW_7_6_4	-0.00176
Ele_11_10_8	0.004988	VdW_4_7_	-0.02952	VdW_7_14_7	0.017917	VdW_6_6_5	0.019012	VdW_9_6_8	0.03313

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VdW_12_12_3	-0.01816	VdW_8_12_1	-0.00609	VdW_11_12_3	0.01594	VdW_5_5_8	-0.0161	Ele_12_9_9	-0.00032
VdW_6_4_2	-0.00299	VdW_12_14_6	0.026061	Ele_11_11_9	0.005928	VdW_6_10_2	0.009417	VdW_4_11_11	0.029645
VdW_12_6_5	0.012996	VdW_12_5_6	-0.00132	VdW_11_8_8	0.030585	VdW_13_13_5	-0.0092	VdW_6_6_12	-0.01499
VdW_12_6_11	-0.02004	Ele_12_10_7	-0.01525	VdW_7_3_9	0.024357	VdW_14_8_11	-0.03213	VdW_6_9_8	0.045305
VdW_8_14_6	0.012813	VdW_10_12_7	-0.01706	VdW_11_9_10	0.013574	VdW_5_13_4	0.003094	VdW_11_3_8	0.04167
VdW_13_6_4	0.007619	VdW_5_14_6	-0.00371	VdW_8_10_10	0.006716	VdW_7_6_3	-0.00634	VdW_13_7_11	-0.04099
VdW_11_6_3	-0.0092	VdW_12_5_4	0.00459	VdW_6_14_6	0.003156	VdW_8_9_12	-0.02469	VdW_7_7_6	-0.00111
VdW_7_14_6	0.000747	Ele_11_10_10	0.019629	VdW_5_5_5	0.002528	VdW_3_9_3	0.007309	VdW_13_6_11	-0.00724

VdW_9_8_6	0.049605	VdW_6_12_12	0.015197	VdW_11_4_7	-0.0034	VdW_15_6_10	-0.01396	VdW_10_7_4	-0.00403
VdW_13_8_4	-0.03692	VdW_10_11_9	0.02129	VdW_4_6_10	0.002835	VdW_6_14_9	-0.01697	VdW_4_8_10	0.01552
VdW_7_13_5	-0.01342	VdW_6_11_3	-0.02577	Ele_11_8_9	0.04453	VdW_6_3_4	-0.00147	VdW_5_13_6	-0.0228
VdW_7_3_7	-0.01242	VdW_9_3_5	-0.00123	VdW_12_7_4	0.018575	VdW_13_13_7	-0.02839	VdW_9_1_5	-0.00773
VdW_12_9_8	-0.01146	VdW_5_4_7	0.010771	Ele_7_11_8	0.025833	VdW_13_7_12	-0.00976	VdW_9_6_9	-0.02202
VdW_7_11_8	0.024087	Ele_7_9_10	-0.02319	VdW_8_4_11	-0.01427	VdW_10_5_9	0.002659	VdW_14_10_7	0.00849
VdW_15_8_10	-0.02629	VdW_17_8_6	0.030793	VdW_4_10_10	0.0066	Ele_9_6_9	-0.00111	VdW_13_8_11	-0.00091
VdW_9_7_7	-0.00496	VdW_10_11_10	-0.02254	Ele_9_9_11	-0.01542	VdW_4_9_7	-0.0042	Ele_9_11_10	0.016261
VdW_13_11_	-0.01514	VdW_9_12	-0.01086	VdW_11_8_1	0.006907	VdW_7_8_13	-0.01835	VdW_7_12_6	0.010175

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VdW_5_12_7	0.006245	VdW_8_13_3	0.008443	VdW_4_9_4	-0.00593	VdW_16_8_12	-0.01466	VdW_13_9_12	0.003526
VdW_6_11_11	-0.00874	VdW_14_8_6	0.017961	VdW_14_7_5	-0.02227	VdW_11_4_5	0.039834	VdW_1_10_4	-0.00617
VdW_12_7_3	0.004419	VdW_5_7_10	0.036003	VdW_16_8_7	-0.00306	VdW_11_5_3	-0.02206	VdW_7_11_6	0.029504
VdW_5_12_4	-0.02211	VdW_13_8_5	0.008026	VdW_7_10_2	-0.01481	VdW_11_13_11	-0.00339	VdW_11_12_4	-0.01349
VdW_13_12_5	-0.00287	VdW_6_10_10	0.036177	VdW_8_14_4	0.00245	VdW_8_7_6	0.00857	VdW_11_7_9	-0.01147
VdW_7_5_5	0.005961	VdW_8_12_8	-0.02343	VdW_4_3_6	-0.03	Ele_12_9_8	-0.00708	VdW_11_11_6	-0.02044
VdW_16_8_5	-0.0119	VdW_9_5_11	-0.02055	VdW_12_6_10	0.004122	VdW_11_8_3	0.013617	Ele_8_9_10	0.01895
Ele_10_10_10	-0.02014	VdW_5_13_7	-0.02912	VdW_14_9_5	-0.00146	VdW_13_4_13	0.013903	VdW_11_8_10	-0.02666

VdW_13_4_9	-0.0263	VdW_10_6_13	-0.00256	Ele_8_7_10	0.020906	VdW_14_5_7	-0.00571	VdW_14_12_11	-0.00637
Ele_11_10_7	0.015642	VdW_5_10_3	-0.01896	VdW_12_4_6	0.02353	Ele_8_9_11	-0.01304	VdW_11_5_4	0.030379
VdW_9_11_10	0.03521	VdW_9_10_6	-0.02026	VdW_12_10_7	0.032267	VdW_7_4_11	-0.01305	VdW_7_13_11	0.014685
VdW_11_3_10	-0.01378	VdW_12_4_11	-0.01913	VdW_8_15_6	0.001974	VdW_5_7_5	0.003339	VdW_7_10_12	0.0056
VdW_10_7_8	-0.01526	VdW_5_7_11	0.015883	VdW_11_2_4	-0.00538	VdW_14_12_4	0.007549	Ele_12_8_8	-0.01776
VdW_14_11_6	-0.02575	VdW_14_12_10	-0.01709	VdW_14_7_10	-0.00173	VdW_8_4_4	0.01302	VdW_11_6_8	-0.00417
VdW_11_10_9	-0.01392	VdW_7_9_12	0.019386	Ele_11_8_8	0.021918	Ele_7_7_10	-0.00263	VdW_13_11_11	0.015569
VdW_4_12_10	0.017219	VdW_13_7_5	0.009749	VdW_6_7_11	-0.00277	VdW_14_6_10	-0.00168	VdW_6_5_10	0.001658
Ele_10_11_9	-0.00355	VdW_15_8	-0.02639	VdW_14_5_1	-0.00461	VdW_6_3_7	-0.0018	VdW_14_8_1	0.010637

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VdW_5_13_9	-0.01548	VdW_14_10_6	0.037437	VdW_7_9_10	-0.01006	VdW_5_11_12	0.015857	VdW_6_8_4	-0.00835
VdW_7_7_14	-0.00574	VdW_10_12_8	0.001151	VdW_7_9_3	0.013402	VdW_11_4_11	0.016254	VdW_7_12_5	-0.00964
VdW_7_14_5	0.010787	VdW_14_5_9	-0.00163	Ele_11_9_7	-0.02282	VdW_13_13_6	0.00615	VdW_13_15_8	-0.02481
VdW_8_5_3	0.011669	VdW_14_8_5	0.001099	VdW_16_6_7	-0.01505	Ele_7_7_9	-0.02329	Ele_9_7_10	0.032405
VdW_13_4_7	0.023853	VdW_6_5_4	0.016108	VdW_11_10_2	0.000479	VdW_14_9_8	0.010421	VdW_7_13_12	-0.00389
VdW_4_6_7	-0.0106	VdW_14_14_9	0.007332	VdW_15_8_11	0.002866	VdW_11_7_4	0.015148	VdW_10_7_3	0.022421
Ele_11_7_8	0.006884	VdW_12_10_8	0.001246	VdW_14_13_6	0.007964	VdW_11_10_13	0.006389	VdW_7_11_9	0.006178
VdW_11_11_8	0.005624	VdW_11_10_8	0.015601	VdW_3_9_6	0.008067	VdW_8_13_12	0.009288	Ele_10_6_9	-0.01991

VdW_11_9_7	-0.00178	VdW_11_10_7	-0.02342	VdW_8_14_5	-0.00334	Ele_10_7_8	-0.00273	VdW_8_14_12	0.031145
VdW_15_12_6	0.015609	VdW_11_14_12	0.001477	VdW_8_10_13	0.021065	Ele_12_9_7	-0.02904	VdW_11_10_6	-0.00774
VdW_6_13_4	-0.01975	VdW_7_12_11	0.017938	VdW_5_4_9	0.028828	VdW_8_4_10	0.031553	VdW_6_3_8	0.017451
VdW_12_13_5	0.022895	VdW_4_7_8	0.026345	VdW_8_3_7	0.012198	VdW_14_9_7	-0.04186	VdW_13_13_10	-0.01031
VdW_15_11_8	-0.00785	VdW_8_7_12	0.029969	VdW_10_9_6	-0.00418	VdW_7_5_9	-0.0007	VdW_12_5_5	-0.00652
VdW_11_8_7	-0.01543	VdW_10_8_6	0.008595	VdW_14_12_7	-0.0015	VdW_6_13_7	0.030931	VdW_13_7_6	0.009167
VdW_9_8_13	-0.0029	VdW_12_8_4	0.023818	VdW_7_4_2	0.020434	VdW_7_15_9	-0.00563	Ele_8_12_7	-0.00656
VdW_12_8_3	-0.00473	VdW_4_7_6	0.008183	VdW_8_11_10	0.020297	VdW_14_5_6	-0.02451	VdW_8_13_4	-0.00943
VdW_15_6_9	0.014431	VdW_8_14	-0.00805	VdW_10_7_7	-0.03018	VdW_7_15_5	-0.02757	Ele_10_9_10	-0.00906

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VdW_5_6_4	0.014512	VdW_6_4_6	-0.00282	VdW_12_11_4	-0.01241	VdW_15_7_6	-0.0181	VdW_12_6_9	-0.02647
VdW_11_10_10	0.042408	VdW_10_11_6	0.003023	VdW_12_12_12	0.01077	VdW_6_10_7	-0.02404	VdW_7_11_11	-0.01557
VdW_8_17_8	-0.02836	VdW_7_11_13	0.028045	VdW_13_12_10	-0.00315	VdW_14_7_4	0.013611	VdW_12_4_9	-0.0125
VdW_12_8_5	-0.00453	VdW_6_7_3	-0.00221	VdW_6_11_12	0.002962	VdW_13_13_4	-0.00374	Ele_6_9_7	-0.0063
VdW_11_8_9	0.013554	VdW_10_10_10	0.029022	VdW_8_4_9	-0.02232	VdW_7_15_10	-0.00036	VdW_4_11_7	0.023312
VdW_13_12_9	0.026107	VdW_14_12_9	0.008371	VdW_11_5_11	-0.0266	VdW_14_13_7	-0.02222	Ele_11_9_10	-0.01068
VdW_14_8_10	0.012573	VdW_8_15_8	-0.00593	Ele_6_10_8	-0.05094	VdW_7_13_3	-0.01131	VdW_11_8_11	-0.01218
VdW_10_6_9	0.028284	VdW_13_5_7	0.014549	VdW_14_12_5	0.013564	VdW_6_4_5	0.004917	VdW_7_6_12	0.00739

VdW_8_8_10	-0.03406	VdW_6_10_4	0.053448	VdW_5_6_10	-0.01096	VdW_6_12_4	0.01025	Ele_9_10_6	0.008036
VdW_9_9_10	0.014593	VdW_4_6_5	-0.00407	VdW_10_13_3	0.017769	VdW_6_12_11	-0.01904	VdW_13_14_10	-0.01649
VdW_12_14_10	0.019585	VdW_13_9_11	0.0287	VdW_13_11_5	0.003853	VdW_8_16_6	-0.00711	VdW_5_11_10	-0.01134
VdW_8_9_10	0.029721	VdW_7_5_4	0.009394	VdW_8_8_12	0.017134	VdW_11_7_3	0.010012	VdW_8_6_10	-0.01946
VdW_15_9_6	0.001745	VdW_6_13_5	0.003515	VdW_5_10_4	-0.02306	VdW_7_13_4	0.015627	VdW_7_5_3	-0.00023
VdW_14_8_4	0.010953	VdW_12_12_11	-0.00365	VdW_11_14_5	-0.02013	VdW_11_13_3	0.01289	VdW_8_5_12	0.008243
VdW_11_14_4	-0.00826	VdW_6_15_5	-0.00154	VdW_4_13_6	-0.01646	VdW_9_14_5	-0.0098	VdW_15_8_9	0.010507
VdW_3_8_6	0.020952	VdW_5_12_10	0.009067	VdW_11_12_13	0.013689	VdW_6_8_13	-0.0183	VdW_12_6_13	-0.00221
VdW_12_6_4	-0.02017	VdW_13_7	-0.00724	VdW_15_7_1	-0.01076	VdW_3_12_7	-0.00111	VdW_2_8_4	0.01696

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Ele_9_9_10	0.005525	VdW_3_12_9	-0.04076	VdW_11_11_7	-0.01571	VdW_13_14_7	0.009422	VdW_10_10_6	-0.03847
VdW_11_11_9	-0.0098	VdW_13_12_8	0.027261	VdW_14_7_6	0.02927	VdW_12_9_7	0.003818	VdW_6_10_8	0.001798
VdW_8_8_13	0.004248	Ele_7_10_10	0.015065	Ele_8_12_9	0.011952	VdW_10_12_3	-0.00721	Ele_10_8_7	0.000924
VdW_7_9_4	0.033852	VdW_11_6_4	0.021651	VdW_14_13_10	-0.0126	VdW_6_4_10	0.016328	VdW_4_14_8	0.009942
VdW_8_8_3	0.003081	VdW_10_6_12	-0.03243	VdW_8_7_4	-0.00458	VdW_11_7_13	0.001058	VdW_10_5_10	0.023667
VdW_10_8_7	-0.03914	VdW_12_11_2	-0.00862	VdW_3_11_10	-0.02212	VdW_11_14_8	-0.03425	VdW_12_3_4	-0.00258
VdW_8_7_13	-0.01059	VdW_6_7_9	-0.01009	VdW_13_13_11	0.017507	VdW_8_3_9	0.003407	VdW_9_14_7	0.013115
VdW_11_7_8	0.028331	VdW_15_9_10	-0.01103	VdW_12_14_5	-0.01348	VdW_9_3_7	0.024065	VdW_8_5_4	-0.00528

VdW_11_8_13	0.015168	VdW_4_8_4	-0.00033	VdW_12_8_12	-0.00362	VdW_12_13_3	-0.00691	VdW_11_15_6	0.004629
VdW_4_12_5	-0.01192	VdW_4_12_7	-0.00494	VdW_3_8_10	0.006139	VdW_12_4_4	-0.00212	VdW_10_8_11	0.016104
VdW_12_9_4	0.008944	VdW_6_8_8	-0.00783	VdW_12_12_10	0.012309	VdW_3_12_8	-0.02802	VdW_4_6_4	0.001006
VdW_6_6_10	0.012582	VdW_12_9_13	0.00721	VdW_6_6_11	-0.00912	VdW_10_5_3	-0.00311	VdW_9_3_8	0.011005
VdW_7_6_11	0.002094	VdW_12_13_10	-0.00766	VdW_11_12_12	0.00689	VdW_9_12_7	-0.02307	Ele_12_10_9	0.027234
VdW_8_15_7	0.033528	VdW_8_13_6	-0.01118	VdW_11_13_5	0.007005	VdW_10_5_4	0.002988	VdW_8_4_7	-0.00967
VdW_11_9_9	-0.01212	VdW_4_8_5	-0.00468	VdW_13_6_5	0.0152	VdW_14_6_5	-0.00036	VdW_7_15_6	-0.00786
VdW_6_14_10	-0.02513	VdW_5_6_3	-0.00591	Ele_8_8_10	-0.02235	VdW_6_9_9	0.023175	VdW_7_13_6	-0.03482
VdW_10_7_9	7.42E-05	VdW_9_4_	0.009424	VdW_8_10_5	0.017753	VdW_14_8_7	0.012886	VdW_8_5_5	-0.00865

		4							
VdW_7_11_7	0.022211	VdW_7_11_4	-0.00849	VdW_8_7_14	0.013837	VdW_6_5_7	0.001305	VdW_6_11_8	0.005554
VdW_12_11_3	0.013611	VdW_6_5_11	0.03833	VdW_5_13_5	0.011596	VdW_3_12_6	-0.02598	VdW_12_8_8	0.007093
VdW_6_13_9	0.027463	VdW_11_4_4	-0.00592	VdW_7_7_3	0.018188	VdW_15_11_7	0.011788	VdW_8_13_11	0.00134
VdW_5_11_3	0.012509	VdW_12_12_4	-0.02673	VdW_4_7_5	0.013492	VdW_7_14_11	0.005602	VdW_10_5_11	-0.01622
VdW_16_12_9	-0.01769	VdW_7_9_9	0.008387	VdW_11_11_3	-0.01252	VdW_5_8_4	-0.03958		
VdW_7_6_1	-0.00292	VdW_4_11_4	-0.0001	VdW_7_3_10	-0.0174	VdW_12_8_13	-0.00665	VdW_15_8_6	0.006747
Ele_7_6_1	0.003745	VdW_5_12_8	0.029165	VdW_11_14_6	-0.01183	VdW_11_13_12	0.00243	VdW_8_16_7	0.006252
VdW_13_9_5	0.02725	VdW_8_13_5	-0.01049	VdW_9_1_6	0.01476	VdW_12_15_5	-0.01144	Ele_6_8_8	-0.03177

VdW_5_8_3	-0.0001	Ele_10_7_9	-0.01432	VdW_13_6_8	-0.01076	VdW_5_8_6	0.007471	VdW_13_5_9	0.030983
VdW_7_3_6	0.005902	VdW_10_9_10	0.007587	VdW_4_7_11	-0.01481	VdW_11_11_13	-0.00728	VdW_9_12_9	-0.04179
VdW_13_10_5	-0.0023	VdW_15_13_9	0.010079	VdW_7_7_12	-0.03553	VdW_7_4_5	0.007444	VdW_12_4_10	-0.00177
VdW_10_2_4	-0.00573	VdW_14_11_5	0.021005	Ele_7_9_9	-0.04703	VdW_7_10_10	-0.00721	VdW_7_6_4	-0.00176
Ele_11_10_8	0.004988	VdW_4_7_10	-0.02952	VdW_7_14_7	0.017917	VdW_6_6_5	0.019012	VdW_9_6_8	0.03313
VdW_12_12_3	-0.01816	VdW_8_12_1	-0.00609	VdW_11_12_3	0.01594	VdW_5_5_8	-0.0161	Ele_12_9_9	-0.00032
VdW_6_4_2	-0.00299	VdW_12_14_6	0.026061	Ele_11_11_9	0.005928	VdW_6_10_2	0.009417	VdW_4_11_11	0.029645
VdW_12_6_5	0.012996	VdW_12_5_6	-0.00132	VdW_11_8_8	0.030585	VdW_13_13_5	-0.0092	VdW_6_6_12	-0.01499
VdW_12_6_11	-0.02004	Ele_12_10_7	-0.01525	VdW_7_3_9	0.024357	VdW_14_8_11	-0.03213	VdW_6_9_8	0.045305

VdW_8_14_6	0.012813	VdW_10_12_7	-0.01706	VdW_11_9_10	0.013574	VdW_5_13_4	0.003094	VdW_11_3_8	0.04167
VdW_13_6_4	0.007619	VdW_5_14_6	-0.00371	VdW_8_10_10	0.006716	VdW_7_6_3	-0.00634	VdW_13_7_11	-0.04099
VdW_11_6_3	-0.0092	VdW_12_5_4	0.00459	VdW_6_14_6	0.003156	VdW_8_9_12	-0.02469	VdW_7_7_6	-0.00111
VdW_7_14_6	0.000747	Ele_11_10_10	0.019629	VdW_5_5_5	0.002528	VdW_3_9_3	0.007309	VdW_13_6_11	-0.00724
VdW_9_8_6	0.049605	VdW_6_12_12	0.015197	VdW_11_4_7	-0.0034	VdW_15_6_10	-0.01396	VdW_10_7_4	-0.00403
VdW_13_8_4	-0.03692	VdW_10_11_9	0.02129	VdW_4_6_10	0.002835	VdW_6_14_9	-0.01697	VdW_4_8_10	0.01552
VdW_7_13_5	-0.01342	VdW_6_11_3	-0.02577	Ele_11_8_9	0.04453	VdW_6_3_4	-0.00147	VdW_5_13_6	-0.0228
VdW_7_3_7	-0.01242	VdW_9_3_5	-0.00123	VdW_12_7_4	0.018575	VdW_13_13_7	-0.02839	VdW_9_1_5	-0.00773
VdW_12_9_8	-0.01146	VdW_5_4_	0.010771	Ele_7_11_8	0.025833	VdW_13_7_1	-0.00976	VdW_9_6_9	-0.02202

		7				2			
VdW_7_11_8	0.024087	Ele_7_9_10	-0.02319	VdW_8_4_11	-0.01427	VdW_10_5_9	0.002659	VdW_14_10_7	0.00849
VdW_15_8_10	-0.02629	VdW_17_8_6	0.030793	VdW_4_10_10	0.0066	Ele_9_6_9	-0.00111	VdW_13_8_11	-0.00091
VdW_9_7_7	-0.00496	VdW_10_11_10	-0.02254	Ele_9_9_11	-0.01542	VdW_4_9_7	-0.0042	Ele_9_11_10	0.016261
VdW_13_11_4	-0.01514	VdW_9_12_8	-0.01086	VdW_11_8_14	0.006907	VdW_7_8_13	-0.01835	VdW_7_12_6	0.010175
VdW_5_12_7	0.006245	VdW_8_13_3	0.008443	VdW_4_9_4	-0.00593	VdW_16_8_12	-0.01466	VdW_13_9_12	0.003526
VdW_6_11_11	-0.00874	VdW_14_8_6	0.017961	VdW_14_7_5	-0.02227	VdW_11_4_5	0.039834	VdW_1_10_4	-0.00617
VdW_12_7_3	0.004419	VdW_5_7_10	0.036003	VdW_16_8_7	-0.00306	VdW_11_5_3	-0.02206	VdW_7_11_6	0.029504
VdW_5_12_4	-0.02211	VdW_13_8_5	0.008026	VdW_7_10_2	-0.01481	VdW_11_13_11	-0.00339	VdW_11_12_4	-0.01349

VdW_13_12_5	-0.00287	VdW_6_10_10	0.036177	VdW_8_14_4	0.00245	VdW_8_7_6	0.00857	VdW_11_7_9	-0.01147
VdW_7_5_5	0.005961	VdW_8_12_8	-0.02343	VdW_4_3_6	-0.03	Ele_12_9_8	-0.00708	VdW_11_11_6	-0.02044
VdW_16_8_5	-0.0119	VdW_9_5_11	-0.02055	VdW_12_6_10	0.004122	VdW_11_8_3	0.013617	Ele_8_9_10	0.01895
Ele_10_10_10	-0.02014	VdW_5_13_7	-0.02912	VdW_14_9_5	-0.00146	VdW_13_4_13	0.013903	VdW_11_8_10	-0.02666
VdW_13_4_9	-0.0263	VdW_10_6_13	-0.00256	Ele_8_7_10	0.020906	VdW_14_5_7	-0.00571	VdW_14_12_11	-0.00637
Ele_11_10_7	0.015642	VdW_5_10_3	-0.01896	VdW_12_4_6	0.02353	Ele_8_9_11	-0.01304	VdW_11_5_4	0.030379
VdW_9_11_10	0.03521	VdW_9_10_6	-0.02026	VdW_12_10_7	0.032267	VdW_7_4_11	-0.01305	VdW_7_13_11	0.014685
VdW_11_3_10	-0.01378	VdW_12_4_11	-0.01913	VdW_8_15_6	0.001974	VdW_5_7_5	0.003339	VdW_7_10_12	0.0056
VdW_10_7_8	-0.01526	VdW_5_7_	0.015883	VdW_11_2_4	-0.00538	VdW_14_12_	0.007549	Ele_12_8_8	-0.01776

		11				4					
VdW_14_11_6	-0.02575	VdW_14_12_10	-0.01709	VdW_14_7_10	-0.00173	VdW_8_4_4	0.01302	VdW_11_6_8	-0.00417		
VdW_11_10_9	-0.01392	VdW_7_9_12	0.019386	Ele_11_8_8	0.021918	Ele_7_7_10	-0.00263	VdW_13_11_11	0.015569		
VdW_4_12_10	0.017219	VdW_13_7_5	0.009749	VdW_6_7_11	-0.00277	VdW_14_6_10	-0.00168	VdW_6_5_10	0.001658		
Ele_10_11_9	-0.00355	VdW_15_8_5	-0.02639	VdW_14_5_10	-0.00461	VdW_6_3_7	-0.0018	VdW_14_8_12	0.010637		
VdW_5_13_9	-0.01548	VdW_14_10_6	0.037437	VdW_7_9_10	-0.01006	VdW_5_11_12	0.015857	VdW_6_8_4	-0.00835		
VdW_7_7_14	-0.00574	VdW_10_12_8	0.001151	VdW_7_9_3	0.013402	VdW_11_4_11	0.016254	VdW_7_12_5	-0.00964		
VdW_7_14_5	0.010787	VdW_14_5_9	-0.00163	Ele_11_9_7	-0.02282	VdW_13_13_6	0.00615	VdW_13_15_8	-0.02481		
VdW_8_5_3	0.011669	VdW_14_8_5	0.001099	VdW_16_6_7	-0.01505	Ele_7_7_9	-0.02329	Ele_9_7_10	0.032405		

VdW_13_4_7	0.023853	VdW_6_5_4	0.016108	VdW_11_10_2	0.000479	VdW_14_9_8	0.010421	VdW_7_13_12	-0.00389
VdW_4_6_7	-0.0106	VdW_14_14_9	0.007332	VdW_15_8_11	0.002866	VdW_11_7_4	0.015148	VdW_10_7_3	0.022421
Ele_11_7_8	0.006884	VdW_12_10_8	0.001246	VdW_14_13_6	0.007964	VdW_11_10_13	0.006389	VdW_7_11_9	0.006178
VdW_11_11_8	0.005624	VdW_11_10_8	0.015601	VdW_3_9_6	0.008067	VdW_8_13_12	0.009288	Ele_10_6_9	-0.01991
VdW_11_9_7	-0.00178	VdW_11_10_7	-0.02342	VdW_8_14_5	-0.00334	Ele_10_7_8	-0.00273	VdW_8_14_12	0.031145
VdW_15_12_6	0.015609	VdW_11_14_12	0.001477	VdW_8_10_13	0.021065	Ele_12_9_7	-0.02904	VdW_11_10_6	-0.00774
VdW_6_13_4	-0.01975	VdW_7_12_11	0.017938	VdW_5_4_9	0.028828	VdW_8_4_10	0.031553	VdW_6_3_8	0.017451
VdW_12_13_5	0.022895	VdW_4_7_8	0.026345	VdW_8_3_7	0.012198	VdW_14_9_7	-0.04186	VdW_13_13_10	-0.01031
VdW_15_11_	-0.00785	VdW_8_7_	0.029969	VdW_10_9_6	-0.00418	VdW_7_5_9	-0.0007	VdW_12_5_5	-0.00652

8		12							
VdW_11_8_7	-0.01543	VdW_10_8_6	0.008595	VdW_14_12_7	-0.0015	VdW_6_13_7	0.030931	VdW_13_7_6	0.009167
VdW_9_8_13	-0.0029	VdW_12_8_4	0.023818	VdW_7_4_2	0.020434	VdW_7_15_9	-0.00563	Ele_8_12_7	-0.00656
VdW_12_8_3	-0.00473	VdW_4_7_6	0.008183	VdW_8_11_10	0.020297	VdW_14_5_6	-0.02451	VdW_8_13_4	-0.00943
VdW_15_6_9	0.014431	VdW_8_14_7	-0.00805	VdW_10_7_7	-0.03018	VdW_7_15_5	-0.02757	Ele_10_9_10	-0.00906
VdW_5_6_4	0.014512	VdW_6_4_6	-0.00282	VdW_12_11_4	-0.01241	VdW_15_7_6	-0.0181	VdW_12_6_9	-0.02647
VdW_11_10_10	0.042408	VdW_10_11_6	0.003023	VdW_12_12_12	0.01077	VdW_6_10_7	-0.02404	VdW_7_11_11	-0.01557
VdW_8_17_8	-0.02836	VdW_7_11_13	0.028045	VdW_13_12_10	-0.00315	VdW_14_7_4	0.013611	VdW_12_4_9	-0.0125
VdW_12_8_5	-0.00453	VdW_6_7_3	-0.00221	VdW_6_11_12	0.002962	VdW_13_13_4	-0.00374	Ele_6_9_7	-0.0063

VdW_11_8_9	0.013554	VdW_10_10_10	0.029022	VdW_8_4_9	-0.02232	VdW_7_15_10	-0.00036	VdW_4_11_7	0.023312
VdW_13_12_9	0.026107	VdW_14_12_9	0.008371	VdW_11_5_11	-0.0266	VdW_14_13_7	-0.02222	Ele_11_9_10	-0.01068
VdW_14_8_10	0.012573	VdW_8_15_8	-0.00593	Ele_6_10_8	-0.05094	VdW_7_13_3	-0.01131	VdW_11_8_11	-0.01218
VdW_10_6_9	0.028284	VdW_13_5_7	0.014549	VdW_14_12_5	0.013564	VdW_6_4_5	0.004917	VdW_7_6_12	0.00739
VdW_8_8_10	-0.03406	VdW_6_10_4	0.053448	VdW_5_6_10	-0.01096	VdW_6_12_4	0.01025	Ele_9_10_6	0.008036
VdW_9_9_10	0.014593	VdW_4_6_5	-0.00407	VdW_10_13_3	0.017769	VdW_6_12_11	-0.01904	VdW_13_14_10	-0.01649
VdW_12_14_10	0.019585	VdW_13_9_11	0.0287	VdW_13_11_5	0.003853	VdW_8_16_6	-0.00711	VdW_5_11_10	-0.01134
VdW_8_9_10	0.029721	VdW_7_5_4	0.009394	VdW_8_8_12	0.017134	VdW_11_7_3	0.010012	VdW_8_6_10	-0.01946
VdW_15_9_6	0.001745	VdW_6_13	0.003515	VdW_5_10_4	-0.02306	VdW_7_13_4	0.015627	VdW_7_5_3	-0.00023

		_5							
VdW_14_8_4	0.010953	VdW_12_12_11	-0.00365	VdW_11_14_5	-0.02013	VdW_11_13_3	0.01289	VdW_8_5_12	0.008243
VdW_11_14_4	-0.00826	VdW_6_15_5	-0.00154	VdW_4_13_6	-0.01646	VdW_9_14_5	-0.0098	VdW_15_8_9	0.010507
VdW_3_8_6	0.020952	VdW_5_12_10	0.009067	VdW_11_12_13	0.013689	VdW_6_8_13	-0.0183	VdW_12_6_13	-0.00221
VdW_12_6_4	-0.02017	VdW_13_7_4	-0.00724	VdW_15_7_10	-0.01076	VdW_3_12_7	-0.00111	VdW_2_8_4	0.01696
Ele_9_9_10	0.005525	VdW_3_12_9	-0.04076	VdW_11_11_7	-0.01571	VdW_13_14_7	0.009422	VdW_10_10_6	-0.03847
VdW_11_11_9	-0.0098	VdW_13_12_8	0.027261	VdW_14_7_6	0.02927	VdW_12_9_7	0.003818	VdW_6_10_8	0.001798
VdW_8_8_13	0.004248	Ele_7_10_10	0.015065	Ele_8_12_9	0.011952	VdW_10_12_3	-0.00721	Ele_10_8_7	0.000924
VdW_7_9_4	0.033852	VdW_11_6_4	0.021651	VdW_14_13_10	-0.0126	VdW_6_4_10	0.016328	VdW_4_14_8	0.009942

VdW_8_8_3	0.003081	VdW_10_6_12	-0.03243	VdW_8_7_4	-0.00458	VdW_11_7_13	0.001058	VdW_10_5_10	0.023667
VdW_10_8_7	-0.03914	VdW_12_11_2	-0.00862	VdW_3_11_10	-0.02212	VdW_11_14_8	-0.03425	VdW_12_3_4	-0.00258
VdW_8_7_13	-0.01059	VdW_6_7_9	-0.01009	VdW_13_13_11	0.017507	VdW_8_3_9	0.003407	VdW_9_14_7	0.013115
VdW_11_7_8	0.028331	VdW_15_9_10	-0.01103	VdW_12_14_5	-0.01348	VdW_9_3_7	0.024065	VdW_8_5_4	-0.00528
VdW_11_8_13	0.015168	VdW_4_8_4	-0.00033	VdW_12_8_12	-0.00362	VdW_12_13_3	-0.00691	VdW_11_15_6	0.004629
VdW_4_12_5	-0.01192	VdW_4_12_7	-0.00494	VdW_3_8_10	0.006139	VdW_12_4_4	-0.00212	VdW_10_8_11	0.016104
VdW_12_9_4	0.008944	VdW_6_8_8	-0.00783	VdW_12_12_10	0.012309	VdW_3_12_8	-0.02802	VdW_4_6_4	0.001006
VdW_6_6_10	0.012582	VdW_12_9_13	0.00721	VdW_6_6_11	-0.00912	VdW_10_5_3	-0.00311	VdW_9_3_8	0.011005
VdW_7_6_11	0.002094	VdW_12_1	-0.00766	VdW_11_12_	0.00689	VdW_9_12_7	-0.02307	Ele_12_10_9	0.027234

		3_10		12					
VdW_8_15_7	0.033528	VdW_8_13_6	-0.01118	VdW_11_13_5	0.007005	VdW_10_5_4	0.002988	VdW_8_4_7	-0.00967
VdW_11_9_9	-0.01212	VdW_4_8_5	-0.00468	VdW_13_6_5	0.0152	VdW_14_6_5	-0.00036	VdW_7_15_6	-0.00786
VdW_6_14_10	-0.02513	VdW_5_6_3	-0.00591	Ele_8_8_10	-0.02235	VdW_6_9_9	0.023175	VdW_7_13_6	-0.03482
VdW_10_7_9	7.42E-05	VdW_9_4_4	0.009424	VdW_8_10_5	0.017753	VdW_14_8_7	0.012886	VdW_8_5_5	-0.00865
VdW_7_11_7	0.022211	VdW_7_11_4	-0.00849	VdW_8_7_14	0.013837	VdW_6_5_7	0.001305	VdW_6_11_8	0.005554
VdW_12_11_3	0.013611	VdW_6_5_11	0.03833	VdW_5_13_5	0.011596	VdW_3_12_6	-0.02598	VdW_12_8_8	0.007093
VdW_6_13_9	0.027463	VdW_11_4_4	-0.00592	VdW_7_7_3	0.018188	VdW_15_11_7	0.011788	VdW_8_13_11	0.00134
VdW_5_11_3	0.012509	VdW_12_12_4	-0.02673	VdW_4_7_5	0.013492	VdW_7_14_11	0.005602	VdW_10_5_11	-0.01622

VdW_16_12_9	-0.01769	VdW_7_9_9	0.008387	VdW_11_11_3	-0.01252	VdW_5_8_4	-0.03958		
VdW_7_6_1	-0.00292	VdW_4_11_4	-0.0001	VdW_7_3_10	-0.0174	VdW_12_8_13	-0.00665	VdW_15_8_6	0.006747
Ele_7_6_1	0.003745	VdW_5_12_8	0.029165	VdW_11_14_6	-0.01183	VdW_11_13_12	0.00243	VdW_8_16_7	0.006252
VdW_13_9_5	0.02725	VdW_8_13_5	-0.01049	VdW_9_1_6	0.01476	VdW_12_15_5	-0.01144	Ele_6_8_8	-0.03177
VdW_5_8_3	-0.0001	Ele_10_7_9	-0.01432	VdW_13_6_8	-0.01076	VdW_5_8_6	0.007471	VdW_13_5_9	0.030983
VdW_7_3_6	0.005902	VdW_10_9_10	0.007587	VdW_4_7_11	-0.01481	VdW_11_11_13	-0.00728	VdW_9_12_9	-0.04179
VdW_13_10_5	-0.0023	VdW_15_13_9	0.010079	VdW_7_7_12	-0.03553	VdW_7_4_5	0.007444	VdW_12_4_10	-0.00177
VdW_10_2_4	-0.00573	VdW_14_11_5	0.021005	Ele_7_9_9	-0.04703	VdW_7_10_10	-0.00721	VdW_7_6_4	-0.00176
Ele_11_10_8	0.004988	VdW_4_7_10	-0.02952	VdW_7_14_7	0.017917	VdW_6_6_5	0.019012	VdW_9_6_8	0.03313

VdW_12_12_3	-0.01816	VdW_8_12_1	-0.00609	VdW_11_12_3	0.01594	VdW_5_5_8	-0.0161	Ele_12_9_9	-0.00032
VdW_6_4_2	-0.00299	VdW_12_14_6	0.026061	Ele_11_11_9	0.005928	VdW_6_10_2	0.009417	VdW_4_11_11	0.029645
VdW_12_6_5	0.012996	VdW_12_5_6	-0.00132	VdW_11_8_8	0.030585	VdW_13_13_5	-0.0092	VdW_6_6_12	-0.01499
VdW_12_6_11	-0.02004	Ele_12_10_7	-0.01525	VdW_7_3_9	0.024357	VdW_14_8_11	-0.03213	VdW_6_9_8	0.045305
VdW_8_14_6	0.012813	VdW_10_12_7	-0.01706	VdW_11_9_10	0.013574	VdW_5_13_4	0.003094	VdW_11_3_8	0.04167
VdW_13_6_4	0.007619	VdW_5_14_6	-0.00371	VdW_8_10_10	0.006716	VdW_7_6_3	-0.00634	VdW_13_7_11	-0.04099
VdW_11_6_3	-0.0092	VdW_12_5_4	0.00459	VdW_6_14_6	0.003156	VdW_8_9_12	-0.02469	VdW_7_7_6	-0.00111
VdW_7_14_6	0.000747	Ele_11_10_10	0.019629	VdW_5_5_5	0.002528	VdW_3_9_3	0.007309	VdW_13_6_11	-0.00724
VdW_9_8_6	0.049605	VdW_6_12	0.015197	VdW_11_4_7	-0.0034	VdW_15_6_1	-0.01396	VdW_10_7_4	-0.00403

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VdW_13_8_4	-0.03692	VdW_10_11_9	0.02129	VdW_4_6_10	0.002835	VdW_6_14_9	-0.01697	VdW_4_8_10	0.01552
VdW_7_13_5	-0.01342	VdW_6_11_3	-0.02577	Ele_11_8_9	0.04453	VdW_6_3_4	-0.00147	VdW_5_13_6	-0.0228
VdW_7_3_7	-0.01242	VdW_9_3_5	-0.00123	VdW_12_7_4	0.018575	VdW_13_13_7	-0.02839	VdW_9_1_5	-0.00773
VdW_12_9_8	-0.01146	VdW_5_4_7	0.010771	Ele_7_11_8	0.025833	VdW_13_7_12	-0.00976	VdW_9_6_9	-0.02202
VdW_7_11_8	0.024087	Ele_7_9_10	-0.02319	VdW_8_4_11	-0.01427	VdW_10_5_9	0.002659	VdW_14_10_7	0.00849
VdW_15_8_10	-0.02629	VdW_17_8_6	0.030793	VdW_4_10_10	0.0066	Ele_9_6_9	-0.00111	VdW_13_8_11	-0.00091
VdW_9_7_7	-0.00496	VdW_10_11_10	-0.02254	Ele_9_9_11	-0.01542	VdW_4_9_7	-0.0042	Ele_9_11_10	0.016261
VdW_13_11_4	-0.01514	VdW_9_12_8	-0.01086	VdW_11_8_14	0.006907	VdW_7_8_13	-0.01835	VdW_7_12_6	0.010175

VdW_5_12_7	0.006245	VdW_8_13_3	0.008443	VdW_4_9_4	-0.00593	VdW_16_8_12	-0.01466	VdW_13_9_12	0.003526
VdW_6_11_11	-0.00874	VdW_14_8_6	0.017961	VdW_14_7_5	-0.02227	VdW_11_4_5	0.039834	VdW_1_10_4	-0.00617
VdW_12_7_3	0.004419	VdW_5_7_10	0.036003	VdW_16_8_7	-0.00306	VdW_11_5_3	-0.02206	VdW_7_11_6	0.029504
VdW_5_12_4	-0.02211	VdW_13_8_5	0.008026	VdW_7_10_2	-0.01481	VdW_11_13_11	-0.00339	VdW_11_12_4	-0.01349
VdW_13_12_5	-0.00287	VdW_6_10_10	0.036177	VdW_8_14_4	0.00245	VdW_8_7_6	0.00857	VdW_11_7_9	-0.01147
VdW_7_5_5	0.005961	VdW_8_12_8	-0.02343	VdW_4_3_6	-0.03	Ele_12_9_8	-0.00708	VdW_11_11_6	-0.02044
VdW_16_8_5	-0.0119	VdW_9_5_11	-0.02055	VdW_12_6_10	0.004122	VdW_11_8_3	0.013617	Ele_8_9_10	0.01895
Ele_10_10_10	-0.02014	VdW_5_13_7	-0.02912	VdW_14_9_5	-0.00146	VdW_13_4_13	0.013903	VdW_11_8_10	-0.02666
VdW_13_4_9	-0.0263	VdW_10_6	-0.00256	Ele_8_7_10	0.020906	VdW_14_5_7	-0.00571	VdW_14_12_	-0.00637

		_13						11	
Ele_11_10_7	0.015642	VdW_5_10_3	-0.01896	VdW_12_4_6	0.02353	Ele_8_9_11	-0.01304	VdW_11_5_4	0.030379
VdW_9_11_10	0.03521	VdW_9_10_6	-0.02026	VdW_12_10_7	0.032267	VdW_7_4_11	-0.01305	VdW_7_13_11	0.014685
VdW_11_3_10	-0.01378	VdW_12_4_11	-0.01913	VdW_8_15_6	0.001974	VdW_5_7_5	0.003339	VdW_7_10_12	0.0056
VdW_10_7_8	-0.01526	VdW_5_7_11	0.015883	VdW_11_2_4	-0.00538	VdW_14_12_4	0.007549	Ele_12_8_8	-0.01776
VdW_14_11_6	-0.02575	VdW_14_12_10	-0.01709	VdW_14_7_10	-0.00173	VdW_8_4_4	0.01302	VdW_11_6_8	-0.00417
VdW_11_10_9	-0.01392	VdW_7_9_12	0.019386	Ele_11_8_8	0.021918	Ele_7_7_10	-0.00263	VdW_13_11_11	0.015569
VdW_4_12_10	0.017219	VdW_13_7_5	0.009749	VdW_6_7_11	-0.00277	VdW_14_6_10	-0.00168	VdW_6_5_10	0.001658
Ele_10_11_9	-0.00355	VdW_15_8_5	-0.02639	VdW_14_5_10	-0.00461	VdW_6_3_7	-0.0018	VdW_14_8_12	0.010637

VdW_5_13_9	-0.01548	VdW_14_10_6	0.037437	VdW_7_9_10	-0.01006	VdW_5_11_12	0.015857	VdW_6_8_4	-0.00835
VdW_7_7_14	-0.00574	VdW_10_12_8	0.001151	VdW_7_9_3	0.013402	VdW_11_4_11	0.016254	VdW_7_12_5	-0.00964
VdW_7_14_5	0.010787	VdW_14_5_9	-0.00163	Ele_11_9_7	-0.02282	VdW_13_13_6	0.00615	VdW_13_15_8	-0.02481
VdW_8_5_3	0.011669	VdW_14_8_5	0.001099	VdW_16_6_7	-0.01505	Ele_7_7_9	-0.02329	Ele_9_7_10	0.032405
VdW_13_4_7	0.023853	VdW_6_5_4	0.016108	VdW_11_10_2	0.000479	VdW_14_9_8	0.010421	VdW_7_13_12	-0.00389
VdW_4_6_7	-0.0106	VdW_14_14_9	0.007332	VdW_15_8_11	0.002866	VdW_11_7_4	0.015148	VdW_10_7_3	0.022421
Ele_11_7_8	0.006884	VdW_12_10_8	0.001246	VdW_14_13_6	0.007964	VdW_11_10_13	0.006389	VdW_7_11_9	0.006178
VdW_11_11_8	0.005624	VdW_11_10_8	0.015601	VdW_3_9_6	0.008067	VdW_8_13_12	0.009288	Ele_10_6_9	-0.01991
VdW_11_9_7	-0.00178	VdW_11_1	-0.02342	VdW_8_14_5	-0.00334	Ele_10_7_8	-0.00273	VdW_8_14_1	0.031145

		0_7								2	
VdW_15_12_6	0.015609	VdW_11_14_12	0.001477	VdW_8_10_13	0.021065	Ele_12_9_7	-0.02904	VdW_11_10_6	-0.00774		
VdW_6_13_4	-0.01975	VdW_7_12_11	0.017938	VdW_5_4_9	0.028828	VdW_8_4_10	0.031553	VdW_6_3_8	0.017451		
VdW_12_13_5	0.022895	VdW_4_7_8	0.026345	VdW_8_3_7	0.012198	VdW_14_9_7	-0.04186	VdW_13_13_10	-0.01031		
VdW_15_11_8	-0.00785	VdW_8_7_12	0.029969	VdW_10_9_6	-0.00418	VdW_7_5_9	-0.0007	VdW_12_5_5	-0.00652		
VdW_11_8_7	-0.01543	VdW_10_8_6	0.008595	VdW_14_12_7	-0.0015	VdW_6_13_7	0.030931	VdW_13_7_6	0.009167		
VdW_9_8_13	-0.0029	VdW_12_8_4	0.023818	VdW_7_4_2	0.020434	VdW_7_15_9	-0.00563	Ele_8_12_7	-0.00656		
VdW_12_8_3	-0.00473	VdW_4_7_6	0.008183	VdW_8_11_10	0.020297	VdW_14_5_6	-0.02451	VdW_8_13_4	-0.00943		
VdW_15_6_9	0.014431	VdW_8_14_7	-0.00805	VdW_10_7_7	-0.03018	VdW_7_15_5	-0.02757	Ele_10_9_10	-0.00906		

VdW_5_6_4	0.014512	VdW_6_4_6	-0.00282	VdW_12_11_4	-0.01241	VdW_15_7_6	-0.0181	VdW_12_6_9	-0.02647
VdW_11_10_10	0.042408	VdW_10_11_6	0.003023	VdW_12_12_12	0.01077	VdW_6_10_7	-0.02404	VdW_7_11_11	-0.01557
VdW_8_17_8	-0.02836	VdW_7_11_13	0.028045	VdW_13_12_10	-0.00315	VdW_14_7_4	0.013611	VdW_12_4_9	-0.0125
VdW_12_8_5	-0.00453	VdW_6_7_3	-0.00221	VdW_6_11_12	0.002962	VdW_13_13_4	-0.00374	Ele_6_9_7	-0.0063
VdW_11_8_9	0.013554	VdW_10_10_10	0.029022	VdW_8_4_9	-0.02232	VdW_7_15_10	-0.00036	VdW_4_11_7	0.023312
VdW_13_12_9	0.026107	VdW_14_12_9	0.008371	VdW_11_5_11	-0.0266	VdW_14_13_7	-0.02222	Ele_11_9_10	-0.01068
VdW_14_8_10	0.012573	VdW_8_15_8	-0.00593	Ele_6_10_8	-0.05094	VdW_7_13_3	-0.01131	VdW_11_8_11	-0.01218
VdW_10_6_9	0.028284	VdW_13_5_7	0.014549	VdW_14_12_5	0.013564	VdW_6_4_5	0.004917	VdW_7_6_12	0.00739
VdW_8_8_10	-0.03406	VdW_6_10	0.053448	VdW_5_6_10	-0.01096	VdW_6_12_4	0.01025	Ele_9_10_6	0.008036

		_4							
VdW_9_9_10	0.014593	VdW_4_6_5	-0.00407	VdW_10_13_3	0.017769	VdW_6_12_11	-0.01904	VdW_13_14_10	-0.01649
VdW_12_14_10	0.019585	VdW_13_9_11	0.0287	VdW_13_11_5	0.003853	VdW_8_16_6	-0.00711	VdW_5_11_10	-0.01134
VdW_8_9_10	0.029721	VdW_7_5_4	0.009394	VdW_8_8_12	0.017134	VdW_11_7_3	0.010012	VdW_8_6_10	-0.01946
VdW_15_9_6	0.001745	VdW_6_13_5	0.003515	VdW_5_10_4	-0.02306	VdW_7_13_4	0.015627	VdW_7_5_3	-0.00023
VdW_14_8_4	0.010953	VdW_12_12_11	-0.00365	VdW_11_14_5	-0.02013	VdW_11_13_3	0.01289	VdW_8_5_12	0.008243
VdW_11_14_4	-0.00826	VdW_6_15_5	-0.00154	VdW_4_13_6	-0.01646	VdW_9_14_5	-0.0098	VdW_15_8_9	0.010507
VdW_3_8_6	0.020952	VdW_5_12_10	0.009067	VdW_11_12_13	0.013689	VdW_6_8_13	-0.0183	VdW_12_6_13	-0.00221
VdW_12_6_4	-0.02017	VdW_13_7_4	-0.00724	VdW_15_7_10	-0.01076	VdW_3_12_7	-0.00111	VdW_2_8_4	0.01696

Ele_9_9_10	0.005525	VdW_3_12_9	-0.04076	VdW_11_11_7	-0.01571	VdW_13_14_7	0.009422	VdW_10_10_6	-0.03847
VdW_11_11_9	-0.0098	VdW_13_12_8	0.027261	VdW_14_7_6	0.02927	VdW_12_9_7	0.003818	VdW_6_10_8	0.001798
VdW_8_8_13	0.004248	Ele_7_10_10	0.015065	Ele_8_12_9	0.011952	VdW_10_12_3	-0.00721	Ele_10_8_7	0.000924
VdW_7_9_4	0.033852	VdW_11_6_4	0.021651	VdW_14_13_10	-0.0126	VdW_6_4_10	0.016328	VdW_4_14_8	0.009942
VdW_8_8_3	0.003081	VdW_10_6_12	-0.03243	VdW_8_7_4	-0.00458	VdW_11_7_13	0.001058	VdW_10_5_10	0.023667
VdW_10_8_7	-0.03914	VdW_12_11_2	-0.00862	VdW_3_11_10	-0.02212	VdW_11_14_8	-0.03425	VdW_12_3_4	-0.00258
VdW_8_7_13	-0.01059	VdW_6_7_9	-0.01009	VdW_13_13_11	0.017507	VdW_8_3_9	0.003407	VdW_9_14_7	0.013115
VdW_11_7_8	0.028331	VdW_15_9_10	-0.01103	VdW_12_14_5	-0.01348	VdW_9_3_7	0.024065	VdW_8_5_4	-0.00528
VdW_11_8_1	0.015168	VdW_4_8_	-0.00033	VdW_12_8_1	-0.00362	VdW_12_13_	-0.00691	VdW_11_15_	0.004629

3		4		2		3		6			
VdW_4_12_5	-0.01192	VdW_4_12_7	-0.00494	VdW_3_8_10	0.006139	VdW_12_4_4	-0.00212	VdW_10_8_11	0.016104		
VdW_12_9_4	0.008944	VdW_6_8_8	-0.00783	VdW_12_12_10	0.012309	VdW_3_12_8	-0.02802	VdW_4_6_4	0.001006		
VdW_6_6_10	0.012582	VdW_12_9_13	0.00721	VdW_6_6_11	-0.00912	VdW_10_5_3	-0.00311	VdW_9_3_8	0.011005		
VdW_7_6_11	0.002094	VdW_12_13_10	-0.00766	VdW_11_12_12	0.00689	VdW_9_12_7	-0.02307	Ele_12_10_9	0.027234		
VdW_8_15_7	0.033528	VdW_8_13_6	-0.01118	VdW_11_13_5	0.007005	VdW_10_5_4	0.002988	VdW_8_4_7	-0.00967		
VdW_11_9_9	-0.01212	VdW_4_8_5	-0.00468	VdW_13_6_5	0.0152	VdW_14_6_5	-0.00036	VdW_7_15_6	-0.00786		
VdW_6_14_10	-0.02513	VdW_5_6_3	-0.00591	Ele_8_8_10	-0.02235	VdW_6_9_9	0.023175	VdW_7_13_6	-0.03482		
VdW_10_7_9	7.42E-05	VdW_9_4_4	0.009424	VdW_8_10_5	0.017753	VdW_14_8_7	0.012886	VdW_8_5_5	-0.00865		

VdW_7_11_7	0.022211	VdW_7_11_4	-0.00849	VdW_8_7_14	0.013837	VdW_6_5_7	0.001305	VdW_6_11_8	0.005554
VdW_12_11_3	0.013611	VdW_6_5_11	0.03833	VdW_5_13_5	0.011596	VdW_3_12_6	-0.02598	VdW_12_8_8	0.007093
VdW_6_13_9	0.027463	VdW_11_4_4	-0.00592	VdW_7_7_3	0.018188	VdW_15_11_7	0.011788	VdW_8_13_11	0.00134
VdW_5_11_3	0.012509	VdW_12_12_4	-0.02673	VdW_4_7_5	0.013492	VdW_7_14_11	0.005602	VdW_10_5_11	-0.01622
VdW_16_12_9	-0.01769	VdW_7_9_9	0.008387	VdW_11_11_3	-0.01252	VdW_5_8_4	-0.03958		
VdW_7_6_1	-0.00292	VdW_4_11_4	-0.0001	VdW_7_3_10	-0.0174	VdW_12_8_13	-0.00665	VdW_15_8_6	0.006747
Ele_7_6_1	0.003745	VdW_5_12_8	0.029165	VdW_11_14_6	-0.01183	VdW_11_13_12	0.00243	VdW_8_16_7	0.006252
VdW_13_9_5	0.02725	VdW_8_13_5	-0.01049	VdW_9_1_6	0.01476	VdW_12_15_5	-0.01144	Ele_6_8_8	-0.03177
VdW_5_8_3	-0.0001	Ele_10_7_9	-0.01432	VdW_13_6_8	-0.01076	VdW_5_8_6	0.007471	VdW_13_5_9	0.030983

VdW_7_3_6	0.005902	VdW_10_9_10	0.007587	VdW_4_7_11	-0.01481	VdW_11_11_13	-0.00728	VdW_9_12_9	-0.04179
VdW_13_10_5	-0.0023	VdW_15_13_9	0.010079	VdW_7_7_12	-0.03553	VdW_7_4_5	0.007444	VdW_12_4_10	-0.00177
VdW_10_2_4	-0.00573	VdW_14_11_5	0.021005	Ele_7_9_9	-0.04703	VdW_7_10_10	-0.00721	VdW_7_6_4	-0.00176
Ele_11_10_8	0.004988	VdW_4_7_10	-0.02952	VdW_7_14_7	0.017917	VdW_6_6_5	0.019012	VdW_9_6_8	0.03313
VdW_12_12_3	-0.01816	VdW_8_12_1	-0.00609	VdW_11_12_3	0.01594	VdW_5_5_8	-0.0161	Ele_12_9_9	-0.00032
VdW_6_4_2	-0.00299	VdW_12_14_6	0.026061	Ele_11_11_9	0.005928	VdW_6_10_2	0.009417	VdW_4_11_11	0.029645
VdW_12_6_5	0.012996	VdW_12_5_6	-0.00132	VdW_11_8_8	0.030585	VdW_13_13_5	-0.0092	VdW_6_6_12	-0.01499
VdW_12_6_11	-0.02004	Ele_12_10_7	-0.01525	VdW_7_3_9	0.024357	VdW_14_8_11	-0.03213	VdW_6_9_8	0.045305
VdW_8_14_6	0.012813	VdW_10_1	-0.01706	VdW_11_9_1	0.013574	VdW_5_13_4	0.003094	VdW_11_3_8	0.04167

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VdW_13_6_4	0.007619	VdW_5_14_6	-0.00371	VdW_8_10_10	0.006716	VdW_7_6_3	-0.00634	VdW_13_7_11	-0.04099
VdW_11_6_3	-0.0092	VdW_12_5_4	0.00459	VdW_6_14_6	0.003156	VdW_8_9_12	-0.02469	VdW_7_7_6	-0.00111
VdW_7_14_6	0.000747	Ele_11_10_10	0.019629	VdW_5_5_5	0.002528	VdW_3_9_3	0.007309	VdW_13_6_11	-0.00724
VdW_9_8_6	0.049605	VdW_6_12_12	0.015197	VdW_11_4_7	-0.0034	VdW_15_6_10	-0.01396	VdW_10_7_4	-0.00403
VdW_13_8_4	-0.03692	VdW_10_11_9	0.02129	VdW_4_6_10	0.002835	VdW_6_14_9	-0.01697	VdW_4_8_10	0.01552
VdW_7_13_5	-0.01342	VdW_6_11_3	-0.02577	Ele_11_8_9	0.04453	VdW_6_3_4	-0.00147	VdW_5_13_6	-0.0228
VdW_7_3_7	-0.01242	VdW_9_3_5	-0.00123	VdW_12_7_4	0.018575	VdW_13_13_7	-0.02839	VdW_9_1_5	-0.00773
VdW_12_9_8	-0.01146	VdW_5_4_7	0.010771	Ele_7_11_8	0.025833	VdW_13_7_12	-0.00976	VdW_9_6_9	-0.02202

VdW_7_11_8	0.024087	Ele_7_9_10	-0.02319	VdW_8_4_11	-0.01427	VdW_10_5_9	0.002659	VdW_14_10_7	0.00849
VdW_15_8_10	-0.02629	VdW_17_8_6	0.030793	VdW_4_10_10	0.0066	Ele_9_6_9	-0.00111	VdW_13_8_11	-0.00091
VdW_9_7_7	-0.00496	VdW_10_11_10	-0.02254	Ele_9_9_11	-0.01542	VdW_4_9_7	-0.0042	Ele_9_11_10	0.016261
VdW_13_11_4	-0.01514	VdW_9_12_8	-0.01086	VdW_11_8_14	0.006907	VdW_7_8_13	-0.01835	VdW_7_12_6	0.010175
VdW_5_12_7	0.006245	VdW_8_13_3	0.008443	VdW_4_9_4	-0.00593	VdW_16_8_12	-0.01466	VdW_13_9_12	0.003526
VdW_6_11_11	-0.00874	VdW_14_8_6	0.017961	VdW_14_7_5	-0.02227	VdW_11_4_5	0.039834	VdW_1_10_4	-0.00617
VdW_12_7_3	0.004419	VdW_5_7_10	0.036003	VdW_16_8_7	-0.00306	VdW_11_5_3	-0.02206	VdW_7_11_6	0.029504
VdW_5_12_4	-0.02211	VdW_13_8_5	0.008026	VdW_7_10_2	-0.01481	VdW_11_13_11	-0.00339	VdW_11_12_4	-0.01349

Table S5. the coefficients and associated variables for the equation of Kw-s 3D QSAR.

Variable	Coefficient	Variable	Coefficient	Variable	Coefficient	Variable	Coefficient	Variable	Coefficient
VdW_11_6_1	-0.02319	VdW_8_13_3	0.010508	VdW_11_4_4	-0.01407	VdW_9_4_4	0.027477	Ele_14_9_8	0.034244
Ele_11_6_1	0.052014	VdW_12_6_1	-0.03382	VdW_12_3_3	0.002549	VdW_17_6_4	0.00158	VdW_14_8_9	-0.02597
VdW_14_6_1	0.01338	VdW_14_10_5	0.009333	VdW_6_3_6	0.024729	VdW_15_12_8	-0.05784	VdW_14_12_7	0.020695
VdW_7_4_2	-0.02712	VdW_13_12_5	-0.03858	Ele_9_10_8	-0.05128	VdW_16_4_8	-0.00418	VdW_3_9_5	-0.03601
VdW_10_7_1	0.007108	VdW_4_10_4	-0.00534	Ele_13_8_4	0.082442	VdW_16_5_6	-0.01626	VdW_3_7_2	0.002863
Ele_7_3_2	0.022777	VdW_10_11_5	0.037783	VdW_16_5_4	-0.00585	VdW_14_4_3	-0.00803	VdW_7_11_7	-0.03367
VdW_15_6_1	0.011249	VdW_8_9_1	-0.05559	Ele_8_9_4	-0.03796	VdW_6_10_10	-0.01538	VdW_9_4_2	0.005881
VdW_12_12	3.20E-05	VdW_3_6_4	-0.05033	VdW_13_6_9	-0.01585	VdW_15_7_8	-0.00374	VdW_15_8_4	0.073266

_2									
VdW_7_10_6	0.042993	VdW_16_12_5	-0.00205	VdW_14_7_5	-0.06145	VdW_3_10_8	0.02699	Ele_7_6_8	-0.12182
VdW_12_6_7	-0.02615	VdW_10_8_9	-0.02489	VdW_7_8_8	0.001854	VdW_14_9_4	0.04614	VdW_10_4_6	-0.02498
VdW_14_9_6	0.013761	VdW_16_11_3	-0.01566	VdW_16_7_5	-0.02397	VdW_13_13_8	-0.04201	VdW_14_7_2	0.023394
VdW_15_6_3	-0.02464	VdW_17_10_7	0.008169	Ele_15_9_6	0.00614	VdW_9_11_5	-0.00624	VdW_11_12_3	0.053148
VdW_7_10_3	0.016903	VdW_6_7_5	0.092958	VdW_14_6_2	-0.05318	VdW_9_11_7	-0.01994	Ele_12_9_3	0.100681
VdW_9_2_4	-0.00758	VdW_15_13_6	0.034699	VdW_14_10_9	0.015685	VdW_9_12_4	0.001659	VdW_10_11_7	0.030572
Ele_11_8_8	-0.05137	VdW_10_10_7	-0.0507	VdW_4_10_3	-0.01534	VdW_9_2_5	-0.01193	VdW_7_11_5	-0.06783
VdW_13_8_4	0.004493	VdW_16_6_4	-0.01628	Ele_6_9_6	-0.00384	VdW_14_7_3	0.027957	VdW_17_5_5	0.007971

Ele_10_8_8	0.017999	VdW_13_3_4	-0.03027	VdW_8_11_9	0.032608	VdW_12_4_5	-0.00553	VdW_8_13_6	0.005196
VdW_13_9_8	0.029874	VdW_10_6_7	0.01496	VdW_8_2_5	0.00278	Ele_11_7_9	0.009096	VdW_8_5_6	-0.03158
VdW_17_7_4	0.013768	VdW_15_5_8	-0.00942	VdW_4_4_5	-0.0012	Ele_12_11_7	0.104709	Ele_6_7_5	-0.03572
VdW_11_8_3	0.007514	VdW_14_7_6	-0.02126	Ele_13_8_8	0.091257	VdW_7_12_3	-0.00445	VdW_15_11_5	-0.02297
VdW_13_10_5	0.02	VdW_7_12_6	0.106322	Ele_14_8_6	-0.01146	VdW_15_9_4	0.034808	Ele_12_6_4	-0.08063
VdW_3_10_4	-0.01048	VdW_12_12_8	-0.01674	VdW_9_7_9	0.007465	VdW_13_11_6	0.057986	VdW_9_11_6	0.005013
VdW_9_10_5	0.006096	VdW_16_11_8	-0.06442	VdW_9_11_8	0.032007	Ele_11_9_3	0.086556	VdW_9_8_3	0.012933
VdW_7_7_8	0.129601	VdW_9_5_5	-0.0205	VdW_5_5_8	0.029384	VdW_16_5_3	0.083978	VdW_10_5_2	0.024442
VdW_11_6_7	-0.00869	VdW_14_7_1	0.065545	VdW_12_10_9	-0.0068	VdW_6_4_9	-0.02638	Ele_10_11_5	-0.03535
Ele_14_6_1	0.020237	VdW_8_8_9	0.031712	VdW_6_8_4	-0.05125	VdW_13_13_	0.002952	VdW_11_4_8	0.023101

						4			
VdW_10_10_6	-0.08803	VdW_7_3_4	0.062339	VdW_4_6_4	0.008043	VdW_7_5_7	-0.05006	Ele_6_6_3	-0.067
Ele_9_9_8	-0.04923	VdW_12_11_7	-0.00958	VdW_13_5_5	-0.01582	VdW_6_12_4	-0.00198	Ele_10_5_6	0.074456
VdW_8_10_8	0.051595	VdW_5_7_9	-0.03017	VdW_14_8_7	-0.02435	VdW_18_10_8	-0.00991	VdW_11_8_10	-0.00024
VdW_12_6_4	0.025405	VdW_7_9_9	-0.04607	VdW_16_4_5	0.067935	VdW_6_10_6	-0.01786	VdW_13_5_3	-0.00584
VdW_7_6_9	-0.02842	VdW_7_10_8	0.014576	VdW_7_10_7	0.028004	VdW_9_10_3	-0.04895	Ele_9_8_9	0.012306
VdW_11_9_8	-0.02153	VdW_4_11_5	-0.03034	Ele_5_9_8	-0.08473	Ele_10_11_6	-0.02385	VdW_14_7_8	-0.00106
VdW_9_8_4	0.016249	Ele_9_10_5	0.030349	Ele_5_9_6	-0.05554	VdW_10_5_5	-0.00566	VdW_7_4_3	0.024525
Ele_12_9_8	0.047995	Ele_7_6_7	-0.04472	VdW_6_4_6	-0.00288	VdW_10_2_6	0.002439	Ele_6_6_5	-0.01776
VdW_13_3_3	-0.02506	VdW_12_5_6	0.01286	VdW_17_6_8	-0.04162	VdW_7_11_3	0.003935	VdW_5_7_5	0.079474
VdW_10_7_	0.018873	Ele_10_10_8	-0.00774	Ele_12_6_5	-0.10601	VdW_10_2_5	0.007845	VdW_10_10_	-0.01923

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VdW_12_6_5	0.03407	VdW_7_9_4	-0.04102	VdW_6_7_8	-0.02123	VdW_7_12_7	0.090875	VdW_13_12_4	0.005942
VdW_9_9_8	-0.05668	VdW_15_6_9	0.030328	VdW_7_7_4	0.019232	VdW_4_5_5	0.011406	VdW_4_8_2	-0.01491
VdW_9_10_6	0.004122	Ele_9_6_5	-0.03307	VdW_6_8_10	0.011102	VdW_14_9_8	-0.02589	Ele_8_7_3	0.042849
VdW_5_11_4	0.025373	Ele_14_10_5	0.020691	VdW_6_3_8	-0.01008	VdW_5_5_2	0.025243	VdW_7_13_4	-0.04173
VdW_3_7_4	-0.00847	VdW_14_5_10	0.042617	VdW_14_7_9	-0.02536	VdW_10_11_6	-0.05166	VdW_11_12_5	-0.06487
VdW_7_6_7	0.074581	VdW_6_5_9	0.008806	Ele_13_6_8	-0.0323	VdW_6_10_5	-0.05481	VdW_11_13_5	0.019081
Ele_10_10_7	-0.10978	VdW_14_5_3	0.025384	Ele_10_11_7	0.117522	Ele_14_7_9	-0.07839	VdW_5_5_7	0.023837
Ele_9_10_7	-0.01675	VdW_5_4_5	0.038465	Ele_8_10_4	-0.058	VdW_11_10_3	-0.0375	Ele_11_6_4	0.011839
VdW_7_6_3	-0.04721	VdW_8_12_8	0.050856	VdW_14_4_8	-0.04816	VdW_12_7_9	0.037715	Ele_11_11_8	0.063261
VdW_18_5_	-0.00989	VdW_12_11_	0.009752	VdW_6_6_10	0.064904	VdW_7_5_6	0.079008	Ele_8_9_9	0.018228

7		5							
VdW_12_9_8	-0.00636	VdW_8_4_2	-0.01689	VdW_6_9_4	0.017265	VdW_12_5_10	0.029541	VdW_10_6_11	-0.07249
VdW_13_4_7	0.079199	VdW_8_9_4	-0.03715	Ele_11_10_8	-0.00539	VdW_12_11_10	-0.00806	Ele_12_6_8	0.03681
VdW_10_12_8	0.005151	VdW_12_6_8	0.035088	VdW_4_12_5	-0.0021	VdW_5_10_8	0.036389	VdW_10_14_5	0.009965
VdW_9_10_7	0.092476	VdW_14_9_5	-0.00737	VdW_13_4_6	0.003349	Ele_13_7_4	-0.03002	VdW_5_6_4	0.017345
VdW_14_10_6	0.030869	VdW_3_7_5	-0.01192	Ele_13_9_4	0.121992	VdW_9_7_3	-0.05988	VdW_14_9_10	0.01928
VdW_7_10_9	-0.00725	VdW_7_3_3	-0.03783	VdW_3_9_4	0.038514	Ele_7_7_4	-0.02896	Ele_15_9_2	0.016164
VdW_9_9_4	0.059677	VdW_14_11_8	0.021418	VdW_4_7_4	-0.02119	VdW_15_3_5	0.088176	VdW_13_10_10	0.008846
Ele_9_10_6	0.006763	Ele_13_9_8	0.012421	Ele_9_5_6	0.114871	Ele_8_7_4	0.039814	VdW_6_3_5	0.011424
VdW_11_10	-0.03934	VdW_17_10_	-0.06587	VdW_13_5_6	-0.09706	Ele_9_5_5	0.021388	VdW_16_8_5	0.005987

_4		4							
VdW_14_9_7	0.001654	Ele_14_7_5	-0.00984	VdW_11_11_11	0.029345	VdW_3_11_6	-0.00574	Ele_14_9_2	0.068282
VdW_6_8_6	-0.01532	VdW_12_5_4	0.037213	VdW_5_6_5	-0.0652	VdW_5_11_3	-0.00241	Ele_12_9_9	0.047341
VdW_13_7_8	-0.00704	Ele_7_10_6	0.089658	VdW_17_10_5	0.007778	VdW_16_9_7	-0.01154	VdW_16_10_5	0.014479
VdW_11_8_8	-0.03026	VdW_17_7_5	0.023258	Ele_13_10_8	0.058635	VdW_9_3_4	0.00886	Ele_9_11_8	-0.0066
VdW_13_10_3	-0.03733	VdW_14_10_7	0.040667	Ele_15_7_6	-0.01663	VdW_12_3_8	-0.00454	Ele_11_5_6	0.063883
VdW_11_6_6	-0.0122	VdW_8_7_9	0.039632	Ele_7_10_7	0.051033	VdW_8_6_11	0.018431	Ele_12_11_6	0.077448
VdW_12_8_3	-0.00975	Ele_10_6_8	0.079589	VdW_13_12_3	-0.03089	VdW_5_8_4	0.009359	VdW_9_11_4	-0.04587
VdW_13_6_11	0.018804	VdW_8_11_7	-0.01846	VdW_4_7_3	0.023936	Ele_14_7_8	-0.03882	VdW_7_7_9	0.010905
VdW_10_2_	0.046579	VdW_6_9_9	-0.02932	Ele_14_8_5	-0.04485	Ele_13_11_6	-0.0428	VdW_17_9_8	-0.03097

4									
Ele_11_10_7	0.060948	VdW_6_7_3	0.015831	VdW_8_5_4	0.073955	VdW_6_8_8	-0.01454	Ele_9_8_3	0.049676
VdW_14_10_2	-0.00233	Ele_12_6_7	0.023449	VdW_14_9_3	0.055369	VdW_5_7_10	0.02466	VdW_7_12_8	0.037457
VdW_15_11_4	0.07462	VdW_12_5_3	-0.00623	Ele_10_5_7	0.013464	VdW_13_4_5	0.04581	Ele_11_11_6	-0.01677
VdW_11_9_3	-0.07003	VdW_3_10_5	-0.0055	VdW_6_12_7	0.048559	VdW_16_7_9	0.002516	VdW_4_6_9	0.00081
VdW_13_6_8	0.031545	VdW_15_4_5	-0.00191	Ele_14_8_8	0.013752	VdW_13_5_2	-0.02061	Ele_13_6_9	-0.05149
VdW_11_10_7	-0.06499	VdW_6_9_7	-0.01726	VdW_6_11_8	0.031975	VdW_12_2_8	-0.04316	VdW_7_2_6	0.012691
VdW_10_10_8	0.008292	VdW_14_10_10	-0.03309	VdW_13_11_4	-0.04319	VdW_11_5_5	-0.0038	VdW_3_11_8	0.023577
VdW_6_7_2	0.004133	VdW_5_5_9	0.004741	VdW_9_5_4	0.029479	VdW_11_4_5	0.015687	VdW_10_4_7	0.010386
Ele_9_8_4	0.0458	VdW_8_11_6	-0.044	Ele_14_6_6	0.036626	VdW_5_11_7	0.064196	VdW_9_2_8	-0.01416
VdW_7_12_	0.007544	Ele_13_7_8	-0.03181	VdW_7_13_5	0.005334	VdW_12_6_9	0.013591	VdW_6_9_5	-0.02337

5									
VdW_5_6_8	-0.01878	VdW_12_5_7	-0.01385	VdW_14_12_3	0.033793	VdW_11_7_9	0.005302	VdW_15_7_6	-0.0098
VdW_9_7_4	0.040788	VdW_12_14_6	-0.01179	VdW_5_12_5	-0.02606	VdW_12_12_10	0.059875	Ele_15_7_4	0.054503
VdW_6_9_3	-0.05908	Ele_6_8_5	-0.01469	VdW_13_10_8	0.08015	VdW_13_4_9	-0.02064	VdW_13_9_9	-0.03444
Ele_14_9_6	0.104807	VdW_3_6_8	-0.01055	VdW_5_13_5	0.048774	VdW_3_6_7	0.015522	VdW_19_7_7	0.00375
VdW_9_6_5	-0.00393	VdW_6_7_6	0.037342	Ele_6_6_7	-0.08246	VdW_12_8_10	0.034708	VdW_4_5_8	0.005412
VdW_11_7_4	0.132634	VdW_11_11_9	0.00352	VdW_10_11_2	0.025489	VdW_4_12_8	0.036089	VdW_6_11_6	-0.0056
VdW_12_10_8	0.066226	VdW_16_10_6	-0.02282	VdW_15_7_2	-0.00158	VdW_11_11_4	0.005698	VdW_13_11_9	-0.03038
VdW_8_5_3	-0.02	Ele_11_9_9	-0.06418	Ele_5_11_5	0.043468	VdW_10_5_6	-0.0923	VdW_9_11_11	0.014874
Ele_13_6_7	0.045797	VdW_5_10_3	-0.02418	VdW_8_12_4	0.036124	VdW_3_4_4	-0.01762	VdW_11_6_8	-0.02165

VdW_7_9_8	-0.0152	VdW_14_12_5	0.002301	VdW_9_3_5	-0.00129	VdW_15_10_7	-0.11552	Ele_12_3_3	-0.04344
VdW_10_6_5	-0.06838	Ele_10_6_5	-0.07892	VdW_16_10_4	-0.04916	VdW_16_5_7	-0.02339	Ele_14_7_1	0.018854
VdW_13_10_7	-0.02262	VdW_11_11_7	0.051144	VdW_15_10_9	0.01658	VdW_3_11_5	0.0348	VdW_5_8_2	0.003664
VdW_7_11_8	0.005973	VdW_10_4_8	0.034292	VdW_16_11_5	-0.05706	VdW_15_6_10	-0.00604	Ele_8_4_6	0.087807
VdW_13_6_5	-0.0114	VdW_8_5_9	0.020413	VdW_7_4_5	-0.05428	VdW_13_7_9	0.002785	VdW_10_12_5	-0.01821
VdW_10_8_8	-0.05384	VdW_6_8_5	-0.00088	VdW_17_10_8	-0.02321	VdW_4_11_6	0.063907	VdW_14_13_8	0.041046
VdW_9_11_1	0.009326	Ele_11_6_7	-0.06202	Ele_9_11_6	-0.01421	VdW_15_9_6	-0.04169	VdW_10_12_6	-0.03321
VdW_14_12_6	-0.00625	VdW_11_11_8	0.019522	VdW_11_10_8	-0.02347	Ele_9_7_4	0.024844	VdW_9_13_4	-0.03828
VdW_7_10_	0.03287	Ele_14_9_5	0.103537	VdW_7_5_10	0.050956	VdW_12_7_3	0.027509	VdW_15_5_2	0.023632

2									
VdW_6_7_9	-0.08224	Ele_10_10_5	-0.05469	VdW_14_11_4	-0.01502	VdW_14_4_4	0.004686	Ele_12_11_5	0.014649
VdW_13_6_7	-0.0218	VdW_9_11_3	0.006155	VdW_2_6_3	0.028047	Ele_13_5_7	-0.04282	Ele_9_9_4	-0.00054
Ele_11_6_5	0.002139	VdW_12_9_3	-0.0985	Ele_10_9_4	-0.00731	VdW_15_6_5	0.10252	VdW_8_3_8	0.04341
VdW_7_4_7	-0.00068	Ele_12_10_8	-0.00514	VdW_15_9_10	-0.00318	Ele_10_11_4	0.079802	VdW_10_3_3	-0.03248
VdW_14_8_6	0.06827	VdW_15_10_10	-0.01052	VdW_4_11_8	-0.05057	VdW_12_5_8	-0.04597	VdW_6_8_2	-0.02215
VdW_12_5_9	0.025903	VdW_15_11_3	0.007213	VdW_6_5_7	-0.02833	VdW_8_8_3	-0.03665	Ele_7_11_6	0.141463
VdW_10_5_9	0.124453	VdW_5_12_8	-0.0532	VdW_14_6_3	0.03808	VdW_6_6_7	0.121993	VdW_7_4_9	0.055978
VdW_16_10_3	0.077293	VdW_14_5_9	-0.01439	VdW_13_5_8	0.069762	VdW_10_9_4	-0.05585	VdW_13_7_3	-0.00633
VdW_16_6_	0.018924	Ele_4_5_2	-0.0343	VdW_5_7_2	-0.00643	VdW_7_3_8	0.048355	VdW_4_8_4	-0.01598

3									
VdW_7_6_8	0.00763	VdW_12_9_9	0.056676	Ele_14_8_7	0.063174	VdW_6_13_6	-0.07895	Ele_10_12_5	0.024482
VdW_4_11_3	0.020847	VdW_11_5_9	0.036538	VdW_11_5_7	-0.00557	VdW_15_9_9	0.009966	VdW_13_6_3	-0.02378
VdW_10_6_6	-0.01311	VdW_12_11_6	0.054557	Ele_9_9_9	-0.00054	VdW_6_6_5	0.076257	Ele_15_6_6	-0.01528
VdW_8_7_4	-0.02968	VdW_14_6_8	-0.00973	Ele_7_8_8	0.005536	VdW_6_10_9	0.015883	Ele_15_6_5	-0.06638
VdW_13_9_4	0.013932	Ele_10_9_8	0.066048	VdW_4_12_6	-0.04392	VdW_15_10_5	0.03947	VdW_4_5_2	0.0064
VdW_10_9_8	-0.07677	VdW_13_10_9	-0.01896	VdW_10_2_8	-0.06227	VdW_6_8_9	-0.01485	VdW_12_14_4	0.00268
VdW_6_12_6	0.044796	VdW_3_13_6	-0.00728	VdW_12_3_6	0.025661	VdW_14_11_9	0.024148	VdW_13_9_2	0.012141
VdW_11_7_10	0.012431	VdW_9_5_7	-0.02833	VdW_15_10_3	0.007166	VdW_2_11_5	-0.00797	Ele_11_10_9	0.001562
VdW_14_6_5	-0.03121	VdW_9_3_9	-0.10129	VdW_9_12_3	0.014752	VdW_15_8_5	-0.01052	Ele_14_8_4	-0.01723

Ele_10_6_6	-0.08079	VdW_7_3_2	-0.00114	VdW_11_11_5	-0.0208	Ele_11_10_5	0.03552	Ele_5_9_7	-0.04348
VdW_9_12_8	-0.02033	VdW_12_11_9	-0.01708	VdW_10_15_3	0.02098	Ele_11_11_5	-0.0002	Ele_11_5_7	0.076419
Ele_14_7_7	-0.04741	VdW_7_8_9	0.085704	VdW_10_11_3	0.042177	VdW_15_8_3	-0.00739	Ele_6_7_6	-0.02594
VdW_13_8_8	0.020145	VdW_5_8_9	-0.04004	Ele_8_5_5	-0.00677	VdW_11_12_4	-0.0164	Ele_9_10_4	-0.08544
VdW_14_5_8	-0.02013	VdW_12_5_5	-0.01347	VdW_14_3_5	-0.00508	Ele_7_7_3	0.070504	Ele_14_7_4	0.074127
VdW_8_2_8	-0.01221	VdW_8_11_5	-0.00978	VdW_10_9_9	-0.08838	VdW_9_4_7	-0.09581	Ele_7_6_3	-0.00112
VdW_16_6_5	0.002957	VdW_9_8_9	0.020925	VdW_5_5_3	-0.06823	Ele_13_6_4	-0.02058	VdW_10_11_4	-0.02327
VdW_6_4_8	-0.02259	VdW_11_11_6	-0.09669	VdW_15_7_9	0.027974	Ele_6_4_2	0.048962	VdW_2_7_6	-0.00334
VdW_12_11_2	0.021601	VdW_8_6_4	0.020366	VdW_12_4_4	-0.04203	VdW_10_5_8	0.012572	VdW_7_5_9	-0.02593

VdW_14_11_3	0.013253	VdW_14_6_7	-0.0125	VdW_9_14_6	-0.00316	VdW_5_9_4	-0.04356	VdW_13_13_6	-0.02473
Ele_6_8_7	0.049656	VdW_11_5_6	0.021752	Ele_13_10_7	-0.03644	VdW_6_6_4	-0.05309	Ele_10_8_9	-0.04586
VdW_10_5_7	-0.00773	Ele_6_9_7	0.089309	Ele_6_9_8	-0.01086	Ele_14_5_6	-0.10626	VdW_9_4_9	0.026017
VdW_15_6_2	-0.02601	VdW_15_7_5	0.049821	VdW_18_7_9	-0.04496	VdW_4_7_9	0.00158	Ele_7_8_2	-0.01991
VdW_9_10_1	-0.05508	VdW_8_4_9	-0.03121	Ele_7_7_8	-0.02957	VdW_12_12_3	0.005334	VdW_15_9_5	0.005068
VdW_13_7_4	-0.02469	VdW_8_11_8	0.019842	VdW_10_11_10	0.037475	VdW_10_4_2	-0.06626	Ele_14_10_6	0.021585
VdW_7_10_4	-0.06986	VdW_8_10_9	0.001088	VdW_2_10_4	0.004738	VdW_7_6_2	0.025392	VdW_6_5_6	0.091778
VdW_8_13_4	-0.00397	VdW_11_2_8	0.024532	VdW_14_9_2	0.033147	VdW_10_4_5	0.04206	Ele_6_8_6	-0.01436
VdW_14_12_8	0.042893	VdW_4_8_5	0.016556	Ele_9_12_4	0.032774	VdW_2_12_8	-0.01612	VdW_10_11_8	0.006872

VdW_14_8_8	0.053025	VdW_12_2_6	0.028345	Ele_6_7_8	0.020976	VdW_14_7_10	0.036983	VdW_9_4_3	0.005868
VdW_12_10_4	-0.06996	VdW_7_6_4	-0.02899	Ele_11_9_8	0.00492	VdW_5_6_7	-0.02305	Ele_13_10_4	0.087866
VdW_11_10_5	-0.00731	VdW_3_7_8	0.015067	Ele_6_7_7	-0.0098	Ele_7_9_8	-0.01388	Ele_5_5_5	0.010148
VdW_7_5_4	-0.07226	VdW_11_6_5	0.040172	VdW_6_7_7	0.108085	VdW_8_13_5	0.03023	Ele_5_7_5	-0.02681
VdW_10_8_3	-0.05024	VdW_6_6_8	0.003477	VdW_6_7_4	0.008239	Ele_12_5_6	0.034197	VdW_10_8_2	-0.01024
VdW_10_7_9	0.099814	VdW_17_11_6	-0.0211	VdW_14_8_4	-0.00114	VdW_6_10_3	0.040079	VdW_15_6_7	-0.01701
Ele_10_10_6	-0.0695	VdW_11_6_9	-0.00885	VdW_15_7_1	-0.00256	Ele_9_5_7	0.023652	VdW_13_7_10	-0.00519
VdW_6_3_4	-0.02976	VdW_16_6_6	0.019747	VdW_8_6_8	-0.08609	Ele_6_10_6	0.057891	Ele_10_9_9	-0.0231
VdW_10_3_5	0.036318	VdW_10_8_4	-0.003	VdW_7_5_5	0.020279	VdW_11_2_6	0.003696	VdW_13_5_9	-0.01991
VdW_6_8_7	0.045938	VdW_11_12_	0.033126	VdW_6_4_3	-0.04199	VdW_14_13_	0.024286	Ele_7_11_7	-0.02193

		8				6			
VdW_8_9_9	-0.01589	VdW_8_5_2	-0.02357	VdW_15_9_3	-0.015	VdW_9_4_5	-0.04176	Ele_7_5_4	0.070542
VdW_10_10_5	0.025587	VdW_9_12_2	-0.0395	VdW_6_6_2	0.026233	VdW_4_6_3	-0.02488	VdW_10_14_8	-0.02982
VdW_11_5_3	0.07327	Ele_8_10_8	-0.01702	VdW_10_6_4	-0.01395	Ele_11_11_7	0.039468	VdW_14_10_4	-0.01321
VdW_13_5_4	0.031058	VdW_9_6_9	0.036898	VdW_5_11_8	0.038707	VdW_10_3_9	-0.02935	VdW_8_7_10	-0.0055
VdW_6_5_3	0.029793	VdW_5_7_8	0.032917	VdW_13_11_2	-0.00573	VdW_10_10_4	-0.07344	VdW_16_4_6	0.034245
Ele_11_6_8	0.01713	VdW_17_9_5	0.006561	VdW_13_8_3	0.031645	VdW_5_7_3	-0.01698	VdW_12_2_5	-0.04449
VdW_14_5_2	-0.01462	VdW_13_6_4	-0.05097	VdW_14_6_10	-0.00897	VdW_11_7_3	0.055894	VdW_9_6_8	-0.04636
VdW_11_11_1	-0.00862	VdW_8_3_4	0.032129	VdW_6_5_4	0.009654	Ele_14_9_7	0.02172	Ele_8_5_4	0.037808
VdW_14_9_9	0.061212	VdW_13_12_6	0.013043	VdW_15_11_8	0.082427	VdW_3_9_8	0.046042	VdW_5_4_8	0.000448

Ele_10_6_7	0.065557	VdW_14_10_8	-0.0619	VdW_8_6_9	0.044025	VdW_14_11_5	-0.05308	VdW_16_7_3	-0.01797
VdW_14_7_4	-0.06116	VdW_4_6_8	-0.01304	VdW_10_5_3	0.005374	Ele_13_6_5	-0.03311	VdW_5_6_6	-0.01302
VdW_8_10_4	-0.06068	VdW_8_5_7	-0.00761	VdW_11_5_8	-0.0427	VdW_15_12_5	-0.00511	VdW_15_4_8	0.041746
Ele_11_6_6	0.10216	VdW_7_5_2	0.04487	VdW_6_6_6	0.064113	VdW_17_6_7	-0.01071	VdW_11_2_5	-0.04012
VdW_6_11_4	0.018043	VdW_13_10_4	0.050683	VdW_9_5_9	0.030469	Ele_13_10_5	0.042438	VdW_16_6_9	-0.02386
VdW_14_8_5	0.023467	VdW_14_6_4	0.008254	VdW_19_7_6	-0.03451	Ele_5_8_5	-0.03561	VdW_13_12_9	-0.04901
VdW_11_6_4	0.000644	Ele_9_6_8	-0.02136	VdW_13_4_3	-0.03419	VdW_10_6_8	-0.03929	VdW_5_9_9	-0.01005
VdW_13_11_8	0.000244	VdW_14_10_3	-0.04918	VdW_8_5_5	-0.02891	VdW_5_4_4	-0.00647	VdW_8_4_4	-0.05669
VdW_16_7_2	0.022453	VdW_7_4_6	0.019145	VdW_6_3_7	-0.03904	VdW_4_9_2	0.029196	VdW_10_6_	0.024279

VdW_7_5_8	-0.01435	VdW_4_11_4	0.046972	VdW_11_8_2	0.018899	VdW_4_10_8	0.028801	VdW_9_10_8	-0.00784
VdW_11_8_9	0.001015	VdW_13_11_3	-0.01342	VdW_6_12_5	0.015439	VdW_10_12_1	0.030477	VdW_6_12_3	-0.05737
VdW_6_5_2	-0.03513	VdW_15_4_6	-0.00396	VdW_12_13_4	-0.00962	VdW_13_11_5	0.037858	VdW_16_7_4	-0.00685
VdW_9_10_4	0.030595	VdW_14_7_7	0.049233	VdW_8_12_3	-0.00793	VdW_4_5_4	-0.054	VdW_10_12_2	-0.01907
VdW_14_3_8	-0.0225	VdW_6_9_6	-0.07876	VdW_13_8_9	0.031795	VdW_16_5_5	-0.04759		
VdW_11_6_1	-0.02319	VdW_8_13_3	0.010508	VdW_11_4_4	-0.01407	VdW_9_4_4	0.027477	Ele_14_9_8	0.034244
Ele_11_6_1	0.052014	VdW_12_6_1	-0.03382	VdW_12_3_3	0.002549	VdW_17_6_4	0.00158	VdW_14_8_9	-0.02597
VdW_14_6_1	0.01338	VdW_14_10_5	0.009333	VdW_6_3_6	0.024729	VdW_15_12_8	-0.05784	VdW_14_12_7	0.020695
VdW_7_4_2	-0.02712	VdW_13_12_5	-0.03858	Ele_9_10_8	-0.05128	VdW_16_4_8	-0.00418	VdW_3_9_5	-0.03601
VdW_10_7_	0.007108	VdW_4_10_4	-0.00534	Ele_13_8_4	0.082442	VdW_16_5_6	-0.01626	VdW_3_7_2	0.002863

1									
Ele_7_3_2	0.022777	VdW_10_11_5	0.037783	VdW_16_5_4	-0.00585	VdW_14_4_3	-0.00803	VdW_7_11_7	-0.03367
VdW_15_6_1	0.011249	VdW_8_9_1	-0.05559	Ele_8_9_4	-0.03796	VdW_6_10_10	-0.01538	VdW_9_4_2	0.005881
VdW_12_12_2	3.20E-05	VdW_3_6_4	-0.05033	VdW_13_6_9	-0.01585	VdW_15_7_8	-0.00374	VdW_15_8_4	0.073266
VdW_7_10_6	0.042993	VdW_16_12_5	-0.00205	VdW_14_7_5	-0.06145	VdW_3_10_8	0.02699	Ele_7_6_8	-0.12182
VdW_12_6_7	-0.02615	VdW_10_8_9	-0.02489	VdW_7_8_8	0.001854	VdW_14_9_4	0.04614	VdW_10_4_6	-0.02498
VdW_14_9_6	0.013761	VdW_16_11_3	-0.01566	VdW_16_7_5	-0.02397	VdW_13_13_8	-0.04201	VdW_14_7_2	0.023394
VdW_15_6_3	-0.02464	VdW_17_10_7	0.008169	Ele_15_9_6	0.00614	VdW_9_11_5	-0.00624	VdW_11_12_3	0.053148
VdW_7_10_3	0.016903	VdW_6_7_5	0.092958	VdW_14_6_2	-0.05318	VdW_9_11_7	-0.01994	Ele_12_9_3	0.100681

VdW_9_2_4	-0.00758	VdW_15_13_6	0.034699	VdW_14_10_9	0.015685	VdW_9_12_4	0.001659	VdW_10_11_7	0.030572
Ele_11_8_8	-0.05137	VdW_10_10_7	-0.0507	VdW_4_10_3	-0.01534	VdW_9_2_5	-0.01193	VdW_7_11_5	-0.06783
VdW_13_8_4	0.004493	VdW_16_6_4	-0.01628	Ele_6_9_6	-0.00384	VdW_14_7_3	0.027957	VdW_17_5_5	0.007971
Ele_10_8_8	0.017999	VdW_13_3_4	-0.03027	VdW_8_11_9	0.032608	VdW_12_4_5	-0.00553	VdW_8_13_6	0.005196
VdW_13_9_8	0.029874	VdW_10_6_7	0.01496	VdW_8_2_5	0.00278	Ele_11_7_9	0.009096	VdW_8_5_6	-0.03158
VdW_17_7_4	0.013768	VdW_15_5_8	-0.00942	VdW_4_4_5	-0.0012	Ele_12_11_7	0.104709	Ele_6_7_5	-0.03572
VdW_11_8_3	0.007514	VdW_14_7_6	-0.02126	Ele_13_8_8	0.091257	VdW_7_12_3	-0.00445	VdW_15_11_5	-0.02297
VdW_13_10_5	0.02	VdW_7_12_6	0.106322	Ele_14_8_6	-0.01146	VdW_15_9_4	0.034808	Ele_12_6_4	-0.08063
VdW_3_10_4	-0.01048	VdW_12_12_8	-0.01674	VdW_9_7_9	0.007465	VdW_13_11_6	0.057986	VdW_9_11_6	0.005013

VdW_9_10_5	0.006096	VdW_16_11_8	-0.06442	VdW_9_11_8	0.032007	Ele_11_9_3	0.086556	VdW_9_8_3	0.012933
VdW_7_7_8	0.129601	VdW_9_5_5	-0.0205	VdW_5_5_8	0.029384	VdW_16_5_3	0.083978	VdW_10_5_2	0.024442
VdW_11_6_7	-0.00869	VdW_14_7_1	0.065545	VdW_12_10_9	-0.0068	VdW_6_4_9	-0.02638	Ele_10_11_5	-0.03535
Ele_14_6_1	0.020237	VdW_8_8_9	0.031712	VdW_6_8_4	-0.05125	VdW_13_13_4	0.002952	VdW_11_4_8	0.023101
VdW_10_10_6	-0.08803	VdW_7_3_4	0.062339	VdW_4_6_4	0.008043	VdW_7_5_7	-0.05006	Ele_6_6_3	-0.067
Ele_9_9_8	-0.04923	VdW_12_11_7	-0.00958	VdW_13_5_5	-0.01582	VdW_6_12_4	-0.00198	Ele_10_5_6	0.074456
VdW_8_10_8	0.051595	VdW_5_7_9	-0.03017	VdW_14_8_7	-0.02435	VdW_18_10_8	-0.00991	VdW_11_8_10	-0.00024
VdW_12_6_4	0.025405	VdW_7_9_9	-0.04607	VdW_16_4_5	0.067935	VdW_6_10_6	-0.01786	VdW_13_5_3	-0.00584
VdW_7_6_9	-0.02842	VdW_7_10_8	0.014576	VdW_7_10_7	0.028004	VdW_9_10_3	-0.04895	Ele_9_8_9	0.012306
VdW_11_9_	-0.02153	VdW_4_11_5	-0.03034	Ele_5_9_8	-0.08473	Ele_10_11_6	-0.02385	VdW_14_7_8	-0.00106

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VdW_9_8_4	0.016249	Ele_9_10_5	0.030349	Ele_5_9_6	-0.05554	VdW_10_5_5	-0.00566	VdW_7_4_3	0.024525
Ele_12_9_8	0.047995	Ele_7_6_7	-0.04472	VdW_6_4_6	-0.00288	VdW_10_2_6	0.002439	Ele_6_6_5	-0.01776
VdW_13_3_3	-0.02506	VdW_12_5_6	0.01286	VdW_17_6_8	-0.04162	VdW_7_11_3	0.003935	VdW_5_7_5	0.079474
VdW_10_7_4	0.018873	Ele_10_10_8	-0.00774	Ele_12_6_5	-0.10601	VdW_10_2_5	0.007845	VdW_10_10_1	-0.01923
VdW_12_6_5	0.03407	VdW_7_9_4	-0.04102	VdW_6_7_8	-0.02123	VdW_7_12_7	0.090875	VdW_13_12_4	0.005942
VdW_9_9_8	-0.05668	VdW_15_6_9	0.030328	VdW_7_7_4	0.019232	VdW_4_5_5	0.011406	VdW_4_8_2	-0.01491
VdW_9_10_6	0.004122	Ele_9_6_5	-0.03307	VdW_6_8_10	0.011102	VdW_14_9_8	-0.02589	Ele_8_7_3	0.042849
VdW_5_11_4	0.025373	Ele_14_10_5	0.020691	VdW_6_3_8	-0.01008	VdW_5_5_2	0.025243	VdW_7_13_4	-0.04173
VdW_3_7_4	-0.00847	VdW_14_5_10	0.042617	VdW_14_7_9	-0.02536	VdW_10_11_6	-0.05166	VdW_11_12_5	-0.06487
VdW_7_6_7	0.074581	VdW_6_5_9	0.008806	Ele_13_6_8	-0.0323	VdW_6_10_5	-0.05481	VdW_11_13_	0.019081

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Ele_10_10_7	-0.10978	VdW_14_5_3	0.025384	Ele_10_11_7	0.117522	Ele_14_7_9	-0.07839	VdW_5_5_7	0.023837
Ele_9_10_7	-0.01675	VdW_5_4_5	0.038465	Ele_8_10_4	-0.058	VdW_11_10_3	-0.0375	Ele_11_6_4	0.011839
VdW_7_6_3	-0.04721	VdW_8_12_8	0.050856	VdW_14_4_8	-0.04816	VdW_12_7_9	0.037715	Ele_11_11_8	0.063261
VdW_18_5_7	-0.00989	VdW_12_11_5	0.009752	VdW_6_6_10	0.064904	VdW_7_5_6	0.079008	Ele_8_9_9	0.018228
VdW_12_9_8	-0.00636	VdW_8_4_2	-0.01689	VdW_6_9_4	0.017265	VdW_12_5_10	0.029541	VdW_10_6_11	-0.07249
VdW_13_4_7	0.079199	VdW_8_9_4	-0.03715	Ele_11_10_8	-0.00539	VdW_12_11_10	-0.00806	Ele_12_6_8	0.03681
VdW_10_12_8	0.005151	VdW_12_6_8	0.035088	VdW_4_12_5	-0.0021	VdW_5_10_8	0.036389	VdW_10_14_5	0.009965
VdW_9_10_7	0.092476	VdW_14_9_5	-0.00737	VdW_13_4_6	0.003349	Ele_13_7_4	-0.03002	VdW_5_6_4	0.017345
VdW_14_10_6	0.030869	VdW_3_7_5	-0.01192	Ele_13_9_4	0.121992	VdW_9_7_3	-0.05988	VdW_14_9_10	0.01928

VdW_7_10_9	-0.00725	VdW_7_3_3	-0.03783	VdW_3_9_4	0.038514	Ele_7_7_4	-0.02896	Ele_15_9_2	0.016164
VdW_9_9_4	0.059677	VdW_14_11_8	0.021418	VdW_4_7_4	-0.02119	VdW_15_3_5	0.088176	VdW_13_10_10	0.008846
Ele_9_10_6	0.006763	Ele_13_9_8	0.012421	Ele_9_5_6	0.114871	Ele_8_7_4	0.039814	VdW_6_3_5	0.011424
VdW_11_10_4	-0.03934	VdW_17_10_4	-0.06587	VdW_13_5_6	-0.09706	Ele_9_5_5	0.021388	VdW_16_8_5	0.005987
VdW_14_9_7	0.001654	Ele_14_7_5	-0.00984	VdW_11_11_11	0.029345	VdW_3_11_6	-0.00574	Ele_14_9_2	0.068282
VdW_6_8_6	-0.01532	VdW_12_5_4	0.037213	VdW_5_6_5	-0.0652	VdW_5_11_3	-0.00241	Ele_12_9_9	0.047341
VdW_13_7_8	-0.00704	Ele_7_10_6	0.089658	VdW_17_10_5	0.007778	VdW_16_9_7	-0.01154	VdW_16_10_5	0.014479
VdW_11_8_8	-0.03026	VdW_17_7_5	0.023258	Ele_13_10_8	0.058635	VdW_9_3_4	0.00886	Ele_9_11_8	-0.0066
VdW_13_10_3	-0.03733	VdW_14_10_7	0.040667	Ele_15_7_6	-0.01663	VdW_12_3_8	-0.00454	Ele_11_5_6	0.063883
VdW_11_6_	-0.0122	VdW_8_7_9	0.039632	Ele_7_10_7	0.051033	VdW_8_6_11	0.018431	Ele_12_11_6	0.077448

6									
VdW_12_8_3	-0.00975	Ele_10_6_8	0.079589	VdW_13_12_3	-0.03089	VdW_5_8_4	0.009359	VdW_9_11_4	-0.04587
VdW_13_6_11	0.018804	VdW_8_11_7	-0.01846	VdW_4_7_3	0.023936	Ele_14_7_8	-0.03882	VdW_7_7_9	0.010905
VdW_10_2_4	0.046579	VdW_6_9_9	-0.02932	Ele_14_8_5	-0.04485	Ele_13_11_6	-0.0428	VdW_17_9_8	-0.03097
Ele_11_10_7	0.060948	VdW_6_7_3	0.015831	VdW_8_5_4	0.073955	VdW_6_8_8	-0.01454	Ele_9_8_3	0.049676
VdW_14_10_2	-0.00233	Ele_12_6_7	0.023449	VdW_14_9_3	0.055369	VdW_5_7_10	0.02466	VdW_7_12_8	0.037457
VdW_15_11_4	0.07462	VdW_12_5_3	-0.00623	Ele_10_5_7	0.013464	VdW_13_4_5	0.04581	Ele_11_11_6	-0.01677
VdW_11_9_3	-0.07003	VdW_3_10_5	-0.0055	VdW_6_12_7	0.048559	VdW_16_7_9	0.002516	VdW_4_6_9	0.00081
VdW_13_6_8	0.031545	VdW_15_4_5	-0.00191	Ele_14_8_8	0.013752	VdW_13_5_2	-0.02061	Ele_13_6_9	-0.05149
VdW_11_10	-0.06499	VdW_6_9_7	-0.01726	VdW_6_11_8	0.031975	VdW_12_2_8	-0.04316	VdW_7_2_6	0.012691

_7									
VdW_10_10_8	0.008292	VdW_14_10_10	-0.03309	VdW_13_11_4	-0.04319	VdW_11_5_5	-0.0038	VdW_3_11_8	0.023577
VdW_6_7_2	0.004133	VdW_5_5_9	0.004741	VdW_9_5_4	0.029479	VdW_11_4_5	0.015687	VdW_10_4_7	0.010386
Ele_9_8_4	0.0458	VdW_8_11_6	-0.044	Ele_14_6_6	0.036626	VdW_5_11_7	0.064196	VdW_9_2_8	-0.01416
VdW_7_12_5	0.007544	Ele_13_7_8	-0.03181	VdW_7_13_5	0.005334	VdW_12_6_9	0.013591	VdW_6_9_5	-0.02337
VdW_5_6_8	-0.01878	VdW_12_5_7	-0.01385	VdW_14_12_3	0.033793	VdW_11_7_9	0.005302	VdW_15_7_6	-0.0098
VdW_9_7_4	0.040788	VdW_12_14_6	-0.01179	VdW_5_12_5	-0.02606	VdW_12_12_10	0.059875	Ele_15_7_4	0.054503
VdW_6_9_3	-0.05908	Ele_6_8_5	-0.01469	VdW_13_10_8	0.08015	VdW_13_4_9	-0.02064	VdW_13_9_9	-0.03444
Ele_14_9_6	0.104807	VdW_3_6_8	-0.01055	VdW_5_13_5	0.048774	VdW_3_6_7	0.015522	VdW_19_7_7	0.00375
VdW_9_6_5	-0.00393	VdW_6_7_6	0.037342	Ele_6_6_7	-0.08246	VdW_12_8_10	0.034708	VdW_4_5_8	0.005412
VdW_11_7_	0.132634	VdW_11_11_	0.00352	VdW_10_11_	0.025489	VdW_4_12_8	0.036089	VdW_6_11_6	-0.0056

4		9		2					
VdW_12_10_8	0.066226	VdW_16_10_6	-0.02282	VdW_15_7_2	-0.00158	VdW_11_11_4	0.005698	VdW_13_11_9	-0.03038
VdW_8_5_3	-0.02	Ele_11_9_9	-0.06418	Ele_5_11_5	0.043468	VdW_10_5_6	-0.0923	VdW_9_11_11	0.014874
Ele_13_6_7	0.045797	VdW_5_10_3	-0.02418	VdW_8_12_4	0.036124	VdW_3_4_4	-0.01762	VdW_11_6_8	-0.02165
VdW_7_9_8	-0.0152	VdW_14_12_5	0.002301	VdW_9_3_5	-0.00129	VdW_15_10_7	-0.11552	Ele_12_3_3	-0.04344
VdW_10_6_5	-0.06838	Ele_10_6_5	-0.07892	VdW_16_10_4	-0.04916	VdW_16_5_7	-0.02339	Ele_14_7_1	0.018854
VdW_13_10_7	-0.02262	VdW_11_11_7	0.051144	VdW_15_10_9	0.01658	VdW_3_11_5	0.0348	VdW_5_8_2	0.003664
VdW_7_11_8	0.005973	VdW_10_4_8	0.034292	VdW_16_11_5	-0.05706	VdW_15_6_10	-0.00604	Ele_8_4_6	0.087807
VdW_13_6_5	-0.0114	VdW_8_5_9	0.020413	VdW_7_4_5	-0.05428	VdW_13_7_9	0.002785	VdW_10_12_5	-0.01821
VdW_10_8_	-0.05384	VdW_6_8_5	-0.00088	VdW_17_10_	-0.02321	VdW_4_11_6	0.063907	VdW_14_13_	0.041046

8				8				8	
VdW_9_11_1	0.009326	Ele_11_6_7	-0.06202	Ele_9_11_6	-0.01421	VdW_15_9_6	-0.04169	VdW_10_12_6	-0.03321
VdW_14_12_6	-0.00625	VdW_11_11_8	0.019522	VdW_11_10_8	-0.02347	Ele_9_7_4	0.024844	VdW_9_13_4	-0.03828
VdW_7_10_2	0.03287	Ele_14_9_5	0.103537	VdW_7_5_10	0.050956	VdW_12_7_3	0.027509	VdW_15_5_2	0.023632
VdW_6_7_9	-0.08224	Ele_10_10_5	-0.05469	VdW_14_11_4	-0.01502	VdW_14_4_4	0.004686	Ele_12_11_5	0.014649
VdW_13_6_7	-0.0218	VdW_9_11_3	0.006155	VdW_2_6_3	0.028047	Ele_13_5_7	-0.04282	Ele_9_9_4	-0.00054
Ele_11_6_5	0.002139	VdW_12_9_3	-0.0985	Ele_10_9_4	-0.00731	VdW_15_6_5	0.10252	VdW_8_3_8	0.04341
VdW_7_4_7	-0.00068	Ele_12_10_8	-0.00514	VdW_15_9_10	-0.00318	Ele_10_11_4	0.079802	VdW_10_3_3	-0.03248
VdW_14_8_6	0.06827	VdW_15_10_10	-0.01052	VdW_4_11_8	-0.05057	VdW_12_5_8	-0.04597	VdW_6_8_2	-0.02215
VdW_12_5_	0.025903	VdW_15_11_	0.007213	VdW_6_5_7	-0.02833	VdW_8_8_3	-0.03665	Ele_7_11_6	0.141463

9		3							
VdW_10_5_9	0.124453	VdW_5_12_8	-0.0532	VdW_14_6_3	0.03808	VdW_6_6_7	0.121993	VdW_7_4_9	0.055978
VdW_16_10_3	0.077293	VdW_14_5_9	-0.01439	VdW_13_5_8	0.069762	VdW_10_9_4	-0.05585	VdW_13_7_3	-0.00633
VdW_16_6_3	0.018924	Ele_4_5_2	-0.0343	VdW_5_7_2	-0.00643	VdW_7_3_8	0.048355	VdW_4_8_4	-0.01598
VdW_7_6_8	0.00763	VdW_12_9_9	0.056676	Ele_14_8_7	0.063174	VdW_6_13_6	-0.07895	Ele_10_12_5	0.024482
VdW_4_11_3	0.020847	VdW_11_5_9	0.036538	VdW_11_5_7	-0.00557	VdW_15_9_9	0.009966	VdW_13_6_3	-0.02378
VdW_10_6_6	-0.01311	VdW_12_11_6	0.054557	Ele_9_9_9	-0.00054	VdW_6_6_5	0.076257	Ele_15_6_6	-0.01528
VdW_8_7_4	-0.02968	VdW_14_6_8	-0.00973	Ele_7_8_8	0.005536	VdW_6_10_9	0.015883	Ele_15_6_5	-0.06638
VdW_13_9_4	0.013932	Ele_10_9_8	0.066048	VdW_4_12_6	-0.04392	VdW_15_10_5	0.03947	VdW_4_5_2	0.0064
VdW_10_9_8	-0.07677	VdW_13_10_9	-0.01896	VdW_10_2_8	-0.06227	VdW_6_8_9	-0.01485	VdW_12_14_4	0.00268

VdW_6_12_6	0.044796	VdW_3_13_6	-0.00728	VdW_12_3_6	0.025661	VdW_14_11_9	0.024148	VdW_13_9_2	0.012141
VdW_11_7_10	0.012431	VdW_9_5_7	-0.02833	VdW_15_10_3	0.007166	VdW_2_11_5	-0.00797	Ele_11_10_9	0.001562
VdW_14_6_5	-0.03121	VdW_9_3_9	-0.10129	VdW_9_12_3	0.014752	VdW_15_8_5	-0.01052	Ele_14_8_4	-0.01723
Ele_10_6_6	-0.08079	VdW_7_3_2	-0.00114	VdW_11_11_5	-0.0208	Ele_11_10_5	0.03552	Ele_5_9_7	-0.04348
VdW_9_12_8	-0.02033	VdW_12_11_9	-0.01708	VdW_10_15_3	0.02098	Ele_11_11_5	-0.0002	Ele_11_5_7	0.076419
Ele_14_7_7	-0.04741	VdW_7_8_9	0.085704	VdW_10_11_3	0.042177	VdW_15_8_3	-0.00739	Ele_6_7_6	-0.02594
VdW_13_8_8	0.020145	VdW_5_8_9	-0.04004	Ele_8_5_5	-0.00677	VdW_11_12_4	-0.0164	Ele_9_10_4	-0.08544
VdW_14_5_8	-0.02013	VdW_12_5_5	-0.01347	VdW_14_3_5	-0.00508	Ele_7_7_3	0.070504	Ele_14_7_4	0.074127
VdW_8_2_8	-0.01221	VdW_8_11_5	-0.00978	VdW_10_9_9	-0.08838	VdW_9_4_7	-0.09581	Ele_7_6_3	-0.00112

VdW_16_6_5	0.002957	VdW_9_8_9	0.020925	VdW_5_5_3	-0.06823	Ele_13_6_4	-0.02058	VdW_10_11_4	-0.02327
VdW_6_4_8	-0.02259	VdW_11_11_6	-0.09669	VdW_15_7_9	0.027974	Ele_6_4_2	0.048962	VdW_2_7_6	-0.00334
VdW_12_11_2	0.021601	VdW_8_6_4	0.020366	VdW_12_4_4	-0.04203	VdW_10_5_8	0.012572	VdW_7_5_9	-0.02593
VdW_14_11_3	0.013253	VdW_14_6_7	-0.0125	VdW_9_14_6	-0.00316	VdW_5_9_4	-0.04356	VdW_13_13_6	-0.02473
Ele_6_8_7	0.049656	VdW_11_5_6	0.021752	Ele_13_10_7	-0.03644	VdW_6_6_4	-0.05309	Ele_10_8_9	-0.04586
VdW_10_5_7	-0.00773	Ele_6_9_7	0.089309	Ele_6_9_8	-0.01086	Ele_14_5_6	-0.10626	VdW_9_4_9	0.026017
VdW_15_6_2	-0.02601	VdW_15_7_5	0.049821	VdW_18_7_9	-0.04496	VdW_4_7_9	0.00158	Ele_7_8_2	-0.01991
VdW_9_10_1	-0.05508	VdW_8_4_9	-0.03121	Ele_7_7_8	-0.02957	VdW_12_12_3	0.005334	VdW_15_9_5	0.005068
VdW_13_7_4	-0.02469	VdW_8_11_8	0.019842	VdW_10_11_10	0.037475	VdW_10_4_2	-0.06626	Ele_14_10_6	0.021585

VdW_7_10_4	-0.06986	VdW_8_10_9	0.001088	VdW_2_10_4	0.004738	VdW_7_6_2	0.025392	VdW_6_5_6	0.091778
VdW_8_13_4	-0.00397	VdW_11_2_8	0.024532	VdW_14_9_2	0.033147	VdW_10_4_5	0.04206	Ele_6_8_6	-0.01436
VdW_14_12_8	0.042893	VdW_4_8_5	0.016556	Ele_9_12_4	0.032774	VdW_2_12_8	-0.01612	VdW_10_11_8	0.006872
VdW_14_8_8	0.053025	VdW_12_2_6	0.028345	Ele_6_7_8	0.020976	VdW_14_7_10	0.036983	VdW_9_4_3	0.005868
VdW_12_10_4	-0.06996	VdW_7_6_4	-0.02899	Ele_11_9_8	0.00492	VdW_5_6_7	-0.02305	Ele_13_10_4	0.087866
VdW_11_10_5	-0.00731	VdW_3_7_8	0.015067	Ele_6_7_7	-0.0098	Ele_7_9_8	-0.01388	Ele_5_5_5	0.010148
VdW_7_5_4	-0.07226	VdW_11_6_5	0.040172	VdW_6_7_7	0.108085	VdW_8_13_5	0.03023	Ele_5_7_5	-0.02681
VdW_10_8_3	-0.05024	VdW_6_6_8	0.003477	VdW_6_7_4	0.008239	Ele_12_5_6	0.034197	VdW_10_8_2	-0.01024
VdW_10_7_9	0.099814	VdW_17_11_6	-0.0211	VdW_14_8_4	-0.00114	VdW_6_10_3	0.040079	VdW_15_6_7	-0.01701

Ele_10_10_6	-0.0695	VdW_11_6_9	-0.00885	VdW_15_7_1	-0.00256	Ele_9_5_7	0.023652	VdW_13_7_10	-0.00519
VdW_6_3_4	-0.02976	VdW_16_6_6	0.019747	VdW_8_6_8	-0.08609	Ele_6_10_6	0.057891	Ele_10_9_9	-0.0231
VdW_10_3_5	0.036318	VdW_10_8_4	-0.003	VdW_7_5_5	0.020279	VdW_11_2_6	0.003696	VdW_13_5_9	-0.01991
VdW_6_8_7	0.045938	VdW_11_12_8	0.033126	VdW_6_4_3	-0.04199	VdW_14_13_6	0.024286	Ele_7_11_7	-0.02193
VdW_8_9_9	-0.01589	VdW_8_5_2	-0.02357	VdW_15_9_3	-0.015	VdW_9_4_5	-0.04176	Ele_7_5_4	0.070542
VdW_10_10_5	0.025587	VdW_9_12_2	-0.0395	VdW_6_6_2	0.026233	VdW_4_6_3	-0.02488	VdW_10_14_8	-0.02982
VdW_11_5_3	0.07327	Ele_8_10_8	-0.01702	VdW_10_6_4	-0.01395	Ele_11_11_7	0.039468	VdW_14_10_4	-0.01321
VdW_13_5_4	0.031058	VdW_9_6_9	0.036898	VdW_5_11_8	0.038707	VdW_10_3_9	-0.02935	VdW_8_7_10	-0.0055
VdW_6_5_3	0.029793	VdW_5_7_8	0.032917	VdW_13_11_2	-0.00573	VdW_10_10_4	-0.07344	VdW_16_4_6	0.034245
Ele_11_6_8	0.01713	VdW_17_9_5	0.006561	VdW_13_8_3	0.031645	VdW_5_7_3	-0.01698	VdW_12_2_5	-0.04449

VdW_14_5_2	-0.01462	VdW_13_6_4	-0.05097	VdW_14_6_10	-0.00897	VdW_11_7_3	0.055894	VdW_9_6_8	-0.04636
VdW_11_11_1	-0.00862	VdW_8_3_4	0.032129	VdW_6_5_4	0.009654	Ele_14_9_7	0.02172	Ele_8_5_4	0.037808
VdW_14_9_9	0.061212	VdW_13_12_6	0.013043	VdW_15_11_8	0.082427	VdW_3_9_8	0.046042	VdW_5_4_8	0.000448
Ele_10_6_7	0.065557	VdW_14_10_8	-0.0619	VdW_8_6_9	0.044025	VdW_14_11_5	-0.05308	VdW_16_7_3	-0.01797
VdW_14_7_4	-0.06116	VdW_4_6_8	-0.01304	VdW_10_5_3	0.005374	Ele_13_6_5	-0.03311	VdW_5_6_6	-0.01302
VdW_8_10_4	-0.06068	VdW_8_5_7	-0.00761	VdW_11_5_8	-0.0427	VdW_15_12_5	-0.00511	VdW_15_4_8	0.041746
Ele_11_6_6	0.10216	VdW_7_5_2	0.04487	VdW_6_6_6	0.064113	VdW_17_6_7	-0.01071	VdW_11_2_5	-0.04012
VdW_6_11_4	0.018043	VdW_13_10_4	0.050683	VdW_9_5_9	0.030469	Ele_13_10_5	0.042438	VdW_16_6_9	-0.02386
VdW_14_8_5	0.023467	VdW_14_6_4	0.008254	VdW_19_7_6	-0.03451	Ele_5_8_5	-0.03561	VdW_13_12_9	-0.04901

VdW_11_6_4	0.000644	Ele_9_6_8	-0.02136	VdW_13_4_3	-0.03419	VdW_10_6_8	-0.03929	VdW_5_9_9	-0.01005
VdW_13_11_8	0.000244	VdW_14_10_3	-0.04918	VdW_8_5_5	-0.02891	VdW_5_4_4	-0.00647	VdW_8_4_4	-0.05669
VdW_16_7_2	0.022453	VdW_7_4_6	0.019145	VdW_6_3_7	-0.03904	VdW_4_9_2	0.029196	VdW_10_6_	0.024279
VdW_7_5_8	-0.01435	VdW_4_11_4	0.046972	VdW_11_8_2	0.018899	VdW_4_10_8	0.028801	VdW_9_10_8	-0.00784
VdW_11_8_9	0.001015	VdW_13_11_3	-0.01342	VdW_6_12_5	0.015439	VdW_10_12_1	0.030477	VdW_6_12_3	-0.05737
VdW_6_5_2	-0.03513	VdW_15_4_6	-0.00396	VdW_12_13_4	-0.00962	VdW_13_11_5	0.037858	VdW_16_7_4	-0.00685
VdW_9_10_4	0.030595	VdW_14_7_7	0.049233	VdW_8_12_3	-0.00793	VdW_4_5_4	-0.054	VdW_10_12_2	-0.01907
VdW_14_3_8	-0.0225	VdW_6_9_6	-0.07876	VdW_13_8_9	0.031795	VdW_16_5_5	-0.04759		

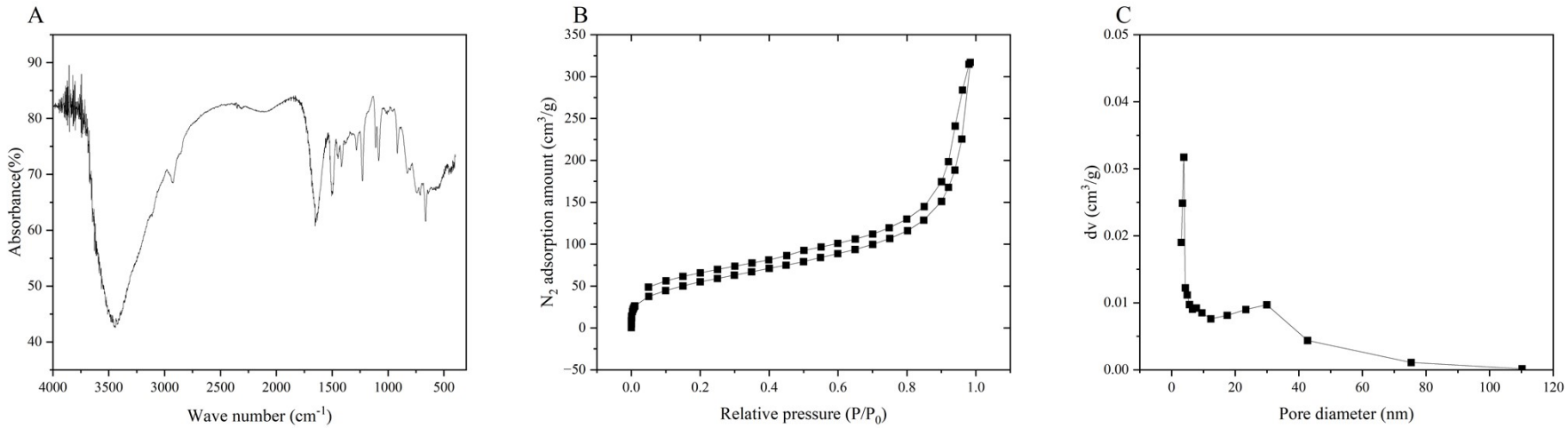

Figure S1 Fourier Transform Infrared (A), N_2 adsorption-desorption isotherms (B) and pore size distribution curves (C) of synthesized solid phase microextraction coatings.

Note: Data were adapted from "Lei, S.; Liang, G.; Ding, M.; Sun, D.; Huang, Z.; Xie, M.-Y., A hydrophilic solid phase microextraction fiber for in vivo monitoring neonicotinoid insecticides in bean sprouts. *Microchemical Journal* **2025,** *215*."

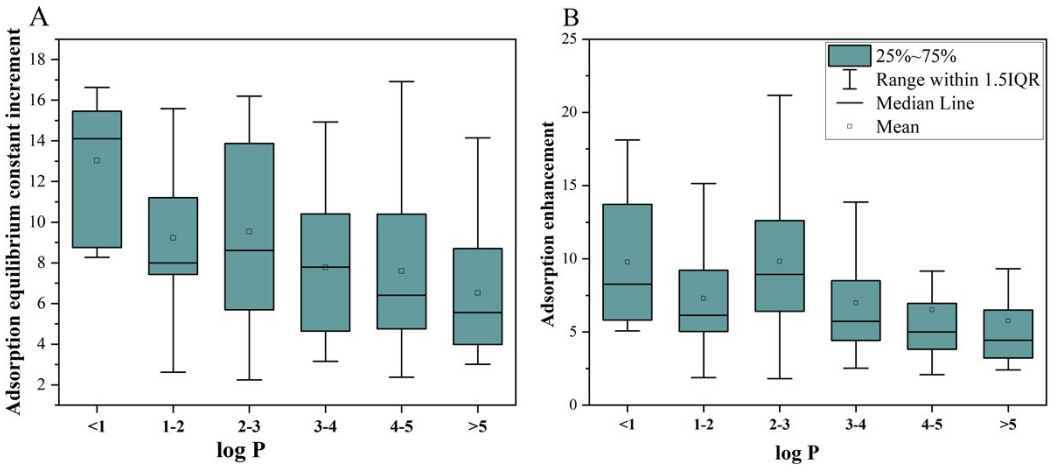

Figure S2. Increases in adsorption equilibrium constants of pesticides with varied hydrophobicity upon acetonitrile addition. Absolute increase (A), relative increase factor (B)

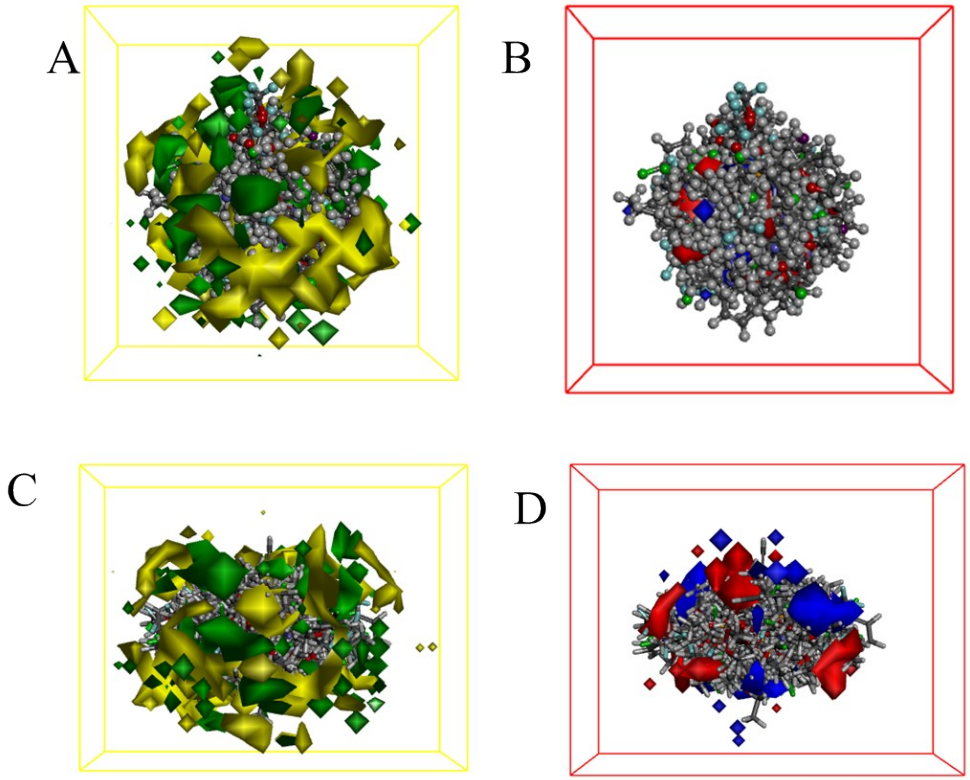

Figure S3. Three-dimensional grid representation of the pesticide model. Van der Waals fields (A, C) and electrostatic fields (B, D) correspond to pure water (A, B) and 1 μg/mL acetonitrile aqueous solution (C, D), respectively.