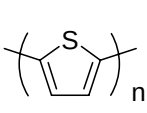
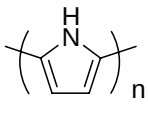
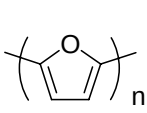
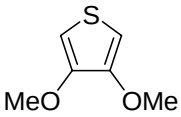
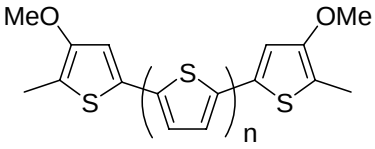
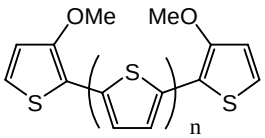
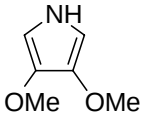
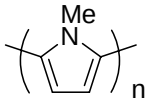
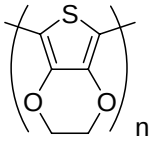
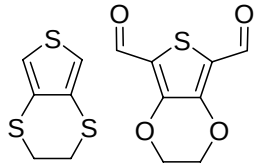
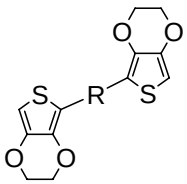
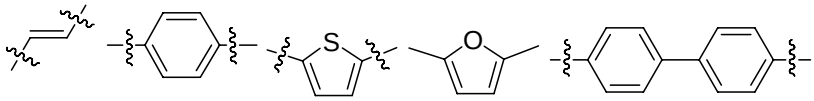
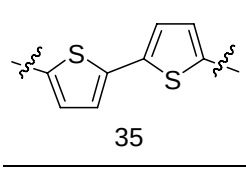
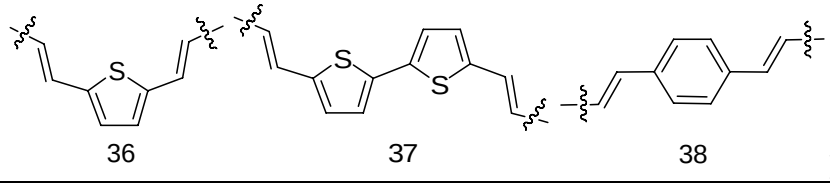
Supplementary Material (ESI) for *PCCP*

Supplementary Information

Improving the accuracy of low level quantum chemical calculation for absorption energies: the neural network and genetic algorithm approach

Ting Gao, Li-Li Shi, Hai-Bin Li, Shan-Shan Zhao, Hui Li, Shi-Ling Sun, Zhong-Min Su* and Ying-Hua Lu*

Table S1 The structure of the 160 organic molecules.

				
1-4 (n=2,4-6)	5-8 (n=2-3, 5, 7)	9-11 (n=2-4)	12	13-15(n=0-2)
				
16-19 (n=0-3)	20	21-25 (n=2-4,6,8)	26-27 (n=2-3)	28	29
					
30-38 R=(	30	31	32	33	34
					
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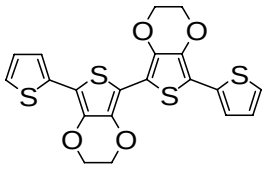

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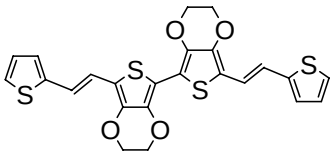

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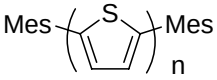
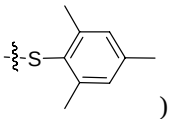
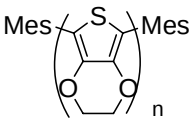


41-44(n=1-4)

(Mes= )



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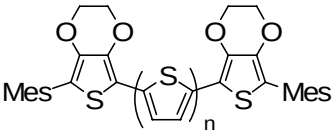
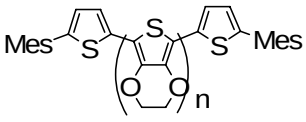


48-49 (n=1-2)



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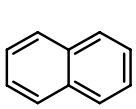

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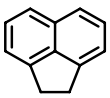

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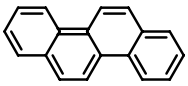

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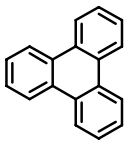

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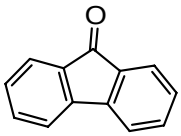

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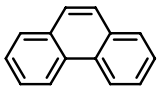

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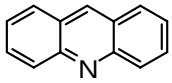

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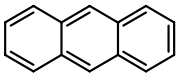

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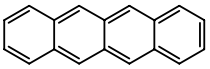

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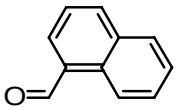

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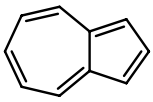

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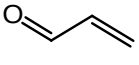

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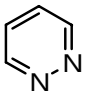

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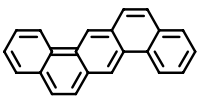

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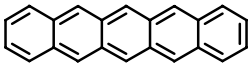

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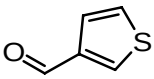

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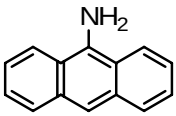

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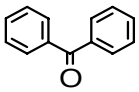

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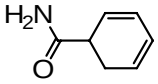

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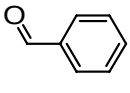

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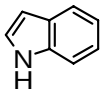

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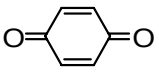

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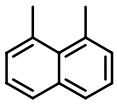

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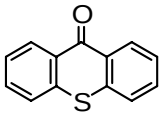

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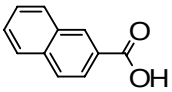

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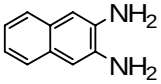

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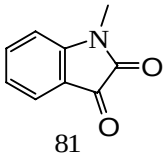

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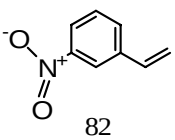

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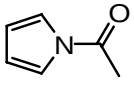

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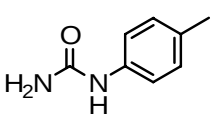

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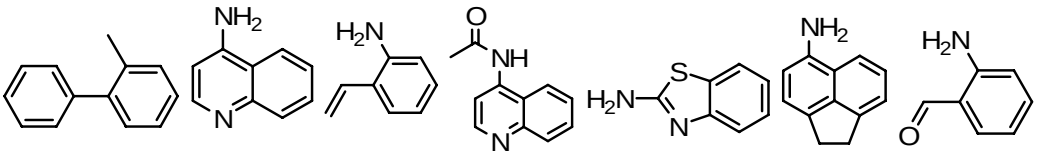

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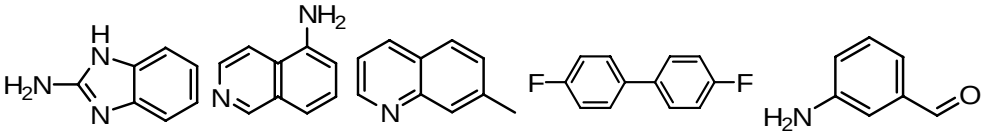

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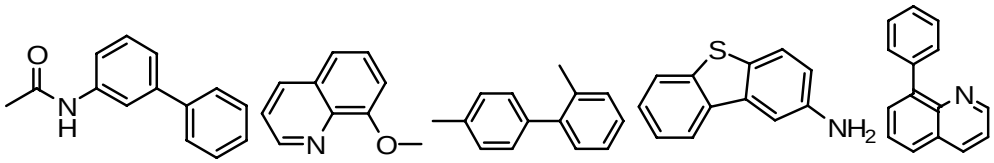

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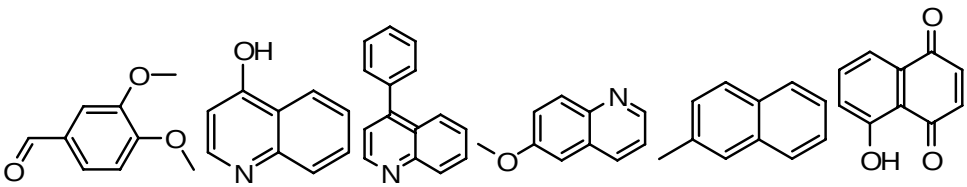

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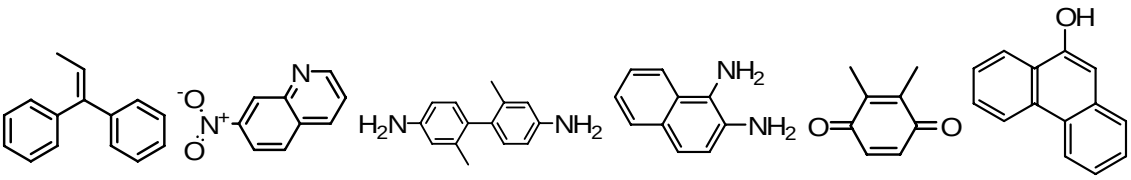

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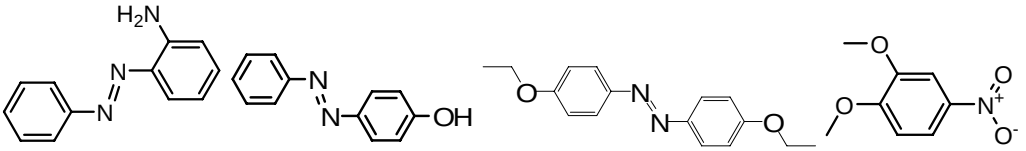

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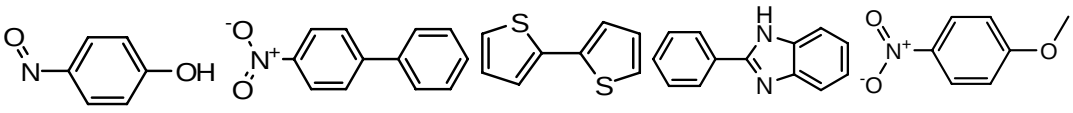

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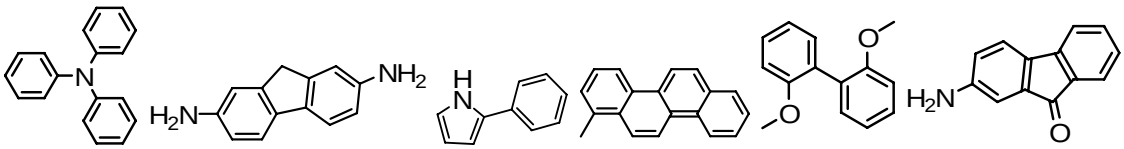

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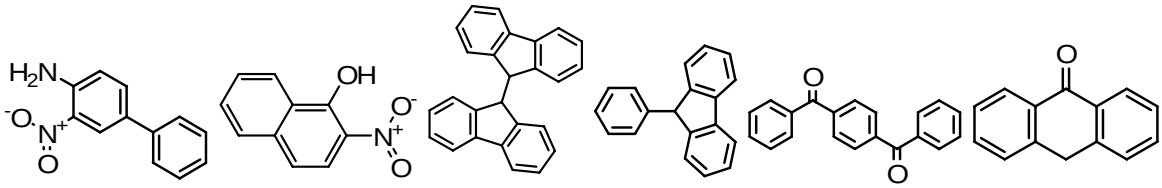
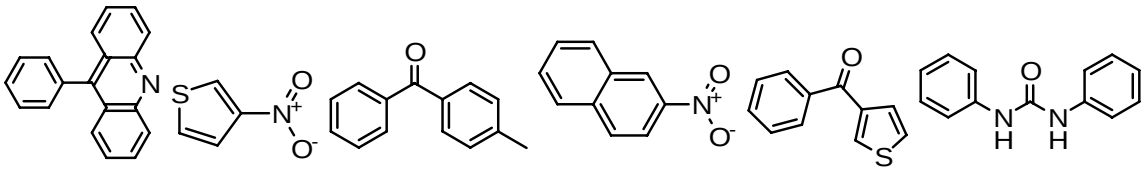
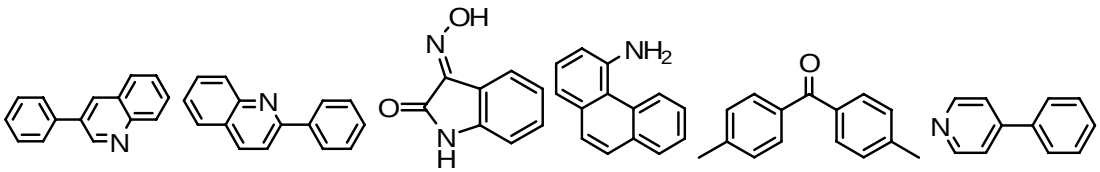


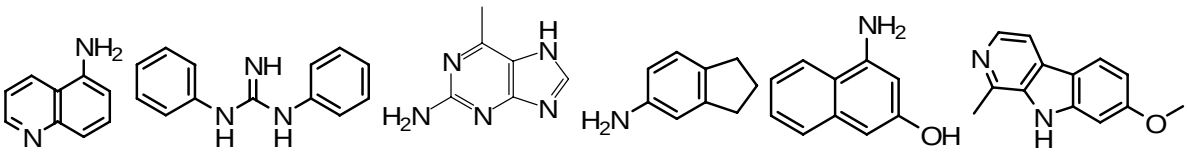
131 132 133 134 135 136



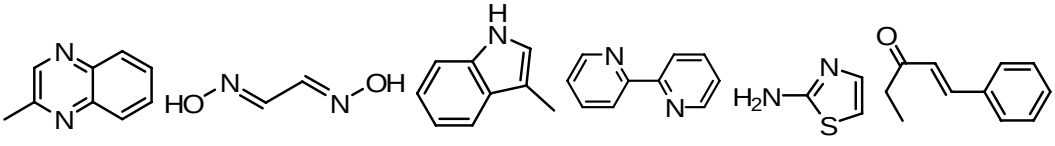
137 138 139 140 141 142



143 144 145 146 147 148



149 150 151 152 153 154



155 156 157 158 159 160

Table S2 The experimental absorption energies and the calculated values of 160 molecules. All data are in units of eV.

		B3LYP/6-31G(d)		B3LYP/STO-3G			ZINDO		
No.	Expt.[a]	Raw[b]	GABP1[c]	Raw[b]	GABP1[c]	GABP2[d]	Raw[b]	GABP1[c]	GABP2[d]
1[f]	4.11	4.03	4.09	4.95	4.21	4.11	3.37	4.10	4.14
2	3.18	2.84	3.10	3.51	3.15	3.12	2.5	3.17	3.17
3	2.98	2.57	2.90	3.18	2.93	2.98	2.31	3.01	2.89
4	2.87	2.38	2.91	2.96	2.84	2.89	2.19	2.93	2.82
5	4.49	4.74	4.53	5.70	4.55	4.58	3.64	4.50	4.43
6[e]	3.91	3.93	3.96	4.70	4.02	3.87	3.1	3.68	3.83
7	3.38	3.21	3.37	3.83	3.34	3.39	2.66	3.33	3.34
8[e]	3.25	2.90	3.40	3.46	3.09	3.39	2.48	3.22	3.37
9	4.40	4.57	4.43	5.58	4.49	4.51	3.52	4.41	4.32
10[e]	3.78	3.71	3.79	4.56	3.94	3.71	2.95	3.59	3.88
11	3.43	3.23	3.35	4.01	3.55	3.32	2.66	3.37	3.35
12[f]	4.90	5.37	4.89	5.74	4.80	4.91	4.46	4.56	4.51
13[e]	3.76	3.56	3.48	4.16	3.63	3.43	3.07	3.95	3.66
14[e]	3.19	3.01	3.12	3.61	3.15	3.15	2.65	3.20	3.21
15[f]	2.96	2.63	2.94	3.13	2.93	3.08	2.41	2.99	2.85
16[f]	3.81	3.78	3.80	4.25	3.76	3.72	3.09	4.00	3.76
17	3.23	3.12	3.22	3.63	3.18	3.23	2.64	3.25	3.26
18	2.99	2.75	3.11	3.25	2.99	3.09	2.4	3.04	2.92
19	2.83	2.51	2.80	2.99	2.83	2.80	2.24	2.89	2.75
20	5.58	6.04	5.87	8.27	5.62	6.05	5.9	5.61	5.89
21[f]	4.96	4.97	4.68	5.89	4.87	4.91	3.89	4.69	4.25
22	4.58	4.66	4.56	5.49	4.64	4.60	3.71	4.55	4.56
23[e]	4.44	4.21	4.37	4.94	4.34	4.20	3.49	4.38	4.26
24[f]	4.34	3.92	4.29	4.66	4.22	3.94	3.34	4.29	4.06
25	4.32	3.82	4.39	4.52	4.32	4.39	3.26	4.26	4.33
26	3.87	3.90	3.83	4.42	3.95	3.89	3.18	3.90	3.79
27	3.10	3.15	3.14	3.54	3.20	3.03	2.63	3.15	3.14
28	4.38	4.69	4.46	5.21	4.52	4.57	4.42	4.53	4.51
29[e,f]	3.83	4.11	3.84	4.69	3.96	4.01	3.54	4.08	3.82
30	3.45	3.44	3.54	3.91	3.43	3.49	2.97	3.42	3.45
31[f]	3.60	3.55	3.65	4.03	3.51	3.25	3.25	3.62	3.83
32[e]	3.32	3.18	3.25	3.69	3.24	3.22	2.69	3.24	3.23
33	3.43	3.29	3.41	3.87	3.40	3.24	2.76	3.33	3.37
34	3.63	3.45	3.59	3.88	3.45	3.44	3.33	3.58	3.53
35	3.01	2.80	3.04	3.30	3.03	3.14	2.44	3.02	3.04
36	2.89	2.68	2.81	3.12	2.88	2.68	2.48	2.92	2.88
37[f]	2.73	2.45	2.71	2.89	2.80	2.93	2.29	2.69	2.76
38	3.15	2.90	3.15	3.34	2.98	3.12	2.9	3.15	3.25
39[e]	2.98	2.78	3.00	3.22	2.99	3.13	2.41	3.01	2.86
40	2.69	2.45	2.72	2.81	2.78	2.71	2.24	2.68	2.76

		B3LYP/6-31G(d)		B3LYP/STO-3G			ZINDO		
No.	Expt.[a]	Raw[b]	GABP1[c]	Raw[b]	GABP1[c]	GABP2[d]	Raw[b]	GABP1[c]	GABP2[d]
41[e,f]	4.11	4.13	4.13	4.51	4.11	4.32	4.05	4.35	4.36
42	3.46	3.34	3.63	3.95	3.56	3.68	3.15	3.58	3.57
43	3.21	2.88	3.21	3.47	3.17	3.32	2.69	3.21	3.33
44	2.95	2.62	2.97	3.17	3.01	3.11	2.45	3.07	3.13
45	4.07	4.12	4.09	4.49	4.11	4.10	3.93	4.21	4.20
46	3.43	3.34	3.34	3.84	3.50	3.46	2.97	3.39	3.28
47	3.09	2.85	3.05	3.25	3.06	3.06	2.51	2.95	3.05
48	3.09	2.88	3.17	3.36	3.03	3.13	2.57	3.03	3.15
49[e,f]	2.71	2.60	2.80	3.09	3.04	2.87	2.37	2.86	2.58
50[e]	3.05	2.84	3.07	3.36	3.13	2.97	2.6	3.11	3.05
51	2.88	2.54	2.85	2.97	2.98	2.85	2.32	2.89	2.86
52	5.63	6.27	5.86	7.18	5.48	5.86	5.27	5.67	5.41
53	5.47	6.06	5.59	7.16	5.67	5.52	5.3	5.44	5.53
54	4.66	4.71	4.49	5.54	4.48	4.43	4.48	4.53	4.59
55	4.83	4.81	4.78	5.65	4.57	4.63	4.58	4.84	4.83
56	5.91	6.04	5.63	7.38	5.83	5.67	5.37	5.78	5.46
57	4.85	4.54	4.73	5.31	4.65	4.73	4.9	5.01	4.69
58[e]	4.96	5.11	4.79	5.78	4.69	4.84	4.73	5.19	4.84
59[e]	4.96	5.37	4.64	6.20	4.88	4.76	4.73	4.77	4.75
60	4.96	5.31	4.64	6.19	4.67	4.65	4.68	5.01	4.60
61	4.54	4.75	4.38	5.52	4.29	4.38	4.28	4.30	4.38
62	5.88	6.15	5.83	7.08	5.78	5.66	5.5	5.53	5.76
63	4.53	5.17	4.75	6.05	4.99	4.87	4.48	4.54	4.74
64	5.99	6.43	5.85	7.67	5.87	5.87	5.89	6.14	5.81
65	4.75	5.52	5.17	6.52	5.17	5.35	4.38	4.74	5.01
66[f]	5.02	5.75	5.32	6.18	5.16	5.29	4.91	5.10	5.03
67	4.13	4.40	4.17	5.28	4.33	4.15	4.15	4.28	4.50
68	4.00	4.34	4.24	5.03	4.06	4.24	3.98	3.94	4.22
69	4.94	5.41	4.98	6.31	5.23	5.31	5.47	5.33	5.31
70	4.28	5.29	4.57	6.19	4.77	4.60	4.66	4.73	4.70
71	4.92	4.75	4.85	5.74	4.95	4.98	4.77	4.96	4.81
72[f]	4.96	5.36	5.05	6.52	4.97	5.52	4.96	4.83	5.14
73[f]	5.15	5.31	5.09	6.49	5.34	5.38	4.88	5.12	5.14
74	5.79	5.93	5.54	7.09	5.70	5.65	5.61	6.01	5.90
75[f]	5.10	4.98	5.06	5.73	4.87	4.91	4.92	5.06	5.10
76	5.44	5.88	5.45	6.98	5.50	5.40	5.18	5.57	5.46
77[e,f]	4.86	5.01	4.91	5.88	4.95	5.01	5.26	5.64	5.23
78	5.39	5.44	5.17	6.47	5.28	5.25	4.92	5.24	5.23
79	5.08	5.45	5.33	6.41	5.27	5.31	4.93	5.10	5.20
80	5.10	5.53	5.13	6.11	5.06	5.05	4.91	5.11	5.17
81	5.12	5.54	5.30	6.40	5.11	5.46	5.89	5.29	5.52
82[e]	5.17	5.29	5.15	5.30	4.63	4.81	4.72	5.18	4.99
83	5.19	5.49	5.04	6.28	5.17	5.25	5.1	5.05	5.12
84[f]	5.17	5.34	4.99	6.07	5.08	5.19	4.62	4.95	4.98
85[e]	5.28	5.90	5.47	5.96	4.92	5.29	4.97	5.24	5.25

		B3LYP/6-31G(d)		B3LYP/STO-3G			ZINDO		
No.	Expt.[a]	Raw[b]	GABP1[c]	Raw[b]	GABP1[c]	GABP2[d]	Raw[b]	GABP1[c]	GABP2[d]
86[e]	5.25	5.35	5.06	6.16	5.12	5.12	4.76	5.35	5.00
87	5.23	5.18	5.12	6.20	5.09	5.15	4.72	5.32	5.23
88	5.32	5.66	5.31	6.32	5.29	5.34	5.14	5.59	5.51
89	5.39	6.10	5.70	7.06	5.69	5.67	5.33	5.21	5.53
90[e]	5.46	5.64	5.43	6.03	5.08	5.15	5.46	5.47	5.67
91	5.69	6.05	5.58	6.80	5.52	5.53	5.84	5.82	5.64
92[f]	5.74	6.12	5.65	7.17	5.79	5.64	5.43	5.88	5.79
93[e]	5.99	6.61	6.06	6.75	5.44	5.58	6.13	5.77	6.06
94[f]	5.99	6.60	6.19	7.38	5.99	5.98	5.52	5.93	5.80
95[e]	6.05	6.30	5.84	7.33	5.86	5.76	5.41	5.88	5.78
96	6.05	5.89	5.49	6.98	5.58	5.45	5.12	5.58	5.52
97	5.06	5.01	4.93	5.61	4.68	4.65	4.48	5.08	5.01
98[e]	5.06	5.75	5.37	6.70	5.38	5.53	5.39	5.05	5.36
99	5.12	5.28	5.17	6.10	5.15	5.03	4.9	5.01	4.93
100	5.17	5.58	5.22	6.24	5.15	5.21	4.97	5.24	5.22
101	5.19	5.10	5.02	6.10	5.07	5.09	4.64	5.02	5.18
102	5.21	5.21	5.07	5.99	5.04	5.14	5.29	5.25	5.01
103	5.32	5.13	5.17	6.11	5.14	5.18	4.97	5.12	5.01
104[e,f]	5.41	5.79	5.33	6.37	5.09	5.45	5.43	5.28	5.56
105	5.51	5.95	5.51	6.47	5.35	5.37	5.17	5.28	5.52
106[e,f]	5.46	5.58	5.53	6.24	5.28	5.32	5.46	5.53	5.31
107	5.56	6.00	5.55	6.37	5.22	5.18	5	5.46	5.41
108	5.56	6.11	5.52	7.06	5.46	5.51	5.19	5.54	5.39
109	5.00	4.84	5.02	5.49	4.78	4.84	4.74	4.89	4.92
110	5.00	4.77	4.92	5.78	4.94	4.99	4.57	4.78	4.83
111	5.00	4.98	4.86	5.04	5.00	4.61	4.55	4.85	4.75
112[f]	5.00	5.53	5.26	6.49	5.37	5.29	5.65	5.31	5.42
113	5.00	5.30	5.00	5.87	4.87	4.88	4.93	5.10	5.05
114	5.00	4.85	4.95	5.64	4.86	4.94	4.8	5.01	4.95
115[e]	5.00	5.01	4.91	6.14	5.03	5.11	4.69	4.80	4.91
116	3.96	3.80	3.89	4.79	4.16	4.19	3.14	3.59	3.85
117[e,f]	3.57	3.59	3.64	4.27	3.62	3.71	3.32	3.76	3.86
118[f]	3.43	3.41	3.48	4.00	3.44	3.46	3.18	3.51	3.68
119	3.84	4.01	3.78	4.66	3.94	4.05	3.6	4.11	3.92
120	4.16	4.21	4.22	4.99	4.31	4.25	3.76	4.20	4.26
121	4.07	3.91	4.09	4.69	4.10	4.08	3.63	4.13	4.08
122	4.12	4.12	4.14	5.03	4.27	4.18	3.44	3.95	4.18
123	4.11	4.24	4.20	5.09	4.39	4.36	3.77	4.25	4.32
124[e]	4.07	4.30	4.18	5.25	4.52	4.38	3.74	4.24	4.10
125	4.18	4.12	4.26	4.79	4.21	4.19	4.13	4.53	4.47
126	4.22	4.30	4.31	4.92	4.29	4.31	3.89	4.20	4.46
127[e]	4.28	4.52	4.48	5.38	4.53	4.53	3.94	4.33	4.49
128	4.43	4.85	4.63	5.81	4.70	4.71	4.48	4.54	4.58
129	4.46	4.60	4.58	4.97	4.39	4.43	4.3	4.69	4.66
130	4.63	4.75	4.63	5.52	4.78	4.75	4.72	4.85	4.69

		B3LYP/6-31G(d)		B3LYP/STO-3G			ZINDO		
No.	Expt.[a]	Raw[b]	GABP1[c]	Raw[b]	GABP1[c]	GABP2[d]	Raw[b]	GABP1[c]	GABP2[d]
131	4.66	4.84	4.87	5.27	4.62	4.66	4.27	4.62	4.71
132	4.66	4.68	4.63	5.41	4.71	4.78	4.31	4.66	4.84
133	4.66	4.53	4.65	5.47	4.82	4.78	4.14	4.49	4.61
134	4.68	4.58	4.76	5.50	4.75	4.78	4.14	4.53	4.47
135[f]	4.71	4.35	4.60	5.34	4.77	4.80	4.56	4.76	4.80
136[f]	4.71	4.66	4.78	5.26	4.64	4.74	4.62	4.85	4.78
137	4.77	5.25	4.89	5.44	4.77	4.81	4.66	4.65	4.69
138	4.77	4.91	4.59	5.11	4.45	4.55	4.76	4.78	4.86
139[e]	4.77	4.61	4.73	5.57	4.86	4.93	4.64	4.84	4.79
140	4.81	4.89	4.80	5.20	4.56	4.69	4.41	4.76	4.86
141[f]	4.82	4.78	4.74	5.45	4.75	4.82	4.83	5.07	4.98
142	4.84	4.91	4.78	5.62	4.86	4.81	4.72	4.84	4.80
143[f]	4.90	4.93	4.86	5.79	4.90	4.90	4.66	4.81	4.78
144	4.92	4.88	4.67	5.74	4.81	4.80	4.57	4.76	4.72
145	4.92	5.26	4.99	5.75	4.84	4.90	4.93	5.11	4.99
146	4.96	5.24	5.12	6.10	5.05	5.11	4.68	4.94	5.12
147[f]	4.70	4.56	4.66	5.53	4.83	4.86	4.59	4.77	4.72
148	4.84	5.03	4.96	6.01	5.05	5.06	4.67	4.90	4.93
149[e]	4.92	5.39	5.09	6.16	5.17	5.22	4.93	5.42	5.39
150	5.12	4.82	4.89	5.40	4.75	4.83	4.72	5.14	4.81
151	6.66	6.39	6.46	6.82	6.66	6.45	5.55	5.96	5.85
152	6.08	6.74	5.98	8.06	6.01	5.99	5.83	5.62	5.82
153	5.12	5.52	5.17	5.90	5.01	5.06	5.05	5.18	5.01
154	5.17	5.25	5.19	5.90	5.17	5.23	4.86	5.34	5.36
155	5.30	5.80	5.44	6.85	5.38	5.38	4.95	5.51	5.50
156	5.32	5.42	5.08	5.83	4.80	4.82	5.13	5.45	5.27
157	5.56	6.13	5.65	7.20	5.77	5.66	5.35	5.82	5.76
158	4.40	4.68	4.61	5.69	4.69	4.74	4.11	4.44	4.48
159[f]	4.84	5.37	4.90	6.32	5.18	5.29	4.36	4.79	4.88
160	4.30	4.42	4.42	5.40	4.66	4.63	4.21	4.33	4.58

[a] Experimental data.

[b] Raw calculated values.

[c] Corrected calculated values after GABP1correction.

[d] Corrected calculated values after GABP2 correction.

[e] Molecules belong to the testing set in GABP1 correction.

[f] Molecules belong to the testing set in GABP2 correction.

Table S3 Synaptic weights Wx_{ij} and Wy_j, biases By_j and Bz for B3LYP/6-31G(d)-GABP1 method.

Weights and biases	y_1	y_2	y_3	y_4
Wx_{1j}	-1.0886	-0.73381	1.9044	1.3932
Wx_{2j}	0.6826	-2.4694	6.8653	-1.3227
Wx_{3j}	-0.06601	1.3449	-3.9795	0.67966
Wx_{4j}	0.066904	-0.44596	0.55725	-0.18936
Wx_{5j}	-1.2813	4.1712	-7.0996	1.3305
Wx_{6j}	0.79617	-3.8915	2.7795	-0.31063
By_j	0.83416	4.0869	1.0647	1.8916

	Z
Wy_1	-0.72976
Wy_2	-99.043
Wy_3	0.16884
Wy_4	1.0141
Bz	98.259

Table S4 Synaptic weights Wx_{ij} and Wy_j, biases By_j and Bz for B3LYP/STO-3G-GABP1 method.

Weights and biases	y_1	y_2	y_3	y_4
Wx_{1j}	1.1198	-1.3019	6.1706	2.5362
Wx_{2j}	0.91431	-1.1807	-16.314	-0.29015
Wx_{3j}	-0.20214	0.25006	-10.335	-0.03535
Wx_{4j}	0.22171	-0.28614	17.469	-0.24977
Wx_{5j}	0.27307	-0.3336	2.568	-0.41078
Wx_{6j}	-0.87915	1.133	30.991	0.85667
By_j	-2.3278	2.0905	-16.146	1.2034

	Z
Wy_1	110.39
Wy_2	51.747
Wy_3	2.996
Wy_4	0.37297
Bz	60.885

Table S5 Synaptic weights Wx_{ij} and Wy_j, biases By_j and Bz for ZINDO-GABP1 method.

Weights and biases	y1	y2	y3	y4
Wx_{1j}	24.608	-0.06339	0.34534	27.25
Wx_{2j}	33.697	-0.22305	-0.07797	84.793
Wx_{3j}	-4.6181	-1.2994	-0.14482	19.343
Wx_{4j}	-61.71	-0.4833	-0.01236	-38.349
Wx_{5j}	-62.451	-0.11055	-0.03262	-51.599
Wx_{6j}	36.825	2.297	0.20474	-113.09
By_j	-56.827	2.7869	-0.02731	-75.378

	Z
Wy_1	0.097383
Wy_2	-14.415
Wy_3	2.1235
Wy_4	-0.1585
Bz	14.047

Table S6 Synaptic weights Wx_{ij} and Wy_j, biases By_j and Bz for B3LYP/STO-3G-GABP2 method.

Weights and biases	y_1	y_2	y_3	y_4
Wx_{1j}	-19.713	-1.1286	0.35008	66.366
Wx_{2j}	-15.287	-0.30304	3.0247	-84.483
Wx_{3j}	-9.7705	0.31049	-5.6704	11.984
Wx_{4j}	7.2324	-0.06519	-4.189	-38.561
Wx_{5j}	2.5447	-0.07894	29.334	-2.0401
Wx_{6j}	-2.1598	0.24323	-32.259	103.08
By_j	5.3127	-0.07127	6.7887	47.813

	Z
Wy_1	-0.23817
Wy_2	-0.99353
Wy_3	-15.494
Wy_4	0.10284
Bz	15.542

Table S7 Synaptic weights Wx_{ij} and Wy_j, biases By_j and Bz for ZINDO-GABP2 method.

Weights and biases	y_1	y_2	y_3	y_4
Wx_{1j}	-2.4399	-195.09	-0.52175	-55.071
Wx_{2j}	-0.27083	-216.26	0.093908	-27.23
Wx_{3j}	-0.31447	-20.598	0.12894	43.938
Wx_{4j}	4.0234	221.53	0.092644	26.21
Wx_{5j}	-7.3457	-14.18	-0.0784	25.958
Wx_{6j}	0.99731	-84.207	-0.26724	-111.54
By_j	2.0124	50.072	-0.44013	-9.95

	Z
Wy_1	0.19802
Wy_2	-0.09134
Wy_3	-2.3525
Wy_4	0.10819
Bz	-1.1367