Table S1 The band gap, each site ion and lattice constant of 2D perovskites

No.	Bandgap (eV)	Bandgap ANN(eV)	A -Site	B-Site	X-Site	Lattice constant					
						a	b	c	A	β	γ
1	1.99	2.17	$CH_3(CH_2)_3NH_3^+$	Pb^{2+}	I^-	8.86	8.68	27.57	90	90	90
2	2.04	2.05	$CH_3NHNH_3^+$	Pb^{2+}	I^-	18.47	19.08	12.64	90	90.03	90
3	2.07	2.05	$CH_3NHNH_3^+$	Pb^{2+}	I^-	18.68	19.19	12.76	90	90	90
4	1.97	2.05	$CH_3NHNH_3^+$	Pb^{2+}	I^-	18.73	6.38	6.4	90	90	90
*5	2.12	2.05	$CH_3NHNH_3^+$	Pb^{2+}	I^-	18.83	6.39	6.4	90	90	90
6	2.79	2.79	$ICHC(I)(CH_2)_2NH_3^+$	Pb^{2+}	Br^-	7.98	8.14	17.63	88.43	85.36	89.87
7	2.22	2.22	$IC_6H_5CH_2NH_3^+$	Pb^{2+}	I^-	16.97	8.88	8.68	90	103.36	90
8	2.22	2.21	$I(CH_2)_6NH_3^+$	Pb^{2+}	I^-	9.22	8.85	31.98	90	90	90
9	2.19	2.21	$I(CH_2)_6NH_3^+$	Pb^{2+}	I^-	9.07	8.89	33.62	90	90	90
*10	2.22	2.21	$I(CH_2)_5NH_3^+$	Pb^{2+}	I^-	16.26	8.9	8.63	90	90.07	90
11	2.28	2.28	$I(CH_2)_4NH_3^+$	Pb^{2+}	I^-	15.37	8.24	9.04	90	91.9	90
12	1.65	1.65	$I(CH_2)_3NH_3^+$	Sn^{2+}	I^-	8.95	8.39	15.39	90	92.27	90
13	2.29	2.29	$I(CH_2)_3NH_3^+$	Pb^{2+}	I^-	14.07	9.04	8.47	90	99.25	90
14	2.37	2.37	$I(CH_2)_2NH_3^+$	Pb^{2+}	I^-	12.55	8.76	8.64	90	97.99	90
*15	2.37	2.37	$I(CH_2)_2NH_3^+$	Pb^{2+}	I^-	8.75	8.75	12.72	90	97.63	90
16	1.66	1.66	$HOOC(CH_2)_3NH_3^+$	Sn^{2+}	I^-	8.89	9.22	24.19	90	90	90
17	2.29	2.29	$HOOC(C_8H1_4)NH_3^+$	Pb^{2+}	I^-	15.04	9.24	8.58	90	106.15	90
18	2.14	2.14	$HO(CH_2)_3NH_3^+$	Pb^{2+}	I^-	10.63	9.2	9.21	90	93.06	90
19	2.16	2.12	$HO(CH_2)_2NH_3^+$	Sn^{2+}	I^-	10.2	9.02	8.93	90	100.36	90
*20	2.09	2.12	$HO(CH_2)_2NH_3^+$	Sn^{2+}	I^-	13.01	19.62	6.39	90	90	90
21	2.16	2.16	$HO(CH_2)_2NH_3^+$	Pb^{2+}	I^-	10.17	9.04	8.93	90	100.57	90
22	2.82	2.82	$HO(CH_2)_2NH_3^+$	Pb^{2+}	Br^-	8.33	8.22	27.62	90	90	90
23	2.25	2.25	$FC_6H_4CH_2NH_3^+$	Pb^{2+}	I^-	8.7	9.24	27.53	90	97.6	90
24	2.03	2.05	$FC_6H_4(CH_2)_2NH_3^+$	Sn^{2+}	I^-	35.07	6.12	12.28	90	108.18	90
*25	2.03	2.05	$FC_6H_4(CH_2)_2NH_3^+$	Sn^{2+}	I^-	34.59	6.1	12.25	90	103.92	90
26	2.09	2.05	$FC_6H_4(CH_2)_2NH_3^+$	Sn^{2+}	I^-	16.65	8.61	8.76	90	98.64	90
27	2.15	2.19	$FC_6H_4(CH_2)_2NH_3^+$	Pb^{2+}	I^-	8.74	8.74	16.9	82.22	82.91	89.6
28	2.13	2.19	$FC_6H_4(CH_2)_2NH_3^+$	Pb^{2+}	I^-	34.64	6.12	12.29	90	103.93	90
29	2.34	2.19	$FC_6H_4(CH_2)_2NH_3^+$	Pb^{2+}	I^-	16.72	8.63	8.8	90	98.78	90
*30	2.11	2.19	$FC_6H_4(CH_2)_2NH_3^+$	Pb^{2+}	I^-	8.74	8.74	16.9	82.22	82.91	89.6
31	2.11	2.19	$FC_6H_4(CH_2)_2NH_3^+$	Pb^{2+}	I^-	34.64	12.23	12.29	90	103.93	90

32	2.28	2.19	$FC_6H_4(CH_2)_2NH_3^+$	Pb^{2+}	I^-	16.53	8.56	8.73	90	99.53	90
33	2.88	2.88	$F_3CCH_2NH^+$	Pb^{2+}	Br^-	8.15	24.49	8.15	90	90	90
34	2.79	2.79	$F_2CHCH_2NH_3^+$	Pb^{2+}	Br^-	8.11	7.95	23.7	90	90	90
*35	2.38	2.34	$F_2C_6H_9NH_3^+$	Pb^{2+}	I^-	29.18	9.5	8.42	90	90	90
36	2.29	2.34	$F_2C_6H_9NH_3^+$	Pb^{2+}	I^-	9.54	8.61	28.92	90	90	90
37	3.34	3.34	$F(CH_2)_2NH_3^+$	Pb^{2+}	Cl^-	7.71	18.46	8.75	90	90	90
38	2.65	2.65	$F(CH_2)_2NH_3^+$	Pb^{2+}	Br^-	12.08	19.53	6.03	90	90	90
39	2.84	2.84	$COOH(CH_2)_3NH_3^+$	Pb^{2+}	Br^-	24.77	8.07	56.96	90	97.14	90
*40	1.79	1.79	$ClC_6H_4(CH_2)_2NH_3^+$	Sn^{2+}	I^-	33.78	6.18	6.19	90	90.42	90
41	2.31	2.31	$ClC_6H_4(CH_2)_2NH_3^+$	Pb^{2+}	I^-	33.33	8.65	8.72	90	93	90
42	2.88	2.88	$CHC(CH_2)_2NH_3^+$	Pb^{2+}	Br^-	12.81	7.82	8.39	90	93.5	90
43	2.08	2.08	$CH_3CH_2CH(CH_3)NH_3^+$	Pb^{2+}	I^-	8.94	8.94	24.96	90	90	90
44	2.28	2.28	$CH_3CH(CH_3)CH_2NH_3^+$	Pb^{2+}	I^-	13.8	8.97	8.76	90	108.25	90
*45	2.12	2.10	$CH_3C_6H_4(CH_2)_2NH_3^+$	Pb^{2+}	I^-	6.13	6.11	17.54	81.58	79.94	89.98
46	2.09	2.10	$CH_3C_6H_4(CH_2)_2NH_3^+$	Pb^{2+}	I^-	6.16	6.17	17.73	80.03	82.27	90
47	2.39	2.30	$CH_3(CH_2)_9NH_3^+$	Pb^{2+}	I^-	8.83	8.49	43.95	90	90	90
48	2.39	2.30	$CH_3(CH_2)_9NH_3^+$	Pb^{2+}	I^-	8.83	8.48	43.97	90	90	90
49	2.28	2.30	$CH_3(CH_2)_9NH_3^+$	Pb^{2+}	I^-	8.97	8.67	42.57	90	90	90
*50	2.28	2.30	$CH_3(CH_2)_9NH_3^+$	Pb^{2+}	I^-	8.98	8.67	42.53	90	90	90
51	2.16	2.30	$CH_3(CH_2)_9NH_3^+$	Pb^{2+}	I^-	8.72	8.71	47.48	90	90	90
52	2.12	2.28	$CH_3(CH_2)_8NH_3^+$	Pb^{2+}	I^-	8.74	8.74	40.03	90	90	90
53	2.35	2.28	$CH_3(CH_2)_8NH_3^+$	Pb^{2+}	I^-	8.71	8.84	19.79	90	96.38	90
54	2.27	2.28	$CH_3(CH_2)_8NH_3^+$	Pb^{2+}	I^-	9.02	8.71	39.76	90	90	90
*55	2.39	2.28	$CH_3(CH_2)_8NH_3^+$	Pb^{2+}	I^-	8.43	8.95	21.33	90	96.11	90
56	2.38	2.32	$CH_3(CH_2)_7NH_3^+$	Pb^{2+}	I^-	8.45	8.99	18.74	90	96.3	90
57	2.28	2.32	$CH_3(CH_2)_7NH_3^+$	Pb^{2+}	I^-	8.98	8.69	37.48	90	90	90
58	2.31	2.30	$CH_3(CH_2)_6NH_3^+$	Pb^{2+}	I^-	8.59	8.94	17.24	90	96.9	90
59	2.26	2.30	$CH_3(CH_2)_6NH_3^+$	Pb^{2+}	I^-	9.01	8.71	34.56	90	90	90
*60	2.29	2.30	$CH_3(CH_2)_6NH_3^+$	Pb^{2+}	I^-	8.86	8.68	36.61	90	90	90

61	2.28	2.28	$CH_3(CH_2)_5NH_3^+$	Pb^{2+}	I^-	8.64	8.85	16.05	90	91.99	90
62	2.29	2.28	$CH_3(CH_2)_5NH_3^+$	Pb^{2+}	I^-	8.94	8.69	32.7	90	90	90
63	2.37	2.33	$CH_3(CH_2)_4NH_3^+$	Pb^{2+}	I^-	8.47	9.01	14.78	90	100.88	90
64	2.32	2.33	$CH_3(CH_2)_4NH_3^+$	Pb^{2+}	I^-	8.67	8.93	14.88	90	100.21	90
*65	2.29	2.33	$CH_3(CH_2)_4NH_3^+$	Pb^{2+}	I^-	9.01	8.73	29.96	90	90	90
66	2.28	2.28	$CH_3(CH_2)_4CH(CH_3)NH_3^+$	Pb^{2+}	I^-	17.46	9.25	8.59	90	103.22	90
67	1.8	1.85	$CH_3(CH_2)_3NH_3^+$	Sn^{2+}	I^-	8.84	8.62	27.56	90	90	90
68	1.77	1.85	$CH_3(CH_2)_3NH_3^+$	Sn^{2+}	I^-	8.81	8.59	27.64	90	90	90
69	2.04	1.85	$CH_3(CH_2)_3NH_3^+$	Sn^{2+}	I^-	8.42	8.93	26.11	90	90	90
*70	1.78	1.85	$CH_3(CH_2)_3NH_3^+$	Sn^{2+}	I^-	8.93	26.02	8.41	90	90	90
71	2.29	2.17	$CH_3(CH_2)_3NH_3^+$	Pb^{2+}	I^-	8.43	8.99	26.23	90	90	90
72	2.27	2.17	$CH_3(CH_2)_3NH_3^+$	Pb^{2+}	I^-	8.88	8.69	27.6	90	90	90
73	2.13	2.17	$CH_3(CH_2)_3NH_3^+$	Pb^{2+}	I^-	8.94	9.06	10.21	90	100.26	90
74	2.82	2.81	$CH_3(CH_2)_3NH_3^+$	Pb^{2+}	Br^-	8.32	8.18	27.66	90	90	90
*75	2.82	2.81	$CH_3(CH_2)_3NH_3^+$	Pb^{2+}	Br^-	8.33	8.22	27.62	90	90	90
76	2.78	2.81	$CH_3(CH_2)_3NH_3^+$	Pb^{2+}	Br^-	8.46	8.65	19.92	90	90	90
77	2.84	2.81	$CH_3(CH_2)_3NH_3^+$	Pb^{2+}	Br^-	8.31	8.18	27.62	90	90	90
78	2.11	2.11	$CH_3(CH_2)_3NH_3^+$	Ge^{2+}	I^-	8.72	8.27	28.01	90	90	90
79	2.31	2.31	$CH_3(CH_2)_3CH(C_2H_5)CH_2NH_3^+$	Pb^{2+}	I^-	18.7	8.85	8.84	90	95.37	90
*80	3.09	3.09	$CH_3(CH_2)_2NH_3^+$	Pb^{2+}	Cl^-	7.82	25.03	7.95	90	90	90
81	2.05	2.05	$CH_3(CH_2)11NH_3^+$	Pb^{2+}	I^-	8.87	8.48	48.84	90	90	90
82	2.77	2.82	$CH_2CH(CH_2)_2NH_3^+$	Pb^{2+}	Br^-	13.53	8.21	8.2	90	96.31	90
83	3.37	3.38	$C_6H_5NH_3^+$	Pb^{2+}	Cl^-	11.12	11.21	17.59	99.17	104.53	90
84	2.03	2.03	$C_6H_5CH_2NH_3^+$	Sn^{2+}	I^-	9.09	8.66	28.76	90	90	90
*85	2.03	2.03	$C_6H_5CH_2NH_3^+$	Sn^{2+}	I^-	9.11	8.68	28.75	90	90	90
86	3.3	3.30	$C_6H_5CH_2NH_3^+$	Sn^{2+}	Cl^-	33.51	7.78	7.77	90	90	90
87	2.72	2.72	$C_6H_5CH_2NH_3^+$	Sn^{2+}	Br^-	33.28	8.11	8.1	90	90	90

88	2.28	2.27	$C_6H_5CH_2NH_3^+$	Pb^{2+}	I^-	9.11	8.63	28.41	90	90	90
89	2.27	2.27	$C_6H_5CH_2NH_3^+$	Pb^{2+}	I^-	9.16	8.69	28.78	90	90	90
90	3.01	3.01	$C_6H_5CH_2NH_3^+$	Pb^{2+}	Cl^-	33.62	7.82	7.73	90	90	90
91	2.91	2.91	$C_6H_5CH_2NH_3^+$	Pb^{2+}	Br^-	33.35	8.15	8.12	90	90	90
92	2.3	2.30	$C_6H_5CH(CH_3)NH_3^+$	Pb^{2+}	I^-	8.79	9.39	14.64	90	100.09	90
93	1.77	1.83	$C_6H_5(CH_2)_2NH_3^+$	Sn^{2+}	I^-	32.3	6.1	6.14	90	93.96	90
94	1.9	1.83	$C_6H_5(CH_2)_2NH_3^+$	Sn^{2+}	I^-	8.65	8.65	32.46	85.15	85.13	89.5
*95	2.68	2.68	$C_6H_5(CH_2)_2NH_3^+$	Sn^{2+}	Br^-	11.5	11.61	17.44	80.45	74.59	90.05
96	2.06	2.11	$C_6H_5(CH_2)_2NH_3^+$	Pb^{2+}	I^-	8.74	8.74	33	84.65	84.66	89.64
97	2.07	2.11	$C_6H_5(CH_2)_2NH_3^+$	Pb^{2+}	I^-	8.68	8.68	16.41	94.45	100.59	90.57
98	2.09	2.11	$C_6H_5(CH_2)_2NH_3^+$	Pb^{2+}	I^-	8.69	8.69	32.39	85.24	85.28	89.45
99	2.05	2.11	$C_6H_5(CH_2)_2NH_3^+$	Pb^{2+}	I^-	8.74	8.74	33.03	84.62	84.63	89.63
*100	2.27	2.11	$C_6H_5(CH_2)_2NH_3^+$	Pb^{2+}	I^-	12.34	12.22	32.24	90	94.3	90
101	2.83	2.79	$C_6H_5(CH_2)_2NH_3^+$	Pb^{2+}	Br^-	11.62	11.63	17.58	99.55	105.72	89.98
102	2.75	2.79	$C_6H_5(CH_2)_2NH_3^+$	Pb^{2+}	Br^-	11.52	11.52	17.27	80.39	73.9	90
103	1.9	1.90	$C_6H_5(CH_2)_2NH_3^+$	Ge^{2+}	I^-	12	12.02	17.47	80.08	73.52	89.96
104	3.24	3.24	$C_6H_5(CH_2)_2NH_3^+$	Cd^{2+}	Cl^-	38.85	7.43	7.37	90	90	90
*105	3.41	3.40	$C_6H11NH_3^+$	Pb^{2+}	Cl^-	11.45	28.31	11.52	90	90.03	90
106	2.91	2.91	$C_6H11NH_3^+$	Pb^{2+}	Br^-	27.79	8.65	8.24	90	90	90
107	2.91	2.91	$C_6H11NH_3^+$	Cd^{2+}	Br^-	26.64	8.67	8.6	90	90	90
108	2.18	2.11	$C_6H11CH_3NH_3^+$	Sn^{2+}	I^-	17.16	8.7	8.68	90	100.81	90
109	2.05	2.11	$C_6H11CH_3NH_3^+$	Sn^{2+}	I^-	34.43	8.74	8.73	90	90	90
*110	2.82	2.82	$C_6H10CH_2NH_3^+$	Pb^{2+}	Br^-	17.06	8.26	8.24	90	99.22	90
111	3.36	3.35	$C_5H_9NH_3^+$	Pb^{2+}	Cl^-	25.84	8.52	7.7	90	90	90
112	2.78	2.78	$C_5H_9NH_3^+$	Pb^{2+}	Br^-	13.43	7.99	8.8	90	106.16	90
113	3.42	3.42	$C_4H_7NH_3^+$	Pb^{2+}	Cl^-	13.22	7.62	8.09	90	106.83	90
114	2.87	2.82	$C_4H_7NH_3^+$	Pb^{2+}	Br^-	13.28	7.95	8.47	90	108.43	90
*115	2.2	2.20	$C_4H_3SCH_2NH_3^+$	Pb^{2+}	I^-	8.84	8.69	29	90	90	90
116	2.25	2.25	$C_4H_3S(CH_2)_2NH_3^+$	Pb^{2+}	I^-	12.28	12.33	31.38	90	90.97	90
117	2.31	2.31	$C_3H_5NH_3^+$	Pb^{2+}	I^-	12.48	8.66	8.75	90	110.28	90
118	3.37	3.37	$C_3H_5NH_3^+$	Pb^{2+}	Cl^-	12.19	7.51	8.05	90	109.14	90
119	2.85	2.85	$C_3H_5NH_3^+$	Pb^{2+}	Br^-	12.4	7.84	8.39	90	108.18	90

*120	2	2.01	$C(NH_2)_3^+$	Sn^{2+}	I^-	13.04	13.57	9.32	90	90	90
121	2.08	2.01	$C(NH_2)_3^+$	Sn^{2+}	I^-	26.89	9.3	12.94	90	90	90
122	1.98	2.01	$C(NH_2)_3^+$	Sn^{2+}	I^-	9.28	26.95	12.81	90	90.75	90
123	1.99	2.01	$C(NH_2)_3^+$	Sn^{2+}	I^-	9.27	12.67	14.44	66.98	85.88	88.26
124	2	2.01	$C(NH_2)_3^+$	Sn^{2+}	I^-	12.83	27.05	9.3	90	90.81	90
*125	2.01	2.07	$C(NH_2)_3^+$	Pb^{2+}	I^-	13.04	13.61	9.36	90	90	90
126	2.18	2.07	$C(NH_2)_3^+$	Pb^{2+}	I^-	27.03	9.31	12.92	90	90	90
127	2.01	2.07	$C(NH_2)_3^+$	Pb^{2+}	I^-	9.21	26.88	12.68	90	91.49	90
128	2.33	2.33	$BrC_6H_5CH_2NH_3^+$	Pb^{2+}	I^-	8.61	8.91	15.87	90	95.14	90
129	2.26	2.26	$BrC_6H_4(CH_2)_2NH_3^+$	Sn^{2+}	I^-	18.54	8.34	8.78	90	93.04	90
*130	2.31	2.31	$BrC_6H_4(CH_2)_2NH_3^+$	Pb^{2+}	I^-	34.15	8.64	8.69	90	91.89	90
131	2.13	2.13	$Br(CH_2)_2NH_3^+$	Pb^{2+}	I^-	12.85	20.77	6.49	90	90	90
132	2.12	2.13	$Br(CH_2)_2NH_3^+$	Pb^{2+}	I^-	9.13	9.14	21.45	90	98.65	90
133	2.14	2.13	$Br(CH_2)_2NH_3^+$	Pb^{2+}	I^-	6.48	12.91	21.14	90	90	90
134	2.83	2.83	$(CH_3)_2CHCH_2NH_3^+$	Pb^{2+}	Br^-	14.2	8.34	8.24	90	105.32	90
*135	2.84	2.83	$(CH_3)_2CHCH_2NH_3^+$	Pb^{2+}	Br^-	28.12	8.31	8.31	90	90	90
136	2.8	2.80	$F_2CHCH_2NH_3^+$	Cd^{2+}	Br^-	7.87	7.66	22.64	90	90	90

Table S2 Value of important features

M_X	M_B	MATS4c	CrippenLogP	Δγ	GATS4e	Band gap
126.9	207.2	0.02107742	0.0284	0	0.893080542	1.99
126.9	207.2	0.188072995	-1.6373	0	0	2.04
126.9	207.2	0.188072995	-1.6373	0	0	2.07
126.9	207.2	0.188072995	-1.6373	0	0	1.97
126.9	207.2	0.188072995	-1.6373	0	0	2.12
79.9	207.2	0.099913248	0.857	0.13	0.816992517	2.79
126.9	207.2	-0.09510933	0.6936	0	1.208165165	2.22
126.9	207.2	0.00440816	1.2237	0	0.802107306	2.22
126.9	207.2	0.00440816	1.2237	0	0.802107306	2.19
126.9	207.2	0.009910949	0.8336	0	0.841181906	2.22
126.9	207.2	0.100907724	0.4435	0	0.915695649	2.28
126.9	118.7	0.183185336	0.0534	0	1.051512029	1.65
126.9	207.2	0.183185336	0.0534	0	1.051512029	2.29
126.9	207.2	0.213035549	-0.3367	0	1.172001033	2.37
126.9	207.2	0.213035549	-0.3367	0	1.172001033	2.37
126.9	118.7	-0.11038621	-0.67301	0	1.041686013	1.66
126.9	207.2	-0.45461794	-0.08272	0	1.951192995	2.29
126.9	207.2	0.228922517	-1.3893	0	0.869517187	2.14
126.9	118.7	-0.37696298	-1.7794	0	1.414689012	2.16
126.9	118.7	-0.37696298	-1.7794	0	1.414689012	2.09
126.9	207.2	-0.37696298	-1.7794	0	1.414689012	2.16

79.9	207.2	-0.37696298	-1.7794	0	1.414689012	2.82
126.9	207.2	-0.16985729	-0.11081	0	1.007285331	2.25
126.9	118.7	0.040020745	0.27119	0	0.805431261	2.03
126.9	118.7	0.040020745	0.27119	0	0.805431261	2.03
126.9	118.7	0.040020745	0.27119	0	0.805431261	2.09
126.9	207.2	0.040020745	0.27119	0.4	0.805431261	2.15
126.9	207.2	0.040020745	0.27119	0	0.805431261	2.13
126.9	207.2	0.040020745	0.27119	0	0.805431261	2.34
126.9	207.2	0.040020745	0.27119	0.4	0.805431261	2.11
126.9	207.2	0.040020745	0.27119	0	0.805431261	2.11
126.9	207.2	0.040020745	0.27119	0	0.805431261	2.28
79.9	207.2	-0.44111349	-0.2094	0	2.502447468	2.88
79.9	207.2	-0.34310461	-0.5066	0	2.123007399	2.79
126.9	207.2	-0.1445384	0.8062	0	1.089315125	2.38
126.9	207.2	-0.1445384	0.8062	0	1.089315125	2.29
35.5	207.2	-0.17600694	-0.8022	0	1.735501284	3.34
79.9	207.2	-0.17600694	-0.8022	0	1.735501284	2.65
79.9	207.2	-0.11038621	-0.9069	0	1.041686013	2.84
126.9	118.7	0.057254733	1.1244	0	0.769741381	1.79
126.9	207.2	0.057254733	1.1244	0	0.769741381	2.31
79.9	207.2	0.146800139	-0.66881	0	0.399824253	2.88
126.9	207.2	-0.01872776	0.0268	0	0.781170801	2.08
126.9	207.2	-0.15973244	-0.1157	0	1.391416345	2.28
126.9	207.2	0.065058224	0.49902	0.02	0.571294379	2.12
126.9	207.2	0.065058224	0.49902	0	0.571294379	2.09
126.9	207.2	0.002005102	2.369	0	0.754623284	2.39
126.9	207.2	0.002005102	2.369	0	0.754623284	2.39
126.9	207.2	0.002005102	2.369	0	0.754623284	2.28
126.9	207.2	0.002005102	2.369	0	0.754623284	2.28
126.9	207.2	0.002005102	2.369	0	0.754623284	2.16
126.9	207.2	0.002102515	1.9789	0	0.756497981	2.12
126.9	207.2	0.002102515	1.9789	0	0.756497981	2.35
126.9	207.2	0.002102515	1.9789	0	0.756497981	2.27
126.9	207.2	0.002102515	1.9789	0	0.756497981	2.39
126.9	207.2	0.002208094	1.5888	0	0.761565322	2.38
126.9	207.2	0.002208094	1.5888	0	0.761565322	2.28
126.9	207.2	0.002254457	1.1987	0	0.771765643	2.31
126.9	207.2	0.002254457	1.1987	0	0.771765643	2.26
126.9	207.2	0.002254457	1.1987	0	0.771765643	2.29
126.9	207.2	0.002317421	0.8086	0	0.790654688	2.28
126.9	207.2	0.002317421	0.8086	0	0.790654688	2.29
126.9	207.2	0.005991826	0.4185	0	0.825438241	2.37
126.9	207.2	0.005991826	0.4185	0	0.825438241	2.32
126.9	207.2	0.005991826	0.4185	0	0.825438241	2.29
126.9	207.2	0.054681846	0.807	0	0.658878907	2.28
126.9	118.7	0.02107742	0.0284	0	0.893080542	1.8
126.9	118.7	0.02107742	0.0284	0	0.893080542	1.77

126.9	118.7	0.02107742	0.0284	0	0.893080542	2.04
126.9	118.7	0.02107742	0.0284	0	0.893080542	1.78
126.9	207.2	0.02107742	0.0284	0	0.893080542	2.29
126.9	207.2	0.02107742	0.0284	0	0.893080542	2.27
126.9	207.2	0.02107742	0.0284	0	0.893080542	2.13
79.9	207.2	0.02107742	0.0284	0	0.893080542	2.82
79.9	207.2	0.02107742	0.0284	0	0.893080542	2.82
79.9	207.2	0.02107742	0.0284	0	0.893080542	2.78
79.9	207.2	0.02107742	0.0284	0	0.893080542	2.84
126.9	72.61	0.02107742	0.0284	0	0.893080542	2.11
126.9	207.2	-0.0389769	1.4447	0	1.163569151	2.31
35.5	207.2	0.02107742	0.0284	0	0.893080542	3.09
126.9	207.2	0.001849515	3.1492	0	0.756335269	2.05
79.9	207.2	0.037151065	-0.26941	0	0.67818858	2.77
35.5	207.2	-0.02658223	0.56	0	0.990198736	3.37
126.9	118.7	-0.05327126	0.089	0	1.166060127	2.03
126.9	118.7	-0.05327126	0.089	0	1.166060127	2.03
35.5	118.7	-0.05327126	0.089	0	1.166060127	3.3
79.9	118.7	-0.05327126	0.089	0	1.166060127	2.72
126.9	207.2	-0.05327126	0.089	0	1.166060127	2.28
126.9	207.2	-0.05327126	0.089	0	1.166060127	2.27
35.5	207.2	-0.05327126	0.089	0	1.166060127	3.01
79.9	207.2	-0.05327126	0.089	0	1.166060127	2.91
126.9	207.2	0.005508771	0.6484	0	0.947756929	2.3
126.9	118.7	0.078271838	0.471	0	0.572875072	1.77
126.9	118.7	0.078271838	0.471	0.5	0.572875072	1.9
79.9	118.7	0.078271838	0.471	0.05	0.572875072	2.68
126.9	207.2	0.078271838	0.471	0.36	0.572875072	2.06
126.9	207.2	0.078271838	0.471	0.57	0.572875072	2.07
126.9	207.2	0.078271838	0.471	0.55	0.572875072	2.09
126.9	207.2	0.078271838	0.471	0.37	0.572875072	2.05
126.9	207.2	0.078271838	0.471	0	0.572875072	2.27
79.9	207.2	0.078271838	0.471	0.02	0.572875072	2.83
79.9	207.2	0.078271838	0.471	0	0.572875072	2.75
126.9	72.61	0.078271838	0.471	0.04	0.572875072	1.9
35.5	112.41	0.078271838	0.471	0	0.572875072	3.24
35.5	207.2	-0.00933481	0.51079	0	0.818782109	3.41
79.9	207.2	-0.00933481	0.51079	0	0.818782109	2.91
79.9	112.41	-0.00933481	0.51079	0	0.818782109	2.91
126.9	118.7	0.046689362	1.5872	0	0.666369656	2.18
126.9	118.7	0.046689362	1.5872	0	0.666369656	2.05
79.9	207.2	0.0035721	0.90089	0	0.788704676	2.82
35.5	207.2	0.046044476	0.12069	0	0.875179357	3.36
79.9	207.2	0.046044476	0.12069	0	0.875179357	2.78
35.5	207.2	0.037151065	-0.26941	0	0.67818858	3.42
79.9	207.2	0.037151065	-0.26941	0	0.67818858	2.87
126.9	207.2	-0.04676287	0.07168	0	0.900827894	2.2

126.9	207.2	0.024553729	0.11418	0	0.672936505	2.25
126.9	207.2	-0.21642911	-0.65951	0	1.075476695	2.31
35.5	207.2	-0.21642911	-0.65951	0	1.075476695	3.37
79.9	207.2	-0.21642911	-0.65951	0	1.075476695	2.85
126.9	118.7	0.388675782	-1.69051	0	0	2
126.9	118.7	0.388675782	-1.69051	0	0	2.08
126.9	118.7	0.388675782	-1.69051	0	0	1.98
126.9	118.7	0.388675782	-1.69051	1.74	0	1.99
126.9	118.7	0.388675782	-1.69051	0	0	2
126.9	207.2	0.388675782	-1.69051	0	0	2.01
126.9	207.2	0.388675782	-1.69051	0	0	2.18
126.9	207.2	0.388675782	-1.69051	0	0	2.01
126.9	207.2	-0.11008709	0.8515	0	1.138856813	2.33
126.9	118.7	0.04540241	1.2335	0	0.726850626	2.26
126.9	207.2	0.04540241	1.2335	0	0.726850626	2.31
126.9	207.2	-0.08769993	-0.3768	0	1.113924416	2.13
126.9	207.2	-0.08769993	-0.3768	0	1.113924416	2.12
126.9	207.2	-0.08769993	-0.3768	0	1.113924416	2.14
79.9	207.2	-0.15973244	-0.1157	0	1.391416345	2.83
79.9	207.2	-0.15973244	-0.1157	0	1.391416345	2.84
79.9	112.41	-0.34310461	-0.5066	0	2.123007399	2.8

Table S3 Parameters of ensemble of regression tree

Name	Minimum leaf size	Number of leaners	Learning rate
Boosted trees	8	30	0.1
Bagged trees	8	30	—

Table S4 Parameters of regression tree

Name	Minimum leaf size	Surrogate decision splits
Complex tree	4	Find all
Medium tree	12	Find all
Simple tree	36	Find all

Table S5 Parameters of support vector machine algorithm

Name	Kernel Function	Box constraint	Epsilon	Kernel scale
Linear SVM	Linear	Auto	Auto	Auto
Quadratic SVM	Quadratic	Auto	Auto	Auto
Cubic SVM	Cubic	Auto	Auto	Auto
Fine Gaussian SVM	Gaussian	Auto	Auto	0.66
Medium Gaussian SVM	Gaussian	Auto	Auto	2.6
Coarse Gaussian SVM	Gaussian	Auto	Auto	11

Table S6 Parameters of Gaussian process regression

Name	Basis Function	Kernel Function	Isotropic Kernel	Kernel mode	Sigma mode	Optimize numeric parameters
Rational Quadratic	Constant	Rational Quadratic	Use	Auto	Auto	Yes
Squared Exponential	Constant	Squared Exponential	Use	Auto	Auto	Yes
Matern 5/2	Constant	Matern 5/2	Use	Auto	Auto	Yes
Exponential	Constant	Exponential	Use	Auto	Auto	Yes

Table S7 Results of multiple stepwise regression

No.	R^2	Q^2	Variable
1[a]	0.868	0.867	M_X

2[b]	0.911	0.909	M_X, M_B
3[c]	0.916	0.914	M_X, M_B, MATS4c
4[d]	0.923	0.920	M_X, M_B, MATS4c, CrippenLogP
5[e]	0.928	0.924	M_X, M_B, MATS4c, CrippenLogP, $\Delta\gamma$
6[f]	0.931	0.927	M_X, M_B, MATS4c, CrippenLogP, $\Delta\gamma$, GATS4e
7[g]	0.935	0.930	M_X, M_B, MATS4c, CrippenLogP, $\Delta\gamma$, GATS4e, E_X
8[h]	0.938	0.932	M_X, M_B, MATS4c, CrippenLogP, $\Delta\gamma$, GATS4e, E_X, nAcid
9[i]	0.940	0.935	M_X, M_B, MATS4c, CrippenLogP, $\Delta\gamma$, GATS4e, E_X, nAcid, MLFER_A

[a] VIF value: 1.00.
[b] VIF value: 1.01 and 1.01.
[c] VIF value: 1.04, 1.01 and 1.03.
[d] VIF value: 1.04, 1.01, 1.13 and 1.12.
[e] VIF value: 1.06, 1.01, 1.16, 1.13 and 1.07.
[f] VIF value: 1.10, 1.02, 3.89, 1.25, 1.08 and 3.69.
[g] VIF value: 4149.93, 1.03, 3.90, 1.26, 1.08, 3.75 and 4141.64.
[h] VIF value: 4176.70, 1.04, 3.91, 1.28, 1.08, 3.75, 4168.28 and 1.04.
[i] VIF value: 4178.13, 1.04, 4.12, 1.70, 1.08, 4.12, 4170.14, 5.84 and 6.61.

Table S8 The name, experimental value of and the predicted value of 2D HOIPs used for verification.

Name	Exp	Pre
$[CH_3(CH_2)_3NH_3]_2PbI_4$	2.3	2.17
$[CH_3NHNH_3]_2PbI_4$	2.12	2.05
$[C_{16}H_9O(CH_2)_3NH_3]_2PbI_4$	2.27	2.21
$[C_{10}H_{70}O(CH_2)_2NH_3]_2PbI_4$	2.39	2.28
$[HO(CH_2)_2NH_3]_2SnI_4$	2.07	2.19
$[F_2C_6H_9NH_3]_2PbI_4$	2.38	2.30
$[ClC_6H_5CH_2NH_3]_2PbI_4$	2.33	2.28
$[CH_3C_6H_4(CH_2)_2NH_3]_2PbI_4$	2.4	2.33
$[CH_3(CH_2)_3CH(C_2H_5)CH_2NH_3]_2PbI_4$	2.38	2.11
$[CH_3(CH_2)_{11}NH_3]_2PbI_4$	2.03	2.11
$[C_6H_9(CH_2)_2NH_3]_2PbBr_4$	2.98	2.91
$[C_6H_5(CH_2)_2NH_3]_2GeI_4$	2.12	2.33