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Supporting Information

Designing Promising Molecules for Organic Solar Cells via Machine Learning Assisted Virtual Screening

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Table S1 Experimental power conversion of efficiency for 300 SM-OPVs reported in the literature. $N_{\mathrm{atom}}^{\mathrm{D}}$, E_{H} and E_{L} represent the number of unsaturated atoms in the main conjugation path, energy of highest occupied molecular orbital (HOMO) and energy of lowest unoccupied molecular orbital (LUMO) of donor molecules. E_{H} and E_{L} of $PC_{71}BM$ ($PC_{61}BM$) are -6.69 (-6.90) and -2.54 (-2.60) eV, respectively.

S No.	Acceptor	PCE (%)	$N_{\mathrm{atom}}^{\mathrm{D}}$	E_{H}	E_{L}	Ref.
1	$PC_{71}BM$	9.84	130	-5.94	-2.39	[2]
2	$PC_{71}BM$	9.54	68	-6.20	-2.05	[3]
3	$PC_{71}BM$	9.45	130	-6.02	-2.40	[2]
4	$PC_{71}BM$	9.36	68	-6.12	-2.01	[4]
5	$PC_{71}BM$	9.09	54	-6.14	-2.31	[5]
6	$PC_{71}BM$	9.05	59	-6.26	-2.27	[6]
7	$PC_{71}BM$	9.01	68	-6.23	-2.07	[7]
8	$PC_{61}BM$	9.00	86	-5.83	-2.44	[8]
9	$PC_{71}BM$	8.95	99	-5.83	-2.11	[9]
10	$PC_{71}BM$	8.91	99	-5.84	-2.10	[10]
11	$PC_{71}BM$	8.90	68	-6.10	-2.02	[11]
12	$PC_{71}BM$	8.85	99	-5.77	-2.05	[12]
13	$PC_{71}BM$	8.54	64	-5.89	-2.07	[13]
14	$PC_{71}BM$	8.50	74	-6.12	-2.03	[14]
15	$PC_{61}BM$	8.34	114	-5.69	-2.47	[15]
16	$PC_{71}BM$	8.34	62	-5.88	-2.06	[16]
17	$PC_{71}BM$	8.33	68	-6.24	-2.05	[17]
18	$PC_{71}BM$	8.27	64	-5.89	-2.07	[10]
19	$PC_{71}BM$	8.26	58	-6.16	-2.02	[18]
20	$PC_{71}BM$	8.24	64	-5.87	-2.10	[13]
21	$PC_{71}BM$	8.23	90	-6.02	-1.97	[19]
22	$PC_{71}BM$	8.13	82	-5.89	-2.46	[20]
23	$PC_{61}BM$	8.04	78	-5.78	-2.40	[21]

24	$PC_{71}BM$	8.02	68	-6.12	-2.01	[22]
25	$PC_{71}BM$	8.02	90	-6.02	-1.97	[23]
26	$PC_{71}BM$	8.02	60	-6.17	-2.35	[24]
27	$PC_{71}BM$	8.00	48	-5.88	-2.07	[25]
28	$PC_{71}BM$	7.95	102	-5.74	-2.27	[26]
29	$PC_{71}BM$	7.91	62	-6.30	-2.26	[27]
30	$PC_{71}BM$	7.85	74	-6.21	-2.05	[14]
31	$PC_{71}BM$	7.83	52	-5.94	-2.10	[28]
32	$PC_{71}BM$	7.83	58	-6.17	-2.03	[29]
33	$PC_{71}BM$	7.81	84	-6.12	-2.20	[30]
34	$PC_{71}BM$	7.80	68	-6.12	-2.01	[31]
35	$PC_{71}BM$	7.79	64	-6.12	-2.04	[32]
36	$PC_{71}BM$	7.75	72	-6.14	-1.97	[33]
37	$PC_{61}BM$	7.74	80	-5.86	-2.19	[34]
38	$PC_{71}BM$	7.72	78	-6.12	-2.01	[31]
39	$PC_{71}BM$	7.70	70	-6.14	-2.16	[35]
40	$PC_{71}BM$	7.61	54	-6.18	-2.30	[24]
41	$PC_{71}BM$	7.60	74	-6.09	-2.01	[36]
42	$PC_{71}BM$	7.55	59	-6.26	-2.27	[6]
43	$PC_{71}BM$	7.54	60	-6.27	-2.17	[37]
44	$PC_{71}BM$	7.47	74	-5.77	-2.32	[20]
45	$PC_{71}BM$	7.44	54	-6.44	-2.39	[38]
46	$PC_{71}BM$	7.36	62	-6.28	-2.07	[39]
47	$PC_{71}BM$	7.35	62	-6.04	-2.20	[40]
48	$PC_{61}BM$	7.30	86	-5.87	-2.30	[41]
49	$PC_{71}BM$	7.24	46	-6.15	-3.10	[42]
50	$PC_{71}BM$	7.21	68	-6.12	-2.01	[43]
51	$PC_{71}BM$	7.21	78	-5.98	-2.09	[44]

52	$PC_{61}BM$	7.20	80	-6.04	-2.26	[34]
53	$PC_{71}BM$	7.18	58	-6.19	-2.04	[31]
54	$PC_{71}BM$	7.06	66	-5.93	-1.92	[45]
55	$PC_{61}BM$	6.98	80	-5.82	-1.99	[46]
56	$PC_{71}BM$	6.91	56	-6.15	-1.76	[47]
57	$PC_{71}BM$	6.89	112	-6.02	-1.98	[48]
58	$PC_{71}BM$	6.86	110	-5.91	-2.32	[49]
59	$PC_{71}BM$	6.86	48	-6.04	-2.14	[50]
60	$PC_{71}BM$	6.84	99	-5.84	-2.13	[9]
61	$PC_{71}BM$	6.83	64	-6.01	-2.37	[51]
62	$PC_{61}BM$	6.83	80	-5.70	-2.37	[52]
63	$PC_{71}BM$	6.75	66	-6.13	-2.02	[53]
64	$PC_{71}BM$	6.73	46	-6.42	-2.26	[38]
65	$PC_{71}BM$	6.71	52	-6.43	-2.32	[54]
66	$PC_{71}BM$	6.67	134	-5.83	-2.12	[10]
67	$PC_{71}BM$	6.67	34	-6.27	-2.23	[55]
68	$PC_{71}BM$	6.59	76	-5.85	-2.48	[56]
69	$PC_{71}BM$	6.59	52	-6.01	-1.93	[57]
70	$PC_{71}BM$	6.59	48	-5.97	-2.10	[50]
71	$PC_{71}BM$	6.52	50	-5.85	-2.05	[58]
72	$PC_{71}BM$	6.49	84	-6.05	-1.83	[59]
73	$PC_{71}BM$	6.47	49	-5.93	-2.01	[60]
74	$PC_{71}BM$	6.43	62	-5.77	-1.89	[16]
75	$PC_{71}BM$	6.42	99	-5.82	-2.14	[12]
76	$PC_{71}BM$	6.40	54	-5.91	-1.99	[61]
77	$PC_{71}BM$	6.40	70	-5.79	-2.06	[62]
78	$PC_{61}BM$	6.38	58	-6.19	-2.04	[63]
79	$PC_{71}BM$	6.37	64	-6.22	-2.26	[27]

80	$PC_{61}BM$	6.30	86	-5.81	-2.23	[41]
81	$PC_{71}BM$	6.30	62	-5.87	-1.76	[64]
82	$PC_{71}BM$	6.30	72	-5.93	-1.74	[65]
83	$PC_{61}BM$	6.30	67	-5.89	-2.32	[66]
84	$PC_{71}BM$	6.27	79	-6.05	-2.28	[67]
85	$PC_{71}BM$	6.26	68	-6.06	-2.01	[43]
86	$PC_{71}BM$	6.23	74	-6.22	-2.44	[68]
87	$PC_{71}BM$	6.20	48	-5.88	-2.05	[69]
88	$PC_{71}BM$	6.20	62	-5.93	-1.71	[35]
89	$PC_{71}BM$	6.17	49	-6.07	-1.98	[70]
90	$PC_{71}BM$	6.15	52	-6.13	-2.07	[71]
91	$PC_{71}BM$	6.15	64	-6.24	-2.26	[37]
92	$PC_{71}BM$	6.14	67	-6.14	-1.90	[72]
93	$PC_{71}BM$	6.11	54	-6.34	-2.29	[73]
94	$PC_{71}BM$	6.11	52	-6.55	-1.96	[74]
95	$PC_{61}BM$	6.10	51	-6.09	-2.01	[75]
96	$PC_{61}BM$	6.10	67	-5.96	-2.32	[66]
97	$PC_{71}BM$	6.07	48	-6.20	-2.13	[76]
98	$PC_{71}BM$	6.07	26	-6.24	-1.82	[77]
99	$PC_{71}BM$	6.05	52	-5.74	-1.72	[78]
100	$PC_{71}BM$	6.04	64	-6.20	-1.85	[59]
101	$PC_{71}BM$	6.02	44	-6.18	-2.13	[79]
102	$PC_{71}BM$	6.00	42	-6.39	-2.29	[80]
103	$PC_{71}BM$	6.00	62	-5.87	-1.91	[81]
104	$PC_{71}BM$	5.98	55	-5.57	-1.92	[82]
105	$PC_{71}BM$	5.95	72	-6.37	-2.71	[17]
106	$PC_{71}BM$	5.94	41	-6.65	-2.90	[83]
107	$PC_{61}BM$	5.93	72	-5.96	-2.05	[84]

108	$PC_{71}BM$	5.89	60	-5.78	-2.02	[62]
109	$PC_{71}BM$	5.88	66	-5.93	-1.94	[85]
110	$PC_{71}BM$	5.87	74	-6.04	-2.20	[86]
111	$PC_{61}BM$	5.84	52	-6.08	-2.01	[87]
112	$PC_{61}BM$	5.80	67	-5.88	-2.27	[66]
113	$PC_{61}BM$	5.80	86	-5.92	-2.44	[66]
114	$PC_{61}BM$	5.79	62	-5.96	-2.04	[88]
115	$PC_{71}BM$	5.76	60	-5.95	-2.09	[89]
116	$PC_{61}BM$	5.70	67	-5.95	-2.41	[66]
117	$PC_{71}BM$	5.69	54	-6.07	-2.19	[90]
118	$PC_{71}BM$	5.67	56	-6.27	-2.06	[53]
119	$PC_{71}BM$	5.67	56	-6.07	-1.90	[85]
120	$PC_{71}BM$	5.67	80	-5.93	-2.15	[91]
121	$PC_{71}BM$	5.66	64	-5.80	-2.00	[13]
122	$PC_{61}BM$	5.65	80	-5.68	-2.41	[92]
123	$PC_{71}BM$	5.65	62	-6.11	-2.13	[93]
124	$PC_{71}BM$	5.62	60	-6.08	-2.30	[94]
125	$PC_{71}BM$	5.61	74	-5.77	-2.01	[95]
126	$PC_{71}BM$	5.60	72	-5.93	-1.60	[65]
127	$PC_{71}BM$	5.58	56	-6.12	-2.02	[96]
128	$PC_{71}BM$	5.56	56	-5.81	-2.00	[62]
129	$PC_{61}BM$	5.51	74	-5.83	-1.98	[46]
130	$PC_{61}BM$	5.50	58	-6.19	-2.07	[97]
131	$PC_{61}BM$	5.50	64	-5.94	-2.05	[98]
132	$PC_{71}BM$	5.50	62	-6.06	-2.15	[99]
133	$PC_{61}BM$	5.50	67	-5.95	-2.32	[66]
134	$PC_{71}BM$	5.47	32	-5.72	-1.59	[100]
135	$PC_{71}BM$	5.45	42	-6.03	-2.16	[101]

136	$PC_{61}BM$	5.44	54	-6.18	-1.97	[102]
137	$PC_{71}BM$	5.44	54	-6.01	-1.96	[103]
138	$PC_{61}BM$	5.42	64	-6.13	-2.06	[104]
139	$PC_{71}BM$	5.40	90	-5.75	-2.08	[105]
140	$PC_{71}BM$	5.37	34	-6.17	-2.17	[106]
141	$PC_{71}BM$	5.37	52	-5.83	-1.90	[28]
142	$PC_{71}BM$	5.30	66	-6.15	-1.97	[107]
143	$PC_{71}BM$	5.30	74	-5.75	-1.69	[108]
144	$PC_{71}BM$	5.28	35	-6.67	-2.92	[83]
145	$PC_{71}BM$	5.26	64	-6.14	-2.05	[109]
146	$PC_{71}BM$	5.25	68	-6.08	-1.79	[110]
147	$PC_{71}BM$	5.24	36	-5.82	-1.93	[111]
148	$PC_{71}BM$	5.23	78	-5.79	-1.95	[44]
149	$PC_{71}BM$	5.22	74	-6.12	-1.85	[59]
150	$PC_{71}BM$	5.21	42	-5.93	-2.15	[101]
151	$PC_{71}BM$	5.21	90	-5.75	-2.08	[49]
152	$PC_{71}BM$	5.19	64	-5.83	-1.84	[112]
153	$PC_{71}BM$	5.16	66	-6.06	-1.95	[107]
154	$PC_{71}BM$	5.15	62	-5.96	-2.03	[113]
155	$PC_{71}BM$	5.11	56	-6.22	-2.04	[53]
156	$PC_{71}BM$	5.10	44	-6.07	-1.89	[114]
157	$PC_{71}BM$	5.09	62	-6.01	-2.04	[115]
158	$PC_{61}BM$	5.07	62	-6.10	-1.79	[97]
159	$PC_{61}BM$	5.07	82	-5.97	-2.18	[116]
160	$PC_{71}BM$	5.05	57	-6.19	-2.08	[117]
161	$PC_{71}BM$	5.05	58	-6.15	-2.09	[118]
162	$PC_{71}BM$	5.05	26	-6.78	-2.42	[119]
163	$PC_{71}BM$	5.04	57	-6.17	-2.04	[120]

164	$PC_{71}BM$	5.03	82	-5.88	-2.11	[121]
165	$PC_{61}BM$	5.03	64	-6.10	-2.29	[122]
166	$PC_{71}BM$	4.99	64	-6.04	-1.95	[123]
167	$PC_{71}BM$	4.97	60	-5.94	-2.14	[124]
168	$PC_{71}BM$	4.97	55	-5.48	-1.82	[82]
169	$PC_{71}BM$	4.96	38	-5.70	-1.56	[125]
170	$PC_{61}BM$	4.93	59	-6.01	-1.95	[126]
171	$PC_{61}BM$	4.92	64	-5.96	-2.01	[127]
172	$PC_{71}BM$	4.91	54	-6.32	-1.87	[59]
173	$PC_{71}BM$	4.90	56	-6.08	-1.98	[96]
174	$PC_{71}BM$	4.88	32	-5.92	-1.74	[100]
175	$PC_{61}BM$	4.86	61	-6.01	-2.00	[128]
176	$PC_{61}BM$	4.84	51	-6.11	-1.82	[129]
177	$PC_{71}BM$	4.83	110	-5.80	-2.04	[49]
178	$PC_{71}BM$	4.80	26	-6.88	-2.28	[119]
179	$PC_{61}BM$	4.80	62	-6.02	-2.12	[130]
180	$PC_{61}BM$	4.78	80	-5.67	-2.31	[131]
181	$PC_{71}BM$	4.76	22	-6.44	-2.21	[132]
182	$PC_{71}BM$	4.75	58	-6.01	-1.99	[115]
183	$PC_{71}BM$	4.73	62	-6.01	-2.21	[133]
184	$PC_{71}BM$	4.72	40	-6.12	-2.36	[42]
185	$PC_{61}BM$	4.70	62	-6.16	-1.96	[97]
186	$PC_{71}BM$	4.68	68	-6.23	-1.94	[134]
187	$PC_{71}BM$	4.67	28	-6.14	-1.63	[77]
188	$PC_{71}BM$	4.66	34	-6.14	-2.14	[135]
189	$PC_{71}BM$	4.65	56	-5.65	-2.02	[136]
190	$PC_{71}BM$	4.65	32	-5.57	-1.48	[137]
191	$PC_{71}BM$	4.65	34	-6.13	-2.12	[135]

192	$PC_{71}BM$	4.64	74	-5.94	-2.09	[86]
193	$PC_{61}BM$	4.63	41	-6.27	-2.09	[138]
194	$PC_{61}BM$	4.62	62	-6.17	-1.78	[139]
195	$PC_{71}BM$	4.61	43	-6.53	-2.87	[140]
196	$PC_{71}BM$	4.60	63	-5.95	-2.19	[141]
197	$PC_{71}BM$	4.60	68	-5.98	-1.95	[142]
198	$PC_{71}BM$	4.58	41	-6.13	-1.96	[93]
199	$PC_{71}BM$	4.57	48	-6.05	-2.20	[143]
200	$PC_{61}BM$	4.56	54	-6.20	-1.99	[63]
201	$PC_{61}BM$	4.56	64	-6.04	-1.95	[123]
202	$PC_{71}BM$	4.56	42	-5.77	-1.73	[78]
203	$PC_{61}BM$	4.54	62	-6.03	-2.10	[127]
204	$PC_{71}BM$	4.52	52	-6.13	-2.01	[71]
205	$PC_{71}BM$	4.50	22	-6.53	-1.99	[144]
206	$PC_{61}BM$	4.46	47	-6.20	-2.01	[145]
207	$PC_{61}BM$	4.45	50	-6.04	-1.93	[146]
208	$PC_{61}BM$	4.43	66	-6.05	-1.98	[147]
209	$PC_{71}BM$	4.40	38	-6.04	-2.06	[148]
210	$PC_{71}BM$	4.40	50	-6.03	-1.95	[149]
211	$PC_{71}BM$	4.40	74	-5.72	-1.77	[108]
212	$PC_{61}BM$	4.40	56	-5.89	-1.93	[150]
213	$PC_{71}BM$	4.40	54	-5.98	-2.02	[151]
214	$PC_{71}BM$	4.36	28	-6.41	-2.20	[152]
215	$PC_{71}BM$	4.34	56	-6.18	-2.19	[153]
216	$PC_{71}BM$	4.33	64	-6.06	-2.29	[154]
217	$PC_{61}BM$	4.32	43	-6.26	-2.35	[155]
218	$PC_{71}BM$	4.32	40	-5.98	-2.07	[156]
219	$PC_{71}BM$	4.25	70	-5.94	-1.92	[157]

220	$PC_{61}BM$	4.25	114	-6.00	-2.10	[158]
221	$PC_{71}BM$	4.25	54	-5.82	-1.92	[159]
222	$PC_{71}BM$	4.24	35	-5.90	-1.97	[160]
223	$PC_{61}BM$	4.21	64	-6.05	-2.10	[161]
224	$PC_{61}BM$	4.20	64	-5.89	-2.07	[162]
225	$PC_{71}BM$	4.20	48	-6.06	-1.97	[163]
226	$PC_{71}BM$	4.19	60	-5.91	-2.06	[62]
227	$PC_{71}BM$	4.18	22	-6.28	-2.16	[164]
228	$PC_{71}BM$	4.18	52	-6.10	-2.05	[115]
229	$PC_{71}BM$	4.18	34	-6.06	-2.07	[135]
230	$PC_{61}BM$	4.16	64	-6.28	-2.17	[165]
231	$PC_{71}BM$	4.15	46	-6.42	-2.08	[53]
232	$PC_{61}BM$	4.14	51	-6.16	-1.96	[128]
233	$PC_{61}BM$	4.12	61	-5.99	-1.92	[128]
234	$PC_{71}BM$	4.09	52	-6.47	-2.14	[166]
235	$PC_{71}BM$	4.08	50	-5.98	-2.12	[90]
236	$PC_{71}BM$	4.07	48	-6.25	-2.02	[57]
237	$PC_{71}BM$	4.06	54	-5.80	-1.90	[167]
238	$PC_{61}BM$	4.05	55	-6.12	-2.04	[168]
239	$PC_{61}BM$	4.04	64	-5.94	-2.01	[161]
240	$PC_{71}BM$	4.04	64	-5.85	-1.77	[112]
241	$PC_{71}BM$	4.02	68	-5.69	-2.23	[169]
242	$PC_{71}BM$	4.00	68	-6.10	-1.96	[170]
243	$PC_{61}BM$	4.00	49	-6.18	-2.02	[168]
244	$PC_{61}BM$	3.97	70	-6.05	-2.11	[171]
245	$PC_{71}BM$	3.97	28	-5.93	-1.84	[111]
246	$PC_{71}BM$	3.96	27	-6.25	-2.20	[172]
247	$PC_{61}BM$	3.95	63	-6.47	-2.47	[173]

248	$PC_{71}BM$	3.94	59	-6.19	-1.91	[72]
249	$PC_{71}BM$	3.91	52	-5.84	-1.81	[174]
250	$PC_{61}BM$	3.83	62	-5.93	-2.02	[127]
251	$PC_{71}BM$	3.76	69	-5.90	-1.95	[70]
252	$PC_{61}BM$	3.75	63	-5.93	-2.08	[46]
253	$PC_{61}BM$	3.73	64	-6.02	-2.07	[127]
254	$PC_{71}BM$	3.73	35	-5.85	-1.96	[160]
255	$PC_{71}BM$	3.70	52	-5.99	-1.87	[175]
256	$PC_{71}BM$	3.70	32	-6.73	-2.55	[176]
257	$PC_{61}BM$	3.66	64	-5.92	-1.98	[127]
258	$PC_{71}BM$	3.64	42	-6.73	-2.47	[54]
259	$PC_{71}BM$	3.59	48	-5.87	-2.08	[124]
260	$PC_{71}BM$	3.54	35	-5.84	-1.86	[160]
261	$PC_{61}BM$	3.53	51	-6.14	-1.86	[128]
262	$PC_{71}BM$	3.51	52	-5.85	-1.76	[174]
263	$PC_{71}BM$	3.47	37	-6.07	-2.42	[177]
264	$PC_{71}BM$	3.45	32	-6.13	-1.72	[178]
265	$PC_{71}BM$	3.40	54	-5.96	-2.08	[162]
266	$PC_{61}BM$	3.40	37	-6.87	-2.36	[179]
267	$PC_{61}BM$	3.40	47	-5.90	-1.73	[129]
268	$PC_{71}BM$	3.34	54	-6.15	-1.97	[123]
269	$PC_{61}BM$	3.27	37	-6.34	-2.06	[168]
270	$PC_{71}BM$	3.26	61	-6.15	-1.83	[180]
271	$PC_{61}BM$	3.26	76	-5.95	-2.09	[181]
272	$PC_{71}BM$	3.24	58	-6.12	-1.98	[182]
273	$PC_{61}BM$	3.23	43	-6.24	-2.32	[155]
274	$PC_{71}BM$	3.21	69	-5.86	-2.07	[183]
275	$PC_{71}BM$	3.20	68	-5.85	-1.86	[142]

276	$PC_{61}BM$	3.14	54	-6.15	-1.97	[123]
277	$PC_{71}BM$	3.10	62	-5.83	-1.76	[174]
278	$PC_{71}BM$	3.09	74	-5.86	-2.03	[95]
279	$PC_{61}BM$	3.07	71	-5.96	-2.06	[168]
280	$PC_{71}BM$	3.07	28	-6.13	-2.29	[184]
281	$PC_{71}BM$	3.04	32	-6.06	-1.69	[185]
282	$PC_{71}BM$	3.02	48	-5.91	-2.06	[50]
283	$PC_{71}BM$	2.89	80	-6.03	-1.73	[186]
284	$PC_{61}BM$	2.70	22	-5.70	-1.73	[187]
285	$PC_{61}BM$	2.59	25	-6.45	-1.87	[188]
286	$PC_{71}BM$	2.56	66	-5.94	-2.23	[189]
287	$PC_{61}BM$	2.50	42	-5.70	-1.89	[190]
288	$PC_{71}BM$	2.38	43	-6.06	-2.47	[177]
289	$PC_{61}BM$	2.33	40	-6.00	-2.13	[191]
290	$PC_{61}BM$	2.30	18	-6.01	-1.36	[192]
291	$PC_{71}BM$	2.30	52	-5.99	-1.78	[193]
292	$PC_{61}BM$	2.10	30	-6.20	-1.93	[194]
293	$PC_{61}BM$	1.76	40	-6.24	-2.05	[195]
294	$PC_{61}BM$	1.74	20	-6.36	-2.04	[196]
295	$PC_{61}BM$	1.54	25	-6.55	-1.94	[196]
296	$PC_{61}BM$	1.34	33	-5.77	-1.79	[197]
297	$PC_{61}BM$	1.17	25	-5.90	-1.67	[197]
298	$PC_{61}BM$	1.00	24	-5.76	-1.68	[198]
299	$PC_{61}BM$	0.52	26	-5.66	-2.11	[199]
300	$PC_{61}BM$	0.50	22	-5.94	-1.82	[200]

1 Descriptors for ML models

For the first time, 13 descriptors related to the energy conversion process are introduced in our recent work,[201] namely, number of unsaturated atoms in the main conjugation path of donor molecules ($N_{\text{atom}}^{\text{D}}$), vertical ionization potential (IP(v)), polarizability, energy of the electronic transition with the largest oscillator strength (E_{g}), reorganization energy for holes (λ_{h}), hole-electron binding energy (E_{bind}), energy of the electronic transition to the lowest-lying triplet state (E_{T_1}), the energetic difference of HOMO of donor and LUMO of acceptor ($E_{\text{HL}}^{\text{DA}}$), the energetic difference of LUMO of donor and LUMO of acceptor ($E_{\text{LL}}^{\text{DA}}$), change in dipole moment in going from the ground state to the first excited state for donor molecules ($\Delta\mu_{\text{ge}}$), the energetic difference of LUMO and LUMO+1 of acceptors ($\Delta_{\text{L}}^{\text{A}}$), and the energetic differences of HOMO and HOMO-1 (Δ_{H}=E_{HOMO}-$E_{\text{HOMO}-1}$) and LUMO and LUMO+1 (Δ_{L}=$E_{\text{LUMO}+1}$-E_{LUMO}) of donors. Detailed descriptions for these 13 descriptors and their relations with the energy conversion process are provided in ref[[201]]. In this work, a number of new descriptors are also taken into account such as

(1) *The largest oscillator strength for the electronic transition*, f_{osc}. It determines the probability of interaction of a molecule with light over a certain range of energy. This parameter is directly related to the photon absorption.

(2,3) *Energy of the first electronic transition*, E_{S_1} and the associated oscillator strength, $f_{\text{osc}}^{\text{S}_1}$. E_{S_1} is the minimum energy of a photon required for absorption by a molecule. Also, in order to examine the energetic condition for the singlet fission process, it is important to consider both E_{S_1} and E_{T_1}as descriptors. Further, it is worth to include $f_{\text{osc}}^{\text{S}_1}$ as a descriptor, as it describes the importance of the first electronic transition.

(4) *Maximal photogenerated current*, J_{ph}. The maximum obtainable current density can be evaluated by assuming that photon absorption occurs at energies $\geq E_{\text{S}_1}$, and it is calculated by numerically integrating with the energy range from E_{S_1} to the superior limit of the sunlight wavelength (AM1.5 condi-

tion) using the following equation,

$$J_{\mathrm{ph}} = e \int_{E_{S_1}}^{\infty} \phi_{\mathrm{ph}}(\lambda) d\lambda. \quad (1)$$

Here, ϕ_{ph} and e are solar photon flux density and elementary charge, respectively. The reference density was obtained from the American Society for Testing and Materials (ASTM G173-03, AM1.5g). This parameter is known to be directly correlated with the J_{SC}.

(5) *Area of absorption spectra for donors*, Δ_{area}. The absorption spectrum was calculated using the following equation with an half-width half-maximum of 3500 cm^{-1} for the first 20 electronic excitations,

$$\varepsilon(\widetilde{\nu}) = \sum_{i=1}^{20} \varepsilon_i(\widetilde{\nu}) = \sum_{i=1}^{20} \frac{\sqrt{\pi} \cdot e^2 \cdot N}{1000 \cdot \ln(10) \cdot c^2 \cdot m_e} \cdot \frac{f_i}{\sigma} exp[-(\frac{\widetilde{\nu} - \widetilde{\nu}_i}{\sigma})^2]. \quad (2)$$

Area of each spectrum was calculated using the composite trapezoidal rule. This descriptor is expected to correlate with the J_{SC}.

(6) *The most favourable excited state for electronic transition in donor molecules*, S_{N}. For many molecules, excitation other the first electronic transition has the largest oscillator strength, and in these cases, there is a high probability of hole-electron recombination. To account this effect, S_{N} is considered as a descriptor.

(7,8) *Contribution of HOMO/HOMO-1 for the* $S_0 \rightarrow S_{\mathrm{N}}$ *transition*, $C_{\mathrm{H}}/C_{\mathrm{H-1}}$. In our previous study,[201] it is noticed that orbitals other than HOMO also contribute to the $S_0 \rightarrow S_{\mathrm{N}}$ transition; thus these two descriptors may be related to the photon absorption.

(9,10) *Contribution of LUMO/LUMO+1 for the* $S_0 \rightarrow S_{\mathrm{N}}$ *transition*, $C_{\mathrm{L}}/C_{\mathrm{L+1}}$. Orbitals energetically close to LUMO also participate in photon absorption, and therefore, these parameters may influence the J_{SC}.

(11) *HOMO-LUMO gap for donors*, Δ_{HL}. It is calculated as the difference of HOMO and LUMO energies of donor molecules, generally used as an optical gap instead of the E_{g} for its low computational cost.

(12) *Fundamental gap for donors*, E_{fund}. It is calculated as the difference between ionization potential and electron affinity, which is related to the energy required for the electron-hole separation.

(13) *Number of π-electrons in donors*, N_{elec}. In OPVs, excitons are formed by excitations of π-electrons from occupied to unoccupied orbitals; thus N_{elec} may be closely related to the energy conversion process.

(14) *Number of heteroatoms present in the main conjugation path for donors*, $N_{\mathrm{het}}^{\mathrm{D}}$. The presence of heteroatoms such as nitrogen, sulfur, and oxygen, in a conjugated molecule may regulate the geometry through non-covalent interactions and influence its photophysical properties.

(15) *Name of acceptors*, *Acceptor*. This is a categorical descriptor to distinguish two acceptors: $PC_{61}BM$ and $PC_{71}BM$.

2 ML models

In our recent work,[201] a number of ML techniques, such as *k*-nearest neighbour (*k*NN), artificial neural network (ANN), random forest (RF) and gradient boosting regression tree (GBRT), were used to build models using 13 descriptors in combination with the stratified sampling technique and 10-fold cross-validation method, and the GBRT model is found to outperform other ML-models with an impressive *r* of 0.77. However, there is an inherent limitation of all tree-based models that they can not predict beyond the data used to train the model. To overcome this limitation, in this work, both GBRT and ANN models are built from 300 experimental data and a set of descriptors carefully chosen from the complete set of 28 descriptors.

At first, we create 8 groups/strata (Table S2) based on the PCE, and the data points are randomly divided within each group to create train (250 data points) and test (50 data points) subsets. The best set of hyper-parameters are obtained by 10-fold cross-validation over the train set in combination with the stratified sampling method. Once ML-models are optimised, the performance of each model is evaluated using the test set (a completely separate dataset). Leave-one-out cross-validation and error analysis are also carried out to further ascertain the stability of models. This procedure is followed to build all the ML-models reported in this work.

Table S2 Division of the dataset to 8 groups of each having a specific range of PCE. *N* represents the number of data points in a group.

	1	2	3	4	5	6	7	8
PCE	$\leq$3%	3-4%	4-5%	5-6%	6-7%	7-8%	8-9%	>9
N	18	41	76	64	47	28	19	7

Selection of a proper set of descriptors is quite challenging as there is a possibility of non-linear correlations between them. In this work, the polarizability of donor molecules is not considered as a descriptor due to its high computational cost and strong correlation with the $N_{\text{atom}}^{\text{D}}$ (r >0.8). We start to build models

using GBRT technique and 12 descriptors (except polarizability) mentioned in our previous work.[201] The performance of this model is found to be increased when Δ_L^A is replaced with a categorical descriptor: *Acceptor*. Then we start to include new descriptors one by one, and reoptimize hyper-parameters of the model to get optimum results. Out of total 28 descriptors used in this process, the best performance for the GBRT model is obtained with the following 13 descriptors: (1) N_{atom}^D, (2) N_{het}^D, (3) E_{LL}^{DA}, (4) λ_h, (5) E_{HL}^{DA}, (6) Δ_H, (7) Δ_L, (8) IP(v), (9) E_g, (10) $\Delta\mu_{ge}$, (11) E_{bind}, (12) E_{T_1} and (13) *Acceptor*. The same set of descriptors was used to build an ANN model. A simple GBRT model (GBRT*) was also built using 7 easily accessible descriptors such as: N_{atom}^D, Δ_H, Δ_L, Δ_{HL}, E_{HL}^{DA}, E_{LL}^{DA} and *Acceptor*.

3 Calculation of PCE using the Scharber model

The PCE of a photovoltaic cell is commonly expressed as

$$\mathrm{PCE} = \frac{V_{\mathrm{OC}} J_{\mathrm{SC}} \mathrm{FF}}{P_{\mathrm{in}}}, \tag{3}$$

where P_{in} is the intensity of incident light. V_{OC} was calculated from the energetic difference of HOMO of donor ($E_{\mathrm{HOMO}}^{\mathrm{Donor}}$) and LUMO of acceptor molecules ($E_{\mathrm{LUMO}}^{\mathrm{Acceptor}}$) with an empirically determined energy loss of 0.3 eV:

$$V_{\mathrm{OC}} = \frac{1}{e}(E_{\mathrm{LUMO}}^{\mathrm{Acceptor}} - E_{\mathrm{HOMO}}^{\mathrm{Donor}} - 0.3)eV. \tag{4}$$

J_{SC} is calculated by assuming absorption of all photons above the first electronic transition (E_{S_1}) of conjugated molecules, given by the expression:

$$J_{\mathrm{SC}} = e \int_{E_{\mathrm{S}_1}(\lambda)}^{\infty} \mathrm{EQE}\Phi_{\mathrm{AirMass1.5}}(\lambda) d\lambda. \tag{5}$$

Both external quantum efficiency (EQE) and FF were set to 0.65. The reference AM1.5g solar spectrum, provided by the American Society for Testing and Materials (ASTM), was used as incident light.

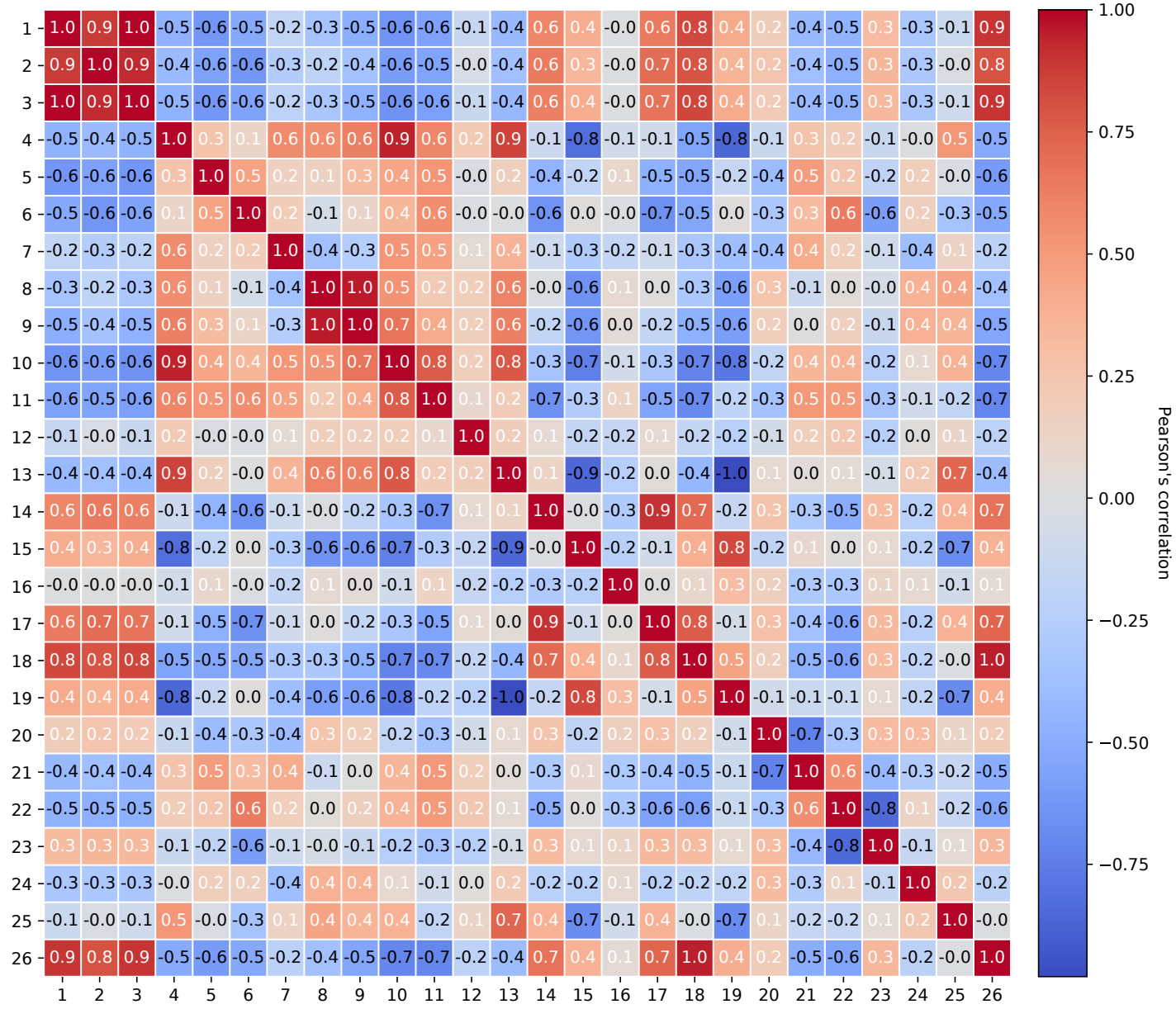

Figure S1 Pearson's correlation coefficient (r) for each possible combination of two descriptors. These are in the following order: 1.$N_{\mathrm{atom}}^{\mathrm{D}}$, 2.$N_{\mathrm{het}}^{\mathrm{D}}$, 3.$N_{\mathrm{elec}}$, 4.$\Delta_{\mathrm{HL}}$, 5.$\Delta_{\mathrm{H}}$, 6.$\Delta_{\mathrm{L}}$, 7.$E_{\mathrm{LL}}^{\mathrm{DA}}$, 8.$E_{\mathrm{HL}}^{\mathrm{DA}}$, 9.IP($v$), 10.$E_{\mathrm{fund}}$, 11.$E_{\mathrm{bind}}$, 12.$\lambda_{\mathrm{h}}$, 13.$E_{\mathrm{S_1}}$, 14.$f_{\mathrm{osc}}^{\mathrm{S_1}}$, 15.$E_{\mathrm{g}}$, 16.$S_{\mathrm{N}}$, 17.$f_{\mathrm{osc}}$, 18.$\Delta_{\mathrm{area}}$, 19.$J_{\mathrm{ph}}$, 20.$C_{\mathrm{H-1}}$, 21.$C_{\mathrm{H}}$, 22.$C_{\mathrm{L}}$, 23.$C_{\mathrm{L+1}}$, 24.$\Delta\mu_{\mathrm{ge}}$, 25.$E_{\mathrm{T_1}}$ and 26. polarizability.

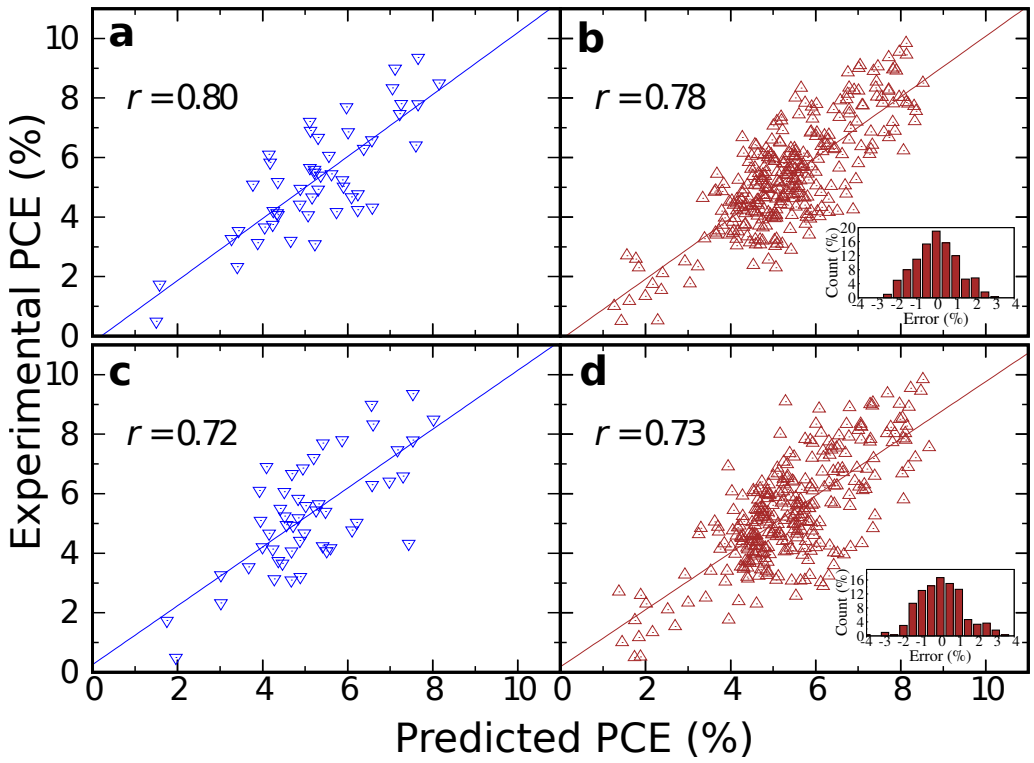

Figure S2 Theoretically predicted vs experimental PCE for the GBRT (a,b) and GBRT* model (c,d). a,c) The test dataset (50 data points) with models trained from 250 data points. b,d) All 300 data points using the LOOCV approach. An inset shows the probability density of prediction errors.

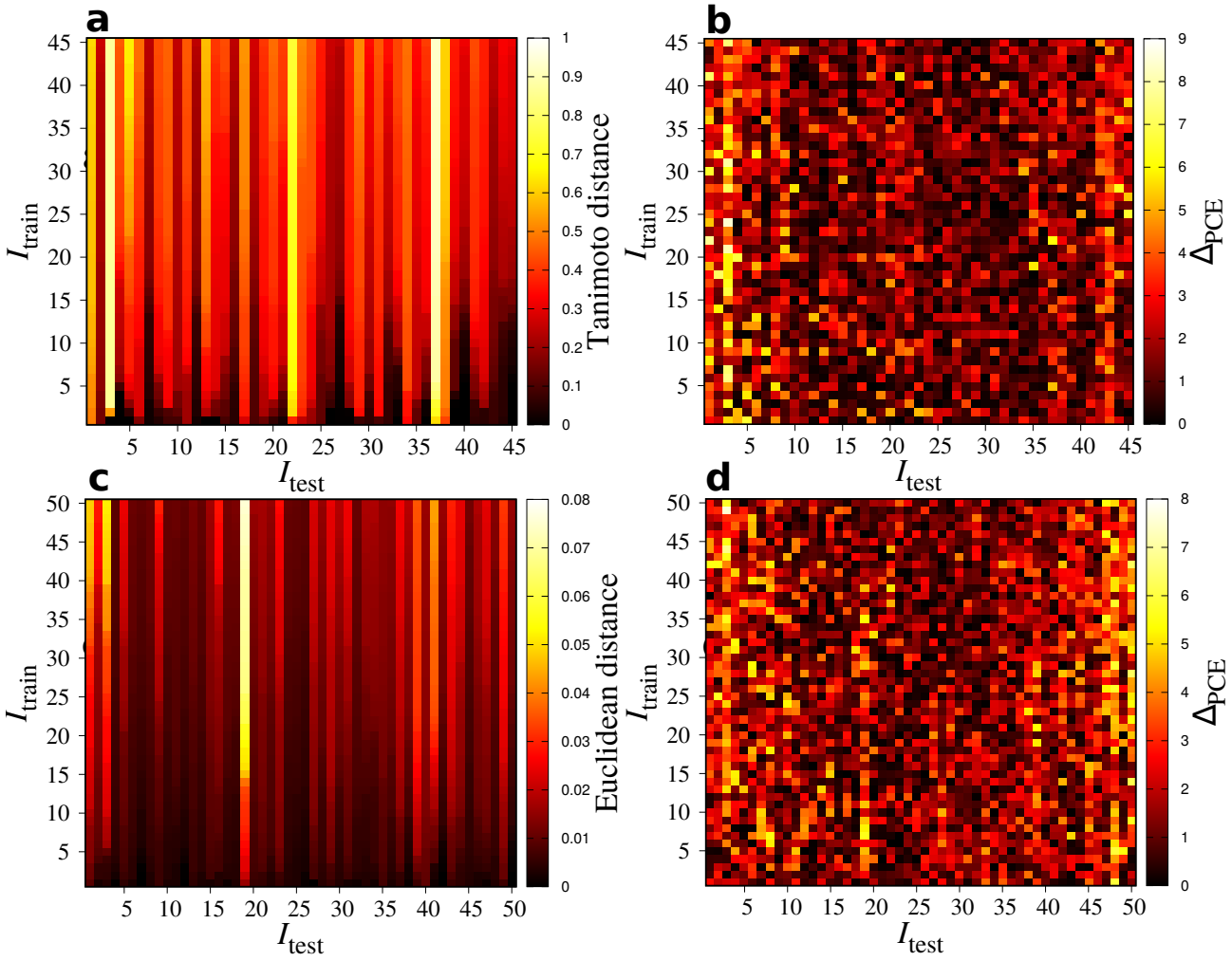

Figure S3 Tanimoto (a) and Euclidean (c) distances of the chemical fingerprints and the normalized features for 45/50 closet datapoints to each sample in the testing set, respectively. The differences of PCE (Δ_{PCE}) of testing samples with respect to the corresponding 45/50 closest training data points are shown in (b, Tanimoto distance) and (d, Euclidean distance). I_{train} and I_{test} are indexes of donor molecules in train and test sets, respectively. Tanimoto distances are calculated by using fingerprints generated by the default set of parameters as implemented in RDKit package.[1]

Table S3 Predicted PCE for chemically different donor molecules than those present in the training set. Predicted PCEs outside and inside the parentheses are computed using GBRT and ANN models.

Donor:Acceptor	Experimental PCE (%)	Predicted PCE (%)	Reference
DR2TDTCz:$PC_{71}BM$	6.75	5.98 (5.78)	[202]
$(DTBT\text{-}TPA)_2An$:$PC_{61}BM$	1.66	3.64 (3.12)	[203]
$(DPP\text{-}TPA)_2An$:$PC_{61}BM$	1.3	2.97 (4.11)	[203]
CAT3STIF:$PC_{71}BM$	4.81	5.74 (5.49)	[204]
CAT3STIF:$PC_{61}BM$	4.06	4.70 (4.97)	[204]
CAT3DBS:$PC_{61}BM$	0.34	4.55 (4.67)	[204]
CAT3STB:$PC_{61}BM$	0.02	4.77 (4.75)	[204]

4 Hypergeometric distribution and z-score

The hypergeometric distribution is a discrete probability distribution that describes the probability of getting k observations in a subpopulation of size n without replacement, given that there are K observations in the entire population of size N.

Z-score is the measure of distance between a data point and the population mean, expressed in standard deviations. For hypergeometric distribution, it is calculated as the difference between the frequency of a molecule in the top set and its expectation value, divided by the standard deviation for the distribution ($\sigma(k)$):

$$z = \frac{k - \langle k \rangle}{\sigma(k)}. \tag{6}$$

Here, $\langle k \rangle$ is the expectation value of k calculated as $\langle k \rangle = nK/N$, and

$$\sigma(k) = \sqrt{\frac{nK(N-n)(N-K)}{N^2(N-1)}}. \tag{7}$$

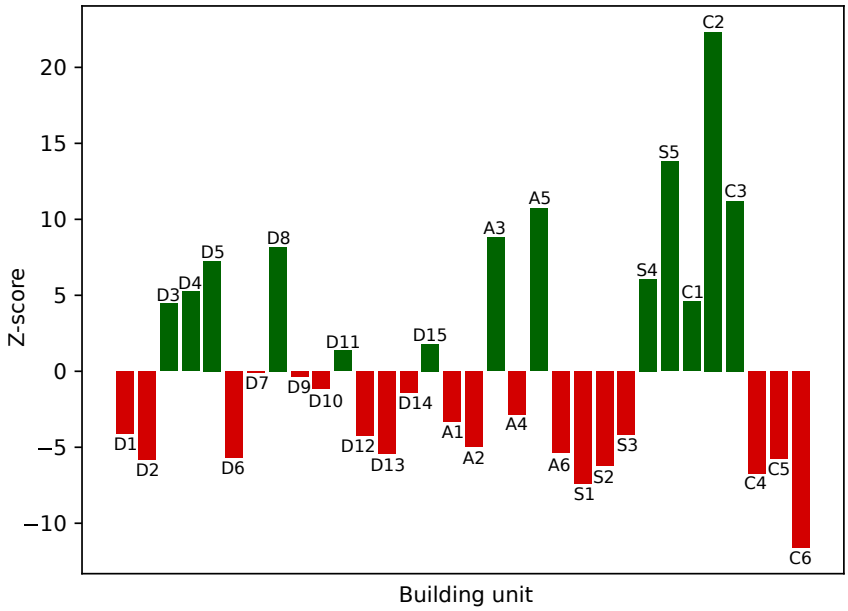

Figure S4 Z-scores for 32 building units.

Table S4 Optical gap of all building units calculated at the M06-2X/6-31G(d) level.

Units	E_g(eV)	E_g(nm)		Units	E_g(eV)	E_g(nm)
D1	5.26	235.8		S1	8.42	147.2
D2	4.83	256.7		S2	7.51	165.0
D3	3.86	321.5		S3	6.22	199.2
D4	4.06	305.2		S4	4.41	281.1
D5	3.86	321.1		S5	3.93	315.5
D6	4.16	297.7		C1	4.38	282.8
D7	4.43	279.6		C2	4.42	280.2
D8	4.03	307.6		C3	4.91	252.4
D9	4.13	300.2		C4	5.36	231.2
D10	3.90	318.1		C5	4.43	279.6
D11	3.56	348.7		C6	4.46	277.7
D12	4.21	294.7				
D13	4.78	259.2				
D14	4.44	279.3				
D15	3.74	331.2				
A1	4.42	280.7				
A2	4.40	281.8				
A3	3.79	327.5				
A4	3.58	346.4				
A5	2.93	422.6				
A6	3.77	328.9				

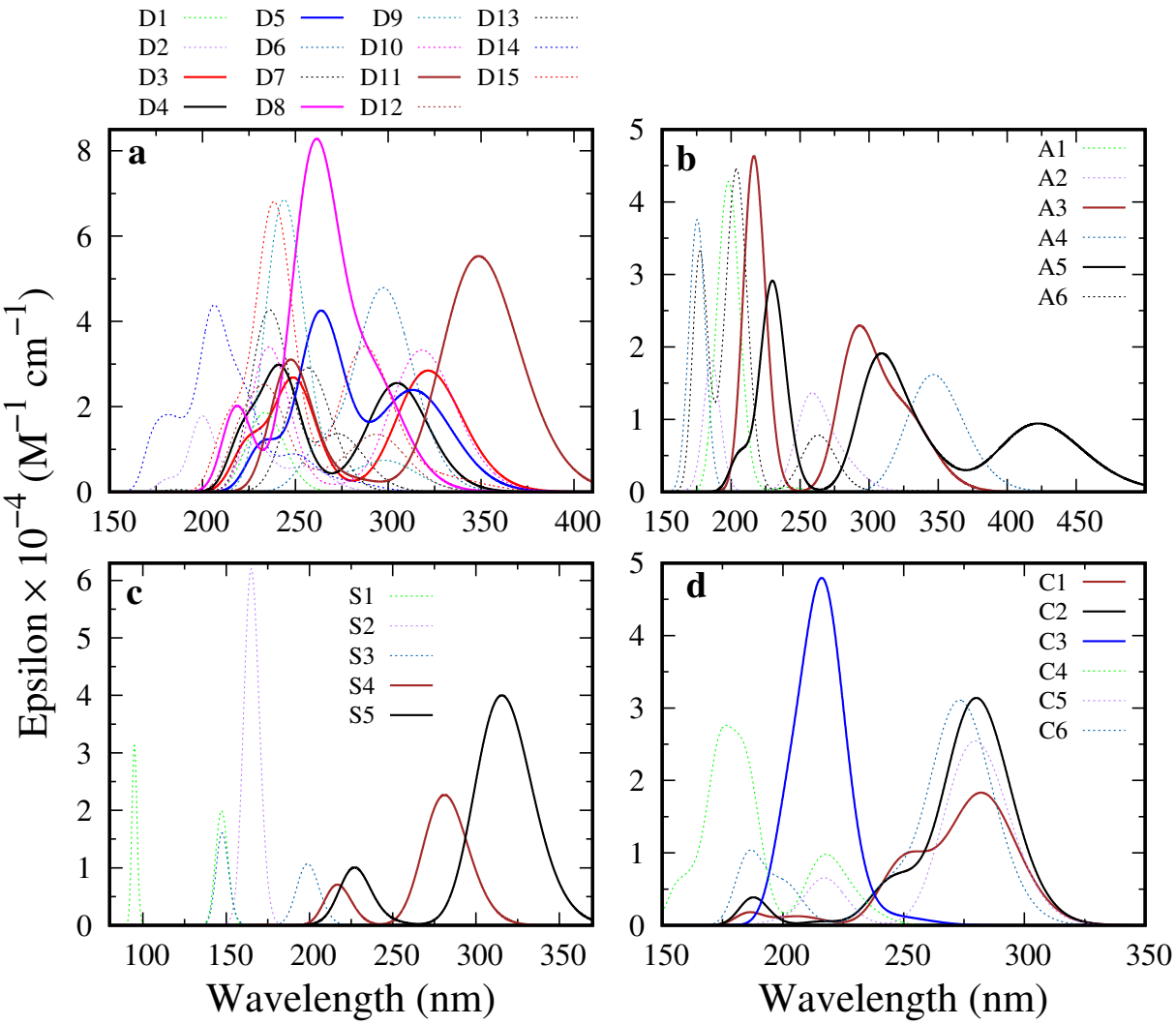

Figure S5 Absorption spectra of building units. Half width at half maximum (HWHM) of each spectrum is 1500 cm^{-1}.

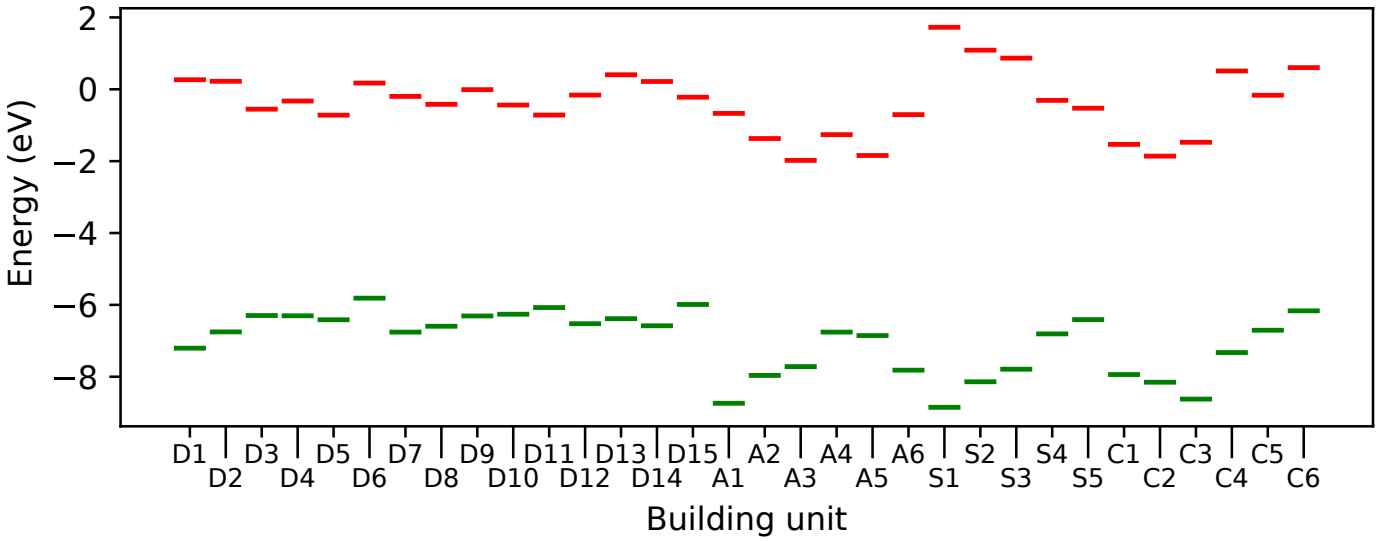

Figure S6 Energies of frontier orbitals of building units.

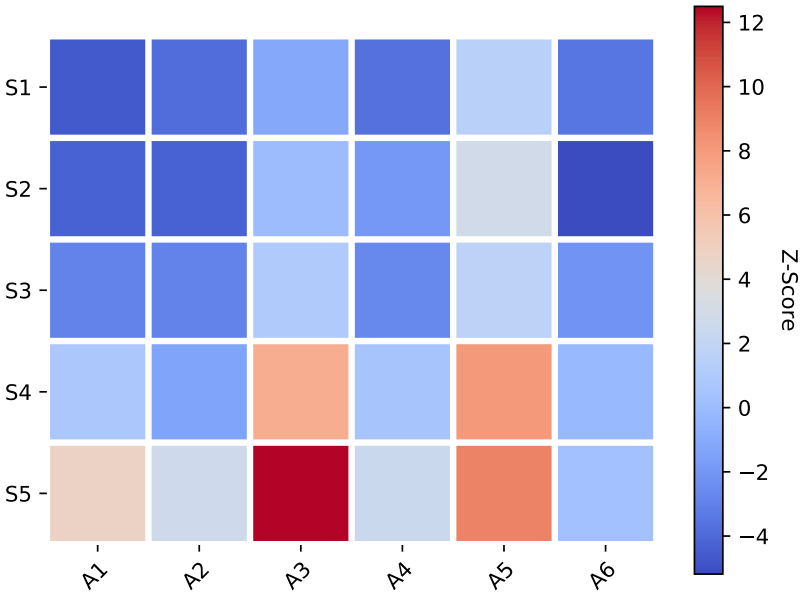

Figure S7 Z-scores for combinations of acceptor and π-spacer units.

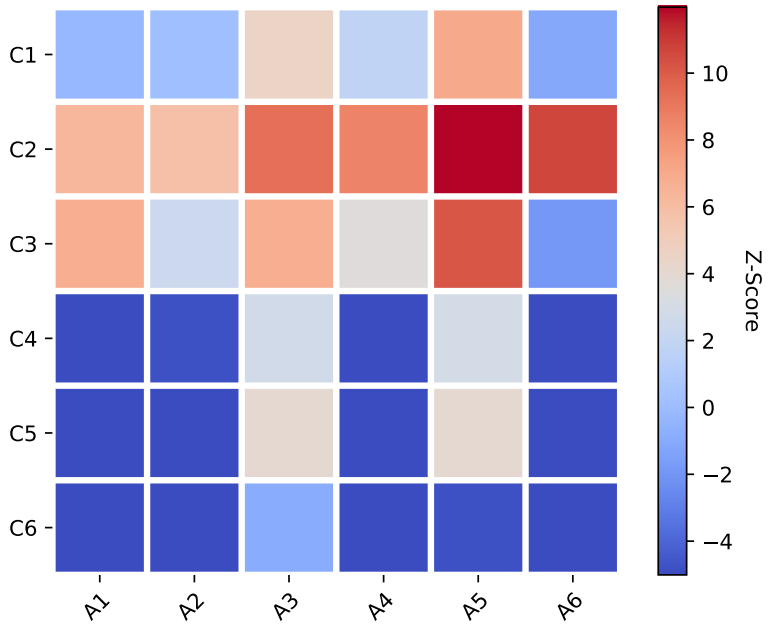

Figure S8 Z-scores for combinations of acceptor and end-capping units.

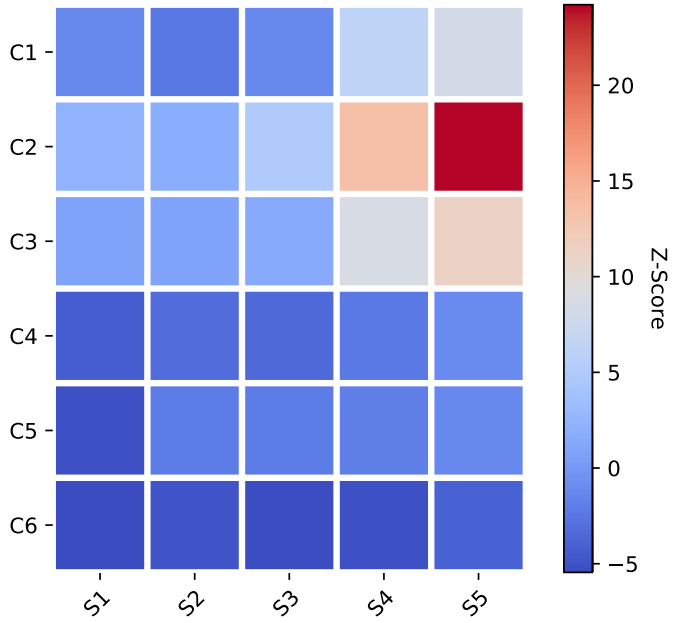

Figure S9 Z-scores for combinations of π-spacer and end-capping units.

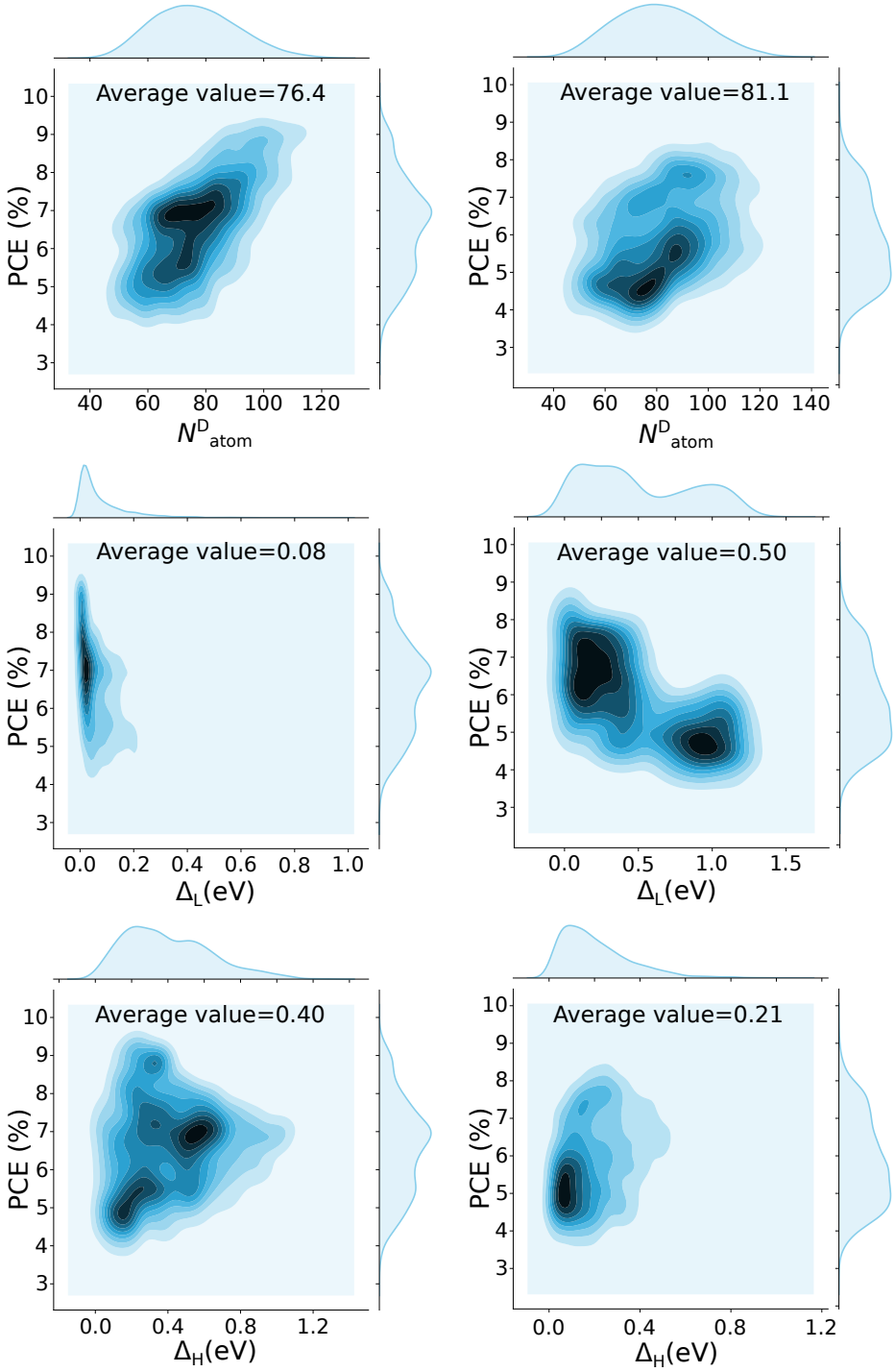

Figure S10 Joint distributions using kernel density estimation for descriptors (N^{D}_{atom}, Δ_L and Δ_H) and the predicted PCEs for CASDSAC (left panel) and CDSASDC (right panel) patterns. The marginal distributions are for the individual variables. The average value of each descriptor is provided in the corresponding subfigure.

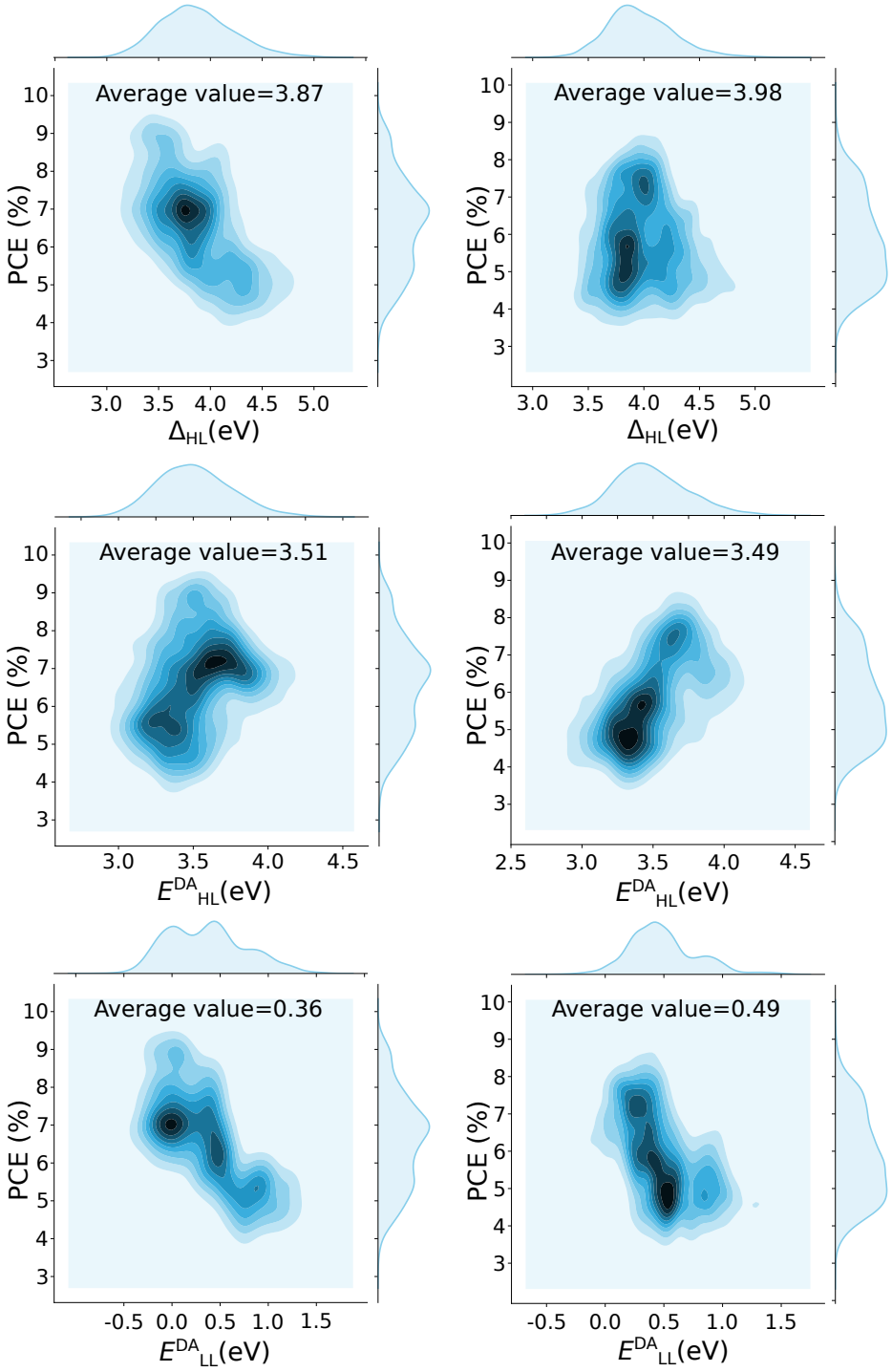

Figure S11 Joint distributions using kernel density estimation for descriptors (Δ_{HL}, E^{DA}_{HL} and E^{DA}_{LL}) and the predicted PCEs for CASDSAC (left panel) and CDSASDC (right panel) patterns. The marginal distributions are for the individual variables. The average value of each descriptor is provided in the corresponding subfigure.

Table S5 Promising molecules for OPVs with predicted PCE $>$ 8.0% selected by screening 1000 candidates using both GBRT and ANN models. Reported values are predicted using the ANN-model.

S No.	molecules	PCE (%)		S No.	molecules	PCE (%)
1	C2-A1-S5-D5-S5-A1-C2	10.8		64	C1-A1-S4-D8-S4-A1-C1	8.7
2	C1-A3-S5-D11-S5-A3-C1	10.7		65	C2-A5-S4-D5-S4-A5-C2	8.7
3	C2-A3-S5-D3-S5-A3-C2	10.7		66	C1-D5-S3-A1-S3-D5-C1	8.7
4	C2-A1-S5-D3-S5-A1-C2	10.5		67	C2-D7-S5-A1-S5-D7-C2	8.7
5	C2-A3-S5-D10-S5-A3-C2	10.4		68	C2-A5-S5-D9-S5-A5-C2	8.6
6	C2-A1-S5-D9-S5-A1-C2	10.4		69	C2-D11-S3-A1-S3-D11-C2	8.6
7	C2-A3-S5-D8-S5-A3-C2	10.3		70	C1-A5-S4-D10-S4-A5-C1	8.6
8	C2-A3-S5-D11-S5-A3-C2	10.2		71	C2-S5-D5-S5-C2	8.6
9	C1-A3-S4-D5-S4-A3-C1	10.1		72	C2-A5-S5-D11-S5-A5-C2	8.5
10	C2-A3-S2-D15-S2-A3-C2	10.1		73	C5-A3-S4-D5-S4-A3-C5	8.5
11	C2-A1-S5-D11-S5-A1-C2	10.1		74	C2-A5-S5-D10-S5-A5-C2	8.5
12	C2-A1-S5-D8-S5-A1-C2	10.0		75	C3-A3-S5-D15-S5-A3-C3	8.5
13	C2-A3-S5-D4-S5-A3-C2	10.0		76	C1-D3-S5-A1-S5-D3-C1	8.5
14	C2-A3-S4-D8-S4-A3-C2	9.9		77	C2-A1-S5-D10-S5-A1-C2	8.5
15	C2-A3-S3-D4-S3-A3-C2	9.9		78	C2-A5-S4-D8-S4-A5-C2	8.4
16	C2-A3-S5-D15-S5-A3-C2	9.8		79	C3-A3-S4-D8-S4-A3-C3	8.4
17	C3-A3-S5-D5-S5-A3-C3	9.6		80	C1-A2-S5-D4-S5-A2-C1	8.4
18	C2-A1-S5-D15-S5-A1-C2	9.6		81	C2-A3-S5-D9-S5-A3-C2	8.4
19	C3-A3-S4-D11-S4-A3-C3	9.6		82	C5-A3-S4-D11-S4-A3-C5	8.4
20	C2-A5-S4-D9-S4-A5-C2	9.6		83	C1-A3-S5-D10-S5-A3-C1	8.4
21	C1-A3-S4-D8-S4-A3-C1	9.5		84	C1-D3-S4-A1-S4-D3-C1	8.4
22	C3-A3-S5-D11-S5-A3-C3	9.4		85	C2-A2-S5-D9-S5-A2-C2	8.4
23	C2-A4-S5-D11-S5-A4-C2	9.4		86	C2-A5-S3-D8-S3-A5-C2	8.4
24	C1-A3-S3-D4-S3-A3-C1	9.4		87	C3-A3-S5-D3-S5-A3-C3	8.4

25	C1-A3-S5-D4-S5-A3-C1	9.4	88	C3-A2-S5-D5-S5-A2-C3	8.3
26	C3-A3-S5-D9-S5-A3-C3	9.3	89	C2-A5-S5-D5-S5-A5-C2	8.3
27	C1-A3-S5-D3-S5-A3-C1	9.3	90	C5-A3-S2-D5-S2-A3-C5	8.3
28	C1-A3-S5-D8-S5-A3-C1	9.3	91	C4-A3-S5-D11-S5-A3-C4	8.3
29	C1-A3-S5-D5-S5-A3-C1	9.3	92	C4-A3-S5-D5-S5-A3-C4	8.3
30	C3-A3-S5-D10-S5-A3-C3	9.3	93	C4-A3-S4-D5-S4-A3-C4	8.3
31	C1-A3-S5-D7-S5-A3-C1	9.2	94	C2-D5-S4-A5-S4-D5-C2	8.3
32	C1-A3-S5-D9-S5-A3-C1	9.2	95	C1-A2-S5-D7-S5-A2-C1	8.3
33	C3-A3-S4-D5-S4-A3-C3	9.2	96	C2-A4-S5-D3-S5-A4-C2	8.3
34	C2-D5-S3-A1-S3-D5-C2	9.2	97	C2-D11-S4-A3-S4-D11-C2	8.3
35	C2-A4-S5-D10-S5-A4-C2	9.2	98	C1-A5-S1-D4-S1-A5-C1	8.3
36	C3-A3-S3-D4-S3-A3-C3	9.2	99	C5-A3-S3-D5-S3-A3-C5	8.2
37	C3-A3-S5-D7-S5-A3-C3	9.1	100	C2-A5-S5-D8-S5-A5-C2	8.2
38	C3-A1-S5-D5-S5-A1-C3	9.1	101	C5-A3-S4-D9-S4-A3-C5	8.2
39	C2-A4-S5-D5-S5-A4-C2	9.1	102	C1-A5-S5-D5-S5-A5-C1	8.2
40	C1-A2-S5-D5-S5-A2-C1	9.0	103	C4-A3-S5-D3-S5-A3-C4	8.2
41	C1-A3-S4-D14-S4-A3-C1	9.0	104	C5-A3-S5-D3-S5-A3-C5	8.2
42	C2-A4-S5-D9-S5-A4-C2	9.0	105	C5-A3-S3-D11-S3-A3-C5	8.2
43	C3-A3-S4-D10-S4-A3-C3	9.0	106	C1-A3-S2-D8-S2-A3-C1	8.2
44	C3-A1-S3-D5-S3-A1-C3	9.0	107	C3-A2-S5-D1-S5-A2-C3	8.2
45	C1-A3-S5-D15-S5-A3-C1	9.0	108	C2-A6-S5-D5-S5-A6-C2	8.2
46	C2-A3-S5-D5-S5-A3-C2	8.9	109	C2-A6-S5-D4-S5-A6-C2	8.2
47	C1-A1-S5-D8-S5-A1-C1	8.9	110	C1-A2-S5-D3-S5-A2-C1	8.1
48	C2-A1-S5-D14-S5-A1-C2	8.8	111	C5-A3-S4-D3-S4-A3-C5	8.1
49	C2-A5-S5-D4-S5-A5-C2	8.8	112	C2-A5-S4-D14-S4-A5-C2	8.1
50	C1-A3-S4-D15-S4-A3-C1	8.8	113	C5-A3-S5-D5-S5-A3-C5	8.1
51	C2-D3-S4-A1-S4-D3-C2	8.8	114	C2-D11-S3-A3-S3-D11-C2	8.1
52	C1-A5-S3-D11-S3-A5-C1	8.8	115	C3-A2-S5-D9-S5-A2-C3	8.1

53	C2-A4-S4-D11-S4-A4-C2	8.8		116	C2-D12-S5-A6-S5-D12-C2	8.1
54	C2-A4-S3-D10-S3-A4-C2	8.8		117	C1-A5-S1-D3-S1-A5-C1	8.1
55	C2-A5-S1-D3-S1-A5-C2	8.8		118	C3-A1-S5-D11-S5-A1-C3	8.1
56	C2-A2-S5-D3-S5-A2-C2	8.8		119	C3-A3-S4-D15-S4-A3-C3	8.1
57	C1-A2-S5-D11-S5-A2-C1	8.7		120	C1-D5-S3-A3-S3-D5-C1	8.1
58	C2-A2-S5-D11-S5-A2-C2	8.7		121	C2-D3-S3-A3-S3-D3-C2	8.1
59	C3-A3-S5-D8-S5-A3-C3	8.7		122	C4-A3-S4-D3-S4-A3-C4	8.1
60	C1-A5-S5-D7-S5-A5-C1	8.7		123	C2-A4-S5-D4-S5-A4-C2	8.1
61	C2-D7-S5-A6-S5-D7-C2	8.7		124	C2-A5-S5-D3-S5-A5-C2	8.0
62	C1-A5-S5-D11-S5-A5-C1	8.7		125	C2-D9-S4-A1-S4-D9-C2	8.0
63	C2-D7-S5-A3-S5-D7-C2	8.7		126	C1-A5-S4-D5-S4-A5-C1	8.0

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