

## Supporting Information

### **Prediction of Carbon Dioxide Adsorption via Deep Learning**

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## **Materials and catalyst characterization**

Vulcan XC605 was purchased from Cabot Corporation, USA. Activated carbon, Darco (AC Darco) was obtained from Aldrich Chemical Company Ltd. Activated Coconut Charcoal (AC Charcoal) was achieved from Fisher Scientific Company. Mesoporous carbons (MC-450, MC-600 and MC-850) was synthesized using enhanced hydrogen-bonding interaction method.<sup>[1]</sup> N<sub>2</sub> adsorption-desorption isotherms were analyzed on a TriStar 3000 volumetric adsorption analyzer manufactured by Micromeritics Instrument Corp. Prior to analysis, all samples were activated at 150 °C for 12 h.

## **CO<sub>2</sub> adsorption procedure**

The samples were dried and subjected to four cycles of pressurization to 5 bar with CO<sub>2</sub> for 0.5 h and then to vacuum at 25 °C until the mass did not change. The mass change between the pressurization and vacuum processes was employed to determine the CO<sub>2</sub> adsorption capacity (mmol CO<sub>2</sub> adsorbed per gram sample). All results are the average data obtained from four cycles.

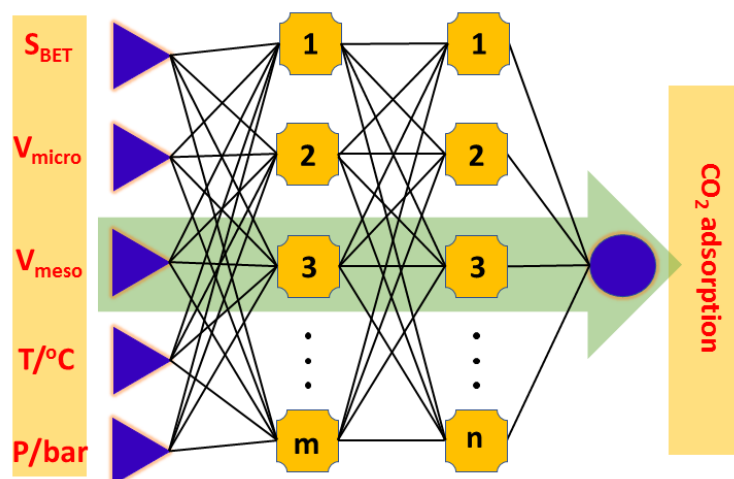
## **Screening textural properties of porous carbons and corresponding CO<sub>2</sub> adsorption capacity**

We screen the porous carbons with different preparation method, pore structure and textural properties. One key rule is that all screened porous carbons almost have no heteroatom N, since the amount of N has been considered as an important influence factor for the CO<sub>2</sub> adsorption capacity. CO<sub>2</sub> adsorption and textural properties (surface area, micropore and mesopore volume) data of 500 porous carbons at different adsorption conditions (temperature and pressure) was collected as the training and predicted set in the literature.<sup>[2,3]</sup>

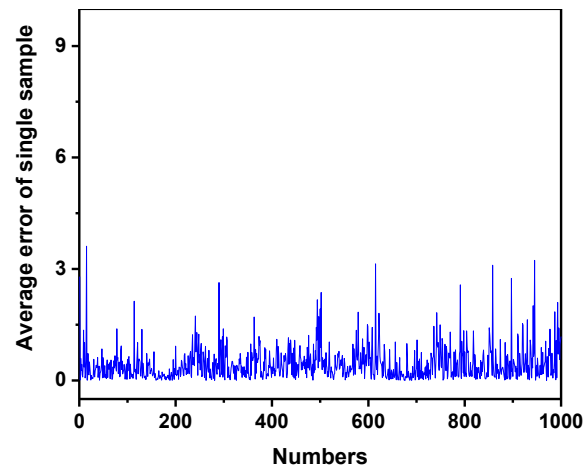
## **Training notes**

The NN and DNN with one and two hidden layers respectively was created in MATLAB R2018a environment using backpropagation algorithm. The weights and biases were the key two parameters to determine neural network structure. The neural network was allowed to adjust the weight and biases value during training to improve their performance. Neurons arranged in layers were needed to be connected each other into a neural network. Each neuron is usually a simple processing unit with many inputs to produce an output. Various network structures with different numbers of neurons and one hidden layer were examined for NN. The numbers of training and testing objectives were 12 and 6 respectively. The selection of neurons was significantly important. In our study, a part of  $S_{\text{BET}}$ ,  $V_{\text{micro}}$  and  $V_{\text{meso}}$  as well as the adsorption conditions (temperature and pressure) were selected as the input neurons. And CO<sub>2</sub> adsorption capacity was chosen as the

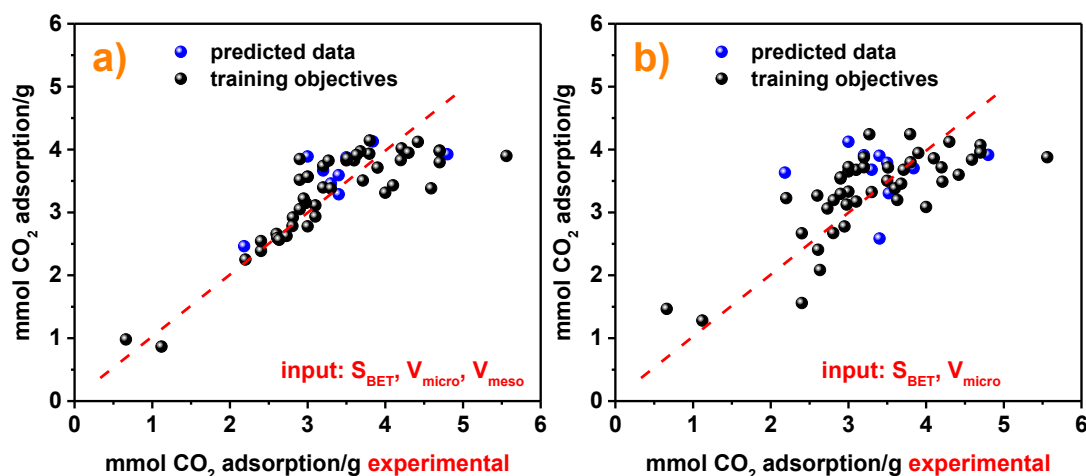
output neuron. Before the creation, the inputs and outputs are normalized in the range of 0 to 1.<sup>[4]</sup> For simplicity, we assume that one hidden layer for NN and two hidden layers for DNN was chosen in our work, and the hidden neuron numbers were optimized by comparing the results derived from different hidden neurons numbers. Since, too little hidden neurons lead to big goal error, and NN became too complicated if the hidden neurons were too many. Backpropagation training method was used to train the neural networks. Training numbers were chosen less than 100000, and goal errors were chosen as 0.001 according to the reported study.<sup>[4]</sup> And then, the predicted data was achieved using linear or nonlinear combination of the input vector, weights, biases and transfer functions.<sup>[4]</sup> Among these analyses, NN-1, NN-2 and NN-3 with five hidden neurons in the hidden layer performed best compared with other networks. For DNN, the selected neuron number of hidden layers was 8 and 8 respectively according to the optimized results.



**Figure S1.** The architecture of deep neural network (DNN) with five neurons as the input.

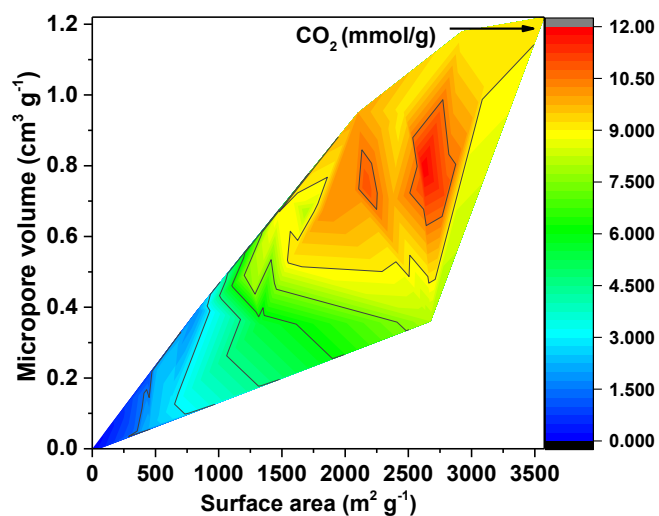


**Figure S2.** Average error of single sample VS training iterations of random 1000 training data



**Figure S3.** The correlations between CO<sub>2</sub> adsorption data achieved from experiment and estimated from NN (a:  $S_{\text{BET}}\text{-}V_{\text{micro}}\text{-}V_{\text{meso}}$ ; b:  $S_{\text{BET}}\text{-}V_{\text{micro}}$ )

We screened out about 80 adsorption data for porous carbons at 25 °C under atmospheric pressure and the corresponding textural properties from Table S2. Then we used  $S_{\text{BET}}\text{-}V_{\text{micro}}$  and  $S_{\text{BET}}\text{-}V_{\text{micro}}\text{-}V_{\text{meso}}$  as variables to train the NN respectively, and then compared the predicted and experimental CO<sub>2</sub> adsorption results. The structure of the NN was the same with the NN-1, NN-2, and NN-3 used in our manuscript. The obtained results are shown in Figure S3. Figure S3a exhibits a better fitting effect than Figure S3b, suggesting that  $V_{\text{meso}}$  should be also an influencing factor for CO<sub>2</sub> adsorption under atmospheric pressure.



**Figure S4.** The correlation between CO<sub>2</sub> uptake, surface area and micropore volume at the same adsorption conditions (25 °C and 5 bar).

The blank area was ascribed to the data unavailable, since it was very difficult to synthesize the porous carbon with both high  $S_{\text{BET}}$  ( $V_{\text{micro}}$ ) and low  $V_{\text{micro}}$  ( $S_{\text{BET}}$ ). The related discussion was also added into the manuscript.



**Table S1.** Porosimetry data for the carbonaceous materials<sup>[1]</sup>

Sample	S <sub>BET</sub> (m <sup>2</sup> /g)	V <sub>total</sub> (cm <sup>3</sup> /g)	V <sub>micro</sub> (cm <sup>3</sup> /g)	V <sub>meso</sub> (cm <sup>3</sup> /g)
AC	798	0.6	0.42	0.18
S300	241	1.1	0.09	1.01
S450	448	1.3	0.21	1.09
S650	826	1.3	0.39	0.91
S800	895	1.3	0.40	0.90
S1000	862	1.3	0.39	0.91
S1200	678	1.4	0.30	1.10
A300	304	1.2	0.14	1.06
A550	500	1.0	0.23	0.77
A800	931	1.4	0.39	1.01
A1000	675	1.4	0.27	1.13
A1200	427	1.1	0.16	0.94

**Table S2.** Porosimetry and CO<sub>2</sub> adsorption data of porous carbons collected in the literature and our lab<sup>[1, 3]</sup>

Entry	S <sub>BET</sub> (m <sup>2</sup> /g)	V <sub>total</sub> (cm <sup>3</sup> /g)	V <sub>micro</sub> (cm <sup>3</sup> /g)	T(°C)	P(bar)	CO <sub>2</sub> uptake (mmol/g)
1	798	0.18	0.42	25	5	2
2	241	1.01	0.09	25	5	0.7
3	448	1.09	0.21	25	5	0.9
4	826	0.91	0.39	25	5	1.8
5	895	0.9	0.4	25	5	2.8
6	862	0.91	0.39	25	5	2.1
7	678	1.1	0.3	25	5	2.3
8	304	1.06	0.14	25	5	0.9
9	500	0.77	0.23	25	5	2.2
10	931	1.01	0.39	25	5	3
11	675	1.13	0.27	25	5	1.8
12	427	0.94	0.16	25	5	1.4
13	451	0.61	0.06	25	5	2.3
14	862	0.91	0.39	25	5	2.1
15	798	0.18	0.42	25	10	2
16	895	0.9	0.4	25	10	3.1
17	862	0.91	0.39	25	10	2.8
18	678	1.1	0.3	25	10	2.9
19	931	1.01	0.39	25	10	3.3
20	675	1.13	0.27	25	5	2.3
21	427	0.94	0.16	25	5	1.8
22	887	0.075	0.347	25	0.04	0.35
23	887	0.075	0.347	25	0.1	0.7
24	887	0.075	0.347	25	0.175	1.05
25	887	0.075	0.347	25	0.35	1.6
26	887	0.075	0.347	25	0.53	1.9
27	887	0.075	0.347	25	0.7	2.21
28	887	0.075	0.347	25	0.87	2.35
29	887	0.075	0.347	25	1	2.6
30	618	1.115	0.217	25	0.04	0.35
31	618	1.115	0.217	25	0.1	0.7
32	618	1.115	0.217	25	0.175	1.05
33	618	1.115	0.217	25	0.35	1.5
34	618	1.115	0.217	25	0.53	1.8
35	618	1.115	0.217	25	0.7	2.1
36	618	1.115	0.217	25	0.87	2.25
37	618	1.115	0.217	25	1	2.4
38	2073	0.138	0.731	0	1	7.17
39	2073	0.138	0.731	25	1	4.21
40	2073	0.138	0.731	50	1	2.47

41	2073	0.138	0.731	0	10	16.44
42	2073	0.138	0.731	25	10	12.74
43	2073	0.138	0.731	0	9	15.2
44	2073	0.138	0.731	0	8	15.5
45	2073	0.138	0.731	0	7	15.2
46	2073	0.138	0.731	0	6	15
47	2073	0.138	0.731	0	5	14.2
48	2073	0.138	0.731	0	4	13
49	2073	0.138	0.731	0	3	12
50	2073	0.138	0.731	0	2	10.4
51	2073	0.138	0.731	0	0.9	6.5
52	2073	0.138	0.731	0	0.8	6
53	2073	0.138	0.731	0	0.7	5.7
54	2073	0.138	0.731	0	0.6	5.2
55	2073	0.138	0.731	0	0.5	4.8
56	2073	0.138	0.731	0	0.4	4.1
57	2073	0.138	0.731	0	0.3	3.4
58	2073	0.138	0.731	0	0.2	2.6
59	2073	0.138	0.731	0	0.1	1.5
60	2073	0.138	0.731	25	0.1	0.7
61	2073	0.138	0.731	25	0.2	1.3
62	2073	0.138	0.731	25	0.3	1.75
63	2073	0.138	0.731	25	0.4	2.25
64	2073	0.138	0.731	25	0.5	2.5
65	2073	0.138	0.731	25	0.6	3
66	2073	0.138	0.731	25	0.7	3.25
67	2073	0.138	0.731	25	0.8	3.6
68	2073	0.138	0.731	25	0.9	3.7
69	2073	0.138	0.731	25	1	4
70	2073	0.138	0.731	25	2	6.8
71	2073	0.138	0.731	25	3	8
72	2073	0.138	0.731	25	4	8.8
73	2073	0.138	0.731	25	5	10.2
74	2073	0.138	0.731	25	6	11
75	2073	0.138	0.731	25	7	11.5
76	2073	0.138	0.731	25	8	12
77	2073	0.138	0.731	25	9	12.5
78	2073	0.138	0.731	25	10	12.6
79	2785	0.644	0.716	0	1	5.09
80	2785	0.644	0.716	25	1	2.81
81	2785	0.644	0.716	50	1	1.52
82	2785	0.644	0.716	0	10	23.27
83	2785	0.644	0.716	0	0.1	0.9
84	2785	0.644	0.716	0	0.2	1.5

85	2785	0.644	0.716	0	0.3	2.1
86	2785	0.644	0.716	0	0.4	2.5
87	2785	0.644	0.716	0	0.5	3
88	2785	0.644	0.716	0	0.6	3.5
89	2785	0.644	0.716	0	0.7	3.9
90	2785	0.644	0.716	0	0.8	4.2
91	2785	0.644	0.716	0	0.9	4.5
92	2785	0.644	0.716	0	2	9.6
93	2785	0.644	0.716	0	3	12.3
94	2785	0.644	0.716	0	4	14
95	2785	0.644	0.716	0	5	17
96	2785	0.644	0.716	0	6	18.5
97	2785	0.644	0.716	0	7	20
98	2785	0.644	0.716	0	8	21.3
99	2785	0.644	0.716	0	9	22
100	2785	0.644	0.716	25	0.1	0.4
101	2785	0.644	0.716	25	0.2	0.7
102	2785	0.644	0.716	25	0.3	1.1
103	2785	0.644	0.716	25	0.4	1.35
104	2785	0.644	0.716	25	0.5	1.6
105	2785	0.644	0.716	25	0.6	1.75
106	2785	0.644	0.716	25	0.7	2
107	2785	0.644	0.716	25	0.8	2.3
108	2785	0.644	0.716	25	0.9	2.5
109	2785	0.644	0.716	25	2	6
110	2785	0.644	0.716	25	3	7.5
111	2785	0.644	0.716	25	4	9
112	2785	0.644	0.716	25	5	11
113	2785	0.644	0.716	25	6	12.5
114	2785	0.644	0.716	25	7	13
115	2785	0.644	0.716	25	8	14
116	2785	0.644	0.716	25	9	15.5
117	2785	0.644	0.716	25	10	16.05
118	1624	0.073	0.589	0	1	7.55
119	1624	0.073	0.589	25	1	4.42
120	1624	0.073	0.589	50	1	2.86
121	1624	0.073	0.589	0	10	13.34
122	1624	0.073	0.589	25	10	11.59
123	1624	0.073	0.589	0	2	9.7
124	1624	0.073	0.589	0	4	11.8
125	1624	0.073	0.589	0	5	12
126	1624	0.073	0.589	0	7	12.5
127	1624	0.073	0.589	0	9	12.7
128	1624	0.073	0.589	0	10	12.9

129	1624	0.073	0.589	0	6	12
130	1624	0.073	0.589	0	8	12.8
131	1624	0.073	0.589	0	3	10.5
132	1624	0.073	0.589	0	0.1	2
133	1624	0.073	0.589	0	0.3	3.7
134	1624	0.073	0.589	0	0.4	4.5
135	1624	0.073	0.589	0	0.6	5.6
136	1624	0.073	0.589	0	0.7	6.2
137	1624	0.073	0.589	0	0.9	7
138	1624	0.073	0.589	0	0.5	5.1
139	1624	0.073	0.589	0	0.8	6.5
140	1624	0.073	0.589	0	0.2	3
141	1624	0.073	0.589	0	2	8.5
142	1624	0.073	0.589	25	0.1	1
143	1624	0.073	0.589	25	0.2	1.6
144	1624	0.073	0.589	25	0.3	2.25
145	1624	0.073	0.589	25	0.4	2.6
146	1624	0.073	0.589	25	0.5	3.01
147	1624	0.073	0.589	25	0.6	3.4
148	1624	0.073	0.589	25	0.7	3.75
149	1624	0.073	0.589	25	0.8	4.05
150	1624	0.073	0.589	25	0.9	4.2
151	1624	0.073	0.589	25	2	6.25
152	1624	0.073	0.589	25	3	7.5
153	1624	0.073	0.589	25	4	8.75
154	1624	0.073	0.589	25	5	9
155	1624	0.073	0.589	25	6	10
156	1624	0.073	0.589	25	7	10.7
157	1624	0.073	0.589	25	8	11
158	1624	0.073	0.589	25	9	11.2
159	1624	0.073	0.589	25	10	11.5
160	2620	0.432	0.793	0	1	6.89
161	2620	0.432	0.793	25	1	4
162	2620	0.432	0.793	50	1	2.38
163	2620	0.432	0.793	0	10	23.26
164	2620	0.432	0.793	25	10	16.81
165	2620	0.432	0.793	0	0.1	1.4
166	2620	0.432	0.793	0	0.2	2.2
167	2620	0.432	0.793	0	0.3	3
168	2620	0.432	0.793	0	0.4	3.4
169	2620	0.432	0.793	0	0.5	4.2
170	2620	0.432	0.793	0	0.6	4.7
171	2620	0.432	0.793	0	0.7	5.4
172	2620	0.432	0.793	0	0.8	5.7

173	2620	0.432	0.793	0	0.9	6.4
174	2620	0.432	0.793	0	2	11
175	2620	0.432	0.793	0	3	13.2
176	2620	0.432	0.793	0	4	16.2
177	2620	0.432	0.793	0	5	18
178	2620	0.432	0.793	0	6	19
179	2620	0.432	0.793	0	7	20.5
180	2620	0.432	0.793	0	8	21.5
181	2620	0.432	0.793	0	9	22.5
182	2620	0.432	0.793	0	10	23
183	2620	0.432	0.793	25	0.1	0.75
184	2620	0.432	0.793	25	0.2	1.25
185	2620	0.432	0.793	25	0.3	1.6
186	2620	0.432	0.793	25	0.4	2.1
187	2620	0.432	0.793	25	0.5	2.5
188	2620	0.432	0.793	25	0.6	2.7
189	2620	0.432	0.793	25	0.7	3.1
190	2620	0.432	0.793	25	0.8	3.48
191	2620	0.432	0.793	25	0.9	3.7
192	2620	0.432	0.793	25	2	7
193	2620	0.432	0.793	25	3	9
194	2620	0.432	0.793	25	4	10.6
195	2620	0.432	0.793	25	5	12
196	2620	0.432	0.793	25	6	13
197	2620	0.432	0.793	25	7	14.5
198	2620	0.432	0.793	25	8	15.5
199	2620	0.432	0.793	25	9	16.25
200	2620	0.432	0.793	25	10	17
201	2162	0.207	0.917	25	0.2	1.13
202	2162	0.207	0.917	25	0.3	1.6
203	2162	0.207	0.917	25	0.5	2.6
204	2162	0.207	0.917	25	0.8	3.5
205	2162	0.207	0.917	25	1	4.1
206	2162	0.207	0.917	25	0.1	0.69
207	2162	0.207	0.917	25	0.4	2.27
208	2162	0.207	0.917	25	0.6	2.82
209	2162	0.207	0.917	25	0.7	3.3
210	2162	0.207	0.917	25	0.9	3.98
211	2180	0.075	0.928	25	0.2	2
212	2180	0.075	0.928	25	0.4	3.18
213	2180	0.075	0.928	25	0.6	4.06
214	2180	0.075	0.928	25	0.8	4.77
215	2180	0.075	0.928	25	1	5.56
216	2180	0.075	0.928	25	0.1	1.14

217	2180	0.075	0.928	25	0.3	2.5
218	2180	0.075	0.928	25	0.5	3.57
219	2318	0.091	0.99	25	1	3.9
220	2318	0.091	0.99	25	0.8	3.3
221	2318	0.091	0.99	25	0.5	2.4
222	2318	0.091	0.99	25	0.3	1.59
223	2318	0.091	0.99	25	0.2	1.13
224	2318	0.091	0.99	25	0.1	0.68
225	2318	0.091	0.99	25	0.4	2.17
226	2318	0.091	0.99	25	0.6	2.79
227	2318	0.091	0.99	25	0.7	3.18
228	2318	0.091	0.99	25	0.9	3.88
229	2350	0.72	0.79	0	1	3.8
230	2350	0.72	0.79	25	1	2.2
231	2350	0.72	0.79	50	1	1.6
232	2350	0.72	0.79	25	0.1	0.35
233	2350	0.72	0.79	25	0.2	0.65
234	2350	0.72	0.79	25	0.4	1.1
235	2350	0.72	0.79	25	0.6	1.47
236	2350	0.72	0.79	25	0.8	1.79
237	970	0.69	0.12	0	1	3.2
238	970	0.69	0.12	25	1	2.4
239	970	0.69	0.12	25	0.1	0.5
240	970	0.69	0.12	25	0.2	0.8
241	970	0.69	0.12	25	0.4	1.37
242	970	0.69	0.12	25	0.5	1.6
243	970	0.69	0.12	25	0.6	1.75
244	970	0.69	0.12	25	0.7	1.85
245	970	0.69	0.12	25	0.8	2.13
246	970	0.69	0.12	25	0.9	2.28
247	1200	0.2	0.48	0	1	4.3
248	1200	0.2	0.48	25	1	2.9
249	1200	0.2	0.48	50	1	2.1
250	1200	0.2	0.48	0	0.2	1.9
251	1200	0.2	0.48	0	0.4	2.75
252	1200	0.2	0.48	0	0.6	3.35
253	1200	0.2	0.48	0	0.8	3.9
254	1200	0.2	0.48	25	0.2	1.15
255	1200	0.2	0.48	25	0.4	1.6
256	1200	0.2	0.48	25	0.6	2.1
257	1200	0.2	0.48	25	0.8	2.51
258	1200	0.2	0.48	50	0.2	0.6
259	1200	0.2	0.48	50	0.4	1.1
260	1200	0.2	0.48	50	0.6	1.45

261	1200	0.2	0.48	50	0.8	1.75
262	1330	0.19	0.54	0	1	5.8
263	1330	0.19	0.54	25	1	3.3
264	1330	0.19	0.54	50	1	2.2
265	1330	0.19	0.54	25	0.1	0.75
266	1330	0.19	0.54	25	0.3	1.54
267	1330	0.19	0.54	25	0.5	2.14
268	1330	0.19	0.54	25	0.6	2.43
269	1330	0.19	0.54	25	0.7	2.6
270	1330	0.19	0.54	25	0.9	3.18
271	1330	0.19	0.54	0	0.2	2.25
272	1330	0.19	0.54	0	0.4	3.25
273	1330	0.19	0.54	0	0.6	3.9
274	1330	0.19	0.54	0	0.8	4.55
275	1330	0.19	0.54	25	0.2	1.25
276	1330	0.19	0.54	25	0.4	1.85
277	1330	0.19	0.54	25	0.6	2.45
278	1330	0.19	0.54	25	0.8	2.9
279	1330	0.19	0.54	50	0.2	0.65
280	1330	0.19	0.54	50	0.4	1.15
281	1330	0.19	0.54	50	0.6	1.52
282	1330	0.19	0.54	50	0.8	1.88
283	1570	0.18	0.65	0	1	4.9
284	1570	0.18	0.65	25	1	3.2
285	1570	0.18	0.65	50	1	2.1
286	1570	0.18	0.65	0	0.2	1.8
287	1570	0.18	0.65	0	0.4	2.8
288	1570	0.18	0.65	0	0.6	3.76
289	1570	0.18	0.65	0	0.8	4.5
290	1570	0.18	0.65	25	0.2	1
291	1570	0.18	0.65	25	0.4	1.7
292	1570	0.18	0.65	25	0.6	2.3
293	1570	0.18	0.65	25	0.8	2.8
294	1570	0.18	0.65	50	0.2	0.2
295	1570	0.18	0.65	50	0.4	0.95
296	1570	0.18	0.65	50	0.6	1.3
297	1570	0.18	0.65	50	0.8	1.8
298	1820	0.2	0.75	0	1	5.4
299	1820	0.2	0.75	25	1	3.4
300	1820	0.2	0.75	50	1	2.1
301	1820	0.2	0.75	50	0.4	0.8
302	1820	0.2	0.75	25	0.4	1.3
303	1820	0.2	0.75	0	0.4	3.2
304	1820	0.2	0.75	50	0.8	1.7



305	1820	0.2	0.75	25	0.8	2.7
306	1820	0.2	0.75	0	0.8	4.7
307	2310	0.28	0.96	0	1	5.6
308	2310	0.28	0.96	25	1	3.1
309	2310	0.28	0.96	50	1	1.9
310	1390	0.29	0.48	0	1	4.9
311	1390	0.29	0.48	25	1	3
312	1390	0.29	0.48	50	1	2.6
313	1545	0.22	0.59	0	1	5
314	1545	0.22	0.59	25	1	3
315	1545	0.22	0.59	50	1	2
316	1450	0.23	0.58	0	1	5.2
317	1450	0.23	0.58	25	1	3.2
318	1450	0.23	0.58	50	1	2
319	1450	0.23	0.58	25	0.1	0.75
320	1450	0.23	0.58	25	0.3	1.48
321	1450	0.23	0.58	25	0.5	2.04
322	1450	0.23	0.58	25	0.6	2.33
323	1450	0.23	0.58	25	0.7	2.5
324	1450	0.23	0.58	25	0.9	3.1
325	1870	0.16	0.77	0	1	5.3
326	1870	0.16	0.77	25	1	3.2
327	1870	0.16	0.77	50	1	2
328	2660	0.35	1.03	0	1	5.4
329	2660	0.35	1.03	25	1	3.1
330	2660	0.35	1.03	50	1	2
331	2660	0.35	1.03	50	0.4	0.8
332	2660	0.35	1.03	25	0.4	1.5
333	2660	0.35	1.03	0	0.4	3
334	2660	0.35	1.03	50	0.8	1.6
335	2660	0.35	1.03	25	0.8	2.6
336	2660	0.35	1.03	0	0.8	4.7
337	2190	0.09	0.92	0	1	5.6
338	2190	0.09	0.92	25	1	3.5
339	2190	0.09	0.92	50	1	2.2
340	2190	0.09	0.92	25	0.3	2.4
341	2190	0.09	0.92	25	0.6	4
342	2190	0.09	0.92	25	0.9	5.3
343	2370	0.12	0.96	0	1	5.8
344	2370	0.12	0.96	25	1	3.5
345	2370	0.12	0.96	50	1	1.8
346	2370	0.12	0.96	25	0.3	2.5
347	2370	0.12	0.96	25	0.6	4.1
348	2370	0.12	0.96	25	0.9	5.5

349	2370	0.24	0.91	0	1	5.2
350	2370	0.24	0.91	25	1	2.9
351	2250	0.12	0.91	0	1	5.5
352	2250	0.12	0.91	25	1	2.9
353	2250	0.12	0.91	50	1	1.8
354	2250	0.12	0.91	25	0.3	2.3
355	2250	0.12	0.91	25	0.6	3.95
356	2250	0.12	0.91	25	0.9	5.2
357	2850	0.12	1.23	0	1	5.2
358	2850	0.12	1.23	25	1	3
359	1260	0.07	0.55	0	1	6.1
360	1260	0.07	0.55	25	1	4.8
361	1260	0.07	0.55	50	1	3.6
362	1260	0.07	0.55	50	0.4	1.7
363	1260	0.07	0.55	25	0.4	2.5
364	1260	0.07	0.55	0	0.4	3.75
365	1260	0.07	0.55	50	0.8	3
366	1260	0.07	0.55	25	0.8	4.1
367	1260	0.07	0.55	0	0.8	5.6
368	1380	0.06	0.61	0	1	6
369	1380	0.06	0.61	25	1	4.7
370	1380	0.06	0.61	50	1	3.3
371	1380	0.06	0.61	50	0.4	1.5
372	1380	0.06	0.61	25	0.4	2.4
373	1380	0.06	0.61	0	0.4	3.6
374	1380	0.06	0.61	50	0.8	2.75
375	1380	0.06	0.61	25	0.8	4
376	1380	0.06	0.61	0	0.8	5.5
377	1390	0.07	0.62	0	1	6.6
378	1390	0.07	0.62	25	1	4.3
379	1390	0.07	0.62	50	1	2.6
380	1390	0.07	0.62	50	0.4	1.25
381	1390	0.07	0.62	25	0.4	2.25
382	1390	0.07	0.62	0	0.4	3.7
383	1390	0.07	0.62	50	0.8	2.2
384	1390	0.07	0.62	25	0.8	3.75
385	1390	0.07	0.62	0	0.8	5.7
386	1940	0.15	0.82	0	1	5.8
387	1940	0.15	0.82	25	1	3.9
388	1940	0.15	0.82	50	1	3.1
389	1940	0.15	0.82	50	0.4	1.25
390	1940	0.15	0.82	25	0.4	2
391	1940	0.15	0.82	0	0.4	3.2
392	1940	0.15	0.82	50	0.8	2.5

393	1940	0.15	0.82	25	0.8	3.25
394	1940	0.15	0.82	0	0.8	5.07
395	3100	0.12	1.45	0	1	5.363
396	3100	0.12	1.45	25	1	2.977
397	3100	0.12	1.45	50	1	1.795
398	2450	0.09	1.03	0	1	8.63
399	2450	0.09	1.03	25	1	4.2
400	2450	0.09	1.03	50	1	2.34
401	2720	0.01	1.21	0	1	5.045
402	2720	0.01	1.21	25	1	3
403	2720	0.01	1.21	50	1	1.75
404	2895	0.14	1.28	0	1	5.5
405	2895	0.14	1.28	25	1	4.59
406	2895	0.14	1.28	50	1	1.977
407	2595	0	1.16	0	1	6.82
408	2595	0	1.16	25	1	3.795
409	2595	0	1.16	50	1	2.295
410	2445	0.05	1.09	0	1	6.18
411	2445	0.05	1.09	25	1	3.27
412	2445	0.05	1.09	50	1	1.95
413	2660	0	1.16	0	1	6.545
414	2660	0	1.16	25	1	4.7
415	2660	0	1.16	50	1	2.886
416	1023	0.011	0.403	0	1	5.39
417	1023	0.011	0.403	25	1	3.6
418	1023	0.011	0.403	50	1	2.33
419	1179	0.039	0.461	0	1	5.8
420	1179	0.039	0.461	25	1	3.68
421	1179	0.039	0.461	50	1	2.36
422	1479	0.037	0.585	0	1	6.05
423	1479	0.037	0.585	25	1	3.84
424	1479	0.037	0.585	50	1	2.3
425	1479	0.037	0.585	0	0.2	2.55
426	1479	0.037	0.585	25	0.2	1.45
427	1479	0.037	0.585	50	0.2	0.75
428	1479	0.037	0.585	0	0.4	3.8
429	1479	0.037	0.585	25	0.4	2.2
430	1479	0.037	0.585	50	0.4	1.25
431	1479	0.037	0.585	0	0.6	4.75
432	1479	0.037	0.585	25	0.6	2.8
433	1479	0.037	0.585	50	0.6	1.7
434	1479	0.037	0.585	0	0.8	5.5
435	1479	0.037	0.585	25	0.8	3.3
436	1479	0.037	0.585	50	0.8	2

437	1735	0.161	0.659	0	1	5.61
438	1735	0.161	0.659	25	1	3.51
439	1735	0.161	0.659	50	1	2.04
440	2307	0.278	0.88	0	1	5.05
441	2307	0.278	0.88	25	1	3.3
442	2307	0.278	0.88	50	1	1.8
443	2750	0.423	1.042	0	1	4.15
444	2750	0.423	1.042	25	1	2.73
445	2750	0.423	1.042	50	1	1.33
446	2750	0.423	1.042	0	0.2	1.1
447	2750	0.423	1.042	25	0.2	0.75
448	2750	0.423	1.042	50	0.2	0.4
449	2750	0.423	1.042	0	0.4	1.95
450	2750	0.423	1.042	25	0.4	1.3
451	2750	0.423	1.042	50	0.4	0.6
452	2750	0.423	1.042	0	0.6	2.75
453	2750	0.423	1.042	25	0.6	1.8
454	2750	0.423	1.042	50	0.6	0.9
455	2750	0.423	1.042	0	0.8	3.05
456	2750	0.423	1.042	25	0.8	2.25
457	2750	0.423	1.042	50	0.8	1.05
458	1770	0.03	0.7	25	0	0
459	1770	0.03	0.7	25	0.2	1.18
460	1770	0.03	0.7	25	0.4	2
461	1770	0.03	0.7	25	0.6	2.73
462	1770	0.03	0.7	25	0.8	3.1818
463	1770	0.03	0.7	25	1	3.8
464	1770	0.03	0.7	25	5	8.63
465	1770	0.03	0.7	25	10	10.2
466	1770	0.03	0.7	25	30	12.9
467	1770	0.03	0.7	25	20	11.8
468	1770	0.03	0.7	25	40	13.6
469	2430	0.14	0.91	25	0.2	0.87
470	2430	0.14	0.91	25	0.4	1.75
471	2430	0.14	0.91	25	0.6	2.5
472	2430	0.14	0.91	25	0.8	3.068
473	2430	0.14	0.91	25	1	3.63
474	2430	0.14	0.91	25	5	9.1
475	2430	0.14	0.91	25	10	13.6
476	2430	0.14	0.91	25	20	15.9
477	2430	0.14	0.91	25	30	18.8
478	2430	0.14	0.91	25	40	20.45
479	2455	0.13	0.96	25	0.2	0.85
480	2455	0.13	0.96	25	0.4	1.7

481	2455	0.13	0.96	25	0.6	2.45
482	2455	0.13	0.96	25	0.8	2.95
483	2455	0.13	0.96	25	1	3.52
484	2455	0.13	0.96	25	5	9.1
485	2455	0.13	0.96	25	10	13.6
486	2455	0.13	0.96	25	20	15.9
487	2455	0.13	0.96	25	30	18.8
488	2455	0.13	0.96	25	40	20.45
489	3125	0.4	1.05	25	0.2	0.68
490	3125	0.4	1.05	25	0.4	1.36
491	3125	0.4	1.05	25	0.6	1.93
492	3125	0.4	1.05	25	0.8	2.47
493	3125	0.4	1.05	25	1	2.95
494	3125	0.4	1.05	25	5	9.1
495	3125	0.4	1.05	25	10	14.3
496	3125	0.4	1.05	25	20	18.2
497	3125	0.4	1.05	25	30	23.8
498	3125	0.4	1.05	25	40	27.3
499	3575	0.61	1.22	25	0.2	0.64
500	3575	0.61	1.22	25	0.4	1.13
501	3575	0.61	1.22	25	0.6	1.7
502	3575	0.61	1.22	25	0.8	2.05
503	3575	0.61	1.22	25	1	2.61
504	3575	0.61	1.22	25	5	9.1
505	3575	0.61	1.22	25	10	14.3
506	3575	0.61	1.22	25	20	18.2
507	3575	0.61	1.22	25	30	27.3
508	3575	0.61	1.22	25	40	31.8
509	460	0.04	0.2	0	0.15	1.3
510	460	0.04	0.2	0	0.4	2
511	460	0.04	0.2	0	0.7	2.5
512	460	0.04	0.2	0	1	2.8
513	763	0.06	0.33	0	0.15	1.9
514	763	0.06	0.33	0	0.4	3.2
515	763	0.06	0.33	0	0.7	4.2
516	763	0.06	0.33	0	1	4.75
517	1160	0.08	0.52	0	0.15	2.4
518	1160	0.08	0.52	25	0.15	1.5
519	1160	0.08	0.52	50	0.15	0.8
520	1160	0.08	0.52	120	0.15	0.2
521	1160	0.08	0.52	0	1	6.3
522	1160	0.08	0.52	25	1	4.7
523	1160	0.08	0.52	50	1	3.1
524	1160	0.08	0.52	120	1	1.1

525	1160	0.08	0.52	0	0.5	4.7
526	1160	0.08	0.52	25	0.5	3.2
527	1160	0.08	0.52	50	0.5	1.9
528	1160	0.08	0.52	120	0.5	0.5
529	2130	0.32	0.78	0	0.15	2
530	2130	0.32	0.78	0	0.4	3.65
531	2130	0.32	0.78	0	0.7	5.5
532	2130	0.32	0.78	0	1	6.7
533	1479	0.16	0.67	25	5	9
534	1479	0.16	0.67	25	10	10.5
535	1479	0.16	0.67	25	15	11.5
536	1479	0.16	0.67	25	20	12
537	1479	0.16	0.67	0	5	10
538	1479	0.16	0.67	0	10	11
539	1479	0.16	0.67	0	15	12
540	1479	0.16	0.67	0	20	12
541	2102	0.23	0.95	25	5	10
542	2102	0.23	0.95	25	10	13
543	2102	0.23	0.95	25	15	14.5
544	2102	0.23	0.95	25	20	15.5
545	2102	0.23	0.95	0	5	13.8
546	2102	0.23	0.95	0	10	16.2
547	2102	0.23	0.95	0	15	17
548	2102	0.23	0.95	0	20	17.5
549	2925	0.38	1.18	25	5	9
550	2925	0.38	1.18	25	10	13.5
551	2925	0.38	1.18	25	15	17.5
552	2925	0.38	1.18	25	20	19.5
553	2925	0.38	1.18	0	5	13.8
554	2925	0.38	1.18	0	10	20
555	2925	0.38	1.18	0	15	22
556	2925	0.38	1.18	0	20	25.5
557	2676	1.52	0.36	25	5	8
558	2676	1.52	0.36	25	10	12.5
559	2676	1.52	0.36	25	15	15
560	2676	1.52	0.36	25	20	17.5
561	2676	1.52	0.36	0	5	11
562	2676	1.52	0.36	0	10	17.5
563	2676	1.52	0.36	0	15	23.5
564	2676	1.52	0.36	0	20	25.5
565	1080	0.08	0.09	0	1	1.265
566	1080	0.08	0.09	25	1	1.12
567	1080	0.08	0.09	50	1	0.796
568	1120	0.26	0.17	0	1	3.755

569	1120	0.26	0.17	25	1	2.634
570	1120	0.26	0.17	50	1	1.743
571	1120	0.26	0.17	0	0.5	2.75
572	1120	0.26	0.17	25	0.5	1.9
573	1120	0.26	0.17	50	0.5	1.2
574	1163	0.13	0.1	0	1	1.054
575	1163	0.13	0.1	25	1	0.661
576	1163	0.13	0.1	50	1	0.393
577	1322	0.55	0.23	0	1	5.184
578	1322	0.55	0.23	25	1	3.401
579	1322	0.55	0.23	50	1	2.293
580	1322	0.55	0.23	0	0.5	3.6
581	1322	0.55	0.23	25	0.5	2.3
582	1322	0.55	0.23	50	0.5	1.5
583	2510	0.5	0.55	0	1	5.229
584	2510	0.5	0.55	25	1	3.712
585	2510	0.5	0.55	50	1	2.343
586	2510	0.5	0.55	50	0.5	1.6
587	2510	0.5	0.55	25	0.5	2.5
588	2510	0.5	0.55	0	0.5	3.6
589	1720	0.41	0.15	0	1	4.182
590	1720	0.41	0.15	25	1	2.805
591	1720	0.41	0.15	50	1	1.976
592	2100	0.49	0.29	0	1	2.818
593	2100	0.49	0.29	25	1	2.183
594	2100	0.49	0.29	50	1	1.72
595	2100	0.49	0.29	0	0.5	2.3
596	2100	0.49	0.29	25	0.5	1.75
597	2100	0.49	0.29	50	0.5	1.3
598	2698	10.073	0.227	25	1	3.7
599	2698	10.073	0.227	25	0.9	3.4
600	2698	10.073	0.227	25	0.8	3.2
601	2698	10.073	0.227	25	0.7	2.8
602	2698	10.073	0.227	25	0.6	2.5
603	2698	10.073	0.227	25	0.5	2.2
604	2698	10.073	0.227	25	0.4	1.8
605	2698	10.073	0.227	25	0.3	1.45
606	2698	10.073	0.227	25	0.2	1
607	2698	10.073	0.227	25	0.1	0.55
608	2772	9.88	0.12	25	1	1.9
609	2772	9.88	0.12	25	0.9	1.75
610	2772	9.88	0.12	25	0.8	1.6
611	2772	9.88	0.12	25	0.7	1.4
612	2772	9.88	0.12	25	0.6	1.2

613	2772	9.88	0.12	25	0.5	1.1
614	2772	9.88	0.12	25	0.4	0.85
615	2772	9.88	0.12	25	0.3	0.65
616	2772	9.88	0.12	25	0.2	0.45
617	2772	9.88	0.12	25	0.1	0.25
618	2560	4.059	0.251	25	1	2.5
619	2560	4.059	0.251	25	0.9	2.25
620	2560	4.059	0.251	25	0.8	2.1
621	2560	4.059	0.251	25	0.7	1.8
622	2560	4.059	0.251	25	0.6	1.6
623	2560	4.059	0.251	25	0.5	1.4
624	2560	4.059	0.251	25	0.4	1.15
625	2560	4.059	0.251	25	0.3	0.9
626	2560	4.059	0.251	25	0.2	0.6
627	2560	4.059	0.251	25	0.1	0.35
628	1948	0.931	0.209	25	1	2.6
629	1948	0.931	0.209	25	0.9	2.45
630	1948	0.931	0.209	25	0.8	2.2
631	1948	0.931	0.209	25	0.7	2
632	1948	0.931	0.209	25	0.6	1.75
633	1948	0.931	0.209	25	0.5	1.6
634	1948	0.931	0.209	25	0.4	1.3
635	1948	0.931	0.209	25	0.3	1.1
636	1948	0.931	0.209	25	0.2	0.75
637	1948	0.931	0.209	25	0.1	0.5
638	1477	4.736	0.014	25	1	1.6
639	1477	4.736	0.014	25	0.9	1.4
640	1477	4.736	0.014	25	0.8	1.3
641	1477	4.736	0.014	25	0.7	1.15
642	1477	4.736	0.014	25	0.6	0.95
643	1477	4.736	0.014	25	0.5	0.8
644	1477	4.736	0.014	25	0.4	0.7
645	1477	4.736	0.014	25	0.3	0.555
646	1477	4.736	0.014	25	0.2	0.4
647	1477	4.736	0.014	25	0.1	0.2
648	1260	2.271	0.139	25	20	10
649	1260	2.271	0.139	25	10	7
650	1260	2.271	0.139	25	6	5
651	1260	2.271	0.139	25	4	4.2
652	1260	2.271	0.139	25	2	2.2
653	1260	2.271	0.139	50	29	9
654	1260	2.271	0.139	50	15	7
655	1260	2.271	0.139	50	10	5.2
656	1260	2.271	0.139	50	6	3.8



657	1260	2.271	0.139	50	4	2.8
658	1260	2.271	0.139	50	2	1.6
659	1828	0.455	0.495	25	20	14.2
660	1828	0.455	0.495	25	10	10.5
661	1828	0.455	0.495	25	6	8.5
662	1828	0.455	0.495	25	4	6.5
663	1828	0.455	0.495	25	2	4
664	1900	0.453	0.547	25	20	15.5
665	1900	0.453	0.547	25	10	11.2
666	1900	0.453	0.547	25	6	9
667	1900	0.453	0.547	25	4	6.6
668	1900	0.453	0.547	25	2	4.05
669	1900	0.453	0.547	50	20	11
670	1900	0.453	0.547	50	10	8
671	1900	0.453	0.547	50	6	6.75
672	1900	0.453	0.547	50	4	5.5
673	1900	0.453	0.547	50	2	3.75
674	2517	4.919	0.611	50	20	14.7
675	2517	4.919	0.611	50	12	10.5
676	2517	4.919	0.611	50	10	8.9
677	2517	4.919	0.611	50	6	6
678	2517	4.919	0.611	50	4	5
679	2517	4.919	0.611	50	2	3
680	2517	4.919	0.611	25	20	19.5
681	2517	4.919	0.611	25	16	17
682	2517	4.919	0.611	25	12	14.6
683	2517	4.919	0.611	25	10	13.2
684	2517	4.919	0.611	25	8	11.8
685	2517	4.919	0.611	25	6	10.2
686	2517	4.919	0.611	25	4	8.1
687	2517	4.919	0.611	25	2	4.9
688	2495	4.834	0.576	25	20	19.2
689	2495	4.834	0.576	25	18	18
690	2495	4.834	0.576	25	16	16.8
691	2495	4.834	0.576	25	12	14.2
692	2495	4.834	0.576	25	10	13
693	2495	4.834	0.576	25	8	11.6
694	2495	4.834	0.576	25	6	10.2
695	2495	4.834	0.576	25	4	8.1
696	2495	4.834	0.576	25	2	4.9
697	2462	3.269	0.521	50	20	14.25
698	2462	3.269	0.521	50	12	10.5
699	2462	3.269	0.521	50	10	8.9
700	2462	3.269	0.521	50	6	6

701	2462	3.269	0.521	50	4	5
702	2462	3.269	0.521	50	2	3
703	2462	3.269	0.521	25	20	19.4
704	2462	3.269	0.521	25	18	18.2
705	2462	3.269	0.521	25	16	16.8
706	2462	3.269	0.521	25	12	14
707	2462	3.269	0.521	25	10	12.6
708	2462	3.269	0.521	25	8	11.2
709	2462	3.269	0.521	25	6	9.8
710	2462	3.269	0.521	25	4	7.8
711	2462	3.269	0.521	25	2	4.6
712	2109	2.811	0.449	25	20	16
713	2109	2.811	0.449	25	18	15
714	2109	2.811	0.449	25	16	14.2
715	2109	2.811	0.449	25	12	12
716	2109	2.811	0.449	25	10	11
717	2109	2.811	0.449	25	8	9.6
718	2109	2.811	0.449	25	6	8.2
719	2109	2.811	0.449	25	4	7
720	2109	2.811	0.449	25	2	4
721	2734	4.634	0.596	25	20	21
722	2734	4.634	0.596	25	16	18.5
723	2734	4.634	0.596	25	12	15.5
724	2734	4.634	0.596	25	10	14
725	2734	4.634	0.596	25	8	12
726	2734	4.634	0.596	25	6	10.5
727	2734	4.634	0.596	25	4	8.3
728	2734	4.634	0.596	25	2	5
729	637	0.097	0.25	0	30	8
730	637	0.097	0.25	0	29	7.5
731	637	0.097	0.25	0	28	7.4
732	637	0.097	0.25	0	27	7.2
733	637	0.097	0.25	0	26	7
734	637	0.097	0.25	0	25	6.8
735	637	0.097	0.25	0	24	6.63
736	637	0.097	0.25	0	23	6.5
737	637	0.097	0.25	0	22	6.4
738	637	0.097	0.25	0	21	6.3
739	637	0.097	0.25	0	20	6.2
740	637	0.097	0.25	0	19	6.17
741	637	0.097	0.25	0	18	6.14
742	637	0.097	0.25	0	17	6.1
743	637	0.097	0.25	0	16	6.05
744	637	0.097	0.25	0	15	6

745	637	0.097	0.25	0	14	5.96
746	637	0.097	0.25	0	13	5.94
747	637	0.097	0.25	0	12	5.9
748	637	0.097	0.25	0	11	5.85
749	637	0.097	0.25	0	10	5.8
750	637	0.097	0.25	0	9	5.78
751	637	0.097	0.25	0	8	5.76
752	637	0.097	0.25	0	7	5.74
753	637	0.097	0.25	0	6	5.72
754	637	0.097	0.25	0	5	5.7
755	637	0.097	0.25	0	4	5.2
756	637	0.097	0.25	0	3	5
757	637	0.097	0.25	0	2	4.5
758	1122	0.092	0.5	0	30	15.5
759	1122	0.092	0.5	0	29	15.1
760	1122	0.092	0.5	0	28	14.6
761	1122	0.092	0.5	0	27	14.2
762	1122	0.092	0.5	0	26	13.7
763	1122	0.092	0.5	0	25	13.2
764	1122	0.092	0.5	0	24	13
765	1122	0.092	0.5	0	23	12.8
766	1122	0.092	0.5	0	22	12.6
767	1122	0.092	0.5	0	21	12.4
768	1122	0.092	0.5	0	20	12.2
769	1122	0.092	0.5	0	19	12.18
770	1122	0.092	0.5	0	18	12.16
771	1122	0.092	0.5	0	17	12.14
772	1122	0.092	0.5	0	16	12.12
773	1122	0.092	0.5	0	15	12
774	1122	0.092	0.5	0	14	11.9
775	1122	0.092	0.5	0	13	11.7
776	1122	0.092	0.5	0	12	11.5
777	1122	0.092	0.5	0	11	11.3
778	1122	0.092	0.5	0	10	11.2
779	1122	0.092	0.5	0	9	11
780	1122	0.092	0.5	0	8	10.8
781	1122	0.092	0.5	0	7	10.6
782	1122	0.092	0.5	0	6	10.4
783	1122	0.092	0.5	0	5	10.2
784	1122	0.092	0.5	0	4	9.8
785	1122	0.092	0.5	0	3	9.2
786	1122	0.092	0.5	0	2	8.5
787	849	0.192	0.31	0	30	10.3
788	849	0.192	0.31	0	29	10

789	849	0.192	0.31	0	28	9.7
790	849	0.192	0.31	0	27	9.4
791	849	0.192	0.31	0	26	9.2
792	849	0.192	0.31	0	25	9
793	849	0.192	0.31	0	24	8.9
794	849	0.192	0.31	0	23	8.8
795	849	0.192	0.31	0	22	8.7
796	849	0.192	0.31	0	21	8.6
797	849	0.192	0.31	0	20	8.5
798	849	0.192	0.31	0	19	8.4
799	849	0.192	0.31	0	18	8.3
800	849	0.192	0.31	0	17	8.2
801	849	0.192	0.31	0	16	8.1
802	849	0.192	0.31	0	15	8
803	849	0.192	0.31	0	14	7.9
804	849	0.192	0.31	0	13	7.7
805	849	0.192	0.31	0	12	7.5
806	849	0.192	0.31	0	11	7.4
807	849	0.192	0.31	0	10	7.2
808	849	0.192	0.31	0	9	7.1
809	849	0.192	0.31	0	8	7
810	849	0.192	0.31	0	7	6.9
811	849	0.192	0.31	0	6	6.7
812	849	0.192	0.31	0	5	6.5
813	849	0.192	0.31	0	4	6.2
814	849	0.192	0.31	0	3	5.8
815	849	0.192	0.31	0	2	5
816	1270	0.01	0.49	25	0.1	0.9
817	1270	0.01	0.49	25	0.15	1.4
818	1270	0.01	0.49	25	0.2	1.65
819	1270	0.01	0.49	25	0.3	2.2
820	1270	0.01	0.49	25	0.4	2.5
821	1270	0.01	0.49	25	0.5	3.05
822	1270	0.01	0.49	25	0.6	3.4
823	1270	0.01	0.49	25	0.7	3.7
824	1270	0.01	0.49	25	0.8	4.05
825	1270	0.01	0.49	25	0.9	4.25
826	1270	0.01	0.49	25	1	4.5
827	1330	0.02	0.51	25	0.1	0.85
828	1330	0.02	0.51	25	0.15	1.2
829	1330	0.02	0.51	25	0.2	1.5
830	1330	0.02	0.51	25	0.3	1.95
831	1330	0.02	0.51	25	0.4	2.35
832	1330	0.02	0.51	25	0.5	2.75

833	1330	0.02	0.51	25	0.6	3.1
834	1330	0.02	0.51	25	0.7	3.42
835	1330	0.02	0.51	25	0.8	3.65
836	1330	0.02	0.51	25	0.9	4
837	1330	0.02	0.51	25	1	4.2
838	1690	0.05	0.67	25	0.1	0.8
839	1690	0.05	0.67	25	0.15	1.1
840	1690	0.05	0.67	25	0.2	1.4
841	1690	0.05	0.67	25	0.3	1.8
842	1690	0.05	0.67	25	0.4	2.25
843	1690	0.05	0.67	25	0.5	2.7
844	1690	0.05	0.67	25	0.6	3.1
845	1690	0.05	0.67	25	0.7	3.42
846	1690	0.05	0.67	25	0.8	3.75
847	1690	0.05	0.67	25	0.9	4.15
848	1690	0.05	0.67	25	1	4.5
849	1690	0.05	0.67	25	5	8
850	1690	0.05	0.67	25	10	11
851	1690	0.05	0.67	25	15	12
852	1690	0.05	0.67	25	20	12.5
853	1690	0.05	0.67	25	25	13.7
854	1690	0.05	0.67	25	30	14.3
855	1690	0.05	0.67	25	35	14.7
856	1690	0.05	0.67	25	40	15
857	1690	0.05	0.67	25	45	15.2
858	1690	0.05	0.67	25	50	15.4
859	670	0.26	0.2	0	0.1	1.175
860	670	0.26	0.2	0	0.2	1.68
861	670	0.26	0.2	0	0.4	2.3
862	670	0.26	0.2	0	0.5	2.65
863	670	0.26	0.2	0	0.7	2.85
864	670	0.26	0.2	0	0.8	3.2
865	670	0.26	0.2	0	1	3.3
866	670	0.26	0.2	25	0.1	0.68
867	670	0.26	0.2	25	0.2	1.05
868	670	0.26	0.2	25	0.4	1.7
869	670	0.26	0.2	25	0.5	2
870	670	0.26	0.2	25	0.7	2.125
871	670	0.26	0.2	25	0.8	2.375
872	670	0.26	0.2	25	1	2.55
873	1281	0.12	0.45	25	0.15	1.3
874	1281	0.12	0.45	25	1	4.5
875	1281	0.12	0.45	25	20	10.3
876	1281	0.12	0.45	25	5	7.8

877	1281	0.12	0.45	25	10	9.2
878	1281	0.12	0.45	25	15	9.9
879	1281	0.12	0.45	25	0.2	1.5
880	1281	0.12	0.45	25	0.4	2.5
881	1281	0.12	0.45	25	0.6	3.3
882	1281	0.12	0.45	25	0.8	3.9
883	1281	0.12	0.45	0	5	9.8
884	1281	0.12	0.45	0	10	10.2
885	1281	0.12	0.45	0	15	10.4
886	1281	0.12	0.45	0	20	10.6
887	1281	0.12	0.45	0	0.2	2.8
888	1281	0.12	0.45	0	0.4	4.1
889	1281	0.12	0.45	0	0.6	5
890	1281	0.12	0.45	0	0.8	6
891	1281	0.12	0.45	0	1	6.3
892	1202	0.16	0.49	25	0.15	1.3
893	1202	0.16	0.49	25	1	4.4
894	1202	0.16	0.49	25	20	9.7
895	1202	0.16	0.49	25	5	7.5
896	1202	0.16	0.49	25	10	8.7
897	1202	0.16	0.49	25	15	9.1
898	1202	0.16	0.49	25	0.2	1.6
899	1202	0.16	0.49	25	0.4	2.5
900	1202	0.16	0.49	25	0.6	3.3
901	1202	0.16	0.49	25	0.8	3.8
902	1202	0.16	0.49	0	5	8.5
903	1202	0.16	0.49	0	10	9.8
904	1202	0.16	0.49	0	15	10.4
905	1202	0.16	0.49	0	20	10.4
906	1202	0.16	0.49	0	0.2	2.8
907	1202	0.16	0.49	0	0.4	4
908	1202	0.16	0.49	0	0.6	4.8
909	1202	0.16	0.49	0	0.8	5.7
910	1202	0.16	0.49	0	1	6
911	1575	0.1	0.7	25	0.15	1.3
912	1575	0.1	0.7	25	1	4.6
913	1575	0.1	0.7	25	20	12.3
914	1575	0.1	0.7	25	5	8.9
915	1575	0.1	0.7	25	10	11
916	1575	0.1	0.7	25	15	11.5
917	1575	0.1	0.7	25	0.2	1.48
918	1575	0.1	0.7	25	0.4	2.4
919	1575	0.1	0.7	25	0.6	3.2
920	1575	0.1	0.7	25	0.8	4

921	1575	0.1	0.7	0	5	11.8
922	1575	0.1	0.7	0	10	12.5
923	1575	0.1	0.7	0	15	12.8
924	1575	0.1	0.7	0	20	13
925	1575	0.1	0.7	0	0.2	2.6
926	1575	0.1	0.7	0	0.4	4.1
927	1575	0.1	0.7	0	0.6	5.5
928	1575	0.1	0.7	0	0.8	6.2
929	1575	0.1	0.7	0	1	7.15
930	1557	0.22	0.53	25	0.15	1.3
931	1557	0.22	0.53	25	1	4.6
932	1557	0.22	0.53	25	20	12.1
933	1557	0.22	0.53	25	5	9.1
934	1557	0.22	0.53	25	10	11
935	1557	0.22	0.53	25	15	11.5
936	1557	0.22	0.53	25	0.2	1.5
937	1557	0.22	0.53	25	0.4	2.5
938	1557	0.22	0.53	25	0.6	3.3
939	1557	0.22	0.53	25	0.8	4.02
940	1557	0.22	0.53	0	5	11.8
941	1557	0.22	0.53	0	10	12.5
942	1557	0.22	0.53	0	15	12.7
943	1557	0.22	0.53	0	20	12.9
944	1557	0.22	0.53	0	0.2	3
945	1557	0.22	0.53	0	0.4	4.5
946	1557	0.22	0.53	0	0.6	5.6
947	1557	0.22	0.53	0	0.8	6.3
948	1557	0.22	0.53	0	1	7.15
949	2274	0.3	0.9	25	0.15	0.8
950	2274	0.3	0.9	25	1	3.6
951	2274	0.3	0.9	25	20	17.5
952	2274	0.3	0.9	25	5	9.8
953	2274	0.3	0.9	25	10	13.5
954	2274	0.3	0.9	25	15	15.1
955	2274	0.3	0.9	25	0.2	1
956	2274	0.3	0.9	25	0.4	1.75
957	2274	0.3	0.9	25	0.6	2.5
958	2274	0.3	0.9	25	0.8	3
959	2274	0.3	0.9	0	5	13.5
960	2274	0.3	0.9	0	10	18
961	2274	0.3	0.9	0	15	20.5
962	2274	0.3	0.9	0	20	22
963	2274	0.3	0.9	0	0.2	1.9
964	2274	0.3	0.9	0	0.4	3

965	2274	0.3	0.9	0	0.6	5.1
966	2274	0.3	0.9	0	0.8	5
967	2377	0.7	0.7	25	0.15	0.8
968	2377	0.7	0.7	25	1	3.6
969	2377	0.7	0.7	25	20	18.1
970	2377	0.7	0.7	25	5	9.82
971	2377	0.7	0.7	25	10	13.6
972	2377	0.7	0.7	25	15	16
973	2377	0.7	0.7	25	0.2	1
974	2377	0.7	0.7	25	0.4	1.75
975	2377	0.7	0.7	25	0.6	2.5
976	2377	0.7	0.7	25	0.8	3
977	2377	0.7	0.7	0	5	14
978	2377	0.7	0.7	0	10	19
979	2377	0.7	0.7	0	15	22
980	2377	0.7	0.7	0	20	24
981	2377	0.7	0.7	0	0.2	2
982	2377	0.7	0.7	0	0.4	3.2
983	2377	0.7	0.7	0	0.6	4.2
984	2377	0.7	0.7	0	0.8	5.2
985	2980	1.8	0.3	25	0.15	0.5
986	2980	1.8	0.3	25	1	2.7
987	2980	1.8	0.3	25	20	21.8
988	2783	1.44	0.36	25	0.15	0.6
989	2783	1.44	0.36	25	1	3
990	2783	1.44	0.36	25	20	21.7
991	1511	0.11	0.54	25	0.15	1.2
992	1511	0.11	0.54	25	1	4.3
993	1511	0.11	0.54	25	20	12
994	1511	0.11	0.54	25	5	8.75
995	1511	0.11	0.54	25	10	10.5
996	1511	0.11	0.54	25	15	11
997	1830	0.11	0.67	25	0.15	1.1
998	1830	0.11	0.67	25	1	4.9
999	1830	0.11	0.67	25	20	14
1000	1830	0.11	0.67	25	5	10.2
1001	1830	0.11	0.67	25	10	12
1002	1830	0.11	0.67	25	15	12.5
1003	2163	0.19	0.74	25	0.15	1.1
1004	2163	0.19	0.74	25	1	4.7
1005	2163	0.19	0.74	25	20	16.8
1006	2163	0.19	0.74	25	5	11
1007	2163	0.19	0.74	25	10	14
1008	2163	0.19	0.74	25	15	15.5



1009	2610	0.41	0.74	25	0.15	0.9
1010	2610	0.41	0.74	25	1	4
1011	2610	0.41	0.74	25	20	19.7
1012	2610	0.41	0.74	25	5	11
1013	2610	0.41	0.74	25	10	15.1
1014	2610	0.41	0.74	25	15	17.5
1015	346	0.46	0.05	25	5	1.36
1016	390	0.55	0.05	25	5	2.02
1017	451	0.61	0.06	25	5	2.25
1018	625	0.43	0.14	25	5	2.79
1019	1327	0.26	0.35	25	5	5.46
1020	55	0.16	0	25	5	0.32

Notes: 1-21<sup>[1]</sup>; 22-37<sup>[3a]</sup>; 38-200<sup>[3b]</sup>; 201-228<sup>[3c]</sup>; 229-336<sup>[3d]</sup>; 337-394<sup>[3e]</sup>; 395-415<sup>[3f]</sup>; 416-457<sup>[3g]</sup>; 458-508<sup>[3h]</sup>; 509-532<sup>[3i]</sup>; 533-564<sup>[3j]</sup>; 565-597<sup>[3k]</sup>; 598-647<sup>[3l]</sup>; 648-728<sup>[3m]</sup>; 729-815<sup>[3n]</sup>; 816-858<sup>[3o]</sup>; 859-872<sup>[3p]</sup>; 873-990<sup>[3q]</sup>; 991-1014<sup>[3r]</sup>; 1015-1020 were performed in our lab. 23, 34, 172, 180, 194, 198, 341, 450, 498, 563, 671, 701, 735, 751, 812, 896, 934, 945, 983, 1016 were chosen as the predicted set randomly.

## Reference

- [1] G. Dura, V. L. Budarin, J. A. Castro-Osma, P. S. Shuttleworth, S. C. Quek, J. H. Clark, M. North, *Angew. Chem. Int. Ed.* **2016**, *55*, 9173-9177.
- [2] C. Liang, S. Dai, *J. Am. Chem. Soc.* **2006**, *128*, 5316-5317.
- [3] a) G. P. Hao, W. C. Li, D. Qian, A. H. Lu, *Adv. Mater.* **2010**, *22*, 853-857; b) W. Travis, S. Gadipelli, Z. Guo, *RSC Adv.* **2015**, *5*, 29558-29562; c) S.-Y. Lee, S.-J. Park, *J. Colloid Interf. Sci.* **2013**, *389*, 230-235; d) M. Sevilla, A. B. Fuertes, *J. Colloid Interf. Sci.* **2012**, *366*, 147-154; e) M. Sevilla, A. B. Fuertes, *Energy Environ. Sci.* **2011**, *4*, 1765-1771; f) A. Wahby, J. M. Ramos-Fernández, M. Martínez-Escandell, A. Sepúlveda-Escribano, J. Silvestre-Albero, F. Rodríguez-Reinoso, *ChemSusChem* **2010**, *3*, 974-981; g) S.-M. Hong, S. W. Choi, S. H. Kim, K. B. Lee, *Carbon* **2016**, *99*, 354-360; h) M. E. Casco, M. Martínez-Escandell, J. Silvestre-Albero, F. Rodríguez-Reinoso, *Carbon* **2014**, *67*, 230-235; i) J. Ludwinowicz, M. Jaroniec, *Carbon* **2015**, *82*, 297-303; j) B. Adeniran, R. Mokaya, *J. Mater. Chem. A* **2015**, *3*, 5148-5161; k) G. K. Parshetti, S. Chowdhury, R. Balasubramanian, *Fuel* **2015**, *148*, 246-254; l) L. Estevez, D. Barpaga, J. Zheng, S. Sabale, R. L. Patel, J. G. Zhang, B. P. McGrail, R. K. Motkuri, *Ind. Eng. Chem. Res.* **2018**, *57*, 1262-1268; m) G. Srinivas, V. Krungleviciute, Z. X. Guo, T. Yildirim, *Energy Environ. Sci.* **2014**, *7*, 335-342; n) G. Singh, I. Y. Kim, K. S. Lakhi, P. Srivastava, R. Naidu, A. Vinu, *Carbon* **2017**, *116*, 448-455; o) M. Sevilla, A. S. M. Al-Jumialy, A. B. Fuertes, R. Mokaya, *ACS Appl. Mater. Interfaces* **2018**, *10*, 1623-1633; p) G. P. Hao, W. C. Li, D. Qian, G. H. Wang, W. P. Zhang, T. Zhang, A. Q. Wang, F. Schüth, H. J. Bongard, A. H. Lu, *J. Am. Chem. Soc.* **2011**, *133*, 11378-11388; q) N. Balahmar, A. S. Al-Jumialy, R. Mokaya, *J. Mater. Chem. A* **2017**, *5*, 12330-12339; r) E. Hirst, A. Taylor, R. Mokaya, *J. Mater. Chem. A* **2018**, *6*, 12393-12403.
- [4] a) J. Behler. *Angew. Chem. Int. Ed.* **2017**, *56*, 12828-12840; b) S. Shakeri, A. Ghassemi, M. Hassani, A. Hajian. *Int. J. Adv. Manuf. Tech.* **2008**, *82*, 549-557; c) G. Chen, K. Fu, Z. Liang, T. Sema, C. Li, P. Tontiwachwuthikul, R. Idem, *Fuel*, **2014**, *126*, 202-212; d) Y. Deng, M. Zhu, D. Xiang, X. Cheng, *Fuel* **2002**, *81*, 1963-1970.