Supporting information

Data-driven Identification of Reaction Network in Oxidative Coupling of Methane Reaction via Experimental Data

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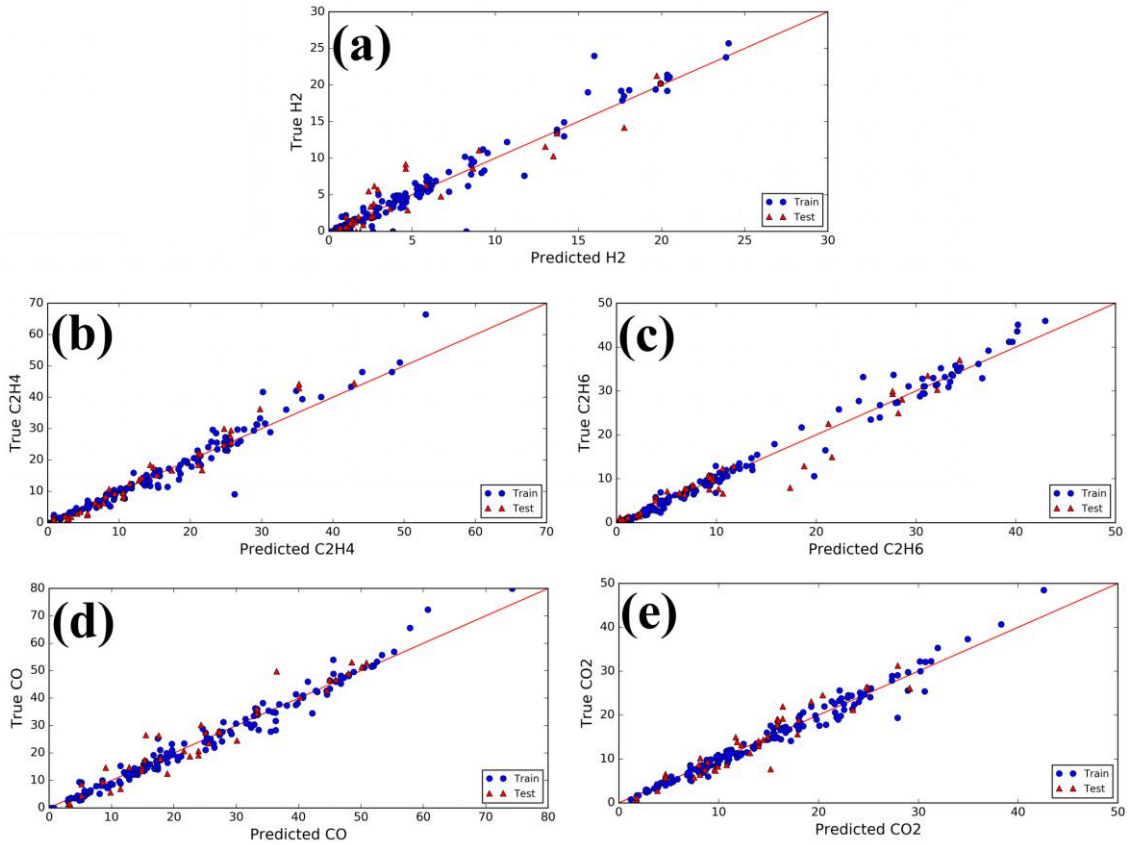

Figure S- 1. "True vs. Predicted" scatter plot in random forest regressors with different target(gas selectivities).

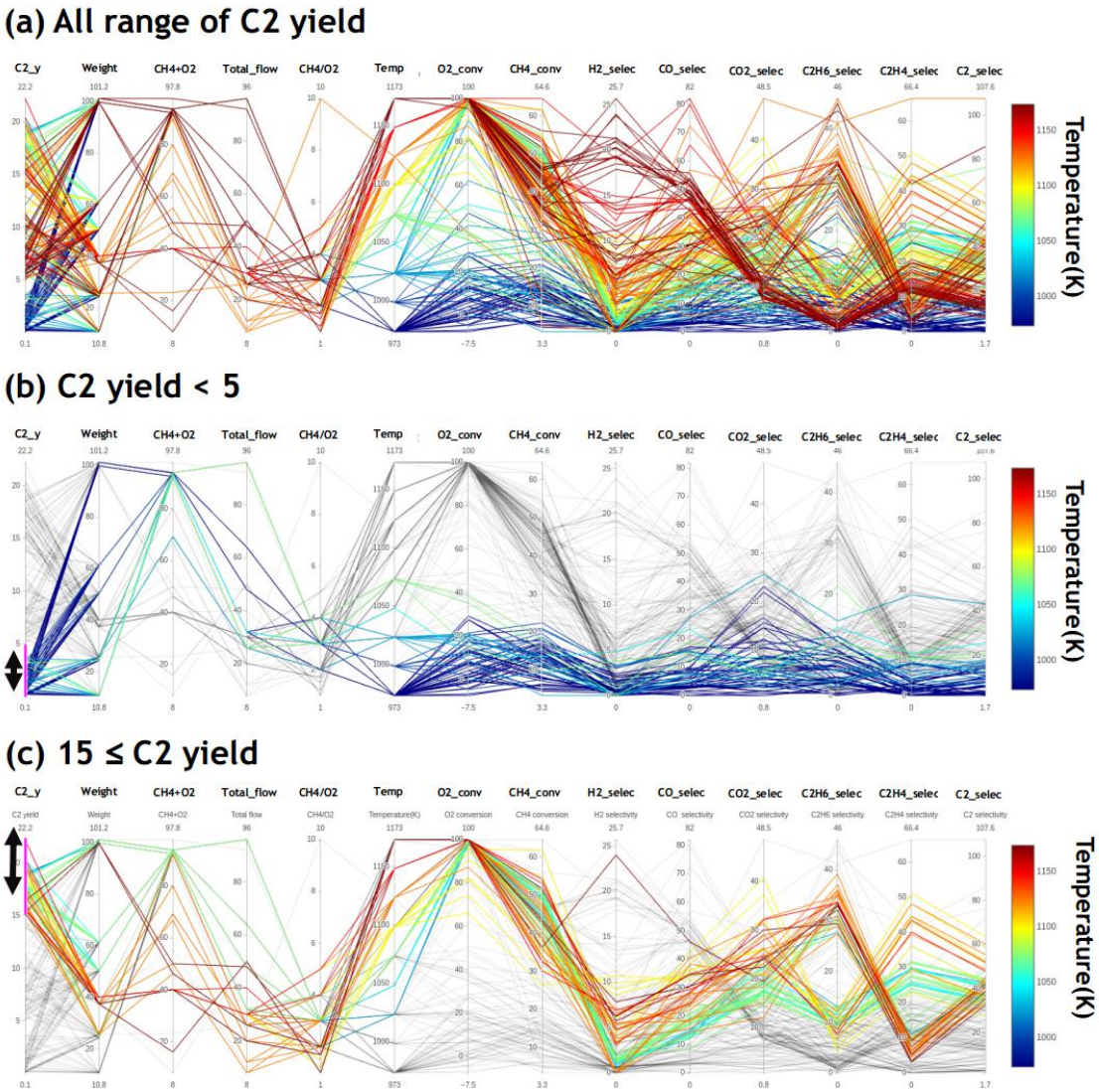

Figure S- 2. Parallel coordinates for all trained valuables against Temperature. (a)All range of C2 yield, (b) selected when C2 yield < 5, and (c) selected when C2 yield ≥ 15.

Table S- 1. Data table of experimental conditions and reaction output. Note that data columns are explained in TABLE Ⅰ. in main article. The original data has already reported in the previous study[1].

No.	Experimental Conditions					Reaction output							
	Weight	CH_4+O_2	Total_flow	CH_4O_2	Temp	O_2_conv	CH_4_conv	H_2 selec	CO selec	C_2H_6 selec	CO_2 selec	C_2H_4 selec	C_2 y
1	37.5	16	50	1	1123	100	4.9	0	31.7	41.2	48.5	66.4	5.2
2	40.1	40	30	5	1098	66.2	26.3	10.7	32.4	12.4	21.2	51.1	16.7
3	40.1	40	30	4	1098	74.4	30.1	9.9	34	10.5	23	48.1	17.6
4	40.1	40	30	5	1123	100	32.8	5.4	22	12	25.1	48.1	19.7
5	40.1	40	30	4	1123	100	35.9	4.8	24.6	10.8	26.3	44.6	19.9
6	40.1	40.1	30	3	1098	81.8	35.3	9.2	36.2	8.6	26.2	44.3	18.7
7	40.1	40	30	5	1148	100	30.1	6.9	29.3	8.5	24.1	43.4	15.6
8	40.1	40.1	30	3	1098	82.6	36.2	8.6	34.6	8.4	26.1	43	18.6
9	37.5	8	50	1	1173	100	11.9	0	27.8	43.6	35.3	42.1	10.2
10	25.7	46.2	26	2	1073	20.1	6.9	0	33.5	34.6	23.8	41.7	5.3
11	40.1	40	30	4	1148	100	32.5	6.3	34.7	7.7	24.7	40.1	15.5
12	40.1	40.1	30	3	1123	100	40.5	4	28.4	9.4	29.1	39.4	19.7
13	40.1	40.1	30	3	1148	100	34.8	6.3	42.8	6.8	26.4	36.3	15
14	40.1	40.1	30	2	1098	90.9	46.4	6.1	35.4	6.3	32.2	36.1	19.7
15	40.1	40.1	30	3	1148	100	35.9	5.7	41.3	6.4	25.9	33.3	14.3
16	101.2	93.8	64	3	1073	100	41.7	1.1	19.4	12.9	16.6	31.7	18.5
17	101.2	93.8	96	3	1073	100	39.1	1.4	23.5	12	15.2	31.4	17
18	101.2	93.7	48	3	1073	100	42.2	1.3	18.8	12.6	18.3	31.2	18.5

19	50.3	93.7	32	3	1048	98.4	49.4	1.6	14.8	10.5	19.1	30	20
20	40.1	40.1	30	1.5	1098	93.9	54.8	4.4	38.1	5.1	37.3	29.8	19.1
21	61.2	93.7	32	3	1048	100	49.4	0.9	13.1	11.4	20.6	29.7	20.3
22	101.2	93.7	32	3	1023	98.1	44	1.2	12.2	13	24.4	29.6	18.8
23	40.1	40.1	30	2	1123	100	47.5	2.9	40.3	7.2	31.3	29.5	17.5
24	101.2	93.7	32	3	1048	100	45	1	14	12.3	22.5	29.4	18.7
25	61.2	93.7	32	4	1073	100	44.2	1.5	12.4	11.6	17.1	28.9	17.9
26	25.7	69.2	26	2	1023	8.8	3.3	0	27.4	14.7	25.6	28.6	1.4
27	61.2	93.7	32	3	1073	100	48.2	1.2	17.5	10.3	18.9	27.7	18.3
28	50.3	93.7	32	3	1073	100	48.9	1.4	18.6	9.7	17.3	27.3	18.1
29	24.3	93.7	32	3	1073	98.6	48.7	2.1	17	9.1	17.6	27.2	17.6
30	61.2	93.7	32	3	1073	100	48.6	1.3	16.9	10	19.4	26.1	17.5
31	101.2	93.7	32	3	1073	100	43.3	1.6	21	10.6	19.9	26.1	15.9
32	25.7	23.1	26	2	1123	37.7	14.1	0	30.8	46	19	25.8	10.1
33	50.3	93.7	32	3	1048	99.3	50.9	1.1	13.6	9.4	17.3	25.6	17.8
34	24.3	93.7	48	3	1073	43.8	23.4	6.2	26.4	12.9	7.7	25.6	9
35	24.3	93.8	96	3	1173	95.4	35.5	8.3	42.6	4.9	7.6	25.5	10.8
36	61.2	93.7	32	3	1048	100	51.6	0.9	12	9.3	17.5	25.2	17.8
37	61.2	93.7	32	3	1073	100	51.3	1.2	13.7	8.5	16.7	25	17.2
38	50.3	93.7	32	3	1048	99.7	50	1	13.5	9.7	17.8	24.9	17.3
39	10.9	93.7	32	3	1098	80.3	36.2	8.1	36	5.8	10.5	24.1	10.8
40	50.3	93.7	32	3	1073	100	49.9	1.3	17.4	8.5	16	23.9	16.2

41	24.3	93.7	32	3	1098	99.4	47	2.4	23.4	7.8	15.9	23.4	14.6
42	50.3	93.7	32	3	1073	100	48.9	1.4	17.5	8.6	16.5	23.1	15.5
43	10.9	93.7	32	3	1123	96.9	40.1	6.3	37.3	5.4	11.8	23	11.4
44	40.1	40	30	1.2	1098	95.7	61.8	3.3	42.3	4.2	40.7	23	16.8
45	50.3	93.7	32	3	1098	100	46.2	2	28.1	7.7	14.1	22.3	13.9
46	61.2	93.7	32	3	1098	100	45.5	2	27.5	7.8	15.2	21.9	13.6
47	61.2	93.7	32	3	1098	100	49	1.8	21.1	7	14.4	21.3	13.8
48	101.2	93.7	32	3	1098	100	40.1	3.3	36.3	6.8	14.5	20.6	11
49	101.2	97.8	92	3	1173	100	35.5	17.9	51.9	2.1	9.8	20.6	8.1
50	40.1	40.1	30	2	1148	100	43	5.4	65.6	3.7	21.4	19.8	10.1
51	10.9	93.7	32	3	1073	36.8	22.9	6.8	31.3	9.9	6.2	19.6	6.7
52	24.3	93.8	64	3	1173	100	36.3	7.6	47.5	3.2	8	19.6	8.3
53	50.3	93.7	32	3	1098	100	47.3	1.9	26.5	6.7	13.2	19.5	12.4
54	24.3	93.8	64	3	1073	25.6	16	4.9	19.9	17.9	6	19.3	5.9
55	40.1	40.1	30	1.5	1123	100	54.1	2.6	56.9	5	29.8	19.1	13
56	61.2	93.7	32	3	1023	41.4	29.2	2	14.9	12.4	13.2	18.5	9
57	50.3	93.7	32	3	1098	100	46.3	2.1	27.6	6.5	13	18.5	11.6
58	101.2	93.8	64	3	1173	100	37.8	21.1	51.7	1.4	10.2	18.5	7.5
59	61.2	93.7	32	2	1073	100	55	1.3	28.8	7.3	22	18.4	14.2
60	37.5	40	20	1.7	1073	34.8	19.4	2.7	33.9	31.5	25.4	17.9	9.6
61	24.3	93.7	48	3	1173	100	37.3	14.2	53.1	1.7	7.6	17.7	7.2
62	101.2	93.7	32	3	1123	100	39.3	10.2	48.9	2.4	10.3	17.3	7.7

63	24.3	93.7	32	3	1123	100	44.3	3.9	37.8	4.4	9.9	17	9.5
64	24.3	93.7	32	3	1048	51.1	32.2	5.7	26.6	7.7	8.3	16.8	7.9
65	101.2	93.7	48	3	1173	100	38.6	23.8	53.3	1	11.3	16.8	6.9
66	50.3	93.7	32	3	1123	100	43.7	5.1	41	3.6	9.4	16.7	8.9
67	10.9	93.7	32	3	1148	98.7	38.6	10.3	51.5	2.3	7.4	16.7	7.4
68	61.2	93.7	32	3	1123	100	43.4	6	41.4	3.2	9.9	16	8.3
69	101.2	93.7	32	3	998	47.2	25.1	1	13	15.5	23.3	15.9	7.9
70	25.7	69.2	26	2	1073	38.2	18.6	0	35.3	29.5	14.1	15.6	8.4
71	101.2	93.7	32	3	1148	100	40.9	19.3	51.1	1.2	11.3	15.3	6.7
72	61.2	93.7	32	3	1123	100	45.8	5.2	37.5	3.1	8.6	15.2	8.4
73	50.3	93.7	32	3	1023	62.1	35.5	5	25.3	6.8	10.6	15.2	7.8
74	50.3	93.7	32	3	1123	100	44.7	5	40.2	3.1	8.7	15.2	8.2
75	24.3	93.7	32	3	1148	100	44.5	11.6	46.7	1.5	7.7	15.2	7.4
76	99.8	92.3	26	4	1073	99.9	34	1.9	8.5	33	14.8	15	16.3
77	50.3	93.7	32	3	1123	100	44.5	5.8	41	2.9	8	14.9	7.9
78	10.9	93.7	32	3	1173	100	40.5	18.5	55.7	1	6.9	14.9	6.4
79	50.3	93.7	32	3	1023	26.7	24.5	2.1	14.7	12.9	10.2	14.7	6.8
80	37.5	91.7	24	10	1123	99	22.7	4.7	5.2	31.3	6.9	14.5	10.4
81	50.3	93.7	32	3	1148	100	44.6	13.4	46.8	1.3	8.7	14.4	7
82	61.2	93.7	32	3	1148	100	44.4	14.9	46.4	1.3	9.8	14.2	6.9
83	61.2	93.7	32	4	1173	100	40.8	19.4	42.7	0.8	8.8	13.8	6
84	99.8	92.3	26	4	1023	81.7	26.5	3.8	14.7	22.6	15.7	13.7	9.6

85	50.3	93.7	32	3	1148	100	45.4	13.5	46.1	1.1	8.1	13.4	6.6
86	24.3	93.7	32	3	1173	100	45.9	19.2	49.6	0.7	8.1	13.4	6.5
87	50.3	93.7	32	3	1148	100	45.4	13.9	46	1.1	7.8	13	6.4
88	101.2	93.7	32	3	1173	100	41.9	25.7	51.5	0.6	13.4	12.9	5.7
89	61.2	93.7	32	3	1148	100	46.4	13	43.4	1.1	7.9	12.6	6.4
90	50.3	93.7	32	3	1173	100	45.8	20.3	49	0.7	9.4	12.5	6
91	61.2	93.7	32	3	1173	100	45.5	21.4	48.2	0.7	10.9	12.3	5.9
92	99.8	92.3	26	3	1073	99.9	40	1.6	12.1	31.1	17.6	12.2	17.4
93	50.3	93.7	32	3	1023	28.4	26.8	2.1	14	9.9	8.6	12.1	5.9
94	10.9	93.7	32	3	1048	11	13.6	4.8	23.3	13.5	4.8	12	3.5
95	40.1	40.1	30	1.5	1148	100	53.6	12.2	79.9	1.2	17.8	11.9	7
96	61.2	93.7	32	3	1173	100	46.2	20.9	47	0.6	10.5	11.8	5.7
97	61.2	93.7	32	3	1023	33.3	28.1	1.5	10.4	10.2	11.3	11.7	6.2
98	50.3	93.7	32	3	1173	100	46.5	20.2	48.5	0.6	9	11.5	5.6
99	24.3	93.8	96	3	1073	14.8	9.6	3.8	15.1	21.7	5	11.4	3.2
100	99.8	92.3	26	3	1023	90	32.7	4.1	19.2	25.8	19	11.2	12.1
101	50.3	93.7	32	3	1173	100	46.5	20.2	48.1	0.6	8.7	11.2	5.5
102	40.1	40	30	1.2	1123	100	61.5	4.1	72.3	2.6	25.6	11.2	8.5
103	99.8	92.3	26	2	1023	99.8	49.2	0.6	14.8	27.7	24.5	11	19
104	25.7	92.3	26	2	1023	21	13	0	12.4	4.9	8.6	11	2.1
105	61.2	93.7	32	3	1173	100	47.5	19.2	45.3	0.1	8.8	11	5.3
106	25.7	92.3	26	4	1073	73	24.4	7.5	21.1	24	11.5	10.8	8.5

107	10.8	92.3	26	4	1073	35.2	15.5	0	12.5	8	5.8	10.7	2.9
108	10.8	92.3	26	3	1073	38.8	18	0.7	18.8	10.6	7.6	10.4	3.8
109	37.5	90	20	5	1123	99.7	31.8	4.3	9.7	33.8	11.8	10.1	14
110	25.7	92.3	26	3	1073	96.4	37.4	4.9	17.1	32.8	17	10	16
111	25.7	92.3	26	2	1073	99.3	49	0	19.2	30	22	9.7	19.5
112	25.7	92.3	26	4	1023	17.3	9.7	0	5.2	2.2	5.4	9.5	1.1
113	25.7	92.3	26	4	1123	99.8	34.2	0	14.3	35.2	12.1	9.5	15.3
114	10.8	92.3	26	2	1073	49.1	25.3	1.3	30.3	12.9	10.2	9.4	5.7
115	99.8	92.3	26	3	973	27.5	12.6	1.7	7.9	2.6	14.7	9.3	1.5
116	25.7	92.3	26	3	1023	19.9	11.2	0	7.2	3	6.3	9.3	1.4
117	37.5	80	20	3	1123	99.8	38.4	3.8	15.4	35.4	19.9	9.3	17.2
118	99.8	92.3	26	2	1073	99.9	48.7	1.4	18.5	27.3	22.6	9.2	17.8
119	10.8	92.3	26	2	1023	20.7	13.9	0	14.4	4.6	4.6	9.2	1.9
120	99.8	92.3	26	4	973	27.4	11.9	1	5.7	1.8	12.4	9.1	1.3
121	99.8	92.3	26	4	1123	99.9	33.2	4.6	12.2	33.2	13.5	9.1	14
122	37.5	16	50	1	1173	100	36.2	24	46	32.9	19.4	9.1	15.2
123	99.8	92.3	26	2	973	29.1	15.6	2.4	11.9	3.3	16.7	8.9	1.9
124	61.2	93.7	32	2	1173	100	56.1	21.3	52.9	0.4	13.9	8.4	5
125	25.7	92.3	26	3	1123	99.9	39	0	18.9	33.5	15	8.4	16.3
126	25.7	92.3	26	2	1073	98.5	50.3	0	20.8	29.4	19.2	8	18.8
127	24.3	93.7	32	3	1023	15.3	20.5	3.3	15.7	9.7	6	8	3.6
128	40.1	40	30	1.2	1148	100	64.6	19	82	0.5	19.8	7.7	5.3

129	99.8	92.3	26	3	1123	99.9	38.7	3.8	16.4	31.1	16	7.6	15
130	25.7	69.2	26	2	1123	99.8	45.7	0	26.9	35.8	23.1	7.3	19.7
131	37.5	40	40	1.7	1148	99.8	54.2	3.2	28.3	33.7	27.9	7.3	22.2
132	37.5	55.6	9	4	1123	99.7	29.1	0	14.5	41.2	19.5	7.2	14.1
133	50.3	93.7	32	3	998	21.3	22.4	3.2	15.3	8.4	8.2	7	3.5
134	10.8	92.3	26	3	1023	19.5	11.7	0	7.7	2.9	3.3	6.9	1.1
135	37.5	66.7	12	3	1123	99.8	35.9	5.5	18	37.1	21.2	6.4	15.6
136	25.7	92.3	26	2	1123	99.9	48.3	0	27.9	27.4	18.4	6.3	16.3
137	37.5	80	20	2	1123	99.8	48.3	3.4	23.6	30.3	24.6	6.3	17.7
138	99.8	46.2	26	4	1173	99.8	26.9	11.2	17.4	45.1	17.6	5.9	13.7
139	25.7	46.2	26	2	1123	87.3	38.4	0	38.2	36.2	20.6	5.9	16.1
140	37.5	50	8	3	1123	99.8	33.7	7.1	18	39.2	24.1	5.9	15.2
141	61.2	93.7	32	3	998	12.8	18.1	0.9	8.8	11.6	11.2	5.6	3.1
142	99.8	92.3	26	2	1123	99.9	47.6	3.1	27.8	25	18.9	5.5	14.5
143	37.5	40	20	1.7	1123	97.6	50.9	6.6	27.7	34.8	32.3	5.4	20.4
144	99.8	50	48	2	1173	99.8	42.6	6.2	34.5	33.2	22.4	5.2	16.4
145	37.5	40	20	1.7	1148	99.8	53	4.7	24.2	33.5	32.1	5.1	20.4
146	37.5	66.7	12	2	1123	99.8	47	0	25.6	28.8	26.1	4.8	15.8
147	10.9	93.7	32	3	1023	-0.5	9.2	3.2	15.9	11.8	4	4.8	1.5
148	61.2	93.7	32	2	973	20.2	20.9	3.2	17	7.7	10.5	4.7	2.6
149	10.8	92.3	26	4	1023	18.5	11.7	0	4.7	1.8	2.4	4.6	0.7
150	50.3	93.7	32	3	998	6.5	16.7	1.2	8.9	10.6	8.3	4.6	2.5

151	37.5	50	8	2	1123	99.8	43.2	5.2	24	30.9	28.9	4.4	15.2
152	61.2	93.7	32	2	973	18	17.6	3	16.3	8.3	12	4.2	2.2
153	101.2	93.7	32	3	973	17.3	14.2	0.6	10	10.7	21.9	3.8	2.1
154	25.7	92.3	26	2	973	13.6	9.2	0	4.5	0.3	4.5	3.5	0.3
155	25.7	92.3	26	4	1173	99.8	32.5	0	25.1	31.1	9.5	3.5	11.2
156	101.2	93.7	32	3	973	17.2	13.6	0.5	9.6	10.6	23.1	3.5	1.9
157	99.8	46.2	26	2	1173	99.8	43.4	7.8	30.4	32.1	24	3.3	15.3
158	25.7	92.3	26	3	1173	99.9	36.5	9.5	34.9	26.8	10.6	3.3	11
159	10.8	92.3	26	2	973	14.9	10.8	0.5	4.2	0.4	1.6	3.3	0.4
160	37.5	40	20	1.7	1173	99.8	51.7	5.7	30.4	29.4	30	3	16.8
161	50.3	93.7	32	3	998	6.4	18.7	0.9	7	7.6	6.5	3	2
162	99.8	92.3	26	4	1173	99.9	31.4	8.6	20.8	28.1	11.4	2.9	9.7
163	61.2	93.7	32	3	973	8.8	17.1	2	9.4	6.9	8.3	2.5	1.6
164	61.2	93.7	32	3	998	11.8	19.6	0.6	5.7	6.7	8.7	2.5	1.8
165	99.8	92.3	26	3	1173	99.9	35.9	8	30.7	23.5	12.7	2.4	9.3
166	25.7	92.3	26	3	973	12.6	8.2	0	2.5	0	3.5	2.4	0.2
167	10.8	92.3	26	3	973	12.9	9.6	0	1.7	0.5	1.2	2.2	0.3
168	24.3	93.7	32	3	998	2	15.2	1.6	8.1	6.4	4.2	2.1	1.3
169	25.7	92.3	26	2	1173	99.9	43.7	9.1	54	16.5	10.9	2	8.1
170	50.3	93.7	32	3	973	5.7	17.1	2.2	9.2	5.8	5.4	2	1.3
171	25.7	92.3	26	4	973	11.4	8.1	0	1.5	0.1	2.8	1.9	0.2
172	50.3	93.7	32	3	973	4	14.9	2	8.6	5.8	6.1	1.7	1.1

173	61.2	93.7	32	4	973	0.6	16.1	1.4	6.2	5.9	6.8	1.6	1.2
174	10.8	92.3	26	4	973	12.5	9.6	0	0.9	1.2	0.8	1.4	0.2
175	101.2	93.7	48	3	973	7.8	7.9	0.6	6.4	9	14.7	1.3	0.8
176	99.8	92.3	26	2	1173	99.9	44.1	11.1	49.8	15	14.4	1.2	7.1
177	101.2	93.7	48	3	973	8	7.7	0.6	6.4	8.8	15.7	1.2	0.8
178	10.9	93.7	32	3	998	-4.8	7.5	1.5	8.1	6.5	2.7	1.1	0.6
179	50.3	93.7	32	3	973	-1.5	13.4	0.6	4.5	5.1	5.8	0.9	0.8
180	61.2	93.7	32	3	973	1	12.5	0.5	4.2	5	8.6	0.8	0.7
181	61.2	93.7	32	3	973	1.1	13.9	0.5	4.2	4.9	7.4	0.8	0.8
182	50.3	93.7	32	3	973	-2	11.4	0.6	4.5	5.1	6.6	0.8	0.7
183	50.3	93.7	32	3	973	-1.4	15.8	0.4	3.1	3	4	0.4	0.5
184	61.2	93.7	32	3	973	2.2	14.6	0.3	3	2.6	6.1	0	0.4
185	61.2	93.7	32	3	973	2.3	16.4	0.3	2.7	2.3	5.2	0	0.4
186	50.3	93.7	32	3	973	-1.3	14.4	0.4	2.9	2.8	4.3	0	0.4
187	24.3	93.7	32	3	973	-4.4	11	0.6	3.4	2.6	3	0	0.3
188	24.3	93.7	32	3	973	-4.2	13	0.6	3.4	2.5	2.5	0	0.3
189	10.9	93.7	32	3	973	-6.8	6.1	0.7	3.4	2.6	1.7	0	0.2
190	10.9	93.7	32	3	973	-7.5	6.3	0.7	3.6	3	1.6	0	0.2
191	24.3	93.7	48	3	973	-0.6	5.1	0.7	3.2	3.7	3	0	0.2
192	24.3	93.7	48	3	973	-0.5	5.7	0.7	2.9	3.6	2.5	0	0.2
193	24.3	93.8	64	3	973	1.4	4.9	0.5	0	2.6	1.7	0	0.1
194	24.3	93.8	96	3	973	4	4.4	0.3	0	1.7	0.8	0	0.1

195	101.2	93.8	64	3	973	7.5	7.1	0.5	4.5	6.5	10.7	0	0.5
196	101.2	93.8	96	3	973	6.9	4.8	0.5	3.5	5.5	9	0	0.3

Table S- 2. Cross validation (CV) result against target selectivity by using experimental condition + X. Note that Avg. Med. And Std. indicates average score, median and standard deviation of CV scores in 10 random states.

Target selectivity	X	Avg.	Med.	Std.
H_2	(None)	0.71	0.67	0.14
	CO	0.73	0.74	0.14
	C_2H_6	0.74	0.75	0.14
	CO_2	0.80	0.79	0.09
	C_2H_4	0.73	0.70	0.12
CO	(None)	0.80	0.83	0.12
	H_2	0.80	0.80	0.08
	C_2H_6	0.90	0.91	0.02
	CO_2	0.78	0.82	0.12
	C_2H_4	0.84	0.87	0.09
C_2H_6	(None)	0.83	0.91	0.12
	H_2	0.80	0.82	0.09
	CO	0.84	0.87	0.07
	CO_2	0.78	0.79	0.11
	C_2H_4	0.82	0.88	0.12
CO_2	(None)	0.77	0.76	0.06
	H_2	0.79	0.78	0.06
	CO	0.78	0.78	0.09
	C_2H_6	0.78	0.80	0.07
	C_2H_4	0.85	0.85	0.04
C_2H_4	(None)	0.77	0.77	0.10
	H_2	0.80	0.79	0.06
	CO	0.76	0.74	0.07
	C_2H_6	0.80	0.79	0.07
	CO_2	0.83	0.84	0.08

Reference

[1] Ohyama, J.; Nishimura, S.; Takahashi, K. Data Driven Determination of Reaction Conditions in Oxidative Coupling of Methane via Machine Learning. ChemCatChem 2019, 11, 4307–4313.