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SUPPORTING INFORMATION

Enhanced Descriptor Identification and Mechanism Understanding for Catalytic Activity using Data-Driven Framework: Revealing the Importance of Interactions between Elementary Steps

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Details of KMC Simulations

The overall reactions were modelled on a 128×128 surface matrix that resembled the Cu(111) and modified Cu(111) surface, where dopant metals (Au, Pd, Pt, Ni) account for 1/9 coverage. Each unit cell consisted of 8 Cu atoms and 1 dopant atom, the associated top sites, hollow sites, and bridge sites was modeled as shown in Figure S1. For each set of kinetic parameters, three kMC simulations were run with different seeds of random number and lasted for more than 10^5 events, and their average value was accepted as final results.

Several assumptions were made to simplify the kMC model. Firstly, the diffusion of surface *H was ignored since it's readily available with the facile activation of H_2 over Cu(111). Secondly, since the major sites on the metal-doped Cu(111) or M-Cu(111) surface are still Cu, the *CO coverage will be limited due to low *CO binding energy, and thus the lateral interaction was ignored. Finally, the desorption of *CH_2O was not included as an elementary step. Although theoretical calculations indicated that the interaction between *CH_2O and Cu(111) is very weak[1], the experimental observation of *CH_2O desorption is rarely reported. It was proposed previously that *CH_2O could be stabilized on step sites and partially oxidized Cu(111) under experimental condition[2]; or *CH_2O could be stabilized by other surface *CH_2O[3] and even undergoes polymerization[4]. These assumptions have described successfully several Cu-based catalytic systems for CO and CO_2 hydrogenation[5-9].

It is worth noted that the major objective of this case study is to test the capability of the data-driven framework and verify the machine-learned results with already established chemical intuitive. The simplified kMC model offered an efficient way to establish the accurate and trusted ML framework. Such framework can be easily enriched with more complex kinetics such as more competitive pathways, detailed site environment and lateral interactions, which will be studied in the next step.

Details of Conventional DRC Calculation

Although the protocol of conventional DRC method is meant for mean-filed microkinetic models, we follow the central concept of this numerical procedure with our kMC simulated results[10]. The nominal DRC coefficient is estimated by finite difference defined as eq. S1[11]. Wherein, χ_i denotes the DRC coefficient of i^{th} elementary step, E_i is the corresponding activation barrier, ΔE refers to a small perturbation of activation energy E_i, and function $f(E_i+\Delta E)$ denotes the kMC simulated methanol TOF when the activation energy of the i^{th} elementary step is perturbated by ΔE and that for other steps was kept the same. The amount of small perturbation ΔE in our case is around 2 kCal · mol^{-1}, so that the induced incremental change of rate constant for i^{th} elementary step, *i.e.*, $\delta k_i/k_i$, would be smaller than 1%[10].

$$\chi_i = \frac{-f(E_i+2\Delta E)+8f(E_i+\Delta E)-8f(E_i-\Delta E)+f(E_i-2\Delta E)}{12\Delta E} + O\left(\Delta E^4\right)$$

(eq. S1)

Details of ML models

For ML models in the present study, they incorporated hyperparameters whose values control the learning process and determine the values of model parameters that a learning algorithm would return. Tuning these hyperparameters not only helped to increase the convergency rate, it also helped to balance the bias and variance thus minimizes the total error when the size of dataset is small[12]. For linear models such as LASSO and SVM, they have limited number of hyperparameters, and the tuning could be quickly optimized with grid-search method. The main hyperparameter for LASSO is the coefficient of *l1*-norm term, which controls cost function's regularization penalty on the non-informative descriptors[13], and the optimized value returned by grid-search between 0 to 1 is 0.27. For SVM with radial basis functional (RBF) kernel, the major hyperparameters are kernel parameter gamma and regularization parameter[14, 15]. The optimized value returned by grid-search is -9.96 and 51.38, respectively.

For tree-based ensemble such as random forest (RF), extra trees (ET) and gradient boosted machine (GBM), they share a similar set of hyperparameters, i.e., number of estimators (n_estimators), the maximum depth of the decision tree(max_depth), the maximum number of leaf nodes in each decision tree (max_leaf_nodes), The minimum number of samples required to split an internal node (min_samples_split) ,the minimum number of samples required to be at a leaf node (min_samples_leaf), and the miminum allowed decrease of impurity for a spilt (min_impurity_decrease)[16]. In principle, increasing the number of estimators (*i.e.*, decision tress) can improve the model's performance by reduce the out-of-bag error in our case since the root mean squared error as criteria, but the computational cost also linearly increased with the number of trees[17]. Max_depth and max_leaf_nodes control the overall depth and shape of decision trees to tune model's complexity in a macroscopic point of view: Increasing max_depth and max_leaf_nodes would increase the tree's complexity and thus lead to a lower bias with higher variacance. Other parameters control the splitting rule of each node to tune model's complexity in a microscopic point of view: increase min_samples_split, min_samples_leaf, and min_impurity_decrease could make each node less likely to split, which would lead to a simpler but more correlated trees that has higher bias and lower variance. The value of these hyperparameters was optimized after the exhaustive grid-search. For RF, the best combination is: n_estimators = 176, max_depth = 661, max_leaf_nodes = 839, min_samples_leaf = 2, min_samples_split = 3, min_impurity_decrease = 0.13; For ET, the best combination is: n_estimators = 556, max_depth = 28, max_leaf_nodes = 1075, min_samples_leaf = 6, min_samples_split = 8, min_impurity_decrease = 0.06; For GBM, the best combination is: n_estimators = 120, max_depth = 6, max_leaf_nodes = 1320, min_samples_leaf = 6, min_samples_split = 3, min_impurity_decrease = 0.02.

Supporting Figures

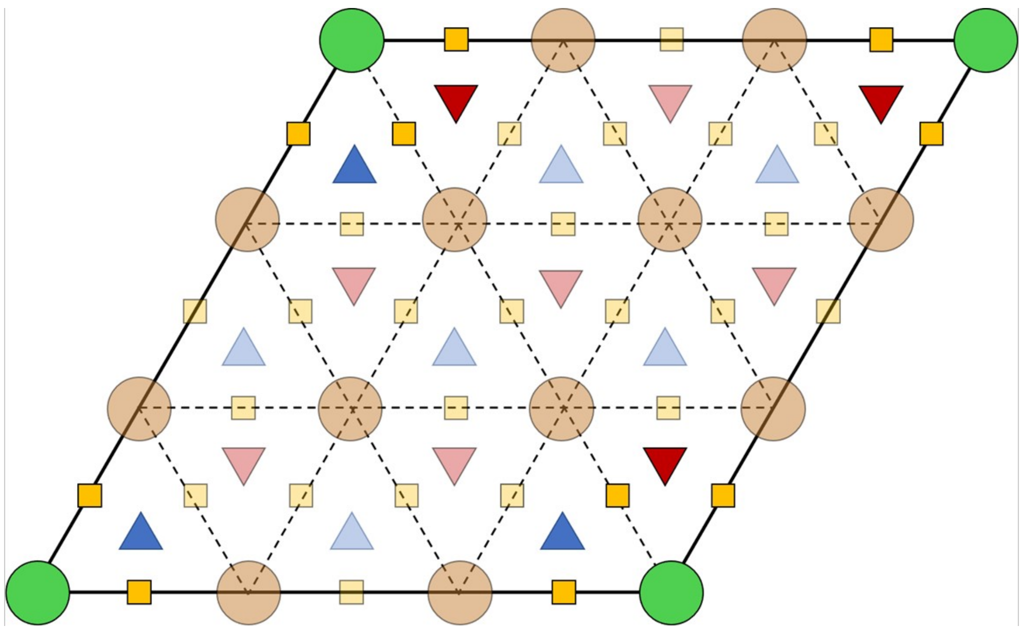

Figure S1. Schematic view of a unit cell in the surface matrix of kMC simulation. Pale solid brown circles indicate Cu-top sites, pale solid blue and red triangles indicate fcc- and hcp-hollow sites around Cu atoms respectively, and pale solid yellow squares indicate Cu-Cu bridge sites; Bold solid green circles indicate a dopant (Au, Pd, Pt, Ni) top site, bold solid blue and red triangles indicate fcc- and hcp-hollow sites around dopant atoms, and bold solid yellow squares indicate bridge sites between dopant and Cu atoms.

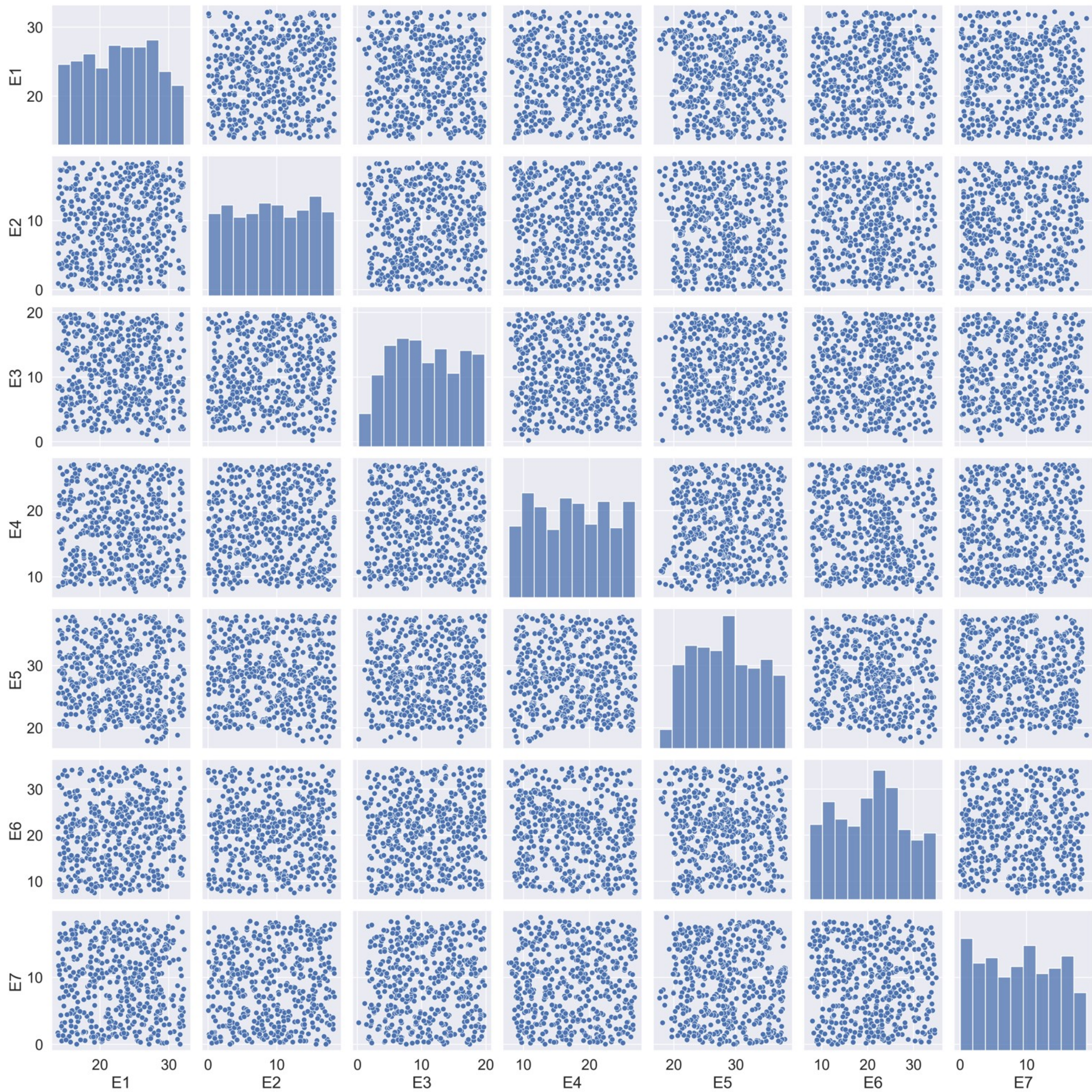

Figure S2. The pair-wise interaction between every two elementary steps.

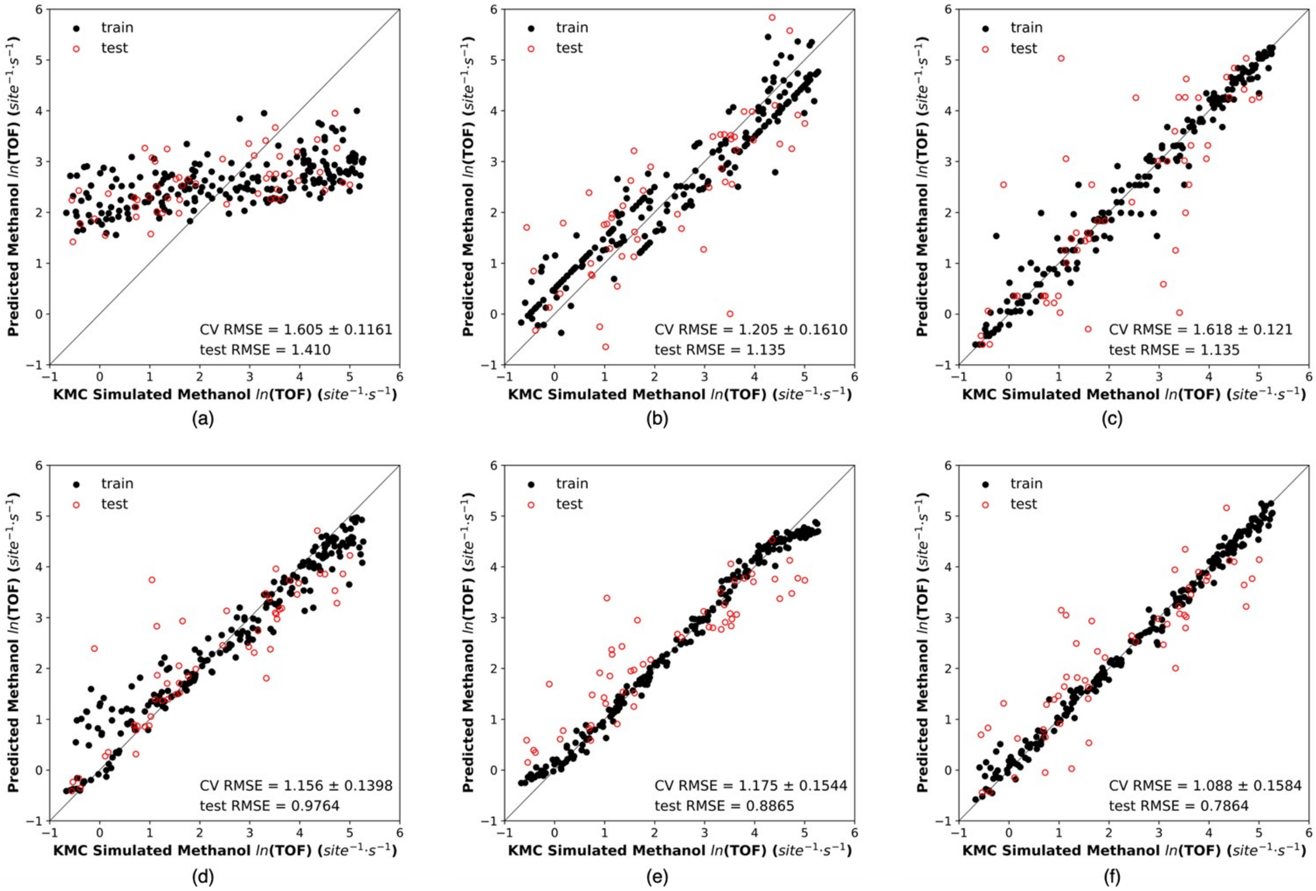

Figure S3. KMC-simulated methanol TOF and on training set (black filled circle) and testing set (red hollow circle) and values predicted by preliminary ML model based on (a) LASSO, (b) SVM, (c) DT, (d) RF, (e) ET, and (f) GBR.

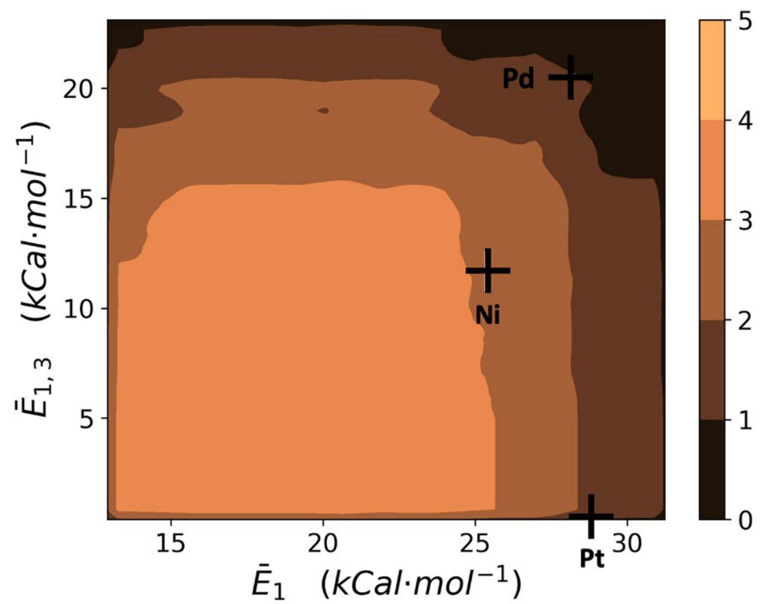

Figure S4. Bivariate partial dependence plots of methanol TOF on $\bar{E}_{1,3}$ based on the retrained ML model.

Supporting Tables

Table S1. DFT calculated activation barriers for elementary steps included in the kMC simulation of CO hydrogenation over M-Cu(111) surface[5].

elementary steps		Ea / kCal·mol^{-1}				
		Cu(111)	Au-Cu(111)	Pd-Cu(111)	Pt-Cu(111)	Ni-Cu(111)
$H_2(g) + 2^* \rightarrow 2^*H$	R_0	89.73†	89.73†	89.73†	89.73†	89.73†
$^*CO + ^*H \rightarrow ^*CHO + ^*$	R_1	23.06	23.06	28.83	28.13	25.14
$^*HCO + ^* \rightarrow ^*CO + ^*H$	R_2	7.15	8.76	15.45	17.53	3.69
$^*HCO + ^*H \rightarrow ^*CH_2O + ^*$	R_3	10.61	10.84	8.23	16.14	7.61
$^*H_2CO + ^*H \rightarrow ^*CH_3O + ^*$	R_4	17.76	12.45	11.99	3.23	7.15
$^*H_3CO + ^*H \rightarrow ^*CH_3OH + ^*$	R_5	28.83	31.59	18.22	12.68	23.06
$^*CO \rightarrow CO(g) + ^*$	R_6	16.60	14.53	27.90	31.82	38.28
$^*CH_3OH \rightarrow CH_3OH(g) + ^*$	R_7	6.23	6.46	6.92	7.15	10.61

†: The activation of hydrogen was considered to take place over Cu, the major component of catalytic surface, and thus its activation barrier was the same in different alloy systems.

Table S2. Site information of intermediates involved in CO hydrogenation over Cu(111) and M-Cu(111).[5]

Surface Species	Adsorption Site	Site Type
$^*H$	η^1-H_{Cu}	hollow site
$^*CO$	η^1-C_{dopant}	top site
$^*CHO$	η^2-$C_{dopant}O_{Cu}$	bridge site
$^*CH_2O$	η^2-$C_{dopant}O_{Cu}$	bridge site
$^*CH_3O$	η^2-$O_{dopant}O_{Cu}$	hollow site

*CH_3OH	η^1-O_{dopant}	top site
*H_2O	η^1-O_{dopant}	top site

Table S3. Reference dataset used for the construction of the machine learning models.

No.	Ea/kCal·mol^{-1}							TOF/site^{-1}·s^{-1}
	E_1	E_2	E_3	E_4	E_5	E_6	E_7	**CH_3OH**
1	20.98	5.73	16.32	20.39	25.90	11.53	10.71	0.77
2	15.98	4.03	13.00	24.99	37.80	21.78	15.86	0.01
3	19.33	0.20	6.38	21.34	34.61	22.28	1.17	0.29
4	18.32	3.29	12.01	26.82	26.69	16.03	7.03	121.65
5	23.65	8.79	12.82	21.34	28.30	14.68	15.15	28.76
6	19.45	14.44	10.59	18.22	25.03	18.03	12.58	1737.76
7	22.02	18.37	9.40	18.26	21.03	10.86	17.95	306.50
8	14.16	17.36	6.00	20.86	32.12	23.77	6.94	2.47
9	22.20	7.19	10.62	12.69	33.82	17.28	3.21	0.63
10	30.47	12.60	13.46	25.52	22.64	24.62	6.66	3.16
11	15.88	17.57	8.57	24.47	27.37	12.73	8.14	203.77
12	25.91	18.21	16.41	10.23	12.68	28.67	15.44	26.75
13	18.95	6.84	19.35	18.57	35.63	8.83	9.36	0.06
14	18.66	8.41	17.18	16.36	21.50	21.76	4.63	325.27
15	22.14	8.64	8.69	21.49	25.58	21.58	17.39	936.22
16	27.63	16.09	11.40	15.87	27.09	24.46	9.95	102.84
17	27.04	17.66	7.70	23.99	23.99	10.50	16.01	2.63
18	28.82	11.64	11.77	19.94	22.76	19.45	3.66	15.69
19	17.51	4.85	14.49	11.44	28.52	12.41	1.77	31.18
20	31.83	14.86	4.53	11.35	24.06	12.87	10.25	0.27
21	27.54	16.30	11.68	19.74	34.21	20.44	13.64	0.48
22	19.77	13.82	8.51	10.58	32.13	12.61	18.25	2.69
23	21.00	8.94	4.82	23.54	21.43	18.75	12.40	4075.09

24	21.84	0.89	14.08	22.32	21.93	22.40	11.49	0.63
25	23.85	12.64	10.10	13.25	28.22	25.79	8.50	99.80
26	15.77	5.45	6.50	17.60	31.62	20.86	10.15	4.23
27	16.22	15.07	8.10	21.81	31.88	23.19	12.71	3.03
28	17.62	14.60	6.98	13.13	28.40	23.33	6.70	90.22
29	25.22	12.47	3.66	19.39	29.02	20.93	10.52	47.98
30	26.81	15.20	1.13	9.77	29.32	27.07	6.12	32.63
31	28.28	18.34	18.50	18.95	26.44	24.63	10.55	36.39
32	20.34	8.11	17.24	23.46	27.48	15.03	0.76	34.69
33	26.35	13.82	18.80	14.53	28.47	25.80	2.97	8.75
34	19.66	18.20	3.39	17.46	24.01	8.97	11.10	362.92
35	28.92	15.76	5.16	25.33	28.09	17.84	5.43	21.54
36	15.41	7.63	15.08	24.04	31.63	19.68	15.67	4.60
37	18.77	1.64	5.18	12.35	32.89	25.82	15.45	1.19
38	30.71	7.36	6.47	22.39	24.59	21.08	7.30	5.68
39	24.69	6.09	12.22	18.06	34.78	8.29	14.95	0.01
40	25.24	4.29	7.41	11.55	23.96	26.41	11.11	81.13
41	20.14	10.14	13.51	25.30	37.34	11.01	11.07	0.03
42	20.87	13.52	18.43	25.20	33.97	15.53	15.97	0.51
43	24.61	5.34	18.59	13.30	25.26	15.67	7.38	0.07
44	29.05	0.84	5.18	21.30	32.62	11.06	14.00	0.01
45	22.82	2.72	3.40	9.67	37.39	22.68	2.71	0.02
46	19.80	11.75	4.22	26.87	28.57	25.07	13.90	59.09
47	21.55	12.26	14.81	23.66	35.41	12.85	11.34	0.16
48	32.12	2.46	2.02	9.66	29.28	19.67	2.75	2.78
49	18.62	5.22	8.85	13.37	27.79	21.52	14.82	165.80
50	28.17	5.71	19.59	22.04	34.66	21.00	4.47	0.00
51	19.40	2.46	10.49	26.95	35.05	9.48	15.66	0.19
52	23.00	0.04	5.25	11.16	27.18	9.07	7.16	0.62
53	32.19	8.62	14.11	10.64	23.00	14.73	8.28	0.00
54	18.09	16.08	14.04	24.60	31.40	15.07	4.19	5.11
55	28.16	8.04	4.01	19.47	36.72	11.06	9.38	0.03
56	31.76	15.44	6.06	11.32	37.53	15.27	5.26	0.01
57	14.06	8.08	2.10	16.78	29.13	10.39	15.39	44.84

58	14.93	10.86	6.13	11.16	23.84	18.70	16.56	4647.59
59	19.18	10.45	11.07	20.05	24.63	16.82	0.32	1904.03
60	25.38	3.02	12.60	26.29	32.47	13.59	9.40	0.15
61	15.49	10.22	9.45	21.62	25.27	15.18	1.23	1369.77
62	29.69	9.13	13.92	9.72	30.20	12.65	0.30	0.03
63	18.59	0.91	15.23	8.92	26.90	10.60	10.49	0.80
64	22.38	16.87	19.32	11.12	22.25	9.31	1.21	8.19
65	20.76	0.78	9.61	17.58	36.22	12.32	4.10	0.07
66	14.28	17.28	4.88	15.05	26.46	12.62	4.37	511.88
67	23.20	1.38	12.45	18.43	29.00	25.22	5.14	1.00
68	24.66	1.90	6.21	16.14	27.67	10.38	9.56	0.80
69	18.59	8.04	14.62	12.87	27.99	14.79	12.35	89.37
70	21.58	8.68	4.32	18.58	36.88	20.58	3.65	0.03
71	17.65	11.12	2.59	10.12	25.37	19.47	4.74	1376.42
72	23.30	15.96	3.17	26.61	31.19	22.38	2.24	6.06
73	22.55	1.62	19.53	18.66	28.68	24.53	9.52	0.01
74	17.56	9.66	13.86	13.86	31.23	18.68	17.58	6.83
75	23.80	11.66	8.48	18.98	22.81	9.66	14.73	19.19
76	16.99	2.98	17.19	26.10	30.32	22.89	14.91	7.75
77	26.71	6.13	18.59	15.50	29.39	21.83	18.42	0.03
78	28.02	9.24	17.05	15.09	31.34	23.97	12.60	0.23
79	19.19	5.69	17.09	12.83	32.30	20.03	0.54	2.63
80	25.47	6.47	17.36	15.16	33.94	17.53	8.53	0.08
81	21.71	4.44	4.62	10.52	31.38	9.05	2.44	3.50
82	23.90	7.02	8.33	18.22	26.69	21.94	7.10	280.01
83	24.96	3.10	4.10	16.47	35.81	17.65	8.99	0.10
84	22.98	17.65	13.22	14.27	25.94	25.73	2.94	693.05
85	27.22	17.15	15.89	13.35	37.59	17.09	7.02	0.02
86	28.43	8.37	4.81	17.29	21.57	18.21	1.38	45.91
87	15.10	4.16	4.34	23.96	31.38	9.17	8.77	5.47
88	23.87	1.27	3.61	10.10	32.83	22.74	14.80	1.45
89	27.35	18.20	3.33	24.65	35.26	12.34	2.30	0.13
90	27.51	13.99	9.75	20.95	35.30	20.51	2.51	0.15
91	16.14	7.03	19.14	12.96	35.70	24.53	4.65	0.11

92	18.51	1.07	10.32	19.14	23.44	16.41	3.54	284.43
93	25.81	16.93	15.74	10.69	33.37	15.39	11.97	283.96
94	29.32	0.53	8.52	11.04	32.22	19.63	0.19	0.08
95	24.10	16.94	16.48	9.65	27.44	17.23	17.76	148.17
96	20.62	16.29	10.62	11.56	24.70	17.62	15.29	2154.79
97	22.68	10.08	7.88	12.68	25.10	18.91	5.44	1381.57
98	27.70	8.11	11.94	18.72	20.99	22.01	14.10	13.94
99	25.42	15.84	12.96	17.12	33.33	11.84	0.59	0.72
100	18.74	3.77	9.80	19.73	31.62	24.98	1.12	4.17
101	18.37	11.34	7.57	26.55	24.71	10.45	8.89	251.53
102	30.22	3.58	10.11	15.40	22.52	20.78	1.78	0.07
103	26.11	14.04	1.39	11.99	22.22	25.88	2.99	541.32
104	23.53	6.98	12.75	13.04	30.24	25.45	10.73	13.38
105	16.58	13.38	18.18	14.08	34.30	8.36	18.16	0.42
106	21.42	4.06	8.80	13.57	37.24	16.96	16.73	0.04
107	28.07	9.44	15.00	11.12	30.00	20.70	13.41	1.28
108	31.69	10.04	4.61	8.63	22.43	11.67	5.15	0.07
109	20.17	3.85	11.01	9.50	29.63	8.92	8.42	1.72
110	26.34	5.57	8.19	19.25	29.14	29.96	15.23	82.28
111	24.95	5.57	14.94	17.18	37.17	22.58	10.61	0.04
112	20.91	9.20	5.31	26.60	28.26	15.24	4.19	79.43
113	23.99	6.71	4.30	18.22	29.08	24.40	3.48	45.26
114	21.41	0.17	9.79	10.54	23.04	10.42	9.29	0.45
115	20.56	0.92	14.18	21.83	36.68	21.30	1.31	1.14
116	18.70	11.16	7.18	24.06	22.86	16.85	11.49	2957.65
117	20.70	10.05	13.32	14.45	20.00	21.96	16.56	3477.05
118	18.43	2.58	19.79	10.57	22.92	19.65	8.80	1.08
119	19.66	7.54	10.54	21.08	29.73	13.61	12.49	23.71
120	17.89	0.96	13.83	17.70	35.70	9.87	1.85	0.03
121	16.97	11.66	19.15	11.57	23.71	10.05	4.07	71.58
122	18.18	10.53	7.49	16.75	31.15	19.97	8.68	6.48
123	13.85	6.69	8.27	19.20	37.31	21.78	1.75	0.02
124	22.37	14.69	13.15	22.81	28.97	12.73	17.23	33.22
125	28.63	10.93	14.46	19.69	28.51	21.66	11.84	3.13

126	23.86	16.08	5.76	18.04	36.84	23.20	16.88	0.04
127	15.64	3.50	12.64	22.13	27.84	14.58	10.23	107.45
128	15.60	0.50	5.07	20.28	31.31	24.55	8.65	5.88
129	32.13	15.34	9.78	18.41	34.98	21.74	4.87	0.23
130	18.78	3.12	2.18	17.46	20.13	7.94	3.49	218.56
131	31.28	17.31	11.42	15.92	37.92	25.54	0.79	0.02
132	18.23	5.00	17.89	19.02	33.11	16.88	11.62	1.25
133	16.64	10.24	13.21	15.99	30.21	18.62	17.63	17.38
134	17.33	8.38	12.08	9.36	33.94	14.64	16.81	0.57
135	22.98	5.90	6.25	23.16	20.48	7.40	14.94	2.24
136	29.77	6.03	9.01	13.50	28.20	21.25	14.77	1.79
137	27.04	5.66	1.79	12.00	22.91	10.75	12.27	3.23
138	20.26	6.76	15.03	20.28	28.27	23.75	16.76	60.07
139	15.03	4.32	15.74	9.07	34.36	21.74	7.90	0.39
140	22.41	15.32	8.26	21.82	35.36	20.38	15.97	0.13
141	15.81	12.74	4.09	26.77	24.73	15.62	17.06	338.59
142	30.73	8.23	4.78	19.40	21.34	14.49	5.77	1.87
143	22.29	1.25	7.75	13.38	20.17	15.92	11.19	67.21
144	29.37	5.20	3.02	18.79	35.55	24.06	5.42	0.12
145	15.78	2.16	18.40	23.05	23.28	21.30	2.75	1.89
146	31.83	14.77	15.95	23.06	37.21	19.26	6.77	0.03
147	26.64	14.67	6.78	19.91	29.03	11.18	14.17	4.88
148	22.94	1.30	17.51	22.72	20.91	20.49	14.85	0.05
149	15.64	3.13	5.75	13.45	27.62	22.08	4.62	188.65
150	27.25	1.77	7.83	26.27	20.59	21.80	5.51	1.90
151	29.53	11.81	6.52	12.12	19.24	31.11	14.21	21.96
152	16.57	13.65	14.50	10.17	35.27	23.17	1.75	0.13
153	14.50	17.34	11.30	15.09	31.14	13.09	3.18	6.74
154	17.53	12.84	18.09	16.93	31.82	22.23	17.82	3.57
155	25.55	1.81	4.30	14.08	28.41	8.86	0.50	0.22
156	28.60	12.00	9.93	23.40	34.35	8.26	8.59	0.02
157	18.91	13.79	13.24	18.15	27.73	23.00	10.17	164.27
158	22.30	5.98	8.72	16.26	33.62	11.67	18.31	0.67
159	27.55	8.83	18.38	26.39	22.89	23.83	12.80	0.12

160	26.93	4.31	5.88	17.28	25.91	19.29	13.78	36.89
161	24.85	16.73	15.69	8.74	26.49	20.83	10.20	353.58
162	28.14	17.14	15.81	9.11	17.67	31.81	6.93	55.20
163	21.35	4.59	12.42	15.00	29.14	13.64	10.94	12.68
164	29.59	15.91	17.93	8.61	19.60	31.11	3.89	2.96
165	20.23	7.14	11.05	16.60	24.46	15.17	2.23	814.64
166	24.65	3.23	6.68	9.15	21.06	27.86	9.27	109.61
167	28.72	11.42	10.98	22.65	36.15	11.19	8.05	0.04
168	21.07	14.02	9.77	26.28	28.09	20.18	4.70	97.30
169	28.19	10.95	19.16	25.60	26.03	22.11	16.74	0.20
170	25.21	3.48	6.62	16.15	22.27	27.22	11.30	81.98
171	28.55	4.34	17.70	13.71	19.86	23.36	10.52	0.00
172	30.04	16.18	12.51	25.26	35.15	24.02	14.44	0.16
173	28.20	17.89	19.10	21.21	23.55	33.01	3.82	19.62
174	16.13	5.15	3.18	13.96	26.63	23.40	10.77	439.40
175	22.96	0.53	18.47	14.86	28.67	24.30	5.66	0.01
176	20.28	3.09	16.94	8.93	33.01	10.29	12.14	0.02
177	23.67	17.00	5.92	19.62	24.99	17.58	9.85	881.41
178	25.25	12.04	11.22	15.72	23.23	21.35	1.25	621.34
179	31.13	16.67	13.10	9.20	15.70	31.52	16.92	5.69
180	24.02	4.19	7.12	14.05	32.86	28.89	8.29	2.06
181	19.89	7.19	15.12	18.50	35.33	24.16	14.39	0.13
182	14.98	18.37	17.81	9.35	37.75	24.14	11.23	0.01
183	16.59	3.81	1.95	10.00	34.73	15.44	14.62	0.21
184	27.82	17.80	12.79	22.08	29.00	10.12	11.28	1.04
185	28.71	7.00	6.10	17.41	26.52	24.32	4.72	30.36
186	22.73	11.90	15.50	15.01	21.35	19.71	16.61	508.00
187	22.06	5.01	3.77	24.28	22.47	8.49	15.45	21.31
188	27.08	18.39	16.53	13.23	27.92	28.92	7.11	72.74
189	21.49	9.74	9.19	18.77	23.53	22.57	11.10	0.00
190	14.67	8.08	18.34	22.82	21.12	17.35	7.12	2034.31
191	17.45	1.47	16.29	22.34	29.66	22.73	11.17	5.50
192	28.49	10.28	17.48	22.45	26.84	10.74	7.50	0.00
193	14.83	3.56	2.19	10.63	28.75	15.02	3.29	66.82

194	15.85	12.06	5.84	10.43	26.87	19.88	1.85	362.75
195	17.62	5.25	6.30	13.39	27.43	22.25	1.89	222.31
196	19.33	13.49	15.96	22.38	23.80	8.76	10.46	60.23
197	23.96	14.98	12.76	23.62	22.11	17.01	14.31	1035.89
198	15.97	14.93	8.85	21.45	24.34	22.50	16.47	2820.91
199	28.71	10.45	17.77	10.69	25.60	22.88	4.98	0.69
200	21.64	7.83	17.04	12.89	28.81	22.08	3.45	15.51
201	27.89	9.94	4.48	15.91	36.09	8.22	1.71	0.00
202	27.39	0.97	12.94	9.56	25.81	24.43	0.91	0.01
203	16.77	13.04	11.13	9.73	27.13	11.96	3.42	280.19
204	14.47	6.77	6.61	14.75	35.23	8.03	15.95	0.15
205	24.23	6.55	4.93	26.17	29.50	18.53	2.48	30.48
206	19.24	8.77	12.56	10.46	35.07	13.37	9.32	0.18
207	16.38	7.33	14.21	25.62	30.44	11.19	15.78	11.07
208	23.48	3.53	7.61	8.25	26.58	26.19	10.90	148.96
209	24.28	0.10	17.45	18.79	26.18	9.31	12.30	0.00
210	19.33	9.01	15.97	16.88	35.85	24.33	18.19	0.08
211	26.20	12.06	6.33	21.29	22.38	11.16	17.39	9.48
212	31.86	14.99	19.69	9.14	26.88	23.79	4.32	0.09
213	30.68	15.75	3.71	26.32	25.52	15.40	15.53	3.45
214	21.78	16.63	19.45	11.91	28.05	25.04	15.81	122.30
215	23.32	5.71	19.83	14.34	37.99	14.92	11.44	0.00
216	17.14	11.33	6.31	16.50	24.19	10.11	0.68	1636.44
217	28.42	11.04	13.21	20.56	26.16	11.40	0.44	0.22
218	30.67	13.77	6.28	17.98	27.52	18.00	12.58	6.57
219	22.45	6.37	17.04	16.08	20.26	23.88	9.32	2.84
220	27.15	15.72	7.59	22.42	27.33	9.28	0.04	1.04
221	20.11	6.00	12.72	12.49	31.60	23.18	0.82	4.79
222	29.72	10.84	7.65	11.61	30.79	8.89	14.22	0.06
223	14.59	11.61	5.68	9.20	20.61	13.88	1.31	36478.09
224	25.89	1.87	9.10	15.89	37.64	7.94	14.66	0.00
225	28.98	4.70	18.35	26.18	20.14	19.05	10.60	0.00
226	16.67	7.48	8.34	24.41	26.43	15.49	1.56	450.28
227	16.61	9.33	2.23	24.86	30.51	22.42	17.83	11.68

228	29.32	7.84	5.36	26.59	21.01	23.11	2.94	28.00
229	23.71	7.43	5.91	15.22	28.13	25.40	1.24	106.82
230	28.71	15.39	2.16	14.28	21.12	27.76	5.89	59.04
231	28.88	15.21	8.91	11.20	18.26	27.21	8.19	51.86
232	23.16	13.79	10.25	16.33	22.85	24.09	6.93	166.17
233	16.15	17.62	10.02	26.95	24.54	7.80	13.08	190.14
234	20.34	13.42	5.55	20.37	28.91	14.11	0.53	53.38
235	31.67	17.14	17.44	16.96	29.88	12.16	0.04	0.07
236	27.88	17.78	11.53	8.67	21.35	11.07	17.17	0.07
237	16.46	4.58	2.27	19.84	22.15	7.85	9.76	1695.05
238	22.90	16.42	16.04	24.05	34.07	25.06	11.79	0.41
239	21.87	5.58	14.28	9.24	30.89	25.60	14.10	6.67
240	27.79	9.57	19.47	22.09	28.60	15.24	9.35	0.01
241	30.34	13.70	7.78	18.54	26.21	14.54	6.80	3.13
242	15.74	11.01	6.75	22.84	22.21	10.31	3.50	4093.19
243	24.37	16.34	14.30	9.72	31.86	19.10	15.79	3.51
244	14.72	7.04	14.55	10.32	29.10	14.51	18.08	44.24
245	14.46	0.49	8.16	14.31	29.58	8.41	9.70	19.27
246	31.94	15.14	2.33	24.09	21.98	24.18	5.47	3.91
247	18.70	2.43	10.22	22.80	20.04	9.30	13.07	6.71
248	14.76	12.77	17.12	21.01	27.77	16.21	11.94	158.60
249	25.18	1.13	18.19	7.81	28.87	31.36	12.18	0.00
250	16.25	7.79	17.01	17.98	34.59	14.97	7.08	0.33
251	19.39	2.16	1.94	24.54	37.63	20.84	9.52	0.02
252	21.38	3.36	6.61	24.03	28.91	14.52	2.32	38.10
253	24.36	8.46	13.17	13.33	34.68	8.09	9.91	0.00
254	29.56	3.87	5.46	21.19	20.53	34.10	16.62	3.05
255	20.88	15.40	7.51	9.73	34.79	13.53	15.61	0.23
256	31.97	0.09	6.31	22.70	25.33	11.38	16.81	0.00
257	25.96	16.25	3.29	10.88	27.52	26.62	8.89	150.87
258	18.24	1.37	3.22	21.11	19.94	8.31	7.80	146.66
259	30.78	12.76	8.60	16.36	35.67	18.42	1.93	0.11
260	24.11	17.65	1.79	11.68	35.17	12.60	4.25	0.18
261	24.67	9.39	17.74	11.20	30.10	24.99	6.85	2.46

262	15.14	17.17	3.97	25.91	20.29	18.24	15.77	834.88
263	17.70	5.62	7.72	11.77	28.80	22.30	4.83	64.48
264	16.60	3.20	13.46	13.27	29.62	13.46	0.05	21.33
265	27.09	16.97	6.36	16.14	24.52	17.23	4.91	129.46
266	21.19	5.10	10.47	21.28	25.17	15.63	4.56	248.11
267	26.79	15.44	7.55	25.79	36.99	19.69	8.82	0.05
268	26.45	7.55	9.94	26.03	29.59	20.05	16.30	18.05
269	27.05	10.21	15.37	23.84	33.38	25.48	7.78	0.84
270	27.79	13.28	13.65	25.20	37.48	25.70	7.92	0.02
271	14.35	3.06	18.73	17.11	23.87	9.36	2.74	0.77
272	23.24	11.05	15.90	18.29	25.68	11.10	13.10	3.83
273	31.44	4.22	9.19	11.80	28.16	20.73	3.06	0.08
274	25.22	17.92	10.76	21.68	31.87	15.33	18.01	3.14
275	28.85	2.22	3.75	14.30	33.76	9.55	16.15	0.01
276	27.41	13.46	12.30	23.20	29.83	13.55	1.13	6.08
277	30.57	5.66	13.92	16.11	24.23	23.51	17.42	0.01
278	29.59	13.00	9.32	17.42	29.71	21.34	12.96	13.25
279	24.30	5.81	8.19	15.96	21.91	26.91	4.97	291.96
280	24.22	1.82	13.10	11.71	26.58	23.91	12.08	0.40
281	28.67	1.20	10.53	15.18	22.28	17.35	12.32	0.03
282	31.66	10.96	8.96	23.31	35.39	25.14	4.12	0.15
283	14.55	7.79	14.18	25.49	25.63	19.05	12.01	558.91
284	18.51	4.25	5.16	26.47	22.38	19.20	14.31	512.84
285	16.63	5.25	16.70	16.04	23.27	14.58	4.15	147.27
286	21.34	15.14	9.10	25.68	21.97	12.10	3.30	400.42
287	27.95	13.36	13.73	10.47	37.82	15.89	9.96	0.02
288	19.15	17.35	6.58	10.91	27.81	14.78	9.52	155.66
289	19.21	9.55	4.73	10.79	27.14	21.88	5.84	289.94
290	15.03	4.20	6.81	11.39	22.11	8.92	0.68	2141.33
291	23.13	11.70	11.01	24.63	27.05	10.66	1.59	32.18
292	30.61	11.36	6.81	10.80	32.52	17.29	15.20	1.38
293	24.07	4.40	17.36	10.20	24.00	22.46	7.74	0.17
294	23.16	10.18	18.39	22.70	32.15	10.54	18.03	0.10
295	24.76	8.33	13.35	20.58	21.52	10.21	5.28	0.31

296	14.50	11.96	18.88	17.25	29.29	23.47	8.57	36.56
297	27.04	2.82	10.80	18.92	20.29	25.65	15.97	0.48
298	17.92	5.64	11.32	19.03	28.68	18.04	17.12	71.54
299	19.69	9.54	16.37	16.32	35.35	20.27	1.44	0.17
300	15.36	4.68	16.71	9.28	36.16	10.95	7.40	0.09
301	30.11	17.53	15.86	8.13	22.77	30.82	12.20	9.37
302	23.59	8.56	6.80	22.13	25.10	23.25	1.07	1079.25
303	28.38	11.71	2.55	21.06	24.43	17.59	4.92	46.80
304	25.71	5.01	6.69	13.41	28.93	25.52	8.08	39.11
305	18.70	11.04	19.66	21.29	21.62	23.13	2.61	413.02
306	14.45	3.82	7.93	15.44	28.74	22.89	2.51	64.77
307	24.47	17.67	8.51	16.42	23.60	13.62	17.09	275.08
308	28.22	12.68	12.84	15.60	12.32	28.41	2.87	33.46
309	30.14	16.28	9.76	24.26	34.05	17.25	15.42	0.41
310	24.02	6.82	11.29	19.82	21.72	16.32	8.23	58.22
311	17.41	18.36	4.55	18.63	22.56	14.43	10.59	8449.02
312	29.19	0.77	3.49	14.35	33.86	24.27	7.12	0.58
313	28.32	14.78	4.57	26.80	33.07	12.31	16.98	0.64
314	24.43	13.58	5.57	9.03	35.71	24.54	11.46	0.10
315	24.93	10.24	6.87	8.97	33.21	14.29	3.26	0.97
316	14.99	18.25	2.95	21.53	30.00	20.67	11.14	19.71
317	17.64	0.74	11.24	16.65	31.18	17.18	1.80	6.71
318	28.61	12.37	5.82	19.08	31.71	24.80	7.83	3.65
319	24.93	15.33	8.32	9.59	26.48	20.37	6.81	402.04
320	24.89	14.92	6.63	21.75	28.66	14.90	4.67	40.59
321	14.08	3.70	8.54	22.23	20.61	9.32	10.46	1914.89
322	28.35	6.69	6.01	11.52	22.30	29.79	8.11	29.81
323	23.89	13.08	8.81	26.40	22.09	22.08	6.49	482.62
324	14.15	15.96	8.54	26.45	35.63	15.93	16.49	0.10
325	20.89	11.09	19.68	19.80	30.20	23.01	17.35	15.16
326	19.02	11.78	18.08	26.26	19.64	20.26	1.14	515.40
327	20.63	8.83	2.95	19.04	20.38	21.78	16.06	513.24
328	22.65	2.06	4.74	21.40	26.22	22.47	10.04	410.63
329	15.34	1.89	6.92	19.97	35.79	16.86	1.07	0.14

330	20.94	15.33	6.18	17.00	31.40	10.65	7.32	4.95
331	24.99	12.61	16.63	25.83	29.94	10.83	3.36	0.96
332	21.97	1.63	3.54	25.05	25.56	20.76	16.07	581.18
333	25.89	15.59	18.72	10.25	38.02	19.57	10.63	0.01
334	28.52	7.52	16.18	9.39	31.39	16.17	2.03	0.04
335	31.55	3.13	13.05	13.07	23.30	20.86	3.14	0.00
336	25.88	4.19	7.68	13.82	22.49	28.28	11.11	33.94
337	16.63	16.52	14.10	15.91	31.30	10.72	12.76	5.99
338	32.03	14.91	8.87	16.60	32.72	19.96	7.25	1.12
339	17.80	9.64	18.07	19.10	33.59	23.55	0.57	0.66
340	13.94	5.29	14.48	19.41	23.95	23.45	1.37	129.06
341	25.65	8.40	8.05	22.11	21.06	9.10	17.11	1.28
342	24.20	15.91	15.60	14.77	35.87	13.66	5.77	0.07
343	25.63	8.90	14.83	15.56	29.21	12.89	9.15	0.90
344	14.71	0.68	2.29	15.50	27.93	12.47	5.73	138.60
345	22.08	9.88	16.58	11.74	32.06	12.66	12.57	2.08
346	17.35	2.93	8.54	11.03	27.47	12.45	10.67	128.15
347	29.40	2.53	5.36	16.25	21.72	17.00	14.57	1.52
348	15.67	12.33	4.19	20.98	37.18	21.18	0.36	0.02
349	27.45	10.76	3.62	9.86	20.34	24.67	11.98	194.12
350	22.96	15.59	16.39	16.60	27.99	15.71	7.92	86.46
351	26.63	13.96	11.38	18.24	27.97	24.49	3.70	90.35
352	28.57	1.19	4.98	21.60	21.96	19.28	12.85	2.80
353	26.31	6.39	10.05	26.53	20.01	16.19	10.45	11.46
354	25.57	11.90	19.15	16.33	24.85	22.88	4.33	3.42
355	27.63	17.60	16.15	8.87	18.64	33.41	7.11	89.71
356	19.18	12.53	2.79	26.85	32.19	7.50	8.60	2.12
357	25.59	12.73	16.46	24.32	28.27	13.07	5.75	4.01
358	28.50	11.28	14.45	10.24	27.42	9.54	15.49	0.02
359	23.52	9.84	6.22	12.89	30.55	20.75	18.20	12.46
360	26.45	13.56	5.84	9.21	28.58	19.83	5.60	66.16
361	26.03	9.42	9.38	25.95	23.44	23.62	17.55	183.97
362	25.02	3.56	7.30	8.26	22.03	34.01	10.61	59.11
363	28.32	2.98	9.80	11.45	23.54	29.58	15.10	0.29

364	27.74	11.17	3.63	17.47	30.02	12.15	13.87	3.28
365	19.19	11.01	6.70	21.21	27.69	24.65	0.32	165.63
366	23.44	14.48	11.76	22.93	24.18	8.28	16.98	7.52
367	31.99	3.27	9.28	16.47	33.31	23.00	3.53	0.01
368	26.91	17.23	16.14	9.43	21.70	29.62	8.32	153.38
369	26.68	12.77	15.01	20.59	26.81	18.53	14.35	27.86
370	18.61	16.17	3.66	22.72	30.37	20.54	9.31	13.91
371	16.63	3.23	8.46	14.35	36.39	25.69	7.66	0.05
372	29.60	16.29	9.54	19.20	24.93	21.92	15.83	30.48
373	29.95	14.48	1.69	16.11	34.82	24.07	17.63	0.25
374	25.45	4.87	19.14	19.14	23.82	16.17	15.67	0.01
375	16.42	14.48	16.33	12.40	25.98	8.81	16.50	308.82
376	22.63	9.10	12.70	19.62	24.10	25.09	7.22	550.92
377	19.20	5.11	13.25	24.41	22.19	25.75	7.22	334.85
378	22.14	14.60	10.94	25.78	25.79	21.07	1.58	454.87
379	28.70	13.39	12.71	13.94	19.93	26.22	7.66	28.21
380	28.39	16.53	17.13	15.32	32.13	30.32	3.52	2.02
381	16.74	7.39	7.58	25.40	31.45	19.47	6.36	4.89
382	28.97	3.44	2.23	25.08	32.67	9.06	0.22	0.08
383	13.94	13.26	1.89	8.58	25.60	19.32	11.77	1134.20
384	24.73	18.16	13.71	22.81	32.95	17.30	3.01	1.20
385	31.71	16.64	2.00	25.92	33.63	21.81	5.50	0.68
386	22.88	6.07	6.31	19.44	23.86	24.53	15.06	71.27
387	30.06	9.19	9.06	12.56	35.39	19.57	2.98	0.18
388	16.81	9.24	18.41	18.62	31.38	22.13	10.30	5.78
389	21.21	5.58	18.39	20.48	29.83	12.06	5.22	0.19
390	21.20	7.89	1.69	21.14	27.91	20.05	0.92	136.18
391	26.72	7.73	5.09	18.26	37.79	23.87	11.45	0.02
392	22.33	3.65	7.77	26.17	22.58	11.91	13.14	23.73
393	28.91	2.66	11.11	11.42	21.29	24.94	7.75	0.06
394	22.76	1.30	3.92	24.02	33.17	18.12	12.41	1.14
395	16.30	10.89	12.63	26.40	37.27	22.95	4.93	0.02
396	22.09	10.73	18.74	9.20	30.64	11.67	2.53	1.75
397	17.66	0.91	3.10	12.81	35.43	16.49	10.73	0.14

398	25.70	4.69	5.74	22.02	24.85	22.66	10.08	179.60
399	25.87	1.22	17.04	14.60	27.80	14.52	0.32	0.00
400	26.54	16.55	16.00	12.40	35.16	25.69	17.23	0.17
401	18.91	0.55	8.48	16.34	20.95	32.03	1.78	554.45
402	25.74	10.17	18.24	21.94	24.36	30.88	1.87	1.01
403	23.07	13.51	7.83	19.88	37.39	31.71	6.54	0.01
404	29.19	16.44	5.19	11.71	18.51	29.31	5.88	35.52
405	20.97	10.89	17.43	16.70	22.69	32.60	16.70	288.69
406	31.28	10.52	17.56	13.95	27.88	26.72	8.77	0.01
407	27.62	17.05	16.18	12.12	37.22	29.65	10.89	0.02
408	13.91	0.92	8.64	19.07	33.69	32.46	13.63	0.55
409	20.40	3.43	5.79	22.74	36.94	29.72	10.00	0.03
410	20.47	16.35	2.03	19.97	34.27	26.94	15.26	0.31
411	16.42	15.26	19.09	11.23	23.69	28.15	2.59	129.32
412	26.07	3.45	11.73	21.74	23.28	26.22	13.75	0.84
413	18.51	16.74	11.11	17.40	21.77	26.89	16.90	394.08
414	26.43	12.16	17.29	17.27	28.56	34.06	14.95	5.24
415	14.39	13.92	2.06	21.70	34.91	30.34	0.54	0.17
416	31.43	13.40	17.83	15.81	24.92	34.38	12.73	0.06
417	31.71	18.29	18.17	11.66	24.00	29.27	11.27	1.55
418	21.49	7.44	9.55	23.90	29.69	30.87	3.99	23.53
419	31.71	3.04	11.52	24.44	33.12	27.75	5.28	0.00
420	21.22	7.98	14.32	21.15	21.33	27.10	2.42	290.47
421	26.14	18.17	11.27	13.24	20.09	26.60	4.01	470.80
422	20.21	2.35	11.71	13.84	27.54	32.04	13.47	39.97
423	21.29	1.78	1.81	10.87	25.67	33.66	1.14	87.08
424	23.98	13.27	14.71	10.42	35.13	28.45	17.79	0.15
425	23.89	10.71	13.69	12.89	23.58	32.37	1.57	252.44
426	21.48	9.61	16.68	25.51	21.70	28.20	2.64	114.96
427	24.13	12.98	12.00	24.19	27.58	28.76	12.16	143.89
428	19.85	15.34	11.98	19.06	22.71	33.15	9.94	302.17
429	17.16	6.31	6.99	22.28	28.69	34.29	13.33	58.40
430	24.40	8.63	14.27	15.64	34.30	26.73	4.35	0.35
431	18.81	13.45	1.72	18.20	35.15	26.31	11.37	0.13

432	19.29	5.14	2.67	11.97	27.35	29.09	15.88	211.13
433	21.86	5.58	15.13	25.86	34.37	26.64	1.53	0.32
434	14.08	14.90	19.09	21.13	31.50	30.83	11.09	3.85
435	19.16	11.55	16.12	11.30	22.61	34.02	14.65	112.17
436	20.22	11.01	15.96	21.75	19.70	34.62	2.15	79.59
437	19.73	13.07	5.24	23.57	32.77	29.05	18.36	1.29
438	22.78	2.63	6.16	16.71	32.27	32.78	15.60	1.99
439	27.91	14.91	14.58	10.31	20.18	29.19	14.91	51.70
440	28.52	8.12	8.40	9.90	36.15	26.06	2.06	0.07
441	15.13	14.66	19.32	24.54	20.63	26.74	14.24	110.27
442	31.66	0.13	4.62	21.07	37.19	27.53	1.47	0.00
443	14.84	10.04	19.43	18.86	24.89	34.04	2.10	104.38
444	14.55	3.11	15.00	8.82	34.31	33.15	12.73	0.34
445	14.97	14.81	15.23	12.55	24.77	28.92	15.64	84.41
446	20.29	6.36	9.34	14.92	34.09	31.66	0.35	0.41
447	16.29	15.23	19.61	13.83	37.08	29.51	17.08	0.03
448	21.31	4.68	7.71	16.21	24.63	26.91	7.22	92.89
449	32.24	9.00	4.21	13.02	28.72	30.23	14.19	1.73
450	23.67	6.00	10.84	25.34	32.28	33.45	11.31	1.99
451	25.09	4.61	8.40	25.13	28.57	33.48	1.83	28.53
452	20.24	17.52	10.34	23.31	33.31	33.34	0.41	0.73
453	28.29	4.78	9.16	20.89	33.86	30.10	3.97	0.38
454	25.74	3.40	6.39	26.72	28.13	26.63	15.24	34.20
455	27.73	6.05	2.74	22.52	30.36	32.12	14.78	9.45
456	21.42	8.92	16.52	8.98	35.66	31.17	6.94	0.10
457	29.23	16.64	18.11	24.77	20.24	27.66	12.92	7.36
458	15.49	17.60	8.06	11.15	23.28	29.27	11.46	171.06
459	17.06	14.50	6.90	10.39	20.22	33.38	4.95	1396.62
460	22.97	10.13	17.49	17.25	31.63	26.96	4.51	3.71
461	23.81	11.49	11.99	23.16	36.94	34.12	9.15	0.03
462	21.99	12.27	4.14	12.92	38.05	32.50	10.87	0.01
463	23.91	18.18	12.36	13.29	36.98	33.86	7.78	0.03
464	15.91	0.03	19.05	11.79	29.78	34.14	5.08	0.27
465	16.97	8.89	9.32	21.84	25.05	28.46	10.85	77.57

466	19.43	1.60	17.73	17.09	23.32	26.26	2.66	0.38
467	20.30	12.56	1.55	18.77	30.65	32.58	10.65	8.63
468	28.21	15.19	0.20	10.75	18.18	28.11	3.24	89.74
469	16.26	2.16	5.72	8.90	32.74	28.45	8.86	1.39
470	23.45	9.17	13.56	17.26	23.23	34.61	1.69	158.42
471	31.29	12.94	7.80	12.59	18.83	24.60	18.99	6.37
472	25.79	3.55	17.26	26.05	25.14	34.02	6.05	0.01
473	20.37	3.86	12.07	9.77	30.92	32.44	14.48	6.76
474	27.78	14.67	13.87	21.69	26.52	25.95	7.22	60.45
475	28.52	14.20	12.94	24.68	36.88	31.48	0.53	0.03
476	29.57	14.06	10.03	26.88	28.52	27.60	14.93	16.70
477	15.17	3.43	13.74	18.68	25.99	32.85	4.47	460.36
478	25.44	3.59	5.99	19.47	33.90	34.51	11.99	0.44
479	27.21	6.68	11.52	13.17	22.05	29.55	16.18	3.65
480	25.57	10.14	3.29	26.24	33.58	31.09	5.89	0.59
481	22.33	8.72	3.05	24.22	24.97	33.11	5.15	74.63
482	17.27	0.88	11.43	10.77	27.60	33.82	17.46	92.83
483	16.66	15.62	6.01	9.61	29.53	29.69	5.40	27.61
484	26.88	13.81	4.22	10.91	17.91	27.91	7.91	239.06
485	24.03	10.37	13.84	15.13	31.65	27.33	14.62	3.92
486	24.66	7.98	12.09	11.74	29.55	32.83	4.56	18.05
487	15.65	14.69	19.65	9.29	23.41	28.44	14.26	245.92
488	22.74	3.58	5.58	17.61	30.05	31.74	17.22	16.54
489	19.03	8.38	15.96	11.86	25.41	29.78	17.42	423.40
490	26.99	10.01	18.99	9.54	37.45	28.84	0.75	0.01
491	29.97	8.53	13.13	26.13	36.09	31.20	17.34	0.03
492	18.47	0.59	6.17	24.21	27.93	31.85	11.57	119.98
493	25.99	16.62	13.69	9.91	27.93	34.93	9.95	94.73
494	25.81	2.46	3.06	14.57	32.63	30.51	5.16	1.48
495	25.42	0.03	10.07	16.89	21.60	33.56	15.12	0.22
496	21.16	13.45	18.29	17.31	26.05	32.91	16.97	405.68
497	31.65	10.34	5.15	20.15	24.86	32.43	2.64	3.08
498	16.52	16.09	9.05	9.91	27.09	27.68	15.13	271.81
499	26.19	18.52	13.01	12.23	14.98	31.23	3.23	16.43

500	33.83	12.34	13.11	23.06	38.13	21.01	7.13	0.09

Table S4. KMC simulated results and calculated nominal DRC coefficients for CO_2 hydrogenation over Cu(111) from the DRC analysis

	kMC simulated methanol TOF / site^{-1}·s^{-1}					DRC coefficients
	$E_i - 2\Delta E$	$E_i - \Delta E$	E_i	$E_i + \Delta E$	$E_i + 2\Delta E$	χ_i
R_1	61.1105	58.9786	40.4718	18.9864	4.0432	0.3010
R_2	11.5611	27.6844	40.4718	51.5580	57.2320	-0.1600
R_3	56.9192	51.2450	40.4718	27.8097	11.4390	0.1557
R_4	40.4818	40.2323	40.4718	39.9813	39.7228	0.0015
R_5	233.0354	145.4736	40.4718	7.0001	0.8212	0.8827
R_6	12.4844	28.1772	40.4718	55.7940	56.3998	-0.1875
R_7	39.9679	40.1809	40.4718	39.9524	39.8091	0.0019

Table S5. Calculated descriptors' value on M-Cu(111) alloys.

Descriptors	Descriptors' value / (kCal·mol^{-1})				
	Au-Cu(111)	Cu(111)	Pd-Cu(111)	Pt-Cu(111)	Ni-Cu(111)
E_1	23.06	23.06	28.83	28.83	25.14
E_5	31.59	28.83	18.22	14.68	23.06
E_6	14.53	16.60	27.90	31.82	34.28

$\bar{E}_{1,3}$	14.75	14.53	0.46	20.51	11.68
$\bar{E}_{1,5}$	26.99	25.78	22.91	18.89	24.08
$\bar{E}_{2,5}$	13.72	11.45	16.72	14.71	6.36

Table S6. Comparison between the kMC simulated methanol production rate and the predicted result from degree of rate control model, simplified machine learning model, and machine learning model.

Models	**Methanol ln(TOF)/site^{-1}·s^{-1}**				
	Au-Cu(111)	**Cu(111)**	**Pd-Cu(111)**	**Pt-Cu(111)**	**Ni-Cu(111)**
kMC	1.4727	3.6904	3.9720	4.0591	3.8223
ML	1.6038	3.4868	3.8709	4.1053	3.7807
Simplified ML	1.2627	3.5320	3.7546	3.8067	4.1256
DRC	1.3992	3.6904	14.9019	18.1721	11.1540

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