

Table S1. The name, reaction temperature (K), quasi-SMILES, the set (active training (+), passive training set (-), calibration set (#), validation set (*)), experimental logK_{O3}, and predicted logK_{O3} of VOCs of Split #1 based on TF2

No.	Name	T (K)	Quasi-SMILES	Set	logK _{O3}	
					Exp.	Prd.
1	alpha-phellandrene	295	<chem>CC(C)C1CC=C(C)C=C1[T24]</chem>	+	-13.92	-13.93
2	bicyclo[2.2.1]-25-heptadiene	297	<chem>C1C2C=CC1C=C2[T24]</chem>	#	-14.33	-14.97
3	bicyclo[2.2.1]-2-heptene	297	<chem>C1CC2CC1C=C2[T24]</chem>	*	-14.67	-14.79
4	3,7-dimethyl-1,3,6-octatriene	298	<chem>CC(C)=CCC=C(C)C=C[T24]</chem>	*	-14.70	-14.80
5	1,3-cyclohexadiene	297	<chem>C1CC=CC=C1[T24]</chem>	+	-14.71	-15.06
6	2,3-dimethyl-2-butene	363	<chem>CC(C)=C(C)C[T37]</chem>	+	-14.85	-14.71
7	3-methylene-7-methyl-1,6-octadiene	295	<chem>CC(C)=CCCC(=C)C=C[T24]</chem>	#	-14.90	-14.60
8	2,3-dimethyl-2-butene	298	<chem>CC(C)=C(C)C[T24]</chem>	*	-14.98	-14.92
9	cyclopentene	294	<chem>C1CC=CC1[T24]</chem>	#	-15.01	-15.70
10	2,3-dimethyl-2-butene	227	<chem>CC(=C(C)C)C[T10]</chem>	#	-15.05	-15.54
11	2,3-dimethyl-2-butene	247	<chem>CC(C)=C(C)C[T13]</chem>	+	-15.08	-15.36
12	2,3-dimethyl-2-butene	284	<chem>CC(C)=C(C)C[T22]</chem>	-	-15.08	-15.05
13	cyclopentene	299	<chem>C1CC=CC1[T25]</chem>	*	-15.09	-15.51
14	1-Methyl-1-cyclopentene	298	<chem>CC1=CCCC1[T24]</chem>	-	-15.17	-15.32
15	d-limonene	295	<chem>CC(=C)C1CCC(=CC1)C[T24]</chem>	+	-15.19	-15.20
16	Dihydromyrcene	298	<chem>CC(CCC=C(C)C)C=C[T24]</chem>	#	-15.20	-14.54
17	trans-3-methyl-2-pentene	299	<chem>C\C(C)=C\C[T25]</chem>	-	-15.25	-15.41
18	carvomenthene	295	<chem>CC(C)C1CCC(=CC1)C[T24]</chem>	*	-15.28	-15.82
19	cis-3-methyl-2-pentene	299	<chem>CC\C(C)=C/C[T25]</chem>	+	-15.34	-15.71
20	linalool	298	<chem>CC(C)=CCCC(C)(O)C=C[T24]</chem>	-	-15.37	-15.62
21	2-methyl-2-butene	298	<chem>CC=C(C)C[T24]</chem>	+	-15.40	-15.46
22	6-methyl-5-hepten-2-one	298	<chem>CC(C)=CCCC(C)=O[T24]</chem>	-	-15.41	-15.50
23	(Z,Z)-2,4-hexadiene	298	<chem>C\C=C/C=C\C[T24]</chem>	#	-15.43	-15.18
24	trans-2,trans-4-hexadiene	294	<chem>C\C=C/C=C/C[T24]</chem>	*	-15.43	-15.48
25	2-methyl-2-butene	284	<chem>CC=C(C)C[T22]</chem>	#	-15.48	-15.58
26	cis-2,trans-4-hexadiene	294	<chem>C\C=C/C=C/C[T24]</chem>	-	-15.50	-15.48
27	cycloheptene	297	<chem>C1CCC=CCC1[T24]</chem>	*	-15.50	-14.75
28	trans-2-pentene	296	<chem>CC/C=C/C[T24]</chem>	*	-15.50	-16.14
29	cis-2-butene	364	<chem>C\C=C/C[T37]</chem>	-	-15.56	-15.87
30	trans-2-butene	336	<chem>C\C=C\C[T31]</chem>	*	-15.56	-16.33
31	trans-2-butene	298	<chem>C\C=C\C[T24]</chem>	#	-15.59	-15.78
32	2-buten-1-ol	289	<chem>CC=CCO[T22]</chem>	#	-15.60	-16.01
33	1,2-Dimethylcyclohexene	298	<chem>CC1=C(C)CCCC1[T24]</chem>	*	-15.68	-15.27
34	cis-2-pentene	296	<chem>CC\C=C/C[T24]</chem>	*	-15.68	-15.92
35	cyclohexene	294	<chem>C1CCC=CC1[T24]</chem>	#	-15.69	-15.72
36	trans-2-butene	309	<chem>C\C=C\C[T27]</chem>	*	-15.69	-15.56

37	2-methyl-2-butene	227	CC=C(C)C[T10]	*	-15.71	-16.07
38	trans-2-butene	314	C\C=C\C[T28]	*	-15.71	-16.33
39	beta-phellandrene	295	CC(C)C1CCC(=C)C=C1[T24]	-	-15.75	-15.88
40	1-methyl-1-cyclohexene	298	CC1=CCCCC1[T24]	#	-15.78	-15.33
41	trans-3-hexene	298	CC\C=C\CC[T24]	#	-15.80	-15.75
42	1,3-cycloheptadiene	294	C1CC=CC=CC1[T24]	-	-15.81	-15.74
43	ethyl vinyl ether	298	CCOC=C[T24]	-	-15.81	-15.99
44	4-acetyl-1-methylcyclohexene	298	CC(=O)C1CCC(=CC1)C[T24]	+	-15.82	-15.88
45	2,4,4-trimethyl-2-pentene	298	CC(C)=CC(C)(C)C[T24]	+	-15.85	-16.09
46	cis-3-hexene	293.3	CC\C=C/CC[T24]	*	-15.85	-15.97
47	cis-2-butene	297	C\C=C/C[T24]	*	-15.86	-16.08
48	cis-2-butene	309	C\C=C/C[T27]	*	-15.86	-15.86
49	cis-2-butene	297	C\C=C/C[T24]	#	-15.86	-16.08
50	cis-2-butene	309	C\C=C/C[T27]	+	-15.86	-15.86
51	cis-2-butene	314	C\C=C/C[T28]	*	-15.87	-16.63
52	trans-4-octene	298	CCC\C=C\CCC[T24]	#	-15.88	-15.79
53	cis-2-butene	298	C\C=C/C[T24]	+	-15.90	-16.08
54	trans-3-hexene	286.5	CC\C=C\CC[T22]	-	-15.91	-15.94
55	cis-5-decene	298	CCCC\C=C/CCCC[T24]	*	-15.94	-16.28
56	trans-2-butene	264	C\C=C\C[T18]	-	-15.94	-15.99
57	trans-2-butene	277	C\C=C\C[T19]	+	-15.94	-15.95
58	trans-2-butene	264	C\C=C\C[T18]	#	-15.94	-15.99
59	trans-2-butene	277	C\C=C\C[T19]	#	-15.94	-15.95
60	cyclohexene	297	C1CCC=CC1[T24]	*	-15.98	-15.72
61	trans-4-octene	290	CCC\C=C\CCC[T22]	+	-16.00	-15.85
62	trans-2-butene	251	C\C=C\C[T14]	-	-16.03	-16.33
63	2-heptene	298	CCCCCC=CC[T24]	-	-16.06	-16.33
64	cis-2-butene	264	C\C=C/C[T18]	*	-16.06	-16.29
65	cis-2-butene	277	C\C=C/C[T19]	-	-16.06	-16.25
66	4-Methyl-1-cyclohexene	298	CC1CCC=CC1[T24]	+	-16.09	-15.87
67	1,3-pentadiene, 2-methyl	298	C\C=C\C(=C)C[T24]	+	-16.10	-15.58
68	2,4-Dimethyl-1,3-butadiene	298	CC=CC(C)=C[T24]	*	-16.10	-16.23
69	1,4-cyclohexadiene	297	C1C=CCC=C1[T24]	+	-16.19	-16.34
70	trans-2-butene	225	C\C=C\C[T10]	#	-16.22	-16.40
71	trans-2-butene	227	C\C=C\C[T10]	+	-16.23	-16.40
72	1,3,5-cycloheptatriene	294	C1C=CC=CC=C1[T24]	#	-16.27	-15.99
73	cis-2-butene	238	C\C=C/C[T12]	*	-16.28	-16.63
74	cis-2-butene	255	C\C=C/C[T15]	-	-16.31	-16.63
75	cis-2-butene	227	C\C=C/C[T10]	-	-16.33	-16.70
76	(E)-1,3-pentadiene	298	C/C=C/C=C[T24]	+	-16.37	-16.28
77	trans-2,2-dimethyl-3-hexene	295.5	CC/C=C/C(C)(C)C[T24]	*	-16.39	-16.38

78	trans-2,5-dimethyl-3-hexene	291	CC(C)\C=C\C(C)C[T22]	#	-16.41	-16.77
79	propene	362	CC=C[T36]	*	-16.42	-17.19
80	trans-2,5-dimethyl-3-hexene	298	CC(C)\C=C\C(C)C[T24]	#	-16.42	-16.47
81	beta-pinene	295	CC1(C)C2CCC(=C)C1C2[T24]	*	-16.44	-16.69
82	trans-2,2-dimethyl-3-hexene	294	CC/C=C/C(C)(C)C[T24]	+	-16.44	-16.38
83	styrene	303	C=Cc1ccccc1[T26]	+	-16.52	-16.71
84	1-butene	363	CCC=C[T37]	-	-16.55	-16.63
85	1,3,5-hexatriene	294	C=CC=CC=C[T24]	+	-16.58	-16.68
86	2,3-dimethyl-1,3-butadiene	298	CC(=C)C(C)=C[T24]	*	-16.58	-15.85
87	trans-2-hexenyl acetate	288.4	CCC/C=C/COC(C)=O[T22]	+	-16.61	-16.56
88	3-penten-2-one	296	CC=CC(C)=O[T24]	#	-16.67	-17.08
89	styrene	296	C=Cc1ccccc1[T24]	*	-16.67	-16.83
90	beta-pinene	296	CC1(C)C2CCC(=C)C1C2[T24]	+	-16.68	-16.69
91	1-penten-3-ol	289	CCC(O)C=C[T22]	*	-16.75	-16.78
92	2-methyl-1,3-butadiene	323	CC(=C)C=C[T29]	#	-16.75	-17.80
93	1-heptene	296	CCCCC=C[T24]	+	-16.76	-17.00
94	2-methyl-1-pentene	296	CCCC(C)=C[T24]	*	-16.77	-17.02
95	1-buten-3-ol	298	CC(O)C=C[T24]	+	-16.79	-16.70
96	2,5-dihydrofuran	294	C1OCC=C1[T24]	#	-16.79	-16.73
97	2-methyl-1-butene	298	CCC(C)=C[T24]	+	-16.80	-16.53
98	pyrrole	295	[nH]1cccc1[T24]	-	-16.80	-17.11
99	2-methylpropene	295	CC(C)=C[T24]	#	-16.84	-17.02
100	2-vinyl pyridine	298	C=Cc1ccccn1[T24]	-	-16.84	-16.92
101	2,5-dimethyl-1,5-hexadiene	298	CC(=C)CCC(C)=C[T24]	#	-16.85	-16.16
102	isoprene	298	CC(=C)C=C[T24]	+	-16.85	-17.25
103	propene	309	CC=C[T27]	#	-16.85	-17.02
104	1-butene	314	CCC=C[T28]	*	-16.86	-17.38
105	2-ethyl-1-butene	287	CCC(=C)CC[T22]	*	-16.86	-18.03
106	2-methylpropene	299	CC(C)=C[T25]	*	-16.87	-16.82
107	2-methyl-1,4-pentadiene	298	CC(=C)CC=C[T24]	-	-16.89	-17.24
108	propene	299	CC=C[T25]	*	-16.89	-17.05
109	1-octene	298	CCCCCCC=C[T24]	+	-16.90	-17.12
110	2-methyl-1,3-butadiene	295	CC(=C)C=C[T24]	-	-16.90	-17.25
111	2-methyl-1-pentene	287	CCCC(C)=C[T22]	-	-16.90	-17.33
112	propene	294	CC=C[T24]	*	-16.90	-17.24
113	propene	298	CC=C[T24]	#	-16.90	-17.24
114	tetramethylhydrazine	296	CN(C)N(C)C[T24]	-	-16.90	-17.10
115	1-butene	299	CCC=C[T25]	#	-16.91	-16.64
116	2-methylpropene	294	CC(C)=C[T24]	+	-16.92	-17.02
117	1-hexene	303	CCCCC=C[T26]	+	-16.95	-16.76
118	1-hexene	299	CCCCC=C[T25]	#	-16.96	-16.68

119	3-methyl-1-butene	298	CC(C)C=C[T24]	-	-16.96	-16.94
120	1-hexene	294	CCCCC=C[T24]	+	-16.97	-16.88
121	1-pentene	299	CCCC=C[T25]	*	-16.97	-16.53
122	4-methyl-1-pentene	296	CC(C)CC=C[T24]	-	-16.98	-17.31
123	propene	296	CC=C[T24]	#	-16.98	-17.24
124	1-butene	303	CCC=C[T26]	+	-16.99	-16.72
125	2,3-dimethyl-1-butene	285	CC(C)C(C)=C[T22]	*	-17.00	-16.60
126	2-methyl-3-buten-2-ol	298	CC(C)(O)C=C[T24]	+	-17.00	-16.85
127	1-hexene	287	CCCCC=C[T22]	*	-17.01	-16.81
128	trimethylamine	296	CN(C)C[T24]	-	-17.01	-17.13
129	1-heptene	287	CCCCCC=C[T22]	+	-17.03	-16.93
130	ethene	362	C=C[T36]	*	-17.04	-18.26
131	methyl methacrylate	291	COC(=O)C(C)=C[T22]	*	-17.12	-18.38
132	vinylcyclohexane	298	C=CC1CCCCC1[T24]	+	-17.12	-17.17
133	1-butene	282	CCC=C[T20]	-	-17.13	-17.38
134	propene	286	CC=C[T22]	#	-17.13	-17.17
135	4-methyl-1-pentene	287	CC(C)CC=C[T22]	+	-17.14	-17.24
136	2-methyl-1,3-butadiene	260	CC(=C)C=C[T17]	+	-17.16	-17.07
137	1,3-butadiene	298	C=CC=C[T24]	+	-17.17	-17.02
138	ethyl vinyl ketone	285	CCC(=O)C=C[T22]	+	-17.22	-17.46
139	ethyl acrylate	298	CCOC(=O)C=C[T24]	-	-17.24	-17.42
140	3-chloro-1-butene	335	CC(Cl)C=C[T31]	-	-17.27	-17.99
141	propene	260	CC=C[T17]	*	-17.29	-17.06
142	2-methylpropene	260	CC(C)=C[T17]	*	-17.30	-16.84
143	3-Buten-1-ol	298	OCCC=C[T24]	+	-17.31	-17.26
144	3-methyl-1-pentene	298	CCC(C)C=C[T24]	#	-17.31	-17.45
145	1-butene	260	CCC=C[T17]	*	-17.32	-16.65
146	methyl vinyl ketone	296	CC(=O)C=C[T24]	+	-17.32	-17.41
147	3-chloro-1-butene	329	CC(Cl)C=C[T30]	+	-17.35	-17.05
148	methyl crotonate	291	COC(=O)\C=C\C[T22]	-	-17.36	-17.54
149	ethene	332	C=C[T30]	#	-17.42	-17.92
150	2-methylpropene	247	CC(C)=C[T13]	#	-17.44	-17.46
151	3-chloro-1-butene	316	CC(Cl)C=C[T28]	#	-17.44	-17.99
152	3-methyl-2-isopropyl-1-butene	298	CC(C)C(=C)C(C)C[T24]	#	-17.48	-17.69
153	1-butene	247	CCC=C[T13]	+	-17.50	-17.27
154	vinyl acetate	298	CC(=O)OC=C[T24]	+	-17.50	-17.44
155	dimethylamine	296	CNC[T24]	+	-17.58	-17.59
156	3-chloro-1-butene	303	CC(Cl)C=C[T26]	#	-17.59	-17.33
157	furan	298	o1cccc1[T24]	-	-17.62	-17.90
158	ethene	309	C=C[T27]	-	-17.63	-18.10
159	ethene	304	C=C[T26]	-	-17.64	-18.20

160	trans-cinnamaldehyde	298	O=C\C=C\Cc1cccc1[T24]	+	-17.66	-17.63
161	propene	250	CC=C[T14]	*	-17.68	-17.79
162	2-chloropropene	393	CC(Cl)=C[T43]	*	-17.70	-19.13
163	trans-2-hexenal	298	CCC/C=C/C=O[T24]	+	-17.70	-17.69
164	2-methylpropene	225	CC(C)=C[T10]	#	-17.71	-17.64
165	ethene	297	C=C[T24]	+	-17.76	-18.32
166	1-butene	225	CCC=C[T10]	*	-17.77	-17.45
167	ethene	294	C=C[T24]	-	-17.78	-18.32
168	ethene	293	C=C[T23]	#	-17.80	-18.86
169	2-chloropropene	374	CC(Cl)=C[T39]	*	-17.81	-19.13
170	ethene	292	C=C[T22]	-	-17.81	-18.11
171	ethene	290	C=C[T22]	-	-17.85	-18.11
172	ethene	288	C=C[T22]	*	-17.86	-18.11
173	ethene	284	C=C[T22]	#	-17.91	-18.11
174	ethene	283	C=C[T21]	-	-17.94	-18.86
175	methacrolein	296	CC(=C)C=O[T24]	*	-17.95	-18.59
176	2-ethyl acrolein	289	CCC(=C)C=O[T22]	+	-17.97	-18.06
177	ethene	286	C=C[T22]	*	-18.03	-18.11
178	crotonaldehyde	296	C/C=C/C=O[T24]	*	-18.05	-17.84
179	trans-crotonaldehyde	298	C/C=C/C=O[T24]	+	-18.05	-17.84
180	vinyl fluoride	294	FC=C[T24]	#	-18.16	-18.77
181	trans-1,3-dichloropropene	295	ClC/C=C/Cl[T24]	-	-18.17	-18.61
182	2-chloropropene	350	CC(Cl)=C[T34]	+	-18.21	-18.07
183	tetrachloroethene	409	ClC(Cl)=C(Cl)Cl[T47]	#	-18.23	-19.38
184	ethene	267	C=C[T18]	-	-18.24	-18.52
185	trans-1,2-dichloroethene	380	Cl\C=C\Cl[T40]	*	-18.25	-18.59
186	trans-1,2-dichloroethene	366	Cl\C=C\Cl[T37]	-	-18.35	-18.68
187	ethene	260	C=C[T17]	*	-18.36	-18.13
188	2-(chloromethyl)-3-chloro-1-propene	295	ClCC(=C)CCl[T24]	#	-18.41	-18.94
189	tetrachloroethene	402	ClC(Cl)=C(Cl)Cl[T44]	*	-18.45	-19.67
190	trans-1,2-dichloroethene	353	Cl\C=C\Cl[T35]	#	-18.45	-19.43
191	m-cresol	298	Cc1cccc(O)c1[T24]	+	-18.50	-18.52
192	trichloroethene	388	ClC=C(Cl)Cl[T42]	*	-18.51	-19.70
193	acrolein	296	C=CC=O[T24]	*	-18.55	-18.95
194	acrolein	286	C=CC=O[T22]	+	-18.59	-18.68
195	o-cresol	296	Cc1ccccc1O[T24]	-	-18.59	-18.84
196	vinyl chloride	298	ClC=C[T24]	*	-18.61	-19.06
197	ethene	235	C=C[T11]	*	-18.65	-18.58
198	2-(5H)-furanone	298	O=C1OCC=C1[T24]	-	-18.66	-18.92
199	ethyl nitrite	324	CCON=O[T29]	*	-18.67	-19.64
200	naphthalene	298	c1ccc2ccccc2c1[T24]	+	-18.70	-18.70

201	methyl nitrite	352	CON=O[T34]	-	-18.71	-19.38
202	1,1-difluoroethene	294	FC(F)=C[T24]	-	-18.72	-19.22
203	2-chloropropene	313	CC(Cl)=C[T28]	-	-18.72	-18.96
204	trans-1,2-dichloroethene	326	Cl\C=C/Cl[T29]	#	-18.75	-19.43
205	ethyl nitrite	310	CCON=O[T27]	-	-18.80	-18.88
206	tetrachloroethene	395	ClC(Cl)=C(Cl)Cl[T43]	-	-18.80	-19.38
207	cis-1,3-dichloropropene	295	ClC\C=C/Cl[T24]	#	-18.82	-18.30
208	trichloroethene	378	ClC=C(Cl)Cl[T40]	-	-18.83	-19.34
209	vinyl fluoride	260	FC=C[T17]	+	-18.85	-18.59
210	ethene	233	C=C[T11]	*	-18.86	-18.58
211	2-chloropropene	294	CC(Cl)=C[T24]	#	-18.96	-18.42
212	Methyl cyanide	298	CC#N[T24]	+	-19.00	-19.00
213	trichloroethene	371	ClC=C(Cl)Cl[T38]	+	-19.02	-19.63
214	trans-1,2-dichloroethene	301	Cl\C=C/Cl[T25]	*	-19.05	-18.34
215	tetrachloroethene	389	ClC(Cl)=C(Cl)Cl[T42]	*	-19.06	-19.67
216	cis-1,2-dichloroethene	382	Cl\C=C/Cl[T40]	*	-19.13	-19.07
217	ethene	225	C=C[T10]	+	-19.14	-18.93
218	ethene	216	C=C[T8]	*	-19.35	-18.86
219	ethene	208	C=C[T6]	#	-19.37	-18.86
220	tetrachloroethene	382	ClC(Cl)=C(Cl)Cl[T40]	+	-19.37	-18.89
221	Benzyl chloride	298	ClCc1ccccc1[T24]	+	-19.40	-19.41
222	cis-1,2-dichloroethene	354	Cl\C=C/Cl[T35]	#	-19.45	-19.91
223	acetaldehyde	298	CC=O[T24]	#	-19.47	-19.17
224	methyl nitrite	326	CON=O[T29]	#	-19.51	-20.28
225	trichloroethene	347	ClC=C(Cl)Cl[T34]	#	-19.61	-18.93
226	cis-1,2-dichloroethene	341	Cl\C=C/Cl[T32]	-	-19.62	-19.91
227	trifluoroethene	260	FC=C(F)F[T17]	+	-19.62	-19.59
228	ethene	198	C=C[T4]	*	-19.74	-18.86
229	cis-1,2-dichloroethene	328	Cl\C=C/Cl[T29]	#	-19.79	-19.91
230	tetrachloroethene	369	ClC(Cl)=C(Cl)Cl[T38]	+	-19.81	-19.18
231	methyl nitrite	298	CON=O[T24]	-	-19.89	-19.73
232	ethene	188	C=C[T2]	-	-19.97	-18.86
233	cis-1,2-dichloroethene	315	Cl\C=C/Cl[T28]	-	-20.04	-19.91
234	ethene	183	C=C[T1]	-	-20.16	-18.86
235	ethene	178	C=C[T0]	+	-20.30	-20.29
236	1,1-dichloroethene	298	ClC(Cl)=C[T24]	-	-20.43	-20.68
237	glyoxal	298	O=CC=O[T24]	+	-20.50	-20.58
238	Isobutane	298	CC(C)C[T24]	*	-22.70	-23.38
239	ethane	298	CC[T24]	#	-23.00	-23.75
240	n-butane	298	CCCC[T24]	*	-23.00	-23.36
241	1,1-Difluoroethane	298	CC(F)F[T24]	*	-24.20	-24.11

242	1,1,1-Trifluoroethane	298	CC(F)(F)F[T24]	+	-25.30	-25.31
243	terpinolene	298	CC(C)=C1CCC(=CC1)C[T24]	*	-14.00	-13.67
244	myrcene	298	CC(C)=CCCC(=C)C=C[T24]	+	-14.90	-14.60
245	2-methyl-2-butene	363	CC=C(C)C[T37]	-	-15.17	-15.24
246	cyclopentene	260	C1CC=CC1[T17]	+	-15.24	-15.52
247	trans-2-butene	364	C\C=C\C[T37]	*	-15.41	-15.57
248	6-methyl-5-hepten-2-one	287	CC(C)=CCCC(C)=O[T22]	*	-15.47	-15.79
249	trans-2-butene	299	C\C=C\C[T25]	*	-15.58	-15.58
250	2-methyl-2-butene	247	CC=C(C)C[T13]	-	-15.65	-15.89
251	cis-2-butene	336	C\C=C/C[T31]	*	-15.71	-16.63
252	cyclohexene	299	C1CCC=CC1[T25]	+	-15.80	-15.52
253	cis-3-hexene	298	CC\C=C/CC[T24]	#	-15.84	-15.97
254	2-pentene, 2,4,4-trimethyl	298	CC(=CC(C)(C)C)C[T24]	-	-15.86	-15.87
255	trans-5-decene	298	CCCC\C=C\CCCC[T24]	+	-15.89	-16.06
256	cyclohexene	260	C1CCC=CC1[T17]	#	-15.93	-15.54
257	cis-2-butene	287	C\C=C/C[T22]	+	-16.00	-16.06
258	cis-4-octene	298	CCC\C=C/CCC[T24]	#	-16.05	-16.01
259	bicyclo[2.2.2]-2-octene	297	C1CC2CCC1C=C2[T24]	#	-16.14	-15.89
260	cis-3-hexen-1-ol	298	CC\C=C/CCO[T24]	-	-16.19	-16.41
261	trans-2,2-dimethyl-3-hexene	296	CC/C=C/C(C)(C)C[T24]	*	-16.36	-16.38
262	trans-2,2-dimethyl-3-hexene	298	CC/C=C/C(C)(C)C[T24]	+	-16.40	-16.38
263	2-methylpropene	363	CC(C)=C[T37]	*	-16.51	-16.81
264	(Z)-1,3-pentadiene	298	C\C=C/C=C[T24]	*	-16.56	-15.97
265	trans-2-hexenyl acetate	288.5	CCC/C=C/COC(C)=O[T22]	*	-16.71	-16.56
266	propene	332	CC=C[T30]	+	-16.75	-16.85
267	1,4-pentadiene	298	C=CCC=C[T24]	-	-16.84	-16.84
268	allyl alcohol	298	OCC=C[T24]	*	-16.84	-17.82
269	1-butene, 2-methyl	298	CCC(=C)C[T24]	*	-16.88	-17.23
270	1-butene	294	CCC=C[T24]	-	-16.90	-16.84
271	1-butene	298	CCC=C[T24]	*	-16.91	-16.84
272	2-methylpropene	298	CC(C)=C[T24]	#	-16.94	-17.02
273	methylenecyclohexane	298	[CH2]=[C]1CC[CH2]CC1[T24]	-	-16.98	-17.17
274	1-butene, 2,3-dimethyl	298	CC(C)C(=C)C[T24]	*	-17.00	-16.97
275	1-decene	298	CCCCCCCCC=C[T24]	#	-17.10	-17.36
276	1,3-butadiene	303	C=CC=C[T26]	*	-17.13	-16.90
277	2-methyl-1,3-butadiene	278	CC(=C)C=C[T20]	*	-17.24	-17.80
278	3,3-dimethyl-1-butene	298	CC(C)(C)C=C[T24]	+	-17.28	-17.37
279	propene	267	CC=C[T18]	+	-17.32	-17.45
280	1-butene, 3,3-dimethyl	298	CC(C)(C)C=C[T24]	*	-17.41	-17.37
281	3-chloro-1-butene	309	CC(Cl)C=C[T27]	#	-17.56	-17.22
282	ethene	303	C=C[T26]	*	-17.59	-18.20

283	3-chloro-1-butene	292	CC(Cl)C=C[T22]	+	-17.70	-17.43
284	ethene	299	C=C[T25]	-	-17.74	-18.12
285	ethene	296	C=C[T24]	-	-17.85	-18.32
286	2-cyclohexen-1-one	296	O=C1CCCC=C1[T24]	#	-17.91	-17.63
287	methyl acrylate	298	COC(=O)C=C[T24]	+	-17.98	-18.00
288	trans-1,2-dichloroethene	394	Cl\C=C\Cl[T43]	*	-18.08	-19.08
289	p-cresol	296	Cc1ccc(O)cc1[T24]	#	-18.33	-18.22
290	2-chloropropene	339	CC(Cl)=C[T32]	-	-18.40	-18.96
291	trans-1,2-dichloroethene	340	Cl\C=C\Cl[T32]	*	-18.58	-19.08
292	ethyl nitrite	328	CCON=O[T29]	*	-18.60	-19.64
293	m-cresol	296	Cc1cccc(O)c1[T24]	#	-18.71	-18.52
294	1,2-propadiene	298	[CH2]=[C]=[CH2][T24]	*	-18.72	-18.28
295	trifluoroethene	294	FC=C(F)F[T24]	*	-18.85	-19.77
296	ethyl nitrite	298	CCON=O[T24]	+	-18.93	-19.10
297	1,1-difluoroethene	290	FC(F)=C[T22]	-	-19.10	-19.01
298	trichloroethene	360	ClC=C(Cl)Cl[T36]	+	-19.24	-19.23
299	ethylamine	296	CCN[T24]	#	-19.56	-19.21
300	ethene	193	C=C[T3]	+	-19.83	-19.88
301	trichloroethene	334	ClC=C(Cl)Cl[T31]	-	-19.97	-19.83
302	propane	298	CCC[T24]	-	-23.20	-23.24

Table S2. The goodness of fit criteria for all models obtained by TF0, TF1, TF2, and TF3 for nine splits

Split	Target Function	Set	n	R ²	CCC	IIC	CII	Q ²	Q ² _{F1}	Q ² _{F2}	Q ² _{F3}	RMSE	MAE	F	\bar{R}_m^2	$\Delta\bar{R}_m^2$	Y-Test	cR ² _p
Split 1	TF0	ATR N	79	0.9856	0.9928	0.7501	0.9888	0.9850				0.200	0.135	5274				0.9779
		PTRN	68	0.9648	0.9692	0.7202	0.9736	0.9628				0.390	0.323	1811				0.9560
		CAL	65	0.6119	0.7718	0.6698	0.7525	0.5802	0.4843	0.4796	0.5363	1.11	0.767	99	0.4758	0.1304		0.6094
		VAL	90	0.8634	0.9177	0.6751	0.9081	0.5862				0.7077	0.5279	556	0.8020	0.0654	0.0132	
	TF1	ATR N	79	0.8280	0.9059	0.8434	0.9022	0.8066				0.691	0.514	371				0.8243
		PTRN	68	0.8187	0.8970	0.8443	0.9112	0.8028				0.683	0.534	298				0.8107
		CAL	65	0.8268	0.9020	0.9093	0.9020	0.8093	0.8200	0.8183	0.8381	0.658	0.535	301	0.7486	0.1520		0.8113
		VAL	90	0.7976	0.8830	0.7702	0.9092	0.7771				0.7891	0.6175	347	0.7093	0.1475	0.0148	
	TF2	ATR N	79	0.9834	0.9916	0.7888	0.9882	0.9825				0.215	0.156	4551				0.9768
		PTRN	68	0.9578	0.9710	0.8675	0.9682	0.9554				0.382	0.289	1498				0.9532
		CAL	65	0.9276	0.9592	0.7878	0.9615	0.9230	0.9129	0.9129	0.9224	0.455	0.359	807	0.8770	0.0709		0.9218
		VAL	90	0.9136	0.9464	0.5804	0.9410	0.9086				0.5730	0.4433	937	0.8698	0.4433	0.0141	
	TF3	ATR N	79	0.8646	0.9274	0.9066	0.9279	0.8491				0.613	0.464	492				0.8614
		PTRN	68	0.8091	0.8938	0.7381	0.9049	0.7926				708	0.549	280				0.8014
		CAL	65	0.8210	0.9060	0.8972	0.8972	0.8039	0.8131	0.8114	0.8319	670	0.524	289	0.7442	0.0022		0.8120
		VAL	90	0.8285	0.9007	0.8151	0.9098	0.8120				0.7455	0.5852	425	0.7537	0.0717	0.0149	
Split 2	TF0	ATR N	79	0.9744	0.9870	0.7081	0.9808	0.9732				0.264	0.168	2931				0.9688
		PTRN	79	0.9560	0.9765	0.9364	0.9659	0.9538				0.348	0.218	1674				0.9537
		CAL	54	0.6221	0.7817	0.6422	0.7842	0.5626	0.4960	0.4960	0.6355	0.987	0.607	86	0.4856	0.1666		0.6098
		VAL	90	0.8548	0.9236	0.8025	0.9055	0.8426				0.7066	0.5005	518	0.7899	0.0763	0.0092	
	TF1	ATR N	79	0.8287	0.9063	0.7241	0.9139	0.8134				0.682	0.539	373				0.8247
		PTRN	79	0.8390	0.9150	0.8752	0.9191	0.8257				0.673	0.527	401				0.8303
		CAL	54	0.8007	0.8749	0.8948	0.9021	0.7858	0.7844	0.7844	0.8440	0.645	0.482	209	0.6557	0.1940		0.7904
		VAL	90	0.8465	0.9105	0.7780	0.9011	0.8368				0.7011	0.5280	485	0.7329	0.1499	0.0086	
	TF2	ATR N	79	0.9650	0.9822	0.9578	0.9749	0.9630				0.308	0.215	2125				0.9568

		PTRN	79	0.9446	0.9662	0.8630	0.9617	0.9416				0.442	0.321	1313				0.9383		
		CAL	54	0.8982	0.9416	0.6120	0.9563	0.8893	0.8894	0.8894	0.9200	0.462	0.367	459	0.8364	0.0978			0.8932	
		VAL	90	0.9037	0.9501	0.8266	0.9324	0.8998				0.5670	0.4319	823	0.8589	0.0555	0.0093			
	TF3	ATR N	79	0.8299	0.9071	0.7627	0.9059	0.8179				0.680	0.546	376					0.8244	
		PTRN	79	0.7809	0.8736	0.6326	0.8846	0.7630				0.865	0.612	274					0.7743	
		CAL	54	0.8382	0.9025	0.9154	0.9240	0.8251	0.8328	0.8328	0.8790	0.568	0.435	269	0.6957	0.1652			0.8265	
		VAL	90	0.8337	0.9127	0.8246	0.9113	0.8211				0.7428	0.5885	441	0.7615	0.0239	0.0092			
	Split 3	TF0	ATR N	88	0.9890	0.9944	0.7915	0.9910	0.9886				0.173	0.116	7704					0.9817
			PTRN	87	0.9659	0.9823	0.8118	0.9728	0.9647				0.369	0.246	2411					0.9618
			CAL	42	0.6650	0.7798	0.7634	0.7977	0.6359	0.6744	0.3863	0.8350	0.736	0.562	79	0.4760	0.2975			0.6595
			VAL	85	0.7879	0.8768	0.6843	0.8758	0.7742				0.7271	0.5168	308	0.6959	0.1543	0.0153		
		TF1	ATR N	88	0.8538	0.9211	0.7022	0.9126	0.8455				0.631	0.502	502					0.8485
PTRN			87	0.8445	0.9184	0.7685	0.9210	0.8323				0.787	0.612	462					0.8383	
CAL			42	0.6816	0.7252	0.8256	0.8281	0.6480	0.5233	0.1017	0.7584	0.891	0.740	86	0.4485	0.3156			0.6680	
VAL			85	0.7314	0.8129	0.7037	0.8847	0.7105				0.8938	0.7251	226	0.6253	0.0570	0.0124			
TF2		ATR N	88	0.9866	0.9932	0.8665	0.9901	0.9860				0.191	0.132	6325					0.9832	
		PTRN	87	0.9574	0.9777	0.8604	0.9695	0.9556				0.411	0.297	1912					0.9532	
		CAL	42	0.9361	0.9231	0.6887	0.9850	0.9268	0.8914	0.7953	0.9450	0.425	0.324	586	0.7224	0.1087			0.9236	
		VAL	85	0.8955	0.9368	0.7375	0.9386	0.8897				0.5178	0.4113	712	0.8149	0.1030	0.0148			
TF3	ATR N	88	0.8490	0.9184	0.8805	0.9066	0.8408				0.641	0.517	484					0.8366		
	PTRN	87	0.8494	0.9187	0.7454	0.9091	0.8411				0.775	0.632	479					0.8444		
	CAL	42	0.6957	0.7335	0.8341	0.8319	0.6636	0.5224	0.1000	0.7580	0.892	0.735	91	0.4313	0.3273			0.6815		
	VAL	85	0.7582	0.8178	0.7614	0.8845	0.7376				0.8754	0.6875	260	0.6604	0.0129	0.0133				
Split 4	TF0	ATR N	84	0.9736	0.9866	0.6384	0.9819	0.9723				0.218	0.154	3020					0.9696	
		PTRN	70	0.9544	0.9739	0.5850	0.9646	0.9520				0.426	0.298	1422					0.9518	
		CAL	61	0.8167	0.8979	0.8413	0.8778	0.8017	0.7747	0.7697	0.6601	0.938	0.637	263	0.7247	0.1665			0.8125	
		VAL	87	0.8030	0.8759	0.5655	0.8957	0.7841				0.7483	0.5206	346	0.6960	0.1804	0.0123			
	TF1	ATR N	84	0.8276	0.9057	0.8674	0.9018	0.8195				0.556	0.454	394					0.8220	

		PTRN	70	0.7877	0.8449	0.6860	0.9008	0.7697				0.908	0.682	252				0.7823	
		CAL	61	0.8122	0.8400	0.9012	0.9064	0.7933	0.7670	0.7619	0.6485	0.954	0.666	255	0.5178	0.2628			0.8055
		VAL	87	0.7415	0.8226	0.8286	0.8969	0.7234				0.7295	0.5510	241	0.5224	0.2688	0.0138		
	TF2	ATR N	84	0.9707	0.9851	0.8956	0.9815	0.9691				0.229	0.166	2713					0.9648
		PTRN	70	0.9509	0.9736	0.9504	0.9630	0.9481				0.431	0.303	1318					0.9487
		CAL	61	0.9495	0.9641	0.6687	0.9769	0.9412	0.9177	0.9159	0.8759	0.567	0.390	1109	0.8105	0.0684			0.9445
		VAL	87	0.8952	0.9334	0.6880	0.9443	0.8872				0.5348	0.4116	747	0.8102	0.1041	0.0138		
	TF3	ATR N	84	0.8256	0.9044	0.8663	0.9024	0.8162				0.559	0.444	388					0.8205
		PTRN	70	0.7960	0.8618	0.6354	0.8834	0.7783				0.872	0.623	265					0.7884
		CAL	61	0.8352	0.8641	0.9137	0.9163	0.8182	0.7934	0.7888	0.6884	0.898	0.614	299	0.5867	0.2153			0.8244
		VAL	87	0.7176	0.8322	0.7158	0.8764	0.6951				0.7347	0.5346	216	0.5817	0.2443	0.0131		
	Split 5	TF0	ATR N	75	0.9719	0.9857	0.9599	0.9788	0.9703				0.249	0.171	2523				
PTRN			80	0.9527	0.9754	0.8165	0.9692	0.9492				0.305	0.208	1570					0.9477
CAL			61	0.7807	0.8785	0.8012	0.8890	0.7487	0.7816	0.7793	0.5448	0.973	0.657	210	0.6867	0.1528			0.7721
VAL			86	0.8774	0.9345	0.8641	0.9213	0.8702				0.5807	0.4392	601	0.8221	0.0202	0.0137		
TF1		ATR N	75	0.8218	0.9022	0.8827	0.9049	0.8021				0.626	0.451	337					0.8171
		PTRN	80	0.7684	0.8734	0.7467	0.8924	0.7560				0.697	0.567	259					0.7647
		CAL	61	0.7598	0.8150	0.8716	0.8805	0.7264	0.7296	0.7268	0.4363	1.08	0.672	187	0.4754	0.2966			0.7502
		VAL	86	0.7459	0.8452	0.7138	0.8937	0.7289				0.8167	0.6025	247	0.6051	0.2290	0.0110		
TF2		ATR N	75	0.9739	0.9868	0.9110	0.9808	0.9725				0.239	0.163	2726					0.9689
		PTRN	80	0.9460	0.9714	0.9139	0.9654	0.9421				0.327	0.223	1365					0.9386
		CAL	61	0.9419	0.9686	0.8129	0.9688	0.9327	0.9415	0.9409	0.8781	0.504	0.361	956	0.8846	0.0587			0.9337
		VAL	86	0.8910	0.9434	0.7194	0.9266	0.8852				0.5330	0.4071	687	0.8412	0.0156	0.0134		
TF3	ATR N	75	0.8055	0.8923	0.8285	0.9141	0.7872				0.654	0.484	302					0.7948	
	PTRN	80	0.7453	0.8554	0.7326	0.8907	0.7321				0.718	0.567	228					0.7399	
	CAL	61	0.7594	0.8075	0.8715	0.9003	0.7274	0.7230	0.7200	0.4224	1.10	0.691	186	0.4550	0.3114			0.7511	
	VAL	86	0.7489	0.8404	0.8361	0.8905	0.7309				0.8130	0.6065	250	0.5725	0.2418	0.0111			
Split 6	TF0	ATR N	84	0.9874	0.9937	0.8612	0.9904	0.9869				0.185	0.129	6441					0.9839

		PTRN	71	0.9663	0.9798	0.8524	0.9745	0.9644				0.332	0.230	1976				0.9571	
		CAL	56	0.7407	0.8412	0.7585	0.8432	0.7128	0.6064	0.5977	0.6754	0.938	0.690	154	0.5805	0.2397			0.7330
		VAL	91	0.8836	0.9179	0.5606	0.9222	0.8761				0.7438	0.5603	679	0.7768	0.1183	0.0105		
	TF1	ATR N	84	0.8209	0.9017	0.8237	0.9161	0.7987				0.700	0.515	376					0.8173
		PTRN	71	0.7850	0.8833	0.8521	0.8989	0.7655				0.773	0.585	252					0.7790
		CAL	56	0.7563	0.8689	0.8697	0.8766	0.7200	0.7512	0.7457	0.7948	0.746	0.567	168	0.6577	0.0511			0.7450
		VAL	91	0.7870	0.8678	0.7126	0.9169	0.7646				0.8103	0.6096	328	0.6480	0.2012	0.0099		
	TF2	ATR N	84	0.9810	0.9904	0.8584	0.9857	0.9801				0.228	0.155	4227					0.9783
		PTRN	71	0.9569	0.9723	0.7565	0.9677	0.9543				0.391	0.282	1532					0.9483
		CAL	56	0.9097	0.9422	0.8120	0.9543	0.9006	0.8668	0.8639	0.8902	0.546	0.432	544	0.7757	0.1033			0.8990
		VAL	91	0.9126	0.9471	0.6621	0.9469	0.9073				0.5758	0.4389	929	0.8488	0.0856	0.0105		
	TF3	ATR N	84	0.8226	0.9027	0.7492	0.9157	0.8012				0.697	0.543	380					0.8192
		PTRN	71	0.7843	0.8823	0.8611	0.9065	0.7642				0.793	0.618	251					0.7803
		CAL	56	0.7689	0.8738	0.8769	0.8900	0.7314	0.7399	0.7342	0.7855	0.763	0.583	180	0.6739	0.0644			0.7613
		VAL	91	0.8136	0.8891	0.8767	0.9229	0.7942				0.7615	0.6086	388	0.7179	0.1700	0.0103		
	Split 7	TF0	ATR N	86	0.9864	0.9932	0.9932	0.9896	0.9859				0.189	0.127	6105				
PTRN			80	0.9632	0.9757	0.9002	0.9719	0.9614				0.379	0.272	2040					0.9568
CAL			43	0.7110	0.7962	0.7729	0.8338	0.6781	0.6921	0.4181	0.7824	0.778	0.578	101	0.5055	0.2808			0.7073
VAL			93	0.8925	0.9298	0.6874	0.9230	0.8883				0.6673	0.5093	756	0.8395	0.1013	0.0122		
TF1		ATR N	86	0.8654	0.9279	0.8090	0.9166	0.8570				0.596	0.469	540					0.8609
		PTRN	80	0.8318	0.9058	0.8323	0.9121	0.8190				0.718	0.569	386					0.8163
		CAL	43	0.7060	0.7601	0.8402	0.8301	0.6733	0.5843	0.2143	0.7062	0.904	0.722	98	0.4352	0.3251			0.6902
		VAL	93	0.8083	0.8711	0.8911	0.9073	0.7898				0.8603	0.7045	383	0.7254	0.1014	0.0130		
TF2		ATR N	86	0.9786	0.9892	0.7470	0.9844	0.9776				0.238	0.156	3842					0.9730
		PTRN	80	0.9546	0.9761	0.8704	0.9667	0.9526				0.370	0.256	1641					0.9529
		CAL	43	0.9124	0.9289	0.5774	0.9727	0.9009	0.9098	0.8295	0.9362	0.421	0.317	427	0.7824	0.1000			0.8968
		VAL	93	0.9085	0.9432	0.5673	0.9365	0.9046				0.5763	0.4287	902	0.8661	0.0266	0.0124		
TF3		ATR N	86	0.8374	0.9115	0.7957	0.9114	0.8228				0.655	0.509	433					0.8326

		PTRN	80	0.8280	0.8962	0.6783	0.9205	0.8151				0.716	0.567	376				0.8244
		CAL	43	0.6441	0.7355	0.8025	0.8393	0.6018	0.5869	0.2192	0.7081	0.901	0.722	74	0.4614	0.3091		0.6358
		VAL	93	0.8087	0.8539	0.7803	0.9118	0.7926				0.8691	0.7122	385	0.6551	0.1911	0.0129	
Split 8	TF0	ATR N	83	0.9903	0.9952	0.9257	0.9920	0.9900				0.167	0.107	8311				0.9859
		PTRN	73	0.9607	0.9738	0.6846	0.9673	0.9591				0.440	0.325	1735				0.9551
		CAL	59	0.6252	0.7559	0.3521	0.7836	0.5524	0.3482	0.3386	0.4858	1.26	0.749	95	0.4524	0.3070		0.6198
		VAL	87	0.8770	0.9267	0.7052	0.9321	0.8662				0.5943	0.4175	602	0.7502	0.1292	0.0119	
	TF1	ATR N	83	0.8212	0.9018	0.7652	0.8985	0.8101				0.721	0.561	372				0.8180
		PTRN	73	0.8218	0.9014	0.8229	0.9000	0.8052				0.815	0.625	327				0.8097
		CAL	59	0.7826	0.8840	0.8846	0.9041	0.7582	0.7799	0.7766	0.8264	0.733	0.591	205	0.6922	0.0595		0.7751
		VAL	87	0.7522	0.8625	0.8338	0.8885	0.7272				0.7404	0.5799	258	0.6519	0.0715	0.0151	
	TF2	ATR N	83	0.9817	0.9907	0.9672	0.9853	0.9808				0.231	0.156	4336				0.9762
		PTRN	73	0.9509	0.9713	0.5904	0.9637	0.9485				0.450	0.319	1375				0.9433
		CAL	59	0.9080	0.9509	0.8728	0.9655	0.8972	0.8983	0.8968	0.9198	0.498	0.408	562	0.8609	0.0876		0.9012
		VAL	87	0.9031	0.9478	0.5651	0.9485	0.8953				0.4817	0.3752	812	0.8387	0.0940	0.0124	
TF3	ATR N	83	0.8129	0.8968	0.5951	0.8964	0.8016				0.737	0.566	352				0.8080	
	PTRN	73	0.8130	0.8980	0.7012	0.9011	0.7979				0.829	0.650	309				0.8028	
	CAL	59	0.7717	0.8779	0.8784	0.9112	0.7471	0.7571	0.7535	0.8084	0.770	0.615	193	0.6783	0.0185		0.7594	
	VAL	87	0.6962	0.8302	0.8285	0.8709	0.6709				0.8561	0.6647	196	0.5809	0.0463	0.6709		
Split 9	TF0	ATR N	91	0.9901	0.9950	0.7134	0.9922	0.9896				0.180	0.120	8857				0.9851
		PTRN	71	0.9901	0.9748	0.1331	0.9929	0.9892				0.354	0.297	6924				0.9861
		CAL	52	0.7115	0.8345	0.8400	0.8405	0.6798	0.6151	0.6140	0.7748	0.803	0.567	123	0.5935	0.2002		0.6935
		VAL	88	0.8945	0.9287	0.6149	0.9274	0.8885				0.6820	0.5083	729	0.8202	0.1026	0.0097	
	TF1	ATR N	91	0.8114	0.8959	0.6756	0.9106	0.7954				0.784	0.618	383				0.8023
		PTRN	71	0.8234	0.8836	0.8042	0.9314	0.8030				0.735	0.615	322				0.8164
		CAL	52	0.7207	0.8401	0.8488	0.8870	0.6877	0.6341	0.6331	0.7859	0.783	0.621	129	0.6069	0.1750		0.7117
		VAL	88	0.7868	0.8581	0.8705	0.9083	0.7625				0.8715	0.7060	317	0.6807	0.1912	0.0095	
TF2	ATR N	91	0.9828	0.9913	0.7435	0.9873	0.9821				0.236	0.163	5099				0.9711	

TF3	PTRN	71	0.9830	0.9797	0.4955	0.9889	0.9812				0.313	0.264	3999				0.9778
	CAL	52	0.8898	0.9395	0.9119	0.9602	0.8794	0.8696	0.8693	0.9237	0.467	0.392	404	0.8274	0.1050		0.8813
	VAL	88	0.9173	0.9501	0.6652	0.9431	0.9142				0.5463	0.4355	954	0.8787	0.0202	0.0097	
	ATR N	91	0.8221	0.9023	0.8122	0.9220	0.8063				0.761	0.584	411				0.8100
	PTRN	71	0.8215	0.8930	0.5411	0.9190	0.8019				0.712	0.558	318				0.8166
	CAL	52	0.7400	0.8505	0.8602	0.8890	0.7117	0.6548	0.6538	0.7980	0.760	0.618	142	0.6308	0.1912		0.7245
	VAL	88	0.7904	0.8721	0.8124	0.9129	0.7688				0.8260	0.6476	324	0.6975	0.1855	0.7688	

Table S3. The name, reaction temperature (K), quasi-SMILES, the set (active training (+), passive training set (-), calibration set (#), validation set (*)), experimental $\log_{K_{O_3}}$, and predicted $\log_{K_{O_3}}$ of VOCs of split 1 based on TF2

No.	SMILES	Experimental $\log_{K_{O_3}}$	Split								
			1	2	3	4	5	6	7	8	9
1	<chem>CC(C)C1CC=C(C)C=C1</chem>	-13.92	+	-	+	#	#	+	+	#	+
2	<chem>C1C2C=CC1C=C2</chem>	-14.33	#	+	-	#	-	-	#	+	-
3	<chem>C1CC2CC1C=C2</chem>	-14.67	*	-	*	-	-	*	*	*	*
4	<chem>CC(C)=CCC=C(C)C=C</chem>	-14.7	*	*	*	#	-	*	*	*	*
5	<chem>C1CC=CC=C1</chem>	-14.71	+	#	-	-	-	+	+	-	+
6	<chem>CC(C)=C(C)C</chem>	-14.85	+	*	+	+	*	+	+	-	+
7	<chem>CC(C)=CCCC(=C)C=C</chem>	-14.9	#	*	-	+	-	-	#	-	+
8	<chem>CC(C)=C(C)C</chem>	-14.98	*	#	*	-	-	*	*	*	*
9	<chem>C1CC=CC1</chem>	-15.01	#	*	#	*	*	#	#	*	#
10	<chem>CC(=C(C)C)C</chem>	-15.05	#	+	#	-	+	#	#	+	#
11	<chem>CC(C)=C(C)C</chem>	-15.08	+	*	*	#	-	+	*	*	+
12	<chem>CC(C)=C(C)C</chem>	-15.08	-	+	*	*	*	*	-	*	*
13	<chem>C1CC=CC1</chem>	-15.09	*	+	*	+	*	*	*	+	*
14	<chem>CC1=CCCC1</chem>	-15.17	-	#	*	*	#	*	*	-	*
15	<chem>CC(=C)C1CCC(=CC1)C</chem>	-15.19	+	+	+	+	+	+	+	+	#

16	CC(CCC=C(C)C)C=C	-15.2	#	-	#	-	+	#	#	-	#
17	CC\C(C)=C\C	-15.25	-	*	-	*	+	-	-	-	-
18	CC(C)C1CCC(=CC1)C	-15.28	*	*	*	-	#	*	*	#	*
19	CC\C(C)=C/C	-15.34	+	-	+	*	*	+	+	*	+
20	CC(C)=CCCC(C)(O)C=C	-15.37	-	-	-	*	-	-	-	#	-
21	CC=C(C)C	-15.4	+	*	+	#	+	+	+	-	+
22	CC(C)=CCCC(C)=O	-15.41	-	-	-	#	+	-	-	-	-
23	C\C=C/C=C\C	-15.43	#	-	#	*	+	#	#	#	#
24	C\C=C/C=C/C	-15.43	*	+	*	-	-	*	*	-	*
25	CC=C(C)C	-15.48	#	+	#	*	*	#	#	+	#
26	C\C=C/C=C/C	-15.5	-	+	-	+	*	-	-	*	-
27	C1CCC=CCC1	-15.5	*	#	*	*	*	*	*	-	*
28	CC/C=C/C	-15.5	*	-	*	-	#	*	*	-	*
29	C\C=C/C	-15.56	-	*	-	*	*	-	-	*	-
30	C\C=C\C	-15.56	*	*	*	+	-	*	*	+	*
31	C\C=C\C	-15.59	#	*	#	*	#	-	#	+	-
32	CC=CCO	-15.6	#	*	#	-	-	+	#	+	+
33	CC1=C(C)CCCC1	-15.68	*	#	*	+	*	*	*	#	*
34	CC\C=C/C	-15.68	*	-	*	+	*	*	*	#	*
35	C1CCC=CC1	-15.69	#	#	#	*	#	+	#	#	+
36	C\C=C\C	-15.69	*	+	*	+	+	*	*	+	*
37	CC=C(C)C	-15.71	*	+	*	*	#	*	*	*	*
38	C\C=C\C	-15.71	*	#	*	-	-	*	*	*	*
39	CC(C)C1CCC(=C)C=C1	-15.75	-	+	-	#	+	-	-	+	-
40	CC1=CCCCC1	-15.78	#	+	#	*	*	+	#	*	+
41	CC\C=C\CC	-15.8	#	-	#	*	+	-	#	+	-
42	C1CC=CC=CC1	-15.81	-	*	-	+	*	-	-	+	-
43	CCOC=C	-15.81	-	+	+	#	*	-	-	#	-
44	CC(=O)C1CCC(=CC1)C	-15.82	+	-	-	-	+	+	+	-	-
45	CC(C)=CC(C)(C)C	-15.85	+	+	+	-	+	+	+	+	-

46	CC\C=C/CC	-15.85	*	*	*	*	-	*	*	#	*
47	C\C=C/C	-15.86	*	*	*	+	-	*	*	+	*
48	C\C=C/C	-15.86	*	#	*	+	-	*	*	+	*
49	C\C=C/C	-15.86	#	+	#	*	#	+	#	#	-
50	C\C=C/C	-15.86	+	+	-	-	#	+	+	+	-
51	C\C=C/C	-15.87	*	*	*	*	#	*	*	+	*
52	CCC\C=C\CCC	-15.88	#	+	-	*	+	+	#	-	-
53	C\C=C/C	-15.9	+	-	+	*	*	+	+	+	+
54	CC\C=C\CC	-15.91	-	-	-	*	-	-	-	-	-
55	CCCC\C=C\CCCC	-15.94	*	*	*	*	+	*	*	*	*
56	C\C=C\C	-15.94	-	-	-	*	+	-	-	*	-
57	C\C=C\C	-15.94	+	*	+	+	-	+	+	+	+
58	C\C=C\C	-15.94	#	#	#	+	*	#	#	#	#
59	C\C=C\C	-15.94	#	+	+	*	#	#	#	*	+
60	C1CCC=CC1	-15.98	*	#	*	+	+	*	*	*	*
61	CCC\C=C\CCC	-16	+	#	+	*	#	+	+	*	+
62	C\C=C\C	-16.03	-	+	-	*	*	-	-	*	+
63	CCCCC=CC	-16.06	-	#	-	-	+	-	-	-	-
64	C\C=C/C	-16.06	*	#	*	+	*	*	*	-	*
65	C\C=C/C	-16.06	-	-	+	+	#	-	-	#	-
66	CC1CCC=CC1	-16.09	+	#	+	*	-	+	+	#	+
67	C\C=C\C(=C)C	-16.1	+	-	+	#	-	+	+	-	+
68	CC=CC(C)=C	-16.1	*	*	*	*	*	*	*	+	*
69	C1C=CCC=C1	-16.19	+	*	+	+	#	+	+	+	+
70	C\C=C\C	-16.22	#	-	#	-	-	#	#	+	#
71	C\C=C\C	-16.23	+	+	+	#	-	+	+	-	+
72	C1C=CC=CC=C1	-16.27	#	+	#	+	+	#	#	-	#
73	C\C=C/C	-16.28	*	-	*	+	+	*	*	+	*
74	C\C=C/C	-16.31	-	*	-	*	+	-	-	*	-
75	C\C=C/C	-16.33	-	-	-	+	+	-	-	+	-

76	C/C=C/C=C	-16.37	+	*	+	-	-	+	+	-	+
77	CC/C=C/C(C)(C)C	-16.39	*	-	*	+	-	*	*	*	*
78	CC(C)\C=C\C(C)C	-16.41	#	*	#	+	*	#	#	+	#
79	CC=C	-16.42	*	*	*	#	+	*	*	-	*
80	CC(C)\C=C\C(C)C	-16.42	#	+	#	+	*	#	#	+	#
81	CC1(C)C2CCC(=C)C1C2	-16.44	*	-	*	#	-	*	*	*	*
82	CC/C=C/C(C)(C)C	-16.44	+	-	+	*	#	+	+	-	+
83	C=Cc1ccccc1	-16.52	+	+	+	+	-	+	+	*	+
84	CCC=C	-16.55	-	*	-	+	*	-	-	#	-
85	C=CC=CC=C	-16.58	+	*	+	*	#	+	+	#	+
86	CC(=C)C(C)=C	-16.58	*	+	*	#	*	*	*	*	*
87	CCC/C=C/COC(C)=O	-16.61	+	+	+	-	+	+	+	-	+
88	CC=CC(C)=O	-16.67	#	*	#	-	-	#	#	-	#
89	C=Cc1ccccc1	-16.67	*	*	*	+	+	*	*	*	*
90	CC1(C)C2CCC(=C)C1C2	-16.68	+	-	+	#	#	+	+	-	+
91	CCC(O)C=C	-16.75	*	*	*	-	#	*	*	-	*
92	CC(=C)C=C	-16.75	#	+	#	*	*	#	#	*	#
93	CCCCCC=C	-16.76	+	*	+	*	*	+	+	+	+
94	CCCC(C)=C	-16.77	*	+	*	+	-	*	*	-	*
95	CC(O)C=C	-16.79	+	-	+	*	#	+	+	-	+
96	C1OCC=C1	-16.79	#	-	#	#	+	#	#	+	#
97	CCC(C)=C	-16.8	+	+	+	#	*	+	+	*	+
98	[nH]1ccccc1	-16.8	-	-	-	-	+	-	-	-	-
99	CC(C)=C	-16.84	#	#	#	+	*	#	#	*	#
100	C=Cc1ccccc1	-16.84	-	+	-	-	-	-	-	+	-
101	CC(=C)CCC(C)=C	-16.85	#	-	#	-	#	#	#	+	#
102	CC(=C)C=C	-16.85	+	#	+	+	-	+	+	+	+
103	CC=C	-16.85	#	+	#	+	*	#	#	*	#
104	CCC=C	-16.86	*	#	*	*	-	*	*	-	*
105	CCC(=C)CC	-16.86	*	*	*	#	+	*	*	#	*

106	CC(C)=C	-16.87	*	#	*	#	+	*	*	+	*
107	CC(=C)CC=C	-16.89	-	-	-	-	*	-	-	+	-
108	CC=C	-16.89	*	+	*	*	*	*	*	*	*
109	CCCCCCC=C	-16.9	+	#	+	-	*	+	+	*	+
110	CC(=C)C=C	-16.9	-	-	-	-	*	-	-	*	-
111	CCCC(C)=C	-16.9	-	#	-	+	-	-	-	*	-
112	CC=C	-16.9	*	+	*	#	-	*	*	#	*
113	CC=C	-16.9	#	#	#	-	+	#	#	#	#
114	CN(C)N(C)C	-16.9	-	-	-	+	-	-	-	#	-
115	CCC=C	-16.91	#	*	#	+	*	#	#	*	#
116	CC(C)=C	-16.92	+	*	+	-	#	+	+	+	+
117	CCCC=C	-16.95	+	-	+	-	#	+	+	+	+
118	CCCC=C	-16.96	#	+	#	*	#	#	#	-	#
119	CC(C)C=C	-16.96	-	#	-	-	-	-	-	+	-
120	CCCC=C	-16.97	+	#	+	*	+	+	+	*	+
121	CCCC=C	-16.97	*	*	*	#	#	*	*	+	*
122	CC(C)CC=C	-16.98	-	*	-	*	*	-	-	#	-
123	CC=C	-16.98	#	*	#	+	+	#	#	-	#
124	CCC=C	-16.99	+	+	+	+	#	+	+	-	+
125	CC(C)C(C)=C	-17	*	+	*	*	+	*	*	*	*
126	CC(C)(O)C=C	-17	+	*	+	+	-	+	+	#	+
127	CCCC=C	-17.01	*	-	*	#	-	*	*	*	*
128	CN(C)C	-17.01	-	-	-	#	#	-	-	+	-
129	CCCCCC=C	-17.03	+	*	+	*	#	+	+	+	+
130	C=C	-17.04	*	+	*	+	*	*	*	-	*
131	COC(=O)C(C)=C	-17.12	*	#	+	#	#	*	*	-	*
132	C=CC1CCCC1	-17.12	+	-	+	#	-	+	+	#	+
133	CCC=C	-17.13	-	*	-	+	+	-	-	*	-
134	CC=C	-17.13	#	*	#	*	+	#	#	#	#
135	CC(C)CC=C	-17.14	+	*	+	+	-	+	+	*	+

136	CC(=C)C=C	-17.16	+	*	+	#	*	+	+	*	+
137	C=CC=C	-17.17	+	*	+	+	*	+	+	+	+
138	CCC(=O)C=C	-17.22	+	#	+	-	#	+	+	*	+
139	CCOC(=O)C=C	-17.24	-	-	-	*	+	-	-	-	-
140	CC(Cl)C=C	-17.27	-	#	-	+	+	-	-	+	-
141	CC=C	-17.29	*	*	*	#	*	*	*	-	*
142	CC(C)=C	-17.3	*	-	*	*	#	*	*	*	*
143	OCCC=C	-17.31	+	-	+	+	+	+	+	#	+
144	CCC(C)C=C	-17.31	#	+	#	+	*	#	#	#	#
145	CCC=C	-17.32	*	*	*	*	-	*	*	-	*
146	CC(=O)C=C	-17.32	+	*	+	-	#	+	+	#	+
147	CC(Cl)C=C	-17.35	+	-	+	*	-	+	+	*	+
148	COC(=O)\C=C\C	-17.36	-	+	-	#	*	-	-	-	-
149	C=C	-17.42	#	+	#	+	+	#	#	#	#
150	CC(C)=C	-17.44	#	#	#	+	+	#	#	*	#
151	CC(Cl)C=C	-17.44	#	*	#	#	*	#	#	*	#
152	CC(C)C(=C)C(C)C	-17.48	#	*	#	#	+	#	#	#	#
153	CCC=C	-17.5	+	+	+	#	*	+	+	+	+
154	CC(=O)OC=C	-17.5	+	+	+	#	-	+	+	+	+
155	CNC	-17.58	+	+	+	*	+	+	+	+	+
156	CC(Cl)C=C	-17.59	#	#	#	*	*	#	#	-	#
157	o1cccc1	-17.62	-	#	-	-	-	-	-	-	-
158	C=C	-17.63	-	+	-	*	*	-	-	+	-
159	C=C	-17.64	-	-	-	#	+	-	-	+	-
160	O=C\C=C\c1cccc1	-17.66	+	*	+	-	-	+	+	*	+
161	CC=C	-17.68	*	*	*	*	-	*	*	#	*
162	CC(Cl)=C	-17.7	*	-	*	*	-	*	*	#	*
163	CCC/C=C/C=O	-17.7	+	-	+	-	+	+	+	*	+
164	CC(C)=C	-17.71	#	+	#	-	+	#	#	*	#
165	C=C	-17.76	+	#	+	#	#	+	+	-	+

166	CCC=C	-17.77	*	+	*	+	#	*	*	*	*
167	C=C	-17.78	-	-	-	*	*	-	-	*	-
168	C=C	-17.8	#	+	#	-	+	#	#	*	#
169	CC(Cl)=C	-17.81	*	-	*	*	-	*	*	*	*
170	C=C	-17.81	-	-	-	+	*	-	-	*	-
171	C=C	-17.85	-	*	-	*	#	-	-	#	-
172	C=C	-17.86	*	#	*	*	*	*	*	*	*
173	C=C	-17.91	#	+	-	+	*	#	-	+	#
174	C=C	-17.94	-	*	-	#	*	-	-	-	-
175	CC(=C)C=O	-17.95	*	-	*	*	*	*	*	*	*
176	CCC(=C)C=O	-17.97	+	*	+	*	*	+	+	+	+
177	C=C	-18.03	*	*	*	-	*	*	*	*	*
178	C/C=C/C=O	-18.05	*	*	*	#	#	*	*	*	*
179	C/C=C/C=O	-18.05	+	*	+	-	#	+	+	#	+
180	FC=C	-18.16	#	+	#	*	-	#	#	#	#
181	ClC/C=C/Cl	-18.17	-	-	-	-	#	-	-	+	-
182	CC(Cl)=C	-18.21	+	*	+	*	+	+	+	*	+
183	ClC(Cl)=C(Cl)Cl	-18.23	#	-	#	-	-	#	#	+	#
184	C=C	-18.24	-	*	-	-	*	-	-	#	-
185	Cl\C=C\Cl	-18.25	*	#	*	#	-	*	*	*	*
186	Cl\C=C\Cl	-18.35	-	#	-	*	-	-	-	+	-
187	C=C	-18.36	*	*	*	+	#	*	*	+	*
188	ClCC(=C)CCl	-18.41	#	*	#	*	+	#	#	-	#
189	ClC(Cl)=C(Cl)Cl	-18.45	*	+	*	+	+	*	*	#	*
190	Cl\C=C\Cl	-18.45	#	*	#	-	*	#	#	+	#
191	Cc1cccc(O)c1	-18.5	+	-	+	*	*	+	+	+	+
192	ClC=C(Cl)Cl	-18.51	*	-	+	*	-	*	*	-	*
193	C=CC=O	-18.55	*	-	*	*	+	*	*	*	*
194	C=CC=O	-18.59	+	+	+	#	+	+	+	+	+
195	Cc1cccc1O	-18.59	-	+	-	#	+	-	-	+	-

196	CIC=C	-18.61	*	#	*	*	+	*	*	-	*
197	C=C	-18.65	*	+	*	+	+	*	*	-	*
198	O=C1OCC=C1	-18.66	-	-	-	*	-	-	-	#	-
199	CCON=O	-18.67	*	#	*	*	+	*	*	-	*
200	c1ccc2ccccc2c1	-18.7	+	+	+	+	#	+	+	#	+
201	CON=O	-18.71	-	-	-	*	*	-	-	-	-
202	FC(F)=C	-18.72	-	*	-	+	*	-	-	*	-
203	CC(Cl)=C	-18.72	-	*	-	-	-	-	-	*	-
204	Cl\C=C\Cl	-18.75	#	-	+	*	*	#	+	+	#
205	CCON=O	-18.8	-	+	-	#	-	-	-	-	-
206	CIC(Cl)=C(Cl)Cl	-18.8	-	+	-	+	#	-	-	-	-
207	CIC\C=C/Cl	-18.82	#	*	+	+	*	#	+	*	#
208	CIC=C(Cl)Cl	-18.83	-	#	-	-	#	-	-	*	-
209	FC=C	-18.85	+	-	+	#	*	+	+	+	+
210	C=C	-18.86	*	#	*	#	*	*	*	-	*
211	CC(Cl)=C	-18.96	#	+	+	*	*	#	+	+	#
212	CC#N	-19	+	-	+	#	-	+	+	*	+
213	CIC=C(Cl)Cl	-19.02	+	+	+	-	*	+	+	*	+
214	Cl\C=C\Cl	-19.05	*	+	*	+	*	*	*	#	*
215	CIC(Cl)=C(Cl)Cl	-19.06	*	-	*	*	*	*	*	#	*
216	Cl\C=C/Cl	-19.13	*	*	*	#	*	*	*	*	*
217	C=C	-19.14	+	-	+	#	+	+	+	-	+
218	C=C	-19.35	*	*	*	-	-	*	*	#	*
219	C=C	-19.37	#	#	+	*	*	#	+	-	#
220	CIC(Cl)=C(Cl)Cl	-19.37	+	+	+	#	+	+	+	-	+
221	ClCc1ccccc1	-19.4	+	*	+	-	-	+	+	-	+
222	Cl\C=C/Cl	-19.45	#	*	-	-	*	#	-	#	#
223	CC=O	-19.47	#	*	-	#	*	#	-	-	#
224	CON=O	-19.51	#	#	-	-	*	#	-	*	#
225	CIC=C(Cl)Cl	-19.61	#	#	-	*	*	#	-	-	#

226	Cl\C=C/Cl	-19.62	-	#	-	*	-	-	-	-	-
227	FC=C(F)F	-19.62	+	#	+	+	*	+	+	+	+
228	C=C	-19.74	*	-	+	*	-	*	*	#	*
229	Cl\C=C/Cl	-19.79	#	-	-	#	#	#	-	*	#
230	ClC(Cl)=C(Cl)Cl	-19.81	+	-	+	+	-	+	+	*	+
231	CON=O	-19.89	-	-	-	+	+	-	-	-	+
232	C=C	-19.97	-	+	-	#	#	-	-	+	+
233	Cl\C=C/Cl	-20.04	-	*	-	-	+	-	-	*	+
234	C=C	-20.16	-	#	-	-	+	-	-	#	+
235	C=C	-20.3	+	-	+	-	-	+	+	+	+
236	ClC(Cl)=C	-20.43	-	-	-	#	#	-	-	+	-
237	O=CC=O	-20.5	+	*	+	+	+	+	+	-	+
238	CC(C)C	-22.7	*	+	*	*	*	*	*	#	*
239	CC	-23	#	*	-	#	#	#	-	-	+
240	CCCC	-23	*	*	+	#	+	*	*	+	*
241	CC(F)F	-24.2	*	-	+	#	#	*	*	-	*
242	CC(F)(F)F	-25.3	+	*	-	-	#	+	+	+	+
243	CC(C)=C1CCC(=CC1)C	-14	*	+	+	+	#	*	*	*	*
244	CC(C)=CCCC(=C)C=C	-14.9	+	-	-	#	#	+	+	#	+
245	CC=C(C)C	-15.17	-	*	-	#	*	-	-	-	-
246	C1CC=CC1	-15.24	+	#	-	+	-	+	+	+	+
247	C\C=C\C	-15.41	*	+	*	*	*	*	*	*	*
248	CC(C)=CCCC(C)=O	-15.47	*	*	*	-	#	*	*	#	*
249	C\C=C\C	-15.58	*	+	*	+	#	*	*	#	*
250	CC=C(C)C	-15.65	-	*	-	+	+	-	-	+	-
251	C\C=C/C	-15.71	*	+	*	*	+	*	*	#	*
252	C1CCC=CC1	-15.8	+	-	#	*	-	+	+	#	+
253	CC\C=C/CC	-15.84	#	-	-	+	+	#	-	*	#
254	CC(=CC(C)(C)C)C	-15.86	-	+	-	#	-	-	-	*	-
255	CCCC\C=C\CCCC	-15.89	+	-	+	*	#	+	+	-	+

256	C1CCC=CC1	-15.93	#	#	#	+	*	#	-	*	#
257	C\C=C/C	-16	+	*	+	-	-	+	+	-	+
258	CCC\C=C/CCC	-16.05	#	+	-	-	-	#	-	*	#
259	C1CC2CCC1C=C2	-16.14	#	+	-	*	*	#	-	#	#
260	CC\C=C/CCO	-16.19	-	*	-	#	-	-	-	#	-
261	CC/C=C/C(C)(C)C	-16.36	*	#	*	-	+	*	*	+	*
262	CC/C=C/C(C)(C)C	-16.4	+	-	+	*	*	+	+	*	+
263	CC(C)=C	-16.51	*	#	*	*	-	*	*	+	*
264	C\C=C/C=C	-16.56	*	*	*	+	-	*	*	*	*
265	CCC/C=C/CO(C)=O	-16.71	*	#	*	+	#	*	*	*	*
266	CC=C	-16.75	+	#	+	-	-	+	+	+	+
267	C=CCC=C	-16.84	-	*	-	*	+	-	-	*	-
268	OCC=C	-16.84	*	-	*	-	+	*	*	+	*
269	CCC(=C)C	-16.88	*	+	*	+	+	*	*	-	*
270	CCC=C	-16.9	-	+	-	+	+	-	-	*	-
271	CCC=C	-16.91	*	*	*	+	+	*	*	+	*
272	CC(C)=C	-16.94	#	-	-	#	#	#	-	+	#
273	[CH2]=[C]1CC[CH2]CC 1	-16.98	-	-	-	-	-	-	-	+	-
274	CC(C)C(=C)C	-17	*	*	*	#	#	*	*	-	+
275	CCCCCCCC=C	-17.1	#	*	+	+	-	#	+	+	+
276	C=CC=C	-17.13	*	*	-	*	-	*	*	#	*
277	CC(=C)C=C	-17.24	*	-	+	-	*	*	*	+	*
278	CC(C)(C)C=C	-17.28	+	+	+	+	+	+	+	#	+
279	CC=C	-17.32	+	*	#	+	-	+	+	+	+
280	CC(C)(C)C=C	-17.41	*	*	*	-	*	*	*	+	*
281	CC(Cl)C=C	-17.56	#	-	+	#	*	#	+	*	#
282	C=C	-17.59	*	-	*	*	#	*	*	*	*
283	CC(Cl)C=C	-17.7	+	+	+	-	#	+	+	*	+
284	C=C	-17.74	-	#	-	-	#	-	-	#	-

285	C=C	-17.85	-	*	-	*	#	-	-	+	-
286	O=C1CCCC=C1	-17.91	#	#	+	#	-	#	+	#	#
287	COC(=O)C=C	-17.98	+	-	+	+	+	+	+	-	+
288	Cl\C=C\Cl	-18.08	*	+	*	+	+	*	*	+	*
289	Cc1ccc(O)cc1	-18.33	#	#	+	-	*	#	+	*	#
290	CC(Cl)=C	-18.4	-	-	-	#	-	-	-	-	-
291	Cl\C=C\Cl	-18.58	*	-	*	-	*	*	*	#	*
292	CCON=O	-18.6	*	+	*	+	#	*	*	#	*
293	Cc1cccc(O)c1	-18.71	#	+	-	+	+	#	-	*	-
294	[CH2]=[C]=[CH2]	-18.72	*	#	*	+	-	*	*	+	+
295	FC=C(F)F	-18.85	*	+	*	-	-	*	*	-	+
296	CCON=O	-18.93	+	*	+	+	*	+	+	#	+
297	FC(F)=C	-19.1	-	*	-	+	-	-	-	+	-
298	ClC=C(Cl)Cl	-19.24	+	-	+	+	-	+	+	-	+
299	CCN	-19.56	#	#	+	+	#	#	-	+	#
300	C=C	-19.83	+	+	-	-	*	+	+	-	+
301	ClC=C(Cl)Cl	-19.97	-	+	-	-	+	-	-	+	-
302	CCC	-23.2	-	+	-	-	*	-	-	*	-

Table S3. Continued

No.	DCW									Predicted log KO3								
	Split 1	Split 2	Split 3	Split 4	Split 5	Split 6	Split 7	Split 8	Split 9	Split 1	Split 2	Split 3	Split 4	Split 5	Split 6	Split 7	Split 8	Split 9
1	26.07	33.41	44.45	30.92	27.41	38.38	30.75	27.24	35.67	-13.93	-13.54	-13.93	-13.85	-14.20	-13.92	-13.92	-14.59	-13.92
2	22.77	30.03	42.01	34.62	27.69	36.87	27.24	28.10	33.70	-14.97	-14.40	-14.37	-12.89	-14.12	-14.29	-14.81	-14.35	-14.40
3	23.34	29.15	35.66	27.56	24.97	30.94	20.53	23.72	28.93	-14.79	-14.62	-15.52	-14.73	-14.87	-15.72	-16.52	-15.59	-15.56
4	23.32	28.68	41.04	29.15	25.00	36.74	27.20	29.02	33.66	-14.80	-14.74	-14.54	-14.31	-14.86	-14.32	-14.82	-14.08	-14.41
5	22.50	25.74	36.70	27.04	25.59	32.46	24.96	24.11	29.26	-15.06	-15.49	-15.33	-14.86	-14.70	-15.35	-15.39	-15.48	-15.48
6	23.60	28.28	41.02	27.68	24.71	35.60	27.57	27.62	32.38	-14.71	-14.84	-14.55	-14.70	-14.94	-14.59	-14.73	-14.48	-14.72
7	23.96	30.67	40.18	26.72	25.16	34.37	28.11	26.70	31.83	-14.60	-14.24	-14.70	-14.95	-14.82	-14.89	-14.59	-14.74	-14.86

8	22.94	25.91	40.23	27.48	25.78	34.73	26.43	26.82	31.43	-14.92	-15.45	-14.69	-14.75	-14.65	-14.80	-15.02	-14.71	-14.95
9	20.46	24.02	36.56	24.35	22.45	30.91	23.11	24.13	28.31	-15.70	-15.93	-15.36	-15.56	-15.57	-15.72	-15.87	-15.47	-15.71
10	20.99	24.85	36.98	24.99	23.71	32.03	24.74	24.97	28.58	-15.54	-15.72	-15.28	-15.40	-15.22	-15.45	-15.45	-15.24	-15.65
11	21.56	23.33	37.14	25.49	23.84	32.59	24.72	24.75	29.55	-15.36	-16.11	-15.25	-15.27	-15.18	-15.32	-15.46	-15.30	-15.41
12	22.54	27.63	38.80	27.20	24.34	33.72	24.63	25.83	30.94	-15.05	-15.01	-14.95	-14.82	-15.04	-15.04	-15.48	-14.99	-15.07
13	21.09	25.59	36.31	24.66	22.66	31.93	23.16	25.16	28.92	-15.51	-15.53	-15.40	-15.48	-15.51	-15.48	-15.85	-15.18	-15.56
14	21.69	24.60	36.15	22.93	21.04	30.41	21.26	24.21	27.22	-15.32	-15.78	-15.43	-15.93	-15.96	-15.84	-16.33	-15.45	-15.98
15	22.05	26.91	37.51	25.56	23.88	33.11	25.81	28.32	30.46	-15.20	-15.19	-15.18	-15.25	-15.17	-15.19	-15.18	-14.28	-15.19
16	24.16	29.75	41.35	26.76	25.26	38.15	28.23	27.18	34.63	-14.54	-14.47	-14.49	-14.94	-14.79	-13.98	-14.56	-14.60	-14.18
17	21.40	27.56	37.27	27.15	22.98	32.61	25.38	24.89	29.47	-15.41	-15.03	-15.23	-14.83	-15.42	-15.31	-15.29	-15.26	-15.43
18	20.08	28.67	42.01	25.56	24.96	30.70	23.43	27.88	27.04	-15.82	-14.75	-14.37	-15.25	-14.87	-15.77	-15.78	-14.41	-16.02
19	20.44	26.94	35.55	25.86	21.73	31.09	24.00	23.73	27.91	-15.71	-15.19	-15.54	-15.17	-15.77	-15.68	-15.64	-15.59	-15.81
20	20.72	27.67	35.11	22.43	22.97	32.37	24.64	25.95	28.88	-15.62	-15.00	-15.62	-16.06	-15.42	-15.37	-15.47	-14.96	-15.57
21	21.25	24.79	36.08	25.78	24.10	32.68	25.13	25.07	29.60	-15.46	-15.74	-15.44	-15.19	-15.11	-15.30	-15.35	-15.21	-15.40
22	21.10	27.54	36.20	26.54	22.83	31.89	25.07	24.53	29.24	-15.50	-15.03	-15.42	-14.99	-15.46	-15.49	-15.37	-15.36	-15.49
23	22.13	27.21	39.25	25.44	24.00	33.86	26.61	25.61	31.01	-15.18	-15.12	-14.87	-15.28	-15.14	-15.01	-14.97	-15.05	-15.06
24	21.18	26.59	37.54	24.16	22.76	32.34	25.22	24.45	29.46	-15.48	-15.28	-15.18	-15.61	-15.48	-15.38	-15.33	-15.38	-15.43
25	20.85	26.51	34.65	25.51	22.67	31.68	23.33	24.08	29.11	-15.58	-15.30	-15.70	-15.26	-15.51	-15.54	-15.81	-15.49	-15.52
26	21.18	26.59	37.54	24.16	22.76	32.34	25.22	24.45	29.46	-15.48	-15.28	-15.18	-15.61	-15.48	-15.38	-15.33	-15.38	-15.43
27	23.49	27.25	39.34	23.21	22.13	33.90	25.10	25.50	29.87	-14.75	-15.11	-14.85	-15.86	-15.65	-15.00	-15.36	-15.08	-15.33
28	19.09	25.69	34.00	24.25	21.48	29.88	23.53	24.27	25.97	-16.14	-15.51	-15.82	-15.59	-15.84	-15.97	-15.76	-15.43	-16.28
29	19.93	25.68	33.39	22.91	20.01	30.56	23.14	22.96	27.58	-15.87	-15.51	-15.93	-15.94	-16.24	-15.81	-15.86	-15.81	-15.89
30	18.50	24.57	32.04	23.61	22.11	29.18	22.01	23.45	27.31	-16.33	-15.79	-16.17	-15.76	-15.66	-16.14	-16.14	-15.67	-15.96
31	20.22	23.92	34.31	23.99	22.33	31.20	23.38	23.32	28.19	-15.78	-15.96	-15.76	-15.66	-15.60	-15.65	-15.80	-15.70	-15.74
32	19.50	19.05	34.01	24.32	22.79	31.58	22.82	23.81	28.89	-16.01	-17.20	-15.82	-15.57	-15.47	-15.56	-15.94	-15.57	-15.57
33	21.83	26.27	35.17	23.82	23.18	32.60	26.18	24.98	29.91	-15.27	-15.36	-15.61	-15.70	-15.37	-15.32	-15.08	-15.23	-15.32
34	19.80	26.39	34.23	23.79	21.46	30.39	23.27	23.21	27.04	-15.92	-15.33	-15.78	-15.71	-15.84	-15.85	-15.82	-15.73	-16.02
35	20.41	23.76	35.64	23.66	22.11	31.12	24.58	23.99	29.04	-15.72	-16.00	-15.52	-15.74	-15.66	-15.67	-15.49	-15.51	-15.54
36	20.92	25.71	35.99	24.62	22.48	32.33	24.59	24.54	27.31	-15.56	-15.50	-15.46	-15.49	-15.56	-15.38	-15.49	-15.36	-15.96
37	19.30	23.72	32.83	23.29	22.03	29.98	23.44	23.21	26.75	-16.07	-16.01	-16.03	-15.84	-15.68	-15.95	-15.78	-15.73	-16.09

38	18.50	23.54	32.04	22.67	21.02	29.18	22.01	23.40	27.27	-16.33	-16.05	-16.17	-16.00	-15.96	-16.14	-16.14	-15.68	-15.97
39	19.91	24.66	34.39	22.74	21.85	30.45	23.61	23.13	27.73	-15.88	-15.77	-15.75	-15.98	-15.73	-15.83	-15.74	-15.76	-15.85
40	21.64	24.34	35.24	22.24	20.70	30.62	22.74	24.08	27.95	-15.33	-15.85	-15.59	-16.11	-16.05	-15.79	-15.96	-15.49	-15.80
41	20.33	26.14	34.01	23.52	21.77	30.56	23.01	23.16	27.25	-15.75	-15.39	-15.82	-15.78	-15.75	-15.81	-15.89	-15.75	-15.97
42	20.36	27.54	39.84	24.87	25.04	32.14	25.66	25.25	29.62	-15.74	-15.03	-14.76	-15.43	-14.85	-15.43	-15.22	-15.16	-15.39
43	19.58	24.47	34.01	23.25	19.32	30.17	23.24	22.16	27.60	-15.99	-15.82	-15.82	-15.85	-16.43	-15.90	-15.83	-16.03	-15.89
44	19.90	25.94	33.92	23.41	22.10	30.54	23.41	23.78	27.05	-15.88	-15.44	-15.83	-15.81	-15.66	-15.81	-15.79	-15.57	-16.02
45	19.24	22.10	31.21	22.30	19.29	28.80	20.77	22.75	25.95	-16.09	-16.42	-16.33	-16.10	-16.44	-16.23	-16.46	-15.86	-16.29
46	19.62	25.44	33.77	23.98	21.79	30.06	23.27	24.22	26.18	-15.97	-15.57	-15.86	-15.66	-15.75	-15.93	-15.82	-15.45	-16.23
47	19.26	23.31	32.60	22.71	21.08	29.69	22.00	22.16	26.63	-16.08	-16.11	-16.07	-15.99	-15.94	-16.02	-16.15	-16.03	-16.12
48	19.96	25.09	34.27	23.34	21.23	30.81	23.21	23.38	25.75	-15.86	-15.66	-15.77	-15.83	-15.90	-15.75	-15.84	-15.69	-16.33
49	19.26	23.31	32.60	22.71	21.08	29.69	22.00	22.16	26.63	-16.08	-16.11	-16.07	-15.99	-15.94	-16.02	-16.15	-16.03	-16.12
50	19.96	25.09	34.27	23.34	21.23	30.81	23.21	23.38	25.75	-15.86	-15.66	-15.77	-15.83	-15.90	-15.75	-15.84	-15.69	-16.33
51	17.54	22.92	30.33	21.38	19.77	27.66	20.62	22.24	25.72	-16.63	-16.21	-16.48	-16.34	-16.31	-16.51	-16.50	-16.01	-16.34
52	20.19	24.56	32.70	21.48	20.79	29.69	21.91	21.82	26.62	-15.79	-15.79	-16.06	-16.31	-16.03	-16.02	-16.17	-16.13	-16.12
53	19.26	23.31	32.60	22.71	21.08	29.69	22.00	22.16	26.63	-16.08	-16.11	-16.07	-15.99	-15.94	-16.02	-16.15	-16.03	-16.12
54	19.71	27.09	35.54	26.02	22.16	30.88	23.81	25.03	28.39	-15.94	-15.15	-15.54	-15.13	-15.65	-15.73	-15.69	-15.22	-15.69
55	18.64	22.54	31.35	20.69	19.82	28.24	21.91	22.76	24.82	-16.28	-16.31	-16.30	-16.52	-16.29	-16.37	-16.17	-15.86	-16.56
56	19.57	23.54	32.04	23.71	21.29	30.42	23.37	22.75	26.81	-15.99	-16.05	-16.17	-15.73	-15.89	-15.84	-15.80	-15.87	-16.08
57	19.70	24.37	33.68	23.35	21.26	30.38	23.40	22.57	27.59	-15.95	-15.84	-15.88	-15.82	-15.90	-15.85	-15.79	-15.92	-15.89
58	19.57	23.54	32.04	23.71	21.29	30.42	23.37	22.75	26.81	-15.99	-16.05	-16.17	-15.73	-15.89	-15.84	-15.80	-15.87	-16.08
59	19.70	24.37	33.68	23.35	21.26	30.38	23.40	22.57	27.59	-15.95	-15.84	-15.88	-15.82	-15.90	-15.85	-15.79	-15.92	-15.89
60	20.41	23.76	35.64	23.66	22.11	31.12	24.58	23.99	29.04	-15.72	-16.00	-15.52	-15.74	-15.66	-15.67	-15.49	-15.51	-15.54
61	20.00	24.73	34.21	25.57	21.43	29.44	22.93	24.51	27.79	-15.85	-15.75	-15.78	-15.25	-15.85	-16.08	-15.91	-15.37	-15.84
62	18.50	23.51	32.04	22.67	21.26	29.18	22.01	22.39	26.97	-16.33	-16.06	-16.17	-16.00	-15.90	-16.14	-16.14	-15.97	-16.04
63	18.50	22.98	33.07	21.47	20.27	28.19	22.12	21.34	25.88	-16.33	-16.20	-15.99	-16.31	-16.17	-16.38	-16.12	-16.27	-16.30
64	18.61	22.92	30.33	22.42	20.04	28.90	21.99	21.59	25.26	-16.29	-16.21	-16.48	-16.07	-16.23	-16.21	-16.15	-16.20	-16.45
65	18.74	23.76	31.97	22.07	20.01	28.86	22.01	21.42	26.03	-16.25	-16.00	-16.19	-16.16	-16.24	-16.22	-16.14	-16.25	-16.27
66	19.93	24.29	33.17	22.02	21.69	29.59	23.75	23.85	26.85	-15.87	-15.86	-15.97	-16.17	-15.78	-16.04	-15.70	-15.55	-16.07
67	20.87	24.75	34.28	24.84	21.38	30.40	24.50	22.77	28.90	-15.58	-15.75	-15.77	-15.44	-15.86	-15.85	-15.51	-15.86	-15.57

68	18.82	22.98	33.93	25.53	23.96	29.03	20.39	23.12	26.90	-16.23	-16.20	-15.83	-15.26	-15.15	-16.18	-16.56	-15.76	-16.06
69	18.47	18.97	30.99	22.20	19.93	28.04	20.99	21.51	24.43	-16.34	-17.22	-16.37	-16.12	-16.26	-16.41	-16.40	-16.22	-16.66
70	18.27	22.86	31.05	21.50	20.26	28.50	21.69	21.46	25.34	-16.40	-16.23	-16.35	-16.31	-16.17	-16.30	-16.23	-16.23	-16.43
71	18.27	22.86	31.05	21.50	20.26	28.50	21.69	21.46	25.34	-16.40	-16.23	-16.35	-16.31	-16.17	-16.30	-16.23	-16.23	-16.43
72	19.57	22.35	31.79	21.98	19.89	31.57	21.56	21.62	28.41	-15.99	-16.36	-16.22	-16.18	-16.27	-15.56	-16.26	-16.19	-15.69
73	17.54	22.92	30.33	21.66	19.82	27.66	20.62	21.31	25.75	-16.63	-16.21	-16.48	-16.26	-16.29	-16.51	-16.50	-16.28	-16.33
74	17.54	22.92	30.33	21.38	19.74	27.66	20.62	21.23	25.75	-16.63	-16.21	-16.48	-16.34	-16.32	-16.51	-16.50	-16.30	-16.33
75	17.31	22.24	29.34	20.22	19.01	26.98	20.31	20.31	23.78	-16.70	-16.39	-16.66	-16.64	-16.52	-16.67	-16.58	-16.56	-16.81
76	18.66	23.08	31.45	20.44	18.58	29.18	21.68	21.96	26.27	-16.28	-16.17	-16.28	-16.58	-16.64	-16.14	-16.23	-16.09	-16.21
77	18.32	22.92	30.67	21.21	19.42	28.14	20.97	20.87	25.51	-16.38	-16.21	-16.42	-16.38	-16.40	-16.39	-16.41	-16.40	-16.39
78	17.10	21.00	30.38	21.49	17.72	30.41	19.68	21.03	27.06	-16.77	-16.70	-16.48	-16.31	-16.87	-15.84	-16.74	-16.36	-16.02
79	15.78	21.71	25.93	21.38	17.88	25.55	18.26	17.42	23.37	-17.19	-16.52	-17.28	-16.34	-16.83	-17.02	-17.10	-17.38	-16.91
80	18.03	22.14	29.47	20.42	19.07	30.32	20.47	20.72	27.35	-16.47	-16.41	-16.64	-16.59	-16.50	-15.87	-16.54	-16.44	-15.95
81	17.35	22.24	29.51	22.11	19.34	26.96	19.88	19.71	24.23	-16.69	-16.39	-16.63	-16.15	-16.43	-16.68	-16.69	-16.73	-16.70
82	18.32	22.92	30.67	21.21	19.42	28.14	20.97	20.87	25.51	-16.38	-16.21	-16.42	-16.38	-16.40	-16.39	-16.41	-16.40	-16.39
83	17.28	21.60	29.09	20.19	19.54	27.11	20.18	18.72	23.95	-16.71	-16.55	-16.71	-16.65	-16.37	-16.64	-16.61	-17.01	-16.77
84	17.55	23.15	29.40	20.15	17.26	27.37	20.69	20.35	24.71	-16.63	-16.15	-16.65	-16.66	-17.00	-16.58	-16.48	-16.55	-16.59
85	17.38	23.92	29.95	19.76	17.87	28.33	19.74	21.28	25.27	-16.68	-15.96	-16.55	-16.76	-16.83	-16.35	-16.72	-16.29	-16.45
86	20.01	22.81	35.58	23.91	21.74	30.00	20.81	21.28	24.90	-15.85	-16.24	-15.53	-15.68	-15.76	-15.94	-16.45	-16.28	-16.54
87	17.76	21.01	29.71	19.93	18.43	27.50	20.20	20.21	24.62	-16.56	-16.70	-16.60	-16.72	-16.68	-16.55	-16.60	-16.59	-16.61
88	16.10	20.69	27.83	19.28	18.64	26.06	19.17	20.36	23.20	-17.08	-16.78	-16.94	-16.88	-16.62	-16.89	-16.87	-16.55	-16.95
89	16.92	19.56	29.13	19.83	17.99	26.50	19.61	18.22	23.53	-16.83	-17.07	-16.70	-16.74	-16.80	-16.79	-16.76	-17.15	-16.87
90	17.35	22.24	29.51	22.11	19.34	26.96	19.88	19.71	24.23	-16.69	-16.39	-16.63	-16.15	-16.43	-16.68	-16.69	-16.73	-16.70
91	17.06	21.97	28.65	19.42	17.71	25.95	19.99	19.41	24.26	-16.78	-16.45	-16.79	-16.85	-16.88	-16.92	-16.66	-16.82	-16.70
92	13.84	19.34	25.88	19.38	16.99	22.99	17.82	19.31	21.23	-17.80	-17.13	-17.29	-16.86	-17.08	-17.63	-17.21	-16.84	-17.43
93	16.37	17.81	27.13	18.05	17.14	25.49	18.39	18.39	22.96	-17.00	-17.52	-17.06	-17.21	-17.04	-17.03	-17.07	-17.11	-17.01
94	16.32	19.41	27.01	19.30	18.10	26.53	17.26	17.77	23.26	-17.02	-17.11	-17.09	-16.88	-16.77	-16.78	-17.36	-17.28	-16.94
95	17.30	20.90	28.97	20.95	18.71	26.78	19.38	18.81	24.74	-16.70	-16.73	-16.73	-16.45	-16.60	-16.72	-16.81	-16.99	-16.58
96	17.23	21.38	27.01	20.02	18.05	25.72	19.22	19.42	23.07	-16.73	-16.61	-17.09	-16.69	-16.78	-16.98	-16.86	-16.81	-16.99
97	17.84	20.97	30.21	21.92	20.19	28.22	19.57	20.83	24.89	-16.53	-16.71	-16.51	-16.20	-16.19	-16.37	-16.77	-16.41	-16.54

98	16.01	20.79	27.22	18.40	18.09	25.16	18.68	19.54	22.28	-17.11	-16.76	-17.05	-17.12	-16.77	-17.11	-16.99	-16.78	-17.18
99	16.29	19.68	27.11	19.31	18.09	26.76	18.29	19.47	23.74	-17.02	-17.04	-17.07	-16.88	-16.77	-16.72	-17.09	-16.80	-16.82
100	16.60	20.50	29.47	20.39	17.92	26.34	19.73	19.16	23.34	-16.92	-16.83	-16.64	-16.60	-16.82	-16.83	-16.72	-16.89	-16.92
101	19.02	22.74	28.68	20.37	20.81	29.82	20.19	20.80	25.50	-16.16	-16.26	-16.79	-16.60	-16.02	-15.99	-16.61	-16.42	-16.39
102	15.57	19.24	26.84	19.00	16.96	25.01	17.94	18.04	22.11	-17.25	-17.15	-17.12	-16.96	-17.09	-17.15	-17.18	-17.21	-17.22
103	16.29	20.27	27.07	18.57	17.37	25.63	18.73	19.57	21.20	-17.02	-16.89	-17.08	-17.07	-16.97	-17.00	-16.98	-16.77	-17.44
104	15.16	20.40	26.34	18.62	17.01	24.46	18.17	19.64	22.85	-17.38	-16.86	-17.21	-17.06	-17.07	-17.28	-17.12	-16.75	-17.04
105	13.11	19.14	24.52	18.93	16.48	22.10	16.53	17.58	20.09	-18.03	-17.18	-17.54	-16.98	-17.22	-17.85	-17.54	-17.34	-17.71
106	16.92	21.25	26.86	19.62	18.30	27.78	18.34	20.51	24.36	-16.82	-16.64	-17.11	-16.80	-16.71	-16.48	-17.08	-16.50	-16.67
107	15.61	20.39	27.76	17.73	18.81	25.00	18.30	18.98	22.51	-17.24	-16.86	-16.95	-17.29	-16.57	-17.15	-17.09	-16.94	-17.12
108	16.22	20.05	25.14	18.26	17.43	25.54	17.58	19.38	22.70	-17.05	-16.95	-17.43	-17.15	-16.96	-17.02	-17.27	-16.82	-17.07
109	15.99	16.42	26.97	18.19	16.93	25.35	18.34	18.57	22.78	-17.12	-17.87	-17.09	-17.17	-17.09	-17.06	-17.08	-17.06	-17.06
110	15.57	19.24	26.84	19.00	16.96	25.01	17.94	18.04	22.11	-17.25	-17.15	-17.12	-16.96	-17.09	-17.15	-17.18	-17.21	-17.22
111	15.31	19.24	25.48	17.76	16.78	23.73	17.87	18.08	21.78	-17.33	-17.15	-17.37	-17.28	-17.13	-17.45	-17.20	-17.20	-17.30
112	15.59	18.48	25.39	17.95	17.22	24.51	17.52	18.35	22.09	-17.24	-17.35	-17.38	-17.23	-17.01	-17.27	-17.29	-17.12	-17.23
113	15.59	18.48	25.39	17.95	17.22	24.51	17.52	18.35	22.09	-17.24	-17.35	-17.38	-17.23	-17.01	-17.27	-17.29	-17.12	-17.23
114	16.06	20.78	27.72	19.04	17.87	25.69	18.84	19.63	22.62	-17.10	-16.76	-16.96	-16.95	-16.83	-16.98	-16.95	-16.75	-17.10
115	17.51	22.35	28.36	20.25	18.54	27.52	19.60	20.59	24.38	-16.64	-16.36	-16.84	-16.63	-16.65	-16.54	-16.76	-16.48	-16.67
116	16.29	19.68	27.11	19.31	18.09	26.76	18.29	19.47	23.74	-17.02	-17.04	-17.07	-16.88	-16.77	-16.72	-17.09	-16.80	-16.82
117	17.12	21.23	27.25	18.27	18.90	26.23	19.01	18.71	23.56	-16.76	-16.64	-17.04	-17.15	-16.55	-16.85	-16.91	-17.01	-16.87
118	17.38	20.77	27.05	18.21	17.56	26.65	18.49	19.25	23.76	-16.68	-16.76	-17.08	-17.16	-16.92	-16.75	-17.04	-16.86	-16.82
119	16.57	18.07	26.56	17.84	15.58	25.00	17.87	17.72	22.92	-16.94	-17.45	-17.17	-17.26	-17.47	-17.15	-17.20	-17.30	-17.02
120	16.75	19.20	27.30	17.90	17.35	25.62	18.44	18.21	23.14	-16.88	-17.16	-17.03	-17.24	-16.98	-17.00	-17.05	-17.16	-16.97
121	17.85	20.70	28.00	19.62	18.34	27.45	18.70	19.54	24.31	-16.53	-16.78	-16.91	-16.80	-16.70	-16.56	-16.99	-16.78	-16.68
122	15.38	21.17	26.10	18.66	16.15	24.80	17.19	18.90	21.90	-17.31	-16.66	-17.25	-17.05	-17.31	-17.20	-17.37	-16.96	-17.27
123	15.59	18.48	25.39	17.95	17.22	24.51	17.52	18.35	22.09	-17.24	-17.35	-17.38	-17.23	-17.01	-17.27	-17.29	-17.12	-17.23
124	17.25	22.81	28.56	20.31	19.88	27.10	20.11	20.06	24.18	-16.72	-16.24	-16.81	-16.62	-16.28	-16.64	-16.63	-16.63	-16.72
125	17.64	21.17	31.76	21.19	18.33	27.89	19.97	21.36	25.21	-16.60	-16.66	-16.23	-16.39	-16.71	-16.45	-16.66	-16.26	-16.47
126	16.85	24.17	28.40	18.86	17.78	25.54	19.05	20.70	23.25	-16.85	-15.89	-16.84	-16.99	-16.86	-17.02	-16.90	-16.45	-16.94
127	16.97	20.20	27.93	17.78	17.13	25.59	19.26	19.11	23.21	-16.81	-16.91	-16.92	-17.28	-17.04	-17.01	-16.85	-16.90	-16.95

128	15.95	20.22	27.14	20.03	17.34	25.06	18.28	18.78	22.01	-17.13	-16.90	-17.06	-16.69	-16.98	-17.14	-17.09	-17.00	-17.24
129	16.60	18.81	27.76	17.92	16.92	25.46	19.21	19.29	23.03	-16.93	-17.26	-16.95	-17.24	-17.10	-17.04	-16.86	-16.85	-17.00
130	12.38	16.35	20.77	16.11	11.81	21.06	14.18	12.65	19.79	-18.26	-17.89	-18.22	-17.71	-18.51	-18.10	-18.14	-18.74	-17.78
131	12.00	16.80	26.51	16.15	14.99	21.77	12.92	16.69	16.71	-18.38	-17.77	-17.18	-17.70	-17.63	-17.93	-18.46	-17.59	-18.53
132	15.82	18.79	26.33	20.10	17.14	25.03	18.16	17.95	22.49	-17.17	-17.27	-17.21	-16.67	-17.03	-17.14	-17.13	-17.23	-17.13
133	15.16	20.40	27.22	18.37	16.79	24.46	18.17	19.48	22.88	-17.38	-16.86	-17.05	-17.12	-17.13	-17.28	-17.12	-16.80	-17.03
134	15.82	19.48	26.02	17.82	17.00	24.49	18.34	19.25	22.16	-17.17	-17.09	-17.27	-17.27	-17.07	-17.27	-17.08	-16.86	-17.21
135	15.60	22.17	26.73	18.54	15.93	24.77	18.00	19.81	21.97	-17.24	-16.40	-17.14	-17.08	-17.37	-17.20	-17.16	-16.70	-17.25
136	16.14	18.85	26.67	19.00	15.89	25.88	18.32	17.32	22.56	-17.07	-17.25	-17.15	-16.96	-17.38	-16.94	-17.08	-17.41	-17.11
137	16.32	19.29	27.28	17.99	16.02	24.49	18.59	17.95	22.94	-17.02	-17.14	-17.04	-17.22	-17.35	-17.27	-17.02	-17.23	-17.02
138	14.91	17.04	26.53	16.52	15.58	24.37	17.47	14.83	21.45	-17.46	-17.71	-17.17	-17.61	-17.47	-17.30	-17.30	-18.12	-17.38
139	15.03	19.65	26.18	14.79	16.66	24.07	17.38	17.78	21.24	-17.42	-17.05	-17.24	-18.06	-17.17	-17.37	-17.32	-17.28	-17.43
140	13.25	16.67	21.18	16.96	14.84	21.20	14.21	17.11	19.67	-17.99	-17.81	-18.14	-17.49	-17.67	-18.07	-18.13	-17.47	-17.81
141	16.17	18.09	25.23	17.95	16.15	25.38	17.90	17.63	22.53	-17.06	-17.44	-17.41	-17.23	-17.31	-17.06	-17.19	-17.32	-17.12
142	16.87	19.30	26.95	19.31	17.02	27.62	18.67	18.75	24.19	-16.84	-17.14	-17.10	-16.88	-17.07	-16.52	-16.99	-17.00	-16.71
143	15.55	18.90	26.56	17.46	16.41	25.14	18.26	18.46	22.57	-17.26	-17.24	-17.17	-17.36	-17.24	-17.11	-17.10	-17.09	-17.11
144	14.93	18.46	22.40	16.33	15.24	24.60	15.87	16.28	21.19	-17.45	-17.35	-17.92	-17.65	-17.56	-17.25	-17.71	-17.71	-17.44
145	17.46	20.40	28.44	19.95	17.26	27.35	19.92	18.84	24.21	-16.65	-16.86	-16.83	-16.71	-17.00	-16.58	-16.68	-16.98	-16.71
146	15.07	16.61	24.41	16.88	14.03	24.13	17.14	16.20	21.82	-17.41	-17.82	-17.56	-17.51	-17.89	-17.36	-17.39	-17.73	-17.29
147	16.21	19.23	26.77	20.64	17.13	25.26	17.89	19.70	22.40	-17.05	-17.15	-17.13	-16.53	-17.04	-17.09	-17.19	-16.73	-17.15
148	14.67	18.50	24.83	17.65	18.25	23.51	16.57	17.26	21.17	-17.54	-17.34	-17.48	-17.31	-16.73	-17.51	-17.53	-17.43	-17.45
149	13.45	16.32	23.56	16.11	13.21	22.06	15.75	15.91	20.36	-17.92	-17.90	-17.71	-17.71	-18.12	-17.86	-17.74	-17.81	-17.65
150	14.92	17.11	24.02	17.32	16.15	24.62	16.58	17.40	21.86	-17.46	-17.70	-17.63	-17.40	-17.31	-17.24	-17.53	-17.39	-17.28
151	13.25	18.22	21.18	16.02	13.75	21.20	14.21	17.06	19.63	-17.99	-17.41	-18.14	-17.74	-17.97	-18.07	-18.13	-17.48	-17.82
152	14.17	18.73	23.78	18.41	15.34	23.37	16.50	18.14	20.68	-17.69	-17.28	-17.67	-17.11	-17.53	-17.54	-17.55	-17.18	-17.57
153	15.51	18.20	25.52	17.95	16.38	24.35	17.83	17.49	21.88	-17.27	-17.42	-17.36	-17.23	-17.24	-17.30	-17.21	-17.36	-17.27
154	14.97	17.88	24.91	18.46	15.80	23.66	16.81	16.98	21.43	-17.44	-17.50	-17.47	-17.10	-17.41	-17.47	-17.47	-17.51	-17.39
155	14.51	17.54	24.25	12.81	15.19	23.27	16.40	16.80	20.68	-17.59	-17.59	-17.59	-18.57	-17.58	-17.57	-17.57	-17.56	-17.57
156	15.33	18.07	23.40	17.58	16.62	23.84	16.15	17.48	20.97	-17.33	-17.45	-17.74	-17.33	-17.18	-17.43	-17.64	-17.36	-17.50
157	13.52	15.87	23.77	16.05	14.99	21.97	15.56	15.72	19.56	-17.90	-18.01	-17.67	-17.73	-17.63	-17.88	-17.79	-17.86	-17.84

158	12.90	14.91	21.91	13.31	11.30	21.15	14.65	14.80	17.62	-18.10	-18.26	-18.01	-18.44	-18.65	-18.08	-18.02	-18.13	-18.31
159	12.57	15.16	20.19	13.04	12.71	20.64	14.01	14.09	18.93	-18.20	-18.19	-18.32	-18.51	-18.26	-18.20	-18.18	-18.33	-17.99
160	14.38	21.69	23.84	16.84	15.41	22.88	16.06	17.84	20.46	-17.63	-16.53	-17.66	-17.52	-17.51	-17.66	-17.66	-17.26	-17.62
161	13.87	18.06	23.12	16.62	16.15	22.49	16.15	17.42	20.87	-17.79	-17.45	-17.79	-17.58	-17.31	-17.76	-17.64	-17.38	-17.52
162	9.63	16.98	16.09	14.24	14.26	22.17	11.58	15.12	15.38	-19.13	-17.73	-19.07	-18.20	-17.83	-17.83	-18.80	-18.04	-18.86
163	14.17	17.78	24.10	16.05	15.65	22.73	15.95	16.68	20.12	-17.69	-17.52	-17.61	-17.73	-17.45	-17.70	-17.69	-17.59	-17.70
164	14.34	18.62	23.85	16.82	16.03	24.06	16.60	17.62	20.89	-17.64	-17.31	-17.66	-17.53	-17.34	-17.38	-17.52	-17.33	-17.52
165	12.20	13.12	20.23	12.68	11.15	20.03	13.44	13.58	18.51	-18.32	-18.71	-18.32	-18.61	-18.69	-18.35	-18.33	-18.47	-18.10
166	14.94	19.72	25.35	17.45	16.26	23.79	17.86	17.70	20.91	-17.45	-17.03	-17.39	-17.36	-17.28	-17.44	-17.20	-17.30	-17.51
167	12.20	13.12	20.23	12.68	11.15	20.03	13.44	13.58	18.51	-18.32	-18.71	-18.32	-18.61	-18.69	-18.35	-18.33	-18.47	-18.10
168	10.48	16.61	17.96	11.35	14.40	18.00	12.07	12.65	17.62	-18.86	-17.82	-18.73	-18.95	-17.79	-18.84	-18.68	-18.74	-18.31
169	9.63	14.04	16.96	11.85	12.89	22.17	11.58	12.01	15.38	-19.13	-18.48	-18.91	-18.82	-18.21	-17.83	-18.80	-18.92	-18.86
170	12.87	15.65	21.26	14.73	12.86	20.75	14.91	16.00	17.80	-18.11	-18.07	-18.13	-18.07	-18.22	-18.17	-17.95	-17.79	-18.27
171	12.87	15.65	21.26	14.73	12.86	20.75	14.91	16.00	17.80	-18.11	-18.07	-18.13	-18.07	-18.22	-18.17	-17.95	-17.79	-18.27
172	12.87	15.65	21.26	14.73	12.86	20.75	14.91	16.00	17.80	-18.11	-18.07	-18.13	-18.07	-18.22	-18.17	-17.95	-17.79	-18.27
173	12.87	15.65	21.26	14.73	12.86	20.75	14.91	16.00	17.80	-18.11	-18.07	-18.13	-18.07	-18.22	-18.17	-17.95	-17.79	-18.27
174	10.48	12.74	17.96	11.35	10.08	18.00	12.07	12.65	17.62	-18.86	-18.81	-18.73	-18.95	-18.99	-18.84	-18.68	-18.74	-18.31
175	11.33	14.74	17.39	12.49	11.94	18.83	11.10	10.99	16.15	-18.59	-18.30	-18.83	-18.66	-18.47	-18.64	-18.92	-19.21	-18.67
176	13.03	15.01	22.04	11.47	11.71	21.00	13.76	14.03	18.87	-18.06	-18.23	-17.99	-18.92	-18.54	-18.11	-18.25	-18.35	-18.01
177	12.87	15.65	21.26	14.73	12.86	20.75	14.91	16.00	17.80	-18.11	-18.07	-18.13	-18.07	-18.22	-18.17	-17.95	-17.79	-18.27
178	13.72	17.53	22.61	14.96	14.04	22.55	15.14	16.03	20.54	-17.84	-17.59	-17.89	-18.01	-17.89	-17.74	-17.89	-17.78	-17.60
179	13.72	17.53	22.61	14.96	14.04	22.55	15.14	16.03	20.54	-17.84	-17.59	-17.89	-18.01	-17.89	-17.74	-17.89	-17.78	-17.60
180	10.77	13.78	15.18	9.59	10.66	18.10	10.21	13.41	16.02	-18.77	-18.54	-19.23	-19.41	-18.83	-18.81	-19.15	-18.52	-18.70
181	11.28	14.21	19.85	13.83	12.05	18.41	12.90	14.63	15.29	-18.61	-18.44	-18.39	-18.31	-18.44	-18.74	-18.46	-18.17	-18.88
182	12.99	15.49	20.15	11.85	12.63	20.81	13.82	12.01	17.85	-18.07	-18.11	-18.33	-18.82	-18.28	-18.16	-18.23	-18.92	-18.25
183	8.84	10.64	14.17	10.26	9.69	15.34	9.35	14.40	13.50	-19.38	-19.35	-19.42	-19.24	-19.10	-19.48	-19.37	-18.24	-19.31
184	11.55	12.74	17.96	12.39	10.11	19.24	13.44	13.01	17.13	-18.52	-18.81	-18.73	-18.68	-18.98	-18.54	-18.33	-18.64	-18.43
185	11.32	12.77	18.89	11.64	12.72	18.27	12.61	10.80	16.03	-18.59	-18.80	-18.56	-18.88	-18.26	-18.77	-18.54	-19.27	-18.70
186	11.06	14.89	20.57	13.16	12.65	18.21	12.85	13.06	15.92	-18.68	-18.26	-18.25	-18.48	-18.28	-18.79	-18.48	-18.62	-18.72
187	12.78	12.74	20.07	12.68	10.08	20.89	13.82	12.86	18.95	-18.13	-18.81	-18.35	-18.61	-18.99	-18.14	-18.23	-18.68	-17.99

188	10.23	10.64	18.67	14.15	12.23	17.32	13.30	12.65	14.68	-18.94	-19.34	-18.60	-18.22	-18.39	-19.00	-18.36	-18.74	-19.03
189	7.90	14.13	14.17	13.42	11.95	12.21	9.35	9.74	10.53	-19.67	-18.45	-19.42	-18.41	-18.47	-20.23	-19.37	-19.57	-20.03
190	8.67	12.14	17.52	11.64	12.87	15.31	10.34	14.14	14.09	-19.43	-18.96	-18.81	-18.88	-18.22	-19.49	-19.12	-18.32	-19.17
191	11.56	13.35	18.30	12.20	10.72	19.00	12.07	13.50	15.57	-18.52	-18.65	-18.67	-18.73	-18.81	-18.60	-18.68	-18.50	-18.81
192	7.82	9.68	19.17	8.01	8.90	12.46	7.77	9.62	11.69	-19.70	-19.59	-18.51	-19.82	-19.31	-20.17	-19.77	-19.60	-19.75
193	10.18	13.46	16.67	10.51	11.12	15.88	10.55	10.73	15.16	-18.95	-18.63	-18.96	-19.17	-18.70	-19.35	-19.06	-19.29	-18.91
194	11.06	13.32	17.94	9.68	10.84	17.98	12.74	13.62	15.91	-18.68	-18.66	-18.73	-19.39	-18.78	-18.84	-18.50	-18.46	-18.73
195	10.55	13.62	17.86	12.61	11.29	18.04	12.09	13.10	14.90	-18.84	-18.59	-18.75	-18.63	-18.65	-18.83	-18.67	-18.61	-18.97
196	9.84	11.40	13.20	9.63	11.37	17.83	9.34	12.47	12.47	-19.06	-19.15	-19.59	-19.40	-18.63	-18.88	-19.37	-18.79	-19.56
197	11.36	14.08	19.28	12.33	11.41	18.98	13.02	13.04	16.91	-18.58	-18.47	-18.49	-18.70	-18.62	-18.60	-18.43	-18.63	-18.48
198	10.30	12.53	17.35	8.65	11.30	17.50	11.51	10.88	14.78	-18.92	-18.86	-18.84	-19.66	-18.65	-18.96	-18.82	-19.24	-19.00
199	8.00	12.10	15.06	12.22	10.84	14.56	10.37	11.23	14.26	-19.64	-18.97	-19.25	-18.73	-18.78	-19.67	-19.11	-19.14	-19.13
200	10.98	13.13	18.14	12.29	8.88	18.58	12.08	10.67	15.98	-18.70	-18.71	-18.70	-18.71	-19.32	-18.70	-18.67	-19.30	-18.71
201	8.84	10.04	14.81	6.59	5.63	15.24	9.42	9.33	13.41	-19.38	-19.50	-19.30	-20.19	-20.22	-19.50	-19.35	-19.68	-19.33
202	9.34	9.71	15.80	10.39	10.02	16.22	10.02	8.99	14.11	-19.22	-19.58	-19.12	-19.20	-19.00	-19.27	-19.20	-19.78	-19.16
203	10.15	15.49	16.73	11.85	12.64	17.27	11.58	13.02	15.34	-18.96	-18.11	-18.95	-18.82	-18.28	-19.01	-18.80	-18.63	-18.87
204	8.67	12.61	18.83	13.34	13.97	15.31	11.59	13.53	14.09	-19.43	-18.84	-18.57	-18.43	-17.91	-19.49	-18.80	-18.49	-19.17
205	10.42	13.79	17.70	12.47	10.96	17.71	11.70	11.17	14.26	-18.88	-18.54	-18.78	-18.66	-18.74	-18.91	-18.77	-19.16	-19.13
206	8.84	13.58	14.17	12.65	11.06	15.34	9.35	12.84	13.50	-19.38	-18.60	-19.42	-18.61	-18.72	-19.48	-19.37	-18.69	-19.31
207	12.24	14.55	17.52	11.88	13.30	19.92	11.53	14.24	16.84	-18.30	-18.35	-18.81	-18.81	-18.10	-18.37	-18.81	-18.29	-18.50
208	8.95	10.32	14.58	8.01	8.97	15.54	9.55	9.62	12.99	-19.34	-19.43	-19.34	-19.82	-19.30	-19.43	-19.32	-19.60	-19.44
209	11.35	13.40	15.02	9.60	9.59	18.96	10.59	12.69	16.46	-18.59	-18.64	-19.26	-19.41	-19.12	-18.61	-19.05	-18.73	-18.59
210	11.36	14.08	19.28	12.33	11.41	18.98	13.02	13.04	16.91	-18.58	-18.47	-18.49	-18.70	-18.62	-18.60	-18.43	-18.63	-18.48
211	11.87	14.42	18.99	13.17	14.26	19.30	12.96	12.94	16.26	-18.42	-18.38	-18.54	-18.48	-17.83	-18.52	-18.45	-18.66	-18.64
212	10.03	11.40	16.43	8.70	10.32	17.37	10.78	10.01	14.74	-19.00	-19.15	-19.01	-19.64	-18.92	-18.99	-19.00	-19.49	-19.01
213	8.03	9.29	13.30	7.70	8.90	14.49	8.37	9.62	12.22	-19.63	-19.69	-19.57	-19.90	-19.31	-19.68	-19.62	-19.60	-19.62
214	12.13	14.08	18.71	13.27	14.15	19.02	12.26	13.30	16.23	-18.34	-18.47	-18.59	-18.45	-17.86	-18.59	-18.63	-18.55	-18.65
215	7.90	10.64	20.95	10.26	9.69	12.21	9.35	9.74	14.14	-19.67	-19.35	-18.19	-19.24	-19.10	-20.23	-19.37	-19.57	-19.16
216	9.83	10.24	12.95	7.40	7.74	16.23	9.55	8.34	12.59	-19.07	-19.45	-19.64	-19.98	-19.63	-19.26	-19.32	-19.97	-19.53
217	10.25	12.06	16.97	10.19	9.08	17.33	11.75	11.73	15.65	-18.93	-18.98	-18.91	-19.26	-19.26	-19.00	-18.76	-19.00	-18.79

218	10.48	12.74	17.96	11.35	10.08	18.00	12.07	12.65	17.62	-18.86	-18.81	-18.73	-18.95	-18.99	-18.84	-18.68	-18.74	-18.31
219	10.48	12.74	14.43	11.35	10.08	18.00	9.38	12.65	17.62	-18.86	-18.81	-19.37	-18.95	-18.99	-18.84	-19.36	-18.74	-18.31
220	10.39	11.27	16.37	10.26	9.76	17.65	11.13	9.74	14.80	-18.89	-19.18	-19.02	-19.24	-19.08	-18.92	-18.92	-19.57	-19.00
221	8.74	15.99	14.40	8.33	8.68	15.75	9.22	9.52	13.11	-19.41	-17.98	-19.37	-19.74	-19.38	-19.38	-19.40	-19.63	-19.41
222	7.17	8.66	11.58	7.40	7.67	13.27	7.28	11.68	10.65	-19.91	-19.85	-19.89	-19.98	-19.65	-19.98	-19.90	-19.02	-20.00
223	9.50	11.41	13.38	10.03	12.62	16.27	8.23	9.44	14.59	-19.17	-19.15	-19.56	-19.30	-18.28	-19.25	-19.65	-19.65	-19.05
224	6.00	10.52	12.71	8.30	7.00	11.70	8.44	11.54	10.94	-20.28	-19.38	-19.68	-19.75	-19.84	-20.36	-19.60	-19.06	-19.93
225	10.24	9.68	15.80	8.01	8.64	16.77	10.01	9.62	14.17	-18.93	-19.59	-19.12	-19.82	-19.39	-19.13	-19.20	-19.60	-19.15
226	7.17	9.59	11.58	7.40	7.46	13.27	7.28	8.87	10.65	-19.91	-19.61	-19.89	-19.98	-19.71	-19.98	-19.90	-19.81	-20.00
227	8.18	12.05	13.29	10.02	9.78	14.76	8.33	10.07	14.05	-19.59	-18.98	-19.58	-19.30	-19.07	-19.62	-19.63	-19.47	-19.18
228	10.48	12.74	12.38	11.35	10.08	18.00	12.07	12.65	17.62	-18.86	-18.81	-19.74	-18.95	-18.99	-18.84	-18.68	-18.74	-18.31
229	7.17	10.07	12.89	9.10	8.56	13.27	8.53	10.54	10.65	-19.91	-19.49	-19.65	-19.54	-19.41	-19.98	-19.58	-19.34	-20.00
230	9.47	10.25	15.09	9.95	9.69	16.60	9.95	9.74	14.03	-19.18	-19.45	-19.25	-19.32	-19.10	-19.18	-19.22	-19.57	-19.18
231	7.72	10.42	13.66	7.92	6.96	13.73	8.56	10.26	11.82	-19.73	-19.40	-19.51	-19.85	-19.85	-19.87	-19.57	-19.42	-19.72
232	10.48	8.13	17.96	11.35	10.08	18.00	12.07	8.33	10.94	-18.86	-19.99	-18.73	-18.95	-18.99	-18.84	-18.68	-19.97	-19.93
233	7.17	8.66	11.58	7.40	7.21	13.27	7.28	9.88	10.62	-19.91	-19.85	-19.89	-19.98	-19.78	-19.98	-19.90	-19.53	-20.01
234	10.48	12.74	17.96	11.35	5.88	18.00	12.07	12.65	10.23	-18.86	-18.81	-18.73	-18.95	-20.15	-18.84	-18.68	-18.74	-20.11
235	5.97	12.74	10.71	11.35	10.08	12.09	5.66	7.11	10.48	-20.29	-18.81	-20.04	-18.95	-18.99	-20.26	-20.31	-20.32	-20.05
236	4.73	5.27	10.34	6.43	7.71	9.67	5.89	7.43	7.28	-20.68	-20.72	-20.11	-20.23	-19.64	-20.85	-20.25	-20.23	-20.82
237	5.04	11.27	7.93	4.63	4.48	10.98	4.69	4.68	8.66	-20.58	-19.18	-20.55	-20.70	-20.54	-20.53	-20.55	-21.01	-20.49
238	-3.82	-3.18	-6.48	-2.39	-3.56	-0.59	-5.12	1.18	-3.14	-23.38	-22.87	-23.16	-22.53	-22.76	-23.32	-23.05	-22.00	-23.36
239	-4.99	-3.08	-8.55	-4.71	-4.30	-1.44	-6.29	-3.11	-2.74	-23.75	-22.85	-23.54	-23.14	-22.96	-23.53	-23.35	-23.22	-23.26
240	-3.77	-3.94	-5.26	-4.25	-3.82	-0.58	-5.57	-1.46	-3.06	-23.36	-23.07	-22.94	-23.02	-22.83	-23.32	-23.17	-22.75	-23.34
241	-6.12	-12.99	-12.23	-18.09	-5.65	-5.50	-9.85	-9.37	-8.82	-24.11	-25.38	-24.20	-26.62	-23.34	-24.51	-24.26	-25.00	-24.74
242	-9.93	-15.46	-19.95	-15.43	-5.73	-8.76	-13.90	-10.39	-11.46	-25.31	-26.00	-25.60	-25.93	-23.36	-25.29	-25.29	-25.29	-25.38
243	26.89	31.10	43.99	30.43	30.47	34.48	23.36	28.26	30.75	-13.67	-14.13	-14.01	-13.98	-13.35	-14.86	-15.80	-14.30	-15.12
244	23.96	30.67	40.18	26.72	25.16	34.37	28.11	26.70	31.83	-14.60	-14.24	-14.70	-14.95	-14.82	-14.89	-14.59	-14.74	-14.86
245	21.92	27.16	36.87	25.98	23.03	33.56	26.27	25.86	30.55	-15.24	-15.13	-15.30	-15.14	-15.41	-15.08	-15.06	-14.98	-15.17
246	21.04	23.64	36.39	24.35	21.38	31.77	23.48	23.41	28.75	-15.52	-16.03	-15.39	-15.56	-15.86	-15.52	-15.77	-15.68	-15.61
247	20.89	26.30	35.10	24.20	21.26	32.08	24.52	24.12	29.14	-15.57	-15.35	-15.62	-15.60	-15.90	-15.44	-15.50	-15.48	-15.51

248	20.20	30.13	38.58	25.10	24.30	35.09	22.50	26.93	27.11	-15.79	-14.37	-14.99	-15.37	-15.06	-14.71	-16.02	-14.68	-16.01
249	20.85	25.49	34.06	24.30	22.54	32.23	23.43	24.36	28.81	-15.58	-15.56	-15.81	-15.58	-15.54	-15.41	-15.78	-15.41	-15.59
250	19.88	22.21	32.99	23.79	22.16	30.55	23.42	23.00	27.72	-15.89	-16.39	-16.00	-15.71	-15.65	-15.81	-15.79	-15.80	-15.86
251	17.54	23.95	30.33	22.33	20.86	27.66	20.62	22.29	25.75	-16.63	-15.95	-16.48	-16.09	-16.01	-16.51	-16.50	-16.00	-16.33
252	21.04	25.32	35.40	23.97	22.32	32.14	24.64	25.03	29.66	-15.52	-15.60	-15.57	-15.66	-15.60	-15.43	-15.48	-15.22	-15.39
253	19.62	25.44	33.77	23.98	21.79	30.06	23.27	24.22	26.18	-15.97	-15.57	-15.86	-15.66	-15.75	-15.93	-15.82	-15.45	-16.23
254	19.95	25.78	36.77	26.46	22.64	30.73	25.14	25.85	28.36	-15.87	-15.48	-15.32	-15.01	-15.51	-15.77	-15.35	-14.98	-15.70
255	19.35	23.24	31.59	20.22	19.80	28.75	21.65	21.70	25.89	-16.06	-16.13	-16.26	-16.64	-16.30	-16.24	-16.24	-16.17	-16.30
256	20.99	23.37	35.48	23.66	21.04	31.98	24.96	23.27	29.48	-15.54	-16.10	-15.55	-15.74	-15.96	-15.47	-15.39	-15.72	-15.43
257	19.35	23.99	33.93	24.43	21.48	30.07	21.95	22.80	27.88	-16.06	-15.94	-15.83	-15.54	-15.84	-15.93	-16.16	-15.85	-15.82
258	19.49	23.86	32.47	21.94	20.81	29.19	22.17	22.88	25.55	-16.01	-15.97	-16.10	-16.19	-16.02	-16.14	-16.10	-15.83	-16.38
259	19.89	24.38	32.03	22.95	22.23	32.15	21.96	21.14	28.89	-15.89	-15.84	-16.18	-15.93	-15.63	-15.42	-16.16	-16.32	-15.57
260	18.23	24.62	31.36	23.09	20.17	28.51	21.65	23.29	25.63	-16.41	-15.78	-16.30	-15.89	-16.20	-16.30	-16.24	-15.71	-16.36
261	18.32	22.92	30.67	21.21	19.42	28.14	20.97	20.87	25.51	-16.38	-16.21	-16.42	-16.38	-16.40	-16.39	-16.41	-16.40	-16.39
262	18.32	22.92	30.67	21.21	19.42	28.14	20.97	20.87	25.51	-16.38	-16.21	-16.42	-16.38	-16.40	-16.39	-16.41	-16.40	-16.39
263	16.96	22.06	27.90	19.51	17.02	27.63	19.43	20.27	24.69	-16.81	-16.43	-16.93	-16.83	-17.07	-16.51	-16.80	-16.57	-16.59
264	19.61	23.69	33.16	21.73	19.82	30.70	23.06	23.12	27.83	-15.97	-16.02	-15.97	-16.25	-16.29	-15.77	-15.88	-15.76	-15.83
265	17.76	21.01	29.71	19.93	18.43	27.50	20.20	20.21	24.62	-16.56	-16.70	-16.60	-16.72	-16.68	-16.55	-16.60	-16.59	-16.61
266	16.84	21.68	28.72	21.38	19.28	26.54	19.83	20.67	23.94	-16.85	-16.53	-16.78	-16.34	-16.44	-16.78	-16.70	-16.46	-16.78
267	16.87	18.93	29.55	19.33	17.86	27.09	19.79	20.92	24.29	-16.84	-17.23	-16.63	-16.87	-16.84	-16.65	-16.71	-16.39	-16.69
268	13.76	20.80	27.28	19.07	17.14	26.46	17.01	19.24	21.41	-17.82	-16.75	-17.04	-16.94	-17.04	-16.80	-17.42	-16.86	-17.39
269	15.64	19.89	27.09	19.22	18.53	24.52	18.69	19.42	21.16	-17.23	-16.98	-17.07	-16.90	-16.65	-17.27	-16.99	-16.81	-17.45
270	16.88	20.78	28.61	19.94	18.33	26.49	19.54	19.55	23.77	-16.84	-16.76	-16.80	-16.71	-16.71	-16.79	-16.77	-16.77	-16.82
271	16.88	20.78	28.61	19.94	18.33	26.49	19.54	19.55	23.77	-16.84	-16.76	-16.80	-16.71	-16.71	-16.79	-16.77	-16.77	-16.82
272	16.29	19.68	27.11	19.31	18.09	26.76	18.29	19.47	23.74	-17.02	-17.04	-17.07	-16.88	-16.77	-16.72	-17.09	-16.80	-16.82
273	15.84	21.50	27.31	18.57	18.18	24.90	18.50	18.74	22.04	-17.17	-16.57	-17.03	-17.07	-16.75	-17.17	-17.04	-17.01	-17.24
274	16.45	20.27	30.17	20.03	17.98	26.99	18.48	19.65	22.96	-16.97	-16.89	-16.51	-16.69	-16.80	-16.67	-17.04	-16.75	-17.01
275	15.24	13.64	26.64	18.48	16.52	25.08	18.25	18.92	22.42	-17.36	-18.58	-17.15	-17.09	-17.21	-17.13	-17.10	-16.95	-17.14
276	16.68	21.32	27.24	18.36	17.57	25.10	19.16	18.46	23.36	-16.90	-16.62	-17.05	-17.13	-16.92	-17.12	-16.87	-17.09	-16.92
277	13.84	18.85	25.45	17.43	15.42	22.99	16.57	17.96	21.23	-17.80	-17.25	-17.37	-17.37	-17.51	-17.63	-17.53	-17.23	-17.43

278	15.21	19.28	25.80	17.40	16.89	24.12	17.58	17.43	21.70	-17.37	-17.14	-17.31	-17.38	-17.11	-17.36	-17.27	-17.38	-17.32
279	14.94	18.09	23.12	17.66	16.18	23.73	17.52	17.78	20.71	-17.45	-17.44	-17.79	-17.31	-17.30	-17.46	-17.29	-17.28	-17.56
280	15.21	19.28	25.80	17.40	16.89	24.12	17.58	17.43	21.70	-17.37	-17.14	-17.31	-17.38	-17.11	-17.36	-17.27	-17.38	-17.32
281	15.67	17.82	25.12	17.97	15.21	24.35	16.79	18.20	19.67	-17.22	-17.51	-17.43	-17.23	-17.57	-17.31	-17.47	-17.16	-17.81
282	12.57	15.16	20.19	13.04	12.71	20.64	14.01	14.09	18.93	-18.20	-18.19	-18.32	-18.51	-18.26	-18.20	-18.18	-18.33	-17.99
283	14.99	16.72	23.84	17.09	14.85	25.05	16.18	17.88	20.63	-17.43	-17.80	-17.66	-17.46	-17.67	-17.14	-17.63	-17.25	-17.58
284	12.83	14.69	19.98	12.99	11.36	21.05	13.50	14.62	19.12	-18.12	-18.31	-18.36	-18.53	-18.63	-18.10	-18.31	-18.18	-17.95
285	12.20	13.12	20.23	12.68	11.15	20.03	13.44	13.58	18.51	-18.32	-18.71	-18.32	-18.61	-18.69	-18.35	-18.33	-18.47	-18.10
286	14.38	16.79	23.48	15.98	14.38	23.65	15.63	17.15	19.70	-17.63	-17.78	-17.73	-17.75	-17.80	-17.47	-17.77	-17.46	-17.81
287	13.21	17.61	22.44	15.73	14.25	21.57	15.24	16.01	18.32	-18.00	-17.57	-17.92	-17.81	-17.84	-17.98	-17.87	-17.78	-18.14
288	9.78	15.08	16.69	14.03	14.03	15.97	10.84	14.44	14.73	-19.08	-18.21	-18.96	-18.25	-17.90	-19.33	-18.99	-18.23	-19.01
289	12.52	15.53	20.18	13.00	13.16	19.43	13.59	14.58	15.11	-18.22	-18.10	-18.33	-18.52	-18.14	-18.49	-18.29	-18.19	-18.92
290	10.15	14.04	16.73	11.85	12.89	17.27	11.58	12.01	15.38	-18.96	-18.48	-18.95	-18.82	-18.21	-19.01	-18.80	-18.92	-18.86
291	9.78	12.13	16.69	11.64	12.87	15.97	10.84	11.33	14.73	-19.08	-18.97	-18.96	-18.88	-18.22	-19.33	-18.99	-19.11	-19.01
292	8.00	12.10	15.06	12.22	10.84	14.56	10.37	11.23	14.26	-19.64	-18.97	-19.25	-18.73	-18.78	-19.67	-19.11	-19.14	-19.13
293	11.56	13.35	18.30	12.20	10.72	19.00	12.07	13.50	15.57	-18.52	-18.65	-18.67	-18.73	-18.81	-18.60	-18.68	-18.50	-18.81
294	12.32	10.82	18.42	12.07	11.37	19.55	10.67	12.75	15.95	-18.28	-19.30	-18.64	-18.77	-18.63	-18.46	-19.03	-18.71	-18.72
295	7.60	12.44	13.45	10.02	10.85	13.90	7.95	10.78	13.61	-19.77	-18.89	-19.55	-19.30	-18.77	-19.83	-19.72	-19.27	-19.29
296	9.72	12.00	16.02	11.84	10.81	16.59	10.49	9.95	15.15	-19.10	-19.00	-19.08	-18.82	-18.79	-19.18	-19.08	-19.51	-18.91
297	10.00	12.23	16.83	12.44	11.73	16.95	11.48	11.41	13.41	-19.01	-18.94	-18.93	-18.67	-18.53	-19.09	-18.82	-19.09	-19.33
298	9.31	13.30	15.19	12.77	10.63	16.29	9.88	9.62	13.86	-19.23	-18.67	-19.23	-18.58	-18.84	-19.25	-19.23	-19.60	-19.22
299	9.37	12.27	13.36	9.12	6.44	9.72	8.14	9.84	14.22	-19.21	-18.93	-19.56	-19.53	-19.99	-20.83	-19.68	-19.54	-19.14
300	7.25	8.80	17.96	11.35	10.08	13.93	7.54	12.65	11.31	-19.88	-19.82	-18.73	-18.95	-18.99	-19.82	-19.83	-18.74	-19.84
301	7.41	10.71	12.39	8.95	9.75	13.23	7.77	10.68	11.69	-19.83	-19.33	-19.74	-19.58	-19.08	-19.99	-19.77	-19.30	-19.75
302	-3.39	-2.55	-5.10	-4.40	-3.61	-0.45	-5.52	-1.64	-2.88	-23.24	-22.71	-22.91	-23.06	-22.77	-23.29	-23.16	-22.80	-23.29

Table S3. Continued

No.	Defect									Applicability Domain								
	Split 1	Split 2	Split 3	Split 4	Split 5	Split 6	Split 7	Split 8	Split 9	Split 1	Split 2	Split 3	Split 4	Split 5	Split 6	Split 7	Split 8	Split 9
1	9.17	2.15	10.28	0.27	0.17	9.22	9.23	0.22	9.24	NO	NO	NO	YES	YES	NO	NO	YES	NO
2	0.11	6.12	5.18	0.14	0.09	3.13	0.14	7.16	9.13	YES	NO	YES	YES	YES	NO	YES	NO	NO
3	0.14	8.15	7.23	0.13	0.10	1.16	4.17	0.20	1.15	YES	NO	No	YES	YES	YES	YES	YES	YES
4	0.15	0.14	0.22	0.17	0.12	0.18	0.21	0.11	0.20	YES	YES	YES	YES	YES	YES	YES	YES	YES
5	0.12	0.09	0.17	0.11	0.09	0.14	0.14	0.09	0.15	YES	YES	YES	YES	YES	YES	YES	YES	YES
6	1.07	0.09	1.11	0.13	0.08	1.10	1.12	0.07	1.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
7	0.15	0.14	0.21	0.20	0.12	0.17	0.20	0.12	0.19	YES	YES	YES	YES	YES	YES	YES	YES	YES
8	0.08	0.09	0.12	0.13	0.08	0.10	0.12	0.06	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
9	0.08	0.09	0.19	0.08	0.07	0.10	0.13	0.09	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
10	0.08	1.09	0.12	0.13	0.08	0.10	0.13	1.06	0.12	YES	YES	YES	YES	YES	YES	YES	YES	YES
11	0.08	0.09	0.12	0.13	1.08	0.10	0.13	1.06	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
12	0.08	0.09	0.14	0.12	0.09	0.09	0.14	0.08	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
13	0.08	0.09	0.21	0.08	0.08	0.10	0.13	0.09	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
14	0.10	0.12	0.19	2.10	0.08	2.12	0.14	0.12	2.13	YES	YES	YES	No	YES	YES	YES	YES	YES
15	5.17	6.15	6.29	2.21	2.13	6.18	5.23	0.17	6.20	NO	NO	YES	NO	NO	NO	YES	YES	NO
16	0.13	0.14	0.27	0.16	0.12	0.14	0.22	0.12	0.17	YES	YES	YES	YES	YES	YES	YES	YES	YES

17	0.10	1.09	0.14	0.15	1.07	0.12	0.13	1.06	0.13	YES	YES	YES	YES	YES	YES	YES	YES	YES
18	14.15	4.16	15.25	0.31	0.21	14.21	14.19	0.27	14.21	No	No	No	YES	YES	No	No	YES	No
19	0.10	1.08	0.14	0.15	1.07	0.12	0.13	1.07	0.13	YES	YES	YES	YES	YES	YES	YES	YES	YES
20	8.16	1.17	10.25	5.22	0.17	9.18	9.23	0.19	9.19	NO	YES	NO	No	YES	NO	NO	YES	NO
21	0.06	0.06	0.09	0.09	0.06	0.08	0.09	0.04	0.09	YES	YES	YES	YES	YES	YES	YES	YES	YES
22	3.14	2.13	3.25	0.22	2.15	3.17	3.24	0.19	3.18	NO	NO	YES	YES	NO	NO	YES	YES	YES
23	0.12	0.09	0.15	0.13	0.07	0.13	0.15	0.06	0.13	YES	YES	YES	YES	YES	YES	YES	YES	YES
24	0.12	0.09	0.15	0.13	0.08	0.13	0.15	0.07	0.13	YES	YES	YES	YES	YES	YES	YES	YES	YES
25	0.06	0.06	0.12	0.08	0.07	0.07	0.10	0.06	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
26	0.12	0.09	0.15	0.13	0.08	0.13	0.15	0.07	0.13	YES	YES	YES	YES	YES	YES	YES	YES	YES
27	6.09	0.12	6.17	0.15	0.13	6.12	6.12	0.17	6.12	No	YES	YES	YES	YES	No	YES	YES	No
28	0.08	0.06	1.10	0.12	0.05	0.11	1.10	0.04	0.10	YES	YES	YES	YES	YES	YES	YES	YES	YES
29	1.06	0.06	1.08	0.09	0.05	1.07	1.08	0.03	1.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
30	0.07	0.06	0.07	1.09	1.05	0.07	0.08	0.03	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
31	0.07	0.06	0.08	0.09	0.05	0.07	0.08	0.03	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
32	0.08	1.07	0.13	0.12	2.09	1.11	0.13	0.10	1.11	YES	YES	YES	YES	NO	YES	YES	YES	YES
33	0.13	0.15	0.24	2.16	0.11	2.15	0.19	0.15	2.17	YES	YES	YES	NO	YES	YES	YES	YES	YES
34	0.09	0.06	0.10	0.12	0.05	0.10	0.10	0.04	0.10	YES	YES	YES	YES	YES	YES	YES	YES	YES
35	0.09	0.11	0.20	0.09	0.08	0.11	0.13	0.11	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
36	0.07	0.07	0.08	0.09	0.05	0.08	0.08	1.03	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
37	0.06	1.06	0.09	0.09	0.06	0.08	0.09	1.04	0.09	YES	YES	YES	YES	YES	YES	YES	YES	YES
38	0.07	0.06	0.07	0.09	0.05	0.07	0.08	1.03	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
39	6.20	5.17	7.32	0.29	3.17	6.23	6.25	3.24	6.25	NO	NO	NO	YES	NO	NO	YES	NO	NO
40	0.11	0.14	0.20	2.11	0.09	2.14	0.15	0.14	2.14	YES	YES	YES	No	YES	YES	YES	YES	YES
41	0.11	0.09	0.13	0.13	0.07	0.12	0.12	0.06	0.12	YES	YES	YES	YES	YES	YES	YES	YES	YES
42	0.13	0.11	0.25	0.10	0.10	0.15	0.17	0.12	0.16	YES	YES	YES	YES	YES	YES	YES	YES	YES
43	3.11	2.08	6.12	0.11	0.09	3.12	6.11	0.09	3.12	NO	NO	YES	YES	YES	NO	YES	YES	YES
44	6.20	3.18	8.28	0.22	0.15	6.24	8.22	0.20	6.23	NO	NO	NO	YES	YES	NO	NO	YES	NO
45	5.12	1.12	5.17	0.19	1.11	5.16	5.16	1.11	4.17	NO	YES	YES	YES	YES	NO	YES	YES	NO
46	0.10	0.08	1.14	0.13	0.06	0.12	1.12	0.06	0.12	YES	YES	YES	YES	YES	YES	YES	YES	YES

47	0.06	0.06	0.08	0.09	0.05	0.08	0.08	0.03	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
48	0.07	0.06	0.09	0.09	0.05	0.08	0.08	1.03	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
49	0.06	0.06	0.08	0.09	0.05	0.08	0.08	0.03	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
50	0.07	0.06	0.09	0.09	0.05	0.08	0.08	1.03	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
51	0.06	0.06	0.08	0.09	0.05	0.07	0.08	1.03	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
52	0.15	0.12	0.20	0.15	0.09	0.15	0.17	0.10	0.16	YES	YES	YES	YES	YES	YES	YES	YES	YES
53	0.06	0.06	0.08	0.09	0.05	0.08	0.08	0.03	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
54	0.11	0.09	0.14	0.12	0.07	0.11	0.13	0.07	0.12	YES	YES	YES	YES	YES	YES	YES	YES	YES
55	0.19	0.16	1.27	0.18	0.11	0.20	1.21	0.14	0.21	YES	YES	YES	YES	YES	YES	YES	YES	YES
56	0.07	0.06	0.07	1.09	1.05	0.08	0.09	0.04	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
57	0.07	1.06	1.07	1.09	0.05	0.08	0.09	0.03	1.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
58	0.07	0.06	0.07	1.09	1.05	0.08	0.09	0.04	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
59	0.07	1.06	1.07	1.09	0.05	0.08	0.09	0.03	1.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
60	0.09	0.11	0.20	0.09	0.08	0.11	0.13	0.11	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
61	0.15	0.13	0.20	0.15	0.10	0.14	0.17	0.11	0.16	YES	YES	YES	YES	YES	YES	YES	YES	YES
62	0.07	1.06	0.07	0.09	0.05	0.07	0.08	0.03	1.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
63	0.11	0.09	0.16	0.11	0.07	0.13	0.12	0.07	0.14	YES	YES	YES	YES	YES	YES	YES	YES	YES
64	0.07	0.06	0.08	1.09	1.05	0.08	0.09	0.04	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
65	0.07	1.06	1.08	1.09	0.05	0.08	0.09	0.03	1.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
66	4.12	0.13	5.21	0.15	0.12	5.16	4.14	0.19	5.15	NO	YES	YES	YES	YES	NO	YES	YES	NO
67	0.14	1.11	0.16	0.16	1.07	0.15	0.15	1.07	0.16	YES	YES	YES	YES	YES	YES	YES	YES	YES
68	0.09	0.10	0.12	0.11	0.07	0.11	0.12	0.06	0.12	YES	YES	YES	YES	YES	YES	YES	YES	YES
69	0.12	0.09	0.18	0.08	0.08	0.13	0.16	0.09	0.14	YES	YES	YES	YES	YES	YES	YES	YES	YES
70	0.07	1.06	0.08	0.09	0.05	0.08	0.09	1.03	0.09	YES	YES	YES	YES	YES	YES	YES	YES	YES
71	0.07	1.06	0.08	0.09	0.05	0.08	0.09	1.03	0.09	YES	YES	YES	YES	YES	YES	YES	YES	YES
72	0.16	0.11	0.21	0.12	0.09	0.17	0.18	0.09	0.18	YES	YES	YES	YES	YES	YES	YES	YES	YES
73	0.06	0.06	0.08	1.09	1.05	0.07	0.08	1.03	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
74	0.06	0.06	0.08	0.09	1.05	0.07	0.08	0.03	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
75	0.07	1.06	0.09	0.09	0.05	0.08	0.09	1.03	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
76	0.08	0.07	0.12	0.10	0.07	0.10	0.12	0.06	0.09	YES	YES	YES	YES	YES	YES	YES	YES	YES

77	5.14	0.12	6.18	1.19	0.10	5.19	6.16	1.11	5.18	No	YES	YES	YES	YES	No	YES	YES	No
78	0.17	3.14	0.32	1.16	1.09	0.17	0.24	3.11	0.20	YES	No	YES	YES	YES	YES	YES	NO	YES
79	1.03	1.04	1.05	0.04	1.05	1.04	1.05	0.02	1.04	YES	YES	YES	YES	YES	YES	YES	YES	YES
80	0.16	3.12	0.31	1.16	1.08	0.17	0.23	3.10	0.20	YES	NO	YES	YES	YES	YES	YES	NO	YES
81	23.18	8.16	28.28	0.31	0.20	24.21	24.22	2.27	24.22	No	NO	No	YES	YES	No	No	No	No
82	5.14	0.12	6.18	1.19	0.10	5.19	6.16	1.11	5.18	NO	YES	YES	YES	YES	NO	YES	YES	NO
83	2.22	2.14	10.23	1.17	2.11	2.20	10.21	2.10	2.23	YES	NO	NO	YES	NO	YES	NO	YES	YES
84	1.05	0.06	1.07	0.07	0.05	1.07	1.06	0.03	1.07	YES	YES	YES	YES	YES	YES	YES	YES	YES
85	1.13	1.09	2.17	0.10	0.07	1.13	2.15	0.06	1.14	YES	YES	YES	YES	YES	YES	YES	YES	YES
86	1.10	0.10	1.16	0.15	0.08	1.11	1.15	0.09	1.13	YES	YES	YES	YES	YES	YES	YES	YES	YES
87	8.20	0.13	12.22	3.22	0.14	8.21	12.21	0.13	8.21	NO	YES	NO	NO	YES	NO	NO	YES	NO
88	0.13	0.09	0.18	0.15	0.13	0.14	0.18	0.17	0.13	YES	YES	YES	YES	YES	YES	YES	YES	YES
89	2.21	2.14	10.23	1.17	2.11	2.20	10.20	2.10	2.22	YES	No	No	YES	NO	YES	No	YES	YES
90	23.18	8.16	28.28	0.31	0.20	24.21	24.22	2.27	24.22	NO	NO	NO	YES	YES	NO	NO	NO	NO
91	2.15	1.09	3.20	1.13	0.12	2.16	3.17	0.12	2.17	YES	YES	YES	YES	YES	YES	YES	YES	YES
92	0.09	0.08	0.13	0.12	0.07	0.10	0.12	0.07	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
93	0.11	0.11	0.17	0.10	0.08	0.13	0.14	0.09	0.13	YES	YES	YES	YES	YES	YES	YES	YES	YES
94	0.08	0.08	0.14	0.11	0.07	0.10	0.13	0.07	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
95	2.11	1.07	3.15	1.11	0.10	2.11	3.14	0.09	2.12	YES	YES	YES	YES	YES	YES	YES	YES	YES
96	0.09	1.07	0.12	0.11	3.07	0.11	0.10	1.09	0.11	YES	YES	YES	YES	NO	YES	YES	YES	YES
97	0.06	0.07	0.08	0.10	0.06	0.08	0.09	0.04	0.09	YES	YES	YES	YES	YES	YES	YES	YES	YES
98	1.15	4.10	16.14	3.12	7.11	1.15	15.13	5.12	2.16	YES	NO	NO	NO	NO	YES	NO	NO	YES
99	0.04	0.06	0.07	0.08	0.06	0.05	0.08	0.04	0.06	YES	YES	YES	YES	YES	YES	YES	YES	YES
100	3.18	8.11	16.21	4.15	8.12	3.18	15.18	9.13	3.19	NO	NO	NO	NO	NO	NO	NO	NO	YES
101	0.12	0.11	0.17	0.17	0.11	0.13	0.18	0.09	0.15	YES	YES	YES	YES	YES	YES	YES	YES	YES
102	0.09	0.08	0.12	0.11	0.07	0.10	0.11	0.07	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
103	0.04	0.05	0.06	0.04	0.05	0.05	0.05	1.02	0.04	YES	YES	YES	YES	YES	YES	YES	YES	YES
104	0.05	0.05	0.07	0.07	0.05	0.07	0.06	1.03	0.07	YES	YES	YES	YES	YES	YES	YES	YES	YES
105	0.12	0.09	0.17	0.14	0.08	0.13	0.14	0.07	0.14	YES	YES	YES	YES	YES	YES	YES	YES	YES
106	0.04	0.06	0.08	0.08	0.06	0.05	0.08	0.04	0.06	YES	YES	YES	YES	YES	YES	YES	YES	YES

107	0.11	0.09	0.15	0.10	0.08	0.11	0.15	0.07	0.12	YES	YES	YES	YES	YES	YES	YES	YES	YES
108	0.03	0.05	0.07	0.04	0.05	0.04	0.06	0.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
109	0.14	0.13	0.20	0.12	0.10	0.15	0.16	0.10	0.16	YES	YES	YES	YES	YES	YES	YES	YES	YES
110	0.09	0.08	0.12	0.11	0.07	0.10	0.11	0.07	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
111	0.11	0.08	0.17	0.13	0.08	0.13	0.15	0.08	0.14	YES	YES	YES	YES	YES	YES	YES	YES	YES
112	0.03	0.04	0.05	0.04	0.05	0.04	0.05	0.02	0.04	YES	YES	YES	YES	YES	YES	YES	YES	YES
113	0.03	0.04	0.05	0.04	0.05	0.04	0.05	0.02	0.04	YES	YES	YES	YES	YES	YES	YES	YES	YES
114	2.06	3.09	5.08	11.11	3.08	2.09	5.09	0.08	2.10	YES	NO	YES	NO	NO	YES	YES	YES	YES
115	0.05	0.05	0.08	0.07	0.05	0.07	0.07	0.03	0.07	YES	YES	YES	YES	YES	YES	YES	YES	YES
116	0.04	0.06	0.07	0.08	0.06	0.05	0.08	0.04	0.06	YES	YES	YES	YES	YES	YES	YES	YES	YES
117	0.09	0.09	0.14	0.09	0.08	0.11	0.12	0.07	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
118	0.09	0.09	0.15	0.09	0.08	0.11	0.12	0.07	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
119	0.08	0.07	0.15	0.09	0.05	0.09	0.12	0.05	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
120	0.09	0.08	0.14	0.09	0.07	0.11	0.11	0.07	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
121	0.07	0.07	0.12	0.08	0.06	0.09	0.10	0.05	0.09	YES	YES	YES	YES	YES	YES	YES	YES	YES
122	4.09	0.08	4.15	0.15	0.11	4.12	4.12	0.11	4.13	NO	YES	YES	YES	YES	NO	YES	YES	NO
123	0.03	0.04	0.05	0.04	0.05	0.04	0.05	0.02	0.04	YES	YES	YES	YES	YES	YES	YES	YES	YES
124	0.06	0.05	0.07	0.07	0.05	0.07	0.07	0.03	0.07	YES	YES	YES	YES	YES	YES	YES	YES	YES
125	0.12	0.09	0.22	0.13	0.08	0.14	0.18	0.08	0.16	YES	YES	YES	YES	YES	YES	YES	YES	YES
126	8.11	2.08	10.16	5.15	0.11	9.13	9.15	0.12	9.14	NO	No	NO	NO	YES	NO	NO	YES	NO
127	0.11	0.08	0.16	0.09	0.08	0.13	0.13	0.08	0.13	YES	YES	YES	YES	YES	YES	YES	YES	YES
128	0.06	0.07	4.07	0.09	0.07	0.08	4.07	5.05	0.09	YES	YES	YES	YES	YES	YES	YES	NO	YES
129	0.13	0.11	0.20	0.11	0.09	0.15	0.15	0.10	0.16	YES	YES	YES	YES	YES	YES	YES	YES	YES
130	1.04	1.03	1.06	0.05	1.03	1.04	1.06	0.03	1.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
131	6.20	0.12	12.23	0.24	0.13	7.20	12.21	1.17	7.21	No	YES	NO	YES	YES	No	No	YES	No
132	6.16	3.17	10.27	0.19	0.14	7.17	8.19	0.25	7.18	NO	NO	NO	YES	YES	NO	NO	YES	NO
133	0.05	0.05	1.07	1.07	1.05	0.07	0.06	1.03	0.07	YES	YES	YES	YES	YES	YES	YES	YES	YES
134	0.05	0.04	0.08	0.05	0.05	0.06	0.07	0.03	0.06	YES	YES	YES	YES	YES	YES	YES	YES	YES
135	4.11	0.08	4.17	0.16	0.12	4.14	4.14	0.12	4.15	NO	YES	YES	YES	YES	NO	YES	YES	NO
136	0.10	0.08	0.13	0.11	0.07	0.11	1.11	1.07	0.12	YES	YES	YES	YES	YES	YES	YES	YES	YES

137	1.08	1.07	2.11	0.07	0.06	1.09	2.09	0.05	1.09	YES	YES	YES	YES	YES	YES	YES	YES	YES
138	2.16	0.11	4.18	0.14	0.08	2.18	4.17	0.11	2.17	YES	YES	YES	YES	YES	YES	YES	YES	YES
139	6.16	0.11	11.17	0.16	0.11	6.16	11.14	0.12	6.16	NO	YES	NO	YES	YES	NO	NO	YES	NO
140	0.13	0.12	0.20	1.14	1.10	0.17	0.17	2.07	0.19	YES	YES	YES	YES	YES	YES	YES	YES	YES
141	0.04	0.04	0.06	0.04	0.05	0.04	1.05	1.02	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
142	0.05	0.06	0.07	0.08	0.06	0.05	1.08	1.04	0.06	YES	YES	YES	YES	YES	YES	YES	YES	YES
143	0.10	1.07	1.16	0.11	2.08	0.11	1.15	0.10	0.12	YES	YES	YES	YES	NO	YES	YES	YES	YES
144	0.10	0.09	0.20	0.11	0.07	0.11	0.15	0.07	0.13	YES	YES	YES	YES	YES	YES	YES	YES	YES
145	0.06	0.05	0.07	0.07	0.05	0.07	1.06	1.03	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
146	2.11	0.10	4.11	0.11	0.07	2.12	4.12	0.09	2.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
147	0.13	0.12	0.20	1.14	1.10	0.18	0.17	2.06	0.19	YES	YES	YES	YES	YES	YES	YES	YES	YES
148	5.21	2.13	11.22	0.23	0.11	6.19	11.21	2.15	6.19	NO	NO	NO	YES	YES	NO	NO	NO	NO
149	0.04	0.04	0.06	1.05	1.03	0.04	0.06	0.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
150	0.04	0.06	0.07	0.08	1.06	0.05	0.08	1.04	0.06	YES	YES	YES	YES	YES	YES	YES	YES	YES
151	0.13	0.10	0.20	0.14	0.08	0.17	0.17	3.05	0.20	YES	YES	YES	YES	YES	YES	YES	No	YES
152	0.18	0.13	0.33	0.20	0.09	0.19	0.25	0.12	0.22	YES	YES	YES	YES	YES	YES	YES	YES	YES
153	0.05	0.05	0.07	0.07	1.05	0.07	0.07	1.03	0.07	YES	YES	YES	YES	YES	YES	YES	YES	YES
154	7.14	5.11	13.13	0.14	3.09	7.14	13.12	3.11	7.14	NO	NO	NO	YES	NO	NO	NO	NO	NO
155	5.06	5.06	9.06	1.07	5.06	5.07	9.05	5.04	5.08	NO	NO	NO	YES	NO	NO	NO	NO	NO
156	0.13	0.12	0.20	0.14	0.08	0.18	0.18	2.07	0.19	YES	YES	YES	YES	YES	YES	YES	YES	YES
157	1.12	0.09	7.13	0.12	0.09	1.12	7.10	0.10	2.13	YES	YES	NO	YES	YES	YES	NO	YES	YES
158	0.04	0.04	0.06	0.05	0.03	0.05	0.06	1.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
159	0.04	0.04	0.06	0.05	0.04	0.04	0.06	0.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
160	5.29	1.19	15.28	1.23	2.12	5.28	15.27	0.16	5.29	NO	YES	NO	YES	NO	NO	NO	YES	NO
161	0.03	1.04	0.05	0.04	0.05	0.04	0.05	0.02	1.04	YES	YES	YES	YES	YES	YES	YES	YES	YES
162	0.07	2.08	0.13	1.09	0.09	0.10	0.11	0.06	0.11	YES	NO	YES	YES	YES	YES	YES	YES	YES
163	0.19	0.12	5.25	0.20	0.12	0.20	5.23	0.19	0.19	YES	YES	YES	YES	YES	YES	YES	YES	YES
164	0.05	1.06	0.07	0.08	0.06	0.05	0.09	1.04	0.07	YES	YES	YES	YES	YES	YES	YES	YES	YES
165	0.04	0.03	0.06	0.05	0.03	0.04	0.06	0.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
166	0.06	1.05	0.08	0.07	0.05	0.07	0.07	1.03	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES

167	0.04	0.03	0.06	0.05	0.03	0.04	0.06	0.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
168	0.04	1.03	0.06	0.05	1.03	0.04	0.06	0.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
169	0.07	1.08	0.10	0.09	0.09	0.10	0.11	0.05	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
170	0.06	0.03	0.09	0.05	0.04	0.06	0.08	0.03	0.07	YES	YES	YES	YES	YES	YES	YES	YES	YES
171	0.06	0.03	0.09	0.05	0.04	0.06	0.08	0.03	0.07	YES	YES	YES	YES	YES	YES	YES	YES	YES
172	0.06	0.03	0.09	0.05	0.04	0.06	0.08	0.03	0.07	YES	YES	YES	YES	YES	YES	YES	YES	YES
173	0.06	0.03	0.09	0.05	0.04	0.06	0.08	0.03	0.07	YES	YES	YES	YES	YES	YES	YES	YES	YES
174	0.04	0.03	0.06	0.05	0.03	0.04	0.06	0.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
175	0.14	0.09	4.18	0.19	0.11	0.14	4.17	0.17	0.15	YES	YES	YES	YES	YES	YES	YES	YES	YES
176	0.17	0.10	4.18	0.17	2.09	0.18	4.16	0.13	0.18	YES	YES	YES	YES	No	YES	YES	YES	YES
177	0.06	0.03	0.09	0.05	0.04	0.06	0.08	0.03	0.07	YES	YES	YES	YES	YES	YES	YES	YES	YES
178	0.14	0.09	4.18	0.17	0.10	0.15	4.18	0.16	0.14	YES	YES	YES	YES	YES	YES	YES	YES	YES
179	0.14	0.09	4.18	0.17	0.10	0.15	4.18	0.16	0.14	YES	YES	YES	YES	YES	YES	YES	YES	YES
180	0.07	1.05	0.06	0.06	0.03	0.06	0.06	0.07	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
181	0.15	0.08	1.17	0.15	0.10	0.22	1.16	1.05	0.25	YES	YES	YES	YES	YES	YES	YES	YES	YES
182	0.08	1.07	1.13	0.09	1.09	0.12	1.14	0.05	0.14	YES	YES	YES	YES	YES	YES	YES	YES	YES
183	0.18	3.11	0.24	0.17	0.12	0.27	0.22	1.09	0.28	YES	NO	YES	YES	YES	YES	YES	YES	YES
184	0.04	0.03	0.06	1.05	1.03	0.04	0.06	0.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
185	1.14	0.10	1.15	0.12	0.10	1.19	1.15	0.04	1.24	YES	YES	YES	YES	YES	YES	YES	YES	YES
186	1.15	0.10	1.16	0.12	0.10	1.20	1.15	0.04	1.24	YES	YES	YES	YES	YES	YES	YES	YES	YES
187	0.04	0.03	0.06	0.05	0.03	0.05	1.06	1.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
188	0.17	1.11	0.23	0.17	5.11	0.23	0.20	2.08	0.26	YES	YES	YES	YES	NO	YES	YES	YES	YES
189	0.18	4.11	0.25	1.17	1.12	0.26	0.23	0.09	0.27	YES	NO	YES	YES	YES	YES	YES	YES	YES
190	0.15	0.10	0.16	0.12	0.09	0.20	0.15	0.04	0.24	YES	YES	YES	YES	YES	YES	YES	YES	YES
191	0.19	1.14	15.22	5.17	10.12	0.20	15.19	8.14	1.22	YES	YES	NO	No	No	YES	NO	NO	YES
192	0.16	0.11	3.18	2.13	0.11	0.22	2.17	2.06	0.22	YES	YES	YES	No	YES	YES	YES	YES	YES
193	1.14	1.08	6.16	0.14	0.09	1.14	6.15	0.15	1.13	YES	YES	YES	YES	YES	YES	YES	YES	YES
194	1.14	1.08	7.14	0.11	2.07	1.14	7.13	0.10	1.14	YES	YES	NO	YES	NO	YES	NO	YES	YES
195	0.18	1.13	9.23	0.22	3.16	1.19	9.21	3.19	1.21	YES	YES	NO	YES	NO	YES	NO	NO	YES
196	0.08	0.08	1.08	1.07	0.09	0.10	1.07	1.04	0.10	YES	YES	YES	YES	YES	YES	YES	YES	YES

197	0.06	0.04	0.09	0.06	1.03	0.06	0.07	0.03	0.06	YES	YES	YES	YES	YES	YES	YES	YES	YES
198	4.12	2.07	9.11	0.14	4.08	4.13	9.11	0.10	4.14	NO	NO	NO	YES	NO	NO	NO	YES	NO
199	0.13	0.09	19.12	0.17	0.16	0.15	19.12	0.14	0.13	YES	YES	No	YES	YES	YES	No	YES	YES
200	6.25	7.15	16.26	6.19	0.11	7.25	15.23	0.13	8.26	NO	NO	NO	NO	YES	NO	NO	YES	NO
201	0.13	0.09	24.12	0.18	2.15	0.14	24.12	0.18	0.12	YES	YES	NO	YES	No	YES	NO	YES	YES
202	2.08	0.06	2.05	3.08	0.03	2.07	2.06	5.09	2.08	YES	YES	YES	NO	YES	YES	YES	No	YES
203	0.08	1.07	0.13	0.10	0.09	0.12	0.14	1.05	0.14	YES	YES	YES	YES	YES	YES	YES	YES	YES
204	0.15	0.10	0.16	0.11	0.10	0.20	0.16	0.04	0.24	YES	YES	YES	YES	YES	YES	YES	YES	YES
205	0.14	0.10	19.12	0.16	0.16	0.16	19.12	1.14	0.13	YES	YES	NO	YES	YES	YES	NO	YES	YES
206	0.18	4.11	0.24	1.17	0.12	0.27	0.22	0.10	0.28	YES	NO	YES	YES	YES	YES	YES	YES	YES
207	0.16	0.08	2.17	1.15	0.09	0.22	2.16	0.05	0.25	YES	YES	YES	YES	YES	YES	YES	YES	YES
208	1.16	0.11	3.18	2.13	0.11	1.23	3.16	2.06	1.23	YES	YES	YES	NO	YES	YES	YES	YES	YES
209	0.07	1.05	0.06	0.06	0.03	0.07	1.06	1.07	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
210	0.06	0.04	0.09	0.06	1.03	0.06	0.07	0.03	0.06	YES	YES	YES	YES	YES	YES	YES	YES	YES
211	0.08	1.08	0.13	0.09	0.07	0.12	0.14	0.06	0.14	YES	YES	YES	YES	YES	YES	YES	YES	YES
212	12.09	0.05	25.09	0.10	5.07	12.08	25.08	6.10	12.08	NO	YES	NO	YES	NO	NO	NO	No	NO
213	1.16	1.11	3.18	3.13	0.11	1.23	3.16	2.06	1.23	YES	YES	YES	NO	YES	YES	YES	YES	YES
214	0.15	0.10	0.17	0.12	0.10	0.20	0.15	0.05	0.24	YES	YES	YES	YES	YES	YES	YES	YES	YES
215	0.18	3.11	1.25	0.16	0.12	0.26	0.23	0.09	0.27	YES	NO	YES	YES	YES	YES	YES	YES	YES
216	1.14	0.09	2.15	0.12	0.10	1.19	2.14	0.04	1.23	YES	YES	YES	YES	YES	YES	YES	YES	YES
217	0.04	1.03	0.07	0.05	0.04	0.05	0.06	1.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
218	0.04	0.03	0.06	0.05	0.03	0.04	0.06	0.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
219	0.04	0.03	1.06	0.05	0.03	0.04	1.06	0.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
220	1.18	3.12	1.24	0.17	0.12	1.27	1.22	0.09	1.28	YES	NO	YES	YES	YES	YES	YES	YES	YES
221	2.26	0.14	11.29	0.20	1.15	2.30	11.24	1.14	2.33	YES	YES	NO	YES	YES	YES	NO	YES	YES
222	0.14	0.09	1.15	0.12	0.10	0.20	1.14	0.05	0.24	YES	YES	YES	YES	YES	YES	YES	YES	YES
223	0.11	1.06	5.13	0.13	2.08	0.11	5.14	1.15	0.11	YES	YES	YES	YES	No	YES	YES	YES	YES
224	0.13	0.09	23.13	0.18	1.16	0.14	23.13	0.18	0.12	YES	YES	NO	YES	YES	YES	NO	YES	YES
225	0.16	0.11	3.18	2.13	1.11	0.23	3.16	2.06	0.23	YES	YES	YES	No	YES	YES	YES	YES	YES
226	0.14	0.09	1.15	0.12	0.10	0.20	1.14	0.04	0.24	YES	YES	YES	YES	YES	YES	YES	YES	YES

227	15.11	0.09	18.05	7.10	2.02	15.08	19.04	18.09	15.10	NO	YES	NO	NO	No	NO	NO	NO	NO
228	0.04	0.03	1.06	0.05	0.03	0.04	0.06	0.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
229	0.14	0.09	1.16	0.12	0.11	0.20	1.15	0.05	0.24	YES	YES	YES	YES	YES	YES	YES	YES	YES
230	1.18	4.11	1.24	1.17	0.12	1.27	1.22	0.09	1.28	YES	NO	YES	YES	YES	YES	YES	YES	YES
231	0.13	0.09	23.13	0.18	1.15	0.14	23.12	0.18	0.12	YES	YES	NO	YES	YES	YES	NO	YES	YES
232	0.04	1.03	0.06	0.05	0.03	0.04	0.06	1.03	1.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
233	0.14	0.09	1.15	0.12	0.10	0.20	1.14	1.04	0.24	YES	YES	YES	YES	YES	YES	YES	YES	YES
234	0.04	0.03	0.06	0.05	1.03	0.04	0.06	0.03	1.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
235	1.04	0.03	1.06	0.05	0.03	1.04	1.06	1.03	1.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
236	0.10	2.08	0.15	0.09	0.09	0.15	0.15	0.06	0.17	YES	NO	YES	YES	YES	YES	YES	YES	YES
237	5.13	1.07	13.13	2.16	3.11	5.13	13.12	2.16	5.12	NO	YES	NO	NO	NO	NO	NO	NO	NO
238	4.11	0.08	6.14	0.16	0.09	4.13	6.12	0.11	5.14	No	YES	YES	YES	YES	No	YES	YES	No
239	0.06	0.04	2.08	0.07	0.03	0.07	2.06	0.04	1.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
240	0.11	0.08	2.15	0.10	0.05	0.12	2.11	0.07	1.13	YES	YES	YES	YES	YES	YES	YES	YES	YES
241	16.06	0.06	18.05	0.07	0.03	16.06	18.05	16.04	16.07	No	YES	NO	YES	YES	No	No	NO	No
242	23.06	0.07	23.04	0.07	0.02	23.06	25.04	23.04	23.07	NO	YES	NO	YES	YES	NO	NO	NO	NO
243	2.16	4.14	4.22	0.22	0.15	2.21	3.21	0.15	2.22	YES	NO	YES	YES	YES	YES	YES	YES	YES
244	0.15	0.14	0.21	0.20	0.12	0.17	0.20	0.12	0.19	YES	YES	YES	YES	YES	YES	YES	YES	YES
245	1.06	0.07	1.09	0.09	0.06	1.08	1.09	0.04	1.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
246	0.09	0.09	0.19	0.07	0.07	0.10	1.13	1.09	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
247	1.07	0.07	1.07	0.09	0.05	1.07	1.08	0.03	1.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
248	1.16	0.13	4.22	0.19	0.13	1.18	4.20	0.14	1.19	YES	YES	YES	YES	YES	YES	YES	YES	YES
249	0.07	0.06	0.09	0.09	0.05	0.08	0.09	0.03	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
250	0.06	0.07	0.09	0.09	1.06	0.08	0.09	1.04	0.09	YES	YES	YES	YES	YES	YES	YES	YES	YES
251	0.06	0.06	0.08	1.09	1.05	0.07	0.08	0.03	0.08	YES	YES	YES	YES	YES	YES	YES	YES	YES
252	0.09	0.11	0.21	0.09	0.08	0.11	0.14	0.11	0.12	YES	YES	YES	YES	YES	YES	YES	YES	YES
253	0.10	0.08	1.14	0.13	0.06	0.12	1.12	0.06	0.12	YES	YES	YES	YES	YES	YES	YES	YES	YES
254	5.12	1.10	5.17	0.19	1.10	5.17	5.15	1.08	4.18	NO	YES	YES	YES	YES	NO	YES	YES	NO
255	0.19	0.16	0.27	0.18	0.12	0.19	0.22	0.14	0.21	YES	YES	YES	YES	YES	YES	YES	YES	YES
256	0.10	0.11	0.20	0.09	0.08	0.11	1.13	1.10	0.12	YES	YES	YES	YES	YES	YES	YES	YES	YES

257	0.06	0.06	0.09	0.08	0.06	0.07	0.09	0.04	0.07	YES	YES	YES	YES	YES	YES	YES	YES	YES
258	0.14	0.12	1.21	0.15	0.09	0.15	1.17	0.10	0.16	YES	YES	YES	YES	YES	YES	YES	YES	YES
259	0.14	7.18	6.26	0.14	0.11	0.17	4.18	0.22	0.17	YES	NO	YES	YES	YES	YES	YES	YES	YES
260	1.15	1.09	5.18	0.21	1.12	2.16	5.19	0.17	2.16	YES	YES	YES	YES	YES	YES	YES	YES	YES
261	5.14	0.12	6.18	1.19	0.10	5.19	6.16	1.11	5.18	No	YES	YES	YES	YES	No	YES	YES	No
262	5.14	0.12	6.18	1.19	0.10	5.19	6.16	1.11	5.18	NO	YES	YES	YES	YES	NO	YES	YES	NO
263	1.04	0.07	1.06	0.08	0.06	1.05	1.08	0.04	1.06	YES	YES	YES	YES	YES	YES	YES	YES	YES
264	0.09	0.08	0.12	0.10	0.07	0.09	0.12	0.06	0.10	YES	YES	YES	YES	YES	YES	YES	YES	YES
265	8.20	0.13	12.22	3.22	0.14	8.21	12.21	0.13	8.21	No	YES	No	NO	YES	No	No	YES	No
266	0.03	0.05	0.05	1.04	1.05	0.04	0.05	0.03	0.04	YES	YES	YES	YES	YES	YES	YES	YES	YES
267	0.09	0.08	0.14	0.07	0.06	0.10	0.12	0.06	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
268	0.10	1.06	2.11	0.10	0.08	0.11	2.11	0.08	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
269	0.09	0.07	0.11	0.12	0.06	0.12	0.10	0.05	0.12	YES	YES	YES	YES	YES	YES	YES	YES	YES
270	0.05	0.05	0.07	0.07	0.05	0.07	0.07	0.03	0.07	YES	YES	YES	YES	YES	YES	YES	YES	YES
271	0.05	0.05	0.07	0.07	0.05	0.07	0.07	0.03	0.07	YES	YES	YES	YES	YES	YES	YES	YES	YES
272	0.04	0.06	0.07	0.08	0.06	0.05	0.08	0.04	0.06	YES	YES	YES	YES	YES	YES	YES	YES	YES
273	2.15	5.15	6.27	3.17	1.12	3.17	4.19	5.18	5.17	YES	NO	YES	NO	YES	NO	YES	NO	NO
274	0.13	0.09	0.21	0.14	0.07	0.14	0.17	0.08	0.16	YES	YES	YES	YES	YES	YES	YES	YES	YES
275	0.19	0.17	0.27	0.16	0.12	0.19	0.21	0.14	0.20	YES	YES	YES	YES	YES	YES	YES	YES	YES
276	1.09	1.07	2.11	0.07	0.06	1.09	2.10	0.05	1.10	YES	YES	YES	YES	YES	YES	YES	YES	YES
277	0.09	0.08	1.12	1.11	1.07	0.10	0.11	1.07	0.11	YES	YES	YES	YES	YES	YES	YES	YES	YES
278	4.09	0.08	4.12	0.13	0.09	4.13	4.11	0.07	4.13	NO	YES	YES	YES	YES	NO	YES	YES	NO
279	0.03	0.04	0.05	1.04	1.05	0.04	0.06	0.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
280	4.09	0.08	4.12	0.13	0.09	4.13	4.11	0.07	4.13	No	YES	YES	YES	YES	No	YES	YES	No
281	0.13	0.12	0.21	0.14	0.08	0.18	0.17	3.06	0.19	YES	YES	YES	YES	YES	YES	YES	No	YES
282	0.04	0.04	0.06	0.05	0.04	0.04	0.06	0.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
283	0.14	0.11	0.22	0.14	0.10	0.19	0.18	2.07	0.21	YES	YES	YES	YES	YES	YES	YES	YES	YES
284	0.04	0.04	0.07	0.05	0.04	0.04	0.06	0.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
285	0.04	0.03	0.06	0.05	0.03	0.04	0.06	0.03	0.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
286	0.13	0.12	3.17	0.14	0.10	0.16	3.15	0.14	0.16	YES	YES	YES	YES	YES	YES	YES	YES	YES

287	6.17	0.11	12.17	0.21	0.10	7.16	12.17	1.14	7.16	NO	YES	NO	YES	YES	NO	NO	YES	NO
288	0.14	1.10	0.15	1.12	0.10	0.19	0.15	0.04	0.24	YES	YES	YES	YES	YES	YES	YES	YES	YES
289	0.19	0.14	15.23	5.16	10.12	0.21	15.20	8.16	0.23	YES	YES	NO	NO	No	YES	NO	No	YES
290	0.08	1.08	0.13	0.10	0.09	0.12	0.14	0.06	0.14	YES	YES	YES	YES	YES	YES	YES	YES	YES
291	0.14	0.10	0.15	0.12	0.09	0.19	0.15	0.04	0.24	YES	YES	YES	YES	YES	YES	YES	YES	YES
292	0.13	0.09	19.12	0.17	0.16	0.15	19.12	0.14	0.13	YES	YES	No	YES	YES	YES	No	YES	YES
293	0.19	1.14	15.22	5.17	10.12	0.20	15.19	8.14	1.22	YES	YES	NO	NO	NO	YES	NO	No	YES
294	0.09	0.07	0.15	4.10	0.05	0.10	0.12	7.06	7.11	YES	YES	YES	NO	YES	YES	YES	NO	NO
295	15.10	0.09	18.05	7.10	2.02	15.08	18.04	17.09	15.10	No	YES	No	NO	NO	No	No	NO	NO
296	0.13	0.09	19.12	0.17	0.16	0.15	19.12	0.14	0.13	YES	YES	NO	YES	YES	YES	NO	YES	YES
297	2.10	0.06	2.08	3.08	0.03	2.09	2.07	5.09	2.10	YES	YES	YES	NO	YES	YES	YES	NO	YES
298	1.16	1.11	3.18	2.14	1.11	1.23	3.16	2.06	1.23	YES	YES	YES	NO	YES	YES	YES	YES	YES
299	0.07	0.05	14.06	7.09	0.06	0.08	7.06	10.04	0.08	YES	YES	NO	NO	YES	YES	NO	NO	YES
300	1.04	1.03	0.06	0.05	0.03	1.04	1.06	0.03	1.05	YES	YES	YES	YES	YES	YES	YES	YES	YES
301	0.16	0.11	2.18	3.13	1.11	0.23	2.16	2.06	0.23	YES	YES	YES	NO	YES	YES	YES	YES	YES
302	0.08	0.06	2.12	0.08	0.04	0.10	2.09	0.06	1.11	YES	YES	YES	YES	YES	YES	YES	YES	YES

Table S4. The correlation weights assigned to each attribute incorporated in the model for Split#1 based on TF2

SAk	CW(SAk)
\$0	-4.87058
\$100	0.76751
\$1,000	0.28427
#####	-1.22714
#####	1.66335
#####	0.71374
#####	1.95006
#####	-0.91024

#####	-0.91566
#####	0.16567
#####	-1.35489
(...C...(...	-0.37126
(...F...(...	-1.34721
(...Cl...(...	-0.04476
(...N...(...	0
(...O...(...	0.13731
(F..=)..2.1.	1.8553
(F..=)..3.1.	0
(F..=)..4.1.	-0.20982
(Cl.=)..1.1.	2.08439
(Cl.=)..2.1.	0
(Cl.=)..3.1.	-0.53081
(Cl.=)..4.1.	2.79869
(N..=)..1.1.	-1.00617
(N..O)..1.2.	0.25562
(O..=)..1.1.	1.19481
(O..=)..1.2.	0.46476
(O..=)..2.1.	0.04739
(O..=)..2.2.	0.24734
/...C...(...	-0.87813
1...C...(...	-0.49437
1...c...(...	1.08295
2...C...(...	1.64741
2...C...1...	0.06723
2...c...1...	1.92647
=...C...(...	-0.10032
=...C.../...	-0.72549
=...C...1...	1.02736

=...C...2...	0
=...O...(...	0.53846
C...(...(...	-0.36842
C...(...1...	0.556
C...(...=...	-0.63553
C...(...C...	1.25512
C.../...C...	1.55608
C...1...(...	-0.16165
C...1...=...	0
C...1...C...	1.36285
C...2...C...	0.81921
C...=...(...	-1.0022
C...=...1...	0
C...=...C...	-0.33355
C...C...#...	0.43657
C...C...(...	-0.49816
C...C.../...	-0.61443
C...C...1...	1.9406
C...C...2...	2.37493
C...C...=...	0.35034
C...C...C...	-0.10756
C...N...(...	0
C...N...C...	0.60359
C...O...(...	-3.14377
C...O...1...	0
C...O...C...	0.46268
C...\...(...	0
C...\...C...	1.018
C...c...1...	-1.68973
BOND00000000	-1.90927

BOND01000000	-1.22786
BOND10000000	3.13365
F...(...(...	-0.88865
F...(...=...	0
F...(...C...	-0.34817
F...(...F...	-0.39603
F...C...(...	0
F...C...=...	-0.63512
EC2-C...10..	0.034
EC2-C...12..	0.27342
EC2-C...13..	-0.73082
EC2-C...14..	0.67107
EC2-C...15..	1.92945
EC2-C...16..	-0.23342
EC2-C...17..	-0.2938
EC2-C...18..	-0.12251
EC2-C...19..	-0.14058
EC2-C...20..	-0.15222
EC2-C...21..	0.68487
EC2-C...22..	-0.29306
EC2-C...23..	0.06171
EC2-C...24..	1.0845
EC2-C...25..	0.24797
EC2-C...26..	0.34052
EC2-C...27..	0.69309
EC2-C...28..	-0.10785
EC2-C...29..	0.47508
EC2-C...30..	-0.55496
EC2-C...31..	1.97682
EC2-C...32..	0.19372

EC2-C...33..	-0.40521
EC2-C...34..	0.59948
EC2-C...35..	-1.16028
EC2-C...36..	-0.82338
EC2-C...37..	1.74603
EC2-C...38..	0
EC2-C...39..	-0.24761
EC2-C...43..	3.24458
EC2-C...44..	1.14685
EC2-F...10..	1.20127
EC2-F...4...	0.42984
EC2-F...5...	0.22746
EC2-F...6...	0.90671
EC2-F...8...	-0.2096
EC2-H...10..	-0.46697
EC2-H...11..	0
EC2-H...12..	-0.63468
EC2-H...13..	-0.74703
EC2-H...3...	-0.83162
EC2-H...4...	0.84859
EC2-H...5...	-0.49541
EC2-H...6...	0.28657
EC2-H...7...	-0.10692
EC2-H...8...	-0.32171
EC2-H...9...	0.07068
EC2-Cl..20..	-0.32367
EC2-Cl..21..	-0.60491
EC2-Cl..22..	0
EC2-Cl..23..	-0.32336
EC2-Cl..24..	1.63359

EC2-Cl..26..	-0.09605
EC2-N...10..	1.48984
EC2-N...11..	-0.05456
EC2-N...14..	0
EC2-N...17..	0
EC2-N...18..	0.97203
EC2-N...20..	0
EC2-N...21..	0
EC2-N...23..	0
EC2-N...26..	0
EC2-O...10..	1.59701
EC2-O...11..	1.63845
EC2-O...12..	0.52193
EC2-O...13..	0.02373
EC2-O...14..	0
EC2-O...15..	-0.14618
EC2-O...5...	-0.14597
EC2-O...6...	-0.31361
EC2-O...7...	0.22172
EC2-O...8...	-1.91859
EC2-O...9...	-0.21062
Cl..(...=...	0.59764
Cl..(...C...	0.6405
Cl..(...Cl..	1.03478
Cl../...C...	0
Cl..C...(...	-1.5333
Cl..C.../...	0
Cl..C...=...	-0.45856
Cl..C...C...	0
Cl..\...C...	0

HALO00000000	1.85347
HALO01000000	-0.57449
HALO10000000	-0.08207
N...#...C...	1.26686
N...(..C...	0
N...C...C...	0
N...O...C...	1.25327
O...(...(...	0.906
O...(..C...	2.02608
O...(..O...	-2.73463
O...1...C...	0
O...=...(...	2.99565
O...=...C...	-1.3697
O...=...N...	0.20482
O...C...(...	-1.15392
O...C.../...	-2.6995
O...C...=...	0.73155
O...C...C...	1.3803
O...N...=...	-0.19816
NNC-C...211.	-0.12136
NNC-C...303.	-0.34849
NNC-C...312.	0.74515
NNC-C...321.	-0.08638
NNC-C...330.	0.47991
NNC-C...404.	-0.56124
NNC-C...413.	-0.70805
NNC-C...422.	-0.50088
NNC-C...431.	-0.63754
NNC-C...440.	0.88883
NNC-F...101.	-0.95309

NNC-F...110.	-0.31363
NNC-F...211.	-0.54067
NNC-H...101.	0.41658
NNC-H...110.	0.42327
NNC-Cl.404.	-0.15105
NNC-Cl.413.	-0.82771
NNC-N...202.	0.08238
NNC-N...211.	-0.36675
NNC-N...303.	0.53127
NNC-N...312.	0
NNC-N...321.	0.59136
NNC-N...330.	0
NNC-O...110.	-1.5942
NNC-O...202.	0.35037
NNC-O...211.	0.02636
NNC-O...220.	1.72537
NOSP00000000	1.56004
NOSP01000000	-0.6214
NOSP10000000	0.62097
NOSP11000000	1.60138
PT2-C...1...	-1.27879
PT2-C...11..	1.14079
PT2-C...12..	0.70266
PT2-C...2...	0.62337
PT2-C...3...	0.40425
PT2-C...4...	-0.55674
PT2-C...5...	0.90665
PT2-C...6...	-0.0155
PT2-C...7...	0.65445
PT2-C...8...	-0.43826

PT2-C...9...	-0.43269
PT2-F...1...	1.16285
PT2-F...2...	0.68167
PT2-F...3...	-0.88279
PT2-H...1...	0.35512
PT2-H...2...	0.19754
PT2-H...3...	-0.24549
PT2-Cl..2...	-0.16531
PT2-Cl..3...	1.62863
PT2-Cl..5...	0.65775
PT2-Cl..6...	0
PT2-N...1...	-0.43716
PT2-N...2...	0.85523
PT2-N...3...	-0.77866
PT2-N...5...	0
PT2-N...6...	0.4847
PT2-N...8...	0
PT2-N...9...	0
PT2-O...1...	-1.00981
PT2-O...2...	-1.18837
PT2-O...3...	-0.46266
PT2-O...4...	1.22108
PT2-O...5...	0.20279
PT2-O...6...	0
PT3-C...0...	-1.96749
PT3-C...1...	-0.25816
PT3-C...10..	0.26506
PT3-C...11..	0.78902
PT3-C...12..	-1.13878
PT3-C...13..	1.19657

PT3-C...14..	0
PT3-C...15..	1.31941
PT3-C...18..	2.45654
PT3-C...2...	-0.21918
PT3-C...20..	0.04322
PT3-C...3...	-0.69985
PT3-C...4...	0.20116
PT3-C...5...	0.54037
PT3-C...6...	0.54679
PT3-C...7...	0.61711
PT3-C...8...	-0.40998
PT3-C...9...	0.15071
PT3-F...2...	1.63292
PT3-F...3...	-0.57219
PT3-F...4...	0.0839
PT3-H...1...	0.35264
PT3-H...2...	-0.18406
PT3-H...3...	-0.02848
PT3-H...4...	0.21985
PT3-H...5...	0.78613
PT3-H...6...	0.91515
PT3-H...7...	0
PT3-H...8...	-0.30656
PT3-H...9...	-0.97917
PT3-Cl..2...	0.24842
PT3-Cl..3...	0
PT3-Cl..5...	-0.2203
PT3-N...1...	-0.60806
PT3-N...3...	1.01546
PT3-N...4...	0.50146

PT3-N...6...	0
PT3-N...9...	0
PT3-O...1...	0.02166
PT3-O...2...	0.30968
PT3-O...3...	-0.83572
PT3-O...4...	-0.78257
PT3-O...5...	1.33997
PT3-O...6...	1.06223
PT3-O...8...	0.76812
VS2-C...10..	-0.43648
VS2-C...11..	-0.35674
VS2-C...12..	-0.83302
VS2-C...13..	-1.24723
VS2-C...14..	-0.14017
VS2-C...15..	0.58225
VS2-C...16..	0.79646
VS2-C...17..	0.70929
VS2-C...2...	1.42378
VS2-C...18..	-0.10524
VS2-C...19..	0.68058
VS2-C...20..	0.41413
VS2-C...21..	-0.49114
VS2-C...22..	0
VS2-C...23..	-1.3638
VS2-C...27..	-0.93697
VS2-C...28..	0.07915
VS2-C...3...	-1.37445
VS2-C...4...	0.40345
VS2-C...5...	-0.04538
VS2-C...6...	0.31818

VS2-C...7...	0.37202
VS2-C...8...	0.31826
VS2-C...9...	0.27267
VS2-F...3...	1.91767
VS2-F...4...	-0.57313
VS2-F...5...	0.42162
VS2-F...6...	0.33436
VS2-F...7...	0.5498
VS2-H...10..	0
VS2-H...11..	-0.91064
VS2-H...12..	-0.48648
VS2-H...2...	-0.62063
VS2-H...3...	0.91885
VS2-H...4...	-0.43643
VS2-H...5...	0.27378
VS2-H...6...	0.03008
VS2-H...7...	-0.16083
VS2-H...8...	-0.36329
VS2-H...9...	-0.30597
VS2-Cl..10..	0.31458
VS2-Cl..4...	-0.43813
VS2-Cl..5...	-0.77851
VS2-Cl..6...	0
VS2-Cl..7...	-0.49815
VS2-Cl..8...	1.78288
VS2-N...11..	0
VS2-N...12..	0
VS2-N...14..	0
VS2-N...17..	0
VS2-N...2...	1.80564

VS2-N...5...	0
VS2-N...6...	0.28182
VS2-N...8...	0
VS2-N...9...	1.41684
VS2-O...10..	0
VS2-O...11..	-0.60684
VS2-O...2...	-1.27354
VS2-O...3...	0.68545
VS2-O...4...	1.66708
VS2-O...5...	0.40712
VS2-O...6...	1.39731
VS2-O...7...	2.00678
VS2-O...8...	0.24444
VS2-O...9...	-1.04225
\...(C...	0
\...(O...	0
\...C...(-0.33483
\...C...=...	0.77123
\...C...C...	-0.86619
\...C...Cl..	0
\...c...1...	-3.01956
[CH2].....	0
[C].....	0
[T10].....	-0.2288
[T13].....	0.34313
[T14].....	0
[T15].....	0
[T17].....	2.29839
[T18].....	1.07112
[T19].....	1.19686

[T20].....	0
[T21].....	0
[T22].....	1.51088
[T23].....	0
[T24].....	1.72016
[T25].....	2.34963
[T26].....	2.08624
[T27].....	2.41887
[T28].....	0
[T29].....	0
[T30].....	2.96535
[T31].....	0
[T32].....	0
[T34].....	2.83907
[T35].....	0
[T36].....	1.90333
[T37].....	2.38554
[T38].....	0.62591
[T40].....	1.54506
[T0].....	-4.51369
[T43].....	0
[T47].....	0
[T1].....	0
[T2].....	0
[T3].....	-3.22736
[T6].....	0
[nH].....	0
c...(O...	-0.20163
c...1..O...	0
c...1...c...	-1.22414

c...2...c...	0.34336
c...C...=...	-1.8247
c...C...Cl..	-1.09234
c...\...C...	-2.93434
c...c...(...	-0.27587
c...c...1...	2.94186
c...c...2...	-0.0355
c...c...c...	0.39071
c...n...1...	0
n...c...c...	0
o...1...c...	0