

SUPPLEMENTAL MATERIAL

Equation 3. Optimization function. $F \equiv$ optimization function value, $SS_{err} \equiv$ sum of squares of residuals, $x_k^* \equiv$ predicted molar flow rate of species k , $x_k \equiv$ experimentally observed molar flow rate of species k . Summation over all experimentally measured species, N .

$$F = SS_{err} = \sum_{k=1}^N (x_k^* - x_k)^2$$

Equation 4. $\bar{x} \equiv$ mean of experimentally observed molar flow rates. Summation over all experimentally measured species, N .

$$\bar{x} = \frac{1}{N} \sum_{k=1}^N x_k$$

Equation 5. $SS_{tot} \equiv$ total sum of squares, $x_k^* \equiv$ predicted molar flow rate of species k , $\bar{x} \equiv$ mean of experimentally observed molar flow rates. Summation over all experimentally measured species, N .

$$SS_{tot} = \sum_{k=1}^N (x_k^* - \bar{x})^2$$

Equation 6. Correlation coefficient. $R^2 \equiv$ coefficient of determination, $SS_{err} \equiv$ sum of squares of residuals, $SS_{tot} \equiv$ total sum of squares.

$$R^2 = 1 - \frac{SS_{err}}{SS_{tot}}$$

Table 8. Division of positional isomers for numerical model. Based upon approximate distributions in [16].

Species	Division
<i>propanol</i>	
propan-1-ol	85%
propan-2-ol	15%
<i>propanediol</i>	
propane-1,2-diol	100%
<i>butanol</i>	
butan-1-ol	95%
butan-2-ol	5%
<i>butanediol</i>	
butane-1,2-diol	60%
butane-2,3-diol	40%
<i>pentanol</i>	
pentan-1-ol	89%
pentan-2-ol	11%
<i>pentanediol</i>	
pentane-1,2-diol	100%
<i>pentanone</i>	
pentan-2-one	100%

<i>hexanol</i>	
hexan-1-ol	45%
hexan-2-ol	45%
hexan-3-ol	10%
<i>hexanediol</i>	
hexane-1,2-diol	100%
<i>hexanetriol</i>	
hexane-1,2,6-triol	100%
<i>hexanone</i>	
hexan-2-one	50%
hexan-3-one	50%
<i>isosorbide and 1,4-sorbitan</i>	
hexahydrofuro[3,2-b]furan-3,6-diol	50%
2-(1,2-dihydroxyethyl)tetrahydrofuran-3,4-diol	50%

Table 9. Reaction network and enthalpy of reaction.

Reaction #	Reaction	Reaction Family	ΔH_R (kJ mol ⁻¹)
1	species784 -> species2 + species514	AcyclicThermalCracking-NParaffin	137.722092
2	species1108 -> species2 + species964	AcyclicThermalCracking-NParaffin	125.328038
3	species1108 -> species247 + species514	AcyclicThermalCracking-NParaffin	83.212061
4	species1147 -> species514 + species784	AcyclicThermalCracking-NParaffin	94.387818
5	species1147 -> species247 + species964	AcyclicThermalCracking-NParaffin	73.018080
6	species1173 -> species514 + species1108	AcyclicThermalCracking-NParaffin	121.313532
7	species1173 -> species784 + species964	AcyclicThermalCracking-NParaffin	108.919478
8	species1173 -> species247 + species1106	AcyclicThermalCracking-NParaffin	99.145110
9	species1178 -> species514 + species1147	AcyclicThermalCracking-NParaffin	124.716798
10	species1178 -> species964 + species1108	AcyclicThermalCracking-NParaffin	114.522816
11	species1178 -> species247 + species1158	AcyclicThermalCracking-NParaffin	105.318979
12	species1178 -> species784 + species1106	AcyclicThermalCracking-NParaffin	113.724091
13	species1 -> species3 + species4	AlcoholCyclization5-Oxygen	-61.145394
14	species1 -> species3 + species5	AlcoholCyclization5-Oxygen	-53.317130
15	species7 -> species3 + species25	AlcoholCyclization5-Oxygen	102.229680
16	species7 -> species3 + species14	AlcoholCyclization5-Oxygen	101.347944
17	species8 -> species3 + species20	AlcoholCyclization5-Oxygen	-53.471102
18	species9 -> species3 + species19	AlcoholCyclization5-Oxygen	-39.829044
19	species23 -> species3 + species116	AlcoholCyclization5-Oxygen	-38.169419
20	species23 -> species3 + species83	AlcoholCyclization5-Oxygen	-45.997641
21	species24 -> species3 + species124	AlcoholCyclization5-Oxygen	-42.460487
22	species24 -> species3 + species84	AlcoholCyclization5-Oxygen	-47.798434
23	species30 -> species3 + species97	AlcoholCyclization5-Oxygen	-34.205539
24	species30 -> species3 + species105	AlcoholCyclization5-Oxygen	-39.826994
25	species43 -> species3 + species131	AlcoholCyclization5-Oxygen	-52.903751
26	species44 -> species3 + species85	AlcoholCyclization5-Oxygen	-37.316636
27	species65 -> species3 + species106	AlcoholCyclization5-Oxygen	-39.802978
28	species93 -> species3 + species292	AlcoholCyclization5-Oxygen	-47.485471
29	species94 -> species3 + species300	AlcoholCyclization5-Oxygen	-34.283738
30	species119 -> species3 + species350	AlcoholCyclization5-Oxygen	-37.780056
31	species119 -> species3 + species262	AlcoholCyclization5-Oxygen	-38.661834
32	species120 -> species3 + species264	AlcoholCyclization5-Oxygen	-39.877997
33	species121 -> species3 + species265	AlcoholCyclization5-Oxygen	-26.233931
34	species139 -> species3 + species290	AlcoholCyclization5-Oxygen	-35.165474
35	species149 -> species3 + species270	AlcoholCyclization5-Oxygen	-45.221090
36	species152 -> species3 + species310	AlcoholCyclization5-Oxygen	-32.610012
37	species153 -> species3 + species311	AlcoholCyclization5-Oxygen	-40.837890
38	species187 -> species3 + species276	AlcoholCyclization5-Oxygen	-44.261281
39	species220 -> species3 + species496	AlcoholCyclization5-Oxygen	-37.538722
40	species252 -> species3 + species349	AlcoholCyclization5-Oxygen	-23.943651

41	species253 -> species3 + species420	AlcoholCyclization5-Oxygen	-30.097646
42	species266 -> species3 + species542	AlcoholCyclization5-Oxygen	-33.323803
43	species267 -> species3 + species416	AlcoholCyclization5-Oxygen	-23.983776
44	species275 -> species3 + species559	AlcoholCyclization5-Oxygen	-43.029093
45	species283 -> species3 + species572	AlcoholCyclization5-Oxygen	-26.601286
46	species302 -> species3 + species604	AlcoholCyclization5-Oxygen	-39.308513
47	species313 -> species3 + species529	AlcoholCyclization5-Oxygen	-38.026200
48	species314 -> species3 + species528	AlcoholCyclization5-Oxygen	-44.285130
49	species326 -> species3 + species317	AlcoholCyclization5-Oxygen	-32.772100
50	species327 -> species3 + species526	AlcoholCyclization5-Oxygen	-38.661834
51	species362 -> species3 + species688	AlcoholCyclization5-Oxygen	-28.867550
52	species362 -> species3 + species536	AlcoholCyclization5-Oxygen	-34.205539
53	species371 -> species3 + species539	AlcoholCyclization5-Oxygen	-27.169808
54	species426 -> species3 + species623	AlcoholCyclization5-Oxygen	-33.569947
55	species437 -> species3 + species624	AlcoholCyclization5-Oxygen	-27.169808
56	species491 -> species3 + species728	AlcoholCyclization5-Oxygen	-31.626103
57	species532 -> species3 + species727	AlcoholCyclization5-Oxygen	-25.512233
58	species533 -> species3 + species822	AlcoholCyclization5-Oxygen	-34.852260
59	species575 -> species3 + species868	AlcoholCyclization5-Oxygen	-31.626103
60	species595 -> species3 + species896	AlcoholCyclization5-Oxygen	-34.852260
61	species632 -> species3 + species814	AlcoholCyclization5-Oxygen	-31.626103
62	species646 -> species3 + species588	AlcoholCyclization5-Oxygen	-25.434076
63	species647 -> species3 + species642	AlcoholCyclization5-Oxygen	-26.650239
64	species648 -> species3 + species641	AlcoholCyclization5-Oxygen	-13.008223
65	species745 -> species3 + species873	AlcoholCyclization5-Oxygen	-16.871896
66	species750 -> species3 + species803	AlcoholCyclization5-Oxygen	-31.626103
67	species794 -> species3 + species965	AlcoholCyclization5-Oxygen	-10.717944
68	species819 -> species3 + species980	AlcoholCyclization5-Oxygen	-26.080797
69	species828 -> species3 + species979	AlcoholCyclization5-Oxygen	-21.055980
70	species829 -> species3 + species1042	AlcoholCyclization5-Oxygen	-30.393999
71	species911 -> species3 + species930	AlcoholCyclization5-Oxygen	-19.382296
72	species912 -> species3 + species1007	AlcoholCyclization5-Oxygen	-27.193866
73	species926 -> species3 + species1028	AlcoholCyclization5-Oxygen	-27.193866
74	species944 -> species3 + species802	AlcoholCyclization5-Oxygen	-25.434076
75	species945 -> species3 + species931	AlcoholCyclization5-Oxygen	-13.942092
76	species990 -> species3 + species1062	AlcoholCyclization5-Oxygen	-18.400395
77	species1032 -> species3 + species1075	AlcoholCyclization5-Oxygen	-21.624544
78	species1078 -> species3 + species1010	AlcoholCyclization5-Oxygen	-18.400395
79	species1143 -> species3 + species1150	AlcoholCyclization5-Oxygen	-17.168249
80	species1154 -> species3 + species1118	AlcoholCyclization5-Oxygen	-13.008223
81	species1 -> species3 + species6	AlcoholCyclization6-Oxygen	-63.450778
82	species7 -> species3 + species31	AlcoholCyclization6-Oxygen	92.098082
83	species23 -> species3 + species117	AlcoholCyclization6-Oxygen	-48.303025
84	species23 -> species3 + species118	AlcoholCyclization6-Oxygen	-48.303025
85	species24 -> species3 + species125	AlcoholCyclization6-Oxygen	-52.592043
86	species30 -> species3 + species148	AlcoholCyclization6-Oxygen	-36.510756
87	species44 -> species3 + species155	AlcoholCyclization6-Oxygen	-47.448234
88	species94 -> species3 + species301	AlcoholCyclization6-Oxygen	-44.415252
89	species119 -> species3 + species363	AlcoholCyclization6-Oxygen	-47.911821
90	species139 -> species3 + species410	AlcoholCyclization6-Oxygen	-44.415252
91	species253 -> species3 + species464	AlcoholCyclization6-Oxygen	-40.229202
92	species266 -> species3 + species543	AlcoholCyclization6-Oxygen	-43.455442
93	species267 -> species3 + species548	AlcoholCyclization6-Oxygen	-34.117382
94	species283 -> species3 + species574	AlcoholCyclization6-Oxygen	-36.732884
95	species313 -> species3 + species631	AlcoholCyclization6-Oxygen	-34.709962
96	species326 -> species3 + species645	AlcoholCyclization6-Oxygen	-35.077317
97	species327 -> species3 + species651	AlcoholCyclization6-Oxygen	-43.455442
98	species362 -> species3 + species696	AlcoholCyclization6-Oxygen	-38.999148
99	species532 -> species3 + species818	AlcoholCyclization6-Oxygen	-35.643831

100	species586 -> species3 + species883	AlcoholCyclization6-Oxygen	-30.820223
101	species643 -> species3 + species936	AlcoholCyclization6-Oxygen	-14.513543
102	species646 -> species3 + species940	AlcoholCyclization6-Oxygen	-34.683896
103	species745 -> species3 + species989	AlcoholCyclization6-Oxygen	-27.003494
104	species808 -> species3 + species1023	AlcoholCyclization6-Oxygen	-26.363970
105	species828 -> species3 + species1038	AlcoholCyclization6-Oxygen	-31.187578
106	species872 -> species3 + species1063	AlcoholCyclization6-Oxygen	-23.139821
107	species893 -> species3 + species1072	AlcoholCyclization6-Oxygen	-16.042000
108	species944 -> species3 + species1102	AlcoholCyclization6-Oxygen	-30.227643
109	species1012 -> species3 + species1124	AlcoholCyclization6-Oxygen	-11.585747
110	species1066 -> species3 + species1151	AlcoholCyclization6-Oxygen	-8.359590
111	species4 -> species3 + species15	AlcoholDehydration-Oxygen	42.196142
112	species4 -> species3 + species16	AlcoholDehydration-Oxygen	35.792894
113	species4 -> species3 + species17	AlcoholDehydration-Oxygen	38.270395
114	species4 -> species3 + species18	AlcoholDehydration-Oxygen	42.196142
115	species5 -> species3 + species26	AlcoholDehydration-Oxygen	17.648652
116	species5 -> species3 + species27	AlcoholDehydration-Oxygen	42.194134
117	species5 -> species3 + species28	AlcoholDehydration-Oxygen	-49.297980
118	species6 -> species3 + species32	AlcoholDehydration-Oxygen	-49.295888
119	species6 -> species3 + species33	AlcoholDehydration-Oxygen	17.650681
120	species6 -> species3 + species34	AlcoholDehydration-Oxygen	42.196142
121	species6 -> species3 + species35	AlcoholDehydration-Oxygen	42.196142
122	species6 -> species3 + species36	AlcoholDehydration-Oxygen	35.792894
123	species6 -> species3 + species37	AlcoholDehydration-Oxygen	42.196142
124	species6 -> species3 + species38	AlcoholDehydration-Oxygen	42.196142
125	species10 -> species3 + species72	AlcoholDehydration-Oxygen	36.044265
126	species13 -> species3 + species81	AlcoholDehydration-Oxygen	35.794923
127	species13 -> species3 + species82	AlcoholDehydration-Oxygen	34.138444
128	species14 -> species3 + species86	AlcoholDehydration-Oxygen	30.261186
129	species14 -> species3 + species87	AlcoholDehydration-Oxygen	42.196142
130	species14 -> species3 + species88	AlcoholDehydration-Oxygen	35.792894
131	species14 -> species3 + species89	AlcoholDehydration-Oxygen	38.270395
132	species14 -> species3 + species90	AlcoholDehydration-Oxygen	42.196142
133	species16 -> species3 + species98	AlcoholDehydration-Oxygen	-26.086152
134	species17 -> species3 + species98	AlcoholDehydration-Oxygen	-28.563624
135	species19 -> species3 + species101	AlcoholDehydration-Oxygen	17.650681
136	species19 -> species3 + species103	AlcoholDehydration-Oxygen	42.196142
137	species19 -> species3 + species99	AlcoholDehydration-Oxygen	35.794923
138	species19 -> species3 + species95	AlcoholDehydration-Oxygen	42.196142
139	species20 -> species3 + species100	AlcoholDehydration-Oxygen	35.792894
140	species20 -> species3 + species96	AlcoholDehydration-Oxygen	42.194134
141	species20 -> species3 + species102	AlcoholDehydration-Oxygen	10.297623
142	species20 -> species3 + species104	AlcoholDehydration-Oxygen	42.194134
143	species25 -> species3 + species132	AlcoholDehydration-Oxygen	2.769457
144	species25 -> species3 + species133	AlcoholDehydration-Oxygen	42.196142
145	species25 -> species3 + species134	AlcoholDehydration-Oxygen	42.196142
146	species25 -> species3 + species135	AlcoholDehydration-Oxygen	17.650681
147	species25 -> species3 + species136	AlcoholDehydration-Oxygen	-49.295888
148	species26 -> species3 + species140	AlcoholDehydration-Oxygen	-51.164044
149	species26 -> species3 + species141	AlcoholDehydration-Oxygen	-49.295888
150	species27 -> species3 + species142	AlcoholDehydration-Oxygen	-65.060782
151	species27 -> species3 + species143	AlcoholDehydration-Oxygen	-129.417396
152	species28 -> species3 + species142	AlcoholDehydration-Oxygen	26.431077
153	species28 -> species3 + species143	AlcoholDehydration-Oxygen	-37.925450
154	species28 -> species3 + species141	AlcoholDehydration-Oxygen	17.650681
155	species28 -> species3 + species144	AlcoholDehydration-Oxygen	-39.875779
156	species29 -> species3 + species145	AlcoholDehydration-Oxygen	-51.815074
157	species29 -> species3 + species146	AlcoholDehydration-Oxygen	-53.265667
158	species30 -> species3 + species149	AlcoholDehydration-Oxygen	41.931881

159	species31 -> species3 + species156	AlcoholDehydration-Oxygen	2.769457
160	species31 -> species3 + species157	AlcoholDehydration-Oxygen	42.196142
161	species31 -> species3 + species158	AlcoholDehydration-Oxygen	35.792894
162	species31 -> species3 + species159	AlcoholDehydration-Oxygen	42.196142
163	species31 -> species3 + species160	AlcoholDehydration-Oxygen	42.196142
164	species31 -> species3 + species161	AlcoholDehydration-Oxygen	42.196142
165	species32 -> species3 + species166	AlcoholDehydration-Oxygen	26.429048
166	species32 -> species3 + species167	AlcoholDehydration-Oxygen	35.792894
167	species32 -> species3 + species168	AlcoholDehydration-Oxygen	42.194134
168	species32 -> species3 + species169	AlcoholDehydration-Oxygen	26.429048
169	species32 -> species3 + species170	AlcoholDehydration-Oxygen	42.194134
170	species33 -> species3 + species175	AlcoholDehydration-Oxygen	-26.620658
171	species33 -> species3 + species176	AlcoholDehydration-Oxygen	35.792894
172	species33 -> species3 + species177	AlcoholDehydration-Oxygen	42.194134
173	species34 -> species3 + species166	AlcoholDehydration-Oxygen	-65.062874
174	species34 -> species3 + species180	AlcoholDehydration-Oxygen	-24.105363
175	species35 -> species3 + species177	AlcoholDehydration-Oxygen	17.648652
176	species35 -> species3 + species168	AlcoholDehydration-Oxygen	-49.297980
177	species36 -> species3 + species180	AlcoholDehydration-Oxygen	-17.702127
178	species36 -> species3 + species176	AlcoholDehydration-Oxygen	17.650681
179	species36 -> species3 + species181	AlcoholDehydration-Oxygen	-22.160389
180	species36 -> species3 + species167	AlcoholDehydration-Oxygen	-49.295888
181	species37 -> species3 + species175	AlcoholDehydration-Oxygen	-51.166136
182	species37 -> species3 + species170	AlcoholDehydration-Oxygen	-49.297980
183	species38 -> species3 + species169	AlcoholDehydration-Oxygen	-65.062874
184	species38 -> species3 + species181	AlcoholDehydration-Oxygen	-28.563624
185	species39 -> species3 + species171	AlcoholDehydration-Oxygen	-51.812982
186	species39 -> species3 + species182	AlcoholDehydration-Oxygen	40.251155
187	species40 -> species3 + species172	AlcoholDehydration-Oxygen	-53.263575
188	species40 -> species3 + species184	AlcoholDehydration-Oxygen	35.792894
189	species40 -> species3 + species183	AlcoholDehydration-Oxygen	35.792894
190	species41 -> species3 + species179	AlcoholDehydration-Oxygen	17.650681
191	species41 -> species3 + species173	AlcoholDehydration-Oxygen	-49.295888
192	species42 -> species3 + species174	AlcoholDehydration-Oxygen	-49.295888
193	species42 -> species3 + species186	AlcoholDehydration-Oxygen	35.792894
194	species42 -> species3 + species178	AlcoholDehydration-Oxygen	17.650681
195	species48 -> species3 + species204	AlcoholDehydration-Oxygen	117.474001
196	species51 -> species3 + species213	AlcoholDehydration-Oxygen	37.004179
197	species59 -> species3 + species227	AlcoholDehydration-Oxygen	116.405993
198	species60 -> species3 + species228	AlcoholDehydration-Oxygen	37.002150
199	species68 -> species3 + species241	AlcoholDehydration-Oxygen	36.520613
200	species68 -> species3 + species242	AlcoholDehydration-Oxygen	36.520613
201	species69 -> species3 + species243	AlcoholDehydration-Oxygen	109.222107
202	species69 -> species3 + species244	AlcoholDehydration-Oxygen	37.002150
203	species73 -> species3 + species248	AlcoholDehydration-Oxygen	61.351415
204	species74 -> species3 + species249	AlcoholDehydration-Oxygen	37.002150
205	species75 -> species3 + species250	AlcoholDehydration-Oxygen	61.353465
206	species81 -> species3 + species256	AlcoholDehydration-Oxygen	34.136415
207	species81 -> species3 + species257	AlcoholDehydration-Oxygen	35.792894
208	species82 -> species3 + species261	AlcoholDehydration-Oxygen	34.138444
209	species82 -> species3 + species256	AlcoholDehydration-Oxygen	35.792894
210	species83 -> species3 + species263	AlcoholDehydration-Oxygen	35.792894
211	species83 -> species3 + species258	AlcoholDehydration-Oxygen	11.681845
212	species84 -> species3 + species268	AlcoholDehydration-Oxygen	42.194134
213	species84 -> species3 + species269	AlcoholDehydration-Oxygen	38.268366
214	species84 -> species3 + species270	AlcoholDehydration-Oxygen	52.086700
215	species84 -> species3 + species271	AlcoholDehydration-Oxygen	-29.758198
216	species84 -> species3 + species259	AlcoholDehydration-Oxygen	35.792894
217	species84 -> species3 + species272	AlcoholDehydration-Oxygen	42.194134

218	species85 -> species3 + species277	AlcoholDehydration-Oxygen	-49.295888
219	species85 -> species3 + species278	AlcoholDehydration-Oxygen	42.196142
220	species85 -> species3 + species279	AlcoholDehydration-Oxygen	35.792894
221	species85 -> species3 + species280	AlcoholDehydration-Oxygen	17.650681
222	species85 -> species3 + species281	AlcoholDehydration-Oxygen	42.196142
223	species86 -> species3 + species285	AlcoholDehydration-Oxygen	42.196142
224	species86 -> species3 + species286	AlcoholDehydration-Oxygen	35.794923
225	species86 -> species3 + species287	AlcoholDehydration-Oxygen	42.196142
226	species87 -> species3 + species285	AlcoholDehydration-Oxygen	30.261186
227	species88 -> species3 + species291	AlcoholDehydration-Oxygen	-26.086152
228	species88 -> species3 + species286	AlcoholDehydration-Oxygen	30.263219
229	species89 -> species3 + species291	AlcoholDehydration-Oxygen	-28.563624
230	species90 -> species3 + species287	AlcoholDehydration-Oxygen	30.261186
231	species91 -> species3 + species288	AlcoholDehydration-Oxygen	30.261186
232	species92 -> species3 + species289	AlcoholDehydration-Oxygen	30.261186
233	species94 -> species3 + species303	AlcoholDehydration-Oxygen	34.600776
234	species97 -> species3 + species263	AlcoholDehydration-Oxygen	35.792894
235	species97 -> species3 + species312	AlcoholDehydration-Oxygen	38.270395
236	species99 -> species3 + species315	AlcoholDehydration-Oxygen	17.648652
237	species100 -> species3 + species316	AlcoholDehydration-Oxygen	10.299657
238	species101 -> species3 + species315	AlcoholDehydration-Oxygen	35.792894
239	species102 -> species3 + species316	AlcoholDehydration-Oxygen	35.794923
240	species105 -> species3 + species270	AlcoholDehydration-Oxygen	36.537705
241	species105 -> species3 + species320	AlcoholDehydration-Oxygen	5.593129
242	species105 -> species3 + species322	AlcoholDehydration-Oxygen	30.138595
243	species105 -> species3 + species308	AlcoholDehydration-Oxygen	30.138595
244	species105 -> species3 + species318	AlcoholDehydration-Oxygen	11.681845
245	species106 -> species3 + species321	AlcoholDehydration-Oxygen	78.847145
246	species106 -> species3 + species323	AlcoholDehydration-Oxygen	91.361113
247	species106 -> species3 + species309	AlcoholDehydration-Oxygen	66.777644
248	species106 -> species3 + species319	AlcoholDehydration-Oxygen	84.959886
249	species116 -> species3 + species351	AlcoholDehydration-Oxygen	-51.815074
250	species116 -> species3 + species352	AlcoholDehydration-Oxygen	17.648652
251	species116 -> species3 + species353	AlcoholDehydration-Oxygen	35.792894
252	species116 -> species3 + species354	AlcoholDehydration-Oxygen	-49.297980
253	species117 -> species3 + species355	AlcoholDehydration-Oxygen	35.792894
254	species117 -> species3 + species356	AlcoholDehydration-Oxygen	42.196142
255	species117 -> species3 + species357	AlcoholDehydration-Oxygen	42.196142
256	species117 -> species3 + species358	AlcoholDehydration-Oxygen	35.792894
257	species117 -> species3 + species359	AlcoholDehydration-Oxygen	-51.812982
258	species118 -> species3 + species364	AlcoholDehydration-Oxygen	35.792894
259	species118 -> species3 + species365	AlcoholDehydration-Oxygen	35.792894
260	species118 -> species3 + species366	AlcoholDehydration-Oxygen	17.650681
261	species118 -> species3 + species355	AlcoholDehydration-Oxygen	35.792894
262	species118 -> species3 + species367	AlcoholDehydration-Oxygen	-49.295888
263	species120 -> species3 + species370	AlcoholDehydration-Oxygen	23.269948
264	species121 -> species3 + species372	AlcoholDehydration-Oxygen	36.522642
265	species121 -> species3 + species373	AlcoholDehydration-Oxygen	42.900728
266	species123 -> species3 + species374	AlcoholDehydration-Oxygen	37.002150
267	species124 -> species3 + species376	AlcoholDehydration-Oxygen	54.265685
268	species124 -> species3 + species377	AlcoholDehydration-Oxygen	42.196142
269	species124 -> species3 + species378	AlcoholDehydration-Oxygen	17.650681
270	species124 -> species3 + species379	AlcoholDehydration-Oxygen	42.196142
271	species124 -> species3 + species380	AlcoholDehydration-Oxygen	-49.295888
272	species125 -> species3 + species383	AlcoholDehydration-Oxygen	35.792894
273	species125 -> species3 + species384	AlcoholDehydration-Oxygen	42.194134
274	species125 -> species3 + species385	AlcoholDehydration-Oxygen	42.194134
275	species125 -> species3 + species386	AlcoholDehydration-Oxygen	42.194134
276	species125 -> species3 + species387	AlcoholDehydration-Oxygen	54.263677

277	species125 -> species3 + species388	AlcoholDehydration-Oxygen	42.194134
278	species126 -> species3 + species374	AlcoholDehydration-Oxygen	35.735071
279	species127 -> species3 + species394	AlcoholDehydration-Oxygen	35.560695
280	species127 -> species3 + species395	AlcoholDehydration-Oxygen	46.397255
281	species129 -> species3 + species397	AlcoholDehydration-Oxygen	37.002150
282	species131 -> species3 + species400	AlcoholDehydration-Oxygen	42.196142
283	species131 -> species3 + species401	AlcoholDehydration-Oxygen	2.769457
284	species132 -> species3 + species403	AlcoholDehydration-Oxygen	-51.164044
285	species132 -> species3 + species404	AlcoholDehydration-Oxygen	-39.875779
286	species133 -> species3 + species405	AlcoholDehydration-Oxygen	-129.417396
287	species134 -> species3 + species406	AlcoholDehydration-Oxygen	-65.060782
288	species135 -> species3 + species403	AlcoholDehydration-Oxygen	-66.045277
289	species136 -> species3 + species405	AlcoholDehydration-Oxygen	-37.925450
290	species136 -> species3 + species404	AlcoholDehydration-Oxygen	12.189461
291	species136 -> species3 + species406	AlcoholDehydration-Oxygen	26.431077
292	species137 -> species3 + species407	AlcoholDehydration-Oxygen	-53.263575
293	species138 -> species3 + species408	AlcoholDehydration-Oxygen	-51.812982
294	species139 -> species3 + species411	AlcoholDehydration-Oxygen	40.012056
295	species142 -> species3 + species417	AlcoholDehydration-Oxygen	-55.643016
296	species143 -> species3 + species417	AlcoholDehydration-Oxygen	8.713665
297	species144 -> species3 + species417	AlcoholDehydration-Oxygen	10.663974
298	species145 -> species3 + species418	AlcoholDehydration-Oxygen	-43.843718
299	species146 -> species3 + species418	AlcoholDehydration-Oxygen	-42.393125
300	species147 -> species3 + species419	AlcoholDehydration-Oxygen	-51.812982
301	species148 -> species3 + species364	AlcoholDehydration-Oxygen	35.792894
302	species148 -> species3 + species421	AlcoholDehydration-Oxygen	42.196142
303	species148 -> species3 + species422	AlcoholDehydration-Oxygen	42.196142
304	species148 -> species3 + species423	AlcoholDehydration-Oxygen	17.650681
305	species148 -> species3 + species424	AlcoholDehydration-Oxygen	-49.295888
306	species150 -> species3 + species428	AlcoholDehydration-Oxygen	41.929872
307	species150 -> species3 + species431	AlcoholDehydration-Oxygen	28.268723
308	species150 -> species3 + species432	AlcoholDehydration-Oxygen	37.002150
309	species151 -> species3 + species427	AlcoholDehydration-Oxygen	41.929872
310	species151 -> species3 + species434	AlcoholDehydration-Oxygen	36.520613
311	species151 -> species3 + species435	AlcoholDehydration-Oxygen	40.381303
312	species152 -> species3 + species430	AlcoholDehydration-Oxygen	35.555795
313	species153 -> species3 + species429	AlcoholDehydration-Oxygen	40.969946
314	species154 -> species3 + species395	AlcoholDehydration-Oxygen	38.452537
315	species155 -> species3 + species441	AlcoholDehydration-Oxygen	35.792894
316	species155 -> species3 + species442	AlcoholDehydration-Oxygen	42.194134
317	species155 -> species3 + species443	AlcoholDehydration-Oxygen	42.194134
318	species156 -> species3 + species445	AlcoholDehydration-Oxygen	-26.620658
319	species156 -> species3 + species446	AlcoholDehydration-Oxygen	42.194134
320	species156 -> species3 + species447	AlcoholDehydration-Oxygen	35.792894
321	species157 -> species3 + species450	AlcoholDehydration-Oxygen	-24.105363
322	species158 -> species3 + species450	AlcoholDehydration-Oxygen	-17.702127
323	species158 -> species3 + species447	AlcoholDehydration-Oxygen	2.769457
324	species158 -> species3 + species451	AlcoholDehydration-Oxygen	-22.160389
325	species159 -> species3 + species446	AlcoholDehydration-Oxygen	2.767427
326	species160 -> species3 + species451	AlcoholDehydration-Oxygen	-28.563624
327	species161 -> species3 + species445	AlcoholDehydration-Oxygen	-66.047369
328	species162 -> species3 + species452	AlcoholDehydration-Oxygen	40.251155
329	species163 -> species3 + species454	AlcoholDehydration-Oxygen	35.792894
330	species163 -> species3 + species453	AlcoholDehydration-Oxygen	35.792894
331	species164 -> species3 + species449	AlcoholDehydration-Oxygen	2.769457
332	species165 -> species3 + species455	AlcoholDehydration-Oxygen	35.792894
333	species165 -> species3 + species448	AlcoholDehydration-Oxygen	2.769457
334	species166 -> species3 + species456	AlcoholDehydration-Oxygen	40.253185
335	species167 -> species3 + species456	AlcoholDehydration-Oxygen	30.889338

336	species167 -> species3 + species457	AlcoholDehydration-Oxygen	-37.925450
337	species169 -> species3 + species457	AlcoholDehydration-Oxygen	-28.561616
338	species171 -> species3 + species458	AlcoholDehydration-Oxygen	40.251155
339	species172 -> species3 + species460	AlcoholDehydration-Oxygen	35.792894
340	species172 -> species3 + species459	AlcoholDehydration-Oxygen	35.792894
341	species174 -> species3 + species461	AlcoholDehydration-Oxygen	88.842596
342	species180 -> species3 + species456	AlcoholDehydration-Oxygen	-0.704335
343	species181 -> species3 + species457	AlcoholDehydration-Oxygen	-65.060782
344	species182 -> species3 + species458	AlcoholDehydration-Oxygen	-51.812982
345	species183 -> species3 + species459	AlcoholDehydration-Oxygen	-53.263575
346	species184 -> species3 + species460	AlcoholDehydration-Oxygen	-53.263575
347	species185 -> species3 + species463	AlcoholDehydration-Oxygen	40.251155
348	species185 -> species3 + species462	AlcoholDehydration-Oxygen	35.792894
349	species186 -> species3 + species461	AlcoholDehydration-Oxygen	3.753952
350	species188 -> species3 + species469	AlcoholDehydration-Oxygen	116.893596
351	species193 -> species3 + species476	AlcoholDehydration-Oxygen	37.004179
352	species195 -> species3 + species477	AlcoholDehydration-Oxygen	37.002150
353	species196 -> species3 + species480	AlcoholDehydration-Oxygen	108.643752
354	species200 -> species3 + species481	AlcoholDehydration-Oxygen	37.002150
355	species201 -> species3 + species484	AlcoholDehydration-Oxygen	35.942250
356	species201 -> species3 + species485	AlcoholDehydration-Oxygen	35.942250
357	species202 -> species3 + species486	AlcoholDehydration-Oxygen	33.912278
358	species205 -> species3 + species480	AlcoholDehydration-Oxygen	116.895646
359	species206 -> species3 + species488	AlcoholDehydration-Oxygen	34.980303
360	species207 -> species3 + species489	AlcoholDehydration-Oxygen	117.474001
361	species214 -> species3 + species494	AlcoholDehydration-Oxygen	37.004179
362	species217 -> species3 + species495	AlcoholDehydration-Oxygen	105.291364
363	species235 -> species3 + species503	AlcoholDehydration-Oxygen	35.560695
364	species235 -> species3 + species504	AlcoholDehydration-Oxygen	46.397255
365	species236 -> species3 + species505	AlcoholDehydration-Oxygen	35.735071
366	species236 -> species3 + species506	AlcoholDehydration-Oxygen	37.002150
367	species243 -> species3 + species512	AlcoholDehydration-Oxygen	37.002150
368	species244 -> species3 + species512	AlcoholDehydration-Oxygen	109.222107
369	species245 -> species3 + species513	AlcoholDehydration-Oxygen	104.223356
370	species246 -> species3 + species514	AlcoholDehydration-Oxygen	88.049184
371	species249 -> species3 + species515	AlcoholDehydration-Oxygen	37.004179
372	species251 -> species3 + species516	AlcoholDehydration-Oxygen	37.002150
373	species252 -> species3 + species517	AlcoholDehydration-Oxygen	41.931881
374	species259 -> species3 + species523	AlcoholDehydration-Oxygen	-26.086152
375	species259 -> species3 + species524	AlcoholDehydration-Oxygen	52.086700
376	species259 -> species3 + species525	AlcoholDehydration-Oxygen	19.408810
377	species260 -> species3 + species527	AlcoholDehydration-Oxygen	34.138444
378	species260 -> species3 + species519	AlcoholDehydration-Oxygen	35.794923
379	species262 -> species3 + species530	AlcoholDehydration-Oxygen	30.261186
380	species262 -> species3 + species531	AlcoholDehydration-Oxygen	35.792894
381	species262 -> species3 + species520	AlcoholDehydration-Oxygen	35.792894
382	species264 -> species3 + species535	AlcoholDehydration-Oxygen	35.792894
383	species264 -> species3 + species521	AlcoholDehydration-Oxygen	35.792894
384	species265 -> species3 + species534	AlcoholDehydration-Oxygen	35.794923
385	species265 -> species3 + species522	AlcoholDehydration-Oxygen	35.794923
386	species266 -> species3 + species544	AlcoholDehydration-Oxygen	40.981083
387	species266 -> species3 + species545	AlcoholDehydration-Oxygen	35.024185
388	species268 -> species3 + species549	AlcoholDehydration-Oxygen	-20.937740
389	species268 -> species3 + species550	AlcoholDehydration-Oxygen	52.088750
390	species269 -> species3 + species523	AlcoholDehydration-Oxygen	-28.561616
391	species269 -> species3 + species551	AlcoholDehydration-Oxygen	13.351700
392	species270 -> species3 + species524	AlcoholDehydration-Oxygen	35.792894
393	species270 -> species3 + species552	AlcoholDehydration-Oxygen	42.196142
394	species270 -> species3 + species551	AlcoholDehydration-Oxygen	-0.466642

395	species270 -> species3 + species550	AlcoholDehydration-Oxygen	42.196142
396	species271 -> species3 + species556	AlcoholDehydration-Oxygen	1.847575
397	species271 -> species3 + species525	AlcoholDehydration-Oxygen	84.959886
398	species271 -> species3 + species549	AlcoholDehydration-Oxygen	51.014592
399	species272 -> species3 + species556	AlcoholDehydration-Oxygen	-70.104594
400	species272 -> species3 + species552	AlcoholDehydration-Oxygen	52.088750
401	species273 -> species3 + species558	AlcoholDehydration-Oxygen	-56.859305
402	species273 -> species3 + species554	AlcoholDehydration-Oxygen	52.086700
403	species274 -> species3 + species557	AlcoholDehydration-Oxygen	-58.309479
404	species274 -> species3 + species553	AlcoholDehydration-Oxygen	52.086700
405	species276 -> species3 + species563	AlcoholDehydration-Oxygen	42.196142
406	species276 -> species3 + species564	AlcoholDehydration-Oxygen	35.792894
407	species276 -> species3 + species565	AlcoholDehydration-Oxygen	2.769457
408	species276 -> species3 + species566	AlcoholDehydration-Oxygen	42.196142
409	species277 -> species3 + species568	AlcoholDehydration-Oxygen	26.429048
410	species277 -> species3 + species569	AlcoholDehydration-Oxygen	35.792894
411	species277 -> species3 + species570	AlcoholDehydration-Oxygen	26.429048
412	species278 -> species3 + species568	AlcoholDehydration-Oxygen	-65.062874
413	species279 -> species3 + species573	AlcoholDehydration-Oxygen	-46.705992
414	species279 -> species3 + species569	AlcoholDehydration-Oxygen	-49.295888
415	species280 -> species3 + species573	AlcoholDehydration-Oxygen	-28.563624
416	species281 -> species3 + species570	AlcoholDehydration-Oxygen	-65.062874
417	species282 -> species3 + species571	AlcoholDehydration-Oxygen	-53.263575
418	species283 -> species3 + species576	AlcoholDehydration-Oxygen	40.012056
419	species284 -> species3 + species579	AlcoholDehydration-Oxygen	38.486603
420	species284 -> species3 + species580	AlcoholDehydration-Oxygen	47.850442
421	species284 -> species3 + species581	AlcoholDehydration-Oxygen	38.486603
422	species290 -> species3 + species584	AlcoholDehydration-Oxygen	30.261186
423	species290 -> species3 + species531	AlcoholDehydration-Oxygen	35.792894
424	species290 -> species3 + species585	AlcoholDehydration-Oxygen	38.270395
425	species292 -> species3 + species589	AlcoholDehydration-Oxygen	54.265685
426	species292 -> species3 + species590	AlcoholDehydration-Oxygen	42.196142
427	species292 -> species3 + species591	AlcoholDehydration-Oxygen	2.769457
428	species292 -> species3 + species592	AlcoholDehydration-Oxygen	42.196142
429	species293 -> species3 + species596	AlcoholDehydration-Oxygen	35.735071
430	species293 -> species3 + species597	AlcoholDehydration-Oxygen	117.474001
431	species294 -> species3 + species598	AlcoholDehydration-Oxygen	35.560695
432	species294 -> species3 + species599	AlcoholDehydration-Oxygen	46.397255
433	species300 -> species3 + species605	AlcoholDehydration-Oxygen	17.650681
434	species300 -> species3 + species606	AlcoholDehydration-Oxygen	35.794923
435	species300 -> species3 + species607	AlcoholDehydration-Oxygen	-49.295888
436	species301 -> species3 + species608	AlcoholDehydration-Oxygen	35.792894
437	species301 -> species3 + species609	AlcoholDehydration-Oxygen	42.196142
438	species301 -> species3 + species610	AlcoholDehydration-Oxygen	42.196142
439	species301 -> species3 + species611	AlcoholDehydration-Oxygen	35.792894
440	species302 -> species3 + species614	AlcoholDehydration-Oxygen	36.520613
441	species304 -> species3 + species618	AlcoholDehydration-Oxygen	36.520613
442	species304 -> species3 + species619	AlcoholDehydration-Oxygen	23.269948
443	species305 -> species3 + species617	AlcoholDehydration-Oxygen	36.522642
444	species305 -> species3 + species621	AlcoholDehydration-Oxygen	36.522642
445	species305 -> species3 + species622	AlcoholDehydration-Oxygen	42.900728
446	species306 -> species3 + species242	AlcoholDehydration-Oxygen	35.560695
447	species307 -> species3 + species243	AlcoholDehydration-Oxygen	117.474001
448	species307 -> species3 + species596	AlcoholDehydration-Oxygen	37.002150
449	species308 -> species3 + species552	AlcoholDehydration-Oxygen	48.595277
450	species310 -> species3 + species534	AlcoholDehydration-Oxygen	35.794923
451	species310 -> species3 + species625	AlcoholDehydration-Oxygen	17.650681
452	species311 -> species3 + species535	AlcoholDehydration-Oxygen	35.792894
453	species311 -> species3 + species628	AlcoholDehydration-Oxygen	10.297623

454	species313 -> species3 + species632	AlcoholDehydration-Oxygen	30.137586
455	species313 -> species3 + species633	AlcoholDehydration-Oxygen	31.106438
456	species313 -> species3 + species634	AlcoholDehydration-Oxygen	28.589029
457	species318 -> species3 + species524	AlcoholDehydration-Oxygen	60.648754
458	species318 -> species3 + species639	AlcoholDehydration-Oxygen	5.593129
459	species319 -> species3 + species640	AlcoholDehydration-Oxygen	78.849195
460	species320 -> species3 + species551	AlcoholDehydration-Oxygen	30.477942
461	species320 -> species3 + species639	AlcoholDehydration-Oxygen	11.681845
462	species321 -> species3 + species640	AlcoholDehydration-Oxygen	84.961936
463	species322 -> species3 + species550	AlcoholDehydration-Oxygen	48.595277
464	species324 -> species3 + species554	AlcoholDehydration-Oxygen	36.537705
465	species325 -> species3 + species553	AlcoholDehydration-Oxygen	36.537705
466	species326 -> species3 + species544	AlcoholDehydration-Oxygen	25.700346
467	species327 -> species3 + species555	AlcoholDehydration-Oxygen	37.473603
468	species332 -> species3 + species662	AlcoholDehydration-Oxygen	35.735071
469	species333 -> species3 + species663	AlcoholDehydration-Oxygen	35.560695
470	species333 -> species3 + species664	AlcoholDehydration-Oxygen	46.397255
471	species334 -> species3 + species665	AlcoholDehydration-Oxygen	109.222107
472	species335 -> species3 + species666	AlcoholDehydration-Oxygen	36.487580
473	species335 -> species3 + species667	AlcoholDehydration-Oxygen	36.520613
474	species337 -> species3 + species666	AlcoholDehydration-Oxygen	22.310029
475	species338 -> species3 + species671	AlcoholDehydration-Oxygen	36.520613
476	species338 -> species3 + species672	AlcoholDehydration-Oxygen	39.421389
477	species340 -> species3 + species662	AlcoholDehydration-Oxygen	37.002150
478	species341 -> species3 + species673	AlcoholDehydration-Oxygen	35.737100
479	species342 -> species3 + species674	AlcoholDehydration-Oxygen	35.562724
480	species342 -> species3 + species675	AlcoholDehydration-Oxygen	46.399305
481	species344 -> species3 + species676	AlcoholDehydration-Oxygen	116.374989
482	species345 -> species3 + species677	AlcoholDehydration-Oxygen	77.567092
483	species347 -> species3 + species673	AlcoholDehydration-Oxygen	37.004179
484	species349 -> species3 + species679	AlcoholDehydration-Oxygen	35.792894
485	species349 -> species3 + species680	AlcoholDehydration-Oxygen	35.792894
486	species350 -> species3 + species683	AlcoholDehydration-Oxygen	-51.812982
487	species350 -> species3 + species606	AlcoholDehydration-Oxygen	35.794923
488	species350 -> species3 + species684	AlcoholDehydration-Oxygen	2.769457
489	species351 -> species3 + species685	AlcoholDehydration-Oxygen	22.545229
490	species351 -> species3 + species686	AlcoholDehydration-Oxygen	17.650681
491	species351 -> species3 + species687	AlcoholDehydration-Oxygen	-39.875779
492	species352 -> species3 + species686	AlcoholDehydration-Oxygen	-51.812982
493	species353 -> species3 + species685	AlcoholDehydration-Oxygen	-65.062874
494	species354 -> species3 + species687	AlcoholDehydration-Oxygen	-42.393125
495	species354 -> species3 + species685	AlcoholDehydration-Oxygen	20.027821
496	species355 -> species3 + species689	AlcoholDehydration-Oxygen	-60.602730
497	species355 -> species3 + species690	AlcoholDehydration-Oxygen	-24.103355
498	species356 -> species3 + species691	AlcoholDehydration-Oxygen	-51.815074
499	species357 -> species3 + species692	AlcoholDehydration-Oxygen	-51.815074
500	species358 -> species3 + species693	AlcoholDehydration-Oxygen	-51.812982
501	species358 -> species3 + species690	AlcoholDehydration-Oxygen	-24.103355
502	species359 -> species3 + species689	AlcoholDehydration-Oxygen	27.003490
503	species359 -> species3 + species691	AlcoholDehydration-Oxygen	42.194134
504	species359 -> species3 + species693	AlcoholDehydration-Oxygen	35.792894
505	species359 -> species3 + species692	AlcoholDehydration-Oxygen	42.194134
506	species360 -> species3 + species694	AlcoholDehydration-Oxygen	-51.812982
507	species361 -> species3 + species695	AlcoholDehydration-Oxygen	-51.812982
508	species363 -> species3 + species697	AlcoholDehydration-Oxygen	35.792894
509	species363 -> species3 + species698	AlcoholDehydration-Oxygen	35.792894
510	species363 -> species3 + species608	AlcoholDehydration-Oxygen	35.792894
511	species363 -> species3 + species699	AlcoholDehydration-Oxygen	2.769457
512	species364 -> species3 + species700	AlcoholDehydration-Oxygen	-46.705992

513	species364 -> species3 + species701	AlcoholDehydration-Oxygen	-49.295888
514	species365 -> species3 + species702	AlcoholDehydration-Oxygen	-49.295888
515	species365 -> species3 + species690	AlcoholDehydration-Oxygen	-24.103355
516	species365 -> species3 + species703	AlcoholDehydration-Oxygen	17.650681
517	species366 -> species3 + species703	AlcoholDehydration-Oxygen	35.792894
518	species366 -> species3 + species700	AlcoholDehydration-Oxygen	-28.563624
519	species367 -> species3 + species702	AlcoholDehydration-Oxygen	35.792894
520	species367 -> species3 + species701	AlcoholDehydration-Oxygen	35.792894
521	species367 -> species3 + species689	AlcoholDehydration-Oxygen	24.486086
522	species371 -> species3 + species705	AlcoholDehydration-Oxygen	46.397255
523	species371 -> species3 + species706	AlcoholDehydration-Oxygen	40.440360
524	species375 -> species3 + species707	AlcoholDehydration-Oxygen	61.318403
525	species376 -> species3 + species708	AlcoholDehydration-Oxygen	-49.297980
526	species376 -> species3 + species709	AlcoholDehydration-Oxygen	-51.166136
527	species377 -> species3 + species710	AlcoholDehydration-Oxygen	-129.419488
528	species378 -> species3 + species709	AlcoholDehydration-Oxygen	-14.551115
529	species379 -> species3 + species711	AlcoholDehydration-Oxygen	-65.062874
530	species380 -> species3 + species708	AlcoholDehydration-Oxygen	54.263677
531	species380 -> species3 + species710	AlcoholDehydration-Oxygen	-37.927500
532	species380 -> species3 + species711	AlcoholDehydration-Oxygen	26.429048
533	species381 -> species3 + species712	AlcoholDehydration-Oxygen	-53.263575
534	species382 -> species3 + species713	AlcoholDehydration-Oxygen	-51.812982
535	species383 -> species3 + species714	AlcoholDehydration-Oxygen	-22.160389
536	species383 -> species3 + species715	AlcoholDehydration-Oxygen	54.265685
537	species383 -> species3 + species716	AlcoholDehydration-Oxygen	42.196142
538	species384 -> species3 + species719	AlcoholDehydration-Oxygen	-10.090846
539	species385 -> species3 + species720	AlcoholDehydration-Oxygen	-14.549107
540	species386 -> species3 + species714	AlcoholDehydration-Oxygen	-28.561616
541	species387 -> species3 + species719	AlcoholDehydration-Oxygen	-22.160389
542	species387 -> species3 + species715	AlcoholDehydration-Oxygen	35.794923
543	species387 -> species3 + species720	AlcoholDehydration-Oxygen	-26.618650
544	species388 -> species3 + species716	AlcoholDehydration-Oxygen	35.794923
545	species389 -> species3 + species721	AlcoholDehydration-Oxygen	54.263677
546	species390 -> species3 + species723	AlcoholDehydration-Oxygen	35.792894
547	species390 -> species3 + species722	AlcoholDehydration-Oxygen	54.263677
548	species391 -> species3 + species724	AlcoholDehydration-Oxygen	35.792894
549	species391 -> species3 + species717	AlcoholDehydration-Oxygen	35.792894
550	species392 -> species3 + species718	AlcoholDehydration-Oxygen	40.251155
551	species393 -> species3 + species707	AlcoholDehydration-Oxygen	55.085582
552	species398 -> species3 + species725	AlcoholDehydration-Oxygen	37.004179
553	species401 -> species3 + species726	AlcoholDehydration-Oxygen	-56.625419
554	species410 -> species3 + species698	AlcoholDehydration-Oxygen	35.792894
555	species410 -> species3 + species729	AlcoholDehydration-Oxygen	42.196142
556	species410 -> species3 + species730	AlcoholDehydration-Oxygen	42.196142
557	species410 -> species3 + species731	AlcoholDehydration-Oxygen	2.769457
558	species412 -> species3 + species734	AlcoholDehydration-Oxygen	41.929872
559	species412 -> species3 + species736	AlcoholDehydration-Oxygen	28.268723
560	species413 -> species3 + species733	AlcoholDehydration-Oxygen	41.929872
561	species413 -> species3 + species737	AlcoholDehydration-Oxygen	36.520613
562	species413 -> species3 + species738	AlcoholDehydration-Oxygen	40.381303
563	species414 -> species3 + species599	AlcoholDehydration-Oxygen	38.452537
564	species415 -> species3 + species735	AlcoholDehydration-Oxygen	41.931881
565	species415 -> species3 + species740	AlcoholDehydration-Oxygen	36.520613
566	species416 -> species3 + species741	AlcoholDehydration-Oxygen	-51.815074
567	species420 -> species3 + species743	AlcoholDehydration-Oxygen	35.792894
568	species420 -> species3 + species744	AlcoholDehydration-Oxygen	35.792894
569	species420 -> species3 + species742	AlcoholDehydration-Oxygen	-51.812982
570	species421 -> species3 + species746	AlcoholDehydration-Oxygen	-129.419488
571	species422 -> species3 + species747	AlcoholDehydration-Oxygen	-65.062874

572	species423 -> species3 + species700	AlcoholDehydration-Oxygen	-28.563624
573	species424 -> species3 + species746	AlcoholDehydration-Oxygen	-37.927500
574	species424 -> species3 + species701	AlcoholDehydration-Oxygen	35.792894
575	species424 -> species3 + species747	AlcoholDehydration-Oxygen	26.429048
576	species425 -> species3 + species748	AlcoholDehydration-Oxygen	-53.263575
577	species426 -> species3 + species750	AlcoholDehydration-Oxygen	34.593848
578	species427 -> species3 + species751	AlcoholDehydration-Oxygen	31.978270
579	species428 -> species3 + species752	AlcoholDehydration-Oxygen	37.004179
580	species431 -> species3 + species756	AlcoholDehydration-Oxygen	49.184803
581	species432 -> species3 + species752	AlcoholDehydration-Oxygen	41.931881
582	species432 -> species3 + species756	AlcoholDehydration-Oxygen	40.451372
583	species433 -> species3 + species753	AlcoholDehydration-Oxygen	41.929872
584	species433 -> species3 + species757	AlcoholDehydration-Oxygen	35.452593
585	species434 -> species3 + species751	AlcoholDehydration-Oxygen	37.387521
586	species436 -> species3 + species677	AlcoholDehydration-Oxygen	70.582281
587	species437 -> species3 + species754	AlcoholDehydration-Oxygen	41.929872
588	species438 -> species3 + species664	AlcoholDehydration-Oxygen	38.452537
589	species439 -> species3 + species675	AlcoholDehydration-Oxygen	38.454567
590	species440 -> species3 + species504	AlcoholDehydration-Oxygen	38.452537
591	species441 -> species3 + species760	AlcoholDehydration-Oxygen	-22.160389
592	species441 -> species3 + species761	AlcoholDehydration-Oxygen	42.196142
593	species441 -> species3 + species762	AlcoholDehydration-Oxygen	35.792894
594	species442 -> species3 + species761	AlcoholDehydration-Oxygen	35.794923
595	species443 -> species3 + species760	AlcoholDehydration-Oxygen	-28.561616
596	species444 -> species3 + species763	AlcoholDehydration-Oxygen	40.251155
597	species464 -> species3 + species764	AlcoholDehydration-Oxygen	35.792894
598	species464 -> species3 + species765	AlcoholDehydration-Oxygen	35.792894
599	species466 -> species3 + species767	AlcoholDehydration-Oxygen	37.004179
600	species474 -> species3 + species770	AlcoholDehydration-Oxygen	37.002150
601	species475 -> species3 + species771	AlcoholDehydration-Oxygen	36.522642
602	species479 -> species3 + species770	AlcoholDehydration-Oxygen	35.735071
603	species483 -> species3 + species772	AlcoholDehydration-Oxygen	46.397255
604	species483 -> species3 + species773	AlcoholDehydration-Oxygen	35.560695
605	species490 -> species3 + species513	AlcoholDehydration-Oxygen	117.440989
606	species491 -> species3 + species777	AlcoholDehydration-Oxygen	36.520613
607	species492 -> species3 + species778	AlcoholDehydration-Oxygen	35.560695
608	species496 -> species3 + species781	AlcoholDehydration-Oxygen	42.194134
609	species496 -> species3 + species782	AlcoholDehydration-Oxygen	35.792894
610	species499 -> species3 + species751	AlcoholDehydration-Oxygen	44.372324
611	species505 -> species3 + species787	AlcoholDehydration-Oxygen	61.353465
612	species506 -> species3 + species787	AlcoholDehydration-Oxygen	60.086382
613	species510 -> species3 + species789	AlcoholDehydration-Oxygen	35.560695
614	species510 -> species3 + species790	AlcoholDehydration-Oxygen	46.397255
615	species511 -> species3 + species791	AlcoholDehydration-Oxygen	26.173723
616	species511 -> species3 + species792	AlcoholDehydration-Oxygen	41.929872
617	species518 -> species3 + species790	AlcoholDehydration-Oxygen	38.452537
618	species520 -> species3 + species798	AlcoholDehydration-Oxygen	30.263219
619	species523 -> species3 + species801	AlcoholDehydration-Oxygen	77.706210
620	species524 -> species3 + species801	AlcoholDehydration-Oxygen	-0.466642
621	species526 -> species3 + species803	AlcoholDehydration-Oxygen	52.086700
622	species526 -> species3 + species804	AlcoholDehydration-Oxygen	-29.758198
623	species526 -> species3 + species805	AlcoholDehydration-Oxygen	35.792894
624	species526 -> species3 + species806	AlcoholDehydration-Oxygen	38.268366
625	species528 -> species3 + species809	AlcoholDehydration-Oxygen	17.650681
626	species528 -> species3 + species810	AlcoholDehydration-Oxygen	42.196142
627	species528 -> species3 + species811	AlcoholDehydration-Oxygen	42.196142
628	species528 -> species3 + species796	AlcoholDehydration-Oxygen	35.792894
629	species529 -> species3 + species814	AlcoholDehydration-Oxygen	36.537705
630	species529 -> species3 + species815	AlcoholDehydration-Oxygen	35.792894

631	species529 -> species3 + species795	AlcoholDehydration-Oxygen	11.681845
632	species530 -> species3 + species817	AlcoholDehydration-Oxygen	35.794923
633	species530 -> species3 + species798	AlcoholDehydration-Oxygen	35.794923
634	species531 -> species3 + species817	AlcoholDehydration-Oxygen	30.263219
635	species532 -> species3 + species372	AlcoholDehydration-Oxygen	29.186630
636	species533 -> species3 + species823	AlcoholDehydration-Oxygen	46.397255
637	species533 -> species3 + species824	AlcoholDehydration-Oxygen	40.440360
638	species536 -> species3 + species814	AlcoholDehydration-Oxygen	52.086700
639	species536 -> species3 + species827	AlcoholDehydration-Oxygen	-32.275585
640	species536 -> species3 + species805	AlcoholDehydration-Oxygen	35.792894
641	species536 -> species3 + species799	AlcoholDehydration-Oxygen	35.792894
642	species538 -> species3 + species832	AlcoholDehydration-Oxygen	23.271977
643	species538 -> species3 + species833	AlcoholDehydration-Oxygen	46.399305
644	species538 -> species3 + species834	AlcoholDehydration-Oxygen	40.442389
645	species539 -> species3 + species826	AlcoholDehydration-Oxygen	84.959886
646	species539 -> species3 + species800	AlcoholDehydration-Oxygen	84.959886
647	species541 -> species3 + species838	AlcoholDehydration-Oxygen	42.898719
648	species541 -> species3 + species839	AlcoholDehydration-Oxygen	36.520613
649	species541 -> species3 + species840	AlcoholDehydration-Oxygen	46.397255
650	species541 -> species3 + species841	AlcoholDehydration-Oxygen	40.440360
651	species542 -> species3 + species842	AlcoholDehydration-Oxygen	17.650681
652	species542 -> species3 + species843	AlcoholDehydration-Oxygen	35.792894
653	species542 -> species3 + species844	AlcoholDehydration-Oxygen	-49.295888
654	species543 -> species3 + species845	AlcoholDehydration-Oxygen	35.792894
655	species543 -> species3 + species846	AlcoholDehydration-Oxygen	42.194134
656	species543 -> species3 + species847	AlcoholDehydration-Oxygen	42.194134
657	species543 -> species3 + species848	AlcoholDehydration-Oxygen	35.792894
658	species546 -> species3 + species852	AlcoholDehydration-Oxygen	46.399305
659	species546 -> species3 + species854	AlcoholDehydration-Oxygen	36.963038
660	species547 -> species3 + species851	AlcoholDehydration-Oxygen	46.399305
661	species547 -> species3 + species853	AlcoholDehydration-Oxygen	47.743331
662	species547 -> species3 + species855	AlcoholDehydration-Oxygen	37.004179
663	species548 -> species3 + species856	AlcoholDehydration-Oxygen	35.792894
664	species548 -> species3 + species857	AlcoholDehydration-Oxygen	35.792894
665	species548 -> species3 + species858	AlcoholDehydration-Oxygen	-51.812982
666	species551 -> species3 + species801	AlcoholDehydration-Oxygen	35.792894
667	species559 -> species3 + species862	AlcoholDehydration-Oxygen	54.263677
668	species559 -> species3 + species863	AlcoholDehydration-Oxygen	42.194134
669	species562 -> species3 + species855	AlcoholDehydration-Oxygen	35.737100
670	species562 -> species3 + species867	AlcoholDehydration-Oxygen	35.562724
671	species562 -> species3 + species859	AlcoholDehydration-Oxygen	46.399305
672	species564 -> species3 + species869	AlcoholDehydration-Oxygen	-61.587225
673	species565 -> species3 + species869	AlcoholDehydration-Oxygen	-28.563624
674	species572 -> species3 + species870	AlcoholDehydration-Oxygen	-49.295888
675	species572 -> species3 + species744	AlcoholDehydration-Oxygen	35.792894
676	species572 -> species3 + species871	AlcoholDehydration-Oxygen	17.650681
677	species574 -> species3 + species765	AlcoholDehydration-Oxygen	35.792894
678	species574 -> species3 + species874	AlcoholDehydration-Oxygen	42.194134
679	species574 -> species3 + species875	AlcoholDehydration-Oxygen	42.194134
680	species574 -> species3 + species876	AlcoholDehydration-Oxygen	35.792894
681	species575 -> species3 + species878	AlcoholDehydration-Oxygen	41.931881
682	species577 -> species3 + species879	AlcoholDehydration-Oxygen	41.929872
683	species577 -> species3 + species880	AlcoholDehydration-Oxygen	36.520613
684	species577 -> species3 + species881	AlcoholDehydration-Oxygen	40.381303
685	species578 -> species3 + species505	AlcoholDehydration-Oxygen	37.002150
686	species584 -> species3 + species817	AlcoholDehydration-Oxygen	35.794923
687	species586 -> species3 + species884	AlcoholDehydration-Oxygen	40.971975
688	species586 -> species3 + species511	AlcoholDehydration-Oxygen	35.562724
689	species586 -> species3 + species885	AlcoholDehydration-Oxygen	41.940834

690	species586 -> species3 + species886	AlcoholDehydration-Oxygen	39.423418
691	species588 -> species3 + species892	AlcoholDehydration-Oxygen	30.261186
692	species589 -> species3 + species895	AlcoholDehydration-Oxygen	-66.047369
693	species591 -> species3 + species895	AlcoholDehydration-Oxygen	-14.551115
694	species595 -> species3 + species897	AlcoholDehydration-Oxygen	36.520613
695	species596 -> species3 + species512	AlcoholDehydration-Oxygen	117.474001
696	species597 -> species3 + species512	AlcoholDehydration-Oxygen	35.735071
697	species604 -> species3 + species899	AlcoholDehydration-Oxygen	35.794923
698	species604 -> species3 + species900	AlcoholDehydration-Oxygen	2.769457
699	species606 -> species3 + species901	AlcoholDehydration-Oxygen	-60.604403
700	species607 -> species3 + species901	AlcoholDehydration-Oxygen	24.486086
701	species608 -> species3 + species902	AlcoholDehydration-Oxygen	-24.103355
702	species611 -> species3 + species902	AlcoholDehydration-Oxygen	-24.103355
703	species615 -> species3 + species484	AlcoholDehydration-Oxygen	34.982332
704	species617 -> species3 + species906	AlcoholDehydration-Oxygen	35.560695
705	species620 -> species3 + species793	AlcoholDehydration-Oxygen	36.520613
706	species620 -> species3 + species908	AlcoholDehydration-Oxygen	46.397255
707	species620 -> species3 + species909	AlcoholDehydration-Oxygen	40.440360
708	species621 -> species3 + species906	AlcoholDehydration-Oxygen	35.560695
709	species623 -> species3 + species803	AlcoholDehydration-Oxygen	36.537705
710	species623 -> species3 + species815	AlcoholDehydration-Oxygen	35.792894
711	species623 -> species3 + species910	AlcoholDehydration-Oxygen	17.648652
712	species624 -> species3 + species826	AlcoholDehydration-Oxygen	84.959886
713	species624 -> species3 + species913	AlcoholDehydration-Oxygen	54.263677
714	species626 -> species3 + species916	AlcoholDehydration-Oxygen	40.969946
715	species626 -> species3 + species917	AlcoholDehydration-Oxygen	38.461470
716	species626 -> species3 + species918	AlcoholDehydration-Oxygen	39.421389
717	species629 -> species3 + species861	AlcoholDehydration-Oxygen	40.971975
718	species629 -> species3 + species921	AlcoholDehydration-Oxygen	35.527666
719	species629 -> species3 + species922	AlcoholDehydration-Oxygen	39.421389
720	species631 -> species3 + species924	AlcoholDehydration-Oxygen	35.792894
721	species631 -> species3 + species856	AlcoholDehydration-Oxygen	35.792894
722	species631 -> species3 + species925	AlcoholDehydration-Oxygen	-51.812982
723	species632 -> species3 + species927	AlcoholDehydration-Oxygen	24.723335
724	species633 -> species3 + species927	AlcoholDehydration-Oxygen	23.754484
725	species635 -> species3 + species928	AlcoholDehydration-Oxygen	36.520613
726	species635 -> species3 + species854	AlcoholDehydration-Oxygen	37.922956
727	species636 -> species3 + species853	AlcoholDehydration-Oxygen	39.491454
728	species636 -> species3 + species929	AlcoholDehydration-Oxygen	37.004179
729	species639 -> species3 + species801	AlcoholDehydration-Oxygen	54.588983
730	species643 -> species3 + species937	AlcoholDehydration-Oxygen	33.038391
731	species645 -> species3 + species941	AlcoholDehydration-Oxygen	17.650681
732	species645 -> species3 + species924	AlcoholDehydration-Oxygen	35.792894
733	species645 -> species3 + species942	AlcoholDehydration-Oxygen	-49.295888
734	species646 -> species3 + species823	AlcoholDehydration-Oxygen	33.038391
735	species647 -> species3 + species833	AlcoholDehydration-Oxygen	38.454567
736	species647 -> species3 + species921	AlcoholDehydration-Oxygen	22.310029
737	species648 -> species3 + species840	AlcoholDehydration-Oxygen	38.452537
738	species648 -> species3 + species946	AlcoholDehydration-Oxygen	36.520613
739	species648 -> species3 + species917	AlcoholDehydration-Oxygen	39.421389
740	species649 -> species3 + species852	AlcoholDehydration-Oxygen	38.454567
741	species650 -> species3 + species851	AlcoholDehydration-Oxygen	38.454567
742	species650 -> species3 + species947	AlcoholDehydration-Oxygen	37.004179
743	species651 -> species3 + species948	AlcoholDehydration-Oxygen	54.263677
744	species651 -> species3 + species949	AlcoholDehydration-Oxygen	42.194134
745	species651 -> species3 + species950	AlcoholDehydration-Oxygen	42.194134
746	species651 -> species3 + species951	AlcoholDehydration-Oxygen	35.792894
747	species652 -> species3 + species947	AlcoholDehydration-Oxygen	35.737100
748	species652 -> species3 + species859	AlcoholDehydration-Oxygen	38.454567

749	species653 -> species3 + species860	AlcoholDehydration-Oxygen	41.931881
750	species653 -> species3 + species953	AlcoholDehydration-Oxygen	28.268723
751	species655 -> species3 + species955	AlcoholDehydration-Oxygen	22.312059
752	species656 -> species3 + species957	AlcoholDehydration-Oxygen	36.520613
753	species656 -> species3 + species958	AlcoholDehydration-Oxygen	37.922956
754	species658 -> species3 + species959	AlcoholDehydration-Oxygen	37.004179
755	species659 -> species3 + species959	AlcoholDehydration-Oxygen	35.737100
756	species660 -> species3 + species955	AlcoholDehydration-Oxygen	35.529695
757	species660 -> species3 + species960	AlcoholDehydration-Oxygen	46.399305
758	species670 -> species3 + species962	AlcoholDehydration-Oxygen	46.397255
759	species670 -> species3 + species958	AlcoholDehydration-Oxygen	36.963038
760	species678 -> species3 + species964	AlcoholDehydration-Oxygen	96.667303
761	species681 -> species3 + species966	AlcoholDehydration-Oxygen	41.929872
762	species681 -> species3 + species967	AlcoholDehydration-Oxygen	46.397255
763	species681 -> species3 + species968	AlcoholDehydration-Oxygen	37.922956
764	species683 -> species3 + species901	AlcoholDehydration-Oxygen	27.003490
765	species683 -> species3 + species970	AlcoholDehydration-Oxygen	12.189461
766	species684 -> species3 + species970	AlcoholDehydration-Oxygen	-42.393125
767	species685 -> species3 + species971	AlcoholDehydration-Oxygen	13.173956
768	species687 -> species3 + species971	AlcoholDehydration-Oxygen	75.594964
769	species688 -> species3 + species972	AlcoholDehydration-Oxygen	-51.812982
770	species688 -> species3 + species973	AlcoholDehydration-Oxygen	54.265685
771	species688 -> species3 + species843	AlcoholDehydration-Oxygen	35.792894
772	species689 -> species3 + species974	AlcoholDehydration-Oxygen	35.792894
773	species690 -> species3 + species974	AlcoholDehydration-Oxygen	-0.706343
774	species693 -> species3 + species974	AlcoholDehydration-Oxygen	27.003490
775	species696 -> species3 + species951	AlcoholDehydration-Oxygen	35.792894
776	species696 -> species3 + species975	AlcoholDehydration-Oxygen	35.792894
777	species696 -> species3 + species976	AlcoholDehydration-Oxygen	54.263677
778	species696 -> species3 + species848	AlcoholDehydration-Oxygen	35.792894
779	species697 -> species3 + species902	AlcoholDehydration-Oxygen	-24.103355
780	species697 -> species3 + species977	AlcoholDehydration-Oxygen	2.769457
781	species698 -> species3 + species978	AlcoholDehydration-Oxygen	-61.587225
782	species699 -> species3 + species978	AlcoholDehydration-Oxygen	-28.563624
783	species699 -> species3 + species977	AlcoholDehydration-Oxygen	35.792894
784	species702 -> species3 + species974	AlcoholDehydration-Oxygen	24.486086
785	species704 -> species3 + species927	AlcoholDehydration-Oxygen	28.221888
786	species727 -> species3 + species981	AlcoholDehydration-Oxygen	-51.812982
787	species728 -> species3 + species982	AlcoholDehydration-Oxygen	35.792894
788	species728 -> species3 + species983	AlcoholDehydration-Oxygen	35.792894
789	species731 -> species3 + species978	AlcoholDehydration-Oxygen	-28.563624
790	species733 -> species3 + species984	AlcoholDehydration-Oxygen	-49.935203
791	species737 -> species3 + species984	AlcoholDehydration-Oxygen	-44.525710
792	species739 -> species3 + species963	AlcoholDehydration-Oxygen	39.414485
793	species741 -> species3 + species986	AlcoholDehydration-Oxygen	-42.393125
794	species742 -> species3 + species987	AlcoholDehydration-Oxygen	35.792894
795	species742 -> species3 + species988	AlcoholDehydration-Oxygen	22.545229
796	species743 -> species3 + species987	AlcoholDehydration-Oxygen	-51.812982
797	species744 -> species3 + species988	AlcoholDehydration-Oxygen	-65.060782
798	species745 -> species3 + species705	AlcoholDehydration-Oxygen	33.036358
799	species750 -> species3 + species992	AlcoholDehydration-Oxygen	41.931881
800	species755 -> species3 + species993	AlcoholDehydration-Oxygen	22.205927
801	species755 -> species3 + species994	AlcoholDehydration-Oxygen	41.929872
802	species758 -> species3 + species960	AlcoholDehydration-Oxygen	38.454567
803	species759 -> species3 + species772	AlcoholDehydration-Oxygen	38.452537
804	species764 -> species3 + species996	AlcoholDehydration-Oxygen	35.792894
805	species764 -> species3 + species997	AlcoholDehydration-Oxygen	35.792894
806	species765 -> species3 + species997	AlcoholDehydration-Oxygen	35.792894
807	species774 -> species3 + species984	AlcoholDehydration-Oxygen	-37.540982

808	species779 -> species3 + species1000	AlcoholDehydration-Oxygen	36.520613
809	species780 -> species3 + species771	AlcoholDehydration-Oxygen	35.562724
810	species782 -> species3 + species1001	AlcoholDehydration-Oxygen	-14.433126
811	species783 -> species3 + species964	AlcoholDehydration-Oxygen	81.458673
812	species786 -> species3 + species1002	AlcoholDehydration-Oxygen	22.205927
813	species786 -> species3 + species1003	AlcoholDehydration-Oxygen	41.931881
814	species793 -> species3 + species1004	AlcoholDehydration-Oxygen	32.189679
815	species794 -> species3 + species967	AlcoholDehydration-Oxygen	38.452537
816	species795 -> species3 + species1005	AlcoholDehydration-Oxygen	60.648754
817	species796 -> species3 + species1006	AlcoholDehydration-Oxygen	-46.705992
818	species799 -> species3 + species1005	AlcoholDehydration-Oxygen	52.086700
819	species799 -> species3 + species1009	AlcoholDehydration-Oxygen	16.891406
820	species802 -> species3 + species1011	AlcoholDehydration-Oxygen	-32.275585
821	species802 -> species3 + species1010	AlcoholDehydration-Oxygen	52.086700
822	species803 -> species3 + species1014	AlcoholDehydration-Oxygen	35.792894
823	species803 -> species3 + species1015	AlcoholDehydration-Oxygen	-0.466642
824	species804 -> species3 + species1018	AlcoholDehydration-Oxygen	-0.097404
825	species805 -> species3 + species1018	AlcoholDehydration-Oxygen	-65.648634
826	species805 -> species3 + species1014	AlcoholDehydration-Oxygen	52.086700
827	species806 -> species3 + species1015	AlcoholDehydration-Oxygen	13.351700
828	species808 -> species3 + species1024	AlcoholDehydration-Oxygen	40.971975
829	species808 -> species3 + species1025	AlcoholDehydration-Oxygen	39.480442
830	species808 -> species3 + species1017	AlcoholDehydration-Oxygen	46.399305
831	species808 -> species3 + species1026	AlcoholDehydration-Oxygen	41.938784
832	species808 -> species3 + species1027	AlcoholDehydration-Oxygen	39.421389
833	species809 -> species3 + species1006	AlcoholDehydration-Oxygen	-28.563624
834	species814 -> species3 + species1014	AlcoholDehydration-Oxygen	35.792894
835	species814 -> species3 + species1005	AlcoholDehydration-Oxygen	35.792894
836	species815 -> species3 + species1014	AlcoholDehydration-Oxygen	36.537705
837	species816 -> species3 + species1029	AlcoholDehydration-Oxygen	34.602785
838	species816 -> species3 + species1008	AlcoholDehydration-Oxygen	11.683874
839	species818 -> species3 + species1030	AlcoholDehydration-Oxygen	35.792894
840	species818 -> species3 + species1031	AlcoholDehydration-Oxygen	35.792894
841	species819 -> species3 + species621	AlcoholDehydration-Oxygen	35.562724
842	species820 -> species3 + species667	AlcoholDehydration-Oxygen	35.560695
843	species821 -> species3 + species671	AlcoholDehydration-Oxygen	35.560695
844	species822 -> species3 + species1034	AlcoholDehydration-Oxygen	2.769457
845	species822 -> species3 + species1035	AlcoholDehydration-Oxygen	35.792894
846	species825 -> species3 + species1036	AlcoholDehydration-Oxygen	46.397255
847	species825 -> species3 + species1037	AlcoholDehydration-Oxygen	36.963038
848	species827 -> species3 + species1018	AlcoholDehydration-Oxygen	2.419988
849	species827 -> species3 + species1009	AlcoholDehydration-Oxygen	84.959886
850	species828 -> species3 + species1039	AlcoholDehydration-Oxygen	30.586940
851	species828 -> species3 + species937	AlcoholDehydration-Oxygen	40.023198
852	species829 -> species3 + species1043	AlcoholDehydration-Oxygen	46.399305
853	species829 -> species3 + species1044	AlcoholDehydration-Oxygen	40.442389
854	species832 -> species3 + species1047	AlcoholDehydration-Oxygen	32.189679
855	species833 -> species3 + species1047	AlcoholDehydration-Oxygen	9.062364
856	species836 -> species3 + species1049	AlcoholDehydration-Oxygen	40.442389
857	species836 -> species3 + species1050	AlcoholDehydration-Oxygen	46.399305
858	species838 -> species3 + species1051	AlcoholDehydration-Oxygen	28.223917
859	species839 -> species3 + species1052	AlcoholDehydration-Oxygen	46.399305
860	species839 -> species3 + species1053	AlcoholDehydration-Oxygen	23.715372
861	species840 -> species3 + species1052	AlcoholDehydration-Oxygen	36.522642
862	species840 -> species3 + species1051	AlcoholDehydration-Oxygen	24.725365
863	species841 -> species3 + species1053	AlcoholDehydration-Oxygen	19.795625
864	species843 -> species3 + species1054	AlcoholDehydration-Oxygen	-60.602730
865	species844 -> species3 + species1054	AlcoholDehydration-Oxygen	24.486086
866	species845 -> species3 + species1055	AlcoholDehydration-Oxygen	-24.105363

867	species848 -> species3 + species1055	AlcoholDehydration-Oxygen	-24.105363
868	species851 -> species3 + species1056	AlcoholDehydration-Oxygen	37.002150
869	species853 -> species3 + species1057	AlcoholDehydration-Oxygen	37.004179
870	species855 -> species3 + species1057	AlcoholDehydration-Oxygen	47.743331
871	species855 -> species3 + species1056	AlcoholDehydration-Oxygen	46.397255
872	species856 -> species3 + species1058	AlcoholDehydration-Oxygen	-51.812982
873	species857 -> species3 + species1059	AlcoholDehydration-Oxygen	-51.812982
874	species858 -> species3 + species1059	AlcoholDehydration-Oxygen	35.792894
875	species858 -> species3 + species1058	AlcoholDehydration-Oxygen	35.792894
876	species859 -> species3 + species1056	AlcoholDehydration-Oxygen	35.735071
877	species861 -> species3 + species1047	AlcoholDehydration-Oxygen	19.762593
878	species862 -> species3 + species1060	AlcoholDehydration-Oxygen	-14.549107
879	species867 -> species3 + species1057	AlcoholDehydration-Oxygen	47.917720
880	species868 -> species3 + species983	AlcoholDehydration-Oxygen	35.792894
881	species868 -> species3 + species1061	AlcoholDehydration-Oxygen	2.769457
882	species870 -> species3 + species988	AlcoholDehydration-Oxygen	20.027821
883	species872 -> species3 + species786	AlcoholDehydration-Oxygen	40.969946
884	species872 -> species3 + species1064	AlcoholDehydration-Oxygen	39.421389
885	species873 -> species3 + species1065	AlcoholDehydration-Oxygen	-51.812982
886	species876 -> species3 + species997	AlcoholDehydration-Oxygen	35.792894
887	species879 -> species3 + species1004	AlcoholDehydration-Oxygen	19.795625
888	species880 -> species3 + species1004	AlcoholDehydration-Oxygen	25.204872
889	species882 -> species3 + species1029	AlcoholDehydration-Oxygen	20.029854
890	species883 -> species3 + species1067	AlcoholDehydration-Oxygen	35.792894
891	species883 -> species3 + species1030	AlcoholDehydration-Oxygen	35.792894
892	species884 -> species3 + species792	AlcoholDehydration-Oxygen	36.520613
893	species884 -> species3 + species1069	AlcoholDehydration-Oxygen	24.723335
894	species885 -> species3 + species1069	AlcoholDehydration-Oxygen	23.754484
895	species886 -> species3 + species791	AlcoholDehydration-Oxygen	22.313029
896	species887 -> species3 + species1070	AlcoholDehydration-Oxygen	36.520613
897	species887 -> species3 + species1037	AlcoholDehydration-Oxygen	37.922956
898	species888 -> species3 + species663	AlcoholDehydration-Oxygen	27.308809
899	species889 -> species3 + species665	AlcoholDehydration-Oxygen	117.474001
900	species891 -> species3 + species789	AlcoholDehydration-Oxygen	35.560695
901	species893 -> species3 + species1073	AlcoholDehydration-Oxygen	38.452537
902	species893 -> species3 + species946	AlcoholDehydration-Oxygen	35.560695
903	species896 -> species3 + species1035	AlcoholDehydration-Oxygen	35.792894
904	species896 -> species3 + species1076	AlcoholDehydration-Oxygen	54.265685
905	species898 -> species3 + species756	AlcoholDehydration-Oxygen	47.917720
906	species904 -> species3 + species791	AlcoholDehydration-Oxygen	19.795625
907	species907 -> species3 + species1069	AlcoholDehydration-Oxygen	28.221888
908	species908 -> species3 + species1004	AlcoholDehydration-Oxygen	22.313029
909	species910 -> species3 + species1015	AlcoholDehydration-Oxygen	18.422416
910	species911 -> species3 + species1078	AlcoholDehydration-Oxygen	35.555795
911	species911 -> species3 + species1017	AlcoholDehydration-Oxygen	33.038391
912	species911 -> species3 + species1079	AlcoholDehydration-Oxygen	33.045291
913	species911 -> species3 + species1080	AlcoholDehydration-Oxygen	34.005209
914	species912 -> species3 + species1016	AlcoholDehydration-Oxygen	40.971975
915	species915 -> species3 + species1083	AlcoholDehydration-Oxygen	40.971975
916	species915 -> species3 + species1084	AlcoholDehydration-Oxygen	36.963038
917	species915 -> species3 + species1085	AlcoholDehydration-Oxygen	39.421389
918	species916 -> species3 + species1051	AlcoholDehydration-Oxygen	21.248042
919	species917 -> species3 + species1051	AlcoholDehydration-Oxygen	23.756514
920	species921 -> species3 + species1047	AlcoholDehydration-Oxygen	25.206901
921	species924 -> species3 + species1087	AlcoholDehydration-Oxygen	-60.602730
922	species925 -> species3 + species1087	AlcoholDehydration-Oxygen	27.003490
923	species925 -> species3 + species1058	AlcoholDehydration-Oxygen	35.792894
924	species926 -> species3 + species1039	AlcoholDehydration-Oxygen	36.963038
925	species926 -> species3 + species1088	AlcoholDehydration-Oxygen	41.938784

926	species929 -> species3 + species1057	AlcoholDehydration-Oxygen	39.491454
927	species930 -> species3 + species1010	AlcoholDehydration-Oxygen	36.537705
928	species932 -> species3 + species1093	AlcoholDehydration-Oxygen	39.423418
929	species932 -> species3 + species1094	AlcoholDehydration-Oxygen	36.522642
930	species933 -> species3 + species1095	AlcoholDehydration-Oxygen	38.454567
931	species934 -> species3 + species1096	AlcoholDehydration-Oxygen	22.310029
932	species935 -> species3 + species1097	AlcoholDehydration-Oxygen	38.452537
933	species936 -> species3 + species1098	AlcoholDehydration-Oxygen	-51.812982
934	species939 -> species3 + species1100	AlcoholDehydration-Oxygen	37.002150
935	species940 -> species3 + species1067	AlcoholDehydration-Oxygen	35.792894
936	species940 -> species3 + species1101	AlcoholDehydration-Oxygen	2.769457
937	species942 -> species3 + species1087	AlcoholDehydration-Oxygen	24.486086
938	species943 -> species3 + species1036	AlcoholDehydration-Oxygen	38.452537
939	species944 -> species3 + species1043	AlcoholDehydration-Oxygen	33.038391
940	species945 -> species3 + species1050	AlcoholDehydration-Oxygen	38.454567
941	species945 -> species3 + species1103	AlcoholDehydration-Oxygen	46.399305
942	species945 -> species3 + species1084	AlcoholDehydration-Oxygen	36.963038
943	species946 -> species3 + species1052	AlcoholDehydration-Oxygen	38.454567
944	species947 -> species3 + species1056	AlcoholDehydration-Oxygen	38.452537
945	species948 -> species3 + species1104	AlcoholDehydration-Oxygen	-28.561616
946	species951 -> species3 + species1104	AlcoholDehydration-Oxygen	-10.090846
947	species956 -> species3 + species1106	AlcoholDehydration-Oxygen	44.798757
948	species956 -> species3 + species1107	AlcoholDehydration-Oxygen	35.307483
949	species961 -> species3 + species1053	AlcoholDehydration-Oxygen	23.715372
950	species966 -> species3 + species1110	AlcoholDehydration-Oxygen	29.343986
951	species967 -> species3 + species1110	AlcoholDehydration-Oxygen	24.876587
952	species972 -> species3 + species1111	AlcoholDehydration-Oxygen	54.263677
953	species972 -> species3 + species1054	AlcoholDehydration-Oxygen	27.003490
954	species973 -> species3 + species1111	AlcoholDehydration-Oxygen	-51.815074
955	species975 -> species3 + species1055	AlcoholDehydration-Oxygen	-24.105363
956	species975 -> species3 + species1112	AlcoholDehydration-Oxygen	54.265685
957	species976 -> species3 + species1112	AlcoholDehydration-Oxygen	35.794923
958	species976 -> species3 + species1104	AlcoholDehydration-Oxygen	-28.561616
959	species979 -> species3 + species1113	AlcoholDehydration-Oxygen	-51.812982
960	species989 -> species3 + species1114	AlcoholDehydration-Oxygen	35.792894
961	species989 -> species3 + species1115	AlcoholDehydration-Oxygen	35.792894
962	species990 -> species3 + species908	AlcoholDehydration-Oxygen	38.452537
963	species990 -> species3 + species880	AlcoholDehydration-Oxygen	35.560695
964	species991 -> species3 + species962	AlcoholDehydration-Oxygen	38.452537
965	species995 -> species3 + species1002	AlcoholDehydration-Oxygen	28.221888
966	species1007 -> species3 + species1119	AlcoholDehydration-Oxygen	35.792894
967	species1007 -> species3 + species1120	AlcoholDehydration-Oxygen	17.650681
968	species1012 -> species3 + species1125	AlcoholDehydration-Oxygen	38.452537
969	species1012 -> species3 + species1126	AlcoholDehydration-Oxygen	36.963038
970	species1012 -> species3 + species1122	AlcoholDehydration-Oxygen	46.397255
971	species1017 -> species3 + species1130	AlcoholDehydration-Oxygen	40.969946
972	species1017 -> species3 + species1131	AlcoholDehydration-Oxygen	23.763417
973	species1017 -> species3 + species1132	AlcoholDehydration-Oxygen	39.421389
974	species1019 -> species3 + species1134	AlcoholDehydration-Oxygen	35.560695
975	species1019 -> species3 + species1129	AlcoholDehydration-Oxygen	46.397255
976	species1020 -> species3 + species1100	AlcoholDehydration-Oxygen	35.735071
977	species1021 -> species3 + species1096	AlcoholDehydration-Oxygen	36.487580
978	species1021 -> species3 + species1135	AlcoholDehydration-Oxygen	37.922956
979	species1022 -> species3 + species1134	AlcoholDehydration-Oxygen	27.308809
980	species1023 -> species3 + species1136	AlcoholDehydration-Oxygen	35.792894
981	species1023 -> species3 + species1137	AlcoholDehydration-Oxygen	35.792894
982	species1024 -> species3 + species1138	AlcoholDehydration-Oxygen	40.440360
983	species1024 -> species3 + species1130	AlcoholDehydration-Oxygen	46.397255
984	species1024 -> species3 + species1139	AlcoholDehydration-Oxygen	24.723335

985	species1025 -> species3 + species1138	AlcoholDehydration-Oxygen	41.931881
986	species1025 -> species3 + species1140	AlcoholDehydration-Oxygen	22.207957
987	species1026 -> species3 + species1131	AlcoholDehydration-Oxygen	28.223917
988	species1026 -> species3 + species1139	AlcoholDehydration-Oxygen	23.756514
989	species1027 -> species3 + species1140	AlcoholDehydration-Oxygen	22.267014
990	species1027 -> species3 + species1132	AlcoholDehydration-Oxygen	46.399305
991	species1028 -> species3 + species1119	AlcoholDehydration-Oxygen	35.792894
992	species1028 -> species3 + species1117	AlcoholDehydration-Oxygen	11.681845
993	species1032 -> species3 + species839	AlcoholDehydration-Oxygen	35.560695
994	species1032 -> species3 + species1073	AlcoholDehydration-Oxygen	46.397255
995	species1032 -> species3 + species1141	AlcoholDehydration-Oxygen	36.963038
996	species1033 -> species3 + species957	AlcoholDehydration-Oxygen	35.560695
997	species1038 -> species3 + species1136	AlcoholDehydration-Oxygen	35.792894
998	species1038 -> species3 + species1142	AlcoholDehydration-Oxygen	35.792894
999	species1040 -> species3 + species1135	AlcoholDehydration-Oxygen	36.963038
1000	species1040 -> species3 + species1097	AlcoholDehydration-Oxygen	46.397255
1001	species1041 -> species3 + species1144	AlcoholDehydration-Oxygen	36.965067
1002	species1041 -> species3 + species1095	AlcoholDehydration-Oxygen	46.399305
1003	species1042 -> species3 + species1145	AlcoholDehydration-Oxygen	54.263677
1004	species1042 -> species3 + species1146	AlcoholDehydration-Oxygen	35.792894
1005	species1046 -> species3 + species1139	AlcoholDehydration-Oxygen	28.221888
1006	species1049 -> species3 + species1148	AlcoholDehydration-Oxygen	28.221888
1007	species1050 -> species3 + species1149	AlcoholDehydration-Oxygen	46.397255
1008	species1050 -> species3 + species1148	AlcoholDehydration-Oxygen	22.264984
1009	species1063 -> species3 + species1114	AlcoholDehydration-Oxygen	35.792894
1010	species1064 -> species3 + species1002	AlcoholDehydration-Oxygen	23.754484
1011	species1066 -> species3 + species1103	AlcoholDehydration-Oxygen	38.454567
1012	species1068 -> species3 + species961	AlcoholDehydration-Oxygen	35.560695
1013	species1068 -> species3 + species1141	AlcoholDehydration-Oxygen	36.963038
1014	species1068 -> species3 + species1152	AlcoholDehydration-Oxygen	41.938784
1015	species1073 -> species3 + species1052	AlcoholDehydration-Oxygen	35.562724
1016	species1078 -> species3 + species1130	AlcoholDehydration-Oxygen	38.452537
1017	species1078 -> species3 + species1131	AlcoholDehydration-Oxygen	21.246009
1018	species1079 -> species3 + species1131	AlcoholDehydration-Oxygen	23.756514
1019	species1080 -> species3 + species1132	AlcoholDehydration-Oxygen	38.454567
1020	species1081 -> species3 + species1129	AlcoholDehydration-Oxygen	38.452537
1021	species1083 -> species3 + species1148	AlcoholDehydration-Oxygen	19.747576
1022	species1084 -> species3 + species1148	AlcoholDehydration-Oxygen	23.756514
1023	species1086 -> species3 + species1144	AlcoholDehydration-Oxygen	37.924985
1024	species1086 -> species3 + species1093	AlcoholDehydration-Oxygen	39.423418
1025	species1089 -> species3 + species1122	AlcoholDehydration-Oxygen	38.454567
1026	species1090 -> species3 + species1156	AlcoholDehydration-Oxygen	40.381303
1027	species1090 -> species3 + species1157	AlcoholDehydration-Oxygen	39.421389
1028	species1090 -> species3 + species1123	AlcoholDehydration-Oxygen	41.929872
1029	species1091 -> species3 + species1158	AlcoholDehydration-Oxygen	92.539243
1030	species1092 -> species3 + species1159	AlcoholDehydration-Oxygen	36.963038
1031	species1092 -> species3 + species1158	AlcoholDehydration-Oxygen	46.397255
1032	species1102 -> species3 + species1162	AlcoholDehydration-Oxygen	54.263677
1033	species1102 -> species3 + species1137	AlcoholDehydration-Oxygen	35.792894
1034	species1103 -> species3 + species1149	AlcoholDehydration-Oxygen	38.452537
1035	species1105 -> species3 + species1140	AlcoholDehydration-Oxygen	19.749610
1036	species1109 -> species3 + species1106	AlcoholDehydration-Oxygen	85.564599
1037	species1122 -> species3 + species1165	AlcoholDehydration-Oxygen	38.452537
1038	species1123 -> species3 + species1166	AlcoholDehydration-Oxygen	21.246009
1039	species1125 -> species3 + species1168	AlcoholDehydration-Oxygen	36.963038
1040	species1125 -> species3 + species1165	AlcoholDehydration-Oxygen	46.397255
1041	species1126 -> species3 + species1168	AlcoholDehydration-Oxygen	38.452537
1042	species1130 -> species3 + species1170	AlcoholDehydration-Oxygen	-63.182584
1043	species1131 -> species3 + species1170	AlcoholDehydration-Oxygen	-45.976302

1044	species1133 -> species3 + species1161	AlcoholDehydration-Oxygen	42.898719
1045	species1133 -> species3 + species1171	AlcoholDehydration-Oxygen	37.922956
1046	species1133 -> species3 + species1172	AlcoholDehydration-Oxygen	40.440360
1047	species1133 -> species3 + species1169	AlcoholDehydration-Oxygen	46.397255
1048	species1139 -> species3 + species1170	AlcoholDehydration-Oxygen	-41.508795
1049	species1141 -> species3 + species1053	AlcoholDehydration-Oxygen	22.313029
1050	species1143 -> species3 + species1125	AlcoholDehydration-Oxygen	46.397255
1051	species1143 -> species3 + species1171	AlcoholDehydration-Oxygen	36.963038
1052	species1153 -> species3 + species1094	AlcoholDehydration-Oxygen	35.562724
1053	species1154 -> species3 + species1169	AlcoholDehydration-Oxygen	38.452537
1054	species1154 -> species3 + species1126	AlcoholDehydration-Oxygen	37.922956
1055	species1154 -> species3 + species1157	AlcoholDehydration-Oxygen	39.421389
1056	species1155 -> species3 + species1159	AlcoholDehydration-Oxygen	37.922956
1057	species1157 -> species3 + species1166	AlcoholDehydration-Oxygen	23.754484
1058	species1161 -> species3 + species1166	AlcoholDehydration-Oxygen	28.221888
1059	species1163 -> species3 + species1174	AlcoholDehydration-Oxygen	63.941896
1060	species1164 -> species3 + species1175	AlcoholDehydration-Oxygen	37.922956
1061	species1164 -> species3 + species1176	AlcoholDehydration-Oxygen	39.421389
1062	species1167 -> species3 + species1174	AlcoholDehydration-Oxygen	14.425696
1063	species1167 -> species3 + species1175	AlcoholDehydration-Oxygen	36.963038
1064	species1169 -> species3 + species1166	AlcoholDehydration-Oxygen	24.723335
1065	species1169 -> species3 + species1168	AlcoholDehydration-Oxygen	37.922956
1066	species1171 -> species3 + species1177	AlcoholDehydration-Oxygen	22.264984
1067	species1171 -> species3 + species1168	AlcoholDehydration-Oxygen	46.397255
1068	species1172 -> species3 + species1177	AlcoholDehydration-Oxygen	19.747576
1069	species4 -> species3 + species13	AlcoholRingClosure-Oxygen	-18.390521
1070	species16 -> species3 + species81	AlcoholRingClosure-Oxygen	-18.388513
1071	species97 -> species3 + species260	AlcoholRingClosure-Oxygen	-18.390521
1072	species105 -> species3 + species260	AlcoholRingClosure-Oxygen	-12.769108
1073	species318 -> species3 + species519	AlcoholRingClosure-Oxygen	11.343987
1074	species623 -> species3 + species797	AlcoholRingClosure-Oxygen	-12.769108
1075	species2 + species7 -> species1	AldehydeHydrogenation-Oxygen	140.434454
1076	species2 + species9 -> species30	AldehydeHydrogenation-Oxygen	-20.506412
1077	species2 + species14 -> species4	AldehydeHydrogenation-Oxygen	-22.058885
1078	species2 + species19 -> species105	AldehydeHydrogenation-Oxygen	-20.504403
1079	species2 + species25 -> species5	AldehydeHydrogenation-Oxygen	-15.112231
1080	species2 + species31 -> species6	AldehydeHydrogenation-Oxygen	-15.114282
1081	species2 + species43 -> species7	AldehydeHydrogenation-Oxygen	-170.247378
1082	species2 + species46 -> species10	AldehydeHydrogenation-Oxygen	-19.546518
1083	species2 + species47 -> species11	AldehydeHydrogenation-Oxygen	-92.247995
1084	species2 + species48 -> species12	AldehydeHydrogenation-Oxygen	-22.058885
1085	species2 + species49 -> species12	AldehydeHydrogenation-Oxygen	-22.058885
1086	species2 + species50 -> species11	AldehydeHydrogenation-Oxygen	-21.098992
1087	species2 + species51 -> species10	AldehydeHydrogenation-Oxygen	-21.098992
1088	species2 + species52 -> species139	AldehydeHydrogenation-Oxygen	-18.586583
1089	species2 + species52 -> species9	AldehydeHydrogenation-Oxygen	-21.098992
1090	species2 + species53 -> species8	AldehydeHydrogenation-Oxygen	-21.098992
1091	species2 + species54 -> species218	AldehydeHydrogenation-Oxygen	-81.576703
1092	species2 + species55 -> species220	AldehydeHydrogenation-Oxygen	-21.098992
1093	species2 + species62 -> species153	AldehydeHydrogenation-Oxygen	-19.546518
1094	species2 + species64 -> species221	AldehydeHydrogenation-Oxygen	-127.328743
1095	species2 + species66 -> species154	AldehydeHydrogenation-Oxygen	-20.506412
1096	species2 + species67 -> species123	AldehydeHydrogenation-Oxygen	-20.506412
1097	species2 + species68 -> species151	AldehydeHydrogenation-Oxygen	-20.506412
1098	species2 + species69 -> species150	AldehydeHydrogenation-Oxygen	-20.506412
1099	species2 + species70 -> species152	AldehydeHydrogenation-Oxygen	-14.130330
1100	species2 + species71 -> species246	AldehydeHydrogenation-Oxygen	-86.625536
1101	species2 + species77 -> species219	AldehydeHydrogenation-Oxygen	-131.350404
1102	species2 + species86 -> species284	AldehydeHydrogenation-Oxygen	-116.204742

1103	species2 + species87 -> species15	AldehydeHydrogenation-Oxygen	-22.058885
1104	species2 + species88 -> species16	AldehydeHydrogenation-Oxygen	-22.058885
1105	species2 + species89 -> species17	AldehydeHydrogenation-Oxygen	-22.058885
1106	species2 + species90 -> species18	AldehydeHydrogenation-Oxygen	-22.058885
1107	species2 + species91 -> species21	AldehydeHydrogenation-Oxygen	-22.058885
1108	species2 + species92 -> species22	AldehydeHydrogenation-Oxygen	-22.058885
1109	species2 + species93 -> species24	AldehydeHydrogenation-Oxygen	-20.139056
1110	species2 + species94 -> species23	AldehydeHydrogenation-Oxygen	-11.226551
1111	species2 + species95 -> species308	AldehydeHydrogenation-Oxygen	-32.561938
1112	species2 + species99 -> species318	AldehydeHydrogenation-Oxygen	-44.617339
1113	species2 + species101 -> species320	AldehydeHydrogenation-Oxygen	-32.561938
1114	species2 + species103 -> species322	AldehydeHydrogenation-Oxygen	-32.561938
1115	species2 + species107 -> species324	AldehydeHydrogenation-Oxygen	-20.504403
1116	species2 + species108 -> species325	AldehydeHydrogenation-Oxygen	-20.504403
1117	species2 + species109 -> species327	AldehydeHydrogenation-Oxygen	-15.090224
1118	species2 + species110 -> species326	AldehydeHydrogenation-Oxygen	-9.672027
1119	species2 + species119 -> species23	AldehydeHydrogenation-Oxygen	-14.722868
1120	species2 + species121 -> species313	AldehydeHydrogenation-Oxygen	-8.712134
1121	species2 + species131 -> species25	AldehydeHydrogenation-Oxygen	-15.114282
1122	species2 + species132 -> species26	AldehydeHydrogenation-Oxygen	-0.233049
1123	species2 + species133 -> species27	AldehydeHydrogenation-Oxygen	-15.114282
1124	species2 + species134 -> species27	AldehydeHydrogenation-Oxygen	-15.114282
1125	species2 + species135 -> species26	AldehydeHydrogenation-Oxygen	-15.114282
1126	species2 + species136 -> species28	AldehydeHydrogenation-Oxygen	-15.114282
1127	species2 + species137 -> species29	AldehydeHydrogenation-Oxygen	-15.112231
1128	species2 + species138 -> species29	AldehydeHydrogenation-Oxygen	-15.112231
1129	species2 + species139 -> species30	AldehydeHydrogenation-Oxygen	-23.018820
1130	species2 + species152 -> species426	AldehydeHydrogenation-Oxygen	-19.544468
1131	species2 + species156 -> species33	AldehydeHydrogenation-Oxygen	-0.233049
1132	species2 + species157 -> species34	AldehydeHydrogenation-Oxygen	-15.114282
1133	species2 + species158 -> species36	AldehydeHydrogenation-Oxygen	-15.114282
1134	species2 + species159 -> species35	AldehydeHydrogenation-Oxygen	-15.114282
1135	species2 + species160 -> species38	AldehydeHydrogenation-Oxygen	-15.114282
1136	species2 + species161 -> species37	AldehydeHydrogenation-Oxygen	-15.114282
1137	species2 + species162 -> species39	AldehydeHydrogenation-Oxygen	-15.114282
1138	species2 + species163 -> species40	AldehydeHydrogenation-Oxygen	-15.114282
1139	species2 + species164 -> species41	AldehydeHydrogenation-Oxygen	-15.114282
1140	species2 + species165 -> species42	AldehydeHydrogenation-Oxygen	-15.114282
1141	species2 + species187 -> species44	AldehydeHydrogenation-Oxygen	-22.058885
1142	species2 + species188 -> species48	AldehydeHydrogenation-Oxygen	-22.058885
1143	species2 + species188 -> species49	AldehydeHydrogenation-Oxygen	-22.058885
1144	species2 + species189 -> species50	AldehydeHydrogenation-Oxygen	-93.207805
1145	species2 + species189 -> species47	AldehydeHydrogenation-Oxygen	-22.058885
1146	species2 + species190 -> species46	AldehydeHydrogenation-Oxygen	-22.058885
1147	species2 + species190 -> species51	AldehydeHydrogenation-Oxygen	-20.506412
1148	species2 + species191 -> species55	AldehydeHydrogenation-Oxygen	-22.058885
1149	species2 + species192 -> species283	AldehydeHydrogenation-Oxygen	-18.586583
1150	species2 + species194 -> species73	AldehydeHydrogenation-Oxygen	-20.506412
1151	species2 + species195 -> species74	AldehydeHydrogenation-Oxygen	-20.506412
1152	species2 + species196 -> species412	AldehydeHydrogenation-Oxygen	-20.504403
1153	species2 + species196 -> species69	AldehydeHydrogenation-Oxygen	-20.504403
1154	species2 + species197 -> species60	AldehydeHydrogenation-Oxygen	-20.506412
1155	species2 + species198 -> species75	AldehydeHydrogenation-Oxygen	-20.506412
1156	species2 + species199 -> species78	AldehydeHydrogenation-Oxygen	-93.207805
1157	species2 + species200 -> species73	AldehydeHydrogenation-Oxygen	-93.207805
1158	species2 + species201 -> species413	AldehydeHydrogenation-Oxygen	-20.504403
1159	species2 + species201 -> species68	AldehydeHydrogenation-Oxygen	-93.205713
1160	species2 + species202 -> species59	AldehydeHydrogenation-Oxygen	-93.207805
1161	species2 + species203 -> species63	AldehydeHydrogenation-Oxygen	-93.174751

1162	species2 + species204 -> species487	AldehydeHydrogenation-Oxygen	-101.459908
1163	species2 + species205 -> species307	AldehydeHydrogenation-Oxygen	-20.504403
1164	species2 + species205 -> species67	AldehydeHydrogenation-Oxygen	-22.056876
1165	species2 + species206 -> species58	AldehydeHydrogenation-Oxygen	-22.058885
1166	species2 + species207 -> species79	AldehydeHydrogenation-Oxygen	-22.058885
1167	species2 + species208 -> species54	AldehydeHydrogenation-Oxygen	-89.277355
1168	species2 + species209 -> species414	AldehydeHydrogenation-Oxygen	-20.504403
1169	species2 + species209 -> species66	AldehydeHydrogenation-Oxygen	-22.056876
1170	species2 + species210 -> species57	AldehydeHydrogenation-Oxygen	-22.058885
1171	species2 + species211 -> species80	AldehydeHydrogenation-Oxygen	-22.058885
1172	species2 + species212 -> species64	AldehydeHydrogenation-Oxygen	-22.058885
1173	species2 + species213 -> species72	AldehydeHydrogenation-Oxygen	-22.058885
1174	species2 + species214 -> species75	AldehydeHydrogenation-Oxygen	-93.207805
1175	species2 + species215 -> species76	AldehydeHydrogenation-Oxygen	-22.058885
1176	species2 + species216 -> species65	AldehydeHydrogenation-Oxygen	-22.058885
1177	species2 + species217 -> species369	AldehydeHydrogenation-Oxygen	-22.058885
1178	species2 + species217 -> species415	AldehydeHydrogenation-Oxygen	-20.506412
1179	species2 + species223 -> species347	AldehydeHydrogenation-Oxygen	-20.506412
1180	species2 + species225 -> species439	AldehydeHydrogenation-Oxygen	-20.506412
1181	species2 + species231 -> species436	AldehydeHydrogenation-Oxygen	-20.506412
1182	species2 + species237 -> species437	AldehydeHydrogenation-Oxygen	-20.506412
1183	species2 + species238 -> species340	AldehydeHydrogenation-Oxygen	-20.506412
1184	species2 + species238 -> species438	AldehydeHydrogenation-Oxygen	-20.506412
1185	species2 + species239 -> species440	AldehydeHydrogenation-Oxygen	-20.506412
1186	species2 + species240 -> species375	AldehydeHydrogenation-Oxygen	-20.506412
1187	species2 + species241 -> species434	AldehydeHydrogenation-Oxygen	-20.506412
1188	species2 + species242 -> species435	AldehydeHydrogenation-Oxygen	-16.645709
1189	species2 + species243 -> species431	AldehydeHydrogenation-Oxygen	-101.459908
1190	species2 + species244 -> species432	AldehydeHydrogenation-Oxygen	-20.506412
1191	species2 + species245 -> species433	AldehydeHydrogenation-Oxygen	-20.506412
1192	species2 + species254 -> species79	AldehydeHydrogenation-Oxygen	-93.207805
1193	species2 + species262 -> species83	AldehydeHydrogenation-Oxygen	-22.058885
1194	species2 + species265 -> species529	AldehydeHydrogenation-Oxygen	-20.504403
1195	species2 + species276 -> species85	AldehydeHydrogenation-Oxygen	-15.114282
1196	species2 + species285 -> species579	AldehydeHydrogenation-Oxygen	-119.914277
1197	species2 + species286 -> species580	AldehydeHydrogenation-Oxygen	-104.149383
1198	species2 + species287 -> species581	AldehydeHydrogenation-Oxygen	-119.914277
1199	species2 + species288 -> species582	AldehydeHydrogenation-Oxygen	-108.117070
1200	species2 + species289 -> species583	AldehydeHydrogenation-Oxygen	-106.666896
1201	species2 + species290 -> species97	AldehydeHydrogenation-Oxygen	-22.058885
1202	species2 + species291 -> species98	AldehydeHydrogenation-Oxygen	-22.058885
1203	species2 + species292 -> species124	AldehydeHydrogenation-Oxygen	-15.114282
1204	species2 + species293 -> species126	AldehydeHydrogenation-Oxygen	-22.058885
1205	species2 + species294 -> species127	AldehydeHydrogenation-Oxygen	-22.058885
1206	species2 + species295 -> species128	AldehydeHydrogenation-Oxygen	-93.207805
1207	species2 + species296 -> species129	AldehydeHydrogenation-Oxygen	-20.506412
1208	species2 + species297 -> species130	AldehydeHydrogenation-Oxygen	-22.058885
1209	species2 + species298 -> species114	AldehydeHydrogenation-Oxygen	-20.139056
1210	species2 + species299 -> species255	AldehydeHydrogenation-Oxygen	-22.058885
1211	species2 + species300 -> species116	AldehydeHydrogenation-Oxygen	-15.112231
1212	species2 + species301 -> species117	AldehydeHydrogenation-Oxygen	-15.114282
1213	species2 + species302 -> species94	AldehydeHydrogenation-Oxygen	-20.139056
1214	species2 + species302 -> species119	AldehydeHydrogenation-Oxygen	-16.642739
1215	species2 + species303 -> species616	AldehydeHydrogenation-Oxygen	-14.128322
1216	species2 + species304 -> species120	AldehydeHydrogenation-Oxygen	-22.058885
1217	species2 + species305 -> species586	AldehydeHydrogenation-Oxygen	-19.546518
1218	species2 + species305 -> species121	AldehydeHydrogenation-Oxygen	-22.058885
1219	species2 + species306 -> species122	AldehydeHydrogenation-Oxygen	-22.058885
1220	species2 + species307 -> species123	AldehydeHydrogenation-Oxygen	-22.058885

1221	species2 + species310 -> species623	AldehydeHydrogenation-Oxygen	-20.504403
1222	species2 + species315 -> species639	AldehydeHydrogenation-Oxygen	-56.673117
1223	species2 + species332 -> species652	AldehydeHydrogenation-Oxygen	-20.506412
1224	species2 + species333 -> species547	AldehydeHydrogenation-Oxygen	-20.506412
1225	species2 + species334 -> species653	AldehydeHydrogenation-Oxygen	-20.506412
1226	species2 + species335 -> species629	AldehydeHydrogenation-Oxygen	-19.546518
1227	species2 + species336 -> species110	AldehydeHydrogenation-Oxygen	-20.139056
1228	species2 + species336 -> species646	AldehydeHydrogenation-Oxygen	-15.090224
1229	species2 + species337 -> species647	AldehydeHydrogenation-Oxygen	-20.506412
1230	species2 + species338 -> species626	AldehydeHydrogenation-Oxygen	-19.546518
1231	species2 + species338 -> species648	AldehydeHydrogenation-Oxygen	-20.506412
1232	species2 + species339 -> species649	AldehydeHydrogenation-Oxygen	-20.506412
1233	species2 + species340 -> species650	AldehydeHydrogenation-Oxygen	-20.506412
1234	species2 + species345 -> species232	AldehydeHydrogenation-Oxygen	-22.058885
1235	species2 + species350 -> species116	AldehydeHydrogenation-Oxygen	-15.112231
1236	species2 + species363 -> species118	AldehydeHydrogenation-Oxygen	-15.114282
1237	species2 + species368 -> species122	AldehydeHydrogenation-Oxygen	-93.207805
1238	species2 + species369 -> species252	AldehydeHydrogenation-Oxygen	-20.506412
1239	species2 + species372 -> species634	AldehydeHydrogenation-Oxygen	-16.645709
1240	species2 + species373 -> species633	AldehydeHydrogenation-Oxygen	-20.506412
1241	species2 + species400 -> species134	AldehydeHydrogenation-Oxygen	-15.114282
1242	species2 + species400 -> species133	AldehydeHydrogenation-Oxygen	-15.114282
1243	species2 + species401 -> species132	AldehydeHydrogenation-Oxygen	-15.114282
1244	species2 + species401 -> species135	AldehydeHydrogenation-Oxygen	-0.233049
1245	species2 + species402 -> species137	AldehydeHydrogenation-Oxygen	-15.114282
1246	species2 + species402 -> species138	AldehydeHydrogenation-Oxygen	-15.114282
1247	species2 + species403 -> species140	AldehydeHydrogenation-Oxygen	-0.233049
1248	species2 + species404 -> species141	AldehydeHydrogenation-Oxygen	-9.653032
1249	species2 + species405 -> species143	AldehydeHydrogenation-Oxygen	-15.114282
1250	species2 + species406 -> species142	AldehydeHydrogenation-Oxygen	-15.114282
1251	species2 + species407 -> species146	AldehydeHydrogenation-Oxygen	-15.114282
1252	species2 + species408 -> species145	AldehydeHydrogenation-Oxygen	-15.114282
1253	species2 + species409 -> species147	AldehydeHydrogenation-Oxygen	-15.114282
1254	species2 + species410 -> species148	AldehydeHydrogenation-Oxygen	-15.114282
1255	species2 + species411 -> species149	AldehydeHydrogenation-Oxygen	-21.098992
1256	species2 + species412 -> species150	AldehydeHydrogenation-Oxygen	-20.506412
1257	species2 + species413 -> species151	AldehydeHydrogenation-Oxygen	-93.207805
1258	species2 + species414 -> species154	AldehydeHydrogenation-Oxygen	-22.058885
1259	species2 + species415 -> species252	AldehydeHydrogenation-Oxygen	-22.058885
1260	species2 + species430 -> species750	AldehydeHydrogenation-Oxygen	-20.506412
1261	species2 + species436 -> species739	AldehydeHydrogenation-Oxygen	-20.506412
1262	species2 + species438 -> species650	AldehydeHydrogenation-Oxygen	-20.506412
1263	species2 + species445 -> species175	AldehydeHydrogenation-Oxygen	-0.233049
1264	species2 + species446 -> species177	AldehydeHydrogenation-Oxygen	-0.233049
1265	species2 + species447 -> species176	AldehydeHydrogenation-Oxygen	-0.233049
1266	species2 + species448 -> species178	AldehydeHydrogenation-Oxygen	-0.233049
1267	species2 + species449 -> species179	AldehydeHydrogenation-Oxygen	-0.233049
1268	species2 + species450 -> species180	AldehydeHydrogenation-Oxygen	-15.114282
1269	species2 + species451 -> species181	AldehydeHydrogenation-Oxygen	-15.114282
1270	species2 + species452 -> species182	AldehydeHydrogenation-Oxygen	-15.114282
1271	species2 + species453 -> species183	AldehydeHydrogenation-Oxygen	-15.114282
1272	species2 + species454 -> species184	AldehydeHydrogenation-Oxygen	-15.114282
1273	species2 + species455 -> species186	AldehydeHydrogenation-Oxygen	-15.114282
1274	species2 + species465 -> species187	AldehydeHydrogenation-Oxygen	-23.018820
1275	species2 + species466 -> species193	AldehydeHydrogenation-Oxygen	-22.058885
1276	species2 + species467 -> species193	AldehydeHydrogenation-Oxygen	-20.506412
1277	species2 + species468 -> species575	AldehydeHydrogenation-Oxygen	-20.506412
1278	species2 + species468 -> species192	AldehydeHydrogenation-Oxygen	-22.058885
1279	species2 + species469 -> species204	AldehydeHydrogenation-Oxygen	-21.478522

1280	species2 + species469 -> species769	AldehydeHydrogenation-Oxygen	-100.879587
1281	species2 + species470 -> species199	AldehydeHydrogenation-Oxygen	-92.625392
1282	species2 + species471 -> species194	AldehydeHydrogenation-Oxygen	-92.625392
1283	species2 + species471 -> species200	AldehydeHydrogenation-Oxygen	-19.923999
1284	species2 + species472 -> species214	AldehydeHydrogenation-Oxygen	-20.506412
1285	species2 + species472 -> species198	AldehydeHydrogenation-Oxygen	-93.207805
1286	species2 + species473 -> species195	AldehydeHydrogenation-Oxygen	-19.923999
1287	species2 + species474 -> species578	AldehydeHydrogenation-Oxygen	-20.506412
1288	species2 + species475 -> species577	AldehydeHydrogenation-Oxygen	-20.504403
1289	species2 + species477 -> species249	AldehydeHydrogenation-Oxygen	-20.506412
1290	species2 + species478 -> species251	AldehydeHydrogenation-Oxygen	-20.506412
1291	species2 + species479 -> species236	AldehydeHydrogenation-Oxygen	-20.506412
1292	species2 + species480 -> species736	AldehydeHydrogenation-Oxygen	-100.879587
1293	species2 + species480 -> species243	AldehydeHydrogenation-Oxygen	-19.926007
1294	species2 + species481 -> species248	AldehydeHydrogenation-Oxygen	-68.858598
1295	species2 + species482 -> species224	AldehydeHydrogenation-Oxygen	-93.207805
1296	species2 + species483 -> species235	AldehydeHydrogenation-Oxygen	-93.207805
1297	species2 + species484 -> species738	AldehydeHydrogenation-Oxygen	-16.065347
1298	species2 + species484 -> species242	AldehydeHydrogenation-Oxygen	-92.627484
1299	species2 + species485 -> species241	AldehydeHydrogenation-Oxygen	-92.627484
1300	species2 + species485 -> species737	AldehydeHydrogenation-Oxygen	-19.926007
1301	species2 + species486 -> species227	AldehydeHydrogenation-Oxygen	-10.714220
1302	species2 + species488 -> species775	AldehydeHydrogenation-Oxygen	-18.966114
1303	species2 + species489 -> species776	AldehydeHydrogenation-Oxygen	-89.277355
1304	species2 + species490 -> species234	AldehydeHydrogenation-Oxygen	-22.058885
1305	species2 + species491 -> species253	AldehydeHydrogenation-Oxygen	-16.642739
1306	species2 + species492 -> species207	AldehydeHydrogenation-Oxygen	-93.207805
1307	species2 + species492 -> species254	AldehydeHydrogenation-Oxygen	-22.058885
1308	species2 + species493 -> species233	AldehydeHydrogenation-Oxygen	-22.058885
1309	species2 + species494 -> species250	AldehydeHydrogenation-Oxygen	-68.858598
1310	species2 + species495 -> species740	AldehydeHydrogenation-Oxygen	-89.277355
1311	species2 + species500 -> species783	AldehydeHydrogenation-Oxygen	-86.625536
1312	species2 + species501 -> species658	AldehydeHydrogenation-Oxygen	-20.506412
1313	species2 + species502 -> species758	AldehydeHydrogenation-Oxygen	-20.506412
1314	species2 + species508 -> species745	AldehydeHydrogenation-Oxygen	-15.090224
1315	species2 + species509 -> species239	AldehydeHydrogenation-Oxygen	-93.205713
1316	species2 + species509 -> species759	AldehydeHydrogenation-Oxygen	-20.504403
1317	species2 + species510 -> species681	AldehydeHydrogenation-Oxygen	-20.506412
1318	species2 + species511 -> species755	AldehydeHydrogenation-Oxygen	-14.128322
1319	species2 + species512 -> species756	AldehydeHydrogenation-Oxygen	-89.277355
1320	species2 + species513 -> species757	AldehydeHydrogenation-Oxygen	-89.277355
1321	species2 + species518 -> species794	AldehydeHydrogenation-Oxygen	-20.506412
1322	species2 + species520 -> species258	AldehydeHydrogenation-Oxygen	-46.170022
1323	species2 + species522 -> species795	AldehydeHydrogenation-Oxygen	-44.617339
1324	species2 + species530 -> species816	AldehydeHydrogenation-Oxygen	-118.722255
1325	species2 + species531 -> species263	AldehydeHydrogenation-Oxygen	-22.058885
1326	species2 + species532 -> species267	AldehydeHydrogenation-Oxygen	-16.640688
1327	species2 + species533 -> species266	AldehydeHydrogenation-Oxygen	-16.642739
1328	species2 + species534 -> species815	AldehydeHydrogenation-Oxygen	-20.506412
1329	species2 + species540 -> species643	AldehydeHydrogenation-Oxygen	-21.466347
1330	species2 + species541 -> species808	AldehydeHydrogenation-Oxygen	-19.546518
1331	species2 + species563 -> species278	AldehydeHydrogenation-Oxygen	-15.114282
1332	species2 + species564 -> species279	AldehydeHydrogenation-Oxygen	-15.114282
1333	species2 + species565 -> species280	AldehydeHydrogenation-Oxygen	-0.233049
1334	species2 + species566 -> species281	AldehydeHydrogenation-Oxygen	-15.114282
1335	species2 + species567 -> species282	AldehydeHydrogenation-Oxygen	-15.114282
1336	species2 + species575 -> species283	AldehydeHydrogenation-Oxygen	-20.139056
1337	species2 + species577 -> species872	AldehydeHydrogenation-Oxygen	-19.546518
1338	species2 + species584 -> species882	AldehydeHydrogenation-Oxygen	-104.149383

1339	species2 + species585 -> species312	AldehydeHydrogenation-Oxygen	-22.058885
1340	species2 + species586 -> species313	AldehydeHydrogenation-Oxygen	-11.224500
1341	species2 + species587 -> species314	AldehydeHydrogenation-Oxygen	-16.642739
1342	species2 + species588 -> species317	AldehydeHydrogenation-Oxygen	-22.058885
1343	species2 + species589 -> species376	AldehydeHydrogenation-Oxygen	-15.114282
1344	species2 + species590 -> species377	AldehydeHydrogenation-Oxygen	-15.114282
1345	species2 + species591 -> species378	AldehydeHydrogenation-Oxygen	-0.233049
1346	species2 + species592 -> species379	AldehydeHydrogenation-Oxygen	-15.114282
1347	species2 + species593 -> species381	AldehydeHydrogenation-Oxygen	-15.114282
1348	species2 + species594 -> species382	AldehydeHydrogenation-Oxygen	-15.114282
1349	species2 + species595 -> species362	AldehydeHydrogenation-Oxygen	-21.098992
1350	species2 + species596 -> species374	AldehydeHydrogenation-Oxygen	-22.058885
1351	species2 + species597 -> species898	AldehydeHydrogenation-Oxygen	-101.459908
1352	species2 + species598 -> species394	AldehydeHydrogenation-Oxygen	-22.058885
1353	species2 + species599 -> species395	AldehydeHydrogenation-Oxygen	-22.058885
1354	species2 + species600 -> species396	AldehydeHydrogenation-Oxygen	-93.207805
1355	species2 + species601 -> species346	AldehydeHydrogenation-Oxygen	-93.207805
1356	species2 + species602 -> species398	AldehydeHydrogenation-Oxygen	-20.506412
1357	species2 + species603 -> species399	AldehydeHydrogenation-Oxygen	-93.207805
1358	species2 + species604 -> species300	AldehydeHydrogenation-Oxygen	-15.114282
1359	species2 + species604 -> species350	AldehydeHydrogenation-Oxygen	-15.114282
1360	species2 + species605 -> species352	AldehydeHydrogenation-Oxygen	-15.114282
1361	species2 + species606 -> species353	AldehydeHydrogenation-Oxygen	-15.114282
1362	species2 + species607 -> species354	AldehydeHydrogenation-Oxygen	-15.114282
1363	species2 + species608 -> species355	AldehydeHydrogenation-Oxygen	-15.114282
1364	species2 + species609 -> species356	AldehydeHydrogenation-Oxygen	-15.114282
1365	species2 + species610 -> species357	AldehydeHydrogenation-Oxygen	-15.114282
1366	species2 + species611 -> species358	AldehydeHydrogenation-Oxygen	-15.114282
1367	species2 + species612 -> species360	AldehydeHydrogenation-Oxygen	-15.114282
1368	species2 + species613 -> species361	AldehydeHydrogenation-Oxygen	-15.114282
1369	species2 + species614 -> species303	AldehydeHydrogenation-Oxygen	-22.058885
1370	species2 + species614 -> species903	AldehydeHydrogenation-Oxygen	-14.128322
1371	species2 + species615 -> species306	AldehydeHydrogenation-Oxygen	-93.205713
1372	species2 + species615 -> species368	AldehydeHydrogenation-Oxygen	-22.056876
1373	species2 + species617 -> species511	AldehydeHydrogenation-Oxygen	-20.506412
1374	species2 + species617 -> species904	AldehydeHydrogenation-Oxygen	-14.128322
1375	species2 + species618 -> species905	AldehydeHydrogenation-Oxygen	-14.128322
1376	species2 + species619 -> species370	AldehydeHydrogenation-Oxygen	-22.058885
1377	species2 + species620 -> species371	AldehydeHydrogenation-Oxygen	-22.058885
1378	species2 + species621 -> species886	AldehydeHydrogenation-Oxygen	-16.645709
1379	species2 + species621 -> species372	AldehydeHydrogenation-Oxygen	-22.058885
1380	species2 + species622 -> species373	AldehydeHydrogenation-Oxygen	-22.058885
1381	species2 + species622 -> species885	AldehydeHydrogenation-Oxygen	-20.506412
1382	species2 + species625 -> species910	AldehydeHydrogenation-Oxygen	-20.506412
1383	species2 + species626 -> species911	AldehydeHydrogenation-Oxygen	-15.090224
1384	species2 + species627 -> species912	AldehydeHydrogenation-Oxygen	-20.506412
1385	species2 + species641 -> species930	AldehydeHydrogenation-Oxygen	-20.504403
1386	species2 + species646 -> species326	AldehydeHydrogenation-Oxygen	-14.720860
1387	species2 + species648 -> species911	AldehydeHydrogenation-Oxygen	-14.130330
1388	species2 + species654 -> species330	AldehydeHydrogenation-Oxygen	-20.139056
1389	species2 + species656 -> species915	AldehydeHydrogenation-Oxygen	-19.546518
1390	species2 + species661 -> species944	AldehydeHydrogenation-Oxygen	-15.090224
1391	species2 + species662 -> species947	AldehydeHydrogenation-Oxygen	-20.504403
1392	species2 + species663 -> species853	AldehydeHydrogenation-Oxygen	-8.323775
1393	species2 + species664 -> species851	AldehydeHydrogenation-Oxygen	-20.504403
1394	species2 + species665 -> species953	AldehydeHydrogenation-Oxygen	-101.459908
1395	species2 + species666 -> species921	AldehydeHydrogenation-Oxygen	-20.506412
1396	species2 + species667 -> species922	AldehydeHydrogenation-Oxygen	-16.645709
1397	species2 + species668 -> species339	AldehydeHydrogenation-Oxygen	-93.207805

1398	species2 + species668 -> species943	AldehydeHydrogenation-Oxygen	-20.506412
1399	species2 + species669 -> species518	AldehydeHydrogenation-Oxygen	-20.504403
1400	species2 + species670 -> species945	AldehydeHydrogenation-Oxygen	-20.506412
1401	species2 + species671 -> species918	AldehydeHydrogenation-Oxygen	-16.645709
1402	species2 + species671 -> species946	AldehydeHydrogenation-Oxygen	-20.506412
1403	species2 + species672 -> species917	AldehydeHydrogenation-Oxygen	-20.506412
1404	species2 + species677 -> species963	AldehydeHydrogenation-Oxygen	-51.674074
1405	species2 + species683 -> species351	AldehydeHydrogenation-Oxygen	-15.114282
1406	species2 + species684 -> species352	AldehydeHydrogenation-Oxygen	-0.233049
1407	species2 + species697 -> species365	AldehydeHydrogenation-Oxygen	-15.114282
1408	species2 + species698 -> species364	AldehydeHydrogenation-Oxygen	-15.114282
1409	species2 + species699 -> species366	AldehydeHydrogenation-Oxygen	-0.233049
1410	species2 + species726 -> species403	AldehydeHydrogenation-Oxygen	-9.653032
1411	species2 + species727 -> species416	AldehydeHydrogenation-Oxygen	-15.112231
1412	species2 + species728 -> species420	AldehydeHydrogenation-Oxygen	-15.114282
1413	species2 + species729 -> species421	AldehydeHydrogenation-Oxygen	-15.114282
1414	species2 + species730 -> species422	AldehydeHydrogenation-Oxygen	-15.114282
1415	species2 + species731 -> species423	AldehydeHydrogenation-Oxygen	-0.233049
1416	species2 + species732 -> species425	AldehydeHydrogenation-Oxygen	-15.114282
1417	species2 + species733 -> species427	AldehydeHydrogenation-Oxygen	-93.207805
1418	species2 + species734 -> species428	AldehydeHydrogenation-Oxygen	-20.506412
1419	species2 + species735 -> species517	AldehydeHydrogenation-Oxygen	-22.058885
1420	species2 + species736 -> species431	AldehydeHydrogenation-Oxygen	-20.506412
1421	species2 + species737 -> species434	AldehydeHydrogenation-Oxygen	-93.207805
1422	species2 + species738 -> species435	AldehydeHydrogenation-Oxygen	-93.207805
1423	species2 + species740 -> species985	AldehydeHydrogenation-Oxygen	-16.645709
1424	species2 + species759 -> species440	AldehydeHydrogenation-Oxygen	-93.207805
1425	species2 + species766 -> species467	AldehydeHydrogenation-Oxygen	-22.058885
1426	species2 + species766 -> species466	AldehydeHydrogenation-Oxygen	-20.506412
1427	species2 + species767 -> species476	AldehydeHydrogenation-Oxygen	-22.058885
1428	species2 + species768 -> species474	AldehydeHydrogenation-Oxygen	-20.504403
1429	species2 + species769 -> species487	AldehydeHydrogenation-Oxygen	-22.058885
1430	species2 + species770 -> species505	AldehydeHydrogenation-Oxygen	-20.506412
1431	species2 + species771 -> species881	AldehydeHydrogenation-Oxygen	-16.645709
1432	species2 + species771 -> species880	AldehydeHydrogenation-Oxygen	-20.506412
1433	species2 + species772 -> species504	AldehydeHydrogenation-Oxygen	-93.207805
1434	species2 + species773 -> species503	AldehydeHydrogenation-Oxygen	-93.207805
1435	species2 + species774 -> species499	AldehydeHydrogenation-Oxygen	-93.207805
1436	species2 + species777 -> species998	AldehydeHydrogenation-Oxygen	-14.128322
1437	species2 + species778 -> species489	AldehydeHydrogenation-Oxygen	-11.294624
1438	species2 + species778 -> species999	AldehydeHydrogenation-Oxygen	-19.546518
1439	species2 + species779 -> species491	AldehydeHydrogenation-Oxygen	-22.058885
1440	species2 + species780 -> species990	AldehydeHydrogenation-Oxygen	-20.504403
1441	species2 + species780 -> species508	AldehydeHydrogenation-Oxygen	-22.056876
1442	species2 + species788 -> species991	AldehydeHydrogenation-Oxygen	-20.506412
1443	species2 + species789 -> species968	AldehydeHydrogenation-Oxygen	-18.144167
1444	species2 + species790 -> species967	AldehydeHydrogenation-Oxygen	-20.506412
1445	species2 + species791 -> species993	AldehydeHydrogenation-Oxygen	-18.096093
1446	species2 + species792 -> species994	AldehydeHydrogenation-Oxygen	-14.128322
1447	species2 + species793 -> species995	AldehydeHydrogenation-Oxygen	-14.128322
1448	species2 + species798 -> species1008	AldehydeHydrogenation-Oxygen	-142.833392
1449	species2 + species817 -> species1029	AldehydeHydrogenation-Oxygen	-119.914277
1450	species2 + species818 -> species548	AldehydeHydrogenation-Oxygen	-15.114282
1451	species2 + species819 -> species532	AldehydeHydrogenation-Oxygen	-15.682804
1452	species2 + species820 -> species537	AldehydeHydrogenation-Oxygen	-21.098992
1453	species2 + species821 -> species893	AldehydeHydrogenation-Oxygen	-20.506412
1454	species2 + species821 -> species540	AldehydeHydrogenation-Oxygen	-15.682804
1455	species2 + species822 -> species542	AldehydeHydrogenation-Oxygen	-15.114282
1456	species2 + species823 -> species544	AldehydeHydrogenation-Oxygen	-22.058885

1457	species2 + species824 -> species545	AldehydeHydrogenation-Oxygen	-22.058885
1458	species2 + species825 -> species546	AldehydeHydrogenation-Oxygen	-93.207805
1459	species2 + species831 -> species935	AldehydeHydrogenation-Oxygen	-20.504403
1460	species2 + species837 -> species933	AldehydeHydrogenation-Oxygen	-20.506412
1461	species2 + species838 -> species1026	AldehydeHydrogenation-Oxygen	-20.506412
1462	species2 + species839 -> species1027	AldehydeHydrogenation-Oxygen	-16.645709
1463	species2 + species840 -> species1017	AldehydeHydrogenation-Oxygen	-19.544468
1464	species2 + species841 -> species1025	AldehydeHydrogenation-Oxygen	-20.506412
1465	species2 + species868 -> species572	AldehydeHydrogenation-Oxygen	-15.114282
1466	species2 + species869 -> species573	AldehydeHydrogenation-Oxygen	-0.233049
1467	species2 + species878 -> species576	AldehydeHydrogenation-Oxygen	-22.058885
1468	species2 + species879 -> species786	AldehydeHydrogenation-Oxygen	-20.506412
1469	species2 + species880 -> species1064	AldehydeHydrogenation-Oxygen	-16.645709
1470	species2 + species881 -> species1064	AldehydeHydrogenation-Oxygen	-20.506412
1471	species2 + species883 -> species631	AldehydeHydrogenation-Oxygen	-15.114282
1472	species2 + species884 -> species632	AldehydeHydrogenation-Oxygen	-22.058885
1473	species2 + species885 -> species633	AldehydeHydrogenation-Oxygen	-22.058885
1474	species2 + species886 -> species634	AldehydeHydrogenation-Oxygen	-22.058885
1475	species2 + species887 -> species635	AldehydeHydrogenation-Oxygen	-93.207805
1476	species2 + species888 -> species636	AldehydeHydrogenation-Oxygen	-20.506412
1477	species2 + species889 -> species637	AldehydeHydrogenation-Oxygen	-22.058885
1478	species2 + species890 -> species638	AldehydeHydrogenation-Oxygen	-22.058885
1479	species2 + species891 -> species682	AldehydeHydrogenation-Oxygen	-22.058885
1480	species2 + species892 -> species1071	AldehydeHydrogenation-Oxygen	-118.722255
1481	species2 + species893 -> species643	AldehydeHydrogenation-Oxygen	-16.642739
1482	species2 + species894 -> species644	AldehydeHydrogenation-Oxygen	-21.098992
1483	species2 + species895 -> species709	AldehydeHydrogenation-Oxygen	-0.233049
1484	species2 + species896 -> species688	AldehydeHydrogenation-Oxygen	-15.114282
1485	species2 + species897 -> species1077	AldehydeHydrogenation-Oxygen	-14.128322
1486	species2 + species899 -> species606	AldehydeHydrogenation-Oxygen	-15.114282
1487	species2 + species900 -> species605	AldehydeHydrogenation-Oxygen	-0.233049
1488	species2 + species900 -> species684	AldehydeHydrogenation-Oxygen	-15.114282
1489	species2 + species901 -> species685	AldehydeHydrogenation-Oxygen	-19.572543
1490	species2 + species902 -> species690	AldehydeHydrogenation-Oxygen	-15.114282
1491	species2 + species903 -> species616	AldehydeHydrogenation-Oxygen	-22.058885
1492	species2 + species904 -> species755	AldehydeHydrogenation-Oxygen	-20.506412
1493	species2 + species906 -> species791	AldehydeHydrogenation-Oxygen	-29.893383
1494	species2 + species907 -> species704	AldehydeHydrogenation-Oxygen	-22.058885
1495	species2 + species908 -> species705	AldehydeHydrogenation-Oxygen	-22.058885
1496	species2 + species909 -> species706	AldehydeHydrogenation-Oxygen	-22.058885
1497	species2 + species916 -> species1078	AldehydeHydrogenation-Oxygen	-20.504403
1498	species2 + species917 -> species1079	AldehydeHydrogenation-Oxygen	-20.506412
1499	species2 + species918 -> species1080	AldehydeHydrogenation-Oxygen	-20.506412
1500	species2 + species919 -> species1081	AldehydeHydrogenation-Oxygen	-20.504403
1501	species2 + species920 -> species939	AldehydeHydrogenation-Oxygen	-20.504403
1502	species2 + species932 -> species1090	AldehydeHydrogenation-Oxygen	-20.504403
1503	species2 + species933 -> species1089	AldehydeHydrogenation-Oxygen	-20.506412
1504	species2 + species940 -> species645	AldehydeHydrogenation-Oxygen	-15.114282
1505	species2 + species943 -> species649	AldehydeHydrogenation-Oxygen	-93.207805
1506	species2 + species946 -> species1080	AldehydeHydrogenation-Oxygen	-16.645709
1507	species2 + species954 -> species657	AldehydeHydrogenation-Oxygen	-93.207805
1508	species2 + species957 -> species1085	AldehydeHydrogenation-Oxygen	-16.645709
1509	species2 + species958 -> species1084	AldehydeHydrogenation-Oxygen	-20.506412
1510	species2 + species961 -> species1105	AldehydeHydrogenation-Oxygen	-14.128322
1511	species2 + species962 -> species1103	AldehydeHydrogenation-Oxygen	-20.504403
1512	species2 + species969 -> species1109	AldehydeHydrogenation-Oxygen	-87.226358
1513	species2 + species970 -> species686	AldehydeHydrogenation-Oxygen	-9.653032
1514	species2 + species977 -> species703	AldehydeHydrogenation-Oxygen	-0.233049
1515	species2 + species978 -> species700	AldehydeHydrogenation-Oxygen	-0.233049

1516	species2 + species980 -> species727	AldehydeHydrogenation-Oxygen	-15.114282
1517	species2 + species981 -> species741	AldehydeHydrogenation-Oxygen	-15.114282
1518	species2 + species982 -> species743	AldehydeHydrogenation-Oxygen	-15.114282
1519	species2 + species983 -> species744	AldehydeHydrogenation-Oxygen	-15.114282
1520	species2 + species984 -> species751	AldehydeHydrogenation-Oxygen	-11.294624
1521	species2 + species990 -> species745	AldehydeHydrogenation-Oxygen	-16.642739
1522	species2 + species991 -> species1066	AldehydeHydrogenation-Oxygen	-20.506412
1523	species2 + species999 -> species776	AldehydeHydrogenation-Oxygen	-81.025252
1524	species2 + species1000 -> species777	AldehydeHydrogenation-Oxygen	-22.058885
1525	species2 + species1000 -> species1116	AldehydeHydrogenation-Oxygen	-14.128322
1526	species2 + species1004 -> species1002	AldehydeHydrogenation-Oxygen	-18.096093
1527	species2 + species1030 -> species856	AldehydeHydrogenation-Oxygen	-15.114282
1528	species2 + species1031 -> species857	AldehydeHydrogenation-Oxygen	-15.114282
1529	species2 + species1032 -> species828	AldehydeHydrogenation-Oxygen	-15.682804
1530	species2 + species1033 -> species835	AldehydeHydrogenation-Oxygen	-21.098992
1531	species2 + species1034 -> species842	AldehydeHydrogenation-Oxygen	-0.233049
1532	species2 + species1035 -> species843	AldehydeHydrogenation-Oxygen	-15.114282
1533	species2 + species1036 -> species852	AldehydeHydrogenation-Oxygen	-93.205713
1534	species2 + species1037 -> species854	AldehydeHydrogenation-Oxygen	-93.207805
1535	species2 + species1041 -> species1012	AldehydeHydrogenation-Oxygen	-20.504403
1536	species2 + species1048 -> species1091	AldehydeHydrogenation-Oxygen	-124.161455
1537	species2 + species1051 -> species1131	AldehydeHydrogenation-Oxygen	-20.506412
1538	species2 + species1052 -> species1132	AldehydeHydrogenation-Oxygen	-16.645709
1539	species2 + species1053 -> species1140	AldehydeHydrogenation-Oxygen	-18.094085
1540	species2 + species1061 -> species871	AldehydeHydrogenation-Oxygen	-0.233049
1541	species2 + species1062 -> species873	AldehydeHydrogenation-Oxygen	-15.114282
1542	species2 + species1067 -> species924	AldehydeHydrogenation-Oxygen	-15.114282
1543	species2 + species1068 -> species926	AldehydeHydrogenation-Oxygen	-22.058885
1544	species2 + species1069 -> species927	AldehydeHydrogenation-Oxygen	-22.058885
1545	species2 + species1070 -> species928	AldehydeHydrogenation-Oxygen	-93.207805
1546	species2 + species1072 -> species936	AldehydeHydrogenation-Oxygen	-15.114282
1547	species2 + species1073 -> species937	AldehydeHydrogenation-Oxygen	-22.056876
1548	species2 + species1074 -> species938	AldehydeHydrogenation-Oxygen	-93.205713
1549	species2 + species1075 -> species979	AldehydeHydrogenation-Oxygen	-15.114282
1550	species2 + species1076 -> species973	AldehydeHydrogenation-Oxygen	-15.114282
1551	species2 + species1086 -> species1154	AldehydeHydrogenation-Oxygen	-20.504403
1552	species2 + species1093 -> species1157	AldehydeHydrogenation-Oxygen	-20.506412
1553	species2 + species1094 -> species1156	AldehydeHydrogenation-Oxygen	-16.645709
1554	species2 + species1095 -> species1122	AldehydeHydrogenation-Oxygen	-20.506412
1555	species2 + species1101 -> species941	AldehydeHydrogenation-Oxygen	-0.233049
1556	species2 + species1116 -> species998	AldehydeHydrogenation-Oxygen	-22.058885
1557	species2 + species1141 -> species1039	AldehydeHydrogenation-Oxygen	-22.058885
1558	species2 + species1144 -> species1126	AldehydeHydrogenation-Oxygen	-20.506412
1559	species2 + species1152 -> species1088	AldehydeHydrogenation-Oxygen	-22.058885
1560	species2 + species1153 -> species1099	AldehydeHydrogenation-Oxygen	-22.056876
1561	species2 + species1160 -> species1163	AldehydeHydrogenation-Oxygen	-77.967166
1562	species2 + species4 -> species23	COHydrogenolysis5-Oxygen	-15.716401
1563	species2 + species4 -> species24	COHydrogenolysis5-Oxygen	-35.086062
1564	species2 + species5 -> species30	COHydrogenolysis5-Oxygen	-35.337102
1565	species2 + species13 -> species83	COHydrogenolysis5-Oxygen	-43.323646
1566	species2 + species13 -> species84	COHydrogenolysis5-Oxygen	-64.494268
1567	species2 + species14 -> species93	COHydrogenolysis5-Oxygen	-37.005890
1568	species2 + species14 -> species94	COHydrogenolysis5-Oxygen	-26.548735
1569	species2 + species19 -> species109	COHydrogenolysis5-Oxygen	-44.015680
1570	species2 + species19 -> species110	COHydrogenolysis5-Oxygen	-34.153030
1571	species2 + species20 -> species113	COHydrogenolysis5-Oxygen	-30.373539
1572	species2 + species20 -> species114	COHydrogenolysis5-Oxygen	-34.686532
1573	species2 + species25 -> species9	COHydrogenolysis5-Oxygen	-29.942880
1574	species2 + species25 -> species139	COHydrogenolysis5-Oxygen	-27.430513

1575	species2 + species81 -> species258	COHydrogenolysis5-Oxygen	-67.436875
1576	species2 + species81 -> species259	COHydrogenolysis5-Oxygen	-64.496360
1577	species2 + species83 -> species266	COHydrogenolysis5-Oxygen	-44.222788
1578	species2 + species83 -> species267	COHydrogenolysis5-Oxygen	-29.902044
1579	species2 + species84 -> species275	COHydrogenolysis5-Oxygen	-37.005890
1580	species2 + species84 -> species266	COHydrogenolysis5-Oxygen	-23.052417
1581	species2 + species85 -> species283	COHydrogenolysis5-Oxygen	-35.112923
1582	species2 + species85 -> species65	COHydrogenolysis5-Oxygen	-45.570036
1583	species2 + species97 -> species313	COHydrogenolysis5-Oxygen	-29.309464
1584	species2 + species97 -> species314	COHydrogenolysis5-Oxygen	-45.775470
1585	species2 + species105 -> species326	COHydrogenolysis5-Oxygen	-23.320654
1586	species2 + species105 -> species327	COHydrogenolysis5-Oxygen	-38.601417
1587	species2 + species106 -> species330	COHydrogenolysis5-Oxygen	-34.177046
1588	species2 + species106 -> species331	COHydrogenolysis5-Oxygen	-42.121583
1589	species2 + species116 -> species313	COHydrogenolysis5-Oxygen	-37.137895
1590	species2 + species116 -> species326	COHydrogenolysis5-Oxygen	-36.770540
1591	species2 + species124 -> species327	COHydrogenolysis5-Oxygen	-28.390406
1592	species2 + species124 -> species314	COHydrogenolysis5-Oxygen	-29.942880
1593	species2 + species131 -> species52	COHydrogenolysis5-Oxygen	-23.958170
1594	species2 + species260 -> species528	COHydrogenolysis5-Oxygen	-71.670246
1595	species2 + species260 -> species529	COHydrogenolysis5-Oxygen	-48.945269
1596	species2 + species260 -> species526	COHydrogenolysis5-Oxygen	-64.494268
1597	species2 + species260 -> species317	COHydrogenolysis5-Oxygen	-43.323646
1598	species2 + species262 -> species532	COHydrogenolysis5-Oxygen	-35.320240
1599	species2 + species262 -> species533	COHydrogenolysis5-Oxygen	-49.638976
1600	species2 + species264 -> species537	COHydrogenolysis5-Oxygen	-48.874141
1601	species2 + species264 -> species538	COHydrogenolysis5-Oxygen	-43.008591
1602	species2 + species265 -> species540	COHydrogenolysis5-Oxygen	-42.922401
1603	species2 + species265 -> species541	COHydrogenolysis5-Oxygen	-56.650523
1604	species2 + species270 -> species544	COHydrogenolysis5-Oxygen	-34.158009
1605	species2 + species270 -> species555	COHydrogenolysis5-Oxygen	-37.665498
1606	species2 + species276 -> species192	COHydrogenolysis5-Oxygen	-31.640621
1607	species2 + species276 -> species216	COHydrogenolysis5-Oxygen	-38.625433
1608	species2 + species290 -> species586	COHydrogenolysis5-Oxygen	-40.143848
1609	species2 + species290 -> species587	COHydrogenolysis5-Oxygen	-51.191658
1610	species2 + species292 -> species109	COHydrogenolysis5-Oxygen	-28.414423
1611	species2 + species292 -> species587	COHydrogenolysis5-Oxygen	-28.414423
1612	species2 + species300 -> species586	COHydrogenolysis5-Oxygen	-41.025584
1613	species2 + species300 -> species110	COHydrogenolysis5-Oxygen	-42.210702
1614	species2 + species310 -> species626	COHydrogenolysis5-Oxygen	-47.746134
1615	species2 + species310 -> species627	COHydrogenolysis5-Oxygen	-57.243396
1616	species2 + species311 -> species629	COHydrogenolysis5-Oxygen	-48.281686
1617	species2 + species311 -> species630	COHydrogenolysis5-Oxygen	-43.601464
1618	species2 + species317 -> species643	COHydrogenolysis5-Oxygen	-49.505925
1619	species2 + species317 -> species644	COHydrogenolysis5-Oxygen	-63.459146
1620	species2 + species349 -> species681	COHydrogenolysis5-Oxygen	-58.940845
1621	species2 + species349 -> species682	COHydrogenolysis5-Oxygen	-60.493527
1622	species2 + species350 -> species646	COHydrogenolysis5-Oxygen	-37.161911
1623	species2 + species350 -> species121	COHydrogenolysis5-Oxygen	-43.537867
1624	species2 + species416 -> species643	COHydrogenolysis5-Oxygen	-57.334189
1625	species2 + species420 -> species371	COHydrogenolysis5-Oxygen	-58.203206
1626	species2 + species420 -> species745	COHydrogenolysis5-Oxygen	-44.842438
1627	species2 + species496 -> species255	COHydrogenolysis5-Oxygen	-46.307675
1628	species2 + species519 -> species795	COHydrogenolysis5-Oxygen	-73.058079
1629	species2 + species519 -> species796	COHydrogenolysis5-Oxygen	-71.671920
1630	species2 + species526 -> species807	COHydrogenolysis5-Oxygen	-50.233522
1631	species2 + species526 -> species808	COHydrogenolysis5-Oxygen	-40.143848
1632	species2 + species528 -> species644	COHydrogenolysis5-Oxygen	-35.112923
1633	species2 + species528 -> species807	COHydrogenolysis5-Oxygen	-43.057544

1634	species2 + species529 -> species643	COHydrogenolysis5-Oxygen	-43.884302
1635	species2 + species529 -> species808	COHydrogenolysis5-Oxygen	-55.692806
1636	species2 + species536 -> species828	COHydrogenolysis5-Oxygen	-35.320240
1637	species2 + species536 -> species829	COHydrogenolysis5-Oxygen	-49.641068
1638	species2 + species539 -> species835	COHydrogenolysis5-Oxygen	-48.364530
1639	species2 + species539 -> species836	COHydrogenolysis5-Oxygen	-55.717073
1640	species2 + species542 -> species808	COHydrogenolysis5-Oxygen	-45.481754
1641	species2 + species542 -> species644	COHydrogenolysis5-Oxygen	-47.626890
1642	species2 + species559 -> species807	COHydrogenolysis5-Oxygen	-31.912791
1643	species2 + species572 -> species872	COHydrogenolysis5-Oxygen	-48.705944
1644	species2 + species572 -> species330	COHydrogenolysis5-Oxygen	-57.835850
1645	species2 + species588 -> species893	COHydrogenolysis5-Oxygen	-54.922113
1646	species2 + species588 -> species894	COHydrogenolysis5-Oxygen	-64.419374
1647	species2 + species604 -> species336	COHydrogenolysis5-Oxygen	-37.185928
1648	species2 + species604 -> species305	COHydrogenolysis5-Oxygen	-36.593348
1649	species2 + species623 -> species911	COHydrogenolysis5-Oxygen	-42.332038
1650	species2 + species623 -> species912	COHydrogenolysis5-Oxygen	-57.245488
1651	species2 + species624 -> species914	COHydrogenolysis5-Oxygen	-57.269337
1652	species2 + species624 -> species915	COHydrogenolysis5-Oxygen	-47.772075
1653	species2 + species641 -> species932	COHydrogenolysis5-Oxygen	-71.430922
1654	species2 + species641 -> species933	COHydrogenolysis5-Oxygen	-62.526114
1655	species2 + species642 -> species934	COHydrogenolysis5-Oxygen	-57.786898
1656	species2 + species642 -> species935	COHydrogenolysis5-Oxygen	-63.059993
1657	species2 + species688 -> species926	COHydrogenolysis5-Oxygen	-47.034436
1658	species2 + species688 -> species944	COHydrogenolysis5-Oxygen	-41.618164
1659	species2 + species727 -> species893	COHydrogenolysis5-Oxygen	-55.803682
1660	species2 + species727 -> species540	COHydrogenolysis5-Oxygen	-50.980366
1661	species2 + species728 -> species620	COHydrogenolysis5-Oxygen	-51.258602
1662	species2 + species728 -> species508	COHydrogenolysis5-Oxygen	-44.866287
1663	species2 + species797 -> species1007	COHydrogenolysis5-Oxygen	-71.670246
1664	species2 + species797 -> species930	COHydrogenolysis5-Oxygen	-48.945269
1665	species2 + species802 -> species1012	COHydrogenolysis5-Oxygen	-54.922113
1666	species2 + species802 -> species1013	COHydrogenolysis5-Oxygen	-64.419374
1667	species2 + species803 -> species1016	COHydrogenolysis5-Oxygen	-52.810866
1668	species2 + species803 -> species1017	COHydrogenolysis5-Oxygen	-45.831118
1669	species2 + species814 -> species937	COHydrogenolysis5-Oxygen	-47.383800
1670	species2 + species814 -> species1024	COHydrogenolysis5-Oxygen	-51.258602
1671	species2 + species822 -> species541	COHydrogenolysis5-Oxygen	-41.049601
1672	species2 + species822 -> species894	COHydrogenolysis5-Oxygen	-41.642180
1673	species2 + species868 -> species577	COHydrogenolysis5-Oxygen	-44.273833
1674	species2 + species868 -> species654	COHydrogenolysis5-Oxygen	-52.810866
1675	species2 + species873 -> species1066	COHydrogenolysis5-Oxygen	-63.486342
1676	species2 + species873 -> species835	COHydrogenolysis5-Oxygen	-72.023376
1677	species2 + species896 -> species661	COHydrogenolysis5-Oxygen	-41.642180
1678	species2 + species896 -> species1068	COHydrogenolysis5-Oxygen	-40.089707
1679	species2 + species930 -> species1089	COHydrogenolysis5-Oxygen	-62.528206
1680	species2 + species930 -> species1090	COHydrogenolysis5-Oxygen	-71.430922
1681	species2 + species931 -> species1091	COHydrogenolysis5-Oxygen	-116.636950
1682	species2 + species931 -> species1092	COHydrogenolysis5-Oxygen	-70.494961
1683	species2 + species965 -> species1109	COHydrogenolysis5-Oxygen	-122.431790
1684	species2 + species979 -> species1012	COHydrogenolysis5-Oxygen	-60.260060
1685	species2 + species979 -> species1099	COHydrogenolysis5-Oxygen	-61.812742
1686	species2 + species980 -> species821	COHydrogenolysis5-Oxygen	-50.411761
1687	species2 + species1007 -> species1121	COHydrogenolysis5-Oxygen	-57.243396
1688	species2 + species1007 -> species1090	COHydrogenolysis5-Oxygen	-48.705944
1689	species2 + species1010 -> species1122	COHydrogenolysis5-Oxygen	-60.611516
1690	species2 + species1010 -> species1123	COHydrogenolysis5-Oxygen	-66.039001
1691	species2 + species1028 -> species1099	COHydrogenolysis5-Oxygen	-49.298398
1692	species2 + species1028 -> species1133	COHydrogenolysis5-Oxygen	-56.650523

1693	species2 + species1042 -> species1133	COHydrogenolysis5-Oxygen	-45.506021
1694	species2 + species1042 -> species1013	COHydrogenolysis5-Oxygen	-46.098475
1695	species2 + species1062 -> species991	COHydrogenolysis5-Oxygen	-58.094003
1696	species2 + species1062 -> species1033	COHydrogenolysis5-Oxygen	-66.039001
1697	species2 + species1075 -> species1041	COHydrogenolysis5-Oxygen	-54.869813
1698	species2 + species1075 -> species1153	COHydrogenolysis5-Oxygen	-54.869813
1699	species2 + species1118 -> species1163	COHydrogenolysis5-Oxygen	-119.987078
1700	species2 + species1118 -> species1164	COHydrogenolysis5-Oxygen	-71.430922
1701	species2 + species1150 -> species1167	COHydrogenolysis5-Oxygen	-59.326191
1702	species2 + species6 -> species30	COHydrogenolysis6-Oxygen	-25.203454
1703	species2 + species6 -> species24	COHydrogenolysis6-Oxygen	-32.780845
1704	species2 + species31 -> species93	COHydrogenolysis6-Oxygen	-27.756028
1705	species2 + species31 -> species9	COHydrogenolysis6-Oxygen	-19.811324
1706	species2 + species117 -> species326	COHydrogenolysis6-Oxygen	-26.636892
1707	species2 + species117 -> species362	COHydrogenolysis6-Oxygen	-46.373782
1708	species2 + species118 -> species313	COHydrogenolysis6-Oxygen	-27.004247
1709	species2 + species118 -> species266	COHydrogenolysis6-Oxygen	-41.917822
1710	species2 + species125 -> species275	COHydrogenolysis6-Oxygen	-32.212281
1711	species2 + species125 -> species314	COHydrogenolysis6-Oxygen	-19.811324
1712	species2 + species148 -> species314	COHydrogenolysis6-Oxygen	-43.470086
1713	species2 + species148 -> species426	COHydrogenolysis6-Oxygen	-31.460542
1714	species2 + species155 -> species65	COHydrogenolysis6-Oxygen	-35.438480
1715	species2 + species301 -> species110	COHydrogenolysis6-Oxygen	-32.079146
1716	species2 + species301 -> species595	COHydrogenolysis6-Oxygen	-40.389198
1717	species2 + species363 -> species533	COHydrogenolysis6-Oxygen	-40.389198
1718	species2 + species363 -> species121	COHydrogenolysis6-Oxygen	-33.406395
1719	species2 + species410 -> species587	COHydrogenolysis6-Oxygen	-41.941671
1720	species2 + species410 -> species152	COHydrogenolysis6-Oxygen	-27.030314
1721	species2 + species464 -> species371	COHydrogenolysis6-Oxygen	-48.071650
1722	species2 + species543 -> species829	COHydrogenolysis6-Oxygen	-44.847459
1723	species2 + species543 -> species644	COHydrogenolysis6-Oxygen	-37.495334
1724	species2 + species548 -> species643	COHydrogenolysis6-Oxygen	-47.200541
1725	species2 + species548 -> species828	COHydrogenolysis6-Oxygen	-54.185310
1726	species2 + species574 -> species330	COHydrogenolysis6-Oxygen	-47.704294
1727	species2 + species574 -> species437	COHydrogenolysis6-Oxygen	-48.071650
1728	species2 + species631 -> species911	COHydrogenolysis6-Oxygen	-45.648277
1729	species2 + species631 -> species926	COHydrogenolysis6-Oxygen	-60.561726
1730	species2 + species645 -> species911	COHydrogenolysis6-Oxygen	-45.648277
1731	species2 + species645 -> species644	COHydrogenolysis6-Oxygen	-61.154181
1732	species2 + species651 -> species912	COHydrogenolysis6-Oxygen	-36.902754
1733	species2 + species651 -> species807	COHydrogenolysis6-Oxygen	-45.439914
1734	species2 + species696 -> species926	COHydrogenolysis6-Oxygen	-36.902754
1735	species2 + species696 -> species829	COHydrogenolysis6-Oxygen	-44.847459
1736	species2 + species818 -> species540	COHydrogenolysis6-Oxygen	-40.848601
1737	species2 + species818 -> species1032	COHydrogenolysis6-Oxygen	-53.617123
1738	species2 + species883 -> species626	COHydrogenolysis6-Oxygen	-45.672126
1739	species2 + species883 -> species1068	COHydrogenolysis6-Oxygen	-53.617123
1740	species2 + species936 -> species1089	COHydrogenolysis6-Oxygen	-65.844445
1741	species2 + species936 -> species1099	COHydrogenolysis6-Oxygen	-75.339614
1742	species2 + species940 -> species894	COHydrogenolysis6-Oxygen	-55.169387
1743	species2 + species940 -> species648	COHydrogenolysis6-Oxygen	-46.631935
1744	species2 + species989 -> species835	COHydrogenolysis6-Oxygen	-61.891820
1745	species2 + species989 -> species945	COHydrogenolysis6-Oxygen	-61.299366
1746	species2 + species1023 -> species1090	COHydrogenolysis6-Oxygen	-51.088314
1747	species2 + species1023 -> species1133	COHydrogenolysis6-Oxygen	-59.033311
1748	species2 + species1038 -> species1099	COHydrogenolysis6-Oxygen	-51.680768
1749	species2 + species1038 -> species1143	COHydrogenolysis6-Oxygen	-58.073083
1750	species2 + species1063 -> species915	COHydrogenolysis6-Oxygen	-61.299366
1751	species2 + species1072 -> species933	COHydrogenolysis6-Oxygen	-60.452524

1752	species2 + species1072 -> species1153	COHydrogenolysis6-Oxygen	-68.397103
1753	species2 + species1102 -> species1154	COHydrogenolysis6-Oxygen	-51.088314
1754	species2 + species1102 -> species1013	COHydrogenolysis6-Oxygen	-59.625766
1755	species2 + species1124 -> species1163	COHydrogenolysis6-Oxygen	-122.369448
1756	species2 + species1124 -> species1167	COHydrogenolysis6-Oxygen	-72.853482
1757	species2 + species1151 -> species1091	COHydrogenolysis6-Oxygen	-130.164240
1758	species7 -> species44 + species45	Decarbonylation-Oxygen	203.020734
1759	species9 -> species45 + species65	Decarbonylation-Oxygen	47.847262
1760	species14 -> species45 + species85	Decarbonylation-Oxygen	64.356196
1761	species19 -> species45 + species106	Decarbonylation-Oxygen	47.873328
1762	species25 -> species45 + species85	Decarbonylation-Oxygen	63.474460
1763	species31 -> species45 + species155	Decarbonylation-Oxygen	63.474460
1764	species43 -> species45 + species187	Decarbonylation-Oxygen	54.832073
1765	species46 -> species45 + species76	Decarbonylation-Oxygen	52.846054
1766	species47 -> species45 + species192	Decarbonylation-Oxygen	-12.392255
1767	species48 -> species45 + species193	Decarbonylation-Oxygen	55.792008
1768	species49 -> species45 + species79	Decarbonylation-Oxygen	55.792008
1769	species50 -> species45 + species79	Decarbonylation-Oxygen	55.792008
1770	species51 -> species45 + species193	Decarbonylation-Oxygen	55.792008
1771	species52 -> species45 + species216	Decarbonylation-Oxygen	48.807197
1772	species52 -> species45 + species192	Decarbonylation-Oxygen	55.792008
1773	species53 -> species45 + species76	Decarbonylation-Oxygen	55.792008
1774	species54 -> species45 + species219	Decarbonylation-Oxygen	24.014486
1775	species55 -> species45 + species221	Decarbonylation-Oxygen	-49.477474
1776	species62 -> species45 + species230	Decarbonylation-Oxygen	48.807197
1777	species64 -> species45 + species218	Decarbonylation-Oxygen	-3.725894
1778	species66 -> species45 + species233	Decarbonylation-Oxygen	47.847262
1779	species67 -> species45 + species234	Decarbonylation-Oxygen	47.880315
1780	species68 -> species45 + species235	Decarbonylation-Oxygen	48.807197
1781	species69 -> species45 + species236	Decarbonylation-Oxygen	48.807197
1782	species70 -> species45 + species237	Decarbonylation-Oxygen	48.809205
1783	species71 -> species45 + species247	Decarbonylation-Oxygen	6.488677
1784	species77 -> species2 + species45	Decarbonylation-Oxygen	-1.943677
1785	species86 -> species45 + species277	Decarbonylation-Oxygen	-15.200765
1786	species87 -> species45 + species278	Decarbonylation-Oxygen	64.356196
1787	species88 -> species45 + species279	Decarbonylation-Oxygen	64.356196
1788	species89 -> species45 + species280	Decarbonylation-Oxygen	43.736482
1789	species90 -> species45 + species281	Decarbonylation-Oxygen	64.356196
1790	species91 -> species45 + species282	Decarbonylation-Oxygen	64.356196
1791	species92 -> species45 + species147	Decarbonylation-Oxygen	64.356196
1792	species93 -> species45 + species65	Decarbonylation-Oxygen	55.792008
1793	species94 -> species45 + species283	Decarbonylation-Oxygen	55.792008
1794	species95 -> species45 + species309	Decarbonylation-Oxygen	72.454788
1795	species99 -> species45 + species319	Decarbonylation-Oxygen	97.038299
1796	species101 -> species45 + species321	Decarbonylation-Oxygen	109.069809
1797	species103 -> species45 + species323	Decarbonylation-Oxygen	97.038299
1798	species107 -> species45 + species328	Decarbonylation-Oxygen	47.873328
1799	species108 -> species45 + species329	Decarbonylation-Oxygen	47.873328
1800	species109 -> species45 + species331	Decarbonylation-Oxygen	49.767090
1801	species110 -> species45 + species330	Decarbonylation-Oxygen	47.849312
1802	species119 -> species45 + species253	Decarbonylation-Oxygen	55.792008
1803	species121 -> species45 + species371	Decarbonylation-Oxygen	48.809205
1804	species131 -> species45 + species276	Decarbonylation-Oxygen	63.474460
1805	species132 -> species45 + species279	Decarbonylation-Oxygen	96.497893
1806	species133 -> species45 + species278	Decarbonylation-Oxygen	63.474460
1807	species134 -> species45 + species281	Decarbonylation-Oxygen	63.474460
1808	species135 -> species45 + species280	Decarbonylation-Oxygen	63.474460
1809	species136 -> species45 + species277	Decarbonylation-Oxygen	63.474460
1810	species137 -> species45 + species282	Decarbonylation-Oxygen	63.474460

1811	species138 -> species45 + species147	Decarbonylation-Oxygen	63.474460
1812	species139 -> species45 + species283	Decarbonylation-Oxygen	55.792008
1813	species152 -> species45 + species437	Decarbonylation-Oxygen	42.433124
1814	species156 -> species45 + species441	Decarbonylation-Oxygen	96.497893
1815	species157 -> species45 + species442	Decarbonylation-Oxygen	63.472410
1816	species158 -> species45 + species441	Decarbonylation-Oxygen	63.474460
1817	species159 -> species45 + species442	Decarbonylation-Oxygen	63.472410
1818	species160 -> species45 + species443	Decarbonylation-Oxygen	63.472410
1819	species161 -> species45 + species443	Decarbonylation-Oxygen	63.472410
1820	species162 -> species45 + species444	Decarbonylation-Oxygen	63.474460
1821	species163 -> species45 + species185	Decarbonylation-Oxygen	63.474460
1822	species164 -> species45 + species444	Decarbonylation-Oxygen	63.474460
1823	species165 -> species45 + species185	Decarbonylation-Oxygen	63.474460
1824	species187 -> species45 + species220	Decarbonylation-Oxygen	56.751902
1825	species188 -> species45 + species207	Decarbonylation-Oxygen	55.792008
1826	species188 -> species45 + species466	Decarbonylation-Oxygen	55.792008
1827	species189 -> species45 + species468	Decarbonylation-Oxygen	-12.392255
1828	species189 -> species45 + species254	Decarbonylation-Oxygen	55.792008
1829	species190 -> species45 + species467	Decarbonylation-Oxygen	55.792008
1830	species190 -> species45 + species215	Decarbonylation-Oxygen	52.846054
1831	species191 -> species45 + species64	Decarbonylation-Oxygen	55.792008
1832	species192 -> species45 + species255	Decarbonylation-Oxygen	48.807197
1833	species194 -> species45 + species224	Decarbonylation-Oxygen	47.880315
1834	species195 -> species45 + species251	Decarbonylation-Oxygen	47.847262
1835	species196 -> species45 + species479	Decarbonylation-Oxygen	48.809205
1836	species196 -> species45 + species245	Decarbonylation-Oxygen	52.848062
1837	species197 -> species45 + species229	Decarbonylation-Oxygen	52.846054
1838	species198 -> species45 + species63	Decarbonylation-Oxygen	47.880315
1839	species199 -> species45 + species239	Decarbonylation-Oxygen	-12.392255
1840	species200 -> species45 + species474	Decarbonylation-Oxygen	-12.392255
1841	species201 -> species45 + species483	Decarbonylation-Oxygen	48.809205
1842	species201 -> species45 + species475	Decarbonylation-Oxygen	-12.392255
1843	species202 -> species45 + species245	Decarbonylation-Oxygen	-12.392255
1844	species203 -> species45 + species71	Decarbonylation-Oxygen	13.666647
1845	species204 -> species45 + species476	Decarbonylation-Oxygen	-24.677818
1846	species205 -> species45 + species490	Decarbonylation-Oxygen	47.882324
1847	species205 -> species45 + species474	Decarbonylation-Oxygen	55.794017
1848	species206 -> species45 + species251	Decarbonylation-Oxygen	55.792008
1849	species207 -> species45 + species75	Decarbonylation-Oxygen	55.792008
1850	species208 -> species45 + species77	Decarbonylation-Oxygen	66.087912
1851	species209 -> species45 + species493	Decarbonylation-Oxygen	47.849312
1852	species209 -> species45 + species239	Decarbonylation-Oxygen	55.794017
1853	species210 -> species45 + species224	Decarbonylation-Oxygen	55.792008
1854	species211 -> species45 + species63	Decarbonylation-Oxygen	50.826270
1855	species212 -> species45 + species54	Decarbonylation-Oxygen	55.792008
1856	species213 -> species45 + species476	Decarbonylation-Oxygen	55.792008
1857	species214 -> species45 + species436	Decarbonylation-Oxygen	-12.392255
1858	species215 -> species45 + species80	Decarbonylation-Oxygen	55.792008
1859	species216 -> species45 + species255	Decarbonylation-Oxygen	55.792008
1860	species217 -> species45 + species436	Decarbonylation-Oxygen	55.792008
1861	species217 -> species45 + species345	Decarbonylation-Oxygen	48.807197
1862	species223 -> species45 + species497	Decarbonylation-Oxygen	47.880315
1863	species225 -> species45 + species498	Decarbonylation-Oxygen	47.847262
1864	species231 -> species45 + species71	Decarbonylation-Oxygen	73.906176
1865	species237 -> species45 + species507	Decarbonylation-Oxygen	48.807197
1866	species238 -> species45 + species502	Decarbonylation-Oxygen	47.880315
1867	species238 -> species45 + species501	Decarbonylation-Oxygen	47.847262
1868	species239 -> species45 + species399	Decarbonylation-Oxygen	47.847262
1869	species240 -> species45 + species348	Decarbonylation-Oxygen	59.838731

1870	species241 -> species45 + species503	Decarbonylation-Oxygen	47.847262
1871	species242 -> species45 + species504	Decarbonylation-Oxygen	58.683822
1872	species243 -> species45 + species505	Decarbonylation-Oxygen	-24.679868
1873	species244 -> species45 + species506	Decarbonylation-Oxygen	48.807197
1874	species245 -> species45 + species393	Decarbonylation-Oxygen	48.807197
1875	species254 -> species45 + species369	Decarbonylation-Oxygen	-12.392255
1876	species262 -> species45 + species420	Decarbonylation-Oxygen	64.356196
1877	species265 -> species45 + species539	Decarbonylation-Oxygen	47.873328
1878	species276 -> species45 + species496	Decarbonylation-Oxygen	63.474460
1879	species285 -> species45 + species568	Decarbonylation-Oxygen	-30.967876
1880	species286 -> species45 + species569	Decarbonylation-Oxygen	-15.202815
1881	species287 -> species45 + species570	Decarbonylation-Oxygen	-30.967876
1882	species288 -> species45 + species571	Decarbonylation-Oxygen	-19.168578
1883	species289 -> species45 + species419	Decarbonylation-Oxygen	-17.718194
1884	species290 -> species45 + species572	Decarbonylation-Oxygen	64.356196
1885	species291 -> species45 + species573	Decarbonylation-Oxygen	43.736482
1886	species292 -> species45 + species106	Decarbonylation-Oxygen	63.474460
1887	species293 -> species45 + species236	Decarbonylation-Oxygen	55.792008
1888	species294 -> species45 + species235	Decarbonylation-Oxygen	55.792008
1889	species295 -> species45 + species237	Decarbonylation-Oxygen	-12.392255
1890	species296 -> species45 + species230	Decarbonylation-Oxygen	52.846054
1891	species297 -> species45 + species233	Decarbonylation-Oxygen	55.792008
1892	species298 -> species45 + species234	Decarbonylation-Oxygen	55.792008
1893	species299 -> species45 + species232	Decarbonylation-Oxygen	55.792008
1894	species300 -> species45 + species572	Decarbonylation-Oxygen	63.474460
1895	species301 -> species45 + species574	Decarbonylation-Oxygen	63.474460
1896	species302 -> species45 + species491	Decarbonylation-Oxygen	55.792008
1897	species302 -> species45 + species575	Decarbonylation-Oxygen	55.792008
1898	species303 -> species45 + species576	Decarbonylation-Oxygen	61.203259
1899	species304 -> species45 + species433	Decarbonylation-Oxygen	55.792008
1900	species305 -> species45 + species620	Decarbonylation-Oxygen	48.809205
1901	species305 -> species45 + species577	Decarbonylation-Oxygen	55.794017
1902	species306 -> species45 + species440	Decarbonylation-Oxygen	55.792008
1903	species307 -> species45 + species578	Decarbonylation-Oxygen	55.792008
1904	species310 -> species45 + species624	Decarbonylation-Oxygen	47.873328
1905	species315 -> species45 + species640	Decarbonylation-Oxygen	158.238838
1906	species332 -> species45 + species659	Decarbonylation-Oxygen	47.847262
1907	species333 -> species45 + species660	Decarbonylation-Oxygen	47.880315
1908	species334 -> species45 + species659	Decarbonylation-Oxygen	48.807197
1909	species335 -> species45 + species660	Decarbonylation-Oxygen	48.807197
1910	species336 -> species45 + species508	Decarbonylation-Oxygen	55.794017
1911	species336 -> species45 + species654	Decarbonylation-Oxygen	47.849312
1912	species337 -> species45 + species655	Decarbonylation-Oxygen	47.847262
1913	species338 -> species45 + species670	Decarbonylation-Oxygen	48.807197
1914	species338 -> species45 + species656	Decarbonylation-Oxygen	47.847262
1915	species339 -> species45 + species657	Decarbonylation-Oxygen	47.847262
1916	species340 -> species45 + species658	Decarbonylation-Oxygen	47.847262
1917	species345 -> species45 + species246	Decarbonylation-Oxygen	14.771779
1918	species350 -> species45 + species420	Decarbonylation-Oxygen	63.474460
1919	species363 -> species45 + species464	Decarbonylation-Oxygen	63.474460
1920	species368 -> species45 + species508	Decarbonylation-Oxygen	-12.392255
1921	species369 -> species45 + species232	Decarbonylation-Oxygen	48.807197
1922	species372 -> species45 + species705	Decarbonylation-Oxygen	58.683822
1923	species373 -> species45 + species706	Decarbonylation-Oxygen	46.348846
1924	species400 -> species45 + species563	Decarbonylation-Oxygen	63.474460
1925	species400 -> species45 + species566	Decarbonylation-Oxygen	63.474460
1926	species401 -> species45 + species565	Decarbonylation-Oxygen	63.474460
1927	species401 -> species45 + species564	Decarbonylation-Oxygen	96.497893
1928	species402 -> species45 + species409	Decarbonylation-Oxygen	63.474460

1929	species402 -> species45 + species567	Decarbonylation-Oxygen	63.474460
1930	species403 -> species45 + species573	Decarbonylation-Oxygen	100.956154
1931	species404 -> species45 + species569	Decarbonylation-Oxygen	87.077868
1932	species405 -> species45 + species568	Decarbonylation-Oxygen	127.828940
1933	species406 -> species45 + species570	Decarbonylation-Oxygen	63.472410
1934	species407 -> species45 + species571	Decarbonylation-Oxygen	63.474460
1935	species408 -> species45 + species419	Decarbonylation-Oxygen	63.474460
1936	species409 -> species45 + species115	Decarbonylation-Oxygen	63.474460
1937	species410 -> species45 + species574	Decarbonylation-Oxygen	63.474460
1938	species411 -> species45 + species576	Decarbonylation-Oxygen	55.792008
1939	species412 -> species45 + species433	Decarbonylation-Oxygen	52.846054
1940	species413 -> species45 + species577	Decarbonylation-Oxygen	-12.392255
1941	species414 -> species45 + species440	Decarbonylation-Oxygen	55.792008
1942	species415 -> species45 + species739	Decarbonylation-Oxygen	55.792008
1943	species430 -> species45 + species754	Decarbonylation-Oxygen	48.807197
1944	species436 -> species45 + species246	Decarbonylation-Oxygen	7.786972
1945	species438 -> species45 + species758	Decarbonylation-Oxygen	47.880315
1946	species445 -> species45 + species760	Decarbonylation-Oxygen	100.958163
1947	species446 -> species45 + species761	Decarbonylation-Oxygen	96.499902
1948	species447 -> species45 + species762	Decarbonylation-Oxygen	96.497893
1949	species448 -> species45 + species462	Decarbonylation-Oxygen	96.497893
1950	species449 -> species45 + species763	Decarbonylation-Oxygen	100.956154
1951	species450 -> species45 + species761	Decarbonylation-Oxygen	123.372688
1952	species451 -> species45 + species760	Decarbonylation-Oxygen	63.474460
1953	species452 -> species45 + species763	Decarbonylation-Oxygen	63.474460
1954	species453 -> species45 + species462	Decarbonylation-Oxygen	63.474460
1955	species454 -> species45 + species463	Decarbonylation-Oxygen	67.932721
1956	species455 -> species45 + species463	Decarbonylation-Oxygen	67.932721
1957	species465 -> species45 + species55	Decarbonylation-Oxygen	54.832073
1958	species466 -> species45 + species75	Decarbonylation-Oxygen	55.792008
1959	species467 -> species45 + species80	Decarbonylation-Oxygen	52.846054
1960	species468 -> species45 + species299	Decarbonylation-Oxygen	48.807197
1961	species468 -> species45 + species369	Decarbonylation-Oxygen	55.792008
1962	species469 -> species45 + species489	Decarbonylation-Oxygen	56.372413
1963	species469 -> species45 + species767	Decarbonylation-Oxygen	-24.097455
1964	species470 -> species45 + species509	Decarbonylation-Oxygen	-11.811892
1965	species471 -> species45 + species768	Decarbonylation-Oxygen	-11.811892
1966	species471 -> species45 + species482	Decarbonylation-Oxygen	48.462728
1967	species472 -> species45 + species203	Decarbonylation-Oxygen	47.847262
1968	species472 -> species45 + species231	Decarbonylation-Oxygen	-12.392255
1969	species473 -> species45 + species478	Decarbonylation-Oxygen	48.429716
1970	species474 -> species45 + species375	Decarbonylation-Oxygen	47.880315
1971	species475 -> species45 + species510	Decarbonylation-Oxygen	48.809205
1972	species477 -> species45 + species516	Decarbonylation-Oxygen	47.847262
1973	species478 -> species45 + species226	Decarbonylation-Oxygen	47.847262
1974	species479 -> species45 + species393	Decarbonylation-Oxygen	52.846054
1975	species480 -> species45 + species770	Decarbonylation-Oxygen	-24.099463
1976	species480 -> species45 + species513	Decarbonylation-Oxygen	48.427666
1977	species481 -> species45 + species770	Decarbonylation-Oxygen	-12.392255
1978	species482 -> species45 + species240	Decarbonylation-Oxygen	-12.392255
1979	species483 -> species45 + species510	Decarbonylation-Oxygen	-12.392255
1980	species484 -> species45 + species772	Decarbonylation-Oxygen	59.264226
1981	species484 -> species45 + species771	Decarbonylation-Oxygen	-11.811892
1982	species485 -> species45 + species771	Decarbonylation-Oxygen	-11.811892
1983	species485 -> species45 + species773	Decarbonylation-Oxygen	48.427666
1984	species486 -> species45 + species513	Decarbonylation-Oxygen	57.918777
1985	species488 -> species45 + species516	Decarbonylation-Oxygen	57.813843
1986	species489 -> species45 + species250	Decarbonylation-Oxygen	-0.328570
1987	species490 -> species45 + species375	Decarbonylation-Oxygen	55.792008

1988	species491 -> species45 + species252	Decarbonylation-Oxygen	55.792008
1989	species492 -> species45 + species217	Decarbonylation-Oxygen	-12.392255
1990	species492 -> species45 + species214	Decarbonylation-Oxygen	55.792008
1991	species493 -> species45 + species399	Decarbonylation-Oxygen	55.792008
1992	species494 -> species45 + species677	Decarbonylation-Oxygen	21.185835
1993	species495 -> species45 + species677	Decarbonylation-Oxygen	21.082917
1994	species500 -> species45 + species784	Decarbonylation-Oxygen	21.267858
1995	species501 -> species45 + species785	Decarbonylation-Oxygen	52.994209
1996	species502 -> species45 + species785	Decarbonylation-Oxygen	52.961156
1997	species508 -> species45 + species682	Decarbonylation-Oxygen	47.847262
1998	species509 -> species45 + species669	Decarbonylation-Oxygen	-12.392255
1999	species509 -> species45 + species603	Decarbonylation-Oxygen	47.849312
2000	species510 -> species45 + species678	Decarbonylation-Oxygen	-4.252534
2001	species511 -> species45 + species786	Decarbonylation-Oxygen	61.201251
2002	species512 -> species45 + species787	Decarbonylation-Oxygen	-0.328570
2003	species513 -> species45 + species707	Decarbonylation-Oxygen	-0.330578
2004	species518 -> species45 + species783	Decarbonylation-Oxygen	3.011405
2005	species520 -> species45 + species743	Decarbonylation-Oxygen	64.356196
2006	species522 -> species45 + species800	Decarbonylation-Oxygen	97.038299
2007	species530 -> species45 + species742	Decarbonylation-Oxygen	-17.718194
2008	species531 -> species45 + species744	Decarbonylation-Oxygen	64.356196
2009	species532 -> species45 + species745	Decarbonylation-Oxygen	54.834123
2010	species533 -> species45 + species371	Decarbonylation-Oxygen	55.792008
2011	species534 -> species45 + species826	Decarbonylation-Oxygen	97.038299
2012	species540 -> species45 + species835	Decarbonylation-Oxygen	42.431074
2013	species541 -> species45 + species836	Decarbonylation-Oxygen	48.807197
2014	species563 -> species45 + species781	Decarbonylation-Oxygen	63.472410
2015	species564 -> species45 + species782	Decarbonylation-Oxygen	63.474460
2016	species565 -> species45 + species782	Decarbonylation-Oxygen	96.497893
2017	species566 -> species45 + species781	Decarbonylation-Oxygen	63.472410
2018	species567 -> species45 + species115	Decarbonylation-Oxygen	63.474460
2019	species575 -> species45 + species252	Decarbonylation-Oxygen	55.792008
2020	species577 -> species45 + species681	Decarbonylation-Oxygen	48.807197
2021	species584 -> species45 + species870	Decarbonylation-Oxygen	-15.200765
2022	species585 -> species45 + species871	Decarbonylation-Oxygen	43.736482
2023	species586 -> species45 + species872	Decarbonylation-Oxygen	55.794017
2024	species587 -> species45 + species330	Decarbonylation-Oxygen	57.711837
2025	species588 -> species45 + species873	Decarbonylation-Oxygen	64.356196
2026	species589 -> species45 + species321	Decarbonylation-Oxygen	88.055920
2027	species590 -> species45 + species323	Decarbonylation-Oxygen	112.639430
2028	species591 -> species45 + species319	Decarbonylation-Oxygen	145.664872
2029	species592 -> species45 + species309	Decarbonylation-Oxygen	88.055920
2030	species593 -> species45 + species328	Decarbonylation-Oxygen	63.474460
2031	species594 -> species45 + species329	Decarbonylation-Oxygen	63.474460
2032	species595 -> species45 + species437	Decarbonylation-Oxygen	55.792008
2033	species596 -> species45 + species505	Decarbonylation-Oxygen	55.792008
2034	species597 -> species45 + species506	Decarbonylation-Oxygen	-24.679868
2035	species598 -> species45 + species503	Decarbonylation-Oxygen	55.792008
2036	species599 -> species45 + species504	Decarbonylation-Oxygen	55.792008
2037	species600 -> species45 + species501	Decarbonylation-Oxygen	-12.392255
2038	species601 -> species45 + species502	Decarbonylation-Oxygen	-12.392255
2039	species602 -> species45 + species498	Decarbonylation-Oxygen	47.847262
2040	species603 -> species45 + species500	Decarbonylation-Oxygen	8.891079
2041	species604 -> species45 + species728	Decarbonylation-Oxygen	63.474460
2042	species604 -> species45 + species868	Decarbonylation-Oxygen	63.474460
2043	species605 -> species45 + species871	Decarbonylation-Oxygen	63.474460
2044	species606 -> species45 + species744	Decarbonylation-Oxygen	63.472410
2045	species607 -> species45 + species870	Decarbonylation-Oxygen	63.474460
2046	species608 -> species45 + species765	Decarbonylation-Oxygen	63.474460

2047	species609 -> species45 + species874	Decarbonylation-Oxygen	63.472410
2048	species610 -> species45 + species875	Decarbonylation-Oxygen	63.472410
2049	species611 -> species45 + species876	Decarbonylation-Oxygen	63.474460
2050	species612 -> species45 + species749	Decarbonylation-Oxygen	63.474460
2051	species613 -> species45 + species877	Decarbonylation-Oxygen	63.474460
2052	species614 -> species45 + species777	Decarbonylation-Oxygen	55.792008
2053	species614 -> species45 + species878	Decarbonylation-Oxygen	61.203259
2054	species615 -> species45 + species780	Decarbonylation-Oxygen	-12.392255
2055	species615 -> species45 + species759	Decarbonylation-Oxygen	55.794017
2056	species617 -> species45 + species793	Decarbonylation-Oxygen	48.807197
2057	species617 -> species45 + species879	Decarbonylation-Oxygen	61.201251
2058	species618 -> species45 + species753	Decarbonylation-Oxygen	61.201251
2059	species619 -> species45 + species757	Decarbonylation-Oxygen	67.974645
2060	species620 -> species45 + species681	Decarbonylation-Oxygen	55.792008
2061	species621 -> species45 + species908	Decarbonylation-Oxygen	58.683822
2062	species621 -> species45 + species880	Decarbonylation-Oxygen	55.792008
2063	species622 -> species45 + species881	Decarbonylation-Oxygen	53.274579
2064	species622 -> species45 + species909	Decarbonylation-Oxygen	46.348846
2065	species625 -> species45 + species913	Decarbonylation-Oxygen	84.486299
2066	species626 -> species45 + species915	Decarbonylation-Oxygen	47.847262
2067	species627 -> species45 + species914	Decarbonylation-Oxygen	47.847262
2068	species641 -> species45 + species931	Decarbonylation-Oxygen	47.873328
2069	species646 -> species45 + species745	Decarbonylation-Oxygen	55.794017
2070	species648 -> species45 + species945	Decarbonylation-Oxygen	48.807197
2071	species654 -> species45 + species682	Decarbonylation-Oxygen	55.792008
2072	species656 -> species45 + species956	Decarbonylation-Oxygen	48.807197
2073	species661 -> species45 + species914	Decarbonylation-Oxygen	47.847262
2074	species662 -> species45 + species959	Decarbonylation-Oxygen	47.849312
2075	species663 -> species45 + species955	Decarbonylation-Oxygen	47.849312
2076	species664 -> species45 + species960	Decarbonylation-Oxygen	47.882324
2077	species665 -> species45 + species959	Decarbonylation-Oxygen	-24.677818
2078	species666 -> species45 + species955	Decarbonylation-Oxygen	47.849312
2079	species667 -> species45 + species960	Decarbonylation-Oxygen	58.685872
2080	species668 -> species45 + species788	Decarbonylation-Oxygen	-12.392255
2081	species668 -> species45 + species954	Decarbonylation-Oxygen	47.847262
2082	species669 -> species45 + species500	Decarbonylation-Oxygen	69.132650
2083	species670 -> species45 + species956	Decarbonylation-Oxygen	47.847262
2084	species671 -> species45 + species962	Decarbonylation-Oxygen	58.683822
2085	species671 -> species45 + species957	Decarbonylation-Oxygen	47.847262
2086	species672 -> species45 + species958	Decarbonylation-Oxygen	46.348846
2087	species677 -> species45 + species514	Decarbonylation-Oxygen	25.253875
2088	species683 -> species45 + species742	Decarbonylation-Oxygen	63.474460
2089	species684 -> species45 + species743	Decarbonylation-Oxygen	96.497893
2090	species697 -> species45 + species764	Decarbonylation-Oxygen	63.474460
2091	species698 -> species45 + species765	Decarbonylation-Oxygen	63.474460
2092	species699 -> species45 + species764	Decarbonylation-Oxygen	96.497893
2093	species726 -> species45 + species869	Decarbonylation-Oxygen	91.536129
2094	species727 -> species45 + species873	Decarbonylation-Oxygen	63.474460
2095	species728 -> species45 + species349	Decarbonylation-Oxygen	63.474460
2096	species729 -> species45 + species874	Decarbonylation-Oxygen	63.472410
2097	species730 -> species45 + species875	Decarbonylation-Oxygen	63.472410
2098	species731 -> species45 + species876	Decarbonylation-Oxygen	96.497893
2099	species732 -> species45 + species749	Decarbonylation-Oxygen	63.474460
2100	species733 -> species45 + species879	Decarbonylation-Oxygen	-12.392255
2101	species734 -> species45 + species753	Decarbonylation-Oxygen	52.846054
2102	species735 -> species45 + species963	Decarbonylation-Oxygen	53.274579
2103	species736 -> species45 + species757	Decarbonylation-Oxygen	60.029898
2104	species737 -> species45 + species880	Decarbonylation-Oxygen	-12.392255
2105	species738 -> species45 + species881	Decarbonylation-Oxygen	-12.392255

2106	species740 -> species45 + species963	Decarbonylation-Oxygen	58.685872
2107	species759 -> species45 + species518	Decarbonylation-Oxygen	-12.392255
2108	species766 -> species45 + species198	Decarbonylation-Oxygen	55.792008
2109	species766 -> species45 + species211	Decarbonylation-Oxygen	52.846054
2110	species767 -> species45 + species250	Decarbonylation-Oxygen	80.141256
2111	species768 -> species45 + species240	Decarbonylation-Oxygen	47.882324
2112	species769 -> species45 + species776	Decarbonylation-Oxygen	67.974645
2113	species770 -> species45 + species707	Decarbonylation-Oxygen	72.196552
2114	species771 -> species45 + species790	Decarbonylation-Oxygen	58.683822
2115	species771 -> species45 + species789	Decarbonylation-Oxygen	47.847262
2116	species772 -> species45 + species790	Decarbonylation-Oxygen	-12.392255
2117	species773 -> species45 + species789	Decarbonylation-Oxygen	-12.392255
2118	species774 -> species45 + species793	Decarbonylation-Oxygen	-12.392255
2119	species777 -> species45 + species517	Decarbonylation-Oxygen	61.203259
2120	species778 -> species45 + species495	Decarbonylation-Oxygen	57.338415
2121	species778 -> species45 + species494	Decarbonylation-Oxygen	57.235488
2122	species779 -> species45 + species415	Decarbonylation-Oxygen	55.792008
2123	species780 -> species45 + species891	Decarbonylation-Oxygen	47.849312
2124	species780 -> species45 + species518	Decarbonylation-Oxygen	55.794017
2125	species788 -> species45 + species969	Decarbonylation-Oxygen	65.856495
2126	species789 -> species45 + species964	Decarbonylation-Oxygen	56.854075
2127	species790 -> species45 + species964	Decarbonylation-Oxygen	46.017515
2128	species791 -> species45 + species1002	Decarbonylation-Oxygen	57.233438
2129	species792 -> species45 + species1003	Decarbonylation-Oxygen	61.203259
2130	species793 -> species45 + species966	Decarbonylation-Oxygen	61.201251
2131	species798 -> species45 + species987	Decarbonylation-Oxygen	-17.720202
2132	species817 -> species45 + species988	Decarbonylation-Oxygen	-30.967876
2133	species818 -> species45 + species989	Decarbonylation-Oxygen	63.474460
2134	species819 -> species45 + species990	Decarbonylation-Oxygen	55.794017
2135	species820 -> species45 + species758	Decarbonylation-Oxygen	55.792008
2136	species821 -> species45 + species1033	Decarbonylation-Oxygen	47.847262
2137	species821 -> species45 + species991	Decarbonylation-Oxygen	55.792008
2138	species822 -> species45 + species539	Decarbonylation-Oxygen	63.474460
2139	species823 -> species45 + species705	Decarbonylation-Oxygen	55.792008
2140	species824 -> species45 + species706	Decarbonylation-Oxygen	55.792008
2141	species825 -> species45 + species670	Decarbonylation-Oxygen	-12.392255
2142	species831 -> species45 + species1045	Decarbonylation-Oxygen	52.091344
2143	species837 -> species45 + species1048	Decarbonylation-Oxygen	97.417704
2144	species838 -> species45 + species1049	Decarbonylation-Oxygen	46.350854
2145	species839 -> species45 + species1050	Decarbonylation-Oxygen	58.685872
2146	species840 -> species45 + species1050	Decarbonylation-Oxygen	48.809205
2147	species841 -> species45 + species1049	Decarbonylation-Oxygen	48.809205
2148	species868 -> species45 + species349	Decarbonylation-Oxygen	63.474460
2149	species869 -> species45 + species1001	Decarbonylation-Oxygen	110.628391
2150	species878 -> species45 + species517	Decarbonylation-Oxygen	55.792008
2151	species879 -> species45 + species966	Decarbonylation-Oxygen	48.807197
2152	species880 -> species45 + species967	Decarbonylation-Oxygen	58.683822
2153	species881 -> species45 + species968	Decarbonylation-Oxygen	46.348846
2154	species883 -> species45 + species1063	Decarbonylation-Oxygen	63.474460
2155	species884 -> species45 + species786	Decarbonylation-Oxygen	55.792008
2156	species885 -> species45 + species1064	Decarbonylation-Oxygen	53.274579
2157	species886 -> species45 + species1064	Decarbonylation-Oxygen	55.792008
2158	species887 -> species45 + species656	Decarbonylation-Oxygen	-12.392255
2159	species888 -> species45 + species655	Decarbonylation-Oxygen	52.846054
2160	species889 -> species45 + species658	Decarbonylation-Oxygen	55.792008
2161	species890 -> species45 + species657	Decarbonylation-Oxygen	55.792008
2162	species891 -> species45 + species783	Decarbonylation-Oxygen	10.956130
2163	species892 -> species45 + species1065	Decarbonylation-Oxygen	-17.718194
2164	species893 -> species45 + species1066	Decarbonylation-Oxygen	55.792008

2165	species894 -> species45 + species835	Decarbonylation-Oxygen	56.751902
2166	species895 -> species45 + species640	Decarbonylation-Oxygen	239.065183
2167	species896 -> species45 + species624	Decarbonylation-Oxygen	63.474460
2168	species897 -> species45 + species754	Decarbonylation-Oxygen	61.201251
2169	species899 -> species45 + species983	Decarbonylation-Oxygen	63.472410
2170	species900 -> species45 + species982	Decarbonylation-Oxygen	96.497893
2171	species900 -> species45 + species1061	Decarbonylation-Oxygen	63.474460
2172	species901 -> species45 + species988	Decarbonylation-Oxygen	59.016157
2173	species902 -> species45 + species997	Decarbonylation-Oxygen	123.370679
2174	species903 -> species45 + species998	Decarbonylation-Oxygen	55.792008
2175	species904 -> species45 + species995	Decarbonylation-Oxygen	48.807197
2176	species906 -> species45 + species1004	Decarbonylation-Oxygen	45.436190
2177	species907 -> species45 + species995	Decarbonylation-Oxygen	53.274579
2178	species908 -> species45 + species967	Decarbonylation-Oxygen	55.792008
2179	species909 -> species45 + species968	Decarbonylation-Oxygen	53.274579
2180	species916 -> species45 + species1083	Decarbonylation-Oxygen	47.849312
2181	species917 -> species45 + species1084	Decarbonylation-Oxygen	46.348846
2182	species918 -> species45 + species1085	Decarbonylation-Oxygen	47.847262
2183	species919 -> species45 + species1082	Decarbonylation-Oxygen	52.524764
2184	species920 -> species45 + species1045	Decarbonylation-Oxygen	52.124398
2185	species932 -> species45 + species1092	Decarbonylation-Oxygen	48.809205
2186	species933 -> species45 + species1091	Decarbonylation-Oxygen	-6.237424
2187	species940 -> species45 + species989	Decarbonylation-Oxygen	63.474460
2188	species943 -> species45 + species991	Decarbonylation-Oxygen	-12.392255
2189	species946 -> species45 + species1103	Decarbonylation-Oxygen	58.685872
2190	species954 -> species45 + species969	Decarbonylation-Oxygen	5.616953
2191	species957 -> species45 + species1106	Decarbonylation-Oxygen	57.085324
2192	species958 -> species45 + species1107	Decarbonylation-Oxygen	46.191737
2193	species961 -> species45 + species1083	Decarbonylation-Oxygen	61.203259
2194	species962 -> species45 + species1106	Decarbonylation-Oxygen	46.248764
2195	species969 -> species45 + species1108	Decarbonylation-Oxygen	25.571972
2196	species970 -> species45 + species987	Decarbonylation-Oxygen	87.077868
2197	species977 -> species45 + species996	Decarbonylation-Oxygen	96.497893
2198	species978 -> species45 + species997	Decarbonylation-Oxygen	160.854424
2199	species980 -> species45 + species1062	Decarbonylation-Oxygen	63.474460
2200	species981 -> species45 + species1065	Decarbonylation-Oxygen	63.474460
2201	species982 -> species45 + species679	Decarbonylation-Oxygen	63.474460
2202	species983 -> species45 + species680	Decarbonylation-Oxygen	63.474460
2203	species984 -> species45 + species1004	Decarbonylation-Oxygen	57.338415
2204	species990 -> species45 + species794	Decarbonylation-Oxygen	55.792008
2205	species991 -> species45 + species1109	Decarbonylation-Oxygen	-0.863285
2206	species999 -> species45 + species740	Decarbonylation-Oxygen	-12.392255
2207	species1000 -> species45 + species740	Decarbonylation-Oxygen	55.792008
2208	species1000 -> species45 + species735	Decarbonylation-Oxygen	61.203259
2209	species1004 -> species45 + species1110	Decarbonylation-Oxygen	58.355545
2210	species1030 -> species45 + species1114	Decarbonylation-Oxygen	63.474460
2211	species1031 -> species45 + species1115	Decarbonylation-Oxygen	63.474460
2212	species1032 -> species45 + species945	Decarbonylation-Oxygen	55.792008
2213	species1033 -> species45 + species1109	Decarbonylation-Oxygen	7.081428
2214	species1034 -> species45 + species800	Decarbonylation-Oxygen	145.664872
2215	species1035 -> species45 + species826	Decarbonylation-Oxygen	112.641439
2216	species1036 -> species45 + species962	Decarbonylation-Oxygen	-12.392255
2217	species1037 -> species45 + species958	Decarbonylation-Oxygen	-12.392255
2218	species1041 -> species45 + species1092	Decarbonylation-Oxygen	47.849312
2219	species1048 -> species45 + species1147	Decarbonylation-Oxygen	-7.159326
2220	species1051 -> species45 + species1148	Decarbonylation-Oxygen	46.348846
2221	species1052 -> species45 + species1149	Decarbonylation-Oxygen	58.683822
2222	species1053 -> species45 + species1148	Decarbonylation-Oxygen	57.235488
2223	species1061 -> species45 + species679	Decarbonylation-Oxygen	96.497893

2224	species1062 -> species45 + species965	Decarbonylation-Oxygen	63.474460
2225	species1067 -> species45 + species1114	Decarbonylation-Oxygen	63.474460
2226	species1068 -> species45 + species915	Decarbonylation-Oxygen	55.792008
2227	species1069 -> species45 + species1002	Decarbonylation-Oxygen	53.274579
2228	species1070 -> species45 + species957	Decarbonylation-Oxygen	-12.392255
2229	species1072 -> species45 + species1151	Decarbonylation-Oxygen	63.474460
2230	species1073 -> species45 + species1103	Decarbonylation-Oxygen	55.794017
2231	species1074 -> species45 + species1048	Decarbonylation-Oxygen	37.178154
2232	species1075 -> species45 + species931	Decarbonylation-Oxygen	63.474460
2233	species1076 -> species45 + species913	Decarbonylation-Oxygen	63.472410
2234	species1086 -> species45 + species1155	Decarbonylation-Oxygen	47.849312
2235	species1093 -> species45 + species1159	Decarbonylation-Oxygen	46.348846
2236	species1094 -> species45 + species1158	Decarbonylation-Oxygen	58.683822
2237	species1095 -> species45 + species1158	Decarbonylation-Oxygen	47.847262
2238	species1101 -> species45 + species1115	Decarbonylation-Oxygen	96.497893
2239	species1116 -> species45 + species985	Decarbonylation-Oxygen	53.274579
2240	species1141 -> species45 + species1084	Decarbonylation-Oxygen	55.792008
2241	species1144 -> species45 + species1159	Decarbonylation-Oxygen	47.847262
2242	species1152 -> species45 + species1085	Decarbonylation-Oxygen	53.274579
2243	species1153 -> species45 + species1091	Decarbonylation-Oxygen	1.707315
2244	species1160 -> species45 + species1173	Decarbonylation-Oxygen	16.513315
2245	species2 + species15 -> species97	FuranRingSaturation2H-Oxygen	-103.910477
2246	species2 + species16 -> species97	FuranRingSaturation2H-Oxygen	-97.507283
2247	species2 + species17 -> species83	FuranRingSaturation2H-Oxygen	-99.984630
2248	species2 + species18 -> species83	FuranRingSaturation2H-Oxygen	-103.910477
2249	species2 + species26 -> species116	FuranRingSaturation2H-Oxygen	-79.362949
2250	species2 + species27 -> species116	FuranRingSaturation2H-Oxygen	-103.908385
2251	species2 + species81 -> species260	FuranRingSaturation2H-Oxygen	-97.508957
2252	species2 + species82 -> species260	FuranRingSaturation2H-Oxygen	-95.852511
2253	species2 + species87 -> species290	FuranRingSaturation2H-Oxygen	-103.910477
2254	species2 + species88 -> species290	FuranRingSaturation2H-Oxygen	-97.507283
2255	species2 + species89 -> species262	FuranRingSaturation2H-Oxygen	-99.984630
2256	species2 + species90 -> species262	FuranRingSaturation2H-Oxygen	-103.910477
2257	species2 + species95 -> species310	FuranRingSaturation2H-Oxygen	-103.910477
2258	species2 + species96 -> species311	FuranRingSaturation2H-Oxygen	-103.908385
2259	species2 + species99 -> species310	FuranRingSaturation2H-Oxygen	-97.508957
2260	species2 + species100 -> species311	FuranRingSaturation2H-Oxygen	-97.507283
2261	species2 + species101 -> species265	FuranRingSaturation2H-Oxygen	-79.365041
2262	species2 + species102 -> species264	FuranRingSaturation2H-Oxygen	-72.011661
2263	species2 + species103 -> species265	FuranRingSaturation2H-Oxygen	-103.910477
2264	species2 + species104 -> species264	FuranRingSaturation2H-Oxygen	-103.908385
2265	species2 + species132 -> species300	FuranRingSaturation2H-Oxygen	-64.483808
2266	species2 + species133 -> species300	FuranRingSaturation2H-Oxygen	-103.910477
2267	species2 + species134 -> species350	FuranRingSaturation2H-Oxygen	-103.910477
2268	species2 + species135 -> species350	FuranRingSaturation2H-Oxygen	-79.365041
2269	species2 + species256 -> species519	FuranRingSaturation2H-Oxygen	-95.850838
2270	species2 + species257 -> species519	FuranRingSaturation2H-Oxygen	-97.507283
2271	species2 + species258 -> species317	FuranRingSaturation2H-Oxygen	-73.396146
2272	species2 + species259 -> species526	FuranRingSaturation2H-Oxygen	-97.507283
2273	species2 + species263 -> species317	FuranRingSaturation2H-Oxygen	-97.507283
2274	species2 + species268 -> species536	FuranRingSaturation2H-Oxygen	-103.908385
2275	species2 + species269 -> species536	FuranRingSaturation2H-Oxygen	-99.982538
2276	species2 + species272 -> species526	FuranRingSaturation2H-Oxygen	-103.908385
2277	species2 + species278 -> species572	FuranRingSaturation2H-Oxygen	-103.910477
2278	species2 + species279 -> species572	FuranRingSaturation2H-Oxygen	-97.507283
2279	species2 + species280 -> species420	FuranRingSaturation2H-Oxygen	-79.365041
2280	species2 + species281 -> species420	FuranRingSaturation2H-Oxygen	-103.910477
2281	species2 + species308 -> species623	FuranRingSaturation2H-Oxygen	-91.853026
2282	species2 + species309 -> species624	FuranRingSaturation2H-Oxygen	-128.491895

2283	species2 + species312 -> species317	FuranRingSaturation2H-Oxygen	-99.984630
2284	species2 + species318 -> species623	FuranRingSaturation2H-Oxygen	-73.396146
2285	species2 + species319 -> species624	FuranRingSaturation2H-Oxygen	-146.674304
2286	species2 + species320 -> species529	FuranRingSaturation2H-Oxygen	-67.307171
2287	species2 + species321 -> species539	FuranRingSaturation2H-Oxygen	-140.561480
2288	species2 + species322 -> species529	FuranRingSaturation2H-Oxygen	-91.853026
2289	species2 + species323 -> species539	FuranRingSaturation2H-Oxygen	-153.075406
2290	species2 + species352 -> species416	FuranRingSaturation2H-Oxygen	-79.362949
2291	species2 + species353 -> species416	FuranRingSaturation2H-Oxygen	-97.507283
2292	species2 + species376 -> species542	FuranRingSaturation2H-Oxygen	-115.980062
2293	species2 + species377 -> species542	FuranRingSaturation2H-Oxygen	-103.910477
2294	species2 + species378 -> species688	FuranRingSaturation2H-Oxygen	-79.365041
2295	species2 + species379 -> species688	FuranRingSaturation2H-Oxygen	-103.910477
2296	species2 + species400 -> species604	FuranRingSaturation2H-Oxygen	-103.910477
2297	species2 + species401 -> species604	FuranRingSaturation2H-Oxygen	-64.483808
2298	species2 + species456 -> species747	FuranRingSaturation2H-Oxygen	-101.967427
2299	species2 + species456 -> species693	FuranRingSaturation2H-Oxygen	-95.121148
2300	species2 + species457 -> species702	FuranRingSaturation2H-Oxygen	-23.788760
2301	species2 + species457 -> species746	FuranRingSaturation2H-Oxygen	-97.508957
2302	species2 + species519 -> species797	FuranRingSaturation2H-Oxygen	-97.508957
2303	species2 + species520 -> species588	FuranRingSaturation2H-Oxygen	-97.507283
2304	species2 + species521 -> species642	FuranRingSaturation2H-Oxygen	-97.507283
2305	species2 + species522 -> species641	FuranRingSaturation2H-Oxygen	-97.508957
2306	species2 + species524 -> species803	FuranRingSaturation2H-Oxygen	-97.507283
2307	species2 + species527 -> species797	FuranRingSaturation2H-Oxygen	-95.852511
2308	species2 + species531 -> species588	FuranRingSaturation2H-Oxygen	-97.507283
2309	species2 + species534 -> species641	FuranRingSaturation2H-Oxygen	-97.508957
2310	species2 + species535 -> species642	FuranRingSaturation2H-Oxygen	-97.507283
2311	species2 + species550 -> species814	FuranRingSaturation2H-Oxygen	-103.910477
2312	species2 + species551 -> species814	FuranRingSaturation2H-Oxygen	-61.247484
2313	species2 + species552 -> species803	FuranRingSaturation2H-Oxygen	-103.910477
2314	species2 + species563 -> species868	FuranRingSaturation2H-Oxygen	-103.910477
2315	species2 + species564 -> species868	FuranRingSaturation2H-Oxygen	-97.507283
2316	species2 + species565 -> species728	FuranRingSaturation2H-Oxygen	-64.483808
2317	species2 + species566 -> species728	FuranRingSaturation2H-Oxygen	-103.910477
2318	species2 + species585 -> species588	FuranRingSaturation2H-Oxygen	-99.984630
2319	species2 + species589 -> species822	FuranRingSaturation2H-Oxygen	-115.980062
2320	species2 + species590 -> species822	FuranRingSaturation2H-Oxygen	-103.910477
2321	species2 + species591 -> species896	FuranRingSaturation2H-Oxygen	-64.483808
2322	species2 + species592 -> species896	FuranRingSaturation2H-Oxygen	-103.910477
2323	species2 + species605 -> species727	FuranRingSaturation2H-Oxygen	-79.365041
2324	species2 + species606 -> species727	FuranRingSaturation2H-Oxygen	-97.508957
2325	species2 + species625 -> species641	FuranRingSaturation2H-Oxygen	-79.365041
2326	species2 + species628 -> species642	FuranRingSaturation2H-Oxygen	-72.011661
2327	species2 + species679 -> species965	FuranRingSaturation2H-Oxygen	-97.507283
2328	species2 + species680 -> species965	FuranRingSaturation2H-Oxygen	-97.507283
2329	species2 + species684 -> species727	FuranRingSaturation2H-Oxygen	-64.483808
2330	species2 + species743 -> species873	FuranRingSaturation2H-Oxygen	-97.507283
2331	species2 + species744 -> species873	FuranRingSaturation2H-Oxygen	-97.507283
2332	species2 + species781 -> species349	FuranRingSaturation2H-Oxygen	-103.908385
2333	species2 + species782 -> species349	FuranRingSaturation2H-Oxygen	-97.507283
2334	species2 + species795 -> species930	FuranRingSaturation2H-Oxygen	-73.396146
2335	species2 + species796 -> species1007	FuranRingSaturation2H-Oxygen	-97.507283
2336	species2 + species799 -> species802	FuranRingSaturation2H-Oxygen	-97.507283
2337	species2 + species800 -> species931	FuranRingSaturation2H-Oxygen	-146.674304
2338	species2 + species805 -> species802	FuranRingSaturation2H-Oxygen	-97.507283
2339	species2 + species806 -> species802	FuranRingSaturation2H-Oxygen	-99.982538
2340	species2 + species809 -> species1028	FuranRingSaturation2H-Oxygen	-79.365041
2341	species2 + species810 -> species1028	FuranRingSaturation2H-Oxygen	-103.910477

2342	species2 + species811 -> species1007	FuranRingSaturation2H-Oxygen	-103.910477
2343	species2 + species815 -> species930	FuranRingSaturation2H-Oxygen	-97.507283
2344	species2 + species826 -> species931	FuranRingSaturation2H-Oxygen	-146.674304
2345	species2 + species842 -> species979	FuranRingSaturation2H-Oxygen	-79.365041
2346	species2 + species843 -> species979	FuranRingSaturation2H-Oxygen	-97.507283
2347	species2 + species862 -> species1042	FuranRingSaturation2H-Oxygen	-115.977970
2348	species2 + species863 -> species1042	FuranRingSaturation2H-Oxygen	-103.908385
2349	species2 + species871 -> species873	FuranRingSaturation2H-Oxygen	-79.365041
2350	species2 + species899 -> species980	FuranRingSaturation2H-Oxygen	-97.508957
2351	species2 + species900 -> species980	FuranRingSaturation2H-Oxygen	-64.483808
2352	species2 + species910 -> species930	FuranRingSaturation2H-Oxygen	-79.362949
2353	species2 + species913 -> species931	FuranRingSaturation2H-Oxygen	-115.977970
2354	species2 + species973 -> species979	FuranRingSaturation2H-Oxygen	-115.980062
2355	species2 + species974 -> species1087	FuranRingSaturation2H-Oxygen	-97.507283
2356	species2 + species974 -> species1059	FuranRingSaturation2H-Oxygen	-88.717536
2357	species2 + species982 -> species1062	FuranRingSaturation2H-Oxygen	-97.507283
2358	species2 + species983 -> species1062	FuranRingSaturation2H-Oxygen	-97.507283
2359	species2 + species1005 -> species1010	FuranRingSaturation2H-Oxygen	-97.507283
2360	species2 + species1014 -> species1010	FuranRingSaturation2H-Oxygen	-97.507283
2361	species2 + species1015 -> species1010	FuranRingSaturation2H-Oxygen	-61.247484
2362	species2 + species1034 -> species1075	FuranRingSaturation2H-Oxygen	-64.483808
2363	species2 + species1035 -> species1075	FuranRingSaturation2H-Oxygen	-97.507283
2364	species2 + species1061 -> species1062	FuranRingSaturation2H-Oxygen	-64.483808
2365	species2 + species1076 -> species1075	FuranRingSaturation2H-Oxygen	-115.980062
2366	species2 + species1117 -> species1118	FuranRingSaturation2H-Oxygen	-73.396146
2367	species2 + species1119 -> species1118	FuranRingSaturation2H-Oxygen	-97.507283
2368	species2 + species1120 -> species1118	FuranRingSaturation2H-Oxygen	-79.365041
2369	species2 + species1145 -> species1150	FuranRingSaturation2H-Oxygen	-115.977970
2370	species2 + species1146 -> species1150	FuranRingSaturation2H-Oxygen	-97.507283
2371	2species2 + species98 -> species317	FuranRingSaturation4H-Oxygen	-133.135298
2372	2species2 + species140 -> species416	FuranRingSaturation4H-Oxygen	-89.912905
2373	2species2 + species291 -> species588	FuranRingSaturation4H-Oxygen	-133.135298
2374	2species2 + species315 -> species641	FuranRingSaturation4H-Oxygen	-176.871906
2375	2species2 + species316 -> species642	FuranRingSaturation4H-Oxygen	-169.521036
2376	2species2 + species403 -> species727	FuranRingSaturation4H-Oxygen	-75.033764
2377	2species2 + species523 -> species802	FuranRingSaturation4H-Oxygen	-133.135298
2378	2species2 + species573 -> species873	FuranRingSaturation4H-Oxygen	-112.515291
2379	2species2 + species639 -> species930	FuranRingSaturation4H-Oxygen	-140.703318
2380	2species2 + species640 -> species931	FuranRingSaturation4H-Oxygen	-287.237458
2381	2species2 + species709 -> species979	FuranRingSaturation4H-Oxygen	-126.527926
2382	2species2 + species726 -> species980	FuranRingSaturation4H-Oxygen	-69.572389
2383	2species2 + species801 -> species1010	FuranRingSaturation4H-Oxygen	-158.754767
2384	2species2 + species869 -> species1062	FuranRingSaturation4H-Oxygen	-97.634477
2385	2species2 + species895 -> species1075	FuranRingSaturation4H-Oxygen	-111.646693
2386	2species2 + species1001 -> species965	FuranRingSaturation4H-Oxygen	-144.788157
2387	2species2 + species1006 -> species1118	FuranRingSaturation4H-Oxygen	-112.515291
2388	2species2 + species1060 -> species1150	FuranRingSaturation4H-Oxygen	-163.142946
2389	species2 + species514 -> species784	Hydrogenation-NOlefin	-137.722218
2390	species2 + species964 -> species1108	Hydrogenation-NOlefin	-125.327954
2391	species2 + species1106 -> species1147	Hydrogenation-NOlefin	-126.729176
2392	species2 + species1107 -> species1147	Hydrogenation-NOlefin	-117.238190
2393	species2 + species1110 -> species1106	Hydrogenation-NOlefin	-110.914074
2394	species2 + species1148 -> species1159	Hydrogenation-NOlefin	-108.193638
2395	species2 + species1148 -> species1158	Hydrogenation-NOlefin	-98.759554
2396	species2 + species1149 -> species1158	Hydrogenation-NOlefin	-122.891611
2397	species2 + species1158 -> species1173	Hydrogenation-NOlefin	-154.225587
2398	species2 + species1159 -> species1173	Hydrogenation-NOlefin	-144.791504
2399	species2 + species1165 -> species1174	Hydrogenation-NOlefin	-154.863229
2400	species2 + species1166 -> species1174	Hydrogenation-NOlefin	-132.229462

2401	species2 + species1166 -> species1176	Hydrogenation-NOlefin	-108.193638
2402	species2 + species1168 -> species1174	Hydrogenation-NOlefin	-145.429146
2403	species2 + species1168 -> species1175	Hydrogenation-NOlefin	-122.891611
2404	species2 + species1170 -> species1165	Hydrogenation-NOlefin	-15.829160
2405	species2 + species1170 -> species1166	Hydrogenation-NOlefin	-38.463010
2406	species2 + species1174 -> species1178	Hydrogenation-NOlefin	-126.827500
2407	species2 + species1175 -> species1178	Hydrogenation-NOlefin	-149.364616
2408	species2 + species1176 -> species1178	Hydrogenation-NOlefin	-150.863325
2409	species2 + species1177 -> species1175	Hydrogenation-NOlefin	-98.759554
2410	species2 + species28 -> species124	Hydrogenation-Oxygen	-36.077293
2411	species2 + species32 -> species125	Hydrogenation-Oxygen	-36.077293
2412	species2 + species72 -> species130	Hydrogenation-Oxygen	-121.441437
2413	species2 + species86 -> species19	Hydrogenation-Oxygen	-99.151177
2414	species2 + species136 -> species292	Hydrogenation-Oxygen	-36.077293
2415	species2 + species141 -> species378	Hydrogenation-Oxygen	-36.077293
2416	species2 + species142 -> species377	Hydrogenation-Oxygen	-20.312190
2417	species2 + species143 -> species379	Hydrogenation-Oxygen	44.044340
2418	species2 + species144 -> species380	Hydrogenation-Oxygen	-45.497234
2419	species2 + species145 -> species381	Hydrogenation-Oxygen	-33.559864
2420	species2 + species146 -> species382	Hydrogenation-Oxygen	-32.109480
2421	species2 + species149 -> species314	Hydrogenation-Oxygen	-121.912974
2422	species2 + species166 -> species388	Hydrogenation-Oxygen	-20.312190
2423	species2 + species167 -> species383	Hydrogenation-Oxygen	-36.077293
2424	species2 + species168 -> species384	Hydrogenation-Oxygen	-36.077293
2425	species2 + species169 -> species386	Hydrogenation-Oxygen	-20.312190
2426	species2 + species170 -> species385	Hydrogenation-Oxygen	-36.077293
2427	species2 + species171 -> species392	Hydrogenation-Oxygen	-33.559864
2428	species2 + species172 -> species391	Hydrogenation-Oxygen	-32.109480
2429	species2 + species173 -> species389	Hydrogenation-Oxygen	-36.077293
2430	species2 + species174 -> species390	Hydrogenation-Oxygen	-36.077293
2431	species2 + species204 -> species66	Hydrogenation-Oxygen	-193.966474
2432	species2 + species213 -> species297	Hydrogenation-Oxygen	-121.441437
2433	species2 + species227 -> species346	Hydrogenation-Oxygen	-206.118066
2434	species2 + species228 -> species343	Hydrogenation-Oxygen	-121.441437
2435	species2 + species241 -> species339	Hydrogenation-Oxygen	-112.055051
2436	species2 + species242 -> species339	Hydrogenation-Oxygen	-112.055051
2437	species2 + species243 -> species340	Hydrogenation-Oxygen	-193.968566
2438	species2 + species244 -> species334	Hydrogenation-Oxygen	-121.441437
2439	species2 + species248 -> species396	Hydrogenation-Oxygen	-145.790643
2440	species2 + species249 -> species398	Hydrogenation-Oxygen	-121.441437
2441	species2 + species250 -> species399	Hydrogenation-Oxygen	-145.790643
2442	species2 + species270 -> species528	Hydrogenation-Oxygen	-120.977013
2443	species2 + species271 -> species528	Hydrogenation-Oxygen	-39.131990
2444	species2 + species277 -> species106	Hydrogenation-Oxygen	-36.077293
2445	species2 + species284 -> species105	Hydrogenation-Oxygen	-3.450838
2446	species2 + species285 -> species95	Hydrogenation-Oxygen	-99.151177
2447	species2 + species286 -> species99	Hydrogenation-Oxygen	-99.151177
2448	species2 + species287 -> species103	Hydrogenation-Oxygen	-99.151177
2449	species2 + species288 -> species108	Hydrogenation-Oxygen	-99.151177
2450	species2 + species289 -> species107	Hydrogenation-Oxygen	-99.151177
2451	species2 + species303 -> species110	Hydrogenation-Oxygen	-111.095242
2452	species2 + species351 -> species542	Hydrogenation-Oxygen	-33.559864
2453	species2 + species354 -> species688	Hydrogenation-Oxygen	-36.077293
2454	species2 + species359 -> species543	Hydrogenation-Oxygen	-33.559864
2455	species2 + species367 -> species696	Hydrogenation-Oxygen	-36.077293
2456	species2 + species370 -> species537	Hydrogenation-Oxygen	-112.021998
2457	species2 + species372 -> species540	Hydrogenation-Oxygen	-105.679054
2458	species2 + species373 -> species540	Hydrogenation-Oxygen	-112.057143
2459	species2 + species374 -> species637	Hydrogenation-Oxygen	-121.441437

2460	species2 + species380 -> species559	Hydrogenation-Oxygen	-36.077293
2461	species2 + species394 -> species638	Hydrogenation-Oxygen	-112.055051
2462	species2 + species395 -> species638	Hydrogenation-Oxygen	-122.891611
2463	species2 + species397 -> species561	Hydrogenation-Oxygen	-121.441437
2464	species2 + species404 -> species591	Hydrogenation-Oxygen	-45.497234
2465	species2 + species405 -> species592	Hydrogenation-Oxygen	44.044340
2466	species2 + species406 -> species590	Hydrogenation-Oxygen	-20.312190
2467	species2 + species407 -> species594	Hydrogenation-Oxygen	-32.109480
2468	species2 + species408 -> species593	Hydrogenation-Oxygen	-33.559864
2469	species2 + species411 -> species587	Hydrogenation-Oxygen	-126.368934
2470	species2 + species417 -> species711	Hydrogenation-Oxygen	-29.732215
2471	species2 + species417 -> species710	Hydrogenation-Oxygen	-94.088537
2472	species2 + species418 -> species712	Hydrogenation-Oxygen	-42.979722
2473	species2 + species418 -> species713	Hydrogenation-Oxygen	-41.529505
2474	species2 + species419 -> species328	Hydrogenation-Oxygen	-33.559864
2475	species2 + species424 -> species651	Hydrogenation-Oxygen	-36.077293
2476	species2 + species427 -> species635	Hydrogenation-Oxygen	-126.368934
2477	species2 + species428 -> species636	Hydrogenation-Oxygen	-126.368934
2478	species2 + species429 -> species630	Hydrogenation-Oxygen	-125.409124
2479	species2 + species430 -> species627	Hydrogenation-Oxygen	-125.409124
2480	species2 + species431 -> species650	Hydrogenation-Oxygen	-113.014861
2481	species2 + species432 -> species653	Hydrogenation-Oxygen	-121.441437
2482	species2 + species434 -> species649	Hydrogenation-Oxygen	-112.055051
2483	species2 + species435 -> species649	Hydrogenation-Oxygen	-115.916046
2484	species2 + species456 -> species716	Hydrogenation-Oxygen	-24.770452
2485	species2 + species457 -> species714	Hydrogenation-Oxygen	-20.312190
2486	species2 + species458 -> species718	Hydrogenation-Oxygen	-33.559864
2487	species2 + species459 -> species717	Hydrogenation-Oxygen	-32.109480
2488	species2 + species460 -> species724	Hydrogenation-Oxygen	-32.109480
2489	species2 + species461 -> species723	Hydrogenation-Oxygen	-89.127150
2490	species2 + species469 -> species209	Hydrogenation-Oxygen	-193.388246
2491	species2 + species476 -> species233	Hydrogenation-Oxygen	-121.441437
2492	species2 + species477 -> species602	Hydrogenation-Oxygen	-121.441437
2493	species2 + species480 -> species238	Hydrogenation-Oxygen	-193.388246
2494	species2 + species481 -> species600	Hydrogenation-Oxygen	-121.441437
2495	species2 + species484 -> species668	Hydrogenation-Oxygen	-111.474730
2496	species2 + species485 -> species668	Hydrogenation-Oxygen	-111.474730
2497	species2 + species486 -> species601	Hydrogenation-Oxygen	-123.624230
2498	species2 + species487 -> species154	Hydrogenation-Oxygen	-113.013187
2499	species2 + species488 -> species225	Hydrogenation-Oxygen	-111.474730
2500	species2 + species489 -> species239	Hydrogenation-Oxygen	-193.966474
2501	species2 + species494 -> species603	Hydrogenation-Oxygen	-121.441437
2502	species2 + species495 -> species669	Hydrogenation-Oxygen	-181.786014
2503	species2 + species499 -> species546	Hydrogenation-Oxygen	-113.014861
2504	species2 + species503 -> species657	Hydrogenation-Oxygen	-112.055051
2505	species2 + species504 -> species657	Hydrogenation-Oxygen	-122.891611
2506	species2 + species505 -> species658	Hydrogenation-Oxygen	-121.441437
2507	species2 + species506 -> species659	Hydrogenation-Oxygen	-121.441437
2508	species2 + species511 -> species626	Hydrogenation-Oxygen	-112.055051
2509	species2 + species512 -> species665	Hydrogenation-Oxygen	-121.441437
2510	species2 + species512 -> species662	Hydrogenation-Oxygen	-193.968566
2511	species2 + species513 -> species502	Hydrogenation-Oxygen	-193.935513
2512	species2 + species515 -> species725	Hydrogenation-Oxygen	-121.441437
2513	species2 + species516 -> species498	Hydrogenation-Oxygen	-121.441437
2514	species2 + species517 -> species682	Hydrogenation-Oxygen	-126.368934
2515	species2 + species524 -> species796	Hydrogenation-Oxygen	-120.977013
2516	species2 + species525 -> species796	Hydrogenation-Oxygen	-88.299136
2517	species2 + species530 -> species265	Hydrogenation-Oxygen	-99.151177
2518	species2 + species544 -> species644	Hydrogenation-Oxygen	-121.931802

2519	species2 + species545 -> species644	Hydrogenation-Oxygen	-115.975041
2520	species2 + species549 -> species810	Hydrogenation-Oxygen	-47.950314
2521	species2 + species550 -> species810	Hydrogenation-Oxygen	-120.977013
2522	species2 + species551 -> species809	Hydrogenation-Oxygen	-102.859456
2523	species2 + species552 -> species811	Hydrogenation-Oxygen	-120.977013
2524	species2 + species553 -> species813	Hydrogenation-Oxygen	-120.977013
2525	species2 + species554 -> species812	Hydrogenation-Oxygen	-120.977013
2526	species2 + species555 -> species807	Hydrogenation-Oxygen	-126.368934
2527	species2 + species556 -> species811	Hydrogenation-Oxygen	1.216586
2528	species2 + species557 -> species813	Hydrogenation-Oxygen	-10.580708
2529	species2 + species558 -> species812	Hydrogenation-Oxygen	-12.031092
2530	species2 + species568 -> species309	Hydrogenation-Oxygen	4.271299
2531	species2 + species569 -> species319	Hydrogenation-Oxygen	13.089732
2532	species2 + species570 -> species323	Hydrogenation-Oxygen	28.854801
2533	species2 + species571 -> species329	Hydrogenation-Oxygen	-32.109480
2534	species2 + species576 -> species330	Hydrogenation-Oxygen	-124.449314
2535	species2 + species579 -> species308	Hydrogenation-Oxygen	-11.798838
2536	species2 + species580 -> species318	Hydrogenation-Oxygen	-39.619468
2537	species2 + species581 -> species322	Hydrogenation-Oxygen	-11.798838
2538	species2 + species582 -> species325	Hydrogenation-Oxygen	-11.538593
2539	species2 + species583 -> species324	Hydrogenation-Oxygen	-12.988977
2540	species2 + species584 -> species310	Hydrogenation-Oxygen	-99.151177
2541	species2 + species596 -> species889	Hydrogenation-Oxygen	-121.441437
2542	species2 + species597 -> species332	Hydrogenation-Oxygen	-193.968566
2543	species2 + species598 -> species890	Hydrogenation-Oxygen	-112.055051
2544	species2 + species599 -> species890	Hydrogenation-Oxygen	-122.891611
2545	species2 + species607 -> species896	Hydrogenation-Oxygen	-36.077293
2546	species2 + species614 -> species336	Hydrogenation-Oxygen	-113.014861
2547	species2 + species616 -> species326	Hydrogenation-Oxygen	-106.638863
2548	species2 + species617 -> species338	Hydrogenation-Oxygen	-113.014861
2549	species2 + species618 -> species337	Hydrogenation-Oxygen	-113.014861
2550	species2 + species619 -> species820	Hydrogenation-Oxygen	-112.982226
2551	species2 + species621 -> species821	Hydrogenation-Oxygen	-112.055051
2552	species2 + species622 -> species821	Hydrogenation-Oxygen	-118.433141
2553	species2 + species632 -> species926	Hydrogenation-Oxygen	-125.409124
2554	species2 + species633 -> species643	Hydrogenation-Oxygen	-113.016953
2555	species2 + species634 -> species643	Hydrogenation-Oxygen	-110.499858
2556	species2 + species662 -> species919	Hydrogenation-Oxygen	-121.441437
2557	species2 + species663 -> species920	Hydrogenation-Oxygen	-112.055051
2558	species2 + species664 -> species920	Hydrogenation-Oxygen	-122.891611
2559	species2 + species665 -> species919	Hydrogenation-Oxygen	-193.968566
2560	species2 + species666 -> species831	Hydrogenation-Oxygen	-112.021998
2561	species2 + species667 -> species831	Hydrogenation-Oxygen	-112.055051
2562	species2 + species671 -> species837	Hydrogenation-Oxygen	-112.055051
2563	species2 + species672 -> species837	Hydrogenation-Oxygen	-114.955818
2564	species2 + species673 -> species865	Hydrogenation-Oxygen	-121.441437
2565	species2 + species674 -> species923	Hydrogenation-Oxygen	-112.055051
2566	species2 + species675 -> species923	Hydrogenation-Oxygen	-122.891611
2567	species2 + species676 -> species830	Hydrogenation-Oxygen	-206.085012
2568	species2 + species677 -> species500	Hydrogenation-Oxygen	-133.736121
2569	species2 + species683 -> species822	Hydrogenation-Oxygen	-33.559864
2570	species2 + species685 -> species843	Hydrogenation-Oxygen	-20.312190
2571	species2 + species686 -> species842	Hydrogenation-Oxygen	-33.559864
2572	species2 + species687 -> species972	Hydrogenation-Oxygen	-45.497234
2573	species2 + species687 -> species844	Hydrogenation-Oxygen	-42.979722
2574	species2 + species689 -> species848	Hydrogenation-Oxygen	-24.770452
2575	species2 + species691 -> species847	Hydrogenation-Oxygen	-33.559864
2576	species2 + species692 -> species846	Hydrogenation-Oxygen	-33.559864
2577	species2 + species693 -> species845	Hydrogenation-Oxygen	-33.559864

2578	species2 + species694 -> species850	Hydrogenation-Oxygen	-33.559864
2579	species2 + species695 -> species849	Hydrogenation-Oxygen	-33.559864
2580	species2 + species701 -> species951	Hydrogenation-Oxygen	-36.077293
2581	species2 + species702 -> species975	Hydrogenation-Oxygen	-36.077293
2582	species2 + species704 -> species828	Hydrogenation-Oxygen	-115.534466
2583	species2 + species705 -> species835	Hydrogenation-Oxygen	-121.931802
2584	species2 + species706 -> species835	Hydrogenation-Oxygen	-115.975041
2585	species2 + species707 -> species785	Hydrogenation-Oxygen	-140.643486
2586	species2 + species708 -> species862	Hydrogenation-Oxygen	-36.077293
2587	species2 + species710 -> species863	Hydrogenation-Oxygen	44.044340
2588	species2 + species711 -> species863	Hydrogenation-Oxygen	-20.312190
2589	species2 + species712 -> species864	Hydrogenation-Oxygen	-32.109480
2590	species2 + species713 -> species864	Hydrogenation-Oxygen	-33.559864
2591	species2 + species725 -> species866	Hydrogenation-Oxygen	-121.441437
2592	species2 + species733 -> species887	Hydrogenation-Oxygen	-126.368934
2593	species2 + species734 -> species888	Hydrogenation-Oxygen	-126.368934
2594	species2 + species735 -> species891	Hydrogenation-Oxygen	-126.368934
2595	species2 + species736 -> species438	Hydrogenation-Oxygen	-113.014861
2596	species2 + species737 -> species943	Hydrogenation-Oxygen	-112.055051
2597	species2 + species738 -> species943	Hydrogenation-Oxygen	-115.916046
2598	species2 + species740 -> species518	Hydrogenation-Oxygen	-113.013187
2599	species2 + species741 -> species979	Hydrogenation-Oxygen	-33.559864
2600	species2 + species742 -> species539	Hydrogenation-Oxygen	-33.559864
2601	species2 + species746 -> species950	Hydrogenation-Oxygen	44.044340
2602	species2 + species747 -> species949	Hydrogenation-Oxygen	-20.312190
2603	species2 + species748 -> species952	Hydrogenation-Oxygen	-32.109480
2604	species2 + species750 -> species912	Hydrogenation-Oxygen	-125.409124
2605	species2 + species751 -> species852	Hydrogenation-Oxygen	-110.988131
2606	species2 + species751 -> species928	Hydrogenation-Oxygen	-121.826783
2607	species2 + species752 -> species860	Hydrogenation-Oxygen	-121.441437
2608	species2 + species752 -> species929	Hydrogenation-Oxygen	-126.368934
2609	species2 + species753 -> species655	Hydrogenation-Oxygen	-126.368934
2610	species2 + species754 -> species914	Hydrogenation-Oxygen	-126.368934
2611	species2 + species755 -> species911	Hydrogenation-Oxygen	-113.016953
2612	species2 + species756 -> species953	Hydrogenation-Oxygen	-133.623990
2613	species2 + species756 -> species947	Hydrogenation-Oxygen	-125.195740
2614	species2 + species757 -> species758	Hydrogenation-Oxygen	-125.164778
2615	species2 + species767 -> species493	Hydrogenation-Oxygen	-121.441437
2616	species2 + species769 -> species414	Hydrogenation-Oxygen	-113.013187
2617	species2 + species770 -> species501	Hydrogenation-Oxygen	-121.441437
2618	species2 + species771 -> species788	Hydrogenation-Oxygen	-112.055051
2619	species2 + species772 -> species954	Hydrogenation-Oxygen	-122.891611
2620	species2 + species773 -> species954	Hydrogenation-Oxygen	-112.055051
2621	species2 + species774 -> species825	Hydrogenation-Oxygen	-113.014861
2622	species2 + species775 -> species439	Hydrogenation-Oxygen	-113.014861
2623	species2 + species776 -> species440	Hydrogenation-Oxygen	-125.195740
2624	species2 + species777 -> species508	Hydrogenation-Oxygen	-113.013187
2625	species2 + species778 -> species509	Hydrogenation-Oxygen	-112.055051
2626	species2 + species786 -> species915	Hydrogenation-Oxygen	-125.409124
2627	species2 + species787 -> species959	Hydrogenation-Oxygen	-145.790643
2628	species2 + species789 -> species969	Hydrogenation-Oxygen	-94.045860
2629	species2 + species790 -> species969	Hydrogenation-Oxygen	-104.882420
2630	species2 + species791 -> species946	Hydrogenation-Oxygen	-102.668247
2631	species2 + species791 -> species918	Hydrogenation-Oxygen	-98.807670
2632	species2 + species792 -> species961	Hydrogenation-Oxygen	-126.368934
2633	species2 + species792 -> species916	Hydrogenation-Oxygen	-113.014861
2634	species2 + species793 -> species670	Hydrogenation-Oxygen	-113.014861
2635	species2 + species798 -> species522	Hydrogenation-Oxygen	-99.151177
2636	species2 + species801 -> species1006	Hydrogenation-Oxygen	-167.216070

2637	species2 + species803 -> species1007	Hydrogenation-Oxygen	-120.977013
2638	species2 + species804 -> species1007	Hydrogenation-Oxygen	-39.131990
2639	species2 + species814 -> species1028	Hydrogenation-Oxygen	-120.977013
2640	species2 + species816 -> species529	Hydrogenation-Oxygen	-0.933450
2641	species2 + species817 -> species534	Hydrogenation-Oxygen	-99.151177
2642	species2 + species823 -> species894	Hydrogenation-Oxygen	-122.891611
2643	species2 + species824 -> species894	Hydrogenation-Oxygen	-116.934850
2644	species2 + species827 -> species1028	Hydrogenation-Oxygen	-36.614602
2645	species2 + species832 -> species1040	Hydrogenation-Oxygen	-112.982226
2646	species2 + species833 -> species934	Hydrogenation-Oxygen	-122.891611
2647	species2 + species834 -> species934	Hydrogenation-Oxygen	-116.934850
2648	species2 + species838 -> species1041	Hydrogenation-Oxygen	-118.433141
2649	species2 + species839 -> species1041	Hydrogenation-Oxygen	-112.055051
2650	species2 + species840 -> species932	Hydrogenation-Oxygen	-122.891611
2651	species2 + species841 -> species932	Hydrogenation-Oxygen	-116.934850
2652	species2 + species844 -> species1042	Hydrogenation-Oxygen	-36.077293
2653	species2 + species851 -> species939	Hydrogenation-Oxygen	-122.891611
2654	species2 + species852 -> species938	Hydrogenation-Oxygen	-122.891611
2655	species2 + species853 -> species939	Hydrogenation-Oxygen	-124.235930
2656	species2 + species854 -> species938	Hydrogenation-Oxygen	-113.455436
2657	species2 + species855 -> species1019	Hydrogenation-Oxygen	-121.441437
2658	species2 + species858 -> species1038	Hydrogenation-Oxygen	-33.559864
2659	species2 + species859 -> species1020	Hydrogenation-Oxygen	-122.891611
2660	species2 + species860 -> species1022	Hydrogenation-Oxygen	-126.368934
2661	species2 + species861 -> species1021	Hydrogenation-Oxygen	-126.368934
2662	species2 + species867 -> species1020	Hydrogenation-Oxygen	-112.055051
2663	species2 + species870 -> species624	Hydrogenation-Oxygen	-36.077293
2664	species2 + species878 -> species654	Hydrogenation-Oxygen	-126.368934
2665	species2 + species879 -> species656	Hydrogenation-Oxygen	-126.368934
2666	species2 + species880 -> species991	Hydrogenation-Oxygen	-112.055051
2667	species2 + species881 -> species991	Hydrogenation-Oxygen	-115.916046
2668	species2 + species882 -> species623	Hydrogenation-Oxygen	-15.506364
2669	species2 + species884 -> species1068	Hydrogenation-Oxygen	-125.409124
2670	species2 + species885 -> species893	Hydrogenation-Oxygen	-118.433141
2671	species2 + species886 -> species893	Hydrogenation-Oxygen	-115.916046
2672	species2 + species892 -> species641	Hydrogenation-Oxygen	-99.151177
2673	species2 + species897 -> species661	Hydrogenation-Oxygen	-113.014861
2674	species2 + species898 -> species652	Hydrogenation-Oxygen	-113.014861
2675	species2 + species901 -> species1035	Hydrogenation-Oxygen	-24.770452
2676	species2 + species903 -> species646	Hydrogenation-Oxygen	-113.977181
2677	species2 + species904 -> species648	Hydrogenation-Oxygen	-119.393369
2678	species2 + species905 -> species647	Hydrogenation-Oxygen	-119.393369
2679	species2 + species906 -> species671	Hydrogenation-Oxygen	-112.055051
2680	species2 + species907 -> species1032	Hydrogenation-Oxygen	-121.910463
2681	species2 + species908 -> species1033	Hydrogenation-Oxygen	-122.891611
2682	species2 + species909 -> species1033	Hydrogenation-Oxygen	-116.934850
2683	species2 + species916 -> species1086	Hydrogenation-Oxygen	-126.368934
2684	species2 + species917 -> species933	Hydrogenation-Oxygen	-114.955818
2685	species2 + species918 -> species933	Hydrogenation-Oxygen	-115.916046
2686	species2 + species921 -> species935	Hydrogenation-Oxygen	-112.019906
2687	species2 + species922 -> species935	Hydrogenation-Oxygen	-115.913954
2688	species2 + species925 -> species1023	Hydrogenation-Oxygen	-33.559864
2689	species2 + species927 -> species937	Hydrogenation-Oxygen	-103.733075
2690	species2 + species927 -> species1088	Hydrogenation-Oxygen	-108.193638
2691	species2 + species928 -> species938	Hydrogenation-Oxygen	-112.052959
2692	species2 + species929 -> species1022	Hydrogenation-Oxygen	-121.441437
2693	species2 + species937 -> species1099	Hydrogenation-Oxygen	-122.891611
2694	species2 + species942 -> species1102	Hydrogenation-Oxygen	-36.077293
2695	species2 + species946 -> species933	Hydrogenation-Oxygen	-112.055051

2696	species2 + species947 -> species1081	Hydrogenation-Oxygen	-121.441437
2697	species2 + species953 -> species1081	Hydrogenation-Oxygen	-113.013187
2698	species2 + species955 -> species1045	Hydrogenation-Oxygen	-107.780258
2699	species2 + species957 -> species1048	Hydrogenation-Oxygen	-62.484693
2700	species2 + species958 -> species1048	Hydrogenation-Oxygen	-63.887170
2701	species2 + species959 -> species1082	Hydrogenation-Oxygen	-116.765817
2702	species2 + species960 -> species1045	Hydrogenation-Oxygen	-118.649454
2703	species2 + species961 -> species1086	Hydrogenation-Oxygen	-113.014861
2704	species2 + species962 -> species1048	Hydrogenation-Oxygen	-73.321253
2705	species2 + species963 -> species783	Hydrogenation-Oxygen	-168.687583
2706	species2 + species966 -> species956	Hydrogenation-Oxygen	-126.368934
2707	species2 + species967 -> species1109	Hydrogenation-Oxygen	-171.602158
2708	species2 + species968 -> species1109	Hydrogenation-Oxygen	-163.127884
2709	species2 + species970 -> species1034	Hydrogenation-Oxygen	-42.979722
2710	species2 + species971 -> species1054	Hydrogenation-Oxygen	-94.088537
2711	species2 + species972 -> species1042	Hydrogenation-Oxygen	-33.559864
2712	species2 + species974 -> species1055	Hydrogenation-Oxygen	-84.668679
2713	species2 + species981 -> species1075	Hydrogenation-Oxygen	-33.559864
2714	species2 + species984 -> species1036	Hydrogenation-Oxygen	-29.076834
2715	species2 + species984 -> species1070	Hydrogenation-Oxygen	-39.913394
2716	species2 + species985 -> species794	Hydrogenation-Oxygen	-116.873764
2717	species2 + species986 -> species1113	Hydrogenation-Oxygen	-42.979722
2718	species2 + species987 -> species800	Hydrogenation-Oxygen	15.607136
2719	species2 + species988 -> species826	Hydrogenation-Oxygen	28.854801
2720	species2 + species992 -> species1016	Hydrogenation-Oxygen	-126.368934
2721	species2 + species993 -> species1080	Hydrogenation-Oxygen	-101.217654
2722	species2 + species994 -> species1105	Hydrogenation-Oxygen	-126.368934
2723	species2 + species994 -> species1078	Hydrogenation-Oxygen	-119.391277
2724	species2 + species995 -> species945	Hydrogenation-Oxygen	-119.393369
2725	species2 + species998 -> species745	Hydrogenation-Oxygen	-113.975089
2726	species2 + species999 -> species759	Hydrogenation-Oxygen	-113.013187
2727	species2 + species1000 -> species780	Hydrogenation-Oxygen	-113.014861
2728	species2 + species1002 -> species1103	Hydrogenation-Oxygen	-101.215562
2729	species2 + species1002 -> species1085	Hydrogenation-Oxygen	-108.193638
2730	species2 + species1003 -> species1083	Hydrogenation-Oxygen	-126.368934
2731	species2 + species1004 -> species957	Hydrogenation-Oxygen	-109.644230
2732	species2 + species1004 -> species962	Hydrogenation-Oxygen	-98.807670
2733	species2 + species1005 -> species1117	Hydrogenation-Oxygen	-145.087731
2734	species2 + species1008 -> species795	Hydrogenation-Oxygen	-0.935459
2735	species2 + species1009 -> species1117	Hydrogenation-Oxygen	-109.892760
2736	species2 + species1010 -> species1118	Hydrogenation-Oxygen	-120.977013
2737	species2 + species1011 -> species1118	Hydrogenation-Oxygen	-36.614602
2738	species2 + species1014 -> species1119	Hydrogenation-Oxygen	-120.977013
2739	species2 + species1015 -> species1120	Hydrogenation-Oxygen	-102.859456
2740	species2 + species1016 -> species1121	Hydrogenation-Oxygen	-125.409124
2741	species2 + species1017 -> species1090	Hydrogenation-Oxygen	-123.851839
2742	species2 + species1018 -> species1119	Hydrogenation-Oxygen	-3.241680
2743	species2 + species1024 -> species1133	Hydrogenation-Oxygen	-126.368934
2744	species2 + species1025 -> species1090	Hydrogenation-Oxygen	-116.932758
2745	species2 + species1026 -> species1012	Hydrogenation-Oxygen	-118.431049
2746	species2 + species1027 -> species1012	Hydrogenation-Oxygen	-115.913954
2747	species2 + species1029 -> species815	Hydrogenation-Oxygen	0.256667
2748	species2 + species1036 -> species1074	Hydrogenation-Oxygen	-122.891611
2749	species2 + species1037 -> species1074	Hydrogenation-Oxygen	-113.457528
2750	species2 + species1039 -> species1099	Hydrogenation-Oxygen	-113.455436
2751	species2 + species1043 -> species1013	Hydrogenation-Oxygen	-122.891611
2752	species2 + species1044 -> species1013	Hydrogenation-Oxygen	-116.934850
2753	species2 + species1046 -> species1143	Hydrogenation-Oxygen	-121.910463
2754	species2 + species1047 -> species1096	Hydrogenation-Oxygen	-109.644230

2755	species2 + species1047 -> species1097	Hydrogenation-Oxygen	-98.774617
2756	species2 + species1049 -> species1092	Hydrogenation-Oxygen	-116.934850
2757	species2 + species1050 -> species1092	Hydrogenation-Oxygen	-122.891611
2758	species2 + species1051 -> species1093	Hydrogenation-Oxygen	-108.193638
2759	species2 + species1051 -> species1095	Hydrogenation-Oxygen	-100.257845
2760	species2 + species1052 -> species1094	Hydrogenation-Oxygen	-122.891611
2761	species2 + species1052 -> species1095	Hydrogenation-Oxygen	-112.055051
2762	species2 + species1053 -> species1094	Hydrogenation-Oxygen	-100.207637
2763	species2 + species1053 -> species1144	Hydrogenation-Oxygen	-98.805578
2764	species2 + species1054 -> species1146	Hydrogenation-Oxygen	-24.770452
2765	species2 + species1056 -> species1129	Hydrogenation-Oxygen	-121.441437
2766	species2 + species1056 -> species1100	Hydrogenation-Oxygen	-122.891611
2767	species2 + species1057 -> species1134	Hydrogenation-Oxygen	-133.623990
2768	species2 + species1057 -> species1100	Hydrogenation-Oxygen	-124.237604
2769	species2 + species1058 -> species1136	Hydrogenation-Oxygen	-33.559864
2770	species2 + species1059 -> species1142	Hydrogenation-Oxygen	-33.559864
2771	species2 + species1064 -> species1066	Hydrogenation-Oxygen	-115.916046
2772	species2 + species1065 -> species931	Hydrogenation-Oxygen	-33.559864
2773	species2 + species1069 -> species1073	Hydrogenation-Oxygen	-103.735167
2774	species2 + species1069 -> species1152	Hydrogenation-Oxygen	-108.193638
2775	species2 + species1070 -> species1074	Hydrogenation-Oxygen	-112.055051
2776	species2 + species1071 -> species930	Hydrogenation-Oxygen	-0.933450
2777	species2 + species1073 -> species1153	Hydrogenation-Oxygen	-122.891611
2778	species2 + species1077 -> species944	Hydrogenation-Oxygen	-113.977181
2779	species2 + species1078 -> species1154	Hydrogenation-Oxygen	-126.368934
2780	species2 + species1079 -> species1089	Hydrogenation-Oxygen	-114.955818
2781	species2 + species1080 -> species1089	Hydrogenation-Oxygen	-115.916046
2782	species2 + species1083 -> species1155	Hydrogenation-Oxygen	-126.368934
2783	species2 + species1084 -> species1091	Hydrogenation-Oxygen	-167.542004
2784	species2 + species1085 -> species1091	Hydrogenation-Oxygen	-170.000522
2785	species2 + species1087 -> species1137	Hydrogenation-Oxygen	-24.770452
2786	species2 + species1088 -> species1099	Hydrogenation-Oxygen	-118.431049
2787	species2 + species1093 -> species1160	Hydrogenation-Oxygen	-114.955818
2788	species2 + species1094 -> species1160	Hydrogenation-Oxygen	-112.055051
2789	species2 + species1095 -> species1160	Hydrogenation-Oxygen	-122.891611
2790	species2 + species1096 -> species1127	Hydrogenation-Oxygen	-111.554645
2791	species2 + species1097 -> species1127	Hydrogenation-Oxygen	-122.424258
2792	species2 + species1098 -> species1124	Hydrogenation-Oxygen	-33.559864
2793	species2 + species1100 -> species1128	Hydrogenation-Oxygen	-121.441437
2794	species2 + species1103 -> species1091	Hydrogenation-Oxygen	-176.978598
2795	species2 + species1105 -> species1154	Hydrogenation-Oxygen	-119.391277
2796	species2 + species1111 -> species1145	Hydrogenation-Oxygen	-33.559864
2797	species2 + species1113 -> species1150	Hydrogenation-Oxygen	-33.559864
2798	species2 + species1116 -> species990	Hydrogenation-Oxygen	-119.391277
2799	species2 + species1122 -> species1163	Hydrogenation-Oxygen	-180.352575
2800	species2 + species1123 -> species1164	Hydrogenation-Oxygen	-126.368934
2801	species2 + species1125 -> species1167	Hydrogenation-Oxygen	-122.891611
2802	species2 + species1126 -> species1163	Hydrogenation-Oxygen	-170.918492
2803	species2 + species1129 -> species1128	Hydrogenation-Oxygen	-122.891611
2804	species2 + species1130 -> species1169	Hydrogenation-Oxygen	-126.368934
2805	species2 + species1130 -> species1123	Hydrogenation-Oxygen	-122.891611
2806	species2 + species1131 -> species1122	Hydrogenation-Oxygen	-100.257845
2807	species2 + species1131 -> species1157	Hydrogenation-Oxygen	-108.193638
2808	species2 + species1132 -> species1122	Hydrogenation-Oxygen	-115.916046
2809	species2 + species1132 -> species1156	Hydrogenation-Oxygen	-122.891611
2810	species2 + species1134 -> species1128	Hydrogenation-Oxygen	-112.055051
2811	species2 + species1135 -> species1127	Hydrogenation-Oxygen	-112.990175
2812	species2 + species1138 -> species1123	Hydrogenation-Oxygen	-116.934850
2813	species2 + species1138 -> species1172	Hydrogenation-Oxygen	-126.368934

2814	species2 + species1139 -> species1125	Hydrogenation-Oxygen	-103.735167
2815	species2 + species1139 -> species1161	Hydrogenation-Oxygen	-108.193638
2816	species2 + species1140 -> species1126	Hydrogenation-Oxygen	-101.217654
2817	species2 + species1140 -> species1156	Hydrogenation-Oxygen	-98.759554
2818	species2 + species1141 -> species1153	Hydrogenation-Oxygen	-113.457528
2819	species2 + species1144 -> species1160	Hydrogenation-Oxygen	-113.457528
2820	species2 + species1152 -> species1153	Hydrogenation-Oxygen	-118.433141
2821	species2 + species1156 -> species1163	Hydrogenation-Oxygen	-173.376592
2822	species2 + species1157 -> species1163	Hydrogenation-Oxygen	-172.416782
2823	species2 + species1161 -> species1167	Hydrogenation-Oxygen	-118.433141
2824	species2 + species1169 -> species1164	Hydrogenation-Oxygen	-122.891611
2825	species2 + species1171 -> species1167	Hydrogenation-Oxygen	-113.457528
2826	species2 + species1172 -> species1164	Hydrogenation-Oxygen	-116.934850
2827	species2 + species8 -> species24	KetoneHydrogenation-Oxygen	-20.620593
2828	species2 + species10 -> species30	KetoneHydrogenation-Oxygen	-17.541671
2829	species2 + species11 -> species23	KetoneHydrogenation-Oxygen	-5.749402
2830	species2 + species12 -> species23	KetoneHydrogenation-Oxygen	-4.789467
2831	species2 + species20 -> species84	KetoneHydrogenation-Oxygen	-14.948177
2832	species2 + species21 -> species97	KetoneHydrogenation-Oxygen	-19.571078
2833	species2 + species22 -> species83	KetoneHydrogenation-Oxygen	-19.571078
2834	species2 + species29 -> species116	KetoneHydrogenation-Oxygen	-19.571078
2835	species2 + species39 -> species117	KetoneHydrogenation-Oxygen	-19.571078
2836	species2 + species40 -> species118	KetoneHydrogenation-Oxygen	-19.571078
2837	species2 + species41 -> species148	KetoneHydrogenation-Oxygen	-19.571078
2838	species2 + species42 -> species118	KetoneHydrogenation-Oxygen	-19.571078
2839	species2 + species46 -> species9	KetoneHydrogenation-Oxygen	-16.581736
2840	species2 + species47 -> species94	KetoneHydrogenation-Oxygen	-86.770721
2841	species2 + species48 -> species94	KetoneHydrogenation-Oxygen	-15.621843
2842	species2 + species49 -> species119	KetoneHydrogenation-Oxygen	-12.125483
2843	species2 + species50 -> species119	KetoneHydrogenation-Oxygen	-12.125483
2844	species2 + species51 -> species139	KetoneHydrogenation-Oxygen	-15.621843
2845	species2 + species53 -> species93	KetoneHydrogenation-Oxygen	-21.580528
2846	species2 + species57 -> species114	KetoneHydrogenation-Oxygen	-15.621843
2847	species2 + species57 -> species127	KetoneHydrogenation-Oxygen	-6.810380
2848	species2 + species58 -> species120	KetoneHydrogenation-Oxygen	-89.328400
2849	species2 + species58 -> species126	KetoneHydrogenation-Oxygen	-93.367215
2850	species2 + species59 -> species120	KetoneHydrogenation-Oxygen	-17.541671
2851	species2 + species59 -> species128	KetoneHydrogenation-Oxygen	-21.580528
2852	species2 + species60 -> species153	KetoneHydrogenation-Oxygen	-16.581736
2853	species2 + species60 -> species129	KetoneHydrogenation-Oxygen	-21.580528
2854	species2 + species61 -> species113	KetoneHydrogenation-Oxygen	-21.580528
2855	species2 + species62 -> species109	KetoneHydrogenation-Oxygen	-21.580528
2856	species2 + species63 -> species232	KetoneHydrogenation-Oxygen	-16.614790
2857	species2 + species66 -> species110	KetoneHydrogenation-Oxygen	-15.623851
2858	species2 + species67 -> species121	KetoneHydrogenation-Oxygen	-7.739312
2859	species2 + species68 -> species121	KetoneHydrogenation-Oxygen	-17.543679
2860	species2 + species69 -> species152	KetoneHydrogenation-Oxygen	-11.167598
2861	species2 + species72 -> species149	KetoneHydrogenation-Oxygen	-11.654030
2862	species2 + species73 -> species123	KetoneHydrogenation-Oxygen	-17.541671
2863	species2 + species73 -> species151	KetoneHydrogenation-Oxygen	-7.737304
2864	species2 + species74 -> species150	KetoneHydrogenation-Oxygen	-94.327025
2865	species2 + species75 -> species252	KetoneHydrogenation-Oxygen	-17.541671
2866	species2 + species76 -> species65	KetoneHydrogenation-Oxygen	-21.580528
2867	species2 + species78 -> species122	KetoneHydrogenation-Oxygen	-17.541671
2868	species2 + species79 -> species253	KetoneHydrogenation-Oxygen	-12.125483
2869	species2 + species80 -> species255	KetoneHydrogenation-Oxygen	-21.580528
2870	species2 + species91 -> species290	KetoneHydrogenation-Oxygen	-19.571078
2871	species2 + species92 -> species262	KetoneHydrogenation-Oxygen	-19.571078
2872	species2 + species96 -> species272	KetoneHydrogenation-Oxygen	-14.948177

2873	species2 + species100 -> species259	KetoneHydrogenation-Oxygen	-14.948177
2874	species2 + species102 -> species269	KetoneHydrogenation-Oxygen	13.022566
2875	species2 + species104 -> species268	KetoneHydrogenation-Oxygen	-14.948177
2876	species2 + species107 -> species265	KetoneHydrogenation-Oxygen	-19.571078
2877	species2 + species108 -> species310	KetoneHydrogenation-Oxygen	-19.571078
2878	species2 + species111 -> species311	KetoneHydrogenation-Oxygen	-19.571078
2879	species2 + species111 -> species274	KetoneHydrogenation-Oxygen	-14.948177
2880	species2 + species112 -> species264	KetoneHydrogenation-Oxygen	-19.571078
2881	species2 + species112 -> species273	KetoneHydrogenation-Oxygen	-14.948177
2882	species2 + species113 -> species275	KetoneHydrogenation-Oxygen	-21.580528
2883	species2 + species114 -> species266	KetoneHydrogenation-Oxygen	-3.314063
2884	species2 + species115 -> species349	KetoneHydrogenation-Oxygen	-19.571078
2885	species2 + species120 -> species362	KetoneHydrogenation-Oxygen	-20.620593
2886	species2 + species122 -> species267	KetoneHydrogenation-Oxygen	-5.749402
2887	species2 + species123 -> species313	KetoneHydrogenation-Oxygen	4.054991
2888	species2 + species126 -> species362	KetoneHydrogenation-Oxygen	-16.581736
2889	species2 + species127 -> species266	KetoneHydrogenation-Oxygen	-12.125483
2890	species2 + species128 -> species362	KetoneHydrogenation-Oxygen	-16.581736
2891	species2 + species129 -> species327	KetoneHydrogenation-Oxygen	-12.125483
2892	species2 + species130 -> species314	KetoneHydrogenation-Oxygen	-12.125483
2893	species2 + species137 -> species300	KetoneHydrogenation-Oxygen	-19.571078
2894	species2 + species138 -> species350	KetoneHydrogenation-Oxygen	-19.571078
2895	species2 + species145 -> species351	KetoneHydrogenation-Oxygen	-19.571078
2896	species2 + species146 -> species354	KetoneHydrogenation-Oxygen	-15.603308
2897	species2 + species147 -> species420	KetoneHydrogenation-Oxygen	-19.571078
2898	species2 + species150 -> species426	KetoneHydrogenation-Oxygen	-10.205655
2899	species2 + species151 -> species313	KetoneHydrogenation-Oxygen	-5.749402
2900	species2 + species153 -> species327	KetoneHydrogenation-Oxygen	-17.124275
2901	species2 + species154 -> species326	KetoneHydrogenation-Oxygen	-4.789467
2902	species2 + species162 -> species301	KetoneHydrogenation-Oxygen	-19.571078
2903	species2 + species163 -> species363	KetoneHydrogenation-Oxygen	-19.571078
2904	species2 + species164 -> species410	KetoneHydrogenation-Oxygen	-19.571078
2905	species2 + species165 -> species363	KetoneHydrogenation-Oxygen	-19.571078
2906	species2 + species171 -> species359	KetoneHydrogenation-Oxygen	-19.571078
2907	species2 + species172 -> species367	KetoneHydrogenation-Oxygen	-15.603308
2908	species2 + species173 -> species424	KetoneHydrogenation-Oxygen	-19.571078
2909	species2 + species174 -> species367	KetoneHydrogenation-Oxygen	-19.571078
2910	species2 + species178 -> species366	KetoneHydrogenation-Oxygen	-19.571078
2911	species2 + species179 -> species423	KetoneHydrogenation-Oxygen	-19.571078
2912	species2 + species182 -> species358	KetoneHydrogenation-Oxygen	-24.029340
2913	species2 + species183 -> species365	KetoneHydrogenation-Oxygen	-19.571078
2914	species2 + species184 -> species364	KetoneHydrogenation-Oxygen	-19.571078
2915	species2 + species185 -> species464	KetoneHydrogenation-Oxygen	-19.571078
2916	species2 + species186 -> species355	KetoneHydrogenation-Oxygen	-19.571078
2917	species2 + species188 -> species302	KetoneHydrogenation-Oxygen	-17.541671
2918	species2 + species189 -> species302	KetoneHydrogenation-Oxygen	-88.690758
2919	species2 + species190 -> species52	KetoneHydrogenation-Oxygen	-17.541671
2920	species2 + species193 -> species283	KetoneHydrogenation-Oxygen	-15.621843
2921	species2 + species194 -> species67	KetoneHydrogenation-Oxygen	-17.541671
2922	species2 + species194 -> species68	KetoneHydrogenation-Oxygen	-7.737304
2923	species2 + species195 -> species412	KetoneHydrogenation-Oxygen	-94.327025
2924	species2 + species195 -> species69	KetoneHydrogenation-Oxygen	-94.327025
2925	species2 + species196 -> species70	KetoneHydrogenation-Oxygen	-17.541671
2926	species2 + species197 -> species296	KetoneHydrogenation-Oxygen	-21.580528
2927	species2 + species197 -> species62	KetoneHydrogenation-Oxygen	-17.541671
2928	species2 + species198 -> species369	KetoneHydrogenation-Oxygen	-17.541671
2929	species2 + species199 -> species368	KetoneHydrogenation-Oxygen	-17.541671
2930	species2 + species199 -> species306	KetoneHydrogenation-Oxygen	-88.690758
2931	species2 + species200 -> species413	KetoneHydrogenation-Oxygen	-7.737304

2932	species2 + species200 -> species307	KetoneHydrogenation-Oxygen	-88.690758
2933	species2 + species201 -> species305	KetoneHydrogenation-Oxygen	-88.690758
2934	species2 + species202 -> species295	KetoneHydrogenation-Oxygen	-21.580528
2935	species2 + species202 -> species304	KetoneHydrogenation-Oxygen	-88.690758
2936	species2 + species203 -> species345	KetoneHydrogenation-Oxygen	-87.730949
2937	species2 + species204 -> species303	KetoneHydrogenation-Oxygen	-98.495126
2938	species2 + species205 -> species305	KetoneHydrogenation-Oxygen	-7.737304
2939	species2 + species206 -> species293	KetoneHydrogenation-Oxygen	-93.367215
2940	species2 + species206 -> species304	KetoneHydrogenation-Oxygen	-89.328400
2941	species2 + species207 -> species491	KetoneHydrogenation-Oxygen	-17.541671
2942	species2 + species209 -> species336	KetoneHydrogenation-Oxygen	-17.541671
2943	species2 + species210 -> species294	KetoneHydrogenation-Oxygen	-6.810380
2944	species2 + species210 -> species298	KetoneHydrogenation-Oxygen	-17.541671
2945	species2 + species211 -> species299	KetoneHydrogenation-Oxygen	-21.580528
2946	species2 + species213 -> species411	KetoneHydrogenation-Oxygen	-12.613965
2947	species2 + species214 -> species415	KetoneHydrogenation-Oxygen	-88.690758
2948	species2 + species215 -> species216	KetoneHydrogenation-Oxygen	-21.580528
2949	species2 + species222 -> species341	KetoneHydrogenation-Oxygen	-93.367215
2950	species2 + species222 -> species344	KetoneHydrogenation-Oxygen	-89.328400
2951	species2 + species222 -> species342	KetoneHydrogenation-Oxygen	-6.810380
2952	species2 + species223 -> species335	KetoneHydrogenation-Oxygen	-7.737304
2953	species2 + species223 -> species333	KetoneHydrogenation-Oxygen	-6.810380
2954	species2 + species224 -> species234	KetoneHydrogenation-Oxygen	-17.541671
2955	species2 + species224 -> species235	KetoneHydrogenation-Oxygen	-6.810380
2956	species2 + species225 -> species337	KetoneHydrogenation-Oxygen	-89.328400
2957	species2 + species225 -> species332	KetoneHydrogenation-Oxygen	-93.367215
2958	species2 + species226 -> species393	KetoneHydrogenation-Oxygen	-88.368172
2959	species2 + species227 -> species370	KetoneHydrogenation-Oxygen	-110.677678
2960	species2 + species227 -> species499	KetoneHydrogenation-Oxygen	-99.913502
2961	species2 + species228 -> species429	KetoneHydrogenation-Oxygen	-12.613965
2962	species2 + species228 -> species397	KetoneHydrogenation-Oxygen	-21.580528
2963	species2 + species229 -> species230	KetoneHydrogenation-Oxygen	-21.580528
2964	species2 + species230 -> species331	KetoneHydrogenation-Oxygen	-20.620593
2965	species2 + species233 -> species330	KetoneHydrogenation-Oxygen	-15.621843
2966	species2 + species234 -> species371	KetoneHydrogenation-Oxygen	-6.810380
2967	species2 + species235 -> species371	KetoneHydrogenation-Oxygen	-17.541671
2968	species2 + species236 -> species437	KetoneHydrogenation-Oxygen	-17.541671
2969	species2 + species238 -> species338	KetoneHydrogenation-Oxygen	-7.737304
2970	species2 + species239 -> species508	KetoneHydrogenation-Oxygen	-17.541671
2971	species2 + species240 -> species510	KetoneHydrogenation-Oxygen	-6.810380
2972	species2 + species241 -> species373	KetoneHydrogenation-Oxygen	-11.163540
2973	species2 + species242 -> species372	KetoneHydrogenation-Oxygen	-17.541671
2974	species2 + species243 -> species511	KetoneHydrogenation-Oxygen	-88.690758
2975	species2 + species244 -> species430	KetoneHydrogenation-Oxygen	-12.613965
2976	species2 + species245 -> species237	KetoneHydrogenation-Oxygen	-21.580528
2977	species2 + species248 -> species374	KetoneHydrogenation-Oxygen	-41.891045
2978	species2 + species248 -> species427	KetoneHydrogenation-Oxygen	-27.158846
2979	species2 + species249 -> species432	KetoneHydrogenation-Oxygen	-94.327025
2980	species2 + species249 -> species428	KetoneHydrogenation-Oxygen	-89.399528
2981	species2 + species250 -> species517	KetoneHydrogenation-Oxygen	-36.963213
2982	species2 + species251 -> species236	KetoneHydrogenation-Oxygen	-93.367215
2983	species2 + species251 -> species433	KetoneHydrogenation-Oxygen	-89.328400
2984	species2 + species254 -> species491	KetoneHydrogenation-Oxygen	-88.690758
2985	species2 + species264 -> species536	KetoneHydrogenation-Oxygen	-14.948177
2986	species2 + species273 -> species536	KetoneHydrogenation-Oxygen	-19.571078
2987	species2 + species274 -> species526	KetoneHydrogenation-Oxygen	-19.571078
2988	species2 + species282 -> species572	KetoneHydrogenation-Oxygen	-19.571078
2989	species2 + species288 -> species584	KetoneHydrogenation-Oxygen	-19.571078
2990	species2 + species289 -> species530	KetoneHydrogenation-Oxygen	-19.571078

2991	species2 + species293 -> species595	KetoneHydrogenation-Oxygen	-17.541671
2992	species2 + species294 -> species533	KetoneHydrogenation-Oxygen	-17.541671
2993	species2 + species295 -> species595	KetoneHydrogenation-Oxygen	-88.690758
2994	species2 + species296 -> species109	KetoneHydrogenation-Oxygen	-17.541671
2995	species2 + species297 -> species587	KetoneHydrogenation-Oxygen	-17.541671
2996	species2 + species298 -> species533	KetoneHydrogenation-Oxygen	-6.810380
2997	species2 + species304 -> species595	KetoneHydrogenation-Oxygen	-21.580528
2998	species2 + species306 -> species532	KetoneHydrogenation-Oxygen	-11.167598
2999	species2 + species307 -> species586	KetoneHydrogenation-Oxygen	-6.779377
3000	species2 + species311 -> species526	KetoneHydrogenation-Oxygen	-14.948177
3001	species2 + species316 -> species523	KetoneHydrogenation-Oxygen	-51.333914
3002	species2 + species324 -> species529	KetoneHydrogenation-Oxygen	-19.571078
3003	species2 + species325 -> species623	KetoneHydrogenation-Oxygen	-19.571078
3004	species2 + species328 -> species539	KetoneHydrogenation-Oxygen	-19.571078
3005	species2 + species329 -> species624	KetoneHydrogenation-Oxygen	-19.571078
3006	species2 + species332 -> species661	KetoneHydrogenation-Oxygen	-17.541671
3007	species2 + species333 -> species541	KetoneHydrogenation-Oxygen	-7.737304
3008	species2 + species334 -> species627	KetoneHydrogenation-Oxygen	-16.581736
3009	species2 + species335 -> species541	KetoneHydrogenation-Oxygen	-6.810380
3010	species2 + species337 -> species661	KetoneHydrogenation-Oxygen	-21.580528
3011	species2 + species339 -> species540	KetoneHydrogenation-Oxygen	-11.165548
3012	species2 + species340 -> species626	KetoneHydrogenation-Oxygen	-6.777369
3013	species2 + species341 -> species560	KetoneHydrogenation-Oxygen	-17.541671
3014	species2 + species341 -> species562	KetoneHydrogenation-Oxygen	-6.810380
3015	species2 + species342 -> species538	KetoneHydrogenation-Oxygen	-89.328400
3016	species2 + species342 -> species562	KetoneHydrogenation-Oxygen	-93.367215
3017	species2 + species343 -> species630	KetoneHydrogenation-Oxygen	-16.581736
3018	species2 + species343 -> species561	KetoneHydrogenation-Oxygen	-21.580528
3019	species2 + species344 -> species538	KetoneHydrogenation-Oxygen	-6.810380
3020	species2 + species344 -> species560	KetoneHydrogenation-Oxygen	-21.580528
3021	species2 + species346 -> species537	KetoneHydrogenation-Oxygen	-16.581736
3022	species2 + species346 -> species546	KetoneHydrogenation-Oxygen	-6.810380
3023	species2 + species347 -> species629	KetoneHydrogenation-Oxygen	-6.777369
3024	species2 + species347 -> species547	KetoneHydrogenation-Oxygen	-6.810380
3025	species2 + species348 -> species678	KetoneHydrogenation-Oxygen	-70.901646
3026	species2 + species360 -> species548	KetoneHydrogenation-Oxygen	-19.571078
3027	species2 + species361 -> species631	KetoneHydrogenation-Oxygen	-19.571078
3028	species2 + species368 -> species532	KetoneHydrogenation-Oxygen	-82.316434
3029	species2 + species370 -> species704	KetoneHydrogenation-Oxygen	2.118142
3030	species2 + species374 -> species632	KetoneHydrogenation-Oxygen	-2.809556
3031	species2 + species375 -> species681	KetoneHydrogenation-Oxygen	-6.810380
3032	species2 + species381 -> species542	KetoneHydrogenation-Oxygen	-19.571078
3033	species2 + species382 -> species688	KetoneHydrogenation-Oxygen	-19.571078
3034	species2 + species389 -> species651	KetoneHydrogenation-Oxygen	-19.571078
3035	species2 + species390 -> species696	KetoneHydrogenation-Oxygen	-19.571078
3036	species2 + species391 -> species696	KetoneHydrogenation-Oxygen	-19.571078
3037	species2 + species392 -> species543	KetoneHydrogenation-Oxygen	-19.571078
3038	species2 + species393 -> species507	KetoneHydrogenation-Oxygen	-21.580528
3039	species2 + species394 -> species545	KetoneHydrogenation-Oxygen	-12.661997
3040	species2 + species395 -> species544	KetoneHydrogenation-Oxygen	-17.541671
3041	species2 + species396 -> species635	KetoneHydrogenation-Oxygen	-7.737304
3042	species2 + species396 -> species637	KetoneHydrogenation-Oxygen	-17.541671
3043	species2 + species397 -> species555	KetoneHydrogenation-Oxygen	-11.654030
3044	species2 + species398 -> species636	KetoneHydrogenation-Oxygen	-94.327025
3045	species2 + species398 -> species653	KetoneHydrogenation-Oxygen	-94.327025
3046	species2 + species399 -> species682	KetoneHydrogenation-Oxygen	-17.541671
3047	species2 + species402 -> species604	KetoneHydrogenation-Oxygen	-19.571078
3048	species2 + species407 -> species607	KetoneHydrogenation-Oxygen	-15.603308
3049	species2 + species408 -> species683	KetoneHydrogenation-Oxygen	-19.571078

3050	species2 + species409 -> species728	KetoneHydrogenation-Oxygen	-19.571078
3051	species2 + species412 -> species152	KetoneHydrogenation-Oxygen	-11.167598
3052	species2 + species413 -> species586	KetoneHydrogenation-Oxygen	-87.732622
3053	species2 + species414 -> species646	KetoneHydrogenation-Oxygen	-12.127491
3054	species2 + species418 -> species687	KetoneHydrogenation-Oxygen	-15.603308
3055	species2 + species419 -> species742	KetoneHydrogenation-Oxygen	-19.571078
3056	species2 + species425 -> species645	KetoneHydrogenation-Oxygen	-19.571078
3057	species2 + species427 -> species632	KetoneHydrogenation-Oxygen	-17.541671
3058	species2 + species428 -> species750	KetoneHydrogenation-Oxygen	-17.541671
3059	species2 + species429 -> species555	KetoneHydrogenation-Oxygen	-20.620593
3060	species2 + species431 -> species755	KetoneHydrogenation-Oxygen	-1.359172
3061	species2 + species432 -> species750	KetoneHydrogenation-Oxygen	-12.613965
3062	species2 + species433 -> species437	KetoneHydrogenation-Oxygen	-21.580528
3063	species2 + species434 -> species633	KetoneHydrogenation-Oxygen	-11.163540
3064	species2 + species435 -> species634	KetoneHydrogenation-Oxygen	-17.541671
3065	species2 + species438 -> species648	KetoneHydrogenation-Oxygen	-7.737304
3066	species2 + species439 -> species647	KetoneHydrogenation-Oxygen	-89.328400
3067	species2 + species439 -> species652	KetoneHydrogenation-Oxygen	-93.367215
3068	species2 + species440 -> species745	KetoneHydrogenation-Oxygen	-12.125483
3069	species2 + species444 -> species574	KetoneHydrogenation-Oxygen	-19.571078
3070	species2 + species448 -> species699	KetoneHydrogenation-Oxygen	-19.571078
3071	species2 + species449 -> species731	KetoneHydrogenation-Oxygen	-19.571078
3072	species2 + species452 -> species611	KetoneHydrogenation-Oxygen	-24.029340
3073	species2 + species453 -> species697	KetoneHydrogenation-Oxygen	-19.571078
3074	species2 + species454 -> species698	KetoneHydrogenation-Oxygen	-19.571078
3075	species2 + species455 -> species608	KetoneHydrogenation-Oxygen	-19.571078
3076	species2 + species458 -> species693	KetoneHydrogenation-Oxygen	-24.029340
3077	species2 + species459 -> species702	KetoneHydrogenation-Oxygen	-15.603308
3078	species2 + species460 -> species701	KetoneHydrogenation-Oxygen	-15.603308
3079	species2 + species461 -> species689	KetoneHydrogenation-Oxygen	-83.927693
3080	species2 + species462 -> species764	KetoneHydrogenation-Oxygen	-19.571078
3081	species2 + species463 -> species765	KetoneHydrogenation-Oxygen	-24.029340
3082	species2 + species466 -> species575	KetoneHydrogenation-Oxygen	-17.541671
3083	species2 + species467 -> species192	KetoneHydrogenation-Oxygen	-17.541671
3084	species2 + species469 -> species614	KetoneHydrogenation-Oxygen	-97.914805
3085	species2 + species470 -> species615	KetoneHydrogenation-Oxygen	-88.110438
3086	species2 + species471 -> species201	KetoneHydrogenation-Oxygen	-7.156899
3087	species2 + species471 -> species205	KetoneHydrogenation-Oxygen	-88.110438
3088	species2 + species472 -> species217	KetoneHydrogenation-Oxygen	-88.690758
3089	species2 + species473 -> species196	KetoneHydrogenation-Oxygen	-93.746704
3090	species2 + species474 -> species577	KetoneHydrogenation-Oxygen	-7.737304
3091	species2 + species476 -> species576	KetoneHydrogenation-Oxygen	-12.613965
3092	species2 + species477 -> species734	KetoneHydrogenation-Oxygen	-89.399528
3093	species2 + species477 -> species244	KetoneHydrogenation-Oxygen	-94.327025
3094	species2 + species478 -> species479	KetoneHydrogenation-Oxygen	-93.367215
3095	species2 + species478 -> species245	KetoneHydrogenation-Oxygen	-89.328400
3096	species2 + species479 -> species237	KetoneHydrogenation-Oxygen	-17.541671
3097	species2 + species480 -> species617	KetoneHydrogenation-Oxygen	-88.110438
3098	species2 + species481 -> species733	KetoneHydrogenation-Oxygen	-2.809556
3099	species2 + species481 -> species596	KetoneHydrogenation-Oxygen	-88.690758
3100	species2 + species482 -> species483	KetoneHydrogenation-Oxygen	-6.810380
3101	species2 + species482 -> species490	KetoneHydrogenation-Oxygen	-88.690758
3102	species2 + species483 -> species620	KetoneHydrogenation-Oxygen	-88.690758
3103	species2 + species484 -> species621	KetoneHydrogenation-Oxygen	-88.110438
3104	species2 + species485 -> species622	KetoneHydrogenation-Oxygen	-81.732348
3105	species2 + species486 -> species619	KetoneHydrogenation-Oxygen	-99.333181
3106	species2 + species486 -> species774	KetoneHydrogenation-Oxygen	-17.419707
3107	species2 + species487 -> species616	KetoneHydrogenation-Oxygen	-11.163540
3108	species2 + species488 -> species597	KetoneHydrogenation-Oxygen	-10.873463

3109	species2 + species488 -> species618	KetoneHydrogenation-Oxygen	-87.787851
3110	species2 + species489 -> species777	KetoneHydrogenation-Oxygen	-98.495126
3111	species2 + species490 -> species620	KetoneHydrogenation-Oxygen	-6.810380
3112	species2 + species492 -> species779	KetoneHydrogenation-Oxygen	-88.690758
3113	species2 + species493 -> species654	KetoneHydrogenation-Oxygen	-17.541671
3114	species2 + species494 -> species735	KetoneHydrogenation-Oxygen	-83.762843
3115	species2 + species497 -> species660	KetoneHydrogenation-Oxygen	-6.810380
3116	species2 + species498 -> species655	KetoneHydrogenation-Oxygen	-89.328400
3117	species2 + species498 -> species659	KetoneHydrogenation-Oxygen	-93.367215
3118	species2 + species499 -> species704	KetoneHydrogenation-Oxygen	-8.646152
3119	species2 + species501 -> species656	KetoneHydrogenation-Oxygen	-7.737304
3120	species2 + species502 -> species670	KetoneHydrogenation-Oxygen	-6.810380
3121	species2 + species503 -> species706	KetoneHydrogenation-Oxygen	-12.661997
3122	species2 + species504 -> species705	KetoneHydrogenation-Oxygen	-17.541671
3123	species2 + species505 -> species786	KetoneHydrogenation-Oxygen	-2.809556
3124	species2 + species506 -> species754	KetoneHydrogenation-Oxygen	-12.613965
3125	species2 + species509 -> species780	KetoneHydrogenation-Oxygen	-88.690758
3126	species2 + species512 -> species792	KetoneHydrogenation-Oxygen	-83.762843
3127	species2 + species513 -> species793	KetoneHydrogenation-Oxygen	-87.730949
3128	species2 + species515 -> species752	KetoneHydrogenation-Oxygen	-89.399528
3129	species2 + species516 -> species506	KetoneHydrogenation-Oxygen	-93.367215
3130	species2 + species516 -> species753	KetoneHydrogenation-Oxygen	-84.400485
3131	species2 + species521 -> species799	KetoneHydrogenation-Oxygen	-14.948177
3132	species2 + species535 -> species805	KetoneHydrogenation-Oxygen	-14.948177
3133	species2 + species537 -> species828	KetoneHydrogenation-Oxygen	-1.394234
3134	species2 + species538 -> species829	KetoneHydrogenation-Oxygen	-21.580528
3135	species2 + species546 -> species828	KetoneHydrogenation-Oxygen	-11.165548
3136	species2 + species547 -> species808	KetoneHydrogenation-Oxygen	-6.777369
3137	species2 + species553 -> species803	KetoneHydrogenation-Oxygen	-19.571078
3138	species2 + species554 -> species814	KetoneHydrogenation-Oxygen	-19.571078
3139	species2 + species557 -> species804	KetoneHydrogenation-Oxygen	8.980215
3140	species2 + species558 -> species827	KetoneHydrogenation-Oxygen	5.012424
3141	species2 + species560 -> species829	KetoneHydrogenation-Oxygen	-6.810380
3142	species2 + species561 -> species807	KetoneHydrogenation-Oxygen	-16.581736
3143	species2 + species562 -> species829	KetoneHydrogenation-Oxygen	-17.541671
3144	species2 + species567 -> species868	KetoneHydrogenation-Oxygen	-19.571078
3145	species2 + species571 -> species870	KetoneHydrogenation-Oxygen	-15.603308
3146	species2 + species578 -> species872	KetoneHydrogenation-Oxygen	-6.777369
3147	species2 + species582 -> species882	KetoneHydrogenation-Oxygen	-15.603308
3148	species2 + species583 -> species816	KetoneHydrogenation-Oxygen	-31.626605
3149	species2 + species593 -> species822	KetoneHydrogenation-Oxygen	-19.571078
3150	species2 + species594 -> species896	KetoneHydrogenation-Oxygen	-19.571078
3151	species2 + species596 -> species884	KetoneHydrogenation-Oxygen	-2.809556
3152	species2 + species597 -> species897	KetoneHydrogenation-Oxygen	-98.495126
3153	species2 + species598 -> species824	KetoneHydrogenation-Oxygen	-12.661997
3154	species2 + species599 -> species823	KetoneHydrogenation-Oxygen	-17.541671
3155	species2 + species600 -> species887	KetoneHydrogenation-Oxygen	-7.737304
3156	species2 + species600 -> species889	KetoneHydrogenation-Oxygen	-88.690758
3157	species2 + species601 -> species825	KetoneHydrogenation-Oxygen	-6.810380
3158	species2 + species601 -> species820	KetoneHydrogenation-Oxygen	-88.690758
3159	species2 + species602 -> species888	KetoneHydrogenation-Oxygen	-94.327025
3160	species2 + species602 -> species334	KetoneHydrogenation-Oxygen	-94.327025
3161	species2 + species603 -> species891	KetoneHydrogenation-Oxygen	-88.690758
3162	species2 + species612 -> species818	KetoneHydrogenation-Oxygen	-19.571078
3163	species2 + species613 -> species883	KetoneHydrogenation-Oxygen	-19.571078
3164	species2 + species615 -> species819	KetoneHydrogenation-Oxygen	-88.690758
3165	species2 + species618 -> species897	KetoneHydrogenation-Oxygen	-21.580528
3166	species2 + species619 -> species907	KetoneHydrogenation-Oxygen	2.118142
3167	species2 + species628 -> species806	KetoneHydrogenation-Oxygen	13.022566

3168	species2 + species629 -> species808	KetoneHydrogenation-Oxygen	-6.810380
3169	species2 + species630 -> species807	KetoneHydrogenation-Oxygen	-21.580528
3170	species2 + species635 -> species926	KetoneHydrogenation-Oxygen	-16.581736
3171	species2 + species636 -> species912	KetoneHydrogenation-Oxygen	-16.581736
3172	species2 + species637 -> species926	KetoneHydrogenation-Oxygen	-6.777369
3173	species2 + species638 -> species644	KetoneHydrogenation-Oxygen	-16.581736
3174	species2 + species642 -> species802	KetoneHydrogenation-Oxygen	-14.948177
3175	species2 + species647 -> species944	KetoneHydrogenation-Oxygen	-16.164340
3176	species2 + species649 -> species643	KetoneHydrogenation-Oxygen	-12.125483
3177	species2 + species650 -> species911	KetoneHydrogenation-Oxygen	-1.361181
3178	species2 + species652 -> species944	KetoneHydrogenation-Oxygen	-12.125483
3179	species2 + species653 -> species912	KetoneHydrogenation-Oxygen	-16.581736
3180	species2 + species655 -> species914	KetoneHydrogenation-Oxygen	-21.580528
3181	species2 + species657 -> species835	KetoneHydrogenation-Oxygen	-16.581736
3182	species2 + species658 -> species915	KetoneHydrogenation-Oxygen	-6.777369
3183	species2 + species659 -> species914	KetoneHydrogenation-Oxygen	-17.541671
3184	species2 + species660 -> species836	KetoneHydrogenation-Oxygen	-6.810380
3185	species2 + species662 -> species916	KetoneHydrogenation-Oxygen	-2.809556
3186	species2 + species663 -> species841	KetoneHydrogenation-Oxygen	-2.857630
3187	species2 + species664 -> species840	KetoneHydrogenation-Oxygen	-7.737304
3188	species2 + species665 -> species961	KetoneHydrogenation-Oxygen	-88.690758
3189	species2 + species666 -> species838	KetoneHydrogenation-Oxygen	-0.399279
3190	species2 + species667 -> species839	KetoneHydrogenation-Oxygen	-6.810380
3191	species2 + species668 -> species821	KetoneHydrogenation-Oxygen	-88.690758
3192	species2 + species673 -> species861	KetoneHydrogenation-Oxygen	-2.809556
3193	species2 + species673 -> species855	KetoneHydrogenation-Oxygen	-6.810380
3194	species2 + species674 -> species834	KetoneHydrogenation-Oxygen	-84.448601
3195	species2 + species674 -> species867	KetoneHydrogenation-Oxygen	-93.367215
3196	species2 + species675 -> species833	KetoneHydrogenation-Oxygen	-89.328400
3197	species2 + species675 -> species859	KetoneHydrogenation-Oxygen	-93.367215
3198	species2 + species676 -> species832	KetoneHydrogenation-Oxygen	-99.913502
3199	species2 + species694 -> species858	KetoneHydrogenation-Oxygen	-19.571078
3200	species2 + species695 -> species925	KetoneHydrogenation-Oxygen	-19.571078
3201	species2 + species707 -> species966	KetoneHydrogenation-Oxygen	-26.198953
3202	species2 + species712 -> species844	KetoneHydrogenation-Oxygen	-15.603308
3203	species2 + species713 -> species972	KetoneHydrogenation-Oxygen	-19.571078
3204	species2 + species717 -> species975	KetoneHydrogenation-Oxygen	-19.571078
3205	species2 + species718 -> species845	KetoneHydrogenation-Oxygen	-24.029340
3206	species2 + species721 -> species948	KetoneHydrogenation-Oxygen	-19.571078
3207	species2 + species722 -> species976	KetoneHydrogenation-Oxygen	-19.571078
3208	species2 + species723 -> species848	KetoneHydrogenation-Oxygen	-19.571078
3209	species2 + species724 -> species951	KetoneHydrogenation-Oxygen	-19.571078
3210	species2 + species725 -> species929	KetoneHydrogenation-Oxygen	-94.327025
3211	species2 + species725 -> species860	KetoneHydrogenation-Oxygen	-89.399528
3212	species2 + species732 -> species940	KetoneHydrogenation-Oxygen	-19.571078
3213	species2 + species733 -> species884	KetoneHydrogenation-Oxygen	-88.690758
3214	species2 + species734 -> species430	KetoneHydrogenation-Oxygen	-17.541671
3215	species2 + species736 -> species904	KetoneHydrogenation-Oxygen	-1.359172
3216	species2 + species737 -> species885	KetoneHydrogenation-Oxygen	-82.312669
3217	species2 + species738 -> species886	KetoneHydrogenation-Oxygen	-88.690758
3218	species2 + species748 -> species942	KetoneHydrogenation-Oxygen	-15.603308
3219	species2 + species749 -> species989	KetoneHydrogenation-Oxygen	-19.571078
3220	species2 + species751 -> species927	KetoneHydrogenation-Oxygen	-24.796602
3221	species2 + species752 -> species992	KetoneHydrogenation-Oxygen	-12.613965
3222	species2 + species753 -> species754	KetoneHydrogenation-Oxygen	-21.580528
3223	species2 + species756 -> species994	KetoneHydrogenation-Oxygen	-8.614103
3224	species2 + species757 -> species995	KetoneHydrogenation-Oxygen	-12.581916
3225	species2 + species758 -> species945	KetoneHydrogenation-Oxygen	-6.810380
3226	species2 + species759 -> species990	KetoneHydrogenation-Oxygen	-88.690758

3227	species2 + species763 -> species876	KetoneHydrogenation-Oxygen	-24.029340
3228	species2 + species766 -> species468	KetoneHydrogenation-Oxygen	-17.541671
3229	species2 + species767 -> species878	KetoneHydrogenation-Oxygen	-12.613965
3230	species2 + species768 -> species475	KetoneHydrogenation-Oxygen	-7.737304
3231	species2 + species769 -> species903	KetoneHydrogenation-Oxygen	-11.163540
3232	species2 + species770 -> species879	KetoneHydrogenation-Oxygen	-2.809556
3233	species2 + species772 -> species908	KetoneHydrogenation-Oxygen	-88.690758
3234	species2 + species773 -> species909	KetoneHydrogenation-Oxygen	-83.810959
3235	species2 + species774 -> species907	KetoneHydrogenation-Oxygen	-79.795156
3236	species2 + species775 -> species898	KetoneHydrogenation-Oxygen	-93.367215
3237	species2 + species775 -> species905	KetoneHydrogenation-Oxygen	-82.950310
3238	species2 + species776 -> species998	KetoneHydrogenation-Oxygen	-23.346218
3239	species2 + species778 -> species1000	KetoneHydrogenation-Oxygen	-87.730949
3240	species2 + species785 -> species956	KetoneHydrogenation-Oxygen	-11.924274
3241	species2 + species787 -> species1003	KetoneHydrogenation-Oxygen	-22.231140
3242	species2 + species812 -> species1028	KetoneHydrogenation-Oxygen	-19.571078
3243	species2 + species813 -> species1007	KetoneHydrogenation-Oxygen	-19.571078
3244	species2 + species820 -> species1032	KetoneHydrogenation-Oxygen	-6.810380
3245	species2 + species825 -> species1032	KetoneHydrogenation-Oxygen	-88.690758
3246	species2 + species830 -> species1040	KetoneHydrogenation-Oxygen	-6.810380
3247	species2 + species831 -> species1041	KetoneHydrogenation-Oxygen	-6.810380
3248	species2 + species832 -> species1046	KetoneHydrogenation-Oxygen	2.118142
3249	species2 + species833 -> species1043	KetoneHydrogenation-Oxygen	-21.580528
3250	species2 + species834 -> species1044	KetoneHydrogenation-Oxygen	-21.580528
3251	species2 + species849 -> species1023	KetoneHydrogenation-Oxygen	-19.571078
3252	species2 + species850 -> species1038	KetoneHydrogenation-Oxygen	-19.571078
3253	species2 + species851 -> species1017	KetoneHydrogenation-Oxygen	-6.777369
3254	species2 + species852 -> species937	KetoneHydrogenation-Oxygen	-17.541671
3255	species2 + species853 -> species1025	KetoneHydrogenation-Oxygen	-15.040267
3256	species2 + species854 -> species1039	KetoneHydrogenation-Oxygen	-17.541671
3257	species2 + species855 -> species1024	KetoneHydrogenation-Oxygen	-2.809556
3258	species2 + species859 -> species1043	KetoneHydrogenation-Oxygen	-17.541671
3259	species2 + species860 -> species1016	KetoneHydrogenation-Oxygen	-17.541671
3260	species2 + species861 -> species1024	KetoneHydrogenation-Oxygen	-6.810380
3261	species2 + species864 -> species1042	KetoneHydrogenation-Oxygen	-19.571078
3262	species2 + species865 -> species1021	KetoneHydrogenation-Oxygen	-7.737304
3263	species2 + species865 -> species1019	KetoneHydrogenation-Oxygen	-6.810380
3264	species2 + species866 -> species1022	KetoneHydrogenation-Oxygen	-94.327025
3265	species2 + species867 -> species1044	KetoneHydrogenation-Oxygen	-12.661997
3266	species2 + species877 -> species1063	KetoneHydrogenation-Oxygen	-19.571078
3267	species2 + species887 -> species1068	KetoneHydrogenation-Oxygen	-87.730949
3268	species2 + species888 -> species627	KetoneHydrogenation-Oxygen	-16.581736
3269	species2 + species889 -> species1068	KetoneHydrogenation-Oxygen	-6.777369
3270	species2 + species890 -> species894	KetoneHydrogenation-Oxygen	-17.541671
3271	species2 + species898 -> species1077	KetoneHydrogenation-Oxygen	-11.163540
3272	species2 + species905 -> species1077	KetoneHydrogenation-Oxygen	-21.580528
3273	species2 + species919 -> species1086	KetoneHydrogenation-Oxygen	-7.737304
3274	species2 + species920 -> species932	KetoneHydrogenation-Oxygen	-7.737304
3275	species2 + species921 -> species1026	KetoneHydrogenation-Oxygen	-0.399279
3276	species2 + species922 -> species1027	KetoneHydrogenation-Oxygen	-6.810380
3277	species2 + species923 -> species934	KetoneHydrogenation-Oxygen	-89.328400
3278	species2 + species923 -> species1020	KetoneHydrogenation-Oxygen	-93.367215
3279	species2 + species928 -> species1088	KetoneHydrogenation-Oxygen	-11.163540
3280	species2 + species929 -> species1016	KetoneHydrogenation-Oxygen	-12.613965
3281	species2 + species934 -> species1013	KetoneHydrogenation-Oxygen	-21.580528
3282	species2 + species935 -> species1012	KetoneHydrogenation-Oxygen	-6.810380
3283	species2 + species938 -> species1099	KetoneHydrogenation-Oxygen	-17.541671
3284	species2 + species939 -> species1090	KetoneHydrogenation-Oxygen	-7.737304
3285	species2 + species943 -> species893	KetoneHydrogenation-Oxygen	-88.690758

3286	species2 + species947 -> species1078	KetoneHydrogenation-Oxygen	-2.809556
3287	species2 + species952 -> species1102	KetoneHydrogenation-Oxygen	-19.571078
3288	species2 + species953 -> species1105	KetoneHydrogenation-Oxygen	-1.359172
3289	species2 + species954 -> species1033	KetoneHydrogenation-Oxygen	-88.690758
3290	species2 + species955 -> species1049	KetoneHydrogenation-Oxygen	-1.897695
3291	species2 + species959 -> species1083	KetoneHydrogenation-Oxygen	-2.809556
3292	species2 + species960 -> species1050	KetoneHydrogenation-Oxygen	-6.810380
3293	species2 + species984 -> species1069	KetoneHydrogenation-Oxygen	-14.032299
3294	species2 + species999 -> species1116	KetoneHydrogenation-Oxygen	-82.312669
3295	species2 + species1019 -> species1133	KetoneHydrogenation-Oxygen	-7.737304
3296	species2 + species1020 -> species1013	KetoneHydrogenation-Oxygen	-17.541671
3297	species2 + species1021 -> species1133	KetoneHydrogenation-Oxygen	-6.810380
3298	species2 + species1022 -> species1121	KetoneHydrogenation-Oxygen	-16.581736
3299	species2 + species1036 -> species1073	KetoneHydrogenation-Oxygen	-88.690758
3300	species2 + species1037 -> species1141	KetoneHydrogenation-Oxygen	-88.690758
3301	species2 + species1040 -> species1143	KetoneHydrogenation-Oxygen	-6.810380
3302	species2 + species1045 -> species1092	KetoneHydrogenation-Oxygen	-11.052454
3303	species2 + species1047 -> species1139	KetoneHydrogenation-Oxygen	-1.849663
3304	species2 + species1056 -> species1130	KetoneHydrogenation-Oxygen	-2.809556
3305	species2 + species1057 -> species1138	KetoneHydrogenation-Oxygen	-10.112561
3306	species2 + species1070 -> species1152	KetoneHydrogenation-Oxygen	-82.312669
3307	species2 + species1074 -> species1153	KetoneHydrogenation-Oxygen	-88.690758
3308	species2 + species1081 -> species1154	KetoneHydrogenation-Oxygen	-7.737304
3309	species2 + species1082 -> species1155	KetoneHydrogenation-Oxygen	-12.412756
3310	species2 + species1096 -> species1161	KetoneHydrogenation-Oxygen	-0.399279
3311	species2 + species1097 -> species1125	KetoneHydrogenation-Oxygen	-6.810380
3312	species2 + species1100 -> species1123	KetoneHydrogenation-Oxygen	-2.809556
3313	species2 + species1127 -> species1167	KetoneHydrogenation-Oxygen	-7.277859
3314	species2 + species1128 -> species1164	KetoneHydrogenation-Oxygen	-7.737304
3315	species2 + species1129 -> species1169	KetoneHydrogenation-Oxygen	-7.737304
3316	species2 + species1134 -> species1172	KetoneHydrogenation-Oxygen	-2.857630
3317	species2 + species1135 -> species1171	KetoneHydrogenation-Oxygen	-6.810380
3318	species1 -> species3 + species8	PinacolRearrangement-Oxygen	-75.610738
3319	species1 -> species3 + species9	PinacolRearrangement-Oxygen	-68.147737
3320	species1 -> species3 + species10	PinacolRearrangement-Oxygen	-71.112519
3321	species1 -> species3 + species11	PinacolRearrangement-Oxygen	-71.112519
3322	species1 -> species3 + species12	PinacolRearrangement-Oxygen	-72.072329
3323	species4 -> species3 + species19	PinacolRearrangement-Oxygen	-46.831094
3324	species4 -> species3 + species20	PinacolRearrangement-Oxygen	-67.936445
3325	species4 -> species3 + species21	PinacolRearrangement-Oxygen	-42.143340
3326	species4 -> species3 + species22	PinacolRearrangement-Oxygen	-42.143340
3327	species5 -> species3 + species29	PinacolRearrangement-Oxygen	-42.143340
3328	species6 -> species3 + species39	PinacolRearrangement-Oxygen	-42.143340
3329	species6 -> species3 + species40	PinacolRearrangement-Oxygen	-42.143340
3330	species6 -> species3 + species41	PinacolRearrangement-Oxygen	-42.143340
3331	species6 -> species3 + species42	PinacolRearrangement-Oxygen	-42.143340
3332	species7 -> species3 + species46	PinacolRearrangement-Oxygen	88.868537
3333	species7 -> species3 + species47	PinacolRearrangement-Oxygen	161.570013
3334	species7 -> species3 + species48	PinacolRearrangement-Oxygen	90.421010
3335	species7 -> species3 + species49	PinacolRearrangement-Oxygen	90.421010
3336	species7 -> species3 + species50	PinacolRearrangement-Oxygen	90.421010
3337	species7 -> species3 + species51	PinacolRearrangement-Oxygen	90.421010
3338	species7 -> species3 + species52	PinacolRearrangement-Oxygen	93.385750
3339	species7 -> species3 + species53	PinacolRearrangement-Oxygen	85.922582
3340	species8 -> species3 + species57	PinacolRearrangement-Oxygen	-72.535916
3341	species8 -> species3 + species58	PinacolRearrangement-Oxygen	14.020998
3342	species8 -> species3 + species59	PinacolRearrangement-Oxygen	-57.765559
3343	species8 -> species3 + species60	PinacolRearrangement-Oxygen	-57.765559
3344	species8 -> species3 + species61	PinacolRearrangement-Oxygen	-62.264196

3345	species8 -> species3 + species62	PinacolRearrangement-Oxygen	-54.800777
3346	species9 -> species3 + species66	PinacolRearrangement-Oxygen	-58.358014
3347	species9 -> species3 + species67	PinacolRearrangement-Oxygen	-67.569926
3348	species9 -> species3 + species68	PinacolRearrangement-Oxygen	-57.765559
3349	species9 -> species3 + species69	PinacolRearrangement-Oxygen	-57.765559
3350	species9 -> species3 + species62	PinacolRearrangement-Oxygen	-62.264196
3351	species9 -> species3 + species70	PinacolRearrangement-Oxygen	-54.802869
3352	species10 -> species3 + species73	PinacolRearrangement-Oxygen	-67.569926
3353	species10 -> species3 + species74	PinacolRearrangement-Oxygen	19.019778
3354	species10 -> species3 + species69	PinacolRearrangement-Oxygen	-54.800777
3355	species10 -> species3 + species60	PinacolRearrangement-Oxygen	-62.264196
3356	species11 -> species3 + species68	PinacolRearrangement-Oxygen	-54.800777
3357	species11 -> species3 + species59	PinacolRearrangement-Oxygen	-62.264196
3358	species11 -> species3 + species73	PinacolRearrangement-Oxygen	-67.569926
3359	species11 -> species3 + species78	PinacolRearrangement-Oxygen	-58.358014
3360	species12 -> species3 + species67	PinacolRearrangement-Oxygen	-63.645334
3361	species12 -> species3 + species58	PinacolRearrangement-Oxygen	10.482485
3362	species12 -> species3 + species57	PinacolRearrangement-Oxygen	-76.074325
3363	species12 -> species3 + species66	PinacolRearrangement-Oxygen	-54.433422
3364	species14 -> species3 + species91	PinacolRearrangement-Oxygen	-42.143340
3365	species14 -> species3 + species92	PinacolRearrangement-Oxygen	-42.143340
3366	species15 -> species3 + species95	PinacolRearrangement-Oxygen	-46.831094
3367	species15 -> species3 + species96	PinacolRearrangement-Oxygen	-67.938537
3368	species16 -> species3 + species99	PinacolRearrangement-Oxygen	-46.829420
3369	species16 -> species3 + species100	PinacolRearrangement-Oxygen	-67.936445
3370	species17 -> species3 + species101	PinacolRearrangement-Oxygen	-67.451101
3371	species17 -> species3 + species102	PinacolRearrangement-Oxygen	-95.909414
3372	species18 -> species3 + species103	PinacolRearrangement-Oxygen	-46.831094
3373	species18 -> species3 + species104	PinacolRearrangement-Oxygen	-67.938537
3374	species19 -> species3 + species107	PinacolRearrangement-Oxygen	-42.143340
3375	species19 -> species3 + species108	PinacolRearrangement-Oxygen	-42.143340
3376	species20 -> species3 + species111	PinacolRearrangement-Oxygen	-42.143340
3377	species20 -> species3 + species112	PinacolRearrangement-Oxygen	-42.143340
3378	species21 -> species3 + species108	PinacolRearrangement-Oxygen	-46.831094
3379	species21 -> species3 + species111	PinacolRearrangement-Oxygen	-67.936445
3380	species22 -> species3 + species107	PinacolRearrangement-Oxygen	-46.831094
3381	species22 -> species3 + species112	PinacolRearrangement-Oxygen	-67.936445
3382	species23 -> species3 + species120	PinacolRearrangement-Oxygen	-74.056382
3383	species23 -> species3 + species121	PinacolRearrangement-Oxygen	-66.595054
3384	species23 -> species3 + species110	PinacolRearrangement-Oxygen	-65.267890
3385	species23 -> species3 + species114	PinacolRearrangement-Oxygen	-86.906701
3386	species23 -> species3 + species122	PinacolRearrangement-Oxygen	-70.150618
3387	species23 -> species3 + species123	PinacolRearrangement-Oxygen	-79.362112
3388	species24 -> species3 + species126	PinacolRearrangement-Oxygen	-58.725369
3389	species24 -> species3 + species127	PinacolRearrangement-Oxygen	-58.725369
3390	species24 -> species3 + species128	PinacolRearrangement-Oxygen	-58.725369
3391	species24 -> species3 + species129	PinacolRearrangement-Oxygen	-58.725369
3392	species24 -> species3 + species130	PinacolRearrangement-Oxygen	-60.278051
3393	species24 -> species3 + species114	PinacolRearrangement-Oxygen	-67.536873
3394	species24 -> species3 + species109	PinacolRearrangement-Oxygen	-55.760586
3395	species24 -> species3 + species113	PinacolRearrangement-Oxygen	-63.224006
3396	species25 -> species3 + species137	PinacolRearrangement-Oxygen	-42.143340
3397	species25 -> species3 + species138	PinacolRearrangement-Oxygen	-42.143340
3398	species28 -> species3 + species145	PinacolRearrangement-Oxygen	-44.660434
3399	species28 -> species3 + species146	PinacolRearrangement-Oxygen	-46.111027
3400	species30 -> species3 + species150	PinacolRearrangement-Oxygen	-57.765559
3401	species30 -> species3 + species151	PinacolRearrangement-Oxygen	-57.765559
3402	species30 -> species3 + species152	PinacolRearrangement-Oxygen	-48.426871
3403	species30 -> species3 + species153	PinacolRearrangement-Oxygen	-61.303968

3404	species30 -> species3 + species123	PinacolRearrangement-Oxygen	-67.569926
3405	species30 -> species3 + species154	PinacolRearrangement-Oxygen	-58.358014
3406	species31 -> species3 + species162	PinacolRearrangement-Oxygen	-42.143340
3407	species31 -> species3 + species163	PinacolRearrangement-Oxygen	-42.143340
3408	species31 -> species3 + species164	PinacolRearrangement-Oxygen	-42.143340
3409	species31 -> species3 + species165	PinacolRearrangement-Oxygen	-42.143340
3410	species32 -> species3 + species171	PinacolRearrangement-Oxygen	-44.660434
3411	species32 -> species3 + species172	PinacolRearrangement-Oxygen	-46.111027
3412	species32 -> species3 + species173	PinacolRearrangement-Oxygen	-42.143340
3413	species32 -> species3 + species174	PinacolRearrangement-Oxygen	-42.143340
3414	species33 -> species3 + species178	PinacolRearrangement-Oxygen	-42.143340
3415	species33 -> species3 + species179	PinacolRearrangement-Oxygen	-42.143340
3416	species36 -> species3 + species182	PinacolRearrangement-Oxygen	-37.684870
3417	species36 -> species3 + species183	PinacolRearrangement-Oxygen	-42.143340
3418	species43 -> species3 + species188	PinacolRearrangement-Oxygen	-57.767651
3419	species43 -> species3 + species189	PinacolRearrangement-Oxygen	13.381357
3420	species43 -> species3 + species190	PinacolRearrangement-Oxygen	-59.320334
3421	species44 -> species3 + species76	PinacolRearrangement-Oxygen	-61.306060
3422	species44 -> species3 + species192	PinacolRearrangement-Oxygen	-53.843059
3423	species44 -> species3 + species193	PinacolRearrangement-Oxygen	-56.807842
3424	species44 -> species3 + species79	PinacolRearrangement-Oxygen	-56.807842
3425	species46 -> species3 + species194	PinacolRearrangement-Oxygen	-66.610117
3426	species46 -> species3 + species195	PinacolRearrangement-Oxygen	19.979692
3427	species46 -> species3 + species196	PinacolRearrangement-Oxygen	-53.843059
3428	species46 -> species3 + species197	PinacolRearrangement-Oxygen	-61.303968
3429	species47 -> species3 + species199	PinacolRearrangement-Oxygen	-57.398204
3430	species47 -> species3 + species200	PinacolRearrangement-Oxygen	-66.610117
3431	species47 -> species3 + species201	PinacolRearrangement-Oxygen	-53.843059
3432	species47 -> species3 + species202	PinacolRearrangement-Oxygen	-61.303968
3433	species48 -> species3 + species205	PinacolRearrangement-Oxygen	-63.647426
3434	species48 -> species3 + species206	PinacolRearrangement-Oxygen	10.482485
3435	species49 -> species3 + species209	PinacolRearrangement-Oxygen	-54.435514
3436	species49 -> species3 + species210	PinacolRearrangement-Oxygen	-76.074325
3437	species50 -> species3 + species199	PinacolRearrangement-Oxygen	13.750741
3438	species50 -> species3 + species194	PinacolRearrangement-Oxygen	-68.162381
3439	species51 -> species3 + species200	PinacolRearrangement-Oxygen	4.538933
3440	species51 -> species3 + species195	PinacolRearrangement-Oxygen	18.427210
3441	species52 -> species3 + species209	PinacolRearrangement-Oxygen	-57.400296
3442	species52 -> species3 + species205	PinacolRearrangement-Oxygen	-66.612209
3443	species52 -> species3 + species201	PinacolRearrangement-Oxygen	14.341275
3444	species52 -> species3 + species196	PinacolRearrangement-Oxygen	-58.360106
3445	species53 -> species3 + species210	PinacolRearrangement-Oxygen	-71.575688
3446	species53 -> species3 + species206	PinacolRearrangement-Oxygen	14.980917
3447	species53 -> species3 + species202	PinacolRearrangement-Oxygen	14.343304
3448	species53 -> species3 + species197	PinacolRearrangement-Oxygen	-58.358014
3449	species55 -> species3 + species198	PinacolRearrangement-Oxygen	-58.360106
3450	species55 -> species3 + species214	PinacolRearrangement-Oxygen	14.341275
3451	species55 -> species3 + species217	PinacolRearrangement-Oxygen	-53.843059
3452	species55 -> species3 + species211	PinacolRearrangement-Oxygen	-61.306060
3453	species57 -> species3 + species222	PinacolRearrangement-Oxygen	10.480456
3454	species57 -> species3 + species223	PinacolRearrangement-Oxygen	-63.647426
3455	species58 -> species3 + species222	PinacolRearrangement-Oxygen	-76.076417
3456	species58 -> species3 + species225	PinacolRearrangement-Oxygen	-54.435514
3457	species61 -> species3 + species222	PinacolRearrangement-Oxygen	0.208765
3458	species62 -> species3 + species223	PinacolRearrangement-Oxygen	-81.382147
3459	species62 -> species3 + species225	PinacolRearrangement-Oxygen	14.386320
3460	species64 -> species3 + species203	PinacolRearrangement-Oxygen	4.844068
3461	species64 -> species3 + species231	PinacolRearrangement-Oxygen	-55.395323
3462	species65 -> species3 + species233	PinacolRearrangement-Oxygen	-58.358014

3463	species65 -> species3 + species234	PinacolRearrangement-Oxygen	-67.536873
3464	species65 -> species3 + species235	PinacolRearrangement-Oxygen	-56.805750
3465	species65 -> species3 + species236	PinacolRearrangement-Oxygen	-56.805750
3466	species65 -> species3 + species230	PinacolRearrangement-Oxygen	-61.303968
3467	species65 -> species3 + species237	PinacolRearrangement-Oxygen	-53.840967
3468	species66 -> species3 + species225	PinacolRearrangement-Oxygen	10.480456
3469	species66 -> species3 + species238	PinacolRearrangement-Oxygen	-63.647426
3470	species67 -> species3 + species223	PinacolRearrangement-Oxygen	-76.076417
3471	species67 -> species3 + species238	PinacolRearrangement-Oxygen	-54.435514
3472	species70 -> species3 + species238	PinacolRearrangement-Oxygen	-67.202571
3473	species72 -> species3 + species248	PinacolRearrangement-Oxygen	-42.263002
3474	species72 -> species3 + species249	PinacolRearrangement-Oxygen	19.977663
3475	species72 -> species3 + species244	PinacolRearrangement-Oxygen	-53.843059
3476	species72 -> species3 + species228	PinacolRearrangement-Oxygen	-61.306060
3477	species76 -> species3 + species224	PinacolRearrangement-Oxygen	-71.575688
3478	species76 -> species3 + species251	PinacolRearrangement-Oxygen	14.980917
3479	species76 -> species3 + species245	PinacolRearrangement-Oxygen	-53.840967
3480	species76 -> species3 + species229	PinacolRearrangement-Oxygen	-61.303968
3481	species79 -> species3 + species224	PinacolRearrangement-Oxygen	-76.074325
3482	species79 -> species3 + species239	PinacolRearrangement-Oxygen	-54.433422
3483	species80 -> species3 + species240	PinacolRearrangement-Oxygen	-68.610906
3484	species80 -> species3 + species226	PinacolRearrangement-Oxygen	5.483705
3485	species83 -> species3 + species264	PinacolRearrangement-Oxygen	-67.936445
3486	species83 -> species3 + species265	PinacolRearrangement-Oxygen	-46.831094
3487	species84 -> species3 + species273	PinacolRearrangement-Oxygen	-42.143340
3488	species84 -> species3 + species274	PinacolRearrangement-Oxygen	-42.143340
3489	species85 -> species3 + species282	PinacolRearrangement-Oxygen	-42.143340
3490	species85 -> species3 + species147	PinacolRearrangement-Oxygen	-42.143340
3491	species86 -> species3 + species288	PinacolRearrangement-Oxygen	-42.143340
3492	species86 -> species3 + species289	PinacolRearrangement-Oxygen	-42.143340
3493	species93 -> species3 + species293	PinacolRearrangement-Oxygen	-56.805750
3494	species93 -> species3 + species294	PinacolRearrangement-Oxygen	-56.805750
3495	species93 -> species3 + species295	PinacolRearrangement-Oxygen	14.343304
3496	species93 -> species3 + species296	PinacolRearrangement-Oxygen	-58.358014
3497	species93 -> species3 + species297	PinacolRearrangement-Oxygen	-58.358014
3498	species93 -> species3 + species298	PinacolRearrangement-Oxygen	-67.536873
3499	species94 -> species3 + species304	PinacolRearrangement-Oxygen	-63.224006
3500	species94 -> species3 + species305	PinacolRearrangement-Oxygen	-55.762678
3501	species94 -> species3 + species306	PinacolRearrangement-Oxygen	-59.318242
3502	species94 -> species3 + species307	PinacolRearrangement-Oxygen	-68.529736
3503	species97 -> species3 + species310	PinacolRearrangement-Oxygen	-46.831094
3504	species97 -> species3 + species311	PinacolRearrangement-Oxygen	-67.936445
3505	species98 -> species3 + species315	PinacolRearrangement-Oxygen	-3.094486
3506	species98 -> species3 + species316	PinacolRearrangement-Oxygen	-31.550707
3507	species105 -> species3 + species324	PinacolRearrangement-Oxygen	-42.143340
3508	species105 -> species3 + species325	PinacolRearrangement-Oxygen	-42.143340
3509	species106 -> species3 + species328	PinacolRearrangement-Oxygen	-42.143340
3510	species106 -> species3 + species329	PinacolRearrangement-Oxygen	-42.143340
3511	species109 -> species3 + species332	PinacolRearrangement-Oxygen	-57.400296
3512	species109 -> species3 + species333	PinacolRearrangement-Oxygen	-66.612209
3513	species109 -> species3 + species334	PinacolRearrangement-Oxygen	-58.360106
3514	species109 -> species3 + species335	PinacolRearrangement-Oxygen	-67.538965
3515	species110 -> species3 + species337	PinacolRearrangement-Oxygen	-63.224006
3516	species110 -> species3 + species338	PinacolRearrangement-Oxygen	-55.760586
3517	species110 -> species3 + species339	PinacolRearrangement-Oxygen	-59.318242
3518	species110 -> species3 + species340	PinacolRearrangement-Oxygen	-68.529736
3519	species113 -> species3 + species341	PinacolRearrangement-Oxygen	-71.577780
3520	species113 -> species3 + species342	PinacolRearrangement-Oxygen	14.978887
3521	species113 -> species3 + species343	PinacolRearrangement-Oxygen	-58.360106

3522	species113 -> species3 + species344	PinacolRearrangement-Oxygen	-67.538965
3523	species114 -> species3 + species344	PinacolRearrangement-Oxygen	-63.226098
3524	species114 -> species3 + species335	PinacolRearrangement-Oxygen	-55.762678
3525	species114 -> species3 + species346	PinacolRearrangement-Oxygen	-59.320334
3526	species114 -> species3 + species347	PinacolRearrangement-Oxygen	-68.531828
3527	species117 -> species3 + species360	PinacolRearrangement-Oxygen	-42.143340
3528	species117 -> species3 + species361	PinacolRearrangement-Oxygen	-42.143340
3529	species119 -> species3 + species336	PinacolRearrangement-Oxygen	-59.851702
3530	species119 -> species3 + species298	PinacolRearrangement-Oxygen	-81.490513
3531	species119 -> species3 + species368	PinacolRearrangement-Oxygen	8.334561
3532	species119 -> species3 + species67	PinacolRearrangement-Oxygen	-73.578569
3533	species120 -> species3 + species337	PinacolRearrangement-Oxygen	-54.435514
3534	species120 -> species3 + species344	PinacolRearrangement-Oxygen	-76.076417
3535	species121 -> species3 + species338	PinacolRearrangement-Oxygen	-54.433422
3536	species121 -> species3 + species335	PinacolRearrangement-Oxygen	-76.074325
3537	species122 -> species3 + species339	PinacolRearrangement-Oxygen	-54.435514
3538	species122 -> species3 + species346	PinacolRearrangement-Oxygen	-76.076417
3539	species123 -> species3 + species340	PinacolRearrangement-Oxygen	-54.435514
3540	species123 -> species3 + species347	PinacolRearrangement-Oxygen	-76.076417
3541	species124 -> species3 + species381	PinacolRearrangement-Oxygen	-42.143340
3542	species124 -> species3 + species382	PinacolRearrangement-Oxygen	-42.143340
3543	species125 -> species3 + species389	PinacolRearrangement-Oxygen	-42.143340
3544	species125 -> species3 + species390	PinacolRearrangement-Oxygen	-42.143340
3545	species125 -> species3 + species391	PinacolRearrangement-Oxygen	-42.143340
3546	species125 -> species3 + species392	PinacolRearrangement-Oxygen	-42.143340
3547	species126 -> species3 + species332	PinacolRearrangement-Oxygen	-54.435514
3548	species126 -> species3 + species341	PinacolRearrangement-Oxygen	-76.076417
3549	species127 -> species3 + species333	PinacolRearrangement-Oxygen	-63.647426
3550	species127 -> species3 + species342	PinacolRearrangement-Oxygen	10.480456
3551	species128 -> species3 + species396	PinacolRearrangement-Oxygen	-68.164473
3552	species128 -> species3 + species346	PinacolRearrangement-Oxygen	-68.131419
3553	species129 -> species3 + species398	PinacolRearrangement-Oxygen	18.425181
3554	species129 -> species3 + species347	PinacolRearrangement-Oxygen	-77.343332
3555	species130 -> species3 + species398	PinacolRearrangement-Oxygen	19.977663
3556	species130 -> species3 + species396	PinacolRearrangement-Oxygen	-66.612209
3557	species130 -> species3 + species334	PinacolRearrangement-Oxygen	-53.843059
3558	species130 -> species3 + species343	PinacolRearrangement-Oxygen	-61.306060
3559	species131 -> species3 + species402	PinacolRearrangement-Oxygen	-42.143340
3560	species136 -> species3 + species407	PinacolRearrangement-Oxygen	-46.111027
3561	species136 -> species3 + species408	PinacolRearrangement-Oxygen	-44.660434
3562	species139 -> species3 + species412	PinacolRearrangement-Oxygen	-60.278051
3563	species139 -> species3 + species413	PinacolRearrangement-Oxygen	12.423472
3564	species139 -> species3 + species307	PinacolRearrangement-Oxygen	-68.529736
3565	species139 -> species3 + species414	PinacolRearrangement-Oxygen	-59.318242
3566	species144 -> species3 + species418	PinacolRearrangement-Oxygen	-48.628540
3567	species148 -> species3 + species425	PinacolRearrangement-Oxygen	-42.143340
3568	species148 -> species3 + species361	PinacolRearrangement-Oxygen	-42.143340
3569	species149 -> species3 + species395	PinacolRearrangement-Oxygen	-61.837428
3570	species149 -> species3 + species374	PinacolRearrangement-Oxygen	-72.499934
3571	species149 -> species3 + species427	PinacolRearrangement-Oxygen	-57.767651
3572	species149 -> species3 + species428	PinacolRearrangement-Oxygen	-57.767651
3573	species149 -> species3 + species429	PinacolRearrangement-Oxygen	-62.266288
3574	species149 -> species3 + species430	PinacolRearrangement-Oxygen	-54.802869
3575	species152 -> species3 + species340	PinacolRearrangement-Oxygen	-73.578569
3576	species152 -> species3 + species438	PinacolRearrangement-Oxygen	-73.578569
3577	species153 -> species3 + species347	PinacolRearrangement-Oxygen	-82.341957
3578	species153 -> species3 + species439	PinacolRearrangement-Oxygen	13.426402
3579	species154 -> species3 + species439	PinacolRearrangement-Oxygen	10.480456
3580	species154 -> species3 + species438	PinacolRearrangement-Oxygen	-63.647426

3581	species155 -> species3 + species444	PinacolRearrangement-Oxygen	-42.143340
3582	species155 -> species3 + species185	PinacolRearrangement-Oxygen	-42.143340
3583	species156 -> species3 + species448	PinacolRearrangement-Oxygen	-42.143340
3584	species156 -> species3 + species449	PinacolRearrangement-Oxygen	-42.143340
3585	species158 -> species3 + species452	PinacolRearrangement-Oxygen	-37.684870
3586	species158 -> species3 + species453	PinacolRearrangement-Oxygen	-42.143340
3587	species167 -> species3 + species458	PinacolRearrangement-Oxygen	-40.202299
3588	species167 -> species3 + species459	PinacolRearrangement-Oxygen	-46.111027
3589	species187 -> species3 + species207	PinacolRearrangement-Oxygen	-56.807842
3590	species187 -> species3 + species466	PinacolRearrangement-Oxygen	-56.807842
3591	species187 -> species3 + species254	PinacolRearrangement-Oxygen	14.341275
3592	species187 -> species3 + species467	PinacolRearrangement-Oxygen	-58.360106
3593	species187 -> species3 + species468	PinacolRearrangement-Oxygen	-53.843059
3594	species187 -> species3 + species215	PinacolRearrangement-Oxygen	-61.306060
3595	species189 -> species3 + species470	PinacolRearrangement-Oxygen	13.168316
3596	species189 -> species3 + species471	PinacolRearrangement-Oxygen	-68.744794
3597	species190 -> species3 + species473	PinacolRearrangement-Oxygen	17.844785
3598	species190 -> species3 + species471	PinacolRearrangement-Oxygen	3.956508
3599	species191 -> species3 + species472	PinacolRearrangement-Oxygen	12.788793
3600	species192 -> species3 + species239	PinacolRearrangement-Oxygen	-57.398204
3601	species192 -> species3 + species474	PinacolRearrangement-Oxygen	-66.610117
3602	species192 -> species3 + species475	PinacolRearrangement-Oxygen	-53.843059
3603	species192 -> species3 + species245	PinacolRearrangement-Oxygen	-61.303968
3604	species193 -> species3 + species474	PinacolRearrangement-Oxygen	-63.645334
3605	species193 -> species3 + species251	PinacolRearrangement-Oxygen	10.482485
3606	species204 -> species3 + species480	PinacolRearrangement-Oxygen	-64.225655
3607	species204 -> species3 + species488	PinacolRearrangement-Oxygen	-72.011242
3608	species213 -> species3 + species481	PinacolRearrangement-Oxygen	4.536904
3609	species213 -> species3 + species477	PinacolRearrangement-Oxygen	18.425181
3610	species215 -> species3 + species482	PinacolRearrangement-Oxygen	-0.426810
3611	species215 -> species3 + species478	PinacolRearrangement-Oxygen	13.428431
3612	species216 -> species3 + species493	PinacolRearrangement-Oxygen	-58.358014
3613	species216 -> species3 + species490	PinacolRearrangement-Oxygen	-67.536873
3614	species216 -> species3 + species483	PinacolRearrangement-Oxygen	14.343304
3615	species216 -> species3 + species479	PinacolRearrangement-Oxygen	-58.358014
3616	species218 -> species3 + species71	PinacolRearrangement-Oxygen	22.236617
3617	species220 -> species3 + species80	PinacolRearrangement-Oxygen	-62.266288
3618	species220 -> species3 + species369	PinacolRearrangement-Oxygen	-54.802869
3619	species220 -> species3 + species75	PinacolRearrangement-Oxygen	-57.767651
3620	species221 -> species3 + species63	PinacolRearrangement-Oxygen	38.997717
3621	species221 -> species3 + species436	PinacolRearrangement-Oxygen	51.426674
3622	species230 -> species3 + species497	PinacolRearrangement-Oxygen	-82.309322
3623	species230 -> species3 + species498	PinacolRearrangement-Oxygen	13.426402
3624	species232 -> species3 + species500	PinacolRearrangement-Oxygen	-34.110102
3625	species232 -> species3 + species348	PinacolRearrangement-Oxygen	-65.042790
3626	species233 -> species3 + species498	PinacolRearrangement-Oxygen	10.480456
3627	species233 -> species3 + species501	PinacolRearrangement-Oxygen	-63.647426
3628	species234 -> species3 + species497	PinacolRearrangement-Oxygen	-76.076417
3629	species234 -> species3 + species502	PinacolRearrangement-Oxygen	-54.435514
3630	species237 -> species3 + species502	PinacolRearrangement-Oxygen	-68.131419
3631	species237 -> species3 + species501	PinacolRearrangement-Oxygen	-68.164473
3632	species252 -> species3 + species518	PinacolRearrangement-Oxygen	-54.433422
3633	species252 -> species3 + species375	PinacolRearrangement-Oxygen	-76.074325
3634	species253 -> species3 + species508	PinacolRearrangement-Oxygen	-59.849610
3635	species253 -> species3 + species234	PinacolRearrangement-Oxygen	-81.490513
3636	species254 -> species3 + species482	PinacolRearrangement-Oxygen	-76.074325
3637	species254 -> species3 + species509	PinacolRearrangement-Oxygen	-54.435514
3638	species255 -> species3 + species399	PinacolRearrangement-Oxygen	-58.358014
3639	species255 -> species3 + species375	PinacolRearrangement-Oxygen	-67.536873

3640	species255 -> species3 + species510	PinacolRearrangement-Oxygen	-53.840967
3641	species255 -> species3 + species393	PinacolRearrangement-Oxygen	-61.303968
3642	species258 -> species3 + species521	PinacolRearrangement-Oxygen	-43.825308
3643	species258 -> species3 + species522	PinacolRearrangement-Oxygen	-22.718200
3644	species263 -> species3 + species534	PinacolRearrangement-Oxygen	-46.829420
3645	species263 -> species3 + species535	PinacolRearrangement-Oxygen	-67.936445
3646	species266 -> species3 + species546	PinacolRearrangement-Oxygen	-62.816484
3647	species266 -> species3 + species547	PinacolRearrangement-Oxygen	-72.028397
3648	species266 -> species3 + species541	PinacolRearrangement-Oxygen	-59.259247
3649	species266 -> species3 + species538	PinacolRearrangement-Oxygen	-66.722248
3650	species267 -> species3 + species537	PinacolRearrangement-Oxygen	-86.908793
3651	species267 -> species3 + species540	PinacolRearrangement-Oxygen	-59.851702
3652	species270 -> species3 + species553	PinacolRearrangement-Oxygen	-42.143340
3653	species270 -> species3 + species554	PinacolRearrangement-Oxygen	-42.143340
3654	species271 -> species3 + species557	PinacolRearrangement-Oxygen	-70.694538
3655	species271 -> species3 + species558	PinacolRearrangement-Oxygen	-69.243945
3656	species275 -> species3 + species560	PinacolRearrangement-Oxygen	-67.538965
3657	species275 -> species3 + species561	PinacolRearrangement-Oxygen	-58.360106
3658	species275 -> species3 + species562	PinacolRearrangement-Oxygen	-56.807842
3659	species276 -> species3 + species567	PinacolRearrangement-Oxygen	-42.143340
3660	species276 -> species3 + species409	PinacolRearrangement-Oxygen	-42.143340
3661	species277 -> species3 + species571	PinacolRearrangement-Oxygen	-46.111027
3662	species277 -> species3 + species419	PinacolRearrangement-Oxygen	-44.660434
3663	species283 -> species3 + species433	PinacolRearrangement-Oxygen	-63.224006
3664	species283 -> species3 + species577	PinacolRearrangement-Oxygen	-55.760586
3665	species283 -> species3 + species440	PinacolRearrangement-Oxygen	-59.318242
3666	species283 -> species3 + species578	PinacolRearrangement-Oxygen	-68.529736
3667	species284 -> species3 + species582	PinacolRearrangement-Oxygen	-34.055417
3668	species284 -> species3 + species583	PinacolRearrangement-Oxygen	-32.605033
3669	species292 -> species3 + species593	PinacolRearrangement-Oxygen	-42.143340
3670	species292 -> species3 + species594	PinacolRearrangement-Oxygen	-42.143340
3671	species295 -> species3 + species600	PinacolRearrangement-Oxygen	-68.164473
3672	species295 -> species3 + species601	PinacolRearrangement-Oxygen	-68.131419
3673	species296 -> species3 + species602	PinacolRearrangement-Oxygen	18.425181
3674	species296 -> species3 + species223	PinacolRearrangement-Oxygen	-77.343332
3675	species297 -> species3 + species602	PinacolRearrangement-Oxygen	18.425181
3676	species297 -> species3 + species600	PinacolRearrangement-Oxygen	4.536904
3677	species298 -> species3 + species601	PinacolRearrangement-Oxygen	13.748708
3678	species298 -> species3 + species223	PinacolRearrangement-Oxygen	-68.164473
3679	species299 -> species3 + species603	PinacolRearrangement-Oxygen	12.790823
3680	species299 -> species3 + species240	PinacolRearrangement-Oxygen	-69.089555
3681	species301 -> species3 + species612	PinacolRearrangement-Oxygen	-42.143340
3682	species301 -> species3 + species613	PinacolRearrangement-Oxygen	-42.143340
3683	species302 -> species3 + species615	PinacolRearrangement-Oxygen	13.748708
3684	species302 -> species3 + species205	PinacolRearrangement-Oxygen	-68.164473
3685	species303 -> species3 + species242	PinacolRearrangement-Oxygen	-58.358014
3686	species303 -> species3 + species243	PinacolRearrangement-Oxygen	14.343304
3687	species303 -> species3 + species617	PinacolRearrangement-Oxygen	-53.840967
3688	species303 -> species3 + species618	PinacolRearrangement-Oxygen	-61.303968
3689	species312 -> species3 + species625	PinacolRearrangement-Oxygen	-67.451101
3690	species312 -> species3 + species628	PinacolRearrangement-Oxygen	-95.909414
3691	species313 -> species3 + species626	PinacolRearrangement-Oxygen	-65.267890
3692	species313 -> species3 + species629	PinacolRearrangement-Oxygen	-86.908793
3693	species314 -> species3 + species635	PinacolRearrangement-Oxygen	-62.224030
3694	species314 -> species3 + species636	PinacolRearrangement-Oxygen	-62.224030
3695	species314 -> species3 + species637	PinacolRearrangement-Oxygen	-72.028397
3696	species314 -> species3 + species638	PinacolRearrangement-Oxygen	-62.816484
3697	species314 -> species3 + species627	PinacolRearrangement-Oxygen	-58.299438
3698	species314 -> species3 + species630	PinacolRearrangement-Oxygen	-65.762438

3699	species317 -> species3 + species641	PinacolRearrangement-Oxygen	-46.831094
3700	species317 -> species3 + species642	PinacolRearrangement-Oxygen	-67.936445
3701	species326 -> species3 + species647	PinacolRearrangement-Oxygen	-74.058474
3702	species326 -> species3 + species648	PinacolRearrangement-Oxygen	-66.595054
3703	species326 -> species3 + species649	PinacolRearrangement-Oxygen	-70.152710
3704	species326 -> species3 + species650	PinacolRearrangement-Oxygen	-79.364204
3705	species327 -> species3 + species652	PinacolRearrangement-Oxygen	-62.816484
3706	species327 -> species3 + species547	PinacolRearrangement-Oxygen	-72.028397
3707	species327 -> species3 + species653	PinacolRearrangement-Oxygen	-63.776294
3708	species327 -> species3 + species629	PinacolRearrangement-Oxygen	-71.995343
3709	species330 -> species3 + species655	PinacolRearrangement-Oxygen	-63.226098
3710	species330 -> species3 + species656	PinacolRearrangement-Oxygen	-55.762678
3711	species330 -> species3 + species657	PinacolRearrangement-Oxygen	-59.320334
3712	species330 -> species3 + species658	PinacolRearrangement-Oxygen	-68.531828
3713	species331 -> species3 + species659	PinacolRearrangement-Oxygen	-59.320334
3714	species331 -> species3 + species660	PinacolRearrangement-Oxygen	-68.498774
3715	species336 -> species3 + species668	PinacolRearrangement-Oxygen	13.750741
3716	species336 -> species3 + species238	PinacolRearrangement-Oxygen	-68.162381
3717	species359 -> species3 + species694	PinacolRearrangement-Oxygen	-42.143340
3718	species359 -> species3 + species695	PinacolRearrangement-Oxygen	-42.143340
3719	species362 -> species3 + species661	PinacolRearrangement-Oxygen	-55.395323
3720	species362 -> species3 + species560	PinacolRearrangement-Oxygen	-77.036226
3721	species362 -> species3 + species537	PinacolRearrangement-Oxygen	-68.131419
3722	species362 -> species3 + species637	PinacolRearrangement-Oxygen	-69.124701
3723	species368 -> species3 + species668	PinacolRearrangement-Oxygen	-54.435514
3724	species368 -> species3 + species601	PinacolRearrangement-Oxygen	-76.076417
3725	species369 -> species3 + species669	PinacolRearrangement-Oxygen	-54.435514
3726	species369 -> species3 + species240	PinacolRearrangement-Oxygen	-76.074325
3727	species370 -> species3 + species666	PinacolRearrangement-Oxygen	-55.395323
3728	species370 -> species3 + species676	PinacolRearrangement-Oxygen	17.028742
3729	species371 -> species3 + species670	PinacolRearrangement-Oxygen	-54.435514
3730	species371 -> species3 + species660	PinacolRearrangement-Oxygen	-76.076417
3731	species372 -> species3 + species671	PinacolRearrangement-Oxygen	-54.435514
3732	species372 -> species3 + species667	PinacolRearrangement-Oxygen	-76.076417
3733	species373 -> species3 + species672	PinacolRearrangement-Oxygen	-57.912836
3734	species373 -> species3 + species666	PinacolRearrangement-Oxygen	-82.487560
3735	species374 -> species3 + species662	PinacolRearrangement-Oxygen	-54.435514
3736	species374 -> species3 + species673	PinacolRearrangement-Oxygen	-76.074325
3737	species380 -> species3 + species712	PinacolRearrangement-Oxygen	-46.111027
3738	species380 -> species3 + species713	PinacolRearrangement-Oxygen	-44.660434
3739	species383 -> species3 + species717	PinacolRearrangement-Oxygen	-42.143340
3740	species383 -> species3 + species718	PinacolRearrangement-Oxygen	-37.684870
3741	species387 -> species3 + species721	PinacolRearrangement-Oxygen	-42.143340
3742	species387 -> species3 + species722	PinacolRearrangement-Oxygen	-42.143340
3743	species394 -> species3 + species663	PinacolRearrangement-Oxygen	-63.647426
3744	species394 -> species3 + species674	PinacolRearrangement-Oxygen	10.482485
3745	species395 -> species3 + species664	PinacolRearrangement-Oxygen	-63.647426
3746	species395 -> species3 + species675	PinacolRearrangement-Oxygen	10.482485
3747	species397 -> species3 + species725	PinacolRearrangement-Oxygen	18.427210
3748	species397 -> species3 + species673	PinacolRearrangement-Oxygen	-77.341240
3749	species410 -> species3 + species732	PinacolRearrangement-Oxygen	-42.143340
3750	species410 -> species3 + species613	PinacolRearrangement-Oxygen	-42.143340
3751	species411 -> species3 + species599	PinacolRearrangement-Oxygen	-60.877618
3752	species411 -> species3 + species596	PinacolRearrangement-Oxygen	-71.539706
3753	species411 -> species3 + species733	PinacolRearrangement-Oxygen	14.341275
3754	species411 -> species3 + species734	PinacolRearrangement-Oxygen	-58.360106
3755	species424 -> species3 + species748	PinacolRearrangement-Oxygen	-46.111027
3756	species424 -> species3 + species695	PinacolRearrangement-Oxygen	-44.660434
3757	species426 -> species3 + species650	PinacolRearrangement-Oxygen	-74.540889

3758	species429 -> species3 + species673	PinacolRearrangement-Oxygen	-86.307970
3759	species429 -> species3 + species675	PinacolRearrangement-Oxygen	10.911023
3760	species430 -> species3 + species662	PinacolRearrangement-Oxygen	-72.132578
3761	species430 -> species3 + species664	PinacolRearrangement-Oxygen	-70.681986
3762	species437 -> species3 + species658	PinacolRearrangement-Oxygen	-68.164473
3763	species437 -> species3 + species758	PinacolRearrangement-Oxygen	-68.131419
3764	species441 -> species3 + species462	PinacolRearrangement-Oxygen	-42.143340
3765	species441 -> species3 + species763	PinacolRearrangement-Oxygen	-37.684870
3766	species465 -> species3 + species492	PinacolRearrangement-Oxygen	13.381357
3767	species465 -> species3 + species766	PinacolRearrangement-Oxygen	-59.320334
3768	species467 -> species3 + species768	PinacolRearrangement-Oxygen	-63.647426
3769	species467 -> species3 + species478	PinacolRearrangement-Oxygen	10.482485
3770	species468 -> species3 + species509	PinacolRearrangement-Oxygen	13.748708
3771	species468 -> species3 + species768	PinacolRearrangement-Oxygen	-68.164473
3772	species476 -> species3 + species770	PinacolRearrangement-Oxygen	-63.647426
3773	species476 -> species3 + species516	PinacolRearrangement-Oxygen	10.480456
3774	species487 -> species3 + species736	PinacolRearrangement-Oxygen	-63.645334
3775	species487 -> species3 + species775	PinacolRearrangement-Oxygen	10.482485
3776	species491 -> species3 + species780	PinacolRearrangement-Oxygen	-54.435514
3777	species491 -> species3 + species490	PinacolRearrangement-Oxygen	-76.074325
3778	species496 -> species3 + species115	PinacolRearrangement-Oxygen	-42.143340
3779	species507 -> species3 + species785	PinacolRearrangement-Oxygen	-63.977544
3780	species508 -> species3 + species788	PinacolRearrangement-Oxygen	-54.435514
3781	species508 -> species3 + species502	PinacolRearrangement-Oxygen	-76.076417
3782	species517 -> species3 + species790	PinacolRearrangement-Oxygen	-57.912836
3783	species517 -> species3 + species707	PinacolRearrangement-Oxygen	-56.687761
3784	species528 -> species3 + species812	PinacolRearrangement-Oxygen	-42.143340
3785	species528 -> species3 + species813	PinacolRearrangement-Oxygen	-42.143340
3786	species532 -> species3 + species820	PinacolRearrangement-Oxygen	-82.450322
3787	species532 -> species3 + species821	PinacolRearrangement-Oxygen	-60.809419
3788	species533 -> species3 + species825	PinacolRearrangement-Oxygen	13.748708
3789	species533 -> species3 + species333	PinacolRearrangement-Oxygen	-68.164473
3790	species537 -> species3 + species830	PinacolRearrangement-Oxygen	-77.034134
3791	species537 -> species3 + species831	PinacolRearrangement-Oxygen	-55.395323
3792	species540 -> species3 + species831	PinacolRearrangement-Oxygen	-82.452414
3793	species540 -> species3 + species837	PinacolRearrangement-Oxygen	-60.811511
3794	species543 -> species3 + species849	PinacolRearrangement-Oxygen	-42.143340
3795	species543 -> species3 + species850	PinacolRearrangement-Oxygen	-42.143340
3796	species544 -> species3 + species851	PinacolRearrangement-Oxygen	-66.610117
3797	species544 -> species3 + species852	PinacolRearrangement-Oxygen	-57.398204
3798	species544 -> species3 + species840	PinacolRearrangement-Oxygen	-53.843059
3799	species544 -> species3 + species833	PinacolRearrangement-Oxygen	-61.303968
3800	species545 -> species3 + species853	PinacolRearrangement-Oxygen	-59.309037
3801	species545 -> species3 + species854	PinacolRearrangement-Oxygen	-60.877618
3802	species545 -> species3 + species841	PinacolRearrangement-Oxygen	-53.843059
3803	species545 -> species3 + species834	PinacolRearrangement-Oxygen	-61.303968
3804	species555 -> species3 + species859	PinacolRearrangement-Oxygen	-61.835336
3805	species555 -> species3 + species855	PinacolRearrangement-Oxygen	-72.497842
3806	species555 -> species3 + species860	PinacolRearrangement-Oxygen	-59.318242
3807	species555 -> species3 + species861	PinacolRearrangement-Oxygen	-68.497101
3808	species559 -> species3 + species864	PinacolRearrangement-Oxygen	-42.143340
3809	species560 -> species3 + species830	PinacolRearrangement-Oxygen	-68.129746
3810	species560 -> species3 + species865	PinacolRearrangement-Oxygen	-68.162381
3811	species561 -> species3 + species865	PinacolRearrangement-Oxygen	-77.341240
3812	species561 -> species3 + species866	PinacolRearrangement-Oxygen	18.427210
3813	species574 -> species3 + species749	PinacolRearrangement-Oxygen	-42.143340
3814	species574 -> species3 + species877	PinacolRearrangement-Oxygen	-42.143340
3815	species575 -> species3 + species759	PinacolRearrangement-Oxygen	13.750741
3816	species575 -> species3 + species474	PinacolRearrangement-Oxygen	-68.162381

3817	species576 -> species3 + species504	PinacolRearrangement-Oxygen	-60.877618
3818	species576 -> species3 + species505	PinacolRearrangement-Oxygen	-71.539706
3819	species576 -> species3 + species879	PinacolRearrangement-Oxygen	-53.843059
3820	species576 -> species3 + species753	PinacolRearrangement-Oxygen	-61.306060
3821	species587 -> species3 + species887	PinacolRearrangement-Oxygen	14.341275
3822	species587 -> species3 + species888	PinacolRearrangement-Oxygen	-58.360106
3823	species587 -> species3 + species889	PinacolRearrangement-Oxygen	-66.612209
3824	species587 -> species3 + species890	PinacolRearrangement-Oxygen	-57.400296
3825	species595 -> species3 + species820	PinacolRearrangement-Oxygen	-68.131419
3826	species595 -> species3 + species889	PinacolRearrangement-Oxygen	-68.164473
3827	species614 -> species3 + species480	PinacolRearrangement-Oxygen	12.210427
3828	species614 -> species3 + species484	PinacolRearrangement-Oxygen	12.210427
3829	species616 -> species3 + species435	PinacolRearrangement-Oxygen	-60.875526
3830	species616 -> species3 + species431	PinacolRearrangement-Oxygen	-72.988206
3831	species616 -> species3 + species904	PinacolRearrangement-Oxygen	-53.840967
3832	species616 -> species3 + species905	PinacolRearrangement-Oxygen	-61.303968
3833	species627 -> species3 + species919	PinacolRearrangement-Oxygen	-68.164473
3834	species627 -> species3 + species920	PinacolRearrangement-Oxygen	-68.164473
3835	species630 -> species3 + species865	PinacolRearrangement-Oxygen	-82.340283
3836	species630 -> species3 + species923	PinacolRearrangement-Oxygen	13.428431
3837	species632 -> species3 + species916	PinacolRearrangement-Oxygen	-54.435514
3838	species632 -> species3 + species861	PinacolRearrangement-Oxygen	-76.074325
3839	species633 -> species3 + species917	PinacolRearrangement-Oxygen	-57.912836
3840	species633 -> species3 + species921	PinacolRearrangement-Oxygen	-82.487560
3841	species634 -> species3 + species918	PinacolRearrangement-Oxygen	-54.435514
3842	species634 -> species3 + species922	PinacolRearrangement-Oxygen	-76.076417
3843	species637 -> species3 + species919	PinacolRearrangement-Oxygen	-54.435514
3844	species637 -> species3 + species865	PinacolRearrangement-Oxygen	-76.074325
3845	species638 -> species3 + species920	PinacolRearrangement-Oxygen	-63.647426
3846	species638 -> species3 + species923	PinacolRearrangement-Oxygen	10.482485
3847	species643 -> species3 + species933	PinacolRearrangement-Oxygen	-59.851702
3848	species643 -> species3 + species935	PinacolRearrangement-Oxygen	-81.490513
3849	species644 -> species3 + species938	PinacolRearrangement-Oxygen	-58.358014
3850	species644 -> species3 + species939	PinacolRearrangement-Oxygen	-67.569926
3851	species644 -> species3 + species932	PinacolRearrangement-Oxygen	-54.802869
3852	species644 -> species3 + species934	PinacolRearrangement-Oxygen	-62.264196
3853	species646 -> species3 + species943	PinacolRearrangement-Oxygen	8.334561
3854	species646 -> species3 + species438	PinacolRearrangement-Oxygen	-73.578569
3855	species651 -> species3 + species849	PinacolRearrangement-Oxygen	-42.143340
3856	species651 -> species3 + species952	PinacolRearrangement-Oxygen	-42.143340
3857	species654 -> species3 + species954	PinacolRearrangement-Oxygen	13.748708
3858	species654 -> species3 + species501	PinacolRearrangement-Oxygen	-68.164473
3859	species661 -> species3 + species831	PinacolRearrangement-Oxygen	-68.131419
3860	species661 -> species3 + species919	PinacolRearrangement-Oxygen	-68.164473
3861	species682 -> species3 + species785	PinacolRearrangement-Oxygen	-70.962314
3862	species682 -> species3 + species969	PinacolRearrangement-Oxygen	-36.426322
3863	species704 -> species3 + species838	PinacolRearrangement-Oxygen	-57.912836
3864	species704 -> species3 + species832	PinacolRearrangement-Oxygen	-85.002981
3865	species705 -> species3 + species962	PinacolRearrangement-Oxygen	-54.435514
3866	species705 -> species3 + species960	PinacolRearrangement-Oxygen	-76.074325
3867	species706 -> species3 + species958	PinacolRearrangement-Oxygen	-57.912836
3868	species706 -> species3 + species955	PinacolRearrangement-Oxygen	-80.986759
3869	species745 -> species3 + species758	PinacolRearrangement-Oxygen	-81.492605
3870	species745 -> species3 + species991	PinacolRearrangement-Oxygen	-59.851702
3871	species750 -> species3 + species851	PinacolRearrangement-Oxygen	-70.679894
3872	species750 -> species3 + species947	PinacolRearrangement-Oxygen	-72.130486
3873	species754 -> species3 + species959	PinacolRearrangement-Oxygen	-73.090296
3874	species754 -> species3 + species960	PinacolRearrangement-Oxygen	-71.607068
3875	species777 -> species3 + species771	PinacolRearrangement-Oxygen	-55.393650

3876	species777 -> species3 + species513	PinacolRearrangement-Oxygen	4.846097
3877	species807 -> species3 + species1019	PinacolRearrangement-Oxygen	-67.569926
3878	species807 -> species3 + species1020	PinacolRearrangement-Oxygen	-58.358014
3879	species807 -> species3 + species1021	PinacolRearrangement-Oxygen	-68.497101
3880	species807 -> species3 + species1022	PinacolRearrangement-Oxygen	-59.318242
3881	species823 -> species3 + species664	PinacolRearrangement-Oxygen	-68.164473
3882	species823 -> species3 + species1036	PinacolRearrangement-Oxygen	13.748708
3883	species824 -> species3 + species663	PinacolRearrangement-Oxygen	-73.044272
3884	species824 -> species3 + species1037	PinacolRearrangement-Oxygen	10.271385
3885	species828 -> species3 + species1040	PinacolRearrangement-Oxygen	-82.450322
3886	species828 -> species3 + species1041	PinacolRearrangement-Oxygen	-60.811511
3887	species829 -> species3 + species1040	PinacolRearrangement-Oxygen	-68.129746
3888	species829 -> species3 + species1019	PinacolRearrangement-Oxygen	-68.162381
3889	species835 -> species3 + species1045	PinacolRearrangement-Oxygen	-72.791977
3890	species835 -> species3 + species1048	PinacolRearrangement-Oxygen	-5.825048
3891	species878 -> species3 + species770	PinacolRearrangement-Oxygen	-73.092388
3892	species878 -> species3 + species772	PinacolRearrangement-Oxygen	10.271385
3893	species894 -> species3 + species1074	PinacolRearrangement-Oxygen	13.748708
3894	species894 -> species3 + species920	PinacolRearrangement-Oxygen	-68.164473
3895	species897 -> species3 + species665	PinacolRearrangement-Oxygen	12.788793
3896	species897 -> species3 + species667	PinacolRearrangement-Oxygen	-69.091647
3897	species903 -> species3 + species736	PinacolRearrangement-Oxygen	-74.540470
3898	species903 -> species3 + species738	PinacolRearrangement-Oxygen	10.273415
3899	species912 -> species3 + species1081	PinacolRearrangement-Oxygen	-68.162381
3900	species912 -> species3 + species939	PinacolRearrangement-Oxygen	-68.162381
3901	species914 -> species3 + species1082	PinacolRearrangement-Oxygen	-63.487179
3902	species914 -> species3 + species1045	PinacolRearrangement-Oxygen	-63.887588
3903	species926 -> species3 + species1086	PinacolRearrangement-Oxygen	-55.395323
3904	species926 -> species3 + species1021	PinacolRearrangement-Oxygen	-77.034134
3905	species927 -> species3 + species1051	PinacolRearrangement-Oxygen	-57.910744
3906	species927 -> species3 + species1047	PinacolRearrangement-Oxygen	-81.034875
3907	species937 -> species3 + species1095	PinacolRearrangement-Oxygen	-54.435514
3908	species937 -> species3 + species1097	PinacolRearrangement-Oxygen	-76.076417
3909	species944 -> species3 + species1081	PinacolRearrangement-Oxygen	-73.578569
3910	species944 -> species3 + species935	PinacolRearrangement-Oxygen	-73.545515
3911	species992 -> species3 + species1056	PinacolRearrangement-Oxygen	-75.609901
3912	species998 -> species3 + species881	PinacolRearrangement-Oxygen	-57.910744
3913	species998 -> species3 + species757	PinacolRearrangement-Oxygen	-70.302915
3914	species1013 -> species3 + species1127	PinacolRearrangement-Oxygen	-67.664066
3915	species1013 -> species3 + species1128	PinacolRearrangement-Oxygen	-68.164473
3916	species1016 -> species3 + species1129	PinacolRearrangement-Oxygen	-70.681986
3917	species1016 -> species3 + species1100	PinacolRearrangement-Oxygen	-72.132578
3918	species1039 -> species3 + species1144	PinacolRearrangement-Oxygen	-54.433422
3919	species1039 -> species3 + species1135	PinacolRearrangement-Oxygen	-76.074325
3920	species1043 -> species3 + species1129	PinacolRearrangement-Oxygen	-68.164473
3921	species1043 -> species3 + species1097	PinacolRearrangement-Oxygen	-68.131419
3922	species1044 -> species3 + species1134	PinacolRearrangement-Oxygen	-73.044272
3923	species1044 -> species3 + species1135	PinacolRearrangement-Oxygen	-71.608742
3924	species1077 -> species3 + species953	PinacolRearrangement-Oxygen	-74.542562
3925	species1077 -> species3 + species922	PinacolRearrangement-Oxygen	-71.608742
3926	species1088 -> species3 + species1096	PinacolRearrangement-Oxygen	-82.485468
3927	species1088 -> species3 + species1093	PinacolRearrangement-Oxygen	-57.910744
3928	species1099 -> species3 + species1160	PinacolRearrangement-Oxygen	-54.435514
3929	species1099 -> species3 + species1127	PinacolRearrangement-Oxygen	-75.608646
3930	species1121 -> species3 + species1128	PinacolRearrangement-Oxygen	-68.164473
3931	species1 -> species2 + species7	PrimaryAlcoholDehydrogenation-Oxygen	-140.434286
3932	species4 -> species2 + species14	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3933	species5 -> species2 + species25	PrimaryAlcoholDehydrogenation-Oxygen	15.112231
3934	species6 -> species2 + species31	PrimaryAlcoholDehydrogenation-Oxygen	15.114261

3935	species7 -> species2 + species43	PrimaryAlcoholDehydrogenation-Oxygen	170.247588
3936	species8 -> species2 + species53	PrimaryAlcoholDehydrogenation-Oxygen	21.098979
3937	species9 -> species2 + species52	PrimaryAlcoholDehydrogenation-Oxygen	21.098979
3938	species10 -> species2 + species51	PrimaryAlcoholDehydrogenation-Oxygen	21.098979
3939	species10 -> species2 + species46	PrimaryAlcoholDehydrogenation-Oxygen	19.546497
3940	species11 -> species2 + species47	PrimaryAlcoholDehydrogenation-Oxygen	92.247995
3941	species11 -> species2 + species50	PrimaryAlcoholDehydrogenation-Oxygen	21.098979
3942	species12 -> species2 + species49	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3943	species12 -> species2 + species48	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3944	species15 -> species2 + species87	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3945	species16 -> species2 + species88	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3946	species17 -> species2 + species89	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3947	species18 -> species2 + species90	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3948	species21 -> species2 + species91	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3949	species22 -> species2 + species92	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3950	species23 -> species2 + species119	PrimaryAlcoholDehydrogenation-Oxygen	14.722885
3951	species23 -> species2 + species94	PrimaryAlcoholDehydrogenation-Oxygen	11.226542
3952	species24 -> species2 + species93	PrimaryAlcoholDehydrogenation-Oxygen	20.139065
3953	species25 -> species2 + species131	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
3954	species26 -> species2 + species132	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
3955	species26 -> species2 + species135	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
3956	species27 -> species2 + species133	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
3957	species27 -> species2 + species134	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
3958	species28 -> species2 + species136	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
3959	species29 -> species2 + species137	PrimaryAlcoholDehydrogenation-Oxygen	15.112231
3960	species29 -> species2 + species138	PrimaryAlcoholDehydrogenation-Oxygen	15.112231
3961	species30 -> species2 + species9	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
3962	species30 -> species2 + species139	PrimaryAlcoholDehydrogenation-Oxygen	23.018816
3963	species33 -> species2 + species156	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
3964	species34 -> species2 + species157	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
3965	species35 -> species2 + species159	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
3966	species36 -> species2 + species158	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
3967	species37 -> species2 + species161	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
3968	species38 -> species2 + species160	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
3969	species39 -> species2 + species162	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
3970	species40 -> species2 + species163	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
3971	species41 -> species2 + species164	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
3972	species42 -> species2 + species165	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
3973	species44 -> species2 + species187	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3974	species46 -> species2 + species190	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3975	species47 -> species2 + species189	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3976	species48 -> species2 + species188	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3977	species49 -> species2 + species188	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3978	species50 -> species2 + species189	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
3979	species51 -> species2 + species190	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
3980	species54 -> species2 + species208	PrimaryAlcoholDehydrogenation-Oxygen	89.277146
3981	species55 -> species2 + species191	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3982	species57 -> species2 + species210	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3983	species58 -> species2 + species206	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3984	species59 -> species2 + species202	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
3985	species60 -> species2 + species197	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
3986	species63 -> species2 + species203	PrimaryAlcoholDehydrogenation-Oxygen	93.174877
3987	species64 -> species2 + species212	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3988	species65 -> species2 + species216	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
3989	species66 -> species2 + species209	PrimaryAlcoholDehydrogenation-Oxygen	22.056868
3990	species67 -> species2 + species205	PrimaryAlcoholDehydrogenation-Oxygen	22.056868
3991	species68 -> species2 + species201	PrimaryAlcoholDehydrogenation-Oxygen	93.205880
3992	species69 -> species2 + species196	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
3993	species72 -> species2 + species213	PrimaryAlcoholDehydrogenation-Oxygen	22.058897

3994	species73 -> species2 + species200	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
3995	species73 -> species2 + species194	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
3996	species74 -> species2 + species195	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
3997	species75 -> species2 + species214	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
3998	species75 -> species2 + species198	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
3999	species76 -> species2 + species215	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4000	species78 -> species2 + species199	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4001	species79 -> species2 + species254	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4002	species79 -> species2 + species207	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4003	species80 -> species2 + species211	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4004	species83 -> species2 + species262	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4005	species85 -> species2 + species276	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4006	species94 -> species2 + species302	PrimaryAlcoholDehydrogenation-Oxygen	20.139065
4007	species97 -> species2 + species290	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4008	species98 -> species2 + species291	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4009	species105 -> species2 + species19	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4010	species110 -> species2 + species336	PrimaryAlcoholDehydrogenation-Oxygen	20.139065
4011	species114 -> species2 + species298	PrimaryAlcoholDehydrogenation-Oxygen	20.139065
4012	species116 -> species2 + species300	PrimaryAlcoholDehydrogenation-Oxygen	15.112231
4013	species116 -> species2 + species350	PrimaryAlcoholDehydrogenation-Oxygen	15.112231
4014	species117 -> species2 + species301	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4015	species118 -> species2 + species363	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4016	species119 -> species2 + species302	PrimaryAlcoholDehydrogenation-Oxygen	16.642722
4017	species120 -> species2 + species304	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4018	species121 -> species2 + species305	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4019	species122 -> species2 + species368	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4020	species122 -> species2 + species306	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4021	species123 -> species2 + species307	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4022	species123 -> species2 + species67	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4023	species124 -> species2 + species292	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4024	species126 -> species2 + species293	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4025	species127 -> species2 + species294	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4026	species128 -> species2 + species295	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4027	species129 -> species2 + species296	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4028	species130 -> species2 + species297	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4029	species132 -> species2 + species401	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4030	species133 -> species2 + species400	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4031	species134 -> species2 + species400	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4032	species135 -> species2 + species401	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4033	species137 -> species2 + species402	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4034	species138 -> species2 + species402	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4035	species139 -> species2 + species52	PrimaryAlcoholDehydrogenation-Oxygen	18.586579
4036	species140 -> species2 + species403	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4037	species141 -> species2 + species404	PrimaryAlcoholDehydrogenation-Oxygen	9.653040
4038	species142 -> species2 + species406	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4039	species143 -> species2 + species405	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4040	species145 -> species2 + species408	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4041	species146 -> species2 + species407	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4042	species147 -> species2 + species409	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4043	species148 -> species2 + species410	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4044	species149 -> species2 + species411	PrimaryAlcoholDehydrogenation-Oxygen	21.098979
4045	species150 -> species2 + species69	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4046	species150 -> species2 + species412	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4047	species151 -> species2 + species413	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4048	species151 -> species2 + species68	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4049	species152 -> species2 + species70	PrimaryAlcoholDehydrogenation-Oxygen	14.130318
4050	species153 -> species2 + species62	PrimaryAlcoholDehydrogenation-Oxygen	19.546497
4051	species154 -> species2 + species414	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4052	species154 -> species2 + species66	PrimaryAlcoholDehydrogenation-Oxygen	20.506416

4053	species175 -> species2 + species445	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4054	species176 -> species2 + species447	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4055	species177 -> species2 + species446	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4056	species178 -> species2 + species448	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4057	species179 -> species2 + species449	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4058	species180 -> species2 + species450	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4059	species181 -> species2 + species451	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4060	species182 -> species2 + species452	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4061	species183 -> species2 + species453	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4062	species184 -> species2 + species454	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4063	species186 -> species2 + species455	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4064	species187 -> species2 + species465	PrimaryAlcoholDehydrogenation-Oxygen	23.018816
4065	species192 -> species2 + species468	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4066	species193 -> species2 + species466	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4067	species193 -> species2 + species467	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4068	species194 -> species2 + species471	PrimaryAlcoholDehydrogenation-Oxygen	92.625476
4069	species195 -> species2 + species473	PrimaryAlcoholDehydrogenation-Oxygen	19.923990
4070	species198 -> species2 + species472	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4071	species199 -> species2 + species470	PrimaryAlcoholDehydrogenation-Oxygen	92.625476
4072	species200 -> species2 + species471	PrimaryAlcoholDehydrogenation-Oxygen	19.923990
4073	species204 -> species2 + species469	PrimaryAlcoholDehydrogenation-Oxygen	21.478505
4074	species207 -> species2 + species492	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4075	species214 -> species2 + species472	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4076	species218 -> species2 + species54	PrimaryAlcoholDehydrogenation-Oxygen	81.576787
4077	species219 -> species2 + species77	PrimaryAlcoholDehydrogenation-Oxygen	131.350613
4078	species220 -> species2 + species55	PrimaryAlcoholDehydrogenation-Oxygen	21.098979
4079	species221 -> species2 + species64	PrimaryAlcoholDehydrogenation-Oxygen	127.328534
4080	species224 -> species2 + species482	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4081	species227 -> species2 + species486	PrimaryAlcoholDehydrogenation-Oxygen	10.714211
4082	species232 -> species2 + species345	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4083	species233 -> species2 + species493	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4084	species234 -> species2 + species490	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4085	species235 -> species2 + species483	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4086	species236 -> species2 + species479	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4087	species239 -> species2 + species509	PrimaryAlcoholDehydrogenation-Oxygen	93.205880
4088	species241 -> species2 + species485	PrimaryAlcoholDehydrogenation-Oxygen	92.627526
4089	species242 -> species2 + species484	PrimaryAlcoholDehydrogenation-Oxygen	92.627526
4090	species243 -> species2 + species480	PrimaryAlcoholDehydrogenation-Oxygen	19.926020
4091	species246 -> species2 + species71	PrimaryAlcoholDehydrogenation-Oxygen	86.625620
4092	species248 -> species2 + species481	PrimaryAlcoholDehydrogenation-Oxygen	68.858640
4093	species249 -> species2 + species477	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4094	species250 -> species2 + species494	PrimaryAlcoholDehydrogenation-Oxygen	68.858640
4095	species251 -> species2 + species478	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4096	species252 -> species2 + species415	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4097	species252 -> species2 + species369	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4098	species253 -> species2 + species491	PrimaryAlcoholDehydrogenation-Oxygen	16.642722
4099	species254 -> species2 + species492	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4100	species255 -> species2 + species299	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4101	species258 -> species2 + species520	PrimaryAlcoholDehydrogenation-Oxygen	46.169938
4102	species263 -> species2 + species531	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4103	species266 -> species2 + species533	PrimaryAlcoholDehydrogenation-Oxygen	16.642722
4104	species267 -> species2 + species532	PrimaryAlcoholDehydrogenation-Oxygen	16.640693
4105	species278 -> species2 + species563	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4106	species279 -> species2 + species564	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4107	species280 -> species2 + species565	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4108	species281 -> species2 + species566	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4109	species282 -> species2 + species567	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4110	species283 -> species2 + species575	PrimaryAlcoholDehydrogenation-Oxygen	20.139065
4111	species283 -> species2 + species192	PrimaryAlcoholDehydrogenation-Oxygen	18.586579

4112	species284 -> species2 + species86	PrimaryAlcoholDehydrogenation-Oxygen	116.204910
4113	species300 -> species2 + species604	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4114	species303 -> species2 + species614	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4115	species306 -> species2 + species615	PrimaryAlcoholDehydrogenation-Oxygen	93.205880
4116	species307 -> species2 + species205	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4117	species308 -> species2 + species95	PrimaryAlcoholDehydrogenation-Oxygen	32.561938
4118	species312 -> species2 + species585	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4119	species313 -> species2 + species121	PrimaryAlcoholDehydrogenation-Oxygen	8.712113
4120	species313 -> species2 + species586	PrimaryAlcoholDehydrogenation-Oxygen	11.224513
4121	species314 -> species2 + species587	PrimaryAlcoholDehydrogenation-Oxygen	16.642722
4122	species317 -> species2 + species588	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4123	species318 -> species2 + species99	PrimaryAlcoholDehydrogenation-Oxygen	44.617465
4124	species320 -> species2 + species101	PrimaryAlcoholDehydrogenation-Oxygen	32.561938
4125	species322 -> species2 + species103	PrimaryAlcoholDehydrogenation-Oxygen	32.561938
4126	species324 -> species2 + species107	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4127	species325 -> species2 + species108	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4128	species326 -> species2 + species646	PrimaryAlcoholDehydrogenation-Oxygen	14.720856
4129	species326 -> species2 + species110	PrimaryAlcoholDehydrogenation-Oxygen	9.672027
4130	species327 -> species2 + species109	PrimaryAlcoholDehydrogenation-Oxygen	15.090236
4131	species330 -> species2 + species654	PrimaryAlcoholDehydrogenation-Oxygen	20.139065
4132	species339 -> species2 + species668	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4133	species340 -> species2 + species238	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4134	species346 -> species2 + species601	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4135	species347 -> species2 + species223	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4136	species350 -> species2 + species604	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4137	species351 -> species2 + species683	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4138	species352 -> species2 + species684	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4139	species352 -> species2 + species605	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4140	species353 -> species2 + species606	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4141	species354 -> species2 + species607	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4142	species355 -> species2 + species608	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4143	species356 -> species2 + species609	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4144	species357 -> species2 + species610	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4145	species358 -> species2 + species611	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4146	species360 -> species2 + species612	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4147	species361 -> species2 + species613	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4148	species362 -> species2 + species595	PrimaryAlcoholDehydrogenation-Oxygen	21.098979
4149	species364 -> species2 + species698	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4150	species365 -> species2 + species697	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4151	species366 -> species2 + species699	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4152	species368 -> species2 + species615	PrimaryAlcoholDehydrogenation-Oxygen	22.056868
4153	species369 -> species2 + species217	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4154	species370 -> species2 + species619	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4155	species371 -> species2 + species620	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4156	species372 -> species2 + species621	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4157	species373 -> species2 + species622	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4158	species374 -> species2 + species596	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4159	species375 -> species2 + species240	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4160	species376 -> species2 + species589	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4161	species377 -> species2 + species590	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4162	species378 -> species2 + species591	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4163	species379 -> species2 + species592	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4164	species381 -> species2 + species593	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4165	species382 -> species2 + species594	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4166	species394 -> species2 + species598	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4167	species395 -> species2 + species599	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4168	species396 -> species2 + species600	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4169	species398 -> species2 + species602	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4170	species399 -> species2 + species603	PrimaryAlcoholDehydrogenation-Oxygen	93.207930

4171	species403 -> species2 + species726	PrimaryAlcoholDehydrogenation-Oxygen	9.653040
4172	species412 -> species2 + species196	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4173	species413 -> species2 + species201	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4174	species414 -> species2 + species209	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4175	species415 -> species2 + species217	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4176	species416 -> species2 + species727	PrimaryAlcoholDehydrogenation-Oxygen	15.112231
4177	species420 -> species2 + species728	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4178	species421 -> species2 + species729	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4179	species422 -> species2 + species730	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4180	species423 -> species2 + species731	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4181	species425 -> species2 + species732	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4182	species426 -> species2 + species152	PrimaryAlcoholDehydrogenation-Oxygen	19.544468
4183	species427 -> species2 + species733	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4184	species428 -> species2 + species734	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4185	species431 -> species2 + species243	PrimaryAlcoholDehydrogenation-Oxygen	101.459824
4186	species431 -> species2 + species736	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4187	species432 -> species2 + species244	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4188	species433 -> species2 + species245	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4189	species434 -> species2 + species737	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4190	species434 -> species2 + species241	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4191	species435 -> species2 + species242	PrimaryAlcoholDehydrogenation-Oxygen	16.645722
4192	species435 -> species2 + species738	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4193	species436 -> species2 + species231	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4194	species437 -> species2 + species237	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4195	species438 -> species2 + species238	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4196	species439 -> species2 + species225	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4197	species440 -> species2 + species759	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4198	species440 -> species2 + species239	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4199	species466 -> species2 + species766	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4200	species467 -> species2 + species766	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4201	species474 -> species2 + species768	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4202	species476 -> species2 + species767	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4203	species487 -> species2 + species204	PrimaryAlcoholDehydrogenation-Oxygen	101.459824
4204	species487 -> species2 + species769	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4205	species489 -> species2 + species778	PrimaryAlcoholDehydrogenation-Oxygen	11.294608
4206	species491 -> species2 + species779	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4207	species499 -> species2 + species774	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4208	species503 -> species2 + species773	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4209	species504 -> species2 + species772	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4210	species505 -> species2 + species770	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4211	species508 -> species2 + species780	PrimaryAlcoholDehydrogenation-Oxygen	22.056868
4212	species511 -> species2 + species617	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4213	species517 -> species2 + species735	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4214	species518 -> species2 + species669	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4215	species529 -> species2 + species265	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4216	species532 -> species2 + species819	PrimaryAlcoholDehydrogenation-Oxygen	15.682804
4217	species537 -> species2 + species820	PrimaryAlcoholDehydrogenation-Oxygen	21.098979
4218	species540 -> species2 + species821	PrimaryAlcoholDehydrogenation-Oxygen	15.682804
4219	species542 -> species2 + species822	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4220	species544 -> species2 + species823	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4221	species545 -> species2 + species824	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4222	species546 -> species2 + species825	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4223	species547 -> species2 + species333	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4224	species548 -> species2 + species818	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4225	species572 -> species2 + species868	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4226	species573 -> species2 + species869	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4227	species575 -> species2 + species468	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4228	species576 -> species2 + species878	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4229	species577 -> species2 + species475	PrimaryAlcoholDehydrogenation-Oxygen	20.504387

4230	species578 -> species2 + species474	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4231	species579 -> species2 + species285	PrimaryAlcoholDehydrogenation-Oxygen	119.914444
4232	species580 -> species2 + species286	PrimaryAlcoholDehydrogenation-Oxygen	104.149383
4233	species581 -> species2 + species287	PrimaryAlcoholDehydrogenation-Oxygen	119.914444
4234	species582 -> species2 + species288	PrimaryAlcoholDehydrogenation-Oxygen	108.117154
4235	species583 -> species2 + species289	PrimaryAlcoholDehydrogenation-Oxygen	106.666770
4236	species586 -> species2 + species305	PrimaryAlcoholDehydrogenation-Oxygen	19.546497
4237	species605 -> species2 + species900	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4238	species606 -> species2 + species899	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4239	species616 -> species2 + species303	PrimaryAlcoholDehydrogenation-Oxygen	14.128318
4240	species616 -> species2 + species903	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4241	species623 -> species2 + species310	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4242	species626 -> species2 + species338	PrimaryAlcoholDehydrogenation-Oxygen	19.546497
4243	species629 -> species2 + species335	PrimaryAlcoholDehydrogenation-Oxygen	19.546497
4244	species631 -> species2 + species883	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4245	species632 -> species2 + species884	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4246	species633 -> species2 + species885	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4247	species633 -> species2 + species373	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4248	species634 -> species2 + species372	PrimaryAlcoholDehydrogenation-Oxygen	16.645722
4249	species634 -> species2 + species886	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4250	species635 -> species2 + species887	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4251	species636 -> species2 + species888	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4252	species637 -> species2 + species889	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4253	species638 -> species2 + species890	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4254	species639 -> species2 + species315	PrimaryAlcoholDehydrogenation-Oxygen	56.672991
4255	species643 -> species2 + species540	PrimaryAlcoholDehydrogenation-Oxygen	21.466334
4256	species643 -> species2 + species893	PrimaryAlcoholDehydrogenation-Oxygen	16.642722
4257	species644 -> species2 + species894	PrimaryAlcoholDehydrogenation-Oxygen	21.098979
4258	species645 -> species2 + species940	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4259	species646 -> species2 + species336	PrimaryAlcoholDehydrogenation-Oxygen	15.090236
4260	species647 -> species2 + species337	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4261	species648 -> species2 + species338	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4262	species649 -> species2 + species943	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4263	species649 -> species2 + species339	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4264	species650 -> species2 + species340	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4265	species650 -> species2 + species438	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4266	species652 -> species2 + species332	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4267	species653 -> species2 + species334	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4268	species657 -> species2 + species954	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4269	species658 -> species2 + species501	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4270	species681 -> species2 + species510	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4271	species682 -> species2 + species891	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4272	species684 -> species2 + species900	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4273	species685 -> species2 + species901	PrimaryAlcoholDehydrogenation-Oxygen	19.572522
4274	species686 -> species2 + species970	PrimaryAlcoholDehydrogenation-Oxygen	9.653040
4275	species688 -> species2 + species896	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4276	species690 -> species2 + species902	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4277	species700 -> species2 + species978	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4278	species703 -> species2 + species977	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4279	species704 -> species2 + species907	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4280	species705 -> species2 + species908	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4281	species706 -> species2 + species909	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4282	species709 -> species2 + species895	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4283	species727 -> species2 + species980	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4284	species736 -> species2 + species480	PrimaryAlcoholDehydrogenation-Oxygen	100.879420
4285	species737 -> species2 + species485	PrimaryAlcoholDehydrogenation-Oxygen	19.926020
4286	species738 -> species2 + species484	PrimaryAlcoholDehydrogenation-Oxygen	16.065330
4287	species739 -> species2 + species436	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4288	species740 -> species2 + species495	PrimaryAlcoholDehydrogenation-Oxygen	89.277146

4289	species741 -> species2 + species981	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4290	species743 -> species2 + species982	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4291	species744 -> species2 + species983	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4292	species745 -> species2 + species990	PrimaryAlcoholDehydrogenation-Oxygen	16.642722
4293	species745 -> species2 + species508	PrimaryAlcoholDehydrogenation-Oxygen	15.090236
4294	species750 -> species2 + species430	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4295	species751 -> species2 + species984	PrimaryAlcoholDehydrogenation-Oxygen	11.294608
4296	species755 -> species2 + species511	PrimaryAlcoholDehydrogenation-Oxygen	14.128318
4297	species755 -> species2 + species904	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4298	species756 -> species2 + species512	PrimaryAlcoholDehydrogenation-Oxygen	89.277146
4299	species757 -> species2 + species513	PrimaryAlcoholDehydrogenation-Oxygen	89.277146
4300	species758 -> species2 + species502	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4301	species759 -> species2 + species509	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4302	species769 -> species2 + species469	PrimaryAlcoholDehydrogenation-Oxygen	100.879420
4303	species775 -> species2 + species488	PrimaryAlcoholDehydrogenation-Oxygen	18.966101
4304	species776 -> species2 + species489	PrimaryAlcoholDehydrogenation-Oxygen	89.277146
4305	species776 -> species2 + species999	PrimaryAlcoholDehydrogenation-Oxygen	81.025294
4306	species777 -> species2 + species1000	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4307	species783 -> species2 + species500	PrimaryAlcoholDehydrogenation-Oxygen	86.625620
4308	species786 -> species2 + species879	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4309	species791 -> species2 + species906	PrimaryAlcoholDehydrogenation-Oxygen	29.893387
4310	species794 -> species2 + species518	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4311	species795 -> species2 + species522	PrimaryAlcoholDehydrogenation-Oxygen	44.617465
4312	species808 -> species2 + species541	PrimaryAlcoholDehydrogenation-Oxygen	19.546497
4313	species815 -> species2 + species534	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4314	species816 -> species2 + species530	PrimaryAlcoholDehydrogenation-Oxygen	118.722297
4315	species828 -> species2 + species1032	PrimaryAlcoholDehydrogenation-Oxygen	15.682804
4316	species835 -> species2 + species1033	PrimaryAlcoholDehydrogenation-Oxygen	21.098979
4317	species842 -> species2 + species1034	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4318	species843 -> species2 + species1035	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4319	species851 -> species2 + species664	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4320	species852 -> species2 + species1036	PrimaryAlcoholDehydrogenation-Oxygen	93.205880
4321	species853 -> species2 + species663	PrimaryAlcoholDehydrogenation-Oxygen	8.323767
4322	species854 -> species2 + species1037	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4323	species856 -> species2 + species1030	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4324	species857 -> species2 + species1031	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4325	species871 -> species2 + species1061	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4326	species872 -> species2 + species577	PrimaryAlcoholDehydrogenation-Oxygen	19.546497
4327	species873 -> species2 + species1062	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4328	species880 -> species2 + species771	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4329	species881 -> species2 + species771	PrimaryAlcoholDehydrogenation-Oxygen	16.645722
4330	species882 -> species2 + species584	PrimaryAlcoholDehydrogenation-Oxygen	104.149383
4331	species885 -> species2 + species622	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4332	species886 -> species2 + species621	PrimaryAlcoholDehydrogenation-Oxygen	16.645722
4333	species893 -> species2 + species821	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4334	species898 -> species2 + species597	PrimaryAlcoholDehydrogenation-Oxygen	101.459824
4335	species903 -> species2 + species614	PrimaryAlcoholDehydrogenation-Oxygen	14.128318
4336	species904 -> species2 + species617	PrimaryAlcoholDehydrogenation-Oxygen	14.128318
4337	species905 -> species2 + species618	PrimaryAlcoholDehydrogenation-Oxygen	14.128318
4338	species910 -> species2 + species625	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4339	species911 -> species2 + species648	PrimaryAlcoholDehydrogenation-Oxygen	14.130318
4340	species911 -> species2 + species626	PrimaryAlcoholDehydrogenation-Oxygen	15.090236
4341	species912 -> species2 + species627	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4342	species915 -> species2 + species656	PrimaryAlcoholDehydrogenation-Oxygen	19.546497
4343	species917 -> species2 + species672	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4344	species918 -> species2 + species671	PrimaryAlcoholDehydrogenation-Oxygen	16.645722
4345	species921 -> species2 + species666	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4346	species922 -> species2 + species667	PrimaryAlcoholDehydrogenation-Oxygen	16.645722
4347	species924 -> species2 + species1067	PrimaryAlcoholDehydrogenation-Oxygen	15.114261

4348	species926 -> species2 + species1068	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4349	species927 -> species2 + species1069	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4350	species928 -> species2 + species1070	PrimaryAlcoholDehydrogenation-Oxygen	93.207930
4351	species930 -> species2 + species641	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4352	species933 -> species2 + species837	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4353	species935 -> species2 + species831	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4354	species936 -> species2 + species1072	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4355	species937 -> species2 + species1073	PrimaryAlcoholDehydrogenation-Oxygen	22.056868
4356	species938 -> species2 + species1074	PrimaryAlcoholDehydrogenation-Oxygen	93.205880
4357	species939 -> species2 + species920	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4358	species941 -> species2 + species1101	PrimaryAlcoholDehydrogenation-Oxygen	0.233032
4359	species943 -> species2 + species668	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4360	species944 -> species2 + species661	PrimaryAlcoholDehydrogenation-Oxygen	15.090236
4361	species945 -> species2 + species670	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4362	species946 -> species2 + species671	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4363	species947 -> species2 + species662	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4364	species953 -> species2 + species665	PrimaryAlcoholDehydrogenation-Oxygen	101.459824
4365	species963 -> species2 + species677	PrimaryAlcoholDehydrogenation-Oxygen	51.674199
4366	species967 -> species2 + species790	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4367	species968 -> species2 + species789	PrimaryAlcoholDehydrogenation-Oxygen	18.144154
4368	species973 -> species2 + species1076	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4369	species979 -> species2 + species1075	PrimaryAlcoholDehydrogenation-Oxygen	15.114261
4370	species985 -> species2 + species740	PrimaryAlcoholDehydrogenation-Oxygen	16.645722
4371	species990 -> species2 + species780	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4372	species991 -> species2 + species788	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4373	species993 -> species2 + species791	PrimaryAlcoholDehydrogenation-Oxygen	18.096110
4374	species994 -> species2 + species792	PrimaryAlcoholDehydrogenation-Oxygen	14.128318
4375	species995 -> species2 + species793	PrimaryAlcoholDehydrogenation-Oxygen	14.128318
4376	species998 -> species2 + species777	PrimaryAlcoholDehydrogenation-Oxygen	14.128318
4377	species998 -> species2 + species1116	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4378	species999 -> species2 + species778	PrimaryAlcoholDehydrogenation-Oxygen	19.546497
4379	species1002 -> species2 + species1004	PrimaryAlcoholDehydrogenation-Oxygen	18.096110
4380	species1008 -> species2 + species798	PrimaryAlcoholDehydrogenation-Oxygen	142.833350
4381	species1012 -> species2 + species1041	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4382	species1017 -> species2 + species840	PrimaryAlcoholDehydrogenation-Oxygen	19.544468
4383	species1025 -> species2 + species841	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4384	species1026 -> species2 + species838	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4385	species1027 -> species2 + species839	PrimaryAlcoholDehydrogenation-Oxygen	16.645722
4386	species1029 -> species2 + species817	PrimaryAlcoholDehydrogenation-Oxygen	119.914444
4387	species1039 -> species2 + species1141	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4388	species1064 -> species2 + species880	PrimaryAlcoholDehydrogenation-Oxygen	16.645722
4389	species1064 -> species2 + species881	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4390	species1066 -> species2 + species991	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4391	species1071 -> species2 + species892	PrimaryAlcoholDehydrogenation-Oxygen	118.722297
4392	species1077 -> species2 + species897	PrimaryAlcoholDehydrogenation-Oxygen	14.128318
4393	species1078 -> species2 + species916	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4394	species1079 -> species2 + species917	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4395	species1080 -> species2 + species946	PrimaryAlcoholDehydrogenation-Oxygen	16.645722
4396	species1080 -> species2 + species918	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4397	species1081 -> species2 + species919	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4398	species1084 -> species2 + species958	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4399	species1085 -> species2 + species957	PrimaryAlcoholDehydrogenation-Oxygen	16.645722
4400	species1088 -> species2 + species1152	PrimaryAlcoholDehydrogenation-Oxygen	22.058897
4401	species1089 -> species2 + species933	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4402	species1090 -> species2 + species932	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4403	species1091 -> species2 + species1048	PrimaryAlcoholDehydrogenation-Oxygen	124.161497
4404	species1099 -> species2 + species1153	PrimaryAlcoholDehydrogenation-Oxygen	22.056868
4405	species1103 -> species2 + species962	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4406	species1105 -> species2 + species961	PrimaryAlcoholDehydrogenation-Oxygen	14.128318

4407	species1109 -> species2 + species969	PrimaryAlcoholDehydrogenation-Oxygen	87.226191
4408	species1116 -> species2 + species1000	PrimaryAlcoholDehydrogenation-Oxygen	14.128318
4409	species1122 -> species2 + species1095	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4410	species1126 -> species2 + species1144	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4411	species1131 -> species2 + species1051	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4412	species1132 -> species2 + species1052	PrimaryAlcoholDehydrogenation-Oxygen	16.645722
4413	species1140 -> species2 + species1053	PrimaryAlcoholDehydrogenation-Oxygen	18.094080
4414	species1154 -> species2 + species1086	PrimaryAlcoholDehydrogenation-Oxygen	20.504387
4415	species1156 -> species2 + species1094	PrimaryAlcoholDehydrogenation-Oxygen	16.645722
4416	species1157 -> species2 + species1093	PrimaryAlcoholDehydrogenation-Oxygen	20.506416
4417	species1163 -> species2 + species1160	PrimaryAlcoholDehydrogenation-Oxygen	77.967334
4418	species2 + species33 -> species117	PyranRingSaturation-Oxygen	-79.365041
4419	species2 + species34 -> species117	PyranRingSaturation-Oxygen	-103.910477
4420	species2 + species35 -> species148	PyranRingSaturation-Oxygen	-103.910477
4421	species2 + species36 -> species148	PyranRingSaturation-Oxygen	-97.507283
4422	species2 + species37 -> species118	PyranRingSaturation-Oxygen	-103.910477
4423	species2 + species38 -> species118	PyranRingSaturation-Oxygen	-103.910477
4424	species2 + species156 -> species301	PyranRingSaturation-Oxygen	-64.483808
4425	species2 + species157 -> species301	PyranRingSaturation-Oxygen	-103.910477
4426	species2 + species158 -> species410	PyranRingSaturation-Oxygen	-97.507283
4427	species2 + species159 -> species410	PyranRingSaturation-Oxygen	-103.910477
4428	species2 + species160 -> species363	PyranRingSaturation-Oxygen	-103.910477
4429	species2 + species161 -> species363	PyranRingSaturation-Oxygen	-103.910477
4430	species2 + species166 -> species359	PyranRingSaturation-Oxygen	-90.660586
4431	species2 + species167 -> species424	PyranRingSaturation-Oxygen	-97.507283
4432	species2 + species168 -> species424	PyranRingSaturation-Oxygen	-103.908385
4433	species2 + species169 -> species367	PyranRingSaturation-Oxygen	-88.143073
4434	species2 + species170 -> species367	PyranRingSaturation-Oxygen	-103.908385
4435	species2 + species175 -> species366	PyranRingSaturation-Oxygen	-35.093551
4436	species2 + species175 -> species356	PyranRingSaturation-Oxygen	-10.548073
4437	species2 + species176 -> species423	PyranRingSaturation-Oxygen	-97.507283
4438	species2 + species176 -> species358	PyranRingSaturation-Oxygen	-79.365041
4439	species2 + species177 -> species423	PyranRingSaturation-Oxygen	-103.908385
4440	species2 + species177 -> species357	PyranRingSaturation-Oxygen	-79.362949
4441	species2 + species178 -> species360	PyranRingSaturation-Oxygen	-79.365041
4442	species2 + species179 -> species361	PyranRingSaturation-Oxygen	-79.365041
4443	species2 + species180 -> species422	PyranRingSaturation-Oxygen	-37.608846
4444	species2 + species180 -> species358	PyranRingSaturation-Oxygen	-44.011914
4445	species2 + species181 -> species365	PyranRingSaturation-Oxygen	-39.553862
4446	species2 + species181 -> species421	PyranRingSaturation-Oxygen	-33.150585
4447	species2 + species182 -> species361	PyranRingSaturation-Oxygen	-101.965335
4448	species2 + species183 -> species425	PyranRingSaturation-Oxygen	-97.507283
4449	species2 + species184 -> species425	PyranRingSaturation-Oxygen	-97.507283
4450	species2 + species186 -> species360	PyranRingSaturation-Oxygen	-97.507283
4451	species2 + species355 -> species548	PyranRingSaturation-Oxygen	-97.507283
4452	species2 + species356 -> species548	PyranRingSaturation-Oxygen	-103.910477
4453	species2 + species357 -> species631	PyranRingSaturation-Oxygen	-103.910477
4454	species2 + species358 -> species631	PyranRingSaturation-Oxygen	-97.507283
4455	species2 + species364 -> species645	PyranRingSaturation-Oxygen	-97.507283
4456	species2 + species365 -> species645	PyranRingSaturation-Oxygen	-97.507283
4457	species2 + species366 -> species548	PyranRingSaturation-Oxygen	-79.365041
4458	species2 + species383 -> species651	PyranRingSaturation-Oxygen	-97.507283
4459	species2 + species384 -> species651	PyranRingSaturation-Oxygen	-103.908385
4460	species2 + species385 -> species696	PyranRingSaturation-Oxygen	-103.908385
4461	species2 + species386 -> species696	PyranRingSaturation-Oxygen	-103.908385
4462	species2 + species387 -> species543	PyranRingSaturation-Oxygen	-115.977970
4463	species2 + species388 -> species543	PyranRingSaturation-Oxygen	-103.908385
4464	species2 + species421 -> species645	PyranRingSaturation-Oxygen	-103.910477
4465	species2 + species422 -> species631	PyranRingSaturation-Oxygen	-103.910477

4466	species2 + species423 -> species631	PyranRingSaturation-Oxygen	-79.365041
4467	species2 + species441 -> species574	PyranRingSaturation-Oxygen	-97.507283
4468	species2 + species442 -> species574	PyranRingSaturation-Oxygen	-103.908385
4469	species2 + species443 -> species464	PyranRingSaturation-Oxygen	-103.908385
4470	species2 + species445 -> species699	PyranRingSaturation-Oxygen	-35.093551
4471	species2 + species445 -> species609	PyranRingSaturation-Oxygen	4.333143
4472	species2 + species446 -> species731	PyranRingSaturation-Oxygen	-103.908385
4473	species2 + species446 -> species610	PyranRingSaturation-Oxygen	-64.481716
4474	species2 + species447 -> species731	PyranRingSaturation-Oxygen	-97.507283
4475	species2 + species447 -> species611	PyranRingSaturation-Oxygen	-64.483808
4476	species2 + species448 -> species612	PyranRingSaturation-Oxygen	-64.483808
4477	species2 + species449 -> species613	PyranRingSaturation-Oxygen	-64.483808
4478	species2 + species450 -> species730	PyranRingSaturation-Oxygen	-37.608846
4479	species2 + species450 -> species611	PyranRingSaturation-Oxygen	-44.011914
4480	species2 + species451 -> species697	PyranRingSaturation-Oxygen	-39.553862
4481	species2 + species451 -> species729	PyranRingSaturation-Oxygen	-33.150585
4482	species2 + species452 -> species613	PyranRingSaturation-Oxygen	-101.965335
4483	species2 + species453 -> species732	PyranRingSaturation-Oxygen	-97.507283
4484	species2 + species454 -> species732	PyranRingSaturation-Oxygen	-97.507283
4485	species2 + species455 -> species612	PyranRingSaturation-Oxygen	-97.507283
4486	species2 + species458 -> species695	PyranRingSaturation-Oxygen	-101.965335
4487	species2 + species459 -> species748	PyranRingSaturation-Oxygen	-97.507283
4488	species2 + species460 -> species748	PyranRingSaturation-Oxygen	-97.507283
4489	species2 + species461 -> species694	PyranRingSaturation-Oxygen	-153.074150
4490	species2 + species462 -> species749	PyranRingSaturation-Oxygen	-97.507283
4491	species2 + species463 -> species749	PyranRingSaturation-Oxygen	-101.965335
4492	species2 + species608 -> species818	PyranRingSaturation-Oxygen	-97.507283
4493	species2 + species609 -> species818	PyranRingSaturation-Oxygen	-103.910477
4494	species2 + species610 -> species883	PyranRingSaturation-Oxygen	-103.910477
4495	species2 + species611 -> species883	PyranRingSaturation-Oxygen	-97.507283
4496	species2 + species689 -> species858	PyranRingSaturation-Oxygen	-88.717536
4497	species2 + species690 -> species924	PyranRingSaturation-Oxygen	-37.610896
4498	species2 + species690 -> species857	PyranRingSaturation-Oxygen	-37.610896
4499	species2 + species691 -> species858	PyranRingSaturation-Oxygen	-103.908385
4500	species2 + species692 -> species925	PyranRingSaturation-Oxygen	-103.908385
4501	species2 + species693 -> species925	PyranRingSaturation-Oxygen	-97.507283
4502	species2 + species697 -> species940	PyranRingSaturation-Oxygen	-97.507283
4503	species2 + species698 -> species940	PyranRingSaturation-Oxygen	-97.507283
4504	species2 + species699 -> species818	PyranRingSaturation-Oxygen	-64.483808
4505	species2 + species700 -> species856	PyranRingSaturation-Oxygen	-15.008385
4506	species2 + species700 -> species941	PyranRingSaturation-Oxygen	-33.150585
4507	species2 + species701 -> species942	PyranRingSaturation-Oxygen	-97.507283
4508	species2 + species702 -> species942	PyranRingSaturation-Oxygen	-97.507283
4509	species2 + species703 -> species857	PyranRingSaturation-Oxygen	-79.365041
4510	species2 + species703 -> species941	PyranRingSaturation-Oxygen	-97.507283
4511	species2 + species714 -> species975	PyranRingSaturation-Oxygen	-39.553862
4512	species2 + species714 -> species950	PyranRingSaturation-Oxygen	-33.152635
4513	species2 + species715 -> species845	PyranRingSaturation-Oxygen	-115.980062
4514	species2 + species715 -> species948	PyranRingSaturation-Oxygen	-97.508957
4515	species2 + species716 -> species845	PyranRingSaturation-Oxygen	-103.910477
4516	species2 + species716 -> species949	PyranRingSaturation-Oxygen	-97.508957
4517	species2 + species717 -> species952	PyranRingSaturation-Oxygen	-97.507283
4518	species2 + species718 -> species849	PyranRingSaturation-Oxygen	-101.965335
4519	species2 + species719 -> species846	PyranRingSaturation-Oxygen	-51.623447
4520	species2 + species719 -> species948	PyranRingSaturation-Oxygen	-39.553862
4521	species2 + species720 -> species847	PyranRingSaturation-Oxygen	-47.164977
4522	species2 + species720 -> species976	PyranRingSaturation-Oxygen	-35.095601
4523	species2 + species721 -> species849	PyranRingSaturation-Oxygen	-115.977970
4524	species2 + species722 -> species850	PyranRingSaturation-Oxygen	-115.977970

4525	species2 + species723 -> species850	PyranRingSaturation-Oxygen	-97.507283
4526	species2 + species724 -> species952	PyranRingSaturation-Oxygen	-97.507283
4527	species2 + species729 -> species940	PyranRingSaturation-Oxygen	-103.910477
4528	species2 + species730 -> species883	PyranRingSaturation-Oxygen	-103.910477
4529	species2 + species731 -> species883	PyranRingSaturation-Oxygen	-64.483808
4530	species2 + species746 -> species942	PyranRingSaturation-Oxygen	-23.786751
4531	species2 + species747 -> species925	PyranRingSaturation-Oxygen	-90.660586
4532	species2 + species760 -> species764	PyranRingSaturation-Oxygen	-39.553862
4533	species2 + species760 -> species874	PyranRingSaturation-Oxygen	-33.152635
4534	species2 + species761 -> species876	PyranRingSaturation-Oxygen	-103.910477
4535	species2 + species761 -> species875	PyranRingSaturation-Oxygen	-97.508957
4536	species2 + species762 -> species876	PyranRingSaturation-Oxygen	-97.507283
4537	species2 + species763 -> species877	PyranRingSaturation-Oxygen	-101.965335
4538	species2 + species764 -> species989	PyranRingSaturation-Oxygen	-97.507283
4539	species2 + species765 -> species989	PyranRingSaturation-Oxygen	-97.507283
4540	species2 + species845 -> species1023	PyranRingSaturation-Oxygen	-97.507283
4541	species2 + species846 -> species1023	PyranRingSaturation-Oxygen	-103.908385
4542	species2 + species847 -> species1038	PyranRingSaturation-Oxygen	-103.908385
4543	species2 + species848 -> species1038	PyranRingSaturation-Oxygen	-97.507283
4544	species2 + species856 -> species936	PyranRingSaturation-Oxygen	-97.507283
4545	species2 + species857 -> species936	PyranRingSaturation-Oxygen	-97.507283
4546	species2 + species874 -> species989	PyranRingSaturation-Oxygen	-103.908385
4547	species2 + species875 -> species1063	PyranRingSaturation-Oxygen	-103.908385
4548	species2 + species876 -> species1063	PyranRingSaturation-Oxygen	-97.507283
4549	species2 + species902 -> species1067	PyranRingSaturation-Oxygen	-37.610896
4550	species2 + species902 -> species1031	PyranRingSaturation-Oxygen	-37.610896
4551	species2 + species924 -> species936	PyranRingSaturation-Oxygen	-97.507283
4552	species2 + species941 -> species936	PyranRingSaturation-Oxygen	-79.365041
4553	species2 + species948 -> species1023	PyranRingSaturation-Oxygen	-115.977970
4554	species2 + species949 -> species1023	PyranRingSaturation-Oxygen	-103.908385
4555	species2 + species950 -> species1102	PyranRingSaturation-Oxygen	-103.908385
4556	species2 + species951 -> species1102	PyranRingSaturation-Oxygen	-97.507283
4557	species2 + species975 -> species1102	PyranRingSaturation-Oxygen	-97.507283
4558	species2 + species976 -> species1038	PyranRingSaturation-Oxygen	-115.977970
4559	species2 + species977 -> species1031	PyranRingSaturation-Oxygen	-64.483808
4560	species2 + species977 -> species1101	PyranRingSaturation-Oxygen	-97.507283
4561	species2 + species978 -> species1030	PyranRingSaturation-Oxygen	-0.127152
4562	species2 + species978 -> species1101	PyranRingSaturation-Oxygen	-33.150585
4563	species2 + species996 -> species1115	PyranRingSaturation-Oxygen	-97.507283
4564	species2 + species997 -> species1115	PyranRingSaturation-Oxygen	-97.507283
4565	species2 + species997 -> species1114	PyranRingSaturation-Oxygen	-97.507283
4566	species2 + species1030 -> species1072	PyranRingSaturation-Oxygen	-97.507283
4567	species2 + species1031 -> species1072	PyranRingSaturation-Oxygen	-97.507283
4568	species2 + species1055 -> species1142	PyranRingSaturation-Oxygen	-37.608846
4569	species2 + species1055 -> species1137	PyranRingSaturation-Oxygen	-37.608846
4570	species2 + species1058 -> species1098	PyranRingSaturation-Oxygen	-97.507283
4571	species2 + species1059 -> species1098	PyranRingSaturation-Oxygen	-97.507283
4572	species2 + species1067 -> species1072	PyranRingSaturation-Oxygen	-97.507283
4573	species2 + species1087 -> species1098	PyranRingSaturation-Oxygen	-88.717536
4574	species2 + species1101 -> species1072	PyranRingSaturation-Oxygen	-64.483808
4575	species2 + species1104 -> species1162	PyranRingSaturation-Oxygen	-33.152635
4576	species2 + species1104 -> species1136	PyranRingSaturation-Oxygen	-51.623447
4577	species2 + species1112 -> species1142	PyranRingSaturation-Oxygen	-115.980062
4578	species2 + species1112 -> species1162	PyranRingSaturation-Oxygen	-97.508957
4579	species2 + species1114 -> species1151	PyranRingSaturation-Oxygen	-97.507283
4580	species2 + species1115 -> species1151	PyranRingSaturation-Oxygen	-97.507283
4581	species2 + species1136 -> species1124	PyranRingSaturation-Oxygen	-97.507283
4582	species2 + species1137 -> species1124	PyranRingSaturation-Oxygen	-97.507283
4583	species2 + species1142 -> species1124	PyranRingSaturation-Oxygen	-97.507283

4584	species2 + species1162 -> species1124	PyranRingSaturation-Oxygen	-115.977970
4585	species7 -> species54 + species55	RetroAldol-Oxygen	149.509131
4586	species8 -> species63 + species64	RetroAldol-Oxygen	-3.645268
4587	species9 -> species55 + species71	RetroAldol-Oxygen	17.882165
4588	species10 -> species54 + species75	RetroAldol-Oxygen	1.320462
4589	species10 -> species76 + species77	RetroAldol-Oxygen	74.336208
4590	species11 -> species63 + species64	RetroAldol-Oxygen	-8.143738
4591	species12 -> species77 + species79	RetroAldol-Oxygen	79.794570
4592	species12 -> species54 + species80	RetroAldol-Oxygen	-2.218064
4593	species21 -> species54 + species115	RetroAldol-Oxygen	11.582371
4594	species29 -> species77 + species147	RetroAldol-Oxygen	80.530327
4595	species40 -> species77 + species185	RetroAldol-Oxygen	80.532377
4596	species43 -> species54 + species191	RetroAldol-Oxygen	1.320462
4597	species46 -> species54 + species198	RetroAldol-Oxygen	2.280376
4598	species47 -> species64 + species203	RetroAldol-Oxygen	-7.216814
4599	species48 -> species77 + species207	RetroAldol-Oxygen	79.794570
4600	species48 -> species80 + species208	RetroAldol-Oxygen	65.000197
4601	species49 -> species54 + species211	RetroAldol-Oxygen	-2.218064
4602	species50 -> species63 + species212	RetroAldol-Oxygen	-7.183802
4603	species50 -> species54 + species198	RetroAldol-Oxygen	0.727895
4604	species51 -> species54 + species214	RetroAldol-Oxygen	73.429409
4605	species51 -> species75 + species208	RetroAldol-Oxygen	69.498625
4606	species51 -> species77 + species215	RetroAldol-Oxygen	75.296143
4607	species52 -> species71 + species191	RetroAldol-Oxygen	18.842083
4608	species52 -> species54 + species217	RetroAldol-Oxygen	2.280376
4609	species53 -> species63 + species212	RetroAldol-Oxygen	-2.685375
4610	species53 -> species54 + species211	RetroAldol-Oxygen	2.280376
4611	species55 -> 2species54	RetroAldol-Oxygen	2.280376
4612	species57 -> species77 + species224	RetroAldol-Oxygen	79.794570
4613	species58 -> species54 + species226	RetroAldol-Oxygen	-7.216814
4614	species59 -> species63 + species203	RetroAldol-Oxygen	58.964401
4615	species60 -> species77 + species229	RetroAldol-Oxygen	75.296143
4616	species61 -> species63 + species203	RetroAldol-Oxygen	63.462828
4617	species62 -> species71 + species211	RetroAldol-Oxygen	18.840050
4618	species62 -> species63 + species231	RetroAldol-Oxygen	-4.239898
4619	species64 -> species54 + species77	RetroAldol-Oxygen	79.794570
4620	species66 -> species77 + species239	RetroAldol-Oxygen	79.794570
4621	species67 -> species54 + species240	RetroAldol-Oxygen	-7.183802
4622	species68 -> species63 + species231	RetroAldol-Oxygen	-8.738326
4623	species68 -> species71 + species198	RetroAldol-Oxygen	17.287568
4624	species69 -> species71 + species214	RetroAldol-Oxygen	89.989054
4625	species69 -> species77 + species245	RetroAldol-Oxygen	75.296143
4626	species70 -> species71 + species217	RetroAldol-Oxygen	18.842083
4627	species72 -> species54 + species250	RetroAldol-Oxygen	26.629658
4628	species73 -> species77 + species224	RetroAldol-Oxygen	70.330404
4629	species74 -> species77 + species251	RetroAldol-Oxygen	70.297350
4630	species75 -> species63 + species77	RetroAldol-Oxygen	70.330404
4631	species76 -> species54 + species63	RetroAldol-Oxygen	-2.685375
4632	species79 -> species54 + species63	RetroAldol-Oxygen	-7.183802
4633	species80 -> species63 + species77	RetroAldol-Oxygen	74.828832
4634	species91 -> species115 + species208	RetroAldol-Oxygen	78.800619
4635	species93 -> species54 + species299	RetroAldol-Oxygen	2.280376
4636	species109 -> species71 + species299	RetroAldol-Oxygen	18.840050
4637	species113 -> species63 + species345	RetroAldol-Oxygen	-2.687383
4638	species114 -> species64 + species348	RetroAldol-Oxygen	2.854798
4639	species119 -> species54 + species369	RetroAldol-Oxygen	-4.688298
4640	species121 -> species71 + species369	RetroAldol-Oxygen	17.289598
4641	species123 -> species54 + species375	RetroAldol-Oxygen	-7.183802
4642	species123 -> species77 + species234	RetroAldol-Oxygen	70.330404

4643	species126 -> species54 + species393	RetroAldol-Oxygen	-2.218064
4644	species127 -> species77 + species235	RetroAldol-Oxygen	79.794570
4645	species127 -> species71 + species80	RetroAldol-Oxygen	21.326430
4646	species128 -> species63 + species345	RetroAldol-Oxygen	-7.185853
4647	species129 -> species71 + species75	RetroAldol-Oxygen	25.824861
4648	species129 -> species77 + species230	RetroAldol-Oxygen	75.296143
4649	species130 -> species54 + species399	RetroAldol-Oxygen	2.280376
4650	species137 -> species77 + species409	RetroAldol-Oxygen	80.532377
4651	species139 -> species54 + species415	RetroAldol-Oxygen	0.360544
4652	species145 -> species77 + species419	RetroAldol-Oxygen	80.532377
4653	species150 -> species77 + species433	RetroAldol-Oxygen	75.296143
4654	species151 -> species63 + species436	RetroAldol-Oxygen	-8.738326
4655	species152 -> species71 + species415	RetroAldol-Oxygen	12.465985
4656	species153 -> species63 + species436	RetroAldol-Oxygen	-5.199792
4657	species154 -> species77 + species440	RetroAldol-Oxygen	79.794570
4658	species183 -> species77 + species462	RetroAldol-Oxygen	80.532377
4659	species184 -> species77 + species463	RetroAldol-Oxygen	84.990638
4660	species187 -> species54 + species64	RetroAldol-Oxygen	2.280376
4661	species188 -> species208 + species211	RetroAldol-Oxygen	65.000197
4662	species189 -> species203 + species212	RetroAldol-Oxygen	-7.216814
4663	species189 -> species54 + species472	RetroAldol-Oxygen	0.727895
4664	species190 -> species198 + species208	RetroAldol-Oxygen	69.498625
4665	species190 -> species54 + species472	RetroAldol-Oxygen	73.429409
4666	species191 -> species54 + species208	RetroAldol-Oxygen	69.498625
4667	species192 -> species64 + species71	RetroAldol-Oxygen	18.842083
4668	species193 -> species75 + species77	RetroAldol-Oxygen	79.794570
4669	species193 -> species77 + species80	RetroAldol-Oxygen	75.296143
4670	species195 -> species77 + species478	RetroAldol-Oxygen	70.297350
4671	species196 -> species71 + species472	RetroAldol-Oxygen	89.991104
4672	species200 -> species77 + species482	RetroAldol-Oxygen	70.330404
4673	species201 -> species71 + species472	RetroAldol-Oxygen	17.289598
4674	species201 -> species203 + species231	RetroAldol-Oxygen	-8.769329
4675	species202 -> 2species203	RetroAldol-Oxygen	58.931389
4676	species204 -> species77 + species489	RetroAldol-Oxygen	79.794570
4677	species205 -> species208 + species240	RetroAldol-Oxygen	60.036509
4678	species206 -> species208 + species226	RetroAldol-Oxygen	60.001447
4679	species207 -> species63 + species208	RetroAldol-Oxygen	60.034459
4680	species213 -> species54 + species494	RetroAldol-Oxygen	73.429409
4681	species213 -> species208 + species250	RetroAldol-Oxygen	93.847915
4682	species214 -> species77 + species203	RetroAldol-Oxygen	70.297350
4683	species215 -> species54 + species203	RetroAldol-Oxygen	68.430617
4684	species215 -> species63 + species208	RetroAldol-Oxygen	64.532886
4685	species216 -> species54 + species345	RetroAldol-Oxygen	2.280376
4686	species217 -> species71 + species208	RetroAldol-Oxygen	86.060361
4687	species230 -> species63 + species71	RetroAldol-Oxygen	20.859110
4688	species233 -> species77 + species399	RetroAldol-Oxygen	79.794570
4689	species234 -> species54 + species348	RetroAldol-Oxygen	4.774634
4690	species235 -> species63 + species71	RetroAldol-Oxygen	16.360683
4691	species236 -> species77 + species393	RetroAldol-Oxygen	75.296143
4692	species237 -> species71 + species345	RetroAldol-Oxygen	18.840050
4693	species243 -> species77 + species513	RetroAldol-Oxygen	70.297350
4694	species244 -> species71 + species494	RetroAldol-Oxygen	89.991104
4695	species245 -> species71 + species203	RetroAldol-Oxygen	84.990303
4696	species249 -> species77 + species516	RetroAldol-Oxygen	70.297350
4697	species251 -> species77 + species226	RetroAldol-Oxygen	70.297350
4698	species254 -> species54 + species203	RetroAldol-Oxygen	-7.216814
4699	species274 -> species71 + species115	RetroAldol-Oxygen	35.126851
4700	species282 -> species77 + species115	RetroAldol-Oxygen	80.532377
4701	species293 -> species208 + species393	RetroAldol-Oxygen	65.000197

4702	species294 -> species71 + species211	RetroAldol-Oxygen	21.326430
4703	species295 -> species203 + species345	RetroAldol-Oxygen	-7.218864
4704	species296 -> species71 + species198	RetroAldol-Oxygen	25.824861
4705	species297 -> species208 + species399	RetroAldol-Oxygen	69.498625
4706	species297 -> species54 + species603	RetroAldol-Oxygen	73.429409
4707	species298 -> species212 + species348	RetroAldol-Oxygen	4.774634
4708	species298 -> species54 + species240	RetroAldol-Oxygen	0.727895
4709	species299 -> species54 + species71	RetroAldol-Oxygen	25.826891
4710	species302 -> species54 + species217	RetroAldol-Oxygen	0.727895
4711	species305 -> species71 + species217	RetroAldol-Oxygen	17.289598
4712	species307 -> species208 + species375	RetroAldol-Oxygen	60.034459
4713	species307 -> species77 + species490	RetroAldol-Oxygen	70.330404
4714	species333 -> species71 + species240	RetroAldol-Oxygen	16.362712
4715	species334 -> species71 + species603	RetroAldol-Oxygen	89.991104
4716	species335 -> species231 + species348	RetroAldol-Oxygen	3.222149
4717	species335 -> species71 + species240	RetroAldol-Oxygen	17.289598
4718	species336 -> species54 + species669	RetroAldol-Oxygen	0.727895
4719	species338 -> species71 + species669	RetroAldol-Oxygen	17.287568
4720	species340 -> species77 + species502	RetroAldol-Oxygen	70.330404
4721	species342 -> species71 + species226	RetroAldol-Oxygen	16.329679
4722	species344 -> species203 + species348	RetroAldol-Oxygen	70.924867
4723	species347 -> species77 + species497	RetroAldol-Oxygen	70.330404
4724	species369 -> species54 + species71	RetroAldol-Oxygen	18.842083
4725	species374 -> species54 + species707	RetroAldol-Oxygen	17.132447
4726	species375 -> species77 + species348	RetroAldol-Oxygen	82.288820
4727	species381 -> species77 + species328	RetroAldol-Oxygen	80.532377
4728	species394 -> species77 + species503	RetroAldol-Oxygen	79.794570
4729	species395 -> species77 + species504	RetroAldol-Oxygen	79.794570
4730	species397 -> species71 + species250	RetroAldol-Oxygen	50.176160
4731	species398 -> species77 + species498	RetroAldol-Oxygen	70.297350
4732	species411 -> species54 + species735	RetroAldol-Oxygen	2.280376
4733	species413 -> species203 + species436	RetroAldol-Oxygen	-8.771338
4734	species425 -> species77 + species749	RetroAldol-Oxygen	80.532377
4735	species427 -> species63 + species677	RetroAldol-Oxygen	19.914108
4736	species428 -> species77 + species753	RetroAldol-Oxygen	75.296143
4737	species429 -> species63 + species677	RetroAldol-Oxygen	24.412535
4738	species430 -> species71 + species735	RetroAldol-Oxygen	18.842083
4739	species431 -> species77 + species757	RetroAldol-Oxygen	82.479987
4740	species436 -> species71 + species77	RetroAldol-Oxygen	96.356265
4741	species465 -> species54 + species212	RetroAldol-Oxygen	1.320462
4742	species466 -> species77 + species211	RetroAldol-Oxygen	75.296143
4743	species467 -> species77 + species198	RetroAldol-Oxygen	79.794570
4744	species468 -> species71 + species212	RetroAldol-Oxygen	18.842083
4745	species468 -> species54 + species231	RetroAldol-Oxygen	0.727895
4746	species474 -> species77 + species240	RetroAldol-Oxygen	70.330404
4747	species475 -> species71 + species231	RetroAldol-Oxygen	17.289598
4748	species476 -> species77 + species250	RetroAldol-Oxygen	104.143860
4749	species483 -> species71 + species203	RetroAldol-Oxygen	16.327650
4750	species487 -> species77 + species776	RetroAldol-Oxygen	91.977207
4751	species490 -> species208 + species348	RetroAldol-Oxygen	71.992916
4752	species492 -> species203 + species208	RetroAldol-Oxygen	60.001447
4753	species505 -> species77 + species707	RetroAldol-Oxygen	94.646641
4754	species510 -> 2species71	RetroAldol-Oxygen	42.386556
4755	species533 -> species54 + species510	RetroAldol-Oxygen	0.727895
4756	species541 -> species71 + species510	RetroAldol-Oxygen	17.289598
4757	species547 -> species71 + species375	RetroAldol-Oxygen	16.362712
4758	species547 -> species77 + species660	RetroAldol-Oxygen	70.330404
4759	species560 -> species345 + species348	RetroAldol-Oxygen	4.774634
4760	species561 -> species71 + species399	RetroAldol-Oxygen	25.826891

4761	species562 -> species71 + species393	RetroAldol-Oxygen	21.328459
4762	species575 -> species54 + species436	RetroAldol-Oxygen	0.727895
4763	species577 -> species71 + species436	RetroAldol-Oxygen	17.287568
4764	species578 -> species77 + species375	RetroAldol-Oxygen	70.330404
4765	species587 -> species54 + species891	RetroAldol-Oxygen	2.280376
4766	species596 -> species208 + species707	RetroAldol-Oxygen	84.350695
4767	species614 -> species54 + species495	RetroAldol-Oxygen	69.498625
4768	species617 -> species71 + species495	RetroAldol-Oxygen	86.058311
4769	species627 -> species71 + species891	RetroAldol-Oxygen	17.882165
4770	species629 -> species348 + species436	RetroAldol-Oxygen	2.262230
4771	species630 -> species63 + species500	RetroAldol-Oxygen	16.085576
4772	species635 -> species63 + species500	RetroAldol-Oxygen	12.547063
4773	species636 -> species77 + species655	RetroAldol-Oxygen	75.296143
4774	species637 -> species54 + species785	RetroAldol-Oxygen	-2.069908
4775	species638 -> species77 + species657	RetroAldol-Oxygen	79.794570
4776	species646 -> species54 + species518	RetroAldol-Oxygen	-4.686247
4777	species648 -> species71 + species518	RetroAldol-Oxygen	17.289598
4778	species650 -> species77 + species758	RetroAldol-Oxygen	70.330404
4779	species654 -> species54 + species500	RetroAldol-Oxygen	22.011242
4780	species656 -> species71 + species500	RetroAldol-Oxygen	38.572945
4781	species658 -> species77 + species785	RetroAldol-Oxygen	75.444256
4782	species660 -> species71 + species348	RetroAldol-Oxygen	28.321145
4783	species733 -> species203 + species677	RetroAldol-Oxygen	19.881075
4784	species823 -> species54 + species790	RetroAldol-Oxygen	0.727895
4785	species824 -> species54 + species789	RetroAldol-Oxygen	-4.151783
4786	species840 -> species71 + species790	RetroAldol-Oxygen	17.289598
4787	species841 -> species71 + species789	RetroAldol-Oxygen	12.409932
4788	species851 -> species77 + species960	RetroAldol-Oxygen	70.330404
4789	species853 -> species77 + species955	RetroAldol-Oxygen	58.116722
4790	species855 -> species71 + species707	RetroAldol-Oxygen	40.676927
4791	species861 -> species348 + species677	RetroAldol-Oxygen	31.872540
4792	species878 -> species54 + species677	RetroAldol-Oxygen	29.378287
4793	species879 -> species71 + species677	RetroAldol-Oxygen	45.939985
4794	species887 -> species203 + species500	RetroAldol-Oxygen	12.514030
4795	species889 -> species208 + species785	RetroAldol-Oxygen	65.148353
4796	species894 -> species54 + species969	RetroAldol-Oxygen	18.737111
4797	species903 -> species54 + species740	RetroAldol-Oxygen	-5.650199
4798	species904 -> species71 + species740	RetroAldol-Oxygen	10.909470
4799	species932 -> species71 + species969	RetroAldol-Oxygen	35.298814
4800	species939 -> species77 + species1045	RetroAldol-Oxygen	74.572436
4801	species1019 -> species71 + species785	RetroAldol-Oxygen	21.474568
4802	species1021 -> species348 + species500	RetroAldol-Oxygen	24.505496
4803	species2 + species56 -> species3 + species45	ReverseWaterGasShift-Oxygen	40.139723
4804	species3 + species45 -> species2 + species56	WaterGasShift-Oxygen	-40.139706

Table 10. Species names and thermodynamic data.

Species #	Rank	MWT	#C	#H	#O	Name	ΔH_f (kJ mol ⁻¹)	ΔG_f (kJ mol ⁻¹)
1	0	182.174	6	14	6	hexane-1,2,3,4,5,6-hexaol	-198.600	-4.200
2	0	2.016	0	2	0	hydrogen	0.000	0.000
3	0	18.015	0	2	1	water	5.549	-34.967
4	1	164.159	6	12	5	2-(1,2-dihydroxyethyl)tetrahydrofuran-3,4-diol	-951.900	-681.334
5	1	164.159	6	12	5	2,5-bis(hydroxymethyl)tetrahydrofuran-3,4-diol	-944.002	-680.061
6	1	164.159	6	12	5	2-(hydroxymethyl)tetrahydro-2H-pyran-3,4,5-triol	-954.226	-683.194
7	1	180.158	6	12	6	2,3,4,5,6-pentahydroxyhexanal	-1117.924	-839.007
8	1	164.159	6	12	5	3,4,5,6-tetrahydroxyhexan-2-one	-966.502	-697.994
9	1	164.159	6	12	5	3,4,5,6-tetrahydroxyhexanal	-959.049	-703.137
10	1	164.159	6	12	5	1,4,5,6-tetrahydroxyhexan-3-one	-962.002	-692.643
11	1	164.159	6	12	5	1,4,5,6-tetrahydroxyhexan-2-one	-962.002	-692.643
12	1	164.159	6	12	5	1,2,5,6-tetrahydroxyhexan-3-one	-962.961	-694.149
13	2	146.144	6	10	4	hexahydrofuro[3,2-b]furan-3,6-diol	-728.983	-506.239
14	2	162.143	6	10	5	2-(3,4-dihydroxytetrahydrofuran-2-yl)-2-hydroxyacetaldehyde	-930.805	-661.951
15	2	146.144	6	10	4	1-(3-hydroxy-2,5-dihydrofuran-2-yl)ethane-1,2-diol	-668.217	-476.393

16	2	146.144	6	10	4 1-(3-hydroxy-2,3-dihydrofuran-2-yl)ethane-1,2-diol	-674.610	-467.160
17	2	146.144	6	10	4 1-(4-hydroxy-4,5-dihydrofuran-2-yl)ethane-1,2-diol	-672.139	-485.501
18	2	146.144	6	10	4 1-(4-hydroxy-2,5-dihydrofuran-2-yl)ethane-1,2-diol	-668.217	-476.393
19	2	146.144	6	10	4 2-(3,4-dihydroxytetrahydrofuran-2-yl)acetaldehyde	-757.596	-518.842
20	2	146.144	6	10	4 1-(3,4-dihydroxytetrahydrofuran-2-yl)ethanone	-778.680	-527.158
21	2	146.144	6	10	4 2-(1,2-dihydroxyethyl)dihydrofuran-3(2H)-one	-752.893	-542.783
22	2	146.144	6	10	4 5-(1,2-dihydroxyethyl)dihydrofuran-3(2H)-one	-752.893	-542.783
23	2	166.175	6	14	5 hexane-1,2,3,5,6-pentaol	-966.812	-703.385
24	2	166.175	6	14	5 hexane-1,2,3,4,5-pentaol	-173.200	-9.200
25	2	162.143	6	10	5 3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-carbaldehyde	-929.845	-670.073
26	2	146.144	6	10	4 (3-hydroxy-2,3-dihydrofuran-2,5-diyl)dimethanol	-684.841	-506.009
27	2	146.144	6	10	4 (3-hydroxy-2,5-dihydrofuran-2,5-diyl)dimethanol	-660.319	-475.120
28	2	146.144	6	10	4 2-(hydroxymethyl)-5-methylenetetrahydrofuran-3,4-diol	-751.635	-571.852
29	2	146.144	6	10	4 2,5-bis(hydroxymethyl)dihydrofuran-3(2H)-one	-744.995	-541.510
30	2	166.175	6	14	5 hexane-1,2,3,4,6-pentaol	-978.593	-719.963
31	2	162.143	6	10	5 3,4,5-trihydroxytetrahydro-2H-pyran-2-carbaldehyde	-940.069	-673.206
32	2	146.144	6	10	4 2-methylenetetrahydro-2H-pyran-3,4,5-triol	-761.859	-574.985
33	2	146.144	6	10	4 6-(hydroxymethyl)-3,4-dihydro-2H-pyran-3,4-diol	-695.065	-509.142
34	2	146.144	6	10	4 6-(hydroxymethyl)-3,6-dihydro-2H-pyran-3,4-diol	-670.543	-478.253
35	2	146.144	6	10	4 2-(hydroxymethyl)-3,6-dihydro-2H-pyran-3,4-diol	-670.543	-478.253
36	2	146.144	6	10	4 2-(hydroxymethyl)-3,4-dihydro-2H-pyran-3,4-diol	-676.936	-469.020
37	2	146.144	6	10	4 2-(hydroxymethyl)-3,6-dihydro-2H-pyran-3,5-diol	-670.543	-478.253
38	2	146.144	6	10	4 6-(hydroxymethyl)-3,6-dihydro-2H-pyran-3,5-diol	-670.543	-478.253
39	2	146.144	6	10	4 5-hydroxy-2-(hydroxymethyl)dihydro-2H-pyran-4(3H)-one	-755.219	-544.643
40	2	146.144	6	10	4 5-hydroxy-2-(hydroxymethyl)dihydro-2H-pyran-3(4H)-one	-755.219	-544.643
41	2	146.144	6	10	4 3-hydroxy-2-(hydroxymethyl)dihydro-2H-pyran-4(3H)-one	-755.219	-544.643
42	2	146.144	6	10	4 5-hydroxy-6-(hydroxymethyl)dihydro-2H-pyran-3(4H)-one	-755.219	-544.643
43	2	178.142	6	10	6 2,3,4,5-tetrahydroxyhexanedial	-1104.158	-830.172
44	2	152.148	5	12	5 pentane-1,2,3,4,5-pentaol	-72.400	-730.584
45	2	28.01	1	0	1 carbon monoxide	5.549	-34.967
46	2	162.143	6	10	5 4,5,6-trihydroxy-3-oxohexanal	-943.417	-677.323
47	2	162.143	6	10	5 4,5,6-trihydroxy-2-oxohexanal	-870.785	-596.759
48	2	162.143	6	10	5 2,5,6-trihydroxy-4-oxohexanal	-941.866	-674.766
49	2	162.143	6	10	5 2,5,6-trihydroxy-3-oxohexanal	-941.866	-674.766
50	2	162.143	6	10	5 2,3,6-trihydroxy-5-oxohexanal	-941.866	-674.766
51	2	162.143	6	10	5 2,3,6-trihydroxy-4-oxohexanal	-941.866	-674.766
52	2	162.143	6	10	5 2,3,4-trihydroxyhexanedial	-377.800	-160.000
53	2	162.143	6	10	5 2,3,4-trihydroxy-5-oxohexanal	-946.366	-680.117
54	2	60.053	2	4	2 2-hydroxyacetaldehyde	-374.244	-291.621
55	2	120.106	4	8	4 2,3,4-trihydroxybutanal	-750.228	-571.341
56	3	44.01	1	0	2 carbon dioxide	-1273.300	-155.634
57	2	146.144	6	10	4 5,6-dihydroxyhexane-2,4-dione	-797.871	-536.128
58	2	146.144	6	10	4 5,6-dihydroxyhexane-2,3-dione	-711.397	-449.593
59	2	146.144	6	10	4 1,4-dihydroxyhexane-2,5-dione	-783.115	-523.205
60	2	146.144	6	10	4 3,6-dihydroxyhexane-2,4-dione	-783.115	-523.205
61	2	146.144	6	10	4 3,4-dihydroxyhexane-2,5-dione	-787.615	-528.556
62	2	146.144	6	10	4 3,4-dihydroxy-5-oxohexanal	-780.162	-533.699
63	2	74.08	3	6	2 1-hydroxypropan-2-one	-408.446	-283.665
64	2	90.079	3	6	3 2,3-dihydroxypropanal	-562.236	-431.481
65	2	136.149	5	12	4 pentane-1,2,3,4-tetraol	-800.095	-587.656
66	2	146.144	6	10	4 5,6-dihydroxy-4-oxohexanal	-776.254	-529.399
67	2	146.144	6	10	4 5,6-dihydroxy-3-oxohexanal	-0.400	72.000
68	2	146.144	6	10	4 3,6-dihydroxy-5-oxohexanal	-775.662	-528.348
69	2	146.144	6	10	4 3,6-dihydroxy-4-oxohexanal	-775.662	-528.348
70	2	146.144	6	10	4 3,4-dihydroxyhexanedial	-104.500	-23.400
71	2	44.053	2	4	1 acetaldehyde	-217.534	-152.756
72	2	146.144	6	10	4 4,5,6-trihydroxyhex-1-en-3-one	-684.475	-468.982
73	2	146.144	6	10	4 1,6-dihydroxyhexane-2,4-dione	-297.400	-527.032
74	2	146.144	6	10	4 1,6-dihydroxyhexane-3,4-dione	-701.903	-442.040
75	2	104.106	4	8	3 1,4-dihydroxybutan-2-one	-586.977	-414.429
76	2	134.133	5	10	4 3,4,5-trihydroxypentan-2-one	109.900	151.900
77	2	30.026	1	2	1 formaldehyde	-175.055	-155.634
78	2	146.144	6	10	4 1,6-dihydroxyhexane-2,5-dione	-779.207	-518.905
79	2	134.133	5	10	4 1,4,5-trihydroxypentan-2-one	-774.969	-554.289
80	2	104.106	4	8	3 3,4-dihydroxybutan-2-one	-591.477	-419.780
81	3	128.128	6	8	3 2,3,3a,6a-tetrahydrofuro[3,2-b]furan-3-ol	-451.693	-292.065
82	3	128.128	6	8	3 2,3,3a,5-tetrahydrofuro[3,2-b]furan-3-ol	-453.350	-304.322
83	3	148.16	6	12	4 1-(4-hydroxytetrahydrofuran-2-yl)ethane-1,2-diol	-771.601	-527.079
84	3	148.16	6	12	4 2-(1-hydroxyethyl)tetrahydrofuran-3,4-diol	-792.680	-538.406
85	3	134.133	5	10	4 2-(hydroxymethyl)tetrahydrofuran-3,4-diol	-755.352	-542.226

86	3	144.128	6	8	4	2-(3,4-dihydroxydihydrofuran-2(3H)-ylidene)acetaldehyde	-659.067	-445.689
87	3	144.128	6	8	4	2-hydroxy-2-(3-hydroxy-2,5-dihydrofuran-2-yl)acetaldehyde	-647.122	-457.010
88	3	144.128	6	8	4	2-hydroxy-2-(3-hydroxy-2,3-dihydrofuran-2-yl)acetaldehyde	-653.515	-447.777
89	3	144.128	6	8	4	2-hydroxy-2-(4-hydroxy-4,5-dihydrofuran-2-yl)acetaldehyde	-651.044	-466.118
90	3	144.128	6	8	4	2-hydroxy-2-(4-hydroxy-2,5-dihydrofuran-2-yl)acetaldehyde	-647.122	-457.010
91	3	144.128	6	8	4	2-hydroxy-2-(3-oxotetrahydrofuran-2-yl)acetaldehyde	-731.798	-523.400
92	3	144.128	6	8	4	2-hydroxy-2-(4-oxotetrahydrofuran-2-yl)acetaldehyde	-731.798	-523.400
93	3	164.159	6	12	5	2,3,4,5-tetrahydroxyhexanal	-966.992	-708.133
94	3	164.159	6	12	5	2,4,5,6-tetrahydroxyhexanal	-956.539	-699.074
95	3	128.128	6	8	3	2-(3-hydroxy-2,5-dihydrofuran-2-yl)acetaldehyde	-473.913	-313.901
96	3	128.128	6	8	3	1-(3-hydroxy-2,5-dihydrofuran-2-yl)ethanone	-317.900	-180.300
97	3	148.16	6	12	4	1-(3-hydroxytetrahydrofuran-2-yl)ethane-1,2-diol	-771.601	-527.079
98	3	128.128	6	8	3	1-(furan-2-yl)ethane-1,2-diol	-459.144	-338.383
99	3	128.128	6	8	3	2-(3-hydroxy-2,3-dihydrofuran-2-yl)acetaldehyde	-480.306	-304.668
100	3	128.128	6	8	3	1-(3-hydroxy-2,3-dihydrofuran-2-yl)ethanone	-501.390	-312.984
101	3	128.128	6	8	3	2-(4-hydroxy-4,5-dihydrofuran-2-yl)acetaldehyde	-498.435	-344.790
102	3	128.128	6	8	3	1-(4-hydroxy-4,5-dihydrofuran-2-yl)ethanone	-526.863	-347.639
103	3	128.128	6	8	3	2-(4-hydroxy-2,5-dihydrofuran-2-yl)acetaldehyde	-473.913	-313.901
104	3	128.128	6	8	3	1-(4-hydroxy-2,5-dihydrofuran-2-yl)ethanone	-84.000	-322.217
105	3	148.16	6	12	4	2-(2-hydroxyethyl)tetrahydrofuran-3,4-diol	-777.140	-535.668
106	3	118.133	5	10	3	2-methyltetrahydrofuran-3,4-diol	-598.618	-404.515
107	3	128.128	6	8	3	2-(4-oxotetrahydrofuran-2-yl)acetaldehyde	-558.589	-380.291
108	3	128.128	6	8	3	2-(3-oxotetrahydrofuran-2-yl)acetaldehyde	-558.589	-380.291
109	3	148.16	6	12	4	3,4,5-trihydroxyhexanal	-800.788	-561.715
110	3	148.16	6	12	4	4,5,6-trihydroxyhexanal	-790.927	-553.707
111	3	128.128	6	8	3	2-acetyldihydrofuran-3(2H)-one	-579.673	-388.607
112	3	128.128	6	8	3	5-acetyldihydrofuran-3(2H)-one	-579.673	-388.607
113	3	148.16	6	12	4	3,4,5-trihydroxyhexan-2-one	-808.241	-556.572
114	3	148.16	6	12	4	4,5,6-trihydroxyhexan-2-one	-812.544	-560.436
115	3	86.091	4	6	2	dihydrofuran-3(2H)-one	-367.695	-265.840
116	3	148.16	6	12	4	(3-hydroxytetrahydrofuran-2,5-diyl)dimethanol	-763.703	-525.806
117	3	148.16	6	12	4	6-(hydroxymethyl)tetrahydro-2H-pyran-3,4-diol	-773.927	-528.939
118	3	148.16	6	12	4	2-(hydroxymethyl)tetrahydro-2H-pyran-3,5-diol	-773.927	-528.939
119	3	164.159	6	12	5	2,3,5,6-tetrahydroxyhexanal	-953.046	-694.550
120	3	148.16	6	12	4	3,5,6-trihydroxyhexan-2-one	-10.000	64.400
121	3	148.16	6	12	4	3,5,6-trihydroxyhexanal	-792.253	-555.668
122	3	148.16	6	12	4	1,5,6-trihydroxyhexan-2-one	-795.798	-546.225
123	3	148.16	6	12	4	1,5,6-trihydroxyhexan-3-one	-805.001	-554.352
124	3	148.16	6	12	4	2-(hydroxymethyl)-5-methyltetrahydrofuran-3,4-diol	-787.268	-542.350
125	3	148.16	6	12	4	2-methyltetrahydro-2H-pyran-3,4,5-triol	-797.492	-545.483
126	3	148.16	6	12	4	2,5,6-trihydroxyhexan-3-one	-803.741	-551.221
127	3	148.16	6	12	4	1,2,5-trihydroxyhexan-3-one	-803.741	-551.221
128	3	148.16	6	12	4	1,4,5-trihydroxyhexan-2-one	-353.600	-163.300
129	3	148.16	6	12	4	1,4,5-trihydroxyhexan-3-one	-803.741	-551.221
130	3	148.16	6	12	4	4,5,6-trihydroxyhexan-3-one	-805.292	-553.778
131	3	160.127	6	8	5	3,4-dihydroxytetrahydrofuran-2,5-dicarbaldehyde	-62.300	-660.085
132	3	144.128	6	8	4	4-hydroxy-5-(hydroxymethyl)-4,5-dihydrofuran-2-carbaldehyde	-685.551	-494.790
133	3	144.128	6	8	4	4-hydroxy-5-(hydroxymethyl)-2,5-dihydrofuran-2-carbaldehyde	-646.162	-465.132
134	3	144.128	6	8	4	3-hydroxy-5-(hydroxymethyl)-2,5-dihydrofuran-2-carbaldehyde	-646.162	-465.132
135	3	144.128	6	8	4	3-hydroxy-5-(hydroxymethyl)-2,3-dihydrofuran-2-carbaldehyde	-670.684	-496.021
136	3	144.128	6	8	4	3,4-dihydroxy-5-methylenetetrahydrofuran-2-carbaldehyde	-737.478	-561.864
137	3	144.128	6	8	4	5-(hydroxymethyl)-4-oxotetrahydrofuran-2-carbaldehyde	-730.838	-531.522
138	3	144.128	6	8	4	5-(hydroxymethyl)-3-oxotetrahydrofuran-2-carbaldehyde	-730.838	-531.522
139	3	164.159	6	12	5	2,3,4,6-tetrahydroxyhexanal	-956.539	-699.074
140	3	128.128	6	8	3	furan-2,5-diyl dimethanol	-494.429	-379.576
141	3	128.128	6	8	3	5-(hydroxymethyl)-2-methylene-2,3-dihydrofuran-3-ol	-492.474	-397.800
142	3	128.128	6	8	3	2-(hydroxymethyl)-5-methylene-2,5-dihydrofuran-3-ol	-483.702	-377.330
143	3	128.128	6	8	3	5-(hydroxymethyl)-2-methylene-2,5-dihydrofuran-3-ol	-547.997	-444.386
144	3	128.128	6	8	3	2,5-dimethylenetetrahydrofuran-3,4-diol	-549.857	-453.545
145	3	128.128	6	8	3	2-(hydroxymethyl)-5-methylenedihydrofuran-3(2H)-one	-555.143	-436.152
146	3	128.128	6	8	3	5-(hydroxymethyl)-2-methylenedihydrofuran-3(2H)-one	-556.592	-437.158
147	3	116.117	5	8	3	5-(hydroxymethyl)dihydrofuran-3(2H)-one	-556.345	-403.675
148	3	148.16	6	12	4	2-(hydroxymethyl)tetrahydro-2H-pyran-3,4-diol	-773.927	-528.939
149	3	148.16	6	12	4	hex-5-ene-1,2,3,4-tetraol	-695.184	-489.433
150	3	148.16	6	12	4	1,4,6-trihydroxyhexan-3-one	-795.206	-545.174
151	3	148.16	6	12	4	1,4,6-trihydroxyhexan-2-one	-795.206	-545.174
152	3	148.16	6	12	4	3,4,6-trihydroxyhexanal	-785.883	-546.626
153	3	148.16	6	12	4	3,4,6-trihydroxyhexan-2-one	-798.747	-549.019
154	3	148.16	6	12	4	1,2,6-trihydroxyhexan-3-one	-795.798	-546.225
155	3	134.133	5	10	4	tetrahydro-2H-pyran-3,4,5-triol	-765.576	-545.359

156	3	144.128	6	8	4	3,4-dihydroxy-3,4-dihydro-2H-pyran-6-carbaldehyde	-695.775	-497.923
157	3	144.128	6	8	4	4,5-dihydroxy-5,6-dihydro-2H-pyran-2-carbaldehyde	-656.386	-468.265
158	3	144.128	6	8	4	3,4-dihydroxy-3,4-dihydro-2H-pyran-2-carbaldehyde	-662.779	-459.032
159	3	144.128	6	8	4	3,4-dihydroxy-3,6-dihydro-2H-pyran-2-carbaldehyde	-656.386	-468.265
160	3	144.128	6	8	4	3,5-dihydroxy-5,6-dihydro-2H-pyran-2-carbaldehyde	-656.386	-468.265
161	3	144.128	6	8	4	3,5-dihydroxy-3,6-dihydro-2H-pyran-2-carbaldehyde	-656.386	-468.265
162	3	144.128	6	8	4	5-hydroxy-4-oxotetrahydro-2H-pyran-2-carbaldehyde	-741.062	-534.655
163	3	144.128	6	8	4	5-hydroxy-3-oxotetrahydro-2H-pyran-2-carbaldehyde	-741.062	-534.655
164	3	144.128	6	8	4	3-hydroxy-4-oxotetrahydro-2H-pyran-2-carbaldehyde	-741.062	-534.655
165	3	144.128	6	8	4	3-hydroxy-5-oxotetrahydro-2H-pyran-2-carbaldehyde	-741.062	-534.655
166	3	128.128	6	8	3	6-methylene-3,6-dihydro-2H-pyran-3,4-diol	-493.926	-380.463
167	3	128.128	6	8	3	2-methylene-3,4-dihydro-2H-pyran-3,4-diol	-484.569	-360.811
168	3	128.128	6	8	3	2-methylene-3,6-dihydro-2H-pyran-3,4-diol	-478.176	-370.044
169	3	128.128	6	8	3	6-methylene-3,6-dihydro-2H-pyran-3,5-diol	-493.926	-380.463
170	3	128.128	6	8	3	2-methylene-3,6-dihydro-2H-pyran-3,5-diol	-478.176	-370.044
171	3	128.128	6	8	3	5-hydroxy-2-methylenedihydro-2H-pyran-4(3H)-one	-565.367	-439.285
172	3	128.128	6	8	3	5-hydroxy-2-methylenedihydro-2H-pyran-3(4H)-one	-566.816	-440.291
173	3	128.128	6	8	3	3-hydroxy-2-methylenedihydro-2H-pyran-4(3H)-one	-562.852	-436.434
174	3	128.128	6	8	3	5-hydroxy-6-methylenedihydro-2H-pyran-3(4H)-one	-562.852	-436.434
175	3	128.128	6	8	3	6-(hydroxymethyl)-2H-pyran-3-ol	-480.131	-351.820
176	3	128.128	6	8	3	2-(hydroxymethyl)-4H-pyran-4-ol	-417.775	-294.968
177	3	128.128	6	8	3	6-(hydroxymethyl)-2H-pyran-4-ol	-411.382	-304.201
178	3	128.128	6	8	3	6-(hydroxymethyl)-2H-pyran-3(4H)-one	-496.058	-370.591
179	3	128.128	6	8	3	6-(hydroxymethyl)-2H-pyran-4(3H)-one	-496.058	-370.591
180	3	128.128	6	8	3	2-(hydroxymethyl)-2H-pyran-4-ol	-453.094	-350.572
181	3	128.128	6	8	3	2-(hydroxymethyl)-2H-pyran-3-ol	-457.548	-331.135
182	3	128.128	6	8	3	2-(hydroxymethyl)-2H-pyran-4(3H)-one	-473.475	-349.906
183	3	128.128	6	8	3	2-(hydroxymethyl)-2H-pyran-3(4H)-one	-477.929	-330.469
184	3	128.128	6	8	3	2-(hydroxymethyl)-2H-pyran-3(6H)-one	-477.929	-330.469
185	3	116.117	5	8	3	5-hydroxydihydro-2H-pyran-3(4H)-one	-566.569	-406.808
186	3	128.128	6	8	3	6-(hydroxymethyl)-2H-pyran-3(6H)-one	-477.929	-330.469
187	3	150.132	5	10	5	2,3,4,5-tetrahydroxypentanal	-938.220	-711.201
188	3	160.127	6	8	5	2,5-dihydroxy-3-oxohexanedial	-920.771	-655.383
189	3	160.127	6	8	5	2,3-dihydroxy-5-oxohexanedial	-849.690	-577.376
190	3	160.127	6	8	5	2,3-dihydroxy-4-oxohexanedial	-922.322	-657.940
191	3	118.09	4	6	4	2,3-dihydroxysuccinaldehyde	-729.133	-551.958
192	3	134.133	5	10	4	3,4,5-trihydroxypentanal	-772.016	-564.783
193	3	134.133	5	10	4	1,2,5-trihydroxypentan-3-one	-774.969	-554.289
194	3	144.128	6	8	4	6-hydroxy-3,5-dioxohexanal	-768.866	-510.206
195	3	144.128	6	8	4	6-hydroxy-3,4-dioxohexanal	-682.359	-425.214
196	3	144.128	6	8	4	3-hydroxy-4-oxohexanedial	-756.118	-511.522
197	3	144.128	6	8	4	4-hydroxy-3,5-dioxohexanal	-763.571	-506.379
198	3	102.09	4	6	3	4-hydroxy-3-oxobutanal	-567.433	-397.603
199	3	144.128	6	8	4	6-hydroxy-2,5-dioxohexanal	-687.031	-421.515
200	3	144.128	6	8	4	6-hydroxy-2,4-dioxohexanal	-696.234	-429.642
201	3	144.128	6	8	4	4-hydroxy-2-oxohexanedial	-683.486	-430.958
202	3	144.128	6	8	4	4-hydroxy-2,5-dioxohexanal	-690.939	-425.815
203	3	72.064	3	4	2	2-oxopropanal	-316.303	-184.732
204	3	144.128	6	8	4	5,6-dihydroxy-4-oxohex-2-enal	-583.097	-364.180
205	3	144.128	6	8	4	2-hydroxy-4-oxohexanedial	-764.362	-518.143
206	3	144.128	6	8	4	2-hydroxy-4,5-dioxohexanal	-690.302	-430.210
207	3	132.117	5	8	4	2,5-dihydroxy-4-oxopentanal	-753.874	-534.906
208	3	58.037	2	2	2	oxalaldehyde	-285.995	-183.645
209	3	144.128	6	8	4	2-hydroxy-3-oxohexanedial	-755.159	-510.016
210	3	144.128	6	8	4	2-hydroxy-3,5-dioxohexanal	-776.776	-516.745
211	3	102.09	4	6	3	2-hydroxy-3-oxobutanal	-570.382	-400.397
212	3	88.063	3	4	3	2-hydroxymalonaldehyde	-541.141	-412.098
213	3	144.128	6	8	4	2,3-dihydroxy-4-oxohex-5-enal	-663.380	-449.599
214	3	102.09	4	6	3	4-hydroxy-2-oxobutanal	-494.801	-317.039
215	3	132.117	5	8	4	2,3-dihydroxy-4-oxopentanal	-758.374	-540.257
216	3	134.133	5	10	4	2,3,4-trihydroxypentanal	-327.400	-168.900
217	3	102.09	4	6	3	2-hydroxysuccinaldehyde	-562.929	-405.540
218	3	62.069	2	6	2	ethane-1,2-diol	-395.339	-311.004
219	3	32.042	1	4	1	methanol	-215.290	-176.140
220	3	122.122	4	10	4	butane-1,2,3,4-tetraol	-770.364	-589.218
221	3	92.095	3	8	3	propane-1,2,3-triol	-583.331	-450.864
222	3	128.128	6	8	3	hexane-2,3,5-trione	-546.307	-291.572
223	3	128.128	6	8	3	3,5-dioxohexanal	-620.367	-379.505
224	3	116.117	5	8	3	1-hydroxypentane-2,4-dione	-609.879	-396.268
225	3	128.128	6	8	3	4,5-dioxohexanal	-524.690	-284.843

226	3	86.091	4	6	2 biacetyl	-344.907	-177.426
227	3	128.128	6	8	3 1-hydroxyhex-3-ene-2,5-dione	-425.413	-225.407
228	3	128.128	6	8	3 3-hydroxyhex-5-ene-2,4-dione	-504.629	-298.038
229	3	116.117	5	8	3 3-hydroxypentane-2,4-dione	-599.623	-388.696
230	3	118.133	5	10	3 3,4-dihydroxypentan-2-one	-620.249	-416.712
231	3	72.064	3	4	2 malonaldehyde	-376.488	-268.237
232	3	76.096	3	8	2 propane-1,2-diol	-424.111	-307.936
233	3	118.133	5	10	3 1,2-dihydroxypentan-3-one	-617.300	-413.918
234	3	118.133	5	10	3 4,5-dihydroxypentan-2-one	-626.470	-423.588
235	3	118.133	5	10	3 1,4-dihydroxypentan-2-one	-615.749	-411.361
236	3	118.133	5	10	3 1,4-dihydroxypentan-3-one	-615.749	-411.361
237	3	118.133	5	10	3 3,4-dihydroxypentanal	-612.796	-421.855
238	3	128.128	6	8	3 3-oxohexanedial	-598.750	-372.776
239	3	116.117	5	8	3 5-hydroxy-4-oxopentanal	-588.262	-389.539
240	3	86.091	4	6	2 3-oxobutanal	-418.934	-266.902
241	3	128.128	6	8	3 6-hydroxy-5-oxohex-3-enal	-497.769	-304.947
242	3	128.128	6	8	3 6-hydroxy-5-oxohex-2-enal	-497.769	-304.947
243	3	128.128	6	8	3 6-hydroxy-4-oxohex-2-enal	-425.137	-224.383
244	3	128.128	6	8	3 3-hydroxy-4-oxohex-5-enal	-497.176	-303.181
245	3	116.117	5	8	3 3-hydroxy-4-oxopentanal	-592.170	-393.839
246	3	46.069	2	6	1 ethanol	-236.119	-168.076
247	3	16.043	1	4	0 methane	-241.830	-293.412
248	3	128.128	6	8	3 1-hydroxyhex-5-ene-2,4-dione	-485.598	-308.912
249	3	128.128	6	8	3 6-hydroxyhex-1-ene-3,4-dione	-423.417	-216.873
250	3	86.091	4	6	2 1-hydroxybut-3-en-2-one	-284.165	-196.309
251	3	116.117	5	8	3 5-hydroxypentane-2,3-dione	-523.405	-309.733
252	3	106.122	4	10	3 butane-1,2,4-triol	-603.568	-441.749
253	3	136.149	5	12	4 pentane-1,2,4,5-tetraol	-786.149	-574.073
254	3	132.117	5	8	4 4,5-dihydroxy-2-oxopentanal	-682.793	-456.899
255	3	106.122	4	10	3 butane-1,2,3-triol	-612.103	-447.796
256	4	110.113	6	6	2 2,6a-dihydrofuro[3,2-b]furan	-176.060	-90.148
257	4	110.113	6	6	2 3a,6a-dihydrofuro[3,2-b]furan	-174.403	-77.891
258	4	130.144	6	10	3 1-(2,3-dihydrofuran-2-yl)ethane-1,2-diol	-518.399	-357.971
259	4	130.144	6	10	3 2-(1-hydroxyethyl)-2,3-dihydrofuran-3-ol	-515.390	-324.232
260	4	130.144	6	10	3 hexahydrofuro[3,2-b]furan-3-ol	-548.684	-351.984
261	4	110.113	6	6	2 2,5-dihydrofuro[3,2-b]furan	-177.717	-102.405
262	4	146.144	6	10	4 2-hydroxy-2-(4-hydroxytetrahydrofuran-2-yl)acetaldehyde	-750.506	-507.696
263	4	130.144	6	10	3 1-(2,5-dihydrofuran-2-yl)ethane-1,2-diol	-494.311	-312.905
264	4	130.144	6	10	3 1-(4-hydroxytetrahydrofuran-2-yl)ethanone	-598.381	-372.903
265	4	130.144	6	10	3 2-(4-hydroxytetrahydrofuran-2-yl)acetaldehyde	-577.297	-364.587
266	4	150.176	6	14	4 hexane-1,2,3,5-tetraol	-814.921	-571.005
267	4	150.176	6	14	4 hexane-1,2,5,6-tetraol	-800.608	-556.967
268	4	130.144	6	10	3 5-(1-hydroxyethyl)-2,5-dihydrofuran-3-ol	-508.997	-333.465
269	4	130.144	6	10	3 5-(1-hydroxyethyl)-2,3-dihydrofuran-3-ol	-512.919	-342.573
270	4	130.144	6	10	3 2-vinyltetrahydrofuran-3,4-diol	-499.118	-311.976
271	4	130.144	6	10	3 2-ethylidenetetrahydrofuran-3,4-diol	-580.904	-402.167
272	4	130.144	6	10	3 2-(1-hydroxyethyl)-2,5-dihydrofuran-3-ol	-508.997	-333.465
273	4	130.144	6	10	3 5-(1-hydroxyethyl)dihydrofuran-3(2H)-one	-593.673	-399.855
274	4	130.144	6	10	3 2-(1-hydroxyethyl)dihydrofuran-3(2H)-one	-593.673	-399.855
275	4	150.176	6	14	4 hexane-2,3,4,5-tetraol	-828.867	-584.588
276	4	132.117	5	8	4 3,4-dihydroxytetrahydrofuran-2-carbaldehyde	-741.195	-532.238
277	4	116.117	5	8	3 2-methylenetetrahydrofuran-3,4-diol	-562.985	-434.017
278	4	116.117	5	8	3 2-(hydroxymethyl)-2,5-dihydrofuran-3-ol	-471.669	-337.285
279	4	116.117	5	8	3 2-(hydroxymethyl)-2,3-dihydrofuran-3-ol	-478.062	-328.052
280	4	116.117	5	8	3 5-(hydroxymethyl)-2,3-dihydrofuran-3-ol	-496.191	-368.174
281	4	116.117	5	8	3 5-(hydroxymethyl)-2,5-dihydrofuran-3-ol	-471.669	-337.285
282	4	116.117	5	8	3 2-(hydroxymethyl)dihydrofuran-3(2H)-one	-556.345	-403.675
283	4	136.149	5	12	4 pentane-1,2,3,5-tetraol	-789.642	-578.597
284	4	146.144	6	10	4 2-(2-hydroxyethylidene)tetrahydrofuran-3,4-diol	-774.218	-592.537
285	4	126.112	6	6	3 2-(3-hydroxyfuran-2(5H)-ylidene)acetaldehyde	-375.384	-240.748
286	4	126.112	6	6	3 2-(3-hydroxyfuran-2(3H)-ylidene)acetaldehyde	-381.777	-231.515
287	4	126.112	6	6	3 2-(4-hydroxyfuran-2(5H)-ylidene)acetaldehyde	-375.384	-240.748
288	4	126.112	6	6	3 2-(3-oxodihydrofuran-2(3H)-ylidene)acetaldehyde	-460.060	-307.138
289	4	126.112	6	6	3 2-(4-oxodihydrofuran-2(3H)-ylidene)acetaldehyde	-460.060	-307.138
290	4	146.144	6	10	4 2-hydroxy-2-(3-hydroxytetrahydrofuran-2-yl)acetaldehyde	-750.506	-507.696
291	4	126.112	6	6	3 2-(furan-2-yl)-2-hydroxyacetaldehyde	-438.049	-319.000
292	4	146.144	6	10	4 3,4-dihydroxy-5-methyltetrahydrofuran-2-carbaldehyde	-773.111	-532.362
293	4	146.144	6	10	4 2,5-dihydroxy-4-oxohexanal	-782.646	-531.838
294	4	146.144	6	10	4 2,5-dihydroxy-3-oxohexanal	-782.646	-531.838
295	4	146.144	6	10	4 4,5-dihydroxy-2-oxohexanal	-711.565	-453.831

296	4	146.144	6	10	4 4,5-dihydroxy-3-oxohexanal	-784.197	-534.395
297	4	146.144	6	10	4 2,3-dihydroxy-4-oxohexanal	-784.197	-534.395
298	4	146.144	6	10	4 2,3-dihydroxy-5-oxohexanal	-793.367	-544.065
299	4	104.106	4	8	3 2,3-dihydroxybutanal	-591.008	-428.413
300	4	146.144	6	10	4 4-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-carbaldehyde	-749.546	-515.818
301	4	146.144	6	10	4 4,5-dihydroxytetrahydro-2H-pyran-2-carbaldehyde	-759.770	-518.951
302	4	162.143	6	10	5 2,3,5-trihydroxyhexanediol	-126.500	-15.600
303	4	146.144	6	10	4 4,5,6-trihydroxyhex-2-enal	-680.564	-478.685
304	4	146.144	6	10	4 2,4-dihydroxy-5-oxohexanal	-778.611	-531.142
305	4	146.144	6	10	4 2,4-dihydroxyhexanediol	-771.158	-536.285
306	4	146.144	6	10	4 2,6-dihydroxy-5-oxohexanal	-774.703	-526.842
307	4	146.144	6	10	4 2,6-dihydroxy-4-oxohexanal	-783.906	-534.969
308	4	130.144	6	10	3 2-(2-hydroxyethyl)-2,5-dihydrofuran-3-ol	-505.501	-353.260
309	4	100.118	5	8	2 2-methyl-2,5-dihydrofuran-3-ol	-688.500	-170.602
310	4	130.144	6	10	3 2-(3-hydroxytetrahydrofuran-2-yl)acetaldehyde	-577.297	-364.587
311	4	130.144	6	10	3 1-(3-hydroxytetrahydrofuran-2-yl)ethanone	-598.381	-372.903
312	4	130.144	6	10	3 1-(4,5-dihydrofuran-2-yl)ethane-1,2-diol	-491.840	-331.246
313	4	150.176	6	14	4 hexane-1,2,4,6-tetraol	-800.016	-555.916
314	4	150.176	6	14	4 hexane-1,2,3,4-tetraol	-816.472	-573.562
315	4	110.113	6	6	2 2-(furan-2-yl)acetaldehyde	-221.145	-130.616
316	4	110.113	6	6	2 1-(furan-2-yl)ethanone	-249.573	-133.465
317	4	132.16	6	12	3 1-(tetrahydrofuran-2-yl)ethane-1,2-diol	-591.302	-372.824
318	4	130.144	6	10	3 2-(2-hydroxyethyl)-2,3-dihydrofuran-3-ol	-523.938	-366.560
319	4	100.118	5	8	2 2-methyl-2,3-dihydrofuran-3-ol	-272.208	-132.397
320	4	130.144	6	10	3 5-(2-hydroxyethyl)-2,3-dihydrofuran-3-ol	-530.023	-384.149
321	4	100.118	5	8	2 5-methyl-2,3-dihydrofuran-3-ol	-278.317	-148.832
322	4	130.144	6	10	3 5-(2-hydroxyethyl)-2,5-dihydrofuran-3-ol	-505.501	-353.260
323	4	100.118	5	8	2 5-methyl-2,5-dihydrofuran-3-ol	-265.815	-141.630
324	4	130.144	6	10	3 5-(2-hydroxyethyl)dihydrofuran-3(2H)-one	-578.133	-397.117
325	4	130.144	6	10	3 2-(2-hydroxyethyl)dihydrofuran-3(2H)-one	-578.133	-397.117
326	4	150.176	6	14	4 hexane-1,2,3,6-tetraol	-799.649	-555.461
327	4	150.176	6	14	4 hexane-1,3,4,5-tetraol	-814.921	-571.005
328	4	100.118	5	8	2 5-methyldihydrofuran-3(2H)-one	-399.611	-265.964
329	4	100.118	5	8	2 2-methyldihydrofuran-3(2H)-one	-399.611	-265.964
330	4	120.149	5	12	3 pentane-1,2,3-triol	-631.973	-438.226
331	4	120.149	5	12	3 pentane-2,3,4-triol	-639.916	-443.222
332	4	130.144	6	10	3 5-hydroxy-4-oxohexanal	-617.034	-386.471
333	4	130.144	6	10	3 5-hydroxy-3-oxohexanal	-626.237	-394.598
334	4	130.144	6	10	3 3-hydroxy-4-oxohexanal	-617.993	-387.977
335	4	130.144	6	10	3 3-hydroxy-5-oxohexanal	-627.163	-397.647
336	4	146.144	6	10	4 2,3-dihydroxyhexanediol	-771.750	-537.336
337	4	130.144	6	10	3 4-hydroxy-5-oxohexanal	-612.999	-385.775
338	4	130.144	6	10	3 3-hydroxyhexanediol	-605.546	-390.918
339	4	130.144	6	10	3 6-hydroxy-5-oxohexanal	-275.700	-156.000
340	4	130.144	6	10	3 6-hydroxy-4-oxohexanal	-618.294	-389.602
341	4	130.144	6	10	3 5-hydroxyhexane-2,4-dione	-638.651	-393.200
342	4	130.144	6	10	3 5-hydroxyhexane-2,3-dione	-552.177	-306.665
343	4	130.144	6	10	3 3-hydroxyhexane-2,4-dione	-625.446	-382.834
344	4	130.144	6	10	3 3-hydroxyhexane-2,5-dione	-634.616	-392.504
345	4	74.08	3	6	2 2-hydroxypropanal	-403.016	-288.553
346	4	130.144	6	10	3 1-hydroxyhexane-2,5-dione	-630.708	-388.204
347	4	130.144	6	10	3 6-hydroxyhexane-2,4-dione	-639.911	-396.331
348	4	58.08	3	6	1 propan-2-one	-260.013	-149.878
349	4	88.107	4	8	2 tetrahydrofuran-3-ol	-386.403	-250.136
350	4	146.144	6	10	4 3-hydroxy-5-(hydroxymethyl)tetrahydrofuran-2-carbaldehyde	-749.546	-515.818
351	4	130.144	6	10	3 2-(hydroxymethyl)-5-methylenetetrahydrofuran-3-ol	-573.851	-420.448
352	4	130.144	6	10	3 (2,3-dihydrofuran-2,5-diyl)dimethanol	-504.542	-351.754
353	4	130.144	6	10	3 (2,5-dihydrofuran-2,5-diyl)dimethanol	-486.413	-311.632
354	4	130.144	6	10	3 5-(hydroxymethyl)-2-methylenetetrahydrofuran-3-ol	-571.336	-417.597
355	4	130.144	6	10	3 6-(hydroxymethyl)-3,6-dihydro-2H-pyran-3-ol	-496.637	-314.765
356	4	130.144	6	10	3 6-(hydroxymethyl)-5,6-dihydro-2H-pyran-3-ol	-490.244	-323.998
357	4	130.144	6	10	3 2-(hydroxymethyl)-3,6-dihydro-2H-pyran-4-ol	-490.244	-323.998
358	4	130.144	6	10	3 2-(hydroxymethyl)-3,4-dihydro-2H-pyran-4-ol	-496.637	-314.765
359	4	130.144	6	10	3 6-methylenetetrahydro-2H-pyran-3,4-diol	-584.075	-423.581
360	4	130.144	6	10	3 6-(hydroxymethyl)dihydro-2H-pyran-3(4H)-one	-574.920	-390.388
361	4	130.144	6	10	3 2-(hydroxymethyl)dihydro-2H-pyran-4(3H)-one	-574.920	-390.388
362	4	150.176	6	14	4 hexane-1,2,4,5-tetraol	-819.373	-577.035
363	4	146.144	6	10	4 3,5-dihydroxytetrahydro-2H-pyran-2-carbaldehyde	-759.770	-518.951
364	4	130.144	6	10	3 2-(hydroxymethyl)-3,6-dihydro-2H-pyran-3-ol	-496.637	-314.765
365	4	130.144	6	10	3 2-(hydroxymethyl)-3,4-dihydro-2H-pyran-3-ol	-496.637	-314.765

366	4	130.144	6	10	3 6-(hydroxymethyl)-3,4-dihydro-2H-pyran-3-ol	-514.766	-354.887
367	4	130.144	6	10	3 2-methylenetetrahydro-2H-pyran-3,5-diol	-581.560	-420.730
368	4	146.144	6	10	4 5,6-dihydroxy-2-oxohexanal	-703.622	-448.835
369	4	104.106	4	8	3 3,4-dihydroxybutanal	-584.024	-424.923
370	4	130.144	6	10	3 5,6-dihydroxyhex-3-en-2-one	-535.051	-335.947
371	4	120.149	5	12	3 pentane-1,2,4-triol	-632.340	-438.681
372	4	130.144	6	10	3 5,6-dihydroxyhex-2-enal	-514.360	-332.267
373	4	130.144	6	10	3 5,6-dihydroxyhex-3-enal	-507.988	-325.898
374	4	130.144	6	10	3 5,6-dihydroxyhex-1-en-3-one	-526.515	-329.185
375	4	88.107	4	8	2 4-hydroxybutan-2-one	-438.478	-283.728
376	4	130.144	6	10	3 2-(hydroxymethyl)-5-methyl-2,3-dihydrofuran-3-ol	-491.527	-315.639
377	4	130.144	6	10	3 2-(hydroxymethyl)-5-methyl-2,5-dihydrofuran-3-ol	-503.585	-337.409
378	4	130.144	6	10	3 5-(hydroxymethyl)-2-methyl-2,3-dihydrofuran-3-ol	-528.107	-368.298
379	4	130.144	6	10	3 5-(hydroxymethyl)-2-methyl-2,5-dihydrofuran-3-ol	-503.585	-337.409
380	4	130.144	6	10	3 2-methyl-5-methylenetetrahydrofuran-3,4-diol	-594.901	-434.141
381	4	130.144	6	10	3 2-(hydroxymethyl)-5-methyldihydrofuran-3(2H)-one	-588.261	-403.799
382	4	130.144	6	10	3 5-(hydroxymethyl)-2-methyldihydrofuran-3(2H)-one	-588.261	-403.799
383	4	130.144	6	10	3 2-methyl-3,4-dihydro-2H-pyran-3,4-diol	-520.202	-331.309
384	4	130.144	6	10	3 2-methyl-3,6-dihydro-2H-pyran-3,4-diol	-513.809	-340.542
385	4	130.144	6	10	3 2-methyl-3,6-dihydro-2H-pyran-3,5-diol	-513.809	-340.542
386	4	130.144	6	10	3 6-methyl-3,6-dihydro-2H-pyran-3,5-diol	-513.809	-340.542
387	4	130.144	6	10	3 6-methyl-3,4-dihydro-2H-pyran-3,4-diol	-501.751	-318.772
388	4	130.144	6	10	3 6-methyl-3,6-dihydro-2H-pyran-3,4-diol	-513.809	-340.542
389	4	130.144	6	10	3 3-hydroxy-2-methyldihydro-2H-pyran-4(3H)-one	-598.485	-406.932
390	4	130.144	6	10	3 5-hydroxy-6-methyldihydro-2H-pyran-3(4H)-one	-598.485	-406.932
391	4	130.144	6	10	3 5-hydroxy-2-methyldihydro-2H-pyran-3(4H)-one	-598.485	-406.932
392	4	130.144	6	10	3 5-hydroxy-2-methyldihydro-2H-pyran-4(3H)-one	-598.485	-406.932
393	4	88.107	4	8	2 3-hydroxybutan-2-one	-432.257	-276.852
394	4	130.144	6	10	3 1,2-dihydroxyhex-4-en-3-one	-526.807	-329.326
395	4	130.144	6	10	3 1,2-dihydroxyhex-5-en-3-one	20.200	74.700
396	4	130.144	6	10	3 1-hydroxyhexane-2,4-dione	-630.741	-386.661
397	4	130.144	6	10	3 4,5-dihydroxyhex-1-en-3-one	-525.255	-326.054
398	4	130.144	6	10	3 1-hydroxyhexane-3,4-dione	-544.234	-301.669
399	4	88.107	4	8	2 1-hydroxybutan-2-one	-429.308	-274.058
400	4	142.112	6	6	4 3-hydroxy-2,5-dihydrofuran-2,5-dicarbaldehyde	-632.005	-455.144
401	4	142.112	6	6	4 3-hydroxy-2,3-dihydrofuran-2,5-dicarbaldehyde	-671.394	-484.802
402	4	142.112	6	6	4 3-oxotetrahydrofuran-2,5-dicarbaldehyde	-716.681	-521.534
403	4	126.112	6	6	3 5-(hydroxymethyl)furan-2-carbaldehyde	-495.139	-368.357
404	4	126.112	6	6	3 4-hydroxy-5-methylene-4,5-dihydrofuran-2-carbaldehyde	-483.773	-376.483
405	4	126.112	6	6	3 4-hydroxy-5-methylene-2,5-dihydrofuran-2-carbaldehyde	-533.840	-434.398
406	4	126.112	6	6	3 3-hydroxy-5-methylene-2,5-dihydrofuran-2-carbaldehyde	-469.545	-367.342
407	4	126.112	6	6	3 5-methylene-4-oxotetrahydrofuran-2-carbaldehyde	-542.435	-427.170
408	4	126.112	6	6	3 5-methylene-3-oxotetrahydrofuran-2-carbaldehyde	-540.986	-426.164
409	4	114.101	5	6	3 4-oxotetrahydrofuran-2-carbaldehyde	-542.188	-393.687
410	4	146.144	6	10	4 3,4-dihydroxytetrahydro-2H-pyran-2-carbaldehyde	-759.770	-518.951
411	4	146.144	6	10	4 2,3,4-trihydroxyhex-5-enal	-675.048	-471.556
412	4	146.144	6	10	4 4,6-dihydroxy-3-oxohexanal	-775.662	-528.348
413	4	146.144	6	10	4 4,6-dihydroxy-2-oxohexanal	-703.030	-447.784
414	4	146.144	6	10	4 2,6-dihydroxy-3-oxohexanal	-774.703	-526.842
415	4	104.106	4	8	3 2,4-dihydroxybutanal	-582.473	-422.366
416	4	132.16	6	12	3 (tetrahydrofuran-2,5-diyl)dimethanol	-583.404	-371.551
417	4	110.113	6	6	2 2,5-dimethylene-2,5-dihydrofuran-3-ol	-297.674	-269.442
418	4	110.113	6	6	2 2,5-dimethylenedihydrofuran-3(2H)-one	-357.329	-321.702
419	4	98.102	5	6	2 5-methylenedihydrofuran-3(2H)-one	-366.493	-298.317
420	4	118.133	5	10	3 5-(hydroxymethyl)tetrahydrofuran-3-ol	-575.053	-387.971
421	4	130.144	6	10	3 2-(hydroxymethyl)-5,6-dihydro-2H-pyran-3-ol	-490.244	-323.998
422	4	130.144	6	10	3 6-(hydroxymethyl)-3,6-dihydro-2H-pyran-4-ol	-490.244	-323.998
423	4	130.144	6	10	3 6-(hydroxymethyl)-3,4-dihydro-2H-pyran-4-ol	-514.766	-354.887
424	4	130.144	6	10	3 2-methylenetetrahydro-2H-pyran-3,4-diol	-581.560	-420.730
425	4	130.144	6	10	3 2-(hydroxymethyl)dihydro-2H-pyran-3(4H)-one	-574.920	-390.388
426	4	150.176	6	14	4 hexane-1,3,4,6-tetraol	-804.468	-561.946
427	4	130.144	6	10	3 1,4-dihydroxyhex-5-en-2-one	-511.797	-314.644
428	4	130.144	6	10	3 1,4-dihydroxyhex-5-en-3-one	-511.797	-314.644
429	4	130.144	6	10	3 3,4-dihydroxyhex-5-en-2-one	-516.297	-319.995
430	4	130.144	6	10	3 3,4-dihydroxyhex-5-enal	-508.844	-325.138
431	4	130.144	6	10	3 1,6-dihydroxyhex-4-en-3-one	-525.557	-328.394
432	4	130.144	6	10	3 4,6-dihydroxyhex-1-en-3-one	-516.720	-320.007
433	4	118.133	5	10	3 3,5-dihydroxypentan-2-one	-611.714	-410.665
434	4	130.144	6	10	3 1,6-dihydroxyhex-3-en-2-one	-517.313	-321.773
435	4	130.144	6	10	3 1,6-dihydroxyhex-4-en-2-one	-513.456	-318.255

436	4	74.08	3	6	2 3-hydroxypropanal	-396.032	-285.063
437	4	120.149	5	12	3 pentane-1,3,4-triol	-632.340	-438.681
438	4	130.144	6	10	3 6-hydroxy-3-oxohexanal	-618.294	-389.602
439	4	130.144	6	10	3 6-hydroxyhexane-2,3-dione	-544.234	-301.669
440	4	118.133	5	10	3 1,5-dihydroxypentan-2-one	-84.700	-32.900
441	4	116.117	5	8	3 3,4-dihydro-2H-pyran-3,4-diol	-488.286	-331.185
442	4	116.117	5	8	3 3,6-dihydro-2H-pyran-3,4-diol	-481.893	-340.418
443	4	116.117	5	8	3 3,6-dihydro-2H-pyran-3,5-diol	-481.893	-340.418
444	4	116.117	5	8	3 3-hydroxydihydro-2H-pyran-4(3H)-one	-566.569	-406.808
445	4	126.112	6	6	3 3-hydroxy-2H-pyran-6-carbaldehyde	-480.841	-340.601
446	4	126.112	6	6	3 4-hydroxy-2H-pyran-6-carbaldehyde	-412.092	-292.982
447	4	126.112	6	6	3 4-hydroxy-4H-pyran-2-carbaldehyde	-418.485	-283.749
448	4	126.112	6	6	3 3-oxo-3,4-dihydro-2H-pyran-6-carbaldehyde	-496.768	-359.372
449	4	126.112	6	6	3 4-oxo-3,4-dihydro-2H-pyran-6-carbaldehyde	-496.768	-359.372
450	4	126.112	6	6	3 4-hydroxy-2H-pyran-2-carbaldehyde	-438.937	-340.584
451	4	126.112	6	6	3 3-hydroxy-2H-pyran-2-carbaldehyde	-443.391	-321.147
452	4	126.112	6	6	3 4-oxo-3,4-dihydro-2H-pyran-2-carbaldehyde	-459.318	-339.918
453	4	126.112	6	6	3 3-oxo-3,4-dihydro-2H-pyran-2-carbaldehyde	-463.772	-320.481
454	4	126.112	6	6	3 3-oxo-3,6-dihydro-2H-pyran-2-carbaldehyde	-463.772	-320.481
455	4	126.112	6	6	3 5-oxo-5,6-dihydro-2H-pyran-2-carbaldehyde	-463.772	-320.481
456	4	110.113	6	6	2 2-methylene-2H-pyran-4-ol	-212.182	-185.726
457	4	110.113	6	6	2 2-methylene-2H-pyran-3-ol	-280.931	-233.345
458	4	110.113	6	6	2 2-methylene-2H-pyran-4(3H)-one	-283.623	-244.548
459	4	110.113	6	6	2 2-methylene-2H-pyran-3(4H)-one	-289.526	-226.117
460	4	110.113	6	6	2 2-methylene-2H-pyran-3(6H)-one	-289.526	-226.117
461	4	110.113	6	6	2 6-methylene-2H-pyran-3(6H)-one	-232.563	-185.060
462	4	98.102	5	6	2 2H-pyran-3(4H)-one	-289.279	-192.634
463	4	98.102	5	6	2 2H-pyran-3(6H)-one	-284.825	-212.071
464	4	118.133	5	10	3 tetrahydro-2H-pyran-3,5-diol	-585.277	-391.104
465	4	148.116	5	8	5 2,3,4-trihydroxypentanedial	-916.166	-690.312
466	4	132.117	5	8	4 2,5-dihydroxy-3-oxopentanal	-753.874	-534.906
467	4	132.117	5	8	4 4,5-dihydroxy-3-oxopentanal	-755.425	-537.463
468	4	132.117	5	8	4 2,3-dihydroxypentanedial	-750.921	-545.400
469	4	142.112	6	6	4 5-hydroxy-4-oxohex-2-enedial	-562.002	-344.797
470	4	142.112	6	6	4 2,5-dioxohexanedial	-594.855	-324.125
471	4	142.112	6	6	4 2,4-dioxohexanedial	-676.690	-412.816
472	4	100.074	4	4	3 2-oxosuccinaldehyde	-475.257	-300.213
473	4	142.112	6	6	4 3,4-dioxohexanedial	-662.815	-408.388
474	4	116.117	5	8	3 5-hydroxy-3-oxopentanal	-597.465	-397.666
475	4	116.117	5	8	3 3-hydroxypentanedial	-584.717	-398.982
476	4	116.117	5	8	3 4,5-dihydroxypent-1-en-3-one	-496.483	-329.122
477	4	126.112	6	6	3 3,4-dioxohex-5-enal	-403.873	-200.047
478	4	114.101	5	6	3 3,4-dioxopentanal	-503.861	-292.907
479	4	116.117	5	8	3 4-hydroxy-3-oxopentanal	-596.205	-394.535
480	4	126.112	6	6	3 4-oxohex-2-enedial	-405.593	-207.557
481	4	126.112	6	6	3 2,4-dioxohex-5-enal	-417.748	-204.475
482	4	114.101	5	6	3 2,4-dioxopentanal	-517.703	-298.878
483	4	116.117	5	8	3 4-hydroxy-2-oxopentanal	-523.573	-313.971
484	4	126.112	6	6	3 5-oxohex-2-enedial	-405.593	-207.557
485	4	126.112	6	6	3 2-oxohex-3-enedial	-405.593	-207.557
486	4	126.112	6	6	3 2,5-dioxohex-3-enal	-415.072	-216.708
487	4	146.144	6	10	4 1,2,6-trihydroxyhex-4-en-3-one	-683.517	-468.191
488	4	126.112	6	6	3 4,5-dioxohex-2-enal	-413.368	-208.315
489	4	114.101	5	6	3 5-hydroxy-4-oxopent-2-enal	-395.105	-224.320
490	4	116.117	5	8	3 2-hydroxy-4-oxopentanal	-605.375	-404.205
491	4	134.133	5	10	4 2,4,5-trihydroxypentanal	-770.465	-562.226
492	4	130.101	5	6	4 2-hydroxy-4-oxopentanedial	-661.698	-437.516
493	4	116.117	5	8	3 2-hydroxy-3-oxopentanal	-596.205	-394.535
494	4	84.075	4	4	2 2-oxobut-3-enal	-216.315	-91.872
495	4	84.075	4	4	2 but-2-enedial	-216.331	-90.989
496	4	104.106	4	8	3 tetrahydrofuran-3,4-diol	-566.702	-404.391
497	4	100.118	5	8	2 pentane-2,4-dione	-461.380	-265.567
498	4	100.118	5	8	2 pentane-2,3-dione	-365.736	-169.362
499	4	130.144	6	10	3 1,5-dihydroxyhex-3-en-2-one	-524.297	-325.263
500	4	58.08	3	6	1 propionaldehyde	-238.363	-144.692
501	4	100.118	5	8	2 3-oxopentanal	-439.796	-257.295
502	4	100.118	5	8	2 4-oxopentanal	-439.763	-258.838
503	4	100.118	5	8	2 1-hydroxypent-3-en-2-one	-338.815	-189.466
504	4	100.118	5	8	2 1-hydroxypent-4-en-2-one	-327.871	-180.192
505	4	100.118	5	8	2 5-hydroxypent-1-en-3-one	-338.523	-189.325

506	4	100.118	5	8	2 4-hydroxypent-1-en-3-one	-337.263	-186.194
507	4	90.123	4	10	2 butane-2,3-diol	-452.883	-304.868
508	4	118.133	5	10	3 4,5-dihydroxypentanal	-604.853	-416.859
509	4	114.101	5	6	3 2-oxopentanedial	-496.086	-292.149
510	4	88.107	4	8	2 3-hydroxybutanal	-424.804	-281.995
511	4	130.144	6	10	3 4,6-dihydroxyhex-2-enal	-512.809	-329.710
512	4	110.113	6	6	2 4-oxohexa-2,5-dienal	-146.651	0.784
513	4	98.102	5	6	2 4-oxopent-2-enal	-246.639	-92.076
514	4	28.054	2	4	0 ethene	5.549	-34.967
515	4	110.113	6	6	2 hexa-1,5-diene-3,4-dione	-144.931	8.294
516	4	98.102	5	6	2 pent-4-ene-2,3-dione	-244.919	-84.566
517	4	88.107	4	8	2 but-3-ene-1,2-diol	-320.159	-211.219
518	4	88.107	4	8	2 4-hydroxybutanal	-416.861	-276.999
519	5	112.129	6	8	2 2,3,3a,6a-tetrahydrofuro[3,2-b]furan	-271.394	-137.810
520	5	128.128	6	8	3 2-(2,3-dihydrofuran-2-yl)-2-hydroxyacetaldehyde	-473.216	-293.522
521	5	112.129	6	8	2 1-(2,3-dihydrofuran-2-yl)ethanone	-321.091	-158.729
522	5	112.129	6	8	2 2-(2,3-dihydrofuran-2-yl)acetaldehyde	-300.007	-150.413
523	5	112.129	6	8	2 1-(furan-2-yl)ethanol	-299.924	-195.455
524	5	112.129	6	8	2 2-vinyl-2,3-dihydrofuran-3-ol	-221.828	-97.802
525	5	112.129	6	8	2 2-ethylidene-2,3-dihydrofuran-3-ol	-254.494	-130.049
526	5	132.16	6	12	3 2-(1-hydroxyethyl)tetrahydrofuran-3-ol	-612.381	-384.151
527	5	112.129	6	8	2 2,3,3a,5-tetrahydrofuro[3,2-b]furan	-273.051	-150.067
528	5	132.16	6	12	3 2-ethyltetrahydrofuran-3,4-diol	-619.471	-395.297
529	5	132.16	6	12	3 5-(2-hydroxyethyl)tetrahydrofuran-3-ol	-596.841	-381.413
530	5	128.128	6	8	3 2-(4-hydroxydihydrofuran-2(3H)-ylidene)acetaldehyde	-478.768	-291.434
531	5	128.128	6	8	3 2-(2,5-dihydrofuran-2-yl)-2-hydroxyacetaldehyde	-473.216	-293.522
532	5	148.16	6	12	4 2,5,6-trihydroxyhexanal	-784.924	-545.120
533	5	148.16	6	12	4 2,3,5-trihydroxyhexanal	-799.237	-559.158
534	5	112.129	6	8	2 2-(2,5-dihydrofuran-2-yl)acetaldehyde	-300.007	-150.413
535	5	112.129	6	8	2 1-(2,5-dihydrofuran-2-yl)ethanone	-321.091	-158.729
536	5	132.16	6	12	3 5-(1-hydroxyethyl)tetrahydrofuran-3-ol	-612.381	-384.151
537	5	132.16	6	12	3 5,6-dihydroxyhexan-2-one	-646.340	-414.018
538	5	132.16	6	12	3 3,5-dihydroxyhexan-2-one	-640.486	-407.597
539	5	102.134	5	10	2 5-methyltetrahydrofuran-3-ol	-418.319	-250.260
540	5	132.16	6	12	3 5,6-dihydroxyhexanal	-619.312	-399.753
541	5	132.16	6	12	3 3,5-dihydroxyhexanal	-633.033	-412.740
542	5	132.16	6	12	3 2-(hydroxymethyl)-5-methyltetrahydrofuran-3-ol	-606.969	-388.095
543	5	132.16	6	12	3 6-methyltetrahydro-2H-pyran-3,4-diol	-617.193	-391.228
544	5	132.16	6	12	3 hex-5-ene-1,2,3-triol	-532.454	-347.372
545	5	132.16	6	12	3 hex-4-ene-1,2,3-triol	-538.523	-351.403
546	5	132.16	6	12	3 1,5-dihydroxyhexan-2-one	-636.578	-403.297
547	5	132.16	6	12	3 1,5-dihydroxyhexan-3-one	-645.781	-411.424
548	5	132.16	6	12	3 6-(hydroxymethyl)tetrahydro-2H-pyran-3-ol	-593.628	-374.684
549	5	112.129	6	8	2 5-ethylidene-2,5-dihydrofuran-3-ol	-288.411	-178.673
550	5	112.129	6	8	2 5-vinyl-2,5-dihydrofuran-3-ol	-215.435	-107.035
551	5	112.129	6	8	2 5-vinyl-2,3-dihydrofuran-3-ol	-258.057	-140.674
552	5	112.129	6	8	2 2-vinyl-2,5-dihydrofuran-3-ol	-215.435	-107.035
553	5	112.129	6	8	2 2-vinyldihydrofuran-3(2H)-one	-300.111	-173.425
554	5	112.129	6	8	2 5-vinyldihydrofuran-3(2H)-one	-300.111	-173.425
555	5	132.16	6	12	3 hex-5-ene-2,3,4-triol	-535.964	-346.505
556	5	112.129	6	8	2 2-ethylidene-2,5-dihydrofuran-3-ol	-337.531	-236.617
557	5	112.129	6	8	2 2-ethylidenedihydrofuran-3(2H)-one	-410.421	-296.445
558	5	112.129	6	8	2 5-ethylidenedihydrofuran-3(2H)-one	-408.972	-295.439
559	5	132.16	6	12	3 2,5-dimethyltetrahydrofuran-3,4-diol	-630.534	-404.639
560	5	132.16	6	12	3 4,5-dihydroxyhexan-2-one	-655.242	-420.520
561	5	132.16	6	12	3 4,5-dihydroxyhexan-3-one	-646.072	-410.850
562	5	132.16	6	12	3 2,5-dihydroxyhexan-3-one	-644.521	-408.293
563	5	114.101	5	6	3 3-hydroxy-2,5-dihydrofuran-2-carbaldehyde	-457.512	-327.297
564	5	114.101	5	6	3 3-hydroxy-2,3-dihydrofuran-2-carbaldehyde	-463.905	-318.064
565	5	114.101	5	6	3 4-hydroxy-4,5-dihydrofuran-2-carbaldehyde	-496.901	-356.955
566	5	114.101	5	6	3 4-hydroxy-2,5-dihydrofuran-2-carbaldehyde	-457.512	-327.297
567	5	114.101	5	6	3 3-oxotetrahydrofuran-2-carbaldehyde	-542.188	-393.687
568	5	98.102	5	6	2 2-methylene-2,5-dihydrofuran-3-ol	-295.052	-239.495
569	5	98.102	5	6	2 2-methylene-2,3-dihydrofuran-3-ol	-285.695	-219.843
570	5	98.102	5	6	2 5-methylene-2,5-dihydrofuran-3-ol	-295.052	-239.495
571	5	98.102	5	6	2 2-methylenedihydrofuran-3(2H)-one	-367.942	-299.323
572	5	118.133	5	10	3 2-(hydroxymethyl)tetrahydrofuran-3-ol	-575.053	-387.971
573	5	98.102	5	6	2 furan-2-ylmethanol	-283.196	-221.056
574	5	118.133	5	10	3 tetrahydro-2H-pyran-3,4-diol	-585.277	-391.104
575	5	134.133	5	10	4 2,3,5-trihydroxypentanal	-770.465	-562.226

576	5	118.133	5	10	3 pent-4-ene-1,2,3-triol	-508.151	-351.079
577	5	118.133	5	10	3 3,5-dihydroxypentanal	-604.261	-415.808
578	5	118.133	5	10	3 1,5-dihydroxypentan-3-one	-617.009	-414.492
579	5	128.128	6	8	3 2-(2-hydroxyethylidene)-2,5-dihydrofuran-3-ol	-494.241	-375.482
580	5	128.128	6	8	3 2-(2-hydroxyethylidene)-2,3-dihydrofuran-3-ol	-484.884	-355.830
581	5	128.128	6	8	3 5-(2-hydroxyethylidene)-2,5-dihydrofuran-3-ol	-494.241	-375.482
582	5	128.128	6	8	3 2-(2-hydroxyethylidene)dihydrofuran-3(2H)-one	-567.131	-435.310
583	5	128.128	6	8	3 5-(2-hydroxyethylidene)dihydrofuran-3(2H)-one	-565.682	-434.304
584	5	128.128	6	8	3 2-(3-hydroxydihydrofuran-2(3H)-ylidene)acetaldehyde	-478.768	-291.434
585	5	128.128	6	8	3 2-(4,5-dihydrofuran-2-yl)-2-hydroxyacetaldehyde	-470.745	-311.863
586	5	148.16	6	12	4 2,4,6-trihydroxyhexanal	-789.743	-551.605
587	5	148.16	6	12	4 2,3,4-trihydroxyhexanal	-800.788	-561.715
588	5	130.144	6	10	3 2-hydroxy-2-(tetrahydrofuran-2-yl)acetaldehyde	-570.207	-353.441
589	5	128.128	6	8	3 3-hydroxy-5-methyl-2,3-dihydrofuran-2-carbaldehyde	-477.370	-305.651
590	5	128.128	6	8	3 3-hydroxy-5-methyl-2,5-dihydrofuran-2-carbaldehyde	-489.428	-327.421
591	5	128.128	6	8	3 4-hydroxy-5-methyl-4,5-dihydrofuran-2-carbaldehyde	-528.817	-357.079
592	5	128.128	6	8	3 4-hydroxy-5-methyl-2,5-dihydrofuran-2-carbaldehyde	-489.428	-327.421
593	5	128.128	6	8	3 5-methyl-3-oxotetrahydrofuran-2-carbaldehyde	-574.104	-393.811
594	5	128.128	6	8	3 5-methyl-4-oxotetrahydrofuran-2-carbaldehyde	-574.104	-393.811
595	5	148.16	6	12	4 2,4,5-trihydroxyhexanal	-799.237	-559.158
596	5	128.128	6	8	3 2-hydroxy-4-oxohex-5-enal	-505.420	-309.802
597	5	128.128	6	8	3 5-hydroxy-4-oxohex-2-enal	-423.877	-221.252
598	5	128.128	6	8	3 2-hydroxy-3-oxohex-4-enal	-505.712	-309.943
599	5	128.128	6	8	3 2-hydroxy-3-oxohex-5-enal	-494.768	-300.669
600	5	128.128	6	8	3 2,4-dioxohexanal	-538.565	-289.271
601	5	128.128	6	8	3 2,5-dioxohexanal	-538.532	-290.814
602	5	128.128	6	8	3 3,4-dioxohexanal	-524.690	-284.843
603	5	86.091	4	6	2 2-oxobutanal	-337.132	-176.668
604	5	144.128	6	8	4 3-hydroxytetrahydrofuran-2,5-dicarbaldehyde	-735.389	-505.830
605	5	128.128	6	8	3 5-(hydroxymethyl)-2,3-dihydrofuran-2-carbaldehyde	-490.385	-341.766
606	5	128.128	6	8	3 5-(hydroxymethyl)-2,5-dihydrofuran-2-carbaldehyde	-472.256	-301.644
607	5	128.128	6	8	3 4-hydroxy-5-methylenetetrahydrofuran-2-carbaldehyde	-557.179	-407.609
608	5	128.128	6	8	3 5-hydroxy-5,6-dihydro-2H-pyran-2-carbaldehyde	-482.480	-304.777
609	5	128.128	6	8	3 5-hydroxy-3,6-dihydro-2H-pyran-2-carbaldehyde	-476.087	-314.010
610	5	128.128	6	8	3 4-hydroxy-3,6-dihydro-2H-pyran-2-carbaldehyde	-476.087	-314.010
611	5	128.128	6	8	3 4-hydroxy-3,4-dihydro-2H-pyran-2-carbaldehyde	-482.480	-304.777
612	5	128.128	6	8	3 5-oxotetrahydro-2H-pyran-2-carbaldehyde	-560.763	-380.400
613	5	128.128	6	8	3 4-oxotetrahydro-2H-pyran-2-carbaldehyde	-560.763	-380.400
614	5	144.128	6	8	4 4,5-dihydroxyhex-2-enedial	-659.469	-459.302
615	5	144.128	6	8	4 2-hydroxy-5-oxohexanedial	-682.527	-429.452
616	5	148.16	6	12	4 hex-4-ene-1,2,3,6-tetraol	-693.736	-489.142
617	5	128.128	6	8	3 4-hydroxyhex-2-enedial	-493.265	-312.884
618	5	128.128	6	8	3 4-hydroxy-5-oxohex-2-enal	-500.718	-307.741
619	5	128.128	6	8	3 2-hydroxy-5-oxohex-3-enal	-513.956	-316.564
620	5	118.133	5	10	3 2,4-dihydroxypentanal	-611.245	-419.298
621	5	128.128	6	8	3 5-hydroxyhex-2-enedial	-493.265	-312.884
622	5	128.128	6	8	3 2-hydroxyhex-3-enedial	-302.700	-171.300
623	5	132.16	6	12	3 2-(2-hydroxyethyl)tetrahydrofuran-3-ol	-596.841	-381.413
624	5	102.134	5	10	2 2-methyltetrahydrofuran-3-ol	-418.319	-250.260
625	5	112.129	6	8	2 2-(4,5-dihydrofuran-2-yl)acetaldehyde	-318.136	-190.535
626	5	132.16	6	12	3 4,6-dihydroxyhexanal	-624.131	-406.238
627	5	132.16	6	12	3 3,4-dihydroxyhexanal	-633.625	-413.791
628	5	112.129	6	8	2 1-(4,5-dihydrofuran-2-yl)ethanone	-346.564	-193.384
629	5	132.16	6	12	3 4,6-dihydroxyhexan-2-one	-645.748	-412.967
630	5	132.16	6	12	3 3,4-dihydroxyhexan-2-one	-641.078	-408.648
631	5	132.16	6	12	3 2-(hydroxymethyl)tetrahydro-2H-pyran-4-ol	-593.628	-374.684
632	5	132.16	6	12	3 hex-5-ene-1,2,4-triol	-528.388	-341.964
633	5	132.16	6	12	3 hex-3-ene-1,2,6-triol	-527.532	-342.724
634	5	132.16	6	12	3 hex-4-ene-1,2,6-triol	-530.047	-345.575
635	5	132.16	6	12	3 1,4-dihydroxyhexan-2-one	-637.537	-404.803
636	5	132.16	6	12	3 1,4-dihydroxyhexan-3-one	-637.537	-404.803
637	5	132.16	6	12	3 5,6-dihydroxyhexan-3-one	-647.332	-413.981
638	5	132.16	6	12	3 1,2-dihydroxyhexan-3-one	-638.129	-405.854
639	5	112.129	6	8	2 2-(furan-2-yl)ethanol	-276.821	-215.041
640	5	82.102	5	6	1 2-methylfuran	48.093	123.286
641	5	114.145	6	10	2 2-(tetrahydrofuran-2-yl)acetaldehyde	-396.998	-210.332
642	5	114.145	6	10	2 1-(tetrahydrofuran-2-yl)ethanone	-418.082	-218.648
643	5	134.176	6	14	3 hexane-1,2,6-triol	-639.815	-418.085
644	5	134.176	6	14	3 hexane-1,2,3-triol	-653.761	-431.668
645	5	132.16	6	12	3 2-(hydroxymethyl)tetrahydro-2H-pyran-3-ol	-593.628	-374.684

646	5	148.16	6	12	4	2,3,6-trihydroxyhexanal	-322.000	-546.626
647	5	132.16	6	12	3	3,6-dihydroxyhexan-2-one	-632.543	-402.601
648	5	132.16	6	12	3	3,6-dihydroxyhexanal	-625.090	-407.744
649	5	132.16	6	12	3	1,6-dihydroxyhexan-2-one	-628.635	-398.301
650	5	132.16	6	12	3	1,6-dihydroxyhexan-3-one	-637.838	-406.428
651	5	132.16	6	12	3	2-methyltetrahydro-2H-pyran-3,4-diol	-617.193	-391.228
652	5	132.16	6	12	3	2,6-dihydroxyhexan-3-one	-636.578	-403.297
653	5	132.16	6	12	3	4,6-dihydroxyhexan-3-one	-637.537	-404.803
654	5	118.133	5	10	3	2,3-dihydroxypentanal	-612.796	-421.855
655	5	102.134	5	10	2	3-hydroxypentan-2-one	-454.045	-270.294
656	5	102.134	5	10	2	3-hydroxypentanal	-446.592	-275.437
657	5	102.134	5	10	2	1-hydroxypentan-2-one	-450.137	-265.994
658	5	102.134	5	10	2	1-hydroxypentan-3-one	-459.340	-274.121
659	5	102.134	5	10	2	2-hydroxypentan-3-one	-458.080	-270.990
660	5	102.134	5	10	2	4-hydroxypentan-2-one	-467.250	-280.660
661	5	132.16	6	12	3	4,5-dihydroxyhexanal	-633.625	-413.791
662	5	112.129	6	8	2	4-oxohex-5-enal	-339.808	-164.435
663	5	112.129	6	8	2	3-oxohex-4-enal	-349.303	-172.703
664	5	112.129	6	8	2	3-oxohex-5-enal	-338.359	-163.429
665	5	112.129	6	8	2	4-oxohex-2-enal	-267.468	-84.012
666	5	112.129	6	8	2	5-oxohex-3-enal	52.500	68.200
667	5	112.129	6	8	2	5-oxohex-2-enal	-349.270	-174.246
668	5	128.128	6	8	3	2-oxohexanediaol	-516.915	-284.085
669	5	86.091	4	6	2	succinaldehyde	-397.317	-260.173
670	5	102.134	5	10	2	4-hydroxypentanal	-445.633	-273.931
671	5	112.129	6	8	2	hex-2-enedial	-327.653	-167.517
672	5	112.129	6	8	2	hex-3-enedial	-324.755	-165.505
673	5	112.129	6	8	2	hex-5-ene-2,4-dione	-361.425	-171.164
674	5	112.129	6	8	2	hex-4-ene-2,3-dione	-275.243	-84.770
675	5	112.129	6	8	2	hex-5-ene-2,3-dione	-264.299	-75.496
676	5	112.129	6	8	2	hex-3-ene-2,5-dione	-276.947	-93.163
677	5	56.064	3	4	1	acrylaldehyde	-117.546	-59.896
678	5	60.096	3	8	1	propan-2-ol	-265.310	-165.426
679	5	70.091	4	6	1	2,3-dihydrofuran	-109.113	-35.962
680	5	70.091	4	6	1	2,5-dihydrofuran	-109.113	-35.962
681	5	90.123	4	10	2	butane-1,3-diol	-444.348	-298.821
682	5	90.123	4	10	2	butane-1,2-diol	-445.899	-301.378
683	5	128.128	6	8	3	3-hydroxy-5-methylenetetrahydrofuran-2-carbaldehyde	-559.694	-410.460
684	5	128.128	6	8	3	5-(hydroxymethyl)-4,5-dihydrofuran-2-carbaldehyde	-505.252	-340.535
685	5	112.129	6	8	2	(5-methylene-2,5-dihydrofuran-2-yl)methanol	-309.796	-213.842
686	5	112.129	6	8	2	(5-methylene-4,5-dihydrofuran-2-yl)methanol	-314.690	-246.396
687	5	112.129	6	8	2	2,5-dimethylenetetrahydrofuran-3-ol	-372.073	-302.141
688	5	132.16	6	12	3	5-(hydroxymethyl)-2-methyltetrahydrofuran-3-ol	-606.969	-388.095
689	5	112.129	6	8	2	6-methylene-3,6-dihydro-2H-pyran-3-ol	-315.566	-236.412
690	5	112.129	6	8	2	(2H-pyran-2-yl)methanol	-279.188	-187.084
691	5	112.129	6	8	2	6-methylene-5,6-dihydro-2H-pyran-3-ol	-300.392	-218.640
692	5	112.129	6	8	2	2-methylene-3,6-dihydro-2H-pyran-4-ol	-300.392	-218.640
693	5	112.129	6	8	2	2-methylene-3,4-dihydro-2H-pyran-4-ol	-306.785	-209.407
694	5	112.129	6	8	2	6-methylenedihydro-2H-pyran-3(4H)-one	-385.068	-285.030
695	5	112.129	6	8	2	2-methylenedihydro-2H-pyran-4(3H)-one	-385.068	-285.030
696	5	132.16	6	12	3	2-methyltetrahydro-2H-pyran-3,5-diol	-617.193	-391.228
697	5	128.128	6	8	3	3-hydroxy-3,4-dihydro-2H-pyran-2-carbaldehyde	-482.480	-304.777
698	5	128.128	6	8	3	3-hydroxy-3,6-dihydro-2H-pyran-2-carbaldehyde	-482.480	-304.777
699	5	128.128	6	8	3	3-hydroxy-3,4-dihydro-2H-pyran-6-carbaldehyde	-515.476	-343.668
700	5	112.129	6	8	2	(2H-pyran-6-yl)methanol	-301.771	-207.769
701	5	112.129	6	8	2	2-methylene-3,6-dihydro-2H-pyran-3-ol	-304.270	-206.556
702	5	112.129	6	8	2	2-methylene-3,4-dihydro-2H-pyran-3-ol	-304.270	-206.556
703	5	112.129	6	8	2	(4H-pyran-2-yl)methanol	-237.476	-140.713
704	5	132.16	6	12	3	hex-3-ene-1,2,5-triol	-532.001	-343.363
705	5	102.134	5	10	2	pent-4-ene-1,2-diol	-344.462	-207.512
706	5	102.134	5	10	2	pent-3-ene-1,2-diol	-350.531	-211.543
707	5	70.091	4	6	1	but-3-en-2-one	-135.699	-64.065
708	5	112.129	6	8	2	5-methyl-2-methylene-2,3-dihydrofuran-3-ol	-299.160	-207.430
709	5	112.129	6	8	2	(5-methylfuran-2-yl)methanol	-301.115	-189.206
710	5	112.129	6	8	2	5-methyl-2-methylene-2,5-dihydrofuran-3-ol	-391.263	-306.675
711	5	112.129	6	8	2	2-methyl-5-methylene-2,5-dihydrofuran-3-ol	-326.968	-239.619
712	5	112.129	6	8	2	5-methyl-2-methylenedihydrofuran-3(2H)-one	-399.858	-299.447
713	5	112.129	6	8	2	2-methyl-5-methylenedihydrofuran-3(2H)-one	-398.409	-298.441
714	5	112.129	6	8	2	2-methyl-2H-pyran-3-ol	-300.814	-193.424
715	5	112.129	6	8	2	2-methyl-4H-pyran-4-ol	-224.461	-104.598

716	5	112.129	6	8	2	2-methyl-2H-pyran-4-ol	-236.519	-126.368
717	5	112.129	6	8	2	2-methyl-2H-pyran-3(4H)-one	-321.195	-192.758
718	5	112.129	6	8	2	2-methyl-2H-pyran-4(3H)-one	-316.741	-212.195
719	5	112.129	6	8	2	6-methyl-2H-pyran-4-ol	-282.363	-180.887
720	5	112.129	6	8	2	6-methyl-2H-pyran-3-ol	-286.817	-161.450
721	5	112.129	6	8	2	6-methyl-2H-pyran-4(3H)-one	-302.744	-180.221
722	5	112.129	6	8	2	6-methyl-2H-pyran-3(4H)-one	-302.744	-180.221
723	5	112.129	6	8	2	6-methyl-2H-pyran-3(6H)-one	-321.195	-192.758
724	5	112.129	6	8	2	2-methyl-2H-pyran-3(6H)-one	-321.195	-192.758
725	5	112.129	6	8	2	hex-1-ene-3,4-dione	-265.748	-76.502
726	5	124.096	6	4	3	furan-2,5-dicarbaldehyde	-486.438	-347.040
727	5	130.144	6	10	3	5-(hydroxymethyl)tetrahydrofuran-2-carbaldehyde	-569.247	-361.563
728	5	116.117	5	8	3	4-hydroxytetrahydrofuran-2-carbaldehyde	-560.896	-377.983
729	5	128.128	6	8	3	3-hydroxy-5,6-dihydro-2H-pyran-2-carbaldehyde	-476.087	-314.010
730	5	128.128	6	8	3	4-hydroxy-5,6-dihydro-2H-pyran-2-carbaldehyde	-476.087	-314.010
731	5	128.128	6	8	3	4-hydroxy-3,4-dihydro-2H-pyran-6-carbaldehyde	-515.476	-343.668
732	5	128.128	6	8	3	3-oxotetrahydro-2H-pyran-2-carbaldehyde	-560.763	-380.400
733	5	128.128	6	8	3	4-hydroxy-2-oxohex-5-enal	-241.200	-306.400
734	5	128.128	6	8	3	4-hydroxy-3-oxohex-5-enal	-492.253	-297.818
735	5	86.091	4	6	2	2-hydroxybut-3-enal	-299.064	-191.836
736	5	128.128	6	8	3	6-hydroxy-3-oxohex-4-enal	-506.013	-311.568
737	5	128.128	6	8	3	6-hydroxy-2-oxohex-3-enal	-425.137	-224.383
738	5	128.128	6	8	3	6-hydroxy-2-oxohex-4-enal	-421.280	-220.865
739	5	76.096	3	8	2	propane-1,3-diol	-415.576	-301.889
740	5	86.091	4	6	2	4-hydroxybut-2-enal	-304.580	-198.965
741	5	114.145	6	10	2	(5-methylenetetrahydrofuran-2-yl)methanol	-393.552	-266.193
742	5	100.118	5	8	2	5-methylenetetrahydrofuran-3-ol	-385.201	-282.613
743	5	100.118	5	8	2	(2,3-dihydrofuran-2-yl)methanol	-297.763	-173.797
744	5	100.118	5	8	2	(2,5-dihydrofuran-2-yl)methanol	-297.763	-173.797
745	5	120.149	5	12	3	pentane-1,2,5-triol	-230.500	-426.149
746	5	112.129	6	8	2	2-methylene-5,6-dihydro-2H-pyran-3-ol	-377.922	-293.264
747	5	112.129	6	8	2	6-methylene-3,6-dihydro-2H-pyran-4-ol	-313.627	-226.208
748	5	112.129	6	8	2	2-methylenedihydro-2H-pyran-3(4H)-one	-386.517	-286.036
749	5	100.118	5	8	2	dihydro-2H-pyran-3(4H)-one	-386.270	-252.553
750	5	132.16	6	12	3	hex-5-ene-1,3,4-triol	-528.388	-341.964
751	5	112.129	6	8	2	1-hydroxyhexa-3,5-dien-2-one	-238.442	-107.133
752	5	112.129	6	8	2	4-hydroxyhexa-1,5-dien-3-one	-233.311	-89.477
753	5	100.118	5	8	2	3-hydroxypent-4-en-2-one	-328.305	-180.135
754	5	102.134	5	10	2	pent-4-ene-2,3-diol	-348.931	-208.151
755	5	132.16	6	12	3	hex-4-ene-1,3,6-triol	-525.981	-340.167
756	5	112.129	6	8	2	6-hydroxyhexa-1,4-dien-3-one	-234.900	-107.192
757	5	100.118	5	8	2	5-hydroxypent-3-en-2-one	-334.888	-200.052
758	5	102.134	5	10	2	5-hydroxypentan-2-one	-459.307	-275.664
759	5	116.117	5	8	3	5-hydroxy-2-oxopentanal	-515.630	-308.975
760	5	98.102	5	6	2	2H-pyran-3-ol	-268.898	-193.300
761	5	98.102	5	6	2	2H-pyran-4-ol	-74.800	-50.800
762	5	98.102	5	6	2	4H-pyran-4-ol	-210.996	-117.011
763	5	98.102	5	6	2	2H-pyran-4(3H)-one	-284.825	-212.071
764	5	100.118	5	8	2	3,4-dihydro-2H-pyran-3-ol	-307.987	-176.930
765	5	100.118	5	8	2	3,6-dihydro-2H-pyran-3-ol	-307.987	-176.930
766	5	130.101	5	6	4	2-hydroxy-3-oxopentanedial	-734.330	-518.080
767	5	114.101	5	6	3	2-hydroxy-3-oxopent-4-enal	-475.388	-309.739
768	5	114.101	5	6	3	3-oxopentanedial	-577.921	-380.840
769	5	144.128	6	8	4	2,6-dihydroxy-3-oxohex-4-enal	-662.422	-448.808
770	5	98.102	5	6	2	3-oxopent-4-enal	-318.979	-172.499
771	5	98.102	5	6	2	pent-2-enedial	-306.824	-175.581
772	5	98.102	5	6	2	2-oxopent-4-enal	-235.695	-82.802
773	5	98.102	5	6	2	2-oxopent-3-enal	-246.639	-92.076
774	5	128.128	6	8	3	5-hydroxy-2-oxohex-3-enal	-432.121	-227.873
775	5	128.128	6	8	3	6-hydroxyhex-4-ene-2,3-dione	-431.953	-223.635
776	5	116.117	5	8	3	1,5-dihydroxypent-3-en-2-one	-483.354	-332.296
777	5	116.117	5	8	3	4,5-dihydroxypent-2-enal	-492.572	-338.825
778	5	112.085	5	4	3	4-oxopent-2-enedial	-384.764	-215.621
779	5	132.117	5	8	4	2,4-dihydroxypentanedial	-749.370	-542.843
780	5	116.117	5	8	3	2-hydroxypentanedial	-583.758	-397.476
781	5	86.091	4	6	2	2,5-dihydrofuran-3-ol	-283.019	-199.450
782	5	86.091	4	6	2	2,3-dihydrofuran-3-ol	-289.412	-190.217
783	5	60.096	3	8	1	propan-1-ol	-257.907	-161.518
784	5	30.07	2	6	0	ethane	-79.409	-29.211
785	5	72.107	4	8	1	butan-2-one	-280.809	-143.357

786	5	102.134	5	10	2 pent-4-ene-1,3-diol	-340.396	-202.104
787	5	82.102	5	6	1 penta-1,4-dien-3-one	-35.711	28.795
788	5	100.118	5	8	2 glutaraldehyde	-418.146	-252.109
789	5	70.091	4	6	1 but-2-enal	-147.870	-60.100
790	5	70.091	4	6	1 but-3-enal	-136.926	-50.826
791	5	112.129	6	8	2 6-hydroxyhexa-2,4-dienal	-245.253	-111.865
792	5	112.129	6	8	2 4-hydroxyhexa-2,5-dienal	-229.400	-99.180
793	5	100.118	5	8	2 4-hydroxypent-2-enal	-333.352	-195.897
794	5	90.123	4	10	2 butane-1,4-diol	-436.405	-293.825
795	6	114.145	6	10	2 2-(2,3-dihydrofuran-2-yl)ethanol	-343.639	-212.305
796	6	114.145	6	10	2 2-ethyl-2,3-dihydrofuran-3-ol	-342.181	-181.123
797	6	114.145	6	10	2 hexahydrofuro[3,2-b]furan	-368.385	-197.729
798	6	110.113	6	6	2 2-(furan-2(3H)-ylidene)acetaldehyde	-201.478	-77.260
799	6	114.145	6	10	2 1-(2,3-dihydrofuran-2-yl)ethanol	-335.091	-169.977
800	6	84.118	5	8	1 2-methyl-2,3-dihydrofuran	-91.909	21.858
801	6	94.113	6	6	1 2-vinylfuran	19.233	73.500
802	6	116.161	6	12	2 1-(tetrahydrofuran-2-yl)ethanol	-432.082	-229.896
803	6	114.145	6	10	2 2-vinyltetrahydrofuran-3-ol	-318.819	-157.721
804	6	114.145	6	10	2 2-ethylidenetetrahydrofuran-3-ol	-400.605	-247.912
805	6	114.145	6	10	2 1-(2,5-dihydrofuran-2-yl)ethanol	-335.091	-169.977
806	6	114.145	6	10	2 1-(4,5-dihydrofuran-2-yl)ethanol	-332.620	-188.318
807	6	134.176	6	14	3 hexane-2,3,4-triol	-661.704	-436.664
808	6	134.176	6	14	3 hexane-1,3,5-triol	-651.618	-428.060
809	6	114.145	6	10	2 5-ethyl-2,3-dihydrofuran-3-ol	-360.310	-221.245
810	6	114.145	6	10	2 5-ethyl-2,5-dihydrofuran-3-ol	-335.788	-190.356
811	6	114.145	6	10	2 2-ethyl-2,5-dihydrofuran-3-ol	-335.788	-190.356
812	6	114.145	6	10	2 5-ethyl-2,5-dihydrofuran-3(2H)-one	-420.464	-256.746
813	6	114.145	6	10	2 2-ethyl-2,5-dihydrofuran-3(2H)-one	-420.464	-256.746
814	6	114.145	6	10	2 5-vinyltetrahydrofuran-3-ol	-318.819	-157.721
815	6	114.145	6	10	2 2-(2,5-dihydrofuran-2-yl)ethanol	-319.551	-167.239
816	6	130.144	6	10	3 5-(2-hydroxyethylidene)tetrahydrofuran-3-ol	-596.434	-441.133
817	6	110.113	6	6	2 2-(furan-2(5H)-ylidene)acetaldehyde	-201.478	-77.260
818	6	130.144	6	10	3 5-hydroxytetrahydro-2H-pyran-2-carbaldehyde	-579.471	-364.696
819	6	146.144	6	10	4 2,5-dihydroxyhexanedial	-770.199	-534.779
820	6	130.144	6	10	3 2-hydroxy-5-oxohexanal	-626.204	-396.141
821	6	130.144	6	10	3 2-hydroxyhexanedial	-604.587	-389.412
822	6	130.144	6	10	3 3-hydroxy-5-methyltetrahydrofuran-2-carbaldehyde	-592.812	-378.107
823	6	130.144	6	10	3 2,3-dihydroxyhex-5-enal	-511.359	-327.989
824	6	130.144	6	10	3 2,3-dihydroxyhex-4-enal	-517.428	-332.020
825	6	130.144	6	10	3 5-hydroxy-2-oxohexanal	-544.402	-305.907
826	6	84.118	5	8	1 2-methyl-2,5-dihydrofuran	-91.909	21.858
827	6	114.145	6	10	2 5-ethylidenetetrahydrofuran-3-ol	-403.120	-250.763
828	6	134.176	6	14	3 hexane-1,2,5-triol	-646.799	-421.575
829	6	134.176	6	14	3 hexane-2,3,5-triol	-661.112	-435.613
830	6	114.145	6	10	2 hexane-2,5-dione	-217.100	-142.100
831	6	114.145	6	10	2 5-oxohexanal	-460.592	-250.774
832	6	114.145	6	10	2 5-hydroxyhex-3-en-2-one	-375.831	-193.019
833	6	114.145	6	10	2 3-hydroxyhex-5-en-2-one	-352.608	-176.428
834	6	114.145	6	10	2 3-hydroxyhex-4-en-2-one	-358.677	-180.459
835	6	104.15	5	12	2 pentane-1,2-diol	-465.769	-291.808
836	6	104.15	5	12	2 pentane-2,4-diol	-473.120	-295.753
837	6	114.145	6	10	2 adipaldehyde	-438.975	-244.045
838	6	114.145	6	10	2 5-hydroxyhex-3-enal	-348.768	-182.970
839	6	114.145	6	10	2 5-hydroxyhex-2-enal	-355.140	-189.339
840	6	114.145	6	10	2 3-hydroxyhex-5-enal	-345.155	-181.571
841	6	114.145	6	10	2 3-hydroxyhex-4-enal	-351.224	-185.602
842	6	114.145	6	10	2 (5-methyl-4,5-dihydrofuran-2-yl)methanol	-347.808	-214.043
843	6	114.145	6	10	2 (5-methyl-2,5-dihydrofuran-2-yl)methanol	-329.679	-173.921
844	6	114.145	6	10	2 5-methyl-2-methylenetetrahydrofuran-3-ol	-414.602	-279.886
845	6	114.145	6	10	2 2-methyl-3,4-dihydro-2H-pyran-4-ol	-339.903	-177.054
846	6	114.145	6	10	2 2-methyl-3,6-dihydro-2H-pyran-4-ol	-333.510	-186.287
847	6	114.145	6	10	2 6-methyl-5,6-dihydro-2H-pyran-3-ol	-333.510	-186.287
848	6	114.145	6	10	2 6-methyl-3,6-dihydro-2H-pyran-3-ol	-339.903	-177.054
849	6	114.145	6	10	2 2-methyldihydro-2H-pyran-4(3H)-one	-418.186	-252.677
850	6	114.145	6	10	2 6-methyldihydro-2H-pyran-3(4H)-one	-418.186	-252.677
851	6	114.145	6	10	2 1-hydroxyhex-5-en-3-one	-357.903	-180.255
852	6	114.145	6	10	2 1-hydroxyhex-5-en-2-one	-348.700	-172.128
853	6	114.145	6	10	2 1-hydroxyhex-4-en-3-one	-356.676	-193.494
854	6	114.145	6	10	2 1-hydroxyhex-4-en-2-one	-358.243	-180.516
855	6	114.145	6	10	2 5-hydroxyhex-1-en-3-one	-367.295	-186.257

856	6	114.145	6	10	2 (3,6-dihydro-2H-pyran-2-yl)methanol	-316.338	-160.510
857	6	114.145	6	10	2 (3,4-dihydro-2H-pyran-2-yl)methanol	-316.338	-160.510
858	6	114.145	6	10	2 6-methylenetetrahydro-2H-pyran-3-ol	-403.776	-269.326
859	6	114.145	6	10	2 2-hydroxyhex-5-en-3-one	-356.643	-177.124
860	6	114.145	6	10	2 4-hydroxyhex-5-en-3-one	-354.128	-174.273
861	6	114.145	6	10	2 4-hydroxyhex-5-en-2-one	-363.298	-183.943
862	6	114.145	6	10	2 2,5-dimethyl-2,3-dihydrofuran-3-ol	-334.793	-177.928
863	6	114.145	6	10	2 2,5-dimethyl-2,5-dihydrofuran-3-ol	-346.851	-199.698
864	6	114.145	6	10	2 2,5-dimethyldihydrofuran-3(2H)-one	-431.527	-266.088
865	6	114.145	6	10	2 hexane-2,4-dione	-482.242	-255.960
866	6	114.145	6	10	2 hexane-3,4-dione	-386.565	-161.298
867	6	114.145	6	10	2 2-hydroxyhex-4-en-3-one	-367.587	-186.398
868	6	116.117	5	8	3 3-hydroxytetrahydrofuran-2-carbaldehyde	-560.896	-377.983
869	6	96.086	5	4	2 furan-2-carbaldehyde	-283.906	-209.837
870	6	100.118	5	8	2 2-methylenetetrahydrofuran-3-ol	-382.686	-279.762
871	6	100.118	5	8	2 (4,5-dihydrofuran-2-yl)methanol	-315.892	-213.919
872	6	120.149	5	12	3 pentane-1,3,5-triol	-622.846	-431.128
873	6	102.134	5	10	2 (tetrahydrofuran-2-yl)methanol	-394.754	-233.716
874	6	100.118	5	8	2 5,6-dihydro-2H-pyran-3-ol	-301.594	-186.163
875	6	100.118	5	8	2 3,6-dihydro-2H-pyran-4-ol	-301.594	-186.163
876	6	100.118	5	8	2 3,4-dihydro-2H-pyran-4-ol	-307.987	-176.930
877	6	100.118	5	8	2 dihydro-2H-pyran-4(3H)-one	-386.270	-252.553
878	6	116.117	5	8	3 2,3-dihydroxypent-4-enal	-487.056	-331.696
879	6	100.118	5	8	2 3-hydroxypent-4-enal	-320.852	-185.278
880	6	100.118	5	8	2 5-hydroxypent-2-enal	-326.368	-192.407
881	6	100.118	5	8	2 5-hydroxypent-3-enal	-322.511	-188.889
882	6	130.144	6	10	3 2-(2-hydroxyethylidene)tetrahydrofuran-3-ol	-581.875	-415.749
883	6	130.144	6	10	3 4-hydroxytetrahydro-2H-pyran-2-carbaldehyde	-579.471	-364.696
884	6	130.144	6	10	3 2,4-dihydroxyhex-5-enal	-507.293	-322.581
885	6	130.144	6	10	3 2,6-dihydroxyhex-3-enal	-506.437	-323.341
886	6	130.144	6	10	3 2,6-dihydroxyhex-4-enal	-508.952	-326.192
887	6	130.144	6	10	3 4-hydroxy-2-oxohexanal	-545.361	-307.413
888	6	130.144	6	10	3 4-hydroxy-3-oxohexanal	-617.993	-387.977
889	6	130.144	6	10	3 2-hydroxy-4-oxohexanal	-626.237	-394.598
890	6	130.144	6	10	3 2-hydroxy-3-oxohexanal	-617.034	-386.471
891	6	88.107	4	8	2 2-hydroxybutanal	-248.000	-154.000
892	6	112.129	6	8	2 2-(dihydrofuran-2(3H)-ylidene)acetaldehyde	-298.469	-137.179
893	6	132.16	6	12	3 2,6-dihydroxyhexanal	-624.131	-406.238
894	6	132.16	6	12	3 2,3-dihydroxyhexanal	-633.625	-413.791
895	6	110.113	6	6	2 5-methylfuran-2-carbaldehyde	-301.825	-177.987
896	6	130.144	6	10	3 4-hydroxy-5-methyltetrahydrofuran-2-carbaldehyde	-592.812	-378.107
897	6	130.144	6	10	3 4,5-dihydroxyhex-2-enal	-521.344	-335.757
898	6	130.144	6	10	3 2,6-dihydroxyhex-4-en-3-one	-524.297	-325.263
899	6	126.112	6	6	3 2,5-dihydrofuran-2,5-dicarbaldehyde	-458.099	-291.656
900	6	126.112	6	6	3 2,3-dihydrofuran-2,5-dicarbaldehyde	-491.095	-330.547
901	6	110.113	6	6	2 5-methylene-2,5-dihydrofuran-2-carbaldehyde	-291.185	-223.291
902	6	110.113	6	6	2 2H-pyran-2-carbaldehyde	-265.031	-177.096
903	6	146.144	6	10	4 2,3,6-trihydroxyhex-4-enal	-297.000	-469.759
904	6	130.144	6	10	3 3,6-dihydroxyhex-4-enal	-506.437	-323.341
905	6	130.144	6	10	3 3,6-dihydroxyhex-4-en-2-one	-513.890	-318.198
906	6	110.113	6	6	2 hexa-2,4-dienedial	-216.331	-90.989
907	6	130.144	6	10	3 2,5-dihydroxyhex-3-enal	-510.906	-323.980
908	6	100.118	5	8	2 2-hydroxypent-4-enal	-323.367	-188.129
909	6	100.118	5	8	2 2-hydroxypent-3-enal	-329.436	-192.160
910	6	114.145	6	10	2 2-(4,5-dihydrofuran-2-yl)ethanol	-337.680	-207.361
911	6	134.176	6	14	3 hexane-1,3,6-triol	-638.264	-415.528
912	6	134.176	6	14	3 hexane-1,3,4-triol	-653.169	-430.617
913	6	84.118	5	8	1 5-methyl-2,3-dihydrofuran	-122.578	-23.549
914	6	104.15	5	12	2 pentane-2,3-diol	-474.671	-298.310
915	6	104.15	5	12	2 pentane-1,3-diol	-465.177	-290.757
916	6	114.145	6	10	2 4-hydroxyhex-5-enal	-341.681	-177.214
917	6	114.145	6	10	2 6-hydroxyhex-3-enal	-344.299	-182.331
918	6	114.145	6	10	2 6-hydroxyhex-4-enal	-343.340	-180.825
919	6	114.145	6	10	2 4-oxohexanal	-460.625	-249.231
920	6	114.145	6	10	2 3-oxohexanal	-460.625	-249.231
921	6	114.145	6	10	2 6-hydroxyhex-3-en-2-one	-368.847	-189.529
922	6	114.145	6	10	2 6-hydroxyhex-4-en-2-one	-364.957	-187.554
923	6	114.145	6	10	2 hexane-2,3-dione	-386.565	-161.298
924	6	114.145	6	10	2 (5,6-dihydro-2H-pyran-2-yl)methanol	-316.338	-160.510
925	6	114.145	6	10	2 2-methylenetetrahydro-2H-pyran-4-ol	-403.776	-269.326

926	6	134.176	6	14	3 hexane-1,2,4-triol	-653.169	-430.617
927	6	114.145	6	10	2 hexa-3,5-diene-1,2-diol	-262.281	-125.125
928	6	114.145	6	10	2 1-hydroxyhex-3-en-2-one	-359.644	-181.402
929	6	114.145	6	10	2 4-hydroxyhex-1-en-3-one	-359.051	-179.636
930	6	116.161	6	12	2 2-(tetrahydrofuran-2-yl)ethanol	-416.542	-227.158
931	6	86.134	5	10	1 2-methyltetrahydrofuran	-238.020	-96.005
932	6	116.161	6	12	2 3-hydroxyhexanal	-467.421	-267.373
933	6	116.161	6	12	2 6-hydroxyhexanal	-458.519	-260.871
934	6	116.161	6	12	2 3-hydroxyhexan-2-one	-474.874	-262.230
935	6	116.161	6	12	2 6-hydroxyhexan-2-one	-480.136	-267.600
936	6	116.161	6	12	2 (tetrahydro-2H-pyran-2-yl)methanol	-413.329	-220.429
937	6	116.161	6	12	2 hex-5-ene-1,2-diol	-365.291	-199.448
938	6	116.161	6	12	2 1-hydroxyhexan-2-one	-470.966	-257.930
939	6	116.161	6	12	2 1-hydroxyhexan-3-one	-480.169	-266.057
940	6	130.144	6	10	3 3-hydroxytetrahydro-2H-pyran-2-carbaldehyde	-579.471	-364.696
941	6	114.145	6	10	2 (3,4-dihydro-2H-pyran-6-yl)methanol	-334.467	-200.632
942	6	114.145	6	10	2 2-methylenetetrahydro-2H-pyran-3-ol	-401.261	-266.475
943	6	130.144	6	10	3 6-hydroxy-2-oxohexanal	-536.459	-300.911
944	6	134.176	6	14	3 hexane-1,4,5-triol	-647.758	-423.081
945	6	104.15	5	12	2 pentane-1,4-diol	-465.177	-290.757
946	6	114.145	6	10	2 6-hydroxyhex-2-enal	-347.197	-184.343
947	6	114.145	6	10	2 6-hydroxyhex-1-en-3-one	-359.352	-181.261
948	6	114.145	6	10	2 6-methyl-3,4-dihydro-2H-pyran-4-ol	-321.452	-164.517
949	6	114.145	6	10	2 6-methyl-3,6-dihydro-2H-pyran-4-ol	-333.510	-186.287
950	6	114.145	6	10	2 2-methyl-5,6-dihydro-2H-pyran-3-ol	-333.510	-186.287
951	6	114.145	6	10	2 2-methyl-3,6-dihydro-2H-pyran-3-ol	-339.903	-177.054
952	6	114.145	6	10	2 2-methyldihydro-2H-pyran-3(4H)-one	-418.186	-252.677
953	6	114.145	6	10	2 6-hydroxyhex-4-en-3-one	-367.888	-188.023
954	6	100.118	5	8	2 2-oxopentanal	-357.961	-168.604
955	6	84.118	5	8	1 pent-3-en-2-one	-190.349	-57.222
956	6	74.123	4	10	1 butan-2-ol	-286.679	-158.450
957	6	84.118	5	8	1 pent-2-enal	-168.699	-52.036
958	6	84.118	5	8	1 pent-3-enal	-167.298	-51.150
959	6	84.118	5	8	1 pent-1-en-3-one	-180.854	-48.954
960	6	84.118	5	8	1 pent-4-en-2-one	-179.372	-49.491
961	6	114.145	6	10	2 4-hydroxyhex-2-enal	-355.140	-189.339
962	6	84.118	5	8	1 pent-4-enal	-157.755	-42.762
963	6	58.08	3	6	1 prop-2-en-1-ol	-134.682	-74.210
964	6	42.081	3	6	0 prop-1-ene	20.531	63.529
965	6	72.107	4	8	1 tetrahydrofuran	-206.104	-95.881
966	6	72.107	4	8	1 but-3-en-2-ol	-160.939	-68.291
967	6	72.107	4	8	1 but-3-en-1-ol	-156.470	-67.652
968	6	72.107	4	8	1 but-2-en-1-ol	-165.054	-74.534
969	6	72.107	4	8	1 butyraldehyde	-259.192	-136.628
970	6	110.113	6	6	2 5-methylene-4,5-dihydrofuran-2-carbaldehyde	-305.989	-225.079
971	6	94.113	6	6	1 2,5-dimethylene-2,5-dihydrofuran	-55.019	-58.335
972	6	114.145	6	10	2 2-methyl-5-methylenetetrahydrofuran-3-ol	-417.117	-282.737
973	6	114.145	6	10	2 (5-methyl-2,3-dihydrofuran-2-yl)methanol	-311.228	-161.384
974	6	94.113	6	6	1 2-methylene-2H-pyran	-38.276	-22.238
975	6	114.145	6	10	2 2-methyl-3,4-dihydro-2H-pyran-3-ol	-339.903	-177.054
976	6	114.145	6	10	2 6-methyl-3,4-dihydro-2H-pyran-3-ol	-321.452	-164.517
977	6	110.113	6	6	2 4H-pyran-2-carbaldehyde	-238.186	-129.494
978	6	110.113	6	6	2 2H-pyran-6-carbaldehyde	-302.481	-196.550
979	6	116.161	6	12	2 (5-methyltetrahydrofuran-2-yl)methanol	-426.670	-233.840
980	6	128.128	6	8	3 tetrahydrofuran-2,5-dicarbaldehyde	-555.090	-351.575
981	6	112.129	6	8	2 5-methylenetetrahydrofuran-2-carbaldehyde	-379.395	-256.205
982	6	98.102	5	6	2 2,3-dihydrofuran-2-carbaldehyde	-283.606	-163.809
983	6	98.102	5	6	2 2,5-dihydrofuran-2-carbaldehyde	-283.606	-163.809
984	6	110.113	6	6	2 2-oxohexa-3,5-dienal	-228.101	-98.434
985	6	88.107	4	8	2 but-2-ene-1,4-diol	-320.267	-212.273
986	6	96.129	6	8	1 2,5-dimethylenetetrahydrofuran	-194.289	-150.737
987	6	82.102	5	6	1 2-methylene-2,3-dihydrofuran	-107.911	-68.439
988	6	82.102	5	6	1 2-methylene-2,5-dihydrofuran	-121.146	-76.007
989	6	102.134	5	10	2 tetrahydro-2H-pyran-3-ol	-404.978	-236.849
990	6	118.133	5	10	3 2,5-dihydroxypentanal	-603.302	-414.302
991	6	102.134	5	10	2 5-hydroxypentanal	-437.690	-268.935
992	6	114.145	6	10	2 hexa-1,5-diene-3,4-diol	-244.979	-111.434
993	6	114.145	6	10	2 hexa-2,4-diene-1,6-diol	-262.389	-126.179
994	6	114.145	6	10	2 hexa-2,5-diene-1,4-diol	-242.572	-109.637
995	6	102.134	5	10	2 pent-2-ene-1,4-diol	-346.524	-206.354

996	6	82.102	5	6	1 4H-pyran	-30.697	37.244
997	6	82.102	5	6	1 2H-pyran	-30.697	37.244
998	6	118.133	5	10	3 pent-3-ene-1,2,5-triol	-505.744	-349.282
999	6	114.101	5	6	3 5-hydroxy-2-oxopent-3-enal	-403.349	-230.941
1000	6	114.101	5	6	3 4-hydroxypent-2-enedial	-471.477	-319.442
1001	6	68.075	4	4	1 furan	-71.963	-62.536
1002	6	84.118	5	8	1 penta-2,4-dien-1-ol	-76.804	11.884
1003	6	84.118	5	8	1 penta-1,4-dien-3-ol	-56.987	28.426
1004	6	82.102	5	6	1 penta-2,4-dienal	-59.668	26.198
1005	7	96.129	6	8	1 2-vinyl-2,3-dihydrofuran	-41.529	56.453
1006	7	96.129	6	8	1 2-ethylfuran	-147.315	-74.127
1007	7	116.161	6	12	2 2-ethyltetrahydrofuran-3-ol	-439.172	-241.042
1008	7	112.129	6	8	2 2-(furan-2(3H)-ylidene)ethanol	-343.232	-272.025
1009	7	96.129	6	8	1 2-ethylidene-2,3-dihydrofuran	-76.710	21.355
1010	7	98.145	6	10	1 2-vinyltetrahydrofuran	-138.520	-3.466
1011	7	98.145	6	10	1 2-ethylidenetetrahydrofuran	-222.821	-96.508
1012	7	118.177	6	14	2 hexane-1,5-diol	-486.006	-282.693
1013	7	118.177	6	14	2 hexane-2,3-diol	-495.500	-290.246
1014	7	96.129	6	8	1 2-vinyl-2,5-dihydrofuran	-41.529	56.453
1015	7	96.129	6	8	1 5-vinyl-2,3-dihydrofuran	-77.758	13.581
1016	7	116.161	6	12	2 hex-1-ene-3,4-diol	-370.719	-201.593
1017	7	116.161	6	12	2 hex-5-ene-1,3-diol	-363.740	-196.891
1018	7	96.129	6	8	1 2-ethylidene-2,5-dihydrofuran	-159.171	-92.566
1019	7	116.161	6	12	2 5-hydroxyhexan-3-one	-488.112	-271.053
1020	7	116.161	6	12	2 2-hydroxyhexan-3-one	-478.909	-262.926
1021	7	116.161	6	12	2 4-hydroxyhexan-2-one	-489.038	-274.102
1022	7	116.161	6	12	2 4-hydroxyhexan-3-one	-479.868	-264.432
1023	7	116.161	6	12	2 2-methyltetrahydro-2H-pyran-4-ol	-436.894	-236.973
1024	7	116.161	6	12	2 hex-5-ene-2,4-diol	-369.168	-199.036
1025	7	116.161	6	12	2 hex-4-ene-1,3-diol	-370.768	-202.428
1026	7	116.161	6	12	2 hex-3-ene-1,5-diol	-368.312	-199.796
1027	7	116.161	6	12	2 hex-2-ene-1,5-diol	-370.827	-202.647
1028	7	116.161	6	12	2 5-ethyltetrahydrofuran-3-ol	-439.172	-241.042
1029	7	112.129	6	8	2 2-(furan-2(5H)-ylidene)ethanol	-320.335	-211.994
1030	7	112.129	6	8	2 3,6-dihydro-2H-pyran-2-carbaldehyde	-302.181	-150.522
1031	7	112.129	6	8	2 3,4-dihydro-2H-pyran-2-carbaldehyde	-302.181	-150.522
1032	7	132.16	6	12	3 2,5-dihydroxyhexanal	-632.074	-411.234
1033	7	102.134	5	10	2 2-hydroxypentanal	-445.633	-273.931
1034	7	112.129	6	8	2 5-methyl-4,5-dihydrofuran-2-carbaldehyde	-348.518	-202.824
1035	7	112.129	6	8	2 5-methyl-2,5-dihydrofuran-2-carbaldehyde	-315.522	-163.933
1036	7	112.129	6	8	2 2-oxohex-5-enal	-256.524	-74.738
1037	7	112.129	6	8	2 2-oxohex-4-enal	-266.067	-83.126
1038	7	116.161	6	12	2 6-methyltetrahydro-2H-pyran-3-ol	-436.894	-236.973
1039	7	116.161	6	12	2 hex-4-ene-1,2-diol	-374.834	-207.836
1040	7	116.161	6	12	2 5-hydroxyhexan-2-one	-488.079	-272.596
1041	7	116.161	6	12	2 5-hydroxyhexanal	-466.462	-265.867
1042	7	116.161	6	12	2 2,5-dimethyltetrahydrofuran-3-ol	-450.235	-250.384
1043	7	116.161	6	12	2 hex-5-ene-2,3-diol	-373.234	-204.444
1044	7	116.161	6	12	2 hex-4-ene-2,3-diol	-379.303	-208.475
1045	7	86.134	5	10	1 pentan-2-one	-301.638	-135.293
1046	7	116.161	6	12	2 hex-3-ene-2,5-diol	-372.781	-200.435
1047	7	96.129	6	8	1 hexa-3,5-dien-2-one	-102.147	29.076
1048	7	86.134	5	10	1 pentanal	-280.021	-128.564
1049	7	86.134	5	10	1 pent-3-en-2-ol	-191.311	-68.615
1050	7	86.134	5	10	1 pent-4-en-2-ol	-185.242	-64.584
1051	7	96.129	6	8	1 hexa-3,5-dienal	-79.048	35.268
1052	7	96.129	6	8	1 hexa-2,5-dienal	-67.262	41.830
1053	7	96.129	6	8	1 hexa-2,4-dienal	-277.100	-174.900
1054	7	96.129	6	8	1 2-methyl-5-methylene-2,5-dihydrofuran	-148.608	-95.568
1055	7	96.129	6	8	1 2-methyl-2H-pyran	-122.454	-49.373
1056	7	96.129	6	8	1 hexa-1,5-dien-3-one	-79.417	44.912
1057	7	96.129	6	8	1 hexa-1,4-dien-3-one	-78.190	31.673
1058	7	96.129	6	8	1 2-methylene-3,6-dihydro-2H-pyran	-126.486	-55.152
1059	7	96.129	6	8	1 2-methylene-3,4-dihydro-2H-pyran	-110.500	-137.230
1060	7	96.129	6	8	1 2,5-dimethylfuran	-107.801	1.164
1061	7	98.102	5	6	2 4,5-dihydrofuran-2-carbaldehyde	-316.602	-202.700
1062	7	100.118	5	8	2 tetrahydrofuran-2-carbaldehyde	-380.597	-223.728
1063	7	102.134	5	10	2 tetrahydro-2H-pyran-4-ol	-404.978	-236.849
1064	7	102.134	5	10	2 pent-2-ene-1,5-diol	-342.055	-205.715
1065	7	84.118	5	8	1 2-methylenetetrahydrofuran	-204.902	-128.358

1066	7	104.15	5	12	2 pentane-1,5-diol	-457.234	-285.761
1067	7	112.129	6	8	2 5,6-dihydro-2H-pyran-2-carbaldehyde	-302.181	-150.522
1068	7	132.16	6	12	3 2,4-dihydroxyhexanal	-632.074	-411.234
1069	7	112.129	6	8	2 2-hydroxyhexa-3,5-dienal	-241.186	-105.742
1070	7	112.129	6	8	2 2-oxohex-3-enal	-267.468	-84.012
1071	7	114.145	6	10	2 2-(dihydrofuran-2(3H)-ylidene)ethanol	-416.135	-286.878
1072	7	114.145	6	10	2 tetrahydro-2H-pyran-2-carbaldehyde	-399.172	-210.441
1073	7	114.145	6	10	2 2-hydroxyhex-5-enal	-344.196	-180.065
1074	7	114.145	6	10	2 2-oxohexanal	-378.790	-160.540
1075	7	114.145	6	10	2 5-methyltetrahydrofuran-2-carbaldehyde	-412.513	-223.852
1076	7	112.129	6	8	2 5-methyl-2,3-dihydrofuran-2-carbaldehyde	-297.071	-151.396
1077	7	132.16	6	12	3 hex-2-ene-1,4,5-triol	-534.516	-346.214
1078	7	116.161	6	12	2 hex-5-ene-1,4-diol	-361.225	-194.040
1079	7	116.161	6	12	2 hex-3-ene-1,6-diol	-363.843	-199.157
1080	7	116.161	6	12	2 hex-2-ene-1,6-diol	-362.884	-197.651
1081	7	116.161	6	12	2 6-hydroxyhexan-3-one	-480.169	-266.057
1082	7	86.134	5	10	1 pentan-3-one	-301.671	-133.75
1083	7	86.134	5	10	1 pent-1-en-3-ol	-182.727	-61.733
1084	7	86.134	5	10	1 pent-3-en-1-ol	-186.842	-67.976
1085	7	86.134	5	10	1 pent-2-en-1-ol	-184.386	-65.344
1086	7	116.161	6	12	2 4-hydroxyhexanal	-467.421	-267.373
1087	7	96.129	6	8	1 6-methylene-3,6-dihydro-2H-pyran	-135.267	-82.157
1088	7	116.161	6	12	2 hex-3-ene-1,2-diol	-369.863	-202.353
1089	7	118.177	6	14	2 hexane-1,6-diol	-478.063	-277.697
1090	7	118.177	6	14	2 hexane-1,3-diol	-486.965	-284.199
1091	7	88.15	5	12	1 pentan-1-ol	-299.565	-145.39
1092	7	88.15	5	12	1 pentan-2-ol	-307.508	-150.386
1093	7	98.145	6	10	1 hex-3-enal	-186.63	-41.96
1094	7	98.145	6	10	1 hex-2-enal	-189.528	-43.972
1095	7	98.145	6	10	1 hex-5-enal	-178.584	-34.698
1096	7	98.145	6	10	1 hex-3-en-2-one	-211.178	-49.158
1097	7	98.145	6	10	1 hex-5-en-2-one	-200.201	-41.427
1098	7	98.145	6	10	1 2-methylenetetrahydro-2H-pyran	-223.477	-115.071
1099	7	118.177	6	14	2 hexane-1,2-diol	-487.557	-285.25
1100	7	98.145	6	10	1 hex-1-en-3-one	-201.683	-40.89
1101	7	112.129	6	8	2 3,4-dihydro-2H-pyran-6-carbaldehyde	-335.177	-189.413
1102	7	116.161	6	12	2 2-methyltetrahydro-2H-pyran-3-ol	-436.894	-236.973
1103	7	86.134	5	10	1 pent-4-en-1-ol	-177.299	-59.588
1104	7	96.129	6	8	1 6-methyl-2H-pyran	-108.457	-17.399
1105	7	116.161	6	12	2 hex-2-ene-1,4-diol	-368.312	-199.796
1106	7	56.108	4	8	0 but-1-ene	1.199	72.719
1107	7	56.108	4	8	0 but-2-ene	-9.841	63.205
1108	7	44.097	3	8	0 propane	-100.238	-21.147
1109	7	74.123	4	10	1 butan-1-ol	-278.736	-153.454
1110	7	54.092	4	6	0 buta-1,3-diene	108.781	149.947
1111	7	96.129	6	8	1 5-methyl-2-methylene-2,3-dihydrofuran	-121.376	-56.026
1112	7	96.129	6	8	1 2-methyl-4H-pyran	-44.162	49.657
1113	7	98.145	6	10	1 2-methyl-5-methylenetetrahydrofuran	-236.818	-128.482
1114	7	84.118	5	8	1 3,6-dihydro-2H-pyran	-191.5	-128.2
1115	7	84.118	5	8	1 3,4-dihydro-2H-pyran	-127.688	-22.675
1116	7	116.117	5	8	3 2,5-dihydroxypent-3-enal	-484.649	-329.899
1117	8	98.145	6	10	1 2-ethyl-2,3-dihydrofuran	-185.97	-71.934
1118	8	100.161	6	12	1 2-ethyltetrahydrofuran	-258.873	-86.787
1119	8	98.145	6	10	1 2-ethyl-2,5-dihydrofuran	-161.882	-26.868
1120	8	98.145	6	10	1 5-ethyl-2,3-dihydrofuran	-180.011	-66.99
1121	8	118.177	6	14	2 hexane-3,4-diol	-495.5	-290.246
1122	8	100.161	6	12	1 hex-5-en-1-ol	-198.128	-51.524
1123	8	100.161	6	12	1 hex-1-en-3-ol	-203.556	-53.669
1124	8	100.161	6	12	1 2-methyltetrahydro-2H-pyran	-256.595	-82.718
1125	8	100.161	6	12	1 hex-5-en-2-ol	-206.071	-56.52
1126	8	100.161	6	12	1 hex-4-en-1-ol	-207.671	-59.912
1127	8	100.161	6	12	1 hexan-2-one	-322.467	-127.229
1128	8	100.161	6	12	1 hexan-3-one	-454.8	-323.2
1129	8	98.145	6	10	1 hex-5-en-3-one	-200.234	-39.884
1130	8	98.145	6	10	1 hexa-1,5-dien-3-ol	-81.29	32.133
1131	8	98.145	6	10	1 hexa-3,5-dien-1-ol	-98.592	18.442
1132	8	98.145	6	10	1 hexa-2,5-dien-1-ol	-82.949	28.522
1133	8	118.177	6	14	2 hexane-2,4-diol	-494.908	-289.195
1134	8	98.145	6	10	1 hex-4-en-3-one	-211.178	-49.158
1135	8	98.145	6	10	1 hex-4-en-2-one	-209.744	-49.815

1136	8	98.145	6	10	1 2-methyl-3,6-dihydro-2H-pyran	-159.604	-22.799
1137	8	98.145	6	10	1 6-methyl-3,6-dihydro-2H-pyran	-159.604	-22.799
1138	8	98.145	6	10	1 hexa-1,4-dien-3-ol	-87.359	28.102
1139	8	98.145	6	10	1 hexa-3,5-dien-2-ol	-103.061	17.803
1140	8	98.145	6	10	1 hexa-2,4-dien-1-ol	-107.176	11.56
1141	8	114.145	6	10	2 2-hydroxyhex-4-enal	-353.739	-188.453
1142	8	98.145	6	10	1 2-methyl-3,4-dihydro-2H-pyran	-159.604	-22.799
1143	8	118.177	6	14	2 hexane-2,5-diol	-493.949	-287.689
1144	8	98.145	6	10	1 hex-4-enal	-188.127	-43.086
1145	8	98.145	6	10	1 2,5-dimethyl-2,3-dihydrofuran	-108.7	-113
1146	8	98.145	6	10	1 2,5-dimethyl-2,5-dihydrofuran	-172.945	-36.21
1147	8	58.124	4	10	0 butane	-121.067	-13.083
1148	8	68.119	5	8	0 penta-1,3-diene	78.409	149.623
1149	8	68.119	5	8	0 penta-1,4-diene	102.636	166.585
1150	8	100.161	6	12	1 2,5-dimethyltetrahydrofuran	-269.936	-96.129
1151	8	86.134	5	10	1 tetrahydro-2H-pyran	-224.679	-82.594
1152	8	114.145	6	10	2 2-hydroxyhex-3-enal	-348.768	-182.97
1153	8	116.161	6	12	2 2-hydroxyhexanal	-466.462	-265.867
1154	8	118.177	6	14	2 hexane-1,4-diol	-486.965	-284.199
1155	8	88.15	5	12	1 pentan-3-ol	-239.1	-166.4
1156	8	100.161	6	12	1 hex-2-en-1-ol	-205.215	-57.28
1157	8	100.161	6	12	1 hex-3-en-1-ol	-206.174	-58.786
1158	8	70.135	5	10	0 pent-1-ene	-19.63	80.783
1159	8	70.135	5	10	0 pent-2-ene	-29.173	72.395
1160	8	100.161	6	12	1 hexanal	-300.85	-120.5
1161	8	100.161	6	12	1 hex-3-en-2-ol	-210.643	-59.425
1162	8	98.145	6	10	1 6-methyl-3,4-dihydro-2H-pyran	-141.153	-10.262
1163	9	102.177	6	14	1 hexan-1-ol	-320.394	-137.326
1164	9	102.177	6	14	1 hexan-3-ol	-329.296	-143.828
1165	9	82.146	6	10	0 hexa-1,5-diene	81.807	174.649
1166	9	82.146	6	10	0 hexa-1,3-diene	59.077	158.813
1167	9	102.177	6	14	1 hexan-2-ol	-328.337	-142.322
1168	9	82.146	6	10	0 hexa-1,4-diene	72.264	166.261
1169	9	100.161	6	12	1 hex-5-en-3-ol	-207.03	-58.026
1170	9	80.13	6	8	0 hexa-1,3,5-triene	96.995	143.385
1171	9	100.161	6	12	1 hex-4-en-2-ol	-215.614	-64.908
1172	9	100.161	6	12	1 hex-4-en-3-ol	-213.099	-62.057
1173	9	72.151	5	12	0 pentane	-141.896	-5.019
1174	10	84.162	6	12	0 hex-1-ene	-40.459	88.847
1175	10	84.162	6	12	0 hex-2-ene	-393.5	-394.4
1176	10	84.162	6	12	0 hex-3-ene	-48.505	81.585
1177	10	82.146	6	10	0 hexa-2,4-diene	48.037	149.299
1178	11	86.178	6	14	0 hexane	-162.725	3.045