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Supplement of

Molecular representation of benzene and phenol secondary organic aerosols

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Supplement S1: Kinetic constant calculation using SAR method

Jenkin et al. (2018) defined the reaction rate of the OH-addition to an aromatic ring $k_{addition}$ as the sum of all partial rate coefficients corresponding to each carbon on the ring.

$$k_{addition} = \sum_{i=1}^{6} k_{part,i} \quad \text{(S1)}$$

where the partial rate coefficient $k_{part,i}$ can be expressed as:

$$k_{part,i} = k_i F_i(\phi) R_i(\phi) \quad \text{(S2)}$$

where k_i ($\mathrm{cm^3\ molecules^{-1}\ s^{-1}}$) is the partial rate coefficient depending on the substitution of the considered carbon, $F_i(\phi)$ is a factor dependent on the neighboring carbons substituted and $R_i(\phi)$ is a factor correcting $F_i(\phi)$ depending on the nature of the substituents. In the following section, the calculation of the trihydroxybenzene hydroxylation kinetic is considered to illustrate the method.

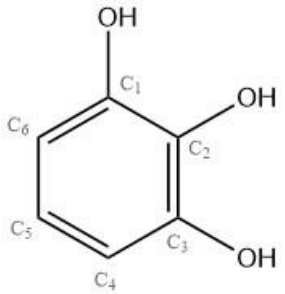

Figure S1: trihydroxybenzene structure.

The values for the parameters $F_i(\phi)$, $R_i(\phi)$ and k_i mentioned above are available in Jenkin et al. (2018). Using trihydroxybenzene as an example, the following values are used for the calculations:

Table S1: k_i values at 298K depending on the carbon i substitution

substitution	name	value ($\mathrm{cm^3\ molecules^{-1}\ s^{-1}}$)
unsubstituted	$k_{i,arom}$	2.0×10^{-13}
substituted	$k_{i,ipso}$	2.8×10^{-13}

The position of the three neighboring hydroxyl groups must be determined for each carbon in order to use the corrected value for $F_i(\phi)$ and $R_i(\phi)$.

Table S2 : $F(\phi)$ values depending on the position of the neighboring substituted carbons and $R(\phi)$ values for each neighboring OH-substituted carbon with a temperature of 298 K.

$F(\phi)$	value	$R(\phi)$	value
F (ortho, ortho)	10.5	R(ortho)	2.6
F (ortho, meta)	34.0	R(para)	2.6
F (ortho, meta, para)	28.0	R(meta)	2.4
F (meta, meta, para)	11.0	R(ipso)	2.4

Table S3: Description of trihydroxybenzene carbons substitution and calculation of partial kinetic constants. In the description of the substitution ϕ, i stands for ipso, o for ortho, m for meta and p for para.

Carbon ID	C1	C1	C1	C1	C1	C1
Substitution	OH	OH	OH	-	-	-
k_i	k_{ipso}	k_{ipso}	k_{ipso}	k_{arom}	k_{arom}	k_{arom}
ϕ	i, o, m	i, o, o	i, o, m	o, m, p	m, m, p	o, m, p
$k_{part,i}$	4.4 × 10−11	1.5 × 10−10	4.4 × 10−11	9.1 × 10−11	3.3 × 10−11	9.1 × 10−11

The sum of all six partial coefficients results in $k_{addition} = 4.58 \times 10^{-10}$ cm^3 molecules^{-1} s^{-1}. To compare, the value given by GECKOA for the hydroxylation rate constant of trihydroxybenzene is $k_{add,GECKOA} = 4.65 \times 10^{-10}$ cm^3 molecules^{-1} s^{-1}.

Supplement S2: Mech 2 – reactions

reaction number	reaction	kinetics
1	HOCH2CHO + OH -> 8.000E-01 HOCH2CO3 + 2.000E-01 GLY + 2.000E-01 HO2	ARR 1.000E-11 0 0
2	HOCH2CHO -> CO + HCHO + 2.000E+00 HO2	EXTRA 91 2.792E-05 0.805 0.338 1.0
3	HOCH2CHO + NO3 -> HNO3 + HOCH2CO3	ARR 1.400E-12 0 1860.00
4	HOCH2CO3 + NO2 -> PHAN	EXTRA 93 21 1.0
5	HOCH2CO3 + NO -> HCHO + HO2 + NO2	ARR 7.500E-12 0 -290.00
6	HOCH2CO3 + NO3 -> HCHO + HO2 + NO2	ARR 4.002E-12 0 0
7	HOCH2CO3 + HO2 -> 4.100E-01 HOCH2CO3H + 1.500E-01 HOCH2CO2H + 1.500E-01 O3 + 4.400E-01 HCHO + 4.400E-01 HO2 + 4.400E-01 OH	ARR 5.200E-13 0 -980.00
8	HOCH2CO3 -> 7.000E-01 HCHO + 7.000E-01 HO2 + 3.000E-01 HOCH2CO2H	RO2 1 ARR 1.000E-11 0 0
9	PHAN -> HOCH2CO3 + NO2	EXTRA 93 22 1.0
10	PHAN + OH -> CO + HCHO + NO2	ARR 1.120E-12 0 0
11	HOCH2CO2H + OH -> HCHO + HO2	ARR 2.730E-12 0 0
12	HOCH2CO3H -> HCHO + HO2 + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
13	HOCH2CO3H + OH -> HOCH2CO3	ARR 6.190E-12 0 0
14	GLYOOA -> 1.800E-01 GLYOO + 1.265E+00 CO + 8.200E-01 HO2 + 5.700E-01 OH + 1.250E-01 HCHO	ARR 1.000E+06 0 0
15	HCOCO3 + NO -> CO + HO2 + NO2	ARR 7.500E-12 0 -290.00
16	HCOCO3 + NO2 -> CO + HO2 + NO3	EXTRA 93 21 1.0
17	HCOCO3 + NO3 -> CO + HO2 + NO2	ARR 4.002E-12 0 0
18	HCOCO3 + HO2 -> 4.100E-01 HCOCO3H + 1.500E-01 HCOCO2H + 1.500E-01 O3 + 4.400E-01 CO + 4.400E-01 HO2 + 4.400E-01 OH	ARR 5.200E-13 0 -980.00
19	HCOCO3 -> 7.000E-01 CO + 7.000E-01 HO2 + 3.000E-01 HCOCO2H	RO2 1 ARR 1.000E-11 0 0
20	HCOCO3H + OH -> HCOCO3	ARR 1.580E-11 0 0
21	HCOCO3H -> CO + HO2 + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
22	HCOCO3H -> CO + HO2 + OH	EXTRA 91 2.792E-05 0.805 0.338 1.0
23	HCOCO2H + OH -> CO + HO2	ARR 1.230E-11 0 0
24	HCOCO2H -> CO + 2.000E+00 HO2	EXTRA 91 1.537E-04 0.170 0.208 1.0
25	GLYOO + SO2 -> GLY + SO3	ARR 7.000E-14 0 0
26	GLYOO + CO -> GLY	ARR 1.200E-15 0 0
27	GLYOO + NO -> GLY + NO2	ARR 1.000E-14 0 0
28	GLYOO + NO2 -> GLY + NO3	ARR 1.000E-15 0 0
29	GLYOO -> GLY + H2O2	TB H2O ARR 6.000E-18 0 0
30	GLYOO -> HCOCO2H	TB H2O ARR 1.000E-17 0 0
31	HCOCH2O2 + NO -> HCOCH2O + NO2	ARR 2.700E-12 0 -360.00
32	HCOCH2O2 + NO3 -> HCOCH2O + NO2	ARR 2.300E-12 0 0
33	HCOCH2O2 + HO2 -> HCOCH2OOH	ARR 1.126E-13 0 -1300.00
34	HCOCH2O2 -> 6.000E-01 HCOCH2O + 2.000E-01 GLY + 2.000E-01 HOCH2CHO	RO2 1 ARR 2.000E-12 0 0
35	HCOCH2O -> CO + HCHO + HO2	ARR 1.000E+06 0 0
36	HCOCH2OOH -> HCOCH2O + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
37	HCOCH2OOH -> CO + HCHO + HO2 + OH	EXTRA 91 2.792E-05 0.805 0.338 1.0
38	HCOCH2OOH + OH -> HCOCH2O2	ARR 1.900E-12 0 -190.00
39	HCOCH2OOH + OH -> GLY + OH	ARR 2.910E-11 0 0
40	BENZENE + OH -> 4.7E-01 BZBIPERO2 + 5.3E-01 PHENOL + 5.3E-01 HO2	ARR 2.300E-12 0 190.00

41	BZBIPERO2 + NO -> 9.180E-01 BZBIPERO + 9.180E-01 NO2 + 8.200E-02 BZBIPERNO3	ARR 2.700E-12 0 -360.00
42	BZBIPERO2 + NO3 -> BZBIPERO + NO2	ARR 2.300E-12 0 0
43	BZBIPERO2 + HO2 -> BZBIPEROOH	ARR 2.241E-13 0 -1300.00
44	BZBIPERO2 -> 6.000E-01 BZBIPERO + 2.000E-01 BZBIPER2OH + 2.000E-01 BZOBIPEROH	RO2 1 ARR 8.800E-13 0 0
45	BZBIPERO -> GLY + HO2 + 6.3E-01 MALDIAL + 3.7E-01 KETENOL	ARR 1.000E+06 0 0
46	BZBIPERNO3 -> BZBIPERO + NO2	EXTRA 91 4.095E-06 1.111 0.316 1.0
47	BZBIPERNO3 + OH -> 5.610E-01 GLY + 5.610E-01 MALDIALONO2 + 2.145E-01 C6DIALPEROHONO2 + 2.145E-01 HO2 + 2.245E-01 BEPOX + 2.245E-01 NO2	ARR 9.77E-11 0 0
48	BZBIPEROOH -> BZBIPERO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
49	BZBIPEROOH + OH -> 0.57 BEPOX + 0.43 BZOBIPEROH + OH	ARR 1.870E-10 0 0
50	BEPOX + OH -> BEPOXOH	ARR 3.03E-11 0 0
51	BEPOXOH + OH ->	ARR 6.03E-11 0 0
52	BEPOXOH + NO3 ->	ARR 2.29E-12 0 0
53	BZBIPER2OH + OH -> BZOBIPEROH + HO2	ARR 1.210E-10 0 0
54	BZOBIPEROH -> GLY + HO2 + MALDIALCO3	EXTRA 91 5.804E-06 1.092 0.377 1.0
55	BZOBIPEROH + OH -> GLY + MALDIALCO3	ARR 8.160E-11 0 0
56	MALDIAL + OH -> 1.700E-01 MALDIALO2 + 8.300E-01 MALDIALCO3	ARR 5.200E-11 0 0
57	MALDIAL -> 8.000E-01 KETENOL + 2.000E-01 ACR	EXTRA 91 1.631E-03 0.244 0.267 1.0
58	MALDIAL + O3 -> GLYOOA + GLY	ARR 2.000E-18 0 0
59	MALDIAL + NO3 -> HNO3 + MALDIALCO3	ARR 5.600E-12 0 1860.00
60	MALDIALO2 + NO -> MALDIALO + NO2	ARR 2.700E-12 0 -360.00
61	MALDIALO2 + NO3 -> MALDIALO + NO2	ARR 2.300E-12 0 0
62	MALDIALO2 + HO2 -> MALDIALOOH	ARR 1.819E-13 0 -1300.00
63	MALDIALO2 -> 6.000E-01 MALDIALO + 2.000E-01 HOCOC4DIAL + 2.000E-01 HOHOC4DIAL	RO2 1 ARR 8.800E-13 0 0
64	MALDIALO -> 2.000E+00 GLY + HO2	ARR 1.000E+06 0 0
65	MALDIALCO3 + NO -> MALDIALCO2 + NO2	ARR 7.500E-12 0 -290.00
66	MALDIALCO3 + NO2 -> MALDIALPAN	EXTRA 93 21 1.0
67	MALDIALCO3 + NO3 -> MALDIALCO2 + NO2	ARR 4.002E-12 0 0
68	MALDIALCO3 + HO2 -> 4.100E-01 MALDALCO3H + 1.500E-01 MALDALCO2H + 1.500E-01 O3 + 4.400E-01 MALDIALCO2 + 4.400E-01 OH	ARR 5.200E-13 0 -980.00
69	MALDIALCO3 -> 7.000E-01 MALDIALCO2 + 3.000E-01 MALDALCO2H	RO2 1 ARR 1.000E-11 0 0
70	MALDIALPAN -> MALDIALCO3 + NO2	EXTRA 93 22 1.0
71	MALDIALPAN + OH -> 2.000E+00 CO + GLY + NO2	ARR 3.700E-11 0 0
72	MALDIALOOH -> MALDIALO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
73	MALDIALOOH -> C32OH13CO + CO + HO2 + OH	EXTRA 91 5.584E-05 0.805 0.338 1.0
74	MALDIALOOH + OH -> MALDIALO2	ARR 1.900E-12 0 -190.00
75	MALDIALOOH + OH -> HOCOC4DIAL + OH	ARR 1.220E-10 0 0
76	HOCOC4DIAL -> CO + HCOCOHCO3 + HO2	EXTRA 91 1.537E-04 0.170 0.208 1.0
77	HOCOC4DIAL -> CO + HCOCOHCO3 + HO2	EXTRA 91 2.792E-05 0.805 0.338 1.0
78	HOCOC4DIAL + OH -> CO2C4DIAL + HO2	ARR 3.670E-11 0 0
79	CO2C4DIAL -> 4.000E+00 CO + 2.000E+00 HO2	EXTRA 91 3.074E-04 0.170 0.208 1.0
80	CO2C4DIAL + OH -> 4.000E+00 CO + HO2	ARR 2.450E-11 0 0
81	HCOCOHCO3 + NO -> GLY + HO2 + NO2	ARR 7.500E-12 0 -290.00
82	HCOCOHCO3 + NO2 -> HCOCOHPAN	EXTRA 93 21 1.0
83	HCOCOHCO3 + NO3 -> GLY + HO2 + NO2	ARR 4.002E-12 0 0

84	HCOCOHCO3 + HO2 -> 5.600E-01 HCOCOHCO3H + 4.400E-01 GLY + 4.400E-01 HO2 + 4.400E-01 OH	ARR 5.200E-13 0 -980.00
85	HCOCOHCO3 -> GLY + HO2	RO2 1 ARR 1.000E-11 0 0
86	HCOCOHPAN -> HCOCOHCO3 + NO2	EXTRA 93 22 1.0
87	HCOCOHPAN + OH -> CO + GLY + NO2	ARR 6.970E-11 0 0
88	HCOCOHCO3H -> GLY + HO2 + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
89	HCOCOHCO3H + OH -> HCOCOHCO3	ARR 7.330E-11 0 0
90	HOHOC4DIAL -> C32OH13CO + CO + 2.000E+00 HO2	EXTRA 91 5.584E-05 0.805 0.338 1.0
91	HOHOC4DIAL + OH -> HO2 + HOCOC4DIAL	ARR 8.130E-11 0 0
92	C32OH13CO -> CO + GLY + 2.000E+00 HO2	EXTRA 91 5.584E-05 0.805 0.338 1.0
93	C32OH13CO + OH -> HCOCOHCO3	ARR 1.360E-10 0 0
94	BZEPOXMUC + O3 -> EPXC4DIAL + GLYOOA	ARR 2.000E-18 0 0
95	BZEPOXMUC -> 1.500E+00 CO + 1.500E+00 HO2 + 5.000E-01 MALDIAL + 5.000E-01 C5DIALO2	EXTRA 91 1.165E-03 0.244 0.267 1.0
96	BZEPOXMUC + NO3 -> BZEMUCCO3 + HNO3	ARR 7.700E-12 0 1860.00
97	BZEPOXMUC + OH -> 6.900E-01 BZEMUCO2 + 3.100E-01 BZEMUCCO3	ARR 6.080E-11 0 0
98	MALANHY + OH -> MALANHYO2	ARR 1.400E-12 0 0
99	MALANHYO2 + NO -> MALANHYO + NO2	ARR 2.700E-12 0 -360.00
100	MALANHYO2 + NO3 -> MALANHYO + NO2	ARR 2.300E-12 0 0
101	MALANHYO2 + HO2 -> MALANHYOOH	ARR 1.819E-13 0 -1300.00
102	MALANHYO2 -> 6.000E-01 MALANHYO + 2.000E-01 MALANHY2OH + 2.000E-01 MALNHYOHCO	RO2 1 ARR 8.800E-13 0 0
103	MALANHYO -> HCOCOHCO3	ARR 1.000E+06 0 0
104	MALANHYOOH -> MALANHYO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
105	MALANHYOOH + OH -> MALNHYOHCO + OH	ARR 4.660E-11 0 0
106	MALANHY2OH + OH -> HO2 + MALNHYOHCO	ARR 2.550E-11 0 0
107	MALNHYOHCO + OH -> 3.000E+00 CO + HO2	ARR 5.680E-12 0 0
108	BZEMUCO2 + NO -> 8.950E-01 BZEMUCO + 8.950E-01 NO2 + 1.050E-01 BZEMUCNO3	ARR 2.700E-12 0 -360.00
109	BZEMUCO2 + NO3 -> BZEMUCO + NO2	ARR 2.300E-12 0 0
110	BZEMUCO2 + HO2 -> BZEMUCOOH	ARR 2.241E-13 0 -1300.00
111	BZEMUCO2 -> 6.000E-01 BZEMUCO + 2.000E-01 BZEMUCOH + 2.000E-01 BZEMUCCO	RO2 1 ARR 8.800E-13 0 0
112	BZEMUCO -> 5.000E-01 C32OH13CO + 5.000E-01 C3DIALO2 + 5.000E-01 EPXC4DIAL + 5.000E-01 GLY + 5.000E-01 HO2	ARR 1.000E+06 0 0
113	BZEMUCNO3 + OH -> BZEMUCCO + NO2	ARR 4.380E-11 0 0
114	BZEMUCNO3 -> EPXC4DIAL + GLY + HO2 + NO2	EXTRA 91 7.914E-05 0.764 0.364 1.0
115	BZEMUCOOH -> BZEMUCO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
116	BZEMUCOOH -> BZEMUCO + OH	EXTRA 91 2.792E-05 0.805 0.338 1.0
117	BZEMUCOOH + OH -> BZEMUCCO + OH	ARR 1.310E-10 0 0
118	BZEMUCOH -> BZEMUCO + HO2	EXTRA 91 5.584E-05 0.805 0.338 1.0
119	BZEMUCOH + OH -> BZEMUCCO + HO2	ARR 8.230E-11 0 0
120	BZEMUCCO -> C3DIALO2 + HCOCOHCO3	EXTRA 91 2.792E-05 0.805 0.338 1.0
121	BZEMUCCO -> C3DIALO2 + HCOCOHCO3	EXTRA 91 5.804E-06 1.092 0.377 1.0
122	BZEMUCCO + OH -> EPXDLCO3 + GLY	ARR 9.200E-11 0 0
123	C3DIALO2 + NO -> C3DIALO + NO2	ARR 2.700E-12 0 -360.00
124	C3DIALO2 + NO3 -> C3DIALO + NO2	ARR 2.300E-12 0 0
125	C3DIALO2 + HO2 -> C3DIALOOH	ARR 1.513E-13 0 -1300.00
126	C3DIALO2 -> 6.000E-01 C3DIALO + 2.000E-01 C32OH13CO + 2.000E-01 C33CO	RO2 1 ARR 8.800E-13 0 0
127	C3DIALO -> CO + GLY + HO2	ARR 1.000E+06 0 0

128	C3DIALOOH -> C3DIALO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
129	C3DIALOOH -> CO + GLY + HO2 + OH	EXTRA 91 5.584E-05 0.805 0.338 1.0
130	C3DIALOOH + OH -> C33CO + OH	ARR 1.440E-10 0 0
131	C33CO -> 3.000E+00 CO + 2.000E+00 HO2	EXTRA 91 5.584E-05 0.805 0.338 1.0
132	C33CO + OH -> 3.000E+00 CO + HO2	ARR 5.770E-11 0 0
133	BZEMUCCO3 + NO -> C5DIALO2 + NO2	ARR 7.500E-12 0 -290.00
134	BZEMUCCO3 + NO2 -> BZEMUCPAN	EXTRA 93 21 1.0
135	BZEMUCCO3 + NO3 -> C5DIALO2 + NO2	ARR 4.002E-12 0 0
136	BZEMUCCO3 + HO2 -> 4.100E-01 BZEMUCCO3H + 1.500E-01 BZEMUCCO2H + 1.500E-01 O3 + 4.400E-01 C5DIALO2 + 4.400E-01 OH	ARR 5.200E-13 0 -980.00
137	BZEMUCCO3 -> 7.000E-01 C5DIALO2 + 3.000E-01 BZEMUCCO2H	RO2 1 ARR 1.000E-11 0 0
138	C5DIALO2 + NO -> C5DIALO + NO2	ARR 2.700E-12 0 -360.00
139	C5DIALO2 + NO3 -> C5DIALO + NO2	ARR 2.300E-12 0 0
140	C5DIALO2 + HO2 -> C5DIALOOH	ARR 2.054E-13 0 -1300.00
141	C5DIALO2 -> 6.000E-01 C5DIALO + 2.000E-01 C5DIALOH + 2.000E-01 C5DIALCO	RO2 1 ARR 8.800E-13 0 0
142	C5DIALO -> CO + HO2 + MALDIAL	ARR 1.000E+06 0 0
143	BZEMUCPAN -> BZEMUCCO3 + NO2	EXTRA 93 22 1.0
144	BZEMUCPAN + OH -> CO + MALDIAL + NO2	ARR 4.050E-11 0 0
145	BZEMUCCO3H -> C5DIALO2 + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
146	BZEMUCCO3H -> C5DIALO2 + OH	EXTRA 91 1.140E-05 0.396 0.298 1.0
147	BZEMUCCO3H -> C5DIALO2 + OH	EXTRA 91 1.140E-05 0.396 0.298 1.0
148	BZEMUCCO3H + OH -> BZEMUCCO3	ARR 4.370E-11 0 0
149	BZEMUCCO2H -> C5DIALO2 + HO2	EXTRA 91 1.140E-05 0.396 0.298 1.0
150	BZEMUCCO2H -> C5DIALO2 + HO2	EXTRA 91 1.140E-05 0.396 0.298 1.0
151	BZEMUCCO2H + OH -> C5DIALO2	ARR 4.060E-11 0 0
152	C5DIALOOH -> C5DIALO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
153	C5DIALOOH -> CO + HO2 + MALDIAL + OH	EXTRA 91 1.140E-05 0.396 0.298 1.0
154	C5DIALOOH -> CO + HO2 + MALDIAL + OH	EXTRA 91 1.140E-05 0.396 0.298 1.0
155	C5DIALOOH + OH -> C5DIALCO + OH	ARR 7.520E-11 0 0
156	C5DIALOH -> CO + 2.000E+00 HO2 + MALDIAL	EXTRA 91 1.140E-05 0.396 0.298 1.0
157	C5DIALOH -> CO + 2.000E+00 HO2 + MALDIAL	EXTRA 91 1.140E-05 0.396 0.298 1.0
158	C5DIALOH + OH -> C5DIALCO + HO2	ARR 7.750E-11 0 0
159	C5DIALCO -> CO + HO2 + MALDIALCO3	EXTRA 91 1.537E-04 0.170 0.208 1.0
160	C5DIALCO -> CO + HO2 + MALDIALCO3	EXTRA 91 1.140E-05 0.396 0.298 1.0
161	C5DIALCO -> CO + HO2 + MALDIALCO3	EXTRA 91 1.140E-05 0.396 0.298 1.0
162	C5DIALCO + OH -> CO + MALDIALCO3	ARR 4.900E-11 0 0
163	EPXC4DIAL -> C3DIALO2 + CO + HO2	EXTRA 91 1.583E-04 0.764 0.364 1.0
164	EPXC4DIAL + OH -> EPXDLCO3	ARR 4.320E-11 0 0
165	EPXC4DIAL + NO3 -> EPXDLCO3 + HNO3	ARR 1.120E-11 0 1860.00
166	EPXDLCO3 + NO -> C3DIALO2 + NO2	ARR 7.500E-12 0 -290.00
167	EPXDLCO3 + NO2 -> EPXDLPAN	EXTRA 93 21 1.0
168	EPXDLCO3 + NO3 -> C3DIALO2 + NO2	ARR 4.002E-12 0 0
169	EPXDLCO3 + HO2 -> 4.100E-01 EPXDLCO3H + 1.500E-01 EPXDLCO2H + 1.500E-01 O3 + 4.400E-01 C3DIALO2 + 4.400E-01 OH	ARR 5.200E-13 0 -980.00
170	EPXDLCO3 -> 7.000E-01 C3DIALO2 + 3.000E-01 EPXDLCO2H	RO2 1 ARR 1.000E-11 0 0
171	EPXDLPAN -> EPXDLCO3 + NO2	EXTRA 93 22 1.0

172	EPXDLPAN + OH -> C33CO + CO + NO2	ARR 2.290E-11 0 0
173	EPXDLCO3H -> C3DIALO2 + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
174	EPXDLCO3H -> C3DIALO2 + OH	EXTRA 91 7.914E-05 0.764 0.364 1.0
175	EPXDLCO3H + OH -> EPXDLCO3	ARR 2.620E-11 0 0
176	EPXDLCO2H -> C3DIALO2 + HO2	EXTRA 91 7.914E-05 0.764 0.364 1.0
177	EPXDLCO2H + OH -> C3DIALO2	ARR 2.310E-11 0 0
178	PBZQONE + OH -> PBZQO2	ARR 4.600E-12 0 0
179	PBZQONE + NO3 -> NBZQO2	ARR 3.000E-13 0 0
180	PBZQO2 + NO -> NO2 + PBZQO	ARR 2.700E-12 0 -360.00
181	PBZQO2 + NO3 -> NO2 + PBZQO	ARR 2.300E-12 0 0
182	PBZQO2 + HO2 -> PBZQOOH	ARR 2.241E-13 0 -1300.00
183	PBZQO2 -> 6.000E-01 PBZQO + 2.000E-01 PBZQOH + 2.000E-01 PBZQCO	RO2 1 ARR 8.800E-13 0 0
184	PBZQO -> C5CO2OHCO3	ARR 1.000E+06 0 0
185	PBZQOOH -> OH + PBZQO	EXTRA 91 7.649E-06 0.682 0.279 1.0
186	PBZQOOH + OH -> OH + PBZQCO	ARR 1.230E-10 0 0
187	PBZQOH + OH -> HO2 + PBZQCO	ARR 9.180E-11 0 0
188	PBZQCO + OH -> C5CO2OHCO3	ARR 6.070E-11 0 0
189	BZFUONE + OH -> BZFUO2	ARR 4.450E-11 0 0
190	BZFUONE + NO3 -> NBZFUO2	ARR 3.000E-13 0 0
191	BZFUONE + O3 -> BZFUONOOA	ARR 2.200E-19 0 0
192	BZFUO2 + NO -> BZFUO + NO2	ARR 2.700E-12 0 -360.00
193	BZFUO2 + NO3 -> BZFUO + NO2	ARR 2.300E-12 0 0
194	BZFUO2 + HO2 -> BZFUOOH	ARR 2.054E-13 0 -1300.00
195	BZFUO2 -> 6.000E-01 BZFUO + 2.000E-01 BZFUOH + 2.000E-01 BZFUCO	RO2 1 ARR 8.800E-13 0 0
196	BZFUO -> CO14O3CHO + HO2	ARR 1.000E+06 0 0
197	BZFUOOH -> BZFUO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
198	BZFUOOH + OH -> BZFUO2	ARR 3.680E-11 0 0
199	BZFUOH + OH -> BZFUCO + HO2	ARR 2.780E-11 0 0
200	BZFUCO + OH -> CO14O3CHO + HO2	ARR 1.780E-11 0 0
201	CO14O3CHO -> CO + HCOCH2O2 + HO2	EXTRA 91 1.537E-04 0.170 0.208 1.0
202	CO14O3CHO + OH -> CO + HCOCH2O2	ARR 3.440E-11 0 0
203	CO14O3CHO + NO3 -> CO + HCOCH2O2 + HNO3	ARR 1.120E-11 0 1860.00
204	PHENOL + OH -> 6.000E-02 C6H5O + 1.26E-01 PHENO2 + 8.000E-01 CATECHOL + 8.1274E-01 HO2 + 1.26E-03 gdBPR_PHEN + 1.274E-02 OXOSORBACID	ARR 4.700E-13 0 -1220.00
205	PHENOL + NO3 -> 7.420E-01 C6H5O + 7.420E-01 HNO3 + 2.580E-01 NPHENO2	ARR 3.800E-12 0 0
206	PHENO -> HO2 + 2.900E-01 PBZQONE + 7.100E-01 GLY + 7.100E-01 MALDALCO2H	ARR 1.000E+06 0 0
207	C6H5O + O3 -> C6H5O2	ARR 2.860E-13 0 0
208	C6H5O + NO2 -> HOC6H4NO2	ARR 2.080E-12 0 0
209	C6H5OOH -> C6H5O + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
210	C6H5OOH + OH -> C6H5O2	ARR 3.600E-12 0 0
211	HOC6H4NO2 + NO3 -> HNO3 + NPHEN1O	ARR 9.000E-14 0 0
212	HOC6H4NO2 + OH -> NPHEN1O	ARR 9.000E-13 0 0
213	NPHEN1O + NO2 -> DNPHEN	ARR 2.080E-12 0 0
214	NPHEN1O + O3 -> NPHEN1O2	ARR 2.860E-13 0 0
215	NPHEN1O2 + NO -> NO2 + NPHEN1O	ARR 2.700E-12 0 -360.00
216	NPHEN1O2 + NO3 -> NO2 + NPHEN1O	ARR 2.300E-12 0 0

217	NPHEN1O2 + HO2 -> NPHEN1OOH	ARR 2.241E-13 0 -1300.00
218	NPHEN1O2 -> NPHEN1O	RO2 1 ARR 2.500E-13 0 0
219	NPHEN1OOH -> NPHEN1O + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
220	NPHEN1OOH + OH -> NPHEN1O2	ARR 9.000E-13 0 0
221	CATECHOL + OH -> 7.000E-02 CATEC1O + 2.2995E-01 BENZ3OH + 2.205E-02 PBZQ1OH + 4.095E-02 CATECBIPERO2 + 3.18525E-01 C6H6O3 + 1.8792975E-01 gdBPR_CAT + 1.3059525E-01 C6H6O4 + 6.7907025E-01 HO2	ARR 1.000E-10 0 0
222	CATECHOL + NO3 -> CATEC1O + HNO3	ARR 9.900E-11 0 0
223	CATECHOL + O3 -> CATECOOA	ARR 9.200E-18 0 0
224	CATECOOA -> HCOCO2H + HO2 + MALDALCO2H + OH	ARR 1.000E+06 0 0
225	CATEC1O + NO2 -> NCATECHOL	ARR 2.080E-12 0 0
226	CATEC1O + O3 -> CATEC1O2	ARR 2.860E-13 0 0
227	CATEC1O2 + NO -> CATEC1O + NO2	ARR 2.700E-12 0 -360.00
228	CATEC1O2 + NO3 -> CATEC1O + NO2	ARR 2.300E-12 0 0
229	CATEC1O2 + HO2 -> CATEC1OOH	ARR 2.241E-13 0 -1300.00
230	CATEC1O2 -> CATEC1O	RO2 1 ARR 8.800E-13 0 0
231	CATEC1OOH -> CATEC1O + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
232	CATEC1OOH + OH -> CATEC1O2	ARR 1.900E-12 0 -190.00
233	NCATECHOL + OH -> NCATECO2	ARR 3.470E-12 0 0
234	NCATECHOL ->	PHOTOLYSIS 1.42398E-04 1.40694E-04 1.35552E-04 1.26744E-04 1.1391E-04 9.651E-05 7.3944E-05 4.6367E-05 2.3588E-05 7.258E-06 0.0000E+00
235	NCATECHOL + NO3 -> NNCATECO2	ARR 2.600E-12 0 0
236	NCATECO2 + NO -> NCATECO + NO2	ARR 2.700E-12 0 -360.00
237	NCATECO2 + NO3 -> NCATECO + NO2	ARR 2.300E-12 0 0
238	NCATECO2 + HO2 -> NCATECOOH	ARR 2.241E-13 0 -1300.00
239	NCATECO2 -> NCATECO	RO2 1 ARR 8.000E-13 0 0
240	NCATECO -> HCOCO2H + HO2 + NC4DCO2H	ARR 1.000E+06 0 0
241	NCATECOOH -> NCATECO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
242	NCATECOOH + OH -> NCATECO2	ARR 1.900E-12 0 -190.00
243	NNCATECO2 + NO -> NNCATECO + NO2	ARR 2.700E-12 0 -360.00
244	NNCATECO2 + NO3 -> NNCATECO + NO2	ARR 2.300E-12 0 0
245	NNCATECO2 + HO2 -> NNCATECOOH	ARR 2.241E-13 0 -1300.00
246	NNCATECO2 -> NNCATECO	RO2 1 ARR 8.000E-13 0 0
247	NNCATECO -> HCOCO2H + NC4DCO2H + NO2	ARR 1.000E+06 0 0
248	NNCATECOOH -> NNCATECO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
249	NNCATECOOH + OH -> NNCATECO2	ARR 1.900E-12 0 -190.00
250	NC4DCO2H + OH -> NC4DCO2	ARR 1.900E-12 0 -190.00
251	NC4DCO2 -> MALANHY + NO2	ARR 1.000E+06 0 0
252	DNPHEN + OH -> DNPHENO2	ARR 3.000E-14 0 0
253	DNPHEN + NO3 -> NDNPHENO2	ARR 2.250E-15 0 0
254	DNPHENO2 + NO -> DNPHENO + NO2	ARR 2.700E-12 0 -360.00
255	DNPHENO2 + NO3 -> DNPHENO + NO2	ARR 2.300E-12 0 0
256	DNPHENO2 + HO2 -> DNPHENOOH	ARR 2.241E-13 0 -1300.00
257	DNPHENO2 -> DNPHENO	RO2 1 ARR 8.000E-13 0 0
258	DNPHENO -> HCOCO2H + NC4DCO2H + NO2	ARR 1.000E+06 0 0
259	DNPHENOOH -> DNPHENO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0

260	DNPHENOOH + OH -> DNPHENO2	ARR 1.900E-12 0 -190.00
261	NDNPHENO2 + NO -> NDNPHENO + NO2	ARR 2.700E-12 0 -360.00
262	NDNPHENO2 + NO3 -> NDNPHENO + NO2	ARR 2.300E-12 0 0
263	NDNPHENO2 + HO2 -> NDNPHENOOH	ARR 2.241E-13 0 -1300.00
264	NDNPHENO2 -> NDNPHENO	RO2 1 ARR 8.000E-13 0 0
265	NDNPHENO -> 2.000E+00 CO + HNO3 + NC4DCO2H + NO2	ARR 1.000E+06 0 0
266	NDNPHENOOH -> NDNPHENO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
267	NDNPHENOOH + OH -> NDNPHENO2	ARR 1.900E-12 0 -190.00
268	PHENO2 + NO -> NO2 + PHENO	ARR 2.700E-12 0 -360.00
269	PHENO2 + NO3 -> NO2 + PHENO	ARR 2.300E-12 0 0
270	PHENO2 + HO2 -> PHENOOH	ARR 2.241E-13 0 -1300.00
271	PHENO2 -> 7.000E-01 PHENO + 3.000E-01 PHENOH	RO2 1 ARR 8.000E-13 0 0
272	PHENOOH -> OH + PHENO	EXTRA 91 7.649E-06 0.682 0.279 1.0
273	PHENOOH + OH -> PHENO2	ARR 1.160E-10 0 0
274	PHENOH + OH -> PHENO	ARR 1.130E-10 0 0
275	NPHENO2 + NO -> NO2 + NPHENO	ARR 2.700E-12 0 -360.00
276	NPHENO2 + NO3 -> NO2 + NPHENO	ARR 2.300E-12 0 0
277	NPHENO2 + HO2 -> NPHENOOH	ARR 2.241E-13 0 -1300.00
278	NPHENO2 -> 7.000E-01 NPHENO + 3.000E-01 NPHENOH	RO2 1 ARR 8.000E-13 0 0
279	NPHENO -> GLY + MALDALCO2H + NO2	ARR 1.000E+06 0 0
280	NPHENOOH -> NPHENO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
281	NPHENOOH + OH -> NPHENO2	ARR 1.070E-10 0 0
282	NPHENOOH -> GLY + MALDALCO2H + NO2 + OH	EXTRA 91 4.095E-06 1.111 0.316 1.0
283	NPHENOH + OH -> NPHENO	ARR 1.040E-10 0 0
284	NPHENOH -> GLY + HO2 + MALDALCO2H + NO2	EXTRA 91 4.095E-06 1.111 0.316 1.0
285	MALDALCO2H -> 2.000E+00 CO + HCOCO2H + 2.000E+00 HO2	EXTRA 91 1.140E-05 0.396 0.298 1.0
286	MALDALCO2H -> 2.000E+00 CO + HCOCO2H + 2.000E+00 HO2	EXTRA 91 1.140E-05 0.396 0.298 1.0
287	MALDALCO2H + OH -> MALDIALCO2	ARR 3.700E-11 0 0
288	MALDALCO3H -> MALDIALCO2 + OH	EXTRA 91 1.520E-03 0.396 0.298 1.0
289	MALDALCO3H + OH -> MALDIALCO3	ARR 4.000E-11 0 0
290	C5CO2OHCO3 + NO -> CO + HO2 + HOCOC4DIAL + NO2	ARR 7.500E-12 0 -290.00
291	C5CO2OHCO3 + NO2 -> C5CO2OHPAN	EXTRA 93 21 1.0
292	C5CO2OHCO3 + NO3 -> CO + HO2 + HOCOC4DIAL + NO2	ARR 4.002E-12 0 0
293	C5CO2OHCO3 + HO2 -> 5.600E-01 C5COOHCO3H + 4.400E-01 CO + 4.400E-01 HO2 + 4.400E-01 HOCOC4DIAL + 4.400E-01 OH	ARR 5.200E-13 0 -980.00
294	C5CO2OHCO3 -> CO + HO2 + HOCOC4DIAL	RO2 1 ARR 1.000E-11 0 0
295	C5CO2OHPAN -> C5CO2OHCO3 + NO2	EXTRA 93 22 1.0
296	C5CO2OHPAN + OH -> 2.000E+00 CO + HOCOC4DIAL + NO2	ARR 7.660E-11 0 0
297	C5COOHCO3H + OH -> C5CO2OHCO3	ARR 8.010E-11 0 0
298	C5COOHCO3H -> CO + HO2 + HOCOC4DIAL + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
299	MALDIALCO2 -> 4.000E-01 CO + 4.000E-01 GLY + HO2 + 6.000E-01 MALANHY	ARR 1.000E+06 0 0
300	NBZFUO2 + NO -> NBZFUO + NO2	ARR 2.700E-12 0 -360.00
301	NBZFUO2 + NO3 -> NBZFUO + NO2	ARR 2.300E-12 0 0
302	NBZFUO2 + HO2 -> NBZFUOOH	ARR 1.819E-13 0 -1300.00
303	NBZFUO2 -> NBZFUO	RO2 1 ARR 8.800E-13 0 0
304	NBZFUO -> 5.000E-01 CO14O3CHO + 5.000E-01 NO2 + 5.000E-01 HO2 + 5.000E-01 NBZFUONE	ARR 1.000E+06 0 0
305	NBZFUONE + OH -> BZFUCO + NO2	ARR 1.160E-12 0 0

306	NBZFUOOH -> NBZFUO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
307	NBZFUOOH + OH -> NBZFUO2	ARR 6.180E-12 0 0
308	BZFUONOOA -> 5.000E-01 BZFUONOO + 5.000E-01 CO + 5.000E-01 HCOCH2O2 + 5.000E-01 OH	ARR 1.000E+06 0 0
309	BZFUONOO + SO2 -> CO14O3CHO + SO3	ARR 7.000E-14 0 0
310	BZFUONOO + CO -> CO14O3CHO	ARR 1.200E-15 0 0
311	BZFUONOO + NO -> CO14O3CHO + NO2	ARR 1.000E-14 0 0
312	BZFUONOO + NO2 -> CO14O3CHO + NO3	ARR 1.000E-15 0 0
313	BZFUONOO -> CO14O3CHO + H2O2	TB H2O ARR 6.000E-18 0 0
314	BZFUONOO -> CO14O3CO2H	TB H2O ARR 1.000E-17 0 0
315	CO14O3CO2H + OH -> HCOCH2O2	ARR 2.190E-11 0 0
316	NBZQO2 + NO -> NBZQO + NO2	ARR 2.700E-12 0 -360.00
317	NBZQO2 + NO3 -> NBZQO + NO2	ARR 2.300E-12 0 0
318	NBZQO2 + HO2 -> NBZQOOH	ARR 2.241E-13 0 -1300.00
319	NBZQO2 -> NBZQO	RO2 1 ARR 8.800E-13 0 0
320	NBZQO -> C6CO4DB + NO2	ARR 1.000E+06 0 0
321	NBZQOOH -> NBZQO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
322	NBZQOOH + OH -> NBZQO2	ARR 6.680E-11 0 0
323	C6CO4DB -> C4CO2DBCO3 + CO + HO2	EXTRA 91 3.074E-04 0.170 0.208 1.0
324	C6CO4DB + OH -> C33CO + 3.000E+00 CO + HO2	ARR 7.700E-11 0 0
325	C4CO2DBCO3 + NO -> C33CO + CO + HO2 + NO2	ARR 7.500E-12 0 -290.00
326	C4CO2DBCO3 + NO2 -> C4CO2DBPAN	EXTRA 93 21 1.0
327	C4CO2DBCO3 + NO3 -> C33CO + CO + HO2 + NO2	ARR 4.002E-12 0 0
328	C4CO2DBCO3 + HO2 -> 5.600E-01 C4CO2DCO3H + 4.400E-01 C33CO + 4.400E-01 CO + 4.400E-01 HO2 + 4.400E-01 OH	ARR 5.200E-13 0 -980.00
329	C4CO2DBCO3 -> C33CO + CO + HO2	RO2 1 ARR 1.000E-11 0 0
330	C4CO2DBPAN -> C4CO2DBCO3 + NO2	EXTRA 93 22 1.0
331	C4CO2DBPAN + OH -> C33CO + CO + NO2	ARR 2.740E-11 0 0
332	C4CO2DCO3H -> C33CO + CO + HO2 + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
333	C4CO2DCO3H -> C33CO + CO + HO2 + OH	EXTRA 91 1.537E-04 0.170 0.208 1.0
334	C4CO2DCO3H + OH -> C4CO2DBCO3	ARR 3.060E-11 0 0
335	C6H5O2 + NO -> C6H5O + NO2	ARR 2.700E-12 0 -360.00
336	C6H5O2 + NO3 -> C6H5O + NO2	ARR 2.300E-12 0 0
337	C6H5O2 + HO2 -> C6H5OOH	ARR 2.241E-13 0 -1300.00
338	C6H5O2 -> C6H5O	RO2 1 ARR 2.500E-13 0 0
339	NO2 -> 0.5 HONO + 0.5 HNO3	EXTRA 95 1.654
340	BENZ3OH + OH -> 7.000E-02 BENZ2OH1O + 7.300E-01 BENZ4OH + 7.300E-01 HO2 + 7.000E-02 PBZQOH + 1.300E-01 BENZ3OHBIPERO2	ARR 4.64E-10 0 0
341	BENZ4OH + OH -> 7.000E-02 BENZ3OH1O + 7.300E-01 BENZ5OH + 7.300E-01 HO2 + 7.000E-02 PBZQ3OH + 1.300E-01 BENZ4OHBIPERO2	ARR 1.05E-09 0 0
342	CATECBIPERO2 + NO -> CATECBIPERO + NO2	ARR 2.700E-12 0 -360.00
343	CATECBIPERO2 + NO3 -> CATECBIPERO + NO2	ARR 2.300E-12 0 0
344	CATECBIPERO2 + HO2 -> CATECBIPEROOH	ARR 2.241E-13 0 -1300.00
345	CATECBIPERO2 -> 7.000E-01 CATECBIPERO + 3.000E-01 CATECBIPER2OH	RO2 1 ARR 8.800E-13 0 0
346	CATECBIPERO -> 0.330 MALDALCO2HOH + 0.330 GLY + 0.165 MALDIAL + 0.165 ACOX + 0.330 MALDALCO2H + 0.330 HCOCO2H + 0.165 MALDIAL2OH + 0.165 GLY + HO2	ARR 1.000E+06 0 0
347	CATECBIPEROOH -> CATECBIPERO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
348	CATECBIPEROOH + OH -> CATECBIPERO2	ARR 1.16E-10 0 0

349	CATECBIPER2OH + OH -> CATECBIPERO	ARR 1.130E-10 0 0
350	BENZ3OHBIPERO2 + NO -> BENZ3OHBIPERO + NO2	ARR 2.700E-12 0 -360.00
351	BENZ3OHBIPERO2 + NO3 -> BENZ3OHBIPERO + NO2	ARR 2.300E-12 0 0
352	BENZ3OHBIPERO2 + HO2 -> BENZ3OHBIPEROOH	ARR 2.241E-13 0 -1300.00
353	BENZ3OHBIPERO2 -> 7.000E-01 BENZ3OHBIPERO + 3.000E-01 BENZ3OHBIPER2OH	RO2 1 ARR 8.800E-13 0 0
354	BENZ3OHBIPERO -> 0.500 MALDALCO2H2OH + 0.500 GLY + 0.250 MALDALCO2HOH + 0.250 HCOCO2H + 0.250 MALDALCO2H + 0.250 ACOX + HO2	ARR 1.000E+06 0 0
355	BENZ3OHBIPEROOH -> BENZ3OHBIPERO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
356	BENZ3OHBIPEROOH + OH -> BENZ3OHBIPERO2	ARR 9.770E-11 0 0
357	BENZ3OHBIPER2OH + OH -> BENZ3OHBIPERO	ARR 1.210E-10 0 0
358	BENZ4OHBIPERO2 + NO -> BENZ4OHBIPERO + NO2	ARR 2.700E-12 0 -360.00
359	BENZ4OHBIPERO2 + NO3 -> BENZ4OHBIPERO + NO2	ARR 2.300E-12 0 0
360	BENZ4OHBIPERO2 + HO2 -> BENZ4OHBIPEROOH	ARR 2.241E-13 0 -1300.00
361	BENZ4OHBIPERO2 -> 7.000E-01 BENZ4OHBIPERO + 3.000E-01 BENZ4OHBIPER2OH	RO2 1 ARR 8.800E-13 0 0
362	BENZ4OHBIPERO -> 0.250 ACMAL2OH + 0.250 GLY + 0.5 MALDALCO2H2OH + 0.5 HCOCO2H + 0.250 MALDALCO2HOH + 0.250 ACOX + HO2	ARR 1.000E+06 0 0
363	BENZ4OHBIPEROOH -> BENZ4OHBIPERO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
364	BENZ4OHBIPEROOH + OH -> BENZ4OHBIPERO2	ARR 9.770E-11 0 0
365	BENZ4OHBIPER2OH + OH -> BENZ4OHBIPERO	ARR 1.210E-10 0 0
366	BENZ2OH1O + NO2 -> NBENZ3OH	ARR 2.080E-12 0 0
367	BENZ2OH1O + O3 -> BENZ2OHO2	ARR 2.860E-13 0 0
368	BENZ2OHO2 + NO -> BENZ2OH1O + NO2	ARR 2.700E-12 0 -360.00
369	BENZ2OHO2 + NO3 -> BENZ2OH1O + NO2	ARR 2.300E-12 0 0
370	BENZ2OHO2 + HO2 -> BENZ2OHOOH	ARR 2.241E-13 0 -1300.00
371	BENZ2OHO2 -> BENZ2OH1O	RO2 1 ARR 8.800E-13 0 0
372	BENZ2OHOOH -> BENZ2OH1O + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
373	BENZ2OHOOH + OH -> BENZ2OHO2	ARR 4.65E-10 0 0
374	NBENZ3OH + OH -> NBENZ3OHO2	ARR 4.59E-11 0 0
375	NBENZ3OH + NO3 -> NNBENZ3OHO2	ARR 2.600E-12 0 0
376	NBENZ3OHO2 + NO -> NBENZ3OHO + NO2	ARR 2.700E-12 0 -360.00
377	NBENZ3OHO2 + NO3 -> NBENZ3OHO + NO2	ARR 2.300E-12 0 0
378	NBENZ3OHO2 + HO2 -> NBENZ3OHOOH	ARR 2.241E-13 0 -1300.00
379	NBENZ3OHO2 -> NBENZ3OHO	RO2 1 ARR 8.000E-13 0 0
380	NBENZ3OHO -> HCOCO2H + HO2 + NC4DCO2HOH	ARR 1.000E+06 0 0
381	NBENZ3OHOOH -> NBENZ3OHO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
382	NBENZ3OHOOH + OH -> NBENZ3OHO2	ARR 1.900E-12 0 -190.00
383	NNBENZ3OHO2 + NO -> NNBENZ3OHO + NO2	ARR 2.700E-12 0 -360.00
384	NNBENZ3OHO2 + NO3 -> NNBENZ3OHO + NO2	ARR 2.300E-12 0 0
385	NNBENZ3OHO2 + HO2 -> NNBENZ3OHOOH	ARR 2.241E-13 0 -1300.00
386	NNBENZ3OHO2 -> NNBENZ3OHO	RO2 1 ARR 8.000E-13 0 0
387	NNBENZ3OHO -> HCOCO2H + NC4DCO2HOH + NO2	ARR 1.000E+06 0 0
388	NNBENZ3OHOOH -> NNBENZ3OHO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
389	NNBENZ3OHOOH + OH -> NNBENZ3OHO2	ARR 1.900E-12 0 -190.00
390	BENZ3OH1O + NO2 -> NBENZ4OH	ARR 2.080E-12 0 0
391	BENZ3OH1O + O3 -> BENZ3OHO2	ARR 2.860E-13 0 0
392	BENZ3OHO2 + NO -> BENZ3OH1O + NO2	ARR 2.700E-12 0 -360.00

393	BENZ3OHO2 + NO3 -> BENZ3OH1O + NO2	ARR 2.300E-12 0 0
394	BENZ3OHO2 + HO2 -> BENZ3OHOOH	ARR 2.241E-13 0 -1300.00
395	BENZ3OHO2 -> BENZ3OH1O	RO2 1 ARR 8.800E-13 0 0
396	BENZ3OHOOH -> BENZ3OH1O + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
397	BENZ3OHOOH + OH -> BENZ3OHO2	ARR 1.900E-12 0 -190.00
398	NBENZ4OH + OH -> NBENZ4OHO2	ARR 3.470E-12 0 0
399	NBENZ4OH + NO3 -> NNBENZ4OHO2	ARR 2.600E-12 0 0
400	NBENZ4OHO2 + NO -> NBENZ4OHO + NO2	ARR 2.700E-12 0 -360.00
401	NBENZ4OHO2 + NO3 -> NBENZ4OHO + NO2	ARR 2.300E-12 0 0
402	NBENZ4OHO2 + HO2 -> NBENZ4OHOOH	ARR 2.241E-13 0 -1300.00
403	NBENZ4OHO2 -> NBENZ4OHO	RO2 1 ARR 8.000E-13 0 0
404	NBENZ4OHO -> ACOX + HO2 + NC4DCO2HOH	ARR 1.000E+06 0 0
405	NBENZ4OHOOH -> NBENZ4OHO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
406	NBENZ4OHOOH + OH -> NBENZ4OHO2	ARR 1.900E-12 0 -190.00
407	NNBENZ4OHO2 + NO -> NNBENZ4OHO + NO2	ARR 2.700E-12 0 -360.00
408	NNBENZ4OHO2 + NO3 -> NNBENZ4OHO + NO2	ARR 2.300E-12 0 0
409	NNBENZ4OHO2 + HO2 -> NNBENZ4OHOOH	ARR 2.241E-13 0 -1300.00
410	NNBENZ4OHO2 -> NNBENZ4OHO	RO2 1 ARR 8.000E-13 0 0
411	NNBENZ4OHO -> ACOX + NC4DCO2HOH + NO2	ARR 1.000E+06 0 0
412	NNBENZ4OHOOH -> NNBENZ4OHO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
413	NNBENZ4OHOOH + OH -> NNBENZ4OHO2	ARR 1.900E-12 0 -190.00
414	BZBIPERO2 -> PC2	ARR 5.00E-3 0 0
415	PC2 -> R1bRO2	ARR 2.3E2 0 0
416	R1bRO2 -> C6H7O7	ARR 2.3E2 0 0
417	C6H7O7 -> C6H7O9	ARR 2E2 0 0
418	C6H7O9 + HO2 -> C6H8O9	ARR 0.266E-12 0 -1300.
419	C6H7O9 + NO -> C6H7O10N	ARR 5.52E-13 0 -360.
420	gdBPR_PHEN + NO ->	ARR 2.542E-12 0 -360.
421	gdBPR_PHEN + HO2 ->	ARR 0.239E-12 0 -1300.
422	gdBPR_PHEN -> C6H7O6	ARR 9400 0 0
423	C6H7O6 -> C6H7O8	ARR 4.4 0 0
424	C6H7O8 + HO2 -> C6H8O8	ARR 0.239E-12 0 -1300.
425	C6H7O8 + NO -> C6H7O9N	ARR 5.19e-13 0 -360.
426	gdBPR_CAT + NO ->	ARR 2.542E-12 0 -360.
427	gdBPR_CAT + HO2 ->	ARR 0.239E-12 0 -1300.
428	gdBPR_CAT -> cat_PC2	ARR 19.2 0 0
429	cat_PC2 -> 0.5 C6H6O7 + 0.5 C6H7O9gd	ARR 3.9 0 0
430	C6H7O9gd -> C6H7O11	ARR 3.6 0 0
431	C6H7O11 + HO2 -> C6H8O11	ARR 0.239E-12 0 -1300.
432	C6H7O11 + NO -> C6H7O12N	ARR 1.28E-13 0 -360.
433	KETENOL -> 0.76 BZFUONE + 0.24 KETB	ARR 3.800E-03 0 0
434	KETB -> MALANHYO2 + HO2	ARR 2.600E-3 0 0
435	MALANHYO2 + HO2 -> MALANHY + HO2 + OH	ARR 2.910E-13 0 -1300.0
436	MALANHYO2 + NO -> 0.85 MALANHY + 0.85 NO2 + 0.85 HO2 + 0.15 MALANHYONO2	ARR 2.700E-12 0 -360.00
437	MALANHYO2 -> MALANHY + HO2	RO2 1 ARR 8.8e-13 0 0
438	KETENOL + OH -> 0.64 MALDALCO2H + 0.64 HO2 + 0.36 ORA1 + 0.36 KETENAL + 0.36 OH	ARR 1.18e-10 0 0

439	KETENOL + O3 -> 0.16 KETENAL + 0.16 OH + 0.16 HO2 + 0.84 GLY + 0.84 ORA1	ARR 1.8e-15 0 0
440	KETENAL + OH -> GLY + OH	ARR 1.0e-12 0 0
441	MALDALCO2H + OH -> 0.62 M1O2A + 0.38 C32OH13CO + 0.38 OH	ARR 2.3e-11 0 0
442	M1O2A + NO -> GLY + HO2 + M1C2O2	ARR 2.700E-12 0 -360.00
443	M1C2O2 + NO -> ORA1 + HO2	ARR 2.700E-12 0 -360.00
444	C2H4 + OH -> HOCH2CH2O2	EXTRA 93 15 1.0
445	C2H4 + O3 -> CH2OOA + HCHO	ARR 9.100E-15 0 2580.00
446	C2H4 + NO3 -> ETHENO3O2	ARR 3.300E-12 0 2880.00
447	HOCH2CH2O2 + NO -> 9.950E-01 HOCH2CH2O + 9.950E-01 NO2 + 5.000E-03 ETHOHNO3	ARR 2.700E-12 0 -360.00
448	HOCH2CH2O2 + NO3 -> HOCH2CH2O + NO2	ARR 2.300E-12 0 0
449	HOCH2CH2O2 + HO2 -> HYETHO2H	ARR 1.530E-13 0 -1300.00
450	HOCH2CH2O2 -> 6.000E-01 HOCH2CH2O + 2.000E-01 ETHGLY + 2.000E-01 HOCH2CHO	RO2 1 ARR 1.7926e-13 0 -682.5
451	HOCH2CH2O -> 2.000E+00 HCHO + HO2	ARR 9.500E+13 0 5988.00
452	HOCH2CH2O -> HO2 + HOCH2CHO	TB O2 ARR 2.500E-14 0 300.00
453	ETHOHNO3 + OH -> HOCH2CHO + NO2	ARR 8.400E-13 0 0
454	HYETHO2H -> HOCH2CH2O + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
455	HYETHO2H + OH -> HOCH2CH2O2	ARR 1.900E-12 0 -190.00
456	HYETHO2H + OH -> HOCH2CHO + OH	ARR 1.380E-11 0 0
457	CH2OO + NO -> HCHO + NO2	ARR 1.000E-14 0 0
458	CH2OO + NO2 -> HCHO + NO3	ARR 1.000E-15 0 0
459	CH2OO + SO2 -> HCHO + SO3	ARR 7.000E-14 0 0
460	CH2OO -> ORA1	TB H2O ARR 1.000E-17 0 0
461	CH2OO -> H2O2 + HCHO	TB H2O ARR 6.000E-18 0 0
462	CH2OO + CO -> HCHO	ARR 1.200E-15 0 0
463	CH2OOA -> 3.700E-01 CH2OO	ARR 1.000E+06 0 0
464	ETHENO3O2 + NO -> ETHENO3O + NO2	ARR 2.700E-12 0 -360.00
465	ETHENO3O2 + HO2 -> ETHO2HNO3	ARR 1.126E-13 0 -1300.00
466	ETHENO3O2 + NO3 -> ETHENO3O + NO2	ARR 2.300E-12 0 0
467	ETHENO3O2 -> 6.000E-01 ETHENO3O + 2.000E-01 ETHOHNO3 + 2.000E-01 NO3CH2CHO	RO2 1 ARR 6.000E-13 0 0
468	ETHENO3O -> HO2 + NO3CH2CHO	TB O2 ARR 2.500E-14 0 300.00
469	ETHENO3O -> 2.000E+00 HCHO + NO2	ARR 7.000E+03 0 0
470	ETHO2HNO3 -> ETHENO3O + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
471	ETHO2HNO3 + OH -> ETHENO3O2	ARR 1.900E-12 0 -190.00
472	ETHO2HNO3 + OH -> NO3CH2CHO + OH	ARR 1.620E-12 0 0
473	NO3CH2CHO -> HCOCH2O + NO2	EXTRA 91 3.246E-05 1.015 0.324 1.0
474	NO3CH2CHO + OH -> NO3CH2CO3	ARR 3.400E-12 0 0
475	NO3CH2CHO + NO3 -> HNO3 + NO3CH2CO3	ARR 1.400E-12 0 1860.00
476	NO3CH2CO3 + NO -> HCHO + 2.000E+00 NO2	ARR 7.500E-12 0 -290.00
477	NO3CH2CO3 + NO2 -> NO3CH2PAN	EXTRA 93 21 1.0
478	NO3CH2CO3 + NO3 -> HCHO + 2.000E+00 NO2	ARR 4.002E-12 0 0
479	NO3CH2CO3 + HO2 -> 4.100E-01 NO3CH2CO3H + 1.500E-01 NO3CH2CO2H + 1.500E-01 O3 + 4.400E-01 HCHO + 4.400E-01 NO2 + 4.400E-01 OH	ARR 5.200E-13 0 -980.00
480	NO3CH2CO3 -> 7.000E-01 HCHO + 7.000E-01 NO2 + 3.000E-01 NO3CH2CO2H	RO2 1 ARR 1.000E-11 0 0
481	NO3CH2PAN -> NO2 + NO3CH2CO3	EXTRA 93 22 1.0
482	NO3CH2PAN + OH -> HCHO + 2.000E+00 NO2	ARR 1.120E-14 0 0

483	NO3CH2CO3H -> HCHO + NO2 + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
484	NO3CH2CO3H + OH -> NO3CH2CO3	ARR 3.630E-12 0 0
485	NO3CH2CO2H + OH -> HCHO + NO2	ARR 1.680E-13 0 0
486	CH2OOB -> 2.400E-01 CH2OO + 7.600E-01 CO + 3.600E-01 HO2 + 3.600E-01 OH	ARR 1.000E+06 0 0
487	HOCH2COCHO -> CO + HO2 + HOCH2CO3	EXTRA 91 1.537E-04 0.170 0.208 1.0
488	HOCH2COCHO + OH -> CO + HOCH2CO3	ARR 1.440E-11 0 0
489	HOCH2COCHO + NO3 -> CO + HNO3 + HOCH2CO3	ARR 3.360E-12 0 1860.00
490	C42AOH -> CO + 2.000E+00 HO2 + NO3CH2CHO	EXTRA 91 2.792E-05 0.805 0.338 1.0
491	C42AOH + OH -> HO2 + NMGLYOX	ARR 2.920E-11 0 0
492	NMGLYOX -> CO + HO2 + NO3CH2CO3	EXTRA 91 1.537E-04 0.170 0.208 1.0
493	NMGLYOX -> 2.000E+00 CO + HCHO + HO2 + NO2	EXTRA 91 2.485E-06 1.196 0.328 1.0
494	NMGLYOX + OH -> CO + NO3CH2CO3	ARR 1.240E-11 0 0
495	NMGLYOX + NO3 -> CO + HNO3 + NO3CH2CO3	ARR 3.360E-12 0 1860.00
496	GLYOOB -> 2.400E-01 GLYOO + 9.200E-01 CO + 7.600E-01 HO2 + 3.600E-01 OH + 2.000E-01 HCHO	ARR 1.000E+06 0 0
497	C3DIOLO2 + NO -> C3DIOLO + NO2	ARR 2.700E-12 0 -360.00
498	C3DIOLO2 + NO3 -> C3DIOLO + NO2	ARR 2.300E-12 0 0
499	C3DIOLO2 + HO2 -> C3DIOLOOH	ARR 1.513E-13 0 -1300.00
500	C3DIOLO2 -> C3DIOLO	RO2 1 ARR 2.000E-12 0 0
501	C3DIOLO -> HCHO + HO2 + HOCH2CHO	ARR 1.000E+06 0 0
502	C3DIOLOOH + OH -> C3DIOLO2	ARR 2.780E-11 0 0
503	C3DIOLOOH -> C3DIOLO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
504	ETHGLY + OH -> HO2 + HOCH2CHO	ARR 1.450E-11 0 0
505	A2PANOO + HO2 -> 4.400E-01 A2PANO + 4.400E-01 OH + 4.100E-01 C2OHOCOOH + 1.500E-01 C2OHOCO2H + 1.500E-01 O3	ARR 5.200E-13 0 -980.00
506	A2PANOO + NO -> A2PANO + NO2	ARR 7.500E-12 0 -290.00
507	A2PANOO + NO3 -> A2PANO + NO2	ARR 4.002E-12 0 0
508	A2PANOO + NO2 -> A2PAN	EXTRA 93 21 1.0
509	A2PANOO -> 7.000E-01 A2PANO + 3.000E-01 C2OHOCO2H	RO2 1 ARR 1.000E-11 0 0
510	ACR + OH -> ACO3	ARR 1.360E-11 0 0
511	ACR + OH -> OCCOHCO2	ARR 1.300E-12 0 0
512	ACR + OH -> ACRO2	ARR 5.100E-12 0 0
513	ACR -> 4.000E-01 C2H4 + 3.000E-01 HCHO + 3.000E-01 ACO3	EXTRA 91 1.140E-05 0.396 0.298 1.0
514	ACR + NO3 -> ACO3 + HNO3	ARR 1.720E-13 0 1190.00
515	ACR + O3 -> CH2OOB + GLY	ARR 1.450E-19 0 0
516	ACR + O3 -> GLYOOB + HCHO	ARR 1.450E-19 0 0
517	OCCOHCO2 + NO -> NO2 + OCCOHCO	ARR 2.565E-12 0 -360.00
518	OCCOHCO2 + NO -> C42AOH	ARR 1.350E-13 0 -360.00
519	OCCOHCO2 + NO3 -> C42AOH + NO2	ARR 2.300E-12 0 0
520	OCCOHCO2 + HO2 -> OCCOHCOOH	ARR 9.079E-14 0 -1300.00
521	OCCOHCO2 + HO2 -> C32OH13CO + 5.200E-01 O3	ARR 6.053E-14 0 -1300.00
522	OCCOHCO2 -> 6.000E-01 OCCOHCO + 2.000E-01 C32OH13CO + 2.000E-01 OCCOHCOH	RO2 1 ARR 2.000E-12 0 0
523	OCCOHCO -> GLY + HCHO + HO2	ARR 1.000E+06 0 0
524	OCCOHCOOH -> OCCOHCO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
525	OCCOHCOOH + OH -> OCCOHCO2	ARR 9.258E-11 0 0
526	OCCOHCOH + OH -> A2PANOO	ARR 6.220E-11 0 0
527	A2PAN -> A2PANOO + NO2	EXTRA 93 22 1.0

528	A2PAN + OH -> CO + HOCH2CHO + NO2	ARR 1.865E-11 0 0
529	C2OHOCOOH -> C3DIOLO2	EXTRA 91 7.649E-06 0.682 0.279 1.0
530	C2OHOCOOH + OH -> A2PANOO	ARR 1.513E-11 0 0
531	C2OHOCO2H + OH -> C3DIOLO2	ARR 1.867E-11 0 0
532	A2PANO -> HO2 + HOCH2CHO	ARR 1.000E+06 0 0
533	ACRO2 + NO -> CHOCOHCO + NO2	ARR 2.700E-12 0 -360.00
534	ACRO2 + NO3 -> CHOCOHCO + NO2	ARR 2.300E-12 0 0
535	ACRO2 + HO2 -> HOCHOCOOH	ARR 1.513E-13 0 -1300.00
536	ACRO2 -> 6.000E-01 CHOCOHCO + 2.000E-01 HOCH2COCHO + 2.000E-01 OCCOHCOH	RO2 1 ARR 8.800E-13 0 0
537	ACRO2 -> CO + HOCH2CHO + OH	ARR 3.000E+07 0 5300.00
538	CHOCOHCO -> CO + HO2 + HOCH2CHO	ARR 1.000E+06 0 0
539	HOCHOCOOH + OH -> HOCH2COCHO + OH	ARR 4.770E-11 0 0
540	HOCHOCOOH -> CHOCOHCO + OH	EXTRA 91 7.649E-06 0.682 0.279 1.0
541	ACOX + OH ->	ARR 5.74E-14 0 -880
542	MALDIAL2OH + OH ->	ARR 3.82E-11 0 0
543	MALDIAL2OH + O3 ->	ARR 3.60E-18 0 0
544	MALDIAL2OH + NO3 ->	ARR 8.35E-12 0 0
545	MALDALCO2HOH + OH ->	ARR 3.82E-11 0 0
546	MALDALCO2HOH + O3 ->	ARR 3.60E-18 0 0
547	MALDALCO2HOH + NO3 ->	ARR 8.35E-12 0 0
548	MALDALCO2H2OH + OH ->	ARR 4.69E-11 0 0
549	MALDALCO2H2OH + NO3 ->	ARR 8.03E-15 0 0
550	ACMAL2OH + OH ->	ARR 2.58E-11 0 0
551	ACMAL2OH + NO3 ->	ARR 3.40E-13 0 0
552	PBZQ1OH + OH ->	ARR 9.180E-11 0 0
553	PBZQ3OH + OH ->	ARR 9.180E-11 0 0
554	NBENZ3OH + OH ->	ARR 0.683E-11 0 0
555	NBENZ3OH + NO3 ->	ARR 0.503E-11 0 0
556	NBENZ4OH + OH ->	ARR 0.683E-11 0 0
557	NBENZ4OH + NO3 ->	ARR 0.503E-11 0 0
558	C6DIALPEROHONO2 + OH ->	ARR 6.75E-11 0 0
559	C6DIALPEROHONO2 + OH ->	ARR 6.75E-11 0 0
560	C6DIALPEROHONO2 + NO3 ->	ARR 5.12E-13 0 0
561	MALDIALONO2 + OH ->	ARR 3.21E-11 0 0
562	MALDIALONO2 + NO3 ->	ARR 4.83E-13 0 0
563	NC4DCO2HOH + OH ->	ARR 5.26E-12 0 -490.00
564	NC4DCO2HOH + NO3 ->	ARR 2.15E-14 0 0
565	C6H6O3 + OH -> C6H6O3_1	ARR 5.038E-12 0 -630.
566	C6H6O3 + O3 -> 0.043 C6H6O3_12 + 0.086 HO2 + 0.043 CO2 + 0.554 C6H6O3_12 + 1.208 HO2 + 0.704 CO2 + 0.043 C6H6O3_12 + 0.086 HO2 + 0.043 CO2 + 0.005 C6H6O3_28 + 0.005 C6H6O3_29 + 0.031 C6H6O3_28 + 0.031 C6H6O3_29 + 0.0156 C6H6O3_2 + 0.0234 CO2 + 0.0156 HO2 + 0.0078 C6H6O3_24 + 0.0156 C6H6O3_19 + 0.0156 CO + 0.100 C6H6O3_2 + 0.050 C6H6O3_24 + 0.100 C6H6O3_19 + 0.100 CO	ARR 3.012E-16 0 1008.
567	C6H6O3 + O3 -> 0.004 C6H6O3_31 + 0.004 C6H6O3_32 + 0.026 C6H6O3_31 + 0.026 C6H6O3_32 + 0.0128 C6H6O3_3 + 0.0192 CO2 + 0.0128 HO2 + 0.0064 C6H6O3_26 + 0.0128 C6H6O3_21 + 0.0128 CO + 0.082 C6H6O3_3 + 0.489 CO2 + 0.326 HO2 + 0.041 C6H6O3_26 + 0.082 C6H6O3_21 + 0.326 CO + 0.0188 C6H6O3_4 + 0.0282 CO2 + 0.0188 HO2 + 0.0094 C6H6O3_23 + 0.0188	ARR 3.012E-16 0 1008.

	C6H6O3_16 + 0.0188 CO + 0.244 C6H6O3_4 + 0.122 C6H6O3_23 + 0.244 C6H6O3_16 + 0.0188 C6H6O3_4 + 0.0282 CO2 + 0.0188 HO2 + 0.0094 C6H6O3_23 + 0.0188 C6H6O3_16 + 0.0188 CO	
568	C6H6O3 + NO3 -> C6H6O3_5	ARR 5.569E-12 0 0
569	C6H6O3_1 + NO -> NO2 + C6H6O3_6	ARR 2.203E-12 0 -360.
570	C6H6O3_1 + NO -> C6H6O3_14	ARR 4.972E-13 0 -360.
571	C6H6O3_1 + HO2 -> 0.920 C6H6O3_10 + 0.080 C6H6O3_6 + 0.080 OH	ARR 2.519E-13 0 -1300.
572	C6H6O3_1 + NO3 -> C6H6O3_6 + NO2	ARR 8.900E-12 0 390.
573	C6H6O3_1 -> 0.600 C6H6O3_6 + 0.200 C6H6O3_35 + 0.200 C6H6O3_40	RO2 1 ARR 1.000E-13 0 -973.
574	C6H6O3_2 -> C6H6O3_7 + GLY	ARR 1.120E+09 0 2768.
575	C6H6O3_3 -> C6H6O3_22 + CO + HO2	ARR 1.120E+09 0 3573.
576	C6H6O3_4 + NO -> MALDALCO2H + CO2 + HO2 + NO2	ARR 7.500E-12 0 -290.
577	C6H6O3_4 + NO2 -> C6H6O3_15	ARR 6.143E-09 0 0
578	C6H6O3_4 + NO3 -> MALDALCO2H + CO2 + HO2 + NO2	ARR 8.900E-12 0 305.
579	C6H6O3_4 + HO2 -> 0.370 C6H6O3_25 + 0.130 C6H6O3_16 + 0.130 O3 + 0.500 MALDALCO2H + 0.500 CO2 + 0.500 HO2 + 0.500 OH	ARR 3.058E-12 0 -730.
580	C6H6O3_4 -> 0.800 MALDALCO2H + 0.800 CO2 + 0.800 HO2 + 0.200 C6H6O3_16	RO2 1 ARR 2.000E-12 0 -508.
581	C6H6O3_5 + NO -> NO2 + C6H6O3_8	ARR 2.175E-12 0 -360.
582	C6H6O3_5 + NO -> C6H6O3_13	ARR 5.248E-13 0 -360.
583	C6H6O3_5 + HO2 -> 0.500 C6H6O3_11 + 0.500 C6H6O3_8 + 0.500 OH	ARR 2.659E-13 0 -1300.
584	C6H6O3_5 + NO3 -> C6H6O3_8 + NO2	ARR 8.900E-12 0 390.
585	C6H6O3_5 -> 0.600 C6H6O3_8 + 0.200 C6H6O3_36 + 0.200 C6H6O3_41	RO2 1 ARR 1.000E-13 0 -611.
586	C6H6O3_6 -> C6H6O3_9 + HO2	ARR 1.120E+09 0 2302.
587	C6H6O3_7 + NO -> HCOCO2H + CO2 + HO2 + NO2	ARR 7.500E-12 0 -290.
588	C6H6O3_7 + NO2 -> C6H6O3_18	ARR 6.143E-09 0 0
589	C6H6O3_7 + NO3 -> HCOCO2H + CO2 + HO2 + NO2	ARR 8.900E-12 0 305.
590	C6H6O3_7 + HO2 -> 0.370 C6H6O3_27 + 0.130 C6H6O3_39 + 0.130 O3 + 0.500 HCOCO2H + 0.500 CO2 + 0.500 HO2 + 0.500 OH	ARR 2.800E-12 0 -730.
591	C6H6O3_7 -> 0.800 HCOCO2H + 0.800 CO2 + 0.800 HO2 + 0.200 C6H6O3_39	RO2 1 ARR 2.000E-12 0 -508.
592	C6H6O3_8 -> C6H6O3_9 + NO2	ARR 1.120E+09 0 4428.
593	C6H6O3_9 + OH ->	ARR 1.173E-11 0 -25.
594	C6H6O3_9 + OH ->	ARR 1.303E-11 0 0
595	C6H6O3_9 + OH ->	ARR 1.823E-12 0 -395.
596	C6H6O3_9 + OH ->	ARR 1.344E-12 0 -910.
597	C6H6O3_9 + O3 ->	ARR 5.950E-18 0 0
598	C6H6O3_9 + NO3 ->	ARR 4.925E-15 0 0
599	C6H6O3_9 + NO3 ->	ARR 2.426E-15 0 0
600	C6H6O3_9 ->	PHOTOLYSIS 1.3993E-05 1.3687E-05 1.2773E-05 1.1268E-05 9.2156E-06 6.7805E-06 4.1825E-06 1.8855E-06 6.5962E-07 1.1592E-07 0.0000E+00
601	C6H6O3_9 ->	PHOTOLYSIS 8.7717E-04 8.7094E-04 8.5109E-04 8.1417E-04 7.5391E-04 6.6369E-04 5.3173E-04 3.4985E-04 1.7813E-04 4.4607E-05 0.0000E+00
602	C6H6O3_9 ->	PHOTOLYSIS 8.7717E-04 8.7094E-04 8.5109E-04 8.1417E-04 7.5391E-04 6.6369E-04 5.3173E-04 3.4985E-04 1.7813E-04 4.4607E-05 0.0000E+00
603	C6H6O3_10 + OH ->	ARR 2.052E-13 0 -1693.
604	C6H6O3_10 + OH ->	ARR 4.477E-12 0 -784.

605	C6H6O3_10 + OH ->	ARR 1.468E-12 0 -910.
606	C6H6O3_10 + O3 ->	ARR 1.560E-18 0 0
607	C6H6O3_10 + NO3 ->	ARR 6.277E-15 0 0
608	C6H6O3_10 + NO3 ->	ARR 3.455E-15 0 0
609	C6H6O3_10 + NO3 ->	ARR 3.455E-15 0 0
610	C6H6O3_10 ->	PHOTOLYSIS 7.1608E-06 7.0590E-06 6.7481E-06 6.2123E-06 5.4266E-06 4.3964E-06 3.1263E-06 1.7392E-06 7.6263E-07 1.7820E-07 0.0000E+00
611	C6H6O3_11 + OH ->	ARR 6.679E-14 0 -1403.
612	C6H6O3_11 + OH ->	ARR 4.591E-12 0 -442.
613	C6H6O3_11 + OH ->	ARR 1.432E-12 0 -910.
614	C6H6O3_11 + O3 ->	ARR 1.560E-18 0 0
615	C6H6O3_11 + NO3 ->	ARR 3.666E-15 0 0
616	C6H6O3_11 + NO3 ->	ARR 3.666E-15 0 0
617	C6H6O3_11 ->	PHOTOLYSIS 3.5767E-06 3.4991E-06 3.2674E-06 2.8868E-06 2.3685E-06 1.7539E-06 1.0960E-06 5.0716E-07 1.8427E-07 3.4435E-08 0.0000E+00
618	C6H6O3_11 ->	PHOTOLYSIS 7.1608E-06 7.0590E-06 6.7481E-06 6.2123E-06 5.4266E-06 4.3964E-06 3.1263E-06 1.7392E-06 7.6263E-07 1.7820E-07 0.0000E+00
619	C6H6O3_12 + OH ->	ARR 1.303E-11 0 0
620	C6H6O3_12 + OH ->	ARR 1.823E-12 0 -395.
621	C6H6O3_12 + OH ->	ARR 1.345E-12 0 -910.
622	C6H6O3_12 + O3 ->	ARR 5.000E-18 0 0
623	C6H6O3_12 + NO3 ->	ARR 2.429E-15 0 0
624	C6H6O3_12 ->	PHOTOLYSIS 1.4998E-04 1.4871E-04 1.4471E-04 1.3738E-04 1.2567E-04 1.0858E-04 8.4431E-05 5.2968E-05 2.5829E-05 6.6301E-06 0.0000E+00
625	C6H6O3_12 ->	PHOTOLYSIS 8.7717E-04 8.7094E-04 8.5109E-04 8.1417E-04 7.5391E-04 6.6369E-04 5.3173E-04 3.4985E-04 1.7813E-04 4.4607E-05 0.0000E+00
626	C6H6O3_12 ->	PHOTOLYSIS 8.7717E-04 8.7094E-04 8.5109E-04 8.1417E-04 7.5391E-04 6.6369E-04 5.3173E-04 3.4985E-04 1.7813E-04 4.4607E-05 0.0000E+00
627	C6H6O3_13 + OH ->	ARR 4.379E-12 0 14.
628	C6H6O3_13 + OH ->	ARR 1.366E-12 0 -910.
629	C6H6O3_13 + O3 ->	ARR 6.864E-20 0 0
630	C6H6O3_13 + NO3 ->	ARR 3.666E-15 0 0
631	C6H6O3_13 + NO3 ->	ARR 3.666E-15 0 0
632	C6H6O3_13 ->	PHOTOLYSIS 3.5767E-06 3.4991E-06 3.2674E-06 2.8868E-06 2.3685E-06 1.7539E-06 1.0960E-06 5.0716E-07 1.8427E-07 3.4435E-08 0.0000E+00
633	C6H6O3_13 ->	PHOTOLYSIS 3.5767E-06 3.4991E-06 3.2674E-06 2.8868E-06 2.3685E-06 1.7539E-06 1.0960E-06 5.0716E-07 1.8427E-07 3.4435E-08 0.0000E+00
634	C6H6O3_14 + OH ->	ARR 4.701E-12 0 -329.
635	C6H6O3_14 + OH ->	ARR 1.542E-12 0 -910.
636	C6H6O3_14 + O3 ->	ARR 6.864E-20 0 0
637	C6H6O3_14 + NO3 ->	ARR 6.277E-15 0 0
638	C6H6O3_14 + NO3 ->	ARR 3.455E-15 0 0

639	C6H6O3_14 + NO3 ->	ARR 3.455E-15 0 0
640	C6H6O3_14 ->	PHOTOLYSIS 3.5767E-06 3.4991E-06 3.2674E-06 2.8868E-06 2.3685E-06 1.7539E-06 1.0960E-06 5.0716E-07 1.8427E-07 3.4435E-08 0.0000E+00
641	C6H6O3_15 ->	ARR 5.200E+16 0 13850.
642	C6H6O3_15 + OH ->	ARR 1.303E-11 0 0
643	C6H6O3_15 + OH ->	ARR 4.098E-12 0 -730.
644	C6H6O3_15 + OH ->	ARR 1.823E-12 0 -395.
645	C6H6O3_15 + O3 ->	ARR 1.666E-18 0 0
646	C6H6O3_15 + NO3 ->	ARR 2.431E-15 0 0
647	C6H6O3_15 + NO3 ->	ARR 3.114E-16 0 0
648	C6H6O3_15 + NO3 ->	ARR 3.114E-16 0 0
649	C6H6O3_15 ->	PHOTOLYSIS 1.1627E-06 1.1412E-06 1.0767E-06 9.6915E-07 8.1900E-07 6.3424E-07 4.2450E-07 2.1828E-07 8.9068E-08 1.9298E-08 0.0000E+00
650	C6H6O3_15 ->	PHOTOLYSIS 4.0033E-06 3.9636E-06 3.8397E-06 3.6166E-06 3.2684E-06 2.7748E-06 2.1033E-06 1.2727E-06 6.0161E-07 1.5165E-07 0.0000E+00
651	C6H6O3_15 ->	PHOTOLYSIS 3.8855E-06 3.8471E-06 3.7268E-06 3.5103E-06 3.1723E-06 2.6932E-06 2.0414E-06 1.2353E-06 5.8391E-07 1.4719E-07 0.0000E+00
652	C6H6O3_15 ->	PHOTOLYSIS 3.8855E-06 3.8471E-06 3.7268E-06 3.5103E-06 3.1723E-06 2.6932E-06 2.0414E-06 1.2353E-06 5.8391E-07 1.4719E-07 0.0000E+00
653	C6H6O3_16 + OH ->	ARR 1.400E-11 0 0
654	C6H6O3_16 + OH ->	ARR 4.187E-12 0 -920.
655	C6H6O3_16 + O3 ->	ARR 1.666E-18 0 0
656	C6H6O3_16 + NO3 ->	ARR 2.431E-15 0 0
657	C6H6O3_16 + NO3 ->	ARR 3.114E-16 0 0
658	C6H6O3_16 + NO3 ->	ARR 3.114E-16 0 0
659	C6H6O3_16 ->	PHOTOLYSIS 4.0033E-06 3.9636E-06 3.8397E-06 3.6166E-06 3.2684E-06 2.7748E-06 2.1033E-06 1.2727E-06 6.0161E-07 1.5165E-07 0.0000E+00
660	C6H6O3_16 ->	PHOTOLYSIS 3.8855E-06 3.8471E-06 3.7268E-06 3.5103E-06 3.1723E-06 2.6932E-06 2.0414E-06 1.2353E-06 5.8391E-07 1.4719E-07 0.0000E+00
661	C6H6O3_16 ->	PHOTOLYSIS 3.8855E-06 3.8471E-06 3.7268E-06 3.5103E-06 3.1723E-06 2.6932E-06 2.0414E-06 1.2353E-06 5.8391E-07 1.4719E-07 0.0000E+00
662	C6H6O3_18 ->	ARR 5.200E+16 0 13850.
663	C6H6O3_18 + OH ->	ARR 1.183E-11 0 -25.
664	C6H6O3_18 + NO3 ->	ARR 4.922E-15 0 0
665	C6H6O3_18 ->	PHOTOLYSIS 1.1627E-06 1.1412E-06 1.0767E-06 9.6915E-07 8.1900E-07 6.3424E-07 4.2450E-07 2.1828E-07 8.9068E-08 1.9298E-08 0.0000E+00
666	C6H6O3_18 ->	PHOTOLYSIS 1.3993E-05 1.3687E-05 1.2773E-05 1.1268E-05 9.2156E-06 6.7805E-06 4.1825E-06 1.8855E-06 6.5962E-07 1.1592E-07 0.0000E+00
667	C6H6O3_19 + OH ->	ARR 1.202E-11 0 -25.
668	C6H6O3_19 + OH ->	ARR 5.218E-12 0 -420.
669	C6H6O3_19 + NO3 ->	ARR 2.318E-14 0 0

670	C6H6O3_19 + NO3 ->	ARR 1.165E-14 0 0
671	C6H6O3_19 ->	PHOTOLYSIS 1.3993E-05 1.3687E-05 1.2773E-05 1.1268E-05 9.2156E-06 6.7805E-06 4.1825E-06 1.8855E-06 6.5962E-07 1.1592E-07 0.0000E+00
672	C6H6O3_19 ->	PHOTOLYSIS 6.3200E-06 6.1814E-06 5.7672E-06 5.0855E-06 4.1552E-06 3.0520E-06 1.8766E-06 8.4112E-07 2.9197E-07 5.0853E-08 0.0000E+00
673	C6H6O3_19 ->	PHOTOLYSIS 2.5975E-05 2.5431E-05 2.3802E-05 2.1107E-05 1.7397E-05 1.2944E-05 8.1150E-06 3.7471E-06 1.3458E-06 2.4407E-07 0.0000E+00
674	C6H6O3_21 + OH ->	ARR 1.302E-11 0 78.
675	C6H6O3_21 + OH ->	ARR 1.980E-12 0 -590.
676	C6H6O3_21 + NO3 ->	ARR 1.087E-14 0 0
677	C6H6O3_21 + NO3 ->	ARR 7.437E-15 0 0
678	C6H6O3_21 + NO3 ->	ARR 6.817E-15 0 0
679	C6H6O3_21 ->	PHOTOLYSIS 2.5975E-05 2.5431E-05 2.3802E-05 2.1107E-05 1.7397E-05 1.2944E-05 8.1150E-06 3.7471E-06 1.3458E-06 2.4407E-07 0.0000E+00
680	C6H6O3_21 ->	PHOTOLYSIS 1.0382E-04 1.0277E-04 9.9520E-05 9.3759E-05 8.4963E-05 7.2773E-05 5.6464E-05 3.6026E-05 1.8062E-05 4.3355E-06 0.0000E+00
681	C6H6O3_21 ->	PHOTOLYSIS 5.7680E-06 5.7096E-06 5.5289E-06 5.2088E-06 4.7202E-06 4.0430E-06 3.1369E-06 2.0014E-06 1.0035E-06 2.4086E-07 0.0000E+00
682	C6H6O3_22 + OH ->	ARR 1.176E-11 0 -25.
683	C6H6O3_22 + OH ->	ARR 1.790E-12 0 -590.
684	C6H6O3_22 + NO3 ->	ARR 1.506E-14 0 0
685	C6H6O3_22 + NO3 ->	ARR 4.747E-15 0 0
686	C6H6O3_22 ->	PHOTOLYSIS 1.3993E-05 1.3687E-05 1.2773E-05 1.1268E-05 9.2156E-06 6.7805E-06 4.1825E-06 1.8855E-06 6.5962E-07 1.1592E-07 0.0000E+00
687	C6H6O3_22 ->	PHOTOLYSIS 1.0382E-04 1.0277E-04 9.9520E-05 9.3759E-05 8.4963E-05 7.2773E-05 5.6464E-05 3.6026E-05 1.8062E-05 4.3355E-06 0.0000E+00
688	C6H6O3_22 ->	PHOTOLYSIS 5.7680E-06 5.7096E-06 5.5289E-06 5.2088E-06 4.7202E-06 4.0430E-06 3.1369E-06 2.0014E-06 1.0035E-06 2.4086E-07 0.0000E+00
689	C6H6O3_23 + OH ->	ARR 6.913E-12 0 -730.
690	C6H6O3_23 + O3 ->	ARR 1.666E-18 0 0
691	C6H6O3_23 + NO3 ->	ARR 5.330E-15 0 0
692	C6H6O3_23 + NO3 ->	ARR 2.626E-15 0 0
693	C6H6O3_23 ->	PHOTOLYSIS 1.3993E-05 1.3687E-05 1.2773E-05 1.1268E-05 9.2156E-06 6.7805E-06 4.1825E-06 1.8855E-06 6.5962E-07 1.1592E-07 0.0000E+00
694	C6H6O3_23 ->	PHOTOLYSIS 4.0033E-06 3.9636E-06 3.8397E-06 3.6166E-06 3.2684E-06 2.7748E-06 2.1033E-06 1.2727E-06 6.0161E-07 1.5165E-07 0.0000E+00
695	C6H6O3_23 ->	PHOTOLYSIS 3.8855E-06 3.8471E-06 3.7268E-06 3.5103E-06 3.1723E-06 2.6932E-06 2.0414E-06 1.2353E-06 5.8391E-07 1.4719E-07 0.0000E+00
696	C6H6O3_23 ->	PHOTOLYSIS 3.8855E-06 3.8471E-06 3.7268E-06 3.5103E-06 3.1723E-06 2.6932E-06 2.0414E-06 1.2353E-06 5.8391E-07 1.4719E-07 0.0000E+00

697	C6H6O3_24 + OH ->	ARR 1.293E-11 0 -25.
698	C6H6O3_24 + OH ->	ARR 1.483E-12 0 -910.
699	C6H6O3_24 + O3 ->	ARR 6.188E-18 0 0
700	C6H6O3_24 + NO3 ->	ARR 5.186E-15 0 0
701	C6H6O3_24 ->	PHOTOLYSIS 1.3993E-05 1.3687E-05 1.2773E-05 1.1268E-05 9.2156E-06 6.7805E-06 4.1825E-06 1.8855E-06 6.5962E-07 1.1592E-07 0.0000E+00
702	C6H6O3_24 ->	PHOTOLYSIS 6.4760E-07 6.4117E-07 6.2110E-07 5.8499E-07 5.2867E-07 4.4890E-07 3.4047E-07 2.0636E-07 9.7703E-08 2.4532E-08 0.0000E+00
703	C6H6O3_24 ->	PHOTOLYSIS 6.4760E-06 6.4117E-06 6.2110E-06 5.8499E-06 5.2867E-06 4.4890E-06 3.4047E-06 2.0636E-06 9.7703E-07 2.4532E-07 0.0000E+00
704	C6H6O3_25 + OH ->	ARR 6.082E-12 0 -730.
705	C6H6O3_25 + O3 ->	ARR 1.666E-18 0 0
706	C6H6O3_25 + NO3 ->	ARR 3.054E-15 0 0
707	C6H6O3_25 ->	PHOTOLYSIS 7.1608E-06 7.0590E-06 6.7481E-06 6.2123E-06 5.4266E-06 4.3964E-06 3.1263E-06 1.7392E-06 7.6263E-07 1.7820E-07 0.0000E+00
708	C6H6O3_25 ->	PHOTOLYSIS 4.0033E-06 3.9636E-06 3.8397E-06 3.6166E-06 3.2684E-06 2.7748E-06 2.1033E-06 1.2727E-06 6.0161E-07 1.5165E-07 0.0000E+00
709	C6H6O3_25 ->	PHOTOLYSIS 3.8855E-06 3.8471E-06 3.7268E-06 3.5103E-06 3.1723E-06 2.6932E-06 2.0414E-06 1.2353E-06 5.8391E-07 1.4719E-07 0.0000E+00
710	C6H6O3_25 ->	PHOTOLYSIS 3.8855E-06 3.8471E-06 3.7268E-06 3.5103E-06 3.1723E-06 2.6932E-06 2.0414E-06 1.2353E-06 5.8391E-07 1.4719E-07 0.0000E+00
711	C6H6O3_26 + OH ->	ARR 5.576E-12 0 -730.
712	C6H6O3_26 + O3 ->	ARR 1.304E-15 0 1690.
713	C6H6O3_26 + NO3 ->	ARR 1.358E-14 0 0
714	C6H6O3_26 ->	PHOTOLYSIS 1.0382E-04 1.0277E-04 9.9520E-05 9.3759E-05 8.4963E-05 7.2773E-05 5.6464E-05 3.6026E-05 1.8062E-05 4.3355E-06 0.0000E+00
715	C6H6O3_26 ->	PHOTOLYSIS 5.7680E-06 5.7096E-06 5.5289E-06 5.2088E-06 4.7202E-06 4.0430E-06 3.1369E-06 2.0014E-06 1.0035E-06 2.4086E-07 0.0000E+00
716	C6H6O3_27 + OH ->	ARR 1.468E-11 0 -25.
717	C6H6O3_27 + NO3 ->	ARR 4.922E-15 0 0
718	C6H6O3_27 ->	PHOTOLYSIS 7.1608E-06 7.0590E-06 6.7481E-06 6.2123E-06 5.4266E-06 4.3964E-06 3.1263E-06 1.7392E-06 7.6263E-07 1.7820E-07 0.0000E+00
719	C6H6O3_27 ->	PHOTOLYSIS 1.3993E-05 1.3687E-05 1.2773E-05 1.1268E-05 9.2156E-06 6.7805E-06 4.1825E-06 1.8855E-06 6.5962E-07 1.1592E-07 0.0000E+00
720	C6H6O3_28 + OH ->	ARR 7.722E-12 0 -490.
721	C6H6O3_28 + NO3 ->	ARR 3.622E-12 0 0
722	C6H6O3_28 ->	PHOTOLYSIS 1.3993E-05 1.3687E-05 1.2773E-05 1.1268E-05 9.2156E-06 6.7805E-06 4.1825E-06 1.8855E-06 6.5962E-07 1.1592E-07 0.0000E+00
723	C6H6O3_28 ->	PHOTOLYSIS 6.3200E-06 6.1814E-06 5.7672E-06 5.0855E-06 4.1552E-06 3.0520E-06 1.8766E-06 8.4112E-07 2.9197E-07 5.0853E-08 0.0000E+00

724	C6H6O3_28 ->	PHOTOLYSIS 6.8267E-05 6.7157E-05 6.3779E-05 5.8001E-05 4.9642E-05 3.8921E-05 2.6222E-05 1.3337E-05 5.2691E-06 1.0571E-06 0.0000E+00
725	C6H6O3_29 + OH ->	ARR 1.202E-11 0 -25.
726	C6H6O3_29 + OH ->	ARR 5.218E-12 0 -420.
727	C6H6O3_29 + NO3 ->	ARR 4.124E-14 0 0
728	C6H6O3_29 ->	PHOTOLYSIS 1.3993E-05 1.3687E-05 1.2773E-05 1.1268E-05 9.2156E-06 6.7805E-06 4.1825E-06 1.8855E-06 6.5962E-07 1.1592E-07 0.0000E+00
729	C6H6O3_29 ->	PHOTOLYSIS 3.1034E-04 3.0825E-04 3.0160E-04 2.8920E-04 2.6889E-04 2.3831E-04 1.9313E-04 1.2954E-04 6.7220E-05 1.6652E-05 0.0000E+00
730	C6H6O3_29 ->	PHOTOLYSIS 2.5975E-05 2.5431E-05 2.3802E-05 2.1107E-05 1.7397E-05 1.2944E-05 8.1150E-06 3.7471E-06 1.3458E-06 2.4407E-07 0.0000E+00
731	C6H6O3_30 + OH ->	ARR 7.760E-12 0 -730.
732	C6H6O3_30 + O3 ->	ARR 1.932E-18 0 0
733	C6H6O3_30 + NO3 ->	ARR 4.283E-15 0 0
734	C6H6O3_30 ->	PHOTOLYSIS 7.1608E-06 7.0590E-06 6.7481E-06 6.2123E-06 5.4266E-06 4.3964E-06 3.1263E-06 1.7392E-06 7.6263E-07 1.7820E-07 0.0000E+00
735	C6H6O3_30 ->	PHOTOLYSIS 4.8066E-06 4.7122E-06 4.4297E-06 3.9632E-06 3.3204E-06 2.5430E-06 1.6791E-06 8.5031E-07 3.4350E-07 7.4208E-08 0.0000E+00
736	C6H6O3_30 ->	PHOTOLYSIS 4.0033E-06 3.9636E-06 3.8397E-06 3.6166E-06 3.2684E-06 2.7748E-06 2.1033E-06 1.2727E-06 6.0161E-07 1.5165E-07 0.0000E+00
737	C6H6O3_30 ->	PHOTOLYSIS 3.8855E-06 3.8471E-06 3.7268E-06 3.5103E-06 3.1723E-06 2.6932E-06 2.0414E-06 1.2353E-06 5.8391E-07 1.4719E-07 0.0000E+00
738	C6H6O3_30 ->	PHOTOLYSIS 3.8855E-06 3.8471E-06 3.7268E-06 3.5103E-06 3.1723E-06 2.6932E-06 2.0414E-06 1.2353E-06 5.8391E-07 1.4719E-07 0.0000E+00
739	C6H6O3_31 + OH ->	ARR 7.754E-12 0 -490.
740	C6H6O3_31 + NO3 ->	ARR 3.638E-12 0 0
741	C6H6O3_31 ->	PHOTOLYSIS 1.0382E-04 1.0277E-04 9.9520E-05 9.3759E-05 8.4963E-05 7.2773E-05 5.6464E-05 3.6026E-05 1.8062E-05 4.3355E-06 0.0000E+00
742	C6H6O3_31 ->	PHOTOLYSIS 5.7680E-06 5.7096E-06 5.5289E-06 5.2088E-06 4.7202E-06 4.0430E-06 3.1369E-06 2.0014E-06 1.0035E-06 2.4086E-07 0.0000E+00
743	C6H6O3_31 ->	PHOTOLYSIS 6.8267E-05 6.7157E-05 6.3779E-05 5.8001E-05 4.9642E-05 3.8921E-05 2.6222E-05 1.3337E-05 5.2691E-06 1.0571E-06 0.0000E+00
744	C6H6O3_32 + OH ->	ARR 8.451E-12 0 -420.
745	C6H6O3_32 + NO3 ->	ARR 2.352E-14 0 0
746	C6H6O3_32 ->	PHOTOLYSIS 2.5975E-05 2.5431E-05 2.3802E-05 2.1107E-05 1.7397E-05 1.2944E-05 8.1150E-06 3.7471E-06 1.3458E-06 2.4407E-07 0.0000E+00
747	C6H6O3_32 ->	PHOTOLYSIS 4.8066E-06 4.7122E-06 4.4297E-06 3.9632E-06 3.3204E-06 2.5430E-06 1.6791E-06 8.5031E-07 3.4350E-07 7.4208E-08 0.0000E+00
748	C6H6O3_32 ->	PHOTOLYSIS 1.0382E-04 1.0277E-04 9.9520E-05 9.3759E-05 8.4963E-05 7.2773E-05

		5.6464E-05 3.6026E-05 1.8062E-05 4.3355E-06 0.0000E+00
749	C6H6O3_32 ->	PHOTOLYSIS 5.7680E-06 5.7096E-06 5.5289E-06 5.2088E-06 4.7202E-06 4.0430E-06 3.1369E-06 2.0014E-06 1.0035E-06 2.4086E-07 0.0000E+00
750	C6H6O3_33 + OH ->	ARR 8.096E-14 0 -2150.
751	C6H6O3_33 + O3 ->	ARR 5.950E-18 0 0
752	C6H6O3_33 + NO3 ->	ARR 6.305E-15 0 0
753	C6H6O3_33 ->	PHOTOLYSIS 7.1608E-06 7.0590E-06 6.7481E-06 6.2123E-06 5.4266E-06 4.3964E-06 3.1263E-06 1.7392E-06 7.6263E-07 1.7820E-07 0.0000E+00
754	C6H6O3_33 ->	PHOTOLYSIS 8.7717E-04 8.7094E-04 8.5109E-04 8.1417E-04 7.5391E-04 6.6369E-04 5.3173E-04 3.4985E-04 1.7813E-04 4.4607E-05 0.0000E+00
755	C6H6O3_33 ->	PHOTOLYSIS 8.7717E-04 8.7094E-04 8.5109E-04 8.1417E-04 7.5391E-04 6.6369E-04 5.3173E-04 3.4985E-04 1.7813E-04 4.4607E-05 0.0000E+00
756	C6H6O3_34 + OH ->	ARR 1.444E-12 0 -1500.
757	C6H6O3_34 + O3 ->	ARR 4.641E-17 0 0
758	C6H6O3_34 + NO3 ->	ARR 5.766E-15 0 0
759	C6H6O3_34 + NO3 ->	ARR 3.559E-15 0 0
760	C6H6O3_34 + NO3 ->	ARR 3.559E-15 0 0
761	C6H6O3_34 ->	PHOTOLYSIS 7.1608E-06 7.0590E-06 6.7481E-06 6.2123E-06 5.4266E-06 4.3964E-06 3.1263E-06 1.7392E-06 7.6263E-07 1.7820E-07 0.0000E+00
762	C6H6O3_34 ->	PHOTOLYSIS 6.4760E-07 6.4117E-07 6.2110E-07 5.8499E-07 5.2867E-07 4.4890E-07 3.4047E-07 2.0636E-07 9.7703E-08 2.4532E-08 0.0000E+00
763	C6H6O3_34 ->	PHOTOLYSIS 6.4760E-06 6.4117E-06 6.2110E-06 5.8499E-06 5.2867E-06 4.4890E-06 3.4047E-06 2.0636E-06 9.7703E-07 2.4532E-07 0.0000E+00
764	C6H6O3_34 ->	PHOTOLYSIS 1.3993E-05 1.3687E-05 1.2773E-05 1.1268E-05 9.2156E-06 6.7805E-06 4.1825E-06 1.8855E-06 6.5962E-07 1.1592E-07 0.0000E+00
765	C6H6O3_35 + OH ->	ARR 2.682E-14 0 -1763.
766	C6H6O3_35 + OH ->	ARR 1.347E-12 0 -910.
767	C6H6O3_35 + OH ->	ARR 1.347E-12 0 -910.
768	C6H6O3_35 + O3 ->	ARR 3.120E-20 0 0
769	C6H6O3_35 + NO3 ->	ARR 2.631E-15 0 0
770	C6H6O3_36 + OH ->	ARR 1.362E-12 0 -910.
771	C6H6O3_36 + OH ->	ARR 1.432E-12 0 -568.
772	C6H6O3_36 + O3 ->	ARR 3.120E-20 0 0
773	C6H6O3_36 + NO3 ->	ARR 1.464E-16 0 0
774	C6H6O3_36 + NO3 ->	ARR 7.299E-17 0 0
775	C6H6O3_36 + NO3 ->	ARR 7.299E-17 0 0
776	C6H6O3_36 ->	PHOTOLYSIS 5.2032E-05 5.1093E-05 4.8258E-05 4.3488E-05 3.6749E-05 2.8358E-05 1.8760E-05 9.3794E-06 3.6776E-06 7.4565E-07 0.0000E+00
777	C6H6O3_37 + OH ->	ARR 6.927E-12 0 -730.
778	C6H6O3_37 + O3 ->	ARR 1.932E-18 0 0
779	C6H6O3_37 + NO3 ->	ARR 1.795E-15 0 0
780	C6H6O3_37 + NO3 ->	ARR 2.805E-15 0 0

781	C6H6O3_37 ->	PHOTOLYSIS 1.0382E-04 1.0277E-04 9.9520E-05 9.3759E-05 8.4963E-05 7.2773E-05 5.6464E-05 3.6026E-05 1.8062E-05 4.3355E-06 0.0000E+00
782	C6H6O3_37 ->	PHOTOLYSIS 5.7680E-06 5.7096E-06 5.5289E-06 5.2088E-06 4.7202E-06 4.0430E-06 3.1369E-06 2.0014E-06 1.0035E-06 2.4086E-07 0.0000E+00
783	C6H6O3_37 ->	PHOTOLYSIS 4.0033E-06 3.9636E-06 3.8397E-06 3.6166E-06 3.2684E-06 2.7748E-06 2.1033E-06 1.2727E-06 6.0161E-07 1.5165E-07 0.0000E+00
784	C6H6O3_37 ->	PHOTOLYSIS 3.8855E-06 3.8471E-06 3.7268E-06 3.5103E-06 3.1723E-06 2.6932E-06 2.0414E-06 1.2353E-06 5.8391E-07 1.4719E-07 0.0000E+00
785	C6H6O3_37 ->	PHOTOLYSIS 3.8855E-06 3.8471E-06 3.7268E-06 3.5103E-06 3.1723E-06 2.6932E-06 2.0414E-06 1.2353E-06 5.8391E-07 1.4719E-07 0.0000E+00
786	C6H6O3_38 + OH ->	ARR 1.568E-12 0 -1500.
787	C6H6O3_38 + O3 ->	ARR 9.408E-17 0 0
788	C6H6O3_38 + NO3 ->	ARR 1.394E-13 0 0
789	C6H6O3_38 + NO3 ->	ARR 1.394E-13 0 0
790	C6H6O3_38 ->	PHOTOLYSIS 7.1608E-06 7.0590E-06 6.7481E-06 6.2123E-06 5.4266E-06 4.3964E-06 3.1263E-06 1.7392E-06 7.6263E-07 1.7820E-07 0.0000E+00
791	C6H6O3_38 ->	PHOTOLYSIS 1.0382E-04 1.0277E-04 9.9520E-05 9.3759E-05 8.4963E-05 7.2773E-05 5.6464E-05 3.6026E-05 1.8062E-05 4.3355E-06 0.0000E+00
792	C6H6O3_38 ->	PHOTOLYSIS 5.7680E-06 5.7096E-06 5.5289E-06 5.2088E-06 4.7202E-06 4.0430E-06 3.1369E-06 2.0014E-06 1.0035E-06 2.4086E-07 0.0000E+00
793	C6H6O3_39 + OH ->	ARR 1.233E-11 0 -25.
794	C6H6O3_39 + NO3 ->	ARR 4.922E-15 0 0
795	C6H6O3_39 ->	PHOTOLYSIS 1.3993E-05 1.3687E-05 1.2773E-05 1.1268E-05 9.2156E-06 6.7805E-06 4.1825E-06 1.8855E-06 6.5962E-07 1.1592E-07 0.0000E+00
796	C6H6O3_40 + OH ->	ARR 2.618E-13 0 -1693.
797	C6H6O3_40 + OH ->	ARR 5.430E-12 0 -920.
798	C6H6O3_40 + O3 ->	ARR 2.184E-18 0 0
799	C6H6O3_40 + NO3 ->	ARR 1.533E-14 0 0
800	C6H6O3_41 + OH ->	ARR 4.693E-12 0 -578.
801	C6H6O3_41 + OH ->	ARR 1.539E-12 0 -910.
802	C6H6O3_41 + O3 ->	ARR 2.184E-18 0 0
803	C6H6O3_41 + NO3 ->	ARR 3.171E-15 0 0
804	C6H6O3_41 + NO3 ->	ARR 3.153E-15 0 0
805	C6H6O3_41 + NO3 ->	ARR 3.153E-15 0 0
806	C6H6O3_41 ->	PHOTOLYSIS 3.5767E-06 3.4991E-06 3.2674E-06 2.8868E-06 2.3685E-06 1.7539E-06 1.0960E-06 5.0716E-07 1.8427E-07 3.4435E-08 0.0000E+00
807	C6H6O3_42 + OH ->	ARR 5.825E-12 0 -730.
808	C6H6O3_42 + O3 ->	ARR 1.932E-18 0 0
809	C6H6O3_42 + NO3 ->	ARR 3.054E-15 0 0
810	C6H6O3_42 ->	PHOTOLYSIS 1.4998E-04 1.4871E-04 1.4471E-04 1.3738E-04 1.2567E-04 1.0858E-04 8.4431E-05 5.2968E-05 2.5829E-05 6.6301E-06 0.0000E+00

811	C6H6O3_42 ->	PHOTOLYSIS 4.0033E-06 3.9636E-06 3.8397E-06 3.6166E-06 3.2684E-06 2.7748E-06 2.1033E-06 1.2727E-06 6.0161E-07 1.5165E-07 0.0000E+00
812	C6H6O3_42 ->	PHOTOLYSIS 3.8855E-06 3.8471E-06 3.7268E-06 3.5103E-06 3.1723E-06 2.6932E-06 2.0414E-06 1.2353E-06 5.8391E-07 1.4719E-07 0.0000E+00
813	C6H6O3_42 ->	PHOTOLYSIS 3.8855E-06 3.8471E-06 3.7268E-06 3.5103E-06 3.1723E-06 2.6932E-06 2.0414E-06 1.2353E-06 5.8391E-07 1.4719E-07 0.0000E+00
814	C6H6O3_43 + OH ->	ARR 2.310E-12 0 -910.
815	C6H6O3_43 + O3 ->	ARR 5.950E-18 0 0
816	C6H6O3_43 + NO3 ->	ARR 2.449E-15 0 0
817	C6H6O3_43 ->	PHOTOLYSIS 8.7717E-04 8.7094E-04 8.5109E-04 8.1417E-04 7.5391E-04 6.6369E-04 5.3173E-04 3.4985E-04 1.7813E-04 4.4607E-05 0.0000E+00
818	C6H6O3_43 ->	PHOTOLYSIS 8.7717E-04 8.7094E-04 8.5109E-04 8.1417E-04 7.5391E-04 6.6369E-04 5.3173E-04 3.4985E-04 1.7813E-04 4.4607E-05 0.0000E+00
819	C6H6O3_44 + OH ->	ARR 2.559E-12 0 -910.
820	C6H6O3_44 + O3 ->	ARR 2.737E-18 0 0
821	C6H6O3_44 + NO3 ->	ARR 4.911E-15 0 0
822	C6H6O3_44 + NO3 ->	ARR 3.406E-15 0 0
823	C6H6O3_44 + NO3 ->	ARR 3.406E-15 0 0
824	C6H6O3_44 ->	PHOTOLYSIS 6.4760E-07 6.4117E-07 6.2110E-07 5.8499E-07 5.2867E-07 4.4890E-07 3.4047E-07 2.0636E-07 9.7703E-08 2.4532E-08 0.0000E+00
825	C6H6O3_44 ->	PHOTOLYSIS 6.4760E-06 6.4117E-06 6.2110E-06 5.8499E-06 5.2867E-06 4.4890E-06 3.4047E-06 2.0636E-06 9.7703E-07 2.4532E-07 0.0000E+00
826	C6H6O3_44 ->	PHOTOLYSIS 1.3993E-05 1.3687E-05 1.2773E-05 1.1268E-05 9.2156E-06 6.7805E-06 4.1825E-06 1.8855E-06 6.5962E-07 1.1592E-07 0.0000E+00
827	C6H6O3_45 + OH ->	ARR 6.331E-12 0 -730.
828	C6H6O3_45 + O3 ->	ARR 3.174E-18 0 0
829	C6H6O3_45 + NO3 ->	ARR 1.555E-13 0 0
830	C6H6O3_45 + NO3 ->	ARR 1.555E-13 0 0
831	C6H6O3_45 ->	PHOTOLYSIS 1.0382E-04 1.0277E-04 9.9520E-05 9.3759E-05 8.4963E-05 7.2773E-05 5.6464E-05 3.6026E-05 1.8062E-05 4.3355E-06 0.0000E+00
832	C6H6O3_45 ->	PHOTOLYSIS 5.7680E-06 5.7096E-06 5.5289E-06 5.2088E-06 4.7202E-06 4.0430E-06 3.1369E-06 2.0014E-06 1.0035E-06 2.4086E-07 0.0000E+00
833	BZBIPERO2 -> BZo_RO2_O7	ARR 0.32 0 0
834	BZBIPERO -> BZeo_RO2_O6	ARR 0.1E-6 0 0
835	BZBIPERO2 -> C5_RO2_O6 + CO	ARR 0.022 0 0
836	BZEMUCO2 -> BZeo_RO2_O8	ARR 0.07 0 0
837	BZEMUCO2 -> C5_RO2_O7 + CO	ARR 0.25 0 0
838	PHENO2 -> BZeo_RO2_O8	ARR 0.07 0 0
839	PHENO2 -> C5_RO2_O7 + CO	ARR 0.25 0 0
840	BZo_RO2_O7 -> BZo_RO2_O9	ARR 1.5 0 0
841	BZo_RO2_O9 -> BZo_RO2_O11	ARR 0.45 0 0

842	BZeo_RO2_O6 -> BZeo_RO2_O8	ARR 0.1 0 0
843	BZeo_RO2_O8 -> BZeo_RO2_O10	ARR 0.01 0 0
844	BZo2_RO_O6 -> BZeo_RO2_O8	ARR 0.90E-6 0 0
845	BZo2_RO_O8 -> BZeo_RO2_O10	ARR 0.85E-6 0 0
846	BZeo2_RO_O5 -> BZo_RO2_O7	ARR 0.90E-6 0 0
847	BZeo2_RO_O7 -> BZo_RO2_O9	ARR 0.90E-6 0 0
848	BZeo2_RO_O9 -> BZo_RO2_O11	ARR 0.40E-6 0 0
849	BZo_RO_O6 -> BZeo_RO2_O8	ARR 0.2E-6 0 0
850	BZo_RO_O8 -> BZeo_RO2_O10	ARR 0.1E-6 0 0
851	BZeo_RO_O5 -> BZo_RO2_O7	ARR 0.45E-6 0 0
852	BZeo_RO_O7 -> BZo_RO2_O9	ARR 0.35E-6 0 0
853	BZeo_RO_O9 -> BZo_RO2_O11	ARR 0.45E-6 0 0
854	C5_RO_O5 -> C5_RO2_O7	ARR 0.90E-6 0 0
855	C5_RO_O6 -> C5_RO2_O8	ARR 0.90E-6 0 0
856	C5_RO_O7 -> C5_RO2_O9	ARR 0.85E-6 0 0
857	C5_RO_O8 -> C5_RO2_O10	ARR 0.70E-6 0 0
858	BZo_RO2_O7 + NO -> BZo_O5_NO3	ARR 0.024E-12 0 -360
859	BZo_RO2_O9 + NO -> BZo_O7_NO3	ARR 0.014E-12 0 -360
860	BZo_RO2_O11 + NO -> BZo_O9_NO3	ARR 0.324E-12 0 -360
861	BZeo_RO2_O6 + NO -> BZeo_O4_NO3	ARR 0.005E-12 0 -360
862	BZeo_RO2_O8 + NO -> BZeo_O6_NO3	ARR 0.016E-12 0 -360
863	BZeo_RO2_O10 + NO -> BZeo_O8_NO3	ARR 0.027E-12 0 -360
864	C5_RO2_O6 + NO -> C5e_O4_NO3	ARR 0.108E-12 0 -360
865	C5_RO2_O7 + NO -> C5_O5_NO3	ARR 0.011E-12 0 -360
866	C5_RO2_O8 + NO -> C5e_O6_NO3	ARR 0.022E-12 0 -360
867	C5_RO2_O9 + NO -> C5_O7_NO3	ARR 0.054E-12 0 -360
868	C5_RO2_O10 + NO -> C5e_O8_NO3	ARR 0.054E-12 0 -360
869	BZo_RO2_O7 + NO -> BZo2_RO_O6 + NO2	ARR 2.422E-12 0 -360
870	BZo_RO2_O9 + NO -> BZo2_RO_O8 + NO2	ARR 2.641E-12 0 -360
871	BZo_RO2_O11 + NO -> BZo2_RO_O10 + NO2	ARR 2.511E-12 0 -360
872	BZeo_RO2_O6 + NO -> BZeo2_RO_O5 + NO2	ARR 2.425E-12 0 -360
873	BZeo_RO2_O8 + NO -> BZeo2_RO_O7 + NO2	ARR 2.414E-12 0 -360
874	BZeo_RO2_O10 + NO -> BZeo2_RO_O9 + NO2	ARR 1.593E-12 0 -360
875	C5_RO2_O6 + NO -> C5_RO_O5 + NO2	ARR 2.592E-12 0 -360
876	C5_RO2_O7 + NO -> C5_RO_O6 + NO2	ARR 2.695E-12 0 -360
877	C5_RO2_O8 + NO -> C5_RO_O7 + NO2	ARR 2.689E-12 0 -360
878	C5_RO2_O9 + NO -> C5_RO_O8 + NO2	ARR 2.646E-12 0 -360
879	C5_RO2_O10 + NO -> C5_RO_O9 + NO2	ARR 2.646E-12 0 -360
880	BZo_RO2_O7 + NO -> BZo_O5_O + NO2 + HO2	ARR 0.27E-12 0 -360
881	BZo_RO2_O9 + NO -> BZo_O7_O + NO2 + HO2	ARR 0.054E-12 0 -360
882	BZo_RO2_O11 + NO -> BZo_O9_O + NO2 + HO2	ARR 0.081E-12 0 -360
883	BZeo_RO2_O6 + NO -> BZeo_O4_O + NO2 + HO2	ARR 0.27E-12 0 -360
884	BZeo_RO2_O8 + NO -> BZeo_O6_O + NO2 + HO2	ARR 0.27E-12 0 -360
885	BZeo_RO2_O10 + NO -> BZeo_O8_O + NO2 + HO2	ARR 1.08E-12 0 -360
886	BZo_RO2_O7 + HO2 -> BZo_O5_OOH	ARR 0.022E-13 0 -1300
887	BZo_RO2_O9 + HO2 -> BZo_O7_OOH	ARR 0.134E-13 0 -1300

888	BZo_RO2_O11 + HO2 -> BZo_O9_OOH	ARR 0.448E-13 0 -1300
889	BZeo_RO2_O6 + HO2 -> BZeo_O4_OOH	ARR 1.344E-13 0 -1300
890	BZeo_RO2_O8 + HO2 -> BZeo_O6_OOH	ARR 0.09E-13 0 -1300
891	BZeo_RO2_O10 + HO2 -> BZeo_O8_OOH	ARR 1.232E-13 0 -1300
892	C5_RO2_O6 + HO2 -> C5e_O4_OOH	ARR 0.01E-13 0 -1300
893	C5_RO2_O7 + HO2 -> C5_O5_OOH	ARR 0.616E-13 0 -1300
894	C5_RO2_O8 + HO2 -> C5e_O6_OOH	ARR 1.233E-13 0 -1300
895	C5_RO2_O9 + HO2 -> C5_O7_OOH	ARR 0.205E-13 0 -1300
896	C5_RO2_O10 + HO2 -> C5e_O8_OOH	ARR 1.233E-13 0 -1300
897	BZo_RO2_O7 + HO2 -> BZo_RO_O6 + OH	ARR 2.218E-13 0 -1300
898	BZo_RO2_O9 + HO2 -> BZo_RO_O8 + OH	ARR 2.061E-13 0 -1300
899	BZo_RO2_O11 + HO2 -> BZo_RO_O10 + OH	ARR 1.905E-13 0 -1300
900	BZeo_RO2_O6 + HO2 -> BZeo_RO_O5 + OH	ARR 0.896E-13 0 -1300
901	BZeo_RO2_O8 + HO2 -> BZeo_RO_O7 + OH	ARR 2.196E-13 0 -1300
902	BZeo_RO2_O10 + HO2 -> BZeo_RO_O9 + OH	ARR 1.008E-13 0 -1300
903	C5_RO2_O6 + HO2 -> MALDIAL + CO + HO2	ARR 2.229E-13 0 -1300
904	C5_RO2_O7 + HO2 -> MALDIAL + CO + HO2	ARR 0.896E-13 0 -1300
905	C5_RO2_O8 + HO2 -> MALDIAL + CO + HO2	ARR 0.896E-13 0 -1300
906	C5_RO2_O9 + HO2 -> MALDIAL + CO + HO2	ARR 2.017E-13 0 -1300
907	C5_RO2_O10 + HO2 -> MALDIAL + CO + HO2	ARR 0.896E-13 0 -1300
908	BZo_RO2_O7 -> BZo_RO_O6	RO2 1 ARR 0.63E-11 0 0
909	BZo_RO2_O9 -> BZo_RO_O8	RO2 1 ARR 1.29E-11 0 0
910	BZo_RO2_O11 -> BZo_RO_O10	RO2 1 ARR 1.95E-11 0 0
911	BZeo_RO2_O6 -> BZeo_RO_O5	RO2 1 ARR 0.3E-11 0 0
912	BZeo_RO2_O8 -> BZeo_RO_O7	RO2 1 ARR 0.96E-11 0 0
913	BZeo_RO2_O10 -> BZeo_RO_O9	RO2 1 ARR 1.62E-11 0 0
914	BZo_RO2_O7 + BZo_RO2_O7 -> BZoO6_BZoO6	ARR 4.17E-11 0 0
915	BZo_RO2_O7 + BZo_RO2_O9 -> BZoO6_BZoO8	ARR 1.0E-10 0 0
916	BZo_RO2_O7 + BZo_RO2_O11 -> BZoO6_BZoO10	ARR 9.69E-11 0 0
917	BZo_RO2_O7 + BZeo_RO2_O6 -> BZoO6_BZeoO5	ARR 2.79E-11 0 0
918	BZo_RO2_O7 + BZeo_RO2_O8 -> BZoO6_BZeoO7	ARR 5.55E-11 0 0
919	BZo_RO2_O7 + BZeo_RO2_O10 -> BZoO6_BZeoO9	ARR 8.31E-11 0 0
920	BZo_RO2_O7 + C5_RO2_O6 -> BZoO6_C5eO5	ARR 4.51E-11 0 0
921	BZo_RO2_O7 + C5_RO2_O7 -> BZoO6_C5O6	ARR 5.89E-11 0 0
922	BZo_RO2_O7 + C5_RO2_O8 -> BZoO6_C5eO7	ARR 7.27E-11 0 0
923	BZo_RO2_O7 + C5_RO2_O9 -> BZoO6_C5O8	ARR 8.65E-11 0 0
924	BZo_RO2_O7 + C5_RO2_O10 -> BZoO6_C5eO9	ARR 1.0E-10 0 0
925	BZo_RO2_O7 + BZBIPERO2 -> BZoO6_BZBI	ARR 0.21E-11 0 0
926	BZo_RO2_O7 + BZEMUCCO3 -> BZoO6_BZMUa	ARR 1.24E-11 0 0
927	BZo_RO2_O7 + BZEMUCO2 -> BZoO6_BZMUb	ARR 2.79E-11 0 0
928	BZo_RO2_O7 + C5DIALO2 -> BZoO6_C5DI	ARR 3.0E-13 0 0
929	BZo_RO2_O7 + NPHENO2 -> BZoO6_NPHa	ARR 6.67E-11 0 0
930	BZo_RO2_O7 + PHENO2 -> BZoO6_PHEN	ARR 2.79E-11 0 0
931	BZo_RO2_O7 + MALDIALCO3 -> BZoO6_MALa	ARR 3.0E-13 0 0
932	BZo_RO2_O7 + EPXDLCO3 -> BZoO6_EPX	ARR 3.0E-13 0 0
933	BZo_RO2_O7 + C3DIALO2 -> BZoO6_C3DI	ARR 3.0E-13 0 0

934	BZo_RO2_O7 + MALDIALO2 -> BZoO6_MALb	ARR 3.0E-13 0 0
935	BZo_RO2_O7 + C6H5O2 -> BZoO6_C6a	ARR 3.0E-13 0 0
936	BZo_RO2_O7 + NBZFUO2 -> BZoO6_NBZa	ARR 3.05E-11 0 0
937	BZo_RO2_O7 + BZFUO2 -> BZoO6_BZFU	ARR 3.0E-13 0 0
938	BZo_RO2_O7 + HCOCOHCO3 -> BZoO6_C3a	ARR 3.0E-13 0 0
939	BZo_RO2_O7 + CATEC1O2 -> BZoO6_CATE	ARR 3.0E-13 0 0
940	BZo_RO2_O7 + HCOCO3 -> BZoO6_C2a	ARR 3.0E-13 0 0
941	BZo_RO2_O7 + HCOCH2O2 -> BZoO6_C2b	ARR 3.0E-13 0 0
942	BZo_RO2_O7 + NPHEN1O2 -> BZoO6_NPHb	ARR 9.78E-12 0 0
943	BZo_RO2_O7 + NNCATECO2 -> BZoO6_NNC	ARR 1.0E-10 0 0
944	BZo_RO2_O7 + NCATECO2 -> BZoO6_NCAT	ARR 8.05E-11 0 0
945	BZo_RO2_O7 + NBZQO2 -> BZoO6_NBZb	ARR 5.12E-11 0 0
946	BZo_RO2_O7 + PBZQO2 -> BZoO6_PBZ	ARR 1.24E-11 0 0
947	BZo_RO2_O7 + MALANHYO2 -> BZoO6_MALc	ARR 3.75E-12 0 0
948	BZo_RO2_O7 + NDNPHENO2 -> BZoO6_NDN	ARR 1.0E-10 0 0
949	BZo_RO2_O7 + DNPHENO2 -> BZoO6_DNP	ARR 1.0E-10 0 0
950	BZo_RO2_O7 + HOCH2CO3 -> BZoO6_C2c	ARR 3.0E-13 0 0
951	BZo_RO2_O7 + C5CO2OHCO3 -> BZoO6_C5a	ARR 2.62E-11 0 0
952	BZo_RO2_O7 + C4CO2DBCO3 -> BZoO6_C4a	ARR 3.0E-13 0 0
953	BZo_RO2_O9 + BZo_RO2_O9 -> BZoO8_BZoO8	ARR 9.69E-11 0 0
954	BZo_RO2_O9 + BZo_RO2_O11 -> BZoO8_BZoO10	ARR 1.0E-10 0 0
955	BZo_RO2_O9 + BZeo_RO2_O6 -> BZoO8_BZeoO5	ARR 5.55E-11 0 0
956	BZo_RO2_O9 + BZeo_RO2_O8 -> BZoO8_BZeoO7	ARR 8.31E-11 0 0
957	BZo_RO2_O9 + BZeo_RO2_O10 -> BZoO8_BZeoO9	ARR 1.0E-10 0 0
958	BZo_RO2_O9 + C5_RO2_O6 -> BZoO8_C5eO5	ARR 7.27E-11 0 0
959	BZo_RO2_O9 + C5_RO2_O7 -> BZoO8_C5O6	ARR 8.65E-11 0 0
960	BZo_RO2_O9 + C5_RO2_O8 -> BZoO8_C5eO7	ARR 1.0E-10 0 0
961	BZo_RO2_O9 + C5_RO2_O9 -> BZoO8_C5O8	ARR 1.0E-10 0 0
962	BZo_RO2_O9 + C5_RO2_O10 -> BZoO8_C5eO9	ARR 1.0E-10 0 0
963	BZo_RO2_O9 + BZBIPERO2 -> BZoO8_BZBI	ARR 2.08E-11 0 0
964	BZo_RO2_O9 + BZEMUCCO3 -> BZoO8_BZMUa	ARR 4.0E-11 0 0
965	BZo_RO2_O9 + BZEMUCO2 -> BZoO8_BZMUb	ARR 5.55E-11 0 0
966	BZo_RO2_O9 + C5DIALO2 -> BZoO8_C5DI	ARR 1.58E-11 0 0
967	BZo_RO2_O9 + NPHENO2 -> BZoO8_NPHa	ARR 9.43E-11 0 0
968	BZo_RO2_O9 + PHENO2 -> BZoO8_PHEN	ARR 5.55E-11 0 0
969	BZo_RO2_O9 + MALDIALCO3 -> BZoO8_MALa	ARR 3.75E-12 0 0
970	BZo_RO2_O9 + EPXDLCO3 -> BZoO8_EPX	ARR 1.75E-11 0 0
971	BZo_RO2_O9 + C3DIALO2 -> BZoO8_C3DI	ARR 3.0E-13 0 0
972	BZo_RO2_O9 + MALDIALO2 -> BZoO8_MALb	ARR 1.93E-11 0 0
973	BZo_RO2_O9 + C6H5O2 -> BZoO8_C6a	ARR 3.0E-13 0 0
974	BZo_RO2_O9 + NBZFUO2 -> BZoO8_NBZa	ARR 5.81E-11 0 0
975	BZo_RO2_O9 + BZFUO2 -> BZoO8_BZFU	ARR 1.93E-11 0 0
976	BZo_RO2_O9 + HCOCOHCO3 -> BZoO8_C3a	ARR 7.2E-12 0 0
977	BZo_RO2_O9 + CATEC1O2 -> BZoO8_CATE	ARR 1.24E-11 0 0
978	BZo_RO2_O9 + HCOCO3 -> BZoO8_C2a	ARR 3.0E-13 0 0
979	BZo_RO2_O9 + HCOCH2O2 -> BZoO8_C2b	ARR 3.0E-13 0 0

980	BZo_RO2_O9 + NPHEN1O2 -> BZoO8_NPHb	ARR 3.74E-11 0 0
981	BZo_RO2_O9 + NNCATECO2 -> BZoO8_NNC	ARR 1.0E-10 0 0
982	BZo_RO2_O9 + NCATECO2 -> BZoO8_NCAT	ARR 1.0E-10 0 0
983	BZo_RO2_O9 + NBZQO2 -> BZoO8_NBZb	ARR 7.87E-11 0 0
984	BZo_RO2_O9 + PBZQO2 -> BZoO8_PBZ	ARR 4.0E-11 0 0
985	BZo_RO2_O9 + MALANHYO2 -> BZoO8_MALc	ARR 3.13E-11 0 0
986	BZo_RO2_O9 + NDNPHENO2 -> BZoO8_NDN	ARR 1.0E-10 0 0
987	BZo_RO2_O9 + DNPHENO2 -> BZoO8_DNP	ARR 1.0E-10 0 0
988	BZo_RO2_O9 + HOCH2CO3 -> BZoO8_C2c	ARR 3.0E-13 0 0
989	BZo_RO2_O9 + C5CO2OHCO3 -> BZoO8_C5a	ARR 5.37E-11 0 0
990	BZo_RO2_O9 + C4CO2DBCO3 -> BZoO8_C4a	ARR 2.79E-11 0 0
991	BZo_RO2_O11 + BZo_RO2_O11 -> BZoO10_BZoO10	ARR 1.0E-10 0 0
992	BZo_RO2_O11 + BZeo_RO2_O6 -> BZoO10_BZeoO5	ARR 8.31E-11 0 0
993	BZo_RO2_O11 + BZeo_RO2_O8 -> BZoO10_BZeoO7	ARR 1.0E-10 0 0
994	BZo_RO2_O11 + BZeo_RO2_O10 -> BZoO10_BZeoO9	ARR 1.0E-10 0 0
995	BZo_RO2_O11 + C5_RO2_O6 -> BZoO10_C5eO5	ARR 1.0E-10 0 0
996	BZo_RO2_O11 + C5_RO2_O7 -> BZoO10_C5O6	ARR 1.0E-10 0 0
997	BZo_RO2_O11 + C5_RO2_O8 -> BZoO10_C5eO7	ARR 1.0E-10 0 0
998	BZo_RO2_O11 + C5_RO2_O9 -> BZoO10_C5O8	ARR 1.0E-10 0 0
999	BZo_RO2_O11 + C5_RO2_O10 -> BZoO10_C5eO9	ARR 1.0E-10 0 0
1000	BZo_RO2_O11 + BZBIPERO2 -> BZoO10_BZBI	ARR 1.0E-10 0 0
1001	BZo_RO2_O11 + BZEMUCCO3 -> BZoO10_BZMUa	ARR 6.75E-11 0 0
1002	BZo_RO2_O11 + BZEMUCO2 -> BZoO10_BZMUb	ARR 8.31E-11 0 0
1003	BZo_RO2_O11 + C5DIALO2 -> BZoO10_C5DI	ARR 4.34E-11 0 0
1004	BZo_RO2_O11 + NPHENO2 -> BZoO10_NPHa	ARR 1.0E-10 0 0
1005	BZo_RO2_O11 + PHENO2 -> BZoO10_PHEN	ARR 8.31E-11 0 0
1006	BZo_RO2_O11 + MALDIALCO3 -> BZoO10_MALa	ARR 3.13E-11 0 0
1007	BZo_RO2_O11 + EPXDLCO3 -> BZoO10_EPX	ARR 4.51E-11 0 0
1008	BZo_RO2_O11 + C3DIALO2 -> BZoO10_C3DI	ARR 2.1E-11 0 0
1009	BZo_RO2_O11 + MALDIALO2 -> BZoO10_MALb	ARR 4.69E-11 0 0
1010	BZo_RO2_O11 + C6H5O2 -> BZoO10_C6a	ARR 2.62E-11 0 0
1011	BZo_RO2_O11 + NBZFUO2 -> BZoO10_NBZa	ARR 8.56E-11 0 0
1012	BZo_RO2_O11 + BZFUO2 -> BZoO10_BZFU	ARR 4.69E-11 0 0
1013	BZo_RO2_O11 + HCOCOHCO3 -> BZoO10_C3a	ARR 3.48E-11 0 0
1014	BZo_RO2_O11 + CATEC1O2 -> BZoO10_CATE	ARR 4.0E-11 0 0
1015	BZo_RO2_O11 + HCOCO3 -> BZoO10_C2a	ARR 8.92E-12 0 0
1016	BZo_RO2_O11 + HCOCH2O2 -> BZoO10_C2b	ARR 3.0E-13 0 0
1017	BZo_RO2_O11 + NPHEN1O2 -> BZoO10_NPHb	ARR 6.5E-11 0 0
1018	BZo_RO2_O11 + NNCATECO2 -> BZoO10_NNC	ARR 1.0E-10 0 0
1019	BZo_RO2_O11 + NCATECO2 -> BZoO10_NCAT	ARR 1.0E-10 0 0
1020	BZo_RO2_O11 + NBZQO2 -> BZoO10_NBZb	ARR 1.0E-10 0 0
1021	BZo_RO2_O11 + PBZQO2 -> BZoO10_PBZ	ARR 6.75E-11 0 0
1022	BZo_RO2_O11 + MALANHYO2 -> BZoO10_MALc	ARR 5.89E-11 0 0
1023	BZo_RO2_O11 + NDNPHENO2 -> BZoO10_NDN	ARR 1.0E-10 0 0
1024	BZo_RO2_O11 + DNPHENO2 -> BZoO10_DNP	ARR 1.0E-10 0 0
1025	BZo_RO2_O11 + HOCH2CO3 -> BZoO10_C2c	ARR 1.06E-11 0 0

1026	BZo_RO2_O11 + C5CO2OHCO3 -> BZoO10_C5a	ARR 8.13E-11 0 0
1027	BZo_RO2_O11 + C4CO2DBCO3 -> BZoO10_C4a	ARR 5.55E-11 0 0
1028	BZeo_RO2_O6 + BZeo_RO2_O6 -> BZeoO5_BZeoO5	ARR 1.41E-11 0 0
1029	BZeo_RO2_O6 + BZeo_RO2_O8 -> BZeoO5_BZeoO7	ARR 4.17E-11 0 0
1030	BZeo_RO2_O6 + BZeo_RO2_O10 -> BZeoO5_BZeoO9	ARR 1.0E-10 0 0
1031	BZeo_RO2_O6 + C5_RO2_O6 -> BZeoO5_C5eO5	ARR 3.13E-11 0 0
1032	BZeo_RO2_O6 + C5_RO2_O7 -> BZeoO5_C5O6	ARR 4.51E-11 0 0
1033	BZeo_RO2_O6 + C5_RO2_O8 -> BZeoO5_C5eO7	ARR 5.89E-11 0 0
1034	BZeo_RO2_O6 + C5_RO2_O9 -> BZeoO5_C5O8	ARR 7.27E-11 0 0
1035	BZeo_RO2_O6 + C5_RO2_O10 -> BZeoO5_C5eO9	ARR 8.65E-11 0 0
1036	BZeo_RO2_O6 + BZBIPERO2 -> BZeoO5_BZBI	ARR 3.0E-13 0 0
1037	BZeo_RO2_O6 + BZEMUCCO3 -> BZeoO5_BZMUa	ARR 3.0E-13 0 0
1038	BZeo_RO2_O6 + BZEMUCO2 -> BZeoO5_BZMUb	ARR 1.41E-11 0 0
1039	BZeo_RO2_O6 + C5DIALO2 -> BZeoO5_C5DI	ARR 3.0E-13 0 0
1040	BZeo_RO2_O6 + NPHENO2 -> BZeoO5_NPHa	ARR 5.29E-11 0 0
1041	BZeo_RO2_O6 + PHENO2 -> BZeoO5_PHEN	ARR 1.41E-11 0 0
1042	BZeo_RO2_O6 + MALDIALCO3 -> BZeoO5_MALa	ARR 3.0E-13 0 0
1043	BZeo_RO2_O6 + EPXDLCO3 -> BZeoO5_EPX	ARR 3.0E-13 0 0
1044	BZeo_RO2_O6 + C3DIALO2 -> BZeoO5_C3DI	ARR 3.0E-13 0 0
1045	BZeo_RO2_O6 + MALDIALO2 -> BZeoO5_MALb	ARR 3.0E-13 0 0
1046	BZeo_RO2_O6 + C6H5O2 -> BZeoO5_C6a	ARR 3.0E-13 0 0
1047	BZeo_RO2_O6 + NBZFUO2 -> BZeoO5_NBZa	ARR 1.67E-11 0 0
1048	BZeo_RO2_O6 + BZFUO2 -> BZeoO5_BZFU	ARR 3.0E-13 0 0
1049	BZeo_RO2_O6 + HCOCOHCO3 -> BZeoO5_C3a	ARR 3.0E-13 0 0
1050	BZeo_RO2_O6 + CATEC1O2 -> BZeoO5_CATE	ARR 3.0E-13 0 0
1051	BZeo_RO2_O6 + HCOCO3 -> BZeoO5_C2a	ARR 3.0E-13 0 0
1052	BZeo_RO2_O6 + HCOCH2O2 -> BZeoO5_C2b	ARR 3.0E-13 0 0
1053	BZeo_RO2_O6 + NPHEN1O2 -> BZeoO5_NPHb	ARR 3.0E-13 0 0
1054	BZeo_RO2_O6 + NNCATECO2 -> BZeoO5_NNC	ARR 1.0E-10 0 0
1055	BZeo_RO2_O6 + NCATECO2 -> BZeoO5_NCAT	ARR 6.67E-11 0 0
1056	BZeo_RO2_O6 + NBZQO2 -> BZeoO5_NBZb	ARR 3.74E-11 0 0
1057	BZeo_RO2_O6 + PBZQO2 -> BZeoO5_PBZ	ARR 3.0E-13 0 0
1058	BZeo_RO2_O6 + MALANHYO2 -> BZeoO5_MALc	ARR 3.0E-13 0 0
1059	BZeo_RO2_O6 + NDNPHENO2 -> BZeoO5_NDN	ARR 1.0E-10 0 0
1060	BZeo_RO2_O6 + DNPHENO2 -> BZeoO5_DNP	ARR 9.17E-11 0 0
1061	BZeo_RO2_O6 + HOCH2CO3 -> BZeoO5_C2c	ARR 3.0E-13 0 0
1062	BZeo_RO2_O6 + C5CO2OHCO3 -> BZeoO5_C5a	ARR 1.24E-11 0 0
1063	BZeo_RO2_O6 + C4CO2DBCO3 -> BZeoO5_C4a	ARR 3.0E-13 0 0
1064	BZeo_RO2_O8 + BZeo_RO2_O8 -> BZeoO7_BZeoO7	ARR 1.0E-10 0 0
1065	BZeo_RO2_O8 + BZeo_RO2_O10 -> BZeoO7_BZeoO9	ARR 9.69E-11 0 0
1066	BZeo_RO2_O8 + C5_RO2_O6 -> BZeoO7_C5eO5	ARR 5.89E-11 0 0
1067	BZeo_RO2_O8 + C5_RO2_O7 -> BZeoO7_C5O6	ARR 7.27E-11 0 0
1068	BZeo_RO2_O8 + C5_RO2_O8 -> BZeoO7_C5eO7	ARR 8.65E-11 0 0
1069	BZeo_RO2_O8 + C5_RO2_O9 -> BZeoO7_C5O8	ARR 1.0E-10 0 0
1070	BZeo_RO2_O8 + C5_RO2_O10 -> BZeoO7_C5eO9	ARR 1.0E-10 0 0
1071	BZeo_RO2_O8 + BZBIPERO2 -> BZeoO7_BZBI	ARR 0.84E-11 0 0

1072	BZeo_RO2_O8 + BZEMUCCO3 -> BZeoO7_BZMUa	ARR 2.62E-11 0 0
1073	BZeo_RO2_O8 + BZEMUCO2 -> BZeoO7_BZMUb	ARR 4.17E-11 0 0
1074	BZeo_RO2_O8 + C5DIALO2 -> BZeoO7_C5DI	ARR 2.02E-12 0 0
1075	BZeo_RO2_O8 + NPHENO2 -> BZeoO7_NPHa	ARR 8.05E-11 0 0
1076	BZeo_RO2_O8 + PHENO2 -> BZeoO7_PHEN	ARR 4.17E-11 0 0
1077	BZeo_RO2_O8 + MALDIALCO3 -> BZeoO7_MALa	ARR 3.0E-13 0 0
1078	BZeo_RO2_O8 + EPXDLCO3 -> BZeoO7_EPX	ARR 3.75E-12 0 0
1079	BZeo_RO2_O8 + C3DIALO2 -> BZeoO7_C3DI	ARR 3.0E-13 0 0
1080	BZeo_RO2_O8 + MALDIALO2 -> BZeoO7_MALb	ARR 5.47E-12 0 0
1081	BZeo_RO2_O8 + C6H5O2 -> BZeoO7_C6a	ARR 3.0E-13 0 0
1082	BZeo_RO2_O8 + NBZFUO2 -> BZeoO7_NBZa	ARR 4.43E-11 0 0
1083	BZeo_RO2_O8 + BZFUO2 -> BZeoO7_BZFU	ARR 5.47E-12 0 0
1084	BZeo_RO2_O8 + HCOCOHCO3 -> BZeoO7_C3a	ARR 3.0E-13 0 0
1085	BZeo_RO2_O8 + CATEC1O2 -> BZeoO7_CATE	ARR 3.0E-13 0 0
1086	BZeo_RO2_O8 + HCOCO3 -> BZeoO7_C2a	ARR 3.0E-13 0 0
1087	BZeo_RO2_O8 + HCOCH2O2 -> BZeoO7_C2b	ARR 3.0E-13 0 0
1088	BZeo_RO2_O8 + NPHEN1O2 -> BZeoO7_NPHb	ARR 2.36E-11 0 0
1089	BZeo_RO2_O8 + NNCATECO2 -> BZeoO7_NNC	ARR 1.0E-10 0 0
1090	BZeo_RO2_O8 + NCATECO2 -> BZeoO7_NCAT	ARR 9.43E-11 0 0
1091	BZeo_RO2_O8 + NBZQO2 -> BZeoO7_NBZb	ARR 6.5E-11 0 0
1092	BZeo_RO2_O8 + PBZQO2 -> BZeoO7_PBZ	ARR 2.62E-11 0 0
1093	BZeo_RO2_O8 + MALANHYO2 -> BZeoO7_MALc	ARR 1.75E-11 0 0
1094	BZeo_RO2_O8 + NDNPHENO2 -> BZeoO7_NDN	ARR 1.0E-10 0 0
1095	BZeo_RO2_O8 + DNPHENO2 -> BZeoO7_DNP	ARR 1.0E-10 0 0
1096	BZeo_RO2_O8 + HOCH2CO3 -> BZeoO7_C2c	ARR 3.0E-13 0 0
1097	BZeo_RO2_O8 + C5CO2OHCO3 -> BZeoO7_C5a	ARR 4.0E-11 0 0
1098	BZeo_RO2_O8 + C4CO2DBCO3 -> BZeoO7_C4a	ARR 1.41E-11 0 0
1099	BZeo_RO2_O10 + BZeo_RO2_O10 -> BZeoO9_BZeoO9	ARR 1.0E-10 0 0
1100	BZeo_RO2_O10 + C5_RO2_O6 -> BZeoO9_C5eO5	ARR 8.65E-11 0 0
1101	BZeo_RO2_O10 + C5_RO2_O7 -> BZeoO9_C5O6	ARR 1.0E-10 0 0
1102	BZeo_RO2_O10 + C5_RO2_O8 -> BZeoO9_C5eO7	ARR 1.0E-10 0 0
1103	BZeo_RO2_O10 + C5_RO2_O9 -> BZeoO9_C5O8	ARR 1.0E-10 0 0
1104	BZeo_RO2_O10 + C5_RO2_O10 -> BZeoO9_C5eO9	ARR 1.0E-10 0 0
1105	BZeo_RO2_O10 + BZBIPERO2 -> BZeoO9_BZBI	ARR 5.55E-11 0 0
1106	BZeo_RO2_O10 + BZEMUCCO3 -> BZeoO9_BZMUa	ARR 5.37E-11 0 0
1107	BZeo_RO2_O10 + BZEMUCO2 -> BZeoO9_BZMUb	ARR 1.0E-10 0 0
1108	BZeo_RO2_O10 + C5DIALO2 -> BZeoO9_C5DI	ARR 2.96E-11 0 0
1109	BZeo_RO2_O10 + NPHENO2 -> BZeoO9_NPHa	ARR 1.0E-10 0 0
1110	BZeo_RO2_O10 + PHENO2 -> BZeoO9_PHEN	ARR 1.0E-10 0 0
1111	BZeo_RO2_O10 + MALDIALCO3 -> BZeoO9_MALa	ARR 1.75E-11 0 0
1112	BZeo_RO2_O10 + EPXDLCO3 -> BZeoO9_EPX	ARR 3.13E-11 0 0
1113	BZeo_RO2_O10 + C3DIALO2 -> BZeoO9_C3DI	ARR 7.2E-12 0 0
1114	BZeo_RO2_O10 + MALDIALO2 -> BZeoO9_MALb	ARR 3.31E-11 0 0
1115	BZeo_RO2_O10 + C6H5O2 -> BZeoO9_C6a	ARR 1.24E-11 0 0
1116	BZeo_RO2_O10 + NBZFUO2 -> BZeoO9_NBZa	ARR 7.19E-11 0 0
1117	BZeo_RO2_O10 + BZFUO2 -> BZeoO9_BZFU	ARR 3.31E-11 0 0

1118	BZeo_RO2_O10 + HCOCOHCO3 -> BZeoO9_C3a	ARR 2.1E-11 0 0
1119	BZeo_RO2_O10 + CATEC1O2 -> BZeoO9_CATE	ARR 2.62E-11 0 0
1120	BZeo_RO2_O10 + HCOCO3 -> BZeoO9_C2a	ARR 3.0E-13 0 0
1121	BZeo_RO2_O10 + HCOCH2O2 -> BZeoO9_C2b	ARR 3.0E-13 0 0
1122	BZeo_RO2_O10 + NPHEN1O2 -> BZeoO9_NPHb	ARR 5.12E-11 0 0
1123	BZeo_RO2_O10 + NNCATECO2 -> BZeoO9_NNC	ARR 1.0E-10 0 0
1124	BZeo_RO2_O10 + NCATECO2 -> BZeoO9_NCAT	ARR 1.0E-10 0 0
1125	BZeo_RO2_O10 + NBZQO2 -> BZeoO9_NBZb	ARR 9.25E-11 0 0
1126	BZeo_RO2_O10 + PBZQO2 -> BZeoO9_PBZ	ARR 5.37E-11 0 0
1127	BZeo_RO2_O10 + MALANHYO2 -> BZeoO9_MALc	ARR 4.51E-11 0 0
1128	BZeo_RO2_O10 + NDNPHENO2 -> BZeoO9_NDN	ARR 1.0E-10 0 0
1129	BZeo_RO2_O10 + DNPHENO2 -> BZeoO9_DNP	ARR 1.0E-10 0 0
1130	BZeo_RO2_O10 + HOCH2CO3 -> BZeoO9_C2c	ARR 3.0E-13 0 0
1131	BZeo_RO2_O10 + C5CO2OHCO3 -> BZeoO9_C5a	ARR 6.75E-11 0 0
1132	BZeo_RO2_O10 + C4CO2DBCO3 -> BZeoO9_C4a	ARR 4.17E-11 0 0
1133	C5_RO2_O6 + C5_RO2_O6 -> C5eO5_C5eO5	ARR 4.86E-11 0 0
1134	C5_RO2_O6 + C5_RO2_O7 -> C5eO5_C5O6	ARR 6.24E-11 0 0
1135	C5_RO2_O6 + C5_RO2_O8 -> C5eO5_C5eO7	ARR 7.62E-11 0 0
1136	C5_RO2_O6 + C5_RO2_O9 -> C5eO5_C5O8	ARR 9.0E-11 0 0
1137	C5_RO2_O6 + C5_RO2_O10 -> C5eO5_C5eO9	ARR 1.0E-10 0 0
1138	C5_RO2_O6 + BZBIPERO2 -> C5eO5_BZBI	ARR 1.75E-11 0 0
1139	C5_RO2_O6 + BZEMUCCO3 -> C5eO5_BZMUa	ARR 1.58E-11 0 0
1140	C5_RO2_O6 + BZEMUCO2 -> C5eO5_BZMUb	ARR 3.13E-11 0 0
1141	C5_RO2_O6 + C5DIALO2 -> C5eO5_C5DI	ARR 3.0E-13 0 0
1142	C5_RO2_O6 + NPHENO2 -> C5eO5_NPHa	ARR 7.01E-11 0 0
1143	C5_RO2_O6 + PHENO2 -> C5eO5_PHEN	ARR 3.13E-11 0 0
1144	C5_RO2_O6 + MALDIALCO3 -> C5eO5_MALa	ARR 3.0E-13 0 0
1145	C5_RO2_O6 + EPXDLCO3 -> C5eO5_EPX	ARR 3.0E-13 0 0
1146	C5_RO2_O6 + C3DIALO2 -> C5eO5_C3DI	ARR 3.0E-13 0 0
1147	C5_RO2_O6 + MALDIALO2 -> C5eO5_MALb	ARR 3.0E-13 0 0
1148	C5_RO2_O6 + C6H5O2 -> C5eO5_C6a	ARR 3.0E-13 0 0
1149	C5_RO2_O6 + NBZFUO2 -> C5eO5_NBZa	ARR 3.39E-11 0 0
1150	C5_RO2_O6 + BZFUO2 -> C5eO5_BZFU	ARR 3.0E-13 0 0
1151	C5_RO2_O6 + HCOCOHCO3 -> C5eO5_C3a	ARR 3.0E-13 0 0
1152	C5_RO2_O6 + CATEC1O2 -> C5eO5_CATE	ARR 3.0E-13 0 0
1153	C5_RO2_O6 + HCOCO3 -> C5eO5_C2a	ARR 3.0E-13 0 0
1154	C5_RO2_O6 + HCOCH2O2 -> C5eO5_C2b	ARR 3.0E-13 0 0
1155	C5_RO2_O6 + NPHEN1O2 -> C5eO5_NPHb	ARR 1.32E-11 0 0
1156	C5_RO2_O6 + NNCATECO2 -> C5eO5_NNC	ARR 1.0E-10 0 0
1157	C5_RO2_O6 + NCATECO2 -> C5eO5_NCAT	ARR 8.39E-11 0 0
1158	C5_RO2_O6 + NBZQO2 -> C5eO5_NBZb	ARR 5.46E-11 0 0
1159	C5_RO2_O6 + PBZQO2 -> C5eO5_PBZ	ARR 1.58E-11 0 0
1160	C5_RO2_O6 + MALANHYO2 -> C5eO5_MALc	ARR 7.2E-12 0 0
1161	C5_RO2_O6 + NDNPHENO2 -> C5eO5_NDN	ARR 1.0E-10 0 0
1162	C5_RO2_O6 + DNPHENO2 -> C5eO5_DNP	ARR 1.0E-10 0 0
1163	C5_RO2_O6 + HOCH2CO3 -> C5eO5_C2c	ARR 3.0E-13 0 0

1164	C5_RO2_O6 + C5CO2OHCO3 -> C5eO5_C5a	ARR 2.96E-11 0 0
1165	C5_RO2_O6 + C4CO2DBCO3 -> C5eO5_C4a	ARR 3.75E-12 0 0
1166	C5_RO2_O7 + C5_RO2_O7 -> C5O6_C5O6	ARR 7.62E-11 0 0
1167	C5_RO2_O7 + C5_RO2_O8 -> C5O6_C5eO7	ARR 9.0E-11 0 0
1168	C5_RO2_O7 + C5_RO2_O9 -> C5O6_C5O8	ARR 1.0E-10 0 0
1169	C5_RO2_O7 + C5_RO2_O10 -> C5O6_C5eO9	ARR 1.0E-10 0 0
1170	C5_RO2_O7 + BZBIPERO2 -> C5O6_BZBI	ARR 3.13E-11 0 0
1171	C5_RO2_O7 + BZEMUCCO3 -> C5O6_BZMUa	ARR 2.96E-11 0 0
1172	C5_RO2_O7 + BZEMUCO2 -> C5O6_BZMUb	ARR 4.51E-11 0 0
1173	C5_RO2_O7 + C5DIALO2 -> C5O6_C5DI	ARR 5.47E-12 0 0
1174	C5_RO2_O7 + NPHENO2 -> C5O6_NPHa	ARR 8.39E-11 0 0
1175	C5_RO2_O7 + PHENO2 -> C5O6_PHEN	ARR 4.51E-11 0 0
1176	C5_RO2_O7 + MALDIALCO3 -> C5O6_MALa	ARR 3.0E-13 0 0
1177	C5_RO2_O7 + EPXDLCO3 -> C5O6_EPX	ARR 7.2E-12 0 0
1178	C5_RO2_O7 + C3DIALO2 -> C5O6_C3DI	ARR 3.0E-13 0 0
1179	C5_RO2_O7 + MALDIALO2 -> C5O6_MALb	ARR 8.92E-12 0 0
1180	C5_RO2_O7 + C6H5O2 -> C5O6_C6a	ARR 3.0E-13 0 0
1181	C5_RO2_O7 + NBZFUO2 -> C5O6_NBZa	ARR 4.77E-11 0 0
1182	C5_RO2_O7 + BZFUO2 -> C5O6_BZFU	ARR 8.92E-12 0 0
1183	C5_RO2_O7 + HCOCOHCO3 -> C5O6_C3a	ARR 3.0E-13 0 0
1184	C5_RO2_O7 + CATEC1O2 -> C5O6_CATE	ARR 2.02E-12 0 0
1185	C5_RO2_O7 + HCOCO3 -> C5O6_C2a	ARR 3.0E-13 0 0
1186	C5_RO2_O7 + HCOCH2O2 -> C5O6_C2b	ARR 3.0E-13 0 0
1187	C5_RO2_O7 + NPHEN1O2 -> C5O6_NPHb	ARR 2.7E-11 0 0
1188	C5_RO2_O7 + NNCATECO2 -> C5O6_NNC	ARR 1.0E-10 0 0
1189	C5_RO2_O7 + NCATECO2 -> C5O6_NCAT	ARR 9.77E-11 0 0
1190	C5_RO2_O7 + NBZQO2 -> C5O6_NBZb	ARR 6.84E-11 0 0
1191	C5_RO2_O7 + PBZQO2 -> C5O6_PBZ	ARR 2.96E-11 0 0
1192	C5_RO2_O7 + MALANHYO2 -> C5O6_MALc	ARR 2.1E-11 0 0
1193	C5_RO2_O7 + NDNPHENO2 -> C5O6_NDN	ARR 1.0E-10 0 0
1194	C5_RO2_O7 + DNPHENO2 -> C5O6_DNP	ARR 1.0E-10 0 0
1195	C5_RO2_O7 + HOCH2CO3 -> C5O6_C2c	ARR 3.0E-13 0 0
1196	C5_RO2_O7 + C5CO2OHCO3 -> C5O6_C5a	ARR 4.34E-11 0 0
1197	C5_RO2_O7 + C4CO2DBCO3 -> C5O6_C4a	ARR 1.75E-11 0 0
1198	C5_RO2_O8 + C5_RO2_O8 -> C5eO7_C5eO7	ARR 1.0E-10 0 0
1199	C5_RO2_O8 + C5_RO2_O9 -> C5eO7_C5O8	ARR 1.0E-10 0 0
1200	C5_RO2_O8 + C5_RO2_O10 -> C5eO7_C5eO9	ARR 1.0E-10 0 0
1201	C5_RO2_O8 + BZBIPERO2 -> C5eO7_BZBI	ARR 1.35E-11 0 0
1202	C5_RO2_O8 + BZEMUCCO3 -> C5eO7_BZMUa	ARR 4.34E-11 0 0
1203	C5_RO2_O8 + BZEMUCO2 -> C5eO7_BZMUb	ARR 5.89E-11 0 0
1204	C5_RO2_O8 + C5DIALO2 -> C5eO7_C5DI	ARR 1.93E-11 0 0
1205	C5_RO2_O8 + NPHENO2 -> C5eO7_NPHa	ARR 9.77E-11 0 0
1206	C5_RO2_O8 + PHENO2 -> C5eO7_PHEN	ARR 5.89E-11 0 0
1207	C5_RO2_O8 + MALDIALCO3 -> C5eO7_MALa	ARR 7.2E-12 0 0
1208	C5_RO2_O8 + EPXDLCO3 -> C5eO7_EPX	ARR 2.1E-11 0 0
1209	C5_RO2_O8 + C3DIALO2 -> C5eO7_C3DI	ARR 3.0E-13 0 0

1210	C5_RO2_O8 + MALDIALO2 -> C5eO7_MALb	ARR 2.27E-11 0 0
1211	C5_RO2_O8 + C6H5O2 -> C5eO7_C6a	ARR 2.02E-12 0 0
1212	C5_RO2_O8 + NBZFUO2 -> C5eO7_NBZa	ARR 6.15E-11 0 0
1213	C5_RO2_O8 + BZFUO2 -> C5eO7_BZFU	ARR 2.27E-11 0 0
1214	C5_RO2_O8 + HCOCOHCO3 -> C5eO7_C3a	ARR 1.06E-11 0 0
1215	C5_RO2_O8 + CATEC1O2 -> C5eO7_CATE	ARR 1.58E-11 0 0
1216	C5_RO2_O8 + HCOCO3 -> C5eO7_C2a	ARR 3.0E-13 0 0
1217	C5_RO2_O8 + HCOCH2O2 -> C5eO7_C2b	ARR 3.0E-13 0 0
1218	C5_RO2_O8 + NPHEN1O2 -> C5eO7_NPHb	ARR 4.08E-11 0 0
1219	C5_RO2_O8 + NNCATECO2 -> C5eO7_NNC	ARR 1.0E-10 0 0
1220	C5_RO2_O8 + NCATECO2 -> C5eO7_NCAT	ARR 1.0E-10 0 0
1221	C5_RO2_O8 + NBZQO2 -> C5eO7_NBZb	ARR 8.22E-11 0 0
1222	C5_RO2_O8 + PBZQO2 -> C5eO7_PBZ	ARR 4.34E-11 0 0
1223	C5_RO2_O8 + MALANHYO2 -> C5eO7_MALc	ARR 3.48E-11 0 0
1224	C5_RO2_O8 + NDNPHENO2 -> C5eO7_NDN	ARR 1.0E-10 0 0
1225	C5_RO2_O8 + DNPHENO2 -> C5eO7_DNP	ARR 1.0E-10 0 0
1226	C5_RO2_O8 + HOCH2CO3 -> C5eO7_C2c	ARR 3.0E-13 0 0
1227	C5_RO2_O8 + C5CO2OHCO3 -> C5eO7_C5a	ARR 5.72E-11 0 0
1228	C5_RO2_O8 + C4CO2DBCO3 -> C5eO7_C4a	ARR 3.13E-11 0 0
1229	C5_RO2_O9 + C5_RO2_O9 -> C5O8_C5O8	ARR 1.0E-10 0 0
1230	C5_RO2_O9 + C5_RO2_O10 -> C5O8_C5eO9	ARR 1.0E-10 0 0
1231	C5_RO2_O9 + BZBIPERO2 -> C5O8_BZBI	ARR 5.89E-11 0 0
1232	C5_RO2_O9 + BZEMUCCO3 -> C5O8_BZMUa	ARR 5.72E-11 0 0
1233	C5_RO2_O9 + BZEMUCO2 -> C5O8_BZMUb	ARR 7.27E-11 0 0
1234	C5_RO2_O9 + C5DIALO2 -> C5O8_C5DI	ARR 3.31E-11 0 0
1235	C5_RO2_O9 + NPHENO2 -> C5O8_NPHa	ARR 1.0E-10 0 0
1236	C5_RO2_O9 + PHENO2 -> C5O8_PHEN	ARR 7.27E-11 0 0
1237	C5_RO2_O9 + MALDIALCO3 -> C5O8_MALa	ARR 2.1E-11 0 0
1238	C5_RO2_O9 + EPXDLCO3 -> C5O8_EPX	ARR 3.48E-11 0 0
1239	C5_RO2_O9 + C3DIALO2 -> C5O8_C3DI	ARR 1.06E-11 0 0
1240	C5_RO2_O9 + MALDIALO2 -> C5O8_MALb	ARR 3.65E-11 0 0
1241	C5_RO2_O9 + C6H5O2 -> C5O8_C6a	ARR 1.58E-11 0 0
1242	C5_RO2_O9 + NBZFUO2 -> C5O8_NBZa	ARR 7.53E-11 0 0
1243	C5_RO2_O9 + BZFUO2 -> C5O8_BZFU	ARR 3.65E-11 0 0
1244	C5_RO2_O9 + HCOCOHCO3 -> C5O8_C3a	ARR 2.44E-11 0 0
1245	C5_RO2_O9 + CATEC1O2 -> C5O8_CATE	ARR 2.96E-11 0 0
1246	C5_RO2_O9 + HCOCO3 -> C5O8_C2a	ARR 3.0E-13 0 0
1247	C5_RO2_O9 + HCOCH2O2 -> C5O8_C2b	ARR 3.0E-13 0 0
1248	C5_RO2_O9 + NPHEN1O2 -> C5O8_NPHb	ARR 5.46E-11 0 0
1249	C5_RO2_O9 + NNCATECO2 -> C5O8_NNC	ARR 1.0E-10 0 0
1250	C5_RO2_O9 + NCATECO2 -> C5O8_NCAT	ARR 1.0E-10 0 0
1251	C5_RO2_O9 + NBZQO2 -> C5O8_NBZb	ARR 9.6E-11 0 0
1252	C5_RO2_O9 + PBZQO2 -> C5O8_PBZ	ARR 5.72E-11 0 0
1253	C5_RO2_O9 + MALANHYO2 -> C5O8_MALc	ARR 4.86E-11 0 0
1254	C5_RO2_O9 + NDNPHENO2 -> C5O8_NDN	ARR 1.0E-10 0 0
1255	C5_RO2_O9 + DNPHENO2 -> C5O8_DNP	ARR 1.0E-10 0 0

1256	C5_RO2_O9 + HOCH2CO3 -> C5O8_C2c	ARR 3.0E-13 0 0
1257	C5_RO2_O9 + C5CO2OHCO3 -> C5O8_C5a	ARR 7.1E-11 0 0
1258	C5_RO2_O9 + C4CO2DBCO3 -> C5O8_C4a	ARR 4.51E-11 0 0
1259	C5_RO2_O10 + C5_RO2_O10 -> C5eO9_C5eO9	ARR 1.0E-10 0 0
1260	C5_RO2_O10 + BZBIPERO2 -> C5eO9_BZBI	ARR 7.27E-11 0 0
1261	C5_RO2_O10 + BZEMUCCO3 -> C5eO9_BZMUa	ARR 7.1E-11 0 0
1262	C5_RO2_O10 + BZEMUCO2 -> C5eO9_BZMUb	ARR 8.65E-11 0 0
1263	C5_RO2_O10 + C5DIALO2 -> C5eO9_C5DI	ARR 4.69E-11 0 0
1264	C5_RO2_O10 + NPHENO2 -> C5eO9_NPHa	ARR 1.0E-10 0 0
1265	C5_RO2_O10 + PHENO2 -> C5eO9_PHEN	ARR 8.65E-11 0 0
1266	C5_RO2_O10 + MALDIALCO3 -> C5eO9_MALa	ARR 3.48E-11 0 0
1267	C5_RO2_O10 + EPXDLCO3 -> C5eO9_EPX	ARR 4.86E-11 0 0
1268	C5_RO2_O10 + C3DIALO2 -> C5eO9_C3DI	ARR 2.44E-11 0 0
1269	C5_RO2_O10 + MALDIALO2 -> C5eO9_MALb	ARR 5.03E-11 0 0
1270	C5_RO2_O10 + C6H5O2 -> C5eO9_C6a	ARR 2.96E-11 0 0
1271	C5_RO2_O10 + NBZFUO2 -> C5eO9_NBZa	ARR 8.91E-11 0 0
1272	C5_RO2_O10 + BZFUO2 -> C5eO9_BZFU	ARR 5.03E-11 0 0
1273	C5_RO2_O10 + HCOCOHCO3 -> C5eO9_C3a	ARR 3.82E-11 0 0
1274	C5_RO2_O10 + CATEC1O2 -> C5eO9_CATE	ARR 4.34E-11 0 0
1275	C5_RO2_O10 + HCOCO3 -> C5eO9_C2a	ARR 1.24E-11 0 0
1276	C5_RO2_O10 + HCOCH2O2 -> C5eO9_C2b	ARR 3.0E-13 0 0
1277	C5_RO2_O10 + NPHEN1O2 -> C5eO9_NPHb	ARR 6.84E-11 0 0
1278	C5_RO2_O10 + NNCATECO2 -> C5eO9_NNC	ARR 1.0E-10 0 0
1279	C5_RO2_O10 + NCATECO2 -> C5eO9_NCAT	ARR 1.0E-10 0 0
1280	C5_RO2_O10 + NBZQO2 -> C5eO9_NBZb	ARR 1.0E-10 0 0
1281	C5_RO2_O10 + PBZQO2 -> C5eO9_PBZ	ARR 7.1E-11 0 0
1282	C5_RO2_O10 + MALANHYO2 -> C5eO9_MALc	ARR 6.24E-11 0 0
1283	C5_RO2_O10 + NDNPHENO2 -> C5eO9_NDN	ARR 1.0E-10 0 0
1284	C5_RO2_O10 + DNPHENO2 -> C5eO9_DNP	ARR 1.0E-10 0 0
1285	C5_RO2_O10 + HOCH2CO3 -> C5eO9_C2c	ARR 1.41E-11 0 0
1286	C5_RO2_O10 + C5CO2OHCO3 -> C5eO9_C5a	ARR 8.48E-11 0 0
1287	C5_RO2_O10 + C4CO2DBCO3 -> C5eO9_C4a	ARR 5.89E-11 0 0
1288	BZBIPERO2 + BZBIPERO2 -> BZBI_BZBI	ARR 2.1E-13 0 0
1289	BZBIPERO2 + BZEMUCCO3 -> BZBI_BZMUa	ARR 3.0E-13 0 0
1290	BZBIPERO2 + BZEMUCO2 -> BZBI_BZMUb	ARR 3.0E-13 0 0
1291	BZBIPERO2 + C5DIALO2 -> BZBI_C5DI	ARR 3.0E-13 0 0
1292	BZBIPERO2 + NPHENO2 -> BZBI_NPHa	ARR 3.91E-11 0 0
1293	BZBIPERO2 + PHENO2 -> BZBI_PHEN	ARR 3.0E-13 0 0
1294	BZBIPERO2 + MALDIALCO3 -> BZBI_MALa	ARR 3.0E-13 0 0
1295	BZBIPERO2 + EPXDLCO3 -> BZBI_EPX	ARR 3.0E-13 0 0
1296	BZBIPERO2 + C3DIALO2 -> BZBI_C3DI	ARR 3.0E-13 0 0
1297	BZBIPERO2 + MALDIALO2 -> BZBI_MALb	ARR 3.0E-13 0 0
1298	BZBIPERO2 + C6H5O2 -> BZBI_C6a	ARR 3.0E-13 0 0
1299	BZBIPERO2 + NBZFUO2 -> BZBI_NBZa	ARR 2.89E-12 0 0
1300	BZBIPERO2 + BZFUO2 -> BZBI_BZFU	ARR 3.0E-13 0 0
1301	BZBIPERO2 + HCOCOHCO3 -> BZBI_C3a	ARR 3.0E-13 0 0

1302	BZBIPERO2 + CATEC1O2 -> BZBI_CATE	ARR 3.0E-13 0 0
1303	BZBIPERO2 + HCOCO3 -> BZBI_C2a	ARR 3.0E-13 0 0
1304	BZBIPERO2 + HCOCH2O2 -> BZBI_C2b	ARR 3.0E-13 0 0
1305	BZBIPERO2 + NPHEN1O2 -> BZBI_NPHb	ARR 3.0E-13 0 0
1306	BZBIPERO2 + NNCATECO2 -> BZBI_NNC	ARR 9.17E-11 0 0
1307	BZBIPERO2 + NCATECO2 -> BZBI_NCAT	ARR 5.29E-11 0 0
1308	BZBIPERO2 + NBZQO2 -> BZBI_NBZb	ARR 2.36E-11 0 0
1309	BZBIPERO2 + PBZQO2 -> BZBI_PBZ	ARR 3.0E-13 0 0
1310	BZBIPERO2 + MALANHYO2 -> BZBI_MALc	ARR 3.0E-13 0 0
1311	BZBIPERO2 + NDNPHENO2 -> BZBI_NDN	ARR 1.0E-10 0 0
1312	BZBIPERO2 + DNPHENO2 -> BZBI_DNP	ARR 7.79E-11 0 0
1313	BZBIPERO2 + HOCH2CO3 -> BZBI_C2c	ARR 3.0E-13 0 0
1314	BZBIPERO2 + C5CO2OHCO3 -> BZBI_C5a	ARR 3.0E-13 0 0
1315	BZBIPERO2 + C4CO2DBCO3 -> BZBI_C4a	ARR 3.0E-13 0 0
1316	BZEMUCCO3 + BZEMUCCO3 -> BZMUa_BZMUa	ARR 3.0E-13 0 0
1317	BZEMUCCO3 + BZEMUCO2 -> BZMUa_BZMUb	ARR 3.0E-13 0 0
1318	BZEMUCCO3 + C5DIALO2 -> BZMUa_C5DI	ARR 3.0E-13 0 0
1319	BZEMUCCO3 + NPHENO2 -> BZMUa_NPHa	ARR 3.74E-11 0 0
1320	BZEMUCCO3 + PHENO2 -> BZMUa_PHEN	ARR 3.0E-13 0 0
1321	BZEMUCCO3 + MALDIALCO3 -> BZMUa_MALa	ARR 3.0E-13 0 0
1322	BZEMUCCO3 + EPXDLCO3 -> BZMUa_EPX	ARR 3.0E-13 0 0
1323	BZEMUCCO3 + C3DIALO2 -> BZMUa_C3DI	ARR 3.0E-13 0 0
1324	BZEMUCCO3 + MALDIALO2 -> BZMUa_MALb	ARR 3.0E-13 0 0
1325	BZEMUCCO3 + C6H5O2 -> BZMUa_C6a	ARR 3.0E-13 0 0
1326	BZEMUCCO3 + NBZFUO2 -> BZMUa_NBZa	ARR 1.16E-12 0 0
1327	BZEMUCCO3 + BZFUO2 -> BZMUa_BZFU	ARR 3.0E-13 0 0
1328	BZEMUCCO3 + HCOCOHCO3 -> BZMUa_C3a	ARR 3.0E-13 0 0
1329	BZEMUCCO3 + CATEC1O2 -> BZMUa_CATE	ARR 3.0E-13 0 0
1330	BZEMUCCO3 + HCOCO3 -> BZMUa_C2a	ARR 3.0E-13 0 0
1331	BZEMUCCO3 + HCOCH2O2 -> BZMUa_C2b	ARR 3.0E-13 0 0
1332	BZEMUCCO3 + NPHEN1O2 -> BZMUa_NPHb	ARR 3.0E-13 0 0
1333	BZEMUCCO3 + NNCATECO2 -> BZMUa_NNC	ARR 9.0E-11 0 0
1334	BZEMUCCO3 + NCATECO2 -> BZMUa_NCAT	ARR 5.12E-11 0 0
1335	BZEMUCCO3 + NBZQO2 -> BZMUa_NBZb	ARR 2.19E-11 0 0
1336	BZEMUCCO3 + PBZQO2 -> BZMUa_PBZ	ARR 3.0E-13 0 0
1337	BZEMUCCO3 + MALANHYO2 -> BZMUa_MALc	ARR 3.0E-13 0 0
1338	BZEMUCCO3 + NDNPHENO2 -> BZMUa_NDN	ARR 1.0E-10 0 0
1339	BZEMUCCO3 + DNPHENO2 -> BZMUa_DNP	ARR 7.62E-11 0 0
1340	BZEMUCCO3 + HOCH2CO3 -> BZMUa_C2c	ARR 3.0E-13 0 0
1341	BZEMUCCO3 + C5CO2OHCO3 -> BZMUa_C5a	ARR 3.0E-13 0 0
1342	BZEMUCCO3 + C4CO2DBCO3 -> BZMUa_C4a	ARR 3.0E-13 0 0
1343	BZEMUCO2 + BZEMUCO2 -> BZMUb_BZMUb	ARR 1.41E-11 0 0
1344	BZEMUCO2 + C5DIALO2 -> BZMUb_C5DI	ARR 3.0E-13 0 0
1345	BZEMUCO2 + NPHENO2 -> BZMUb_NPHa	ARR 5.29E-11 0 0
1346	BZEMUCO2 + PHENO2 -> BZMUb_PHEN	ARR 1.41E-11 0 0
1347	BZEMUCO2 + MALDIALCO3 -> BZMUb_MALa	ARR 3.0E-13 0 0

1348	BZEMUCO2 + EPXDLCO3 -> BZMUb_EPX	ARR 3.0E-13 0 0
1349	BZEMUCO2 + C3DIALO2 -> BZMUb_C3DI	ARR 3.0E-13 0 0
1350	BZEMUCO2 + MALDIALO2 -> BZMUb_MALb	ARR 3.0E-13 0 0
1351	BZEMUCO2 + C6H5O2 -> BZMUb_C6a	ARR 3.0E-13 0 0
1352	BZEMUCO2 + NBZFUO2 -> BZMUb_NBZa	ARR 1.67E-11 0 0
1353	BZEMUCO2 + BZFUO2 -> BZMUb_BZFU	ARR 3.0E-13 0 0
1354	BZEMUCO2 + HCOCOHCO3 -> BZMUb_C3a	ARR 3.0E-13 0 0
1355	BZEMUCO2 + CATEC1O2 -> BZMUb_CATE	ARR 3.0E-13 0 0
1356	BZEMUCO2 + HCOCO3 -> BZMUb_C2a	ARR 3.0E-13 0 0
1357	BZEMUCO2 + HCOCH2O2 -> BZMUb_C2b	ARR 3.0E-13 0 0
1358	BZEMUCO2 + NPHEN1O2 -> BZMUb_NPHb	ARR 3.0E-13 0 0
1359	BZEMUCO2 + NNCATECO2 -> BZMUb_NNC	ARR 1.0E-10 0 0
1360	BZEMUCO2 + NCATECO2 -> BZMUb_NCAT	ARR 6.67E-11 0 0
1361	BZEMUCO2 + NBZQO2 -> BZMUb_NBZb	ARR 3.74E-11 0 0
1362	BZEMUCO2 + PBZQO2 -> BZMUb_PBZ	ARR 3.0E-13 0 0
1363	BZEMUCO2 + MALANHYO2 -> BZMUb_MALc	ARR 3.0E-13 0 0
1364	BZEMUCO2 + NDNPHENO2 -> BZMUb_NDN	ARR 1.0E-10 0 0
1365	BZEMUCO2 + DNPHENO2 -> BZMUb_DNP	ARR 9.17E-11 0 0
1366	BZEMUCO2 + HOCH2CO3 -> BZMUb_C2c	ARR 3.0E-13 0 0
1367	BZEMUCO2 + C5CO2OHCO3 -> BZMUb_C5a	ARR 1.24E-11 0 0
1368	BZEMUCO2 + C4CO2DBCO3 -> BZMUb_C4a	ARR 3.0E-13 0 0
1369	C5DIALO2 + C5DIALO2 -> C5DI_C5DI	ARR 3.0E-13 0 0
1370	C5DIALO2 + NPHENO2 -> C5DI_NPHa	ARR 1.32E-11 0 0
1371	C5DIALO2 + PHENO2 -> C5DI_PHEN	ARR 3.0E-13 0 0
1372	C5DIALO2 + MALDIALCO3 -> C5DI_MALa	ARR 3.0E-13 0 0
1373	C5DIALO2 + EPXDLCO3 -> C5DI_EPX	ARR 3.0E-13 0 0
1374	C5DIALO2 + C3DIALO2 -> C5DI_C3DI	ARR 3.0E-13 0 0
1375	C5DIALO2 + MALDIALO2 -> C5DI_MALb	ARR 3.0E-13 0 0
1376	C5DIALO2 + C6H5O2 -> C5DI_C6a	ARR 3.0E-13 0 0
1377	C5DIALO2 + NBZFUO2 -> C5DI_NBZa	ARR 3.0E-13 0 0
1378	C5DIALO2 + BZFUO2 -> C5DI_BZFU	ARR 3.0E-13 0 0
1379	C5DIALO2 + HCOCOHCO3 -> C5DI_C3a	ARR 3.0E-13 0 0
1380	C5DIALO2 + CATEC1O2 -> C5DI_CATE	ARR 3.0E-13 0 0
1381	C5DIALO2 + HCOCO3 -> C5DI_C2a	ARR 3.0E-13 0 0
1382	C5DIALO2 + HCOCH2O2 -> C5DI_C2b	ARR 3.0E-13 0 0
1383	C5DIALO2 + NPHEN1O2 -> C5DI_NPHb	ARR 3.0E-13 0 0
1384	C5DIALO2 + NNCATECO2 -> C5DI_NNC	ARR 6.58E-11 0 0
1385	C5DIALO2 + NCATECO2 -> C5DI_NCAT	ARR 2.7E-11 0 0
1386	C5DIALO2 + NBZQO2 -> C5DI_NBZb	ARR 3.0E-13 0 0
1387	C5DIALO2 + PBZQO2 -> C5DI_PBZ	ARR 3.0E-13 0 0
1388	C5DIALO2 + MALANHYO2 -> C5DI_MALc	ARR 3.0E-13 0 0
1389	C5DIALO2 + NDNPHENO2 -> C5DI_NDN	ARR 9.08E-11 0 0
1390	C5DIALO2 + DNPHENO2 -> C5DI_DNP	ARR 5.2E-11 0 0
1391	C5DIALO2 + HOCH2CO3 -> C5DI_C2c	ARR 3.0E-13 0 0
1392	C5DIALO2 + C5CO2OHCO3 -> C5DI_C5a	ARR 3.0E-13 0 0
1393	C5DIALO2 + C4CO2DBCO3 -> C5DI_C4a	ARR 3.0E-13 0 0

1394	NPHENO2 + NPHENO2 -> NPHa_NPHa	ARR 9.17E-11 0 0
1395	NPHENO2 + PHENO2 -> NPHa_PHEN	ARR 5.29E-11 0 0
1396	NPHENO2 + MALDIALCO3 -> NPHa_MALa	ARR 1.16E-12 0 0
1397	NPHENO2 + EPXDLCO3 -> NPHa_EPX	ARR 1.5E-11 0 0
1398	NPHENO2 + C3DIALO2 -> NPHa_C3DI	ARR 3.0E-13 0 0
1399	NPHENO2 + MALDIALO2 -> NPHa_MALb	ARR 1.67E-11 0 0
1400	NPHENO2 + C6H5O2 -> NPHa_C6a	ARR 3.0E-13 0 0
1401	NPHENO2 + NBZFUO2 -> NPHa_NBZa	ARR 5.55E-11 0 0
1402	NPHENO2 + BZFUO2 -> NPHa_BZFU	ARR 1.67E-11 0 0
1403	NPHENO2 + HCOCOHCO3 -> NPHa_C3a	ARR 4.61E-12 0 0
1404	NPHENO2 + CATEC1O2 -> NPHa_CATE	ARR 9.78E-12 0 0
1405	NPHENO2 + HCOCO3 -> NPHa_C2a	ARR 3.0E-13 0 0
1406	NPHENO2 + HCOCH2O2 -> NPHa_C2b	ARR 3.0E-13 0 0
1407	NPHENO2 + NPHEN1O2 -> NPHa_NPHb	ARR 3.48E-11 0 0
1408	NPHENO2 + NNCATECO2 -> NPHa_NNC	ARR 1.0E-10 0 0
1409	NPHENO2 + NCATECO2 -> NPHa_NCAT	ARR 1.0E-10 0 0
1410	NPHENO2 + NBZQO2 -> NPHa_NBZb	ARR 7.62E-11 0 0
1411	NPHENO2 + PBZQO2 -> NPHa_PBZ	ARR 3.74E-11 0 0
1412	NPHENO2 + MALANHYO2 -> NPHa_MALc	ARR 2.87E-11 0 0
1413	NPHENO2 + NDNPHENO2 -> NPHa_NDN	ARR 1.0E-10 0 0
1414	NPHENO2 + DNPHENO2 -> NPHa_DNP	ARR 1.0E-10 0 0
1415	NPHENO2 + HOCH2CO3 -> NPHa_C2c	ARR 3.0E-13 0 0
1416	NPHENO2 + C5CO2OHCO3 -> NPHa_C5a	ARR 5.12E-11 0 0
1417	NPHENO2 + C4CO2DBCO3 -> NPHa_C4a	ARR 2.53E-11 0 0
1418	PHENO2 + PHENO2 -> PHEN_PHEN	ARR 1.41E-11 0 0
1419	PHENO2 + MALDIALCO3 -> PHEN_MALa	ARR 3.0E-13 0 0
1420	PHENO2 + EPXDLCO3 -> PHEN_EPX	ARR 3.0E-13 0 0
1421	PHENO2 + C3DIALO2 -> PHEN_C3DI	ARR 3.0E-13 0 0
1422	PHENO2 + MALDIALO2 -> PHEN_MALb	ARR 3.0E-13 0 0
1423	PHENO2 + C6H5O2 -> PHEN_C6a	ARR 3.0E-13 0 0
1424	PHENO2 + NBZFUO2 -> PHEN_NBZa	ARR 1.67E-11 0 0
1425	PHENO2 + BZFUO2 -> PHEN_BZFU	ARR 3.0E-13 0 0
1426	PHENO2 + HCOCOHCO3 -> PHEN_C3a	ARR 3.0E-13 0 0
1427	PHENO2 + CATEC1O2 -> PHEN_CATE	ARR 3.0E-13 0 0
1428	PHENO2 + HCOCO3 -> PHEN_C2a	ARR 3.0E-13 0 0
1429	PHENO2 + HCOCH2O2 -> PHEN_C2b	ARR 3.0E-13 0 0
1430	PHENO2 + NPHEN1O2 -> PHEN_NPHb	ARR 3.0E-13 0 0
1431	PHENO2 + NNCATECO2 -> PHEN_NNC	ARR 1.0E-10 0 0
1432	PHENO2 + NCATECO2 -> PHEN_NCAT	ARR 6.67E-11 0 0
1433	PHENO2 + NBZQO2 -> PHEN_NBZb	ARR 3.74E-11 0 0
1434	PHENO2 + PBZQO2 -> PHEN_PBZ	ARR 3.0E-13 0 0
1435	PHENO2 + MALANHYO2 -> PHEN_MALc	ARR 3.0E-13 0 0
1436	PHENO2 + NDNPHENO2 -> PHEN_NDN	ARR 1.0E-10 0 0
1437	PHENO2 + DNPHENO2 -> PHEN_DNP	ARR 9.17E-11 0 0
1438	PHENO2 + HOCH2CO3 -> PHEN_C2c	ARR 3.0E-13 0 0
1439	PHENO2 + C5CO2OHCO3 -> PHEN_C5a	ARR 1.24E-11 0 0

1440	PHENO2 + C4CO2DBCO3 -> PHEN_C4a	ARR 3.0E-13 0 0
1441	MALDIALCO3 + MALDIALCO3 -> MALa_MALa	ARR 3.0E-13 0 0
1442	MALDIALCO3 + EPXDLCO3 -> MALa_EPX	ARR 3.0E-13 0 0
1443	MALDIALCO3 + C3DIALO2 -> MALa_C3DI	ARR 3.0E-13 0 0
1444	MALDIALCO3 + MALDIALO2 -> MALa_MALb	ARR 3.0E-13 0 0
1445	MALDIALCO3 + C6H5O2 -> MALa_C6a	ARR 3.0E-13 0 0
1446	MALDIALCO3 + NBZFUO2 -> MALa_NBZa	ARR 3.0E-13 0 0
1447	MALDIALCO3 + BZFUO2 -> MALa_BZFU	ARR 3.0E-13 0 0
1448	MALDIALCO3 + HCOCOHCO3 -> MALa_C3a	ARR 3.0E-13 0 0
1449	MALDIALCO3 + CATEC1O2 -> MALa_CATE	ARR 3.0E-13 0 0
1450	MALDIALCO3 + HCOCO3 -> MALa_C2a	ARR 3.0E-13 0 0
1451	MALDIALCO3 + HCOCH2O2 -> MALa_C2b	ARR 3.0E-13 0 0
1452	MALDIALCO3 + NPHEN1O2 -> MALa_NPHb	ARR 3.0E-13 0 0
1453	MALDIALCO3 + NNCATECO2 -> MALa_NNC	ARR 5.37E-11 0 0
1454	MALDIALCO3 + NCATECO2 -> MALa_NCAT	ARR 1.5E-11 0 0
1455	MALDIALCO3 + NBZQO2 -> MALa_NBZb	ARR 3.0E-13 0 0
1456	MALDIALCO3 + PBZQO2 -> MALa_PBZ	ARR 3.0E-13 0 0
1457	MALDIALCO3 + MALANHYO2 -> MALa_MALc	ARR 3.0E-13 0 0
1458	MALDIALCO3 + NDNPHENO2 -> MALa_NDN	ARR 7.87E-11 0 0
1459	MALDIALCO3 + DNPHENO2 -> MALa_DNP	ARR 4.0E-11 0 0
1460	MALDIALCO3 + HOCH2CO3 -> MALa_C2c	ARR 3.0E-13 0 0
1461	MALDIALCO3 + C5CO2OHCO3 -> MALa_C5a	ARR 3.0E-13 0 0
1462	MALDIALCO3 + C4CO2DBCO3 -> MALa_C4a	ARR 3.0E-13 0 0
1463	EPXDLCO3 + EPXDLCO3 -> EPX_EPX	ARR 3.0E-13 0 0
1464	EPXDLCO3 + C3DIALO2 -> EPX_C3DI	ARR 3.0E-13 0 0
1465	EPXDLCO3 + MALDIALO2 -> EPX_MALb	ARR 3.0E-13 0 0
1466	EPXDLCO3 + C6H5O2 -> EPX_C6a	ARR 3.0E-13 0 0
1467	EPXDLCO3 + NBZFUO2 -> EPX_NBZa	ARR 3.0E-13 0 0
1468	EPXDLCO3 + BZFUO2 -> EPX_BZFU	ARR 3.0E-13 0 0
1469	EPXDLCO3 + HCOCOHCO3 -> EPX_C3a	ARR 3.0E-13 0 0
1470	EPXDLCO3 + CATEC1O2 -> EPX_CATE	ARR 3.0E-13 0 0
1471	EPXDLCO3 + HCOCO3 -> EPX_C2a	ARR 3.0E-13 0 0
1472	EPXDLCO3 + HCOCH2O2 -> EPX_C2b	ARR 3.0E-13 0 0
1473	EPXDLCO3 + NPHEN1O2 -> EPX_NPHb	ARR 3.0E-13 0 0
1474	EPXDLCO3 + NNCATECO2 -> EPX_NNC	ARR 6.75E-11 0 0
1475	EPXDLCO3 + NCATECO2 -> EPX_NCAT	ARR 2.87E-11 0 0
1476	EPXDLCO3 + NBZQO2 -> EPX_NBZb	ARR 3.0E-13 0 0
1477	EPXDLCO3 + PBZQO2 -> EPX_PBZ	ARR 3.0E-13 0 0
1478	EPXDLCO3 + MALANHYO2 -> EPX_MALc	ARR 3.0E-13 0 0
1479	EPXDLCO3 + NDNPHENO2 -> EPX_NDN	ARR 9.25E-11 0 0
1480	EPXDLCO3 + DNPHENO2 -> EPX_DNP	ARR 5.37E-11 0 0
1481	EPXDLCO3 + HOCH2CO3 -> EPX_C2c	ARR 3.0E-13 0 0
1482	EPXDLCO3 + C5CO2OHCO3 -> EPX_C5a	ARR 3.0E-13 0 0
1483	EPXDLCO3 + C4CO2DBCO3 -> EPX_C4a	ARR 3.0E-13 0 0
1484	C3DIALO2 + C3DIALO2 -> C3DI_C3DI	ARR 3.0E-13 0 0
1485	C3DIALO2 + MALDIALO2 -> C3DI_MALb	ARR 3.0E-13 0 0

1486	C3DIALO2 + C6H5O2 -> C3DI_C6a	ARR 3.0E-13 0 0
1487	C3DIALO2 + NBZFUO2 -> C3DI_NBZa	ARR 3.0E-13 0 0
1488	C3DIALO2 + BZFUO2 -> C3DI_BZFU	ARR 3.0E-13 0 0
1489	C3DIALO2 + HCOCOHCO3 -> C3DI_C3a	ARR 3.0E-13 0 0
1490	C3DIALO2 + CATEC1O2 -> C3DI_CATE	ARR 3.0E-13 0 0
1491	C3DIALO2 + HCOCO3 -> C3DI_C2a	ARR 3.0E-13 0 0
1492	C3DIALO2 + HCOCH2O2 -> C3DI_C2b	ARR 3.0E-13 0 0
1493	C3DIALO2 + NPHEN1O2 -> C3DI_NPHb	ARR 3.0E-13 0 0
1494	C3DIALO2 + NNCATECO2 -> C3DI_NNC	ARR 4.34E-11 0 0
1495	C3DIALO2 + NCATECO2 -> C3DI_NCAT	ARR 4.61E-12 0 0
1496	C3DIALO2 + NBZQO2 -> C3DI_NBZb	ARR 3.0E-13 0 0
1497	C3DIALO2 + PBZQO2 -> C3DI_PBZ	ARR 3.0E-13 0 0
1498	C3DIALO2 + MALANHYO2 -> C3DI_MALc	ARR 3.0E-13 0 0
1499	C3DIALO2 + NDNPHENO2 -> C3DI_NDN	ARR 6.84E-11 0 0
1500	C3DIALO2 + DNPHENO2 -> C3DI_DNP	ARR 2.96E-11 0 0
1501	C3DIALO2 + HOCH2CO3 -> C3DI_C2c	ARR 3.0E-13 0 0
1502	C3DIALO2 + C5CO2OHCO3 -> C3DI_C5a	ARR 3.0E-13 0 0
1503	C3DIALO2 + C4CO2DBCO3 -> C3DI_C4a	ARR 3.0E-13 0 0
1504	MALDIALO2 + MALDIALO2 -> MALb_MALb	ARR 3.0E-13 0 0
1505	MALDIALO2 + C6H5O2 -> MALb_C6a	ARR 3.0E-13 0 0
1506	MALDIALO2 + NBZFUO2 -> MALb_NBZa	ARR 3.0E-13 0 0
1507	MALDIALO2 + BZFUO2 -> MALb_BZFU	ARR 3.0E-13 0 0
1508	MALDIALO2 + HCOCOHCO3 -> MALb_C3a	ARR 3.0E-13 0 0
1509	MALDIALO2 + CATEC1O2 -> MALb_CATE	ARR 3.0E-13 0 0
1510	MALDIALO2 + HCOCO3 -> MALb_C2a	ARR 3.0E-13 0 0
1511	MALDIALO2 + HCOCH2O2 -> MALb_C2b	ARR 3.0E-13 0 0
1512	MALDIALO2 + NPHEN1O2 -> MALb_NPHb	ARR 3.0E-13 0 0
1513	MALDIALO2 + NNCATECO2 -> MALb_NNC	ARR 6.93E-11 0 0
1514	MALDIALO2 + NCATECO2 -> MALb_NCAT	ARR 3.05E-11 0 0
1515	MALDIALO2 + NBZQO2 -> MALb_NBZb	ARR 1.16E-12 0 0
1516	MALDIALO2 + PBZQO2 -> MALb_PBZ	ARR 3.0E-13 0 0
1517	MALDIALO2 + MALANHYO2 -> MALb_MALc	ARR 3.0E-13 0 0
1518	MALDIALO2 + NDNPHENO2 -> MALb_NDN	ARR 9.43E-11 0 0
1519	MALDIALO2 + DNPHENO2 -> MALb_DNP	ARR 5.55E-11 0 0
1520	MALDIALO2 + HOCH2CO3 -> MALb_C2c	ARR 3.0E-13 0 0
1521	MALDIALO2 + C5CO2OHCO3 -> MALb_C5a	ARR 3.0E-13 0 0
1522	MALDIALO2 + C4CO2DBCO3 -> MALb_C4a	ARR 3.0E-13 0 0
1523	C6H5O2 + C6H5O2 -> C6a_C6a	ARR 3.0E-13 0 0
1524	C6H5O2 + NBZFUO2 -> C6a_NBZa	ARR 3.0E-13 0 0
1525	C6H5O2 + BZFUO2 -> C6a_BZFU	ARR 3.0E-13 0 0
1526	C6H5O2 + HCOCOHCO3 -> C6a_C3a	ARR 3.0E-13 0 0
1527	C6H5O2 + CATEC1O2 -> C6a_CATE	ARR 3.0E-13 0 0
1528	C6H5O2 + HCOCO3 -> C6a_C2a	ARR 3.0E-13 0 0
1529	C6H5O2 + HCOCH2O2 -> C6a_C2b	ARR 3.0E-13 0 0
1530	C6H5O2 + NPHEN1O2 -> C6a_NPHb	ARR 3.0E-13 0 0
1531	C6H5O2 + NNCATECO2 -> C6a_NNC	ARR 4.86E-11 0 0

1532	C6H5O2 + NCATECO2 -> C6a_NCAT	ARR 9.78E-12 0 0
1533	C6H5O2 + NBZQO2 -> C6a_NBZb	ARR 3.0E-13 0 0
1534	C6H5O2 + PBZQO2 -> C6a_PBZ	ARR 3.0E-13 0 0
1535	C6H5O2 + MALANHYO2 -> C6a_MALc	ARR 3.0E-13 0 0
1536	C6H5O2 + NDNPHENO2 -> C6a_NDN	ARR 7.36E-11 0 0
1537	C6H5O2 + DNPHENO2 -> C6a_DNP	ARR 3.48E-11 0 0
1538	C6H5O2 + HOCH2CO3 -> C6a_C2c	ARR 3.0E-13 0 0
1539	C6H5O2 + C5CO2OHCO3 -> C6a_C5a	ARR 3.0E-13 0 0
1540	C6H5O2 + C4CO2DBCO3 -> C6a_C4a	ARR 3.0E-13 0 0
1541	NBZFUO2 + NBZFUO2 -> NBZa_NBZa	ARR 1.93E-11 0 0
1542	NBZFUO2 + BZFUO2 -> NBZa_BZFU	ARR 3.0E-13 0 0
1543	NBZFUO2 + HCOCOHCO3 -> NBZa_C3a	ARR 3.0E-13 0 0
1544	NBZFUO2 + CATEC1O2 -> NBZa_CATE	ARR 3.0E-13 0 0
1545	NBZFUO2 + HCOCO3 -> NBZa_C2a	ARR 3.0E-13 0 0
1546	NBZFUO2 + HCOCH2O2 -> NBZa_C2b	ARR 3.0E-13 0 0
1547	NBZFUO2 + NPHEN1O2 -> NBZa_NPHb	ARR 3.0E-13 0 0
1548	NBZFUO2 + NNCATECO2 -> NBZa_NNC	ARR 1.0E-10 0 0
1549	NBZFUO2 + NCATECO2 -> NBZa_NCAT	ARR 6.93E-11 0 0
1550	NBZFUO2 + NBZQO2 -> NBZa_NBZb	ARR 4.0E-11 0 0
1551	NBZFUO2 + PBZQO2 -> NBZa_PBZ	ARR 1.16E-12 0 0
1552	NBZFUO2 + MALANHYO2 -> NBZa_MALc	ARR 3.0E-13 0 0
1553	NBZFUO2 + NDNPHENO2 -> NBZa_NDN	ARR 1.0E-10 0 0
1554	NBZFUO2 + DNPHENO2 -> NBZa_DNP	ARR 9.43E-11 0 0
1555	NBZFUO2 + HOCH2CO3 -> NBZa_C2c	ARR 3.0E-13 0 0
1556	NBZFUO2 + C5CO2OHCO3 -> NBZa_C5a	ARR 1.5E-11 0 0
1557	NBZFUO2 + C4CO2DBCO3 -> NBZa_C4a	ARR 3.0E-13 0 0
1558	BZFUO2 + BZFUO2 -> BZFU_BZFU	ARR 3.0E-13 0 0
1559	BZFUO2 + HCOCOHCO3 -> BZFU_C3a	ARR 3.0E-13 0 0
1560	BZFUO2 + CATEC1O2 -> BZFU_CATE	ARR 3.0E-13 0 0
1561	BZFUO2 + HCOCO3 -> BZFU_C2a	ARR 3.0E-13 0 0
1562	BZFUO2 + HCOCH2O2 -> BZFU_C2b	ARR 3.0E-13 0 0
1563	BZFUO2 + NPHEN1O2 -> BZFU_NPHb	ARR 3.0E-13 0 0
1564	BZFUO2 + NNCATECO2 -> BZFU_NNC	ARR 6.93E-11 0 0
1565	BZFUO2 + NCATECO2 -> BZFU_NCAT	ARR 3.05E-11 0 0
1566	BZFUO2 + NBZQO2 -> BZFU_NBZb	ARR 1.16E-12 0 0
1567	BZFUO2 + PBZQO2 -> BZFU_PBZ	ARR 3.0E-13 0 0
1568	BZFUO2 + MALANHYO2 -> BZFU_MALc	ARR 3.0E-13 0 0
1569	BZFUO2 + NDNPHENO2 -> BZFU_NDN	ARR 9.43E-11 0 0
1570	BZFUO2 + DNPHENO2 -> BZFU_DNP	ARR 5.55E-11 0 0
1571	BZFUO2 + HOCH2CO3 -> BZFU_C2c	ARR 3.0E-13 0 0
1572	BZFUO2 + C5CO2OHCO3 -> BZFU_C5a	ARR 3.0E-13 0 0
1573	BZFUO2 + C4CO2DBCO3 -> BZFU_C4a	ARR 3.0E-13 0 0
1574	HCOCOHCO3 + HCOCOHCO3 -> C3a_C3a	ARR 3.0E-13 0 0
1575	HCOCOHCO3 + CATEC1O2 -> C3a_CATE	ARR 3.0E-13 0 0
1576	HCOCOHCO3 + HCOCO3 -> C3a_C2a	ARR 3.0E-13 0 0
1577	HCOCOHCO3 + HCOCH2O2 -> C3a_C2b	ARR 3.0E-13 0 0

1578	HCOCOHCO3 + NPHEN1O2 -> C3a_NPHb	ARR 3.0E-13 0 0
1579	HCOCOHCO3 + NNCATECO2 -> C3a_NNC	ARR 5.72E-11 0 0
1580	HCOCOHCO3 + NCATECO2 -> C3a_NCAT	ARR 1.84E-11 0 0
1581	HCOCOHCO3 + NBZQO2 -> C3a_NBZb	ARR 3.0E-13 0 0
1582	HCOCOHCO3 + PBZQO2 -> C3a_PBZ	ARR 3.0E-13 0 0
1583	HCOCOHCO3 + MALANHYO2 -> C3a_MALc	ARR 3.0E-13 0 0
1584	HCOCOHCO3 + NDNPHENO2 -> C3a_NDN	ARR 8.22E-11 0 0
1585	HCOCOHCO3 + DNPHENO2 -> C3a_DNP	ARR 4.34E-11 0 0
1586	HCOCOHCO3 + HOCH2CO3 -> C3a_C2c	ARR 3.0E-13 0 0
1587	HCOCOHCO3 + C5CO2OHCO3 -> C3a_C5a	ARR 3.0E-13 0 0
1588	HCOCOHCO3 + C4CO2DBCO3 -> C3a_C4a	ARR 3.0E-13 0 0
1589	CATEC1O2 + CATEC1O2 -> CATE_CATE	ARR 3.0E-13 0 0
1590	CATEC1O2 + HCOCO3 -> CATE_C2a	ARR 3.0E-13 0 0
1591	CATEC1O2 + HCOCH2O2 -> CATE_C2b	ARR 3.0E-13 0 0
1592	CATEC1O2 + NPHEN1O2 -> CATE_NPHb	ARR 3.0E-13 0 0
1593	CATEC1O2 + NNCATECO2 -> CATE_NNC	ARR 6.24E-11 0 0
1594	CATEC1O2 + NCATECO2 -> CATE_NCAT	ARR 2.36E-11 0 0
1595	CATEC1O2 + NBZQO2 -> CATE_NBZb	ARR 3.0E-13 0 0
1596	CATEC1O2 + PBZQO2 -> CATE_PBZ	ARR 3.0E-13 0 0
1597	CATEC1O2 + MALANHYO2 -> CATE_MALc	ARR 3.0E-13 0 0
1598	CATEC1O2 + NDNPHENO2 -> CATE_NDN	ARR 8.74E-11 0 0
1599	CATEC1O2 + DNPHENO2 -> CATE_DNP	ARR 4.86E-11 0 0
1600	CATEC1O2 + HOCH2CO3 -> CATE_C2c	ARR 3.0E-13 0 0
1601	CATEC1O2 + C5CO2OHCO3 -> CATE_C5a	ARR 3.0E-13 0 0
1602	CATEC1O2 + C4CO2DBCO3 -> CATE_C4a	ARR 3.0E-13 0 0
1603	HCOCO3 + HCOCO3 -> C2a_C2a	ARR 3.0E-13 0 0
1604	HCOCO3 + HCOCH2O2 -> C2a_C2b	ARR 3.0E-13 0 0
1605	HCOCO3 + NPHEN1O2 -> C2a_NPHb	ARR 3.0E-13 0 0
1606	HCOCO3 + NNCATECO2 -> C2a_NNC	ARR 3.13E-11 0 0
1607	HCOCO3 + NCATECO2 -> C2a_NCAT	ARR 3.0E-13 0 0
1608	HCOCO3 + NBZQO2 -> C2a_NBZb	ARR 3.0E-13 0 0
1609	HCOCO3 + PBZQO2 -> C2a_PBZ	ARR 3.0E-13 0 0
1610	HCOCO3 + MALANHYO2 -> C2a_MALc	ARR 3.0E-13 0 0
1611	HCOCO3 + NDNPHENO2 -> C2a_NDN	ARR 5.63E-11 0 0
1612	HCOCO3 + DNPHENO2 -> C2a_DNP	ARR 1.75E-11 0 0
1613	HCOCO3 + HOCH2CO3 -> C2a_C2c	ARR 3.0E-13 0 0
1614	HCOCO3 + C5CO2OHCO3 -> C2a_C5a	ARR 3.0E-13 0 0
1615	HCOCO3 + C4CO2DBCO3 -> C2a_C4a	ARR 3.0E-13 0 0
1616	HCOCH2O2 + HCOCH2O2 -> C2b_C2b	ARR 3.0E-13 0 0
1617	HCOCH2O2 + NPHEN1O2 -> C2b_NPHb	ARR 3.0E-13 0 0
1618	HCOCH2O2 + NNCATECO2 -> C2b_NNC	ARR 1.93E-11 0 0
1619	HCOCH2O2 + NCATECO2 -> C2b_NCAT	ARR 3.0E-13 0 0
1620	HCOCH2O2 + NBZQO2 -> C2b_NBZb	ARR 3.0E-13 0 0
1621	HCOCH2O2 + PBZQO2 -> C2b_PBZ	ARR 3.0E-13 0 0
1622	HCOCH2O2 + MALANHYO2 -> C2b_MALc	ARR 3.0E-13 0 0
1623	HCOCH2O2 + NDNPHENO2 -> C2b_NDN	ARR 4.43E-11 0 0

1624	HCOCH2O2 + DNPHENO2 -> C2b_DNP	ARR 5.47E-12 0 0
1625	HCOCH2O2 + HOCH2CO3 -> C2b_C2c	ARR 3.0E-13 0 0
1626	HCOCH2O2 + C5CO2OHCO3 -> C2b_C5a	ARR 3.0E-13 0 0
1627	HCOCH2O2 + C4CO2DBCO3 -> C2b_C4a	ARR 3.0E-13 0 0
1628	NPHEN1O2 + NPHEN1O2 -> NPHb_NPHb	ARR 3.0E-13 0 0
1629	NPHEN1O2 + NNCATECO2 -> NPHb_NNC	ARR 8.74E-11 0 0
1630	NPHEN1O2 + NCATECO2 -> NPHb_NCAT	ARR 4.86E-11 0 0
1631	NPHEN1O2 + NBZQO2 -> NPHb_NBZb	ARR 1.93E-11 0 0
1632	NPHEN1O2 + PBZQO2 -> NPHb_PBZ	ARR 3.0E-13 0 0
1633	NPHEN1O2 + MALANHYO2 -> NPHb_MALc	ARR 3.0E-13 0 0
1634	NPHEN1O2 + NDNPHENO2 -> NPHb_NDN	ARR 1.0E-10 0 0
1635	NPHEN1O2 + DNPHENO2 -> NPHb_DNP	ARR 7.36E-11 0 0
1636	NPHEN1O2 + HOCH2CO3 -> NPHb_C2c	ARR 3.0E-13 0 0
1637	NPHEN1O2 + C5CO2OHCO3 -> NPHb_C5a	ARR 3.0E-13 0 0
1638	NPHEN1O2 + C4CO2DBCO3 -> NPHb_C4a	ARR 3.0E-13 0 0
1639	NNCATECO2 + NNCATECO2 -> NNC_NNC	ARR 1.0E-10 0 0
1640	NNCATECO2 + NCATECO2 -> NNC_NCAT	ARR 1.0E-10 0 0
1641	NNCATECO2 + NBZQO2 -> NNC_NBZb	ARR 1.0E-10 0 0
1642	NNCATECO2 + PBZQO2 -> NNC_PBZ	ARR 9.0E-11 0 0
1643	NNCATECO2 + MALANHYO2 -> NNC_MALc	ARR 8.13E-11 0 0
1644	NNCATECO2 + NDNPHENO2 -> NNC_NDN	ARR 1.0E-10 0 0
1645	NNCATECO2 + DNPHENO2 -> NNC_DNP	ARR 1.0E-10 0 0
1646	NNCATECO2 + HOCH2CO3 -> NNC_C2c	ARR 3.31E-11 0 0
1647	NNCATECO2 + C5CO2OHCO3 -> NNC_C5a	ARR 1.0E-10 0 0
1648	NNCATECO2 + C4CO2DBCO3 -> NNC_C4a	ARR 7.79E-11 0 0
1649	NCATECO2 + NCATECO2 -> NCAT_NCAT	ARR 1.0E-10 0 0
1650	NCATECO2 + NBZQO2 -> NCAT_NBZb	ARR 9.0E-11 0 0
1651	NCATECO2 + PBZQO2 -> NCAT_PBZ	ARR 5.12E-11 0 0
1652	NCATECO2 + MALANHYO2 -> NCAT_MALc	ARR 4.25E-11 0 0
1653	NCATECO2 + NDNPHENO2 -> NCAT_NDN	ARR 1.0E-10 0 0
1654	NCATECO2 + DNPHENO2 -> NCAT_DNP	ARR 1.0E-10 0 0
1655	NCATECO2 + HOCH2CO3 -> NCAT_C2c	ARR 3.0E-13 0 0
1656	NCATECO2 + C5CO2OHCO3 -> NCAT_C5a	ARR 6.5E-11 0 0
1657	NCATECO2 + C4CO2DBCO3 -> NCAT_C4a	ARR 3.91E-11 0 0
1658	NBZQO2 + NBZQO2 -> NBZb_NBZb	ARR 6.06E-11 0 0
1659	NBZQO2 + PBZQO2 -> NBZb_PBZ	ARR 2.19E-11 0 0
1660	NBZQO2 + MALANHYO2 -> NBZb_MALc	ARR 1.32E-11 0 0
1661	NBZQO2 + NDNPHENO2 -> NBZb_NDN	ARR 1.0E-10 0 0
1662	NBZQO2 + DNPHENO2 -> NBZb_DNP	ARR 1.0E-10 0 0
1663	NBZQO2 + HOCH2CO3 -> NBZb_C2c	ARR 3.0E-13 0 0
1664	NBZQO2 + C5CO2OHCO3 -> NBZb_C5a	ARR 3.56E-11 0 0
1665	NBZQO2 + C4CO2DBCO3 -> NBZb_C4a	ARR 9.78E-12 0 0
1666	PBZQO2 + PBZQO2 -> PBZ_PBZ	ARR 3.0E-13 0 0
1667	PBZQO2 + MALANHYO2 -> PBZ_MALc	ARR 3.0E-13 0 0
1668	PBZQO2 + NDNPHENO2 -> PBZ_NDN	ARR 1.0E-10 0 0
1669	PBZQO2 + DNPHENO2 -> PBZ_DNP	ARR 7.62E-11 0 0

1670	PBZQO2 + HOCH2CO3 -> PBZ_C2c	ARR 3.0E-13 0 0
1671	PBZQO2 + C5CO2OHCO3 -> PBZ_C5a	ARR 3.0E-13 0 0
1672	PBZQO2 + C4CO2DBCO3 -> PBZ_C4a	ARR 3.0E-13 0 0
1673	MALANHYO2 + MALANHYO2 -> MALc_MALc	ARR 3.0E-13 0 0
1674	MALANHYO2 + NDNPHENO2 -> MALc_NDN	ARR 1.0E-10 0 0
1675	MALANHYO2 + DNPHENO2 -> MALc_DNP	ARR 6.75E-11 0 0
1676	MALANHYO2 + HOCH2CO3 -> MALc_C2c	ARR 3.0E-13 0 0
1677	MALANHYO2 + C5CO2OHCO3 -> MALc_C5a	ARR 3.0E-13 0 0
1678	MALANHYO2 + C4CO2DBCO3 -> MALc_C4a	ARR 3.0E-13 0 0
1679	NDNPHENO2 + NDNPHENO2 -> NDN_NDN	ARR 1.0E-10 0 0
1680	NDNPHENO2 + DNPHENO2 -> NDN_DNP	ARR 1.0E-10 0 0
1681	NDNPHENO2 + HOCH2CO3 -> NDN_C2c	ARR 5.81E-11 0 0
1682	NDNPHENO2 + C5CO2OHCO3 -> NDN_C5a	ARR 1.0E-10 0 0
1683	NDNPHENO2 + C4CO2DBCO3 -> NDN_C4a	ARR 1.0E-10 0 0
1684	DNPHENO2 + DNPHENO2 -> DNP_DNP	ARR 1.0E-10 0 0
1685	DNPHENO2 + HOCH2CO3 -> DNP_C2c	ARR 1.93E-11 0 0
1686	DNPHENO2 + C5CO2OHCO3 -> DNP_C5a	ARR 9.0E-11 0 0
1687	DNPHENO2 + C4CO2DBCO3 -> DNP_C4a	ARR 6.41E-11 0 0
1688	HOCH2CO3 + HOCH2CO3 -> C2c_C2c	ARR 3.0E-13 0 0
1689	HOCH2CO3 + C5CO2OHCO3 -> C2c_C5a	ARR 3.0E-13 0 0
1690	HOCH2CO3 + C4CO2DBCO3 -> C2c_C4a	ARR 3.0E-13 0 0
1691	C5CO2OHCO3 + C5CO2OHCO3 -> C5a_C5a	ARR 1.06E-11 0 0
1692	C5CO2OHCO3 + C4CO2DBCO3 -> C5a_C4a	ARR 3.0E-13 0 0
1693	C4CO2DBCO3 + C4CO2DBCO3 -> C4a_C4a	ARR 3.0E-13 0 0
1694	BZo_RO2_O7 -> BZo_O4_2OH	RO2 1 ARR 0.22E-11 0 0
1695	BZo_RO2_O9 -> BZo_O6_2OH	RO2 1 ARR 0.45E-11 0 0
1696	BZo_RO2_O11 -> BZo_O8_2OH	RO2 1 ARR 0.68E-11 0 0
1697	BZeo_RO2_O6 -> BZeo_O3_2OH	RO2 1 ARR 0.1E-11 0 0
1698	BZeo_RO2_O8 -> BZeo_O5_2OH	RO2 1 ARR 0.34E-11 0 0
1699	BZeo_RO2_O10 -> BZeo_O7_2OH	RO2 1 ARR 0.57E-11 0 0
1700	C5_RO2_O6 -> C5e_O3_2OH	RO2 1 ARR 0.25E-11 0 0
1701	C5_RO2_O7 -> C5_O4_2OH	RO2 1 ARR 0.36E-11 0 0
1702	C5_RO2_O8 -> C5e_O5_2OH	RO2 1 ARR 0.48E-11 0 0
1703	C5_RO2_O9 -> C5_O6_2OH	RO2 1 ARR 0.6E-11 0 0
1704	C5_RO2_O10 -> C5e_O7_2OH	RO2 1 ARR 0.71E-11 0 0
1705	BZo_RO2_O7 -> BZo_O5_O	RO2 1 ARR 0.21E-11 0 0
1706	BZo_RO2_O9 -> BZo_O7_O	RO2 1 ARR 0.43E-11 0 0
1707	BZo_RO2_O11 -> BZo_O9_O	RO2 1 ARR 0.65E-11 0 0
1708	BZeo_RO2_O6 -> BZeo_O4_O	RO2 1 ARR 0.1E-11 0 0
1709	BZeo_RO2_O8 -> BZeo_O6_O	RO2 1 ARR 0.32E-11 0 0
1710	BZeo_RO2_O10 -> BZeo_O8_O	RO2 1 ARR 0.54E-11 0 0
1711	C5_RO2_O6 -> C5e_O4_O	RO2 1 ARR 0.24E-11 0 0
1712	C5_RO2_O7 -> C5_O5_O	RO2 1 ARR 0.35E-11 0 0
1713	C5_RO2_O8 -> C5e_O6_O	RO2 1 ARR 0.46E-11 0 0
1714	C5_RO2_O9 -> C5_O7_O	RO2 1 ARR 0.57E-11 0 0
1715	C5_RO2_O10 -> C5e_O8_O	RO2 1 ARR 0.68E-11 0 0

1716	BZo2_RO_O6 -> GLY + MALDIAL + HO2	ARR 0.05E-6 0 0
1717	BZo2_RO_O8 -> GLY + MALDIAL + HO2	ARR 0.05E-6 0 0
1718	BZo2_RO_O10 -> GLY + MALDIAL + HO2	ARR 0.05E-6 0 0
1719	BZeo2_RO_O5 -> GLY + MALDIAL + HO2	ARR 0.05E-6 0 0
1720	BZeo2_RO_O7 -> GLY + MALDIAL + HO2	ARR 0.05E-6 0 0
1721	BZeo2_RO_O9 -> GLY + MALDIAL + HO2	ARR 0.05E-6 0 0
1722	BZo_RO_O6 -> GLY + MALDIAL + HO2	ARR 0.8E-6 0 0
1723	BZo_RO_O8 -> GLY + MALDIAL + HO2	ARR 0.88E-6 0 0
1724	BZo_RO_O10 -> GLY + MALDIAL + HO2	ARR 0.43E-6 0 0
1725	BZeo_RO_O5 -> GLY + MALDIAL + HO2	ARR 0.1E-6 0 0
1726	BZeo_RO_O7 -> GLY + MALDIAL + HO2	ARR 0.64E-6 0 0
1727	BZeo_RO_O9 -> GLY + MALDIAL + HO2	ARR 0.1E-6 0 0
1728	C5_RO_O5 -> MALDIAL + CO + HO2	ARR 0.05E-6 0 0
1729	C5_RO_O6 -> MALDIAL + CO + HO2	ARR 0.05E-6 0 0
1730	C5_RO_O7 -> MALDIAL + CO + HO2	ARR 0.05E-6 0 0
1731	C5_RO_O8 -> MALDIAL + CO + HO2	ARR 0.05E-6 0 0
1732	C5_RO_O9 -> MALDIAL + CO + HO2	ARR 0.05E-6 0 0
1733	BZo_RO2_O7 -> BZouni_O6_O + OH	ARR 0.01 0 0
1734	BZo_RO2_O9 -> BZouni_O8_O + OH	ARR 0.01 0 0
1735	BZo_RO2_O11 -> BZouni_O10_O + OH	ARR 0.01 0 0
1736	BZeo_RO2_O6 -> BZeouni_O5_O + HO2	ARR 0.01 0 0
1737	BZeo_RO2_O8 -> BZeouni_O7_O + HO2	ARR 0.01 0 0
1738	BZeo_RO2_O10 -> BZeouni_O9_O + HO2	ARR 0.01 0 0
1739	C5_RO2_O6 -> C5euni_O5_O + OH	ARR 0.3 0 0
1740	C5_RO2_O7 -> C5uni_O6_O + OH	ARR 0.8 0 0
1741	C5_RO2_O8 -> C5euni_O7_O + OH	ARR 0.8 0 0
1742	C5_RO2_O9 -> C5uni_O8_O + HO2	ARR 0.01 0 0
1743	C5_RO2_O10 -> C5euni_O9_O + HO2	ARR 0.01 0 0
1744	BZo2_RO_O6 -> ROCS_O5_O + HO2	ARR 0.05E-6 0 0
1745	BZo2_RO_O8 -> ROCS_O7_O + HO2	ARR 0.10E-6 0 0
1746	BZo2_RO_O10 -> ROCS_O9_O + HO2	ARR 0.60E-6 0 0
1747	BZo2_RO_O10 -> ROCS_O8_O + HO2	ARR 0.35E-6 0 0
1748	BZeo2_RO_O5 -> ROCS_O4_O + HO2	ARR 0.05E-6 0 0
1749	BZeo2_RO_O7 -> ROCS_O6_O + HO2	ARR 0.05E-6 0 0
1750	BZeo2_RO_O9 -> ROCS_O8_O + HO2	ARR 0.55E-6 0 0
1751	BZo_RO_O6 -> ROCS_O5_O + HO2	ARR 0.004E-6 0 0
1752	BZo_RO_O8 -> ROCS_O7_O + HO2	ARR 0.001E-6 0 0
1753	BZo_RO_O10 -> ROCS_O9_O + HO2	ARR 0.02E-6 0 0
1754	BZeo_RO_O5 -> ROCS_O4_O + HO2	ARR 0.45E-6 0 0
1755	BZeo_RO_O7 -> ROCS_O6_O + HO2	ARR 0.007E-6 0 0
1756	BZeo_RO_O9 -> ROCS_O8_O + HO2	ARR 0.45E-6 0 0
1757	C5_RO_O5 -> C5e_O4_O + HO2	ARR 0.05E-6 0 0
1758	C5_RO_O6 -> C5_O5_O + HO2	ARR 0.05E-6 0 0
1759	C5_RO_O7 -> C5e_O6_O + HO2	ARR 0.10E-6 0 0
1760	C5_RO_O8 -> C5_O7_O + HO2	ARR 0.25E-6 0 0
1761	C5_RO_O9 -> C5e_O8_O + HO2	ARR 0.50E-6 0 0

1762	C5_RO_O9 -> C5_O7_O + HO2	ARR 0.45E-6 0 0
1763	BZo_RO2_O7 -> C5_RO2_O8 + CO	ARR 0.6 0 0
1764	BZo_RO2_O9 -> C5_RO2_O10 + CO	ARR 0.014 0 0
1765	BZeo_RO2_O6 -> C5_RO2_O7 + CO	ARR 0.8 0 0
1766	BZeo_RO2_O8 -> C5_RO2_O9 + CO	ARR 0.06 0 0

Supplement S3: Mech 2 – species

name	SMILES	molar weight ($g.mol^{-1}$)	Psat (torr)	dHvap ($kJ.mol^{-1}$)	Henry constant ($M.atm^{-1}$)
A2PAN	OCC(O)C(=O)OON(=O)=O	167.1	1.21E-03	8.35E+01	4.99E+06
A2PANO	OCC(O)C(=O)[O]	105.1			
A2PANOO	OCC(O)C(=O)O[O]	121.1			
ACMAL2OH	O=C(O)C(O)=C(O)C(=O)O	148.1	5.24E-07	1.23E+02	1.13E+12
ACO3	[O]OC(=O)C=C	87.1			
ACOX	O=C(O)C(=O)O	90.0	4.76E-03	7.56E+01	3.04E+07
ACR	C=CC=O	56.1	2.72E+02	3.05E+01	4.61E+00
ACRO2	OCC(O[O])C=O	105.1			
BENZ2OH1O	Oc1cccc([O])c1O	125.1			
BENZ2OHO2	c1(O[O])cccc(O)c1O	141.1			
BENZ2OHOOH	OOc1cccc(O)c1O	142.1	3.79E-06	1.08E+02	2.44E+10
BENZ3OH	Oc1cccc(O)c1O	126.1	1.33E-04	9.09E+01	1.56E+10
BENZ3OH1O	Oc1ccc([O])c(O)c1O	141.1			
BENZ3OHBP2OH	OC2=CC1OOC(O)(C1O)C2(O)O	192.1	1.37E-08	1.40E+02	8.45E+11
BENZ3OHBPO	[O]C1(O)C(O)=CC2OOC1(O)C2O	191.1			
BENZ3OHBPO2	[O]OC1(O)C(O)=CC2OOC1(O)C2O	207.1			
BENZ3OHBPOOH	OOC1(O)C(O)=CC2OOC1(O)C2O	208.1	1.89E-10	1.59E+02	1.42E+13
BENZ3OHO2	c1(O[O])ccc(O)c(O)c1O	157.1			
BENZ3OHOOH	OOc1ccc(O)c(O)c1O	158.1	1.36E-08	1.33E+02	2.63E+14
BENZ4OH	Oc1ccc(O)c(O)c1O	142.1	7.33E-07	1.14E+02	8.43E+13
BENZ4OHBP2OH	OC2=CC1(O)OOC(O)(C1O)C2(O)O	208.1	1.26E-10	1.63E+02	1.66E+14
BENZ4OHBPO	[O]C1(O)C(O)=CC2(O)OOC1(O)C2O	207.1			
BENZ4OHBPO2	[O]OC1(O)C(O)=CC2(O)OOC1(O)C2O	223.1			
BENZ4OHBPOOH	OOC1(O)C(O)=CC2(O)OOC1(O)C2O	224.1	1.30E-12	1.83E+02	3.82E+15
BENZ5OH	Oc1cc(O)c(O)c(O)c1O	158.1	2.51E-09	1.41E+02	6.91E+17

BENZENE	c1ccccc1	78.1	5.00E+01	3.56E+01	3.50E-01
BEPOX	OC1C3OOC1C2OC2C3O	160.1	7.87E-04	8.67E+01	4.40E+05
BEPOXOH	OC2C1OOC(O)(C1O)C3OC23	176.1	1.87E-05	1.05E+02	4.36E+07
BZBI_BZBI	O(C1C=CC2OOC1C2O)OC1C=CC2OOC1C2O	286.2	1.23E-05	1.05E+02	2.22E+05
BZBI_BZFU	O(C1C=CC2OOC1C2O)OC1C(O)COC1=O	260.2	1.09E-06	1.13E+02	2.23E+07
BZBI_BZMUa	O(C1C=CC2OOC1C2O)OC(=O)C1OC1C=CC=O	284.2	8.13E-04	8.54E+01	7.88E+03
BZBI_BZMUb	O=CC(O)C(OOC1C=CC2OOC1C2O)C1OC1C=O	302.2	3.06E-08	1.32E+02	1.40E+09
BZBI_C2a	O(C1C=CC2OOC1C2O)OC(=O)C=O	216.1	4.76E-01	5.96E+01	4.41E+02
BZBI_C2b	O(C1C=CC2OOC1C2O)OCC=O	202.2	2.82E-02	7.01E+01	3.22E+03
BZBI_C2c	OCC(=O)(OOC1C=CC2OOC1C2O)	218.2	5.85E-02	6.96E+01	3.98E+03
BZBI_C3a	OC(C=O)C(=O)(OOC1C=CC2OOC1C2O)	246.2	3.41E-03	8.22E+01	7.85E+04
BZBI_C3DI	O(C1C=CC2OOC1C2O)OC(C=O)C=O	230.2	7.74E-04	8.55E+01	1.79E+05
BZBI_C4a	O(C1C=CC2OOC1C2O)OC(=O)C=CC(=O)C=O	270.2	1.69E-03	8.20E+01	1.99E+04
BZBI_C5a	OC(C=O)C(=O)C=CC(=O)(OOC1C=CC2OOC1C2O)	300.2	5.10E-06	1.09E+02	1.04E+07
BZBI_C5DI	O=CC=CC(OOC1C=CC2OOC1C2O)C=O	256.2	6.97E-05	9.53E+01	3.34E+05
BZBI_C6a	O(C1C=CC2OOC1C2O)Oc1ccccc1	236.2	2.04E-03	7.95E+01	2.42E+02
BZBI_CATE	O(C1C=CC2OOC1C2O)Oc1ccccc1O	252.2	5.51E-05	9.59E+01	1.47E+05
BZBI_DNP	O(C1C=CC2OOC1C2O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	392.2	1.47E-12	1.79E+02	1.27E+13
BZBI_EPX	O(C1C=CC2OOC1C2O)OC(=O)C1OC1C=O	258.2	8.76E-03	7.59E+01	4.64E+03
BZBI_MALa	O(C1C=CC2OOC1C2O)OC(=O)C=CC=O	242.2	3.30E-02	6.96E+01	1.02E+03
BZBI_MALb	O(C1C=CC2OOC1C2O)OC(C=O)C(O)C=O	260.2	2.80E-06	1.12E+02	6.57E+07
BZBI_MALc	O(C1C=CC2OOC1C2O)OC1C(=O)OC(=O)C1O	274.2	3.69E-06	1.11E+02	9.00E+06
BZBI_NBZa	O(C1C=CC2OOC1C2O)OC1C(=O)OCC1ON(=O)=O	305.2	5.41E-07	1.16E+02	1.02E+07
BZBI_NBZb	O(C1C=CC2OOC1C2O)OC1C(=O)C=CC(=O)C1ON(=O)=O	329.2	8.24E-08	1.25E+02	3.83E+07
BZBI_NCAT	O(C1C=CC2OOC1C2O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	363.2	2.50E-12	1.78E+02	3.62E+13
BZBI_NDN	O(C1C=CC2OOC1C2O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	437.2	7.84E-13	1.81E+02	6.60E+12
BZBI_NNC	O(C1C=CC2OOC1C2O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	408.2	1.17E-12	1.80E+02	2.67E+13
BZBI_NPHa	O(C1C=CC2OOC1C2O)OC1(O)C=CC2OOC1C2ON(=O)=O	347.2	6.81E-08	1.29E+02	4.54E+07
BZBI_NPHb	O(C1C=CC2OOC1C2O)Oc1ccccc1N(=O)=O	281.2	1.90E-05	9.92E+01	7.49E+03
BZBI_PBZ	O(C1C=CC2OOC1C2O)OC1C(=O)C=CC(=O)C1O	284.2	1.77E-07	1.22E+02	8.52E+07

BZBI_PHEN	O(C1C=CC2OOC1C2O)OC1(O)C=CC2OOC1C2O	302.2	1.76E-07	1.25E+02	6.63E+07
BZBIPER2OH	OC1C=CC2OOC1C2O	144.1	5.99E-03	7.80E+01	6.84E+04
BZBIPERNO3	O=N(=O)OC1C=CC2OOC1C2O	189.1	2.48E-03	8.10E+01	5.40E+04
BZBIPERO	[O]C1C=CC2OOC1C2O	143.1			
BZBIPERO2	[O]OC1C=CC2OOC1C2O	159.1			
BZBIPERO2bis	[O]OC1C=CC2OOC1C2O	159.1			
BZBIPEROOH	OOC1C=CC2OOC1C2O	160.1	3.48E-04	8.96E+01	5.46E+05
BZEMUCCO	O=CC1OC1C(=O)C(O)C=O	158.1	1.06E-04	9.36E+01	2.85E+07
BZEMUCCO2H	O=CC=CC1OC1C(=O)O	142.1	3.89E-04	8.78E+01	6.88E+06
BZEMUCCO3	[O]OC(=O)C1OC1C=CC=O	157.1			
BZEMUCCO3H	OOC(=O)C1OC1C=CC=O	158.1	1.62E-03	8.14E+01	4.90E+05
BZEMUCNO3	O=CC1OC1C(ON(=O)=O)C(O)C=O	205.1	4.30E-06	1.09E+02	3.62E+08
BZEMUCO	O=CC(O)C([O])C1OC1C=O	159.1			
BZEMUCO2	O=CC(O)C(O[O])C1OC1C=O	175.1			
BZEMUCOH	O=CC(O)C(O)C1OC1C=O	160.1	8.20E-06	1.07E+02	3.77E+08
BZEMUCOOH	O=CC(O)C(OO)C1OC1C=O	176.1	3.78E-07	1.20E+02	2.04E+09
BZEMUCPAN	O=CC=CC1OC1C(=O)OON(=O)=O	203.1	5.11E-03	7.47E+01	1.45E+04
BZeo_O3_2OH	OC1C2OC2C3OOC1C3(O)	160.1	7.87E-04	8.67E+01	4.40E+05
BZeo_O4_NO3	O=N(=O)OC1C2OC2C3OOC1C3(O)	205.1	3.19E-04	8.97E+01	3.78E+05
BZeo_O4_O	O=C1C2OC2C3OOC1C3(O)	158.1	4.88E-03	7.67E+01	6.26E+04
BZeo_O4_OOH	OOC1C2OC2C3OOC1C3(O)	176.1	4.39E-05	9.87E+01	4.79E+06
BZeo_O5_2OH	O=C=CC(OO)C(O)C(O)C(=O)O	192.1	4.63E-07	1.24E+02	2.83E+10
BZeo_O6_NO3	O=C=CC(OO)C(O)C(O)C(=O)ON(=O)=O	237.1	3.51E+00	5.88E+01	8.95E+02
BZeo_O6_O	O=C=CC(OO)C(=O)C(O)C(=O)O	190.1	6.66E-06	1.10E+02	1.83E+09
BZeo_O6_OOH	O=C=CC(OO)C(O)C(O)C(=O)OO	208.1	2.42E-06	1.17E+02	3.84E+09
BZeo_O7_2OH	O=C(O)C(O)C(=O)CC(OO)C(=O)OO	224.1	4.43E-13	1.84E+02	2.66E+16
BZeo_O8_NO3	O=C(ON(=O)=O)C(O)C(=O)CC(OO)C(=O)OO	269.1	2.07E-04	9.65E+01	3.36E+07
BZeo_O8_O	O=C(O)C(=O)C(=O)CC(OO)C(=O)OO	222.1	1.81E-11	1.65E+02	1.05E+15
BZeo_O8_OOH	O=C(OO)C(O)C(=O)CC(OO)C(=O)OO	240.1	4.63E-12	1.73E+02	1.22E+16
BZeo_RO_O5	[O]C1C2OC2C3OOC1C3(O)	159.1			

BZeo_RO_O7	O=C=CC(OO)C(O)C(O)C(=O)[O]	191.1			
BZeo_RO_O9	O=C([O])C(O)C(=O)CC(OO)C(=O)OO	223.1			
BZeo_RO2_O10	O=C(O[O])C(O)C(=O)CC(OO)C(=O)OO	239.1			
BZeo_RO2_O6	[O]OC1C2OC2C3OOC1C3(O)	175.1			
BZeo_RO2_O8	O=C=CC(OO)C(O)C(O)C(=O)O[O]	207.1			
BZeo2_RO_O5	[O]C1C2OC2C3OOC1C3(O)	159.1			
BZeo2_RO_O7	O=C=CC(OO)C(O)C(O)C(=O)[O]	191.1			
BZeo2_RO_O9	O=C([O])C(O)C(=O)CC(OO)C(=O)OO	223.1			
BZeoO5_5	O(C1C2OC2C3OOC1C3(O))OC1C2OC2C3OOC1C3(O)	318.2	2.26E-07	1.22E+02	9.30E+06
BZeoO5_7	O=C=CC(OO)C(O)C(O)C(=O)(OOC1C2OC2C3OOC1C3(O))	350.2	1.30E-07	1.31E+02	7.50E+08
BZeoO5_9	O=C(OOC1C2OC2C3OOC1C3(O))C(O)C(=O)CC(OO)C(=O)OO	382.2	7.74E-13	1.83E+02	2.46E+14
BZeoO5_BZBI	O(C1C2OC2C3OOC1C3(O))OC1C=CC2OOC1C2O	302.2	1.64E-06	1.14E+02	1.57E+06
BZeoO5_BZFU	O(C1C2OC2C3OOC1C3(O))OC1C(O)COC1=O	276.2	1.10E-07	1.24E+02	2.26E+08
BZeoO5_BZMUa	O(C1C2OC2C3OOC1C3(O))OC(=O)C1OC1C=CC=O	300.2	1.36E-04	9.29E+01	5.44E+04
BZeoO5_BZMUb	O=CC(O)C(OOC1C2OC2C3OOC1C3(O))C1OC1C=O	318.2	3.53E-09	1.41E+02	1.32E+10
BZeoO5_C2a	O(C1C2OC2C3OOC1C3(O))OC(=O)C=O	232.1	7.77E-02	6.72E+01	3.04E+03
BZeoO5_C2b	O(C1C2OC2C3OOC1C3(O))OCC=O	218.2	4.05E-03	7.84E+01	2.60E+04
BZeoO5_C2c	OCC(=O)(OOC1C2OC2C3OOC1C3(O))	234.2	9.35E-03	7.75E+01	2.36E+04
BZeoO5_C3a	OC(C=O)C(=O)(OOC1C2OC2C3OOC1C3(O))	262.2	4.63E-04	9.09E+01	5.77E+05
BZeoO5_C3DI	O(C1C2OC2C3OOC1C3(O))OC(C=O)C=O	246.2	1.18E-04	9.38E+01	1.48E+06
BZeoO5_C4a	O(C1C2OC2C3OOC1C3(O))OC(=O)C=CC(=O)C=O	286.2	2.33E-04	9.09E+01	1.74E+05
BZeoO5_C5a	OC(C=O)C(=O)C=CC(=O)(OOC1C2OC2C3OOC1C3(O))	316.2	5.71E-07	1.19E+02	1.01E+08
BZeoO5_C5DI	O=CC=CC(OOC1C2OC2C3OOC1C3(O))C=O	272.2	1.03E-05	1.04E+02	2.92E+06
BZeoO5_C5eO5	O=CC(OOC1C2OC2C3OOC1C3(O))C(O)C(O)C=O	306.2	4.04E-10	1.53E+02	6.01E+11
BZeoO5_C5eO7	O=CC(OO)C(O)C(O)C(=O)(OOC1C2OC2C3OOC1C3(O))	338.2	6.61E-11	1.63E+02	1.80E+12
BZeoO5_C5eO9	O=C(OOC1C2OC2C3OOC1C3(O))C(OO)C(O)C(O)C(OO)=O	370.2	1.58E-13	1.92E+02	1.80E+15
BZeoO5_C5O6	OOC=CC(O)C(O)C(=O)(OOC1C2OC2C3OOC1C3(O))	322.2	9.01E-10	1.51E+02	5.35E+10
BZeoO5_C5O8	O=C(OOC1C2OC2C3OOC1C3(O))C(O)C(O)C(O)C(=O)OO	354.2	4.80E-12	1.77E+02	6.52E+13
BZeoO5_C6a	O(C1C2OC2C3OOC1C3(O))Oc1ccccc1	252.2	3.28E-04	8.75E+01	1.55E+03
BZeoO5_CATE	O(C1C2OC2C3OOC1C3(O))Oc1ccccc1O	268.2	7.67E-06	1.05E+02	9.64E+05

BZeoO5_DNP	O(C1C2OC2C3OOC1C3(O))OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	408.2	1.24E-13	1.90E+02	1.25E+14
BZeoO5_EPX	O(C1C2OC2C3OOC1C3(O))OC(=O)C1OC1C=O	274.2	1.47E-03	8.32E+01	2.98E+04
BZeoO5_MALa	O(C1C2OC2C3OOC1C3(O))OC(=O)C=CC=O	258.2	5.30E-03	7.75E+01	7.66E+03
BZeoO5_MALb	O(C1C2OC2C3OOC1C3(O))OC(C=O)C(O)C=O	276.2	3.27E-07	1.21E+02	6.27E+08
BZeoO5_MALc	O(C1C2OC2C3OOC1C3(O))OC1C(=O)OC(=O)C1O	290.2	4.50E-07	1.21E+02	7.95E+07
BZeoO5_NBZa	O(C1C2OC2C3OOC1C3(O))OC1C(=O)OCC1ON(=O)=O	321.2	5.31E-08	1.27E+02	1.14E+08
BZeoO5_NBZb	O(C1C2OC2C3OOC1C3(O))OC1C(=O)C=CC(=O)C1ON(=O)=O	345.2	7.61E-09	1.36E+02	4.20E+08
BZeoO5_NCAT	O(C1C2OC2C3OOC1C3(O))OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	379.2	2.01E-13	1.89E+02	3.64E+14
BZeoO5_NDN	O(C1C2OC2C3OOC1C3(O))OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	453.2	6.86E-14	1.93E+02	6.42E+13
BZeoO5_NNC	O(C1C2OC2C3OOC1C3(O))OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	424.2	9.74E-14	1.92E+02	2.67E+14
BZeoO5_NPHa	O(C1C2OC2C3OOC1C3(O))OC1(O)C=CC2OOC1C2ON(=O)=O	363.2	7.90E-09	1.39E+02	3.53E+08
BZeoO5_NPHb	O(C1C2OC2C3OOC1C3(O))Oc1ccccc1N(=O)=O	297.2	2.76E-06	1.08E+02	7.57E+04
BZeoO5_PBZ	O(C1C2OC2C3OOC1C3(O))OC1C(=O)C=CC(=O)C1O	300.2	1.63E-08	1.33E+02	8.95E+08
BZeoO5_PHEN	O(C1C2OC2C3OOC1C3(O))OC1(O)C=CC2OOC1C2O	318.2	1.95E-08	1.35E+02	5.23E+08
BZeoO7_7	O=C=CC(OO)C(O)C(O)C(=O)(OO(C(=O)C(O)C(O)C(OO)C=C=O))	382.2	1.26E-07	1.37E+02	6.50E+09
BZeoO7_9	O=C=CC(OO)C(O)C(O)C(=O)(OO(C(C(O)C(=O)CC(OO)C(=O)OO)=O))	414.2	4.39E-13	1.90E+02	3.06E+15
BZeoO7_BZBI	O=C=CC(OO)C(O)C(O)C(=O)(OOC1C=CC2OOC1C2O)	334.2	1.17E-06	1.21E+02	8.43E+07
BZeoO7_BZFU	O=C=CC(OO)C(O)C(O)C(=O)(OOC1C(O)COC1=O)	308.2	8.26E-08	1.31E+02	4.25E+09
BZeoO7_BZMUa	O=C=CC(OO)C(O)C(O)C(=O)(OOC(=O)C1OC1C=CC=O)	332.2	1.02E-04	1.01E+02	4.64E+05
BZeoO7_BZMUb	O=C=CC(OO)C(O)C(O)C(=O)(OO(C(C1OC1C=O)C(O)C=O))	350.2	2.27E-09	1.49E+02	2.43E+11
BZeoO7_C2a	O=C=CC(OO)C(O)C(O)C(=O)(OOC(=O)C=O)	264.1	1.42E-01	7.18E+01	5.89E+03
BZeoO7_C2b	O=C=CC(OO)C(O)C(O)C(=O)(OOCC=O)	250.2	6.66E-03	8.30E+01	2.43E+05
BZeoO7_C2c	O=C=CC(OO)C(O)C(O)C(=O)(OO(C(=O)CO))	266.2	1.60E-02	8.22E+01	8.57E+04
BZeoO7_C3a	O=C=CC(OO)C(O)C(O)C(=O)(OO(C(=O)C(C=O)O))	294.2	6.73E-04	9.59E+01	1.44E+06
BZeoO7_C3DI	O=C=CC(OO)C(O)C(O)C(=O)(OOC(C=O)C=O)	278.2	1.63E-04	9.86E+01	1.01E+07
BZeoO7_C4a	O=C=CC(OO)C(O)C(O)C(=O)(OOC(=O)C=CC(=O)C=O)	318.2	2.16E-04	9.72E+01	8.78E+05
BZeoO7_C5a	O=C=CC(OO)C(O)C(O)C(=O)(OO(C(=O)C=CC(=O)C(C=O)O))	348.2	4.22E-07	1.26E+02	5.63E+08
BZeoO7_C5DI	O=C=CC(OO)C(O)C(O)C(=O)(OO(C(C=O)C=CC=O))	304.2	9.68E-06	1.10E+02	4.08E+07
BZeoO7_C5eO5	O=C=CC(OO)C(O)C(O)C(=O)(OO(C(C(O)C(O)C=O)C=O))	338.2	3.84E-10	1.58E+02	5.96E+12
BZeoO7_C5eO7	O=C=CC(OO)C(O)C(O)C(=O)(OO(C(=O)C(O)C(O)C(OO)C=O))	370.2	5.90E-11	1.69E+02	1.38E+13

BZeoO7_C5eO9	O=C=CC(OO)C(O)C(O)C(=O)(OO(C(C(OO)C(O)C(O)C(OO)=O)=O))	402.2	1.23E-13	1.98E+02	1.61E+16
BZeoO7_C5O6	O=C=CC(OO)C(O)C(O)C(=O)(OO(C(=O)C(O)C(O)C=COO))	354.2	8.77E-10	1.57E+02	4.52E+11
BZeoO7_C5O8	O=C=CC(OO)C(O)C(O)C(=O)(OO(C(C(O)C(O)C(O)C(=O)OO)=O))	386.2	4.48E-12	1.82E+02	3.59E+14
BZeoO7_C6a	O=C=CC(OO)C(O)C(O)C(=O)(OOc1ccccc1)	284.2	2.60E-04	9.46E+01	1.06E+05
BZeoO7_CATE	O=C=CC(OO)C(O)C(O)C(=O)(OOc1ccccc1O)	300.2	5.53E-06	1.12E+02	5.58E+07
BZeoO7_DNP	O=C=CC(OO)C(O)C(O)C(=O)(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O)	440.2	4.06E-14	1.99E+02	8.02E+15
BZeoO7_EPX	O=C=CC(OO)C(O)C(O)C(=O)(OOC(=O)C1OC1C=O)	306.2	1.61E-03	8.99E+01	1.34E+05
BZeoO7_MALa	O=C=CC(OO)C(O)C(O)C(=O)(OOC(=O)C=CC=O)	290.2	6.50E-03	8.33E+01	2.92E+04
BZeoO7_MALb	O=C=CC(OO)C(O)C(O)C(=O)(OOC(C=O)C(O)C=O)	308.2	3.63E-07	1.27E+02	5.28E+09
BZeoO7_MALc	O=C=CC(OO)C(O)C(O)C(=O)(OOC1C(=O)OC(=O)C1O)	322.2	3.93E-07	1.27E+02	7.41E+08
BZeoO7_NBZa	O=C=CC(OO)C(O)C(O)C(=O)(OOC1C(=O)OCC1ON(=O)=O)	353.2	2.72E-08	1.35E+02	5.80E+09
BZeoO7_NBZb	O=C=CC(OO)C(O)C(O)C(=O)(OOC1C(=O)C=CC(=O)C1ON(=O)=O)	377.2	3.32E-09	1.44E+02	5.52E+10
BZeoO7_NCAT	O=C=CC(OO)C(O)C(O)C(=O)(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)O)	411.2	1.07E-13	1.97E+02	9.76E+15
BZeoO7_NDN	O=C=CC(OO)C(O)C(O)C(=O)(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)	485.2	1.48E-14	2.03E+02	9.71E+15
BZeoO7_NNC	O=C=CC(OO)C(O)C(O)C(=O)(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)	456.2	3.32E-14	2.01E+02	1.42E+16
BZeoO7_NPHa	O=C=CC(OO)C(O)C(O)C(=O)(OOC1(O)C=CC2OOC1C2ON(=O)=O)	395.2	3.81E-09	1.47E+02	2.55E+10
BZeoO7_NPHb	O=C=CC(OO)C(O)C(O)C(=O)(OOc1ccccc1N(=O)=O)	329.2	1.29E-06	1.17E+02	5.49E+06
BZeoO7_PBZ	O=C=CC(OO)C(O)C(O)C(=O)(OOC1C(=O)C=CC(=O)C1O)	332.2	1.04E-08	1.40E+02	3.83E+10
BZeoO7_PHEN	O=C=CC(OO)C(O)C(O)C(=O)(OOC1(O)C=CC2OOC1C2O)	350.2	1.46E-08	1.42E+02	1.54E+10
BZeoO9_9	O=C(OO(C(C(O)C(=O)CC(OO)C(=O)OO)=O))C(O)C(=O)CC(OO)C(=O)OO	446.2	3.55E-19	2.54E+02	1.72E+22
BZeoO9_BZBI	O=C(OOC1C=CC2OOC1C2O)C(O)C(=O)CC(OO)C(=O)OO	366.2	1.01E-11	1.71E+02	1.75E+13
BZeoO9_BZFU	O=C(OOC1C(O)COC1=O)C(O)C(=O)CC(OO)C(=O)OO	340.2	2.55E-13	1.87E+02	2.46E+15
BZeoO9_BZMUa	O=C(OOC(=O)C1OC1C=CC=O)C(O)C(=O)CC(OO)C(=O)OO	364.2	2.55E-09	1.45E+02	2.52E+10
BZeoO9_BZMUb	O=C(OO(C(C1OC1C=O)C(O)C=O))C(O)C(=O)CC(OO)C(=O)OO	382.2	6.21E-15	2.06E+02	6.02E+16
BZeoO9_C2a	O=C(OOC(=O)C=O)C(O)C(=O)CC(OO)C(=O)OO	296.1	5.72E-06	1.12E+02	1.75E+08
BZeoO9_C2b	O=C(OOCC=O)C(O)C(=O)CC(OO)C(=O)OO	282.2	1.30E-07	1.27E+02	1.63E+10
BZeoO9_C2c	O=C(OO(C(=O)CO))C(O)C(=O)CC(OO)C(=O)OO	298.2	2.94E-07	1.26E+02	7.43E+09
BZeoO9_C3a	O=C(OO(C(=O)C(C=O)O))C(O)C(=O)CC(OO)C(=O)OO	326.2	8.38E-09	1.42E+02	1.05E+11
BZeoO9_C3DI	O=C(OOC(C=O)C=O)C(O)C(=O)CC(OO)C(=O)OO	310.2	2.27E-09	1.46E+02	5.60E+11
BZeoO9_C4a	O=C(OOC(=O)C=CC(=O)C=O)C(O)C(=O)CC(OO)C(=O)OO	350.2	5.63E-09	1.42E+02	4.20E+10

BZeoO9_C5a	O=C(OO(C(=O)C=CC(=O)C(C=O)O))C(O)C(=O)CC(OO)C(=O)OO	380.2	3.24E-12	1.77E+02	6.82E+13
BZeoO9_C5DI	O=C(OO(C(C=O)C=CC=O))C(O)C(=O)CC(OO)C(=O)OO	336.2	1.27E-10	1.58E+02	2.50E+12
BZeoO9_C5eO5	O=C(OO(C(C(O)C(O)C=O)C=O))C(O)C(=O)CC(OO)C(=O)OO	370.2	4.54E-16	2.19E+02	2.90E+18
BZeoO9_C5eO7	O=C(OO(C(=O)C(O)C(O)C(OO)C=O))C(O)C(=O)CC(OO)C(=O)OO	402.2	4.84E-17	2.31E+02	1.86E+19
BZeoO9_C5eO9	O=C(OO(C(C(OO)C(O)C(O)C(OO)=O)=O))C(O)C(=O)CC(OO)C(=O)OO	434.2	4.64E-20	2.65E+02	1.91E+23
BZeoO9_C5O6	O=C(OO(C(=O)C(O)C(O)C=COO))C(O)C(=O)CC(OO)C(=O)OO	386.2	9.72E-16	2.17E+02	6.57E+17
BZeoO9_C5O8	O=C(OO(C(C(O)C(O)C(O)C(=O)OO)=O))C(O)C(=O)CC(OO)C(=O)OO	418.2	2.37E-18	2.47E+02	2.03E+21
BZeoO9_C6a	O=C(OOc1ccccc1)C(O)C(=O)CC(OO)C(=O)OO	316.2	6.93E-09	1.39E+02	4.78E+09
BZeoO9_CATE	O=C(OOc1ccccc1O)C(O)C(=O)CC(OO)C(=O)OO	332.2	8.34E-11	1.60E+02	1.09E+13
BZeoO9_DNP	O=C(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O)C(O)C(=O)CC(OO)C(=O)OO	472.2	3.96E-20	2.64E+02	1.01E+22
BZeoO9_EPX	O=C(OOC(=O)C1OC1C=O)C(O)C(=O)CC(OO)C(=O)OO	338.2	4.41E-08	1.33E+02	6.33E+09
BZeoO9_MALa	O=C(OOC(=O)C=CC=O)C(O)C(=O)CC(OO)C(=O)OO	322.2	2.41E-07	1.25E+02	9.82E+08
BZeoO9_MALb	O=C(OOC(C=O)C(O)C=O)C(O)C(=O)CC(OO)C(=O)OO	340.2	1.47E-12	1.80E+02	8.46E+14
BZeoO9_MALc	O=C(OOC1C(=O)OC(=O)C1O)C(O)C(=O)CC(OO)C(=O)OO	354.2	1.79E-12	1.80E+02	2.77E+14
BZeoO9_NBZa	O=C(OOC1C(=O)OCC1ON(=O)=O)C(O)C(=O)CC(OO)C(=O)OO	385.2	1.37E-13	1.89E+02	3.19E+15
BZeoO9_NBZb	O=C(OOC1C(=O)C=CC(=O)C1ON(=O)=O)C(O)C(=O)CC(OO)C(=O)OO	409.2	2.14E-14	1.98E+02	2.14E+16
BZeoO9_NCAT	O=C(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)O)C(O)C(=O)CC(OO)C(=O)OO	443.2	6.07E-20	2.63E+02	1.65E+22
BZeoO9_NDN	O=C(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)C(O)C(=O)CC(OO)C(=O)OO	517.2	2.32E-20	2.66E+02	1.03E+22
BZeoO9_NNC	O=C(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)C(O)C(=O)CC(OO)C(=O)OO	488.2	3.18E-20	2.65E+02	1.76E+22
BZeoO9_NPHa	O=C(OOC1(O)C=CC2OOC1C2ON(=O)=O)C(O)C(=O)CC(OO)C(=O)OO	427.2	1.92E-14	2.01E+02	8.62E+15
BZeoO9_NPHb	O=C(OOc1ccccc1N(=O)=O)C(O)C(=O)CC(OO)C(=O)OO	361.2	4.12E-11	1.62E+02	1.45E+11
BZeoO9_PBZ	O=C(OOC1C(=O)C=CC(=O)C1O)C(O)C(=O)CC(OO)C(=O)OO	364.2	4.02E-14	1.96E+02	1.63E+16
BZeoO9_PHEN	O=C(OOC1(O)C=CC2OOC1C2O)C(O)C(=O)CC(OO)C(=O)OO	382.2	4.42E-14	1.98E+02	6.34E+15
BZeouni_O5_O	OOC1C2OC2C3OOC1C3(=O)	174.1	3.33E-04	8.79E+01	1.02E+06
BZeouni_O7_O	O=C=CC(OO)C(=O)C(O)C(=O)OO	206.1	2.81E-05	1.04E+02	6.43E+08
BZeouni_O9_O	O=C(OO)C(=O)C(=O)CC(OO)C(=O)OO	238.1	1.47E-10	1.56E+02	9.17E+14
BZEPOXMUC	O=CC=CC1OC1C=O	126.1	3.89E-02	6.61E+01	9.87E+03
BZFU_BZFU	O(C1C(O)COC1=O)OC1C(O)COC1=O	234.2	3.38E-08	1.28E+02	4.68E+09
BZFU_C2a	O(C1C(O)COC1=O)OC(=O)C=O	190.1	5.73E-02	6.61E+01	2.01E+04
BZFU_C2b	O(C1C(O)COC1=O)OCC=O	176.1	2.25E-03	7.85E+01	2.46E+05

BZFU_C2c	OCC(=O)(OOC1C(O)COC1=O)	192.1	6.38E-03	7.61E+01	2.49E+05
BZFU_C3a	OC(C=O)C(=O)(OOC1C(O)COC1=O)	220.1	2.88E-04	9.06E+01	5.09E+06
BZFU_C4a	O(C1C(O)COC1=O)OC(=O)C=CC(=O)C=O	244.2	1.31E-04	9.18E+01	1.60E+06
BZFU_C5a	OC(C=O)C(=O)C=CC(=O)(OOC1C(O)COC1=O)	274.2	2.84E-07	1.20E+02	1.13E+09
BZFU_CATE	O(C1C(O)COC1=O)Oc1ccccc1O	226.2	6.55E-06	1.04E+02	5.88E+06
BZFU_DNP	O(C1C(O)COC1=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	366.2	6.09E-14	1.92E+02	2.24E+15
BZFU_MALc	O(C1C(O)COC1=O)OC1C(=O)OC(=O)C1O	248.1	2.45E-07	1.21E+02	7.41E+08
BZFU_NBZb	O(C1C(O)COC1=O)OC1C(=O)C=CC(=O)C1ON(=O)=O	303.2	2.54E-09	1.40E+02	1.21E+10
BZFU_NCAT	O(C1C(O)COC1=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	337.2	7.92E-14	1.92E+02	7.08E+15
BZFU_NDN	O(C1C(O)COC1=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	411.2	4.26E-14	1.94E+02	1.03E+15
BZFU_NNC	O(C1C(O)COC1=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	382.2	5.01E-14	1.94E+02	4.26E+15
BZFU_NPHb	O(C1C(O)COC1=O)Oc1ccccc1N(=O)=O	255.2	1.79E-06	1.08E+02	6.15E+05
BZFU_PBZ	O(C1C(O)COC1=O)OC1C(=O)C=CC(=O)C1O	258.2	4.94E-09	1.37E+02	2.39E+10
BZFUCO	OC1COC(=O)C1=O	116.1	8.19E-04	8.20E+01	2.60E+06
BZFUO	[O]C1C(O)COC1=O	117.1			
BZFUO2	[O]OC1C(O)COC1=O	133.1			
BZFUOH	OC1C(O)COC1=O	118.1	2.18E-04	8.82E+01	1.13E+07
BZFUONE	C1OC(=O)C=C1	84.1	5.47E-01	5.28E+01	2.98E+02
BZFUONOO	[O-][O+]=CC(=O)OCC=O	132.1			
BZFUONOOA	[O-][O+]=CC(=O)OCC=O	132.1			
BZFUOOH	OOC1C(O)COC1=O	134.1	1.13E-05	1.01E+02	5.74E+07
BZMUa_BZFU	O(C(=O)C1OC1C=CC=O)OC1C(O)COC1=O	258.2	8.47E-05	9.37E+01	5.49E+05
BZMUa_BZMUa	O(C(=O)C1OC1C=CC=O)OC(=O)C1OC1C=CC=O	282.2	2.35E-02	6.91E+01	1.14E+02
BZMUa_BZMUb	O=CC(O)C(OOC(=O)C1OC1C=CC=O)C1OC1C=O	300.2	3.10E-06	1.10E+02	3.01E+07
BZMUa_C2a	O(C(=O)C1OC1C=CC=O)OC(=O)C=O	214.1	6.03E+00	4.77E+01	1.59E+01
BZMUa_C2b	O(C(=O)C1OC1C=CC=O)OCC=O	200.2	5.30E-01	5.65E+01	3.51E+02
BZMUa_C2c	OCC(=O)(OOC(=O)C1OC1C=CC=O)	216.1	1.80E+00	5.43E+01	1.04E+02
BZMUa_C3a	OC(C=O)C(=O)(OOC(=O)C1OC1C=CC=O)	244.2	1.02E-01	6.68E+01	1.77E+03
BZMUa_C3DI	O(C(=O)C1OC1C=CC=O)OC(C=O)C=O	228.2	2.20E-02	7.00E+01	9.72E+03
BZMUa_C4a	O(C(=O)C1OC1C=CC=O)OC(=O)C=CC(=O)C=O	268.2	4.21E-02	6.73E+01	3.26E+02

BZMUa_C5a	OC(C=O)C(=O)C=CC(=O)(OOC(=O)C1OC1C=CC=O)	298.2	2.74E-04	9.06E+01	1.12E+05
BZMUa_C5DI	O=CC=CC(OOC(=O)C1OC1C=CC=O)C=O	254.2	2.48E-03	7.86E+01	1.33E+04
BZMUa_C6a	O(C(=O)C1OC1C=CC=O)Oc1ccccc1	234.2	6.59E-02	6.32E+01	1.25E+01
BZMUa_CATE	O(C(=O)C1OC1C=CC=O)Oc1ccccc1O	250.2	3.00E-03	7.73E+01	1.01E+04
BZMUa_DNP	O(C(=O)C1OC1C=CC=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	390.2	4.07E-10	1.52E+02	1.02E+11
BZMUa_EPX	O(C(=O)C1OC1C=CC=O)OC(=O)C1OC1C=O	256.2	1.96E-01	6.08E+01	9.74E+01
BZMUa_MALa	O(C(=O)C1OC1C=CC=O)OC(=O)C=CC=O	240.2	5.50E-01	5.64E+01	2.49E+01
BZMUa_MALb	O(C(=O)C1OC1C=CC=O)OC(C=O)C(O)C=O	258.2	1.75E-04	9.27E+01	2.09E+06
BZMUa_MALc	O(C(=O)C1OC1C=CC=O)OC1C(=O)OC(=O)C1O	272.2	3.17E-04	9.07E+01	1.48E+05
BZMUa_NBZa	O(C(=O)C1OC1C=CC=O)OC1C(=O)OCC1ON(=O)=O	303.2	3.14E-05	9.73E+01	2.98E+05
BZMUa_NBZb	O(C(=O)C1OC1C=CC=O)OC1C(=O)C=CC(=O)C1ON(=O)=O	327.2	6.39E-06	1.05E+02	9.82E+05
BZMUa_NCAT	O(C(=O)C1OC1C=CC=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	361.2	7.77E-10	1.51E+02	2.40E+11
BZMUa_NDN	O(C(=O)C1OC1C=CC=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	435.2	1.89E-10	1.55E+02	6.19E+10
BZMUa_NNC	O(C(=O)C1OC1C=CC=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	406.2	3.10E-10	1.54E+02	2.16E+11
BZMUa_NPHa	O(C(=O)C1OC1C=CC=O)OC1(O)C=CC2OOC1C2ON(=O)=O	345.2	6.72E-06	1.07E+02	1.04E+06
BZMUa_NPHb	O(C(=O)C1OC1C=CC=O)Oc1ccccc1N(=O)=O	279.2	1.01E-03	8.04E+01	1.30E+02
BZMUa_PBZ	O(C(=O)C1OC1C=CC=O)OC1C(=O)C=CC(=O)C1O	282.2	1.67E-05	1.01E+02	2.02E+06
BZMUa_PHEN	O(C(=O)C1OC1C=CC=O)OC1(O)C=CC2OOC1C2O	300.2	2.00E-05	1.04E+02	1.30E+06
BZMUb_BZFU	O=CC(O)C(OOC1C(O)COC1=O)C1OC1C=O	276.2	1.22E-09	1.45E+02	2.04E+11
BZMUb_BZMUb	O=CC(O)C(OO(C(C1OC1C=O)C(O)C=O))C1OC1C=O	318.2	2.64E-11	1.64E+02	1.68E+13
BZMUb_C2a	O=CC(O)C(OOC(=O)C=O)C1OC1C=O	232.1	2.05E-03	8.29E+01	9.27E+05
BZMUb_C2b	O=CC(O)C(OOCC=O)C1OC1C=O	218.2	6.29E-05	9.66E+01	1.76E+07
BZMUb_C2c	O=CC(O)C(OO(C(=O)CO))C1OC1C=O	234.2	2.74E-04	9.28E+01	9.63E+06
BZMUb_C3a	O=CC(O)C(OO(C(=O)C(C=O)O))C1OC1C=O	262.2	8.43E-06	1.08E+02	2.56E+08
BZMUb_C3DI	O=CC(O)C(OOC(C=O)C=O)C1OC1C=O	246.2	1.39E-06	1.14E+02	8.93E+08
BZMUb_C4a	O=CC(O)C(OOC(=O)C=CC(=O)C=O)C1OC1C=O	286.2	5.71E-06	1.07E+02	6.40E+07
BZMUb_C5a	O=CC(O)C(OO(C(=O)C=CC(=O)C(C=O)O))C1OC1C=O	316.2	8.87E-09	1.38E+02	5.52E+10
BZMUb_C5DI	O=CC(O)C(OO(C(C=O)C=CC=O))C1OC1C=O	272.2	1.22E-07	1.24E+02	1.95E+09
BZMUb_C6a	O=CC(O)C(OOc1ccccc1)C1OC1C=O	252.2	8.17E-06	1.04E+02	1.10E+06
BZMUb_CATE	O=CC(O)C(OOc1ccccc1O)C1OC1C=O	268.2	1.44E-07	1.23E+02	5.37E+08

BZMUb_DNP	O=CC(O)C(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O)C1OC1C=O	408.2	9.54E-16	2.13E+02	1.72E+17
BZMUb_EPX	O=CC(O)C(OOC(=O)C1OC1C=O)C1OC1C=O	274.2	3.60E-05	9.97E+01	1.44E+07
BZMUb_MALa	O=CC(O)C(OOC(=O)C=CC=O)C1OC1C=O	258.2	1.31E-04	9.38E+01	2.79E+06
BZMUb_MALb	O=CC(O)C(OOC(C=O)C(O)C=O)C1OC1C=O	276.2	2.61E-09	1.43E+02	5.85E+11
BZMUb_MALc	O=CC(O)C(OOC1C(=O)OC(=O)C1O)C1OC1C=O	290.2	6.44E-09	1.40E+02	3.78E+10
BZMUb_NBZa	O=CC(O)C(OOC1C(=O)OCC1ON(=O)=O)C1OC1C=O	321.2	7.12E-10	1.47E+02	1.21E+11
BZMUb_NBZb	O=CC(O)C(OOC1C(=O)C=CC(=O)C1ON(=O)=O)C1OC1C=O	345.2	1.25E-10	1.55E+02	5.21E+11
BZMUb_NCAT	O=CC(O)C(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)O)C1OC1C=O	379.2	1.38E-15	2.13E+02	4.19E+17
BZMUb_NDN	O=CC(O)C(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)C1OC1C=O	453.2	5.96E-16	2.15E+02	1.04E+17
BZMUb_NNC	O=CC(O)C(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)C1OC1C=O	424.2	7.78E-16	2.15E+02	3.10E+17
BZMUb_NPHa	O=CC(O)C(OOC1(O)C=CC2OOC1C2ON(=O)=O)C1OC1C=O	363.2	1.19E-10	1.58E+02	3.50E+11
BZMUb_NPHb	O=CC(O)C(OOc1ccccc1N(=O)=O)C1OC1C=O	297.2	5.64E-08	1.26E+02	3.68E+07
BZMUb_PBZ	O=CC(O)C(OOC1C(=O)C=CC(=O)C1O)C1OC1C=O	300.2	2.25E-10	1.53E+02	8.17E+11
BZMUb_PHEN	O=CC(O)C(OOC1(O)C=CC2OOC1C2O)C1OC1C=O	318.2	2.59E-10	1.55E+02	4.37E+11
BZo_O4_2OH	O=CC(O)C(O)C1OC1C(O)=O	176.1	8.81E-09	1.39E+02	1.66E+12
BZo_O5_NO3	O=CC(O)C(O)C1OC1C(ON(=O)=O)=O	221.1	3.42E-01	6.48E+01	6.87E+03
BZo_O5_O	O=CC(=O)C(O)C1OC1C(O)=O	174.1	1.81E-07	1.23E+02	7.52E+10
BZo_O5_OOH	O=CC(O)C(O)C1OC1C(OO)=O	192.1	6.81E-08	1.29E+02	2.60E+10
BZo_O6_2OH	O=C(O)C(O)C(O)C1OC1C(OO)=O	208.1	3.51E-11	1.65E+02	1.21E+14
BZo_O7_NO3	O=C(ON(=O)=O)C(O)C(O)C1OC1C(OO)=O	253.1	5.68E-03	8.38E+01	4.48E+05
BZo_O7_O	O=C(O)C(=O)C(O)C1OC1C(OO)=O	206.1	9.09E-10	1.48E+02	6.29E+12
BZo_O7_OOH	O=C(OO)C(O)C(O)C1OC1C(OO)=O	224.1	3.12E-10	1.55E+02	4.29E+13
BZo_O8_2OH	O=C(OO)C(O)C(O)C(=O)C(O)C(=O)OO	240.1	1.74E-13	1.90E+02	1.52E+17
BZo_O9_NO3	O=C(OO)C(O)C(O)C(=O)C(ON(=O)=O)C(=O)OO	285.1	1.46E-13	1.90E+02	1.60E+17
BZo_O9_O	O=C(OO)C(O)C(O)C(=O)C(=O)C(=O)OO	238.1	6.32E-12	1.72E+02	6.36E+15
BZo_O9_OOH	O=C(OO)C(O)C(O)C(=O)C(OO)C(=O)OO	256.1	3.81E-15	2.08E+02	1.73E+19
BZo_RO_O10	O=C(OO)C(O)C(O)C(=O)C([O])C(=O)OO	239.1			
BZo_RO_O6	O=CC(O)C(O)C1OC1C([O])=O	175.1			
BZo_RO_O8	O=C([O])C(O)C(O)C1OC1C(OO)=O	207.1			
BZo_RO2_O11	O=C(OO)C(O)C(O)C(=O)C(O[O])C(=O)OO	255.1			

BZo_RO2_O7	O=CC(O)C(O)C1OC1C(O[O])=O	191.1			
BZo_RO2_O9	O=C(O[O])C(O)C(O)C1OC1C(OO)=O	223.1			
BZo2_RO_O10	O=C(OO)C(O)C(O)C(=O)C([O])C(=O)OO	239.1			
BZo2_RO_O6	O=CC(O)C(O)C1OC1C([O])=O	175.1			
BZo2_RO_O8	O=C([O])C(O)C(O)C1OC1C(OO)=O	207.1			
BZOBIPEROH	O=C1C=CC2OOC1C2O	142.1	3.07E-02	6.79E+01	1.08E+04
BZoO10_10	O=C(OO)C(O)C(O)C(=O)C(OO(C(C(=O)OO)C(=O)C(O)C(O)C(OO)=O))C(=O)OO	478.2	1.54E-30	3.84E+02	1.68E+35
BZoO10_5	O=C(OO)C(O)C(O)C(=O)C(OOC1C2OC2C3OOC1C3(O))C(=O)OO	398.2	1.93E-17	2.34E+02	4.21E+19
BZoO10_7	O=C(OO)C(O)C(O)C(=O)C(OO(C(=O)C(O)C(O)C(OO)C=C=O))C(=O)OO	430.2	9.89E-18	2.40E+02	1.43E+21
BZoO10_9	O=C(OO)C(O)C(O)C(=O)C(OO(C(C(O)C(=O)CC(OO)C(=O)OO)=O))C(=O)OO	462.2	1.56E-24	3.14E+02	5.37E+28
BZoO10_BZBI	O=C(OO)C(O)C(O)C(=O)C(OOC1C=CC2OOC1C2O)C(=O)OO	382.2	3.45E-16	2.20E+02	2.49E+18
BZoO10_BZFU	O=C(OO)C(O)C(O)C(=O)C(OOC1C(O)COC1=O)C(=O)OO	356.2	3.67E-18	2.41E+02	8.11E+20
BZoO10_BZMUa	O=C(OO)C(O)C(O)C(=O)C(OOC(=O)C1OC1C=CC=O)C(=O)OO	380.2	2.33E-13	1.89E+02	4.98E+15
BZoO10_BZMUb	O=C(OO)C(O)C(O)C(=O)C(OO(C(C1OC1C=O)C(O)C=O))C(=O)OO	398.2	7.14E-20	2.61E+02	1.60E+22
BZoO10_C2a	O=C(OO)C(O)C(O)C(=O)C(OOC(=O)C=O)C(=O)OO	312.1	1.05E-09	1.51E+02	1.06E+13
BZoO10_C2b	O=C(OO)C(O)C(O)C(=O)C(OOCC=O)C(=O)OO	298.2	1.07E-11	1.70E+02	6.88E+14
BZoO10_C2c	O=C(OO)C(O)C(O)C(=O)C(OO(C(=O)CO))C(=O)OO	314.2	2.77E-11	1.68E+02	9.96E+14
BZoO10_C3a	O=C(OO)C(O)C(O)C(=O)C(OO(C(=O)C(C=O)O))C(=O)OO	342.2	5.28E-13	1.87E+02	1.68E+16
BZoO10_C3DI	O=C(OO)C(O)C(O)C(=O)C(OOC(C=O)C=O)C(=O)OO	326.2	1.21E-13	1.91E+02	3.09E+16
BZoO10_C4a	O=C(OO)C(O)C(O)C(=O)C(OOC(=O)C=CC(=O)C=O)C(=O)OO	366.2	5.10E-13	1.85E+02	7.13E+15
BZoO10_C5a	O=C(OO)C(O)C(O)C(=O)C(OO(C(=O)C=CC(=O)C(C=O)O))C(=O)OO	396.2	9.73E-17	2.26E+02	3.05E+19
BZoO10_C5DI	O=C(OO)C(O)C(O)C(=O)C(OO(C(C=O)C=CC=O))C(=O)OO	352.2	5.63E-15	2.05E+02	2.11E+17
BZoO10_C5eO5	O=C(OO)C(O)C(O)C(=O)C(OO(C(C(O)C(O)C=O)C=O))C(=O)OO	386.2	2.75E-21	2.77E+02	1.23E+24
BZoO10_C5eO7	O=C(OO)C(O)C(O)C(=O)C(OO(C(=O)C(O)C(O)C(OO)C=O))C(=O)OO	418.2	2.51E-22	2.90E+02	3.30E+25
BZoO10_C5eO9	O=C(OO)C(O)C(O)C(=O)C(OO(C(C(OO)C(O)C(O)C(OO)=O)=O))C(=O)OO	450.2	1.27E-25	3.27E+02	7.62E+29
BZoO10_C5O6	O=C(OO)C(O)C(O)C(=O)C(OO(C(=O)C(O)C(O)C=COO))C(=O)OO	402.2	6.89E-21	2.74E+02	1.16E+24
BZoO10_C5O8	O=C(OO)C(O)C(O)C(=O)C(OO(C(C(O)C(O)C(O)C(=O)OO)=O))C(=O)OO	434.2	9.54E-24	3.06E+02	4.99E+27
BZoO10_C6a	O=C(OO)C(O)C(O)C(=O)C(OOc1ccccc1)C(=O)OO	332.2	5.93E-13	1.83E+02	1.94E+14
BZoO10_CATE	O=C(OO)C(O)C(O)C(=O)C(OOc1ccccc1O)C(=O)OO	348.2	4.31E-15	2.06E+02	8.17E+17
BZoO10_DNP	O=C(OO)C(O)C(O)C(=O)C(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O)C(=O)OO	488.2	1.62E-25	3.25E+02	8.92E+27

BZoO10_EPX	O=C(OO)C(O)C(O)C(=O)C(OOC(=O)C1OC1C=O)C(=O)OO	354.2	4.99E-12	1.75E+02	7.50E+14
BZoO10_MALa	O=C(OO)C(O)C(O)C(=O)C(OOC(=O)C=CC=O)C(=O)OO	338.2	3.41E-11	1.66E+02	1.07E+14
BZoO10_MALb	O=C(OO)C(O)C(O)C(=O)C(OOC(C=O)C(O)C=O)C(=O)OO	356.2	2.64E-17	2.32E+02	1.29E+20
BZoO10_MALc	O=C(OO)C(O)C(O)C(=O)C(OOC1C(=O)OC(=O)C1O)C(=O)OO	370.2	3.81E-17	2.31E+02	6.93E+19
BZoO10_NBZa	O=C(OO)C(O)C(O)C(=O)C(OOC1C(=O)OCC1ON(=O)=O)C(=O)OO	401.2	2.94E-18	2.41E+02	8.11E+20
BZoO10_NBZb	O=C(OO)C(O)C(O)C(=O)C(OOC1C(=O)C=CC(=O)C1ON(=O)=O)C(=O)OO	425.2	4.00E-19	2.51E+02	5.81E+21
BZoO10_NCAT	O=C(OO)C(O)C(O)C(=O)C(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)O)C(=O)OO	459.2	1.91E-25	3.25E+02	1.60E+28
BZoO10_NDN	O=C(OO)C(O)C(O)C(=O)C(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)C(=O)OO	533.2	1.30E-25	3.26E+02	7.63E+27
BZoO10_NNC	O=C(OO)C(O)C(O)C(=O)C(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)C(=O)OO	504.2	1.40E-25	3.26E+02	1.37E+28
BZoO10_NPHa	O=C(OO)C(O)C(O)C(=O)C(OOC1(O)C=CC2OOC1C2ON(=O)=O)C(=O)OO	443.2	3.87E-19	2.53E+02	1.94E+21
BZoO10_NPHb	O=C(OO)C(O)C(O)C(=O)C(OOc1ccccc1N(=O)=O)C(=O)OO	377.2	1.73E-15	2.10E+02	1.25E+16
BZoO10_PBZ	O=C(OO)C(O)C(O)C(=O)C(OOC1C(=O)C=CC(=O)C1O)C(=O)OO	380.2	5.31E-19	2.50E+02	5.39E+21
BZoO10_PHEN	O=C(OO)C(O)C(O)C(=O)C(OOC1(O)C=CC2OOC1C2O)C(=O)OO	398.2	6.42E-19	2.51E+02	1.72E+21
BZoO6_BZBI	O=CC(O)C(O)C1OC1C(=O)(OOC1C=CC2OOC1C2O)	318.2	1.00E-07	1.29E+02	7.74E+08
BZoO6_BZeoO5	O=CC(O)C(O)C1OC1C(=O)(OOC1C2OC2C3OOC1C3(O))	334.2	1.09E-08	1.39E+02	6.51E+09
BZoO6_BZeoO7	O=CC(O)C(O)C1OC1C(=O)(OO(C(=O)C(O)C(O)C(OO)C=C=O))	366.2	8.34E-09	1.46E+02	3.81E+10
BZoO6_BZeoO9	O=CC(O)C(O)C1OC1C(=O)(OO(C(C(O)C(=O)CC(OO)C(=O)OO)=O))	398.2	2.15E-14	2.02E+02	1.17E+16
BZoO6_BZFU	O=CC(O)C(O)C1OC1C(=O)(OOC1C(O)COC1=O)	292.2	4.85E-09	1.41E+02	9.85E+10
BZoO6_BZMUa	O=CC(O)C(O)C1OC1C(=O)(OOC(=O)C1OC1C=CC=O)	316.2	9.81E-06	1.08E+02	6.22E+06
BZoO6_BZMUb	O=CC(O)C(O)C1OC1C(=O)(OO(C(C1OC1C=O)C(O)C=O))	334.2	1.15E-10	1.60E+02	6.20E+12
BZoO6_BZoO10	O=CC(O)C(O)C1OC1C(=O)(OO(C(C(=O)OO)C(=O)C(O)C(O)C(OO)=O))	414.2	3.01E-19	2.55E+02	8.73E+21
BZoO6_BZoO6	O=CC(O)C(O)C1OC1C(=O)(OO(C(=O)C1OC1C(O)C(O)C=O))	350.2	4.62E-10	1.56E+02	1.02E+12
BZoO6_BZoO8	O=CC(O)C(O)C1OC1C(=O)(OO(C(C(O)C(O)C1OC1C(OO)=O)=O))	382.2	1.53E-12	1.83E+02	1.24E+14
BZoO6_C2a	O=CC(O)C(O)C1OC1C(=O)(OOC(=O)C=O)	248.1	1.06E-02	7.92E+01	1.13E+05
BZoO6_C2b	O=CC(O)C(O)C1OC1C(=O)(OOCC=O)	234.2	3.87E-04	9.18E+01	4.46E+06
BZoO6_C2c	O=CC(O)C(O)C1OC1C(=O)(OO(C(=O)CO))	250.2	1.26E-03	8.95E+01	1.30E+06
BZoO6_C3a	O=CC(O)C(O)C1OC1C(=O)(OO(C(=O)C(C=O)O))	278.2	4.18E-05	1.05E+02	3.47E+07
BZoO6_C3DI	O=CC(O)C(O)C1OC1C(=O)(OOC(C=O)C=O)	262.2	8.43E-06	1.08E+02	2.56E+08
BZoO6_C4a	O=CC(O)C(O)C1OC1C(=O)(OOC(=O)C=CC(=O)C=O)	302.2	1.90E-05	1.05E+02	1.36E+07
BZoO6_C5a	O=CC(O)C(O)C1OC1C(=O)(OO(C(=O)C=CC(=O)C(C=O)O))	332.2	2.99E-08	1.35E+02	1.17E+10

BZoO6_C5DI	O=CC(O)C(O)C1OC1C(=O)(OO(C(C=O)C=CC=O))	288.2	5.82E-07	1.19E+02	8.41E+08
BZoO6_C5eO5	O=CC(O)C(O)C1OC1C(=O)(OO(C(C(O)C(O)C=O)C=O))	322.2	1.29E-11	1.71E+02	2.27E+14
BZoO6_C5eO7	O=CC(O)C(O)C1OC1C(=O)(OO(C(=O)C(O)C(O)C(OO)C=O))	354.2	2.23E-12	1.81E+02	1.79E+14
BZoO6_C5eO9	O=CC(O)C(O)C1OC1C(=O)(OO(C(C(OO)C(O)C(O)C(OO)=O)=O))	386.2	4.52E-15	2.11E+02	8.40E+16
BZoO6_C5O6	O=CC(O)C(O)C1OC1C(=O)(OO(C(=O)C(O)C(O)C=COO))	338.2	4.04E-11	1.68E+02	3.88E+12
BZoO6_C5O8	O=CC(O)C(O)C1OC1C(=O)(OO(C(C(O)C(O)C(O)C(=O)OO)=O))	370.2	1.71E-13	1.94E+02	4.59E+15
BZoO6_C6a	O=CC(O)C(O)C1OC1C(=O)(OOc1ccccc1)	268.2	2.75E-05	1.01E+02	6.83E+05
BZoO6_CATE	O=CC(O)C(O)C1OC1C(=O)(OOc1ccccc1O)	284.2	4.77E-07	1.20E+02	2.52E+08
BZoO6_DNP	O=CC(O)C(O)C1OC1C(=O)(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O)	424.2	2.64E-15	2.10E+02	1.11E+17
BZoO6_EPX	O=CC(O)C(O)C1OC1C(=O)(OOC(=O)C1OC1C=O)	290.2	1.36E-04	9.69E+01	2.19E+06
BZoO6_MALa	O=CC(O)C(O)C1OC1C(=O)(OOC(=O)C=CC=O)	274.2	5.47E-04	9.06E+01	4.73E+05
BZoO6_MALb	O=CC(O)C(O)C1OC1C(=O)(OOC(C=O)C(O)C=O)	292.2	1.54E-08	1.38E+02	1.61E+11
BZoO6_MALc	O=CC(O)C(O)C1OC1C(=O)(OOC1C(=O)OC(=O)C1O)	306.2	2.62E-08	1.36E+02	2.22E+10
BZoO6_NBZa	O=CC(O)C(O)C1OC1C(=O)(OOC1C(=O)OCC1ON(=O)=O)	337.2	2.14E-09	1.44E+02	8.32E+10
BZoO6_NBZb	O=CC(O)C(O)C1OC1C(=O)(OOC1C(=O)C=CC(=O)C1ON(=O)=O)	361.2	2.91E-10	1.54E+02	4.32E+11
BZoO6_NCAT	O=CC(O)C(O)C1OC1C(=O)(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)O)	395.2	5.07E-15	2.09E+02	2.01E+17
BZoO6_NDN	O=CC(O)C(O)C1OC1C(=O)(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)	469.2	1.28E-15	2.13E+02	9.00E+16
BZoO6_NNC	O=CC(O)C(O)C1OC1C(=O)(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)	440.2	2.16E-15	2.12E+02	2.01E+17
BZoO6_NPHa	O=CC(O)C(O)C1OC1C(=O)(OOC1(O)C=CC2OOC1C2ON(=O)=O)	379.2	3.32E-10	1.55E+02	2.35E+11
BZoO6_NPHb	O=CC(O)C(O)C1OC1C(=O)(OOc1ccccc1N(=O)=O)	313.2	1.41E-07	1.24E+02	4.25E+07
BZoO6_PBZ	O=CC(O)C(O)C1OC1C(=O)(OOC1C(=O)C=CC(=O)C1O)	316.2	6.91E-10	1.50E+02	4.82E+11
BZoO6_PHEN	O=CC(O)C(O)C1OC1C(=O)(OOC1(O)C=CC2OOC1C2O)	334.2	9.46E-10	1.52E+02	2.16E+11
BZoO8_BZBI	O=C(OOC1C=CC2OOC1C2O)C(O)C(O)C1OC1C(OO)=O	350.2	4.62E-10	1.55E+02	2.00E+11
BZoO8_BZeoO5	O=C(OOC1C2OC2C3OOC1C3(O))C(O)C(O)C1OC1C(OO)=O	366.2	4.39E-11	1.65E+02	1.89E+12
BZoO8_BZeoO7	O=C(OO(C(=O)C(O)C(O)C(OO)C=C=O))C(O)C(O)C1OC1C(OO)=O	398.2	2.87E-11	1.72E+02	1.66E+13
BZoO8_BZeoO9	O=C(OO(C(C(O)C(=O)CC(OO)C(=O)OO)=O))C(O)C(O)C1OC1C(OO)=O	430.2	3.37E-17	2.33E+02	5.38E+19
BZoO8_BZFU	O=C(OOC1C(O)COC1=O)C(O)C(O)C1OC1C(OO)=O	324.2	1.67E-11	1.68E+02	2.32E+13
BZoO8_BZMUa	O=C(OOC(=O)C1OC1C=CC=O)C(O)C(O)C1OC1C(OO)=O	348.2	9.06E-08	1.30E+02	4.43E+08
BZoO8_BZMUb	O=C(OO(C(C1OC1C=O)C(O)C=O))C(O)C(O)C1OC1C(OO)=O	366.2	4.13E-13	1.87E+02	6.56E+14
BZoO8_BZoO10	O=C(OO(C(C(=O)OO)C(=O)C(O)C(O)C(OO)=O))C(O)C(O)C1OC1C(OO)=O	446.2	2.46E-22	2.90E+02	8.64E+25

BZoO8_BZoO8	O=C(OO(C(C(O)C(O)C1OC1C(OO)=O)=O))C(O)C(O)C1OC1C(OO)=O	414.2	3.27E-15	2.12E+02	2.03E+17
BZoO8_C2a	O=C(OOC(=O)C=O)C(O)C(O)C1OC1C(OO)=O	280.1	1.63E-04	9.87E+01	3.36E+06
BZoO8_C2b	O=C(OOCC=O)C(O)C(O)C1OC1C(OO)=O	266.2	4.34E-06	1.13E+02	2.47E+08
BZoO8_C2c	O=C(OO(C(=O)CO))C(O)C(O)C1OC1C(OO)=O	282.2	1.12E-05	1.11E+02	1.02E+08
BZoO8_C3a	O=C(OO(C(=O)C(C=O)O))C(O)C(O)C1OC1C(OO)=O	310.2	3.43E-07	1.27E+02	1.68E+09
BZoO8_C3DI	O=C(OOC(C=O)C=O)C(O)C(O)C1OC1C(OO)=O	294.2	8.20E-08	1.30E+02	9.70E+09
BZoO8_C4a	O=C(OOC(=O)C=CC(=O)C=O)C(O)C(O)C1OC1C(OO)=O	334.2	1.70E-07	1.27E+02	8.78E+08
BZoO8_C5a	O=C(OO(C(=O)C=CC(=O)C(C=O)O))C(O)C(O)C1OC1C(OO)=O	364.2	1.43E-10	1.60E+02	1.16E+12
BZoO8_C5DI	O=C(OO(C(C=O)C=CC=O))C(O)C(O)C1OC1C(OO)=O	320.2	4.68E-09	1.42E+02	4.87E+10
BZoO8_C5eO5	O=C(OO(C(C(O)C(O)C=O)C=O))C(O)C(O)C1OC1C(OO)=O	354.2	3.54E-14	1.99E+02	2.93E+16
BZoO8_C5eO7	O=C(OO(C(=O)C(O)C(O)C(OO)C=O))C(O)C(O)C1OC1C(OO)=O	386.2	4.52E-15	2.11E+02	8.40E+16
BZoO8_C5eO9	O=C(OO(C(C(OO)C(O)C(O)C(OO)=O)=O))C(O)C(O)C1OC1C(OO)=O	418.2	5.92E-18	2.43E+02	4.04E+20
BZoO8_C5O6	O=C(OO(C(=O)C(O)C(O)C=COO))C(O)C(O)C1OC1C(OO)=O	370.2	8.53E-14	1.97E+02	2.98E+15
BZoO8_C5O8	O=C(OO(C(C(O)C(O)C(O)C(=O)OO)=O))C(O)C(O)C1OC1C(OO)=O	402.2	2.75E-16	2.25E+02	7.24E+18
BZoO8_C6a	O=C(OOc1ccccc1)C(O)C(O)C1OC1C(OO)=O	300.2	2.18E-07	1.24E+02	5.57E+07
BZoO8_CATE	O=C(OOc1ccccc1O)C(O)C(O)C1OC1C(OO)=O	316.2	3.63E-09	1.43E+02	8.03E+10
BZoO8_DNP	O=C(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O)C(O)C(O)C1OC1C(OO)=O	456.2	3.48E-18	2.43E+02	6.76E+19
BZoO8_EPX	O=C(OOC(=O)C1OC1C=O)C(O)C(O)C1OC1C(OO)=O	322.2	1.51E-06	1.18E+02	1.02E+08
BZoO8_MALa	O=C(OOC(=O)C=CC=O)C(O)C(O)C1OC1C(OO)=O	306.2	6.92E-06	1.11E+02	2.16E+07
BZoO8_MALb	O=C(OOC(C=O)C(O)C=O)C(O)C(O)C1OC1C(OO)=O	324.2	7.83E-11	1.63E+02	1.13E+13
BZoO8_MALc	O=C(OOC1C(=O)OC(=O)C1O)C(O)C(O)C1OC1C(OO)=O	338.2	9.92E-11	1.62E+02	3.98E+12
BZoO8_NBZa	O=C(OOC1C(=O)OCC1ON(=O)=O)C(O)C(O)C1OC1C(OO)=O	369.2	7.90E-12	1.71E+02	2.76E+13
BZoO8_NBZb	O=C(OOC1C(=O)C=CC(=O)C1ON(=O)=O)C(O)C(O)C1OC1C(OO)=O	393.2	9.02E-13	1.81E+02	2.21E+14
BZoO8_NCAT	O=C(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)O)C(O)C(O)C1OC1C(OO)=O	427.2	6.40E-18	2.41E+02	1.05E+20
BZoO8_NDN	O=C(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)C(O)C(O)C1OC1C(OO)=O	501.2	1.77E-18	2.45E+02	6.72E+19
BZoO8_NNC	O=C(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)C(O)C(O)C1OC1C(OO)=O	472.2	2.87E-18	2.44E+02	1.15E+20
BZoO8_NPHa	O=C(OOC1(O)C=CC2OOC1C2ON(=O)=O)C(O)C(O)C1OC1C(OO)=O	411.2	1.04E-12	1.83E+02	8.28E+13
BZoO8_NPHb	O=C(OOc1ccccc1N(=O)=O)C(O)C(O)C1OC1C(OO)=O	345.2	7.74E-10	1.49E+02	3.66E+09
BZoO8_PBZ	O=C(OOC1C(=O)C=CC(=O)C1O)C(O)C(O)C1OC1C(OO)=O	348.2	1.99E-12	1.78E+02	1.76E+14
BZoO8_PHEN	O=C(OOC1(O)C=CC2OOC1C2O)C(O)C(O)C1OC1C(OO)=O	366.2	2.80E-12	1.79E+02	6.17E+13

BZouni_O10_O	O=C(OO)C(=O)C(O)C(=O)C(OO)C(=O)OO	254.1	1.71E-13	1.88E+02	9.04E+17
BZouni_O6_O	O=CC(=O)C(O)C1OC1C(OO)=O	190.1	1.09E-06	1.15E+02	1.90E+09
BZouni_O8_O	O=C(OO)C(=O)C(O)C1OC1C(OO)=O	222.1	6.43E-09	1.39E+02	4.15E+12
C2a_C2a	O(C(=O)C=O)OC(=O)C=O	146.1	1.54E+03	2.78E+01	1.78E+00
C2a_C2b	O(C(=O)C=O)OCC=O	132.1	1.43E+02	3.57E+01	4.16E+01
C2a_C2c	OCC(=O)(OOC(=O)C=O)	148.1	1.22E+03	3.04E+01	4.30E+00
C2a_C4a	O(C(=O)C=O)OC(=O)C=CC(=O)C=O	200.1	1.46E+01	4.43E+01	2.94E+01
C2a_C5a	OC(C=O)C(=O)C=CC(=O)(OOC(=O)C=O)	230.1	1.79E-01	6.41E+01	4.15E+03
C2a_DNP	O(C(=O)C=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	322.1	6.04E-07	1.20E+02	1.38E+09
C2a_MALc	O(C(=O)C=O)OC1C(=O)OC(=O)C1O	204.1	2.82E-01	6.33E+01	3.39E+03
C2a_NBZb	O(C(=O)C=O)OC1C(=O)C=CC(=O)C1ON(=O)=O	259.1	4.26E-03	7.68E+01	7.65E+04
C2a_NCAT	O(C(=O)C=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	293.1	1.69E-06	1.17E+02	1.57E+09
C2a_NDN	O(C(=O)C=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	367.1	2.24E-07	1.23E+02	1.52E+09
C2a_NNC	O(C(=O)C=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	338.1	5.20E-07	1.21E+02	2.39E+09
C2a_NPHb	O(C(=O)C=O)Oc1ccccc1N(=O)=O	211.1	2.61E-01	5.70E+01	2.18E+01
C2a_PBZ	O(C(=O)C=O)OC1C(=O)C=CC(=O)C1O	214.1	1.48E-02	7.25E+01	6.68E+04
C2b_C2b	O(CC=O)OCC=O	118.1	7.61E+00	4.60E+01	3.99E+02
C2b_C2c	OCC(=O)(OOCC=O)	134.1	1.05E+02	3.85E+01	6.33E+01
C2b_C4a	O(CC=O)OC(=O)C=CC(=O)C=O	186.1	1.34E+00	5.28E+01	5.98E+02
C2b_C5a	OC(C=O)C(=O)C=CC(=O)(OOCC=O)	216.1	1.03E-02	7.48E+01	1.13E+05
C2b_DNP	O(CC=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	308.2	1.53E-08	1.35E+02	2.79E+10
C2b_MALc	O(CC=O)OC1C(=O)OC(=O)C1O	190.1	1.24E-02	7.49E+01	4.10E+04
C2b_NBZb	O(CC=O)OC1C(=O)C=CC(=O)C1ON(=O)=O	245.1	2.38E-04	8.82E+01	5.32E+05
C2b_NCAT	O(CC=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	279.2	3.30E-08	1.33E+02	4.40E+10
C2b_NDN	O(CC=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	353.2	7.35E-09	1.38E+02	2.23E+10
C2b_NNC	O(CC=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	324.2	1.36E-08	1.37E+02	4.79E+10
C2b_NPHb	O(CC=O)Oc1ccccc1N(=O)=O	197.1	1.93E-02	6.69E+01	1.47E+02
C2b_PBZ	O(CC=O)OC1C(=O)C=CC(=O)C1O	200.2	6.47E-04	8.46E+01	6.86E+05
C2c_C2c	OCC(=O)(OO(C(=O)CO))	150.1	2.50E+02	3.79E+01	2.06E+01
C2c_C4a	OCC(=O)(OOC(=O)C=CC(=O)C=O)	202.1	4.10E+00	5.07E+01	2.14E+02

C2c_C5a	OCC(=O)(OO(C(=O)C=CC(=O)C(C=O)O))	232.1	2.85E-02	7.31E+01	4.15E+04
C2H4	C=C	28.1	1.42E+04	1.68E+01	7.55E-02
C2OHOCO2H	OCC(O)C(=O)O	106.1	1.05E-05	1.07E+02	5.62E+09
C2OHOCOOH	OCC(O)C(=O)OO	122.1	9.78E-05	9.72E+01	1.45E+08
C32OH13CO	O=CC(O)C=O	88.1	1.67E-01	6.35E+01	5.87E+04
C33CO	O=CC(=O)C=O	86.0	2.11E+00	5.11E+01	3.94E+03
C3a_C2a	OC(C=O)C(=O)(OOC(=O)C=O)	176.1	6.19E+01	4.25E+01	6.15E+01
C3a_C2b	OC(C=O)C(=O)(OOCC=O)	162.1	4.02E+00	5.20E+01	1.50E+03
C3a_C2c	OC(C=O)C(=O)(OO(C(=O)CO))	178.1	1.85E+01	4.89E+01	3.05E+02
C3a_C3a	OC(C=O)C(=O)(OO(C(=O)C(C=O)O))	206.1	8.19E-01	6.19E+01	5.39E+03
C3a_C4a	OC(C=O)C(=O)(OOC(=O)C=CC(=O)C=O)	230.1	2.34E-01	6.32E+01	3.18E+03
C3a_C5a	OC(C=O)C(=O)(OO(C(=O)C=CC(=O)C(C=O)O))	260.2	1.23E-03	8.70E+01	8.25E+05
C3a_CATE	OC(C=O)C(=O)(OOc1ccccc1O)	212.2	1.11E-02	7.47E+01	5.21E+04
C3a_DNP	OC(C=O)C(=O)(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O)	352.2	8.57E-10	1.50E+02	1.13E+12
C3a_MALc	OC(C=O)C(=O)(OOC1C(=O)OC(=O)C1O)	234.1	1.49E-03	8.71E+01	9.91E+05
C3a_NBZb	OC(C=O)C(=O)(OOC1C(=O)C=CC(=O)C1ON(=O)=O)	289.2	1.93E-05	1.02E+02	2.39E+07
C3a_NCAT	OC(C=O)C(=O)(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)O)	323.2	2.17E-09	1.48E+02	1.40E+12
C3a_NDN	OC(C=O)C(=O)(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)	397.2	3.44E-10	1.54E+02	1.18E+12
C3a_NNC	OC(C=O)C(=O)(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)	368.2	7.41E-10	1.52E+02	1.89E+12
C3a_NPHb	OC(C=O)C(=O)(OOc1ccccc1N(=O)=O)	241.2	2.65E-03	7.89E+01	5.79E+03
C3a_PBZ	OC(C=O)C(=O)(OOC1C(=O)C=CC(=O)C1O)	244.2	5.93E-05	9.80E+01	1.92E+07
C3DI_BZFU	O(C(C=O)C=O)OC1C(O)COC1=O	204.1	5.46E-05	9.52E+01	1.29E+07
C3DI_C2a	O(C(C=O)C=O)OC(=O)C=O	160.1	5.67E+00	4.85E+01	7.34E+02
C3DI_C2b	O(C(C=O)C=O)OCC=O	146.1	2.45E-01	6.00E+01	1.22E+04
C3DI_C2c	OCC(=O)(OOC(C=O)C=O)	162.1	2.77E+00	5.30E+01	3.32E+03
C3DI_C3a	OC(C=O)C(=O)(OOC(C=O)C=O)	190.1	1.08E-01	6.67E+01	5.52E+04
C3DI_C3DI	O(C(C=O)C=O)OC(C=O)C=O	174.1	8.14E-03	7.43E+01	2.87E+05
C3DI_C4a	O(C(C=O)C=O)OC(=O)C=CC(=O)C=O	214.1	5.10E-02	6.65E+01	1.46E+04
C3DI_C5a	OC(C=O)C(=O)C=CC(=O)(OOC(C=O)C=O)	244.2	2.93E-04	9.02E+01	4.35E+06
C3DI_C6a	O(C(C=O)C=O)Oc1ccccc1	180.2	4.20E-02	6.52E+01	4.92E+02

C3DI_CATE	O(C(C=O)C=O)Oc1ccccc1O	196.2	2.24E-03	7.82E+01	1.83E+05
C3DI_DNP	O(C(C=O)C=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	336.2	2.73E-10	1.53E+02	1.86E+12
C3DI_MALb	O(C(C=O)C=O)OC(C=O)C(O)C=O	204.1	7.36E-05	9.63E+01	5.19E+07
C3DI_MALc	O(C(C=O)C=O)OC1C(=O)OC(=O)C1O	218.1	2.62E-04	9.14E+01	2.06E+06
C3DI_NBZa	O(C(C=O)C=O)OC1C(=O)OCC1ON(=O)=O	249.1	2.12E-05	9.87E+01	1.04E+07
C3DI_NBZb	O(C(C=O)C=O)OC1C(=O)C=CC(=O)C1ON(=O)=O	273.2	7.14E-06	1.04E+02	2.55E+07
C3DI_NCAT	O(C(C=O)C=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	307.2	5.34E-10	1.52E+02	3.07E+12
C3DI_NDN	O(C(C=O)C=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	381.2	1.33E-10	1.56E+02	1.50E+12
C3DI_NNC	O(C(C=O)C=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	352.2	2.37E-10	1.55E+02	3.05E+12
C3DI_NPHb	O(C(C=O)C=O)Oc1ccccc1N(=O)=O	225.2	7.43E-04	8.14E+01	4.07E+03
C3DI_PBZ	O(C(C=O)C=O)OC1C(=O)C=CC(=O)C1O	228.2	1.74E-05	1.01E+02	3.34E+07
C3DIALO	O=CC([O])C=O	87.1			
C3DIALO2	[O]OC(C=O)C=O	103.1			
C3DIALOOH	OOC(C=O)C=O	104.1	9.98E-03	7.45E+01	2.56E+05
C3DIOLO	OCC(O)C[O]	91.1			
C3DIOLO2	[O]OCC(O)CO	107.1			
C3DIOLOOH	OOCC(O)CO	108.1	2.38E-05	1.02E+02	1.93E+08
C42AOH	O=CC(O)CON(=O)=O	135.1	2.33E-02	7.21E+01	2.22E+05
C4a_C4a	O(C(=O)C=CC(=O)C=O)OC(=O)C=CC(=O)C=O	254.2	9.41E-02	6.37E+01	6.85E+02
C4CO2DBCO3	[O]OC(=O)C=CC(=O)C=O	143.1			
C4CO2DBPAN	O=CC(=O)C=CC(=O)OON(=O)=O	189.1	7.15E-03	7.38E+01	3.54E+04
C4CO2DCO3H	OOC(=O)C=CC(=O)C=O	144.1	4.28E-03	7.69E+01	6.15E+05
C5_O4_2OH	OOC=CC(O)C(O)C(=O)O	164.1	2.19E-10	1.56E+02	2.95E+13
C5_O5_NO3	OOC=CC(O)C(O)C(=O)ON(=O)=O	209.1	1.02E-01	7.16E+01	1.45E+04
C5_O5_O	OOC=CC(=O)C(O)C(=O)O	162.1	5.09E-09	1.40E+02	1.07E+12
C5_O5_OOH	OOC=CC(O)C(O)C(=O)OO	180.1	2.59E-09	1.45E+02	1.85E+12
C5_O6_2OH	O=C(O)C(O)C(O)C(O)C(=O)OO	196.1	1.68E-12	1.80E+02	6.98E+15
C5_O7_NO3	O=C(ON(=O)=O)C(O)C(O)C(O)C(=O)OO	241.1	2.17E-03	9.02E+01	3.17E+06
C5_O7_O	O=C(O)C(=O)C(O)C(O)C(=O)OO	194.1	6.76E-11	1.61E+02	1.96E+14
C5_O7_OOH	O=C(OO)C(O)C(O)C(O)C(=O)OO	212.1	2.05E-11	1.68E+02	1.29E+15

C5_RO_O5	O=CC([O])C(O)C(O)C=O	147.1			
C5_RO_O6	OOC=CC(O)C(O)C(=O)[O]	163.1			
C5_RO_O7	O=CC(OO)C(O)C(O)C([O])=O	179.1			
C5_RO_O8	O=C([O])C(O)C(O)C(O)C(=O)OO	195.1			
C5_RO_O9	O=C([O])C(OO)C(O)C(O)C(OO)=O	211.1			
C5_RO2_O10	O=C([O])C(OO)C(O)C(O)C(OO)=O	227.1			
C5_RO2_O6	O=CC(O[O])C(O)C(O)C=O	163.1			
C5_RO2_O7	OOC=CC(O)C(O)C(=O)O[O]	179.1			
C5_RO2_O8	O=CC(OO)C(O)C(O)C(O[O])=O	195.1			
C5_RO2_O9	O=C(O[O])C(O)C(O)C(O)C(=O)OO	211.1			
C5a_C4a	OC(C=O)C(=O)C=CC(=O)(OOC(=O)C=CC(=O)C=O)	284.2	6.11E-04	8.69E+01	2.19E+05
C5a_C5a	OC(C=O)C(=O)C=CC(=O)(OO(C(=O)C=CC(=O)C(C=O)O))	314.2	1.69E-06	1.14E+02	1.25E+08
C5CO2OHCO3	OC(C=O)C(=O)C=CC(=O)O[O]	173.1			
C5CO2OHPAN	O=CC(O)C(=O)C=CC(=O)OON(=O)=O	219.1	2.79E-05	9.88E+01	2.41E+07
C5COOHCO3H	OC(C=O)C(=O)C=CC(=O)OO	174.1	5.98E-06	1.07E+02	3.15E+08
C5DI_BZFU	O=CC=CC(OOC1C(O)COC1=O)C=O	230.2	5.04E-06	1.05E+02	2.61E+07
C5DI_C2a	O=CC=CC(OOC(=O)C=O)C=O	186.1	6.06E-01	5.65E+01	1.23E+03
C5DI_C2b	O=CC=CC(OOCC=O)C=O	172.1	2.87E-02	6.80E+01	1.56E+04
C5DI_C2c	O=CC=CC(OO(C(=O)CO))C=O	188.1	2.22E-01	6.22E+01	7.67E+03
C5DI_C3a	O=CC=CC(OO(C(=O)C(C=O)O))C=O	216.1	9.03E-03	7.62E+01	1.41E+05
C5DI_C3DI	O=CC=CC(OOC(C=O)C=O)C=O	200.2	9.89E-04	8.25E+01	4.27E+05
C5DI_C4a	O=CC=CC(OOC(=O)C=CC(=O)C=O)C=O	240.2	5.36E-03	7.53E+01	2.36E+04
C5DI_C5a	O=CC=CC(OO(C(=O)C=CC(=O)C(C=O)O))C=O	270.2	2.51E-05	1.00E+02	9.90E+06
C5DI_C5DI	O=CC=CC(OO(C(C=O)C=CC=O))C=O	226.2	1.22E-04	9.10E+01	6.12E+05
C5DI_C6a	O=CC=CC(OOc1ccccc1)C=O	206.2	5.23E-03	7.34E+01	6.00E+02
C5DI_CATE	O=CC=CC(OOc1ccccc1O)C=O	222.2	2.44E-04	8.73E+01	3.06E+05
C5DI_DNP	O=CC=CC(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O)C=O	362.2	1.85E-11	1.65E+02	6.20E+12
C5DI_EPX	O=CC=CC(OOC(=O)C1OC1C=O)C=O	228.2	2.20E-02	7.00E+01	9.72E+03
C5DI_MALa	O=CC=CC(OOC(=O)C=CC=O)C=O	212.2	5.39E-02	6.55E+01	2.35E+03
C5DI_MALb	O=CC=CC(OOC(C=O)C(O)C=O)C=O	230.2	6.74E-06	1.06E+02	1.18E+08

C5DI_MALc	O=CC=CC(OOC1C(=O)OC(=O)C1O)C=O	244.2	2.06E-05	1.02E+02	5.43E+06
C5DI_NBZa	O=CC=CC(OOC1C(=O)OCC1ON(=O)=O)C=O	275.2	2.22E-06	1.08E+02	1.48E+07
C5DI_NBZb	O=CC=CC(OOC1C(=O)C=CC(=O)C1ON(=O)=O)C=O	299.2	6.71E-07	1.14E+02	3.70E+07
C5DI_NCAT	O=CC=CC(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)O)C=O	333.2	3.04E-11	1.65E+02	1.46E+13
C5DI_NDN	O=CC=CC(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)C=O	407.2	9.99E-12	1.68E+02	3.72E+12
C5DI_NNC	O=CC=CC(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)C=O	378.2	1.50E-11	1.67E+02	1.13E+13
C5DI_NPHa	O=CC=CC(OOC1(O)C=CC2OOC1C2ON(=O)=O)C=O	317.2	5.18E-07	1.18E+02	4.52E+07
C5DI_NPHb	O=CC=CC(OOc1ccccc1N(=O)=O)C=O	251.2	9.40E-05	9.00E+01	4.30E+03
C5DI_PBZ	O=CC=CC(OOC1C(=O)C=CC(=O)C1O)C=O	254.2	1.43E-06	1.11E+02	7.17E+07
C5DI_PHEN	O=CC=CC(OOC1(O)C=CC2OOC1C2O)C=O	272.2	1.34E-06	1.15E+02	5.59E+07
C5DIALCO	O=CC=CC(=O)C=O	112.1	1.49E-01	6.08E+01	9.86E+03
C5DIALO	O=CC=CC([O])C=O	113.1			
C5DIALO2	O=CC=CC(O[O])C=O	129.1			
C5DIALOH	O=CC=CC(O)C=O	114.1	1.41E-02	7.27E+01	1.53E+05
C5DIALOOH	O=CC=CC(OO)C=O	130.1	8.97E-04	8.39E+01	5.74E+05
C5e_O3_2OH	O=CC(O)C(O)C(O)C=O	148.1	1.17E-06	1.17E+02	9.33E+09
C5e_O4_NO3	O=CC(ON(=O)=O)C(O)C(O)C=O	193.1	7.23E-07	1.18E+02	7.86E+09
C5e_O4_O	O=CC(=O)C(O)C(O)C=O	146.1	2.34E-05	1.02E+02	4.29E+08
C5e_O4_OOH	O=CC(OO)C(O)C(O)C=O	164.1	4.11E-08	1.31E+02	7.32E+10
C5e_O5_2OH	O=CC(OO)C(O)C(O)C(O)=O	180.1	1.53E-11	1.68E+02	9.58E+14
C5e_O6_NO3	O=CC(OO)C(O)C(O)C(ON(=O)=O)=O	225.1	1.26E-02	8.04E+01	2.34E+05
C5e_O6_O	O=CC(OO)C(=O)C(O)C(O)=O	178.1	6.15E-10	1.50E+02	2.08E+13
C5e_O6_OOH	O=CC(OO)C(O)C(O)C(OO)=O	196.1	1.89E-10	1.57E+02	2.60E+13
C5e_O7_2OH	O=C(O)C(OO)C(O)C(O)C(OO)=O	212.1	3.42E-14	1.98E+02	4.51E+17
C5e_O8_NO3	O=C(ON(=O)=O)C(OO)C(O)C(O)C(OO)=O	257.1	1.12E-04	1.02E+02	8.29E+07
C5e_O8_O	O=C(O)C(OO)C(=O)C(O)C(OO)=O	210.1	1.69E-12	1.78E+02	1.39E+16
C5e_O8_OOH	O=C(OO)C(OO)C(O)C(O)C(OO)=O	228.1	4.82E-13	1.85E+02	1.37E+17
C5eO5_BZBI	O=CC(OOC1C=CC2OOC1C2O)C(O)C(O)C=O	290.2	4.37E-09	1.42E+02	5.41E+10
C5eO5_BZFU	O=CC(OOC1C(O)COC1=O)C(O)C(O)C=O	264.2	1.25E-10	1.57E+02	9.85E+12
C5eO5_BZMUa	O=CC(OOC(=O)C1OC1C=CC=O)C(O)C(O)C=O	288.2	5.82E-07	1.19E+02	8.41E+08

C5eO5_BZMUb	O=CC(OO(C(C1OC1C=O)C(O)C=O))C(O)C(O)C=O	306.2	2.14E-12	1.77E+02	8.61E+14
C5eO5_C2a	O=CC(OOC(=O)C=O)C(O)C(O)C=O	220.1	7.11E-04	8.97E+01	9.61E+06
C5eO5_C2b	O=CC(OOCC=O)C(O)C(O)C=O	206.2	1.41E-05	1.05E+02	3.03E+08
C5eO5_C2c	O=CC(OO(C(=O)CO))C(O)C(O)C=O	222.2	7.89E-05	1.00E+02	1.27E+08
C5eO5_C3a	O=CC(OO(C(=O)C(C=O)O))C(O)C(O)C=O	250.2	1.95E-06	1.17E+02	4.05E+09
C5eO5_C3DI	O=CC(OOC(C=O)C=O)C(O)C(O)C=O	234.2	2.30E-07	1.23E+02	2.07E+10
C5eO5_C4a	O=CC(OOC(=O)C=CC(=O)C=O)C(O)C(O)C=O	274.2	1.28E-06	1.16E+02	1.32E+09
C5eO5_C5a	O=CC(OO(C(=O)C=CC(=O)C(C=O)O))C(O)C(O)C=O	304.2	1.32E-09	1.48E+02	1.64E+12
C5eO5_C5DI	O=CC(OO(C(C=O)C=CC=O))C(O)C(O)C=O	260.2	1.68E-08	1.34E+02	6.74E+10
C5eO5_C5eO5	O=CC(OO(C(C(O)C(O)C=O)C=O))C(O)C(O)C=O	294.2	1.65E-13	1.90E+02	4.27E+16
C5eO5_C5eO7	O=CC(OO(C(=O)C(O)C(O)C(OO)C=O))C(O)C(O)C=O	326.2	3.77E-14	1.99E+02	7.32E+16
C5eO5_C5eO9	O=CC(OO(C(C(OO)C(O)C(O)C(OO)=O)=O))C(O)C(O)C=O	358.2	6.37E-17	2.30E+02	2.91E+19
C5eO5_C5O6	O=CC(OO(C(=O)C(O)C(O)C=COO))C(O)C(O)C=O	310.2	8.79E-13	1.84E+02	1.32E+15
C5eO5_C5O8	O=CC(OO(C(C(O)C(O)C(O)C(=O)OO)=O))C(O)C(O)C=O	342.2	2.88E-15	2.12E+02	1.35E+18
C5eO5_C6a	O=CC(OOc1ccccc1)C(O)C(O)C=O	240.2	1.50E-06	1.13E+02	3.64E+07
C5eO5_CATE	O=CC(OOc1ccccc1O)C(O)C(O)C=O	256.2	1.94E-08	1.33E+02	1.62E+10
C5eO5_DNP	O=CC(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O)C(O)C(O)C=O	396.2	5.46E-17	2.28E+02	1.42E+19
C5eO5_EPX	O=CC(OOC(=O)C1OC1C=O)C(O)C(O)C=O	262.2	8.43E-06	1.08E+02	2.56E+08
C5eO5_MALa	O=CC(OOC(=O)C=CC=O)C(O)C(O)C=O	246.2	3.48E-05	1.02E+02	4.86E+07
C5eO5_MALb	O=CC(OOC(C=O)C(O)C=O)C(O)C(O)C=O	264.2	2.94E-10	1.55E+02	1.97E+13
C5eO5_MALc	O=CC(OOC1C(=O)OC(=O)C1O)C(O)C(O)C=O	278.2	8.36E-10	1.50E+02	1.54E+12
C5eO5_NBZa	O=CC(OOC1C(=O)OCC1ON(=O)=O)C(O)C(O)C=O	309.2	7.70E-11	1.58E+02	6.37E+12
C5eO5_NBZb	O=CC(OOC1C(=O)C=CC(=O)C1ON(=O)=O)C(O)C(O)C=O	333.2	1.36E-11	1.67E+02	2.72E+13
C5eO5_NCAT	O=CC(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)O)C(O)C(O)C=O	367.2	8.52E-17	2.27E+02	2.90E+19
C5eO5_NDN	O=CC(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)C(O)C(O)C=O	441.2	3.45E-17	2.30E+02	9.39E+18
C5eO5_NNC	O=CC(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)C(O)C(O)C=O	412.2	4.90E-17	2.29E+02	2.22E+19
C5eO5_NPHa	O=CC(OOC1(O)C=CC2OOC1C2ON(=O)=O)C(O)C(O)C=O	351.2	1.33E-11	1.69E+02	1.70E+13
C5eO5_NPHb	O=CC(OOc1ccccc1N(=O)=O)C(O)C(O)C=O	285.2	6.69E-09	1.37E+02	2.19E+09
C5eO5_PBZ	O=CC(OOC1C(=O)C=CC(=O)C1O)C(O)C(O)C=O	288.2	2.41E-11	1.65E+02	3.75E+13
C5eO5_PHEN	O=CC(OOC1(O)C=CC2OOC1C2O)C(O)C(O)C=O	306.2	2.90E-11	1.66E+02	1.91E+13

C5eO7_BZBI	O=CC(OO)C(O)C(O)C(=O)(OOC1C=CC2OOC1C2O)	322.2	7.82E-10	1.52E+02	1.45E+11
C5eO7_BZFU	O=CC(OO)C(O)C(O)C(=O)(OOC1C(O)COC1=O)	296.2	2.44E-11	1.66E+02	1.59E+13
C5eO7_BZMUa	O=CC(OO)C(O)C(O)C(=O)(OOC(=O)C1OC1C=CC=O)	320.2	1.36E-07	1.28E+02	4.04E+08
C5eO7_BZMUb	O=CC(OO)C(O)C(O)C(=O)(OO(C(C1OC1C=O)C(O)C=O))	338.2	4.39E-13	1.86E+02	1.52E+15
C5eO7_C2a	O=CC(OO)C(O)C(O)C(=O)(OOC(=O)C=O)	252.1	2.81E-04	9.64E+01	3.20E+06
C5eO7_C2b	O=CC(OO)C(O)C(O)C(=O)(OOCC=O)	238.2	5.99E-06	1.11E+02	2.91E+08
C5eO7_C2c	O=CC(OO)C(O)C(O)C(=O)(OO(C(=O)CO))	254.2	2.23E-05	1.08E+02	7.00E+07
C5eO7_C3a	O=CC(OO)C(O)C(O)C(=O)(OO(C(=O)C(C=O)O))	282.2	5.70E-07	1.25E+02	1.95E+09
C5eO7_C3DI	O=CC(OO)C(O)C(O)C(=O)(OOC(C=O)C=O)	266.2	9.33E-08	1.30E+02	1.93E+10
C5eO7_C4a	O=CC(OO)C(O)C(O)C(=O)(OOC(=O)C=CC(=O)C=O)	306.2	2.99E-07	1.25E+02	6.95E+08
C5eO7_C5a	O=CC(OO)C(O)C(O)C(=O)(OO(C(=O)C=CC(=O)C(C=O)O))	336.2	2.37E-10	1.58E+02	1.16E+12
C5eO7_C5DI	O=CC(OO)C(O)C(O)C(=O)(OO(C(C=O)C=CC=O))	292.2	5.29E-09	1.42E+02	8.26E+10
C5eO7_C5eO7	O=CC(OO)C(O)C(O)C(=O)(OO(C(=O)C(O)C(O)C(OO)C=O))	358.2	6.26E-15	2.09E+02	1.36E+17
C5eO7_C5eO9	O=CC(OO)C(O)C(O)C(=O)(OO(C(C(OO)C(O)C(O)C(OO)=O)=O))	390.2	7.73E-18	2.41E+02	1.72E+20
C5eO7_C5O8	O=CC(OO)C(O)C(O)C(=O)(OO(C(C(O)C(O)C(O)C(=O)OO)=O))	374.2	3.85E-16	2.23E+02	3.54E+18
C5eO7_C6a	O=CC(OO)C(O)C(O)C(=O)(OOc1ccccc1)	272.2	3.62E-07	1.22E+02	8.27E+07
C5eO7_CATE	O=CC(OO)C(O)C(O)C(=O)(OOc1ccccc1O)	288.2	3.94E-09	1.43E+02	7.48E+10
C5eO7_DNP	O=CC(OO)C(O)C(O)C(=O)(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O)	428.2	5.13E-18	2.41E+02	7.21E+19
C5eO7_EPX	O=CC(OO)C(O)C(O)C(=O)(OOC(=O)C1OC1C=O)	294.2	2.38E-06	1.16E+02	1.04E+08
C5eO7_MALa	O=CC(OO)C(O)C(O)C(=O)(OOC(=O)C=CC=O)	278.2	1.12E-05	1.09E+02	1.85E+07
C5eO7_MALb	O=CC(OO)C(O)C(O)C(=O)(OOC(C=O)C(O)C=O)	296.2	8.71E-11	1.62E+02	2.55E+13
C5eO7_MALc	O=CC(OO)C(O)C(O)C(=O)(OOC1C(=O)OC(=O)C1O)	310.2	1.61E-10	1.60E+02	1.87E+12
C5eO7_NBZa	O=CC(OO)C(O)C(O)C(=O)(OOC1C(=O)OCC1ON(=O)=O)	341.2	1.26E-11	1.69E+02	1.29E+13
C5eO7_NBZb	O=CC(OO)C(O)C(O)C(=O)(OOC1C(=O)C=CC(=O)C1ON(=O)=O)	365.2	1.63E-12	1.78E+02	1.15E+14
C5eO7_NCAT	O=CC(OO)C(O)C(O)C(=O)(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)O)	399.2	9.40E-18	2.39E+02	1.26E+20
C5eO7_NDN	O=CC(OO)C(O)C(O)C(=O)(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)	473.2	2.76E-18	2.43E+02	5.72E+19
C5eO7_NNC	O=CC(OO)C(O)C(O)C(=O)(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)	444.2	4.51E-18	2.42E+02	1.16E+20
C5eO7_NPHa	O=CC(OO)C(O)C(O)C(=O)(OOC1(O)C=CC2OOC1C2ON(=O)=O)	383.2	1.78E-12	1.80E+02	6.10E+13
C5eO7_NPHb	O=CC(OO)C(O)C(O)C(=O)(OOc1ccccc1N(=O)=O)	317.2	1.14E-09	1.47E+02	6.16E+09
C5eO7_PBZ	O=CC(OO)C(O)C(O)C(=O)(OOC1C(=O)C=CC(=O)C1O)	320.2	3.39E-12	1.76E+02	1.28E+14

C5eO7_PHEN	O=CC(OO)C(O)C(O)C(=O)(OOC1(O)C=CC2OOC1C2O)	338.2	4.58E-12	1.77E+02	5.66E+13
C5eO9_BZBI	O=C(OOC1C=CC2OOC1C2O)C(OO)C(O)C(O)C(OO)=O	354.2	2.09E-12	1.80E+02	1.36E+14
C5eO9_BZFU	O=C(OOC1C(O)COC1=O)C(OO)C(O)C(O)C(OO)=O	328.2	4.87E-14	1.96E+02	1.98E+16
C5eO9_BZMUa	O=C(OOC(=O)C1OC1C=CC=O)C(OO)C(O)C(O)C(OO)=O	352.2	7.60E-10	1.53E+02	1.45E+11
C5eO9_BZMUb	O=C(OO(C(C1OC1C=O)C(O)C=O))C(OO)C(O)C(O)C(OO)=O	370.2	9.73E-16	2.16E+02	5.60E+17
C5eO9_C2a	O=C(OOC(=O)C=O)C(OO)C(O)C(O)C(OO)=O	284.1	2.51E-06	1.18E+02	5.77E+08
C5eO9_C2b	O=C(OOCC=O)C(OO)C(O)C(O)C(OO)=O	270.2	3.84E-08	1.35E+02	7.76E+10
C5eO9_C2c	O=C(OO(C(=O)CO))C(OO)C(O)C(O)C(OO)=O	286.2	1.11E-07	1.33E+02	2.92E+10
C5eO9_C3a	O=C(OO(C(=O)C(C=O)O))C(OO)C(O)C(O)C(OO)=O	314.2	2.76E-09	1.50E+02	4.66E+11
C5eO9_C3DI	O=C(OOC(C=O)C=O)C(OO)C(O)C(O)C(OO)=O	298.2	5.47E-10	1.54E+02	3.24E+12
C5eO9_C4a	O=C(OOC(=O)C=CC(=O)C=O)C(OO)C(O)C(O)C(OO)=O	338.2	1.61E-09	1.49E+02	2.41E+11
C5eO9_C5a	O=C(OO(C(=O)C=CC(=O)C(C=O)O))C(OO)C(O)C(O)C(OO)=O	368.2	6.90E-13	1.86E+02	5.20E+14
C5eO9_C5DI	O=C(OO(C(C=O)C=CC=O))C(OO)C(O)C(O)C(OO)=O	324.2	2.59E-11	1.67E+02	1.92E+13
C5eO9_C5eO9	O=C(OO(C(C(OO)C(O)C(O)C(OO)=O)=O))C(OO)C(O)C(O)C(OO)=O	422.2	6.19E-21	2.76E+02	1.87E+24
C5eO9_C6a	O=C(OOc1ccccc1)C(OO)C(O)C(O)C(OO)=O	304.2	1.60E-09	1.48E+02	3.52E+10
C5eO9_CATE	O=C(OOc1ccccc1O)C(OO)C(O)C(O)C(OO)=O	320.2	1.79E-11	1.69E+02	8.11E+13
C5eO9_DNP	O=C(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O)C(OO)C(O)C(O)C(OO)=O	460.2	4.08E-21	2.76E+02	1.45E+23
C5eO9_EPX	O=C(OOC(=O)C1OC1C=O)C(OO)C(O)C(O)C(OO)=O	326.2	1.58E-08	1.40E+02	2.68E+10
C5eO9_MALa	O=C(OOC(=O)C=CC=O)C(OO)C(O)C(O)C(OO)=O	310.2	8.36E-08	1.32E+02	4.64E+09
C5eO9_MALb	O=C(OOC(C=O)C(O)C=O)C(OO)C(O)C(O)C(OO)=O	328.2	2.70E-13	1.90E+02	6.46E+15
C5eO9_MALc	O=C(OOC1C(=O)OC(=O)C1O)C(OO)C(O)C(O)C(OO)=O	342.2	3.49E-13	1.89E+02	2.27E+15
C5eO9_NBZa	O=C(OOC1C(=O)OCC1ON(=O)=O)C(OO)C(O)C(O)C(OO)=O	373.2	2.72E-14	1.98E+02	2.54E+16
C5eO9_NBZb	O=C(OOC1C(=O)C=CC(=O)C1ON(=O)=O)C(OO)C(O)C(O)C(OO)=O	397.2	3.00E-15	2.09E+02	2.45E+17
C5eO9_NCAT	O=C(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)O)C(OO)C(O)C(O)C(OO)=O	431.2	7.14E-21	2.74E+02	2.01E+23
C5eO9_NDN	O=C(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)C(OO)C(O)C(O)C(OO)=O	505.2	2.31E-21	2.78E+02	1.57E+23
C5eO9_NNC	O=C(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)C(OO)C(O)C(O)C(OO)=O	476.2	3.64E-21	2.77E+02	2.24E+23
C5eO9_NPHa	O=C(OOC1(O)C=CC2OOC1C2ON(=O)=O)C(OO)C(O)C(O)C(OO)=O	415.2	3.32E-15	2.11E+02	7.87E+16
C5eO9_NPHb	O=C(OOc1ccccc1N(=O)=O)C(OO)C(O)C(O)C(OO)=O	349.2	3.64E-12	1.75E+02	3.08E+12
C5eO9_PBZ	O=C(OOC1C(=O)C=CC(=O)C1O)C(OO)C(O)C(O)C(OO)=O	352.2	5.74E-15	2.06E+02	1.77E+17
C5eO9_PHEN	O=C(OOC1(O)C=CC2OOC1C2O)C(OO)C(O)C(O)C(OO)=O	370.2	7.99E-15	2.07E+02	5.39E+16

C5euni_O5_O	O=CC(OO)C(=O)C(O)C=O	162.1	9.91E-07	1.15E+02	2.72E+09
C5euni_O7_O	O=CC(OO)C(=O)C(O)C(OO)=O	194.1	5.51E-09	1.40E+02	1.25E+12
C5euni_O9_O	O=C(OO)C(OO)C(=O)C(O)C(OO)=O	226.1	1.80E-11	1.67E+02	8.59E+15
C5O6_BZBI	OOC=CC(O)C(O)C(=O)(OOC1C=CC2OOC1C2O)	306.2	9.56E-09	1.41E+02	4.83E+09
C5O6_BZFU	OOC=CC(O)C(O)C(=O)(OOC1C(O)COC1=O)	280.2	3.72E-10	1.53E+02	4.59E+11
C5O6_BZMUa	OOC=CC(O)C(O)C(=O)(OOC(=O)C1OC1C=CC=O)	304.2	1.67E-06	1.17E+02	1.20E+07
C5O6_BZMUb	OOC=CC(O)C(O)C(=O)(OO(C(C1OC1C=O)C(O)C=O))	322.2	8.79E-12	1.73E+02	2.97E+13
C5O6_C2a	OOC=CC(O)C(O)C(=O)(OOC(=O)C=O)	236.1	3.26E-03	8.60E+01	1.14E+05
C5O6_C2b	OOC=CC(O)C(O)C(=O)(OOCC=O)	222.2	8.18E-05	1.00E+02	8.87E+06
C5O6_C2c	OOC=CC(O)C(O)C(=O)(OO(C(=O)CO))	238.2	2.28E-04	9.84E+01	2.79E+06
C5O6_C3a	OOC=CC(O)C(O)C(=O)(OO(C(=O)C(C=O)O))	266.2	7.92E-06	1.13E+02	5.81E+07
C5O6_C3DI	OOC=CC(O)C(O)C(=O)(OOC(C=O)C=O)	250.2	1.51E-06	1.17E+02	4.91E+08
C5O6_C4a	OOC=CC(O)C(O)C(=O)(OOC(=O)C=CC(=O)C=O)	290.2	3.61E-06	1.14E+02	2.24E+07
C5O6_C5a	OOC=CC(O)C(O)C(=O)(OO(C(=O)C=CC(=O)C(C=O)O))	320.2	3.54E-09	1.46E+02	3.04E+10
C5O6_C5DI	OOC=CC(O)C(O)C(=O)(OO(C(C=O)C=CC=O))	276.2	8.50E-08	1.29E+02	2.00E+09
C5O6_C5eO7	OOC=CC(O)C(O)C(=O)(OO(C(=O)C(O)C(O)C(OO)C=O))	342.2	1.37E-13	1.95E+02	2.83E+15
C5O6_C5eO9	OOC=CC(O)C(O)C(=O)(OO(C(C(OO)C(O)C(O)C(OO)=O)=O))	374.2	1.73E-16	2.27E+02	5.84E+18
C5O6_C5O6	OOC=CC(O)C(O)C(=O)(OO(C(=O)C(O)C(O)C=COO))	326.2	2.44E-12	1.82E+02	7.61E+13
C5O6_C5O8	OOC=CC(O)C(O)C(=O)(OO(C(C(O)C(O)C(O)C(=O)OO)=O))	358.2	8.08E-15	2.09E+02	1.10E+17
C5O6_C6a	OOC=CC(O)C(O)C(=O)(OOc1ccccc1)	256.2	3.52E-06	1.12E+02	3.39E+06
C5O6_CATE	OOC=CC(O)C(O)C(=O)(OOc1ccccc1O)	272.2	4.65E-08	1.32E+02	3.14E+09
C5O6_DNP	OOC=CC(O)C(O)C(=O)(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O)	412.2	9.78E-17	2.27E+02	1.74E+18
C5O6_EPX	OOC=CC(O)C(O)C(=O)(OOC(=O)C1OC1C=O)	278.2	2.88E-05	1.06E+02	3.31E+06
C5O6_MALa	OOC=CC(O)C(O)C(=O)(OOC(=O)C=CC=O)	262.2	1.31E-04	9.84E+01	6.16E+05
C5O6_MALb	OOC=CC(O)C(O)C(=O)(OOC(C=O)C(O)C=O)	280.2	1.68E-09	1.49E+02	5.47E+11
C5O6_MALc	OOC=CC(O)C(O)C(=O)(OOC1C(=O)OC(=O)C1O)	294.2	2.18E-09	1.48E+02	6.62E+10
C5O6_NBZa	OOC=CC(O)C(O)C(=O)(OOC1C(=O)OCC1ON(=O)=O)	325.2	1.83E-10	1.56E+02	3.93E+11
C5O6_NBZb	OOC=CC(O)C(O)C(=O)(OOC1C(=O)C=CC(=O)C1ON(=O)=O)	349.2	2.26E-11	1.66E+02	3.55E+12
C5O6_NCAT	OOC=CC(O)C(O)C(=O)(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)O)	383.2	1.93E-16	2.25E+02	2.99E+18
C5O6_NDN	OOC=CC(O)C(O)C(=O)(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)	457.2	4.96E-17	2.29E+02	1.43E+18

C5O6_NNC	OOC=CC(O)C(O)C(=O)(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)	428.2	8.72E-17	2.28E+02	2.85E+18
C5O6_NPHa	OOC=CC(O)C(O)C(=O)(OOC1(O)C=CC2OOC1C2ON(=O)=O)	367.2	2.48E-11	1.68E+02	1.88E+12
C5O6_NPHb	OOC=CC(O)C(O)C(=O)(OOc1ccccc1N(=O)=O)	301.2	1.29E-08	1.36E+02	2.10E+08
C5O6_PBZ	OOC=CC(O)C(O)C(=O)(OOC1C(=O)C=CC(=O)C1O)	304.2	4.98E-11	1.63E+02	3.77E+12
C5O6_PHEN	OOC=CC(O)C(O)C(=O)(OOC1(O)C=CC2OOC1C2O)	322.2	6.80E-11	1.65E+02	1.68E+12
C5O8_BZBI	O=C(OOC1C=CC2OOC1C2O)C(O)C(O)C(O)C(=O)OO	338.2	5.95E-11	1.65E+02	5.99E+12
C5O8_BZFU	O=C(OOC1C(O)COC1=O)C(O)C(O)C(O)C(=O)OO	312.2	1.61E-12	1.80E+02	8.61E+14
C5O8_BZMUa	O=C(OOC(=O)C1OC1C=CC=O)C(O)C(O)C(O)C(=O)OO	336.2	1.66E-08	1.40E+02	9.98E+09
C5O8_BZMUb	O=C(OO(C(C1OC1C=O)C(O)C=O))C(O)C(O)C(O)C(=O)OO	354.2	3.54E-14	1.99E+02	2.93E+16
C5O8_C2a	O=C(OOC(=O)C=O)C(O)C(O)C(O)C(=O)OO	268.1	5.19E-05	1.06E+02	3.67E+07
C5O8_C2b	O=C(OOCC=O)C(O)C(O)C(O)C(=O)OO	254.2	9.33E-07	1.22E+02	3.62E+09
C5O8_C2c	O=C(OO(C(=O)CO))C(O)C(O)C(O)C(=O)OO	270.2	2.78E-06	1.20E+02	1.44E+09
C5O8_C3a	O=C(OO(C(=O)C(C=O)O))C(O)C(O)C(O)C(=O)OO	298.2	7.48E-08	1.36E+02	2.88E+10
C5O8_C3DI	O=C(OOC(C=O)C=O)C(O)C(O)C(O)C(=O)OO	282.2	1.42E-08	1.40E+02	1.90E+11
C5O8_C4a	O=C(OOC(=O)C=CC(=O)C=O)C(O)C(O)C(O)C(=O)OO	322.2	3.56E-08	1.36E+02	1.61E+10
C5O8_C5a	O=C(OO(C(=O)C=CC(=O)C(C=O)O))C(O)C(O)C(O)C(=O)OO	352.2	2.02E-11	1.70E+02	3.34E+13
C5O8_C5DI	O=C(OO(C(C=O)C=CC=O))C(O)C(O)C(O)C(=O)OO	308.2	6.67E-10	1.53E+02	1.28E+12
C5O8_C5eO9	O=C(OO(C(C(OO)C(O)C(O)C(OO)=O)=O))C(O)C(O)C(O)C(=O)OO	406.2	3.79E-19	2.57E+02	1.64E+22
C5O8_C5O8	O=C(OO(C(C(O)C(O)C(O)C(=O)OO)=O))C(O)C(O)C(O)C(=O)OO	390.2	2.17E-17	2.38E+02	2.86E+20
C5O8_C6a	O=C(OOc1ccccc1)C(O)C(O)C(O)C(=O)OO	288.2	3.48E-08	1.34E+02	1.27E+09
C5O8_CATE	O=C(OOc1ccccc1O)C(O)C(O)C(O)C(=O)OO	304.2	4.73E-10	1.54E+02	1.73E+12
C5O8_DNP	O=C(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O)C(O)C(O)C(O)C(=O)OO	444.2	1.89E-19	2.57E+02	4.79E+21
C5O8_EPX	O=C(OOC(=O)C1OC1C=O)C(O)C(O)C(O)C(=O)OO	310.2	3.43E-07	1.27E+02	1.68E+09
C5O8_MALa	O=C(OOC(=O)C=CC=O)C(O)C(O)C(O)C(=O)OO	294.2	1.72E-06	1.19E+02	3.34E+08
C5O8_MALb	O=C(OOC(C=O)C(O)C=O)C(O)C(O)C(O)C(=O)OO	312.2	9.23E-12	1.74E+02	3.44E+14
C5O8_MALc	O=C(OOC1C(=O)OC(=O)C1O)C(O)C(O)C(O)C(=O)OO	326.2	1.17E-11	1.74E+02	1.25E+14
C5O8_NBZa	O=C(OOC1C(=O)OCC1ON(=O)=O)C(O)C(O)C(O)C(=O)OO	357.2	7.85E-13	1.83E+02	9.24E+14
C5O8_NBZb	O=C(OOC1C(=O)C=CC(=O)C1ON(=O)=O)C(O)C(O)C(O)C(=O)OO	381.2	8.95E-14	1.93E+02	7.46E+15
C5O8_NCAT	O=C(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)O)C(O)C(O)C(O)C(=O)OO	415.2	3.81E-19	2.55E+02	6.71E+21
C5O8_NDN	O=C(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)C(O)C(O)C(O)C(=O)OO	489.2	9.54E-20	2.60E+02	4.67E+21

C5O8_NNC	O=C(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)C(O)C(O)C(O)C(=O)OO	460.2	1.71E-19	2.58E+02	7.22E+21
C5O8_NPHa	O=C(OOC1(O)C=CC2OOC1C2ON(=O)=O)C(O)C(O)C(O)C(=O)OO	399.2	1.06E-13	1.95E+02	3.11E+15
C5O8_NPHb	O=C(OOc1ccccc1N(=O)=O)C(O)C(O)C(O)C(=O)OO	333.2	8.57E-11	1.61E+02	1.29E+11
C5O8_PBZ	O=C(OOC1C(=O)C=CC(=O)C1O)C(O)C(O)C(O)C(=O)OO	336.2	1.96E-13	1.90E+02	6.42E+15
C5O8_PHEN	O=C(OOC1(O)C=CC2OOC1C2O)C(O)C(O)C(O)C(=O)OO	354.2	2.92E-13	1.91E+02	2.32E+15
C5uni_O6_O	OOC=CC(=O)C(O)C(=O)OO	178.1	4.45E-08	1.30E+02	1.98E+11
C5uni_O8_O	O=C(OO)C(=O)C(O)C(O)C(=O)OO	210.1	6.18E-10	1.51E+02	6.51E+13
C6a_BZFU	O(c1ccccc1)OC1C(O)COC1=O	210.2	2.50E-04	8.63E+01	1.61E+04
C6a_C2a	O(c1ccccc1)OC(=O)C=O	166.1	1.90E+01	4.05E+01	1.86E+00
C6a_C2b	O(c1ccccc1)OCC=O	152.2	1.71E+00	4.92E+01	8.35E+00
C6a_C2c	OCC(=O)(OOc1ccccc1)	168.2	4.23E+00	4.88E+01	1.28E+01
C6a_C3a	OC(C=O)C(=O)(OOc1ccccc1)	196.2	3.12E-01	6.00E+01	2.01E+02
C6a_C4a	O(c1ccccc1)OC(=O)C=CC(=O)C=O	220.2	1.45E-01	5.99E+01	3.24E+01
C6a_C5a	OC(C=O)C(=O)C=CC(=O)(OOc1ccccc1)	250.2	9.25E-04	8.32E+01	1.17E+04
C6a_C6a	O(c1ccccc1)Oc1ccccc1	186.2	1.58E-01	5.73E+01	2.53E-01
C6a_CATE	O(c1ccccc1)Oc1ccccc1O	202.2	6.99E-03	7.15E+01	7.30E+02
C6a_DNP	O(c1ccccc1)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	342.2	1.15E-09	1.46E+02	3.80E+09
C6a_MALc	O(c1ccccc1)OC1C(=O)OC(=O)C1O	224.2	7.51E-04	8.51E+01	6.21E+03
C6a_NBZa	O(c1ccccc1)OC1C(=O)OCC1ON(=O)=O	255.2	8.05E-05	9.13E+01	6.30E+03
C6a_NBZb	O(c1ccccc1)OC1C(=O)C=CC(=O)C1ON(=O)=O	279.2	2.35E-05	9.69E+01	1.25E+04
C6a_NCAT	O(c1ccccc1)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	313.2	1.86E-09	1.45E+02	1.20E+10
C6a_NDN	O(c1ccccc1)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	387.2	6.51E-10	1.48E+02	1.56E+09
C6a_NNC	O(c1ccccc1)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	358.2	9.16E-10	1.48E+02	8.12E+09
C6a_NPHb	O(c1ccccc1)Oc1ccccc1N(=O)=O	231.2	2.70E-03	7.41E+01	5.81E+00
C6a_PBZ	O(c1ccccc1)OC1C(=O)C=CC(=O)C1O	234.2	5.05E-05	9.41E+01	5.85E+04
C6CO4DB	O=CC(=O)C=CC(=O)C=O	140.1	1.11E-02	7.13E+01	1.32E+05
C6DIALPERO4N	O=CC1OOC(C(C=O)ON(=O)=O)C1O	221.1	1.26E-05	1.04E+02	1.23E+08
C6H5O	[O]c1ccccc1	93.1			
C6H5O2	[O]Oc1ccccc1	109.1			
C6H5OOH	OOc1ccccc1	110.1	5.30E-02	6.55E+01	8.28E+02

C6H6O3	C1=CC(=O)C(C=C1)(O)O	126.1	4.12E-03	7.74E+01	3.86E+05
C6H6O3_1	C1(O)(O)C(=O)C=CC(O[O])C1(O)	175.1			
C6H6O3_10	C1(O)C(OO)C=CC(=O)C1(O)(O)	176.1	3.31E-09	1.43E+02	6.33E+11
C6H6O3_11	C1(O)(O)C(ON(=O)(=O))C(OO)C=CC1(=O)	221.1	2.55E-09	1.44E+02	4.25E+11
C6H6O3_12	C(=O)(O)C(=O)C=CC(=O)	128.1	1.11E-03	8.29E+01	9.65E+06
C6H6O3_13	C1(O)(O)C(ON(=O)(=O))C(ON(=O)(=O))C=CC1(=O)	250.1	3.44E-08	1.32E+02	4.75E+10
C6H6O3_14	C1(O)C(ON(=O)(=O))C=CC(=O)C1(O)(O)	205.1	6.71E-08	1.29E+02	4.99E+10
C6H6O3_15	C(=O)(OON(=O)(=O))C(O)(O)C=CC(=O)	207.1	6.26E-05	9.72E+01	3.20E+07
C6H6O3_16	C(=O)(O)C(O)(O)C=CC(=O)	146.1	1.18E-06	1.17E+02	2.87E+10
C6H6O3_18	C(=O)(OON(=O)(=O))C(O)(O)C(=O)	181.1	9.61E-04	8.60E+01	5.97E+06
C6H6O3_19	C(=O)C(O)(O)C(=O)CC(=O)	146.1	9.48E-05	9.59E+01	1.40E+08
C6H6O3_2	C(=O)C(O)(O)C(=O)C([O])C(=O)	161.1			
C6H6O3_21	C(=O)CC(O)(O)C(=O)C(=O)	146.1	9.48E-05	9.59E+01	1.21E+08
C6H6O3_22	C(=O)C(O)(O)C(=O)C(=O)	132.1	3.38E-04	9.06E+01	4.39E+07
C6H6O3_23	C(=O)C(O)(O)C=CC(=O)	130.1	6.55E-04	8.78E+01	8.08E+06
C6H6O3_24	C(=O)C(O)(O)C(=O)C=C	130.1	2.56E-03	8.09E+01	2.02E+06
C6H6O3_25	C(=O)(OO)C(O)(O)C=CC(=O)	162.1	7.86E-06	1.08E+02	4.10E+08
C6H6O3_26	C(=O)C(=O)C(O)(O)C=C	130.1	3.80E-03	7.95E+01	1.36E+06
C6H6O3_27	C(=O)(OO)C(O)(O)C(=O)	136.1	1.50E-04	9.65E+01	5.71E+07
C6H6O3_28	C(=O)C(O)(O)C(=O)C1OC1C(=O)	174.1	2.55E-06	1.12E+02	2.38E+09
C6H6O3_29	C(=O)C(O)(O)C(=O)C(=O)CC(=O)	174.1	2.13E-06	1.12E+02	6.21E+09
C6H6O3_3	C(=O)C(=O)C(O)(O)C([O])C(=O)	161.1			
C6H6O3_30	C(O)(OO)C(=O)C(O)(O)C=CC(=O)	192.1	1.36E-10	1.58E+02	2.67E+13
C6H6O3_31	C(=O)C(=O)C(O)(O)C1OC1C(=O)	174.1	2.55E-06	1.12E+02	2.38E+09
C6H6O3_32	C(=O)CC(=O)C(O)(O)C(=O)C(=O)	174.1	2.13E-06	1.12E+02	6.21E+09
C6H6O3_33	C(O)(OO)C(O)(O)C(=O)C=CC(=O)	192.1	8.35E-11	1.60E+02	4.35E+13
C6H6O3_34	C(O)(OO)C=CC(=O)C(O)(O)C(=O)	192.1	1.36E-10	1.58E+02	2.67E+13
C6H6O3_35	C1(O)(O)C(=O)C=CC(=O)C1(O)	158.1	1.20E-06	1.14E+02	5.43E+09
C6H6O3_36	C1(O)(O)C(ON(=O)(=O))C(=O)C=CC1(=O)	203.1	6.47E-07	1.17E+02	5.31E+09
C6H6O3_37	C(=O)C(=O)C(O)(O)C=CC(=O)	158.1	1.99E-05	1.02E+02	2.66E+08

C6H6O3_38	C(O)(OO)C=CC(O)(O)C(=O)C(=O)	192.1	2.21E-10	1.56E+02	1.64E+13
C6H6O3_39	C(=O)(O)C(O)(O)C(=O)	120.1	2.17E-05	1.05E+02	3.37E+09
C6H6O3_4	C(=O)C=CC(O)(O)C(=O)(O[O])	161.1			
C6H6O3_40	C1(O)C(O)(O)C(=O)C=CC1(O)	160.1	1.05E-07	1.27E+02	6.49E+10
C6H6O3_41	C1(O)(O)C(ON(=O)(=O))C(O)C=CC1(=O)	205.1	6.71E-08	1.29E+02	4.99E+10
C6H6O3_42	C(=O)(O)C(=O)C(O)(O)C=CC(=O)	174.1	1.99E-08	1.34E+02	1.70E+12
C6H6O3_43	C(=O)(O)C(O)(O)C(=O)C=CC(=O)	174.1	1.26E-08	1.36E+02	2.69E+12
C6H6O3_44	C(=O)(O)C=CC(=O)C(O)(O)C(=O)	174.1	1.26E-08	1.36E+02	2.69E+12
C6H6O3_45	C(=O)(O)C=CC(O)(O)C(=O)C(=O)	174.1	1.99E-08	1.34E+02	1.70E+12
C6H6O3_5	C1(O)(O)C(ON(=O)(=O))C(O[O])C=CC1(=O)	220.1			
C6H6O3_6	C1(O)(O)C(=O)C=CC([O])C1(O)	159.1			
C6H6O3_7	C(=O)C(O)(O)C(=O)(O[O])	135.1			
C6H6O3_8	C1(O)(O)C(ON(=O)(=O))C([O])C=CC1(=O)	204.1			
C6H6O3_9	C(=O)C(O)(O)C(=O)C=CC(=O)	158.1	1.33E-05	1.04E+02	3.98E+08
C6H6O4	C(=CC=O)C=C(C(=O)O)O	142.1	2.29E-05	1.02E+02	4.55E+08
C6H6O7	C(=CC(C(=O)O)OO)C(=O)C(=O)O	190.1	5.10E-11	1.61E+02	1.70E+14
C6H7O10N	O=CC(=O)C(OO)C(OO)C(C=O)ON(=O)=O	253.1	2.17E-11	1.65E+02	6.20E+13
C6H7O11	C(=O)(C(C(C(C(=O)O)OO)OO)O[O])C(=O)O	255.1			
C6H7O12N	C(=O)(C(C(C(C(=O)O)OO)OO)ON(=O)=O)C(=O)O	285.1	4.63E-19	2.50E+02	3.47E+22
C6H7O6	C(=CC(C(C(=O)O)O)O[O])C=O	175.1			
C6H7O7	O=CC([O])=CC(OO)C(C=O)OO	191.1			
C6H7O8	C(=CC(=O)O[O])C(C(C(=O)O)O)OO	207.1			
C6H7O9	O=CC(=O)C(OO)C(OO)C(C=O)O[O]	223.1			
C6H7O9gd	C(=C(C(=O)O)O)C(C(C(=O)O)OO)O[O]	223.1			
C6H7O9N	C(=CC(=O)OO)C(C(C(=O)O)O)ON(=O)=O	237.1	3.07E-10	1.54E+02	1.00E+13
C6H8O11	C(=O)(C(C(C(C(=O)O)OO)OO)OO)C(=O)O	256.1	2.89E-21	2.75E+02	1.44E+25
C6H8O8	C(=CC(=O)OO)C(C(C(=O)O)O)OO	208.1	8.48E-12	1.70E+02	7.22E+14
C6H8O9	O=CC(=O)C(OO)C(OO)C(C=O)OO	224.1	6.95E-13	1.81E+02	5.25E+15
cat_PC2	C(=CC(C(=O)O)O[O])C(C(=O)O)O	191.1			
CATE_C2a	O(c1ccccc1O)OC(=O)C=O	182.1	1.14E+00	5.29E+01	8.32E+02

CATE_C2b	O(c1ccccc1O)OCC=O	168.2	7.18E-02	6.32E+01	6.35E+03
CATE_C2c	OCC(=O)(OOc1ccccc1O)	184.2	1.87E-01	6.24E+01	4.17E+03
CATE_C4a	O(c1ccccc1O)OC(=O)C=CC(=O)C=O	236.2	5.31E-03	7.47E+01	3.00E+04
CATE_C5a	OC(C=O)C(=O)C=CC(=O)(OOc1ccccc1O)	266.2	2.09E-05	1.01E+02	5.82E+06
CATE_CATE	O(c1ccccc1O)Oc1ccccc1O	218.2	8.38E-05	9.17E+01	3.50E+06
CATE_DNP	O(c1ccccc1O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	358.2	1.10E-11	1.68E+02	2.92E+12
CATE_MALc	O(c1ccccc1O)OC1C(=O)OC(=O)C1O	240.2	1.62E-05	1.02E+02	1.99E+06
CATE_NBZb	O(c1ccccc1O)OC1C(=O)C=CC(=O)C1ON(=O)=O	295.2	3.45E-07	1.17E+02	9.03E+07
CATE_NCAT	O(c1ccccc1O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	329.2	1.62E-11	1.67E+02	7.34E+12
CATE_NDN	O(c1ccccc1O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	403.2	6.83E-12	1.69E+02	2.01E+12
CATE_NNC	O(c1ccccc1O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	374.2	8.83E-12	1.69E+02	6.01E+12
CATE_NPHb	O(c1ccccc1O)Oc1ccccc1N(=O)=O	247.2	1.04E-04	8.98E+01	1.00E+04
CATE_PBZ	O(c1ccccc1O)OC1C(=O)C=CC(=O)C1O	250.2	7.07E-07	1.14E+02	6.42E+07
CATEC1O	[O]c1ccccc1O	109.1			
CATEC1O2	[O]Oc1ccccc1O	125.1			
CATEC1OOH	OOc1ccccc1O	126.1	9.86E-04	8.30E+01	2.18E+06
CATECBIPERO	[O]C1(O)C(O)=CC2OOC1C2O	175.1			
CATECBIPERO2	[O]OC1(O)C(O)=CC2OOC1C2O	191.1			
CATECBP2OH	OC2=CC1OOC(C1O)C2(O)O	176.1	1.07E-06	1.19E+02	5.69E+09
CATECBPOOH	OOC1(O)C(O)=CC2OOC1C2O	192.1	1.97E-08	1.36E+02	7.18E+10
CATECHOL	Oc1ccccc1O	110.1	2.17E-02	6.84E+01	2.87E+06
CATECOOA	[O-][O+]=C(O)C=CC=CC(=O)O	158.1			
CH2OO	[O-][O+]=C	46.0			
CH2OOA	[O-][O+]=C	46.0			
CH2OOB	[O-][O+]=C	46.0			
CHOCOHCO	[O]C(CO)C=O	89.1			
CO14O3CHO	O=CCOC(=O)C=O	116.1	4.55E-01	5.71E+01	3.60E+03
CO14O3CO2H	O=CCOC(=O)C(=O)O	132.1	6.51E-03	7.70E+01	1.35E+06
CO2C4DIAL	O=CC(=O)C(=O)C=O	114.1	1.15E-01	6.20E+01	7.23E+04
DNP_C2c	OCC(=O)(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O)	324.2	2.80E-08	1.34E+02	4.02E+10

DNP_C4a	O(C1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O)OC(=O)C=CC(=O)C=O	376.2	8.28E-10	1.48E+02	2.30E+11
DNP_C5a	OC(C=O)C(=O)C=CC(=O)(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O)	406.2	4.66E-13	1.84E+02	5.39E+14
DNP_DNP	O(C1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	498.2	6.87E-21	2.72E+02	1.28E+22
DNPHEN	O=N(=O)c1ccc(O)c(c1)N(=O)=O	184.1	2.51E-04	8.58E+01	8.40E+04
DNPHENO	O=N(=O)C1=CC2(OOC(C2O)C1([O])O)N(=O)=O	249.1			
DNPHENO2	[O]OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	265.1			
DNPHENOOH	OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	266.1	2.77E-11	1.64E+02	2.00E+13
EPX_BZFU	O(C(=O)C1OC1C=O)OC1C(O)COC1=O	232.1	9.32E-04	8.38E+01	2.89E+05
EPX_C2a	O(C(=O)C1OC1C=O)OC(=O)C=O	188.1	5.70E+01	3.97E+01	1.16E+01
EPX_C2b	O(C(=O)C1OC1C=O)OCC=O	174.1	5.12E+00	4.81E+01	2.90E+02
EPX_C2c	OCC(=O)(OOC(=O)C1OC1C=O)	190.1	2.09E+01	4.54E+01	5.58E+01
EPX_C3a	OC(C=O)C(=O)(OOC(=O)C1OC1C=O)	218.1	1.20E+00	5.76E+01	8.26E+02
EPX_C3DI	O(C(=O)C1OC1C=O)OC(C=O)C=O	202.1	2.06E-01	6.14E+01	6.85E+03
EPX_C4a	O(C(=O)C1OC1C=O)OC(=O)C=CC(=O)C=O	242.1	3.84E-01	5.88E+01	2.49E+02
EPX_C5a	OC(C=O)C(=O)C=CC(=O)(OOC(=O)C1OC1C=O)	272.2	3.09E-03	8.09E+01	5.83E+04
EPX_C6a	O(C(=O)C1OC1C=O)Oc1ccccc1	208.2	5.44E-01	5.50E+01	1.14E+01
EPX_CATE	O(C(=O)C1OC1C=O)Oc1ccccc1O	224.2	2.79E-02	6.84E+01	6.69E+03
EPX_DNP	O(C(=O)C1OC1C=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	364.2	5.92E-09	1.40E+02	3.27E+10
EPX_EPX	O(C(=O)C1OC1C=O)OC(=O)C1OC1C=O	230.1	1.70E+00	5.25E+01	7.99E+01
EPX_MALb	O(C(=O)C1OC1C=O)OC(C=O)C(O)C=O	232.1	2.05E-03	8.29E+01	9.27E+05
EPX_MALc	O(C(=O)C1OC1C=O)OC1C(=O)OC(=O)C1O	246.1	3.97E-03	8.06E+01	6.25E+04
EPX_NBZa	O(C(=O)C1OC1C=O)OC1C(=O)OCC1ON(=O)=O	277.1	3.03E-04	8.79E+01	2.35E+05
EPX_NBZb	O(C(=O)C1OC1C=O)OC1C(=O)C=CC(=O)C1ON(=O)=O	301.2	6.52E-05	9.51E+01	8.15E+05
EPX_NCAT	O(C(=O)C1OC1C=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	335.2	1.34E-08	1.38E+02	5.36E+10
EPX_NDN	O(C(=O)C1OC1C=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	409.2	2.46E-09	1.43E+02	2.75E+10
EPX_NNC	O(C(=O)C1OC1C=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	380.2	4.76E-09	1.42E+02	6.37E+10
EPX_NPHb	O(C(=O)C1OC1C=O)Oc1ccccc1N(=O)=O	253.2	8.09E-03	7.19E+01	1.46E+02
EPX_PBZ	O(C(=O)C1OC1C=O)OC1C(=O)C=CC(=O)C1O	256.2	1.94E-04	9.12E+01	1.08E+06
EPXC4DIAL	O=CC1OC1C=O	100.1	3.53E-01	5.77E+01	7.96E+03
EPXDLCO2H	O=CC1OC1C(=O)O	116.1	5.43E-03	7.73E+01	2.54E+06

EPXDLCO3	[O]OC(=O)C1OC1C=O	131.1			
EPXDLCO3H	OOC(=O)C1OC1C=O	132.1	2.18E-02	7.12E+01	1.45E+05
EPXDLPAN	O=CC1OC1C(=O)OON(=O)=O	177.1	5.27E-02	6.55E+01	7.49E+03
ETHENO3O	[O]CCON(=O)=O	106.1			
ETHENO3O2	[O]OCCON(=O)=O	122.1			
ETHGLY	OCCO	62.1	7.29E-02	6.56E+01	1.49E+05
ETHO2HNO3	OOCCON(=O)=O	123.1	4.50E-02	6.89E+01	7.95E+04
ETHOHNO3	OCCON(=O)=O	107.1	2.95E-01	6.13E+01	1.48E+04
gdBPR_CAT	C1=CC(C2(C(C1OO2)(O)O)O)O[O]	191.1			
gdBPR_PHEN	C1=CC2C(C(C1O[O])OO2)(O)O	175.1			
GLY	O=CC=O	58.0	2.89E+00	5.03E+01	2.88E+03
GLYOO	[O-][O+]=CC=O	74.0			
GLYOOA	[O-][O+]=CC=O	74.0			
GLYOOB	[O-][O+]=CC=O	74.0			
HCHO	C=O	30.0	3.73E+03	2.22E+01	5.35E-06
HCOCH2O	[O]CC=O	59.0			
HCOCH2O2	[O]OCC=O	75.0			
HCOCH2OOH	OOCC=O	76.1	1.12E+00	5.49E+01	3.33E+03
HCOCO	O=[C]C=O	57.0	2.91E+04	1.58E+01	5.30E-01
HCOCO2H	O=CC(=O)O	74.0	5.89E-01	5.81E+01	7.15E+04
HCOCO3	[O]OC(=O)C=O	89.0			
HCOCO3H	OOC(=O)C=O	90.0	2.07E+00	5.28E+01	4.56E+03
HCOCOHCO3	OC(C=O)C(=O)O[O]	119.1			
HCOCOHCO3H	OC(C=O)C(=O)OO	120.1	6.25E-03	7.87E+01	1.00E+06
HCOCOHPAN	O=CC(O)C(=O)OON(=O)=O	165.1	2.41E-02	7.03E+01	1.15E+05
HOC6H4NO2	O=N(=O)c1ccccc1O	139.1	6.62E-02	6.32E+01	2.97E+03
HOCH2CH2O	OCC[O]	61.1			
HOCH2CH2O2	OCCO[O]	77.1			
HOCH2CHO	OCC=O	60.1	7.69E+00	4.74E+01	1.84E+03
HOCH2CO2H	OCC(=O)O	76.1	8.90E-03	7.67E+01	6.69E+06

HOCH2CO3	OCC(=O)O[O]	91.0			
HOCH2CO3H	OCC(=O)OO	92.1	5.93E-02	6.88E+01	3.83E+05
HOCH2COCHO	OCC(=O)C=O	88.1	2.66E-01	5.96E+01	4.57E+04
HOCHOCOOH	OCC(OO)C=O	106.1	7.31E-04	8.63E+01	6.38E+06
HOCOC4DIAL	O=CC(=O)C(O)C=O	116.1	1.07E-02	7.41E+01	9.16E+05
HOHOC4DIAL	O=CC(O)C(O)C=O	118.1	7.34E-04	8.77E+01	1.37E+07
HYETHO2H	OCCOO	78.1	1.44E-02	7.27E+01	3.83E+05
KETB	O=C=CCC=O	84.1	5.26E+03	2.15E+01	1.37E+00
KETENAL	C(=C=O)C=O	70.1	1.46E+04	1.80E+01	1.06E+00
KETENOL	O=C=CC=CO	84.1	1.42E+05	1.47E+01	5.17E-02
M1C2O2	O=C(O)C(O)O[O]	107.0			
M1O2A	OC(=O)C(O)C(C=O)O[O]	149.1			
MALa_BZFU	O(C(=O)C=CC=O)OC1C(O)COC1=O	216.1	3.90E-03	7.67E+01	5.38E+04
MALa_C2a	O(C(=O)C=CC=O)OC(=O)C=O	172.1	1.17E+02	3.61E+01	3.67E+00
MALa_C2b	O(C(=O)C=CC=O)OCC=O	158.1	1.07E+01	4.45E+01	7.48E+01
MALa_C2c	OCC(=O)(OOC(=O)C=CC=O)	174.1	6.87E+01	4.00E+01	1.28E+01
MALa_C3a	OC(C=O)C(=O)(OOC(=O)C=CC=O)	202.1	3.69E+00	5.23E+01	2.02E+02
MALa_C3DI	O(C(=O)C=CC=O)OC(C=O)C=O	186.1	4.63E-01	5.74E+01	1.61E+03
MALa_C4a	O(C(=O)C=CC=O)OC(=O)C=CC(=O)C=O	226.1	1.22E+00	5.32E+01	5.29E+01
MALa_C5a	OC(C=O)C(=O)C=CC(=O)(OOC(=O)C=CC=O)	256.2	1.20E-02	7.43E+01	1.11E+04
MALa_C6a	O(C(=O)C=CC=O)Oc1ccccc1	192.2	1.77E+00	4.92E+01	2.65E+00
MALa_CATE	O(C(=O)C=CC=O)Oc1ccccc1O	208.2	9.46E-02	6.23E+01	1.69E+03
MALa_DNP	O(C(=O)C=CC=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	348.2	3.16E-08	1.32E+02	6.02E+09
MALa_EPX	O(C(=O)C=CC=O)OC(=O)C1OC1C=O	214.1	4.76E+00	4.84E+01	2.01E+01
MALa_MALa	O(C(=O)C=CC=O)OC(=O)C=CC=O	198.1	1.04E+01	4.45E+01	6.20E+00
MALa_MALb	O(C(=O)C=CC=O)OC(C=O)C(O)C=O	216.1	6.71E-03	7.72E+01	1.90E+05
MALa_MALc	O(C(=O)C=CC=O)OC1C(=O)OC(=O)C1O	230.1	1.60E-02	7.40E+01	1.21E+04
MALa_NBZa	O(C(=O)C=CC=O)OC1C(=O)OCC1ON(=O)=O	261.1	1.22E-03	8.10E+01	4.03E+04
MALa_NBZb	O(C(=O)C=CC=O)OC1C(=O)C=CC(=O)C1ON(=O)=O	285.2	3.29E-04	8.71E+01	1.14E+05
MALa_NCAT	O(C(=O)C=CC=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	319.2	7.07E-08	1.30E+02	1.05E+10

MALa_NDN	O(C(=O)C=CC=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	393.2	1.36E-08	1.35E+02	4.50E+09
MALa_NNC	O(C(=O)C=CC=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	364.2	2.56E-08	1.34E+02	1.15E+10
MALa_NPHb	O(C(=O)C=CC=O)Oc1ccccc1N(=O)=O	237.2	2.69E-02	6.58E+01	2.43E+01
MALa_PBZ	O(C(=O)C=CC=O)OC1C(=O)C=CC(=O)C1O	240.2	9.48E-04	8.34E+01	1.74E+05
MALANHY	O=C1C=CC(=O)O1	98.1	4.72E+05	6.48E+00	3.19E-04
MALANHY2OH	O=C1OC(=O)C(O)C1O	132.1	1.82E-03	8.41E+01	1.54E+06
MALANHYO	O=C1OC(=O)C(O)C1[O]	131.1			
MALANHYO2	[O]OC1C(=O)OC(=O)C1O	147.1			
MALANHYONO2	OONOC1C(=O)OC(=O)C1O	179.1	6.66E+00	5.06E+01	1.44E+02
MALANHYOOH	OOC1C(=O)OC(=O)C1O	148.1	8.59E-05	9.67E+01	5.26E+06
MALb_BZFU	O(C(C=O)C(O)C=O)OC1C(O)COC1=O	234.2	1.27E-07	1.24E+02	7.45E+09
MALb_C2a	O(C(C=O)C(O)C=O)OC(=O)C=O	190.1	1.08E-01	6.67E+01	5.52E+04
MALb_C2b	O(C(C=O)C(O)C=O)OCC=O	176.1	3.35E-03	7.99E+01	1.15E+06
MALb_C2c	OCC(=O)(OOC(C=O)C(O)C=O)	192.1	2.28E-02	7.46E+01	4.07E+05
MALb_C3a	OC(C=O)C(=O)(OOC(C=O)C(O)C=O)	220.1	7.11E-04	8.97E+01	9.61E+06
MALb_C4a	O(C(C=O)C(O)C=O)OC(=O)C=CC(=O)C=O	244.2	3.92E-04	8.92E+01	3.25E+06
MALb_C5a	OC(C=O)C(=O)C=CC(=O)(OOC(C=O)C(O)C=O)	274.2	9.28E-07	1.17E+02	1.82E+09
MALb_C6a	O(C(C=O)C(O)C=O)Oc1ccccc1	210.2	4.47E-04	8.66E+01	8.75E+04
MALb_CATE	O(C(C=O)C(O)C=O)Oc1ccccc1O	226.2	1.04E-05	1.04E+02	3.10E+07
MALb_DNP	O(C(C=O)C(O)C=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	366.2	1.79E-13	1.89E+02	3.50E+15
MALb_MALb	O(C(C=O)C(O)C=O)OC(C=O)C(O)C=O	234.2	2.30E-07	1.23E+02	2.07E+10
MALb_MALc	O(C(C=O)C(O)C=O)OC1C(=O)OC(=O)C1O	248.1	7.17E-07	1.19E+02	1.21E+09
MALb_NBZa	O(C(C=O)C(O)C=O)OC1C(=O)OCC1ON(=O)=O	279.2	6.46E-08	1.26E+02	5.53E+09
MALb_NBZb	O(C(C=O)C(O)C=O)OC1C(=O)C=CC(=O)C1ON(=O)=O	303.2	1.48E-08	1.33E+02	1.94E+10
MALb_NCAT	O(C(C=O)C(O)C=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	337.2	3.11E-13	1.87E+02	6.44E+15
MALb_NDN	O(C(C=O)C(O)C=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	411.2	1.01E-13	1.91E+02	2.55E+15
MALb_NNC	O(C(C=O)C(O)C=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	382.2	1.57E-13	1.90E+02	5.64E+15
MALb_NPHb	O(C(C=O)C(O)C=O)Oc1ccccc1N(=O)=O	255.2	3.49E-06	1.07E+02	2.42E+06
MALb_PBZ	O(C(C=O)C(O)C=O)OC1C(=O)C=CC(=O)C1O	258.2	3.05E-08	1.31E+02	2.39E+10
MALc_C2c	OCC(=O)(OOC1C(=O)OC(=O)C1O)	206.1	2.94E-02	7.39E+01	6.87E+04

MALc_C4a	O(C1C(=O)OC(=O)C1O)OC(=O)C=CC(=O)C=O	258.1	6.92E-04	8.71E+01	2.80E+05
MALc_C5a	OC(C=O)C(=O)C=CC(=O)(OOC1C(=O)OC(=O)C1O)	288.2	1.54E-06	1.15E+02	2.20E+08
MALc_DNP	O(C1C(=O)OC(=O)C1O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	380.2	2.27E-13	1.88E+02	8.06E+14
MALc_MALc	O(C1C(=O)OC(=O)C1O)OC1C(=O)OC(=O)C1O	262.1	1.03E-06	1.18E+02	1.77E+08
MALc_NDN	O(C1C(=O)OC(=O)C1O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	425.2	1.22E-13	1.90E+02	4.57E+14
MALDALCO2H	O=CC=CC(=O)O	100.1	2.30E-02	7.03E+01	4.66E+05
MALDALCO2HOH	O=CC=C(O)C(=O)O	116.1	1.31E-04	9.46E+01	2.97E+08
MALDALCO3H	OOC(=O)C=CC=O	116.1	8.77E-02	6.44E+01	3.00E+04
MALDIAL	O=CC=CC=O	84.1	4.32E-01	5.65E+01	3.40E+03
MALDIAL2OH	O=CC(O)=C(O)C=O	116.1	1.58E-01	6.71E+01	1.14E+05
MALDIALCO2	O=CC=CC(=O)[O]	99.1			
MALDIALCO3	[O]OC(=O)C=CC=O	115.1			
MALDIALO	O=CC(O)C([O])C=O	117.1			
MALDIALO2	[O]OC(C=O)C(O)C=O	133.1			
MALDIALOH	O=CC=C(O)C=O	100.1	2.49E-02	7.07E+01	2.58E+05
MALDIALONO2	O=CC(O)C(C=O)ON(=O)=O	163.1	3.21E-04	9.03E+01	1.75E+07
MALDIALOOH	OOC(C=O)C(O)C=O	134.1	3.34E-05	1.00E+02	8.06E+07
MALDIALPAN	O=CC=CC(=O)OON(=O)=O	161.1	1.88E-01	5.92E+01	1.35E+03
MALNHYOHCO	O=C1OC(=O)C(O)C1=O	130.1	1.61E-02	7.20E+01	1.20E+05
MDALCO2H2OH	O=C(O)C=C(O)C=O	132.1	1.31E-04	9.46E+01	2.97E+08
NBENZ3OH	O=N(=O)c1ccc(O)c(O)c1O	171.1	3.96E-06	1.07E+02	3.74E+10
NBENZ3OHO	O=N(=O)C12C=C(O)C(O)([O])C(O)(OO1)C2O	236.1			
NBENZ3OHO2	O=N(=O)C12C=C(O)C(O)(O[O])C(O)(OO1)C2O	252.1			
NBENZ3OHOOH	O=N(=O)C12C=C(O)C(O)(OO)C(O)(OO1)C2O	253.1	3.09E-13	1.88E+02	9.60E+15
NBENZ4OH	O=N(=O)c1c(O)cc(O)c(O)c1O	187.1	1.75E-08	1.31E+02	2.16E+14
NBENZ4OHO	O=N(=O)C12OOC(O)(C1O)C(O)([O])C(O)=C2O	252.1			
NBENZ4OHO2	O=N(=O)C12OOC(O)(C1O)C(O)(O[O])C(O)=C2O	268.1			
NBENZ4OHOOH	O=N(=O)C12OOC(O)(C1O)C(O)(OO)C(O)=C2O	269.1	3.30E-16	2.21E+02	2.96E+19
NBZa_BZFU	O(C1C(=O)OCC1ON(=O)=O)OC1C(O)COC1=O	279.2	1.83E-08	1.30E+02	2.29E+09
NBZa_C2a	O(C1C(=O)OCC1ON(=O)=O)OC(=O)C=O	235.1	1.49E-02	7.11E+01	2.46E+04

NBZa_C2b	O(C1C(=O)OCC1ON(=O)=O)OCC=O	221.1	7.61E-04	8.27E+01	2.08E+05
NBZa_C2c	OCC(=O)(OOC1C(=O)OCC1ON(=O)=O)	237.1	2.12E-03	8.00E+01	2.58E+05
NBZa_C3a	OC(C=O)C(=O)(OOC1C(=O)OCC1ON(=O)=O)	265.1	9.53E-05	9.45E+01	5.92E+06
NBZa_C4a	O(C1C(=O)OCC1ON(=O)=O)OC(=O)C=CC(=O)C=O	289.2	4.23E-05	9.62E+01	1.16E+06
NBZa_C5a	OC(C=O)C(=O)C=CC(=O)(OOC1C(=O)OCC1ON(=O)=O)	319.2	1.17E-07	1.24E+02	8.52E+08
NBZa_CATE	O(C1C(=O)OCC1ON(=O)=O)Oc1ccccc1O	271.2	3.96E-06	1.06E+02	4.21E+06
NBZa_DNP	O(C1C(=O)OCC1ON(=O)=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	411.2	4.26E-14	1.94E+02	1.03E+15
NBZa_MALc	O(C1C(=O)OCC1ON(=O)=O)OC1C(=O)OC(=O)C1O	293.1	1.24E-07	1.23E+02	3.66E+08
NBZa_NBZa	O(C1C(=O)OCC1ON(=O)=O)OC1C(=O)OCC1ON(=O)=O	324.2	5.60E-09	1.36E+02	1.17E+09
NBZa_NBZb	O(C1C(=O)OCC1ON(=O)=O)OC1C(=O)C=CC(=O)C1ON(=O)=O	348.2	1.05E-09	1.44E+02	3.86E+09
NBZa_NCAT	O(C1C(=O)OCC1ON(=O)=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	382.2	5.01E-14	1.94E+02	4.26E+15
NBZa_NDN	O(C1C(=O)OCC1ON(=O)=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	456.2	2.95E-14	1.95E+02	3.72E+14
NBZa_NNC	O(C1C(=O)OCC1ON(=O)=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	427.2	3.11E-14	1.96E+02	2.34E+15
NBZa_NPHb	O(C1C(=O)OCC1ON(=O)=O)Oc1ccccc1N(=O)=O	300.2	9.82E-07	1.11E+02	1.30E+05
NBZa_PBZ	O(C1C(=O)OCC1ON(=O)=O)OC1C(=O)C=CC(=O)C1O	303.2	2.54E-09	1.40E+02	1.21E+10
NBZb_C2c	OCC(=O)(OOC1C(=O)C=CC(=O)C1ON(=O)=O)	261.1	3.95E-04	8.80E+01	9.64E+05
NBZb_C4a	O(C1C(=O)C=CC(=O)C1ON(=O)=O)OC(=O)C=CC(=O)C=O	313.2	1.54E-05	1.01E+02	2.43E+06
NBZb_C5a	OC(C=O)C(=O)C=CC(=O)(OOC1C(=O)C=CC(=O)C1ON(=O)=O)	343.2	2.88E-08	1.30E+02	2.61E+09
NBZb_DNP	O(C1C(=O)C=CC(=O)C1ON(=O)=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	435.2	4.44E-15	2.05E+02	6.55E+15
NBZb_MALc	O(C1C(=O)C=CC(=O)C1ON(=O)=O)OC1C(=O)OC(=O)C1O	317.2	1.84E-08	1.33E+02	2.03E+09
NBZb_NBZb	O(C1C(=O)C=CC(=O)C1ON(=O)=O)OC1C(=O)C=CC(=O)C1ON(=O)=O	372.2	5.53E-10	1.47E+02	3.35E+09
NBZb_NDN	O(C1C(=O)C=CC(=O)C1ON(=O)=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	480.2	2.91E-15	2.06E+02	2.29E+15
NBZb_PBZ	O(C1C(=O)C=CC(=O)C1ON(=O)=O)OC1C(=O)C=CC(=O)C1O	327.2	9.77E-10	1.45E+02	2.02E+10
NBZFUO	O=N(=O)OC1COC(=O)C1[O]	162.1			
NBZFUO2	[O]OC1C(=O)OCC1ON(=O)=O	178.1			
NBZFUONE	O=N(=O)OC1C(=O)COC1=O	161.1	2.00E-04	8.93E+01	2.26E+06
NBZFUOOH	OOC1C(=O)OCC1ON(=O)=O	179.1	9.26E-06	1.02E+02	5.97E+07
NBZQO	O=N(=O)OC1C(=O)C=CC(=O)C1[O]	186.1			
NBZQO2	[O]OC1C(=O)C=CC(=O)C1ON(=O)=O	202.1			
NBZQOOH	OOC1C(=O)C=CC(=O)C1ON(=O)=O	203.1	2.05E-06	1.10E+02	3.05E+08

NC4DCO2	O=CC(=CC(=O)[O])N(=O)=O	144.1			
NC4DCO2H	O=CC(=CC(=O)O)N(=O)=O	145.1	5.83E-05	9.58E+01	2.49E+08
NC4DCO2HOH	O=CC(=C(O)C(=O)O)N(=O)=O	161.1	1.49E-04	9.55E+01	3.20E+08
NCAT_C2c	OCC(=O)(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)O)	295.2	7.75E-08	1.32E+02	4.87E+10
NCAT_C4a	O(C1(O)C(=CC2(OOC1C2O)N(=O)=O)O)OC(=O)C=CC(=O)C=O	347.2	1.62E-09	1.47E+02	4.60E+11
NCAT_C5a	OC(C=O)C(=O)C=CC(=O)(OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)O)	377.2	8.17E-13	1.83E+02	1.14E+15
NCAT_DNP	O(C1(O)C(=CC2(OOC1C2O)N(=O)=O)O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	469.2	7.99E-21	2.71E+02	4.40E+22
NCAT_MALc	O(C1(O)C(=CC2(OOC1C2O)N(=O)=O)O)OC1C(=O)OC(=O)C1O	351.2	4.04E-13	1.87E+02	1.91E+15
NCAT_NBZb	O(C1(O)C(=CC2(OOC1C2O)N(=O)=O)O)OC1C(=O)C=CC(=O)C1ON(=O)=O	406.2	5.29E-15	2.05E+02	2.84E+16
NCAT_NCAT	O(C1(O)C(=CC2(OOC1C2O)N(=O)=O)O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	440.2	1.14E-20	2.71E+02	1.08E+23
NCAT_NDN	O(C1(O)C(=CC2(OOC1C2O)N(=O)=O)O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	514.2	5.06E-21	2.73E+02	2.74E+22
NCAT_PBZ	O(C1(O)C(=CC2(OOC1C2O)N(=O)=O)O)OC1C(=O)C=CC(=O)C1O	361.2	9.00E-15	2.03E+02	4.38E+16
NCATECHOL	O=N(=O)c1ccc(O)c(O)c1	155.1	5.54E-04	8.43E+01	1.01E+07
NCATECO	O=N(=O)C12OOC(C2O)C(O)([O])C(=C1)O	220.1			
NCATECO2	[O]OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	236.1			
NCATECOOH	OOC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	237.1	4.68E-11	1.63E+02	3.41E+13
NDN_C2c	OCC(=O)(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)	369.2	1.07E-08	1.38E+02	4.25E+10
NDN_C4a	O(C1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)OC(=O)C=CC(=O)C=O	421.2	3.78E-10	1.51E+02	1.62E+11
NDN_C5a	OC(C=O)C(=O)C=CC(=O)(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)	451.2	2.35E-13	1.87E+02	3.82E+14
NDN_DNP	O(C1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	543.2	4.82E-21	2.73E+02	6.29E+21
NDN_NDN	O(C1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	588.2	3.39E-21	2.75E+02	2.60E+21
NDNPHENO	O=N(=O)OC1C2OOC1(C=C(N(=O)=O)C2([O])O)N(=O)=O	294.1			
NDNPHENO2	[O]OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	310.1			
NDNPHENOOH	OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	311.1	1.95E-11	1.65E+02	1.52E+13
NMGLYOX	O=CC(=O)CON(=O)=O	133.1	1.96E-01	6.10E+01	1.89E+04
NNBENZ3OHO	O=N(=O)OC1C2(O)OOC1(N(=O)=O)C=C(O)C2(O)[O]	281.1			
NNBENZ3OHO2	O=N(=O)OC1C2(O)OOC1(N(=O)=O)C=C(O)C2(O)O[O]	297.1			
NNBENZ3OHOOH	O=N(=O)OC1C2(O)OOC1(N(=O)=O)C=C(O)C2(O)OO	298.1	2.19E-13	1.89E+02	6.76E+15
NNBENZ4OHO	O=N(=O)OC1C2(O)OOC1(N(=O)=O)C(O)=C(O)C2(O)[O]	297.1			
NNBENZ4OHO2	O=N(=O)OC1C2(O)OOC1(N(=O)=O)C(O)=C(O)C2(O)O[O]	313.1			

NNBENZ4OHOOH	O=N(=O)OC1C2(O)OOC1(N(=O)=O)C(O)=C(O)C2(O)OO	314.1	2.73E-16	2.22E+02	1.81E+19
NNC_C2c	OCC(=O)(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)	340.2	2.51E-08	1.36E+02	6.85E+10
NNC_C4a	O(C1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)OC(=O)C=CC(=O)C=O	392.2	6.36E-10	1.51E+02	4.62E+11
NNC_C5a	OC(C=O)C(=O)C=CC(=O)(OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)	422.2	3.59E-13	1.86E+02	1.05E+15
NNC_DNP	O(C1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	514.2	5.06E-21	2.73E+02	2.74E+22
NNC_MALc	O(C1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)OC1C(=O)OC(=O)C1O	396.2	1.92E-13	1.89E+02	1.44E+15
NNC_NBZb	O(C1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)OC1C(=O)C=CC(=O)C1ON(=O)=O	451.2	3.10E-15	2.07E+02	1.63E+16
NNC_NCAT	O(C1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	485.2	6.54E-21	2.73E+02	8.03E+22
NNC_NDN	O(C1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	559.2	3.19E-21	2.75E+02	1.58E+22
NNC_NNC	O(C1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	530.2	3.70E-21	2.75E+02	5.83E+22
NNC_PBZ	O(C1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)OC1C(=O)C=CC(=O)C1O	406.2	5.29E-15	2.05E+02	2.84E+16
NNCATECO	O=N(=O)OC1C2OOC1(C=C(O)C2([O])O)N(=O)=O	265.1			
NNCATECO2	[O]OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	281.1			
NNCATECOOH	OOC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	282.1	3.14E-11	1.65E+02	2.62E+13
NO3CH2CHO	O=CCON(=O)=O	105.0	4.15E+00	4.86E+01	1.73E+03
NO3CH2CO2H	OC(=O)CON(=O)=O	121.0	2.29E-02	7.23E+01	1.20E+06
NO3CH2CO3	[O]OC(=O)CON(=O)=O	136.0			
NO3CH2CO3H	OOC(=O)CON(=O)=O	137.0	7.83E-02	6.69E+01	3.05E+05
NO3CH2PAN	O=C(CON(=O)=O)OON(=O)=O	182.0	1.39E-01	6.23E+01	6.29E+03
NPHa_BZFU	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC1C(O)COC1=O	321.2	5.31E-09	1.39E+02	5.07E+09
NPHa_C2a	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC(=O)C=O	277.1	5.07E-03	7.96E+01	4.29E+04
NPHa_C2b	O(C1(O)C=CC2OOC1C2ON(=O)=O)OCC=O	263.2	2.55E-04	9.12E+01	3.88E+05
NPHa_C2c	OCC(=O)(OOC1(O)C=CC2OOC1C2ON(=O)=O)	279.2	4.72E-04	9.11E+01	5.78E+05
NPHa_C3a	OC(C=O)C(=O)(OOC1(O)C=CC2OOC1C2ON(=O)=O)	307.2	2.22E-05	1.05E+02	1.22E+07
NPHa_C3DI	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC(C=O)C=O	291.2	6.24E-06	1.08E+02	2.12E+07
NPHa_C4a	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC(=O)C=CC(=O)C=O	331.2	1.37E-05	1.04E+02	2.67E+06
NPHa_C5a	OC(C=O)C(=O)C=CC(=O)(OOC1(O)C=CC2OOC1C2ON(=O)=O)	361.2	2.48E-08	1.34E+02	2.27E+09
NPHa_C6a	O(C1(O)C=CC2OOC1C2ON(=O)=O)Oc1ccccc1	297.2	1.92E-05	1.01E+02	3.02E+04
NPHa_CATE	O(C1(O)C=CC2OOC1C2ON(=O)=O)Oc1ccccc1O	313.2	3.82E-07	1.19E+02	2.26E+07
NPHa_DNP	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	453.2	3.03E-15	2.08E+02	6.55E+15

NPHa_EPX	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC(=O)C1OC1C=O	319.2	7.86E-05	9.72E+01	5.39E+05
NPHa_MALa	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC(=O)C=CC=O	303.2	3.34E-04	9.03E+01	1.10E+05
NPHa_MALb	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC(C=O)C(O)C=O	321.2	1.37E-08	1.36E+02	1.28E+10
NPHa_MALc	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC1C(=O)OC(=O)C1O	335.2	1.71E-08	1.36E+02	2.05E+09
NPHa_NBZa	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC1C(=O)OCC1ON(=O)=O	366.2	2.76E-09	1.41E+02	2.29E+09
NPHa_NBZb	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC1C(=O)C=CC(=O)C1ON(=O)=O	390.2	3.54E-10	1.51E+02	1.06E+10
NPHa_NCAT	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	424.2	4.65E-15	2.08E+02	2.02E+16
NPHa_NDN	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	498.2	1.66E-15	2.11E+02	3.36E+15
NPHa_NNC	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	469.2	2.24E-15	2.10E+02	1.48E+16
NPHa_NPHa	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC1(O)C=CC2OOC1C2ON(=O)=O	408.2	2.67E-10	1.55E+02	1.28E+10
NPHa_NPHb	O(C1(O)C=CC2OOC1C2ON(=O)=O)Oc1ccccc1N(=O)=O	342.2	1.41E-07	1.22E+02	1.06E+06
NPHa_PBZ	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC1C(=O)C=CC(=O)C1O	345.2	7.20E-10	1.48E+02	2.40E+10
NPHa_PHEN	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC1(O)C=CC2OOC1C2O	363.2	6.50E-10	1.51E+02	1.94E+10
NPHb_C2c	OCC(=O)(OOc1ccccc1N(=O)=O)	213.1	4.21E-02	6.66E+01	5.00E+02
NPHb_C4a	O(c1ccccc1N(=O)=O)OC(=O)C=CC(=O)C=O	265.2	5.92E-03	7.31E+01	1.11E+02
NPHb_C5a	OC(C=O)C(=O)C=CC(=O)(OOc1ccccc1N(=O)=O)	295.2	1.66E-05	1.00E+02	1.32E+05
NPHb_DNP	O(c1ccccc1N(=O)=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	387.2	4.73E-12	1.71E+02	2.58E+11
NPHb_MALc	O(c1ccccc1N(=O)=O)OC1C(=O)OC(=O)C1O	269.2	5.17E-06	1.06E+02	1.83E+05
NPHb_NBZb	O(c1ccccc1N(=O)=O)OC1C(=O)C=CC(=O)C1ON(=O)=O	324.2	1.69E-06	1.09E+02	4.27E+04
NPHb_NCAT	O(c1ccccc1N(=O)=O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	358.2	5.74E-12	1.71E+02	1.15E+12
NPHb_NDN	O(c1ccccc1N(=O)=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	432.2	3.23E-12	1.72E+02	7.97E+10
NPHb_NNC	O(c1ccccc1N(=O)=O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	403.2	3.47E-12	1.73E+02	5.73E+11
NPHb_NPHb	O(c1ccccc1N(=O)=O)Oc1ccccc1N(=O)=O	276.2	3.58E-05	9.25E+01	1.10E+02
NPHb_PBZ	O(c1ccccc1N(=O)=O)OC1C(=O)C=CC(=O)C1O	279.2	2.05E-06	1.09E+02	3.75E+05
NPHEN1O	O=N(=O)c1ccccc1[O]	138.1			
NPHEN1O2	[O]Oc1ccccc1N(=O)=O	154.1			
NPHEN1OOH	OOc1ccccc1N(=O)=O	155.1	3.04E-04	8.65E+01	2.30E+04
NPHENO	O=N(=O)OC1C2OOC1C([O])(O)C=C2	204.1			
NPHENO2	[O]OC1(O)C=CC2OOC1C2ON(=O)=O	220.1			
NPHENOH	O=N(=O)OC1C2OOC1C(O)(O)C=C2	205.1	6.93E-05	9.82E+01	1.09E+07

NPHENOOH	OOC1(O)C=CC2OOC1C2ON(=O)=O	221.1	2.27E-06	1.13E+02	8.45E+07
OCCOHCO	OC(C[O])C=O	89.1			
OCCOHCO2	OC(CO[O])C=O	105.1			
OCCOHCOH	OC(CO)C=O	90.1	1.66E-02	7.37E+01	7.73E+05
OCCOHCOOH	OC(COO)C=O	106.1	2.42E-03	8.18E+01	1.28E+06
OXOSORBACID	C(=CC=O)C=CC(=O)O	126.1	2.79E-03	7.90E+01	6.88E+05
PBZ_C2c	OCC(=O)(OOC1C(=O)C=CC(=O)C1O)	216.1	1.28E-03	8.38E+01	8.63E+05
PBZ_C4a	O(C1C(=O)C=CC(=O)C1O)OC(=O)C=CC(=O)C=O	268.2	4.05E-05	9.70E+01	4.07E+06
PBZ_C5a	OC(C=O)C(=O)C=CC(=O)(OOC1C(=O)C=CC(=O)C1O)	298.2	6.68E-08	1.27E+02	3.55E+09
PBZ_DNP	O(C1C(=O)C=CC(=O)C1O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	390.2	6.79E-15	2.03E+02	1.36E+16
PBZ_MALc	O(C1C(=O)C=CC(=O)C1O)OC1C(=O)OC(=O)C1O	272.2	3.96E-08	1.30E+02	3.79E+09
PBZ_NDN	O(C1C(=O)C=CC(=O)C1O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	435.2	4.44E-15	2.05E+02	6.55E+15
PBZ_PBZ	O(C1C(=O)C=CC(=O)C1O)OC1C(=O)C=CC(=O)C1O	282.2	1.75E-09	1.42E+02	4.55E+10
PBZQ1OH	O=c1ccc(=O)c(O)c1	124.1	8.93E-03	7.18E+01	1.82E+05
PBZQ3OH	O=c1cc(O)c(=O)c(O)c1O	156.1	4.12E-07	1.19E+02	5.37E+10
PBZQCO	O=C1C=CC(=O)C(O)C1=O	140.1	1.20E-03	8.02E+01	1.61E+06
PBZQO	O=C1C=CC(=O)C(O)C1[O]	141.1			
PBZQO2	[O]OC1C(=O)C=CC(=O)C1O	157.1			
PBZQOH	O=C1C=CC(=O)C(O)C1O	142.1	7.25E-05	9.44E+01	2.69E+07
PBZQONE	O=C1C=CC(=O)C=C1	108.1	5.06E-01	5.27E+01	2.36E+02
PBZQOOH	OOC1C(=O)C=CC(=O)C1O	158.1	3.52E-06	1.07E+02	2.34E+08
PC2	O=CC(O)C=CC(C=O)(O[O])	159.1			
PHAN	OCC(=O)OON(=O)=O	137.0	2.98E-01	5.80E+01	1.63E+04
PHEN_BZFU	O(C1(O)C=CC2OOC1C2O)OC1C(O)COC1=O	276.2	1.04E-08	1.36E+02	8.40E+09
PHEN_C2a	O(C1(O)C=CC2OOC1C2O)OC(=O)C=O	232.1	2.07E-02	7.51E+01	2.72E+04
PHEN_C2b	O(C1(O)C=CC2OOC1C2O)OCC=O	218.2	7.97E-04	8.75E+01	3.45E+05
PHEN_C2c	OCC(=O)(OOC1(O)C=CC2OOC1C2O)	234.2	1.84E-03	8.65E+01	3.92E+05
PHEN_C3a	OC(C=O)C(=O)(OOC1(O)C=CC2OOC1C2O)	262.2	8.16E-05	1.00E+02	8.21E+06
PHEN_C3DI	O(C1(O)C=CC2OOC1C2O)OC(C=O)C=O	246.2	1.86E-05	1.04E+02	1.88E+07
PHEN_C4a	O(C1(O)C=CC2OOC1C2O)OC(=O)C=CC(=O)C=O	286.2	4.20E-05	1.00E+02	2.85E+06

PHEN_C5a	OC(C=O)C(=O)C=CC(=O)(OOC1(O)C=CC2OOC1C2O)	316.2	6.80E-08	1.30E+02	2.40E+09
PHEN_C6a	O(C1(O)C=CC2OOC1C2O)Oc1ccccc1	252.2	4.59E-05	9.80E+01	5.75E+04
PHEN_CATE	O(C1(O)C=CC2OOC1C2O)Oc1ccccc1O	268.2	8.56E-07	1.16E+02	2.45E+07
PHEN_DNP	O(C1(O)C=CC2OOC1C2O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)N(=O)=O	408.2	5.64E-15	2.06E+02	1.05E+16
PHEN_EPX	O(C1(O)C=CC2OOC1C2O)OC(=O)C1OC1C=O	274.2	2.69E-04	9.31E+01	4.76E+05
PHEN_MALa	O(C1(O)C=CC2OOC1C2O)OC(=O)C=CC=O	258.2	1.12E-03	8.63E+01	1.07E+05
PHEN_MALb	O(C1(O)C=CC2OOC1C2O)OC(C=O)C(O)C=O	276.2	3.44E-08	1.33E+02	1.28E+10
PHEN_MALc	O(C1(O)C=CC2OOC1C2O)OC1C(=O)OC(=O)C1O	290.2	4.42E-08	1.33E+02	2.70E+09
PHEN_NBZa	O(C1(O)C=CC2OOC1C2O)OC1C(=O)OCC1ON(=O)=O	321.2	5.31E-09	1.39E+02	5.07E+09
PHEN_NBZb	O(C1(O)C=CC2OOC1C2O)OC1C(=O)C=CC(=O)C1ON(=O)=O	345.2	7.20E-10	1.48E+02	2.40E+10
PHEN_NCAT	O(C1(O)C=CC2OOC1C2O)OC1(O)C(=CC2(OOC1C2O)N(=O)=O)O	379.2	9.80E-15	2.05E+02	2.50E+16
PHEN_NDN	O(C1(O)C=CC2OOC1C2O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)N(=O)=O	453.2	3.03E-15	2.08E+02	6.55E+15
PHEN_NNC	O(C1(O)C=CC2OOC1C2O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	424.2	4.65E-15	2.08E+02	2.02E+16
PHEN_NPHb	O(C1(O)C=CC2OOC1C2O)Oc1ccccc1N(=O)=O	297.2	2.77E-07	1.20E+02	2.69E+06
PHEN_PBZ	O(C1(O)C=CC2OOC1C2O)OC1C(=O)C=CC(=O)C1O	300.2	1.51E-09	1.45E+02	3.83E+10
PHEN_PHEN	O(C1(O)C=CC2OOC1C2O)OC1(O)C=CC2OOC1C2O	318.2	1.66E-09	1.48E+02	2.35E+10
PHENO	OC1C2OOC1C([O])(O)C=C2	159.1			
PHENO2	[O]OC1(O)C=CC2OOC1C2O	175.1			
PHENOH	OC1C2OOC1C(O)(O)C=C2	160.1	1.73E-04	9.51E+01	9.68E+06
PHENOL	Oc1ccccc1	94.1	1.53E+00	5.05E+01	9.90E+02
PHENOOH	OOC1(O)C=CC2OOC1C2O	176.1	4.51E-06	1.10E+02	8.21E+07
R1bRO2	O=CC(O)=CC(O[O])C(C=O)OO	191.1			
ROCS_O4_O	O=C1C2OC2C3OOC1C3(O)	158.1	4.88E-03	7.67E+01	6.26E+04
ROCS_O5_O	O=CC(=O)C(O)C1OC1C(O)=O	174.1	1.81E-07	1.23E+02	7.52E+10
ROCS_O6_O	O=C=CC(OO)C(=O)C(O)C(=O)O	190.1	6.66E-06	1.10E+02	1.83E+09
ROCS_O7_O	O=C(O)C(=O)C(O)C1OC1C(OO)=O	206.1	9.09E-10	1.48E+02	6.29E+12
ROCS_O8_O	O=C(O)C(=O)C(=O)CC(OO)C(=O)OO	222.1	1.81E-11	1.65E+02	1.05E+15
ROCS_O9_O	O=C(OO)C(O)C(O)C(=O)C(=O)C(=O)OO	238.1	6.32E-12	1.72E+02	6.36E+15

Supplement S4: reduced mechanism - reactions

1	BENZENE + OH -> 5.300E-01 PHENOL + 3.520E-01 BZBIPERO2	KINETIC ARR2 2.300E-12 190.00
2	BZBIPERO2 + NO ->	KINETIC ARR2 2.700E-12 -360.00
3	PHENOL + OH -> 8.000E-01 CATECHOL + 1.260E-01 BZBIPERO2	KINETIC ARR2 4.700E-13 -1220.00
4	PHENOL + NO3 -> 2.580E-01 NPHENO2	KINETIC ARR1 3.800E-12
5	CATECHOL + OH -> 3.187E-01 C6H6O3 + 2.298E-01 BENZ3OH + 1.878E-01 C6H7O10N + 1.309E-01 C6H6O4 + 6.993E-02 CATEC1O	KINETIC ARR1 1.000E-10
6	C6H6O3 + NO -> 1.840E-01 C6H6O3_14	KINETIC ARR2 2.700E-12 -360.00
7	CATECHOL + NO3 -> CATEC1O	KINETIC ARR1 9.900E-11
8	CATEC1O + NO2 -> NCATECHOL	KINETIC ARR1 2.080E-12
9	CATEC1O + O3 -> CATEC1O2	KINETIC ARR1 2.860E-13
10	CATEC1O2 + NO -> CATEC1O	KINETIC ARR2 2.700E-12 -360.00
11	CATEC1O2 + HO2 ->	KINETIC ARR2 2.241E-13 -1300.00
12	NCATECHOL ->	KINETIC PHOTOLYSIS 1.42398E-04 1.40694E-04 1.35552E-04 1.26744E-04 1.1391E-04 9.651E-05 7.3944E-05 4.6367E-05 2.3588E-05 7.258E-06 0.0000E+00
13	NCATECHOL + NO3 -> NNCATECO2	KINETIC ARR1 2.600E-12
14	NNCATECO2 + NO -> NC4DCO2H	KINETIC ARR2 2.700E-12 -360.00
15	NC4DCO2H + OH ->	KINETIC ARR2 1.900E-12 -190.00
16	NPHENO2 + NO ->	KINETIC ARR2 2.700E-12 -360.00
17	BENZ3OH + OH -> 7.300E-01 BENZ4OH	KINETIC ARR1 4.600E-10
18	BZBIPERO2 -> BZo_RO2_O7	KINETIC ARR1 2.929E-01
19	C6H7O10N -> 5.000E-01 C6H7O12N + 5.000E-01 C6H6O7	KINETIC ARR1 1.780E+01
20	BZo_RO2_O7 -> 8.711E-01 BZo_RO2_O9 + 1.289E-01 BZouni_O6_O	KINETIC ARR1 2.410E+00
21	BZo_RO2_O9 -> 5.125E-01 C5uni_O6_O + 4.875E-01 BZo_RO2_O11	KINETIC ARR1 5.850E-01
22	BZo_RO2_O9 + NO ->	KINETIC ARR2 2.420E-12 -360.00
23	BZo_RO2_O11 + NO -> 8.610E-01 BZo2_RO_O10 + 1.390E-01 BZo_O9_NO3	KINETIC ARR2 2.920E-12 -360.00
24	BZo_RO2_O7 + NO ->	KINETIC ARR2 2.700E-12 -360.00
25	NPHENO2 + NPHENO2 -> NPHa_NPHa	KINETIC ARR1 9.17E-11
26	NNCATECO2 + NNCATECO2 -> NNC_NNC	KINETIC ARR1 1.0E-10
27	BZo2_RO_O10 -> 9.500E-01 BZouni_O10_O	KINETIC ARR1 1.000E-06
28	BZo_RO2_O11 -> BZouni_O10_O	KINETIC ARR1 0.01

Supplement S5: reduced mechanism – gas phase species

nom	SMILES	molar weight ($g.mol^{-1}$)	Psat (torr)	dHvap ($kJ.mol^{-1}$)	Henry constant ($M.atm^{-1}$)
BENZ3OH	Oc1cccc(O)c1O	126.1	1.33E-04	9.09E+01	1.56E+10
BENZ4OH	Oc1ccc(O)c(O)c1O	142.1	7.33E-07	1.14E+02	8.43E+13
BENZENE	c1ccccc1	78.1	5.00E+01	3.56E+01	3.50E-01
BZBIPERO2	[O]OC1C=CC2OOC1C2O	159.1			
BZo_O9_NO3	O=C(OO)C(O)C(O)C(=O)C(ON(=O)=O)C(=O)OO	285.1	1.46E-13	1.90E+02	1.60E+17
BZo_RO2_O11	O=C(OO)C(O)C(O)C(=O)C(O[O])C(=O)OO	255.1			
BZo_RO2_O7	O=CC(O)C(O)C1OC1C(O[O])=O	191.1			
BZo_RO2_O9	O=C(O[O])C(O)C(O)C1OC1C(OO)=O	223.1			
BZo2_RO_O10	O=C(OO)C(O)C(O)C(=O)C([O])C(=O)OO	239.1			
BZouni_O10_O	O=C(OO)C(=O)C(O)C(=O)C(OO)C(=O)OO	254.1	1.71E-13	1.88E+02	9.04E+17
BZouni_O6_O	O=CC(=O)C(O)C1OC1C(OO)=O	190.1	1.09E-06	1.15E+02	1.90E+09
C5uni_O6_O	OOC=CC(=O)C(O)C(=O)OO	178.1	4.45E-08	1.30E+02	1.98E+11
C6H6O3	C1=CC(=O)C(C=C1)(O)O	126.1	4.12E-03	7.74E+01	3.86E+05
C6H6O3_14	C1(O)C(ON(=O)(=O))C=CC(=O)C1(O)(O)	205.1	6.71E-08	1.29E+02	4.99E+10
C6H6O4	C(=CC=O)C=C(C(=O)O)O	142.1	2.29E-05	1.02E+02	4.55E+08
C6H6O7	C(=CC(C(=O)O)OO)C(=O)C(=O)O	190.1	5.10E-11	1.61E+02	1.70E+14
C6H7O10N	O=CC(=O)C(OO)C(OO)C(C=O)ON(=O)=O	253.1	2.17E-11	1.65E+02	6.20E+13
C6H7O12N	C(=O)(C(C(C(C(=O)O)OO)OO)ON(=O)=O)C(=O)O	285.1	4.63E-19	2.50E+02	3.47E+22
CATEC1O	[O]c1ccccc1O	109.1			
CATEC1O2	[O]Oc1ccccc1O	125.1			
CATECHOL	Oc1ccccc1O	110.1	2.17E-02	6.84E+01	2.87E+06
NC4DCO2H	O=CC(=CC(=O)O)N(=O)=O	145.1	5.83E-05	9.58E+01	2.49E+08
NCATECHOL	O=N(=O)c1ccc(O)c(O)c1	155.1	5.54E-04	8.43E+01	1.01E+07
NNC_NNC	O(C1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O)OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	530.2	3.70E-21	2.75E+02	5.83E+22
NNCATECO2	[O]OC1(O)C(=CC2(OOC1C2ON(=O)=O)N(=O)=O)O	281.1			

NPHa_NPHa	O(C1(O)C=CC2OOC1C2ON(=O)=O)OC1(O)C=CC2OOC1C2ON(=O)=O	408.2	2.67E-10	1.55E+02	1.28E+10
NPHENO2	[O]OC1(O)C=CC2OOC1C2ON(=O)=O	220.1			
PHENOL	Oc1ccccc1	94.1	1.53E+00	5.05E+01	9.90E+02

Supplement S6: Influence of non-ideality on simulated concentrations of chamber experiments

Gas–particle partitioning of semi-volatile organic compounds in aerosol models is commonly described using activity coefficients, which account for non-ideal interactions in the condensed phase. These coefficients quantify deviations from ideal solution behavior and directly affect effective saturation concentrations during condensation and evaporation. In the ideal case, activity coefficients are set to unity, implicitly assuming ideal mixing and neglecting intermolecular interactions within the particle phase. To assess the sensitivity of the results to this assumption, the chamber experiments are reproduced in SSH-aerosol using different activity-coefficient models, while retaining the quasi-explicit chemical scheme including the germinal diol pathway (Mech 2). In addition to the ideal formulation, simulations were performed using UNIFAC, which estimates activity coefficients based on group-contribution theory and accounts for non-ideal organic-organic interactions, and AIOMFAC, which extends this approach by including inorganic-organic interactions. AIOMFAC therefore provides a more comprehensive representation of aerosol-phase thermodynamics, particularly under conditions where inorganic species contribute significantly to particle composition. Figure S2 shows that using UNIFAC rather than assuming ideality tends to increase the simulated SOA concentrations by up to 15 %, whereas AIOMFAC leads to lower SOA concentrations, especially in the experiments with high concentrations of neutral seeds (experiments 5,6 and 14). The influence of non-ideality on SOA concentrations concerns mostly species originating from multi-hydroxylation, as they have higher volatility than those formed from autoxidation. These trends are consistent with those reported by Kim et al. (2019) when comparing ideal, UNIFAC, and AIOMFAC impacts. Overall, the influence of non-ideal gas–particle partitioning remains much smaller than that of introducing additional chemical pathways in the SOA formation scheme.

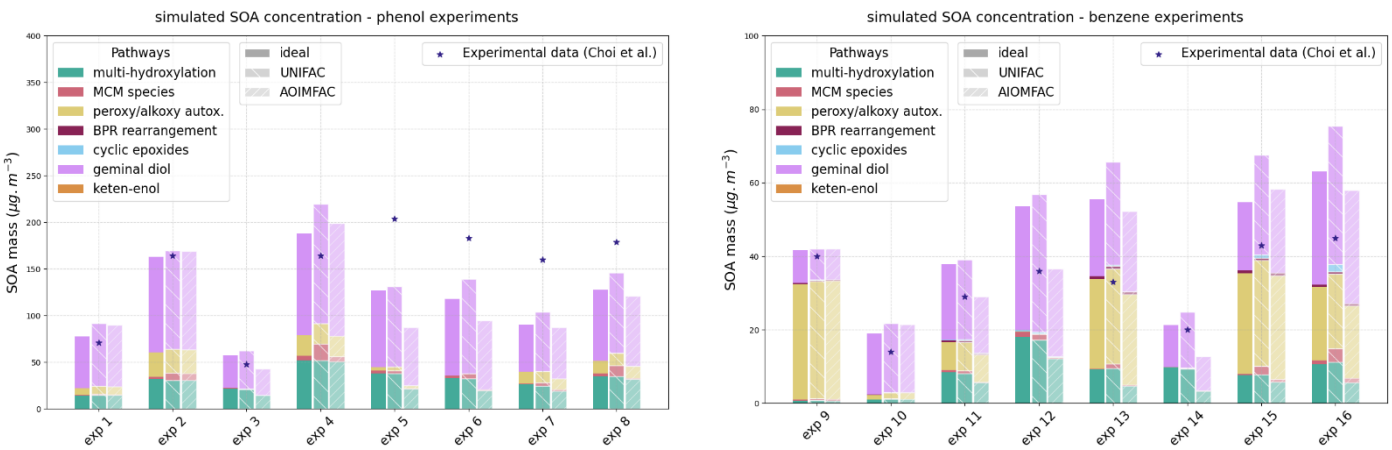

Figure S2: SOA concentrations simulated using Mech 2 and different activity models (ideal for the left bars, UNIFAC for the middle bars and AIOMFAC for the right bars) and comparison to experimental concentrations (stars on the graph). The left panel represents experiments using phenol as the precursor, while the right panel shows experiments using benzene.

Supplement S7: Influence of nitrophenol saturation vapor pressure

In SSH-aerosol v2.0, saturation vapor pressures (P^{sat}) are estimated using UManSysProp (Topping et al., 2016) and the SMILES structure associated with each species. For certain compounds, P^{sat} values are obtained experimentally and may differ from these calculated values: for nitrophenol, experiments conducted by Bannan et al. (2017) yielded a value of 3.86E-5 torr, also used in other modeling studies (Lanzafame et al., 2022) and compared to the 6.63E−2 torr estimated using UManSysProp. In order to evaluate the influence of the P^{sat} for nitrophenol on simulated SOA formation, additional simulations are performed using the value observed by Bannan et al. (2017).

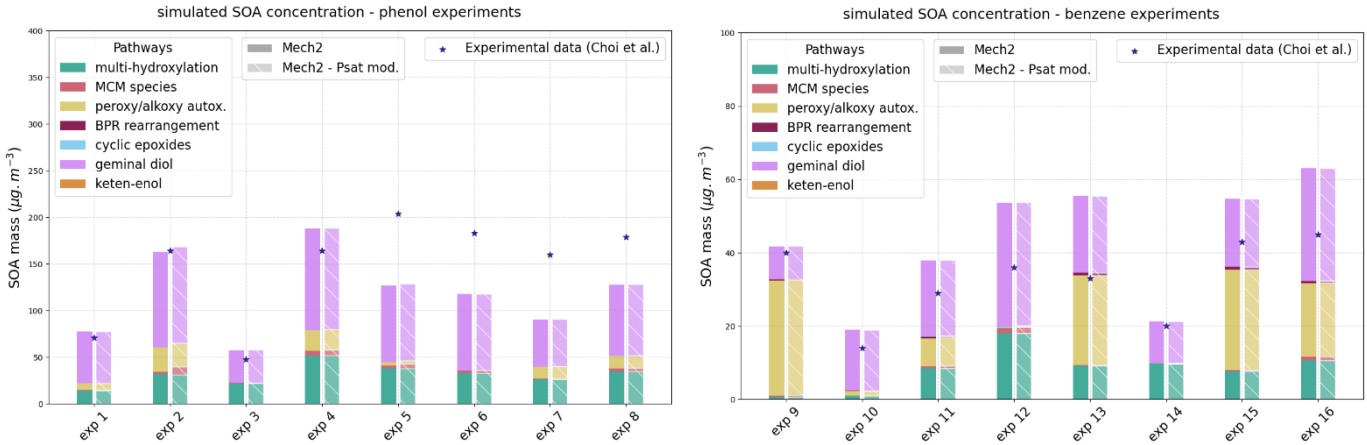

Figure S3: SOA concentrations simulated using Mech 2 with different PVS for nitrophenol compound and comparison to experimental concentrations (stars on the graph). The left panel represents experiments using phenol as the precursor, while the right panel shows experiments using benzene.

Overall, the impact of the modified P^{sat} of nitrophenol on simulated SOA concentrations remains small, for most experimental conditions, only minor changes in aerosol mass are observed (see Figure S3). However, more pronounced effects are obtained in simulations where OH and NO2 concentrations are higher, where nitrophenol compounds contribute significantly to the organic aerosol fraction. Under these conditions, using the observed P^{sat} value slightly enhance the partitioning of nitrophenol and thus the contribution of the MCM pathway to SOA mass formation.

Supplement S8: SOA composition in contrasted environments - 12 a.m.

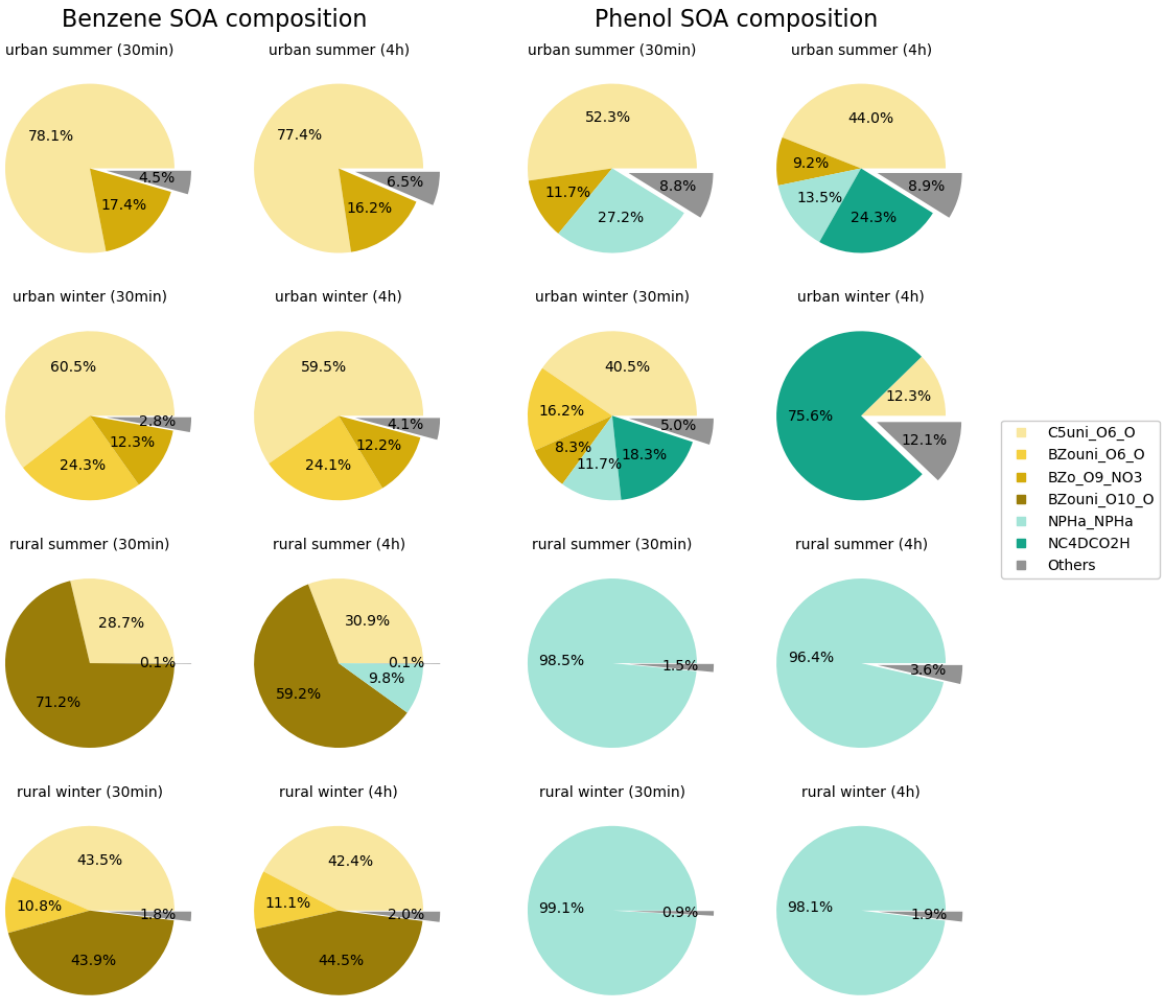

Figure S4: Benzene and phenol SOA composition after short (30 min) and longer (4 h) simulation times in a winter/summer and rural/urban conditions with initial time 12am. Compounds representing under 5 % of the SOA mass are aggregated in the "Others" category.

Supplement S9: RO2/RO autoxidation scheme

Set of reactions applied to peroxy radicals in the autoAPRAM framework (Pichelstorfer et al., 2024).

RO2 (H-shift + O2 addition) -> RO2

RO2 + NO -> RONO2505

RO2 + NO -> RO + NO2

RO2 + NO -> RO + NO2 -> RCHO + NO2 + HO2

RO2 + HO2 -> ROOH

RO2 + HO2 -> RO + O2 + OH

RO2 (+ R'O2) -> RO510

RO2 + R'O2 -> ROOR'

RO2 -> ROH

RO2 (+ R'O2) -> RCHO

RO2 (H-shift) -> RCHO

RO2 (H-shift) -> C5RO2 + CO

Set of reactions applied to the alkoxy radicals in the autoAPRAM framework (Pichelstorfer et al. 2024).

RO (H-shift + O2 addition) -> RO2

RO (H-shift) -> RCHO

RO fragmentation -> C2-C4 carbonyls

Supplement S10: Comparison of SOA functional group composition

Functional groups represented follow the UNIFAC nomenclature (RC alkyl, C═C carbon double bond, OH hydroxyl, CO–OH hydroperoxide, RCO carbonyl, COOH acid, COOOH peroxyacetyl acid, PAN peroxyacyl nitrates, RCOO esther, NO3 nitroaromatics and nitrates, COOC peroxide)

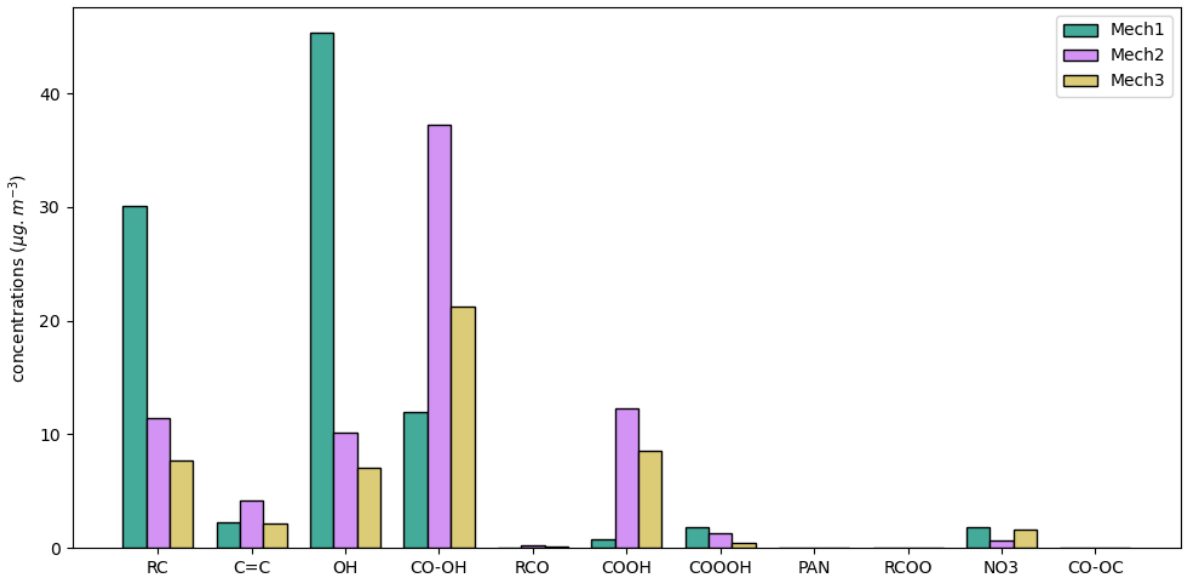

Figure S5: SOA mass concentration attributed to the corresponding functional group using Mech1, Mech2 and Mech3 for experiment 1.

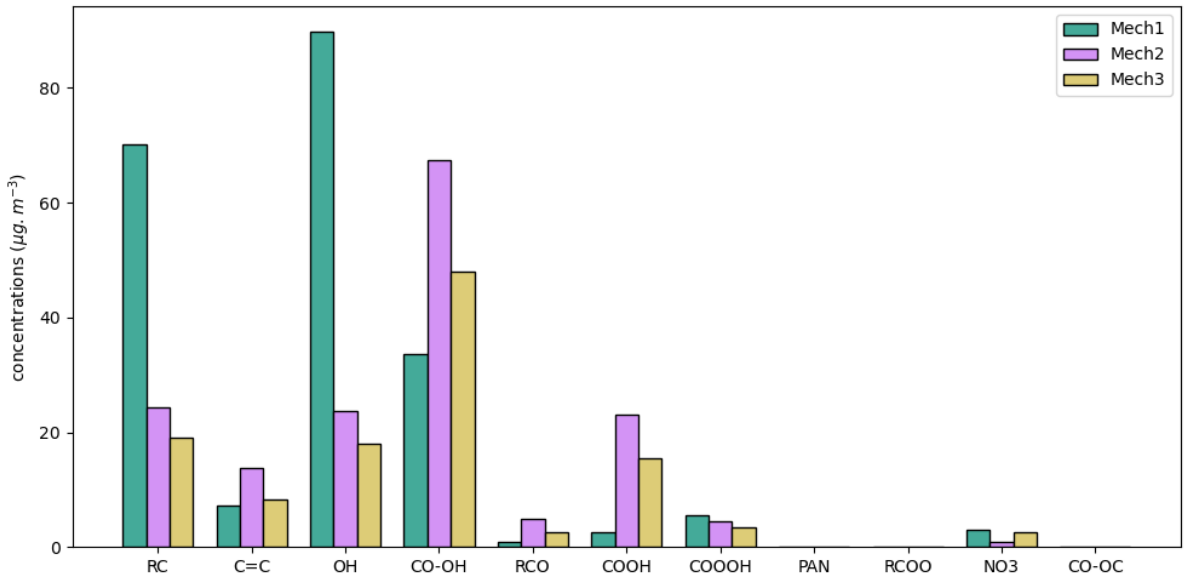

Figure S6: SOA mass concentration attributed to the corresponding functional group using Mech1, Mech2 and Mech3 for experiment 2.

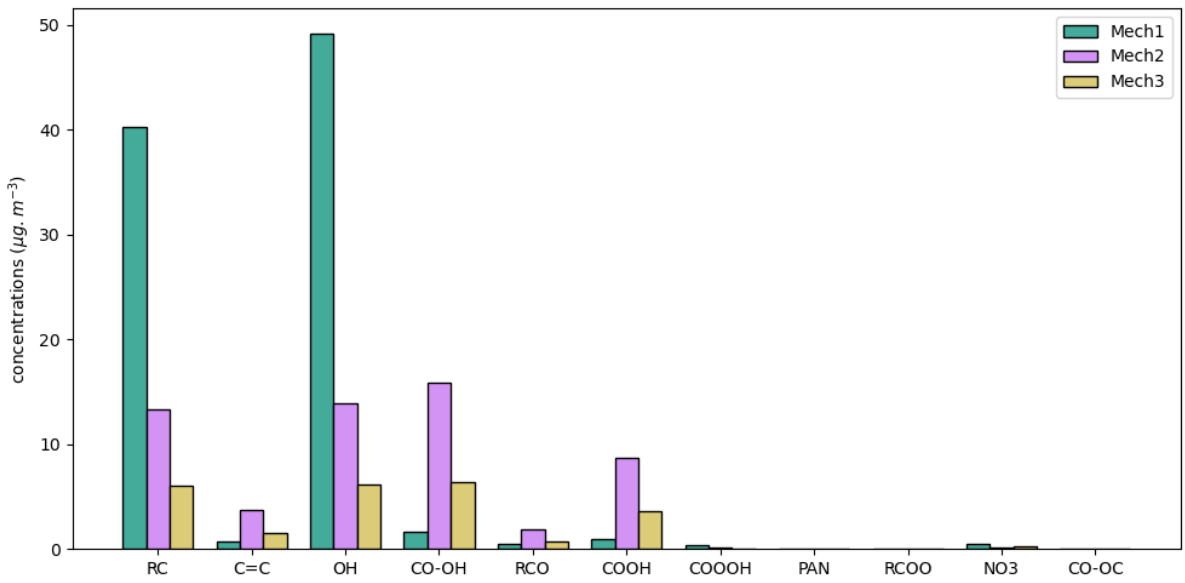

Figure S7: SOA mass concentration attributed to the corresponding functional group using Mech1, Mech2 and Mech3 for experiment 3.

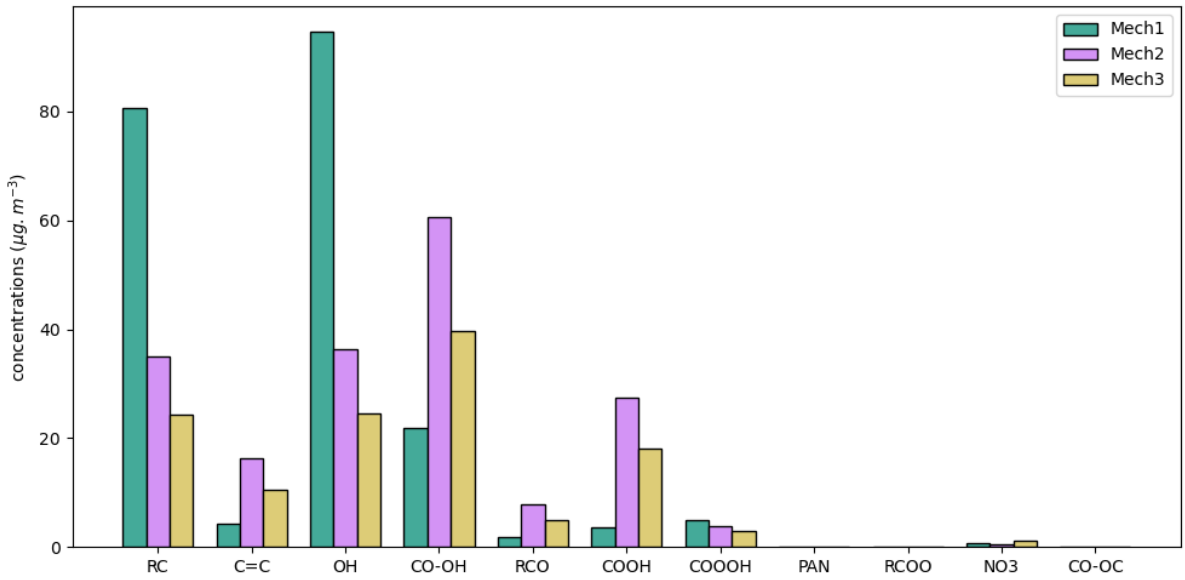

Figure S8: SOA mass concentration attributed to the corresponding functional group using Mech1, Mech2 and Mech3 for experiment 4.

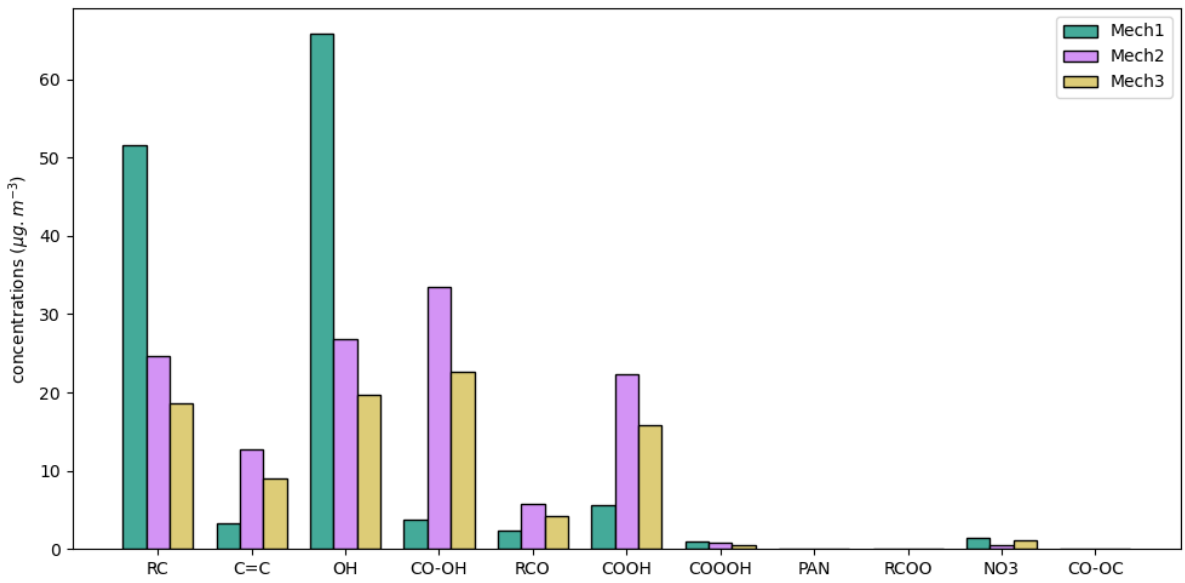

Figure S9: SOA mass concentration attributed to the corresponding functional group using Mech1, Mech2 and Mech3 for experiment 5.

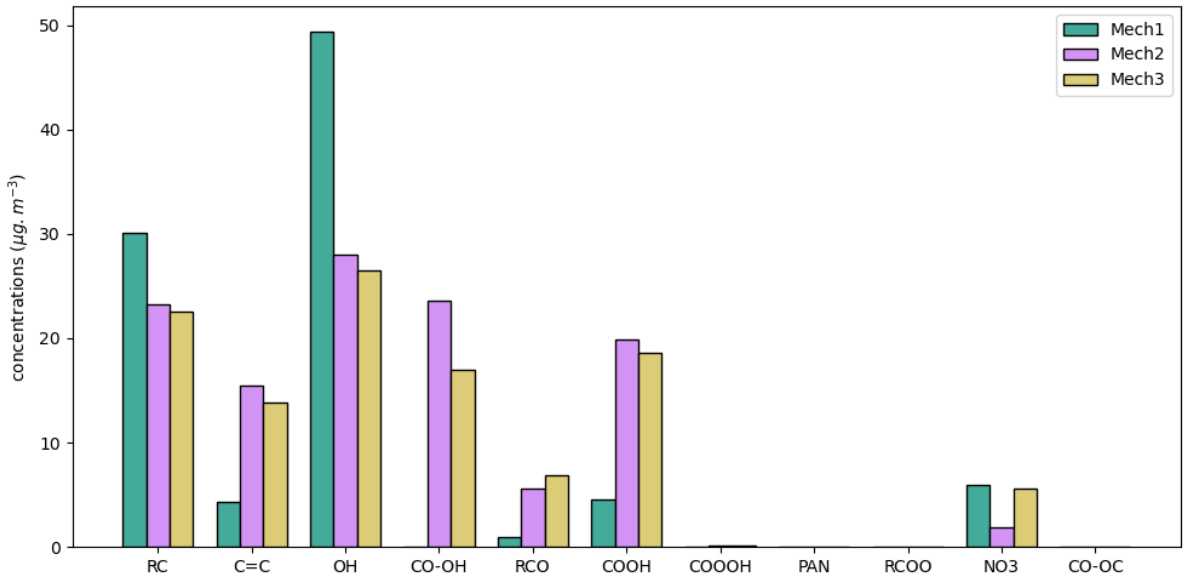

Figure S10: SOA mass concentration attributed to the corresponding functional group using Mech1, Mech2 and Mech3 for experiment 6.

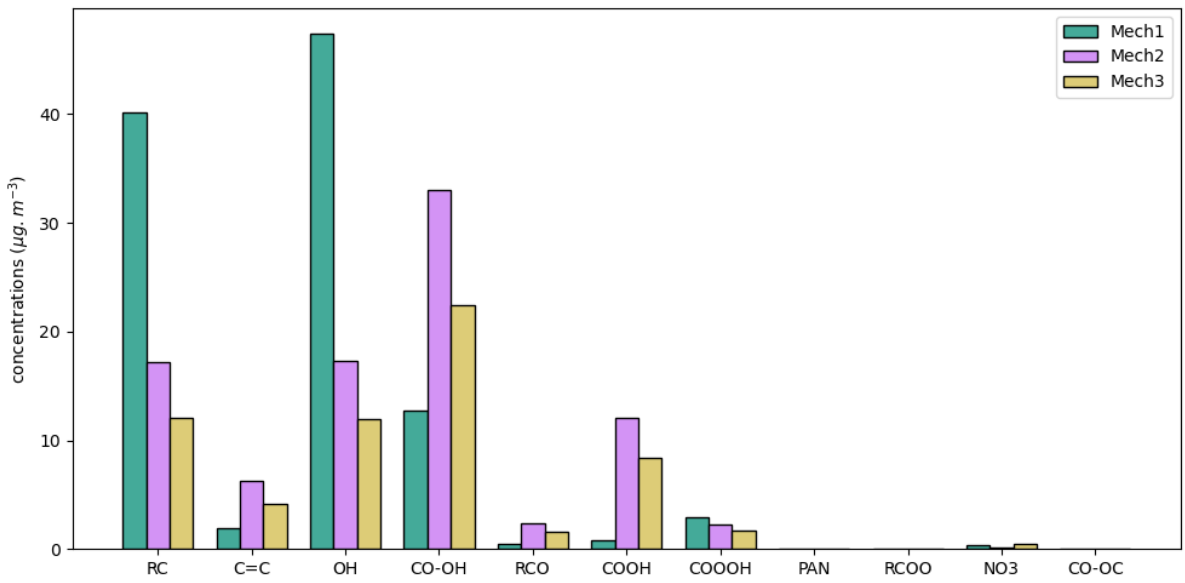

Figure S11: SOA mass concentration attributed to the corresponding functional group using Mech1, Mech2 and Mech3 for experiment 7.

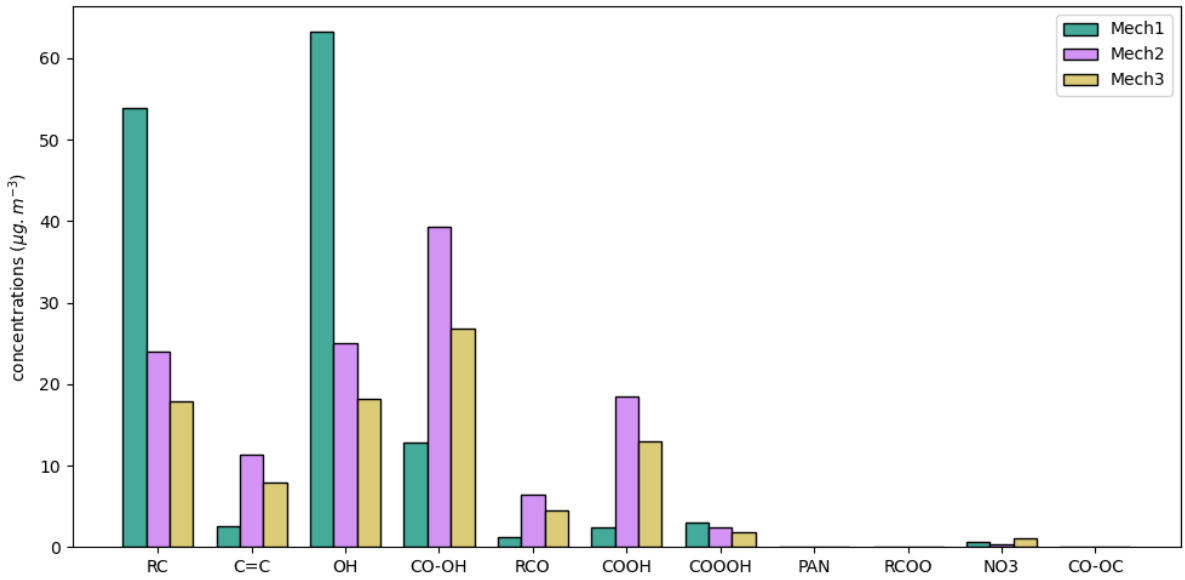

Figure S12: SOA mass concentration attributed to the corresponding functional group using Mech1, Mech2 and Mech3 for experiment 8.

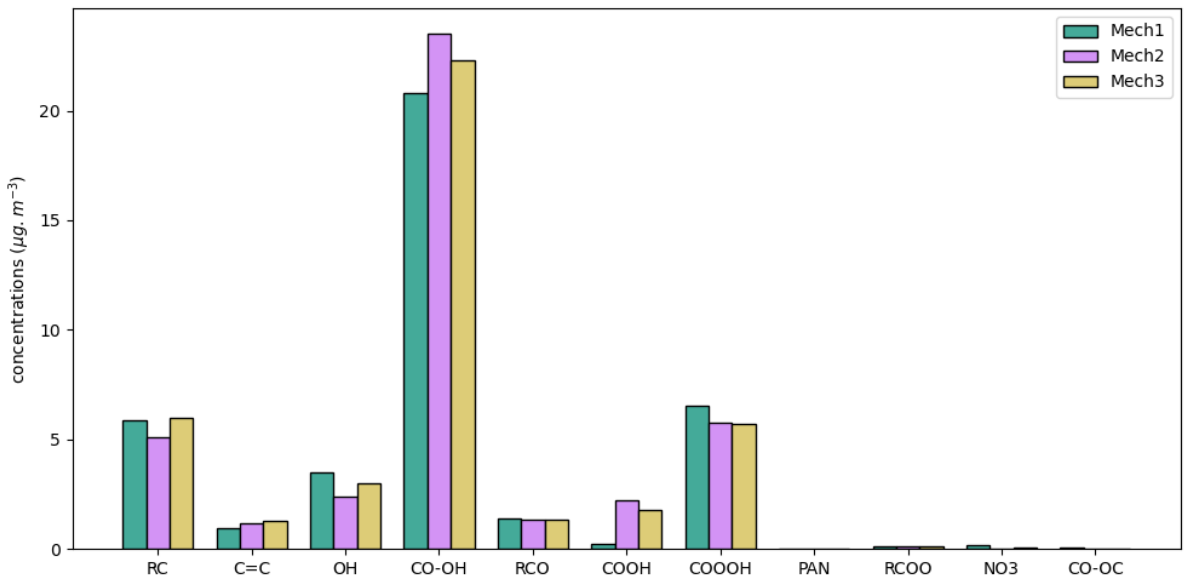

Figure S13: SOA mass concentration attributed to the corresponding functional group using Mech1, Mech2 and Mech3 for experiment 9.

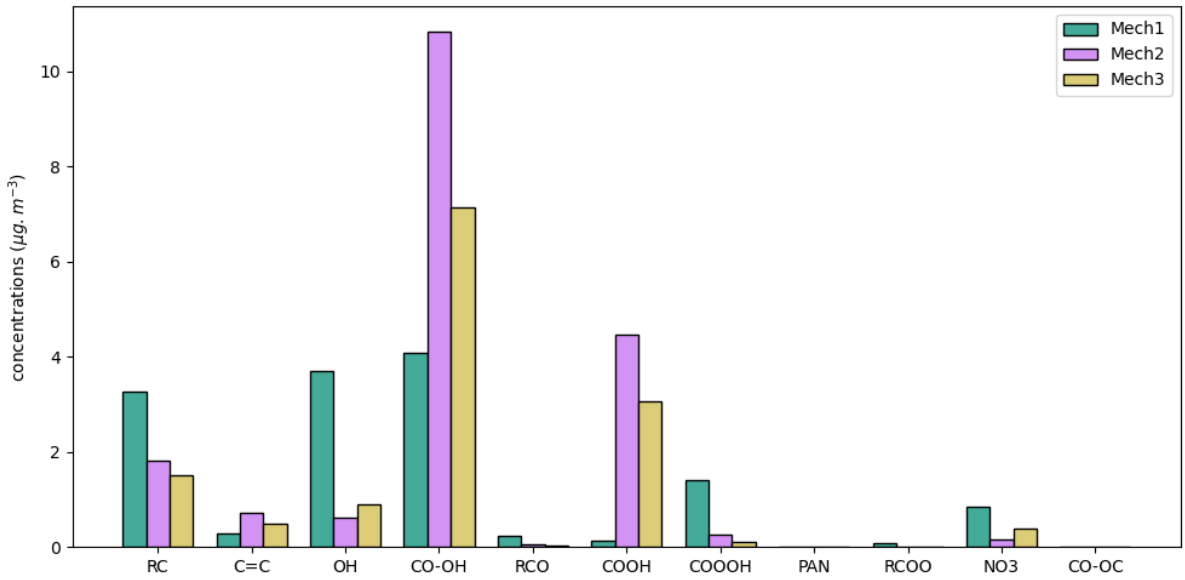

Figure S14: SOA mass concentration attributed to the corresponding functional group using Mech1, Mech2 and Mech3 for experiment 10.

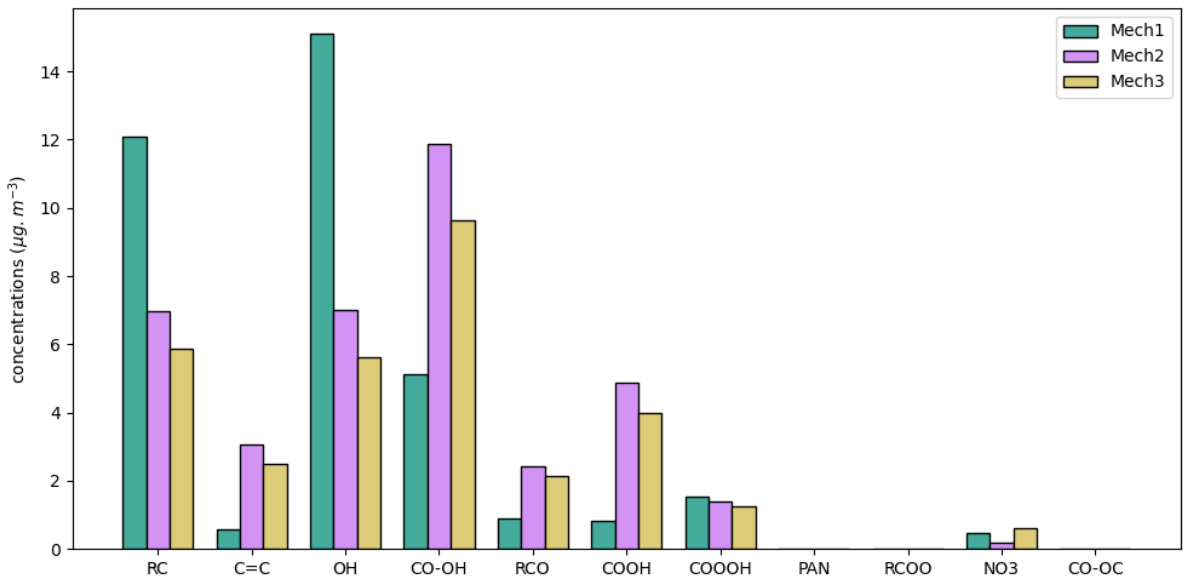

Figure S15: SOA mass concentration attributed to the corresponding functional group using Mech1, Mech2 and Mech3 for experiment 11.

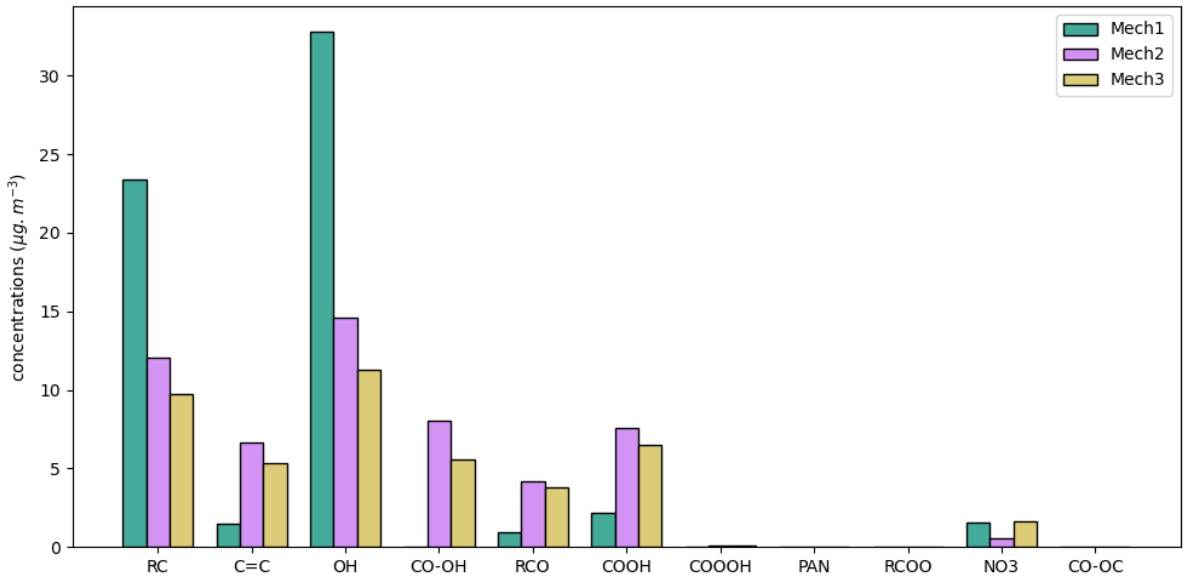

Figure S16: SOA mass concentration attributed to the corresponding functional group using Mech1, Mech2 and Mech3 for experiment 12.

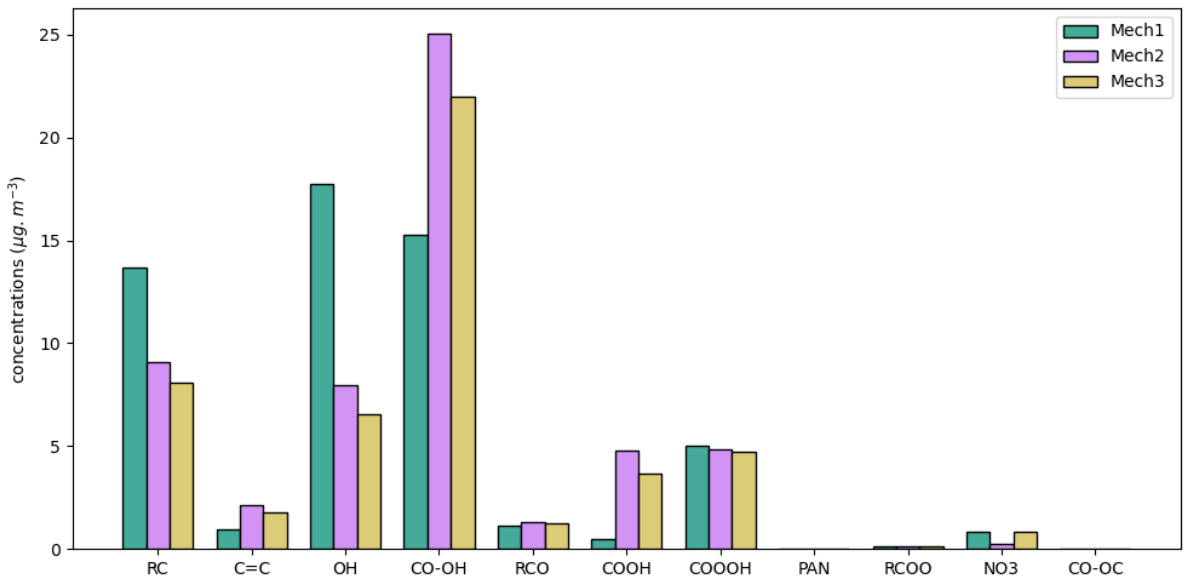

Figure S17: SOA mass concentration attributed to the corresponding functional group using Mech1, Mech2 and Mech3 for experiment 13.

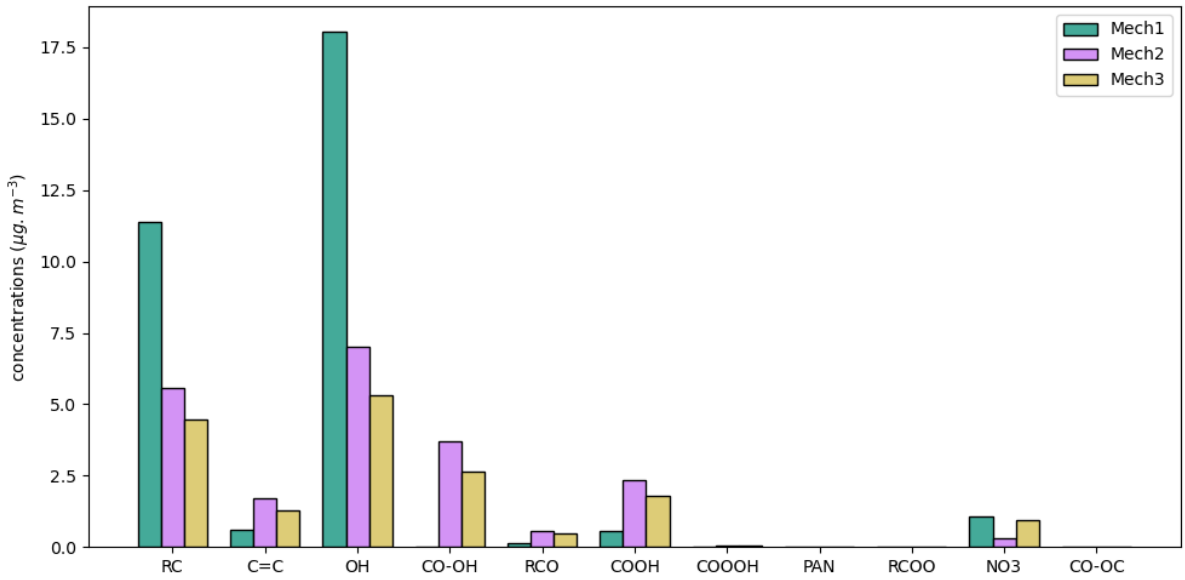

Figure S18 SOA mass concentration attributed to the corresponding functional group using Mech1, Mech2 and Mech3 for experiment 14.

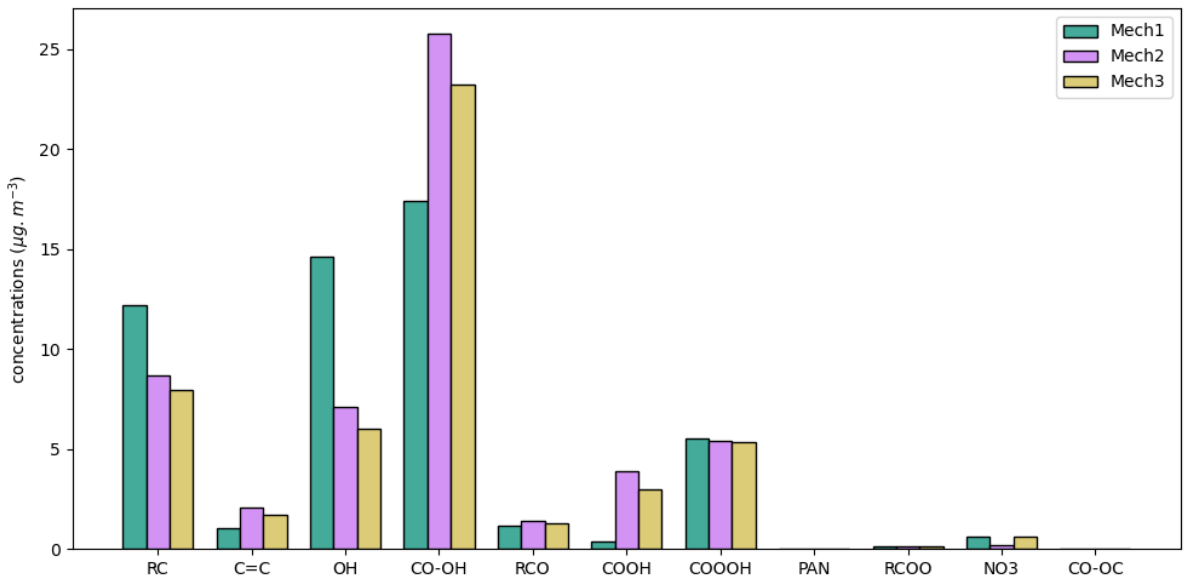

Figure S19: SOA mass concentration attributed to the corresponding functional group using Mech1, Mech2 and Mech3 for experiment 15.

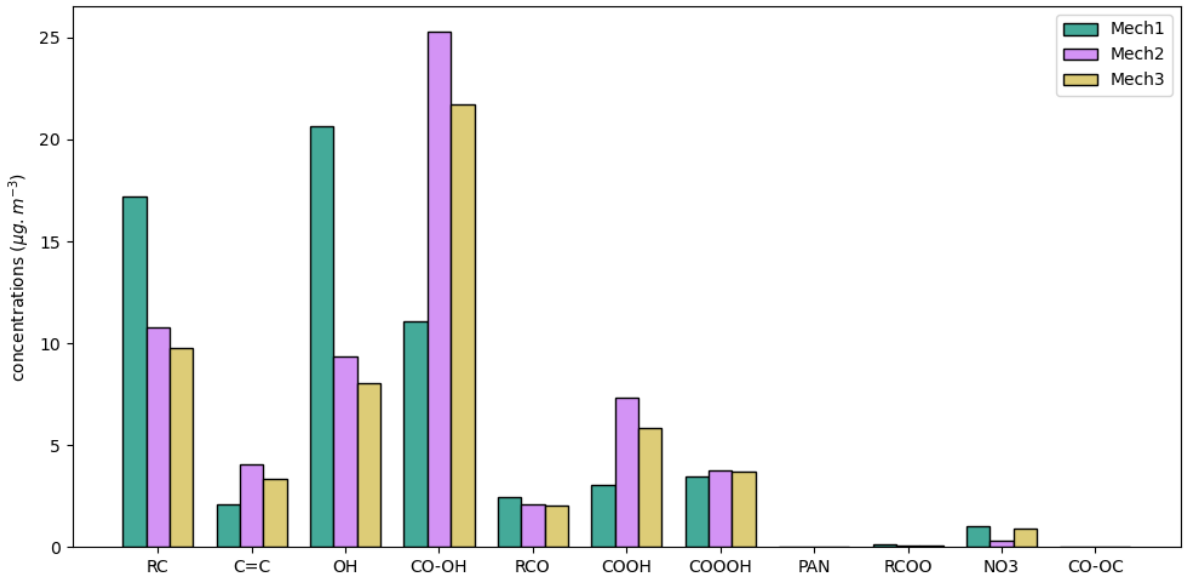

Figure S20: SOA mass concentration attributed to the corresponding functional group using Mech1, Mech2 and Mech3 for experiment 16.

Supplement S11: SOA functional group composition from Borrás et al. (2012)

In the article from Borrás et al. (2012), benzene photooxidation is investigated in the EUPHORE simulation chamber under various OH concentrations, obtained by adding oxidants (H2O2, NO or HONO) under natural irradiation and in the absence of seed aerosol. Gaseous products and particle-phase products are monitored, with the condensed-phase products chemically characterized by GC–MS. Several multi-oxygenated products are identified, including dicarboxylic acids, providing additional information on the chemical composition of benzene SOA. Figure S21 and Figure S22 compare the functional group composition obtained by Borrás et al. (2012) for benzene and phenol experiments, respectively for H2O2 experiments (exp 3 and 14) and NO/HONO experiments (exp 8 and 15).

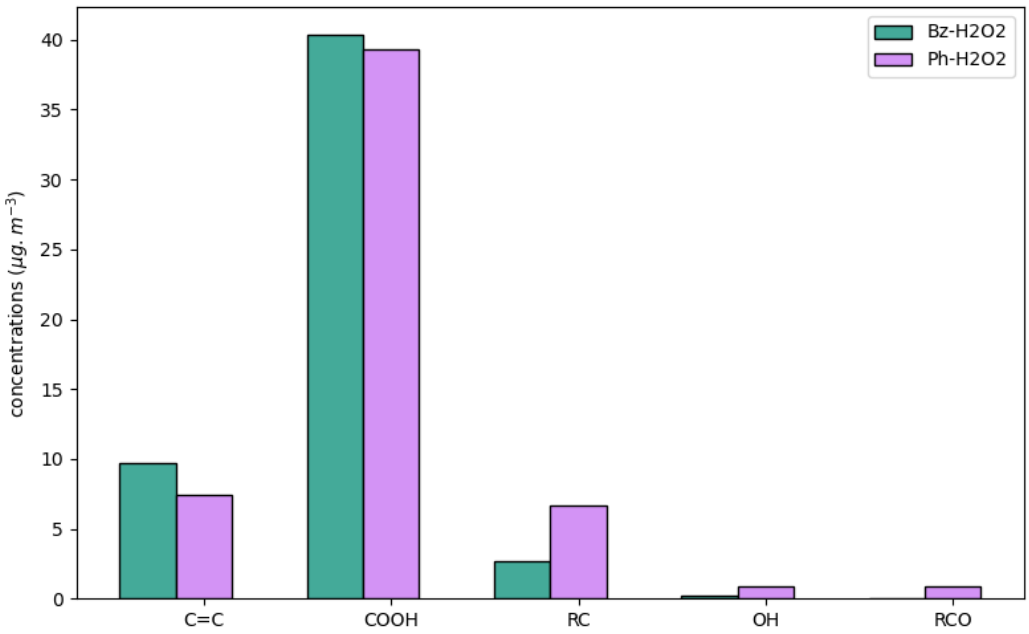

Figure S21: Proportion of each functional group in SOA concentration for experiments 3 and 14 from Borrás et al. (2012).

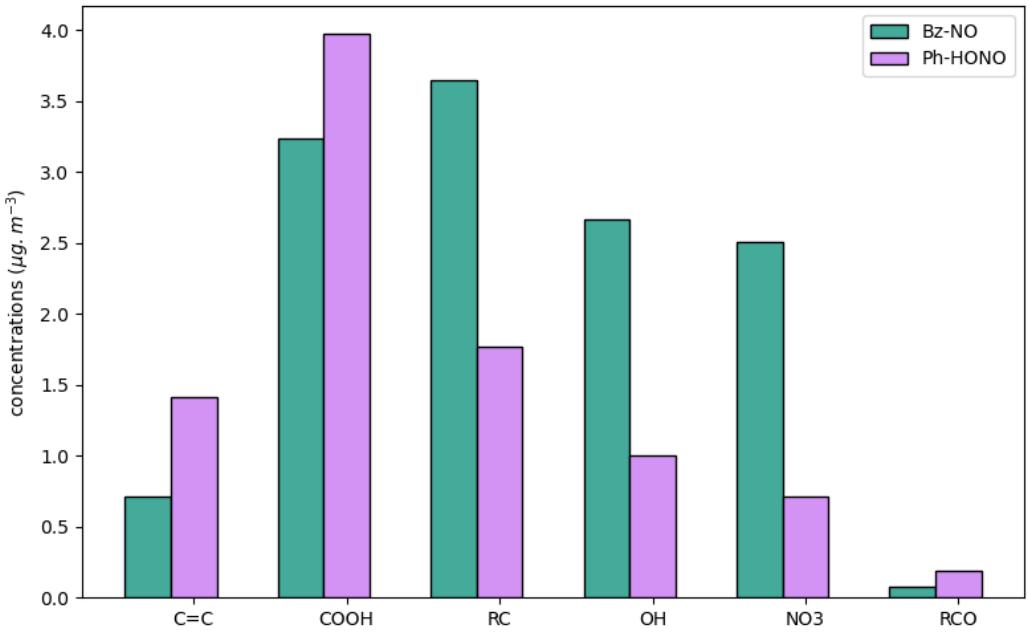

Figure S22: Proportion of each functional group in SOA concentration for experiments 8 and 15 from Borrás et al. (2012).

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