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# Supplementary information for "Quantifying the impact of relative humidity on human exposure to gas phase squalene ozonolysis products"

Pascale S. J. Lakey[1,*], Andreas Zuend[2], Glenn C. Morrison[3], Thomas Berkemeier[4], Jake Wilson[4], Caleb Arata[5], Allen H. Goldstein[5], Kevin R. Wilson[6], Nijing Wang[7], Jonathan Williams[7], Jonathan P. D. Abbatt[8], Manabu Shiraiwa[1,*]

[1] Department of Chemistry, University of California, Irvine, CA 92697, USA

[2] Department of Atmospheric and Oceanic Sciences, McGill University, Montreal, Quebec, Canada

[3] Gillings School of Global Public Health, University of North Carolina, Chapel Hill, NC, USA

[4] Multiphase Chemistry Department, Max Planck Institute for Chemistry, Mainz, Germany

[5] Department of Environmental Science, Policy and Management, University of California, Berkeley, USA.

[6] Chemical Sciences Division, Lawrence Berkeley National Laboratory, CA, USA

[7] Air Chemistry Department, Max Planck Institute for Chemistry, Mainz, Germany

[8] Department of Chemistry, University of Toronto, ON, Canada

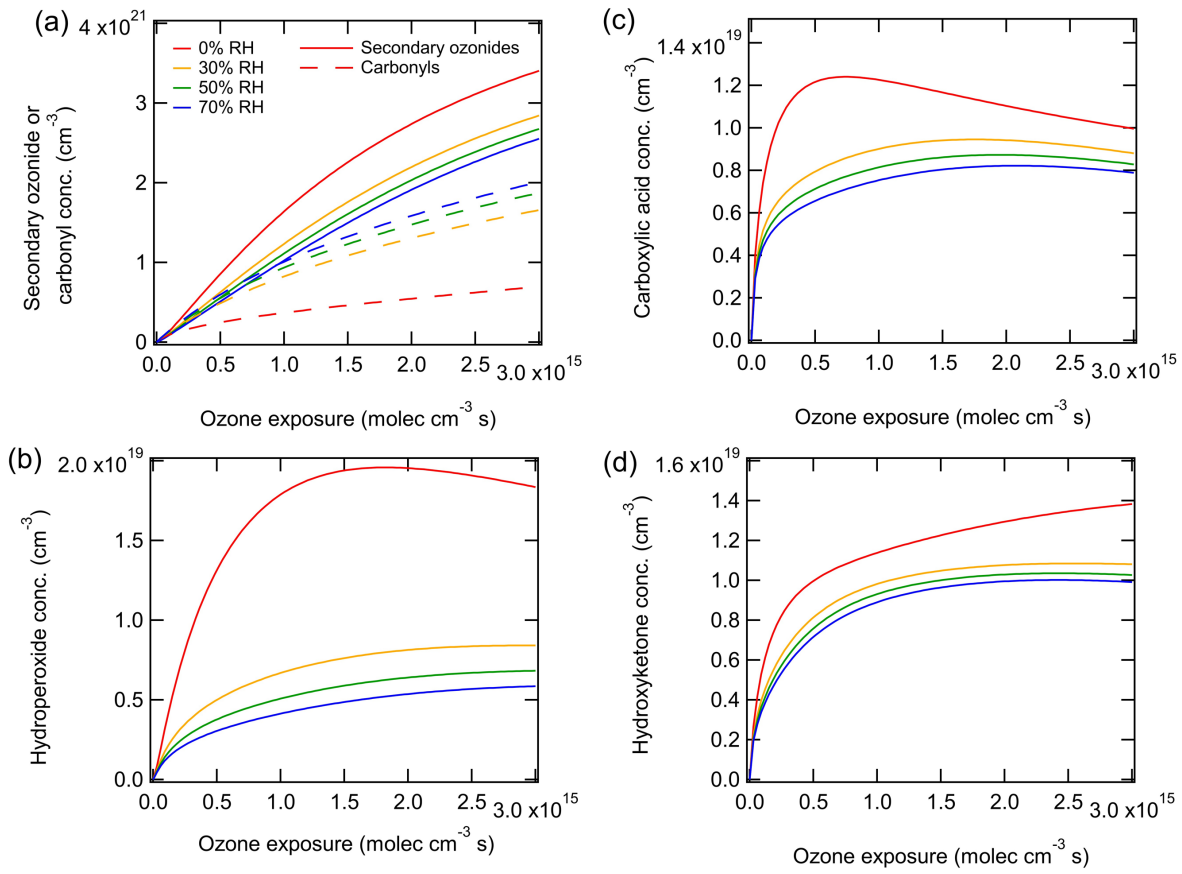


**Figure S1:** Model estimates of (a) secondary ozonide and carbonyl, (b) hydroperoxide, (c) carboxylic acid and (d) hydroxyketone concentrations in squalene particles as a function of ozone exposure and RH for the scenario shown in Figure 2.

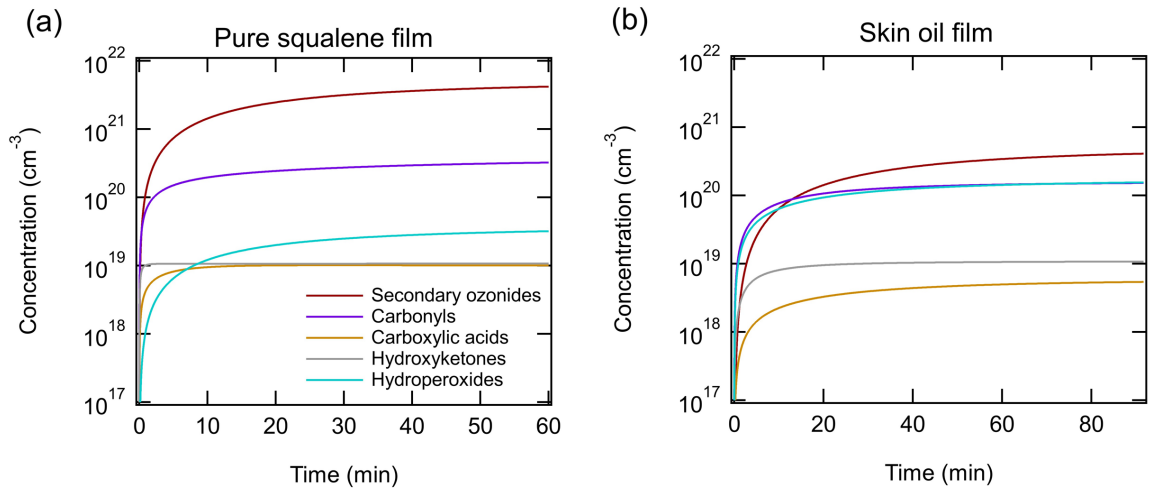


**Figure S2:** Model estimates of secondary ozonide, carbonyl, hydroperoxide, carboxylic acid and hydroxyketone concentrations as a function of time in (a) squalene films for the scenario shown in Figure 3 and (b) skin oil films for the scenario shown in Figure 4.

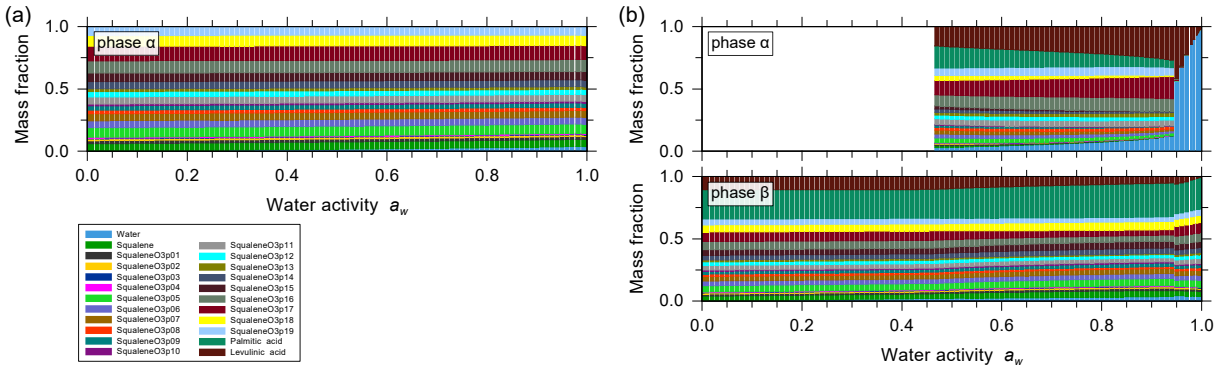


**Figure S3:** AIOMFAC-LLE predictions of the equilibrium water uptake and phase compositions in mass fractions for (a) the squalene ozonolysis system (a surrogate mixture) listed in Table S4 and (b) the same system but including also palmitic acid and levulinic acid. (a) A single liquid phase predicted. (b) The grey shaded area represents typical indoor RHs.overall (dry) system composition is a 1 : 1 : 1 molar ratio for the surrogate mixture : palmitic acid : levulinic acid amounts. (b) LLPS is predicted at water activities above 0.47.

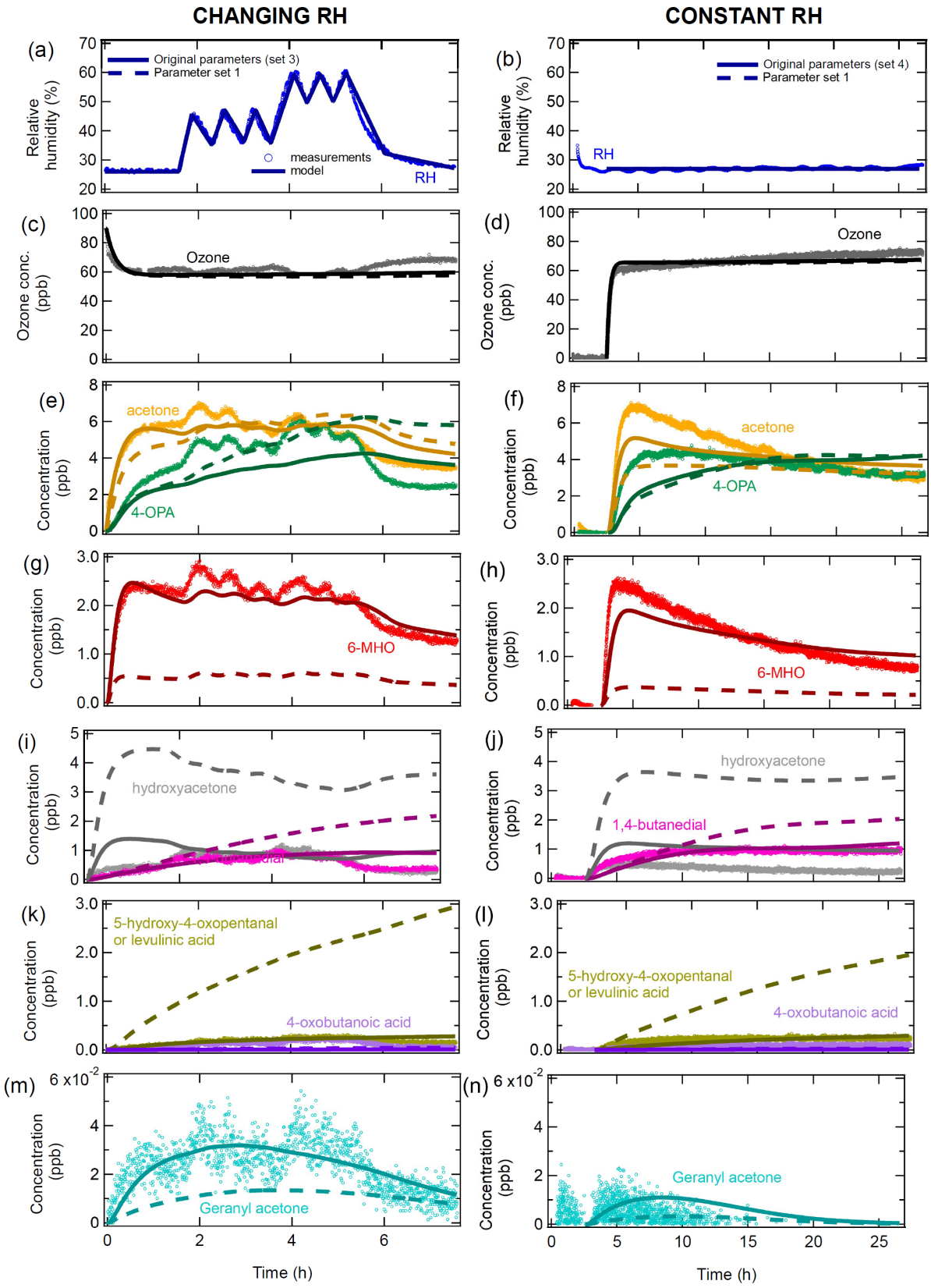


**Figure S4:** Sensitivity test showing the impact of using parameter set 1 (which was used when fitting Figure 1, dashed lines) compared to parameter sets 3 and 4 (used for Figure 5, solid lines). Parameters which were changed when performing the sensitivity test were $k_{4,bulk}$, $k_{5,bulk}$, $k_{1,gas}$, $k_{2,gas}$, $k_{3,gas}$ and $k_{4,gas}$.

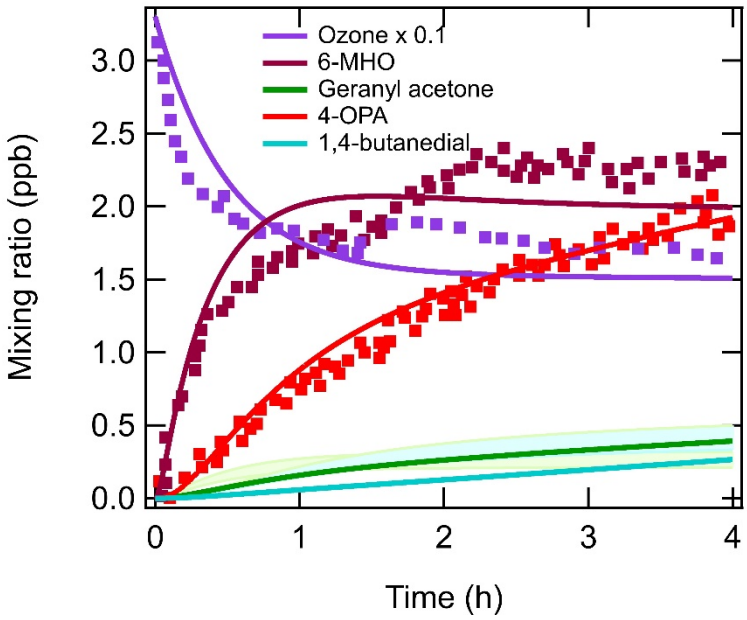


**Figure S5:** Measurements (markers) and outputs from KM-SUB-Skin-Clothing (lines) of the temporal evolution of squalene ozonolysis products when two people enter a 30 $m^3$ chamber containing 33 ppb ozone at a temperature of 23 °C. Measurements are from Wisthaler et al.[1]

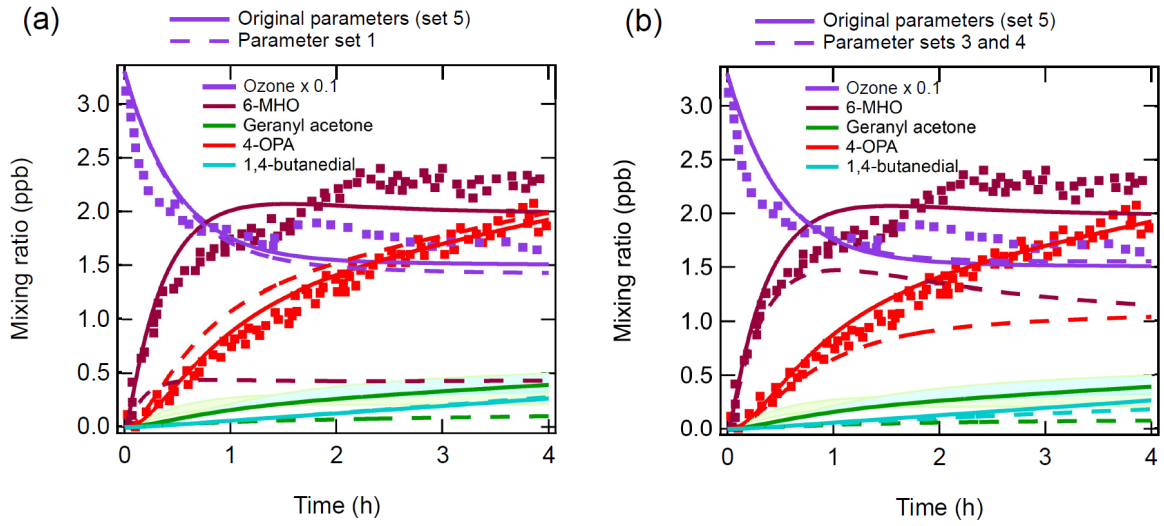


**Figure S6:** Sensitivity test showing the impact of using (a) parameter set 1 (which was used when fitting Figure 2, dashed lines) and (b) parameter sets 3 and 4 (which were used when fitting Figure 5, dashed lines) compared to parameter set 5 which was used to fit Figure S5. In panel (a) $k_{4,bulk}$, $k_{5,bulk}$, $k_{1,gas}$, $k_{2,gas}$, $k_{3,gas}$ and $k_{4,gas}$ were changed while in panel (b) $k_{5,bulk}$, $K_{H2O}$ and $K_{clothing,GA}$ were changed.

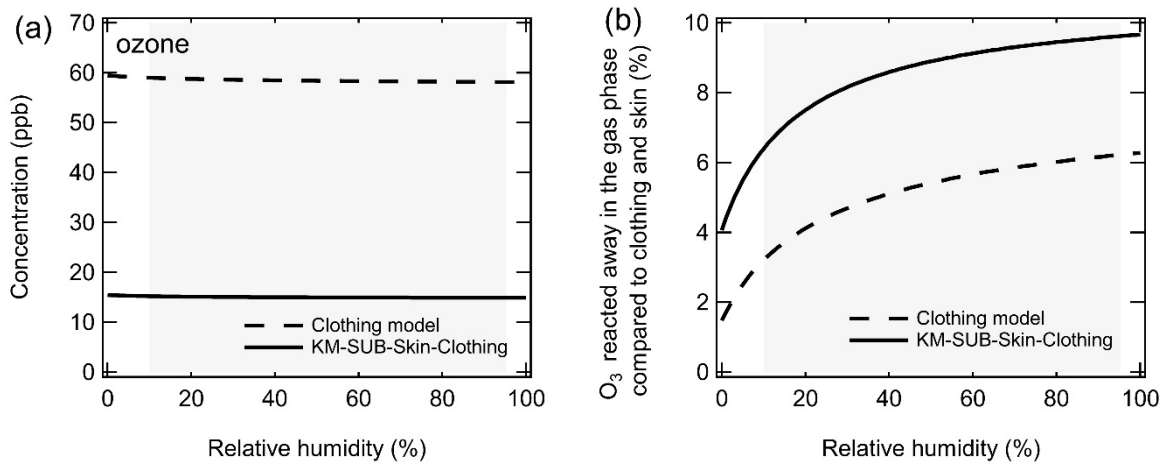


**Figure S7:** The impact of prolonged RH on the (a) gas-phase concentrations of ozone and (b) the percentage of $O_3$ reacted away in the gas phase compared to the clothing and skin. Ozone concentrations were calculated after four hours at a fixed RH using the conditions and parameters used in the clothing model to fit the ICHEAR data shown in the left-hand side panels of Fig. 5 (dashed lines) and the conditions and parameters used in the KM-SUB-Skin-Clothing model to fit the data in Fig. S5 (solid lines).

**Table S1:** The full squalene ozonolysis mechanism implemented in the kinetic models

**General scheme:**

O3 + double bond → ½ (BR1 primary CI + BR1 secondary carbonyl + BR2 secondary CI + BR2 primary carbonyl)

CI + $H_2O$ → Carbonyl + $H_2O_2$ (R2)

CI + $O_3$ → Carbonyl (R3)

CI → Carboxylic acid or Hydroxy ketone (R4)

CI + Carbonyl → Secondary ozonide (R5)

CI + Carboxylic acid → Hydroperoxide (R6)

**Legend**

| | |
|---|---|
| allCI | all Criegee Intermediates |
| allR'C(=O)OH | all carboxylic acids |
| allR'C(=O)R'' | all carbonyls |
| BR1 | branching ratio 1 (Gas phase value = 1, Condensed phase value = 0.2) |
| BR2 | branching ratio 2 (Gas phase value = 1, Condensed phase value = 1.8) |

**Notes:**

1) Note that although the following species appear in the clothing and KM-SUB-Skin-Clothing model in these models they are treated as a generic 'Product' that does not react further and does not impact the species of interest: CI7 (only treated in the gas-phase), CI8 (only treated in the gas-phase), CI9 (only treated in the gas-phase), CI10, CI11, CI13, CI14, CI15, CI17, CI18, CI19, CI20, CI21, CI23, CI26, CI27, SO1, HP1, SO13, HP13, SO17, HP17, SO19, HP19, SO11, SO12, SO13, SO15, SO16, SO18, SO20, HP20, SO21, SO23, HP23, SO34, SO35, SO37, SOSO1, HPSO1, SOSO2, HPSO2, SOHP2, HPHP2, SOSO3, HPSO3, SOSO4, HPSO4, SOSO5, HPSO5, SOHP5, HPHP5, SOSO6, HPSO6, SOSO7, HPSO7, CISO1, CIHP1, CISO3, CIHP3, CISO4, CIHP4, CISO7, CIHP7, CISO8, CIHP8, CA3, HK6

2) SO (secondary ozonides) and HP (hydroperoxides) are grouped together in the clothing and KM-SUB-Skin-Clothing models

**Full mechanism:**

| Reaction number | Rate | Occurs in the gas phase (Y/N) | Sensitive in the squalene particle model (Figure 1) | Included in clothing and KM-SUB-Skin-Clothing models (Y/N) | Reaction |
|---|---|---|---|---|---|
| 1 | k1×6 | N | Y | Y | Squalene+O3->(1/6)((BR2)CI1+(BR2)CI2+(BR2)CI3+(BR1)CI4+(BR1)CI5+(BR1)CI6+(BR2)TOT+(BR2)TOP+(BR2)TTT+(BR1)Geranylacetone+(BR1)6-MHO+(BR1)acetone) |
| 2 | k1 | Y | Y | Y | 6-MHO+O3->(1/2)((BR2)CI1+(BR1)CI7+(BR1)acetone+(BR2)4-OPA) |
| 3 | k1×2 | Y | Y | Y | Geranylacetone+O3->(1/4)((BR2)CI1+(BR2)CI2+(BR1)CI7+(BR1)CI8+(BR1)acetone+(BR1)6-MHO+(BR2)4-MON+(BR2)4-OPA) |
| 4 | k1×3 | N | Y | Y | TTT+O3->(1/6)((BR2)CI1+(BR2)CI2+(BR2)CI3+((BR1)CI9+(BR1)CI10+(BR1)CI11+(BR1)acetone+(BR1)6-MHO+(BR1)Geranylacetone+(BR2)ProductA+(BR2)4-MOD+(BR2)butanedial) |
| 5 | k1 | Y | Y | Y | 4-MON+O3->(1/2)((BR1)CI7+(BR2)CI12+(BR2)4-OPA+(BR1)4-OPA) |
| 6 | k1 | Y | Y | Y | 4-MOD+O3->(1/2)((BR1)CI9+(BR2)CI12+(BR1)4-OPA+(BR2)butanedial) |
| 7 | k1×2 | Y | Y | Y (but not in the gas phase) | ProductA+O3->(1/4)((BR1)CI9+(BR1)CI10+(BR2)CI12+(BR2)CI16+(BR1)4-OPA+(BR1)4-MON+(BR2)4-MOD+(BR2)butanedial) |
| 8 | k1×4 | N | Y | Y | TOP+O3->(1/8)((BR2)CI1+(BR2)CI2+(BR2)CI3+(BR1)CI4+(BR2)CI12+(BR1)CI13+(BR1)CI14+(BR1)CI15+(BR1)acetone+(BR1)6-MHO+(BR1)Geranylacetone+(BR2)TTT+(BR1)4-OPA+(BR2)4-MOD+(BR2)ProductB+(BR2)ProductC) |
| 9 | k1×2 | Y | Y | Y (but not in the gas phase) | ProductB+O3->(1/4)((BR2)CI12+(BR2)CI12+(BR1)CI13+(BR1)CI13+((BR1)4-OPA+(BR1)4-OPA+(BR2)4-MOD+(BR2)4-MOD) |
| 10 | k1×3 | N | Y | Y | ProductC+O3->(1/6)((BR2)CI12+(BR2)CI12+(BR1)CI13+(BR1)CI14+(BR2)CI16+(BR1)CI17+(BR1)4-OPA+(BR1)4-OPA+(BR1)4-MON+(BR2)ProductA+(BR2)4-MOD+(BR2)ProductB) |
| 11 | k1×5 | N | Y | Y | TOT+O3->(1/10)((BR2)CI1+(BR2)CI2+(BR2)CI3+(BR1)CI4+(BR1)CI5+(BR2)CI12+(BR2)CI16+(BR1)CI17+(BR1)CI18+(BR1)CI19+(BR1)acetone+(BR1)6-MHO+(BR1)Geranylacetone+(BR2)TTT+(BR2)TOP+(BR2)ProductD+(BR2)ProductC+(BR2)ProductA+(BR1)4-MON+(BR1)4-OPA) |
| 12 | k1×4 | N | Y | Y | ProductD+O3->(1/4)((BR2)CI12+(BR2)CI16+(BR1)CI17+(BR1)CI18+(BR1)4-OPA+(BR1)4-MON+(BR2)ProductA+(BR2)ProductC) |
| 13 | k1 | Y | Y | Y | HK3+O3->(1/2)((BR2)CI1+(BR1)CI20+(BR1)acetone+(BR2)HK2) |
| 14 | k1 | N | Y | N | HK4+O3->(1/2)((BR2)CI12+(BR1)CI20+(BR1)4-OPA+(BR2)HK2) |
| 15 | k1×2 | Y | Y | Y (but not in the gas phase) | HK5+O3->(1/4)((BR2)CI1+(BR2)CI2+(BR1)CI20+(BR1)CI21+(BR1)acetone+(BR1)6-MHO+(BR2)HK2+(BR2)HK4) |
| 16 | k1 | N | Y | N | CA3+O3->(1/2)((BR1)CI7+(BR2)CI22+(BR2)4-OPA+(BR1)CA1) |
| 17 | k1 | N | Y | N | CA4+O3->(1/2)((BR1)CI9+(BR2)CI22+(BR1)CA1+(BR2)butanedial) |
| 18 | k1 | N | Y | N | CA5+O3->(1/2)((BR2)CI12+(BR1)CI23+(BR2)CA2+(BR1)4-OPA) |
| 19 | k1×2 | N | Y | N | CA6+O3->(1/4)((BR1)CI9+(BR1)CI10+(BR2)CI22+(BR2)CI24+(BR1)CA1+(BR1)CA3+(BR2)4-MOD+(BR2)butanedial) |
| 20 | k1×2 | N | Y | N | CA7+O3->(1/4)((BR2)CI12+(BR1)CI13+(BR2)CI22+(BR1)CI25+(BR1)CA1+(BR2)CA4+(BR2)4-MOD+(BR1)4-OPA) |
| 21 | k1×2 | N | Y | N | CA8+O3->(1/4)((BR2)CI12+(BR2)CI16+(BR1)CI23+(BR1)CI26+(BR2)CA2+(BR2)CA5+(BR1)4-OPA+(BR1)4-MON) |
| 22 | k1×3 | N | Y | Y | CA9+O3->(1/6)((BR2)CI1+(BR2)CI2+(BR2)CI3+(BR1)CI23+(BR1)CI26+(BR1)CI27+(BR1)acetone+(BR1)6-MHO+(BR1)Geranylacetone+(BR2)CA2+(BR2)CA5+(BR2)CA8) |
| 23 | k1×3 | N | N | N | CA10+O3->(1/6)((BR2)CI12+(BR1)CI14+(BR1)CI13+(BR2)CI22+(BR2)CI24+(BR1)CI28+(BR1)CA1+(BR1)CA3+(BR2)CA6+(BR2)ProductB+(BR2)4-MOD+(BR1)4-OPA) |
| 24 | k1×3 | N | Y | N | CA11+O3->(1/6)((BR2)CI12+(BR2)CI16+(BR1)CI17+(BR2)CI22+(BR1)CI25+(BR1)CI29+(BR1)CA1+(BR2)CA4+(BR2)CA7+(BR2)ProductA+(BR1)4-MON+(BR1)4-OPA) |
| 25 | k1×4 | N | Y | N | CA12+O3->(1/8)((BR2)CI1+(BR2)CI2+(BR2)CI3+(BR1)CI4+(BR2)CI22+(BR1)CI25+(BR1)CI29+(BR1)CI30+(BR1)acetone+(BR1)6-MHO+(BR1)Geranylacetone+(BR2)TTT+(BR1)CA1+(BR2)CA4+(BR2)CA7+(BR2)CA11) |
| 26 | k1×4 | N | N | N | CA13+O3->(1/8)((BR2)CI12+(BR2)CI16+(BR1)CI18+(BR1)CI17+(BR2)CI22+(BR2)CI24+(BR1)CI28+(BR1)CI31+(BR1)CA1+(BR1)CA3+(BR2)CA6+(BR2)CA10+(BR2)ProductA+(BR2)ProductC+(BR1)4-MON+(BR1)4-OPA) |
| 27 | k1×5 | N | N | N | CA14+O3->(1/10)((BR2)CI1+(BR2)CI2+(BR2)CI3+(BR1)CI4+(BR1)CI5+(BR2)CI22+(BR2)CI24+(BR1)CI28+(BR1)CI31+(BR1)CI32+(BR1)CA1+(BR1)CA3+(BR2)CA6+(BR2)CA10+(BR2)CA13+(BR1)acetone+(BR1)6-MHO+(BR1)Geranylacetone+(BR2)TTT+(BR2)TOP) |
| 28 | k1 | N | N | N | HK7+O3->(1/2)((BR1)CI20+(BR2)CI22+(BR2)HK2+(BR1)CA1) |
| 29 | k1 | N | N | N | CA16+O3->(1/2)((BR2)CI22+(BR1)CI23+(BR1)CA1+(BR2)CA2) |
| 30 | k1×2 | N | N | N | CA17+O3->(1/4)((BR2)CI22+(BR1)CI23+(BR2)CI24+(BR1)CI26+(BR1)CA1+(BR2)CA2+(BR1)CA3+(BR2)CA5) |
| 31 | k1×2 | N | N | N | CA18+O3->(1/4)((BR2)CI22+(BR2)CI22+(BR1)CI25+(BR1)CI25+(BR1)CA1+(BR1)CA1+(BR2)CA4+(BR2)CA4) |
| 32 | k1×3 | N | N | N | CA19+O3->(1/6)((BR2)CI22+(BR2)CI22+(BR2)CI24+(BR1)CI25+(BR1)CI28+(BR1)CI29+(BR1)CA1+(BR1)CA1+(BR1)CA3+(BR2)CA4+(BR2)CA6+(BR2)CA7) |
| 33 | k1×4 | N | N | N | CA20+O3->(1/8)((BR2)CI22+(BR2)CI22+(BR2)CI24+(BR2)CI24+(BR1)CI28+(BR1)CI28+(BR1)CI31+(BR1)CI31+(BR1)CA1+(BR1)CA1+(BR1)CA3+(BR1)CA3+(BR2)CA6+(BR2)CA6+(BR2)CA10+(BR2)CA10) |
| 34 | k2 | Y | Y | Y | CI1+H2O->acetone |
| 35 | k3 | Y | Y | Y | CI1+O3->acetone |
| 36 | k4 | Y | Y | Y | CI1->HK1 |
| 37 | k5 | Y | Y | Y (but not in the gas phase) | CI1+allR'C(=O)R''->SO1 |
| 38 | k6 | Y | N | Y (but not in the gas phase) | CI1+allR'C(=O)OH->HP1 |
| 39 | k2 | Y | Y | Y (only in the gas-phase) | CI7+H2O->4-OPA |
| 40 | k3 | Y | Y | Y (only in the gas-phase) | CI7+O3->4-OPA |
| 41 | k4 | Y | Y | Y (only in the gas-phase) | CI7->CA1 |
| 42 | k5 | Y | Y | N | CI7+allR'C(=O)R''->SO2 |
| 43 | k6 | Y | N | N | CI7+allR'C(=O)OH->HP2 |
| 44 | k2 | Y | Y | Y (only in the gas-phase) | CI9+H2O->butanedial |
| 45 | k3 | Y | Y | Y (only in the gas-phase) | CI9+O3->butanedial |
| 46 | k4 | Y | Y | Y (only in the gas-phase) | CI9->CA2 |
| 47 | k5 | Y | Y | N | CI9+allR'C(=O)R''->SO3 |
| 48 | k6 | Y | N | N | CI9+allR'C(=O)OH->HP3 |
| 49 | k2 | Y | Y | Y | CI12+H2O->4-OPA |
| 50 | k3 | Y | Y | Y | CI12+O3->4-OPA |
| 51 | k4 | Y | Y | Y | CI12->HK2 |
| 52 | k5 | Y | Y | Y (but not in the gas phase) | CI12+allR'C(=O)R''->SO4 |
| 53 | k6 | Y | N | Y (but not in the gas phase) | CI12+allR'C(=O)OH->HP4 |
| 54 | k2 | Y | Y | Y | CI2+H2O->6-MHO |
| 55 | k3 | Y | Y | Y | CI2+O3->6-MHO |
| 56 | k4 | Y | Y | Y | CI2->HK3 |
| 57 | k5 | Y | Y | Y (but not in the gas phase) | CI2+allR'C(=O)R''->SO5 |
| 58 | k6 | Y | N | Y (but not in the gas phase) | CI2+allR'C(=O)OH->HP5 |
| 59 | k2 | Y | Y | Y (only in the gas-phase) | CI8+H2O->4-MON |
| 60 | k3 | Y | Y | Y (only in the gas-phase) | CI8+O3->4-MON |
| 61 | k4 | Y | Y | Y (only in the gas-phase) | CI8->CA3 |
| 62 | k5 | Y | Y | N | CI8+allR'C(=O)R''->SO6 |
| 63 | k6 | Y | N | N | CI8+allR'C(=O)OH->HP6 |

| | | | | | |
|---|---|---|---|---|---|
| 64 | k2 | Y | Y | N | CI10+H2O->4-MOD |
| 65 | k3 | Y | Y | N | CI10+O3->4-MOD |
| 66 | k4 | Y | Y | N | CI10->CA4 |
| 67 | k5 | Y | Y | N | CI10+allR'C(=O)R''->SO7 |
| 68 | k6 | Y | N | N | CI10+allR'C(=O)OH->HP7 |
| 69 | k2 | Y | Y | N | CI13+H2O->4-MOD |
| 70 | k3 | Y | Y | N | CI13+O3->4-MOD |
| 71 | k4 | Y | Y | N | CI13->CA5 |
| 72 | k5 | Y | Y | N | CI13+allR'C(=O)R''->SO8 |
| 73 | k6 | Y | N | N | CI13+allR'C(=O)OH->HP8 |
| 74 | k2 | Y | Y | Y (but not in the gas phase) | CI16+H2O->4-MON |
| 75 | k3 | Y | Y | Y (but not in the gas phase) | CI16+O3->4-MON |
| 76 | k4 | Y | Y | Y (but not in the gas phase) | CI16->HK4 |
| 77 | k5 | Y | Y | Y (but not in the gas phase) | CI16+allR'C(=O)R''->SO9 |
| 78 | k6 | Y | N | Y (but not in the gas phase) | CI16+allR'C(=O)OH->HP9 |
| 79 | k2 | N | Y | Y (but not in the gas phase) | CI3+H2O->Geranylacetone |
| 80 | k3 | N | Y | Y (but not in the gas phase) | CI3+O3->Geranylacetone |
| 81 | k4 | N | Y | Y (but not in the gas phase) | CI3->HK5 |
| 82 | k5 | N | Y | Y (but not in the gas phase) | CI3+allR'C(=O)R''->SO10 |
| 83 | k6 | N | N | Y (but not in the gas phase) | CI3+allR'C(=O)OH->HP10 |
| 84 | k2 | N | Y | N | CI11+H2O->ProductA |
| 85 | k3 | N | Y | N | CI11+O3->ProductA |
| 86 | k4 | N | Y | N | CI11->CA6 |
| 87 | k5 | N | Y | N | CI11+allR'C(=O)R''->SO11 |
| 88 | k6 | N | N | N | CI11+allR'C(=O)OH->HP11 |
| 89 | k2 | N | Y | N | CI14+H2O->ProductB |
| 90 | k3 | N | Y | N | CI14+O3->ProductB |
| 91 | k4 | N | Y | N | CI14->CA7 |
| 92 | k5 | N | Y | N | CI14+allR'C(=O)R''->SO12 |
| 93 | k6 | N | N | N | CI14+allR'C(=O)OH->HP12 |
| 94 | k2 | N | Y | N | CI17+H2O->ProductA |
| 95 | k3 | N | Y | N | CI17+O3->ProductA |
| 96 | k4 | N | Y | N | CI17->CA8 |
| 97 | k5 | N | Y | N | CI17+allR'C(=O)R''->SO13 |
| 98 | k6 | N | N | N | CI17+allR'C(=O)OH->HP13 |
| 99 | k2 | N | Y | Y | CI4+H2O->TTT |
| 100 | k3 | N | Y | Y | CI4+O3->TTT |
| 101 | k4 | N | Y | Y | CI4->CA9 |
| 102 | k5 | N | Y | Y | CI4+allR'C(=O)R''->SO14 |
| 103 | k6 | N | N | Y | CI4+allR'C(=O)OH->HP14 |
| 104 | k2 | N | N | N | CI15+H2O->ProductC |
| 105 | k3 | N | N | N | CI15+O3->ProductC |
| 106 | k4 | N | N | N | CI15->CA10 |
| 107 | k5 | N | N | N | CI15+allR'C(=O)R''->SO15 |
| 108 | k6 | N | N | N | CI15+allR'C(=O)OH->HP15 |
| 109 | k2 | N | Y | N | CI18+H2O->ProductC |
| 110 | k3 | N | Y | N | CI18+O3->ProductC |
| 111 | k4 | N | Y | N | CI18->CA11 |
| 112 | k5 | N | Y | N | CI18+allR'C(=O)R''->SO16 |
| 113 | k6 | N | N | N | CI18+allR'C(=O)OH->HP16 |
| 114 | k2 | N | Y | Y | CI5+H2O->TOP |
| 115 | k3 | N | Y | Y | CI5+O3->TOP |
| 116 | k4 | N | Y | Y | CI5->CA12 |
| 117 | k5 | N | Y | Y | CI5+allR'C(=O)R''->SO17 |
| 118 | k6 | N | N | Y | CI5+allR'C(=O)OH->HP17 |
| 119 | k2 | N | N | N | CI19+H2O->ProductD |
| 120 | k3 | N | N | N | CI19+O3->ProductD |
| 121 | k4 | N | N | N | CI19->CA13 |
| 122 | k5 | N | N | N | CI19+allR'C(=O)R''->SO18 |
| 123 | k6 | N | N | N | CI19+allR'C(=O)OH->HP18 |
| 124 | k2 | N | Y | Y | CI6+H2O->TOT |
| 125 | k3 | N | Y | Y | CI6+O3->TOT |
| 126 | k4 | N | Y | Y | CI6->CA14 |
| 127 | k5 | N | Y | Y | CI6+allR'C(=O)R''->SO19 |
| 128 | k6 | N | N | Y | CI6+allR'C(=O)OH->HP19 |
| 129 | k2 | Y | Y | Y (only in the gas-phase) | CI20+H2O->HK2 |
| 130 | k3 | Y | Y | Y (only in the gas-phase) | CI20+O3->HK2 |
| 131 | k4 | Y | Y | Y (only in the gas-phase) | CI20->HK6 |
| 132 | k5 | Y | Y | N | CI20+allR'C(=O)R''->SO20 |
| 133 | k6 | Y | N | N | CI20+allR'C(=O)OH->HP20 |
| 134 | k2 | N | Y | N | CI22+H2O->CA1 |
| 135 | k3 | N | Y | N | CI22+O3->CA1 |
| 136 | k4 | N | Y | N | CI22->HK6 |
| 137 | k5 | N | Y | N | CI22+allR'C(=O)R''->SO21 |
| 138 | k6 | N | N | N | CI22+allR'C(=O)OH->HP21 |
| 139 | k2 | N | Y | N | CI23+H2O->CA2 |
| 140 | k3 | N | Y | N | CI23+O3->CA2 |
| 141 | k4 | N | Y | N | CI23->CA15 |
| 142 | k5 | N | Y | N | CI23+allR'C(=O)R''->SO22 |
| 143 | k6 | N | N | N | CI23+allR'C(=O)OH->HP22 |
| 144 | k2 | Y | Y | N | CI21+H2O->HK4 |
| 145 | k3 | Y | Y | N | CI21+O3->HK4 |
| 146 | k4 | Y | Y | N | CI21->HK7 |
| 147 | k5 | Y | Y | N | CI21+allR'C(=O)R''->SO23 |
| 148 | k6 | Y | N | N | CI21+allR'C(=O)OH->HP23 |
| 149 | k2 | N | N | N | CI24+H2O->CA3 |
| 150 | k3 | N | N | N | CI24+O3->CA3 |
| 151 | k4 | N | N | N | CI24->HK7 |
| 152 | k5 | N | N | N | CI24+allR'C(=O)R''->SO24 |
| 153 | k6 | N | N | N | CI24+allR'C(=O)OH->HP24 |
| 154 | k2 | N | N | N | CI25+H2O->CA4 |

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|---|---|---|---|---|---|---|
| 155 | k3 | N | N | N | CI25+O3->CA4 | |
| 156 | k4 | N | N | N | CI25->CA16 | |
| 157 | k5 | N | N | N | CI25+allR'C(=O)R''->SO25 | |
| 158 | k6 | N | N | N | CI25+allR'C(=O)OH->HP25 | |
| 159 | k2 | N | N | N | CI26+H2O->CA5 | |
| 160 | k3 | N | N | N | CI26+O3->CA5 | |
| 161 | k4 | N | N | N | CI26->CA16 | |
| 162 | k5 | N | N | N | CI26+allR'C(=O)R''->SO26 | |
| 163 | k6 | N | N | N | CI26+allR'C(=O)OH->HP26 | |
| 164 | k2 | N | N | N | CI27+H2O->CA8 | |
| 165 | k3 | N | N | N | CI27+O3->CA8 | |
| 166 | k4 | N | N | N | CI27->CA17 | |
| 167 | k5 | N | N | N | CI27+allR'C(=O)R''->SO27 | |
| 168 | k6 | N | N | N | CI27+allR'C(=O)OH->HP27 | |
| 169 | k2 | N | N | N | CI28+H2O->CA6 | |
| 170 | k3 | N | N | N | CI28+O3->CA6 | |
| 171 | k4 | N | N | N | CI28->CA17 | |
| 172 | k5 | N | N | N | CI28+allR'C(=O)R''->SO28 | |
| 173 | k6 | N | N | N | CI28+allR'C(=O)OH->HP28 | |
| 174 | k2 | N | N | N | CI29+H2O->CA7 | |
| 175 | k3 | N | N | N | CI29+O3->CA7 | |
| 176 | k4 | N | N | N | CI29->CA18 | |
| 177 | k5 | N | N | N | CI29+allR'C(=O)R''->SO29 | |
| 178 | k6 | N | N | N | CI29+allR'C(=O)OH->HP29 | |
| 179 | k2 | N | N | N | CI30+H2O->CA11 | |
| 180 | k3 | N | N | N | CI30+O3->CA11 | |
| 181 | k4 | N | N | N | CI30->CA19 | |
| 182 | k5 | N | N | N | CI30+allR'C(=O)R''->SO30 | |
| 183 | k6 | N | N | N | CI30+allR'C(=O)OH->HP30 | |
| 184 | k2 | N | N | N | CI31+H2O->CA10 | |
| 185 | k3 | N | N | N | CI31+O3->CA10 | |
| 186 | k4 | N | N | N | CI31->CA19 | |
| 187 | k5 | N | N | N | CI31+allR'C(=O)R''->SO31 | |
| 188 | k6 | N | N | N | CI31+allR'C(=O)OH->HP31 | |
| 189 | k2 | N | N | N | CI32+H2O->CA13 | |
| 190 | k3 | N | N | N | CI32+O3->CA13 | |
| 191 | k4 | N | N | N | CI32->CA20 | |
| 192 | k5 | N | N | N | CI32+allR'C(=O)R''->SO32 | |
| 193 | k6 | N | N | N | CI32+allR'C(=O)OH->HP32 | |
| 194 | k6 | Y | N | N | CA1+allCI->HP2 | |
| 195 | k6 | Y | N | N | CA2+allCI->HP3 | |
| 196 | k6 | N | N | N | CA3+allCI->HP6 | |
| 197 | k6 | N | N | N | CA4+allCI->HP7 | |
| 198 | k6 | N | N | N | CA5+allCI->HP8 | |
| 199 | k6 | N | N | N | CA6+allCI->HP11 | |
| 200 | k6 | N | N | N | CA7+allCI->HP12 | |
| 201 | k6 | N | N | N | CA8+allCI->HP13 | |
| 202 | k6 | N | N | N | CA9+allCI->HP14 | |
| 203 | k6 | N | N | N | CA10+allCI->HP15 | |
| 204 | k6 | N | N | N | CA11+allCI->HP16 | |
| 205 | k6 | N | N | N | CA12+allCI->HP17 | |
| 206 | k6 | N | N | N | CA13+allCI->HP18 | |
| 207 | k6 | N | N | N | CA14+allCI->HP19 | |
| 208 | k6×2 | Y | N | N | CA15+allCI->HP22 | |
| 209 | k6×2 | N | N | N | CA16+allCI->(1/2)(HP25+HP26) | |
| 210 | k6×2 | N | N | N | CA17+allCI->(1/2)(HP27+HP28) | |
| 211 | k6×2 | N | N | N | CA18+allCI->HP29 | |
| 212 | k6×2 | N | N | N | CA19+allCI->(1/2)(HP30+HP31) | |
| 213 | k6×2 | N | N | N | CA20+allCI->HP32 | |
| 214 | k6 | N | N | N | HK6+allCI->HP20 | |
| 215 | k6 | N | N | N | HK7+allCI->HP23 | |
| 216 | k5 | Y | Y (gas phase only) | N | acetone+allCI->SO1 | |
| 217 | k5 | Y | Y | Y (but not in the gas phase) | 6-MHO+allCI->SO5 | |
| 218 | k5 | Y | Y | Y (but not in the gas phase) | Geranylacetone+allCI->SO10 | |
| 219 | k5 | N | Y | Y | TTT+allCI->SO14 | |
| 220 | k5 | N | Y | Y | TOP+allCI->SO17 | |
| 221 | k5 | N | Y | Y | TOT+allCI->SO19 | |
| 222 | k5×2 | Y | Y (gas phase only) | N | 4-OPA+allCI->(1/2)(SO2+SO4) | |
| 223 | k5×2 | Y | Y | Y (but not in the gas phase) | 4-MON+allCI->(1/2)(SO6+SO9) | |
| 224 | k5×2 | Y | Y | Y (but not in the gas phase) | 4-MOD+allCI->(1/2)(SO7+SO8) | |
| 225 | k5 | Y | Y (gas phase only) | N | butanedial+allCI->SO3 | |
| 226 | k5×2 | Y | Y | Y (but not in the gas phase) | ProductA+allCI->(1/2)(SO11+SO13) | |
| 227 | k5 | Y | Y | Y (but not in the gas phase) | ProductB+allCI->SO12 | |
| 228 | k5×2 | N | Y | Y | ProductC+allCI->(1/2)SO15+SO16 | |
| 229 | k5 | N | Y | Y | ProductD+allCI->SO18 | |
| 230 | k5 | Y | Y | Y (but not in the gas phase) | CA1+allCI->SO21 | |
| 231 | k5 | Y | Y | Y (but not in the gas phase) | CA2+allCI->SO22 | |
| 232 | k5 | N | Y | N | CA3+allCI->SO24 | |
| 233 | k5 | N | Y | N | CA4+allCI->SO25 | |
| 234 | k5 | N | Y | N | CA5+allCI->SO26 | |
| 235 | k5 | N | Y | N | CA6+allCI->SO28 | |
| 236 | k5 | N | Y | N | CA7+allCI->SO29 | |
| 237 | k5 | N | Y | N | CA8+allCI->SO27 | |
| 238 | k5 | N | N | N | CA10+allCI->SO31 | |
| 239 | k5 | N | Y | N | CA11+allCI->SO30 | |
| 240 | k5 | N | N | N | CA13+allCI->SO32 | |
| 241 | k5 | Y | Y | N | HK1+allCI->SO33 | |
| 242 | k5×2 | Y | Y | Y (but not in the gas phase) | HK2+allCI->(1/2)(SO20+SO34) | |
| 243 | k5 | Y | Y | Y (but not in the gas phase) | HK3+allCI->SO35 | |
| 244 | k5×2 | N | Y | N | HK4+allCI->(1/2)(SO23+SO36) | |
| 245 | k5 | Y | Y | Y (but not in the gas phase) | HK5+allCI->SO37 | |

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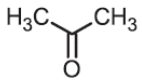
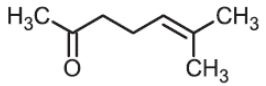
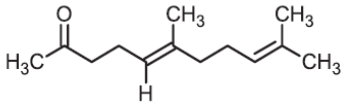
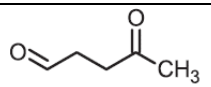
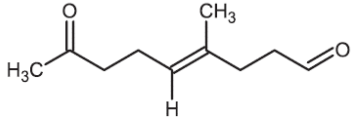
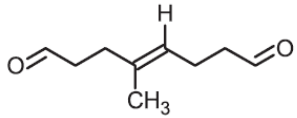
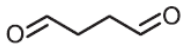
|---|---|---|---|---|---|
| 246 | k5 | N | N | N | HK6+allCl->SO38 |
| 247 | k5 | N | N | N | HK7+allCl->SO39 |
| 248 | k1 | N | Y | Y | SO5+O3->(1/2)((BR1)acetone+(BR2)SO4+(BR1)ClSO1+(BR2)Cl1) |
| 249 | k1 | N | N | Y | HP5+O3->(1/2)((BR1)acetone+(BR2)HP4+(BR1)ClHP1+(BR2)Cl1) |
| 250 | k1 | N | Y | Y | SO6+O3->(1/2)((BR2)4-OPA+(BR1)Cl7+(BR1)SO2+(BR2)ClSO2) |
| 251 | k1 | N | N | Y | HP6+O3->(1/2)((BR2)4-OPA+(BR1)Cl7+(BR1)HP2+(BR2)ClHP2) |
| 252 | k1 | N | Y | Y | SO7+O3->(1/2)((BR2)butanedial+(BR1)Cl9+(BR1)SO2+(BR2)ClSO2) |
| 253 | k1 | N | N | Y | HP7+O3->(1/2)((BR2)butanedial+(BR1)Cl9+(BR1)HP2+(BR2)ClHP2) |
| 254 | k1 | N | Y | Y | SO8+O3->(1/2)((BR1)4-OPA+(BR2)Cl12+(BR2)SO3+(BR1)ClSO3) |
| 255 | k1 | N | N | Y | HP8+O3->(1/2)((BR1)4-OPA+(BR2)Cl12+(BR2)HP3+(BR1)ClHP3) |
| 256 | k1 | N | Y | Y | SO9+O3->(1/2)((BR1)4-OPA+(BR2)Cl12+(BR2)SO4+(BR1)ClSO1) |
| 257 | k1 | N | N | Y | HP9+O3->(1/2)((BR1)4-OPA+(BR2)Cl12+(BR2)HP4+(BR1)ClHP1) |
| 258 | k1×2 | N | Y | Y | SO10+O3->(1/4)((BR1)acetone+(BR1)6-MHO+(BR2)Cl1+(BR2)Cl2+(BR2)SO4+(BR2)SO9+(BR1)ClSO1+(BR1)ClSO4) |
| 259 | k1×2 | N | N | Y | HP10+O3->(1/4)((BR1)acetone+(BR1)6-MHO+(BR2)Cl1+(BR2)Cl2+(BR2)HP4+(BR2)HP9+(BR1)ClHP1+(BR1)ClHP4) |
| 260 | k1×2 | N | Y | N | SO11+O3->(1/4)(((BR2)4-MOD+(BR2)butanedial+(BR1)Cl9+(BR1)Cl10+(BR1)SO2+(BR1)SO6+(BR2)ClSO5+(BR2)ClSO2) |
| 261 | k1×2 | N | N | N | HP11+O3->(1/4)((BR2)4-MOD+(BR2)butanedial+(BR1)Cl9+(BR1)Cl10+(BR1)HP2+(BR1)HP6+(BR2)ClHP5+(BR2)ClHP2) |
| 262 | k1×2 | N | Y | N | SO12+O3->(1/4)((BR1)4-OPA+(BR2)4-MOD+(BR2)Cl12+(BR1)Cl13+(BR1)SO2+(BR2)SO7+(BR2)ClSO2+(BR1)ClSO6) |
| 263 | k1×2 | N | N | N | HP12+O3->(1/4)((BR1)4-OPA+(BR2)4-MOD+(BR2)Cl12+(BR1)Cl13+(BR1)HP2+(BR2)HP7+(BR2)ClHP2+(BR1)ClHP6) |
| 264 | k1×2 | N | Y | N | SO13+O3->(1/4)((BR1)4-OPA+(BR1)4-MON+(BR2)Cl12+(BR2)Cl16+(BR2)SO3+(BR2)SO8+(BR1)ClSO3+(BR1)ClSO7) |
| 265 | k1×2 | N | N | N | HP13+O3->(1/4)((BR1)4-OPA+(BR1)4-MON+(BR2)Cl12+(BR2)Cl16+(BR2)HP3+(BR2)HP8+(BR1)ClHP3+(BR1)ClHP7) |
| 266 | k1×3 | N | Y | Y | SO14+O3->(1/6)((BR1)acetone+(BR1)6-MHO+(BR1)Geranylacetone+(BR2)Cl1+(BR2)Cl2+(BR2)Cl3+(BR2)SO3+(BR2)SO8+(BR2)SO13+(BR1)ClSO3+(BR1)ClSO7+(BR1)ClSO8) |
| 267 | k1×3 | N | N | Y | HP14+O3->(1/6)((BR1)acetone+(BR1)6-MHO+(BR1)Geranylacetone+(BR2)Cl1+(BR2)Cl2+(BR2)Cl3+(BR2)HP3+(BR2)HP8+(BR2)HP13+(BR1)ClHP3+(BR1)ClHP7+(BR1)ClHP8) |
| 268 | k1×3 | N | Y | N | SO15+O3->(1/6)((BR1)4-OPA+(BR2)4-MOD+(BR2)ProductB+(BR2)Cl12+(BR1)Cl13+(BR1)Cl14+(BR1)SO2+(BR1)SO6+(BR2)SO11+(BR2)ClSO2+(BR2)ClSO5+(BR1)ClSO9) |
| 269 | k1×3 | N | N | N | HP15+O3->(1/6)((BR1)4-OPA+(BR2)4-MOD+(BR2)ProductB+(BR2)Cl12+(BR1)Cl13+(BR1)Cl14+(BR1)HP2+(BR1)HP6+(BR2)HP11+(BR2)ClHP2+(BR2)ClHP5+(BR1)ClHP9) |
| 270 | k1×3 | N | Y | N | SO16+O3->(1/6)((BR1)4-OPA+(BR1)4-MON+(BR2)ProductA+(BR2)Cl12+(BR2)Cl16+(BR1)Cl17+(BR1)SO2+(BR2)SO7+(BR2)SO12+(BR2)ClSO2+(BR1)ClSO6+(BR1)ClSO10) |
| 271 | k1×3 | N | N | N | HP16+O3->(1/6)((BR1)4-OPA+(BR1)4-MON+(BR2)ProductA+(BR2)Cl12+(BR2)Cl16+(BR1)Cl17+(BR1)HP2+(BR2)HP7+(BR2)HP12+(BR2)ClHP2+(BR1)ClHP6+(BR1)ClHP10) |
| 272 | k1×4 | N | Y | N | SO17+O3->(1/8)((BR1)acetone+(BR1)6-MHO+(BR1)Geranylacetone+(BR2)TTT+(BR2)Cl1+(BR2)Cl2+(BR2)Cl3+(BR1)Cl4+(BR1)SO2+(BR2)SO7+(BR2)SO12+(BR2)SO16+(BR2)ClSO2+(BR1)ClSO6+(BR1)ClSO10+(BR1)ClSO11) |
| 273 | k1×4 | N | N | N | HP17+O3->(1/8)((BR1)acetone+(BR1)6-MHO+(BR1)Geranylacetone+(BR2)TTT+(BR2)Cl1+(BR2)Cl2+(BR2)Cl3+(BR1)Cl4+(BR1)HP2+(BR2)HP7+(BR2)HP12+(BR2)HP16+(BR2)ClHP2+(BR1)ClHP6+(BR1)ClHP10+(BR1)ClHP11) |
| 274 | k1×4 | N | Y | N | SO18+O3->(1/8)((BR1)4-OPA+(BR1)4-MON+(BR2)ProductA+(BR2)ProductC+(BR2)Cl12+(BR2)Cl16+(BR1)Cl17+(BR1)Cl18+(BR1)SO2+(BR1)SO6+(BR2)SO11+(BR2)SO15+(BR2)ClSO2+(BR2)ClSO5+(BR1)ClSO9+(BR1)ClSO12) |
| 275 | k1×4 | N | N | N | HP18+O3->(1/8)((BR1)4-OPA+(BR1)4-MON+(BR2)ProductA+(BR2)ProductC+(BR2)Cl12+(BR2)Cl16+(BR1)Cl17+(BR1)Cl18+(BR1)HP2+(BR1)HP6+(BR2)HP11+(BR2)HP15+(BR2)ClHP2+(BR2)ClHP5+(BR1)ClHP9+(BR1)ClHP12) |
| 276 | k1×5 | N | Y | N | SO19+O3->(1/10)((BR1)acetone+(BR1)6-MHO+(BR1)Geranylacetone+(BR2)TTT+(BR2)TOP+(BR2)Cl1+(BR2)Cl2+(BR2)Cl3+(BR1)Cl4+(BR1)Cl5+(BR1)SO2+(BR1)SO6+(BR2)SO11+(BR2)SO15+(BR2)ClSO2+(BR2)ClSO5+(BR1)ClSO9+(BR1)ClSO12+(BR1)ClSO13) |
| 277 | k1×5 | N | N | N | HP19+O3->(1/10)((BR1)acetone+(BR1)6-MHO+(BR1)Geranylacetone+(BR2)TTT+(BR2)TOP+(BR2)Cl1+(BR2)Cl2+(BR2)Cl3+(BR1)Cl4+(BR1)Cl5+(BR1)HP2+(BR1)HP6+(BR2)HP11+(BR2)HP15+(BR2)HP18+(BR2)ClHP2+(BR2)ClHP5+(BR1)ClHP9+(BR1)ClHP12+(BR1)ClHP13) |
| 278 | k1 | N | N | N | SO23+O3->(1/2)((BR2)HK2+(BR1)Cl20+(BR1)SO2+(BR2)ClSO2) |
| 279 | k1 | N | N | N | HP23+O3->(1/2)((BR2)HK2+(BR1)Cl20+(BR1)HP2+(BR2)ClHP2) |
| 280 | k1 | N | N | N | SO24+O3->(1/2)((BR1)CA1+(BR2)Cl22+(BR2)SO4+(BR1)ClSO1) |
| 281 | k1 | N | N | N | HP24+O3->(1/2)((BR1)CA1+(BR2)Cl22+(BR2)HP4+(BR1)ClHP1) |
| 282 | k1 | N | N | N | SO25+O3->(1/2)((BR1)CA1+(BR2)Cl22+(BR2)SO3+(BR1)ClSO3) |
| 283 | k1 | N | N | N | HP25+O3->(1/2)((BR1)CA1+(BR2)Cl22+(BR2)HP3+(BR1)ClHP3) |
| 284 | k1 | N | N | N | SO26+O3->(1/2)((BR2)CA2+(BR1)Cl23+(BR1)SO2+(BR2)ClSO2) |
| 285 | k1 | N | N | N | HP26+O3->(1/2)((BR2)CA2+(BR1)Cl23+(BR1)HP2+(BR2)ClHP2) |
| 286 | k1×2 | N | N | N | SO27+O3->(1/4)((BR2)CA2+(BR2)CA5+(BR1)Cl23+(BR1)Cl26+(BR1)SO2+(BR1)SO6+(BR2)ClSO2+(BR2)ClSO5) |
| 287 | k1×2 | N | N | N | HP27+O3->(1/4)((BR2)CA2+(BR2)CA5+(BR1)Cl23+(BR1)Cl26+(BR1)HP2+(BR1)HP6+(BR2)ClHP2+(BR2)ClHP5) |
| 288 | k1×2 | N | N | N | SO28+O3->(1/4)((BR1)CA1+(BR1)CA3+(BR2)Cl22+(BR2)Cl24+(BR2)SO3+(BR2)SO8+(BR1)ClSO3+(BR1)ClSO7) |
| 289 | k1×2 | N | N | N | HP28+O3->(1/4)((BR1)CA1+(BR1)CA3+(BR2)Cl22+(BR2)Cl24+(BR2)HP3+(BR2)HP8+(BR1)ClHP3+(BR1)ClHP7) |
| 290 | k1×2 | N | N | N | SO29+O3->(1/4)((BR1)CA1+(BR2)CA4+(BR2)Cl22+(BR1)Cl25+(BR1)SO2+(BR2)SO7+(BR2)ClSO2+(BR1)ClSO6) |
| 291 | k1×2 | N | N | N | HP29+O3->(1/4)((BR1)CA1+(BR2)CA4+(BR2)Cl22+(BR1)Cl25+(BR1)HP2+(BR2)HP7+(BR2)ClHP2+(BR1)ClHP6) |
| 292 | k1×3 | N | N | N | SO30+O3->(1/6)((BR1)CA1+(BR2)CA4+(BR2)CA7+(BR2)Cl22+(BR1)Cl25+(BR1)Cl29+(BR1)SO2+(BR1)SO6+(BR2)SO11+(BR2)ClSO2+(BR2)ClSO5+(BR1)ClSO9) |
| 293 | k1×3 | N | N | N | HP30+O3->(1/6)((BR1)CA1+(BR2)CA4+(BR2)CA7+(BR2)Cl22+(BR1)Cl25+(BR1)Cl29+(BR1)HP2+(BR1)HP6+(BR2)HP11+(BR2)ClHP2+(BR2)ClHP5+(BR1)ClHP9) |
| 294 | k1×3 | N | N | N | SO31+O3->(1/6)((BR1)CA1+(BR1)CA3+(BR2)CA6+(BR2)Cl22+(BR2)Cl24+(BR1)Cl28+(BR1)SO2+(BR2)SO7+(BR2)SO12+(BR2)ClSO2+(BR1)ClSO6+(BR1)ClSO10) |
| 295 | k1×3 | N | N | N | HP31+O3->(1/6)((BR1)CA1+(BR1)CA3+(BR2)CA6+(BR2)Cl22+(BR2)Cl24+(BR1)Cl28+(BR1)HP2+(BR2)HP7+(BR2)HP12+(BR2)ClHP2+(BR1)ClHP6+(BR1)ClHP10) |
| 296 | k1×4 | N | N | N | SO32+O3->(1/8)((BR1)CA1+(BR1)CA3+(BR2)CA6+(BR2)CA10+(BR2)Cl22+(BR2)Cl24+(BR1)Cl28+(BR1)Cl31+(BR1)SO2+(BR1)SO6+(BR2)SO11+(BR2)SO15+(BR2)ClSO2+(BR2)ClSO5+(BR1)ClSO9+(BR1)ClSO12) |
| 297 | k1×4 | N | N | N | HP32+O3->(1/8)((BR1)CA1+(BR1)CA3+(BR2)CA6+(BR2)CA10+(BR2)Cl22+(BR2)Cl24+(BR1)Cl28+(BR1)Cl31+(BR1)HP2+(BR1)HP6+(BR2)HP11+(BR2)HP15+(BR2)ClHP2+(BR2)ClHP5+(BR1)ClHP9+(BR1)ClHP12) |
| 298 | k1 | N | N | N | SO35+O3->(1/2)((BR1)acetone+(BR2)Cl1+(BR2)SO34+(BR1)ClSO14) |
| 299 | k1 | N | N | N | SO36+O3->(1/2)((BR1)4-OPA+(BR2)Cl12+(BR2)SO34+(BR1)ClSO14) |
| 300 | k1×2 | N | N | N | SO37+O3->(1/4)((BR1)acetone+(BR1)6-MHO+(BR2)Cl1+(BR2)Cl2+(BR2)SO34+(BR2)SO36+(BR1)ClSO14+(BR1)ClSO15) |
| 301 | k1 | N | N | N | SO39+O3->(1/2)((BR1)CA1+(BR2)Cl22+(BR2)SO34+(BR1)ClSO14) |
| 302 | k2 | N | Y | N | ClSO1+H2O->SO4 |
| 303 | k3 | N | Y | N | ClSO1+O3->SO4 |
| 304 | k4 | N | Y | N | ClSO1->SO21 |
| 305 | k5 | N | Y | N | ClSO1+allR'C(=O)R"->SOSO1 |
| 306 | k6 | N | N | N | ClSO1+allR'C(=O)OH->SOHP1 |
| 307 | k2 | N | N | N | ClHP1+H2O->HP4 |
| 308 | k3 | N | N | N | ClHP1+O3->HP4 |
| 309 | k4 | N | N | N | ClHP1->HP21 |
| 310 | k5 | N | N | N | ClHP1+allR'C(=O)R"->HPSO1 |
| 311 | k6 | N | N | N | ClHP1+allR'C(=O)OH->HPHP1 |
| 312 | k2 | N | Y | Y | ClSO2+H2O->SO2 |
| 313 | k3 | N | Y | Y | ClSO2+O3->SO2 |
| 314 | k4 | N | Y | Y | ClSO2->SO20 |
| 315 | k5 | N | Y | Y | ClSO2+allR'C(=O)R"->SOSO2 |
| 316 | k6 | N | N | Y | ClSO2+allR'C(=O)OH->SOHP2 |
| 317 | k2 | N | N | Y | ClHP2+H2O->HP2 |
| 318 | k3 | N | N | Y | ClHP2+O3->HP2 |
| 319 | k4 | N | N | Y | ClHP2->HP20 |
| 320 | k5 | N | N | Y | ClHP2+allR'C(=O)R"->HPSO2 |
| 321 | k6 | N | N | Y | ClHP2+allR'C(=O)OH->HPHP2 |
| 322 | k2 | N | Y | N | ClSO3+H2O->SO3 |
| 323 | k3 | N | Y | N | ClSO3+O3->SO3 |
| 324 | k4 | N | Y | N | ClSO3->SO22 |
| 325 | k5 | N | Y | N | ClSO3+allR'C(=O)R"->SOSO3 |
| 326 | k6 | N | N | N | ClSO3+allR'C(=O)OH->SOHP3 |
| 327 | k2 | N | N | N | ClHP3+H2O->HP3 |
| 328 | k3 | N | N | N | ClHP3+O3->HP3 |
| 329 | k4 | N | N | N | ClHP3->HP22 |
| 330 | k5 | N | N | N | ClHP3+allR'C(=O)R"->HPSO3 |
| 331 | k6 | N | N | N | ClHP3+allR'C(=O)OH->HPHP3 |
| 332 | k2 | N | Y | N | ClSO4+H2O->SO9 |
| 333 | k3 | N | Y | N | ClSO4+O3->SO9 |
| 334 | k4 | N | Y | N | ClSO4->SO24 |
| 335 | k5 | N | Y | N | ClSO4+allR'C(=O)R"->SOSO4 |
| 336 | k6 | N | N | N | ClSO4+allR'C(=O)OH->SOHP4 |

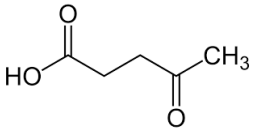
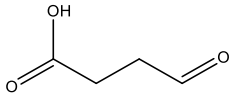
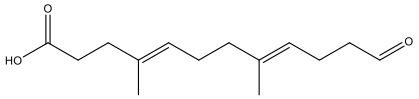
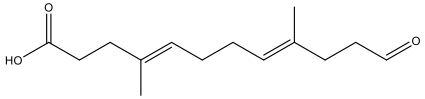
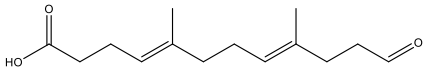
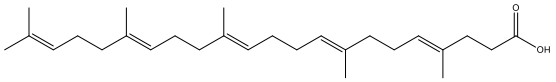
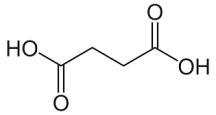
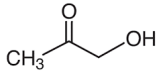
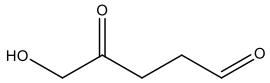
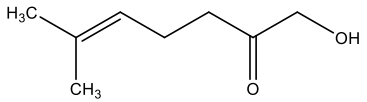
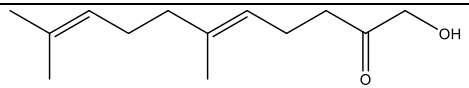
| | | | | | |
|---|---|---|---|---|---|
| 337 | k2 | N | N | N | ClHP4+H2O->HP9 |
| 338 | k3 | N | N | N | ClHP4+O3->HP9 |
| 339 | k4 | N | N | N | ClHP4->HP24 |
| 340 | k5 | N | N | N | ClHP4+allR'C(=O)R''->HPSO4 |
| 341 | k6 | N | N | N | ClHP4+allR'C(=O)OH->HPHP4 |
| 342 | k2 | N | Y | Y | ClSO5+H2O->SO6 |
| 343 | k3 | N | Y | Y | ClSO5+O3->SO6 |
| 344 | k4 | N | Y | Y | ClSO5->SO23 |
| 345 | k5 | N | Y | Y | ClSO5+allR'C(=O)R''->SOSO5 |
| 346 | k6 | N | N | Y | ClSO5+allR'C(=O)OH->SOHP5 |
| 347 | k2 | N | N | Y | ClHP5+H2O->HP6 |
| 348 | k3 | N | N | Y | ClHP5+O3->HP6 |
| 349 | k4 | N | N | Y | ClHP5->HP23 |
| 350 | k5 | N | N | Y | ClHP5+allR'C(=O)R''->HPSO5 |
| 351 | k6 | N | N | Y | ClHP5+allR'C(=O)OH->HPHP5 |
| 352 | k2 | N | Y | N | ClSO6+H2O->SO7 |
| 353 | k3 | N | Y | N | ClSO6+O3->SO7 |
| 354 | k4 | N | Y | N | ClSO6->SO26 |
| 355 | k5 | N | Y | N | ClSO6+allR'C(=O)R''->SOSO6 |
| 356 | k6 | N | N | N | ClSO6+allR'C(=O)OH->SOHP6 |
| 357 | k2 | N | N | N | ClHP6+H2O->HP7 |
| 358 | k3 | N | N | N | ClHP6+O3->HP7 |
| 359 | k4 | N | N | N | ClHP6->HP26 |
| 360 | k5 | N | N | N | ClHP6+allR'C(=O)R''->HPSO6 |
| 361 | k6 | N | N | N | ClHP6+allR'C(=O)OH->HPHP6 |
| 362 | k2 | N | Y | N | ClSO7+H2O->SO8 |
| 363 | k3 | N | Y | N | ClSO7+O3->SO8 |
| 364 | k4 | N | Y | N | ClSO7->SO25 |
| 365 | k5 | N | Y | N | ClSO7+allR'C(=O)R''->SOSO7 |
| 366 | k6 | N | N | N | ClSO7+allR'C(=O)OH->SOHP7 |
| 367 | k2 | N | N | N | ClHP7+H2O->HP8 |
| 368 | k3 | N | N | N | ClHP7+O3->HP8 |
| 369 | k4 | N | N | N | ClHP7->HP25 |
| 370 | k5 | N | N | N | ClHP7+allR'C(=O)R''->HPSO7 |
| 371 | k6 | N | N | N | ClHP7+allR'C(=O)OH->HPHP7 |
| 372 | k2 | N | N | N | ClSO8+H2O->SO13 |
| 373 | k3 | N | N | N | ClSO8+O3->SO13 |
| 374 | k4 | N | N | N | ClSO8->SO28 |
| 375 | k5 | N | N | N | ClSO8+allR'C(=O)R''->SOSO8 |
| 376 | k6 | N | N | N | ClSO8+allR'C(=O)OH->SOHP8 |
| 377 | k2 | N | N | N | ClHP8+H2O->HP13 |
| 378 | k3 | N | N | N | ClHP8+O3->HP13 |
| 379 | k4 | N | N | N | ClHP8->HP28 |
| 380 | k5 | N | N | N | ClHP8+allR'C(=O)R''->HPSO8 |
| 381 | k6 | N | N | N | ClHP8+allR'C(=O)OH->HPHP8 |
| 382 | k2 | N | N | N | ClSO9+H2O->SO11 |
| 383 | k3 | N | N | N | ClSO9+O3->SO11 |
| 384 | k4 | N | N | N | ClSO9->SO27 |
| 385 | k5 | N | N | N | ClSO9+allR'C(=O)R''->SOSO9 |
| 386 | k6 | N | N | N | ClSO9+allR'C(=O)OH->SOHP9 |
| 387 | k2 | N | N | N | ClHP9+H2O->HP11 |
| 388 | k3 | N | N | N | ClHP9+O3->HP11 |
| 389 | k4 | N | N | N | ClHP9->HP27 |
| 390 | k5 | N | N | N | ClHP9+allR'C(=O)R''->HPSO9 |
| 391 | k6 | N | N | N | ClHP9+allR'C(=O)OH->HPHP9 |
| 392 | k2 | N | N | N | ClSO10+H2O->SO12 |
| 393 | k3 | N | N | N | ClSO10+O3->SO12 |
| 394 | k4 | N | N | N | ClSO10->SO29 |
| 395 | k5 | N | N | N | ClSO10+allR'C(=O)R''->SOSO10 |
| 396 | k6 | N | N | N | ClSO10+allR'C(=O)OH->SOHP10 |
| 397 | k2 | N | N | N | ClHP10+H2O->HP12 |
| 398 | k3 | N | N | N | ClHP10+O3->HP12 |
| 399 | k4 | N | N | N | ClHP10->HP29 |
| 400 | k5 | N | N | N | ClHP10+allR'C(=O)R''->HPSO10 |
| 401 | k6 | N | N | N | ClHP10+allR'C(=O)OH->HPHP10 |
| 402 | k2 | N | N | N | ClSO11+H2O->SO16 |
| 403 | k3 | N | N | N | ClSO11+O3->SO16 |
| 404 | k4 | N | N | N | ClSO11->SO31 |
| 405 | k5 | N | N | N | ClSO11+allR'C(=O)R''->SOSO11 |
| 406 | k6 | N | N | N | ClSO11+allR'C(=O)OH->SOHP11 |
| 407 | k2 | N | N | N | ClHP11+H2O->HP16 |
| 408 | k3 | N | N | N | ClHP11+O3->HP16 |
| 409 | k4 | N | N | N | ClHP11->HP31 |
| 410 | k5 | N | N | N | ClHP11+allR'C(=O)R''->HPSO11 |
| 411 | k6 | N | N | N | ClHP11+allR'C(=O)OH->HPHP11 |
| 412 | k2 | N | N | N | ClSO12+H2O->SO15 |
| 413 | k3 | N | N | N | ClSO12+O3->SO15 |
| 414 | k4 | N | N | N | ClSO12->SO30 |
| 415 | k5 | N | N | N | ClSO12+allR'C(=O)R''->SOSO12 |
| 416 | k6 | N | N | N | ClSO12+allR'C(=O)OH->SOHP12 |
| 417 | k2 | N | N | N | ClHP12+H2O->HP15 |
| 418 | k3 | N | N | N | ClHP12+O3->HP15 |
| 419 | k4 | N | N | N | ClHP12->HP30 |
| 420 | k5 | N | N | N | ClHP12+allR'C(=O)R''->HPSO12 |
| 421 | k6 | N | N | N | ClHP12+allR'C(=O)OH->HPHP12 |
| 422 | k2 | N | N | N | ClSO13+H2O->SO18 |
| 423 | k3 | N | N | N | ClSO13+O3->SO18 |
| 424 | k4 | N | N | N | ClSO13->SO32 |
| 425 | k5 | N | N | N | ClSO13+allR'C(=O)R''->SOSO13 |
| 426 | k6 | N | N | N | ClSO13+allR'C(=O)OH->SOHP13 |
| 427 | k2 | N | N | N | ClHP13+H2O->HP18 |

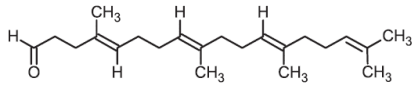
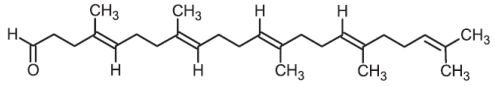
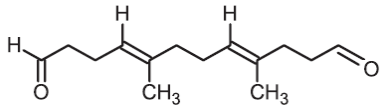
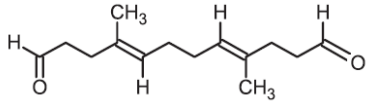
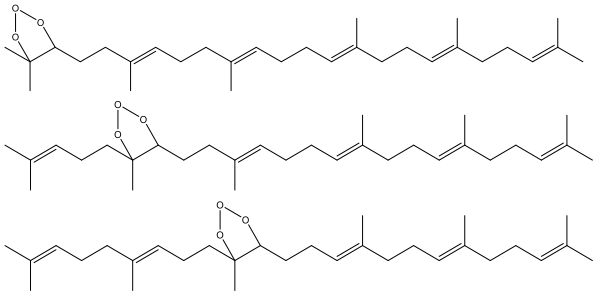
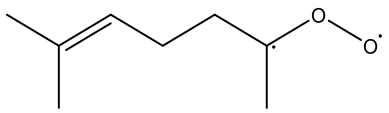
| | | | | | | |
|---|---|---|---|---|---|---|
| | 428 | k3 | N | N | N | ClHP13+O3->HP18 |
| | 429 | k4 | N | N | N | ClHP13->HP32 |
| | 430 | k5 | N | N | N | ClHP13+allR'C(=O)R''->HPSO13 |
| | 431 | k6 | N | N | N | ClHP13+allR'C(=O)OH->HPHP13 |
| | 432 | k2 | N | N | N | ClSO14+H2O->SO34 |
| | 433 | k3 | N | N | N | ClSO14+O3->SO34 |
| | 434 | k4 | N | N | N | ClSO14->SO38 |
| | 435 | k5 | N | N | N | ClSO14+allR'C(=O)R''->SOSO14 |
| | 436 | k6 | N | N | N | ClSO14+allR'C(=O)OH->SOHP14 |
| | 437 | k2 | N | N | N | ClSO15+H2O->SO36 |
| | 438 | k3 | N | N | N | ClSO15+O3->SO36 |
| | 439 | k4 | N | N | N | ClSO15->SO39 |
| | 440 | k5 | N | N | N | ClSO15+allR'C(=O)R''->SOSO15 |
| | 441 | k6 | N | N | N | ClSO15+allR'C(=O)OH->SOHP15 |
| | 442 | k5 | N | Y | Y | SO2+allCl->SOSO2 |
| | 443 | k5 | N | N | Y | HP2+allCl->HPSO2 |
| | 444 | k5 | N | Y | Y | SO3+allCl->SOSO3 |
| | 445 | k5 | N | N | Y | HP3+allCl->HPSO3 |
| | 446 | k5 | N | Y | Y | SO4+allCl->SOSO1 |
| | 447 | k5 | N | N | Y | HP4+allCl->HPSO1 |
| | 448 | k5 | N | Y | Y | SO6+allCl->SOSO5 |
| | 449 | k5 | N | N | Y | HP6+allCl->HPSO5 |
| | 450 | k5 | N | Y | Y | SO7+allCl->SOSO6 |
| | 451 | k5 | N | N | Y | HP7+allCl->HPSO6 |
| | 452 | k5 | N | Y | Y | SO8+allCl->SOSO7 |
| | 453 | k5 | N | N | Y | HP8+allCl->HPSO7 |
| | 454 | k5 | N | Y | Y | SO9+allCl->SOSO4 |
| | 455 | k5 | N | N | Y | HP9+allCl->HPSO4 |
| | 456 | k5 | N | Y | N | SO11+allCl->SOSO9 |
| | 457 | k5 | N | N | N | HP11+allCl->HPSO9 |
| | 458 | k5 | N | Y | N | SO12+allCl->SOSO10 |
| | 459 | k5 | N | N | N | HP12+allCl->HPSO10 |
| | 460 | k5 | N | Y | N | SO13+allCl->SOSO8 |
| | 461 | k5 | N | N | N | HP13+allCl->HPSO8 |
| | 462 | k5 | N | Y | N | SO15+allCl->SOSO12 |
| | 463 | k5 | N | N | N | HP15+allCl->HPSO12 |
| | 464 | k5 | N | Y | N | SO16+allCl->SOSO11 |
| | 465 | k5 | N | N | N | HP16+allCl->HPSO11 |
| | 466 | k5 | N | Y | N | SO18+allCl->SOSO13 |
| | 467 | k5 | N | N | N | HP18+allCl->HPSO13 |
| | 468 | k5 | N | Y | N | SO20+allCl->SOSO14 |
| | 469 | k5 | N | N | N | HP20+allCl->HPSO14 |
| | 470 | k5 | N | Y | N | SO23+allCl->SOSO15 |
| | 471 | k5 | N | N | N | HP23+allCl->HPSO15 |
| | 472 | k5 | N | N | N | SO36+allCl->SOSO15 |
| | 473 | k6 | N | N | N | SO21+allCl->SOHP1 |
| | 474 | k6 | N | N | N | HP21+allCl->HPHP1 |
| | 475 | k6 | N | N | N | SO22+allCl->SOHP3 |
| | 476 | k6 | N | N | N | HP22+allCl->HPHP3 |
| | 477 | k6 | N | N | N | SO24+allCl->SOHP4 |
| | 478 | k6 | N | N | N | HP24+allCl->HPHP4 |
| | 479 | k6 | N | N | N | SO25+allCl->SOHP7 |
| | 480 | k6 | N | N | N | HP25+allCl->HPHP7 |
| | 481 | k6 | N | N | N | SO26+allCl->SOHP6 |
| | 482 | k6 | N | N | N | HP26+allCl->HPHP6 |
| | 483 | k6 | N | N | N | SO27+allCl->SOHP9 |
| | 484 | k6 | N | N | N | HP27+allCl->HPHP9 |
| | 485 | k6 | N | N | N | SO28+allCl->SOHP8 |
| | 486 | k6 | N | N | N | HP28+allCl->HPHP8 |
| | 487 | k6 | N | N | N | SO29+allCl->SOHP10 |
| | 488 | k6 | N | N | N | HP29+allCl->HPHP10 |
| | 489 | k6 | N | N | N | SO30+allCl->SOHP12 |
| | 490 | k6 | N | N | N | HP30+allCl->HPHP12 |
| | 491 | k6 | N | N | N | SO31+allCl->SOHP11 |
| | 492 | k6 | N | N | N | HP31+allCl->HPHP11 |
| | 493 | k6 | N | N | N | SO32+allCl->SOHP13 |
| | 494 | k6 | N | N | N | HP32+allCl->HPHP13 |
| | 495 | k6 | N | N | N | SO38+allCl->SOHP14 |
| | 496 | k6 | N | N | N | SO39+allCl->SOHP15 |
| | 497 | k1 | N | N | N | SOSO4+O3->(1/2)((BR2)SO4+(BR1)ClSO1+(BR2)ClSO2+(BR1)SO2) |
| | 498 | k1 | N | N | N | HPSO4+O3->(1/2)((BR2)HP4+(BR1)ClHP1+(BR2)ClSO2+(BR1)SO2) |
| | 499 | k1 | N | N | N | SOHP4+O3->(1/2)((BR2)SO4+(BR1)ClSO1+(BR2)ClHP2+(BR1)HP2) |
| | 500 | k1 | N | N | N | HPHP4+O3->(1/2)((BR2)HP4+(BR1)ClHP1+(BR2)ClHP2+(BR1)HP2) |
| | 501 | k1 | N | N | N | SOSO5+O3->(1/2)((BR1)SO2+(BR2)ClSO2+(BR1)ClSO1+(BR2)SO4) |
| | 502 | k1 | N | N | N | HPSO5+O3->(1/2)((BR1)HP2+(BR2)ClHP2+(BR1)ClSO1+(BR2)SO4) |
| | 503 | k1 | N | N | N | SOHP5+O3->(1/2)((BR1)SO2+(BR2)ClSO2+(BR1)ClHP1+(BR2)HP4) |
| | 504 | k1 | N | N | N | HPHP5+O3->(1/2)((BR1)HP2+(BR2)ClHP2+(BR1)ClHP1+(BR2)HP4) |
| | 505 | k1 | N | N | N | SOSO6+O3->(1/2)((BR1)SO2+(BR2)ClSO2+(BR1)ClSO3+(BR2)SO3) |
| | 506 | k1 | N | N | N | HPSO6+O3->(1/2)((BR1)HP2+(BR2)ClHP2+(BR1)ClSO3+(BR2)SO3) |
| | 507 | k1 | N | N | N | SOHP6+O3->(1/2)((BR1)SO2+(BR2)ClSO2+(BR1)ClHP3+(BR2)HP3) |
| | 508 | k1 | N | N | N | HPHP6+O3->(1/2)((BR1)HP2+(BR2)ClHP2+(BR1)ClHP3+(BR2)HP3) |
| | 509 | k1 | N | N | N | SOSO7+O3->(1/2)((BR2)SO3+(BR1)ClSO3+(BR2)ClSO2+(BR1)SO2) |
| | 510 | k1 | N | N | N | HPSO7+O3->(1/2)((BR2)HP3+(BR1)ClHP3+(BR2)ClSO2+(BR1)SO2) |
| | 511 | k1 | N | N | N | SOHP7+O3->(1/2)((BR2)SO3+(BR1)ClSO3+(BR2)ClHP2+(BR1)HP2) |
| | 512 | k1 | N | N | N | HPHP7+O3->(1/2)((BR2)HP3+(BR1)ClHP3+(BR2)ClHP2+(BR1)HP2) |
| | 513 | k1×2 | N | N | N | SOSO8+O3->(1/4)((BR2)SO3+(BR2)SO8+(BR1)ClSO3+(BR1)ClSO7+(BR2)ClSO5+(BR2)ClSO2+(BR1)SO6+(BR1)SO2) |
| | 514 | k1×2 | N | N | N | HPSO8+O3->(1/4)((BR2)HP3+(BR2)HP8+(BR1)ClHP3+(BR1)ClHP7+(BR2)ClSO5+(BR2)ClSO2+(BR1)SO6+(BR1)SO2) |
| | 515 | k1×2 | N | N | N | SOHP8+O3->(1/4)((BR2)SO3+(BR2)SO8+(BR1)ClSO3+(BR1)ClSO7+(BR2)ClHP5+(BR2)ClHP2+(BR1)HP6+(BR1)HP2) |
| | 516 | k1×2 | N | N | N | HPHP8+O3->(1/4)((BR2)HP3+(BR2)HP8+(BR1)ClHP3+(BR1)ClHP7+(BR2)ClHP5+(BR2)ClHP2+(BR1)HP6+(BR1)HP2) |
| | 517 | k1×2 | N | N | N | SOSO9+O3->(1/4)((BR1)SO2+(BR1)SO6+(BR2)ClSO2+(BR2)ClSO5+(BR1)ClSO7+(BR1)ClSO3+(BR2)SO8+(BR2)SO3) |
| | 518 | k1×2 | N | N | N | HPSO9+O3->(1/4)((BR1)HP2+(BR1)HP6+(BR2)ClHP2+(BR2)ClHP5+(BR1)ClSO7+(BR1)ClSO3+(BR2)SO8+(BR2)SO3) |

| | | | | | |
|---|---|---|---|---|---|
| 519 | k1×2 | N | N | N | SOHP9+O3->(1/4)((BR1)SO2+(BR1)SO6+BR2)CISO2+(BR2)CISO5+(BR1)CIHP7+(BR1)CIHP3+(BR2)HP8+(BR2)HP3) |
| 520 | k1×2 | N | N | N | HPHP9+O3->(1/4)((BR1)HP2+(BR1)HP6+(BR2)CIHP2+(BR2)CIHP5+(BR1)CIHP7+(BR1)CIHP3+(BR2)HP8+(BR2)HP3) |
| 521 | k1×2 | N | N | N | SOSO10+O3->(1/4)((BR1)SO2+(BR2)SO7+(BR2)CISO2+(BR1)CISO6+(BR1)CISO6+(BR2)CISO2+(BR2)SO7+(BR1)SO2) |
| 522 | k1×2 | N | N | N | HPSO10+O3->(1/4)((BR1)HP2+(BR2)HP7+(BR2)CIHP2+(BR1)CIHP6+(BR1)CISO6+(BR2)CISO2+(BR2)SO7+(BR1)SO2) |
| 523 | k1×2 | N | N | N | SOHP10+O3->(1/4)((BR1)SO2+(BR2)SO7+(BR2)CISO2+(BR1)CISO6+(BR1)CIHP6+(BR2)CIHP2+(BR2)HP7+(BR1)HP2) |
| 524 | k1×2 | N | N | N | HPHP10+O3->(1/4)((BR1)HP2+(BR2)HP7+(BR2)CIHP2+(BR1)CIHP6+(BR1)CIHP6+(BR2)CIHP2+(BR2)HP7+(BR1)HP2) |
| 525 | k1×3 | N | N | N | SOSO11+O3->(1/6)((BR1)SO2+(BR2)SO7+(BR2)SO12+(BR2)CISO2+(BR1)CISO6+(BR1)CISO10+(BR1)CISO9+(BR2)CISO5+(BR2)CISO2+(BR2)SO11+(BR1)SO6+(BR1)SO2) |
| 526 | k1×3 | N | N | N | HPSO11+O3->(1/6)((BR1)HP2+(BR2)HP7+(BR2)HP12+(BR2)CIHP2+(BR1)CIHP6+(BR1)CIHP10+(BR1)CISO9+(BR2)CISO5+(BR2)CISO2+(BR2)SO11+(BR1)SO6+(BR1)SO2) |
| 527 | k1×3 | N | N | N | SOHP11+O3->(1/6)((BR1)SO2+(BR2)SO7+(BR2)SO12+(BR2)CISO2+(BR1)CISO6+(BR1)CISO10+(BR1)CIHP9+(BR2)CIHP5+(BR2)CIHP2+(BR2)HP11+(BR1)HP6+(BR1)HP2) |
| 528 | k1×3 | N | N | N | HPHP11+O3->(1/6)((BR1)HP2+(BR2)HP7+(BR2)HP12+(BR2)CIHP2+(BR1)CIHP6+(BR1)CIHP10+(BR1)CIHP9+(BR2)CIHP5+(BR2)CIHP2+(BR2)HP11+(BR1)HP6+(BR1)HP2) |
| 529 | k1×3 | N | N | N | SOSO12+O3->(1/6)((BR1)SO2+(BR1)SO6+(BR2)SO11+(BR2)CISO2+(BR2)CISO5+(BR1)CISO9+(BR1)CISO10+(BR1)CISO6+(BR2)CISO2+(BR2)SO12+(BR2)SO7+(BR1)SO2) |
| 530 | k1×3 | N | N | N | HPSO12+O3->(1/6)((BR1)HP2+(BR1)HP6+(BR2)HP11+(BR2)CIHP2+(BR2)CIHP5+(BR1)CIHP9+(BR1)CISO10+(BR1)CISO6+(BR2)CISO2+(BR2)SO12+(BR2)SO7+(BR1)SO2) |
| 531 | k1×3 | N | N | N | SOHP12+O3->(1/6)((BR1)SO2+(BR1)SO6+(BR2)SO11+(BR2)CISO2+(BR2)CISO5+(BR1)CISO9+(BR1)CIHP10+(BR1)CIHP6+(BR2)CIHP2+(BR2)HP12+(BR2)HP7+(BR1)HP2) |
| 532 | k1×3 | N | N | N | HPHP12+O3->(1/6)((BR1)HP2+(BR1)HP6+(BR2)HP11+(BR2)CIHP2+(BR2)CIHP5+(BR1)CIHP9+(BR1)CIHP10+(BR1)CIHP6+(BR2)CIHP2+(BR2)HP12+(BR2)HP7+(BR1)HP2) |
| 533 | k1×4 | N | N | N | SOSO13+O3->(1/8)((BR1)SO2+(BR1)SO6+(BR2)SO11+(BR2)SO15+(BR2)CISO2+(BR2)CISO5+(BR1)CISO9+(BR1)CISO12+(BR1)CISO12+(BR1)CISO9+(BR2)CISO5+(BR2)CISO2+(BR2)SO15+(BR2)SO11+(BR1)SO6+(BR1)SO2) |
| 534 | k1×4 | N | N | N | HPSO13+O3->(1/8)((BR1)HP2+(BR1)HP6+(BR2)HP11+(BR2)HP15+(BR2)CIHP2+(BR2)CIHP5+(BR1)CIHP9+(BR1)CIHP12+(BR1)CISO12+(BR1)CISO9+(BR2)CISO5+(BR2)CISO2+(BR2)SO15+(BR2)SO11+(BR1)SO6+(BR1)SO2) |
| 535 | k1×4 | N | N | N | SOHP13+O3->(1/8)((BR1)SO2+(BR1)SO6+(BR2)SO11+(BR2)SO15+(BR2)CISO2+(BR2)CISO5+(BR1)CISO9+(BR1)CISO12+(BR1)CIHP12+(BR1)CIHP9+(BR2)CIHP5+(BR2)CIHP2+(BR2)HP15+(BR2)HP11+(BR1)HP6+(BR1)HP2) |
| 536 | k1×4 | N | N | N | HPHP13+O3->(1/8)((BR1)HP2+(BR1)HP6+(BR2)HP11+(BR2)HP15+(BR2)CIHP2+(BR2)CIHP5+(BR1)CIHP9+(BR1)CIHP12+(BR1)CIHP12+(BR1)CIHP9+(BR2)CIHP5+(BR2)CIHP2+(BR2)HP15+(BR2)HP11+(BR1)HP6+(BR1)HP2) |
| 537 | k1 | N | N | N | SOSO15+O3->(1/2)((BR2)SO34+(BR1)CISO14+(BR2)CISO2+(BR1)SO2) |
| 538 | k1 | N | N | N | SOHP15+O3->(1/2)((BR2)SO34+(BR1)CISO14+(BR2)CIHP2+(BR1)HP2) |
| 539 | k6 | N | N | Y | Palmitic acid or skin oil acids+allCl->Paproducts |
| 540 | k1 | Only included in the clothing and KM-SUB-Skin-Clothing models. Not included in the gas phase. | | | Other double bonds+O3->CIDB+*Product* |
| 541 | k2 | | | | CIDB+H2O->carbonylproduct |
| 542 | k3 | | | | CIDB+O3->carbonylproduct |
| 543 | k4 | | | | CIDB->skin oil acids |
| 544 | k5 | | | | CIDB+allR'C(=O)R''->*Product* |
| 545 | k5 | | | | carbonylproduct+zallCl->*Product* |

**Table S2:** The names, structures, SMILES and volatility information for squalene ozonolysis products which have been mentioned in the main text.

| **Abbreviation or name used in the mechanism** | **Other names** | **Structure** | **SMILES** | **Can it partition to the gas-phase** |
|---|---|---|---|---|
| acetone | N/A |  | O=C(C)C | Yes |
| 6-MHO | 6-methyl-5-hepten-2-one |  | C(C)(C)=CCCC(=O)(C) | Yes |
| GA | geranyl acetone |  | C(C)(C)=CCCC(C)=CCCC(=O)(C) | Yes |
| 4-OPA | 4-oxopentanal |  | O=C(C)CCC=O | Yes |
| 4-MON | 4-methyl-8-oxo-4-nonenal |  | C(C)(=CCCC(=O)(C))CCC=O | Yes |
| 4-MOD | 4-methyl-4-octene-1,8-dial |  | C(C)(=CCCC(=O))CCC=O | Yes |
| 1,4 butanedial | succinic dialdehyde |  | O=CCCC=O | Yes |

| | | | | |
|---|---|---|---|---|
| CA1 | levulinic acid or 4-oxopentanoic acid |  | O=C(O)CCC(=O)(C) | Yes[a] |
| CA2 | 4-oxobutanoic acid |  | O=C(O)CCC=O | Yes |
| CA6 | C14 aldehydic acid |  | O=CCCC=C(C)CCC=C(C)CCC(=O)(O) | No |
| CA7 | C14 aldehydic acid |  | O=CCCC(C)=CCCC=C(C)CCC(=O)(O) | No |
| CA8 | C14 aldehydic acid |  | O=CCCC(C)=CCCC(C)=CCCC(=O)(O) | No |
| CA14 | C27-acid |  | O=C(O)CCC(C)=CCCC(C)=CCCC=C(C)CCC=C(C)CCC=C(C)C | No |
| CA15 | succinic acid |  | O=C(O)CCC(=O)O | Yes[a] |
| HK1 | hydroxyacetone |  | O=C(C)CO | Yes |
| HK2 | 5-hydroxy-4-oxo-pentanal |  | O=C(CCC(=O))CO | Yes |
| HK3 | 6-methyl-5-ene-2-oxo-heptanol |  | C(C)(C)=CCCC(=O)CO | Yes |
| HK5 | OH-geranyl acetone |  | CC(C)=CCCC(C)=CCCC(=O)(CO) | Yes[b] |

| | | | | |
|---|---|---|---|---|
| TOP | C22-aldehyde |  | C(C)(C)=CCCC(C)=CCCC(C)=CCCC=C(C)CCC=O | No |
| TOT | C27-aldehyde |  | C(C)(C)=CCCC(C)=CCCC(C)=CCCC=C(C)CCC=C(C)CCC=O | No |
| Product A | C14-dialdehyde |  | C(C)(=CCCC(C)=CCCC(=O))CCC=O | Yes[b] |
| Product B | C14-dialdehyde |  | C(C)(=CCCC=C(C)CCC(=O))CCC=O | Yes[b] |
| $C_{30,SOZ}$ | C30-secondary ozonide |  | CC(C1CCC(C)=CCCC(C)=CCCC=C(CCC=C(CCC=C(C)C)C)C)(OOO1)C and CC(C)=CCCC(C1CCC(C)=CCCC=C(CCC=C(CCC=C(C)C)C)C)(OOO1)C and CC(C)=CCCC(C)=CCCC(C1CCC=C(CCC=C(CCC=C(C)C)C)C)(OOO1)C | No |
| CI2 | N/A |  | N/A | No |

[a] Treated as non-volatile in Figures 3 and 4 as this was measured in the bulk and it otherwise completely partitions to the gas-phase in the model.

[b]Treated as non-volatile under the conditions in Figures 5, 6 and S5.

**Table S3:** Parameters used in the kinetic models to reproduce experimental measurements shown in Figures 1-4 and S3.

| Parameter | Parameter description | Value | | | | | Comments |
|---|---|---|---|---|---|---|---|
| | | **Parameter set 1 (used for Fig. 2)** | **Parameter set 2 (used for Fig.s 3 and 4)** | **Parameter set 3 (used for Fig. 5 changing RH experiments)** | **Parameter set 4 (used for Fig. 5, stable RH experiments)** | **Parameter set 5 (used for Fig. S5, KM-SUB-Skin-Clothing)** | |
| $T$ (°C) | Temperature | Room temperature (assumed to be 25 °C) | Room temperature (assumed to be 25 °C) | 27.4 – 28.3 (assumed to be 27.5 °C for modeling purposes) | | 23 | |
| $RH$ (%) | Relative humidity | See panels (a) and (e) | 0 | See panels (a) and (b) | | 22.5 (average of 20 -25 % measured range) | From experimental measurements |
| $k_{1,bulk}$ ($cm^3$ $s^{-1}$) | Second order bulk rate coefficient of ozone with double bonds | $2.2 \times 10^{-17}$ | | | | | Same as Lakey et al.[2, 3] where measurements were able to be reproduced reasonably well using this value. Note that this value is about a factor of 10 smaller than used in Heine et al.[4] which is based on work reported in Razumovskii and Lisitsyn[5] and is the only measured rate coefficient of squalene with ozone to our knowledge. However, the rate coefficient was measured in chloroform, and it is possible that it would be different in other substrates such as pure squalene and skin oil. Increasing the rate coefficient caused a larger discrepancy between the value of $K_{O3}$ used in the model and the value determined by molecular dynamics simulations (see below). |

| | | | | | | |
|---|---|---|---|---|---|---|
| | | | | | | $k_{1,bulk}$ and $K_{O3}$ were codependent. Note that as more measurements or theoretical calculations of the rate coefficient of squalene with ozone and the partitioning coefficient of ozone into squalene and skin oil become available, we will be able to update the model and ideally resolve the apparent discrepancy between this rate coefficient and the partitioning coefficient of ozone. |
| $k_{2,bulk}$ ($cm^3$ $s^{-1}$) | Second order bulk rate coefficient of CIs with water | $5.7 \times 10^{-19}$ | Insensitive (dry experiments) | $5.7 \times 10^{-19}$ | $5.7 \times 10^{-19}$ | Determined by the MCGA and optimization. Within the range given in the literature. Note that this rate coefficient and $K_{H2O}$ are codependent and that the same results can be obtained if one of these parameters is increased by a certain factor by decreasing the other one by the same factor. |
| $k_{3,bulk}$ ($cm^3$ $s^{-1}$) | Second order bulk rate coefficient of CIs with ozone | $1.0 \times 10^{-14}$ | Insensitive in the range of 0 - $1.0 \times 10^{-14}$. | Insensitive in the range of 0 - $1.0 \times 10^{-14}$. | Insensitive in the range of 0 - $1.0 \times 10^{-14}$. | Determined by the MCGA and optimization. The original MCGA range was set to be fast based on the theoretically determined value of ~$1 \times 10^{-12}$ $cm^3$ $s^{-1}$ in the gas phase.[6] However, the bulk rate may be smaller (see text). |
| $k_{4,bulk}$ ($s^{-1}$) | First order bulk rate coefficient for the rearrangement of CIs | 3 | 3 | 0.44 | 0.44 | Determined by the MCGA and optimization. Very important for fitting the concentrations of carboxylic acids and hydroxyketones. |
| $k_{5,bulk}$ ($cm^3$ $s^{-1}$) | Second order bulk rate coefficient of CIs with carbonyls | $8.5 \times 10^{-20}$ | $1.7 \times 10^{-19}$ | $7.6 \times 10^{-19}$ | $1.0 \times 10^{-20}$ | Determined by the MCGA and optimization. All values are within two orders of magnitude of those used in Heine et al.[4] |
| $k_{6,bulk}$ ($cm^3$ $s^{-1}$) | Second order bulk rate coefficient of CIs with carboxylic acids | $2.7 \times 10^{-20}$ | $2.7 \times 10^{-20}$ | $2.7 \times 10^{-20}$ | $2.7 \times 10^{-20}$ | Determined by fitting data in Figure 4 and set to the same value in other models. |
| $k_{1,gas}$ ($cm^3$ $s^{-1}$) | Second order gas phase rate coefficient of ozone with double bonds | $2.0 \times 10^{-15}$ | Insensitive | $4.0 \times 10^{-16}$ | $4.0 \times 10^{-16}$ | Determined by the MCGA and optimization. All within a factor of 5 of the values used in Lakey et al.[2, 3] which were based on EPIWIN gas-phase rate constants. |
| $k_{2,gas}$ ($cm^3$ $s^{-1}$) | Second order gas phase rate coefficient of CIs with water | $2.5 \times 10^{-16}$ | Insensitive | $4.4 \times 10^{-16}$ | $4.4 \times 10^{-16}$ | Determined by the MCGA and optimization. Within the range given in the literature.[7] |
| $k_{3,gas}$ ($cm^3$ $s^{-1}$) | Second order gas phase rate coefficient of CIs with ozone | $1.0 \times 10^{-14}$ | Insensitive | $2.4 \times 10^{-14}$ | $2.4 \times 10^{-14}$ | Determined by the MCGA and optimization. Theoretical calculations have previously |

| | | | | | | |
|---|---|---|---|---|---|---|
| | | | | | | predicted fast gas phase rate coefficients (~ 1 × $10^{-12}$ $cm^3$ $s^{-1}$)[6] so the rate was fixed to be relatively fast and within 2 orders of magnitude of this value in the MCGA. |
| $k_{4,gas}$ ($s^{-1}$) | First order gas phase rate coefficient for the rearrangement of CIs | 1 | Insensitive | 1.1 | 1.1 | Determined by the MCGA and optimization. |
| $k_{5,gas}$ ($cm^3$ $s^{-1}$) | Second order gas phase rate coefficient of CIs with carbonyls | 1.3 × $10^{-19}$ | Insensitive | Insensitive | Insensitive | Determined by the MCGA and optimization. Assumed to be slow like in the bulk. |
| $k_{6,gas}$ ($cm^3$ $s^{-1}$) | Second order gas phase rate coefficient of CIs with carboxylic acids | Insensitive | Insensitive | Insensitive | Insensitive | N/A |
| $BR_{bulk}$ | Branching ratio of primary and secondary carbonyls in the bulk for reaction 1 | BR1 = 0.2, BR2 =1.8 (i.e. for every double bond which reacts with ozone on average (0.2/ 2) primary CIs and secondary carbonyls and (1.8/ 2) secondary CIs and primary carbonyls form) | | | | Fixed to be the same as for Heine et al. [4] |
| $BR_{gas}$ | Branching ratio of primary and secondary carbonyls in the gas phase for reaction 1 | BR1 = 1, BR2 =1 (i.e. for every double bond which reacts with ozone on average (1/ 2) primary CIs and secondary carbonyls and (1/ 2) secondary CIs and primary carbonyl form) | | | | Expected to be approximately equal. [4, 8] |
| $K_{O3}$ (mol $cm^{-3}$ $atm^{-1}$) | Equilibrium partitioning coefficient of ozone from the gas phase into a bulk liquid phase | 6.4 × $10^{-4}$ | | | | Determined by the MCGA and optimization. Fixed in the MCGA to be approximately a maximum of a factor of 5 different from the molecular dynamic value of 3.3 × $10^{-3}$ mol $cm^{-3}$ $atm^{-1}$.[9] |
| $K_{H2O}$ (mol $cm^{-3}$ $atm^{-1}$) | Equilibrium partitioning coefficient of water from the gas phase into a bulk liquid phase | O:C ratio × 0.18 | Dry experiments | 3.2 × $10^{-4}$ | 4.2 × $10^{-4}$ | Determined by the MCGA and optimization for skin oil and clothing. AIOMFAC calculations determined that the partitioning of water into pure squalene should be negligible but would increase as oxygenated molecules formed and the kinetic model is consistent with the results. The partitioning of water into skin oil is expected to be controlled by the concentration of molecules such as glycerols in the skin and we therefore assume a constant partitioning value.[10] |
| $K_{clothing,4MOD}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of 4MOD for clothing | Partitioning coefficients between the gas phase and particles or skin oil were | | 105 | 105 | Determined by the MCGA and optimization but also constrained to be generally consistent with the saturation vapor pressures of the |

| | | | | | |
|---|---|---|---|---|---|
| | | insensitive parameters when trying to reproduce these experiments as under the experimental conditions the concentration of volatile products in the particles or film will be almost negligible. This is in agreement with Heine et al. for the pure squalene particles. | | | molecules (e.g. acetone has the lowest partitioning coefficient and geranyl acetone has the highest one).[4] Note that all of the hydroxy ketones have slightly higher partitioning coefficients compared to other molecules than may be expected based solely on the saturation vapor pressures of the molecules but the reason for this is unknown. [4] |
| $K_{clothing,4MON}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of 4MON for clothing | | 35.0 | 35.0 | |
| $K_{clothing,4OPA}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of 4OPA for clothing | | 0.40 | 0.40 | |
| $K_{clothing,6MHO}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of 6MHO for clothing | | 0.60 | 0.60 | |
| $K_{clothing,CA1}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of CA1 for clothing | | 18.3 | 18.3 | |
| $K_{clothing,CA2}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of CA2 for clothing | | 27.1 | 27.1 | |
| $K_{clothing,GA}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of geranyl acetone for clothing | | $1.3 \times 10^3$ | 325 | |
| $K_{clothing,HK1}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of HK1 for clothing | | 1.18 | 1.18 | |
| $K_{clothing,HK2}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of HK2 for clothing | | 52.7 | 52.7 | |
| $K_{clothing,HK3}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of HK3 for clothing | | 40.2 | 40.2 | |
| $K_{clothing,acetone}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of acetone for clothing | | 0.0013 | 0.0013 | |
| $K_{clothing,1,4butanedial}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of 1,4 butanedial for clothing | | 0.13 | 0.13 | |
| $K_{skin,4MOD}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of 4MOD for skin | | N/A | 0.27 | From von Domaros et al. [9] |
| $K_{skin,4MON}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of 4MON for skin | | N/A | 0.47 | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| $K_{skin,4OPA}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of 4OPA for skin | | | N/A | | $7.5 \times 10^{-3}$ | |
| $K_{skin,6MHO}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of 6MHO for skin | | | N/A | | 0.083 | |
| $K_{skin,CA1}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of CA1 for skin | | | N/A | | 0.37 | Assumed to be about a factor of 50 lower than for clothing based on the values for the other molecules. |
| $K_{skin,CA2}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of CA2 for skin | | | N/A | | 0.54 | |
| $K_{skin,GA}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of geranyl acetone for skin | | | N/A | | 5.8 | From von Domaros et al. [9] |
| $K_{skin,HK1}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of HK1 for skin | | | N/A | | 0.024 | Assumed to be about a factor of 50 lower than for clothing based on the values for the other molecules. |
| $K_{skin,HK2}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of HK2 for skin | | | N/A | | 1.05 | |
| $K_{skin,HK3}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of HK3 for skin | | | N/A | | 0.80 | |
| $K_{skin,acetone}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of acetone for skin | | | N/A | | $5.4 \times 10^{-4}$ | From von Domaros et al. [9] |
| $K_{skin,1,4butanedial}$ (mol $cm^{-3}$ $atm^{-1}$) | Partitioning coefficient of 1,4 butanedial for skin | | | N/A | | $2.4 \times 10^{-3}$ | |
| [Sq] ($cm^{-3}$) | Initial squalene concentration | $1.3 \times 10^{21}$ | $1.3 \times 10^{21}$ (pure squalene, fig. 3) $1.3 \times 10^{20}$ (skin oil, fig. 4) | $1.6 \times 10^{18}$ | $6.3 \times 10^{17}$ | $1.3 \times 10^{20}$ (skin oil) $6.5 \times 10^{18}$ (stratum corneum) $5.0 \times 10^{18}$ (in clothing skin oil and other substances) | For pure squalene the values are based on the density and molecular weight of squalene. Skin oil should consist of approximately 10% squalene,[10] so the concentration of pure squalene was divided by 10. Concentrations in clothing were determined using the MCGA and optimization. Skin oil concentrations are kept constant as replenishment is assumed. |
| [CA] ($cm^{-3}$) | Initial carboxylic acid concentration | 0 | 0 (pure squalene, fig.3) $7.9 \times 10^{19}$ (palmitic acid fig. 4) $2.4 \times 10^{20}$ (other acids, fig. 4) | $4.0 \times 10^{18}$ | $1.6 \times 10^{18}$ | $3.3 \times 10^{20}$ (skin oil) $3.3 \times 10^{20}$ (stratum corneum) $1.3 \times 10^{19}$(in clothing skin | Assumed to be 2.5 times the concentration of squalene.[10] Palmitic acid is expected to account for approximately a quarter of the carboxylic acids in skin oil.[10] Skin oil concentrations are kept constant as replenishment is assumed. |

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| | | | | | | oil and other substances) | |
| [OS] ($cm^{-3}$) | Initial concentration of other reactive double bonds | 0 | 0 | $1.3 \times 10^{19}$ | $1.8 \times 10^{18}$ | $6.5 \times 10^{19}$ (skin oil) $6.5 \times 10^{19}$(stratum corneum) $2.5 \times 10^{18}$ (in clothing skin oil and other substances) | Determined by the MCGA and optimization. Skin oil concentrations are kept constant as replenishment is assumed. |
| $V_{chamber}$ ($m^3$) | Volume of the chamber or room | Note: The particle concentration was assumed to be 1000 µg $m^{-3}$ with the initial diameter of the particles being 300 nm and a spherical assumption assumed. | Not used in the model. Note that the model was set up so that all volatile molecules partitioned to the gas phase. | 22 | 22 | 28.5 | From measurements |
| $S$ ($cm^2$) | Initial surface area of the particles (fig 2) or surface area of the clothing (figs. 5 and S5) | | | 4 t-shirts: 6000 $cm^2$ per t-shirt | 4 t-shirts: 6000 $cm^2$ per t-shirt | 2 people: $3.4 \times 10^4$ | Same as Lakey et al. |
| $BL_{O3}$ (cm) | Boundary layer next to clothing | N/A | N/A | 0.65 | 1.01 | 1.2 | Determined by the MCGA and optimization |
| $T_{clothing}$ (mm) | Thickness of the clothing | N/A | | 1 | 1 | 1 | Same as Lakey et al. [2] |
| $T_{film}$ (nm) | Thickness of the film | N/A | Squalene film = 12<br>Skin oil film = 39 | N/A | N/A | N/A | A density of 0.858 g $cm^{-3}$ is assumed. For the squalene film 40 ng were deposited on a 4 $mm^2$ capillary.[11] The skin oil film was produced by people touching the capillary. A typical fingerprint has been estimated to weigh |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | | | | | | 10 μg[12] and has a surface area of approximately 3 $cm^2$. |
| *AER* ($h^{-1}$) | air exchange rate | N/A | | 3 | 3 | 1 | From measurements |
| $P_{O3}$ (ppb $cm^{-3}$ $s^{-1}$) | Ozone production rate | N/A (constant ozone concentrations set in the model. | N/A (a constant ozone concentration of 50 ppb was set in the model) | $8.33 \times 10^{-2}$ | $8.33 \times 10^{-2}$ | $9.2 \times 10^{-3}$ | To maintain the correct ozone concentration in the empty chamber when considering air exchange. |
| *t* (s) | measurement timepoint | 37 | Continuous (see figures) | Continuous (see figures) | Continuous (see figures) | Continuous (see figures) | From measurements |
| $\varepsilon$ | porosity factor of the clothing | N/A | | 0.6 | 0.6 | 0.6 | Same as Lakey et al. [2] |
| $V_{air}$ | volume fraction of air in the clothing | N/A | | 0.75 | 0.75 | 0.75 | Same as Lakey et al. [2] |
| $V_{oil+other}$ (%) | volume percentage of skin oil and other substances in the clothing | N/A | | 3.8 | 16.7 | 1 | Determined by the MCGA and optimization |
| $[LS]_{clothing}$ ($cm^{-3}$) | Effective conc. of laundering species in the clothing skin oil and other substances | N/A | | Set to zero for simplicity | | | N/A |
| $k_{SO,cl}$ and $k_{cl,SO}$ (cm $s^{-1}$) | Contact transfer rate from skin oil to clothing or clothing to skin oil | N/A | | N/A | N/A | $2.8 \times 10^{-10}$ | Same as in Lakey et al.[2] |
| $k_{OS}$ ($cm^3$ $s^{-1}$) | Rate coefficient of other reactive species with ozone | N/A | | same as $k_{1,bulk}$ | same as $k_{1,bulk}$ | same as $k_{1,bulk}$ | N/A |
| $k_{O3,wall}$ ($s^{-1}$) | First order rate coefficient of ozone loss to the chamber walls | N/A | | $9.3 \times 10^{-5}$ | $9.3 \times 10^{-5}$ | Assumed to be negligible (for simplicity) | Values were assumed. |
| *Other parameters* | For example, gas phase and bulk diffusion coefficients | Values can be found in previous publications.[2, 3] | | | | | |

**Table S4:** System of squalene and 19 squalene ozonolysis products used for the water uptake predictions with the AIOMFAC-LLE model. The mole fractions of the different compounds were obtained from a kinetic reaction simulation under the following conditions: $T$ = 298 K, RH = 70%, $O_3$ exposure = $3\times10^{15}$ molecules $cm^3$ s.

| No. | Component | SMILES[a] | *M* [g/mol] | Mole fraction (dry mixture) | *A* coeff. [b] | *B* coeff. [b] | AIOMFAC subgroups |
|---|---|---|---|---|---|---|---|
| 2 | Squalene | C/C(C)=C\CC/C(C)=C/CC/C(C)=C/CC/C=C(CC/C=C(C)/CC/C=C(C)\C)\C | 410.73 | 5.18% | 4.51490 | -86630.36 | (CH3)_8 (CH2)_10 (CH=C)_6 |
| 3 | SqualeneO3p01 | C/C(CCC1OC(C)(C)OO1)=C\CC/C=C(CC/C=C(C)/CCC=O)\C | 364.53 | 2.40% | 4.75983 | -80542.76 | (CH3)_5 (CH2)_7 (CH=C)_3 (CH2O[ether])_1 (CHO[ald]_1 (CHOOC[perox])_1 |
| 4 | SqualeneO3p02 | C/C(CCC1OC(C)(C)OO1)=C\CC/C=C(CC/C=C(C)/CC/C=C(C)/C)\C | 390.61 | 1.28% | 4.75130 | -81843.42 | (CH3)_7 (CH2)_7 (CH=C)_4 (CH2O[ether])_1 (CHOOC[perox])_1 |
| 5 | SqualeneO3p03 | C/C(CCC=O)=C\CC/C=C(C)/CC/C=C(CCC=O)\C | 290.45 | 0.72% | 4.10138 | -69921.74 | (CH3)_3(CH2)_8(CH=C)_3(CHO)_2 |
| 6 | SqualeneO3p04 | C/C(CCC=O)=C\CC/C=C(C)/CC/C=C(CC/C=C(C)/C)\C | 316.53 | 0.76% | 4.20853 | -71222.40 | (CH3)_5(CH2)_8(CH=C)_4(CHO)_1 |
| 7 | SqualeneO3p05 | C/C(CCC1OC(C)(OO1)C)=C\CCC2(C)OC(C)(OO2)C | 316.39 | 8.76% | 4.72699 | -62648.57 | (CH3)_6(CH2)_2(CH=C)_1(CH2O[ether])_2 (CHOOC[perox])_1(COOC[perox])_1 |
| 8 | SqualeneO3p06 | C/C(CCC1OC(C)(OO1)C)=C\CCC2OC(C)(OO2)C | 302.36 | 6.66% | 4.67280 | -62949.18 | (CH3)_5(CH2)_2(CH=C)_1(CH2O[ether])_2 (CHOOC[perox])_2 |
| 9 | SqualeneO3p07 | C/C(CC/C=C(CCC=O)\C)=C\CCC1OC(C)(OO1)C | 296.41 | 6.78% | 4.44493 | -66435.46 | (CH3)_4 (CH2)_5 (CH=C)_2 (CHO)[ald])_1 (CH2O[ether])_1 (CHOOC[perox])_1 |
| 10 | SqualeneO3p08 | O=C(C)CC/C=C(CCC1OC(CCC=O)(OO1)C)\C | 284.35 | 3.54% | 4.53302 | -67956.26 | (CH3)_2 (CH2)_5 (CH=C)_1 (CH3CO[ket])_1 (CHO[ald])_1 (CHOOC)_1 (CH2O[ether])_1 |
| 11 | SqualeneO3p09 | CC1(CCC=O)OC(CC/C=C(CC/C=C(CC/C=C(C)\C)\C)\C)OO1 | 364.53 | 3.48% | 4.75983 | -80542.76 | (CH3)_5(CH2)_7(CH=C)_3 (CHO[ald])_1 (CHOOC)_1 (CH2O[ether])_1 |
| 12 | SqualeneO3p10 | O=CCC/C=C(CC/C=C(C)/CC/C=C(C)\C)\C | 248.41 | 2.08% | 3.89363 | -57115.10 | (CH3)_4(CH2)_6(CH=C)_3(CHO)_1 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 13 | SqualeneO3p11 | O=CCC/C(C)=C/CC1OC(OO1)(C)CCC=O | 256.30 | 7.56% | 4.40706 | -62313.34 | (CH3)_2(CH2)_5(CH=C)_1 (CHO[ald])_2 (CHOOC)_1 (CH2O[ether])_1 |
| 14 | SqualeneO3p12 | O=CCCC(OO1)(C)OC1(C)CC/C=C(CCC=O)\C | 284.35 | 5.34% | 4.52423 | -64834.19 | (CH3)_3(CH2)_5(CH=C)_1 (CHO[ald])_2 (COOC)_1 (CH2O[ether])_1 |
| 15 | SqualeneO3p13 | O=CCCC(OO1)(C)OC1CCC2OC(CCC=O)(C)O O2 | 318.32 | 2.55% | 5.15360 | -74455.16 | (CH3)_2(CH2)_4 (CHO[ald])_2 (CHOOC)_2 (CH2O[ether])_2 |
| 16 | SqualeneO3p14 | CC(CC/C=C(C)\C)(OO1)OC1CCC2OC(CC/C=C (C)/C)(C)OO2 | 370.49 | 5.52% | 4.98770 | -77056.48 | (CH3)_6 (CH2)_4 (CH=C)_2 (CHOOC)_2 (CH2O[ether])_2 |
| 17 | SqualeneO3p15 | CC(CC/C=C(CC/C=C(C)\C)/C)(OO1)OC1CCC2( C)OC(CC/C=C(CC/C=C(C)/C)\C)(C)OO2 | 520.75 | 4.74% | 5.67169 | -104970.47 | (CH3)_9 (CH2)_8 (CH=C)_4 (CHOOC)_1 (COOC)_1 (CH2O[ether])_2 |
| 18 | SqualeneO3p16 | O=CCCC1OOC(CCC2OC(OO2)CCC=O)(C)O1 | 304.30 | 8.79% | 5.09941 | -74755.77 | (CH3)_1(CH2)_4 (CHO)[ald])_2 (CHOOC[perox])_2 (CH2O[ether])_2 |
| 19 | SqualeneO3p17 | O=C(C)CCC1OOC(CCC2OC(OO2)CCC(C)=O)( C)O1 | 332.35 | 12.60% | 5.22537 | -80398.69 | (CH3)_1 (CH2)_4 (CH3CO)_2 (CHOOCH[perox])_1 (CHOOC[perox])_1 (CH2O[ether])_2 |
| 20 | SqualeneO3p18 | CC1(CCC2OC(OO2)(C)CCC3OC(CC/C=C(C)/C) (C)OO3)OC(OO1)(C)C/C=C(C)\C | 486.60 | 6.22% | 5.84511 | -97362.07 | (CH3)_8 (CH2)_5 (CH=C)_2 (CHOOC)_2 (COOC)_1 (CH2O[ether])_3 |
| 21 | SqualeneO3p19 | CC1(CCC2OC(OO2)(C)CCC3OC(CC/C(C)=C/C CC=O)OO3)OC(OO1)(C)CCC=O | 502.56 | 5.04% | 6.46696 | -111990.12 | (CH3)_4 (CH2)_7 (CH=C)_1 (CHO[ald])_2 (CHOOCH)_1 (CHOOC)_1 (COOC)_1 (CH2O[ether])_3 |

[a] The two sides of the secondary ozonides which contain different functional groups and were treated separately in the kinetic model were combined to create molecules from which SMILES could be generated.

[b] $A$ and $B$ are the coefficients for the temperature-dependent liquid-state pure component saturation vapor pressure, $p_i^0$, as predicted by the EVAPORATION model [13] using the following expression: $\log_{10}\left(\frac{p_i^0}{[\text{atm}]}\right) = A_i + \frac{B_i}{T^{1.5}}$, where $T$ is the absolute temperature in K.

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