

S1. Materials and reagents

- 5 Ultratrace H₂O₂ (≥30%), no stabilizers added, (1R,2S,5R)-(-)-Menthol (≥99%), (+)-Borneol (≥98%), water for LC/MS (gradient-grade) were purchased from Sigma-Merck (Schnelldorf, Germany). (+)-Fenchol was purchased from Alfa Aesar; Chemat (Gdańsk, Poland). (+)-Fenchone (>98%), and (1S,2S,5S)-(-)-2-hydroxy-3-
- 10 pinanone were purchased from TCI. Camphor (>99.76%) and (±)Camphorquinone (>99.90%) were purchased from Ambeed. Menthone (≥97%), (±)-exo,exo-2,3-Camphanediol (≥97%), and Dimethyl phthalate (≥99%) were purchased from Sigma-Merck (Schnelldorf, Germany). Sodium chloride and extra pure were purchased from Thermo. Ethyl acetate (≥99.5%), was purchased from Honeywell (Avantor Performance Materials, Gliwice, Poland).
- Ultra-high purity (UHP) gases: helium (≥ 99.9999%) was supplied by Multax (Stare Babice, Poland), methane (≥ 99.9995%) was purchased from AirProducts (Warsaw, Poland), and ammonia (99.999%) was obtained from Air Liquid (Warsaw, Poland).

S2. Kinetic box models

- Reactions 1-5 in Table S2-S4 describe the generation of OH via photolysis of H₂O₂ (Tan et al., 2009). The k values of Reactions 1-5 in Tables S2-S4 reflect the first-order rate of disappearance of H₂O₂. This value was obtained by fitting the model data to the experimentally measured rate of H₂O₂ photolysis, which was obtained by visual titration with potassium permanganate. The majority of k values used in the models were predicted with the structure-activity relationship (SAR) (Witkowski et al., 2024).

Table S1. Reactions used in the model for the aqueous OH oxidation of fenchol (R1).

Reaction number	Reaction	k (M ⁻¹ s ⁻¹)
1	H ₂ O ₂ = OH + OH	5.4×10 ⁻⁶
2	OH + H ₂ O ₂ = HO ₂ + H ₂ O	2.7×10 ⁷
3	HO ₂ +H ₂ O ₂ =OH + H ₂ O	3.7
4	HO ₂ + HO ₂ = H ₂ O ₂ + O ₂	8.3×10 ⁵
5	OH + HO ₂ = H ₂ O+O ₂	7.1×10 ⁹
6	FCH + OH = Pr1	8.0×10 ⁷
7	FCH + OH = Fenchone	5.6×10 ⁸
8	FCH + OH = P1	3.8×10 ⁸
9	FCH + OH = P2	2.0×10 ⁹
10	P1 + OH = Pr2	6.0×10 ⁷
11	P1 + OH = P3	2.9×10 ⁹
12	P3 + OH = Pr3	2.0×10 ⁹
13	P2 + OH = Pr4	5.0×10 ⁷
14	P2 + OH = P4	4.1×10 ⁹

15	P4 + OH = Pr5	2.0×10^8
18	P4 + OH = P6	1.2×10^9
19	P4 + OH = P5	1.4×10^9
20	P6 + OH = Pr6	6.0×10^7
21	P6 + OH = P7	2.8×10^9
22	P5 + OH = Pr7	1.8×10^9
23	P7 + OH = Pr8	1.6×10^9
24	Fenchone + OH = Pr9	1.9×10^9
25	Fenchone + OH = P8	3.2×10^8
26	Fenchone + OH = P10	2.1×10^8
27	Fenchone + OH = P9	2.7×10^8
28	P8 + OH = Pr10	1.5×10^9
29	P10 + OH = Pr11	3.3×10^9
30	P9 + OH = Pr12	3.0×10^9

20 **Table S2** Reactions used in the model for the aqueous OH oxidation of borneol (R2)

Reaction number	Reaction	k (M ⁻¹ s ⁻¹)
1	H2O2 = OH + OH	5.3×10^{-6}
2	OH + H2O2 = HO2 + H2O	2.7×10^7
3	HO2+H2O2=OH + H2O	3.7
4	HO2 + HO2 = H2O2 + O2	8.3×10^5
5	OH + HO2 = H2O+O2	7.1×10^9
6	BNL+ OH = Pr1	9.0×10^7
7	BNL + OH = Camphor	6.6×10^8
8	BNL + OH = P1	5.3×10^8
9	BNL + OH = P2	4.9×10^8
10	BNL + OH = P6	1.2×10^9
11	BNL + OH = P7	3.3×10^8
12	BNL + OH = P12	6.0×10^7
13	P12 + OH = Pr2	2.6×10^9
14	P1 + OH = Pr3	2.6×10^9
15	P6 + OH = Pr4	2.4×10^9
18	P2 + OH = Pr5	8.0×10^7
19	P2 + OH = P3	3.6×10^9
20	P7 + OH = Pr6	1.0×10^8
21	P7 + OH = P8	3.2×10^9

22	P3 + OH = Pr7	9.0×10^7
23	P3 + OH = P4	8.8×10^8
24	P3 + OH = P5	7.9×10^8
25	P4 + OH = Pr8	1.7×10^9
26	P5 + OH = Pr9	1.4×10^9
27	P8 + OH = Pr10	9.0×10^7
28	P8 + OH = P9	7.5×10^8
29	P8 + OH = P10	6.7×10^8
30	P9 + OH = Pr11	1.7×10^9
31	P10 + OH = Pr12	1.4×10^9
32	Camphor + OH = Pr13	1.9×10^9
33	Camphor + OH = CA	2.4×10^8
34	Camphor + OH = P14	2.9×10^8
35	CA + OH = Pr14	2.0×10^9
36	P14 + OH = Pr15	2.0×10^9

Table S3 Reactions used in the model for the aqueous OH oxidation of menthol (R3)

Reaction number	Reaction	k (M ⁻¹ s ⁻¹)
1	H2O2 = OH + OH	4.0×10^{-6}
2	OH + H2O2 = HO2 + H2O	2.7×10^7
3	HO2+H2O2=OH + H2O	3.7
4	HO2 + HO2 = H2O2 + O2	8.3×10^5
5	OH + HO2 = H2O+O2	7.1×10^9
6	MTH + OH = Pr1	1.6×10^8
7	MTH + OH = Menthone	2.7×10^8
8	MTH + OH = P1	2.3×10^9
9	MTH + OH = P2	5.9×10^8
10	MTH + OH = P7	3.5×10^8
11	MTH + OH = P8	3.1×10^8
12	P1 + OH = Pr2	4.3×10^9
13	P2 + OH = Pr3	3.5×10^8
14	P2 + OH = P3	4.0×10^9
15	P3 + OH = Pr4	4.4×10^8
18	P3 + OH = P4	4.0×10^9
19	P4 + OH = Pr5	1.5×10^8
20	P4 + OH = P6	1.5×10^9

21	P4 + OH = P5	1.3×10^9
22	P6 + OH = Pr6	2.8×10^9
23	P5 + OH = Pr7	2.3×10^9
24	P7+ OH = Pr8	4.1×10^9
25	P8 + OH = Pr9	1.2×10^8
26	P8 + OH = P9	5.6×10^9
27	P9 + OH = Pr10	2.1×10^8
28	P9 + OH = P10	4.0×10^9
29	P10 + OH = Pr11	1.3×10^8
30	P10 + OH = P12	1.3×10^9
31	P10 + OH = P11	1.1×10^9
32	P12 + OH = Pr12	2.7×10^{10}
33	P11 + OH = Pr13	2.3×10^{10}
34	Menthone + OH = Pr14	2.9×10^9
35	Menthone + OH = P13	4.3×10^8
36	Menthone + OH = P16	6.4×10^8
37	Menthone + OH = P17	3.0×10^8
38	P13 + OH = Pr15	3.3×10^9
39	P16 + OH = Pr16	3.6×10^9
40	P17 + OH = Pr17	3.2×10^9

Table S4 Henry's Law constant values for the reactants of R1

Name	$M \times \text{atm}^{-1}$	H^{cc}
Fenchol	21.0×10^2	5.14×10^3
Fenchone	14.3	3.50×10^2
P1	3.91×10^5	9.57×10^6
P2	4.08×10^3	9.98×10^4
P6	2.51×10^3	6.14×10^4
P5	1.30×10^8	3.18×10^9
P3	3.75×10^4	9.17×10^5
P8	1.49×10^6	3.65×10^7
P10	8.40×10^{11}	2.06×10^{13}
P9	3.08×10^{10}	7.54×10^{11}
P4	3.91×10^5	9.57×10^6
P7	1.25×10^7	3.06×10^8

Table S5 Henry's Law constant values for the reactants of R2

Name	$M \times \text{atm}^{-1}$	H^{cc}
Borneol	46.0	1.13×10^3
Camphor	14.3	3.50×10^2
P1	3.91×10^5	9.57×10^6
P3	3.75×10^4	9.17×10^5
P2	4.08×10^3	9.98×10^4
P4	2.40×10^5	5.87×10^6
P5	1.25×10^7	3.06×10^8
P6	3.91×10^5	9.57×10^6
P8	3.75×10^4	9.17×10^5
P7	4.08×10^3	9.98×10^4
P9	2.40×10^5	5.87×10^6
P10	1.25×10^7	3.06×10^8
P12	2.66×10^7	6.51×10^8
P14	2.55×10^6	6.24×10^7
CA	7.63×10^7	1.87×10^9

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Table S6. Henry's Law constant values for the reactants of R3.

Name	$M \times \text{atm}^{-1}$	H^{cc}
Menthol	66.9	1.64×10^3
Menthone	6.29	1.54×10^2
P1	1.72×10^5	4.21×10^6
P2	1.80×10^3	4.40×10^4
P3	1.72×10^5	4.21×10^6
P4	1.65×10^4	4.04×10^5
P6	1.06×10^5	2.59×10^6
P5	5.49×10^6	1.34×10^8
P7	1.72×10^5	4.21×10^6
P8	1.80×10^3	4.40×10^4
P9	1.72×10^5	4.21×10^6
P10	1.65×10^4	4.04×10^5
P12	1.06×10^5	2.59×10^6
P11	5.49×10^6	1.34×10^8
P16	1.13×10^6	2.76×10^7
P17	4.95×10^5	1.21×10^7
P13	3.38×10^7	8.27×10^8

28 **Table S7.** The modeled and measured yields of the products from the reactions R1 - R3.

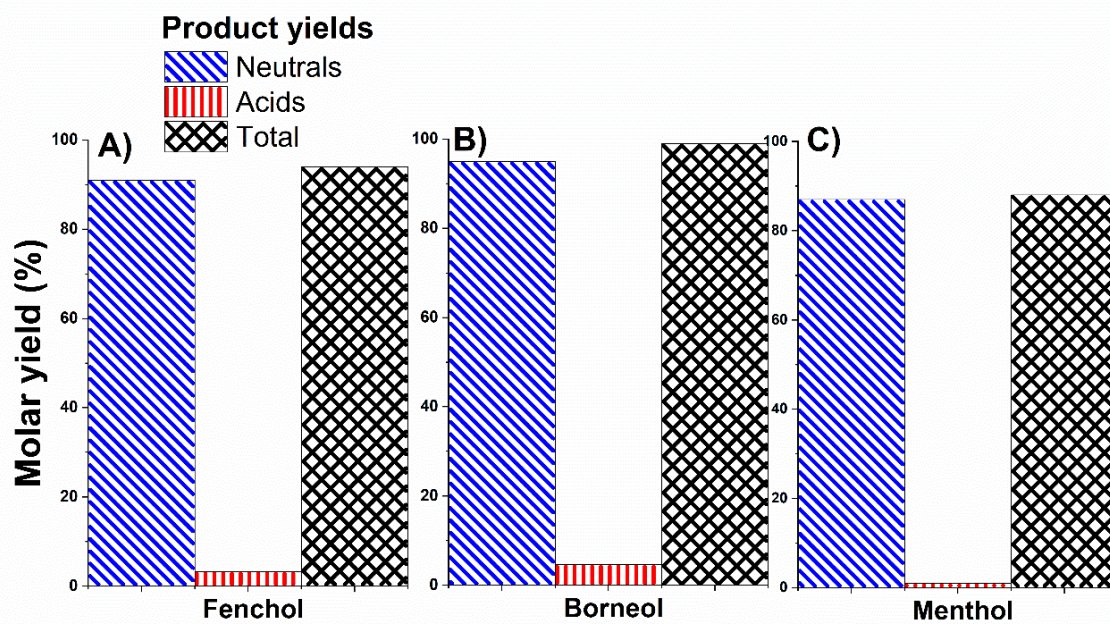
Molar yield ^a					
<i>Products formed directly from FCH (R1)</i>		<i>Products formed directly from BNL (R2)</i>		<i>Products formed directly from MTH (R3)</i>	
Fenchone	0.11±0.01	Camphor	0.12±0.02	Menthone	0.03±0.003
P1	0.05±0.003	P1	0.10±0.01	P1	0.17±0.01
P2	0.22±0.01	P2 ^b	0.15	P2	0.02±0.003
P3	0.07±0.01	P3	0.10±0.003	P3	0.16±0.004
P4	0.12±0.01	P4 ^b	0.03±0.02	P4	0.04±0.01
P5	0.16±0.001	P5	0.02±0.01	P5	0.04±0.001
P6	0.16±0.01	P6	0.15±0.01	P6	0.04±0.001
P7	0.02±0.01	P7 ^b	0.10	P7	0.19±0.01
		P8	0.16±0.02	P8 ^b	0.08
		P9 ^b	0.005	P9 ^b	0.08
		P10 ^b	0.0045	P10	0.02±0.01
		P12 ^b	0.02	P11 ^b	0.0002
				P12 ^b	0.0002

29 ^aUncertainties are 2σ values from triplicate measurements ^bValues derived by fitting the model to the
 30 experimental data

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 32 **Table S8.** The modeled yields of terpenoic acids (second-generation products) formed from fenchone, camphor,
 33 and menthone.

<i>Products formed from fenchone</i>			<i>Products formed from camphor</i>			<i>Products formed from menthone</i>		
Name	Yield (effective, from FCH)	Yield (from fenchone)	Name	Yield (effective, from BNL)	Yield (from camphor)	Name	Yield (effective, from MTH)	Yield (from menthone)
P8 ^b	0.01	0.12	P13 ^b	0.01	0.1	P13 ^b	0.003	0.1
P9 ^b	0.01	0.1	P15 ^b	0.01	0.12	P16 ^b	0.004	0.15
P10 ^b	0.01	0.08				P17 ^b	0.002	0.07

34 ^aUncertainties are 2σ values from triplicate measurements ^bValues derived by fitting the model to the
 35 experimental data



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Figure S1. Yields of neutral and acidic products formed in reactions R1 – 3 in Fig. 1.

S3 Chromatographic analyses

GC/MS analyses were conducted using a GC/MS-2010 Ultra gas chromatograph coupled with a single quadrupole mass spectrometer (Shimadzu) equipped with electron ionization (EI) or negative chemical ionization (NCI) ion sources – see section 2.7.1 in the main text.

S3.1 Gas chromatography coupled with electron-ionization mass spectrometry

Table S9. Retention times for and ions monitored in SIM mode for the reactants of R1 studied with the GC-EI/MS instrument.

Name	Elemental composition	Retention time (min)	Column	Ions monitored in selected SIM mode (m/z)	Concentration range (µg/L)	R ^{2,a}
(+)-Fenchol	C ₁₀ H ₁₈ O	18.16	VF-WAX plus	154, 139, 136, 125, 123, 121, 111, 107, 105, 97, 91, 85, 84, 81, 80, 72, 71, 69, 67, 57, 55, 53	(3.78-4.31) × 10 ⁴	0.984
(+)-Fenchone	C ₁₀ H ₁₆ O	17.45		153, 152, 137, 134, 123, 119, 109, 97, 95, 91, 82, 81, 80		0.987
(±)-exo,exo-2,3-Camphanediol	C ₁₀ H ₁₈ O ₂	20.84		152, 139, 137, 122, 121, 119, 112, 111, 110, 109, 107, 99, 96, 95, 94, 85, 84, 83, 82, 81		0.989
(±)Camphorquinone	C ₁₀ H ₁₄ O ₂	19.36		167, 166, 139, 138, 124, 123, 111, 110, 109, 105, 96, 95, 91, 84, 83		0.997
(1S,2S,5S)-(-)-2-hydroxy-3-pinanone	C ₁₀ H ₁₆ O ₂	18.49		168, 140, 126, 125, 122, 119, 111, 108, 107, 100, 99, 97, 93, 92, 91, 85, 84, 83		0.9974
Product 1	-	18.65		167, 164, 150, 149, 139, 137, 135, 127, 126, 125, 124, 123, 121, 111, 110, 109, 108, 107, 98, 97, 95, 94, 93, 91, 85, 84, 83, 82, 81, 80, 79, 77		HP
Product 2	-	18.74		139, 138, 123, 110, 109, 105, 97, 96, 95, 94, 91, 82, 81, 80, 79, 77, 70, 6		HP

				9	
Product 3	-	19.12		168,153,150,135,126,125,123, 122,113,112,111,109,108,107, 100,97,96,95,94,93,91,85,84,8 3,82,81,80,79	CQ
Product 4	-	19.22		139,136,125,123,122,121,111, 108,107,105,100,99,98,97,96,9 5,94,93,92,91,85,84,83,82,81,8 0,79,77	CQ
Product 5	-	19.30		139,136,125,123,122,121,111, 108,107,105,100,99,98,97,96,9 5,94,93,92,91,85,84,83,82,81,8 0,79,77	CQ
Product 6	-	19.38		154,137,136,125,124,123,121, 112,111,110,109,108,107,98,9 7,96,95,94,93,91,85,84,83,82,8 1,80,79	CQ
Product 7	-	19.54		139,138,124,123,121,109,108, 107,105,97,96,95,94,93,92,91, 83,82,81,79,77	CQ
Product 8	-	19.73		153,151,150,136,135,125,122, 121,111,110,109,108,107,98,9 7,96,95,94,93,91,84,83,82,81,8 0,79	CQ
Product 9	-	19.93		154,139,136,123,122,121,112, 111,110,109,108,107,106,105, 99,97,96,95,94,93,92,91,85,84, 83,82,81,80,79	CQ
Product 10	-	20.54		154,153,139,129,127,123,121, 113,112,111,110,105,99,98,97, 95,94,91,85,83,82,81,80,79,77	CND
Product 11	-	20.66		226,139,137,129,128,123,121, 111,110,109,108,107,106,105,	CND

				100,99,98,97,96,95,93,86,85,84,83,82,81,79	
Product 12	-	20.81		184,166,155,138,137,124,123,115,114,113,110,109,100,99,97,96,95,85,83,82,81,80,79	CND
Product 13	-	20.91		154,137,136,124,123,122,121,119,113,110,108,107,106,105,98,97,96,95,94,93,84,83,82,81,80,79	CND
Product 14	-	21.40		183,182,167,166,154,140,139,126,125,123,121,112,111,97,95,85,84,83,77	CND
Dimethyl phthalate	IS	17.75		162,163, 134, 133, 120, 105, 104, 92, 77, 76, 50, 49	-

45 ^aSurrogate standards used for quantification: HP = 2-hydroxy-3-pinane, CQ = Camphorquinone, CND= Camphanediol

Table S10. Retention times for precursor menthol, and its products were monitored in SIM mode with the GC-EI/MS instrument.

Name	Elemental composition	Retention time (min)	Column	Ions monitored in selected SIM mode (m/z)	Concentration range (µg/L)	R ^{2,a}
(-)-Menthol	C ₁₀ H ₂₀ O	12.53	VF-WAX plus	139, 138, 123, 110, 109, 96, 95, 83, 82, 81, 80, 71, 69, 68, 67, 57, 56, 55	(3.38-3.64) × 10 ⁴	0.9952
Menthone	C ₁₀ H ₁₈ O	11.07		155,154,140,139,125,121,113,112,111,110,109,98,97,96,95,94,93		0.9951
(±)-exo,exo-2,3-Camphanediol	C ₁₀ H ₁₈ O ₂	20.84		152,139,137,122,121,119,112,111,110,109,107,99,96,95,94,85,84,83,82,81		0.9784
(1S,2S,5S)-(-)-2-hydroxy-3-pinane	C ₁₀ H ₁₆ O ₂	18.49		168,140,126,125,122,119,111,108,107,100,99,97,93,92,91,85,84,83		0.9974
Product 1	-	19.04		170,152,140,137,126,125,12		HP

				4,123,110,109,98,97,96,95,9 1,86,85,84,83,82,81,79	
Product 2	-	19.40		169,168,167,153,139,138,13 7,127,126,125,124,123,113,1 12,111,110,109,107,99,98,97 ,96,95,93,85,84,83,82,81,80, 79	HP
Product 3	-	19.96		172,154,141,140,139,136,12 9,125,122,121,112,111,107,9 9,98,97,96,95,93,87,85,84,81 ,71,70,69	HP
Product 4	-	20.84		152,142,139,137,126,124,12 3,122,121,119,113,112,111,1 10,109,107,99,97,96,95,94,8 5,84,83,82,81	CND
Dimethyl phthalate	IS	17.75		162,163,134,133, 120, 105, 104, 92, 77, 76, 50, 49	-

*Surrogate standards used for quantification: HP = 2-hydroxy-3-pinane, CND= Camphanediol

50 **Table S11.** Retention times for Borneol, and its products were monitored in SIM mode with the GC-EI/MS instrument.

Name	Elemental composition	Retention time (min)	Column	Ions monitored in selected SIM mode (m/z)	Concentration range (µg/L)	R ^{2,a}
(+)-Borneol	C ₁₀ H ₁₈ O	13.16		140, 139, 136, 121, 111, 110, 96, 95, 83, 81, 82, 83, 79, 77, 71, 69, 67, 57, 55, 53	(3.51-3.74) × 10 ⁴	0.9964
Camphor	C ₁₀ H ₁₆ O	11.70		153,152,147,137,123,119, 110,109,108,107,105,97,9 6,95,93,91		0.9961
(±)-exo,exo-2,3- Camphanediol	C ₁₀ H ₁₈ O ₂	20.84		152,139,137,122,121,119, 112,111,110,109,107,99,9 6,95,94,85,84,83,82,81		0.9899
(±)Camphorquino	C ₁₀ H ₁₄ O ₂	19.36		167,166,139,138,124,123,		0.9982

ne			VF-WAX plus	111,110,109,105,96,95,91, ,84,83	
(1S,2S,5S)-(-)-2-hydroxy-3-pinanone	C ₁₀ H ₁₆ O ₂	18.49		168,140,126,125,122,119, 111,108,107,100,99,97,93, ,92,91,85,84,83	0.9974
Product 1	-	16.17		153,152,147,137,123,119, 110,109,108,95,93,83,82, 81,80	Camph or
Product 2	-	16.59		139,136,121,111,110,105, 99,95,93,83,82,81	Camph or
Product 3	-	18.75		167,166,151,138,125,123, 110,109,107,106,95,93,83, ,81,77,70,69	HP
Product 4	-	19.02		139,138,125,123,113,110, 109,96,95,91,84,82,81,80, 79	HP
Product 5	-	19.22		139,138,124,123,110,109, 105,97,96,95,94,93,91,82, 81,80,79,77	HP
Product 6	-	19.48		167,166,153,151,140,139, 138,135,126,125,124,123, 121,111,110,109,107,98,9 7,96,95,93,91,86,85,84,83 ,82,81,79	CQ
Product 7	-	19.76		153,150,149,137,136,125, 121,112,111,110,109,107, 97,96,95	CQ
Product 8	-	19.87		139,138,123,121,109,105, 96,95,94,93,91,83,81,79,7 7	CQ
Product 9	-	20.10	168,154,153,150,137,135, 125,124,123,110,109,108, 107,106,95,93	CND	

Product 10	-	20.27		155,154,150,144,140,139, 137,136,126,125,123,122, 121,119,113,112,111,110, 109,108,107,106,105,103, 96,95		CND
Product 11	-	21.05		169,168,153,150,139,135, 125,124,123,111,110,109, 108,107		CND
Dimethyl phthalate	IS	17.75		162,163, 134, 133, 120, 105, 104, 92, 77, 76, 50, 49		-

^aSurrogate standards used for quantification: HP = 2-hydroxy-3-pinanone, CQ = Camphorquinone, CND= Camphanediol

S3.2 Gas chromatography coupled with negative chemical ionization mass spectrometry

Table S12 Retention times with the elemental composition for TACs formed in FCH+OH reaction (R1) obtained using the LC-ToF/MS instrument

t_r (min)	Name	m/z (Da)	Elemental composition	Difference (Da)
9.93	P10	215.0920	C ₁₀ H ₁₆ O ₅	0.0001
12.10	P8	169.0868	C ₉ H ₁₄ O ₃	0.0003
13.15	P9	199.0971	C ₁₀ H ₁₆ O ₄	0.0001

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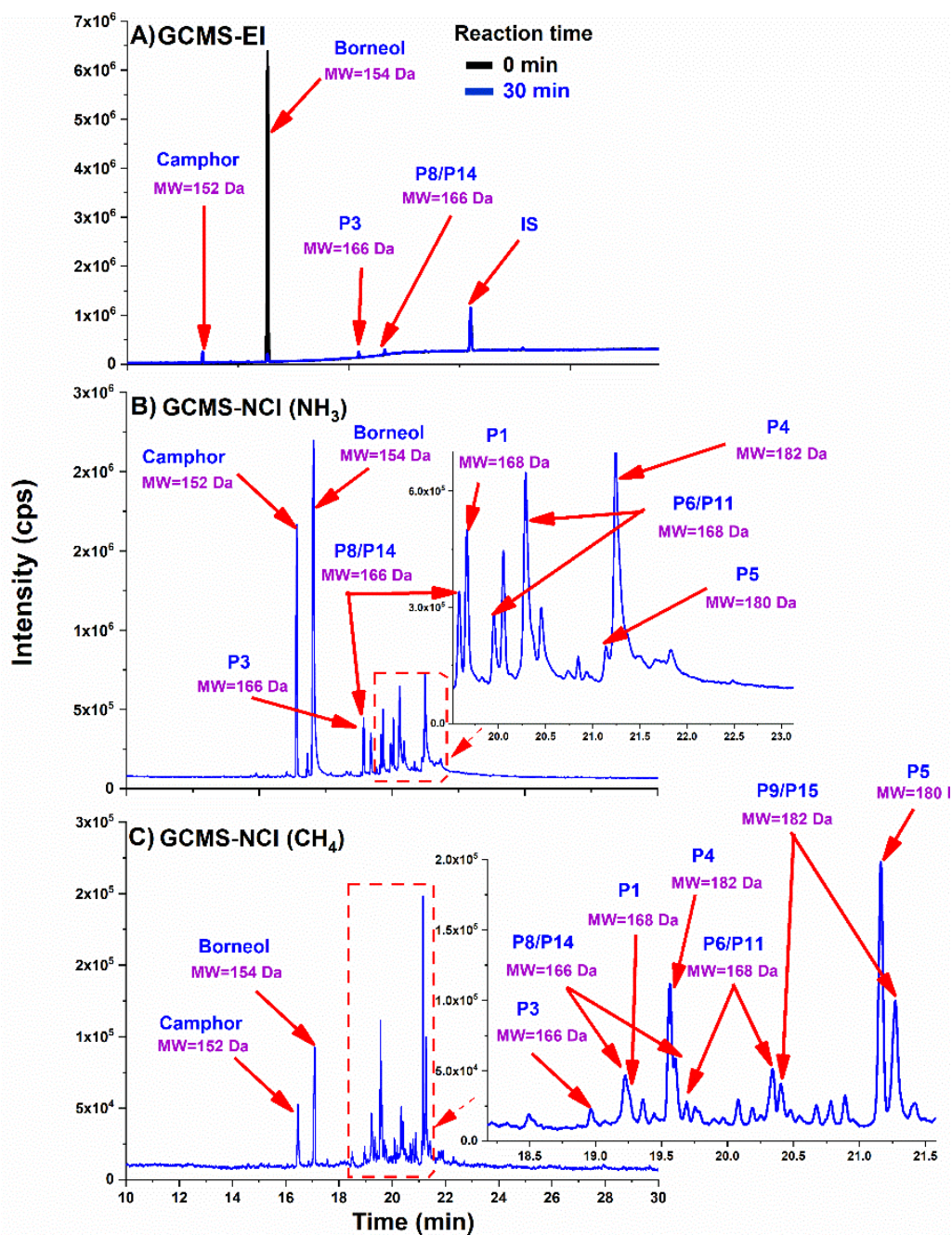
Table S13 Retention times with their elemental composition for TACs formed from BNL + _{aq}OH (R2) with the LC-ToF/MS instrument

t_r (min)	Name	m/z (Da)	Elemental composition	Difference (Da)
12.38	Camphoric acid	199.0970	C ₁₀ H ₁₆ O ₄	0.0000
13.15	P15	181.0864	C ₁₀ H ₁₄ O ₃	-0.0001
13.96	P12	183.1022	C ₁₀ H ₁₆ O ₃	0.0001

Table S14 Retention times with the elemental composition for TACs formed from MTH + _{aq}OH reaction (R3) obtained with the LC-ToF/MS instrument

60

t_r (min)	Name	m/z (Da)	Elemental composition	Difference (Da)
15.27	P13	201.1130	C ₁₀ H ₁₈ O ₄	0.0003
16.17	P17	185.1184	C ₁₀ H ₁₈ O ₃	0.0006
16.33	P16	183.1024	C ₁₀ H ₁₆ O ₃	0.0003



65 **Figure S2:** GC/MS chromatograms of the neutral products of borneol + OH reaction (R2) detected with EI (A) and (-)NCI using NH₃ (B), and CH₄ (C) as reagent gases. Note that different chromatographic columns were used for GC-EI/MS and GC-NCI/MS analyses (section 2.7.1), resulting in different retention times between panels (A), (B), and (C).

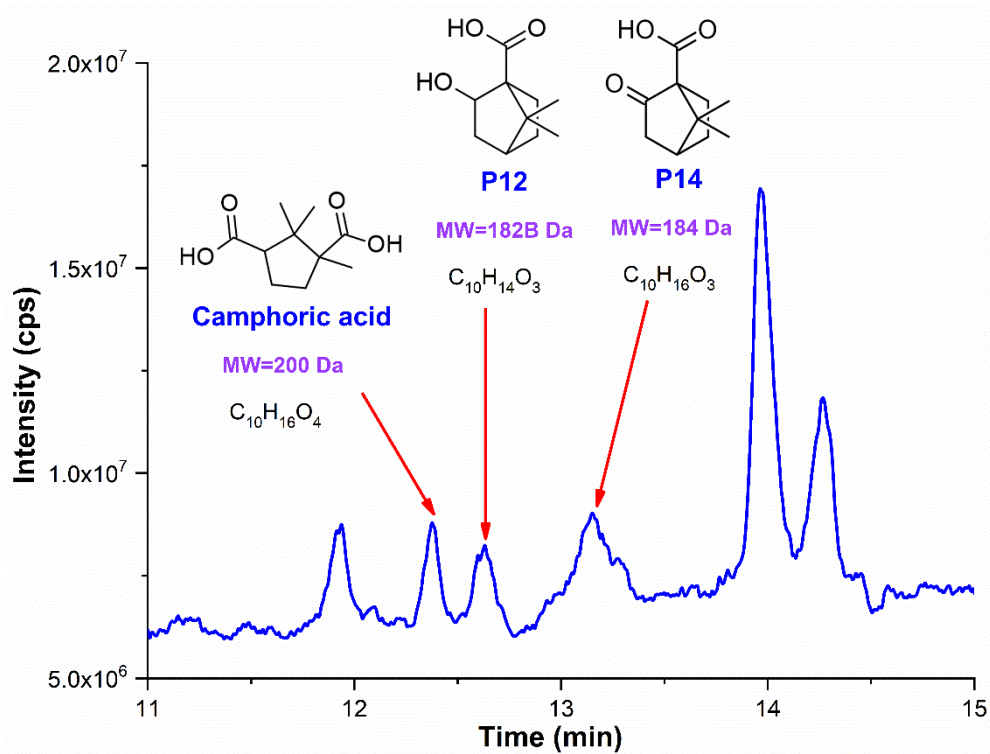
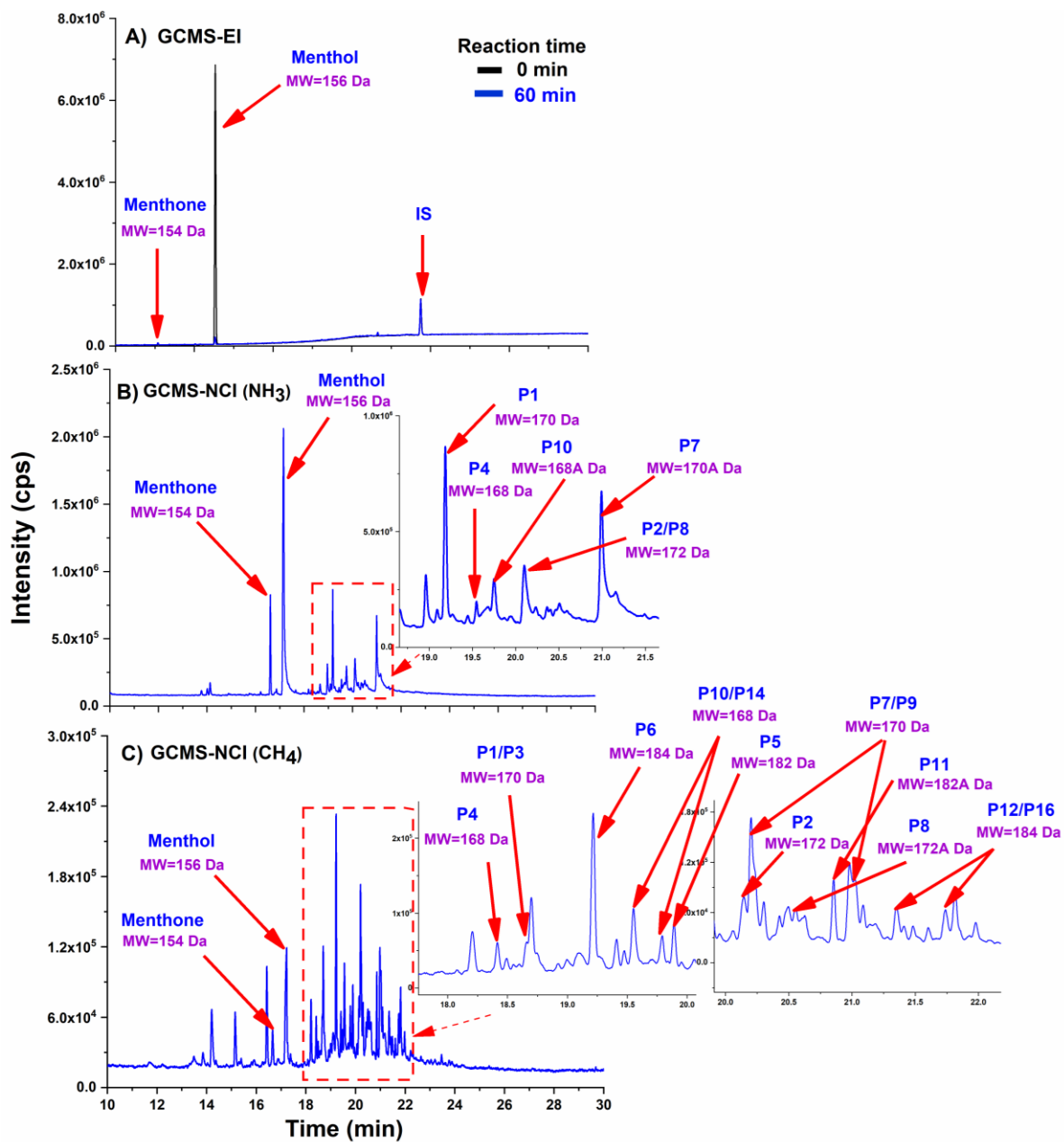


Figure S3: LC-ToF/MS chromatogram of TACs formed from OH reaction with borneol – R2 in the main text.



70 **Figure S4: GC/MS chromatograms of the neutral products of menthol + OH reaction (R3) detected with EI (A) and, (-)NCI using NH₃ (B), and CH₄ (C) as reagent gases. Note that different chromatographic columns were used for GC-EI/MS and GC-NCI/MS analyses (section 2.7.1), resulting in different retention times between panel (A) and panels (B) and (C).**

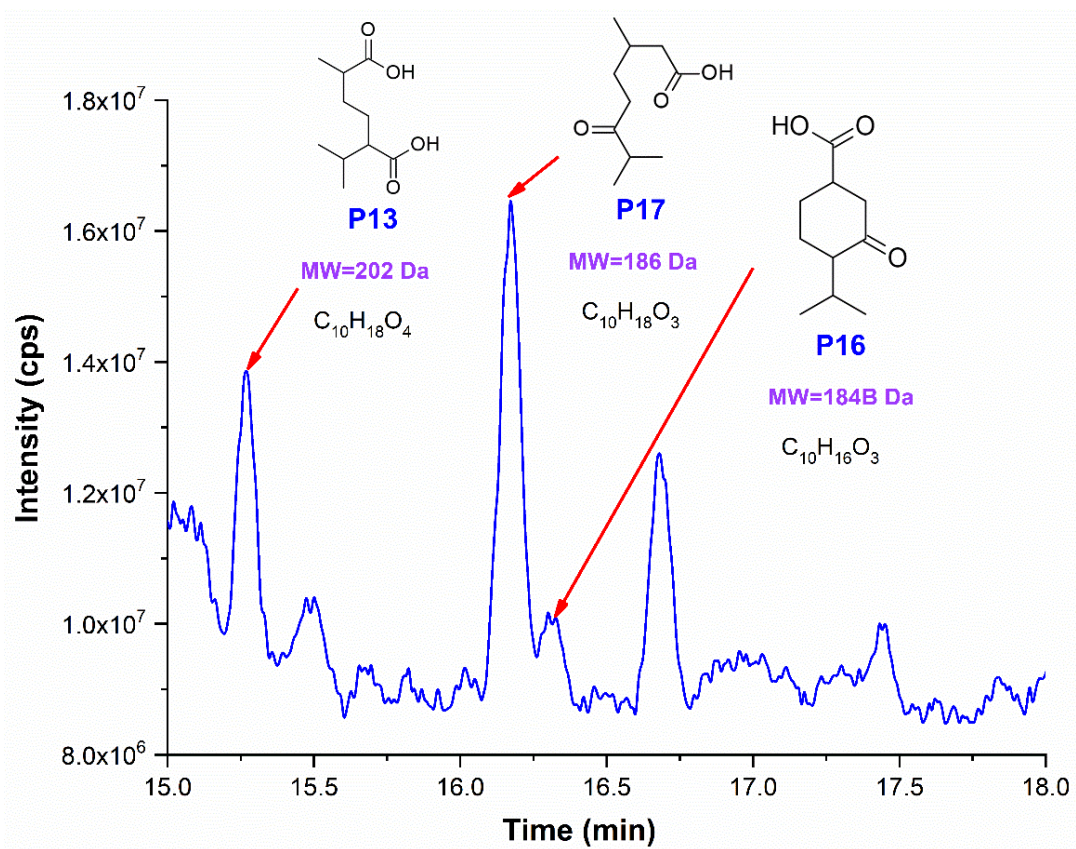
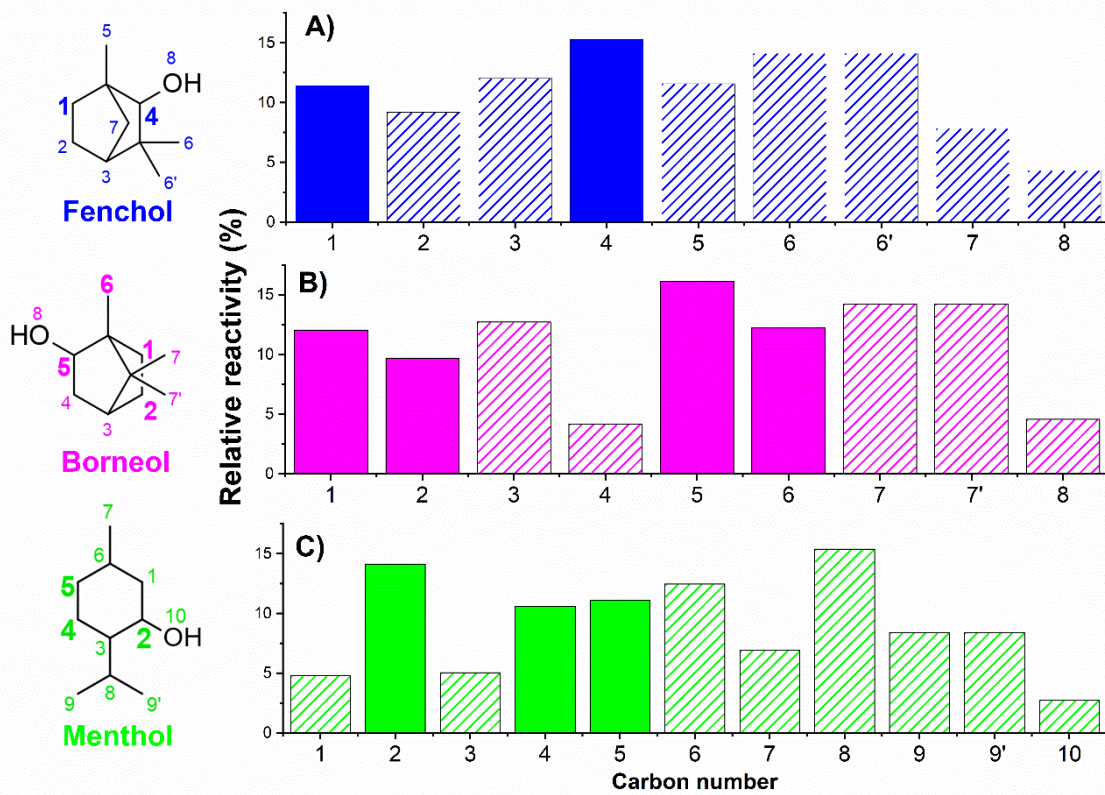
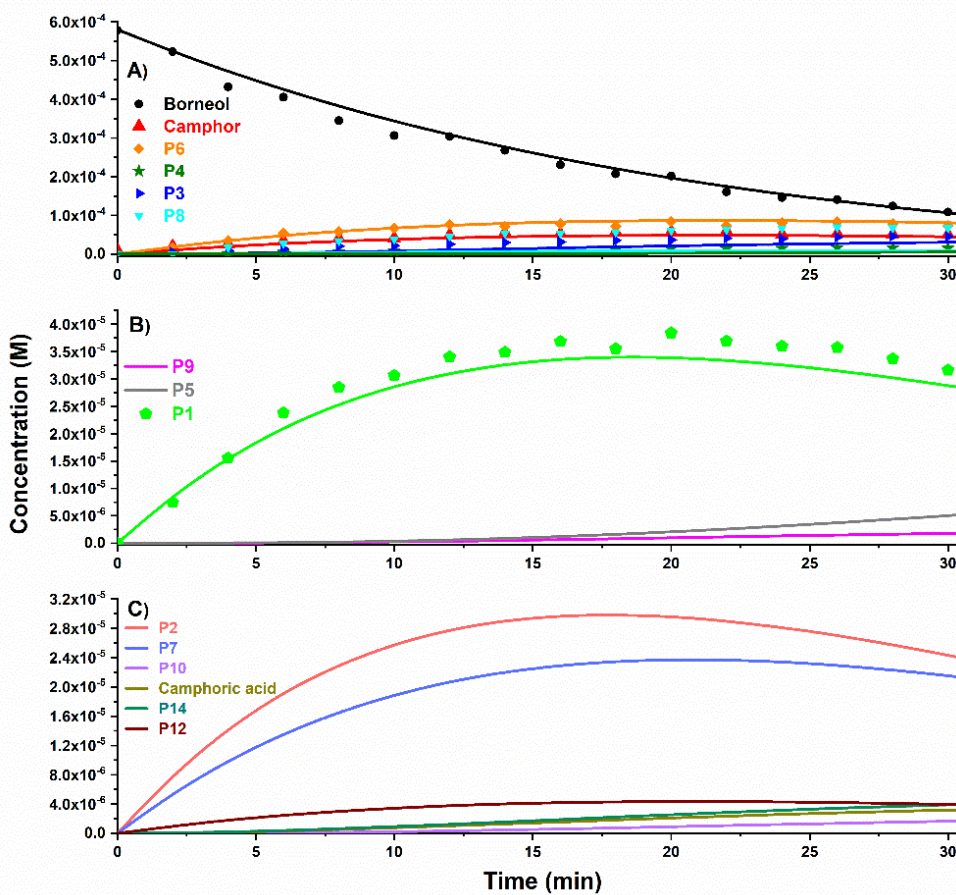


Figure S5: LC-ToF/MS chromatogram of TACs formed from OH reaction with menthol – R3 in Fig. 1.



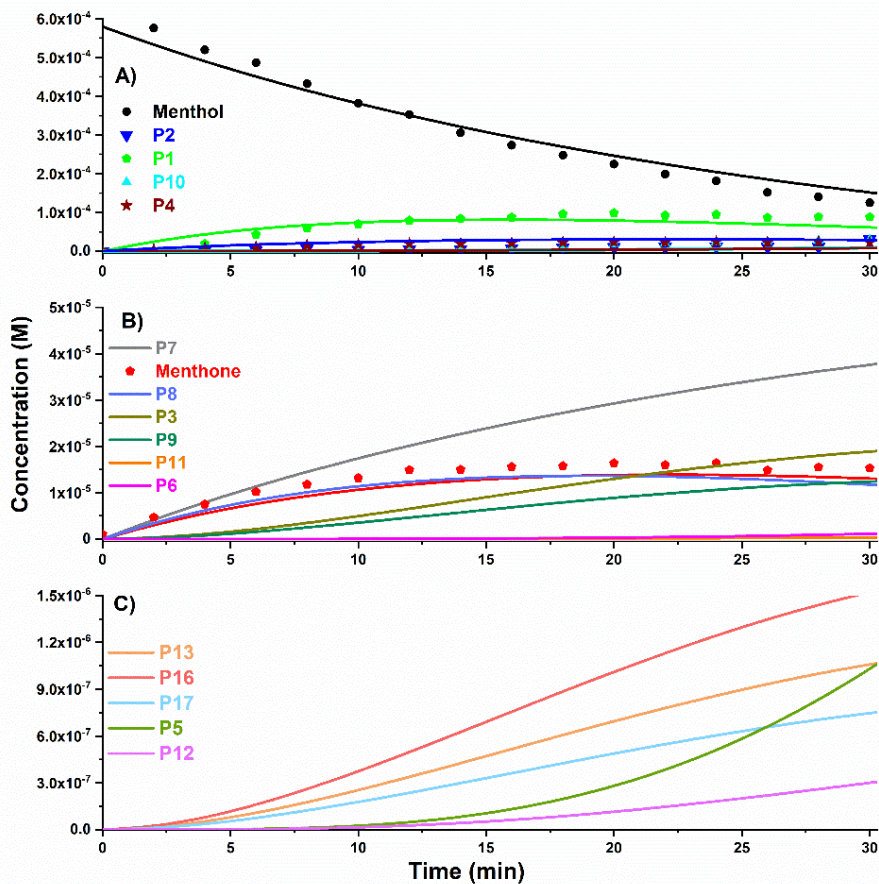
80 **Figure S6: The partial rate coefficients for the aliphatic H-atom abstraction from fenchol (A), borneol (B), and menthol (C) predicted with SAR. The H-atom abstraction sites shown in Schemes 1-7, in the main text, are shown in bold.**



85 **Figure S7: Temporal concentration profiles of the BNL and products of R2: points - experiment, and lines - model; A) precursor (BNL), camphor, structures of products P3, P4, P6 and P8 (stable carbonyl products), B) structures of products P1, P5 and P9 (stable carbonyl products), C) structures of stable carbonyl products P2, P7, P10, TAC products are camphoric acid, P12, P14 are shown in Schemes 3-5 (main text).**

For R2, the temporal profiles of some of the products were also reproduced accurately by the box model - Fig. S7. For products camphor, P1, P3, P4, P6, P8, experimental agrees well with the results generated by the model- Fig. S7A, B. However, for products P2, P5, P7, P9, P10, P12, P14, camphoric acid, only the model-generated data is presented in Figs. S7B, C (section 3.5). For R2, the yield of acidic products was approx. 5%, and the yield of 95±10% corresponded to the 90 carbonyl products – Table 1 and Figure S1.

Similar results were obtained for R3 – Fig. S8.



95 **Figure S8: Temporal concentration profiles of the MTH and products of R3: points - experiment, and lines - model; A) precursor (MTH), P1, P2, P4, P10; B) structures of products menthone, P3, P6, P7, P8, P9, P11 (stable carbonyl products), C) structures of stable carbonyl products P5, P12, TAC products are P13, P16, P17 are shown in Schemes 6 and 7.**

The box model for R3 accurately reproduced the temporal evolution of products menthone, P1, P2, P4, and P10 - Fig. S8A, B. For products P3, P5-P9, P11-P13, P16, and P17, only data generated by the model is presented- Figs. S8B and C (section 3.5). For R3, the yields of acidic and stable carbonyl products were 1% and ($87 \pm 5\%$), respectively- Table 1 and Fig. S1.

100 References

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