SUPPORTING INFORMATION

Overcoming the lack of authentic standards for the quantification of biogenic secondary organic aerosol markers

Pinic acid synthesis

In a round-bottomed flask fitted with a dropping funnel, pinonic acid (5.00 g, 27.14 mmol) was dissolved in a mixture of water:1,4-dioxane (1:5, 400 mL) and stirred rapidly. Meanwhile, in a beaker, bromine (4.60 mL, 89.56 mmol) was added dropwise to a solution of NaOH (14.11 g, 352.82 mmol) in water (136 mL) dropwise over 3 min at 0 °C. The solution was allowed to stir at 0 °C for 30 min (during this time, the solution should turn from yellow to colourless). The newly formed NaOBr and NaOH solution, was added to the dropping funnel and the reaction mixture was cooled to 0 °C. The NaOBr solution was then added dropwise over 30 min at 0 °C. The reaction mixture was then allowed to warm to room temperature slowly (without removal of the cooling bath) over 16 h, and then stirred at room temperature for a further 24 h. At this point, the reaction mixture was transferred into a separating funnel. The reaction mixture was washed with CH_2Cl_2 (3 x 100 mL) to remove any organic compounds (1,4-dioxane and water are miscible and therefore stay in the same phase). The CH_2Cl_2 organic layer was discarded, and the remaining aqueous layer was acidified to pH1 using concentrated HCl (37%). **Warning: addition of HCl to the aqueous layer causes effervescence and an exotherm.** The acidic aqueous layer was then extracted with CH2Cl2 (100 mL × 3) and the combined organic layers were washed with brine (100 mL), dried (Na2SO4), filtered and concentrated under reduced pressure via rotary evaporator. Brine was produced by adding NaCl to deionised water until no further solids cold be dissolved. Solid NaCl is left in the bottom of the Winchester in order to maintain the saturation. The reaction mixture was purified by flash column chromatography (silica, *n*-hexane 100% for 6 min, then a gradient to 20% EtOAc in *n*hexane for 5 min, then 20% EtOAc in *n*hexane for 10 min, then a gradient to n-hexane 100% to 40% EtOAc in hexane to yield pinic acid as a white solid (3.79 g, 75%). 1H NMR (400 MHz, CHLOROFORM-D) δ 2.79 (dd, J = 10.4, 7.8 Hz, 1H), 2.44–2.32 (m, 3H), 2.19 – 2.08 (m, 1H), 1.99 – 1.88 (m, 1H), 1.26 (s, 3H), 1.02 (s, 3H). 13C NMR (101 MHz, CHLOROFORM-D) δ 179.0, 178.7, 46.2, 43.1, 38.1, 35.2, 30.1, 24.4, 17.7. ESI-neg-MS (m/z): [M]- calcd. for $C_9H_{14}O_4$, 185.0819; found 185.0821. Elemental Analysis. Calculated for $C_9H_{14}O_4$: C, 58.05; H, 7.58; N, 0; Found: C, 57.51; H, 7.43; N, 0. Purity > 99 %.

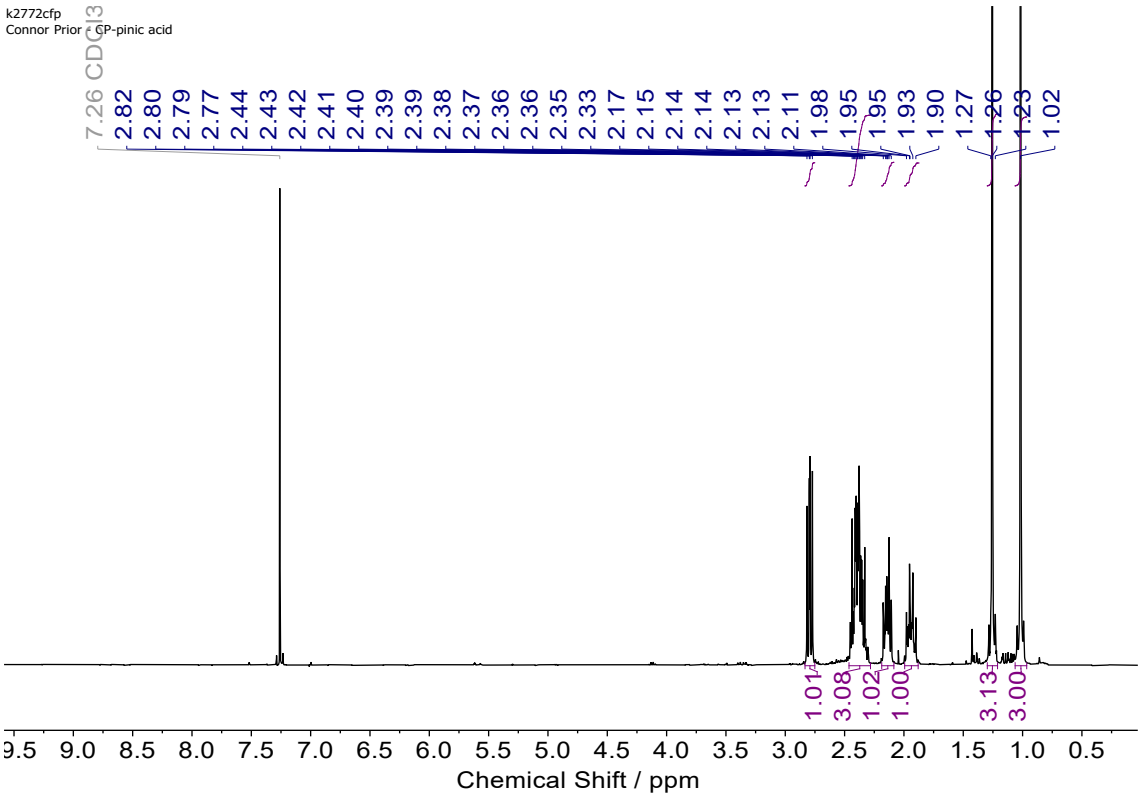

Figure S1. Synthesised pinic acid ^{1}H NRM spectrum.

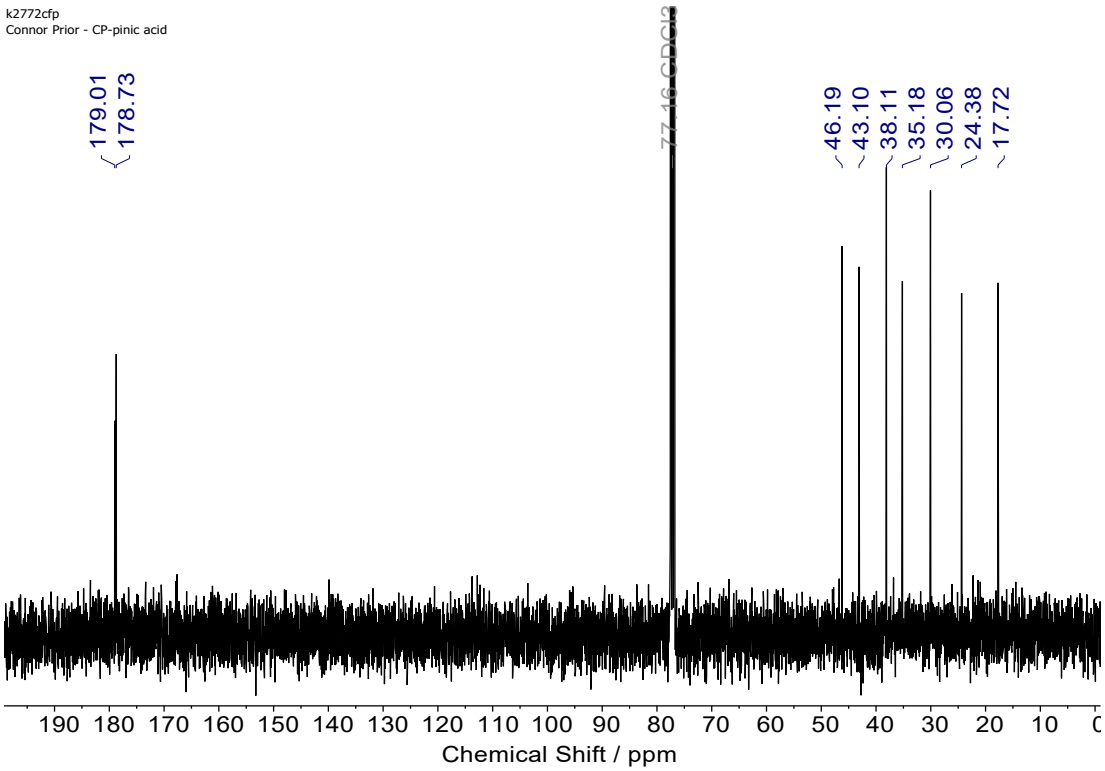

Figure S2. Synthesised pinic acid ^{13}C NMR spectrum

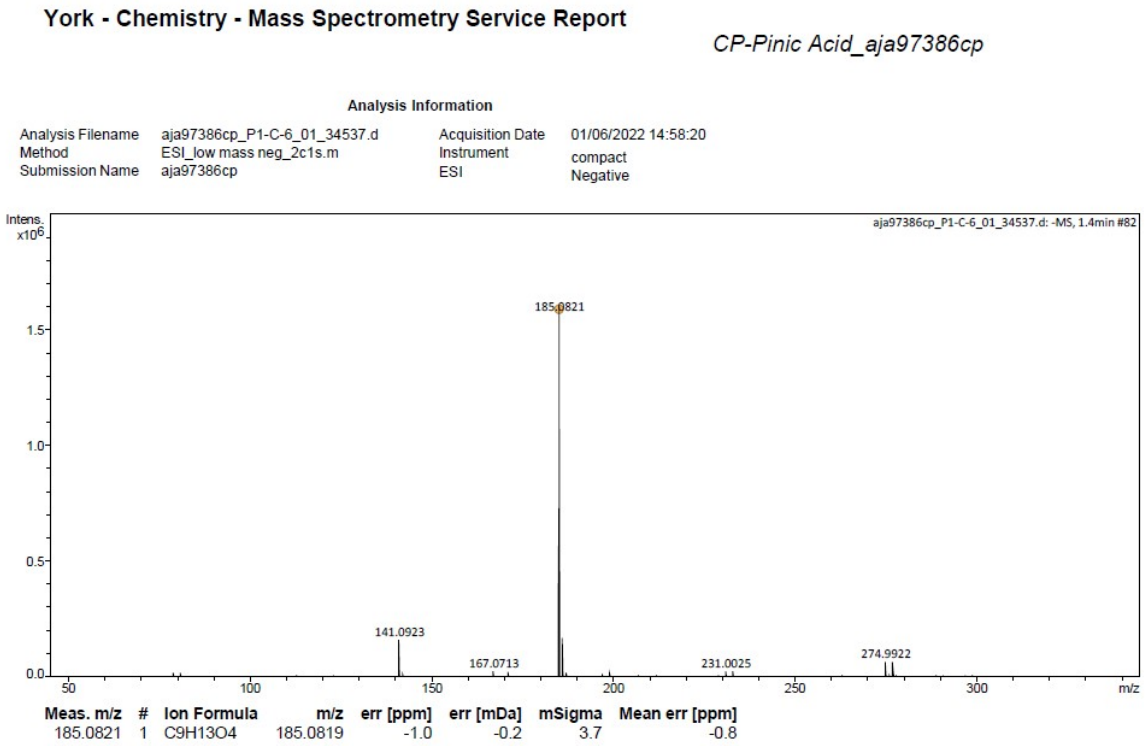

Figure S3. Synthesised pinic acid ESI mass spectrometry data

Table S1. Measured ($logRIE_M$) and predicted ($logRIE_P$) logRIE values for the 89 standards used for the development of the random forest model. Predicted logRIE values have an error range of ± 0.59. Alongside their molecular formulas, SMILE formula, retention times (RT), the likely dominant functionality facilitating ionisation, purity and manufacturer. * For some standards the manufacturer was not available, but all standards are at least 95 % pure.

Compound	Formula	SMILE	RT	Functionality	$logRIE_M$	$logRIE_P$	Purity	Manufacturer
2,6 dimethyl-4-nitrophenol	$C_8H_9NO_3$	CC1=CC(=CC(=C1O)C)[N+](=O)[O-]	12.71	-OH	1.75	0.33	98	Sigma
4-nitro-1-naphthol	$C_{10}H_7NO_3$	C1=CC=C2C(=C1)C(=CC=C2O)[N+](=O)[O-]	14.99	-OH	1.75	1.17	98	TCI Chemicals
2-methyl-4-nitrophenol	$C_7H_7NO_3$	CC1=C(C=CC(=C1)[N+](=O)[O-])O	10.42	-OH	1.72	1.39	97	Sigma
Isoborneolacetic acid	$C_{13}H_{22}O_3$	CC1(C2(CCC1(C(C2CC(=O)O)O)C)C)C	14.87	-OOH	1.62	0.81	99	Sigma
2-fluro nitrophenol	$C_6H_4FNO_3$	C1=CC(=C(C=C1[N+](=O)[O-])F)O	7.16	-OH	1.6	1.22	99	fluorochem
3-methyl-4-nitrophenol	$C_7H_7NO_3$	CC1=C(C=CC(=C1)O)[N+](=O)[O-]	9.3	-OH	1.57	1.43	99	fluorochem
Sebacic acid	$C_{10}H_{18}O_4$	C(CCCCC(=O)O)CCCC(=O)O	13.14	-OOH	1.46	1.15	99	Sigma
4-nitrocatechol	$C_6H_5NO_4$	C1=CC(=C(C=C1[N+](=O)[O-])O)O	4.76	-OH	1.36	1.03	96	Sigma
4-nitrobenzene-1,3-diol	$C_6H_5NO_4$	C1=CC(=C(C=C1O)O)[N+](=O)[O-]	6.73	-OH	1.34	0.31	95	Fluorochem
Azelaic acid	$C_9H_{16}O_4$	C(CCCC(=O)O)CCCC(=O)O	10.51	-OH	1.33	1.25	98	Sigma
2-methyl-5-nitrophenol	$C_7H_7NO_3$	CC1=C(C=C(C=C1)[N+](=O)[O-])O	11	-OH	1.33	1.34	98	Sigma
2-methyl-3-nitrophenol	$C_7H_7NO_3$	CC1=C(C=CC=C1O)[N+](=O)[O-]	9.77	-OH	1.31	1.08	98	Fluorochem
2,4-dinitrophenol	$C_6H_4N_2O_5$	C1=CC(=C(C=C1[N+](=O)[O-])[N+](=O)[O-])O	7.42	-OH	1.3	0.4	98	Sigma
Suberic acid	$C_8H_{14}O_4$	C(CCCC(=O)O)CCC(=O)O	7.56	-OH	1.29	0.94	98	Sigma
4-hydroxybenzaldehyde	$C_7H_6O_2$	C1=CC(=CC=C1C=O)O	4.2	-CHO/-OH	1.26	0.39	98	Alfa Aesar
3-nitrophenol	$C_6H_5NO_3$	C1=CC(=CC(=C1)O)[N+](=O)[O-]	9.89	-OH	1.23	1.12	99	Thermo Sci
4-methyl-3-nitrophenol	$C_7H_7NO_3$	CC1=C(C=C(C=C1)O)[N+](=O)[O-]	9.89	-OH	1.23	1.34	97	Fluorochem
Camphoric acid	$C_{10}H_{16}O_4$	CC1(C(CCC1(C)C(=O)O)C(=O)O)C	9.04	-OOH	1.2	0.9	98	Alfa Aesar
2-Hydroxyhexanoic acid	$C_6H_{12}O_3$	CCCCC(C(=O)O)O	5.68	-OOH	1.14	0.32	95	*
3,3-dimethyl glutaric acid	$C_9H_{16}O_4$	CC(C)(CC(=O)O)CC(=O)O	4.43	-OOH	1.13	0.65	98	Sigma
p-coumaric acid	$C_9H_8O_3$	C1=CC(=CC=C1C=CC(=O)O)O	6.4	-OOH	1.13	0.8	98	Sigma
2,3-napthalenedicarboxylic acid	$C_{12}H_6O_3$	O=C(O)C1CC2CCCCC2(CC1(C(=O)O))	10.68	-CO	1.03	0.75	95	Sigma
2-hydroxy-3-methylbutyric acid	$C_5H_{10}O_3$	CC(C)C(C(=O)O)O	2.39	-OOH	1.01	-0.07	99	Sigma
Pimelic acid	$C_7H_{12}O_4$	C(CCC(=O)O)CCC(=O)O	4.63	-OOH	0.92	0.8	98	Thermo Sci
Isophthalic acid	$C_8H_6O_4$	C1=CC(=CC(=C1)C(=O)O)C(=O)O	6.24	-OOH	0.92	0.62	95	*
Citraconic acid	$C_5H_6O_4$	CC(=CC(=O)O)C(=O)O	1.17	-OOH	0.91	0.34	98	Sigma

2,5-dihydroxybenzoic acid	$C_7H_6O_4$	C1=CC(=C(C=C1O)C(=O)O)O	2.91	-OOH	0.91	0.42	95	*
2-Methoxy-4-nitrophenol	$C_7H_7NO_4$	COC1=C(C=CC(=C1)[N+](=O)[O-])O	7.61	-OH	0.91	0.19	97	Sigma
Cholic acid	$C_{24}H_{40}O_5$	CC(CCC(=O)O)C1CCC2C1(C(CC3C2C(CC4C3(CCC(C4)O)C)O)O)C	20.4	-OOH	0.91	0.88	95	*
Diphenolic acid	$C_{17}H_{18}O_4$	CC(CCC(=O)O)(C1=CC=C(C=C1)O)C2=CC=C(C=C2)O	11.52	-OOH	0.87	0.91	95	Sigma
1,2,4-Butanetricarboxylic acid	$C_7H_{10}O_6$	C(CC(=O)O)C(CC(=O)O)C(=O)O	1.23	-OOH	0.8	0.45	97	Activate Scientific
3,4-Dihydroxy benzoic acid	$C_7H_6O_4$	C1=CC(=C(C=C1C(=O)O)O)O	1.82	-OOH	0.77	0.58	97	Sigma
Sinapic acid	$C_{11}H_{12}O_5$	COC1=CC(=CC(=C1O)OC)C=CC(=O)O	7.85	-OOH	0.76	0.52	98	Santa Cruz Biotechnology
Adipic acid	$C_6H_{10}O_4$	C(CCC(=O)O)CC(=O)O	2.33	-OOH	0.75	0.69	99	Sigma
Levulinic acid	$C_5H_8O_3$	CC(=O)CCC(=O)O	1.22	-OOH	0.72	-0.58	98	Sigma
Hippuric acid	$C_9H_9NO_3$	C1=CC=C(C=C1)C(=O)NCC(=O)O	3.57	-OOH	0.63	0.82	98	Thermo Sci
3-methyl adipic acid	$C_7H_{12}O_4$	CC(CCC(=O)O)CC(=O)O	4.54	-OOH	0.62	0.8	95	*
Succinic acid	$C_4H_6O_4$	C(CC(=O)O)C(=O)O	0.97	-OOH	0.6	0.5	99	Sigma
3-nitrobenzoic acid	$C_7H_5NO_4$	C1=CC(=CC(=C1)[N+](=O)[O-])C(=O)O	7.53	-OOH	0.59	0.79	95	*
1,4-cyclohexanedicarboxylic acid	$C_8H_{12}O_4$	C1CC(CCC1C(=O)O)C(=O)O	5.83	-OOH	0.58	0.88	99	Sigma
Glutaric acid	$C_5H_8O_4$	C(CC(=O)O)CC(=O)O	1.31	-OOH	0.57	0.75	99	Sigma
4-methyl-catechol	$C_7H_8O_2$	CC1=CC(=C(C=C1)O)O	4.65	-OH	0.56	0.44	95	*
4-hydroxy benzoic acid	$C_7H_6O_3$	C1=CC(=CC=C1C(=O)O)O	3.38	-OOH	0.5	0.62	99	Sigma
2-Methylsuccinic acid	$C_5H_8O_4$	CC(CC(=O)O)C(=O)O	1.76	-OOH	0.49	0.55	95	*
3-hydroxy benzoic acid	$C_7H_6O_3$	C1=CC(=CC(=C1)O)C(=O)O	4.42	-OOH	0.41	0.42	95	*
Itaconic acid	$C_5H_6O_4$	C=C(CC(=O)O)C(=O)O	1.48	-OOH	0.39	0.55	95	*
Malic acid	$C_4H_6O_5$	C(C(C(=O)O)O)C(=O)O	0.72	-OOH	0.3	-0.2	99	Sigma
Citric acid	$C_6H_8O_7$	C(C(=O)O)C(CC(=O)O)(C(=O)O)O	0.93	-OOH	0.28	0.45	95	*
Mandelic acid	$C_8H_8O_3$	C1=CC=C(C=C1)C(C(=O)O)O	3.33	-OOH	0.27	0.55	99	Thermo Sci
Maleic acid	$C_4H_4O_4$	C(=CC(=O)O)C(=O)O	0.75	-OOH	0.26	0.47	99	Sigma
trans,trans,1,3-butadiene-1,4-dicarboxylic acid	$C_6H_6O_4$	C(=CC(=O)O)C=CC(=O)O	2.11	-OOH	0.19	0.63	95	*
DL-tartaric acid	$C_4H_6O_6$	C(C(C(=O)O)O)(C(=O)O)O	0.72	-OOH	0.15	-0.25	95	*
Shikimic acid	$C_7H_{10}O_5$	C1C(C(C(C=C1C(=O)O)O)O)O	0.74	-OOH	0.1	0.29	98	Alfa Aesar

O-toluic acid	$C_8H_8O_2$	CC1=CC=CC=C1C(=O)O	10.74	-OOH	0.1	-0.62	99	Sigma
Vanillin	$C_8H_8O_3$	COC1=C(C=CC(=C1)C=O)O	5.55	-CHO/-OH	0.09	0.05	99	Thermo Sci
4-nitrocinnamic acid	$C_9H_7NO_4$	C1=CC(=CC=C1C=CC(=O)O)[N+](=O)[O-]	10.97	-OOH	0.03	0	95	*
Nonanoic acid	$C_9H_{18}O_2$	CCCCCCCCC(=O)O	19.46	-OOH	-0.11	-0.32	97	Alfa Aesar
Dodecanoic acid	$C_{12}H_{24}O_2$	CCCCCCCCCCCC(=O)O	23.62	-OOH	-0.14	-0.51	98	Sigma
Benzoic acid	$C_7H_6O_2$	C1=CC=C(C=C1)C(=O)O	7.93	-OOH	-0.19	-0.7	99.5	Sigma
Methylmalonic acid	$C_4H_6O_4$	CC(C(=O)O)C(=O)O	1.05	-OOH	-0.21	-0.89	95	*
Vanillic acid	$C_8H_8O_4$	COC1=C(C=CC(=C1)C(=O)O)O	4.34	-OOH	-0.25	1.02	95	*
2-nitro-1-naphthol	$C_{10}H_7NO_3$	C1=CC=C2C(=C1)C=CC(=C2O)[N+](=O)[O-]	18.83	-OH	-0.34	-0.48	95	Sigma
m-toluic acid	$C_8H_8O_2$	CC1=CC(=CC=C1)C(=O)O	11.42	-OOH	-0.38	-0.47	99	Sigma
2-nitroresorcinol	$C_6H_5NO_4$	C1=CC(=C(C(=C1)O)[N+](=O)[O-])O	5.41	-OH	-0.4	-0.49	98	Sigma
Valeric acid	$C_5H_{10}O_2$	CCCCC(=O)O	2.31	-OOH	-0.46	-1.1	99	Sigma
p-toluic acid	$C_8H_8O_2$	CC1=CC=C(C=C1)C(=O)O	11.45	-OOH	-0.47	-0.95	98	Sigma
2-nitrobenzoic acid	$C_7H_5NO_4$	C1=CC=C(C(=C1)C(=O)O)[N+](=O)[O-]	2.94	-OOH	-0.49	0.15	95	*
2-nitrophenol	$C_6H_5NO_3$	C1=CC=C(C(=C1)[N+](=O)[O-])O	10.84	-OH	-0.54	-0.6	98	*
pyruvic acid	$C_3H_4O_3$	CC(=O)C(=O)O	0.78	-OOH	-0.57	-1.6	98	Sigma
4-methoxy-benzoic acid	$C_8H_8O_3$	COC1=CC=C(C=C1)C(=O)O	9.09	-OOH	-0.57	-0.02	95	*
5-methyl-2-nitrophenol	$C_7H_7NO_3$	CC1=CC(=C(C=C1)[N+](=O)[O-])O	12.92	-OH	-0.59	-0.01	97	Sigma
DL-isoleucine	$C_6H_{13}NO_2$	CCC(C)C(C(=O)O)N	0.99	-OOH	-0.64	-0.49	95	*
Trans-cinnamic acid	$C_9H_8O_2$	C1=CC=C(C=C1)C=CC(=O)O	11.76	-OOH	-0.67	-0.5	98	Sigma
Malonic acid	$C_3H_4O_4$	C(C(=O)O)C(=O)O	0.76	-OOH	-0.7	-0.54	99	Sigma
4-methyl-2-nitrophenol	$C_7H_7NO_3$	CC1=CC(=C(C=C1)O)[N+](=O)[O-]	12.86	-OH	-0.75	0.03	99	Sigma
2-methyl-6-nitrophenol	$C_7H_7NO_3$	CC1=C(C(=CC=C1)[N+](=O)[O-])O	14.54	-OH	-0.75	-0.58	98	Fluorochem
4-methoxy-2-nitrophenol	$C_7H_7NO_4$	COC1=CC(=C(C=C1)O)[N+](=O)[O-]	11.75	-OH	-0.76	-0.47	98	Sigma
4-Phenylbutyric acid	$C_{10}H_{12}O_2$	C1=CC=C(C=C1)CCCC(=O)O	13.37	-OOH	-0.77	-0.65	95	*
Acetoxyacetic acid	$C_4H_6O_4$	CC(=O)OCC(=O)O	1.17	-OOH	-0.78	-0.05	99	Sigma
Ketopinic acid	$C_{10}H_{14}O_3$	CC1(C2CCC1(C(=O)C2)C(=O)O)C	8.66	-OOH	-0.85	-0.38	99	Sigma

3,4-dimethyl-benzoic acid	$C_9H_{10}O_2$	CC1=C(C=C(C=C1)C(=O)O)C	14.14	-OOH	-1.03	-0.67	95	*
Furoic acid	$C_5H_4O_3$	C1=COC(=C1)C(=O)O	3.21	-OOH	-1.23	-0.93	98	Apollo Scientific
4-hydroxycinnamic acid	$C_9H_8O_3$	C1=CC(=CC=C1C=CC(=O)O)O	6.38	-OOH	-1.29	-0.48	95	*
Aconitic acid	$C_6H_6O_6$	C(C(=CC(=O)O)C(=O)O)C(=O)O	1	-OOH	-1.39	0.49	98	Thermo Sci
Crotonic acid	$C_4H_6O_2$	CC=CC(=O)O	1.05	-OOH	-1.76	-1.92	95	*
Sorbic acid	$C_6H_8O_2$	CC=CC=CC(=O)O	7.88	-OOH	-1.8	-0.96	95	*
Phenyl acetic acid	$C_8H_8O_2$	C1=CC=C(C=C1)CC(=O)O	4.96	-OOH	-2.09	-0.7	95	*
Butyric acid	$C_4H_8O_2$	CCCC(=O)O	3.16	-OOH	-2.34	-1.33	99	Sigma
3,3-dimethyl acrylic acid	$C_5H_8O_2$	CC(=CC(=O)O)C	5.04	-OOH	-2.84	-1.38	95	*

Table S2. Contains descriptors obtained from Chemdes which had a R correlation greater than 0.3 to the logRIE values of the standards in Table S1. Package from which the descriptor as obtained and the description of the descriptor.

Descriptor	Package	Description
ATSm5	Chemopy	Broto-Moreau autocorrelation of a topological structure-lag5/weighted by atomic masses
ZMIC5	PaDEL	Z-modified information content index (neighbourhood symmetry of 5-order)
EstateVSA1	Chemopy	MOE-type descriptors using Estate indices and surface area contributions
SpMAD_Dzp	PaDEL	Spectral mean absolute deviation from Barysz matrix / weighted by polarizabilities
PEOE_VSA13	RDKit	MOE Charge VSA Descriptor 13 (0.25 <= x < 0.30)
AATS6s	PaDEL	averaged moreau-broto autocorrelation of lag 6 weighted by intrinsic state
AATS7i	PaDEL	Average Broto-Moreau autocorrelation - lag 7 / weighted by first ionization potential
MLFER_A	PaDEL	Overall or summation solute hydrogen bond acidity
MATS1p	PaDEL	moran coefficient of lag 1 weighted by polarizability
AATS6e	PaDEL	Average Broto-Moreau autocorrelation - lag 6 / weighted by Sanderson electronegativities
MLFER_S	PaDEL	combined dipolarity/polarizability
JGI4	PaDEL	Mean topological charge index of order 4
EState_VSA10	RDKit	MOE-type descriptors using EState indices and surface area contributions
MATSm6	Chemopy	Moran autocorrelation-lag6/weighted by atomic masses
AATS6v	PaDEL	Average Broto-Moreau autocorrelation - lag 6 / weighted by van der Waals volumes
PEOE_VSA2	RDKit	MOE Charge VSA Descriptor 2 (-0.30 <= x < -0.25)

Table S3. Compound tag and reference (superscript number), molecular formula (MF,) predicted RIE factor, minimum predicted RIE (RIE_{min}), maximum predicted RIE (RIE_{max}) and Simplified Input Line Entry System (SMILES) formulas for the structures of the previously proposed BSOA markers. Based on the RMSE uncertainty of 0.59, the predicted RIE values have an uncertainty range, as shown by the minimum and maximum RIE values. *Markers that have been structurally confirmed by comparison to an authentic standard or MS^2 data in the BSOA chamber samples.

TAG	MF	RIE	RIE_{min}	RIE_{max}	SMILE
***Pinene_169**[1]	$C_9H_{14}O_3$	0.33	0.09	1.29	CC1(C)C(CC=O)CC1C(O)=O
***Pinene_171a**[1]	$C_8H_{12}O_4$	0.58	0.15	2.27	CC1(C)C(C(C)=O)CC1C(O)=O
***Pinene_171b**[1]	$C_8H_{12}O_4$	2.24	0.57	8.70	CC1(OC(CC1CC(O)=O)=O)C
***Pinene_185a**[1]	$C_9H_{14}O_4$	7.27	1.87	28.26	CC1(C)C(C(O)=O)CC1CC(O)=O
Pinene_185b[2]	$C_{10}H_{18}O_3$	12.06	3.10	46.92	CC1(C)C(C(C)O)CC1CC(O)=O
Pinene_189[1]	$C_8H_{14}O_5$	3.41	0.88	13.27	CC(O)(C(CC(O)=O)CC(O)=O)C
***Pinene_197**[1]	$C_{10}H_{14}O_4$	0.61	0.16	2.38	CC1(C)C(C(C=O)=O)CC1CC(O)=O
***Pinene_199a**[1]	$C_{10}H_{16}O_4$	5.69	1.46	22.13	CC1(C)C(C(CO)=O)CC1CC(O)=O
***Pinene_199b**[1]	$C_{10}H_{16}O_4$	5.24	1.35	20.38	CC1(C(CC1CC(O)=O)C(C)=O)CO
***Pinene_213**[1]	$C_{10}H_{14}O_5$	4.06	1.04	15.80	OC(C(C1CC(CC(O)=O)C1(C)C)=O)=O
Pinene_231[1]	$C_{10}H_{16}O_6$	4.77	1.23	18.57	CC(OC(C)(C(CC(O)=O)CC(O)=O)C)=O
Pinene_309[1]	$C_{17}H_{26}O_5$	0.74	0.19	2.88	OC(C1CC(CC(OC2CC(CC=O)C2(C)C)=O)C1(C)C)=O
Pinene_313[1]	$C_{16}H_{26}O_6$	5.82	1.50	22.66	OC(C1CC(CC(OCC(C(C)(O)C)CC=O)=O)C1(C)C)=O
Pinene_325[1]	$C_{17}H_{26}O_6$	9.67	2.49	37.64	OC(C1CC(CC(OCC2CC(C(O)=O)C2(C)C)=O)C1(C)C)=O
Pinene_343a[1]	$C_{16}H_{24}O_8$	5.21	1.34	20.28	CC(OC1=O)(C(CC(OC(C)(C(CC(O)=O)CC(O)=O)C)=O)C1)C
Pinene_343b[2]	$C_{16}H_{24}O_8$	5.19	1.33	20.20	O=C(C1CC(CC(OC(C)(C(C(O)=O)CC(O)=O)C)=O)C1(C)C)O
Pinene_351[2]	$C_{20}H_{32}O_5$	0.79	0.20	3.09	CC(C1CC(CC(OC(C2CC(CC(O)=O)C2(C)C)C)=O)C1(C)C)=O
Pinene_353a[2]	$C_{19}H_{30}O_6$	12.69	3.26	49.36	OC(C1CC(CC(OC(C2CC(CC(O)=O)C2(C)C)C)=O)C1(C)C)=O
Pinene_353b[2]	$C_{20}H_{34}O_5$	12.72	3.27	49.51	CC(O)C1CC(CC(OC(C2CC(CC(O)=O)C2(C)C)C)=O)C1(C)C
Pinene_357[1]	$C_{17}H_{26}O_8$	1.72	0.44	6.70	OC(CC(CC(O)=O)C(C)(OC(C1CC(CC(O)=O)C1(C)C)=O)C)=O
***Pinene_367**[1]	$C_{19}H_{28}O_7$	8.58	2.21	33.39	OC(C1CC(CC(OCC(C2CC(CC(O)=O)C2(C)C)=O)=O)C1(C)C)=O
Bcary_171a[3]	$C_8H_{12}O_4$	4.56	1.17	17.74	CC1(C)CC(C(O)=O)C1C(O)=O
***Bcary_171b**[3]	$C_9H_{16}O_3$	7.09	1.82	27.59	CC1(C)CC(C(O)=O)C1CCO
Bcary_183a[3]	$C_{10}H_{16}O_3$	0.44	0.11	1.72	CC1(C)CC(C(O)=O)C1CCC=O
Bcary_183b[3]	$C_{10}H_{16}O_3$	7.20	1.85	28.02	CC1(C)CC(C(CC(O)=O)=C)C1O
Bcary_185[3]	$C_9H_{14}O_4$	6.59	1.69	25.63	CC1(C)CC(C(O)=O)C1CC(O)=O
***Bcary_197**[3]	$C_{11}H_{18}O_3$	0.54	0.14	2.11	CC1(C)CC(C(O)=O)C1CCC(C)=O
Bcary_199[3]	$C_{10}H_{16}O_4$	11.09	2.85	43.13	CC1(C(CCC(O)=O)C(C(O)=O)C1)C
Bcary_225[3]	$C_{12}H_{18}O_4$	11.44	2.94	44.51	CC1(C)CC(C(C(O)=O)=C)C1CCC(O)=O
***Bcary_237**[3]	$C_{14}H_{22}O_3$	0.45	0.12	1.75	CC1(C)CC(C(CCC=O)=C)C1CCC(O)=O
***Bcary_241**[3]	$C_{13}H_{22}O_4$	6.51	1.67	25.34	CC1(C)CC(C(CCO)=C)C1C(O)CC(O)=O
Bcary_251a[4]	$C_{14}H_{20}O_4$	0.67	0.17	2.63	CC1(C)CC2C1C=C(C(C)=O)OC2CCC(O)=O

***Bcary_251b**[3]	$C_{15}H_{24}O_5$	0.60	0.15	2.32	CC1(C)CC(C(CCC(O)=O)=C)C1CCC(C)=O
Bcary_253a[3]	$C_{14}H_{22}O_4$	0.74	0.19	2.86	CC1(C)CC(C(CCC(O)=O)=O)C1CCC(C)=O
***Bcary_253b**[3]	$C_{14}H_{22}O_4$	13.54	3.48	52.69	CC1(C)CC(C(CCC(O)=O)=C)C1CCC(O)=O
***Bcary_255a**[3]	$C_{13}H_{20}O_5$	9.08	2.33	35.31	CC1(C)CC(C(CCC(O)=O)=O)C1CCC(O)=O
Bcary_255b[4]	$C_{14}H_{24}O_4$	10.12	2.60	39.38	CC1(C)CC(C(CC(O)=O)=C)C1CCC(O)(O)C
Bcary_265[4]	$C_{15}H_{22}O_4$	0.77	0.20	3.00	CC1(C)CC(C(CCC(O)=O)=C)C1CCC(C=O)=O
Bcary_267a[4]	$C_{14}H_{20}O_5$	0.75	0.19	2.93	CC1(C)CC(C(CCC(O)=O)=O)C1CCC(C=O)=O
Bcary_267b[3]	$C_{15}H_{24}O_4$	0.72	0.18	2.79	CC1(CC(C1C(O)CC(C)=O)C(CCC(O)=O)=C)C
Bcary_267c[3]	$C_{15}H_{24}O_4$	11.36	2.92	44.18	CC1(C)CC(C(CCC(O)=O)=C)C1CCC(CO)=O
Bcary_269a[4]	$C_{14}H_{22}O_5$	5.71	1.47	22.22	CC1(C)CC(C(CCC(O)=O)=O)C1CCC(CO)=O
Bcary_269b[4]	$C_{15}H_{26}O_4$	10.68	2.74	41.54	CC1(C)CC(C(CCC(O)=O)=C)C1CCC(O)(O)C
Bcary_271a[4]	$C_{14}H_{24}O_5$	8.83	2.27	34.36	CC1(C)CC(C(CCC(O)=O)=O)C1CCC(O)(O)C
Bcary_271b[3]	$C_{14}H_{24}O_5$	5.43	1.40	21.14	CC1(C)CC(C(CCC(O)=O)=O)C1C(O)CC(O)=O
Bcary_271c[3]	$C_{14}H_{24}O_5$	0.64	0.16	2.49	CC1(C)CC(C(CCC(O)=O)=O)C1CCC(OO)=O
Bcary_283[4]	$C_{15}H_{24}O_5$	11.83	3.04	46.04	CC1(C)CC(C(CCC(O)=O)=C)C1CCC(C(O)O)=O
Bcary_285a[4]	$C_{14}H_{22}O_6$	0.85	0.22	3.31	CC1(CC(C1CCC(CO)=O)C(C(O)CC(O)=O)=O)C
Bcary_285b[4]	$C_{15}H_{26}O_5$	10.44	2.68	40.62	CC1(CC(C1CCC(O)(O)CO)C(CCC(O)=O)=C)C
Bcary_287a[3]	$C_{14}H_{24}O_6$	8.40	2.16	32.67	CC1(C)CC(C(CCC(OO)O)=C)C1C(O)CC(O)=O
Bcary_287b[3]	$C_{14}H_{24}O_6$	0.86	0.22	3.36	CC1(CC(C1C(CC(OC)=O)O)C(C(O)CCO)=O)C
Lim_157a[5]	$C_7H_{10}O_4$	0.63	0.16	2.43	CC(CC(CCC(O)=O)=O)=O
Lim_157b[5]	$C_7H_{10}O_4$	2.64	0.68	10.25	O=CCC(CC(O)=O)C(C)=O
Lim_157c[5]	$C_7H_{10}O_4$	1.59	0.41	6.18	O=CC(C(C)=O)CCC(O)=O
Lim_157d[5]	$C_7H_{10}O_4$	0.69	0.18	2.69	CC(CCC(CC(O)=O)=O)=O
Lim_171a[5]	$C_8H_{12}O_4$	1.58	0.41	6.16	OC(CCC(C(C)=O)CC=O)=O
Lim_171b[5]	$C_8H_{12}O_4$	2.91	0.75	11.33	OC(C(CC(CO)C(C)=C)=O)=O
***Lim_173a**[5]	$C_7H_{10}O_5$	5.00	1.28	19.44	OC(CCC(CCC(O)=O)=O)=O
Lim_173b[5]	$C_7H_{10}O_5$	3.21	0.82	12.48	OC(CC(C(C)=O)CC(O)=O)=O
Lim_173c[5]	$C_7H_{10}O_5$	1.37	0.35	5.32	OC(C(CC(CO)C(C)=O)=O)=O
***Lim_183**[6]	$C_{10}H_{16}O_3$	0.27	0.07	1.04	CC(CCC(C(C)=C)CC(O)=O)=O
***Lim_185a**[6]	$C_9H_{14}O_4$	0.69	0.18	2.68	CC(CCC(CC(O)=O)C(C)=O)=O
***Lim_185b**[6]	$C_9H_{14}O_4$	6.33	1.63	24.63	OC(CCC(C(C)=C)CC(O)=O)=O
***Lim_187a**[6]	$C_8H_{12}O_5$	5.11	1.31	19.87	OC(CCC(C(C)=O)CC(O)=O)=O
***Lim_187b**[6]	$C_8H_{12}O_5$	1.20	0.31	4.69	CC(C(CC(C(C)=O)C(O)=O)O)=O
***Lim_187c**[6]	$C_8H_{12}O_5$	0.71	0.18	2.76	OCCC(CC(C(O)=O)CC=O)=O
Lim_189[5]	$C_7H_{10}O_6$	5.29	1.36	20.59	OC(CC(CCC(O)=O)C(O)=O)=O
Lim_199a[5]	$C_{10}H_{16}O_4$	0.68	0.18	2.66	CC(CCC(C(CO)=C)C(C=O)O)=O
Lim_199b[5]	$C_{10}H_{16}O_4$	0.64	0.16	2.48	CC(C(O)CC(C(C=O)O)C(C)=C)=O
Lim_199c[5]	$C_{10}H_{16}O_4$	0.62	0.16	2.39	OCC(CC(C(C(C)=C)CC=O)O)=O
Lim_199d[5]	$C_{10}H_{16}O_4$	0.64	0.16	2.48	CC(C(CC(C(O)C=O)C(C)=C)O)=O
Lim_199e[5]	$C_{10}H_{16}O_4$	4.56	1.17	17.75	OCC(CCC(CC(O)=O)C(C)=C)=O
Lim_199f[5]	$C_{10}H_{16}O_4$	0.68	0.18	2.66	CC(CCC(C(CO)=C)C(O)C=O)=O
Lim_199g[5]	$C_{10}H_{16}O_4$	0.64	0.16	2.48	CC(C(O)CC(C(C=O)O)C(C)=C)=O
Lim_199h[5]	$C_{10}H_{16}O_4$	0.62	0.16	2.39	OCC(CC(C(C(C)=C)CC=O)O)=O
Lim_199i[5]	$C_{10}H_{16}O_4$	0.64	0.16	2.48	CC(C(CC(C(O)C=O)C(C)=C)O)=O
Lim_199j[5]	$C_{10}H_{16}O_4$	3.35	0.86	13.03	CC(CCC(C(C)=C)C(O)C(O)=O)=O
Lim_201a[5]	$C_9H_{14}O_5$	2.12	0.54	8.23	CC(C(CC(CC(O)=O)C(C)=O)O)=O

Lim_201b[5]	$C_9H_{14}O_5$	2.50	0.64	9.74	OCC(CCC(CC(O)=O)C(C)=O)=O
Lim_201c[5]	$C_9H_{14}O_5$	0.84	0.21	3.25	OOC(CC(C(C)=C)CCC(O)=O)=O
***Lim_203**[5]	$C_8H_{12}O_6$	5.31	1.37	20.67	OC(CC(CCCC(O)=O)C(O)=O)=O
Lim_213[5]	$C_{10}H_{14}O_5$	4.64	1.19	18.05	OC(CC/C(C)=C(CC(O)=O)/C(C)=O)=O
Lim_215[5]	$C_{10}H_{16}O_5$	0.48	0.12	1.85	CC(CCC(C(C)=C)C(C(O)=O)OO)=O
***Lim_339a**[5]	$C_{18}H_{28}O_6$	0.67	0.17	2.60	CC(CCC(C(OC(CC(CCC(C)=O)C(C)=O)=O)O)C(C)=C)=O
Lim_339b[5]	$C_{18}H_{28}O_6$	0.73	0.19	2.86	O=CC(C(C)=C)CCC(CC(C)(CCC(CC(O)=O)C(C)=O)O)=O
Lim_367a[6]	$C_{19}H_{28}O_7$	8.41	2.16	32.71	OC(CCC(CC(OCC(CCC(CC(O)=O)C(C)=C)=O)=C)C(C)=C)=O
Lim_367b[6]	$C_{19}H_{28}O_7$	7.70	1.98	29.95	CC(C(CCC(OCC(CCC(CC(O)=O)C(C)=C)=O)=O)CC(O)=O)=C

Table S4. Filter sampling start and end datetimes used for the quantification of BSOA markers.

Sample.ID	Start time	End time
150	24/05/2017 17:40	25/05/2017 08:29
151	25/05/2017 08:37	25/05/2017 11:30
152	25/05/2017 11:38	25/05/2017 14:30
153	25/05/2017 14:40	25/05/2017 17:31
154	25/05/2017 17:40	26/05/2017 08:33
155	26/05/2017 08:45	26/05/2017 11:20
156	26/05/2017 11:27	26/05/2017 14:31
157	26/05/2017 14:41	26/05/2017 17:30
159	27/05/2017 08:28	27/05/2017 11:22
160	27/05/2017 11:35	27/05/2017 14:20
161	27/05/2017 14:30	27/05/2017 17:20
162	27/05/2017 17:31	28/05/2017 08:24
163	28/05/2017 08:33	28/05/2017 11:24
164	28/05/2017 11:33	28/05/2017 14:23
165	28/05/2017 14:33	28/05/2017 17:28
166	28/05/2017 17:40	29/05/2017 08:26
167	29/05/2017 08:35	29/05/2017 11:26
168	29/05/2017 11:35	29/05/2017 14:39
169	29/05/2017 14:49	29/05/2017 17:26
170	29/05/2017 17:35	30/05/2017 08:25
171	30/05/2017 08:35	30/05/2017 11:24
172	30/05/2017 11:35	30/05/2017 14:24
173	30/05/2017 14:35	30/05/2017 17:18

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