Supplementary Information

Experimental data from SOA formation from chamber experiments

In this section we present detailed experimental information of chamber experiments for SOA formation gathered from literature for α-pinene, limonene and isoprene. For each study we explain important information on the way some parameters are calculated and what assumptions were made to develop our experimental datasets.

α-pinene

Experimental information collected regarding α-pinene oxidation for SOA formation derived from three different studies. In Kim et al. (2012) the oxidation time for α-pinene was 4–4.5 hours without specifying, so a 4.25-hour oxidation time is selected that corresponds to 15300 seconds. Temperature and RH varied throughout the experiments and O_3 concentrations were calculated based on the O_3/VOC ratio. In Liu et al. (2013) 30 degrees Celsius and 50 % relative humidity was established in all experiments. A 0.2 ppm level of ozone was also established in the chamber. The oxidation duration was 4 hours (14400 seconds). In Presto & Donahue (2006) no data on RH was available.

Study	Experiment number	VOC concentration [μg/m^3]	T [°C]	time [s]	RH [%]	OH [molecules/cm^3]	NO_x [ppb]	O_3 [ppm]	SOA measured [μg/m^3]
(Kim et al., 2012)	A-PIN1	363.46	42	15300	14	N/A	22	0.042	25
	A-PIN2	347.91	37	15300	15	N/A	22	0.042	26
	A-PIN3	574.79	33	15300	16	N/A	32	0.069	102
	A-PIN4	420.21	35	15300	17	N/A	96	0.045	18
	A-PIN5	642.31	37	15300	15	N/A	125	0.076	77
(Liu et al., 2013)	A-PIN6	854.29	30	14400	50	N/A	76.01	0.2	33.82
	A-PIN7	870.72	30	14400	50	N/A	77.1	0.2	65.10
	A-PIN8	799.53	30	14400	50	N/A	78.04	0.2	40.28
	A-PIN9	1188.35	30	14400	50	N/A	97.81	0.2	92.44
	A-PIN10	1171.92	30	14400	50	N/A	111.08	0.2	65.26
	A-PIN11	1122.63	30	14400	50	N/A	95.27	0.2	66.91
	A-PIN12	1182.87	30	14400	50	N/A	102.87	0.2	76.64
	A-PIN13	1144.54	30	14400	50	N/A	103.08	0.2	73.90
	A-PIN14	1418.35	30	14400	50	N/A	132.01	0.2	122.70
	A-PIN15	1330.73	30	14400	50	N/A	121.82	0.2	110.35
	A-PIN16	1347.16	30	14400	50	N/A	122.5	0.2	88.79
	A-PIN17	1610.02	30	14400	50	N/A	130.01	0.2	91.13
	A-PIN18	1352.63	30	14400	50	N/A	119.34	0.2	88.543
	A-PIN19	1599.07	30	14400	50	N/A	146.67	0.2	149.14
	A-PIN20	1631.92	30	14400	50	N/A	152.09	0.2	89.31
(Presto & Donahue, 2006)	A-PIN21	63.55	22	14400	N/A	N/A	26	0.22	0.21
	A-PIN22	35.43	22	14400	N/A	N/A	6	0.28	2.68
	A-PIN23	137.80	22	14400	N/A	N/A	5.3	0.34	10.70
	A-PIN24	64.68	22	14400	N/A	N/A	41	0.29	0.70
	A-PIN25	75.37	22	14400	N/A	N/A	5.5	0.26	6.43
	A-PIN26	246.36	22	14400	N/A	N/A	5	0.35	46.60

Table S1. Experimental information for α-pinene

Limonene

Experimental information regarding limonene oxidation for SOA formation was collected from two different studies. Hammes et al. (2019) performed experiments in chambers. In Table S2 it is shown that the experiments were performed under NO_x-free conditions. To account for that, in the model we used NO_x level of 0.0001 ppb to select a low NO_x Yield from GECKO-A model based on the NOx parameterization explained in section 3.2. Under Dry conditions we used a RH of 0%. In the study of Kim et al. (2012) no information for OH concentration could be attained. The O_3 levels were calculated based on the O_3/VOC ratio.

Study	Experiment number	VOC concentration [µg/m3]	T [°C]	time [s]	RH [%]	OH [molecules/cm^3]	NO_x [ppb]	O_3 [ppm]	SOA measured [µg/m^3]
(Hammes et al., 2019)	LIM1	84.94881	20	240	40	8.71E+06	NOx-free	0.4	2.6
	LIM2	226.5301	20	240	40	8.51E+06	NOx-free	0.4	4.2
	LIM3	849.4881	20	240	40	8.10E+06	NOx-free	0.4	32
	LIM4	84.94881	20	240	Dry	8.82E+06	NOx-free	0.4	0.04
	LIM5	226.5301	20	240	Dry	8.61E+06	NOx-free	0.4	0.8
	LIM6	849.4881	20	240	dry	7.48E+06	NOx-free	0.4	12
	LIM7	84.94881	20	240	40	1.64E+07	NOx-free	1	4.7
	LIM8	226.5301	20	240	40	1.61E+07	NOx-free	1	7.3
	LIM9	849.4881	20	240	40	1.56E+07	NOx-free	1	25
	LIM10	84.94881	20	240	Dry	1.66E+07	NOx-free	1	0.04
	LIM11	226.5301	20	240	Dry	1.64E+07	NOx-free	1	1.4
	LIM12	849.4881	20	240	dry	1.58E+07	NOx-free	1	19
	LIM13	84.94881	20	240	40	2.48E+07	NOx-free	5	4
	LIM14	226.5301	20	240	40	2.60E+07	NOx-free	5	10
	LIM15	849.4881	20	240	40	2.59E+07	NOx-free	5	56
	LIM16	84.94881	20	240	Dry	2.54E+07	NOx-free	5	4
	LIM17	226.5301	20	240	Dry	2.67E+07	NOx-free	5	5.7
	LIM18	849.4881	20	240	Dry	2.65E+07	NOx-free	5	22
(Kim et al., 2012)	LIM19	321.1613	37	18000	18	N/A	20	0.036	79.2
	LIM20	354.7917	31	18000	17	N/A	20	0.04	109
	LIM21	414.8333	35	18000	19	N/A	40	0.04	117
	LIM22	409.375	31	18000	21	N/A	56	0.038	136
	LIM23	388.2415	39	18000	14	N/A	78	0.032	103
	LIM24	382.9231	39	18000	14	N/A	115	0.03	110

Table S2. Experimental information for limonene

Isoprene

This section presents the experimental information gathered for the case of isoprene. In the study of Song et al. (2019) each experiment lasted 240 minutes (14400 seconds) and the O_3 concentration in the chamber was 0.005 ppm. Temperature was constant at 25 degrees celcius and the conditions were dry (<10% RH). In Xu et al. (2014) all the experiments were conducted under dry conditions (RH<5%) and at 25 degrees celcius. A full experiment cycle lasted 1200 minutes (72000 seconds). Before every experiment the chambers were filled with purified air so that the O_3 concentrations was less than 1 ppb. Kroll et al. (2005) conducted chamber experiments for isoprene oxidation and examined the formation of SOA. RH and Temperature was different for each experiment, and no information on OH

concentration was found. Brégonzio-Rozier et al. (2015) examined isoprene oxidation for SOA formation, with two different sets of experiments in terms of OH production, one from HONO and one from NO_x. The experiments from HONO had an average OH concentration of $4x10^6$ and the NO_x around $1.9x10^6$. The experiments lasted 7 hours (25200 seconds), the temperature ranged and the conditions were dry (<5% RH). Dommen et al. (2006) conducted 15-hour experimens and the RH ranged from 0-85%.

Study	Experiment number	VOC concentration [μg/m^3]	T [°C]	time [s]	RH [%]	OH [molecules/cm^3]	NO_x [ppb]	O_3 [ppm]	SOA measured [μg/m^3]
(Song et al., 2019)	ISO1	427.6403	25	14400	<10	1.78E+07	NOx-free	0.005	197.1
	ISO2	466.8963	25	14400	<10	1.49E+07	NOx-free	0.005	166.5
	ISO3	414.2765	25	14400	<10	1.13E+06	NOx-free	0.005	70.2
	ISO4	437.1063	25	14400	<10	9.89E+06	NOx-free	0.005	49.3
	ISO5	545.13	25	14400	<10	1.03E+07	NOx-free	0.005	88.9
	ISO6	235.8147	25	14400	<10	1.24E+07	NOx-free	0.005	48.9
	ISO7	108.0237	25	14400	<10	1.36E+07	NOx-free	0.005	17.4
	ISO8	89.64855	25	14400	<10	1.67E+07	NOx-free	0.005	4
	ISO9	40.09128	25	14400	<10	1.65E+07	NOx-free	0.005	2.9
(Xu et al., 2014)	ISO10	126.6773	25	72000	<5	1.04E+06	<0.01	<0.001	6.3
	ISO11	218.2747	25	72000	<5	8.20E+05	<0.01	<0.001	14.7
	ISO12	402.8616	25	72000	<5	4.40E+05	<0.01	<0.001	30.2
	ISO13	270.3377	25	72000	<5	4.64E+06	68.1	<0.001	19.7
	ISO14	254.4682	25	72000	<5	4.40E+06	114.8	<0.001	19.7
	ISO15	319.0597	25	72000	<5	3.58E+06	338.2	<0.001	27
	ISO16	293.7243	25	72000	<5	3.35E+06	466.2	<0.001	10.9
	ISO17	280.0821	25	72000	<5	2.72E+06	738.1	<0.001	4.2
(Kroll et al., 2005)	ISO18	707.6652	20.1	10800	42.4	N/A	242	0.07	11.9
	ISO19	283.2594	19.9	10800	47.3	N/A	240	0.004	4.4
	ISO20	141.1958	20.8	10800	46.6	N/A	213	0.01	0.9
	ISO21	70.57389	20.9	10800	41.1	N/A	202	0.025	0.5
	ISO22	495.1967	20.2	10800	44.2	N/A	240	0.119	5.5
	ISO23	1060.051	20.5	10800	49.5	N/A	239	0.213	16.3
	ISO24	211.0037	21.9	10800	48.1	N/A	255	0.032	2.3
	ISO25	169.2046	21.2	10800	43.1	N/A	249	0.024	1.5
(Brégonzio-Rozier et al., 2015)	ISO26	1348.101	18.1	25200	<5	4.00E+06	151	0.347	8.4
	ISO27	1433.425	16.4	25200	<5	4.00E+06	93	0.546	4.7
	ISO28	1389.462	16.6	25200	<5	4.00E+06	77	0.397	1.6
	ISO29	1316.706	20	25200	<5	4.00E+06	114	0.495	12.4
	ISO30	1292.034	21.1	25200	<5	4.00E+06	140	0.3	7.3
	ISO31	1313.121	20.8	25200	<5	4.00E+06	112	0.286	5.5
	ISO32	1299.783	21.9	25200	<5	4.00E+06	132	0.359	6.2
	ISO33	1273.809	21.4	25200	<5	4.00E+06	101	0.174	7.8
	ISO34	1257.499	20.6	25200	<5	4.00E+06	117	0.175	4.4
	ISO35	1252.966	21	25200	<5	4.00E+06	111	0.113	0.3
	ISO36	1225.105	24.3	25200	<5	4.00E+06	97	0.131	0.1

	ISO37	2372.511	18.3	25200	<5	1.90E+06	133	0.201	2.8
	ISO38	2399.036	17.5	25200	<5	1.90E+06	66	0.054	2.4
	ISO39	2273.292	19.7	25200	<5	1.90E+06	185	0.081	0.15
	ISO40	509.6928	20	54000	47	N/A	79	0.158	1
	ISO41	574.8203	20	54000	51	N/A	40	0.1	0.7
	ISO42	993.901	20	54000	52	N/A	166	0.214	5
	ISO43	1042.039	20	54000	84	N/A	144	0.175	3.7
	ISO44	1277.064	20	54000	51	N/A	169	0.192	12.9
	ISO45	1330.865	20	54000	53	N/A	80	0.203	10
(Domm	ISO46	1339.359	20	54000	<2	N/A	100	0.234	22.6
en et al.,	ISO47	1339.359	20	54000	9	N/A	115	0.25	9.2
2006)	ISO48	1359.181	20	54000	<2	N/A	162	0.235	16.8
	ISO49	1359.181	20	54000	52	N/A	178	0.257	9.6
	ISO50	1427.14	20	54000	<2	N/A	164	0.25	17.5
	ISO51	2367.24	20	54000	50	N/A	579	0.391	86.5
	ISO52	3128.948	20	54000	53	N/A	491	0.337	50.7
	ISO53	4859.072	20	54000	50	N/A	825	0.45	177.4
	ISO54	5026.138	20	54000	49	N/A	934	0.458	217

Table S3. Experimental information for isoprene

SOMA model experimental fitting

This section presents the multi variable linear regression analysis performed for experimental fitting of SOMA for the case of α-pinene, limonene, and isoprene. We show the regression graphs between SOA_{exp}/SOA_{orig} and O_{3exp}/O_{3gecko}, T_{exp}/T_{gecko} and RH_{exp}/RH_{gecko} for every compound taken from Tables S1–S3. Here, SOA_{orig} represents the SOA predicted by the model under initial experimental conditions without applying correction factors, while SOA_{exp} is the experimentally measured SOA. The aim of this analysis is to develop correction factors for the model's SOA yield parameter by assessing how the SOA_{orig}/SOA_{exp} ratio varies with changes in the O_{3exp}/O_{3gecko}, T_{exp}/T_{gecko} and RH_{exp}/RH_{gecko} ratios. GECKO–A assumes constant conditions of O_{3gecko}= 0.04 ppm, T_{gecko}= 25°C and RH_{gecko} =70% in SOA yield production. This approach addresses a key limitation of the current SOA model, which selects yield values based solely on NO_x levels. The resulting correction factors will enable the model to better account for varying environmental conditions, ultimately improving its ability to capture the effects of O_3, T, and RH on SOA formation.

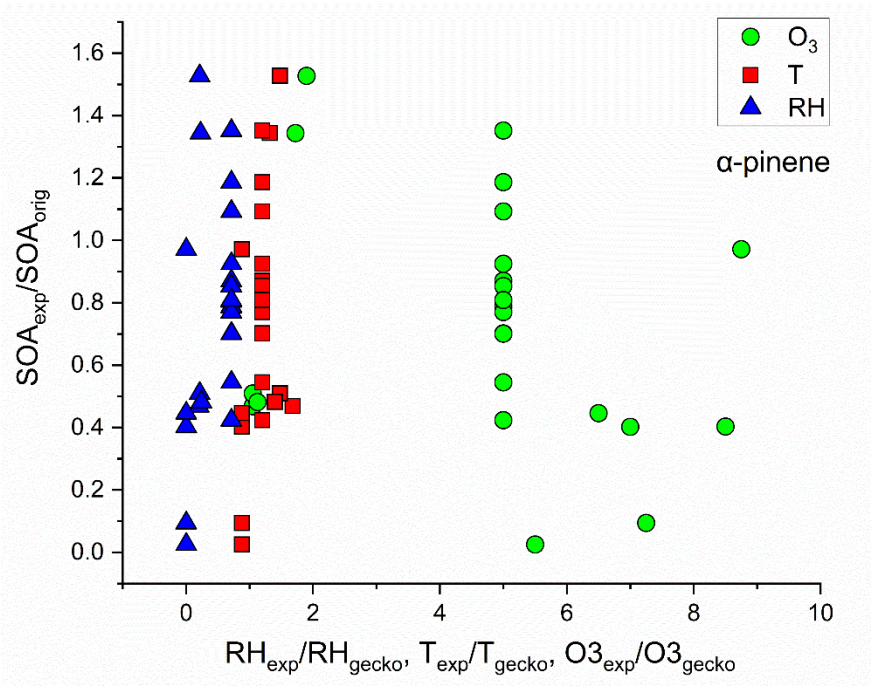

Figure S1. Regression analysis for α-pinene

Equation produced by multivariable linear regression analysis for the case of α-pinene:

$$\frac{SOA_{exp}}{SOA_{orig}} = -0.8 + 0.1 \times \frac{O_{3\,exp}}{O_{3\,gecko}} + 1 \times \frac{T_{exp}}{T_{gecko}} + 0.3 \times \frac{RH_{exp}}{RH_{gecko}} \quad (18)$$

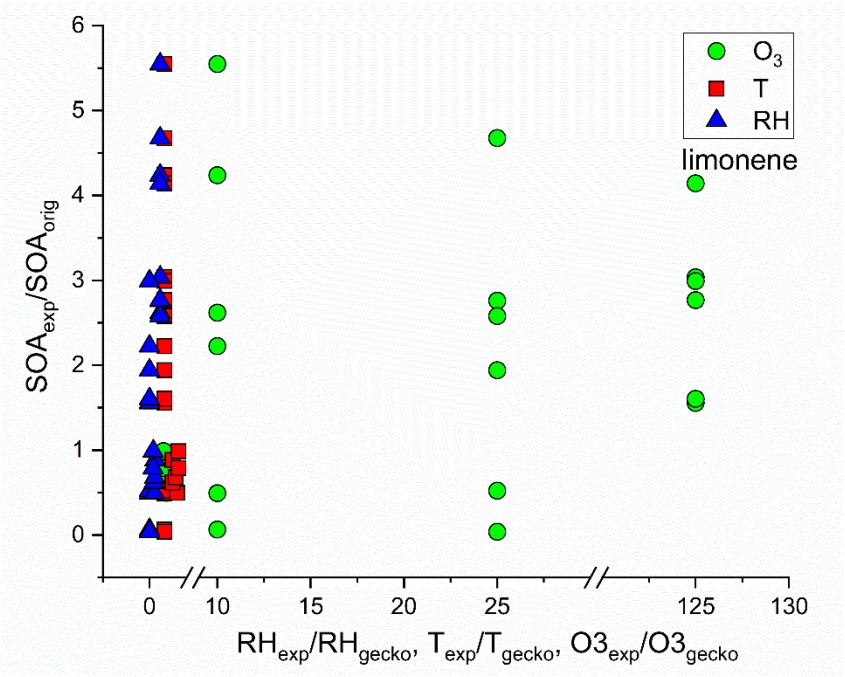

Figure S2. Regression analysis for limonene

Equation produced by multivariable linear regression analysis for the case of limonene:

$$\frac{SOA_{exp}}{SOA_{orig}} = 2.7 + 0.01 \times \frac{O_{3\,exp}}{O_{3\,gecko}} - 1.9 \times \frac{T_{exp}}{T_{gecko}} + 4 \times \frac{RH_{exp}}{RH_{gecko}} \quad (19)$$

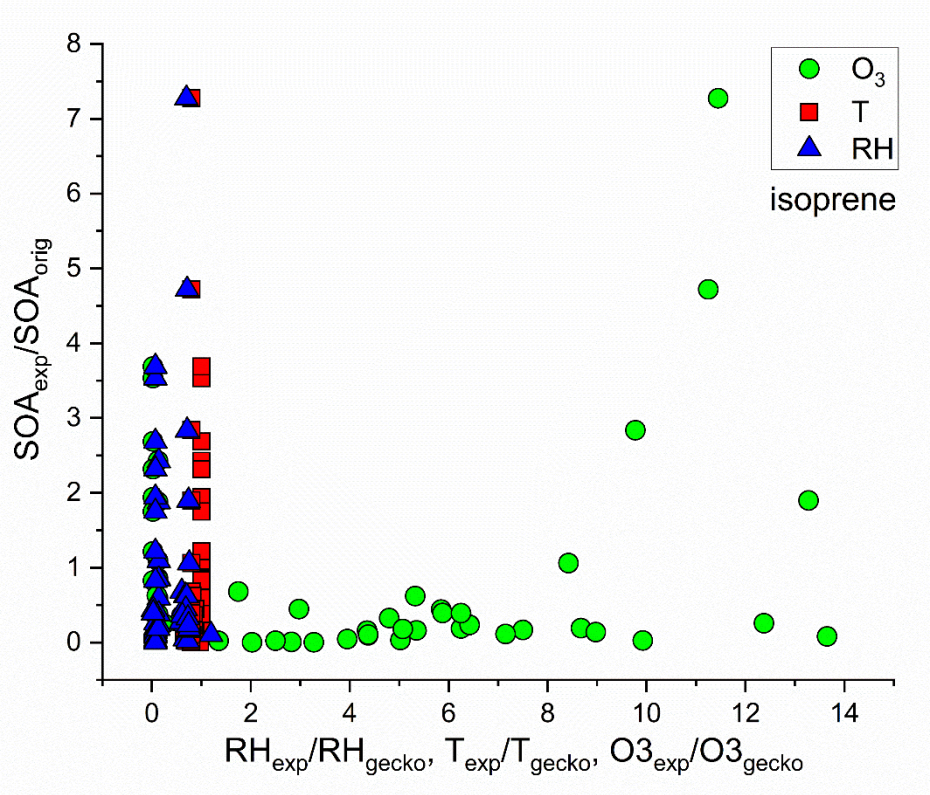

Figure S3. Regression analysis for isoprene

Equation produced by multivariable linear regression analysis for the case of isoprene:

$$\frac{SOA_{exp}}{SOA_{orig}} = -8.9 + 0.2 \times \frac{O_{3\,exp}}{O_{3\,gecko}} + 10.2 \times \frac{T_{exp}}{T_{gecko}} + 1.1 \times \frac{RH_{exp}}{RH_{gecko}} \qquad (20)$$

SOMA model calibration

This section presents the corrections applied to the SOMA for α-pinene, limonene and isoprene. Figure S4 illustrates the comparison between the experimental SOA values, the uncorrected model predictions, and the model outputs after incorporating corrections for O_3, RH, and T in the case of α-pinene. The deviation from the experimental data was 17% for the original model, which improved to 4% with the correction. Figure S5 compares the model outputs before and after corrections, with experimental results for limonene. The initial model showed a 14.2% deviation from experimental values, which was reduced to 13.7% after the correction. In Figure S6, the same analysis is conducted for isoprene. The original model exhibited an average 39% deviation from experimental data, which was reduced to 32% after the usage of correction factors derived from regression analysis. While the corrections for isoprene did not achieve the desired accuracy, incorporating additional experimental data could improve the calibration of the model for this compound.

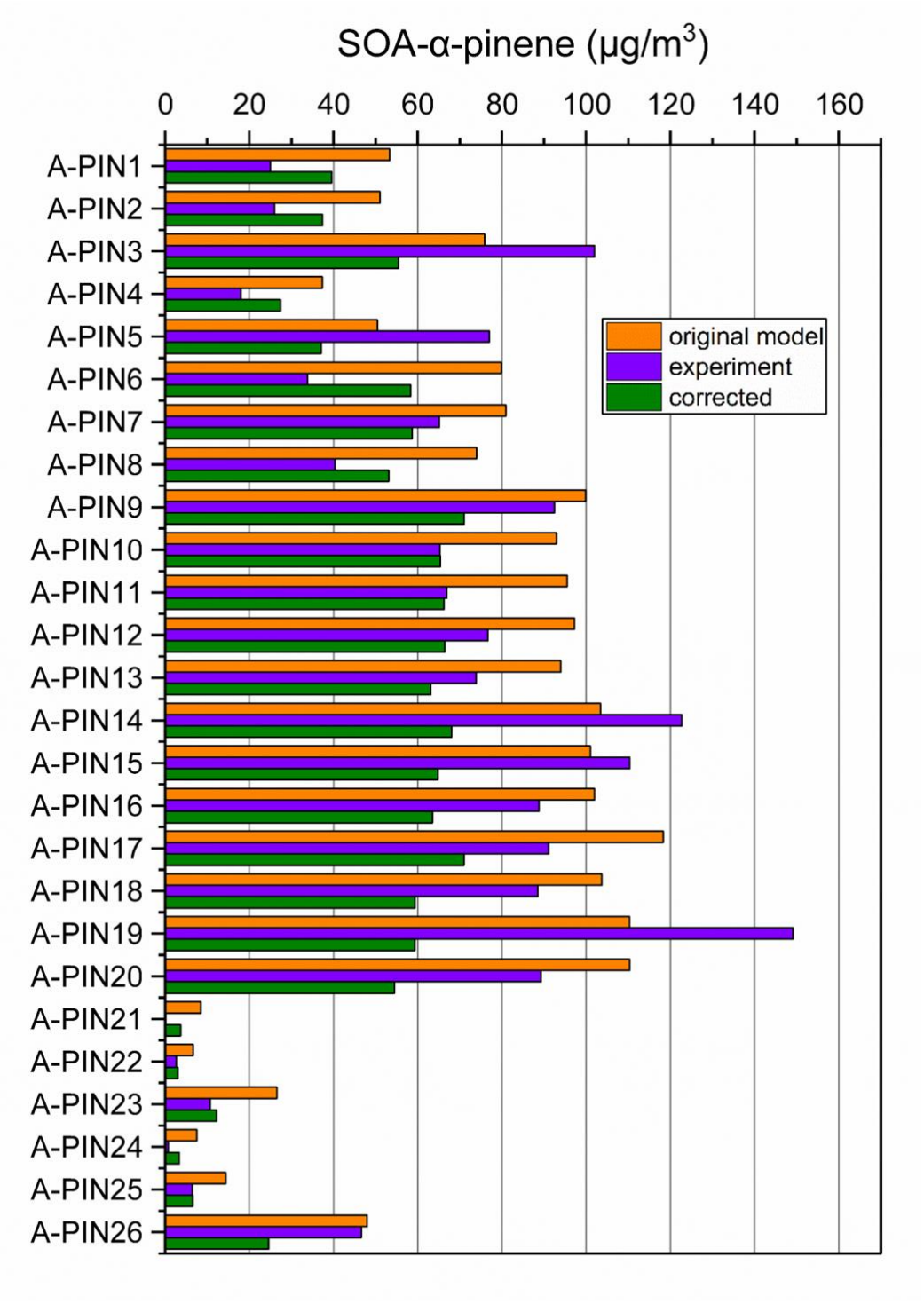

Figure S4. SOMA model correction for α-pinene

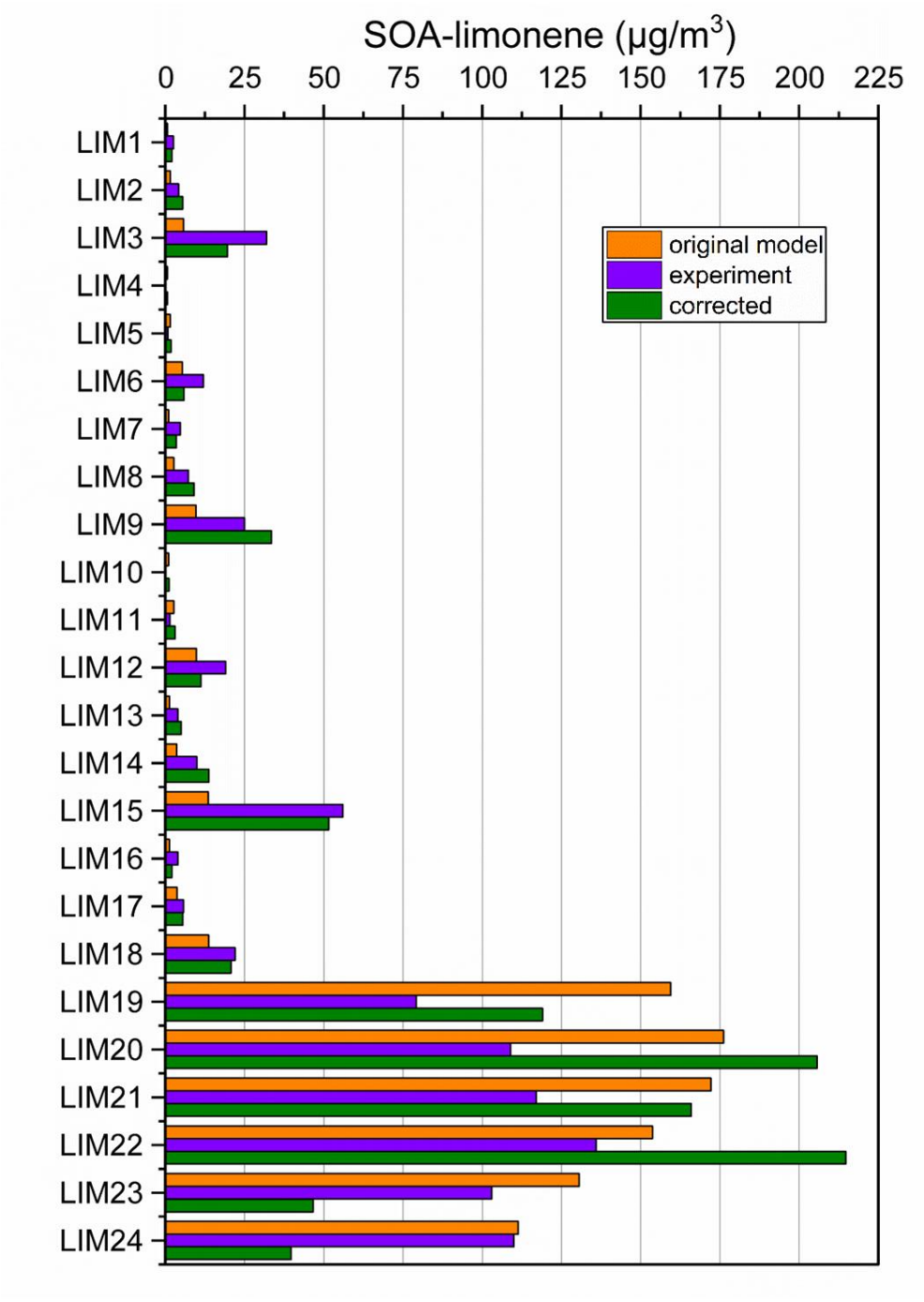

Figure S5. SOMA model correction for limonene

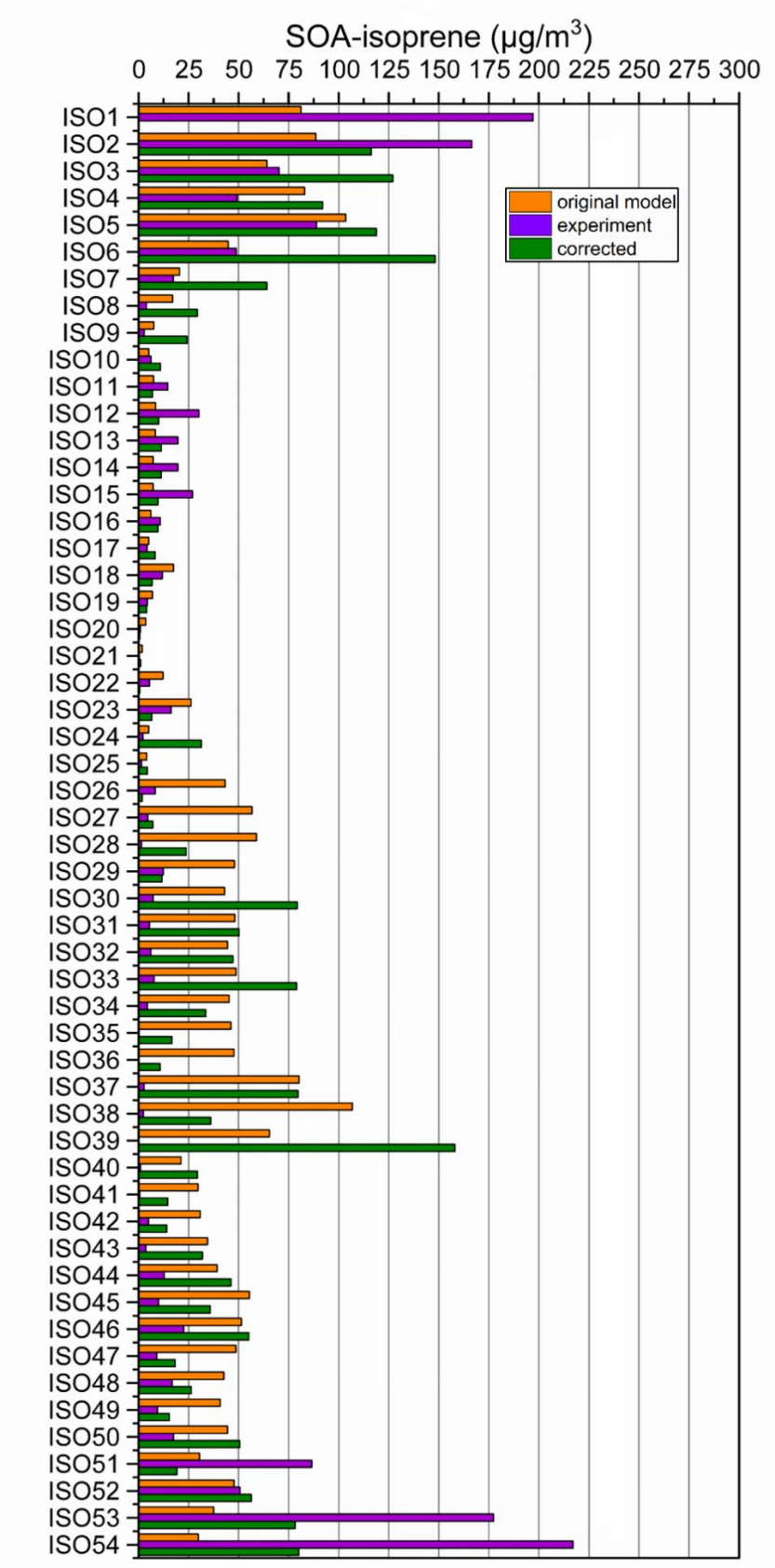

Figure S6. SOMA model correction for isoprene