COBRA: A Computational Brewing Application for Predicting the Molecular Composition of Organic Aerosols

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Supplementary Material

Table S1: Molecular formulas of constituents in isoprene high-NOx SOA detected by high-resolution negative ion mode ESI-MS, for comparison with molecular formulas predicted by COBRA. "Predicted structures" indicates the number of structural or stereo isomers predicted for each molecular formula.

Molecular Mass (Da)	Signal to Noise	# C	# H	# O	# N	Predicted structures
72.021	1.7	3	4	2	0	0
74.037	9.6	3	6	2	0	0
76.016	10.5	2	4	3	0	0
86.037	4.2	4	6	2	0	0
88.016	82.2	3	4	3	0	0
88.052	2.5	4	8	2	0	0
90.032	7.5	3	6	3	0	0
102.032	19.2	4	6	3	0	2
104.011	1.9	3	4	4	0	0
104.047	1.4	4	8	3	0	0
114.032	2.2	5	6	3	0	2
116.047	4.8	5	8	3	0	3
118.027	7.4	4	6	4	0	3
120.042	386.4	4	8	4	0	2
126.068	1.3	7	10	2	0	0
128.047	2.1	6	8	3	0	4
130.027	3.2	5	6	4	0	4
132.042	16.3	5	8	4	0	9
136.037	2.1	4	8	5	0	2
142.063	1.2	7	10	3	0	2
146.022	2.3	5	6	5	0	8
148.037	62.8	5	8	5	0	6
150.053	20.9	5	10	5	0	2
156.042	1.7	7	8	4	0	2
156.079	1.1	8	12	3	0	0
158.058	4	7	10	4	0	8
160.037	11.1	6	8	5	0	16
162.053	217.5	6	10	5	0	17
164.032	2.6	5	8	6	0	6
164.059	1.1	8	8	2	2	0
165.027	3.4	4	7	6	1	0

168.079	1.7	9	12	3	0	0
170.058	2.9	8	10	4	0	2
172.037	2.1	7	8	5	0	8
172.074	4.1	8	12	4	0	5
174.016	1.2	6	6	6	0	4
174.053	14.1	7	10	5	0	25
176.032	16.9	6	8	6	0	19
176.068	86.6	7	12	5	0	21
178.048	27.6	6	10	6	0	20
184.074	1.6	9	12	4	0	1
184.11	1.5	10	16	3	0	0
186.053	4	8	10	5	0	9
186.089	13.4	9	14	4	0	2
188.032	1.8	7	8	6	0	12
188.068	13	8	12	5	0	23
190.048	157.5	7	10	6	0	42
190.084	8.9	8	14	5	0	11
192.027	1.4	6	8	7	0	4
192.063	31.1	7	12	6	0	37
194.043	2.7	6	10	7	0	9
200.068	3.5	9	12	5	0	5
202.048	5.6	8	10	6	0	24
202.084	8.2	9	14	5	0	4
204.027	1.2	7	8	7	0	15
204.063	176.4	8	12	6	0	47
204.1	3.3	9	16	5	0	1
206.043	17.3	7	10	7	0	38
206.069	1.1	10	10	3	2	0
206.079	27.3	8	14	6	0	20
208.058	17.5	7	12	7	0	25
210.074	3.6	7	14	7	0	6
212.105	1.7	11	16	4	0	0
214.048	1.2	9	10	6	0	5
214.084	2.6	10	14	5	0	0
216.063	12.5	9	12	6	0	20
216.1	4.2	10	16	5	0	0
218.043	9.8	8	10	7	0	36
218.079	24	9	14	6	0	22
218.115	5.4	10	18	5	0	0
220.058	61.6	8	12	7	0	56

220.095	25.9	9	16	6	0	10
222.038	1.3	7	10	8	0	13
222.064	1.5	10	10	4	2	0
222.074	328.9	8	14	7	0	37
222.085	1.1	7	14	6	2	0
224.08	3.1	10	12	4	2	0
228.063	1	10	12	6	0	5
228.075	1.2	9	12	5	2	0
228.1	1.8	11	16	5	0	0
230.043	1.2	9	10	7	0	15
230.079	6	10	14	6	0	7
230.115	1.8	11	18	5	0	0
232.058	30.5	9	12	7	0	59
232.095	10.6	10	16	6	0	8
232.131	1.1	11	20	5	0	0
234.038	1.9	8	10	8	0	33
234.074	86.5	9	14	7	0	66
234.11	2.2	10	18	6	0	5
236.053	6.1	8	12	8	0	41
236.09	12	9	16	7	0	28
236.178	1.7	15	24	2	0	0
238.069	18.4	8	14	8	0	21
238.105	4.5	9	18	7	0	8
240.085	1	8	16	8	0	9
242.115	1	12	18	5	0	0
244.058	2.2	10	12	7	0	36
244.095	4.8	11	16	6	0	2
244.131	1.2	12	20	5	0	0
246.074	15.8	10	14	7	0	78
246.11	4.9	11	18	6	0	0
248.053	11.3	9	12	8	0	81
248.09	15.6	10	16	7	0	41
249.048	1.2	8	11	8	1	2
250.069	185.4	9	14	8	0	99
250.105	2.5	10	18	7	0	8
251.064	6.3	8	13	8	1	0
252.075	1.8	11	12	5	2	0
252.085	33.3	9	16	8	0	34
252.173	1.3	15	24	3	0	0
253.043	1.2	7	11	9	1	0

257.163	1	13	23	4	1	0
258.074	2.7	11	14	7	0	42
260.053	1.7	10	12	8	0	83
260.09	8	11	16	7	0	48
260.126	3.4	12	20	6	0	0
262.069	18	10	14	8	0	156
262.105	22.6	11	18	7	0	13
262.142	1.6	12	22	6	0	0
264.048	1.7	9	12	9	0	45
264.085	294.9	10	16	8	0	74
264.1	1.1	14	16	5	0	0
265.08	2.1	9	15	8	1	0
266.064	5.9	9	14	9	0	40
266.1	3.9	10	18	8	0	12
267.059	248.7	8	13	9	1	4
268.079	1.7	9	16	9	0	15
270.085	1.5	11	14	6	2	0
272.09	3.2	12	16	7	0	16
272.126	1.4	13	20	6	0	0
274.069	3.5	11	14	8	0	126
274.105	6.9	12	18	7	0	12
274.142	2.4	13	22	6	0	0
276.048	1	10	12	9	0	117
276.085	24.2	11	16	8	0	152
276.121	5.3	12	20	7	0	0
278.064	19.1	10	14	9	0	162
278.1	63.5	11	18	8	0	56
279.059	3.1	9	13	9	1	6
280.079	38.6	10	16	9	0	77
280.116	2.3	11	20	8	0	0
281.075	7.4	9	15	9	1	4
282.095	2.3	10	18	9	0	10
283.054	4.6	8	13	10	1	4
283.09	11.5	9	17	9	1	2
286.069	1.2	12	14	8	0	26
286.105	1.4	13	18	7	0	8
286.142	1.3	14	22	6	0	0
288.085	4.3	12	16	8	0	110
288.121	18.7	13	20	7	0	4
290.064	3	11	14	9	0	225

290.1	20.5	12	18	8	0	128
290.137	3	13	22	7	0	0
292.079	117.1	11	16	9	0	323
292.116	11.3	12	20	8	0	52
292.131	1.8	16	20	5	0	0
293.075	1.1	10	15	9	1	0
294.059	7	10	14	10	0	80
294.095	37.5	11	18	9	0	144
294.147	1.5	16	22	5	0	0
295.054	11.2	9	13	10	1	10
296.074	7	10	16	10	0	24
296.111	1.5	11	20	9	0	2
296.162	1.8	16	24	5	0	0
297.07	15.3	9	15	10	1	4
298.178	2.4	16	26	5	0	0
299.085	8.8	9	17	10	1	0
300.096	2.2	12	16	7	2	0
300.121	1.1	14	20	7	0	4
302.1	4.5	13	18	8	0	78
302.137	4.5	14	22	7	0	0
304.079	7	12	16	9	0	286
304.116	11.4	13	20	8	0	67
304.152	1.9	14	24	7	0	0
306.059	1.8	11	14	10	0	219
306.095	101.6	12	18	9	0	383
306.131	6.6	13	22	8	0	20
307.09	1.1	11	17	9	1	0
308.074	32.4	11	16	10	0	237
308.111	17.7	12	20	9	0	112
309.07	21.1	10	15	10	1	0
310.09	27.2	11	18	10	0	126
310.126	1.7	12	22	9	0	1
311.085	2.6	10	17	10	1	0
312.044	7.7	8	12	11	2	0
312.106	2.7	11	20	10	0	2
313.065	1.2	9	15	11	1	0
316.079	1.3	13	16	9	0	64
316.116	3.4	14	20	8	0	13
316.152	1.2	15	24	7	0	0
318.095	9.9	13	18	9	0	255

318.131	7.2	14	22	8	0	6
320.074	8.6	12	16	10	0	438
320.111	28	13	20	9	0	194
320.147	6.9	14	24	8	0	0
322.09	92.6	12	18	10	0	529
322.126	18.7	13	22	9	0	47
323.085	3.6	11	17	10	1	0
323.122	1.5	12	21	9	1	0
324.069	2.6	11	16	11	0	112
324.106	170.4	12	20	10	0	184
325.065	5.5	10	15	11	1	4
325.101	2.7	11	19	10	1	0
326.085	1.6	11	18	11	0	33
326.121	1.1	12	22	10	0	3
327.08	1.5	10	17	11	1	0
328.075	15.5	9	16	11	2	0
330.095	1.4	14	18	9	0	33
330.106	1.4	13	18	8	2	0
330.131	2.2	15	22	8	0	0
332.074	1.4	13	16	10	0	183
332.111	7.9	14	20	9	0	98
332.147	2.6	15	24	8	0	0
334.09	21.9	13	18	10	0	536
334.126	13.1	14	22	9	0	69
335.085	2	12	17	10	1	4
336.069	3.2	12	16	11	0	309
336.106	71	13	20	10	0	550
336.142	5.1	14	24	9	0	32
337.065	3	11	15	11	1	22
337.101	1.8	12	19	10	1	0
338.085	13.8	12	18	11	0	405
338.121	9.2	13	22	10	0	170
339.08	8.1	11	17	11	1	20
339.091	1.6	10	17	10	3	0
340.101	22.4	12	20	11	0	173
340.137	2.6	13	24	10	0	2
341.096	2.9	11	19	11	1	0
342.055	1.6	9	14	12	2	0
342.106	1.3	14	18	8	2	0
344.07	2.4	9	16	12	2	0

344.111	1.1	15	20	9	0	12
344.147	1.2	16	24	8	0	0
346.126	5.1	15	22	9	0	35
346.163	1.3	16	26	8	0	0
348.069	1	13	16	11	0	275
348.106	15.2	14	20	10	0	443
349.101	1.7	13	19	10	1	0
350.085	16.6	13	18	11	0	781
350.121	20.9	14	22	10	0	370
350.158	1.3	15	26	9	0	16
351.08	3.7	12	17	11	1	28
351.117	2.4	13	21	10	1	0
352.091	1.3	15	16	8	2	0
352.101	209.7	13	20	11	0	691
352.137	3.3	14	24	10	0	108
353.059	2	11	15	12	1	14
353.096	21.5	12	19	11	1	8
354.08	1	12	18	12	0	122
354.116	20.1	13	22	11	0	232
355.075	4.2	11	17	12	1	10
355.111	1.5	12	21	11	1	0
356.095	1	12	20	12	0	72
357.091	6.4	11	19	12	1	0
358.101	1.4	14	18	9	2	0
360.106	3	15	20	10	0	126
360.142	2.5	16	24	9	0	0
362.085	2.6	14	18	11	0	450
362.121	10.1	15	22	10	0	190
362.158	3.8	16	26	9	0	0
363.117	1.1	14	21	10	1	0
364.101	24.9	14	20	11	0	966
364.137	16.4	15	24	10	0	105
364.173	1.3	16	28	9	0	0
365.096	3.8	13	19	11	1	0
365.132	2.8	14	23	10	1	0
366.08	4.5	13	18	12	0	576
366.106	1.3	16	18	8	2	0
366.116	264.6	14	22	11	0	780
366.153	1.2	15	26	10	0	2
367.075	4.8	12	17	12	1	30

367.111	8.6	13	21	11	1	0
368.095	9.2	13	20	12	0	549
368.132	4	14	24	11	0	191
369.081	1.2	14	15	9	3	0
369.091	250.9	12	19	12	1	10
369.102	1	11	19	11	3	0
370.111	4	13	22	12	0	144
371.106	1.3	12	21	12	1	0
372.117	2.1	15	20	9	2	0
374.121	2.4	16	22	10	0	37
374.158	1.3	17	26	9	0	0
376.101	4.4	15	20	11	0	486
376.137	6.7	16	24	10	0	44
376.173	2.3	17	28	9	0	0
378.08	1.8	14	18	12	0	656
378.116	24.8	15	22	11	0	775
378.153	6.3	16	26	10	0	12
379.111	3	14	21	11	1	0
380.095	34.3	14	20	12	0	1204
380.132	41	15	24	11	0	518
381.091	9.7	13	19	12	1	30
381.127	5.4	14	23	11	1	0
382.096	1.2	10	22	15		0
382.111	44.3	14	22	12	0	1069
382.148	2.4	15	26	11	0	166
383.07	1.5	12	17	13	1	26
383.106	13.9	13	21	12	1	16
384.127	3.4	14	24	12	0	389
385.086	8.4	12	19	13	1	14
385.122	15.9	13	23	12	1	0
386.081	1.2	11	18	13	2	0
387.101	2.1	12	21	13	1	2
388.137	1.7	17	24	10	0	17
388.173	1	18	28	9	0	0
389.117	1.3	12	23	13	1	0
390.116	4	16	22	11	0	320
390.153	14.4	17	26	10	0	15
392.095	5.1	15	20	12	0	1037
392.132	16.8	16	24	11	0	440
392.168	3	17	28	10	0	0

393.127	1.4	15	23	11	1	0
394.111	134.7	15	22	12	0	1710
394.148	8.5	16	26	11	0	233
395.106	4.7	14	21	12	1	26
396.09	9.1	14	20	13	0	848
396.127	37.7	15	24	12	0	1166
397.086	25.2	13	19	13	1	54
397.122	2.7	14	23	12	1	16
398.106	6.7	14	22	13	0	693
398.142	1.6	15	26	12	0	272
399.101	27.2	13	21	13	1	22
401.117	16.7	13	23	13	1	0
402.153	1.1	18	26	10	0	6
404.132	3.7	17	24	11	0	158
404.168	3.5	18	28	10	0	2
406.111	8.2	16	22	12	0	1112
406.148	9.5	17	26	11	0	154
406.184	1.5	18	30	10	0	0
408.09	3.6	15	20	13	0	1294
408.127	73.5	16	24	12	0	1382
408.163	6.7	17	28	11	0	52
409.086	1.3	14	19	13	1	46
409.122	4.1	15	23	12	1	0
410.106	34.3	15	22	13	0	2007
410.142	13.5	16	26	12	0	726
411.101	40	14	21	13	1	44
411.138	1	15	25	12	1	0
412.122	20.1	15	24	13	0	1411
412.158	1.2	16	28	12	0	130
413.081	2.6	13	19	14	1	12
413.117	4.6	14	23	13	1	2
414.076	13	12	18	14	2	0
414.137	3.3	15	26	13	0	400
415.096	2.4	13	21	14	1	0
415.133	2.2	14	25	13	1	0
417.112	2.5	13	23	14	1	0
418.107	1.3	12	22	14	2	0
418.148	3.2	18	26	11	0	50
420.127	8	17	24	12	0	694
420.163	5.5	18	28	11	0	38

422.106	13	16	22	13	0	2017
422.142	20.3	17	26	12	0	757
422.179	5	18	30	11	0	8
423.101	2	15	21	13	1	18
424.122	81.4	16	24	13	0	2588
424.158	7.9	17	28	12	0	369
425.081	1.8	14	19	14	1	42
425.117	6.2	15	23	13	1	8
425.153	1.2	16	27	12	1	0
426.101	3.4	15	22	14	0	1313
426.137	94.7	16	26	13	0	1549
427.096	16.6	14	21	14	1	68
427.169	2	16	29	12	1	0
428.091	2.2	13	20	14	2	0
428.117	1.9	15	24	14	0	964
428.153	1.1	16	28	13	0	380
429.112	3.8	14	23	14	1	44
430.071	1.5	12	18	15	2	0
430.107	28.8	13	22	14	2	0
432.163	1.9	19	28	11	0	10
434.106	1.1	17	22	13	0	653
434.142	6	18	26	12	0	311
434.179	2	19	30	11	0	5
435.138	1.1	17	25	12	1	0
436.122	21.5	17	24	13	0	1685
436.158	9.5	18	28	12	0	321
436.194	1.2	19	32	11	0	0
437.117	2.3	16	23	13	1	12
437.153	1.1	17	27	12	1	0
438.101	4.6	16	22	14	0	2086
438.137	48.7	17	26	13	0	2038
438.174	4.3	18	30	12	0	170
439.096	6	15	21	14	1	96
440.117	14.4	16	24	14	0	2485
440.153	6	17	28	13	0	1110
441.112	14	15	23	14	1	76
441.148	1.1	16	27	13	1	0
442.071	1.1	13	18	15	2	0
442.132	17	16	26	14	0	1495
442.169	1.5	17	30	13	0	275

443.091	1.5	14	21	15	1	40
443.128	4.5	15	25	14	1	18
444.086	4	13	20	15	2	0
444.123	1.3	14	24	14	2	0
444.148	1.1	16	28	14	0	526
446.102	5.9	13	22	15	2	0
448.122	2.1	18	24	13	0	317
448.158	3.5	19	28	12	0	75
450.101	1.5	17	22	14	0	968
450.137	12.1	18	26	13	0	901
450.174	4.1	19	30	12	0	59
451.133	1.9	17	25	13	1	2
451.169	1	18	29	12	1	0
452.117	16.4	17	24	14	0	2425
452.153	15	18	28	13	0	983
453.112	5.4	16	23	14	1	52
453.148	2.8	17	27	13	1	0
454.132	128.6	17	26	14	0	2838
454.169	2.3	18	30	13	0	432
455.091	3.5	15	21	15	1	122
455.128	20.2	16	25	14	1	20
456.086	1.6	14	20	15	2	0
456.112	1.4	16	24	15	0	1271
456.148	17.2	17	28	14	0	1718
457.107	7.5	15	23	15	1	78
458.07	1.6	18	18	14	0	0
458.102	3	14	22	15	2	0
458.127	1.2	16	26	15	0	877
459.122	8.6	15	25	15	1	14
460.118	3.3	14	24	15	2	0
462.174	2	20	30	12	0	16
464.117	2.6	18	24	14	0	725
464.153	6.7	19	28	13	0	333
464.189	2.8	20	32	12	0	15
465.112	1	17	23	14	1	12
465.148	1.5	18	27	13	1	0
466.132	21.9	18	26	14	0	1818
466.169	8.9	19	30	13	0	313
468.112	4.5	17	24	15	0	1772
468.133	1.2	14	28	17	0	0

468.148	146.5	18	28	14	0	1974
468.159	1.1	17	28	13	2	0
469.107	7.2	16	23	15	1	142
470.127	7.3	17	26	15	0	2114
470.164	3	18	30	14	0	1003
471.122	162.1	16	25	15	1	118
471.134	1.8	15	25	14	3	0
472.081	1.1	14	20	16	2	0
472.143	4.1	17	28	15	0	1287
473.138	2.2	16	27	15	1	38
475.092	1.9	13	21	16	3	0
475.154	1.2	16	29	15	1	0
476.113	1.4	14	24	16	2	0
476.153	1.4	20	28	13	0	25
476.189	1	21	32	12	0	0
478.132	3.5	19	26	14	0	293
478.169	4.2	20	30	13	0	77
478.205	1.6	21	34	12	0	0
480.112	2.5	18	24	15	0	887
480.148	17.4	19	28	14	0	772
480.184	4.4	20	32	13	0	78
481.107	1.2	17	23	15	1	76
482.127	20.7	18	26	15	0	2004
482.164	19.8	19	30	14	0	760
483.122	11.5	17	25	15	1	132
484.143	29.7	18	28	15	0	2054
484.179	2	19	32	14	0	332
485.102	3.4	16	23	16	1	152
485.138	10.7	17	27	15	1	100
486.097	1.1	15	22	16	2	0
486.158	3.7	18	30	15	0	1054
487.117	7.6	16	25	16	1	132
487.154	8.2	17	29	15	1	32
488.113	2	15	24	16	2	0
489.133	3.1	16	27	16	1	74
491.149	1.7	16	29	16	1	8
492.148	2.7	20	28	14	0	71
492.184	6.7	21	32	13	0	0
492.221	1.1	22	36	12	0	0
494.127	4.7	19	26	15	0	484

494.164	9.8	20	30	14	0	196
494.2	2	21	34	13	0	0
495.122	1.4	18	25	15	1	24
496.143	67.9	19	28	15	0	995
496.179	5.8	20	32	14	0	177
497.102	1.3	17	23	16	1	114
498.122	7.1	18	26	16	0	1116
498.158	25.9	19	30	15	0	1060
499.117	21.7	17	25	16	1	210
500.138	5.1	18	28	16	0	1076
500.174	1.2	19	32	15	0	486