Method development and application for the analysis of chiral organic marker species in ice cores – Supplementary information

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Figure S1. Schematic experimental setup of the chamber experiments with α-pinene.

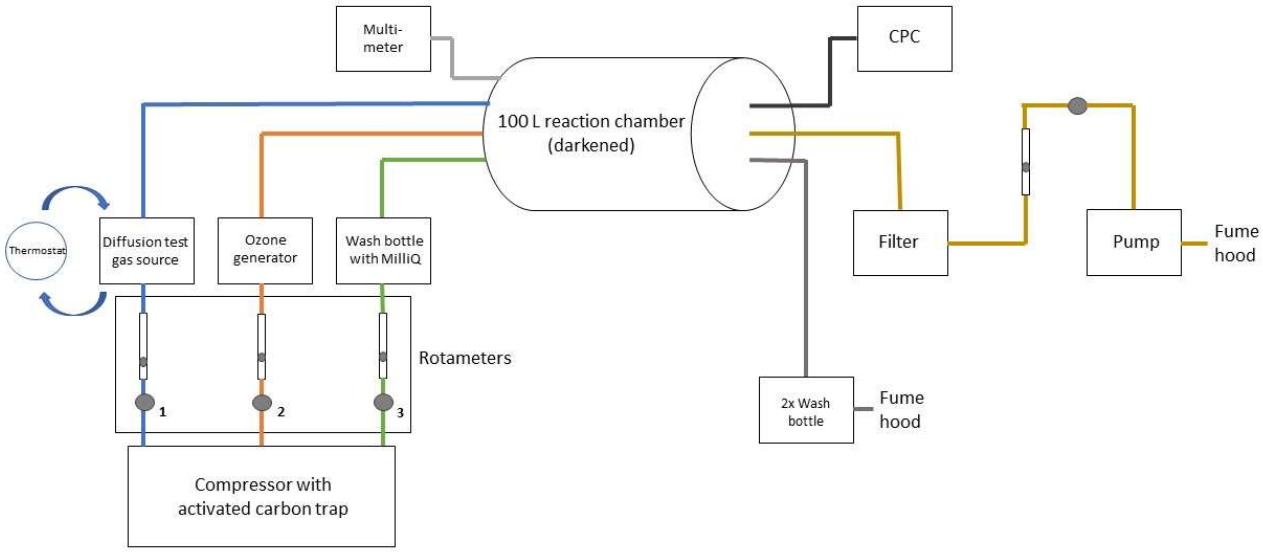

Table S1. Tested conditions during 1D-LC method development with the chiral column, with tested eluents, column oven temperature T, flowrate and flowrate of the PCF.

	Eluent A (%)	Eluent B (%)	*T* (°C)	Flowrate (μL/min)	Flowrate PCF (μL/min)
Eluent	98% H_2O, 20% ACN, 0.04%formic acid	98% ACN, 2% H_2O			50mM NH_4OH in MeOH
1	80	20	25	200	
2	90	10	25	200	
3	85	15	25	200	
4	85	15	30	200	
5	75	25	30	200	
6	80	20	30	150	
7	80	20	30	250	
8	75–>90	25–>10	30	200	
9	75–>80	25–>20	30	200	
10	80	20	40	200	
Eluent	MeOH	ACN			
1	10	90	30	200	
2	5	95	30	200	
3	2	98	30	200	
4	20	80	30	200	
5	50	50	30	200	
6	10	90	30	200	100
Eluent	IPA	ACN			
1	10	90	30	200	100
2	20	80	30	200	100
3	5	95	30	200	100
4	2	98	30	200	100
5	40	60	30	200	100

Table S2. Tested conditions during 2D-LC method development with the PFP (pump 1) and chiral column (pump 2), with eluent composition and flowrate of each pump, column oven temperature T, flow rate of the PCF and the tested time windows for peak transfer.

Sample loop volume (µL)	Pump 1 (PFP) B (%)	Pump 1 (PFP) Flowrate (µL/min)	Pump 2 (chiral) B (%)	Pump 2 (chiral) Flowrate (µL/min)	Temp (°C)	Pin t(cut) (min)	Pinon t(cut) (min)	PCF (µL/min)
100	20	300	20	200	40	1.75-2.00	2.55-2.80	
100	20	300	20	200	40	1.55-1.80	2.35-2.60	
100	20	300	20	200	40	1.45-1.70	2.35-2.60	
100	20	300	20	200	40	1.65-1.90	2.40-2.65	
100	20	300	20	300	40	1.65-1.90	2.40-2.65	
				while rinsing				
100	20	300	20	400	40	1.65-1.90	2.40-2.65	
				while rinsing				
50	20	300	20	200	40	1.70-1.85	2.45-2.60	
50	20	300	20	200	40	1.75-1.90	2.40-2.55	
50	20	300	20	200	40	1.725-1.875	2.425-2.575	
50	20	300	20	200	40	1.70-1.85	2.40-2.55	
				300 while rinsing				
50	20	300	20	300	40	1.70-1.85	2.40-2.55	
				400 while rinsing				
50	20	300	10	200	40	1.70-1.85	2.40-2.55	
50	20	300	10	400	40	1.70-1.85	2.40-2.55	
				200 at 5.5min				
50	20	300	15	350	40	1.70-1.85	2.40-2.55	
				200 at 5.5min				
50	20	300	20	200	40	1.70-1.85	2.40-2.55	100
50	20	300	10	400	40	1.70-1.85	2.40-2.55	100
				200 at 5.5min				
20	20	200	20	200	40	2.745-2.845	3.775-3.875	
20	20	200	20	200	40	2.75-2.85	3.75-3.85	
20	20	200	15	200	40	2.80-2.90	3.75-3.85	
20	20	200	15	200	40	2.65-2.75	3.75-3.85	
20	20	200	15	200	40	2.725-2.825	3.75-3.85	
20	20	200	15	200	40	2.70-2.80	2.77-3.87	
20	20	200	15	200	40	2.70-2.80	3.76-3.86	