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

Johanna Schäfer[1], Anja Beschnitt[1], Francois Burgay[2], Thomas Singer[2], Margit Schwikowski[2], Thorsten Hoffmann[1]

[1]Department of Chemistry, Johannes Gutenberg University, Mainz, 55099, Germany
[2]Laboratory of Environmental Chemistry (LUC), Paul Scherrer Institute, Villigen PSI, 5232, Switzerland

Correspondence to: Thorsten Hoffmann (t.hoffmann@uni-mainz.de)

Figure S1. Schematic experimental setup of the chamber experiments with α-pinene.
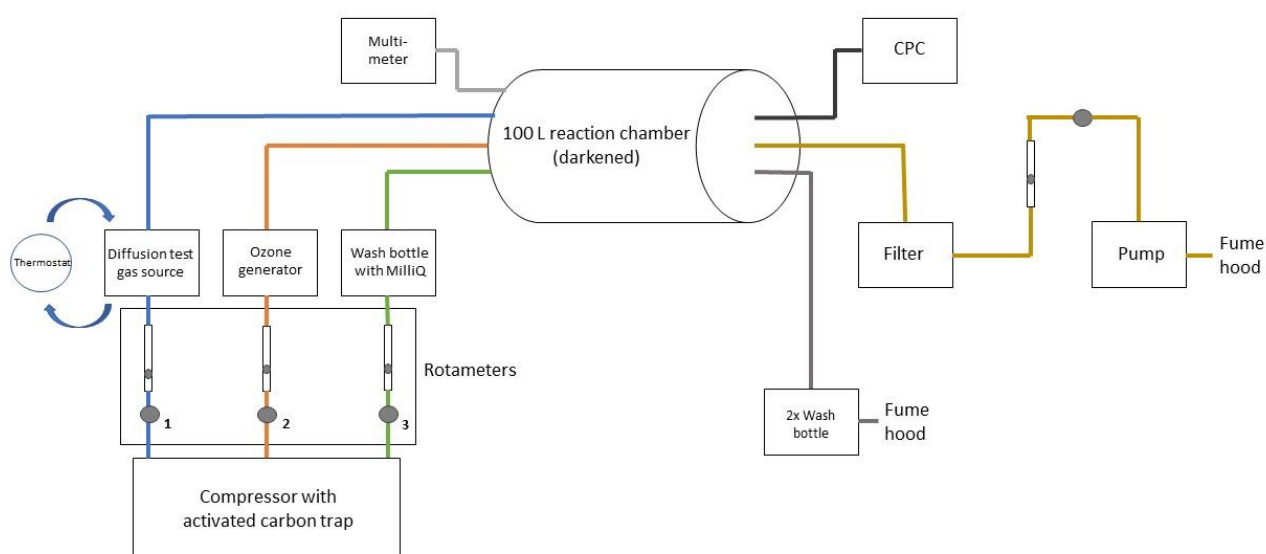
Table S1. Tested conditions during 1D-LC method development with the chiral column, with tested eluents, column oven temperature T, flowrate and flowrate of the PCF.

	Eluent A (%)	Eluent B (%)	T (˚C)	Flowrate (μL/min)	Flowrate PCF (μL/min)
Eluent	98% H$_2$O, 20% ACN, 0.04%formic acid	98% ACN, 2% H$_2$O			50mM NH$_4$OH 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 while rinsing	40	1.65-1.90	2.40-2.65	
100	20	300	20	400 while rinsing	40	1.65-1.90	2.40-2.65	
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	200 300 while rinsing	40	1.70-1.85	2.40-2.55	
50	20	300	20	300 400 while rinsing	40	1.70-1.85	2.40-2.55	
50	20	300	10	200	40	1.70-1.85	2.40-2.55	
50	20	300	10	400 200 at 5.5min	40	1.70-1.85	2.40-2.55	
50	20	300	15	350 200 at 5.5min	40	1.70-1.85	2.40-2.55	
50	20	300	20	200	40	1.70-1.85	2.40-2.55	100
50	20	300	10	400 200 at 5.5min	40	1.70-1.85	2.40-2.55	100
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	

Table S3. Dating and depth from the top of the ice core of the analysed Belukha ice core samples.

Depth (cm)	Age
3402.77	1962
3756.92	1953
4451.95	1936
4795.83	1927
5326.95	1912
6030.70	1888
6418.82	1873

Table S4. Accuracy (Acc.) of different concentrations (25 ppb, 50 ppb and 250 ppb) as percent relative deviation with respect to the standard concentration.

Compound	Acc.(25 ppb) (%)	Acc.(50 ppb) (%)	Acc.(250 ppb) (%)
Pinic acid E1	3.4	7.2	4.6
Pinic acid E2	5.6	7.4	5.4
Pinonic acid E2	14.0	6.4	4.1
Pinonic acid E2	9.6	7.1	5.3