Addition of a fast GC to SIFT-MS for analyses of individual monoterpenes in mixtures

Supplementary Material

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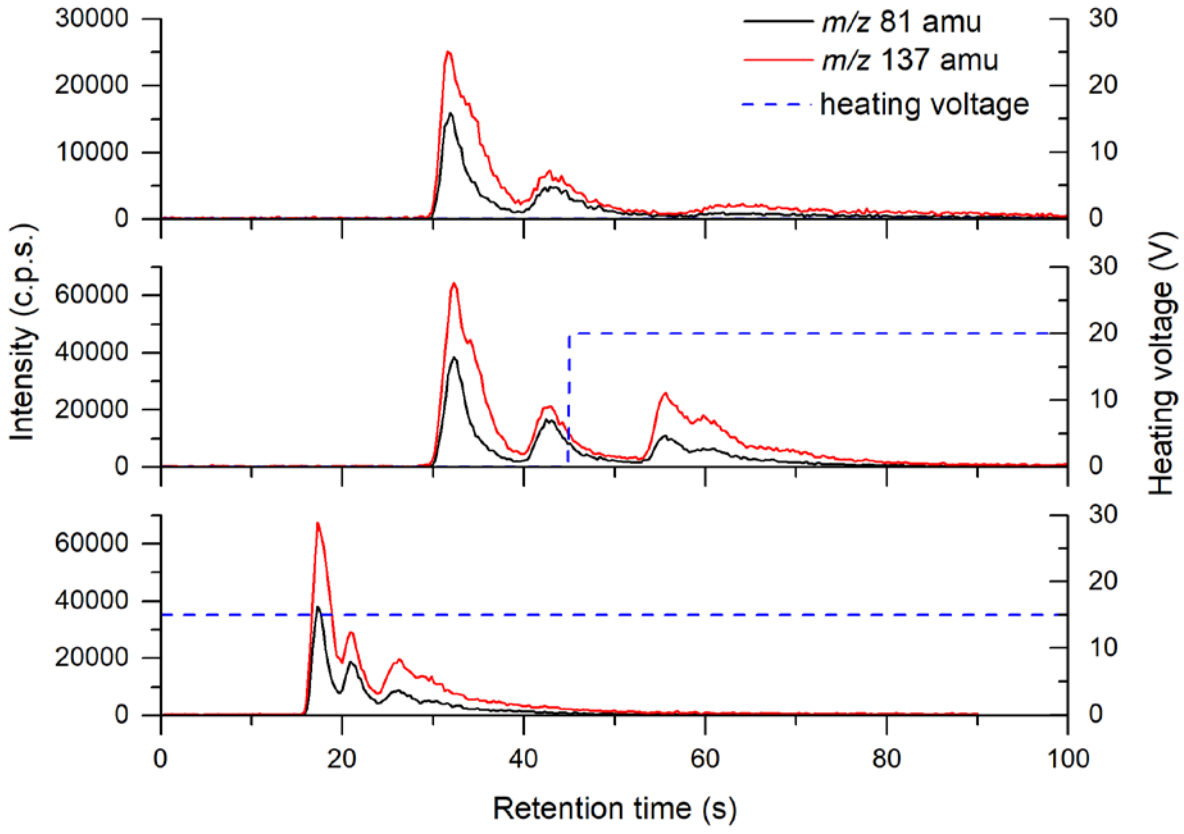

Figure S1: Chromatograms of a monoterpene mixture analysed by the MXT-1 column for different profiles of the heating voltage. Profiles were analysed by SIFT-MS using the H_3O^+ reagent ion.

Table S1: Summary of reaction rate constants and branching ratios of investigated monoterpenes. All presented rate constants have units of $10^{-9}cm^3s^{-1}$. Only significant products are given, for witch branching ratios are at least 10%.

	H_3O^+		NO^+		$O_2^{+\cdot}$	
	rate	Products (b.r.)	k	Products (b.r.)	k	Products (b.r.)
α-pinene	2.3[a], 2.4 [a*]	$C_6H_9^+$ (30[a], 39[b]), $C_{10}H_{17}^+$ (67[a], 61[b])	2.0[a], 2.0[a*], 2.3[b]	$C_7H_8^+$ (16[b]), $C_{10}H_{16}^+$ (85[a], 77[b])	2.0[a], 1.9[a*], 2.1[b]	$C_7H_8^+$ (18[a], 22[b]), $C_7H_9^+$ (52[a], 56[b]), $C_9H_{13}^+$ (12[a], 12[b])
β-pinene	2.4[a], 2.6 [a*]	$C_6H_9^+$ (33[a], 40[b]), $C_{10}H_{17}^+$ (64[a], 60[b])	2.1[a], 2.2[a*], 2.1[b]	$C_{10}H_{16}^+$ (93[a], 89[b])	2.1[a], 2.1[a*], 2.0[b]	$C_7H_9^+$ (56[a], 19[b]), $C_9H_{13}^+$ (49[b]), $C_{10}H_{16}^+$ (11[a])
R-limonene	2.6[a], 2.6[a*]	$C_6H_9^+$ (22[a], 29[b]), $C_{10}H_{17}^+$ (73[a], 68[b])	2.2[a], 2.2[a*], 2.2[b]	$C_{10}H_{16}^+$ (91[a], 89[b])	2.2[a], 2.1[a*], 2.2[b]	$C_5H_8^+$ (10[b]), $C_7H_8^+$ (10[b]), $C_7H_9^+$ (26[a], 30[b]), $C_7H_{10}^+$ (11[a], 12[b]), $C_8H_{11}^+$ (11[b]), $C_9H_{13}^+$ (14[a], 13[b]), $C_{10}H_{16}^+$ (11[a], 11[b])
3-carene	2.3[a], 2.4[a*]	$C_6H_9^+$ (19[a], 24[b]), $C_{10}H_{17}^+$ (78[a], 76[b])	2.1[a], 2.0[a*], 2.2[b]	$C_{10}H_{16}^+$ (86[a], 81[b])	2.0[a], 2.0[a*], 1.9[b]	$C_7H_8^+$ (11[b]), $C_7H_9^+$ (41[a], 45[b]), $C_9H_{13}^+$ (20[a], 20[b]), $C_{10}H_{16}^+$ (14[a])
myrcene	2.6[a], 2.7[a*]	$C_6H_9^+$ (26[a], 30[b]), $C_{10}H_{17}^+$ (59[a], 58[b])	2.3[a], 2.2[a*], 2.2[b]	$C_7H_8^+$ (11[b]), $C_7H_9^+$ (22[a], 34[b]), $C_{10}H_{16}^+$ (61[a], 55[b])	2.2[a], 2.2[a*], 2.2[b]	$C_5H_9^+$ (10[b]), $C_7H_8^+$ (70[b]), $C_7H_9^+$ (61[a])
camphene	2.4[a], 2.6[a*]	$C_6H_9^+$ (14[b]), $C_{10}H_{17}^+$ (88[a], 86[b])	2.1[a], 2.1[a*], 2.3[b]	$C_{10}H_{16}^+$ (87[a], 79[b]), $NO^+C_{10}H_{16}$ (11[b])	2.0[a], 2.1[a*], 2.2[b]	$C_7H_9^+$ (13[a], 19[b]), $C_8H_{11}^+$ (10[b]), $C_9H_{13}^+$ (44[a], 49[b])
α-terpinene		$C_6H_9^+$ (10[b]), $C_{10}H_{17}^+$ (87[b])	2.0[b]	$C_{10}H_{16}^+$ (87[a], 99[b]),	2.0[b]	$C_7H_9^+$ (16[b]), $C_9H_{13}^+$ (42[b]), $C_{10}H_{16}^+$ (33[b])
γ-terpinene		$C_6H_9^+$ (17[b]), $C_{10}H_{17}^+$ (81[b])	2.1[b]	$C_{10}H_{15}^+$ (18[b]), $C_{10}H_{16}^+$ (87[a], 75[b]),	1.9[b]	$C_7H_8^+$ (12[b]), $C_7H_9^+$ (46[b]), $C_9H_{13}^+$ (21[b]), $C_{10}H_{16}^+$ (14[b])

[a] (Schoon et al., 2003); [b] (Wang et al., 2003); [c] Present result based on SIFT-MS measurements; [d] Present result based on fastGC-SIFT-MS measurements; * theoretical data based on the method of Su and Chesnavitch (Su and Chesnavich, 1982); b.r. stands for branching ratio; Dimension of rate constants is $10^{-9}cm^3s^{-1}$.

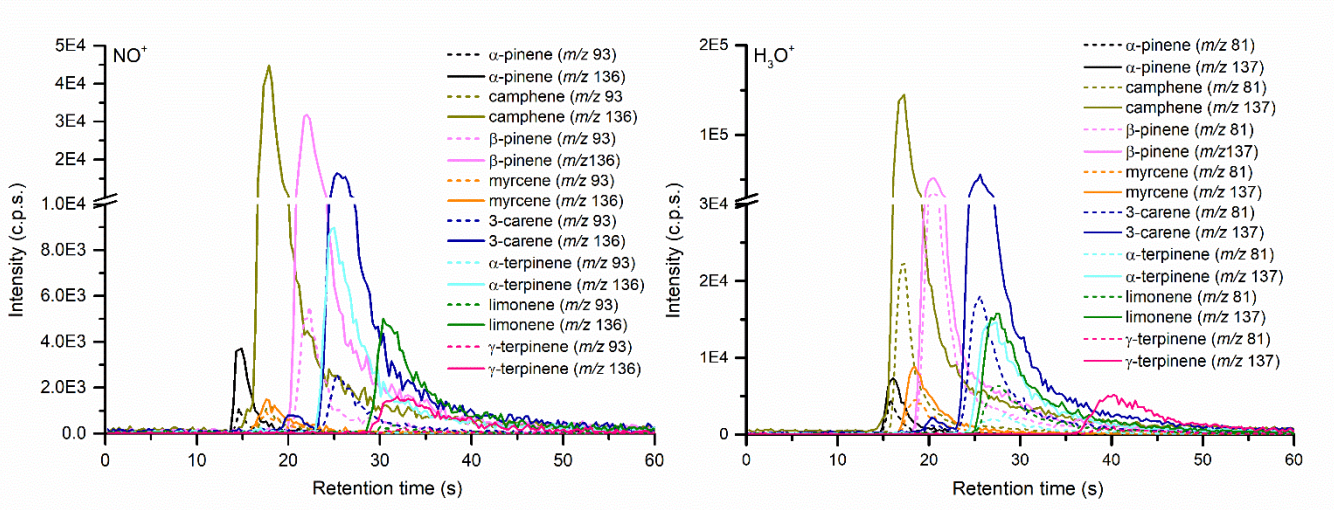

Figure S2: Chromatograms of individual monoterpenes analysed using the MXT-1 column at a constant temperature of column ~40 °C. The profile is associated with the profile shown in the bottom of Figure S1. Profiles were analysed by SIFT-MS using the H_3O^+ reagent ion. Intensity of α-pinene was reduced.

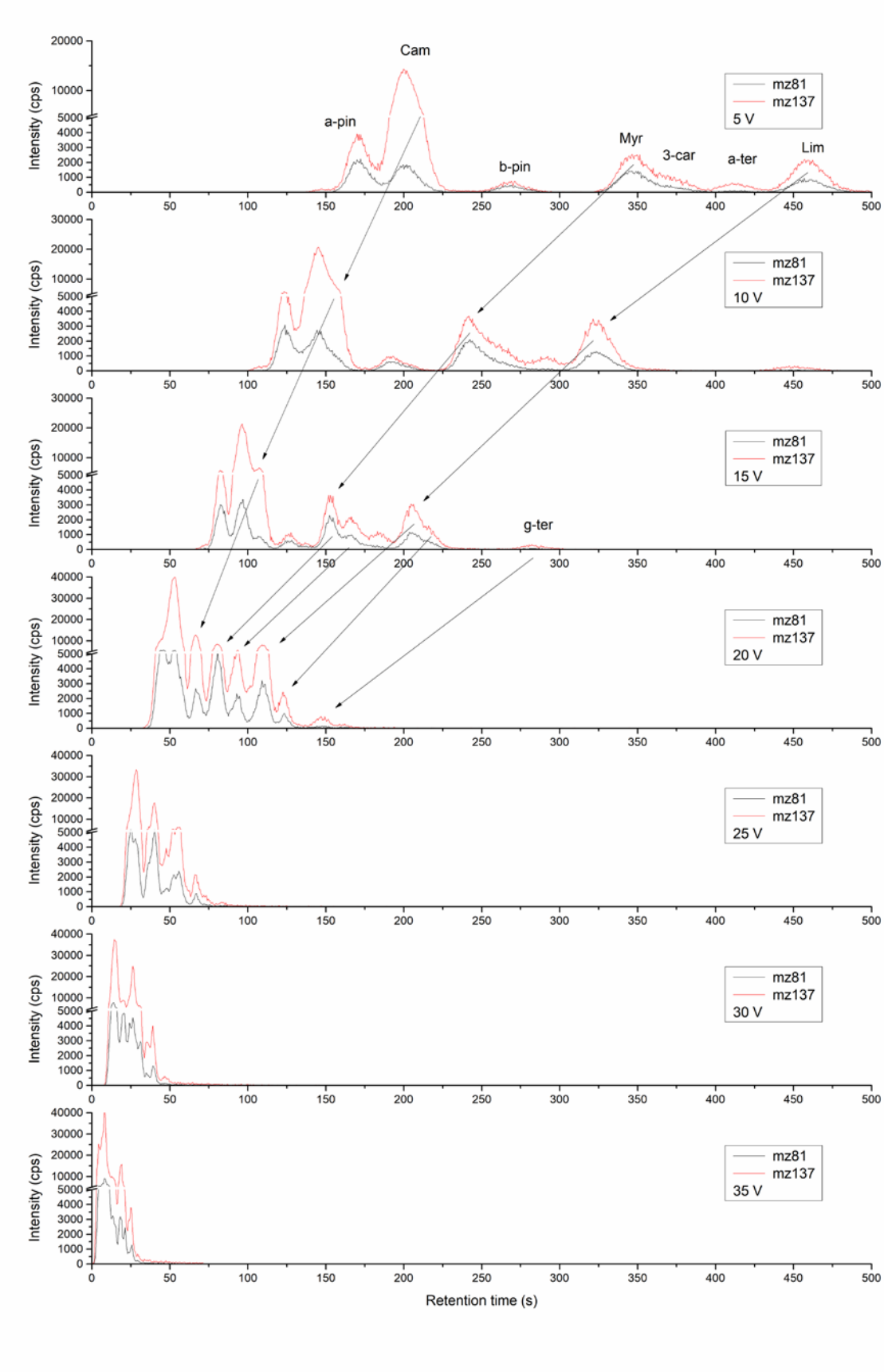

Figure S3: Chromatograms of a monoterpene mixture analysed by the MXT- Volatiles column for different heating voltages. Profiles were analysed by SIFT-MS using the H_3O^+ reagent ion.

Figure S4: Sample no. 1 (Pincea punges)

Figure S5: Sample no. 2 (Abies concolor)

Figure S6: Sample no. 3 (Pinus nigra)

References

Schoon, N., Amelynck, C., Vereecken, L., and Arijs, E.: A selected ion flow tube study of the reactions of H_3O^+, NO^+ and O_2^+ with a series of monoterpenes, International Journal of Mass Spectrometry, 229, 231-240, 2003.

Su, T., and Chesnavich, W. J.: Parametrization of the ion–polar molecule collision rate constant by trajectory calculations, The Journal of Chemical Physics, 76, 5183-5185, 1982.

Wang, T., Španěl, P., and Smith, D.: Selected ion flow tube, SIFT, studies of the reactions of H_3O^+, NO^+ and O_2^+ with eleven $C_{10}H_{16}$ monoterpenes, Int. J. Mass Spec., 228, 117-126, 2003.