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Addition of fast gas chromatography to selected ion flow tube mass spectrometry for analysis of individual monoterpenes in mixtures

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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^+**			**$O_2^{+\cdot}$**		
	k	*m/z*	Products (b.r.)	*k*	*m/z*	Products (b.r.)	*k*	*m/z*	Products (b.r.)
α-pinene	2.3^{a},	81	$C_6H_9^+$ (30^{a}, 39^{b}),	2.0^{a},	92	$C_7H_8^+$ (16^{b}),	2.0^{a},	92	$C_7H_8^+$ (18^{a}, 22^{b}),
	2.4^{a*}	137	$C_{10}H_{17}^+$ (67^{a}, 61^{b})	2.0^{a*},	136	$C_{10}H_{16}^+$ (85^{a}, 77^{b})	1.9^{a*},	93	$C_7H_9^+$ (52^{a}, 56^{b}),
				2.3^{b}			2.1^{b}	121	$C_9H_{13}^+$ (12^{a}, 12^{b})
β-pinene	2.4^{a},	81	$C_6H_9^+$ (33^{a}, 40^{b}),	2.1^{a},	136	$C_{10}H_{16}^+$ (93^{a}, 89^{b})	2.1^{a},	93	$C_7H_9^+$ (56^{a}, 19^{b}),
	2.6^{a*}	137	$C_{10}H_{17}^+$ (64^{a}, 60^{b})	2.2^{a*},			2.1^{a*},	121	$C_9H_{13}^+$ (49^{b}),
				2.1^{b}			2.0^{b}	136	$C_{10}H_{16}^+$ (11^{a})
R-limonene	2.6^{a},	81	$C_6H_9^+$ (22^{a}, 29^{b}),	2.2^{a},	136	$C_{10}H_{16}^+$ (91^{a}, 89^{b})	2.2^{a},	68	$C_5H_8^+$ (10^{b}),
	2.6^{a*}	137	$C_{10}H_{17}^+$ (73^{a}, 68^{b})	2.2^{a*},			2.1^{a*},	92	$C_7H_8^+$ (10^{b}),
				2.2^{b}			2.2^{b}	93	$C_7H_9^+$ (26^{a}, 30^{b}),
								94	$C_7H_{10}^+$ (11^{a}, 12^{b}),
								107	$C_8H_{11}^+$ (11^{b}),
								121	$C_9H_{13}^+$ (14^{a}, 13^{b}),
								136	$C_{10}H_{16}^+$ (11^{a}, 11^{b})
3-carene	2.3^{a},	81	$C_6H_9^+$ (19^{a}, 24^{b}),	2.1^{a},	136	$C_{10}H_{16}^+$ (86^{a}, 81^{b})	2.0^{a},	92	$C_7H_8^+$ (11^{b}),
	2.4^{a*}	137	$C_{10}H_{17}^+$ (78^{a}, 76^{b})	2.0^{a*},			2.0^{a*},	93	$C_7H_9^+$ (41^{a}, 45^{b}),
				2.2^{b}			1.9^{b}	121	$C_9H_{13}^+$ (20^{a}, 20^{b}),
								136	$C_{10}H_{16}^+$ (14^{a})
myrcene	2.6^{a},	81	$C_6H_9^+$ (26^{a}, 30^{b}),	2.3^{a},	92	$C_7H_8^+$ (11^{b}),	2.2^{a},	69	$C_5H_9^+$ (10^{b}),
	2.7^{a*}	137	$C_{10}H_{17}^+$ (59^{a}, 58^{b})	2.2^{a*},	93	$C_7H_9^+$ (22^{a}, 34^{b}),	2.2^{a*},	92	$C_7H_8^+$ (70^{b}),
				2.2^{b}	136	$C_{10}H_{16}^+$ (61^{a}, 55^{b})	2.2^{b}	93	$C_7H_9^+$ (61^{a})
camphene	2.4^{a},	81	$C_6H_9^+$ (14^{b}),	2.1^{a},	136	$C_{10}H_{16}^+$ (87^{a}, 79^{b}),	2.0^{a},	93	$C_7H_9^+$ (13^{a}, 19^{b}),
	2.6^{a*}	137	$C_{10}H_{17}^+$ (88^{a}, 86^{b})	2.1^{a*},	166	$NO^+C_{10}H_{16}$ (11^{b})	2.1^{a*},	107	$C_8H_{11}^+$ (10^{b}),
				2.3^{b}			2.2^{b}	121	$C_9H_{13}^+$ (44^{a}, 49^{b})
α-terpinene		81	$C_6H_9^+$ (10^{b}),	2.0^{b}	136	$C_{10}H_{16}^+$ (87^{a}, 99^{b}),	2.0^{b}	93	$C_7H_9^+$ (16^{b}),
		137	$C_{10}H_{17}^+$ (87^{b})					121	$C_9H_{13}^+$ (42^{b}),
								136	$C_{10}H_{16}^+$ (33^{b})
γ-terpinene		81	$C_6H_9^+$ (17^{b}),	2.1^{b}	135	$C_{10}H_{15}^+$ (18^{b}),	1.9^{b}	92	$C_7H_8^+$ (12^{b}),
		137	$C_{10}H_{17}^+$ (81^{b})		136	$C_{10}H_{16}^+$ (87^{a}, 75^{b}),		93	$C_7H_9^+$ (46^{b}),
								121	$C_9H_{13}^+$ (21^{b}),
								136	$C_{10}H_{16}^+$ (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 $10^{-9}cm^3s^{-1}$.

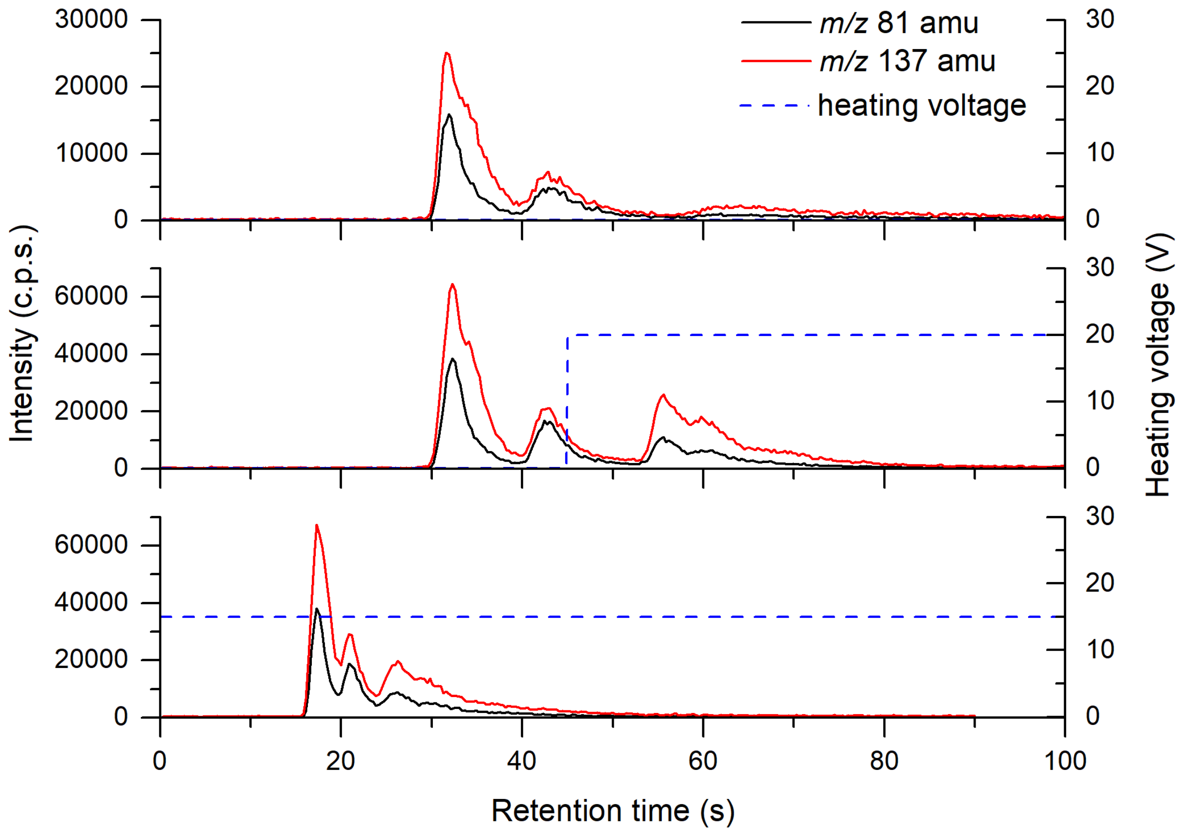

Figure S1: Chromatograms of a monoterpene mixture analysed by the MXT-1 column for different profiles of the heating voltage. Profiles were analysed by SIFT-MS using the H_3O^+ reagent ion.

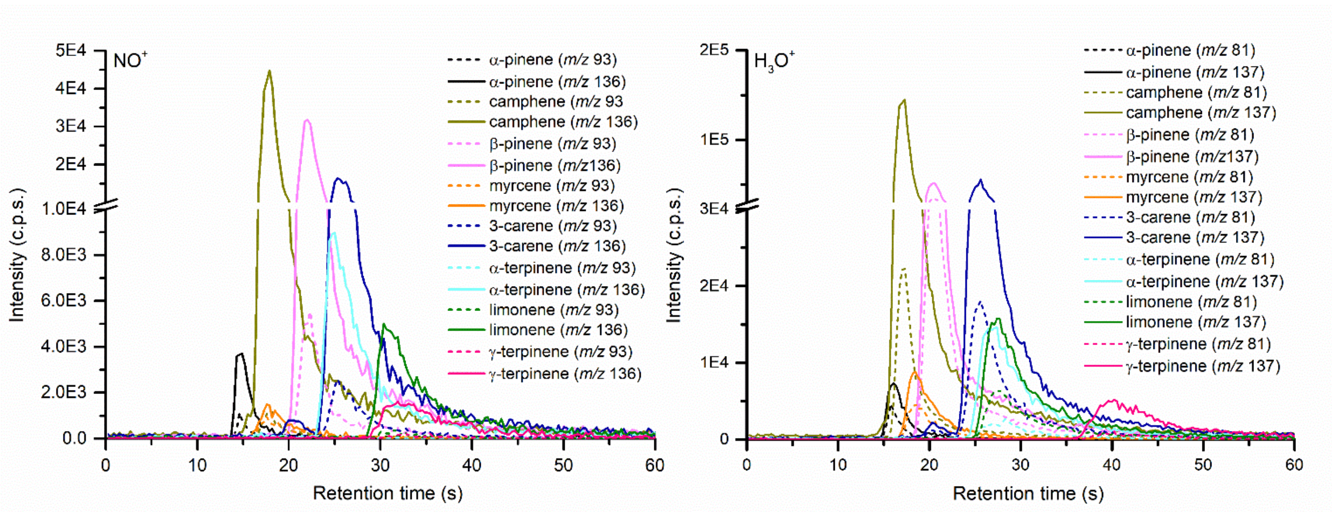

Figure S2: Chromatograms of individual monoterpenes analysed using the MXT-1 column at a constant temperature of column ~40 °C. The profile is associated with the profile shown in the bottom of Figure S1. Profiles were analysed by SIFT-MS using the H_3O^+ reagent ion. Intensity of α-pinene was reduced.

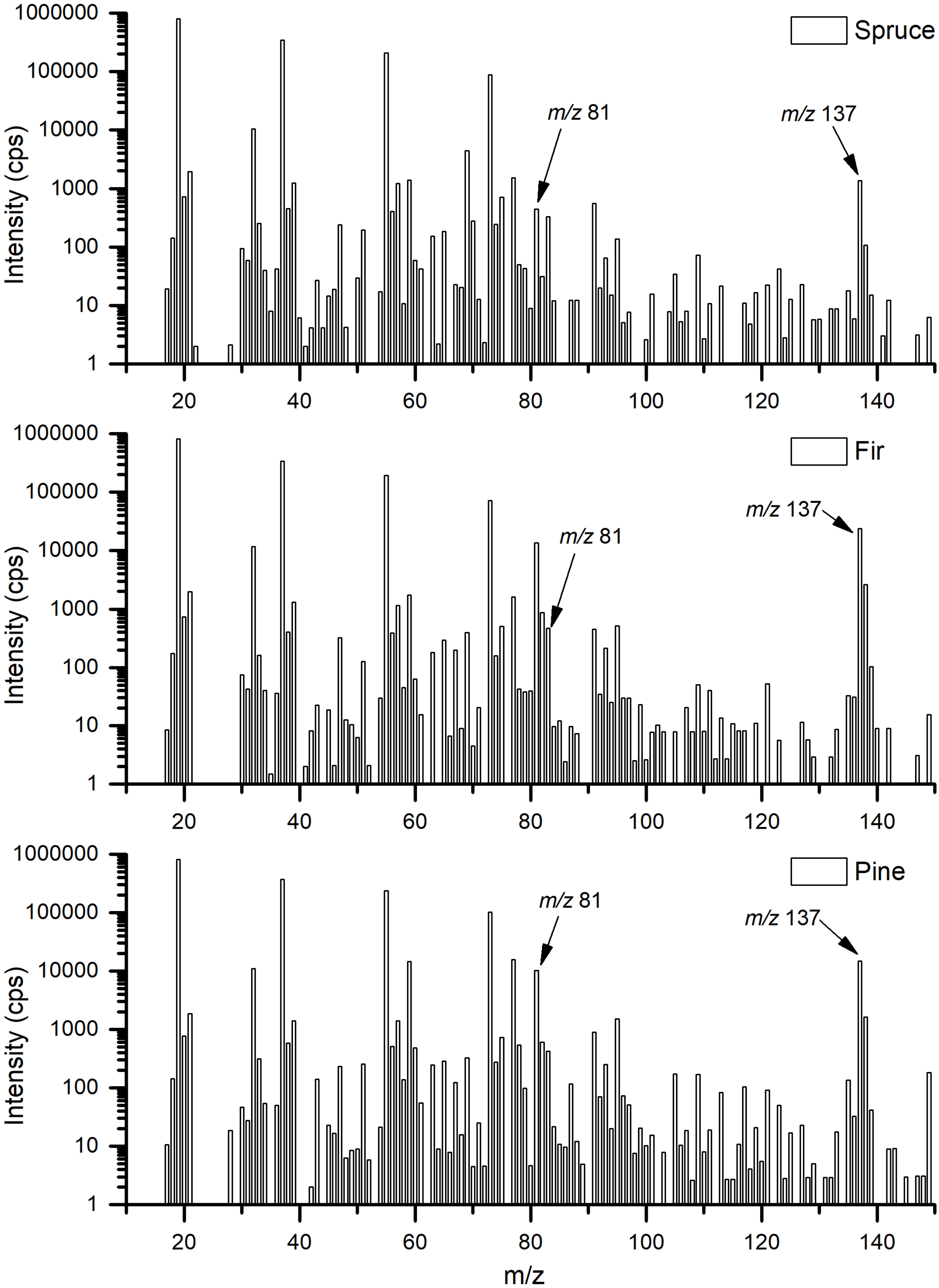

Figure S3: SIFT-MS spectra of coniferous samples analysed by H_3O^+ reagent ions. The marked ions with m/z 81 and m/z 137 were used for analysis of monoterpenes.

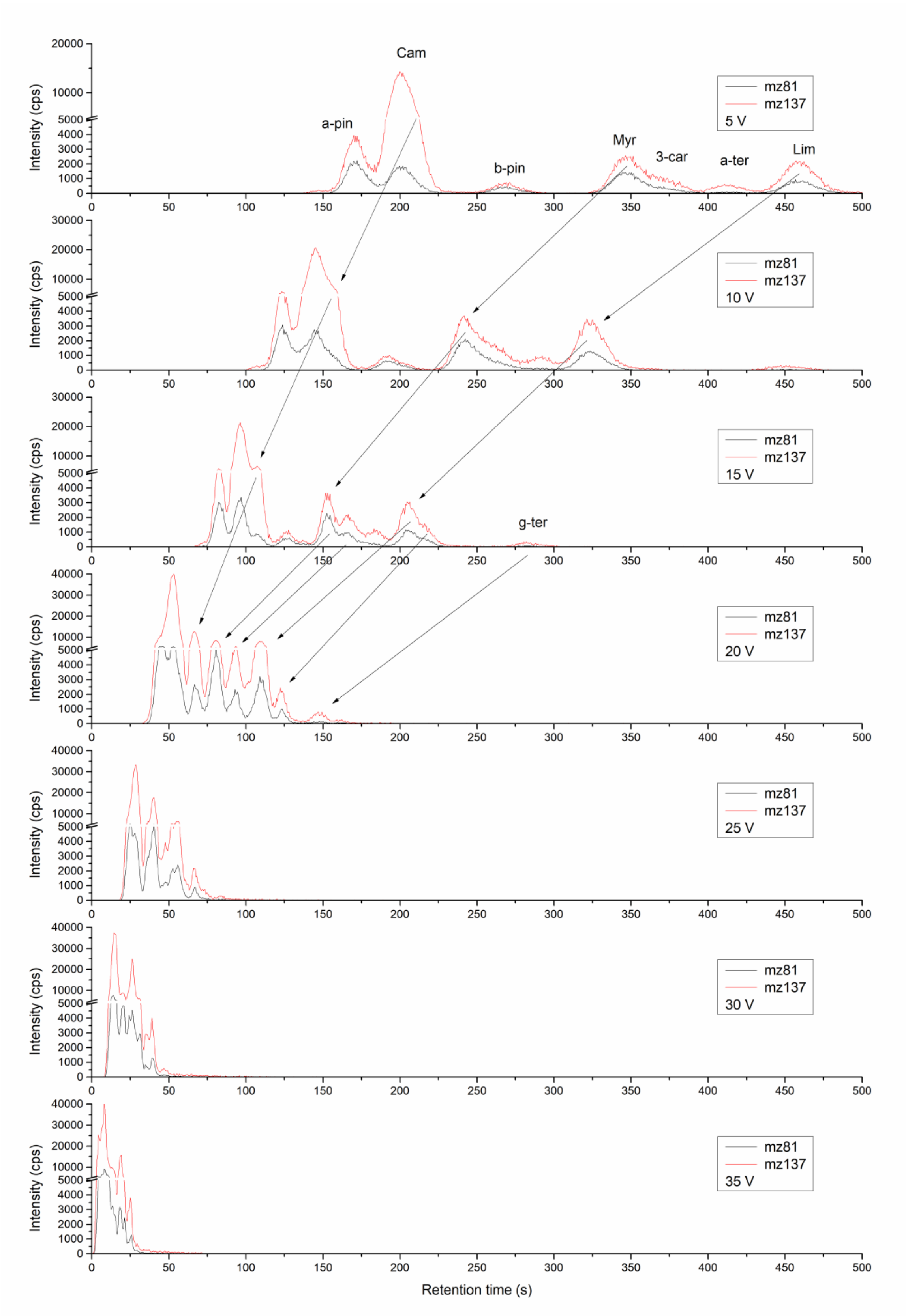

Figure S4: Chromatograms of a monoterpene mixture analysed by the MXT- Volatiles column for different heating voltages. Profiles were analysed by SIFT-MS using the H_3O^+ reagent ion.

Figure S5: Sample no. 1 (Pincea punges)

Figure S6: Sample no. 2 (Abies concolor)

Figure S7: Sample no. 3 (Pinus nigra)

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