

LC-MS/MS Evaluation of Pyrrolizidine Alkaloids Profile in Relation to Safety of Comfrey Roots and Leaves from Polish Sources

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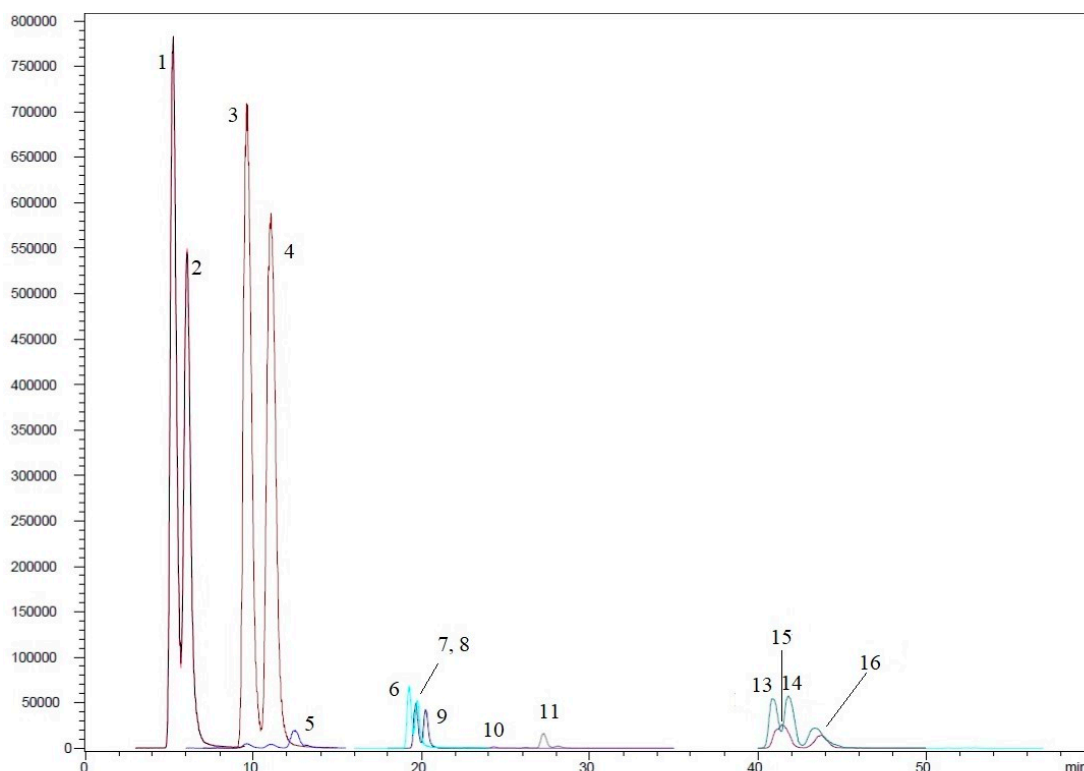


Figure S1: HPLC-MS/MS base peak chromatogram (MRM mode) of pyrrolizidine alkaloids present in methanol extract of comfrey (*Symphytum officinale*) root obtained from the herbal store (HR2) – the numbering of the peaks corresponds to numbers of PAs given in Table 1.

Table S1: Validation data for quantitative analysis of pyrrolizidine alkaloids by proposed HPLC-MS/MS method

Validation parameter		Intermedine	Lycopsamine	Intermedine N-oxide	Lycopsamine N-oxide
Correlation coefficients	Roots	0.9818-0.9923	0.9824-0.9984	0.9973-0.9997	_*
	Leaves	0.9810-0.9905	0.9909-0.9944	0.9901-0.9983	_*
LOD [$\mu\text{g/mL}$]	Roots	0.0026-0.0045	0.0028-0.0054	0.0027-0.0048	0.0026-0.0063
	Leaves	0.010-0.013	0.0028-0.0048	0.0032-0.0061	0.0026-0.0031
LOQ [$\mu\text{g/mL}$]	Roots	0.0086-0.015	0.0094-0.018	0.0089-0.016	0.0086-0.021
	Leaves	0.0030-0.0038	0.0094-0.016	0.0103-0.0204	0.0087-0.010
Recovery \pm CV [%] ¹	50%	105 \pm 12	111 \pm 3	112 \pm 11	-
	100%	117 \pm 22	112 \pm 8	114 \pm 12	-
Precision [CV%] ²	Intra-day	0.63	0.67	0.97	-
	Inter-day	1.18	0.98	1.00	-

*Results based on calibration curve for intermedine N-oxide; ¹Measured for comfrey leaf sample (HL2) (n-2); ²Measured for comfrey leaf sample (HL2) (intra-day: n-6, interday: n-3)

Table S2: Mean IC₅₀ values of intermedine, lycopsamine, intermedine N-oxide and lycopsamine N-oxide in HepD and HepG2 cells reported by Wang et al [12] calculated to $\mu\text{g/mL}$.

	HepD	HepG2
Intermedine	71.66	56.61
Lycopsamine	81.36	65.11
Intermedine N-oxide	49.11	46.43
Lycopsamine N-oxide	56.38	57.32