Supporting data 1 to the Manuscript:

Risk assessment of (herbal) teas containing pyrrolizidine alkaloids (PAs) based on margin of exposure approach and relative potency (REP) factors

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Supplemental tables

Table S1. Mass parameters for individual PA compounds.

Compound	Precursor ion (m/z)	Cone voltage (V)	Product ion 1 (m/z)	Product ion 2 (m/z)	Product ion 3 (m/z)	RT (min)
7-Acetylintermedine	342.2	30	120	180	94	8.80
7-Acetylintermedine N-oxide	358.2	30	137	214	180	5.90
7-Acetyllycopsamine	342.2	30	120	180	94	8.85
7-Acetyllycopsamine N-oxide	358.2	30	137	214	180	5.90
Acetylpetasitenine	424.2	30	122	168	150	9.10
Adonifoline	366.2	40	94	338	120	5.55
Amabiline	284.2	30	122	140	94	3.30
Atropine	290.2	40	124	93	94	4.15
Echimidine	398.2	30	120	220	83	10.55
Echimidine N-oxide	414.2	30	254	352	94	7.40
Echinatine	300.2	30	138	156	94	6.45
Echinatine N-oxide	316.2	30	111	172	94	3.75
Erucifoline	350.2	40	94	120	138	7.30
Erucifoline N-oxide	366.2	40	94	118	120	3.25
Europine	330.2	30	94	138	156	6.15
Europine N-oxide	346.2	30	172	111	256	3.55
Florosenine	424.2	30	122	168	150	8.40
Heliosupine	398.2	30	120	220	336	10.40
Heliosupine N-oxide	414.2	30	94	254	138	7.10
Heliotrine	314.2	30	138	156	94	8.10
Heliotrine N-oxide	330.2	30	111	172	94	5.50
Indicine N-oxide	316.2	30	94	172	111	3.55
Integerrimine	336.2	40	94	120	138	9.95
Integerrimine N-oxide	352.2	40	94	120	136	6.50
Intermedine	300.2	30	94	156	138	5.45
Intermedine N-oxide	316.2	30	94	172	111	3.40
Jacobine	352.2	40	120	155	94	7.65
Jacobine N-oxide	368.2	40	120	296	119	4.40
Jacoline	370.2	40	94	138	120	5.35
Jacoline N-oxide	386.2	40	94	120	138	2.60
Jaconine	388.2	40	94	120	138	8.75
Jaconine N-oxide	404.2	40	94	120	118	4.90
Lasiocarpine	412.2	30	120	220	336	11.25
Lasiocarpine N-oxide	428.2	30	138	254	94	8.25
Lycopsamine	300.2	30	94	156	138	5.50

Lycopsamine N-oxide	316.2	30	94	172	111	3.45
Merenskine	388.2	40	94	120	138	9.05
Merenskine N-oxide	404.2	40	94	120	118	5.10
Merepoxine	352.2	40	94	120	138	8.20
Merepoxine N-oxide	368.2	40	94	120	119	5.00
Monocrotaline	326.2	40	94	120	121	5.60
Monocrotaline N-oxide	342.2	40	120	137	94	2.45
Neosenkirkine	366.2	30	122	168	150	6.85
Otosenine	382.2	30	122	168	150	4.55
Petasitenine	382.2	30	122	168	150	5.90
Retrorsine	352.2	40	94	120	138	8.55
Retrorsine N-oxide	368.2	40	94	120	119	5.40
Riddelliine	350.2	40	94	120	138	7.80
Riddelliine N-oxide	366.2	40	94	118	120	4.50
Rinderine	300.2	30	138	156	94	6.60
Rinderine N-oxide	316.2	30	111	172	94	3.85
Sceleratine	370.2	40	94	138	120	5.75
Sceleratine N-oxide	386.2	40	94	120	138	2.80
Scopolamine	304.2	30	138	156	94	2.95
Senecionine	336.2	40	94	120	138	10.25
Senecionine N-oxide	352.2	40	94	120	136	6.70
Seneciphylline	334.2	40	120	138	94	9.25
Seneciphylline N-oxide	350.2	40	94	138	118	5.80
Senecivernine	336.2	40	94	120	138	10.40
Senecivernine N-oxide	352.2	40	94	120	136	6.75
Senkirkine	366.2	30	122	168	150	7.00
Spartioidine	334.2	40	120	138	94	8.95
Spartioidine N-oxide	350.2	40	94	120	118	5.70
Supinine	284.2	30	122	140	110	6.90
Supinine N-oxide	300.2	30	120	156	140	4.95
Trichodesmine	354.2	40	120	222	121	8.65
Trichodesmine N-oxide	370.2	40	137	238	94	5.30
Usaramine	352.2	40	94	120	138	8.30
Usaramine N-oxide	368.2	40	94	120	119	5.25

Table S2. The REP factors of individual PA and their *N*-ox congeners in this study according to Merz and Schrenk (2016) [1].

PA and their *N*-ox congeners	REP factor	PA and their *N*-ox congeners	REP factor
7-Acetylintermedine	0.1	Lycopsamine *N*-ox	0.01
7-Acetyllycopsamine	0.1	Merenskine	1
7-Acetyllycopsamine/intermedine *N*-ox	0.1	Merenskine *N*-ox	1
Acetylpetasitenine	1	Merepoxine	1
Adonifoline	1	Merepoxine *N*-ox	1
Amabiline	0.01	Monocrotaline	1
Atropine	0	Monocrotaline *N*-ox	1
Echimidine	0.1	Neosenkirkine	1
Echimidine *N*-ox	0.1	Otosenine	1
Echinatine	0.3	Petasitenine	1
Echinatine *N*-ox	0.3	Retrorsine	1
Erucifoline	1	Retrorsine *N*-ox	1
Erucifoline *N*-ox	1	Riddelliine	1
Europine	0.3	Riddelliine *N*-ox	1
Europine *N*-ox	0.3	Rinderine	0.3
Florosenine	1	Rinderine *N*-ox	0.3
Heliosupine	1	Sceleratine	1
Heliosupine *N*-ox	1	Sceleratine *N*-ox	1
Heliotrine	0.3	Scopolamine	0
Heliotrine *N*-ox	0.3	Senecionine	1
Indicine *N*-ox	0.01	Senecionine *N*-ox	1
Integerrimine	1	Seneciphylline	1
Integerrimine *N*-ox	1	Seneciphylline *N*-ox	1
Intermedine	0.01	Senecivernine	1
Intermedine *N*-ox	0.01	Senecivernine *N*-ox	1
Jacobine	1	Senkirkine	1
Jacobine *N*-ox	1	Spartioidine	1
Jacoline	1	Spartioidine *N*-ox	1
Jacoline *N*-ox	1	Supinine	0.01
Jaconine	1	Supinine *N*-ox	0.01
Jaconine *N*-ox	1	Trichodesmine	1
Lasiocarpine	1	Trichodesmine *N*-ox	1
Lasiocarpine *N*-ox	1	Usaramine	1
Lycopsamine	0.01	Usaramine *N*-ox	1

References

1. Merz, K.-H.; Schrenk, D. Interim Relative Potency Factors for the Toxicological Risk Assessment of Pyrrolizidine Alkaloids in Food and Herbal Medicines. *Toxicol. Lett.* **2016**, *263*, 44–57, doi:10.1016/j.toxlet.2016.05.002.