Accurate mass analysis and structure elucidation of selenium metabolites by liquid chromatography electrospray time-of-flight mass spectrometry

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Electronic Supplementary Data

Accurate mass analysis performed on the studied selenized compounds (*m/z* 661, *m/z* 425.9 and *m/z* 513) and their characteristic fragment ions are included in the following tables

Table captions

Table S1. Accurate mass analysis of doubly selenised species with *m/z* 661, detected at 17.65 minutes. Elemental composition calculator tool: C [0-50]; H [0-100]; O [0-30]; N [0-25]; S [0-0] and Se [2-2].

Table S2. Accurate mass analysis of the fragment ions from in-source CID fragmentation of *m/z* 661: *m/z* 526, *m/z* 508, *m/z* 410, *m/z* 330 and *m/z* 136. Elemental composition calculator tool: C [0-50]; H [0-100]; O [0-30]; N [0-25]; S [0-0] (except for *m/z* 330, S [0-2]) and Se [0-0],[1-1] or [2-2] depending on the isotopic profile.

Table S3. Accurate mass analysis of unknown doubly selenised species with *m/z* 425.9, detected at 20.0 minutes. Elemental composition calculator tool: C [0-50]; H [0-100]; O [0-30]; N [0-25]; S [0-2] and Se [2-2].

Table S4. Accurate mass analysis of in-source fragment ions from selenized species with *m/z* 425.9. Elemental composition calculator tool: C [0-50]; H [0-100]; O [0-30]; N [0-25]; S [0-0] and Se [0-0],[1-1] or [2-2] depending on the isotopic profile.

Table S5. Accurate mass analysis of unknown doubly selenised species with *m/z* 513 detected at 10.7 minutes. Elemental composition calculator tool: C [0-50]; H [0-100]; O [0-30]; N [0-25]; S [0-2] and Se [2-2].

Table S6. Accurate mass analysis of fragment ions from *m/z* 513. Elemental composition calculator tool: C [0-50]; H [0-100]; O [0-30]; N [0-25]; S [0-0] and Se [0-0], [1-1] or [2-2] depending on the isotopic profile. Both odd and even electron states are included.

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Table S1. Accurate mass analysis of doubly selenised species with *m/z* 661, detected at 17.65 minutes. Elemental composition calculator tool: C [0-50]; H [0-100]; O [0-30]; N [0-25]; S [0-0] and Se [2-2].

	Formula	**Calculated *m/z***	**Error (mDa)**	**Error (ppm)**	**DBE**
***m/z* 661.0283**					
	$C_{20}H_{25}N_{10}O_6Se_2$	**661.0283**	**-0.0463**	**-0.0701**	**15.5**
	$C_5H_{21}N_{22}O_7Se_2$	661.0288	-0.5489	-0.8303	8.5
	$C_4H_{25}N_{18}O_{11}Se_2$	661.0275	0.7883	1.1926	3.5
	$C_{19}H_{29}N_6O_{10}Se_2$	661.027	1.2909	1.9529	10.5
	$C_{23}H_3O_{12}Se_2$	661.0296	-1.3944	-2.1094	9.5
	$C_8H_{29}N_{12}O_{13}Se_2$	661.0301	-1.8969	-2.87	2.5
	$C_{18}H_{33}N_2O_{14}Se_2$	661.0256	2.639	3.9923	5.5
	$C_{16}H_{21}N_{16}O_4Se_2$	661.0256	2.639	3.992	16.5
	$C_{24}H_{29}N_4O_8Se_2$	661.031	-2.73	-4.13	14.5
	$C_9H_{25}N_{16}O_9Se_2$	661.0315	-3.234	-4.892	7.5
	$H_{21}N_{24}O_9Se_2$	661.0248	3.4737	5.255	4.5
	$C_{15}H_{25}N_{12}O_8Se_2$	661.0243	3.976	6.015	11.5
	$C_{25}H_{25}N_8O_4Se_2$	661.0323	-4.069	-6.15	19.5
	$C_{30}H_{29}O_7Se_2$	661.0238	4.4789	6.777	18.5
	$C_{10}H_{21}N_{20}O_5Se_2$	661.0328	-4.5716	-6.9159	12.5
	$C_{12}H_{33}N_6O_{15}Se_2$	661.0328	-4.5823	-6.9322	1.5
	$C_{14}H_{29}N_8O_{12}Se_2$	661.0256	5.3132	-0.070	6.5
	$C_{12}H_{17}N_{22}O_2Se_2$	661.0229	5.32	8.05	17.5
	$C_{11}H_{17}N_{24}OSe_2$	661.0342	-5.9089	-8.94	17.5
	$C_{13}H_{29}N_{10}O_{11}Se_2$	661.0342	-5.9196	-8.95	6.5

Table S2. Accurate mass analysis of the fragment ions from in-source CID fragmentation of *m/z* 661: *m/z* 526, *m/z* 508, *m/z* 410, *m/z* 330 and *m/z* 136. Elemental composition calculator tool: C [0-50]; H [0-100]; O [0-30]; N [0-25]; S [0-0] (except for *m/z* 330, S [0-2]) and Se [0-0],[1-1] or [2-2] depending on the isotopic profile.

	Formula	**Calculated *m/z***	**Error (mDa)**	**Error (ppm)**	**DBE**
***m/z* 525.9749**					
	$C_{16}H_{16}N_9O_2Se_2$	525.9751	-0.2884	-0.5483	15.5
	$H_{16}N_{17}O_7Se_2$	525.9743	0.5463	1.0386	3.5
	$CH_{12}N_{21}O_3Se_2$	525.9756	-0.7909	-1.5038	8.5
	$C_{15}H_{20}N_5O_6Se_2$	**525.9738**	**1.0489**	**1.9941**	**10.5**
	$C_4H_{20}N_{11}O_9Se_2$	525.977	-2.139	-4.067	2.5
	$C_{14}H_{24}NO_{10}Se_2$	525.9725	2.3862	4.537	5.5
	$C_{12}H_{12}N_{15}Se_2$	525.9725	2.3969	4.557	16.5
	$C_{20}H_{20}N_3O_4Se_2$	525.9778	-2.9738	-5.65	14.5
	$C_5H_{16}N_{15}O_5Se_2$	525.9783	-3.4763	-6.61	7.5
	$C_{11}H_{16}N_{11}O_4Se_2$	525.9711	3.7342	7.10	11.5
	$C_{21}H_{16}N_7Se_2$	525.9792	-4.311	-8.20	19.5
	$C_6H_{12}N_{19}OSe_2$	525.9797	-4.8136	-9.15	12.5
	$C_8H_{24}N_5O_{11}Se_2$	525.9797	-4.8244	-9.17	1.5
	$C_{10}H_{20}N_7O_8Se_2$	525.9698	-4.069	9.64	6.5
***m/z* 507.9621**					
	$C_{14}H_{22}NO_9Se_2$	507.9619	0.1509	-0.297	6.5
	$C_{15}H_{18}N_5O_5Se_2$	**507.9632**	**-1.1863**	**-2.33**	**11.5**
	$C_{11}H_{14}N_{11}O_3Se_2$	507.9606	1.499	2.95	12.5
	$H_{14}N_{17}O_6Se_2$	507.9637	-1.6889	-3.3249	4.5
	$C_{16}H_{14}N_9OSe_2$	507.9646	-2.52	-4.968	16.5
	$C_{10}H_{18}N_7O_7Se_2$	507.9592	2.83	5.584	7.5
	$CH_{10}N_{21}O_2Se_2$	507.9651	-3.02	-5.957	9.5
	$C_9H_{22}N_3O_{11}Se_2$	507.9579	4.1736	8.22	2.5
	$C_7H_{10}N_{17}OSe_2$	507.9579	4.1844	8.24	13.5
	$C_4H_{18}N_{11}O_8Se_2$	507.9664	-4.3743	-8.61	3.5

***m/z* 409.9276**					
	$C_{10}H_{12}N_5O_3Se_2$	**409.9265**	**1.0931**	**2.66**	**9.5**
	$C_9H_{16}NO_7Se_2$	409.9251	2.43	5.93	4.5
	$C_{15}H_{12}N_3OSe_2$	409.9305	-2.93	-7.15	13.5
	$H_8N_{15}O_2Se_2$	409.931	-3.43	-8.37	6.5
	$C_6H_8N_{11}OSe_2$	409.9238	3.78	9.22	10.5
***m/z* 330.0096**					
	$C_{10}H_{20}NO_2S_2Se$	330.0095	0.0803	0.24	2.5
	$C_{12}H_{16}N_7O_5SSe$	330.0093	0.2643	0.80	-0.5
	$C_{10}H_{12}N_5O_3Se$	**330.0099**	**-0.3863**	**-1.17**	**8.5**
	$C_9H_{16}NO_7Se$	330.0086	0.9509	2.88	3.5
	$C_3H_{12}N_{11}OSSe$	330.0106	-1.0729	-3.25	4.5
	$C_6H_8N_{11}OSe$	330.0073	2.299	6.966	9.5
	$C_6H_{16}N_7S_2Se$	330.0068	2.7657	8.381	3.5
***m/z* 136.0621**					
	$C_5H_6N_5$	**136.0617**	**0.33**	**2.4**	**5.5**

Table S3. Accurate mass analysis of unknown doubly selenised species with *m/z* 425.9, detected at 20.0 minutes. Elemental composition calculator tool: C [0-50]; H [0-100]; O [0-30]; N [0-25]; S [0-2] and Se [2-2].

	Formula	**Calculated *m/z***	**Error (mDa)**	**Error (ppm)**	**DBE**
***m/z* 425.9585**					
	$C_4H_{16}N_{11}OSSe_2$	425.9584	0.0064	0.015	4.5
	$C_{11}H_{16}N_5O_3Se_2$	**425.9578**	**0.693**	**1.63**	**8.5**
	$C_{11}H_{24}NO_2S_2Se_2$	425.9573	1.16	2.72	2.5
	$C_3H_{20}N_7O_5SSe_2$	425.9571	1.34	3.15	-0.5
	$C_{10}H_{20}NO_7Se_2$	425.9564	2.03	4.77	3.5
	$H_{16}N_{11}O_6Se_2$	425.9609	-2.49	-5.86	0.5
	$C_8H_{20}N_5O_3SSe_2$	425.9611	-2.68	-6.29	3.5
	$C_{16}H_{16}N_3OSe_2$	425.9618	-3.33	-7.82	12.5
	$CH_{20}N_{11}OSe_2$	425.9618	-3.36	-7.90	-0.5
	$C_7H_{12}N_{11}OSe_2$	425.9551	3.38	7.93	9.5
	$CH_{12}N_{15}O_2Se_2$	425.9623	-3.83	-9.00	5.5
	$C_7H_{20}N_7S_2Se_2$	425.9546	3.84	9.03	3.5

Table S4. Accurate mass analysis of in-source fragment ions from selenized species with *m/z* 425.9. Elemental composition calculator tool: C [0-50]; H [0-100]; O [0-30]; N [0-25]; S [0-0] and Se [0-0],[1-1] or [2-2] depending on the isotopic profile.

	Formula	**Calculated *m/z***	**Error (mDa)**	**Error (ppm)**	**DBE**
***m/z* 309.9100**					
	$C_6H_8N_5Se_2$	**309.91046**	**-0.46**	**-1.49**	**7.5**
	$C_5H_{12}NO_4Se_2$	309.90912	0.87	2.82	2.5
***m/z* 290.9020**					
	$C_6H_{11}O_3Se_2$	**290.9033**	**-1.31**	**-4.51**	**3.5**
	$C_2H_7N_6OSe_2$	290.9006	1.37	4.72	4.5
	$CH_{11}N_2O_5Se_2$	290.8992	2.71	9.32	-0.5
***m/z* 229.9937**					
	$C_6H_8N_5Se$	**229.9939**	**-0.24**	**-1.05**	**6.5**
	$C_5H_{12}NO_4Se$	229.9926	1.095	4.76	1.5
***m/z* 174.8560**					
	CH_3Se_2	**174.85596**	**0.032**	**0.18**	**2.5**
***m/z* 136.0614**					
	$C_5H_6N_5$	**136.0617**	**-0.37**	**-2.73**	**5.5**

Table S5. Accurate mass analysis of unknown doubly selenised species with *m/z* 513 detected at 10.7 minutes. Elemental composition calculator tool: C [0-50]; H [0-100]; O [0-30]; N [0-25]; S [0-2] and Se [2-2].

	Formula	**Calculated *m/z***	**Error (mDa)**	**Error (ppm)**	**DBE**
***m/z* 512.9900**					
	$C_{22}H_{25}O_2SSe_2$	512.99001	-0.0195	-0.038	12.5
	$C_{14}H_{21}N_6O_5Se_2$	**512.98983**	**0.164**	**0.32**	**9.5**
	$C_7H_{21}N_{12}O_3SSe_2$	512.99052	-0.52	-1.02	5.5
	$C_{14}H_{29}N_2O_4S_2Se_2$	512.98936	0.63	1.23	3.5
	$C_{15}H_{25}N_6S_2Se_2$	512.9907	-0.706	-1.376	8.5
	$C_6H_{25}N_8O_7SSe_2$	512.98918	0.815	1.589	0.5
	$C_{15}H_{17}N_{10}OSe_2$	512.99117	-1.17	-2.28	14.5
	$H_{21}N_{18}OS_2Se_2$	512.9912	-1.208	-2.356	1.5
	$C_{13}H_{25}N_2O_9Se_2$	512.98849	1.50	2.927	4.5
	$H_{13}N_{22}O_2Se_2$	512.99167	-1.675	-3.26	7.5
	$C_3H_{17}N_{18}O_5Se_2$	512.98783	2.163	4.21	6.5
	$C_{18}H_{25}O_7Se_2$	512.99252	-2.521	-4.91	8.5

Table S6. Accurate mass analysis of fragment ions from *m/z* 513. Elemental composition calculator tool: C [0-50]; H [0-100]; O [0-30]; N [0-25]; S [0-0] and Se [0-0], [1-1] or [2-2] depending on the isotopic profile. Both odd and even electron states are included.

	Formula	**Calculated *m/z***	**Error (mDa)**	**Error (ppm)**	**DBE**
***m/z* 410.9358**					
	$C_{12}H_{15}N_2O_4Se_2$	410.93567	0.125	0.30	8.5
	$C_{13}H_{11}N_6Se_2$	410.93701	-1.21	-2.95	13.5
	$C_{10}H_{13}N_5O_3Se_2$	**410.93433**	**1.47**	**3.57**	**9**
	$C_{15}H_{13}N_3OSe_2$	410.93835	-2.55	-6.22	13
	$C_9H_{17}NO_7Se_2$	410.93299	2.805	6.83	4
	$C_8H_{11}N_8O_2Se_2$	410.93298	2.811	6.84	9.5
	$H_9N_{15}O_2Se_2$	410.93885	-3.057	-7.44	6
	$CH_{15}N_8O_7Se_2$	410.93886	-3.062	-7.45	0.5
	$C_{17}H_{15}O_2Se_2$	410.93969	-3.90	-9.48	12.5
***m/z* 181.9710**					
	$C_4H_8NO_2Se$	**181.97147**	**-0.47**	**2.61**	**2.5**
	$C_2H_6N_4OSe$	181.97013	0.867	4.76	3
***m/z* 136.0615**					
	$C_5H_6N_5$	**136.0617**	**-0.27**	**-2.0**	**5.5**