Supporting Information

Automated LC-HRMS(/MS) approach for the annotation of fragment ions derived from stable isotope labeling-assisted untargeted metabolomics

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Keywords: LC-HRMS/MS, LTQ Orbitrap XL, metabolite identification, stable isotope labeling, tandem mass spectrometry

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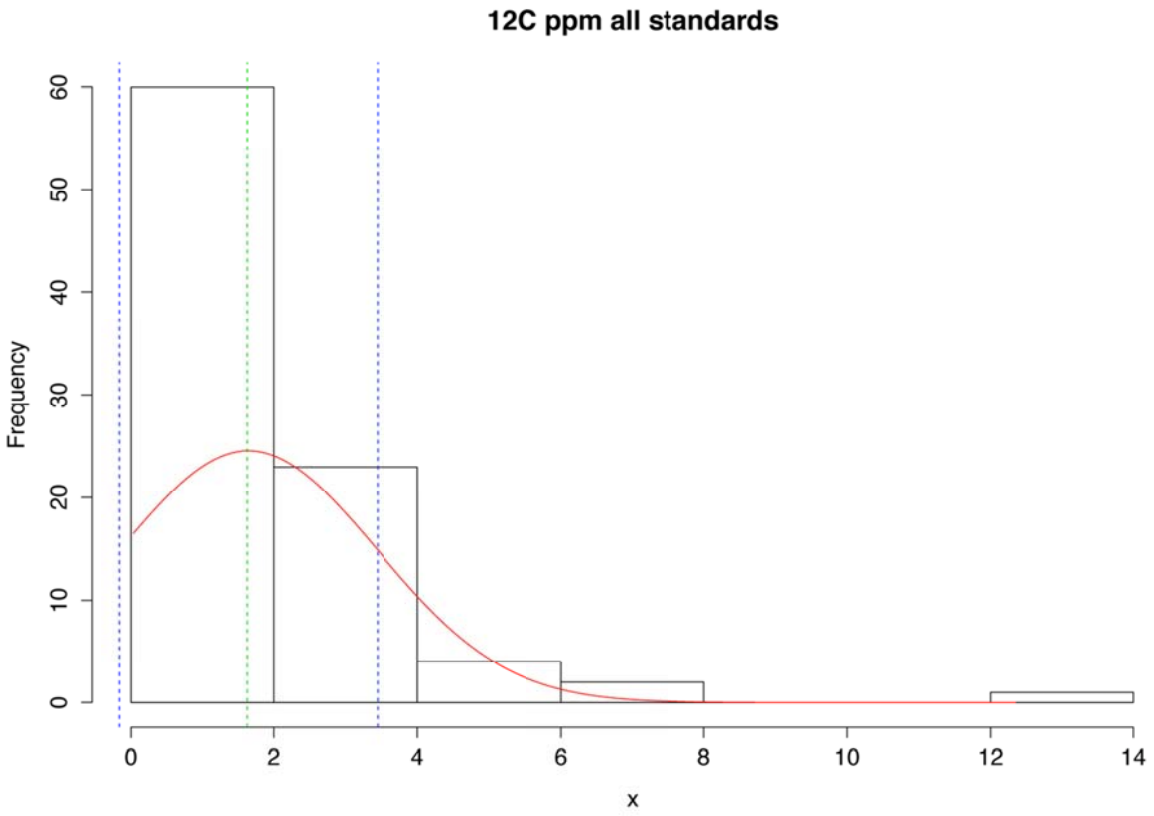


Figure S-1. Distribution of mass accuracy intervals of ^{12}C fragment signals. The histogram shows the distribution of all calculated mass deviations [ppm] of all manually annotated signals. The mass accuracy was calculated by comparing the measured mass of the fragment signal to the calculated exact mass. This was done for all manually annotated fragment signals of all product ion spectra (all standard substances). The green dashed line depicts the mean of a normal distribution of all ppm errors. The blue dashed lines show the mean ± 1 * the standard deviation.

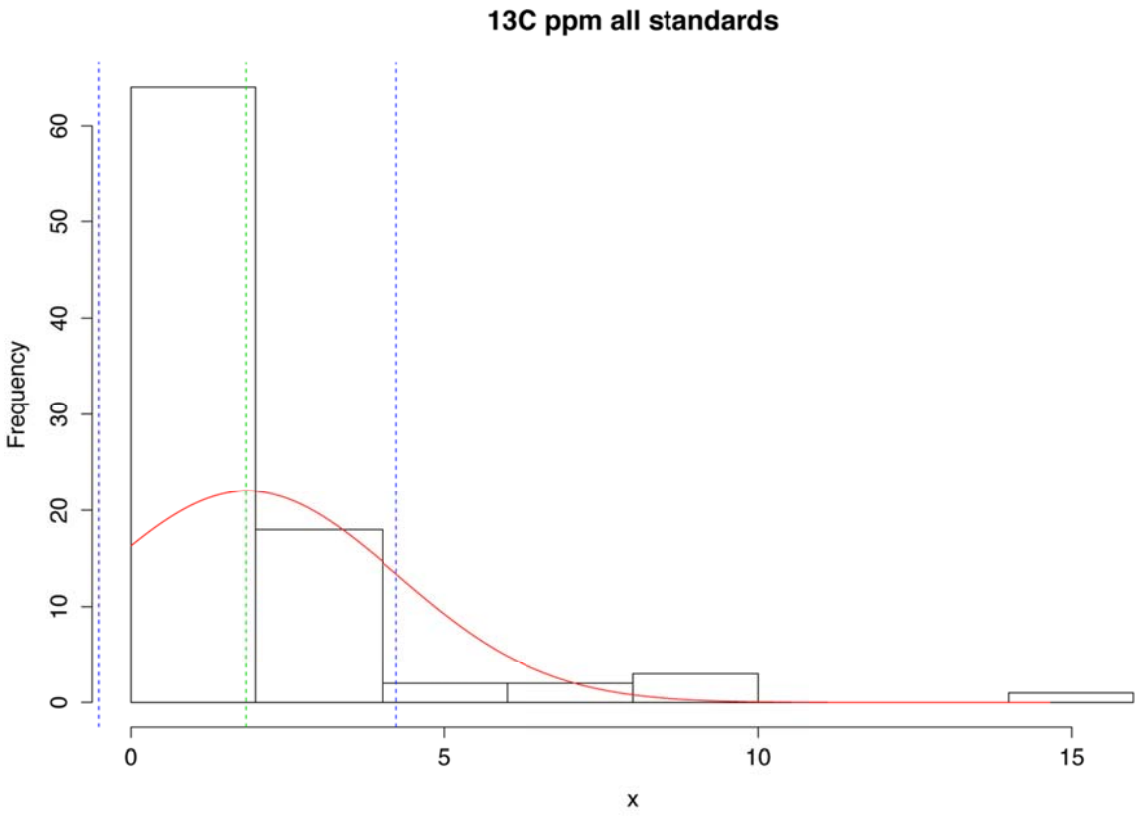


Figure S-2. Distribution of mass accuracy of ^{13}C fragment signals. The histogram shows the distribution of all calculated mass deviations [ppm] of all manually annotated signals. The mass accuracy was calculated by comparing the accurate mass of the fragment signal to the exact mass, which was calculated based on the molecular formula of the fragment signal. This was done for all manually annotated fragment signals of all product ion spectra. The green dashed line depicts the mean of a normal distribution of all ppm errors. The blue dashed lines show the mean ± 1 * the standard deviation.

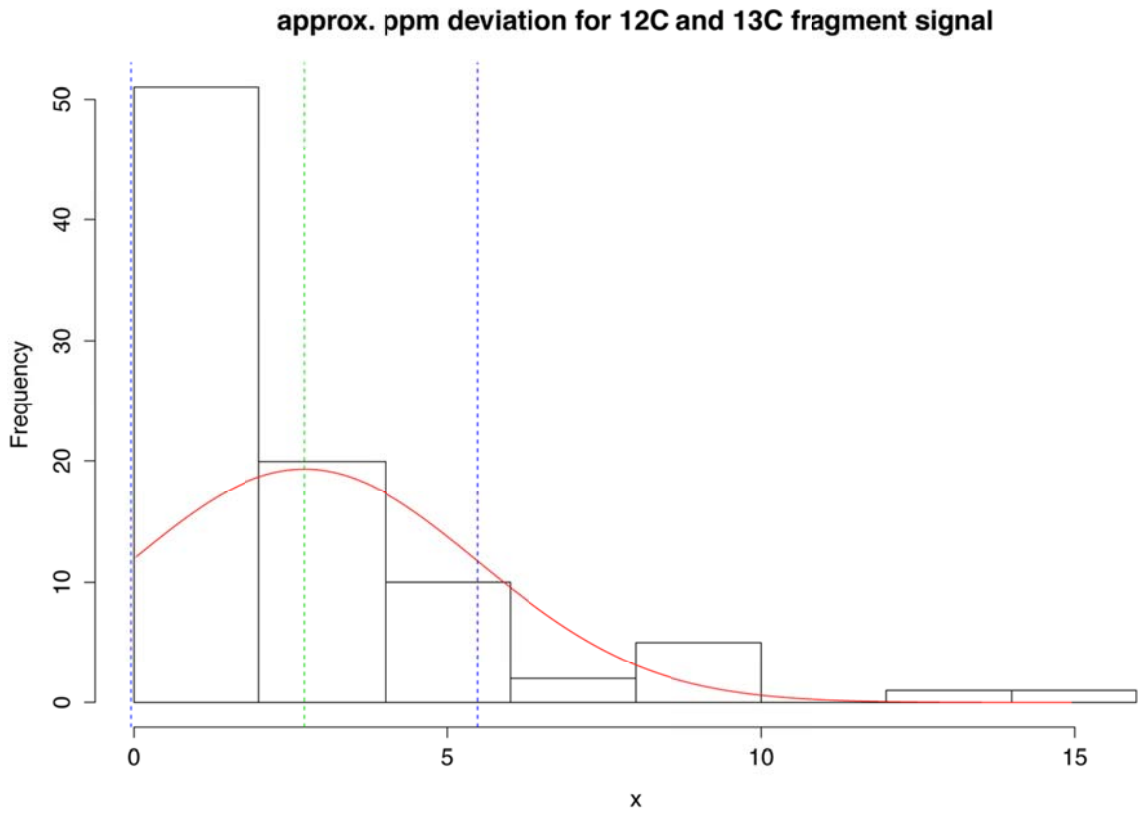


Figure S-3. Distribution of mass accuracy intervals of ^{12}C and ^{13}C fragment signals based on the rules of error propagation. For the inter-spectrum comparison, the tolerance of the *m/z* difference window between ^{12}C and potentially corresponding MS/MS signals has to be chosen based on the fragment mass accuracies of both ^{12}C and corresponding U-^{13}C fragment ions. Here the distribution of mass accuracy intervals of the *m/z* values is shown.

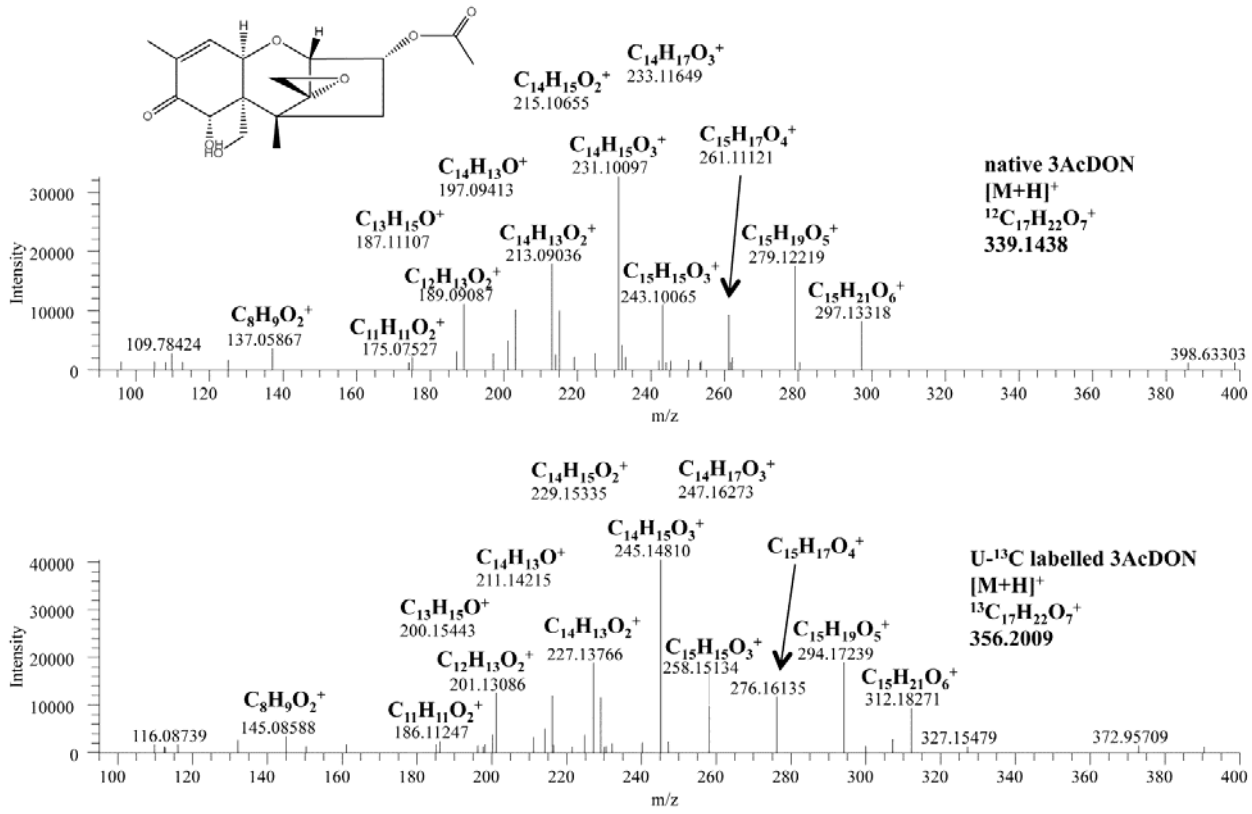


Figure S-4. Collision-induced dissociation (CID) product ion spectra of native 3AcDON and U-^{13}C-labeled 3AcDON standard. Molecular formulas for selected fragment signals are given for mass deviations below 10 ppm and were determined manually. Structure formula of 3AcDON is shown in the upper left corner.

Table S-1. Fragments and corresponding elemental compositions for MS/MS fragments of 3AcDON ($C_{17}H_{22}O_7$) derived from automated data evaluation by FragExtract, all of which have been manually verified.

No.	Molecular formula	Relative abundan	m/z_{meas} [a]	Δ m/z [ppm]	n(C)
1	$C_{12}H_{13}O$	4.5	173.0950	6.2	12
2	$C_{11}H_{11}O_2$	7.5	175.0754	0.2	11
3	$C_{13}H_{15}O$	8.4	187.1109	4.6	13
4	$C_{12}H_{13}O_2$	30.8	189.0905	2.7	12
5	$C_{14}H_{13}O$	6.0	197.0957	2.2	14
6	$C_{13}H_{13}O_2$	9.1	201.0905	2.6	13
7	$C_{13}H_{15}O_2$	26.4	203.1054	6.2	13
8	$C_{14}H_{13}O_2$	45.1	213.0901	4.48	14
9	$C_{14}H_{15}O_2$	29.8	215.1055	5.2	14
10	$C_{15}H_{13}O_2$	5.2	225.0916	2.6	15
11	$C_{14}H_{15}O_3$	100.0	231.1009	3.0	14
12	$C_{14}H_{17}O_3$	6.9	233.1169	1.5	14
13	$C_{15}H_{15}O_3$	21.9	243.1009	2.7	15
14	$C_{15}H_{17}O_4$	30.4	261.1115	2.4	15
15	$C_{15}H_{19}O_5$	46.6	279.1219	2.7	15
16	$C_{16}H_{19}O_5$	5.6	291.1226	0.3	16
17	$C_{16}H_{21}O_5$	2.2	293.1357	9.0	16
18	$C_{15}H_{21}O_6$	21.5	297.1325	1.6	15

[a] m/z_{meas} = measured m/z of fragment in MS/MS spectrum; The fragment number (No.) corresponds to the fragments highlighted in Figure 1. Molecular formulas were calculated by FragExtract with the element list of C, H, N, O, Cl, S and P. The maximum atom count of those 7 elements was derived as described in Table 1 by Kind and Fiehn [1](m/z < 500 Da: max. C: 39, max. H: 72, max. N: 20, max. O: 20, max. P: 9, max. S: 10; m/z < 1000 Da: max. C: 78, max. H: 126, max. N: 20, max. O: 27, max. P: 9, max. S: 14).

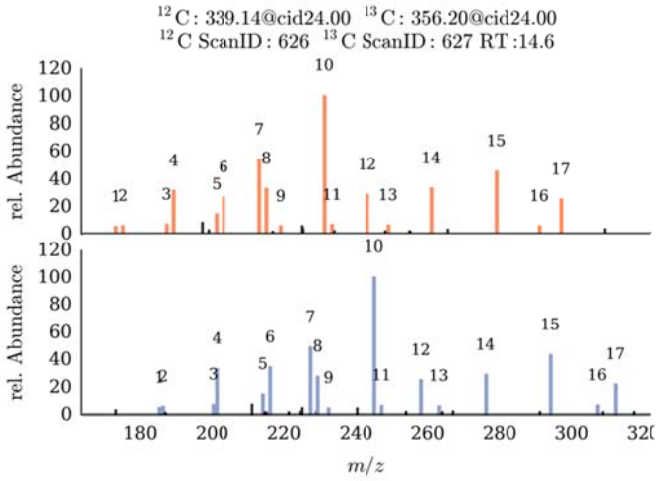
Table S-2 Summary of results for spiked *Fusarium* culture filtrates.

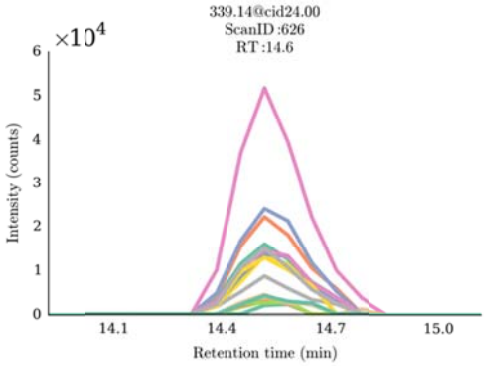
Standard compound	High concentration (c = 1mg/L)	Lowest concentration (mg/L)
	# detected/ # annotated	concentration /# detected/ # annotated
3AcDON	39/ 17	0.1/ 16/ 1
DIAS	26/ 3	0.7/ 26/ 1
T-2	74/ 10	0.001/ 15/ 1
HT-2	41/ 4	0.001/ 15/ 1
ZEN	87 / 12	0.02/ 12/ 1
FB3	15/ 7	0.4/ 11/ 2
GRIS	40/ 7	0.001/ 18/ 1
STER	29/ 6	0.02/ 21/ 2
FB1	63/ 15	0.007/ 19/ 2
FB2	48/ 12	0.007/ 17/ 2

The number of signals that were detected in the raw LC-HRMS/MS spectra at the highest concentration level (c= ~1 mg/L) compared to the number of signals annotated by FragExtract is shown. Additionally the lowest concentration for each compound for which at least one fragment was still annotated is presented together with the total number of observed signals vs. the number of annotated fragments.

3AcDON

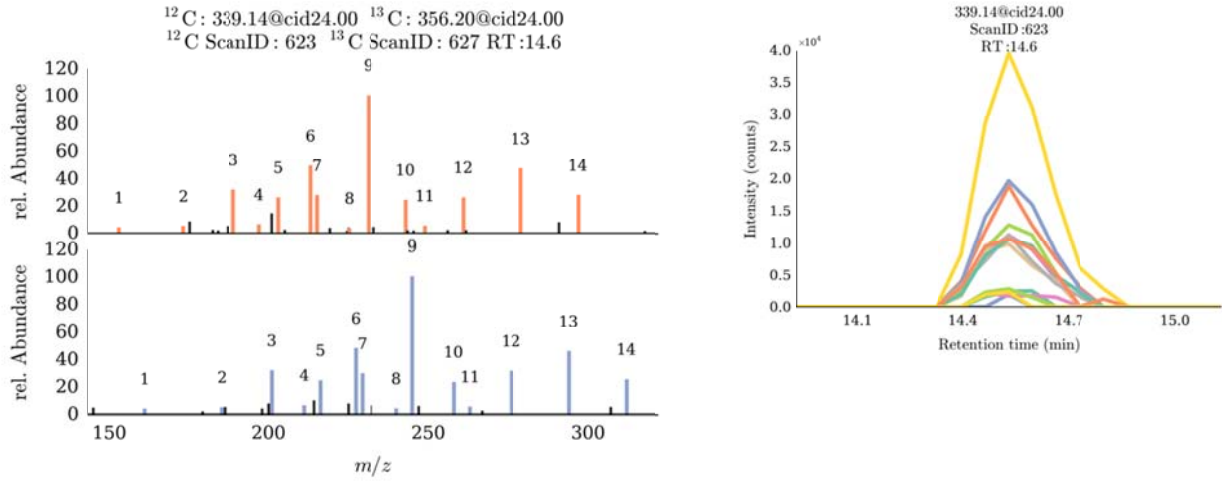
Figure S-5. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for 3AcDON at a concentration level of c = 1.0 mg/L





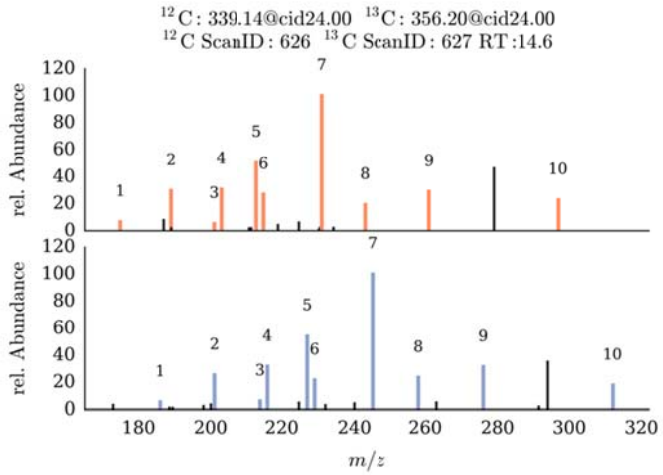
No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{12}H_{13}O$	4.17	173.0966	185.1363	2.2	12
2	$C_{11}H_{11}O_2$	4.81	175.0759	186.1123	1.9	11
3	$C_{13}H_{15}O$	5.83	187.1123	200.1555	2.9	13
34	$C_{12}H_{13}O_2$	30.77	189.0916	201.1311	0.7	12
5	$C_{13}H_{13}O_2$	13.47	201.0916	214.1353	1.1	13
6	$C_{13}H_{15}O_2$	26.02	203.1072	216.1507	0.7	13
7	$C_{14}H_{13}O_2$	53.55	213.0916	227.1380	0.2	14
8	$C_{14}H_{15}O_2$	32.40	215.1072	229.1539	0.4	14
9	$C_{13}H_{15}O_3$	4.57	219.1021	232.1462	3.5	13
10	$C_{14}H_{15}O_3$	100.00	231.1021	245.1487	0.4	14
11	$C_{14}H_{17}O_3$	5.54	233.1178	247.1647	3.0	14
12	$C_{15}H_{15}O_3$	27.97	243.1021	258.1512	1.2	15
13	$C_{14}H_{17}O_4$	5.29	249.1127	263.1593	1.7	14
14	$C_{15}H_{17}O_4$	32.63	261.1127	276.1628	2.7	15
15	$C_{15}H_{19}O_5$	45.15	279.1233	294.1734	1.5	15
16	$C_{16}H_{19}O_5$	4.67	291.1233	307.1761	0.2	16
17	$C_{15}H_{21}O_6$	24.41	297.1338	312.1830	0.4	15

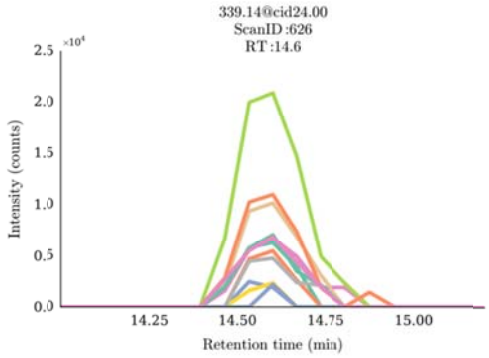
Figure S-6. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for 3AcDON at a concentration level of c = 0.7 mg/L



No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_8H_9O_3$	3.09	153.0553	161.0819	4.5	8
2	$C_{12}H_{13}O$	4.07	173.0965	185.1358	2.3	12
3	$C_{12}H_{13}O_2$	30.87	189.0913	201.1317	1.4	12
4	$C_{14}H_{13}O$	5.25	197.0957	211.1428	2.0	14
5	$C_{13}H_{15}O_2$	25.17	203.1073	216.1505	3.0	13
6	$C_{14}H_{13}O_2$	48.66	213.0910	227.1383	0.1	14
7	$C_{14}H_{15}O_2$	26.73	215.1068	229.1536	0.7	14
8	$C_{15}H_{13}O_2$	2.44	225.0911	240.1399	0.3	15
9	$C_{14}H_{15}O_3$	100.00	231.1019	245.1487	1.3	14
10	$C_{15}H_{15}O_3$	23.26	243.1014	258.1519	0.6	15
11	$C_{14}H_{17}O_4$	4.29	249.1115	263.1591	2.7	14
12	$C_{15}H_{17}O_4$	25.17	261.1127	276.1624	2.2	15
13	$C_{15}H_{19}O_5$	46.57	279.1231	294.1732	1.5	15
14	$C_{15}H_{21}O_6$	26.94	297.1337	312.1847	1.5	15

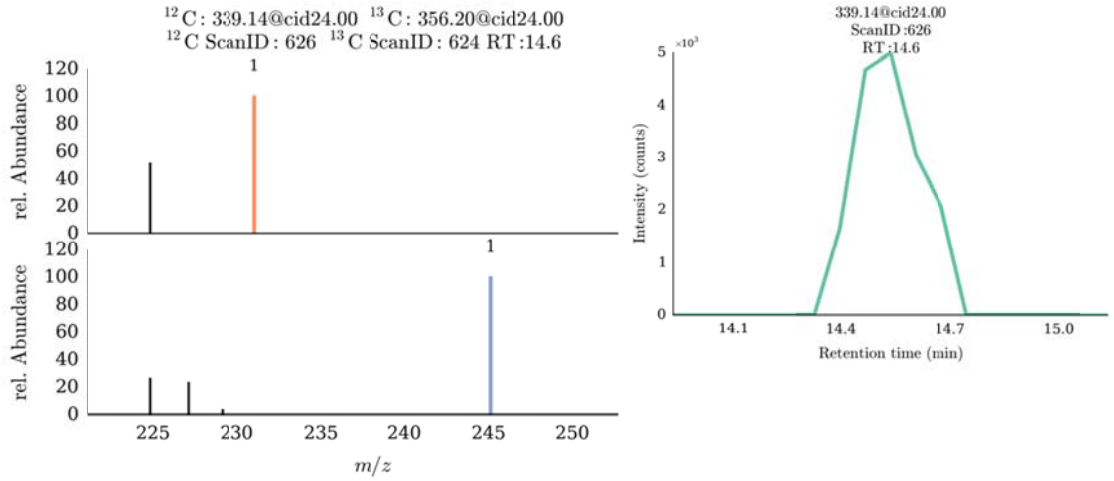
Figure S-7. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for 3AcDON at a concentration level of c = 0.4 mg/L





No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{11}H_{11}O_2$	6.70	175.0764	186.1128	5.9	11
2	$C_{12}H_{13}O_2$	29.79	189.0907	201.1308	1.4	12
3	$C_{13}H_{13}O_2$	5.27	201.0923	214.1356	6.3	13
4	$C_{13}H_{15}O_2$	30.81	203.1065	216.1503	0.8	13
5	$C_{14}H_{13}O_2$	50.48	213.0911	227.1380	0.3	14
6	$C_{14}H_{15}O_2$	27.09	215.1067	229.1532	0.3	14
7	$C_{14}H_{15}O_3$	100.00	231.1015	245.1485	0.1	14
8	$C_{15}H_{15}O_3$	19.44	243.1014	258.1522	0.7	15
9	$C_{15}H_{17}O_4$	29.11	261.1114	276.1626	2.7	15
10	$C_{15}H_{21}O_6$	22.98	297.1331	312.1839	0.5	15

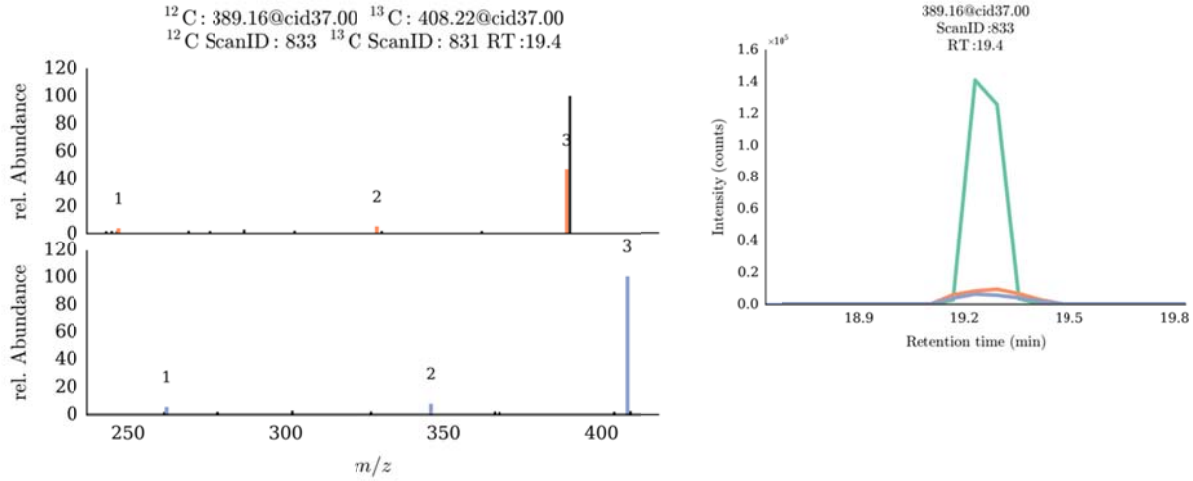
Figure S-8. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for 3AcDON at a concentration level of c = 0.1 mg/L



No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{14}H_{15}O_3$	100.00	231.0996	245.1488	8.5	14

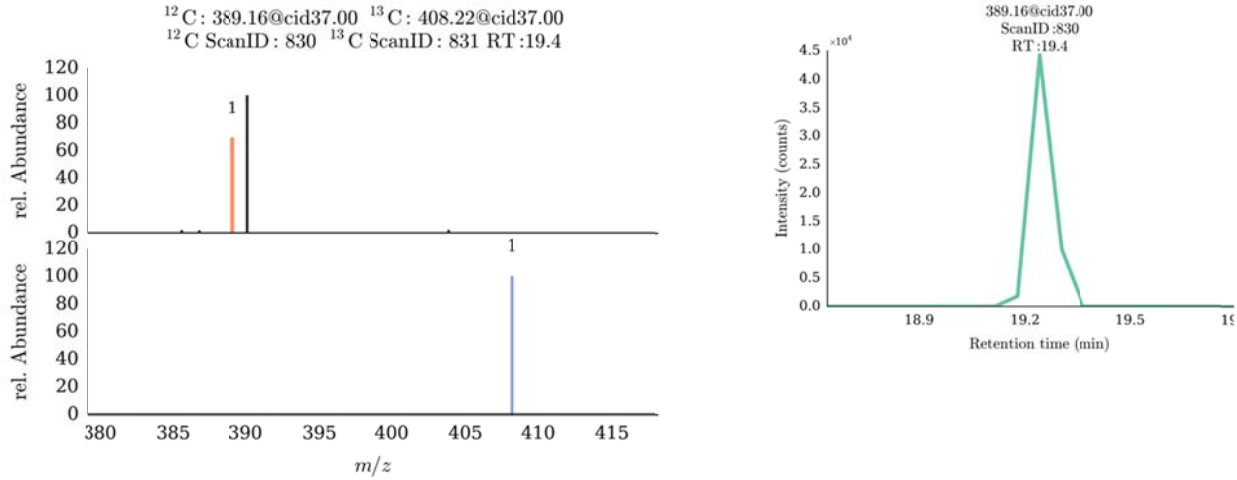
DIAS

Figure S-9. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for DIAS at a concentration level of c = 1.0 mg/L



No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{15}H_{19}O_3$	4.45	247.1321	262.1822	3.1	15
2	$C_{17}H_{22}O_5Na$	7.42	329.1364	346.1921	1.5	17
3	$C_{19}H_{26}O_7Na$	100.00	389.1564	408.2207	1.7	19

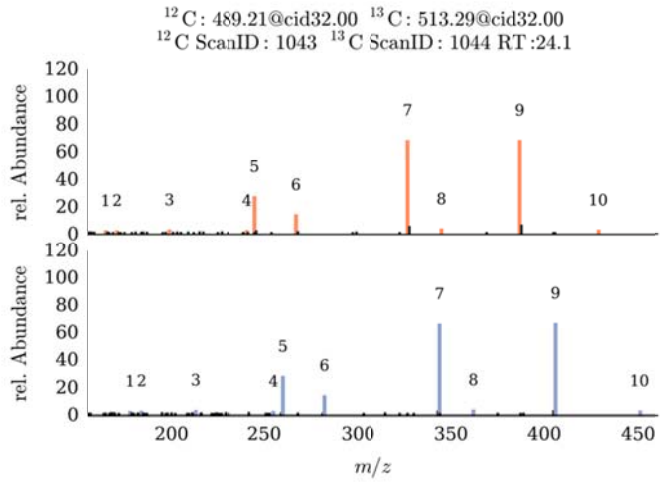
Figure S-10. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for DIAS at a concentration level of c = 0.7 mg/L

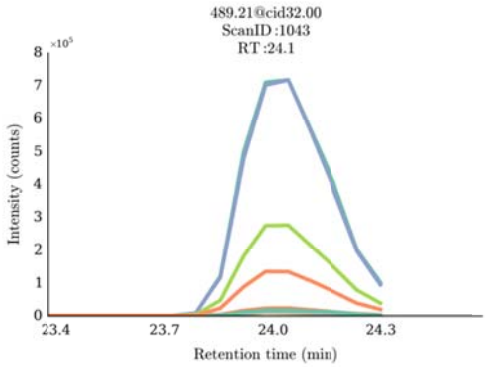


No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{19}H_{26}O_7Na$	100.00	389.1565	408.2198	1.58	19

T-2 toxin

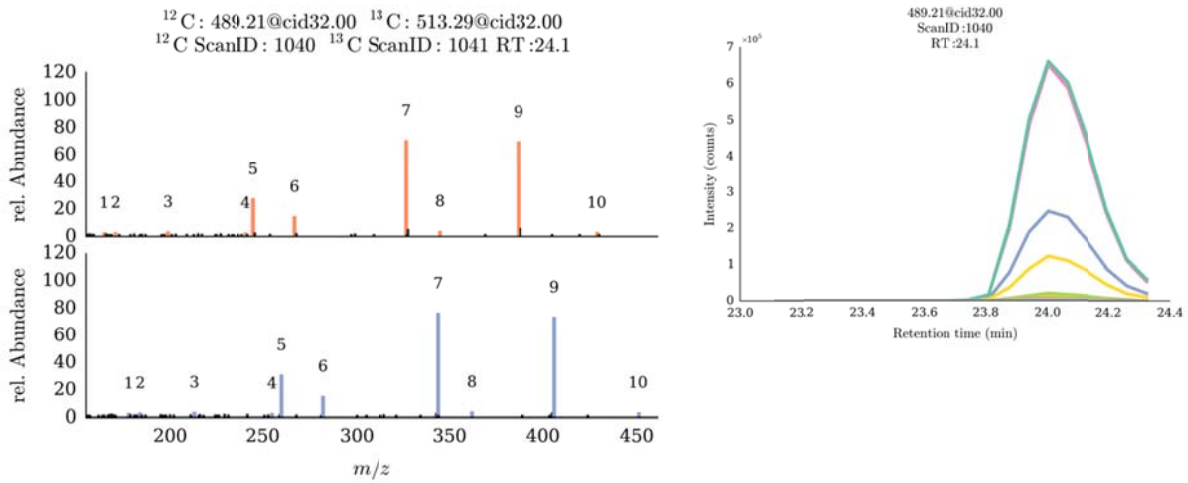
Figure S-11. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for T-2 toxin at a concentration level of c = 1.0 mg/L





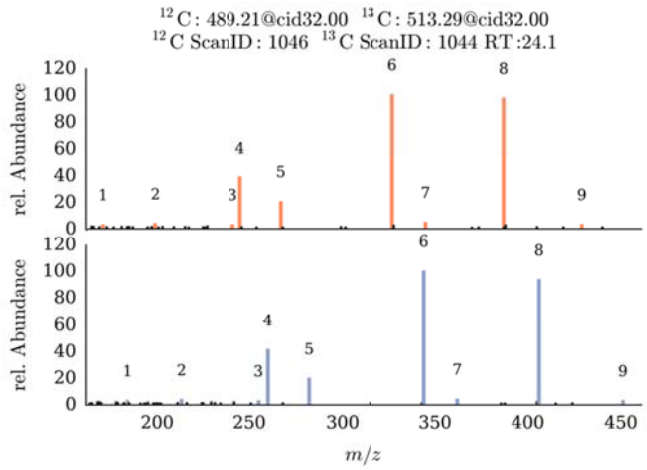
No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{13}H_9$	2.03	165.0695	178.1130	2.4	13
2	$C_{13}H_{15}$	2.22	171.1163	184.1602	3.2	13
3	$C_{14}H_{15}O$	3.05	199.1114	213.1585	1.9	14
4	$C_{14}H_{18}O_2Na$	2.25	241.1192	255.1668	2.8	14
5	$C_{15}H_{17}O_3$	39.08	245.1171	260.1673	0.6	15
6	$C_{15}H_{16}O_3Na$	19.40	267.0990	282.1494	0.6	15
7	$C_{17}H_{20}O_5Na$	100.00	327.1202	344.1773	0.4	17
8	$C_{17}H_{22}O_6Na$	3.98	345.1305	362.1879	1.2	17
9	$C_{19}H_{24}O_7Na$	99.93	387.1415	406.2050	0.1	19
10	$C_{22}H_{30}O_7Na$	2.76	429.1876	451.2633	1.8	22

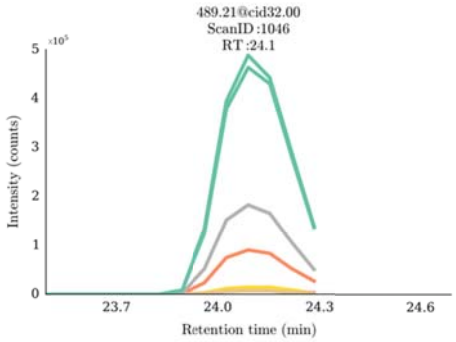
Figure S-12. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for T-2 toxin at a concentration level of c = 0.7 mg/L



No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{13}H_9$	2.15	165.0696	178.1133	1.9	13
2	$C_{13}H_{15}$	2.39	171.1161	184.1598	4.1	13
3	$C_{14}H_{15}O$	3.21	199.1113	213.1582	2.4	14
4	$C_{14}H_{18}O_2Na$	2.21	241.1196	255.1664	1.1	14
5	$C_{15}H_{17}O_3$	38.13	245.1168	260.1673	1.6	15
6	$C_{15}H_{16}O_3Na$	19.35	267.0988	282.1493	1.3	15
7	$C_{17}H_{20}O_5Na$	100.00	327.1200	344.1773	1.0	17
8	$C_{17}H_{22}O_6Na$	3.87	345.1304	362.1877	1.3	17
9	$C_{19}H_{24}O_7Na$	98.65	387.1412	406.2051	0.6	19
10	$C_{22}H_{30}O_7Na$	2.53	429.1874	451.2619	2.3	22

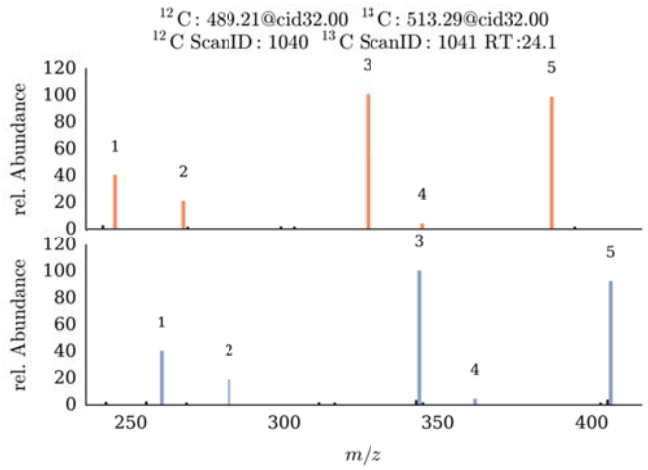
Figure S-13. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for T-2 toxin at a concentration level of c = 0.4 mg/L

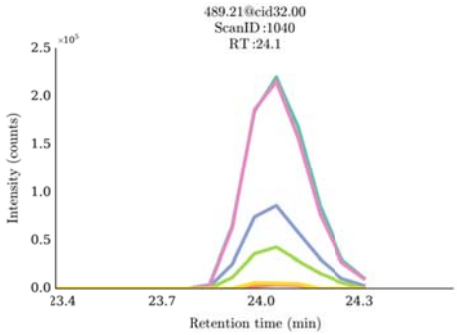




No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{13}H_{15}$	2.34	171.1168	184.1601	0.1	13
2	$C_{14}H_{15}O$	3.03	199.1112	213.1582	2.7	14
3	$C_{14}H_{18}O_2Na$	2.29	241.1203	255.1668	1.5	14
4	$C_{15}H_{17}O_3$	38.01	245.1175	260.1676	1.2	15
5	$C_{15}H_{16}O_3Na$	19.55	267.0994	282.1496	0.9	15
6	$C_{17}H_{20}O_5Na$	100.00	327.1207	344.1775	1.1	17
7	$C_{17}H_{22}O_6Na$	3.97	345.1309	362.1880	0.0	17
8	$C_{19}H_{24}O_7Na$	97.29	387.1420	406.2053	1.4	19
9	$C_{22}H_{30}O_7Na$	2.46	429.1877	451.2622	1.5	22

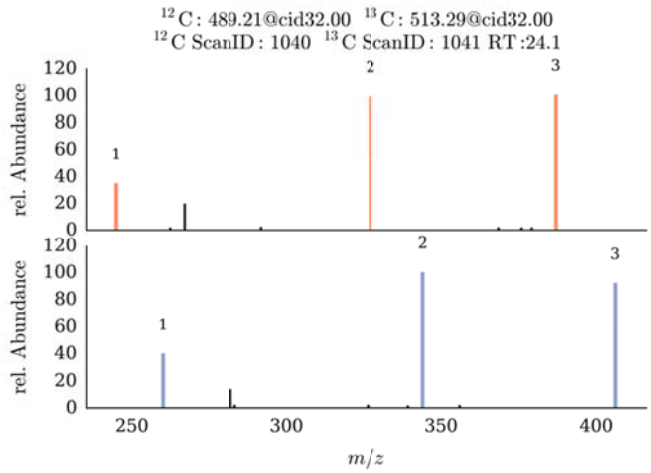
Figure S-14. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for T-2 toxin at a concentration level of c = 0.1 mg/L

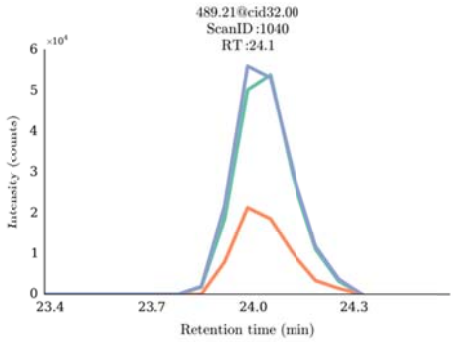




No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{15}H_{17}O_3$	39.28	245.1173	260.1678	0.3	15
2	$C_{15}H_{16}O_3Na$	19.77	267.0991	282.1500	0.3	15
3	$C_{17}H_{20}O_5Na$	100.00	327.1204	344.1776	0.3	17
4	$C_{17}H_{22}O_6Na$	2.96	345.1301	362.1896	2.2	17
5	$C_{19}H_{24}O_7Na$	98.09	387.1417	406.2053	0.6	19

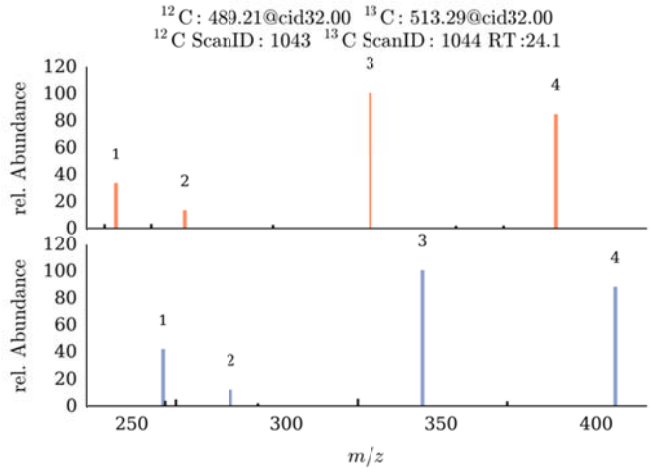
Figure S-15. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for T-2 toxin at a concentration level of c = 0.02 mg/L

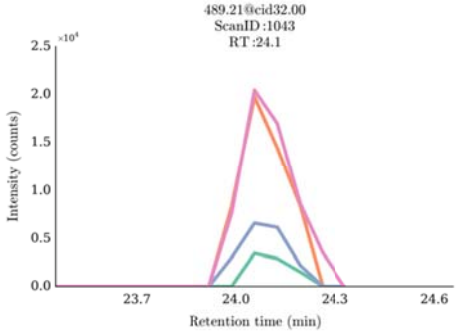




No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{15}H_{17}O_3$	33.91	245.1171	260.1677	0.7	15
2	$C_{17}H_{20}O_5Na$	98.69	327.1204	344.1772	0.2	17
3	$C_{19}H_{24}O_7Na$	100.00	387.1414	406.2048	0.0	19

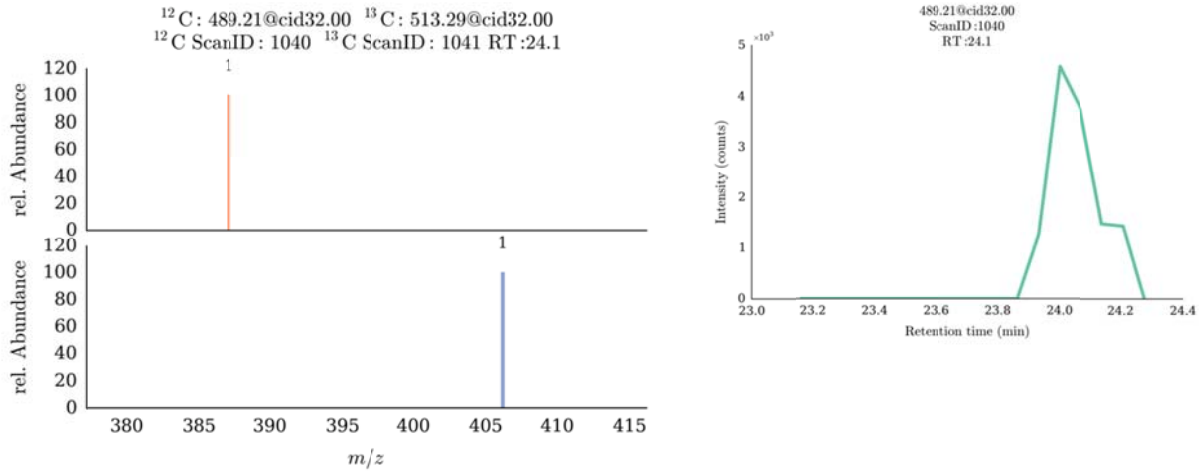
Figure S-16. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for T-2 toxin at a concentration level of c = 0.007 mg/L





No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{15}H_{17}O_3$	32.43	245.1164	260.1668	3.3	15
2	$C_{15}H_{16}O_3Na$	12.26	267.0991	282.1492	0.2	15
3	$C_{17}H_{20}O_5Na$	100.00	327.1205	344.1768	0.5	17
4	$C_{19}H_{24}O_7Na$	84.15	387.1414	406.2053	0.1	19

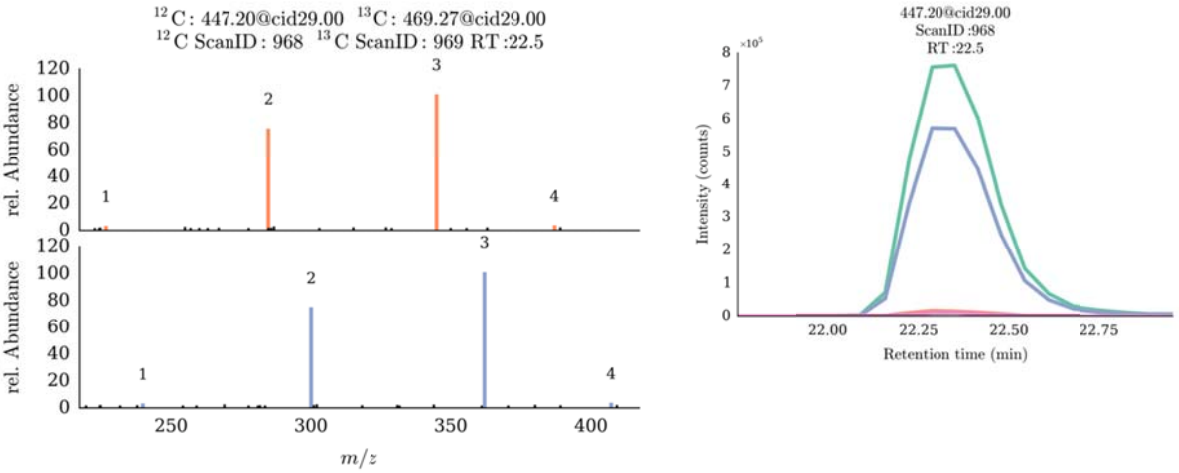
Figure S-17. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for T-2 toxin at a concentration level of c = 0.001 mg/L



No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{19}H_{24}O_7Na$	100.00	387.1415	406.2051	0.1	19

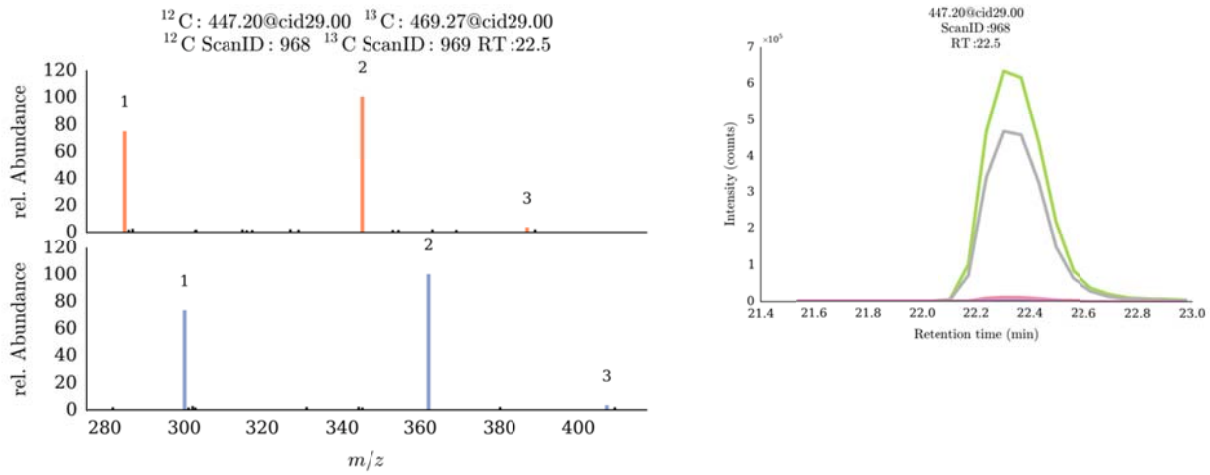
HT-2 toxin

Figure S-18. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for HT-2 toxin at a concentration level of c = 1.0 mg/L



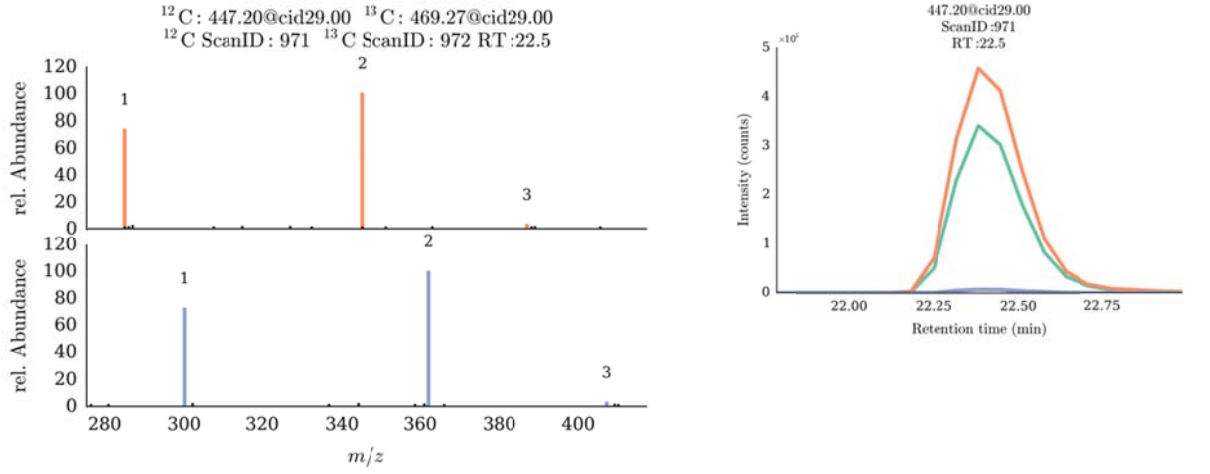
No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{13}H_{16}O_2Na$	2.09	227.1039	240.1475	1.8	13
2	$C_{15}H_{18}O_4Na$	74.75	285.1098	300.1599	0.3	15
3	$C_{17}H_{22}O_6Na$	100.00	345.1310	362.1879	0.3	17
4	$C_{20}H_{28}O_6Na$	2.52	387.1777	407.2443	0.3	20

Figure S-19. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for HT-2 toxin at a concentration level of c = 0.7 mg/L



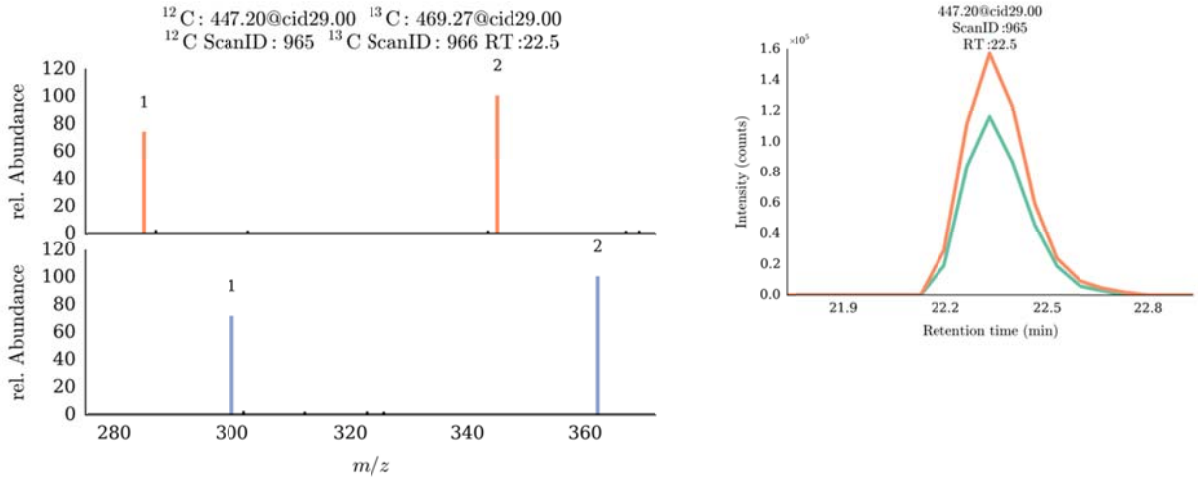
No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{15}H_{18}O_4Na$	74.56	285.1100	300.1602	0.8	15
2	$C_{17}H_{22}O_6Na$	100.00	345.1311	362.1883	0.7	17
3	$C_{20}H_{28}O_6Na$	2.37	387.1772	407.2449	1.6	20

Figure S-20. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for HT-2 toxin at a concentration level of c = 0.4 mg/L



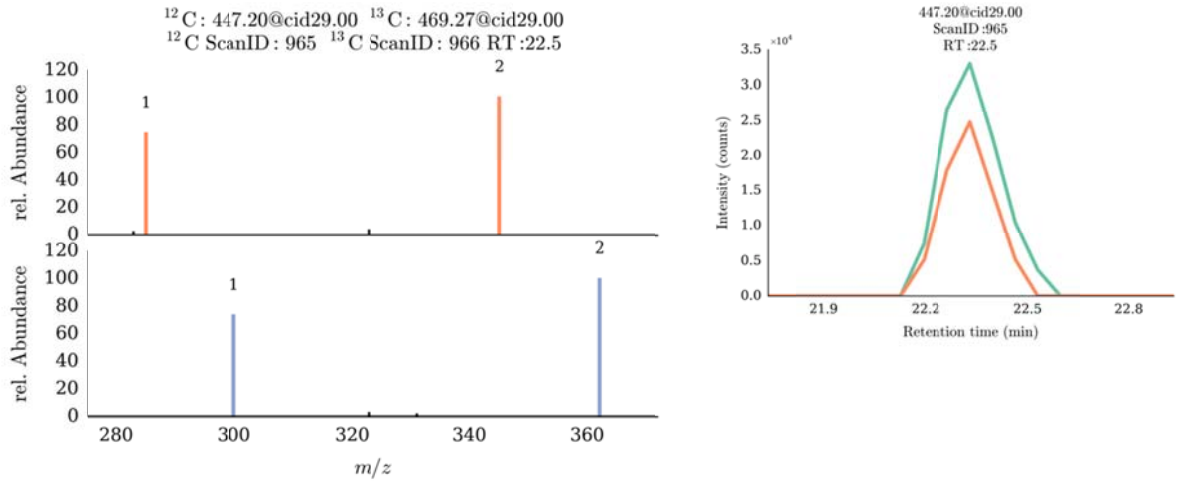
No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{15}H_{18}O_4Na$	73.27	285.1101	300.1606	1.2	15
2	$C_{17}H_{22}O_6Na$	100.00	345.1313	362.1887	1.1	17
3	$C_{20}H_{28}O_6Na$	2.20	387.1785	407.2442	1.8	20

Figure S-21. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for HT-2 toxin at a concentration level of c = 0.1 mg/L



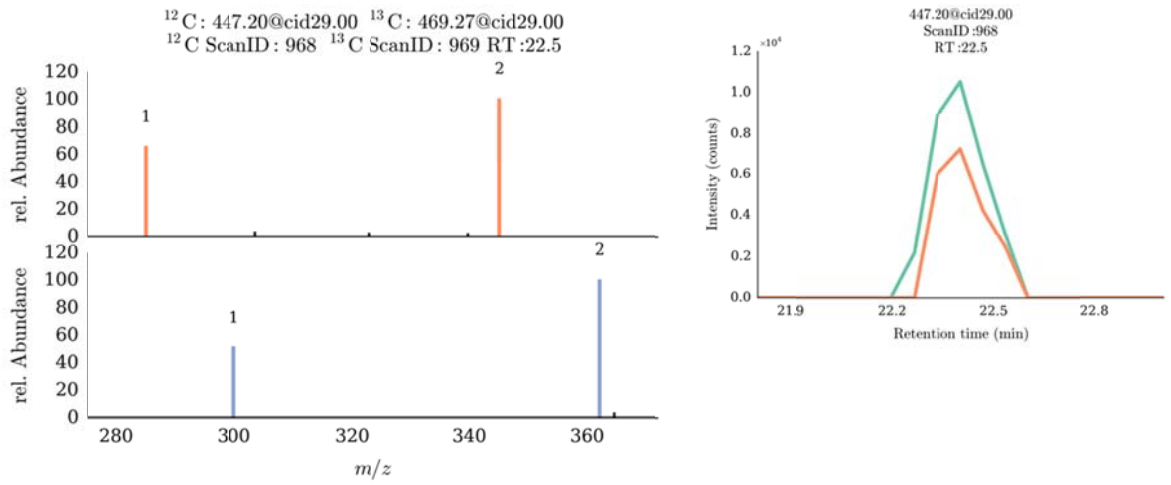
No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{15}H_{18}O_4Na$	73.59	285.1100	300.1606	0.8	15
2	$C_{17}H_{22}O_6Na$	100.00	345.1310	362.1887	0.5	17

Figure S-22. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for HT-2 toxin at a concentration level of c = 0.02 mg/L



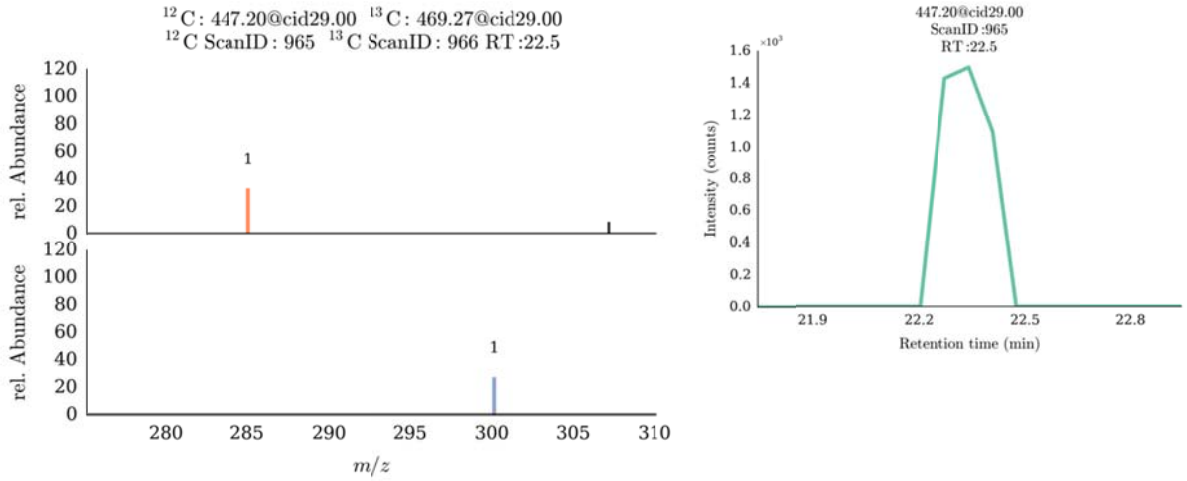
No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{15}H_{18}O_4Na$	74.04	285.1096	300.1598	0.6	15
2	$C_{17}H_{22}O_6Na$	100.00	345.1304	362.1881	1.3	17

Figure S-23. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for HT-2 toxin at a concentration level of c = 0.007 mg/L



No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	13C *m/z*	ppm	n(C)
1	$C_{15}H_{18}O_4Na$	65.56	285.1102	300.1593	1.7	15
2	$C_{15}H_{18}O_4Na$	100.00	345.1316	362.1873	2.0	17

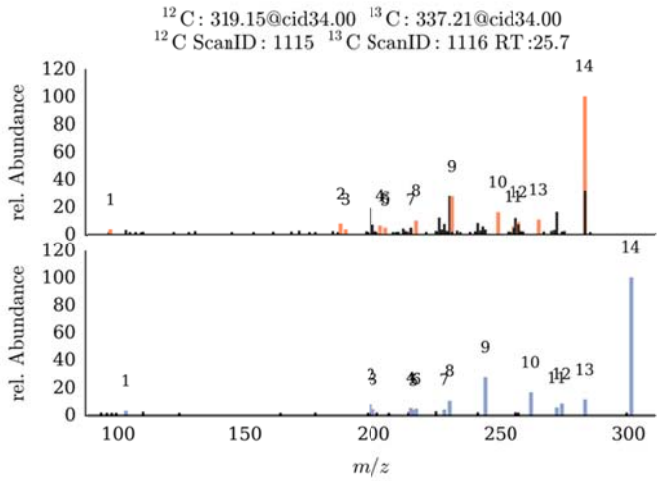
Figure S-24. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for HT-2 toxin at a concentration level of c = 0.001 mg/L

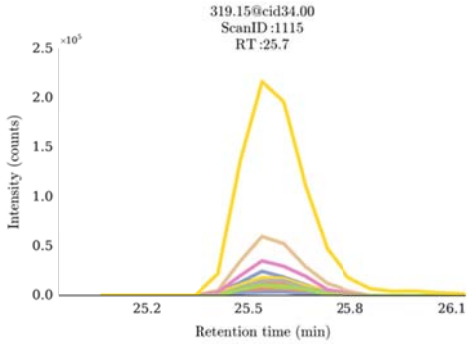


No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{15}H_{18}O_4Na$	31.84	285.1107	300.1596	3.5	15

ZEN

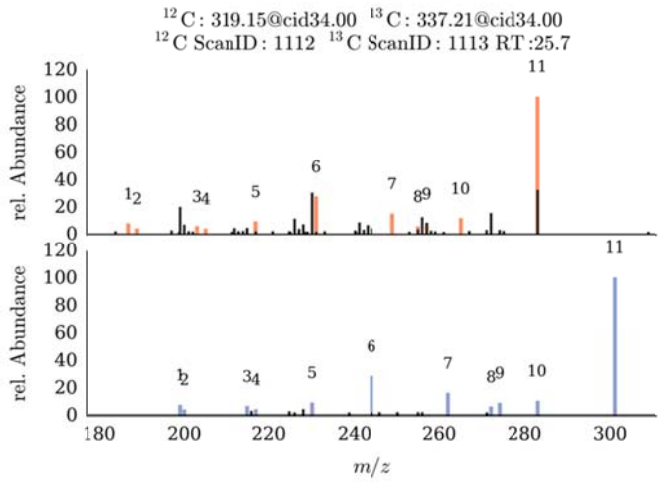
Figure S-25. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for ZEN at a concentration level of c = 1.0 mg/L

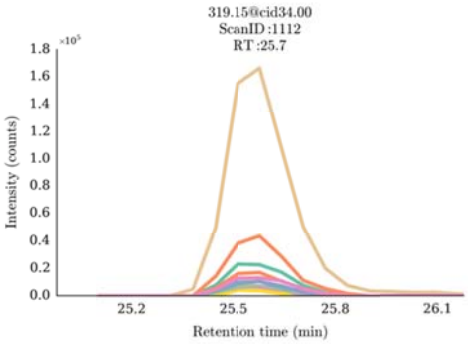




No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	C_6H_9O	2.56	97.0648	103.0841	0.0	6
2	$C_{12}H_{11}O_2$	6.78	187.0759	199.1156	3.1	12
3	$C_{11}H_9O_3$	2.67	189.0544	200.0921	0.9	11
4	$C_{12}H_{11}O_3$	5.23	203.0704	215.1109	0.6	12
5	$C_{11}H_9O_4$	2.20	205.0489	216.0867	3.2	11
6	$C_{12}H_{13}O_3$	3.84	205.0857	217.1261	1.0	12
7	$C_{13}H_{11}O_3$	2.57	215.0699	228.1125	1.5	13
8	$C_{13}H_{13}O_3$	8.98	217.0859	230.1296	0.0	13
9	$C_{13}H_{11}O_4$	26.72	231.0651	244.1088	0.2	13
10	$C_{13}H_{13}O_5$	15.21	249.0760	262.1191	0.9	13
11	$C_{17}H_{19}O_2$	4.72	255.1376	272.1955	1.4	17
12	$C_{17}H_{21}O_2$	7.97	257.1536	274.2106	0.1	17
13	$C_{18}H_{17}O_2$	9.72	265.1216	283.1831	2.5	18
14	$C_{18}H_{19}O_3$	100.00	283.1332	301.1935	1.1	18

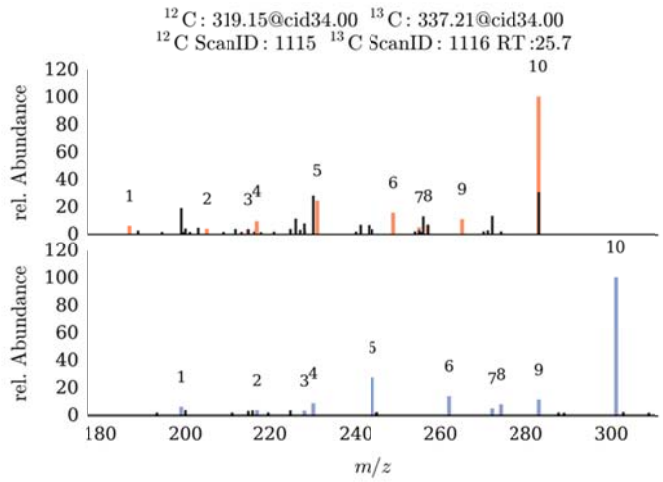
Figure S-26. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for ZEN at a concentration level of c =0.7 mg/L

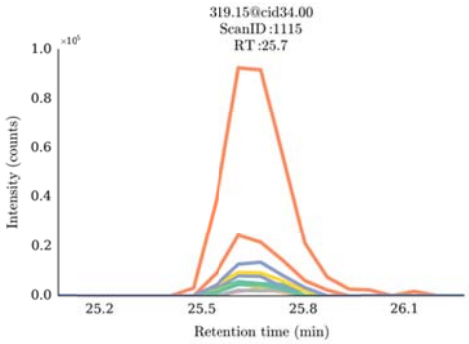




No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{12}H_{11}O_2$	6.77	187.0758	199.1155	2.4	12
2	$C_{11}H_9O_3$	3.17	189.0550	200.0910	2.0	11
3	$C_{12}H_{11}O_3$	4.71	203.0700	215.1108	1.2	12
4	$C_{13}H_{11}O_3$	2.67	215.0707	228.1135	1.8	13
5	$C_{13}H_{13}O_3$	8.28	217.0859	230.1296	0.2	13
6	$C_{13}H_{11}O_4$	26.63	231.0652	244.1086	0.1	13
7	$C_{13}H_{13}O_5$	14.03	249.0759	262.1190	0.5	13
8	$C_{17}H_{19}O_2$	4.66	255.1378	272.1948	0.8	17
9	$C_{17}H_{21}O_2$	6.62	257.1543	274.2109	2.8	17
10	$C_{18}H_{17}O_2$	10.61	265.1224	283.1822	0.3	18
11	$C_{18}H_{19}O_3$	100.00	283.1332	301.1933	1.2	18

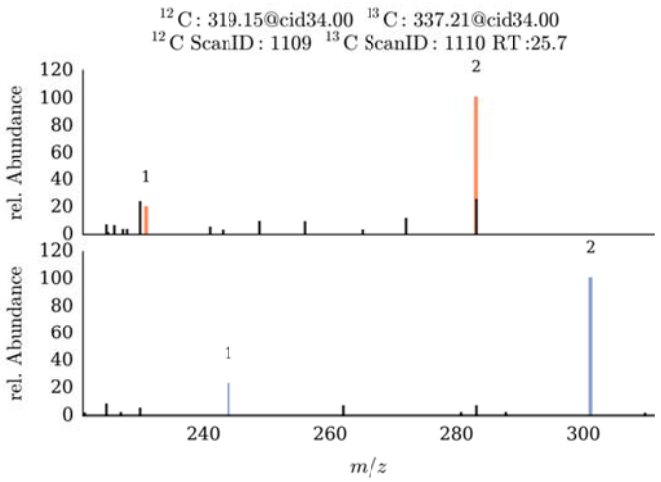
Figure S-27. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for ZEN at a concentration level of c = 0.4 mg/L

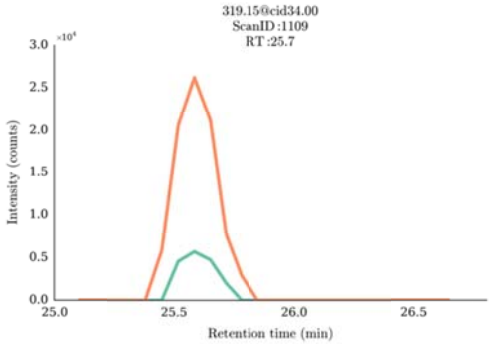




No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{12}H_{11}O_2$	5.06	187.0747	199.1155	3.7	12
2	$C_{12}H_{13}O_3$	2.98	205.0843	217.1235	7.7	12
3	$C_{13}H_{11}O_3$	2.58	215.0700	228.1142	1.2	13
4	$C_{13}H_{13}O_3$	8.47	217.0855	230.1300	1.8	13
5	$C_{13}H_{11}O_4$	23.60	231.0653	244.1087	0.3	13
6	$C_{13}H_{13}O_5$	14.70	249.0758	262.1197	0.3	13
7	$C_{17}H_{19}O_2$	3.95	255.1376	272.1937	1.3	17
8	$C_{17}H_{21}O_2$	5.21	257.1538	274.2097	0.9	17
9	$C_{18}H_{17}O_2$	9.99	265.1220	283.1830	1.1	18
10	$C_{18}H_{19}O_3$	100.00	283.1331	301.1934	0.9	18

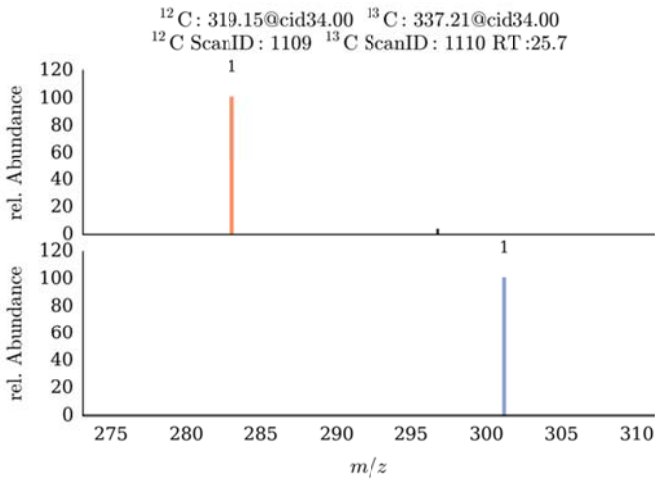
Figure S-28. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for ZEN at a concentration level of c = 0.1 mg/L

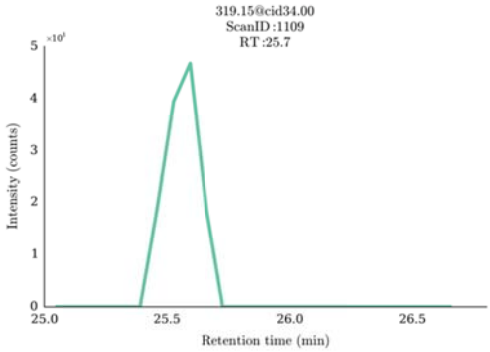




No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{13}H_{11}O_4$	19.36	231.0661	244.1088	4.1	13
2	$C_{18}H_{19}O_3$	100.00	283.1333	301.1932	1.5	18

Figure S-29. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for ZEN at a concentration level of c = 0.02 mg/L

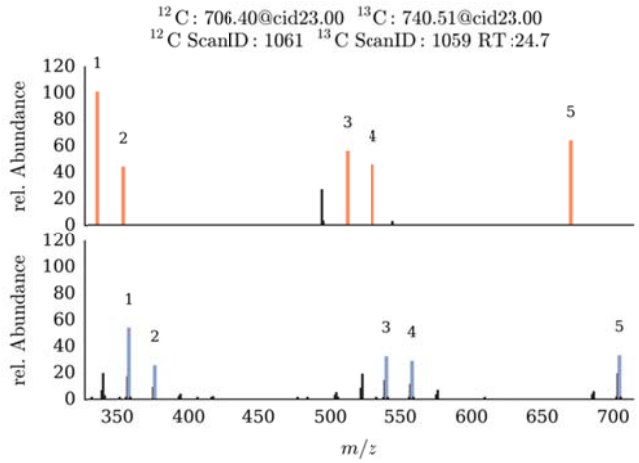


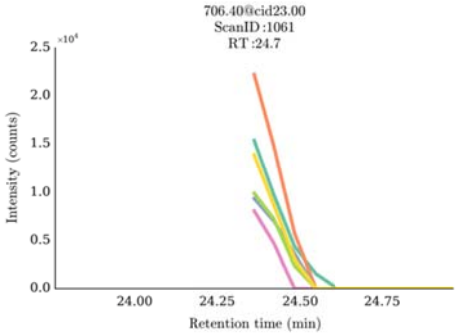


No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{18}H_{19}O_3$	100.00	283.1327	301.1919	0.5	18

FB3

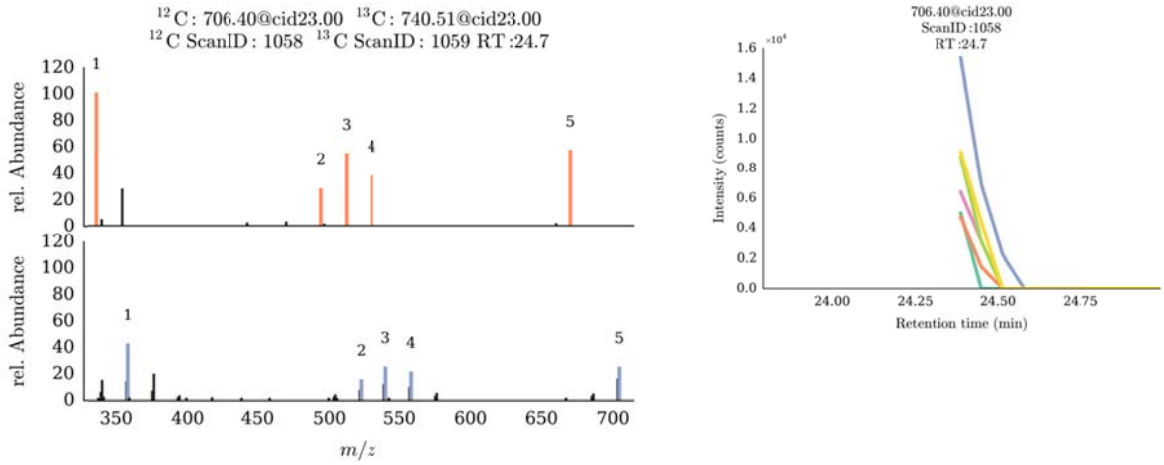
Figure S-30. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for FB3 at a concentration level of c = 1.0 mg/L





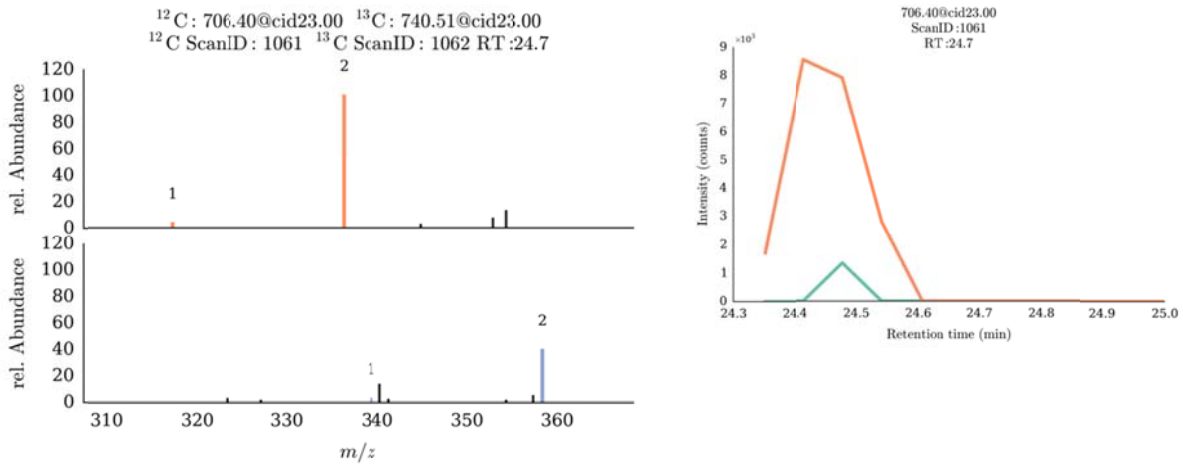
No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{22}H_{42}ON$	100.00	336.3259	358.3999	0.6	22
2	$C_{22}H_{44}O_2N$	42.98	354.3378	376.4104	3.2	22
3	$C_{28}H_{50}O_7N$	55.11	512.3582	540.4523	0.1	28
4	$C_{28}H_{52}O_8N$	44.53	530.3705	558.4633	3.3	28
5	$C_{34}H_{56}O_{12}N$	63.04	670.3845	704.4944	7.2	34

Figure S-31. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for FB3 at a concentration level of c = 0.7 mg/L



No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{22}H_{42}ON$	100.00	336.3278	358.4001	5.1	22
2	$C_{28}H_{48}O_6N$	27.45	494.3472	522.4424	0.8	28
3	$C_{28}H_{50}O_7N$	53.70	512.3576	540.4526	1.1	28
4	$C_{28}H_{52}O_8N$	37.34	530.3693	558.4636	1.1	28
5	$C_{34}H_{56}O_{12}N$	56.28	670.3816	704.4946	2.8	34

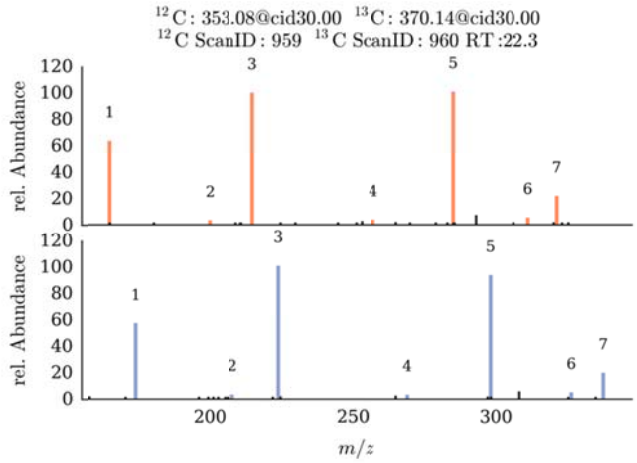
Figure S-32. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for FB3 at a concentration level of c = 0.4 mg/L

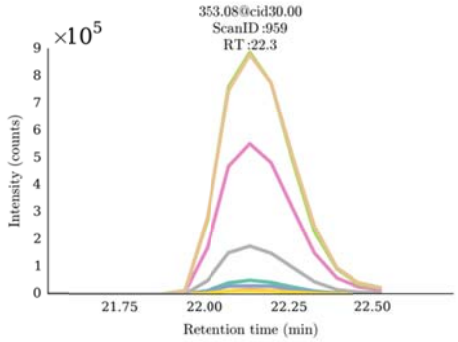


No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{22}H_{39}N$	3.03	317.3095	339.3860	5.7	22
2	$C_{22}H_{42}ON$	100.00	336.3251	358.4002	3.0	22

GRIS

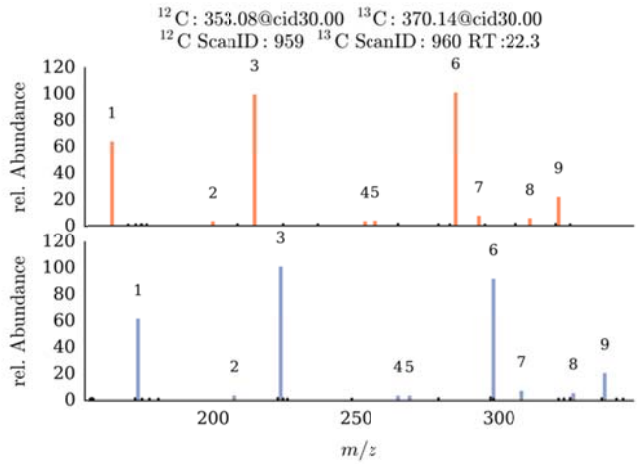
Figure S-33. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for GRIS at a concentration level of c = 1.0 mg/L

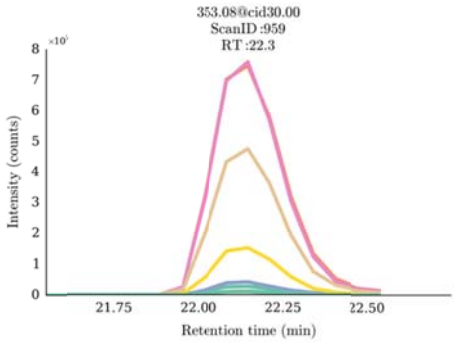




No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_9H_9O_3$	62.71	165.0544	174.0844	1.5	9
2	$C_8H_5O_4Cl$	2.22	199.9870	208.0145	0.4	8
3	$C_9H_8O_4Cl$	99.13	215.0106	224.0405	0.1	9
4	$C_{12}H_{14}O_4Cl$	2.64	257.0576	269.0972	0.5	12
5	$C_{13}H_{14}O_5Cl$	100.00	285.0526	298.0959	0.5	13
6	$C_{15}H_{16}O_5Cl$	4.27	311.0685	326.1187	1.3	15
7	$C_{16}H_{14}O_5Cl$	20.67	321.0525	337.1059	0.3	16

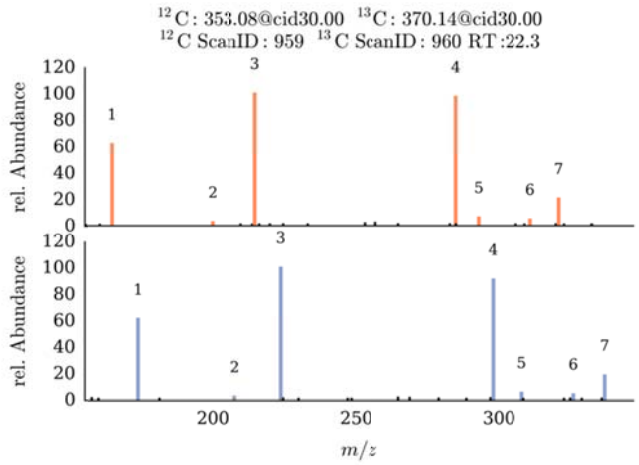
Figure S-34. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for GRIS at a concentration level of c = 0.7 mg/L

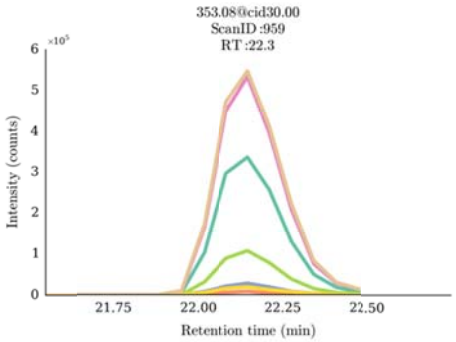




No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_9H_9O_3$	62.89	165.0544	174.0847	1.4	9
2	$C_8H_5O_4Cl$	2.06	199.9867	208.0137	1.8	8
3	$C_9H_8O_4Cl$	98.46	215.0106	224.0408	0.1	9
4	$C_{12}H_{10}O_4Cl$	2.15	253.0259	265.0667	1.2	12
5	$C_{12}H_{14}O_4Cl$	2.45	257.0568	269.0975	2.8	12
6	$C_{13}H_{14}O_5Cl$	100.00	285.0526	298.0963	0.5	13
7	$C_{15}H_{14}O_4Cl$	6.27	293.0575	308.1083	0.2	15
8	$C_{15}H_{16}O_5Cl$	4.42	311.0684	326.1182	1.1	15
9	$C_{16}H_{14}O_5Cl$	20.75	321.0524	337.1061	0.0	16

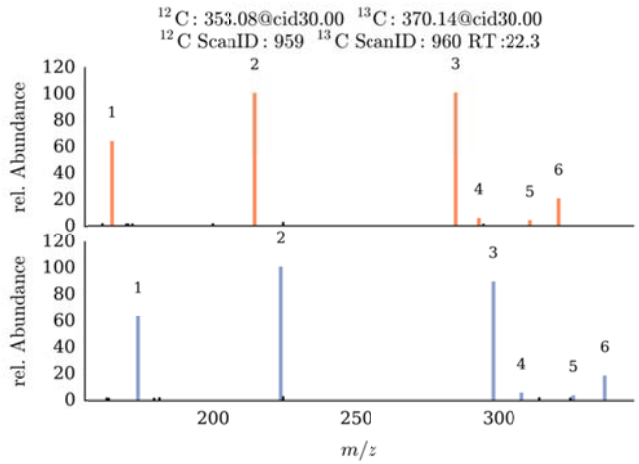
Figure S-35. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for GRIS at a concentration level of c = 0.4 mg/L

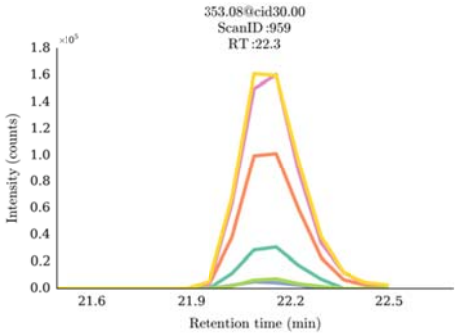




No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_9H_9O_3$	61.71	165.0546	174.0850	0.3	9
2	$C_8H_5O_4Cl$	2.27	199.9870	208.0143	0.5	8
3	$C_9H_8O_4Cl$	100.00	215.0108	224.0411	1.0	9
4	$C_{13}H_{14}O_5Cl$	97.46	285.0528	298.0967	1.4	13
5	$C_{15}H_{14}O_4Cl$	5.87	293.0576	308.1082	0.4	15
6	$C_{15}H_{16}O_5Cl$	4.27	311.0683	326.1189	0.8	15
7	$C_{16}H_{14}O_5Cl$	20.21	321.0526	337.1066	0.7	16

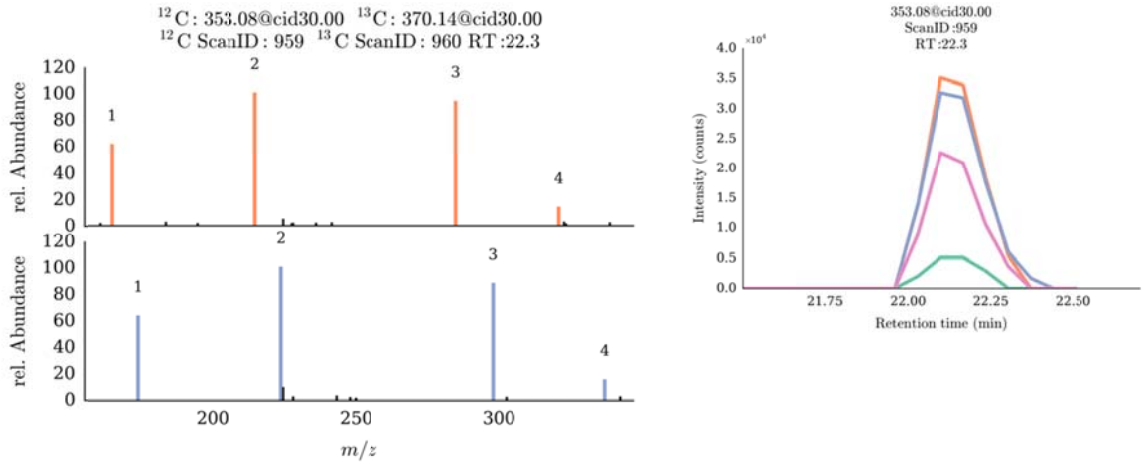
Figure S-36. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for GRIS at a concentration level of c = 0.1 mg/L





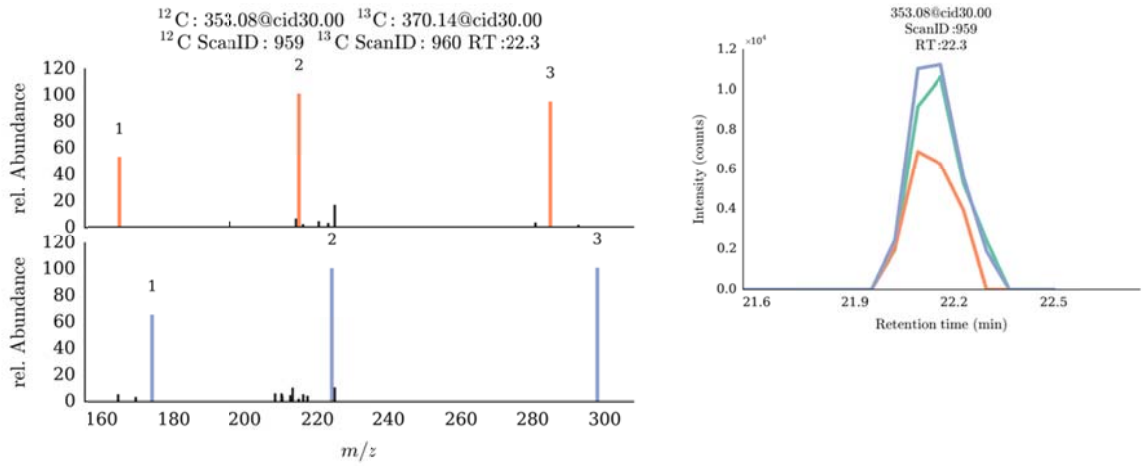
No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_9H_9O_3$	63.31	165.0546	174.0847	0.3	9
2	$C_9H_8O_4Cl$	99.63	215.0107	224.0408	0.7	9
3	$C_{13}H_{14}O_5Cl$	100.00	285.0527	298.0963	1.1	13
4	$C_{15}H_{14}O_4Cl$	4.85	293.0578	308.1084	1.1	15
5	$C_{15}H_{16}O_5Cl$	3.04	311.0688	326.1174	2.2	15
6	$C_{16}H_{14}O_5Cl$	19.50	321.0524	337.1064	0.2	16

Figure S-37. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for GRIS at a concentration level of c = 0.02 mg/L



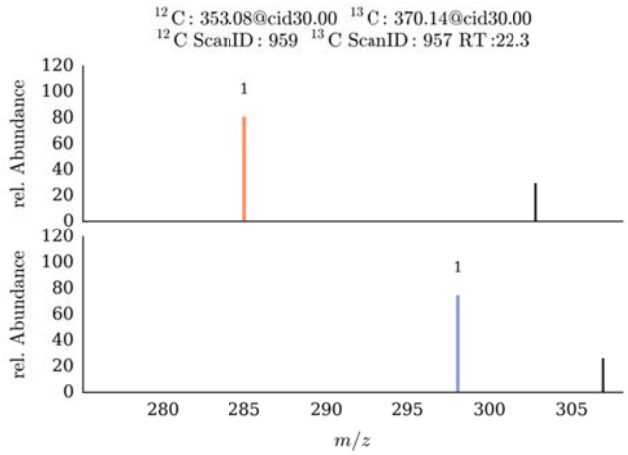
No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_9H_9O_3$	60.86	165.0545	174.0846	1.0	9
2	$C_9H_8O_4Cl$	100.00	215.0107	224.0408	0.6	9
3	$C_{13}H_{14}O_5Cl$	93.65	285.0524	298.0960	0.0	13
4	$C_{16}H_{14}O_5Cl$	13.31	321.0533	337.1042	2.8	16

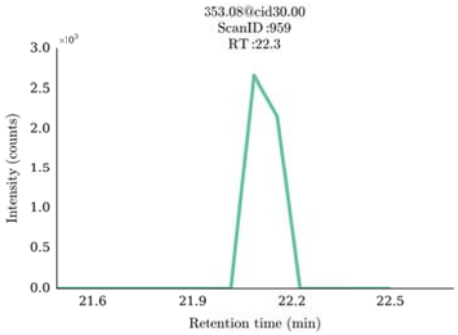
Figure S-38. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for GRIS at a concentration level of c = 0.007 mg/L



No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_9H_9O_3$	51.70	165.0547	174.0845	0.5	9
2	$C_9H_8O_4Cl$	100.00	215.0102	224.0413	1.7	9
3	$C_{13}H_{14}O_5Cl$	94.04	285.0519	298.0966	1.7	13

Figure S-39. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for GRIS at a concentration level of c = 0.001 mg/L

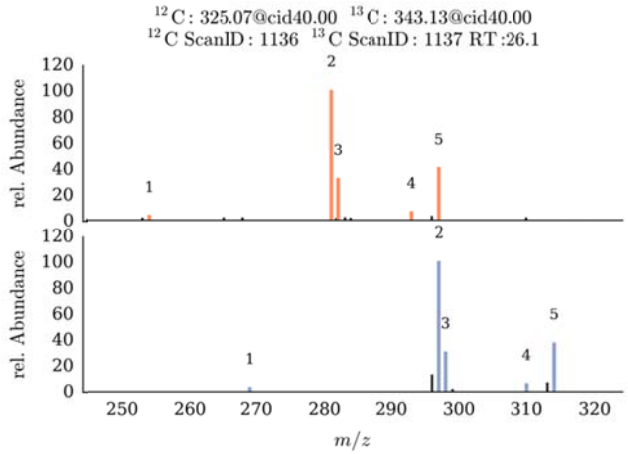


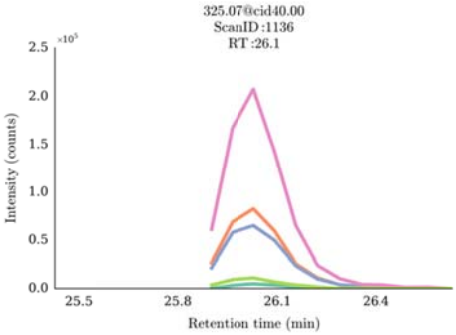


No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{13}H_{14}O_5Cl$	80.03	285.0532	298.0967	9.2	13

STER

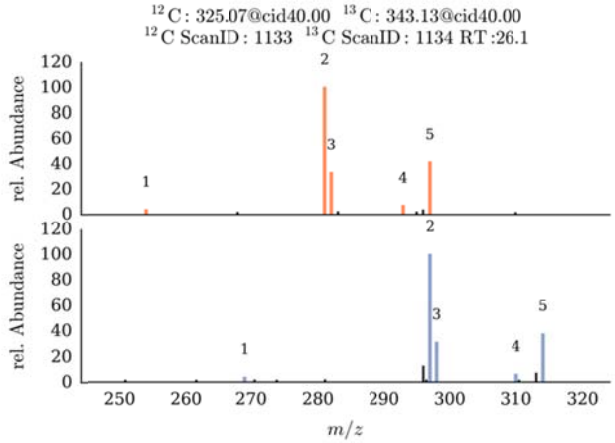
Figure S-40. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for STER at a concentration level of c = 1.0 mg/L

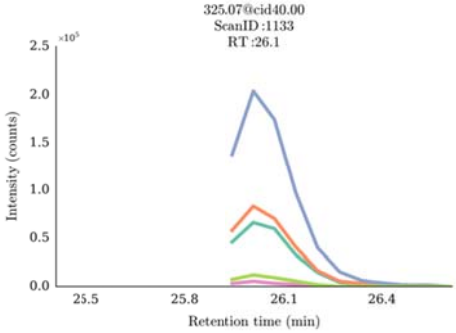




No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{15}H_{10}O_4$	2.85	254.0564	269.1068	4.0	15
2	$C_{16}H_9O_5$	100.00	281.0446	297.0984	0.7	16
3	$C_{16}H_{10}O_5$	31.73	282.0522	298.1061	0.4	16
4	$C_{17}H_9O_5$	5.78	293.0443	310.1017	0.7	17
5	$C_{17}H_{13}O_5$	40.13	297.0758	314.1331	0.3	17

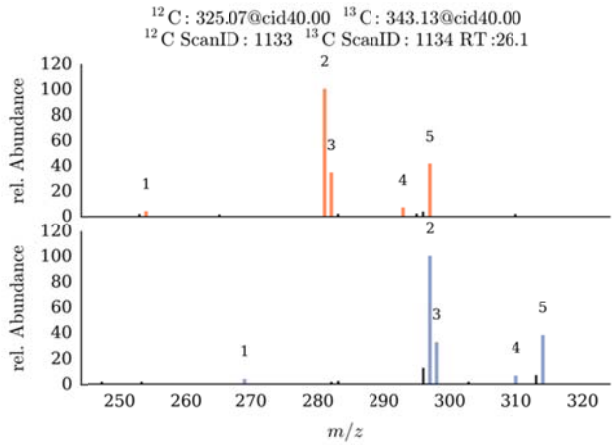
Figure S-41. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for STER at a concentration level of c = 0.7 mg/L

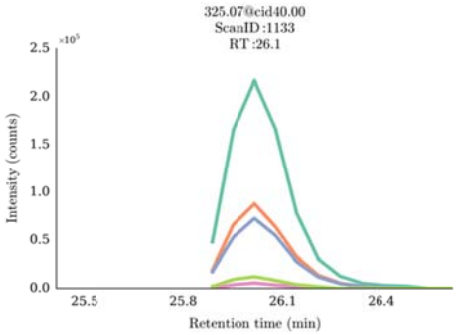




No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{15}H_{10}O_4$	3.18	254.0583	269.1083	3.8	15
2	$C_{16}H_9O_5$	100.00	281.0448	297.0983	1.1	16
3	$C_{16}H_{10}O_5$	32.74	282.0522	298.1058	0.3	16
4	$C_{17}H_9O_5$	6.38	293.0447	310.1012	0.8	17
5	$C_{17}H_{13}O_5$	41.02	297.0760	314.1328	1.0	17

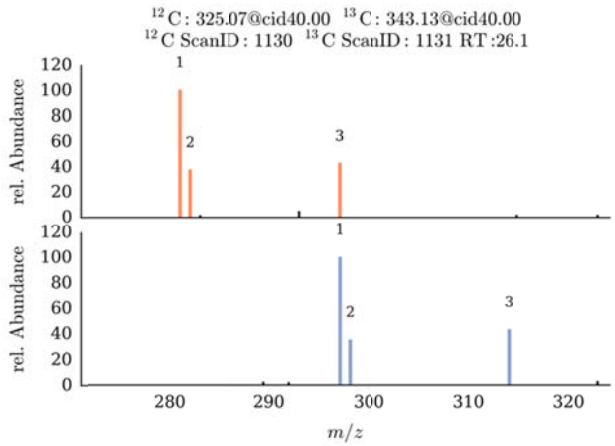
Figure S-42. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for STER at a concentration level of c = 0.4 mg/L

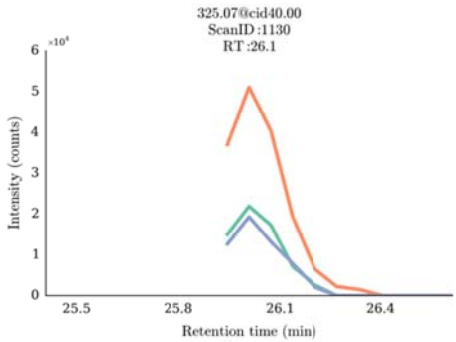




No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{15}H_{10}O_4$	3.08	254.0577	269.1071	1.4	15
2	$C_{16}H_9O_5$	100.00	281.0447	297.0985	1.0	16
3	$C_{16}H_{10}O_5$	33.86	282.0523	298.1061	0.1	16
4	$C_{17}H_9O_5$	6.07	293.0445	310.1028	0.0	17
5	$C_{17}H_{13}O_5$	40.85	297.0760	314.1331	0.8	17

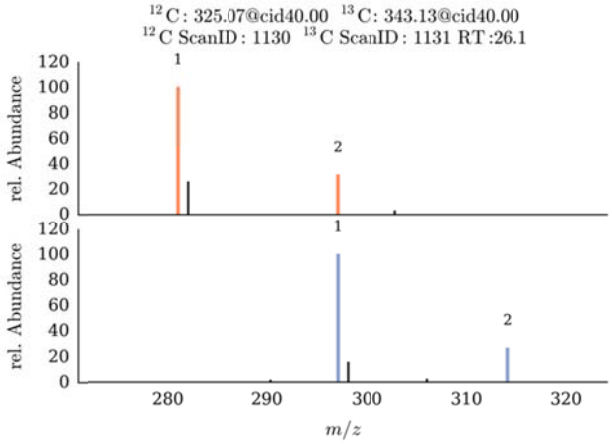
Figure S-43. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for STER at a concentration level of c = 0.1 mg/L

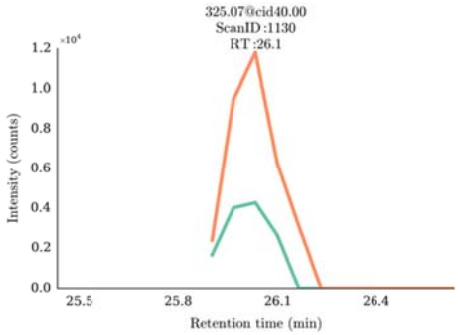




No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{16}H_9O_5$	100.00	281.0445	297.0981	0.3	16
2	$C_{16}H_{10}O_5$	37.04	282.0520	298.1059	1.1	16
3	$C_{17}H_{13}O_5$	42.17	297.0755	314.1328	0.7	17

Figure S-44. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for STER at a concentration level of c = 0.02 mg/L

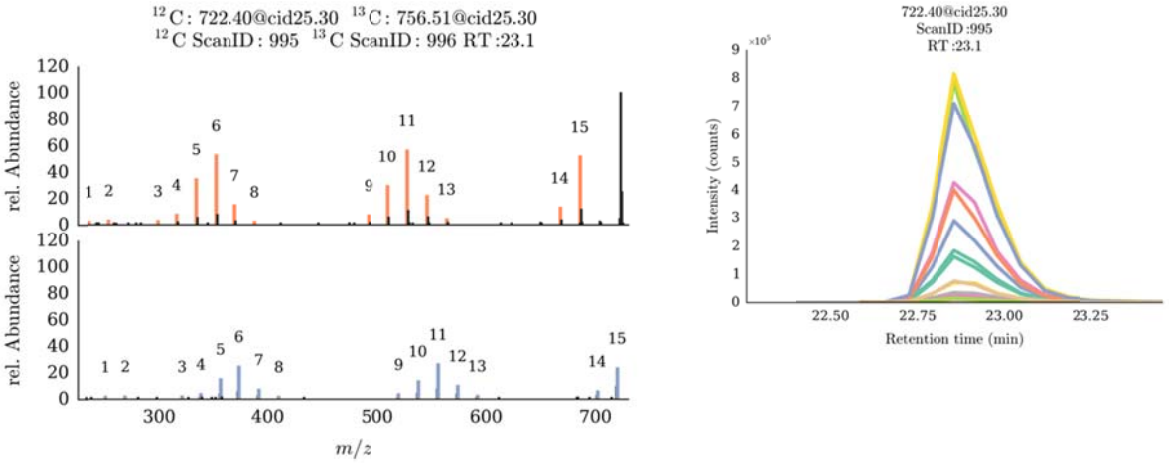




No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{16}H_9O_5$	100.00	281.0442	297.0977	1.0	16
2	$C_{17}H_{13}O_5$	30.81	297.0747	314.1331	3.6	17

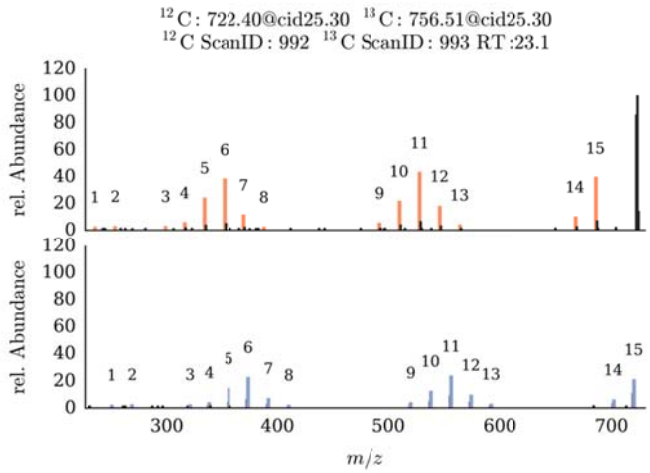
FB1

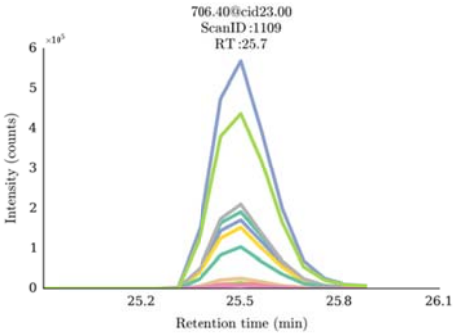
Figure S-45. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for FB1 at a concentration level of c = 1.0 mg/L



No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{15}H_{26}ON$	2.42	236.2009	251.2507	0.1	15
2	$C_{15}H_{28}O2N$	4.16	254.2112	269.2610	0.9	15
3	$C_{22}H_{35}$	3.53	299.2733	321.3478	0.2	22
4	$C_{22}H_{38}N$	12.05	316.2999	338.3737	0.1	22
5	$C_{22}H_{40}ON$	60.56	334.3106	356.3846	0.4	22
6	$C_{22}H_{42}O_2N$	93.22	352.3214	374.3953	1.0	22
7	$C_{22}H_{44}O_3N$	24.84	370.3317	392.4058	0.4	22
8	$C_{22}H_{46}O_4N$	2.39	388.3423	410.4200	0.5	22
9	$C_{28}H_{46}O_6N$	11.22	492.3322	520.4266	0.4	28
10	$C_{28}H_{48}O_7N$	51.05	510.3429	538.4374	0.8	28
11	$C_{28}H_{50}O_8N$	100.00	528.3535	556.4478	0.8	28
12	$C_{28}H_{52}O_9N$	37.54	546.3638	574.4581	0.3	28
13	$C_{28}H_{54}O_{10}N$	5.96	564.3754	592.4683	2.0	28
14	$C_{34}H_{54}O_{12}N$	21.60	668.3654	702.4793	2.0	34
15	$C_{34}H_{56}O_{13}N$	91.54	686.3762	720.4902	2.3	34

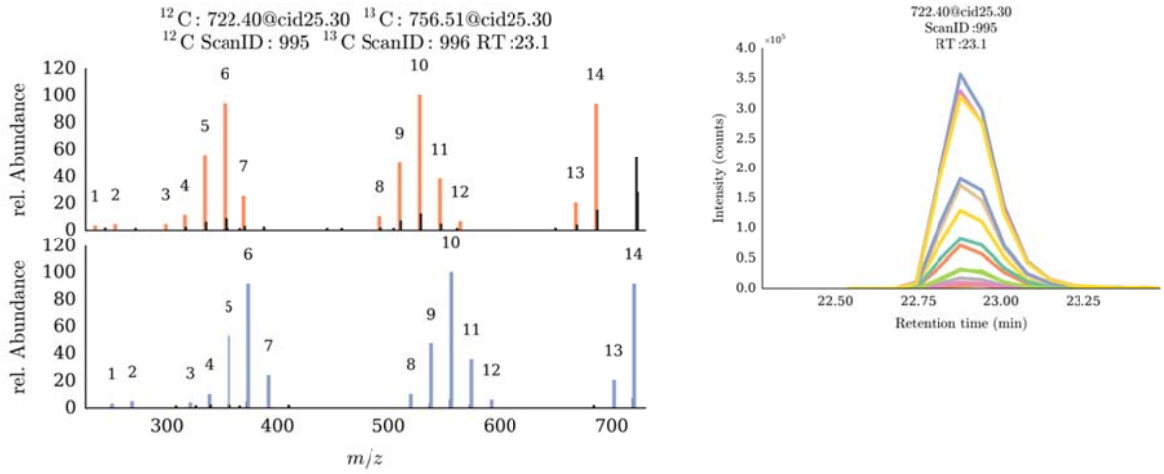
Figure S-46. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for FB1 at a concentration level of c = 0.7 mg/L





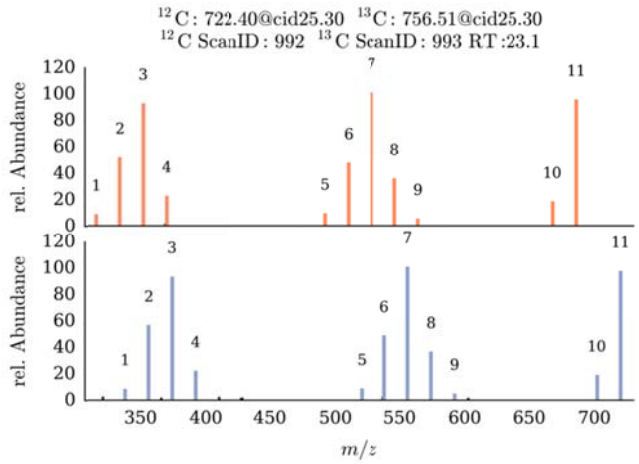
No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{15}H_{26}ON$	2.14	236.2007	251.2519	0.9	15
2	$C_{15}H_{28}O_2N$	3.36	254.2115	269.2615	0.0	15
3	$C_{22}H_{35}$	3.24	299.2734	321.3474	0.2	22
4	$C_{22}H_{38}N$	9.98	316.3001	338.3740	0.8	22
5	$C_{22}H_{40}ON$	54.14	334.3107	356.3849	0.9	22
6	$C_{22}H_{42}O_2N$	87.89	352.3215	374.3955	1.3	22
7	$C_{22}H_{44}O_3N$	23.69	370.3318	392.4060	0.7	22
8	$C_{22}H_{46}O_4N$	2.15	388.3419	410.4159	0.5	22
9	$C_{28}H_{46}O_6N$	9.43	492.3324	520.4269	0.9	28
10	$C_{28}H_{48}O_7N$	48.27	510.3431	538.4376	1.2	28
11	$C_{28}H_{50}O_8N$	100.00	528.3538	556.4480	1.3	28
12	$C_{28}H_{52}O_9N$	39.22	546.3643	574.4585	1.1	28
13	$C_{28}H_{54}O_{10}N$	5.98	564.3750	592.4686	1.4	28
14	$C_{34}H_{54}O_{12}N$	20.13	668.3653	702.4792	1.9	34
15	$C_{34}H_{56}O_{13}N$	90.94	686.3765	720.4905	2.8	34

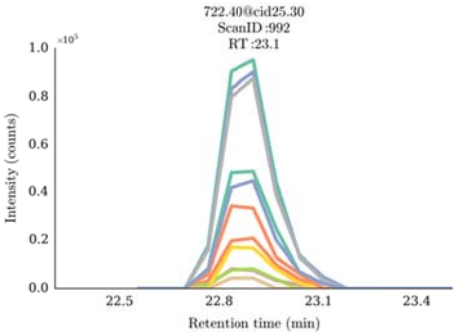
Figure S-47. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for FB1 at a concentration level of c = 0.4 mg/L



No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{15}H_{26}ON$	2.41	236.2016	251.2514	2.9	15
2	$C_{15}H_{28}O_2N$	3.36	254.2112	269.2622	0.8	15
3	$C_{22}H_{35}$	3.43	299.2737	321.3462	1.4	22
4	$C_{22}H_{38}N$	10.31	316.2999	338.3737	0.1	22
5	$C_{22}H_{40}ON$	54.94	334.3107	356.3847	0.8	22
6	$C_{22}H_{42}O_2N$	93.49	352.3215	374.3952	1.3	22
7	$C_{22}H_{44}O_3N$	24.52	370.3317	392.4052	0.4	22
8	$C_{28}H_{46}O_6N$	9.37	492.3320	520.4259	0.1	28
9	$C_{28}H_{48}O_7N$	49.30	510.3427	538.4369	0.4	28
10	$C_{28}H_{50}O_8N$	100.00	528.3534	556.4471	0.6	28
11	$C_{28}H_{52}O_9N$	37.45	546.3640	574.4578	0.7	28
12	$C_{28}H_{54}O_{10}N$	5.55	564.3744	592.4662	0.3	28
13	$C_{34}H_{54}O_{12}N$	19.58	668.3643	702.4782	0.4	34
14	$C_{34}H_{56}O_{13}N$	93.17	686.3759	720.4894	1.8	34

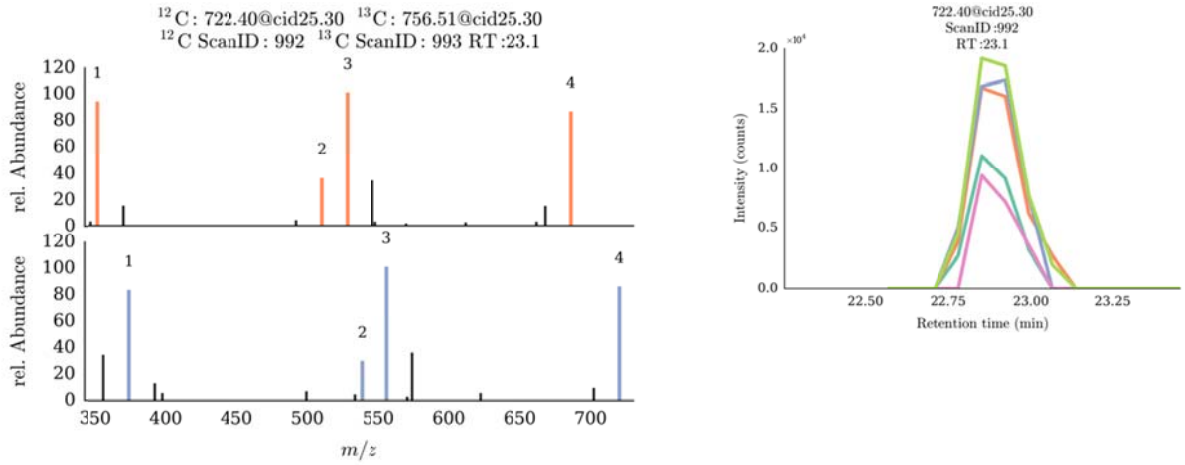
Figure S-48. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for FB1 at a concentration level of c = 0.1 mg/L





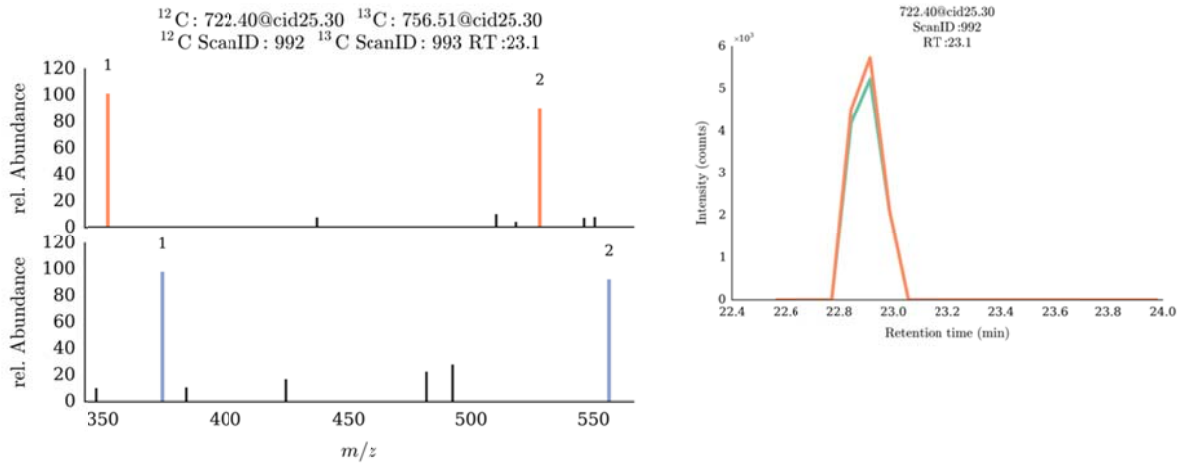
No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{22}H_{38}N$	7.72	316.2995	338.3751	1.1	22
2	$C_{22}H_{40}ON$	50.89	334.3109	356.3846	1.5	22
3	$C_{22}H_{42}O_2N$	91.86	352.3219	374.3950	2.5	22
4	$C_{22}H_{44}O_3N$	21.57	370.3324	392.4059	2.2	22
5	$C_{28}H_{46}O_6N$	8.31	492.3325	520.4254	1.1	28
6	$C_{28}H_{48}O_7N$	46.74	510.3434	538.4369	1.6	28
7	$C_{28}H_{50}O_8N$	100.00	528.3534	556.4467	0.6	28
8	$C_{28}H_{52}O_9N$	34.78	546.3650	574.4587	2.4	28
9	$C_{28}H_{54}O_{10}N$	4.32	564.3765	592.4726	4.0	28
10	$C_{34}H_{54}O_{12}N$	17.33	668.3646	702.4775	0.9	34
11	$C_{34}H_{56}O_{13}N$	94.70	686.3762	720.4894	2.3	34

Figure S-49. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for FB1 at a concentration level of c = 0.02 mg/L



No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{22}H_{42}O_2N$	93.21	352.3217	374.3943	2.0	22
2	$C_{28}H_{48}O_7N$	35.27	510.3388	538.4343	7.2	28
3	$C_{28}H_{50}O_8N$	100.00	528.3520	556.4437	2.1	28
4	$C_{34}H_{56}O_{13}N$	85.60	686.3760	720.4894	2.1	34

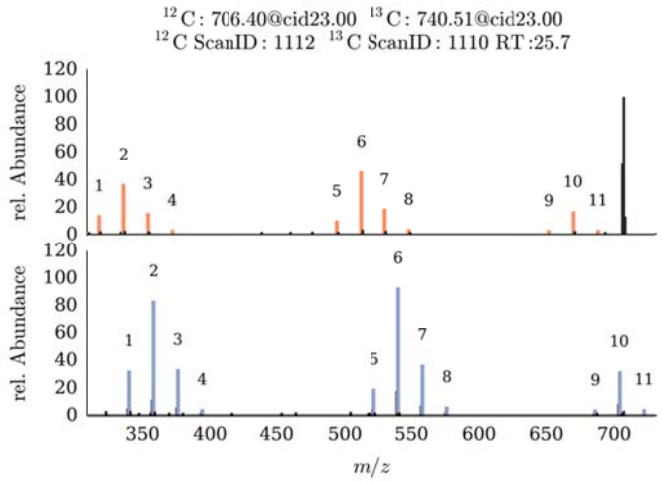
Figure S-50. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for FB1 at a concentration level of c = 0.007 mg/L

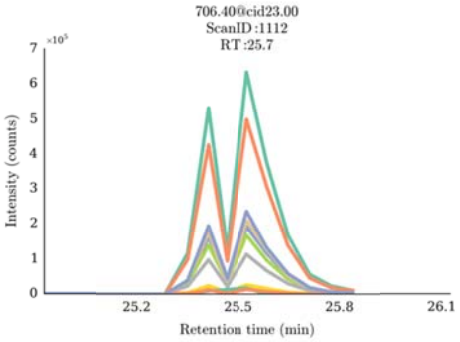


No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{22}H_{42}O_2N$	100.00	352.3227	374.3944	4.9	22
2	$C_{28}H_{50}O_8N$	88.81	528.3536	556.4446	1.0	28

FB2

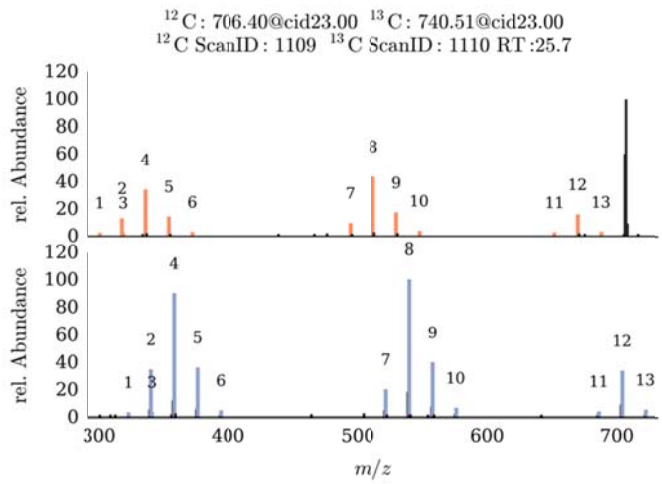
Figure S-51. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for FB2 at a concentration level of c = 1.0 mg/L

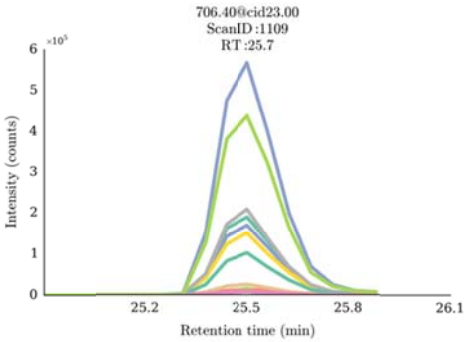




No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{22}H_{40}N$	27.40	318.3158	340.3900	1.0	22
2	$C_{22}H_{42}ON$	79.01	336.3267	358.4003	1.8	22
3	$C_{22}H_{44}O_2N$	31.13	354.3372	376.4109	1.4	22
4	$C_{22}H_{46}O_3N$	3.46	372.3475	394.4218	0.8	22
5	$C_{28}H_{48}O_6N$	18.72	494.3483	522.4427	1.4	28
6	$C_{28}H_{50}O_7N$	100.00	512.3594	540.4532	2.5	28
7	$C_{28}H_{52}O_8N$	37.94	530.3699	558.4637	2.1	28
8	$C_{28}H_{54}O_9N$	4.93	548.3791	576.4744	0.4	28
9	$C_{34}H_{54}O_{11}N$	2.90	652.3701	686.4835	1.5	34
10	$C_{34}H_{56}O_{12}N$	33.88	670.3817	704.4951	3.0	34
11	$C_{34}H_{58}O_{13}N$	3.49	688.3928	722.5065	3.6	34

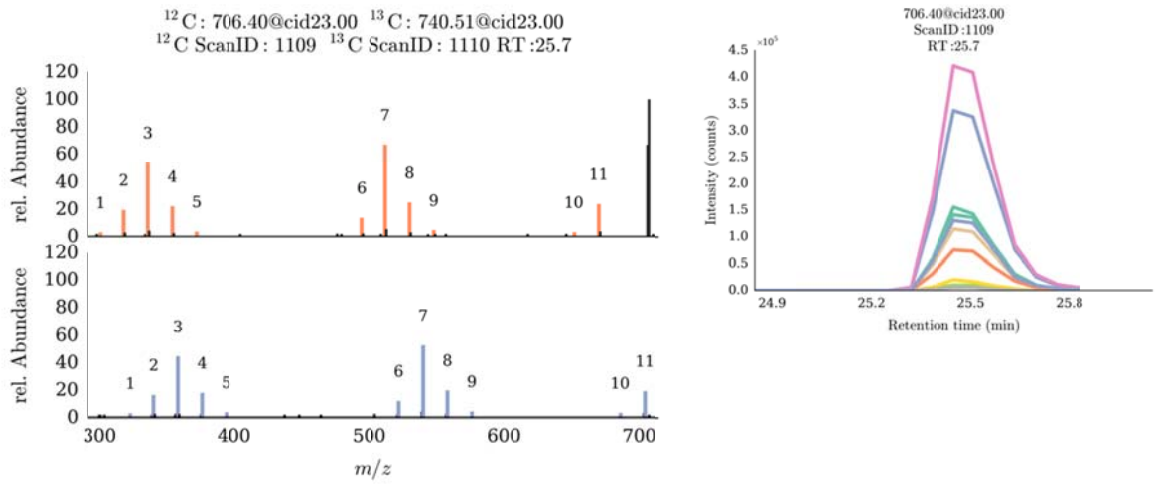
Figure S-52. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for FB2 at a concentration level of c = 0.7 mg/L





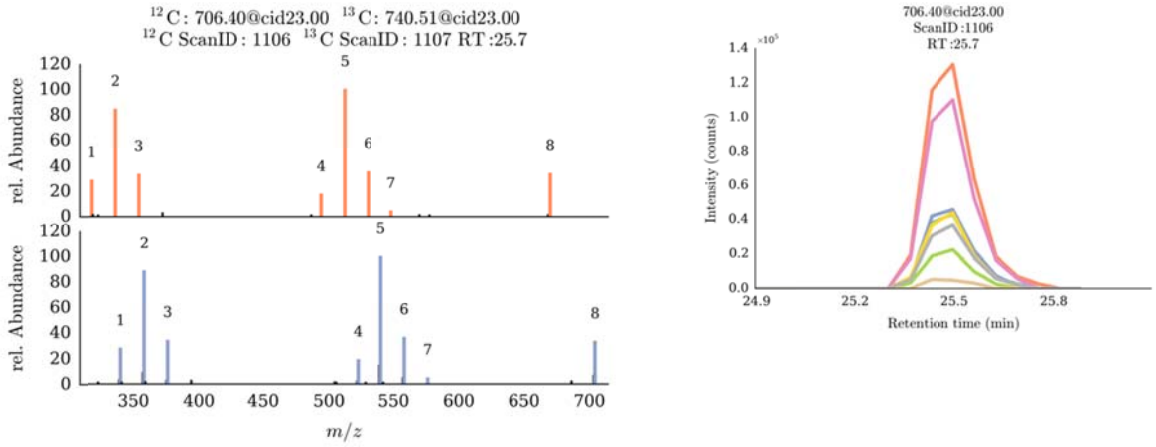
No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{22}H_{37}$	2.04	301.2881	323.3633	3.1	22
2	$C_{22}H_{40}N$	27.21	318.3155	340.3898	0.2	22
3	$C_{22}H_{39}O$	2.16	319.3016	341.3730	6.6	22
4	$C_{22}H_{42}ON$	77.29	336.3263	358.4001	0.6	22
5	$C_{22}H_{44}O_2N$	30.43	354.3367	376.4107	0.1	22
6	$C_{22}H_{46}O_3N$	3.17	372.3472	394.4213	0.0	22
7	$C_{28}H_{48}O_6N$	18.71	494.3478	522.4424	0.5	28
8	$C_{28}H_{50}O_7N$	100.00	512.3589	540.4529	1.4	28
9	$C_{28}H_{52}O_8N$	37.30	530.3694	558.4636	1.3	28
10	$C_{28}H_{54}O_9N$	5.21	548.3796	576.4747	0.5	28
11	$C_{34}H_{54}O_{11}N$	2.49	652.3708	686.4841	2.5	34
12	$C_{34}H_{56}O_{12}N$	33.97	670.3809	704.4947	1.8	34
13	$C_{34}H_{58}O_{13}N$	3.45	688.3921	722.5059	2.6	34

Figure S-53. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for FB2 at a concentration level of c = 0.4 mg/L



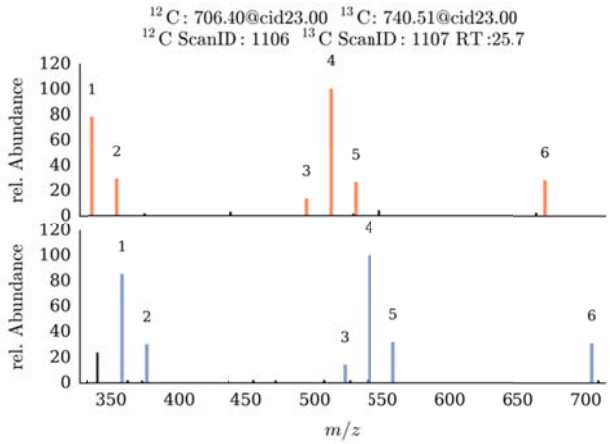
No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{22}H_{37}$	2.07	301.2891	323.3621	0.3	22
2	$C_{22}H_{40}N$	27.26	318.3159	340.3897	1.0	22
3	$C_{22}H_{42}ON$	79.98	336.3269	358.4001	2.3	22
4	$C_{22}H_{44}O_2N$	31.26	354.3373	376.4106	1.8	22
5	$C_{22}H_{46}O_3N$	3.06	372.3481	394.4213	2.5	22
6	$C_{28}H_{48}O_6N$	18.48	494.3484	522.4421	1.6	28
7	$C_{28}H_{50}O_7N$	100.00	512.3594	540.4527	2.3	28
8	$C_{28}H_{52}O_8N$	35.43	530.3698	558.4636	2.0	28
9	$C_{28}H_{54}O_9N$	4.68	548.3798	576.4735	0.9	28
10	$C_{34}H_{54}O_{11}N$	2.52	652.3707	686.4854	2.4	34
11	$C_{34}H_{56}O_{12}N$	33.77	670.3813	704.4948	2.4	34

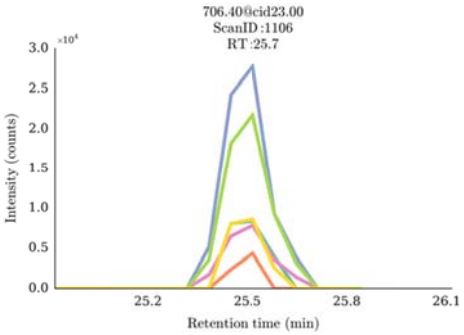
Figure S-54. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for FB2 at a concentration level of c = 0.1 mg/L



No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{22}H_{40}N$	28.29	318.3159	340.3900	1.2	22
2	$C_{22}H_{42}ON$	84.47	336.3268	358.4003	2.2	22
3	$C_{22}H_{44}O_2N$	33.09	354.3373	376.4109	1.9	22
4	$C_{28}H_{48}O_6N$	17.28	494.3477	522.4423	0.3	28
5	$C_{28}H_{50}O_7N$	100.00	512.3589	540.4526	1.4	28
6	$C_{28}H_{52}O_8N$	35.07	530.3696	558.4637	1.6	28
7	$C_{28}H_{54}O_9N$	3.80	548.3776	576.4756	3.1	28
8	$C_{34}H_{56}O_{12}N$	33.61	670.3804	704.4946	1.0	34

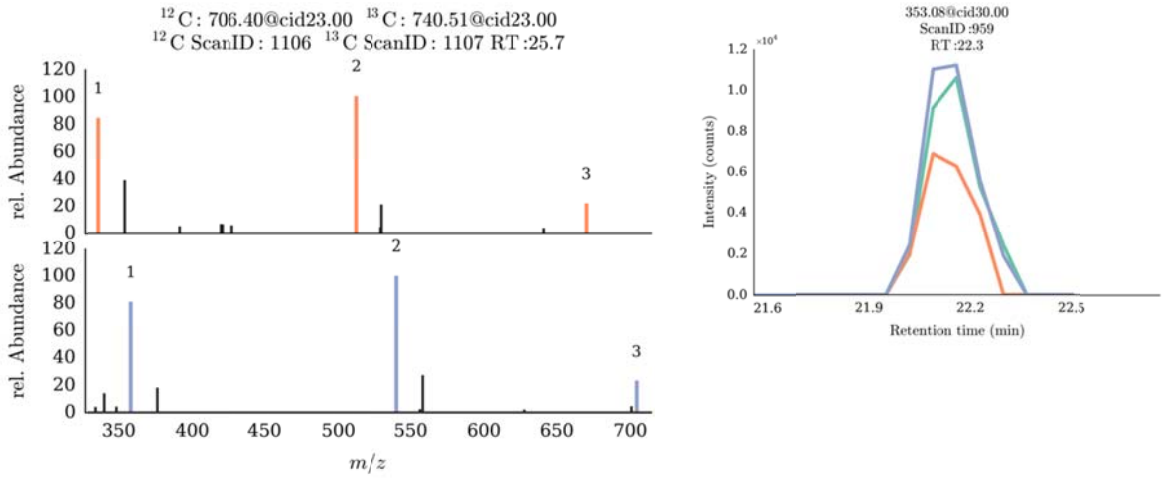
Figure S-55. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for FB2 at a concentration level of c = 0.02 mg/L





No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{22}H_{42}ON$	77.54	336.3266	358.4006	1.4	22
2	$C_{22}H_{44}O_2N$	28.24	354.3366	376.4102	0.1	22
3	$C_{28}H_{48}O_6N$	12.57	494.3481	522.4402	0.9	28
4	$C_{28}H_{50}O_7N$	100.00	512.3586	540.4522	0.8	28
5	$C_{28}H_{52}O_8N$	25.46	530.3685	558.4645	0.5	28
6	$C_{34}H_{56}O_{12}N$	27.36	670.3788	704.4922	1.3	34

Figure S-56. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for FB2 at a concentration level of c = 0.007 mg/L



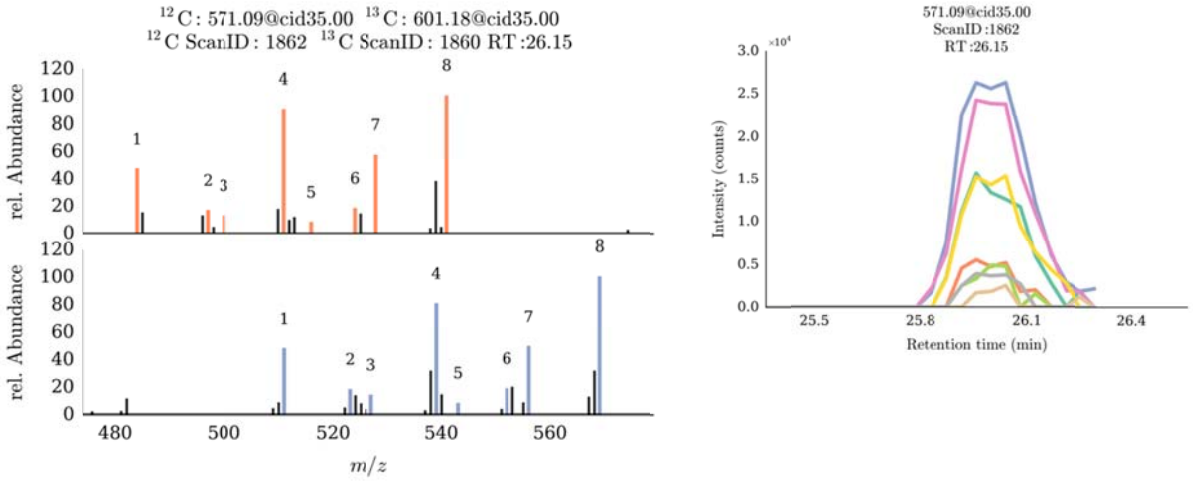
No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{22}H_{42}ON$	84.16	336.3280	358.3999	5.7	22
2	$C_{28}H_{50}O_7N$	100.00	512.3586	540.4524	0.9	28
3	$C_{34}H_{56}O_{12}N$	20.59	670.3787	704.4961	1.6	34

Table S-3. Overview of all precursor ions of biological compounds which had been chosen from a metabolomics LC-HRMS dataset for LC-HRMS/MS measurements and subsequent data processing by FragExtract used together with the annotated elemental composition

^{12}C *m/z*	^{13}C *m/z*	n(C)	Ion species	Rt[min]	Possible molecular formula	Annotated molecular formula
571.0856	601.1863	30	$[M+H]^+$	26.15	$C_{30}H_{19}O_{12}$, $C_{30}H_{24}O_5NP_3$	$C_{30}H_{19}O_{12}$, $C_{30}H_{24}O_5NP_3$
611.2491	637.3363	26	$[M+H]^+$	10.45	$C_{26}H_{46}N7P_5$, $C_{26}H_{41}O_7N_6P_2$, $C_{26}H_{34}O_5N_{11}P$	$C_{26}H_{41}O_7N_6P_2$, $C_{26}H_{34}O_5N_{11}P$
647.3724	677.4731	30	$[M+Na]^+$	23.9	$C_{30}H_{52}O_8N_6Na$, $C_{30}H_{57}ON_7P_3Na$	$C_{30}H_{52}O_8N_6Na$
647.3724	677.4731	30	$[M+Na]^+$	26.74	$C_{30}H_{52}O_8N_6Na$, $C_{30}H_{57}ON_7P_3Na$	$C_{30}H_{52}O_8N_6Na$
651.5653	690.6961	39	unknown	35.39	$C_{39}H_{75}O_5N_2$	$C_{39}H_{75}O_5N_2$
761.3612	791.4619	30	$[M+H]^+$	12.74	$C_{30}H_{48}O_7N_{15}P$, $C_{30}H_{60}O_2N_{11}P_5$, $C_{30}H_{75}O_4NP_8$, $C_{30}H_{70}O_{11}P_5$, $C_{30}H_{55}O_9N_{10}P_2$	$C_{30}H_{48}O_7N_{15}P$, $C_{30}H_{55}O_9N_{10}P_2$
787.5031	822.6205	35	$[M+H]^+$	22.31	$C_{35}H_{67}O_{10}N_{10}$, $C_{35}H_{72}O_3N_{11}P_3$, $C_{35}H_{82}O_{12}P_3$	$C_{35}H_{67}O_{10}N_{10}$
877.375	916.5058	39	$[M+H]^+$	17.01	$C_{39}H_{64}O_4N_9P_5$, $C_{39}H_{59}O_{11}N_8P_2$, $C_{39}H_{52}O_9N_{13}P$, $C_{39}H_{57}O_2N_{14}P_4$, $C_{39}H_{62}O_{18}N_2P$	$C_{39}H_{59}O_{11}N_8P_2$, $C_{39}H_{52}O_9N_{13}P$
790.3163	820.4168	30	$[M+H]^+$	13.25	$C_{30}H_{54}O_{13}N_8Fe$, $C_{30}H_{59}O_6N_9P_3Fe$, $C_{30}H_{44}O_4N_{19}Fe$, $C_{30}H_{71}ON_5P_7Fe$, $C_{30}H_{66}O_8N_4P_4Fe$, $C_{30}H_{61}O_{15}N_3PFe$	$C_{30}H_{54}O_{13}N_8Fe$, $C_{30}H_{66}O_8N_4P_4Fe$

To obtain the possible molecular formulas for the precursor ions a ±3 ppm window was allowed. For pairing of the corresponding fragment ions an inter-spectrum mass deviation of ±10 ppm and a Relative abundance deviation of 30% was allowed. Rt is the approximate measured retention time as taken from the preceding LC-HRMS full scan measurements. n(C) is the number of carbon atoms that was calculated by FragExtract for the precursor ion and was compared to the detected number of carbon atoms by MetExtract. The ion species was obtained by analyzing the LC-HRMS full scan data with MetExtract[2, 3].

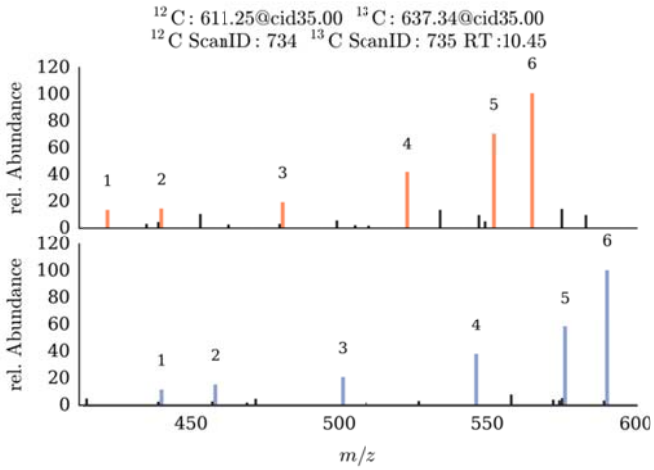
Figure S-57. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for *m/z* 571.0856 (aurofusarin) at a CE of 35%

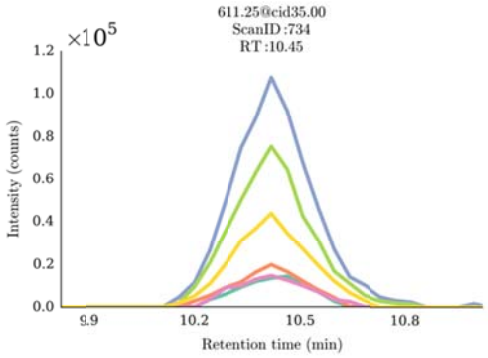


No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{27}H_{21}O_2NP_3$, $C_{27}H_{16}O_9$	46.49	484.0774	511.1716	1.1/3.0	27
2	$C_{26}H_7O_5N_7$,*	15.83	497.0484	523.1320	3.9/*	26
3	$C_{27}H_{21}O_3NP_3$, $C_{27}H_{16}O_{10}$	11.87	500.0730	527.1638	0.2/1.7	27
4	$C_{28}H_{15}O_{10}$, $C_{28}H_{20}O_3NP_3$	90.11	511.0663	539.1609	0.5/2.3	28
5	$C_{27}H_{16}O_{11}$, $C_{27}H_{21}O_4NP_3$	7.06	516.0702	543.1566	2.9/4.6	27
6	$C_{28}H_{12}O_{11}$, $C_{28}H_{17}O_4NP_3$	17.35	524.0387	552.1304	2.4/4.2	28
7	$C_{28}H_{21}O_4NP_3$, $C_{28}H_{16}O_{11}$	57.09	528.0682	556.1622	0.7/1.0	28
8	$C_{28}H_{13}O_{12}$, $C_{28}H_{18}O_5NP_3$	100.00	541.0403	569.1337	0.2/1.9	28

'*' no elemental composition could be calculated for the neutral loss mass, molecular formula with the lowest mass deviation is presented

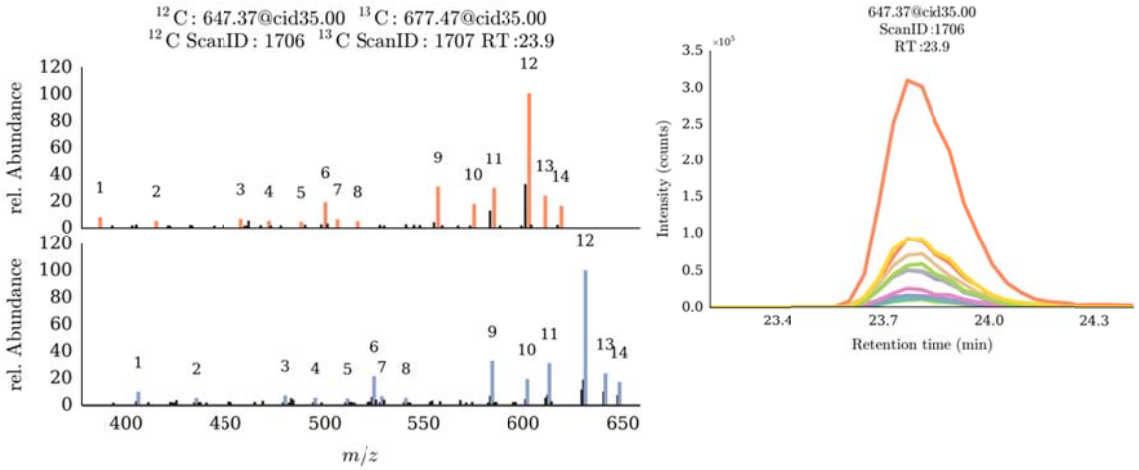
Figure S-58. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for *m/z* 611.2491 at a CE of 35%





No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{18}H_{26}O_3N_5P_2$, $C_{18}H_{19}ON_{10}P$	12.28	422.1492	440.2112	3.2/3.9	18
2	$C_{18}H_{28}O_4N_5P_2$, $C_{18}H_{21}O_2N_{10}P$	13.33	440.1602	458.2239	2.0/4.9	18
3	$C_{20}H_{31}O_4N_6P_2$, $C_{20}H_{24}O_2N_{11}P$	18.12	481.1871	501.2555	1.2/5.0	20
4	$C_{23}H_{37}O_4N_6P_2$, $C_{23}H_{30}O_2N_{11}P$	40.53	523.2343	546.3108	0.7/5.1	23
5	$C_{24}H_{36}O_6N_5P_2$, $C_{24}H_{29}O_4N_{10}P$	69.80	552.2128	576.2931	1.3/4.2	24
6	$C_{25}H_{39}O_5N_6P_2$, $C_{25}H_{32}O_3N_{11}P$	100.00	565.2445	590.3284	1.2/4.1	25

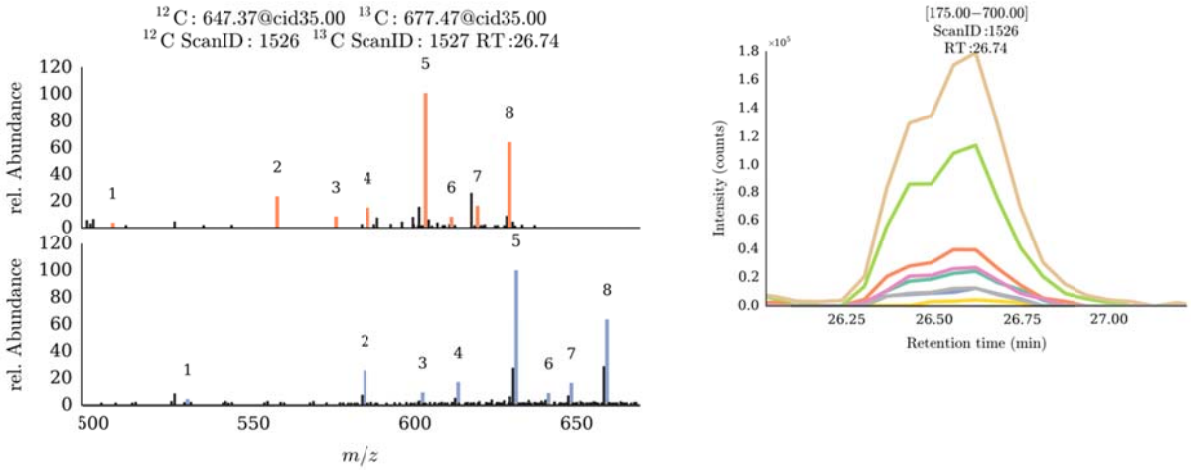
Figure S-59. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for *m/z* 647.3724 (RT: 23.9) at a CE of 35%



No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{19}H_{32}O_3N_4Na$	7.02	387.2374	406.3004	1.9	19
2	$C_{20}H_{29}O_3N_7$,*	4.10	415.2335	435.2995	2.1/*	20
3	$C_{22}H_{37}O_4N_5Na$	5.62	458.2743	480.3471	1.1	22
4	$C_{23}H_{39}O_4N_5Na$	4.26	472.2878	495.3670	3.4	23
5	$C_{23}H_{46}O_7PNa$,*	3.28	488.2874	511.3609	0.1/*	23
6	$C_{25}H_{40}O_3N_8$,*	18.08	500.3213	525.4047	1/*	25
7	$C_{23}H_{53}ONP_4Na$,*	5.44	506.2969	529.3708	0.2/*	23
8	$C_{25}H_{43}O_5N_5Na$	3.87	516.3135	541.3983	4.1	25
9	$C_{27}H_{46}O_5N_6Na$	29.73	557.3425	584.4333	0.5	27
10	$C_{27}H_{48}O_6N_6Na$	16.72	575.3534	602.4434	1.1	27
11	$C_{28}H_{46}O_6N_6Na$	28.66	585.3370	613.4308	0.1	28
12	$C_{28}H_{48}O_7N_6Na$	100.00	603.3485	631.4424	1.4	28
13	$C_{30}H_{48}O_6N_6Na$	23.14	611.3530	641.4531	0.4	30
14	$C_{29}H_{52}O_7N_6Na$	15.52	619.3808	648.4758	3.0	29

'*' no elemental composition could be calculated for the neutral loss mass, molecular formula with the lowest mass deviation is presented

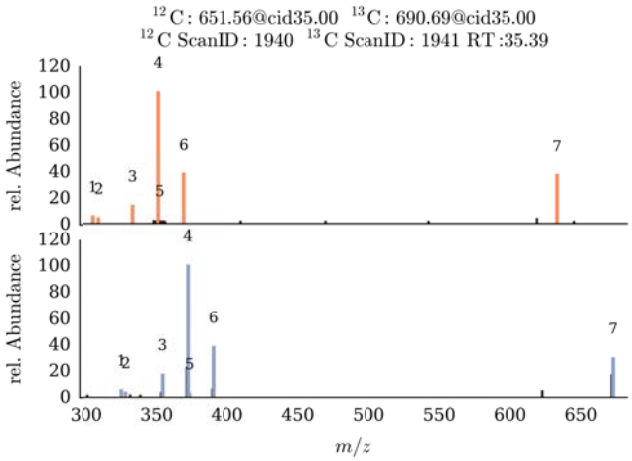
Figure S-60. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for *m/z* 647.3724 (RT: 26.74) at a CE of 35%

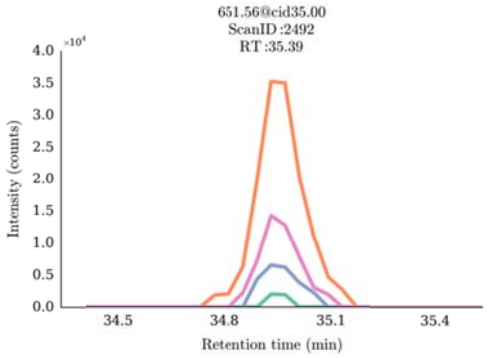


No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{23}H_{41}O_6N_5Na$, *	2.59	506.2959	529.3726	1.9/*	23
2	$C_{27}H_{46}O_5N_6Na$	22.47	557.3431	584.4341	1.6	27
3	$C_{27}H_{48}O_6N_6Na$	7.25	575.3558	602.4443	5.2	27
4	$C_{28}H_{46}O_6N_6Na$	13.94	585.3367	613.4315	0.6	28
5	$C_{28}H_{48}O_7N_6Na$	100.00	603.3486	631.4435	1.5	28
6	$C_{30}H_{48}O_6N_6Na$	7.21	611.3503	641.4539	3.9	30
7	$C_{29}H_{52}O_7N_6Na$	15.38	619.3798	648.4776	1.4	29
8	$C_{30}H_{50}O_7N_6Na$	63.58	629.3629	659.4656	0.6	30

'*' no elemental composition could be calculated for the neutral loss mass, molecular formula with the lowest mass deviation is presented

Figure S-61. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for *m/z* 651.5653 at a CE of 35%

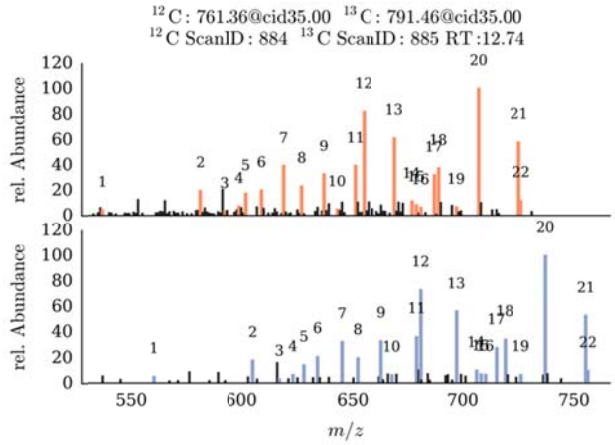


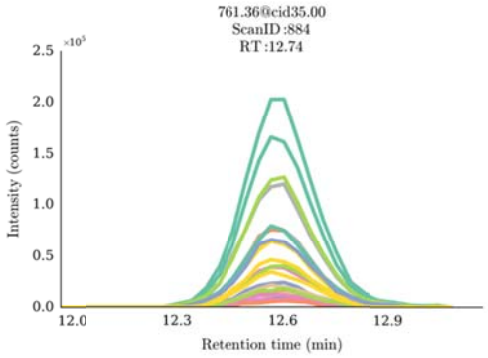


No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{20}H_{37}N_2$	5.06	305.2939	325.3613	4.1	20
2	$C_{19}H_{37}ON_2$	3.60	309.2904	328.3551	1.2	19
3	$C_{21}H_{37}ON_2$	13.17	333.2897	354.3604	1.1	21
4	$C_{21}H_{39}O_2N_2$	100.00	351.3009	372.3715	0.8	21
5	$C_{21}H_{38}O_3N$	2.02	352.2849	373.3563	0.7	21
6	$C_{21}H_{41}O_3N_2$	37.64	369.3119	390.3821	1.9	21
7	$C_{39}H_{73}O_4N_2$	36.65	633.5590	672.6896	4.0	39

'*' no elemental composition could be calculated for the neutral loss mass, molecular formula with the lowest mass deviation is presented

Figure S-62. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for *m/z* 761.3612 at a CE of 35%

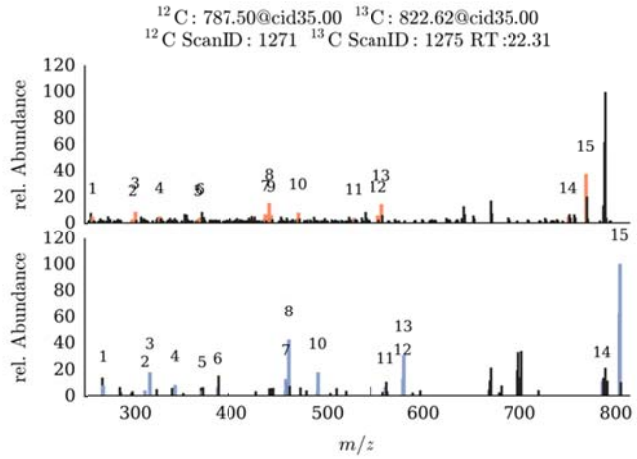


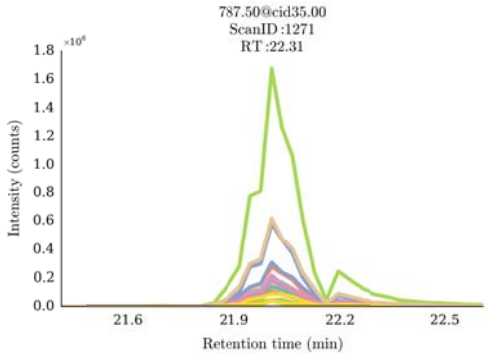


No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{23}H_{46}O_5N_3P_3$,*	3.84	537.2636	560.3390	1.6/*	23
2	$C_{24}H_{39}O_5N_8P_2$, $C_{24}H_{32}O_3N_{13}P$	19.23	581.2509	605.3289	0.7/4.5	24
3	$C_{25}H_{36}O_6N_7P_2$, $C_{25}H_{29}O_4N_{12}P$	2.89	592.2191	617.2988	1.1/4.0	25
4	$C_{24}H_{34}O_4N_{13}P$, $C_{24}H_{41}O_6N_8P_2$	6.82	599.2596	623.3440	1.3/3.7	24
5	$C_{26}H_{34}O_6N_7P_2$, $C_{26}H_{27}O_4N_{12}P$	17.03	602.2032	628.2947	1.4/3.6	26
6	$C_{25}H_{32}O_4N_{13}P$, $C_{25}H_{39}O_6N_8P_2$	19.53	609.2457	634.3286	4.0/0.9	25
7	$C_{26}H_{37}O_6N_8P_2$, $C_{26}H_{30}O_4N_{13}P$	38.99	619.2302	645.3178	0.7/4.2	26
8	$C_{25}H_{41}O_7N_8P_2$, $C_{25}H_{34}O_5N_{13}P$	22.79	627.2562	652.3403	1.01/3.8	25
9	$C_{26}H_{32}O_5N_{13}P$, $C_{26}H_{39}O_7N_8P_2$	32.38	637.2405	663.3270	1.0/3.8	26
10	$C_{25}H_{48}O_{10}N_3P_3$	4.40	643.2547	668.3333	0.0	25
11	$C_{28}H_{49}O_4N_{10}P_2$	39.10	651.3401	679.4352	1.1	28
12	$C_{26}H_{41}O_8N_8P_2$, $C_{26}H_{34}O_6N_{13}P$	81.82	655.2512	681.3387	0.8/3.8	26
13	$C_{28}H_{43}O_5N_{15}$	61.11	669.3512	697.4460	8.1	28
14	$C_{29}H_{39}O_5N_{15}$	10.77	677.3213	706.4132	5.9	29
15	$C_{29}H_{42}O_3N_{15}P$	8.03	679.3322	708.4325	0.8	29
16	$C_{29}H_{43}O_5N_{15}$	5.92	681.3550	710.4467	2.3	29
17	$C_{28}H_{45}O_6N_{15}$	31.72	687.3615	715.4541	8.2	28
18	$C_{30}H_{39}O_5N_{15}$	37.26	689.3188	719.4215	9.4	30
19	$C_{29}H_{44}O_4N_{15}P$	6.22	697.3442	726.4453	1.3	29
20	$C_{30}H_{41}O_6N_{15}$	100.00	707.3299	737.4301	8.5	30
21	$C_{30}H_{43}O_7N_{15}$	57.90	725.3409	755.4415	7.6	30
22	$C_{30}H_{50}O_8N_9P_2$	11.49	726.3251	756.4257	0.1	30

'*' no elemental composition could be calculated for the neutral loss mass, molecular formula with the lowest mass deviation is presented

Figure S-63. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for *m/z* 787.5031 at a CE of 35%

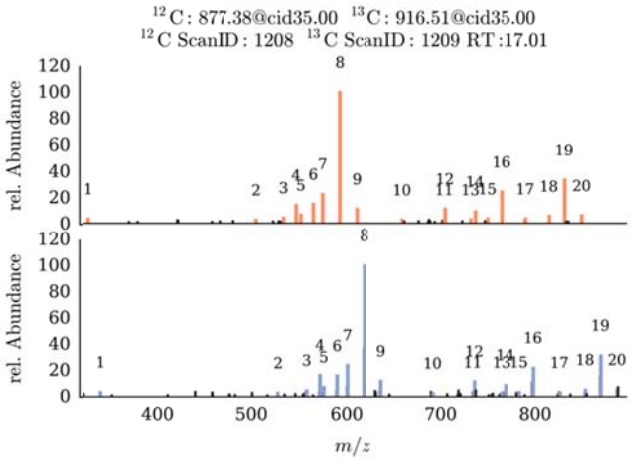


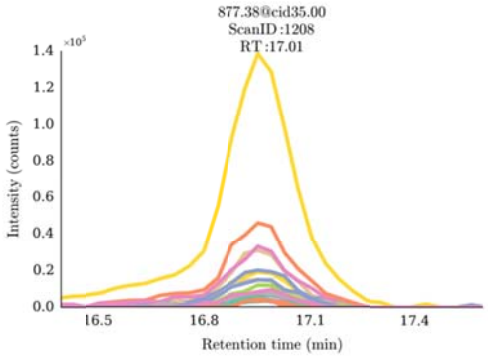


No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{11}H_{18}O_4N_3$	7.55	256.1297	267.1664	1.9	11
2	$C_{13}H_{21}O_4N_4$	2.75	297.1548	310.1974	3.0	13
3	$C_{15}H_{30}O_3N_3$	18.77	300.2287	315.2783	1.8	15
4	$C_{16}H_{29}O_3N_4$	8.61	325.2236	341.2797	0.7	16
5	$C_4H_{31}O_{10}N_9$	3.02	365.2190	369.2298	0.5	4
6	$C_{18}H_{31}O_4N_4$	6.58	367.2341	385.2920	0.2	18
7	$C_{21}H_{34}O_5N_5$	13.28	436.2581	457.3263	6.1	21
8	$C_{20}H_{34}O_6N_5$	37.30	440.2508	460.3174	0.9	20
9	$C_{15}H_{39}O_5N_8P$, *	11.71	442.2780	457.3263	1.1/*	15
10	$C_{20}H_{36}O_6N_7$	16.73	470.2727	490.3398	1.2	20
11	$C_{34}H_{35}N_6$	5.61	527.2935	561.4027	3.3	34
12	$C_{26}H_{45}O_7N_6$	10.81	553.3348	579.4205	0.7	26
13	$C_{23}H_{41}O_8N_8$	35.09	557.3046	580.3846	0.8	23
14	$C_{35}H_{63}O_8N_{10}$	8.70	751.4826	786.5923	0.2	35
15	$C_{35}H_{65}O_9N_{10}$	100.00	769.4943	804.6111	1.6	35

'*' no elemental composition could be calculated for the neutral loss mass, molecular formula with the lowest mass deviation is presented

Figure S-64. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for *m/z* 877.375 at a CE of 35%

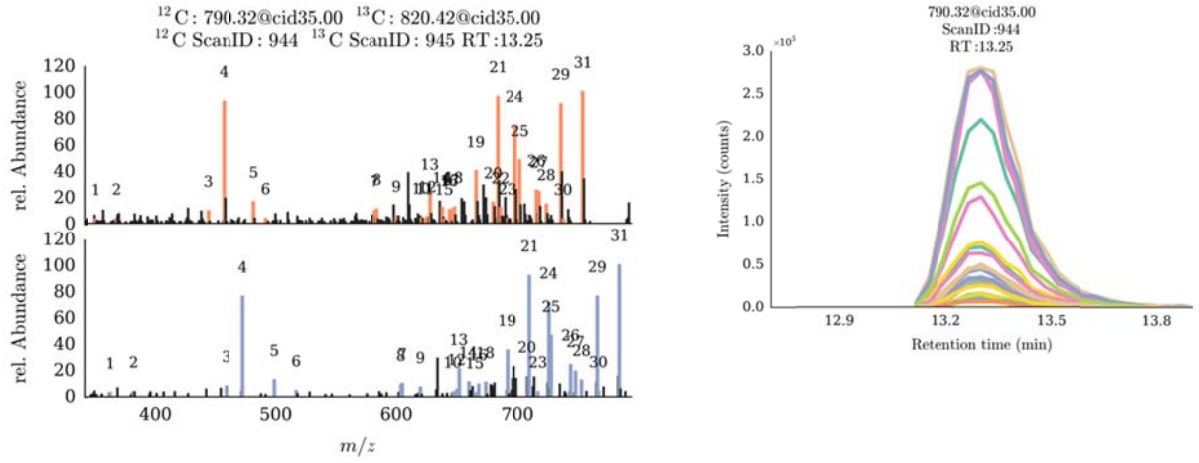




No.	Molecular formula	Relative abundance [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{13}H_{21}O_2N_4P_2$	3.18	327.1135	340.1575	0.3	13
2	$C_{23}H_{38}O_{10}P$	2.28	505.2199	528.2996	0.3	23
3	$C_{24}H_{34}O_5N_5P_2$	3.95	534.2030	558.2822	0.1	24
4	$C_{25}H_{37}O_4N_6P_2$	13.77	547.2343	572.3174	0.5	25
5	$C_{24}H_{36}O_6N_5P_2$	6.07	552.2122	576.2914	2.4	24
6	$C_{25}H_{39}O_5N_6P_2$	14.47	565.2446	590.3286	1.0	25
7	$C_{26}H_{37}O_5N_6P_2$	22.24	575.2289	601.3160	1.1	26
8	$C_{26}H_{39}O_6N_6P_2$	100.00	593.2394	619.3262	1.2	26
9	$C_{26}H_{41}O_7N_6P_2$	10.66	611.2505	637.3368	0.2	26
10	$C_{32}H_{46}O_7N_4P_2$	2.41	660.2834	692.3959	0.4	32
11	$C_{30}H_{58}ON_6P_6$,*	2.45	704.3085	734.4025	1.1/*	30
12	$C_{31}H_{47}O_7N_8P_2$	10.83	705.2997	736.4063	5.7	31
13	$C_{33}H_{61}ON_3P_7$,*	2.52	732.2970	765.4107	0.4/*	33
14	$C_{32}H_{51}O_8N_8P_2$,*	8.66	737.3309	769.4375	1.2/*	32
15	$C_{33}H_{57}O_{11}N_2P_3$,*	3.21	750.3168	783.4226	0.3/*	33
16	$C_{33}H_{56}O_2N_9P_5$,*	23.86	765.3242	798.4343	0.3/*	33
17	$C_{36}H_{54}O_9N_7P_2$	3.22	790.3392	826.4662	7.7	36
18	$C_{38}H_{57}O_8N_8P_2$	5.23	815.3688	853.5005	9.9	38
19	$C_{38}H_{57}O_9N_8P_2$	33.15	831.3703	869.4990	1.8	38
20	$C_{37}H_{75}O_9P_6$,*	5.64	849.3829	886.5046	0.2/*	37

'*' no elemental composition could be calculated for the neutral loss mass, molecular formula with the lowest mass deviation is presented

Figure S-65. Product ion spectra, fragment ion EICs and list of all FragExtract derived fragment ions for *m/z* 790.3163 at a CE of 35%



No.	Molecular formula	rel. intensity [%]	^{12}C *m/z*	^{13}C *m/z*	ppm	n(C)
1	$C_{12}H_{13}O_6N_3Fe$	2.58	351.0153	363.0555	1.32	12
2	$C_{14}H_{18}N_9Fe$,*	2.85	368.1026	382.1494	9.0/*	14
3	$C_{15}H_{22}O_9N_7$	8.86	444.1444	459.1927	6.6	15
4	$C_{16}H_{27}O_7N_5Fe$, $C_{16}H_{39}O_2NP_4Fe$	92.88	457.1258	473.1788	0.8/3.7	16
5	$C_{17}H_{26}O_7N_6Fe$, $C_{17}H_{38}O_2N_2P_4Fe$	15.70	482.1207	499.1785	0.1/4.2	17
6	$C_{25}H_{14}O_5N_7$, $C_{25}H_{26}N_3P_4$	3.11	492.1054	517.1887	0.6/3.6	25
7	$C_{23}H_{50}O_3N_2P_4Fe$, $C_{23}H_{38}O_8N_6Fe$	8.87	582.2112	605.2850	0.7/2.9	23
8	$C_{20}H_{28}O_{11}N_6Fe$, $C_{20}H_{40}O_6N_2P_4Fe$	10.15	584.1156	604.1823	0.7/4.3	20
9	$C_{20}H_{54}O_7NP_4Fe$, $C_{20}H_{42}O_{12}N_5Fe$	5.06	600.2189	620.2891	0.9/2.6	20
10	$C_{26}H_{37}O_{10}N_4Fe$, $C_{26}H_{49}O_5P_4Fe$	3.43	621.1844	647.2700	1.5/4.8	26
11	$C_{23}H_{34}N_{14}P_2Fe$,*	3.11	624.1911	647.2700	0.2/*	23
12	$C_{24}H_{50}O_5N_2P_4Fe$, $C_{24}H_{38}O_{10}N_6Fe$	4.60	626.2012	650.2781	0.3/3.0	24
13	$C_{24}H_{40}O_{10}N_6Fe$, $C_{24}H_{52}O_5N_2P_4Fe$	21.88	628.2158	652.2931	1.2/2.1	24
14	$C_{22}H_{44}O_2N_8P_6$,*	11.60	638.2008	660.2736	0.1/*	22
15	$C_{25}H_{52}O_5N_2P_4Fe$, $C_{25}H_{40}O_{10}N_6Fe$	2.66	640.2162	665.3029	1.4/1.9	25
16	$C_{24}H_{52}O_6N_2P_4Fe$, $C_{24}H_{40}O_{11}N_6Fe$	9.45	644.2112	668.2872	1.252.1	24
17	$C_{23}H_{51}O_6N_3P_4Fe$, $C_{23}H_{39}O_{11}N_7Fe$	9.96	645.2077	668.2872	0.7/4.0	23
18	$C_{26}H_{31}O_{11}N_7P$,*	11.75	648.1819	674.2719	0.9/*	26
19	$C_{26}H_{38}O_{11}N_6Fe$, $C_{26}H_{50}O_6N_2P_4Fe$	39.41	666.1948	692.2816	0.8/2.4	26
20	$C_{28}H_{48}O_8N_8Fe$, $C_{28}H_{60}O_3N_4P_4Fe$	15.30	680.2938	708.3848	0.1/3.2	28
21	$C_{26}H_{40}O_{12}N_6Fe$	96.33	684.2048	710.2918	0.0	26
22	$C_{22}H_{44}O_{14}N_{11}$	11.41	686.3064	708.3848	0.0	22
23	$C_{25}H_{61}O_{11}P_5$	3.07	692.2897	717.3715	0.1	25
24	$C_{28}H_{50}O_9N_8Fe$, $C_{28}H_{62}O_4N_4P_4Fe$	73.88	698.3050	726.3978	0.8/2.2	28

25	$C_{26}H_{42}O_{13}N_6Fe$, $C_{26}H_{54}O_8N_2P_4Fe$	47.79	702.2152	728.3026	0.2/3.2	26
26	$C_{28}H_{52}O_{10}N_8Fe$	24.63	716.3150	744.4077	0.0	28
27	$C_{30}H_{46}O_9N_8Fe$	23.38	718.2735	748.3731	0.5	30
28	$C_{29}H_{48}O_{10}N_8Fe$	13.80	724.2837	753.3824	0.1	29
29	$C_{30}H_{48}O_{10}N_8Fe$	90.80	736.2837	766.3844	0.1	30
30	$C_{29}H_{58}O_6N_4P_4Fe$	2.68	738.2684	767.3695	4.5	29
31	$C_{30}H_{50}O_{11}N_8Fe$, $C_{30}H_{62}O_6N_4P_4Fe$	100.00	754.2943	784.3955	0.1/2.8	30

'*' no elemental composition could be calculated for the neutral loss mass, molecular formula with the lowest mass deviation is presented

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(1) Kind, T.; Fiehn, O. *BMC Bioinformatics* **2007**, *8*, 105.

(2) Bueschl, C.; Kluger, B.; Berthiller, F.; Lirk, G.; Winkler, S.; Krska, R.; Schuhmacher, R. *Bioinformatics* **2012**, *28*, 736-738.

(3) Bueschl, C.; Kluger, B.; Lemmens, M.; Adam, G.; Wiesenberger, G.; Maschietto, V.; Marocco, A.; Strauss, J.; Bödi, S.; Thallinger, G.; Krska, R.; Schuhmacher, R. *Metabolomics* **2013**, 1-16.