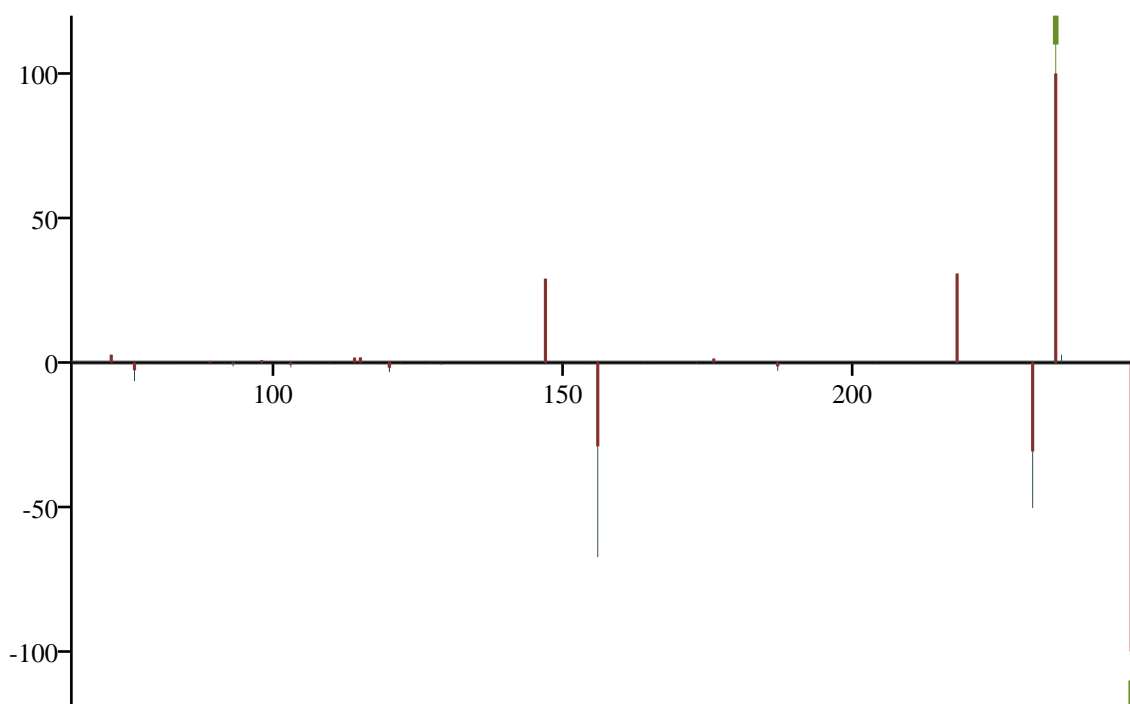


ID	1
Target name	CouPut
LC-HRMS/MS file	12C13C_Wheat_Fg_conc_MSMS_CID25_Set1.mzML
Sum formula	C13H19N2O2
Adduct	[M] ⁺ (-0.0006)
<hr/>	
Native precursor m/z	235.1441
Cn	13
Charge count	1.0
Retention time [min]	7.30 - 8.20
MS scan event	FTMS + p ESI Full ms [100.00-1000.00]
Native MS/MS scan event	FTMS + c ESI w Full ms2 235.14@cid25.00 [60.00-250.00]
Labelled MS/MS scan event	FTMS + c ESI w Full ms2 248.19@cid25.00 [65.00-250.00]
Selected native MS/MS scan id	788
Selected labelled MS/MS scan id	786
<hr/>	

FragExtract version beta_v2.6.2

Num	mz	relInt	Cn	sumFormula	deviation [ppm]	Adduct	NeutralLoss
0	72.0807	2.7	4	C4H10N	1.08	[M] ⁺	C9H9NO2
1	89.1072	0.5	4	C4H13N2	1.80	[M] ⁺	C9H6O2
2	98.0600	0.7	5	C5H8ON	0.66	[M] ⁺	C8H11NO
3	114.0912	1.7	6	C6H12ON	1.07	[M] ⁺	C7H7NO
4	115.0865	1.8	5	C5H11ON2	0.95	[M] ⁺	C8H8O
5	147.0441	29.0	9	C9H7O2	-0.08	[M] ⁺	C4H12N2
6	176.1071	1.4	11	C11H14ON	-0.81	[M] ⁺	C2H5NO
7	218.1179	30.8	13	C13H16O2N	-1.54	[M] ⁺	H3N
8	235.1444	100.0	13	C13H19O2N2	-1.24	[M] ⁺	Parent

Mass spectra



EICs

