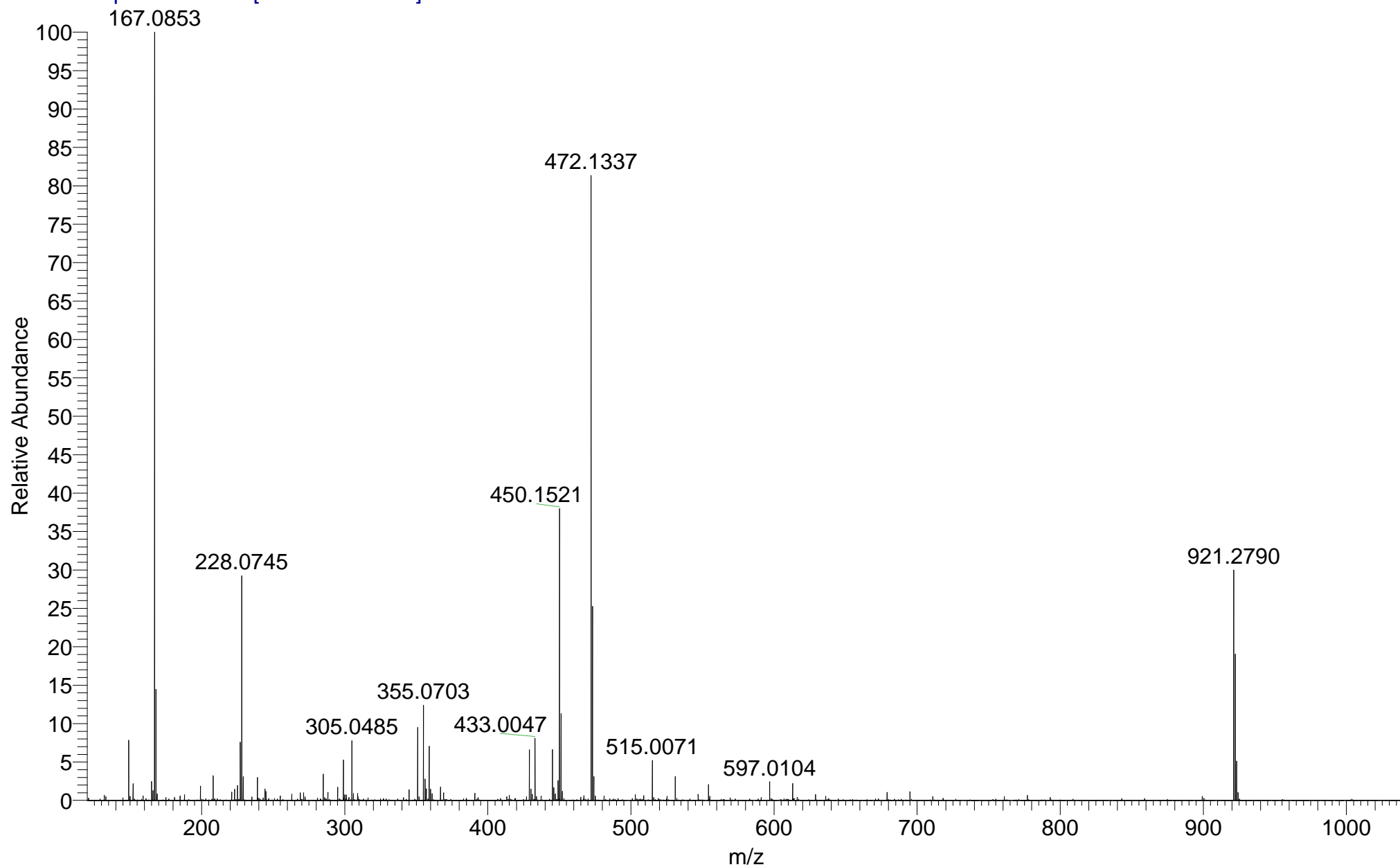


EM018
(DCM)/MeOH + NH₄OAc
C₂₉H₂₃NO₂S

EPSRC National Facility Swansea
LTQ Orbitrap XL

STATAY
28/06/2017 16:08:32

STATAY_CWE3V_29788 #44-57 RT: 0.74-1.03 AV: 11 SM: 7G NL: 1.50E6
T: FTMS + p NSI Full ms [120.00-1935.00]

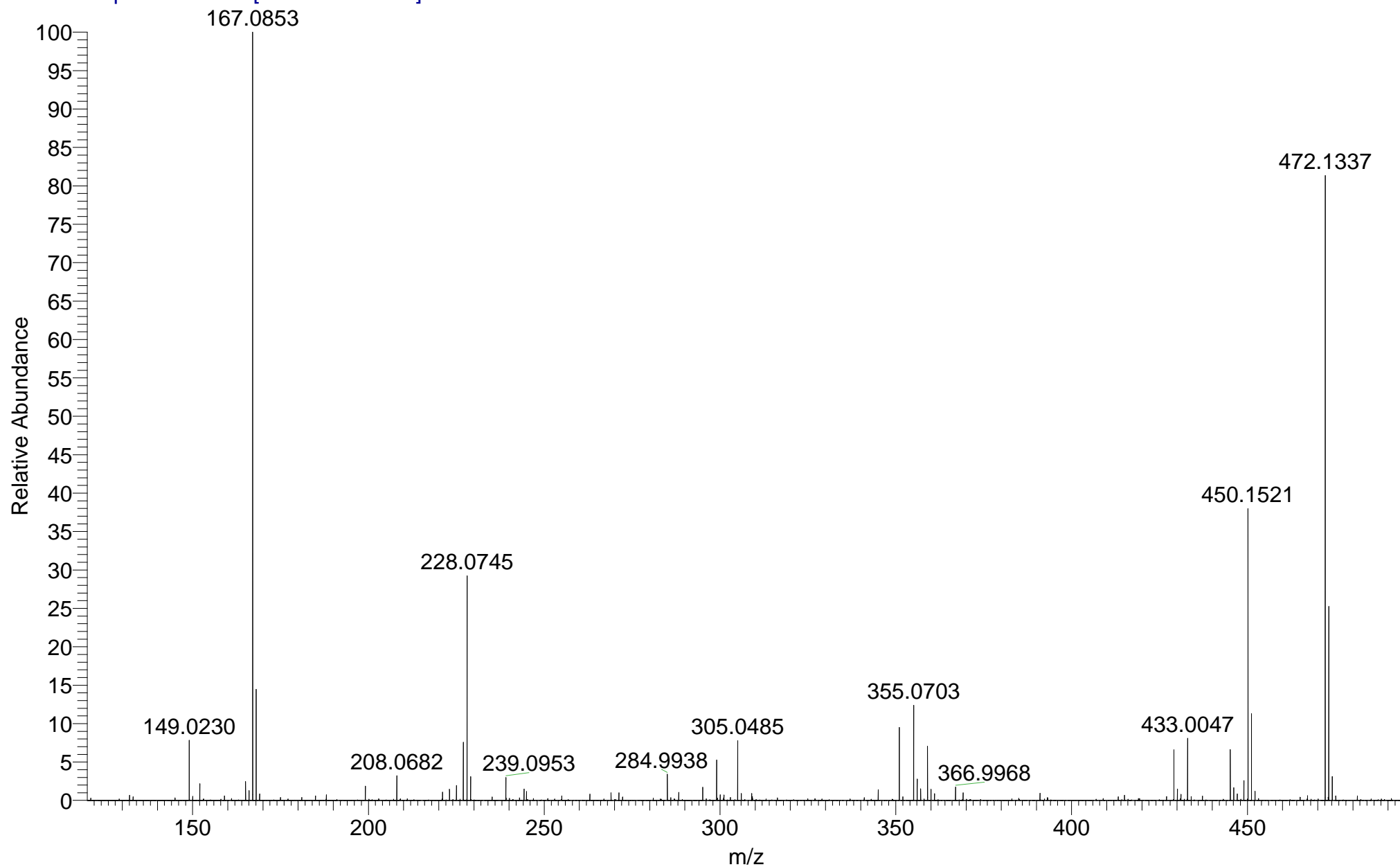


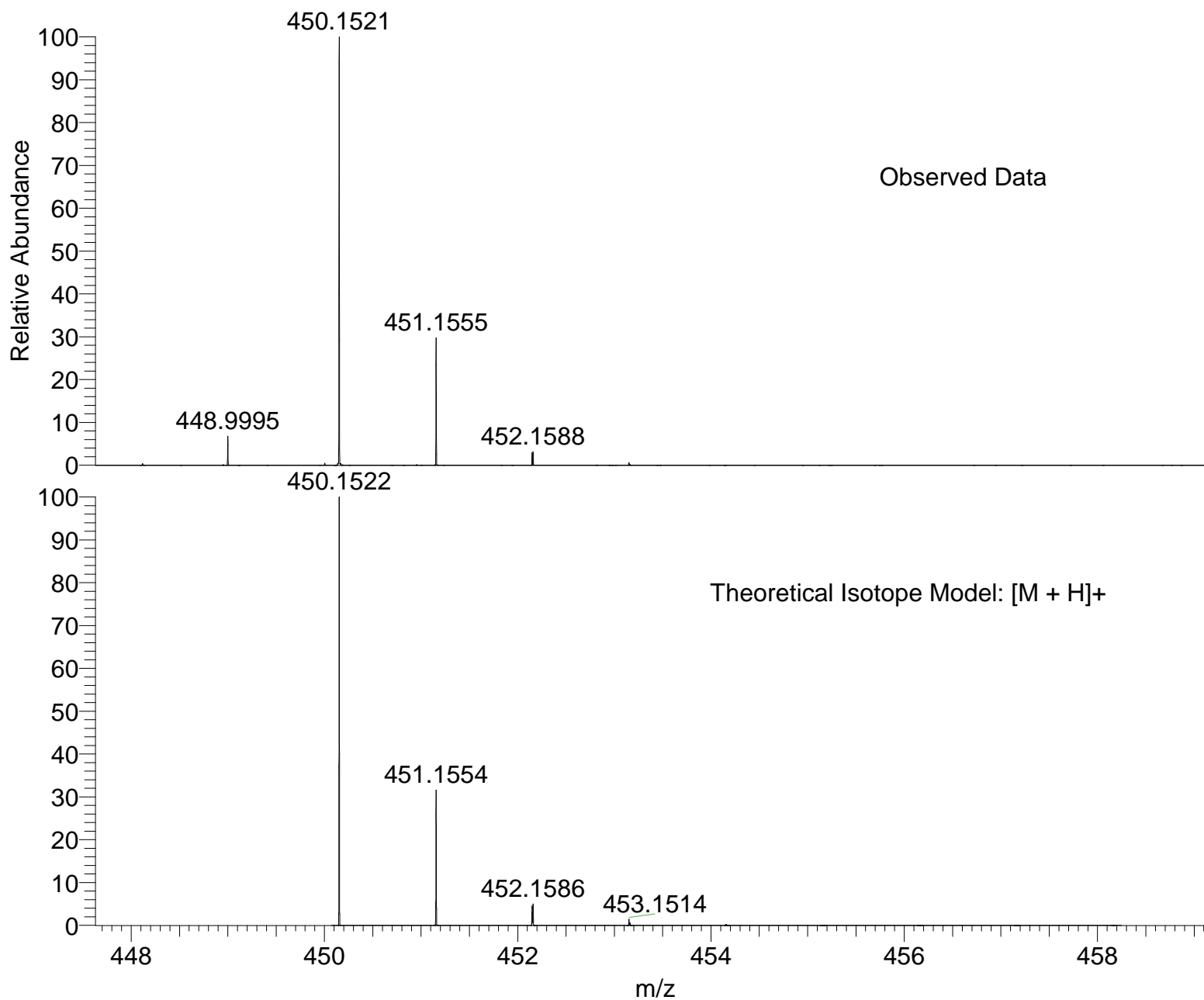
EM018
(DCM)/MeOH + NH₄OAc
C₂₉H₂₃NO₂S

EPSRC National Facility Swansea
LTQ Orbitrap XL

STATAY
28/06/2017 16:08:32

STATAY_CWE3V_29788 #44-57 RT: 0.74-1.03 AV: 11 SM: 7G NL: 1.50E6
T: FTMS + p NSI Full ms [120.00-1935.00]





NL:
5.69E5
STATAY_CWE3V_29788#44-
57 RT: 0.74-1.03 AV: 11 T:
FTMS + p NSI Full ms
[120.00-1935.00]

NL:
1.61E4
C₂₉H₂₃NO₂SH:
C₂₉H₂₄N₁O₂S₁
p (gss, s /p:40) Chrg 1
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....15
 16 O 0....15
 12 C 0....60
 1 H 0....70
 23 Na 0....0
 32 S 0....5
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 150

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
450.1521	450.1521	0.0	-3.0	C ₇ H ₃₀ O ₁₀ N ₈ S ₂
	450.1521	0.1	2.5	C ₆ H ₂₄ O ₅ N ₁₅ S ₂
	450.1520	0.1	10.0	C ₂₂ H ₂₆ O ₁₀
	450.1520	0.1	15.5	C ₂₁ H ₂₀ O ₅ N ₇
	450.1520	0.1	21.0	C ₂₀ H ₁₄ N ₁₄
	450.1522	-0.3	18.5	C ₂₉ H ₂₄ O ₂ N ₁ S ₁
	450.1523	-0.4	5.5	C ₁₄ H ₂₈ O ₂ N ₉ S ₃
	450.1523	-0.4	0.0	C ₁₅ H ₃₄ O ₇ N ₂ S ₃
	450.1518	0.7	-0.5	C ₁₄ H ₃₆ O ₁ N ₅ S ₅
	450.1526	-1.0	3.0	C ₇ H ₂₂ O ₁₁ N ₁₂
	450.1516	1.2	9.5	C ₂₁ H ₂₈ O ₄ N ₃ S ₂
	450.1527	-1.4	11.5	C ₁₄ H ₂₀ O ₃ N ₁₃ S ₁
	450.1527	-1.4	6.0	C ₁₅ H ₂₆ O ₈ N ₆ S ₁
	450.1514	1.6	1.0	C ₁₄ H ₃₀ O ₁₂ N ₂ S ₁
	450.1514	1.6	6.5	C ₁₃ H ₂₄ O ₇ N ₉ S ₁
	450.1529	-1.8	14.5	C ₂₂ H ₂₄ N ₇ S ₂
	450.1529	-1.8	9.0	C ₂₃ H ₃₀ O ₅ S ₂
	450.1529	-1.9	1.5	C ₇ H ₂₈ N ₁₅ S ₄
	450.1512	2.0	-2.0	C ₆ H ₂₆ O ₁₅ N ₈
	450.1512	2.0	3.5	C ₅ H ₂₀ O ₁₀ N ₁₅
	450.1531	-2.3	-1.0	C ₁₆ H ₃₈ O ₂ N ₂ S ₅
	450.1509	2.6	0.5	C ₁₃ H ₃₂ O ₆ N ₅ S ₃
	450.1509	2.6	6.0	C ₁₂ H ₂₆ O ₁ N ₁₂ S ₃
	450.1509	2.7	19.0	C ₂₇ H ₂₂ O ₁ N ₄ S ₁
	450.1534	-2.8	20.5	C ₂₂ H ₁₆ O ₁ N ₁₁
	450.1534	-2.9	15.0	C ₂₃ H ₂₂ O ₆ N ₄
	450.1534	-2.9	2.0	C ₈ H ₂₆ O ₆ N ₁₂ S ₂
	450.1507	3.0	-2.5	C ₅ H ₂₈ O ₉ N ₁₁ S ₂
	450.1507	3.1	10.5	C ₂₀ H ₂₄ O ₉ N ₃
	450.1507	3.1	16.0	C ₁₉ H ₁₈ O ₄ N ₁₀
	450.1536	-3.3	5.0	C ₁₆ H ₃₀ O ₃ N ₆ S ₃

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
	450.1504	3.7	0.0	C ₁₂ H ₃₄ N ₈ S ₅
	450.1504	3.7	13.0	C ₂₇ H ₃₀ S ₃
	450.1538	-3.7	8.0	C ₂₄ H ₃₄ S ₄
	450.1539	-4.0	2.5	C ₉ H ₂₄ O ₁₂ N ₉
	450.1503	4.1	-3.0	C ₄ H ₃₀ O ₃ N ₁₄ S ₄
	450.1502	4.2	10.0	C ₁₉ H ₂₆ O ₃ N ₆ S ₂
	450.1541	-4.4	11.0	C ₁₆ H ₂₂ O ₄ N ₁₀ S ₁
	450.1541	-4.4	5.5	C ₁₇ H ₂₈ O ₉ N ₃ S ₁
	450.1501	4.5	1.5	C ₁₂ H ₂₈ O ₁₁ N ₅ S ₁
	450.1500	4.6	7.0	C ₁₁ H ₂₂ O ₆ N ₁₂ S ₁
	450.1543	-4.8	14.0	C ₂₄ H ₂₆ O ₁ N ₄ S ₂
	450.1543	-4.9	1.0	C ₉ H ₃₀ O ₁ N ₁₂ S ₄
	450.1499	5.0	-1.5	C ₄ H ₂₄ O ₁₄ N ₁₁