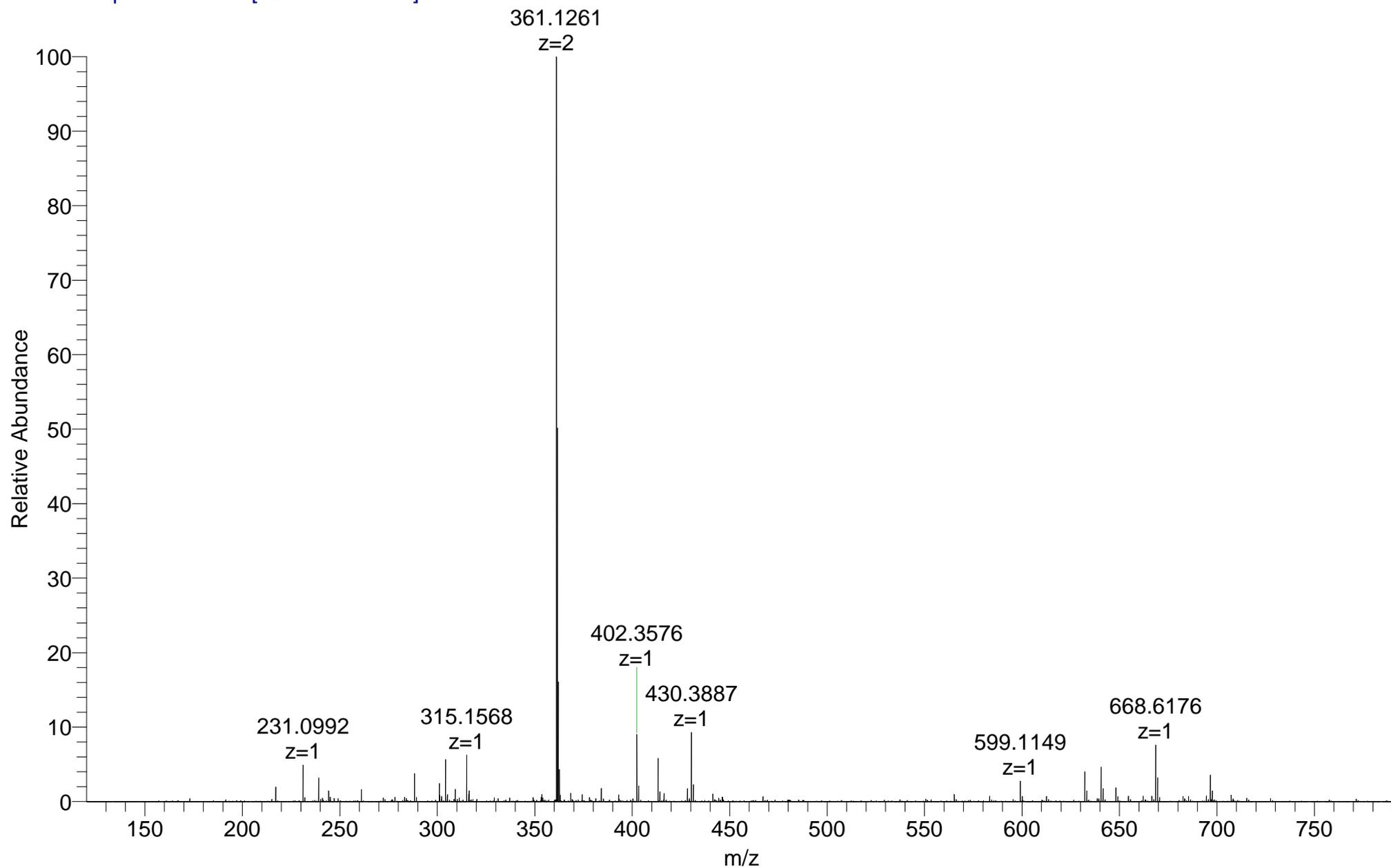


MAR-57
(MeCN)/(MeOH)
C47H38F12N4P2S2

EPSRC National Facility Swansea
LTQ Orbitrap XL

UEAFIL
10/25/16 14:29:45

UEAFIL_BRPZT_96 #20-28 RT: 0.67-1.05 AV: 8 SM: 7G NL: 1.67E6
T: FTMS + p NSI Full ms [120.00-1935.00]

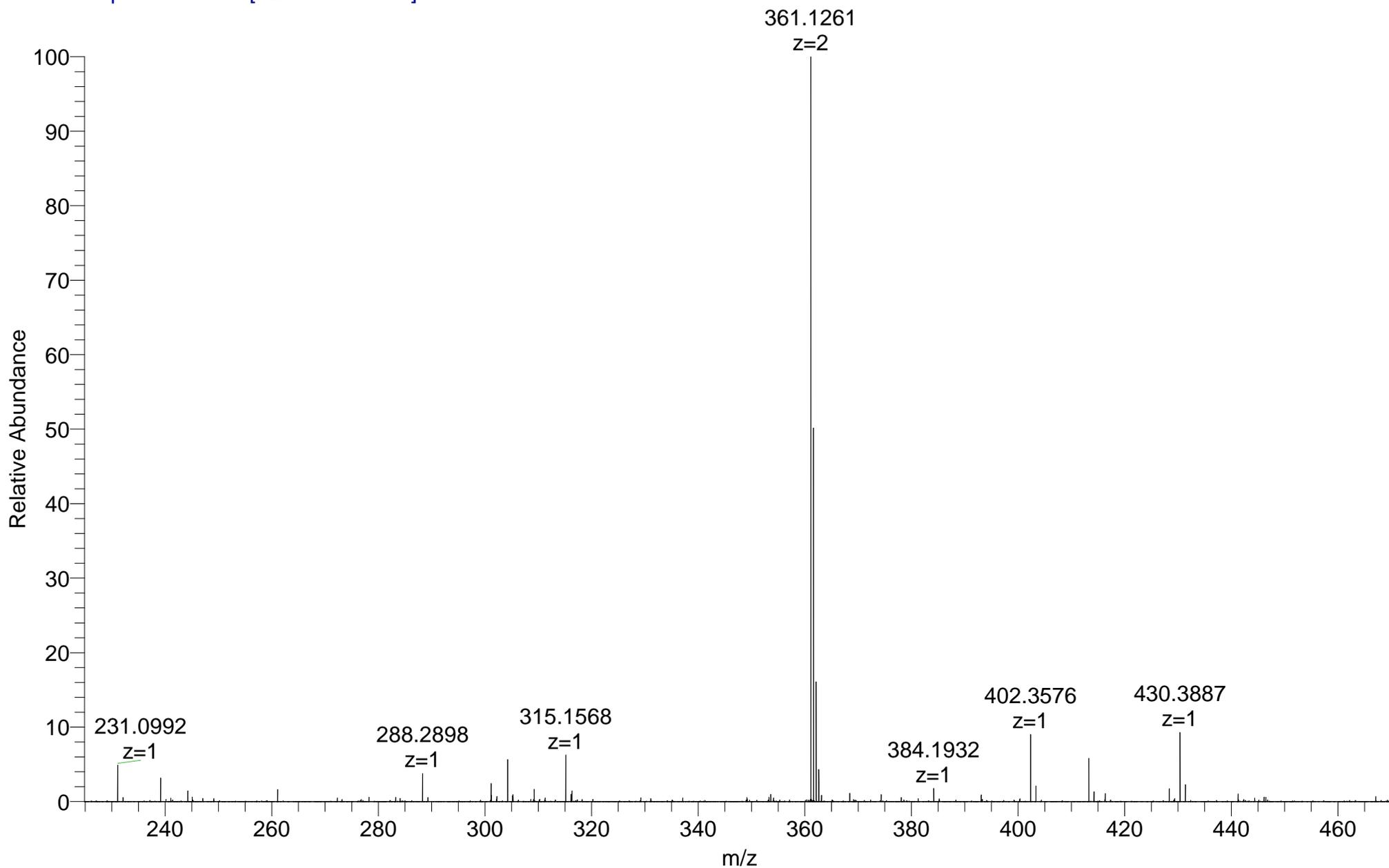


MAR-57
(MeCN)/(MeOH)
C47H38F12N4P2S2

EPSRC National Facility Swansea
LTQ Orbitrap XL

UEAFIL
10/25/16 14:29:45

UEAFIL_BRPZT_96 #20-28 RT: 0.67-1.05 AV: 8 SM: 7G NL: 1.67E6
T: FTMS + p NSI Full ms [120.00-1935.00]

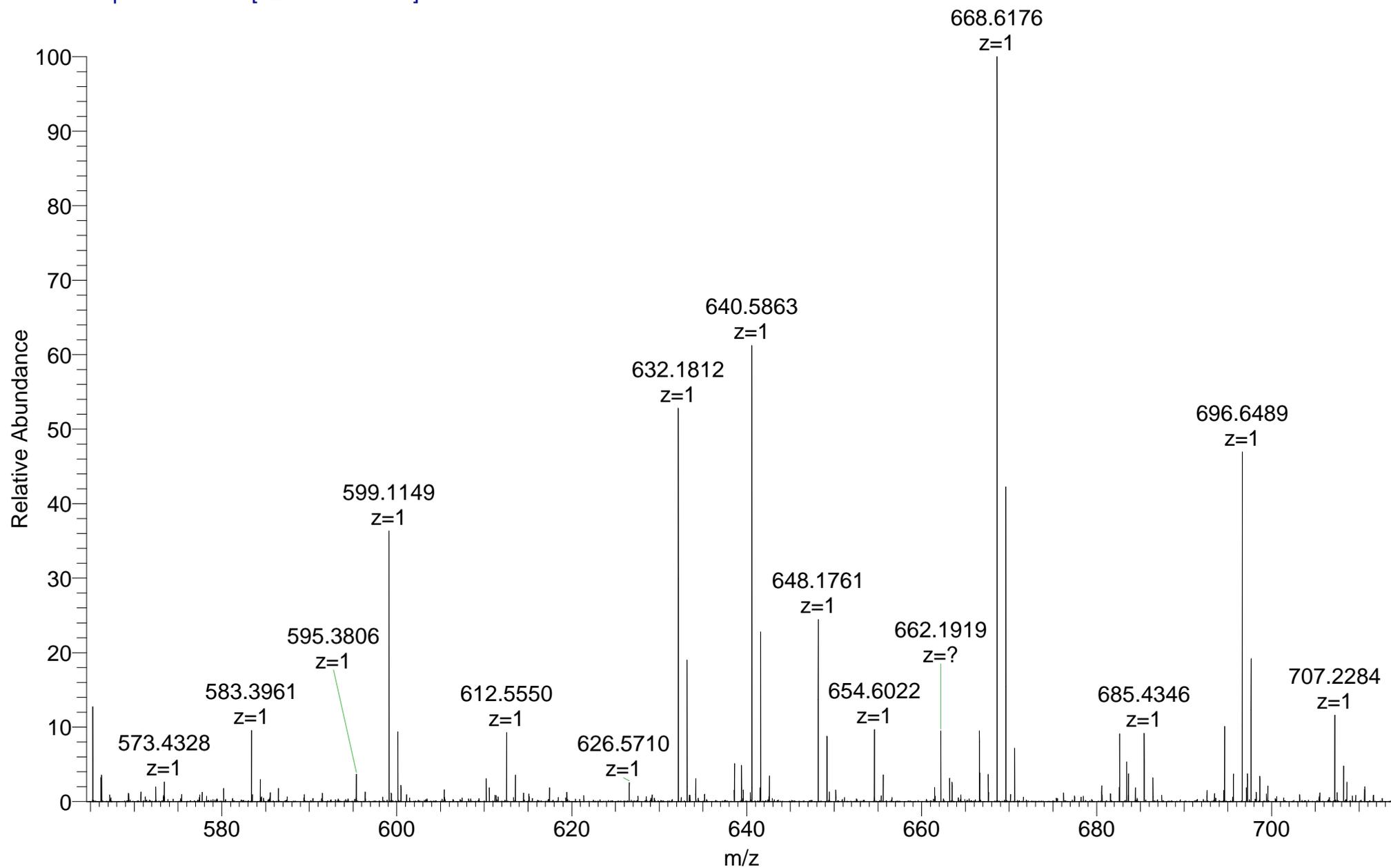


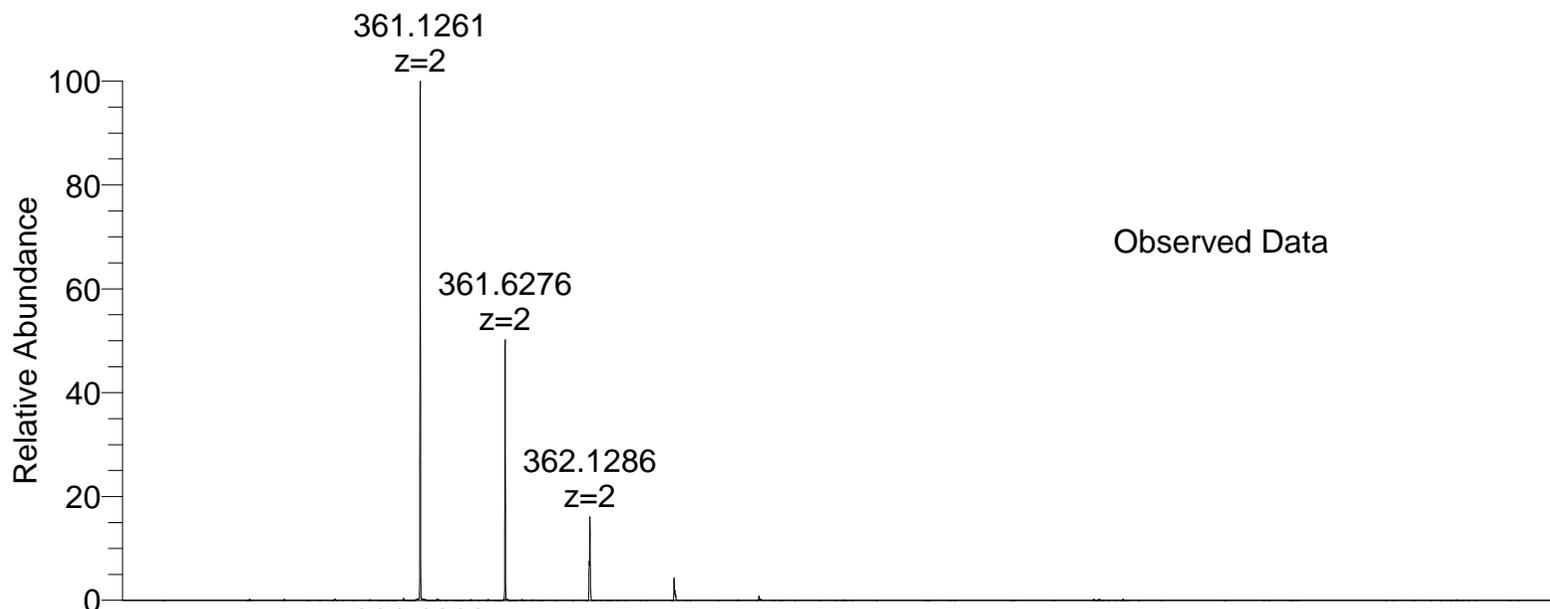
MAR-57
(MeCN)/(MeOH)
C47H38F12N4P2S2

EPSRC National Facility Swansea
LTQ Orbitrap XL

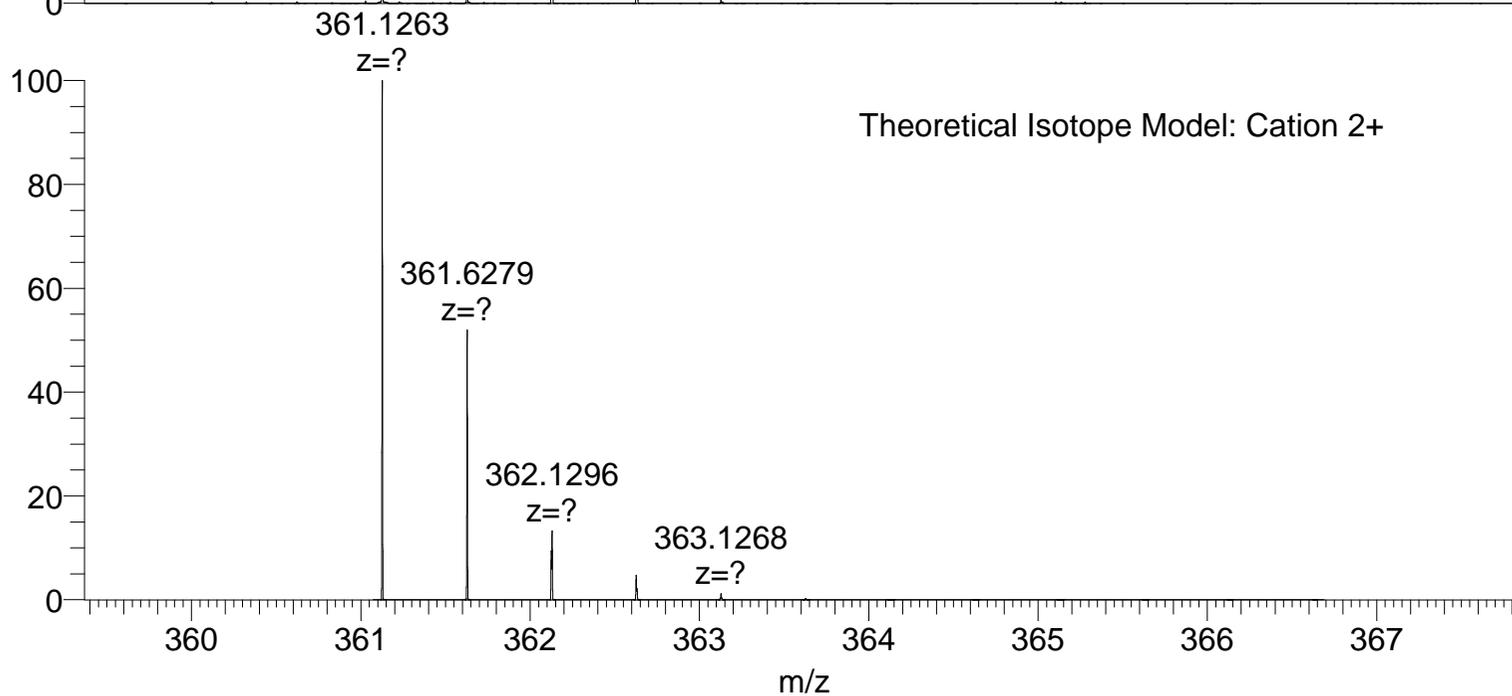
UEAFIL
10/25/16 14:29:45

UEAFIL_BRPZT_96 #20-28 RT: 0.67-1.05 AV: 8 SM: 7G NL: 1.27E5
T: FTMS + p NSI Full ms [120.00-1935.00]





NL:
1.67E6
UEAFIL_BRPZT_96#20-28
RT: 0.67-1.05 AV: 8 T: FTMS
+ p NSI Full ms
[120.00-1935.00]



NL:
1.25E4
C₄₇ H₃₈ N₄ S₂:
C₄₇ H₃₈ N₄ S₂
p (gss, s /p:40) Chrg 2
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.
 14 N 0....15
 16 O 0....15
 12 C 0....50
 1 H 0....70
 23 Na 0....0
 32 S 0....5
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 100

N-Rule: Do not use
 Charge: 2

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
361.1261	361.1260	0.2	-2.0	C ₂₆ H ₅₈ O ₁₂ S ₅
	361.1260	0.2	3.5	C ₂₅ H ₅₂ O ₇ N ₇ S ₅
	361.1260	0.2	9.0	C ₂₄ H ₄₆ O ₂ N ₁₄ S ₅
	361.1262	-0.2	19.5	C ₃₂ H ₃₆ O ₁₁ N ₉
	361.1260	0.2	22.0	C ₃₉ H ₄₂ O ₂ N ₆ S ₃
	361.1259	0.4	0.5	C ₃₉ H ₄₂ O ₁₀ N ₁₃ S ₄
	361.1263	-0.4	28.0	C ₃₉ H ₃₄ O ₃ N ₁₀ S ₁
	361.1263	-0.4	22.5	C ₄₀ H ₄₀ O ₈ N ₃ S ₁
	361.1259	0.5	13.5	C ₃₂ H ₄₄ O ₁₀ N ₅ S ₂
	361.1259	0.5	19.0	C ₃₁ H ₃₈ O ₅ N ₁₂ S ₂
	361.1263	-0.5	9.5	C ₂₅ H ₄₄ O ₈ N ₁₁ S ₃
	361.1263	-0.5	4.0	C ₂₆ H ₅₀ O ₁₃ N ₄ S ₃
	361.1259	0.5	32.0	C ₄₆ H ₃₄ O ₅ N ₄
	361.1259	0.5	37.5	C ₄₅ H ₂₆ N ₁₁
	361.1263	-0.7	31.0	C ₄₇ H ₃₈ N ₄ S ₂
	361.1258	0.7	10.5	C ₂₄ H ₄₀ O ₁₃ N ₁₁ S ₁
	361.1264	-0.7	18.0	C ₃₂ H ₄₂ N ₁₂ S ₄
	361.1264	-0.7	12.5	C ₃₃ H ₄₈ O ₅ N ₅ S ₄
	361.1258	0.9	16.0	C ₃₉ H ₅₀ O ₁ N ₂ S ₅
	361.1257	1.1	7.5	C ₃₂ H ₅₂ O ₉ N ₁ S ₄
	361.1257	1.1	13.0	C ₃₁ H ₄₆ O ₄ N ₈ S ₄
	361.1265	-1.1	15.5	C ₂₅ H ₃₆ O ₉ N ₁₅ S ₁
	361.1265	-1.1	10.0	C ₂₆ H ₄₂ O ₁₄ N ₈ S ₁
	361.1257	1.2	26.0	C ₄₆ H ₄₂ O ₄ S ₂
	361.1266	-1.3	37.0	C ₄₇ H ₃₀ O ₁ N ₈
	361.1266	-1.3	31.5	C ₄₈ H ₃₆ O ₆ N ₁
	361.1256	1.4	4.5	C ₂₄ H ₄₈ O ₁₂ N ₇ S ₃
	361.1256	1.4	10.0	C ₂₃ H ₄₂ O ₇ N ₁₄ S ₃
	361.1266	-1.4	18.5	C ₃₃ H ₄₀ O ₆ N ₉ S ₂
	361.1266	-1.4	13.0	C ₃₄ H ₄₆ O ₁₁ N ₂ S ₂
	361.1256	1.4	23.0	C ₃₈ H ₃₈ O ₇ N ₆ S ₁

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
361.1256	361.1256	1.4	28.5	C ₃₇ H ₃₂ O ₂ N ₁₃ S ₁
361.1266	361.1266	-1.4	0.0	C ₁₉ H ₅₀ O ₁₁ N ₁₀ S ₄
361.1255	361.1255	1.6	1.5	C ₁₆ H ₄₄ O ₁₅ N ₁₃ S ₂
361.1267	361.1267	-1.6	21.5	C ₄₁ H ₄₄ O ₃ N ₃ S ₃
361.1255	361.1255	1.7	14.5	C ₃₁ H ₄₀ O ₁₅ N ₅
361.1255	361.1255	1.7	20.0	C ₃₀ H ₃₄ O ₁₀ N ₁₂
361.1267	361.1267	-1.7	8.5	C ₂₆ H ₄₈ O ₃ N ₁₁ S ₅
361.1267	361.1267	-1.7	3.0	C ₂₇ H ₅₄ O ₈ N ₄ S ₅
361.1254	361.1254	2.0	-1.5	C ₂₄ H ₅₆ O ₁₁ N ₃ S ₅
361.1254	361.1254	2.0	4.0	C ₂₃ H ₅₀ O ₆ N ₁₀ S ₅
361.1268	361.1268	-2.0	24.5	C ₃₃ H ₃₂ O ₇ N ₁₃
361.1268	361.1268	-2.0	19.0	C ₃₄ H ₃₈ O ₁₂ N ₆
361.1254	361.1254	2.1	17.0	C ₃₈ H ₄₆ O ₆ N ₂ S ₃
361.1253	361.1253	2.1	22.5	C ₃₇ H ₄₀ O ₁ N ₉ S ₃
361.1269	361.1269	-2.1	6.0	C ₁₉ H ₄₂ O ₁₂ N ₁₄ S ₂
361.1269	361.1269	-2.3	27.5	C ₄₁ H ₃₆ O ₄ N ₇ S ₁
361.1269	361.1269	-2.3	22.0	C ₄₂ H ₄₂ O ₉ S ₁
361.1253	361.1253	2.3	8.5	C ₃₁ H ₄₈ O ₁₄ N ₁ S ₂
361.1253	361.1253	2.3	14.0	C ₃₀ H ₄₂ O ₉ N ₈ S ₂
361.1269	361.1269	-2.3	14.5	C ₂₆ H ₄₀ O ₄ N ₁₅ S ₃
361.1253	361.1253	2.3	19.5	C ₂₉ H ₃₆ O ₄ N ₁₅ S ₂
361.1269	361.1269	-2.3	9.0	C ₂₇ H ₄₆ O ₉ N ₈ S ₃
361.1269	361.1269	-2.3	3.5	C ₂₈ H ₅₂ O ₁₄ N ₁ S ₃
361.1252	361.1252	2.4	27.0	C ₄₅ H ₃₈ O ₉
361.1252	361.1252	2.4	32.5	C ₄₄ H ₃₂ O ₄ N ₇
361.1270	361.1270	-2.5	30.5	C ₄₉ H ₄₀ O ₁ N ₁ S ₂
361.1252	361.1252	2.6	11.0	C ₂₂ H ₃₈ O ₁₂ N ₁₄ S ₁
361.1270	361.1270	-2.6	17.5	C ₃₄ H ₄₄ O ₁ N ₉ S ₄
361.1270	361.1270	-2.6	12.0	C ₃₅ H ₅₀ O ₆ N ₂ S ₄
361.1251	361.1251	2.7	16.5	C ₃₇ H ₄₈ N ₅ S ₅
361.1250	361.1250	3.0	8.0	C ₃₀ H ₅₀ O ₈ N ₄ S ₄
361.1250	361.1250	3.0	13.5	C ₂₉ H ₄₄ O ₃ N ₁₁ S ₄
361.1272	361.1272	-3.0	15.0	C ₂₇ H ₃₈ O ₁₀ N ₁₂ S ₁
361.1272	361.1272	-3.0	9.5	C ₂₈ H ₄₄ O ₁₅ N ₅ S ₁
361.1250	361.1250	3.0	26.5	C ₄₄ H ₄₀ O ₃ N ₃ S ₂
361.1273	361.1273	-3.2	36.5	C ₄₉ H ₃₂ O ₂ N ₅
361.1249	361.1249	3.2	5.0	C ₂₂ H ₄₆ O ₁₁ N ₁₀ S ₃
361.1273	361.1273	-3.2	23.5	C ₃₄ H ₃₆ O ₂ N ₁₃ S ₂
361.1273	361.1273	-3.2	18.0	C ₃₅ H ₄₂ O ₇ N ₆ S ₂
361.1249	361.1249	3.3	18.0	C ₃₇ H ₄₂ O ₁₁ N ₂ S ₁
361.1249	361.1249	3.3	23.5	C ₃₆ H ₃₆ O ₆ N ₉ S ₁
361.1273	361.1273	-3.3	5.0	C ₂₀ H ₄₆ O ₇ N ₁₄ S ₄
361.1273	361.1273	-3.3	-0.5	C ₂₁ H ₅₂ O ₁₂ N ₇ S ₄

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
361.1274	361.1274	-3.5	21.0	C ₄₃ H ₄₆ O ₄ S ₃
361.1248	361.1248	3.5	15.0	C ₂₉ H ₃₈ O ₁₄ N ₈
361.1248	361.1248	3.5	20.5	C ₂₈ H ₃₂ O ₉ N ₁₅
361.1274	361.1274	-3.5	8.0	C ₂₈ H ₅₀ O ₄ N ₈ S ₅
361.1274	361.1274	-3.5	2.5	C ₂₉ H ₅₆ O ₉ N ₁ S ₅
361.1247	361.1247	3.9	-1.0	C ₂₂ H ₅₄ O ₁₀ N ₆ S ₅
361.1247	361.1247	3.9	4.5	C ₂₁ H ₄₈ O ₅ N ₁₃ S ₅
361.1275	361.1275	-3.9	24.0	C ₃₅ H ₃₄ O ₈ N ₁₀
361.1275	361.1275	-3.9	18.5	C ₃₆ H ₄₀ O ₁₃ N ₃
361.1247	361.1247	3.9	17.5	C ₃₆ H ₄₄ O ₅ N ₅ S ₃
361.1247	361.1247	3.9	23.0	C ₃₅ H ₃₈ N ₁₂ S ₃
361.1275	361.1275	-3.9	5.5	C ₂₁ H ₄₄ O ₁₃ N ₁₁ S ₂
361.1247	361.1247	4.0	36.0	C ₅₀ H ₃₄ N ₄ S ₁
361.1276	361.1276	-4.1	32.5	C ₄₂ H ₃₂ N ₁₁ S ₁
361.1276	361.1276	-4.1	27.0	C ₄₃ H ₃₈ O ₅ N ₄ S ₁
361.1246	361.1246	4.2	9.0	C ₂₉ H ₄₆ O ₁₃ N ₄ S ₂
361.1246	361.1246	4.2	14.5	C ₂₈ H ₄₀ O ₈ N ₁₁ S ₂
361.1276	361.1276	-4.2	14.0	C ₂₈ H ₄₂ O ₅ N ₁₂ S ₃
361.1276	361.1276	-4.2	8.5	C ₂₉ H ₄₈ O ₁₀ N ₅ S ₃
361.1246	361.1246	4.2	27.5	C ₄₃ H ₃₆ O ₈ N ₃
361.1246	361.1246	4.2	33.0	C ₄₂ H ₃₀ O ₃ N ₁₀
361.1277	361.1277	-4.4	17.0	C ₃₆ H ₄₆ O ₂ N ₆ S ₄
361.1244	361.1244	4.6	11.5	C ₃₆ H ₅₂ O ₄ N ₁ S ₅
361.1278	361.1278	-4.6	11.5	C ₂₁ H ₃₆ O ₁₄ N ₁₅
361.1244	361.1244	4.8	3.0	C ₂₉ H ₅₄ O ₁₂ S ₄
361.1244	361.1244	4.8	8.5	C ₂₈ H ₄₈ O ₇ N ₇ S ₄