

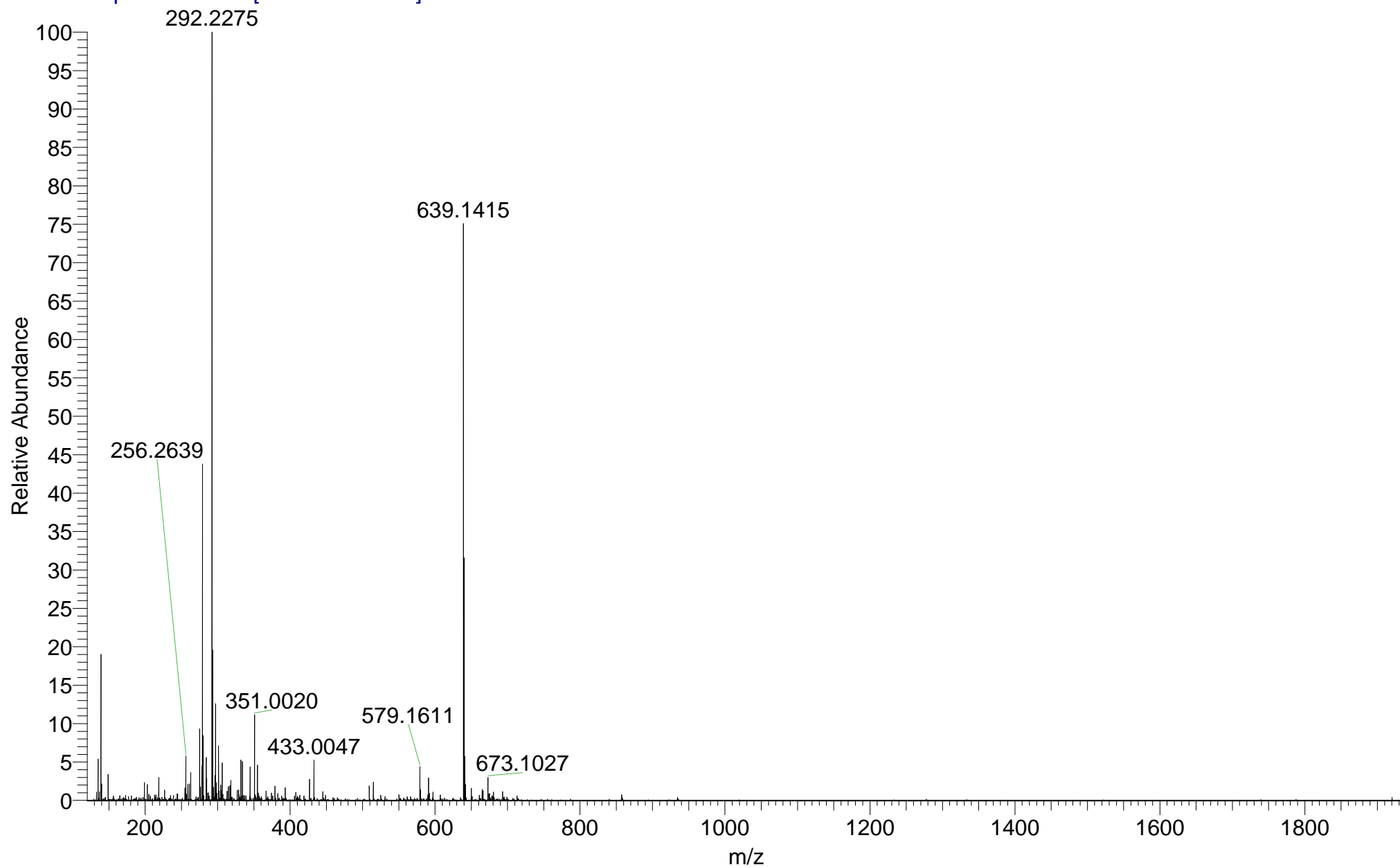
MAR17
(DCM)/MeOH + NH₄OAc
C39H22N6S2

EPSRC National Facility Swansea
LTQ Orbitrap XL

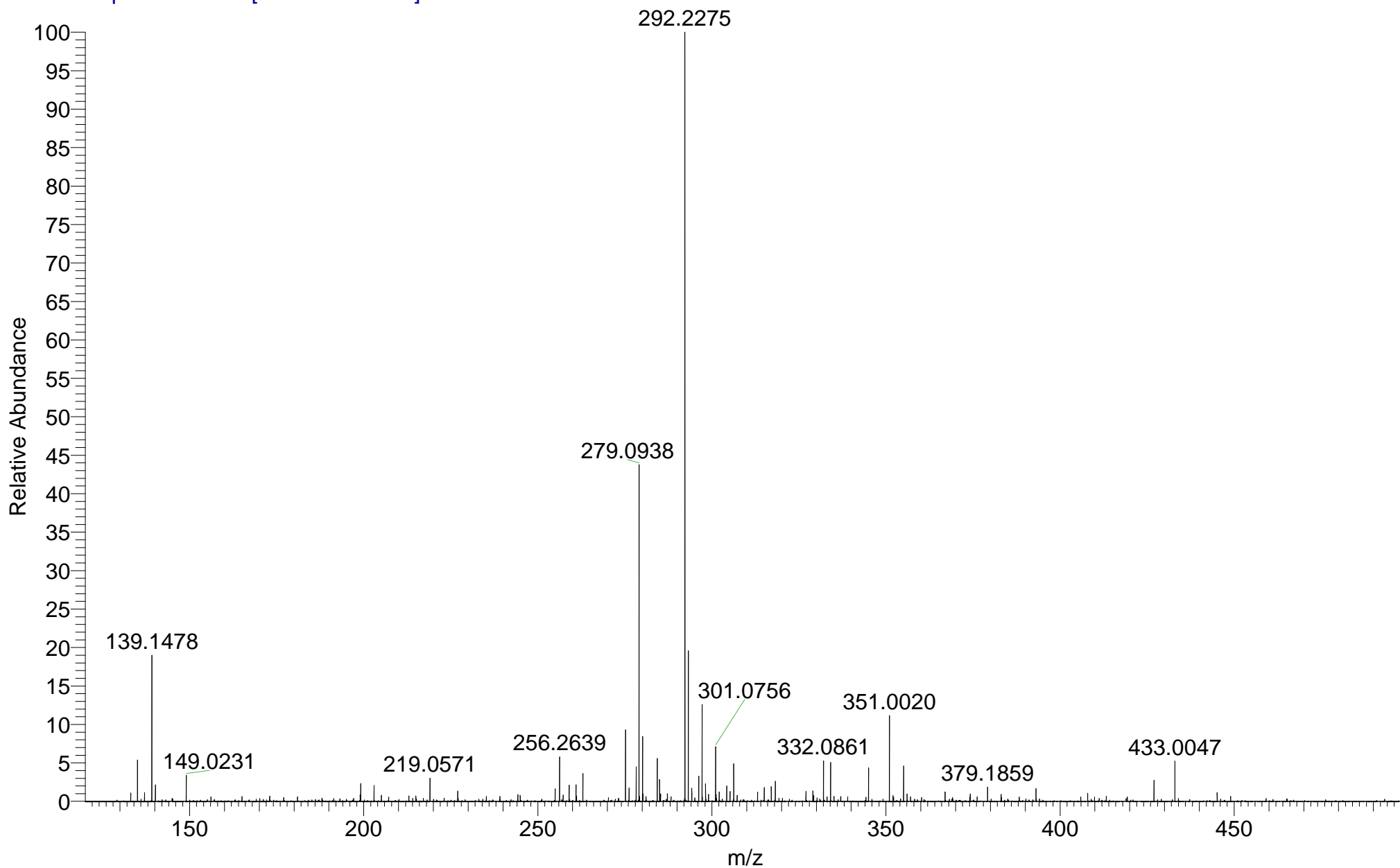
UEAFIL
16/05/2016 09:03:38

UEAFIL_V174W_53 #34-46 RT: 0.74-1.04 AV: 12 SM: 7G NL: 7.15E6

T: FTMS + p NSI Full ms [120.00-1935.00]



UEAFIL_V174W_53 #34-46 RT: 0.74-1.04 AV: 12 SM: 7G NL: 7.15E6
T: FTMS + p NSI Full ms [120.00-1935.00]

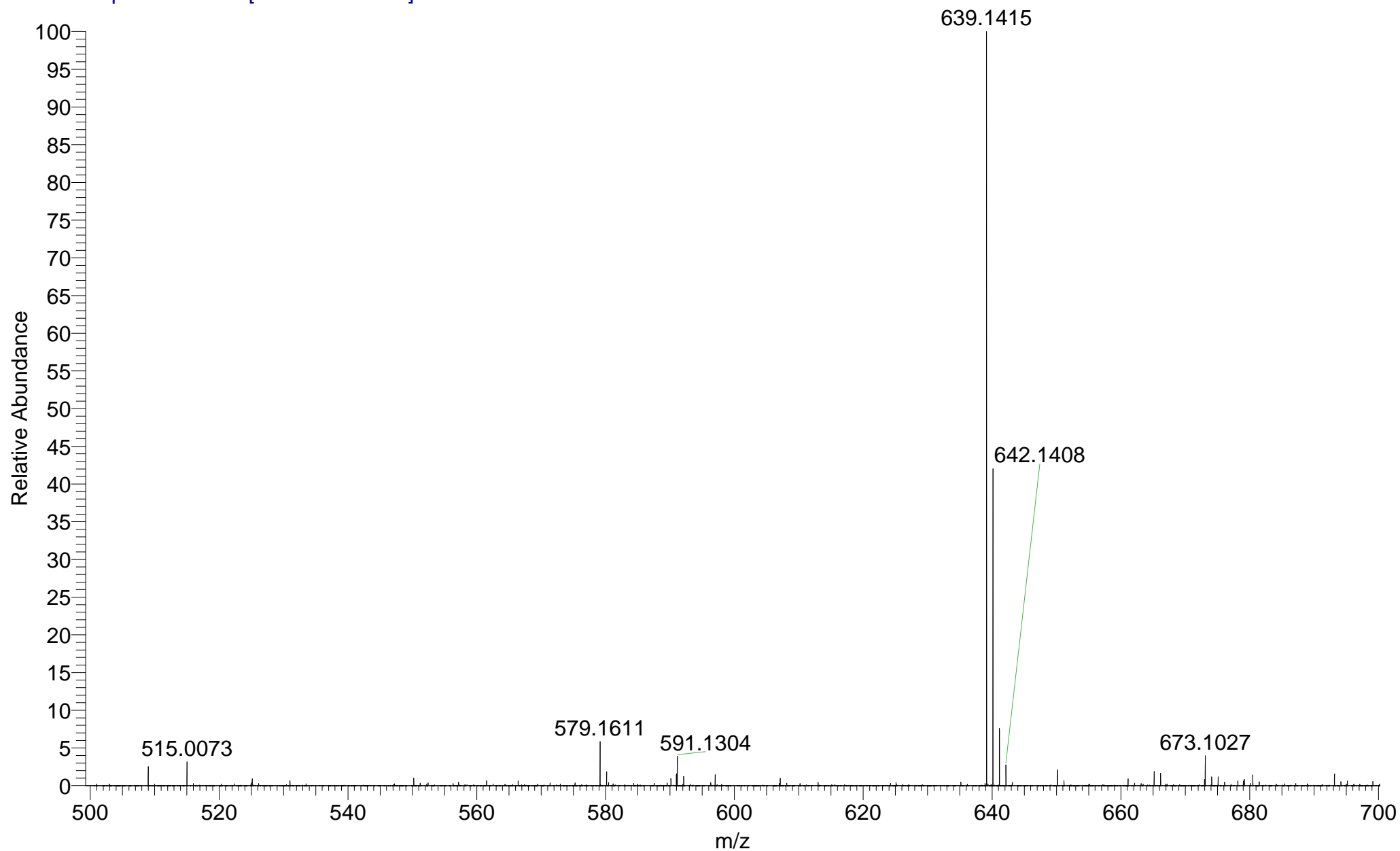


MAR17
(DCM)/MeOH + NH₄OAc
C₃₉H₂₂N₆S₂

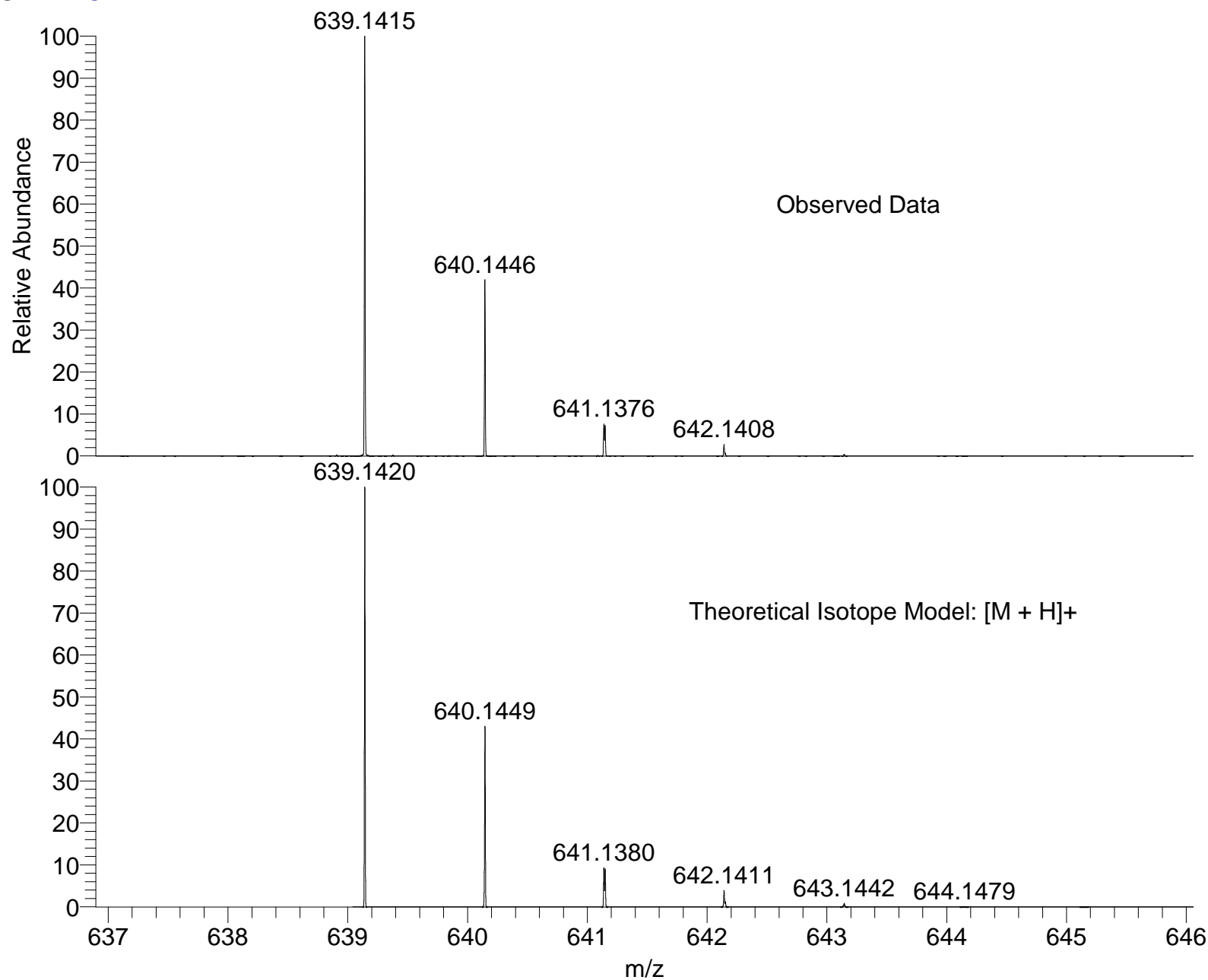
EPSRC National Facility Swansea
LTQ Orbitrap XL

UEAFIL
16/05/2016 09:03:38

UEAFIL_V174W_53 #34-46 RT: 0.74-1.04 AV: 12 SM: 7G NL: 5.37E6
T: FTMS + p NSI Full ms [120.00-1935.00]



SM: 7G



NL:
5.37E6
UEAFIL_V174W_53#34-46
RT: 0.74-1.04 AV: 12 T: FTMS
+ p NSI Full ms
[120.00-1935.00]

NL:
1.36E4
C₃₉H₂₂N₆S₂H:
C₃₉H₂₃N₆S₂
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....80
 1 H 0....100
 23 Na 0....0
 32 S 0....2
 Tolerance Window: +- 5.00 ppm
 Db/Ring Equiv: -3.. 100
 Fits: 700

N-Rule: Do not use
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
639.1415	639.1417	-0.2	20.0	C ₂₄ H ₂₁ O ₁₁ N ₁₁
	639.1413	0.3	35.5	C ₄₆ H ₂₃ O ₂ S ₁
	639.1412	0.5	8.5	C ₂₅ H ₃₅ O ₁₅ S ₂
	639.1412	0.5	14.0	C ₂₄ H ₂₉ O ₁₀ N ₇ S ₂
	639.1412	0.5	19.5	C ₂₃ H ₂₃ O ₅ N ₁₄ S ₂
	639.1418	-0.5	28.5	C ₂₃ H ₂₃ O ₅ N ₁₄ S ₂
	639.1418	-0.5	23.0	C ₃₁ H ₁₉ O ₃ N ₁₂ S ₁
	639.1418	-0.5	23.0	C ₃₂ H ₂₅ O ₈ N ₅ S ₁
	639.1411	0.6	32.5	C ₃₈ H ₁₉ O ₅ N ₆
	639.1411	0.6	38.0	C ₃₇ H ₁₃ N ₁₃
	639.1410	0.8	11.0	C ₁₆ H ₂₅ O ₁₃ N ₁₃ S ₁
	639.1420	-0.8	31.5	C ₃₉ H ₂₃ N ₆ S ₂
	639.1407	1.3	26.5	C ₃₈ H ₂₇ O ₄ N ₂ S ₂
	639.1423	-1.3	10.5	C ₁₈ H ₂₇ O ₁₄ N ₁₀ S ₁
	639.1425	-1.5	37.5	C ₃₉ H ₁₅ O ₁ N ₁₀
	639.1425	-1.5	32.0	C ₄₀ H ₂₁ O ₆ N ₃
	639.1405	1.6	18.0	C ₃₁ H ₂₉ O ₁₂ N ₁ S ₁
	639.1405	1.6	23.5	C ₃₀ H ₂₃ O ₇ N ₈ S ₁
	639.1405	1.6	29.0	C ₂₉ H ₁₇ O ₂ N ₁₅ S ₁
	639.1425	-1.6	19.0	C ₂₅ H ₂₅ O ₆ N ₁₁ S ₂
	639.1425	-1.6	13.5	C ₂₆ H ₃₁ O ₁₁ N ₄ S ₂
	639.1403	1.8	2.0	C ₈ H ₂₉ O ₁₅ N ₁₅ S ₂
	639.1403	1.9	15.0	C ₂₃ H ₂₅ O ₁₅ N ₇
	639.1403	1.9	20.5	C ₂₂ H ₁₉ O ₁₀ N ₁₄
	639.1430	-2.3	25.0	C ₂₅ H ₁₇ O ₇ N ₁₅
	639.1430	-2.3	19.5	C ₂₆ H ₂₃ O ₁₂ N ₈
	639.1400	2.4	36.0	C ₄₄ H ₂₁ O ₁ N ₃ S ₁
	639.1398	2.6	9.0	C ₂₃ H ₃₃ O ₁₄ N ₃ S ₂
	639.1398	2.6	14.5	C ₂₂ H ₂₇ O ₉ N ₁₀ S ₂
	639.1432	-2.6	28.0	C ₃₃ H ₂₁ O ₄ N ₉ S ₁
	639.1432	-2.6	22.5	C ₃₄ H ₂₇ O ₉ N ₂ S ₁
	639.1398	2.6	27.5	C ₃₇ H ₂₃ O ₉ N ₂

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
	639.1398	2.7	33.0	C ₃₆ H ₁₇ O ₄ N ₉
	639.1434	-2.9	31.0	C ₄₁ H ₂₅ O ₁ N ₃ S ₂
	639.1393	3.4	27.0	C ₃₆ H ₂₅ O ₃ N ₅ S ₂
	639.1437	-3.4	15.5	C ₁₉ H ₂₃ O ₁₀ N ₁₄ S ₁
	639.1437	-3.4	10.0	C ₂₀ H ₂₉ O ₁₅ N ₇ S ₁
	639.1438	-3.6	37.0	C ₄₁ H ₁₇ O ₂ N ₇
	639.1438	-3.6	31.5	C ₄₂ H ₂₃ O ₇
	639.1392	3.7	18.5	C ₂₉ H ₂₇ O ₁₁ N ₄ S ₁
	639.1391	3.7	24.0	C ₂₈ H ₂₁ O ₆ N ₁₁ S ₁
	639.1439	-3.7	24.0	C ₂₆ H ₂₁ O ₂ N ₁₅ S ₂
	639.1439	-3.7	18.5	C ₂₇ H ₂₇ O ₇ N ₈ S ₂
	639.1439	-3.7	13.0	C ₂₈ H ₃₃ O ₁₂ N ₁ S ₂
	639.1390	4.0	15.5	C ₂₁ H ₂₃ O ₁₄ N ₁₀
	639.1443	-4.4	24.5	C ₂₇ H ₁₉ O ₈ N ₁₂
	639.1443	-4.4	19.0	C ₂₈ H ₂₅ O ₁₃ N ₅
	639.1386	4.5	36.5	C ₄₂ H ₁₉ N ₆ S ₁
	639.1444	-4.5	6.0	C ₁₃ H ₂₉ O ₁₃ N ₁₃ S ₂
	639.1385	4.7	9.5	C ₂₁ H ₃₁ O ₁₃ N ₆ S ₂
	639.1385	4.7	15.0	C ₂₀ H ₂₅ O ₈ N ₁₃ S ₂
	639.1445	-4.7	33.0	C ₃₄ H ₁₇ N ₁₃ S ₁
	639.1445	-4.7	27.5	C ₃₅ H ₂₃ O ₅ N ₆ S ₁
	639.1385	4.8	28.0	C ₃₅ H ₂₁ O ₈ N ₅
	639.1385	4.8	33.5	C ₃₄ H ₁₅ O ₃ N ₁₂