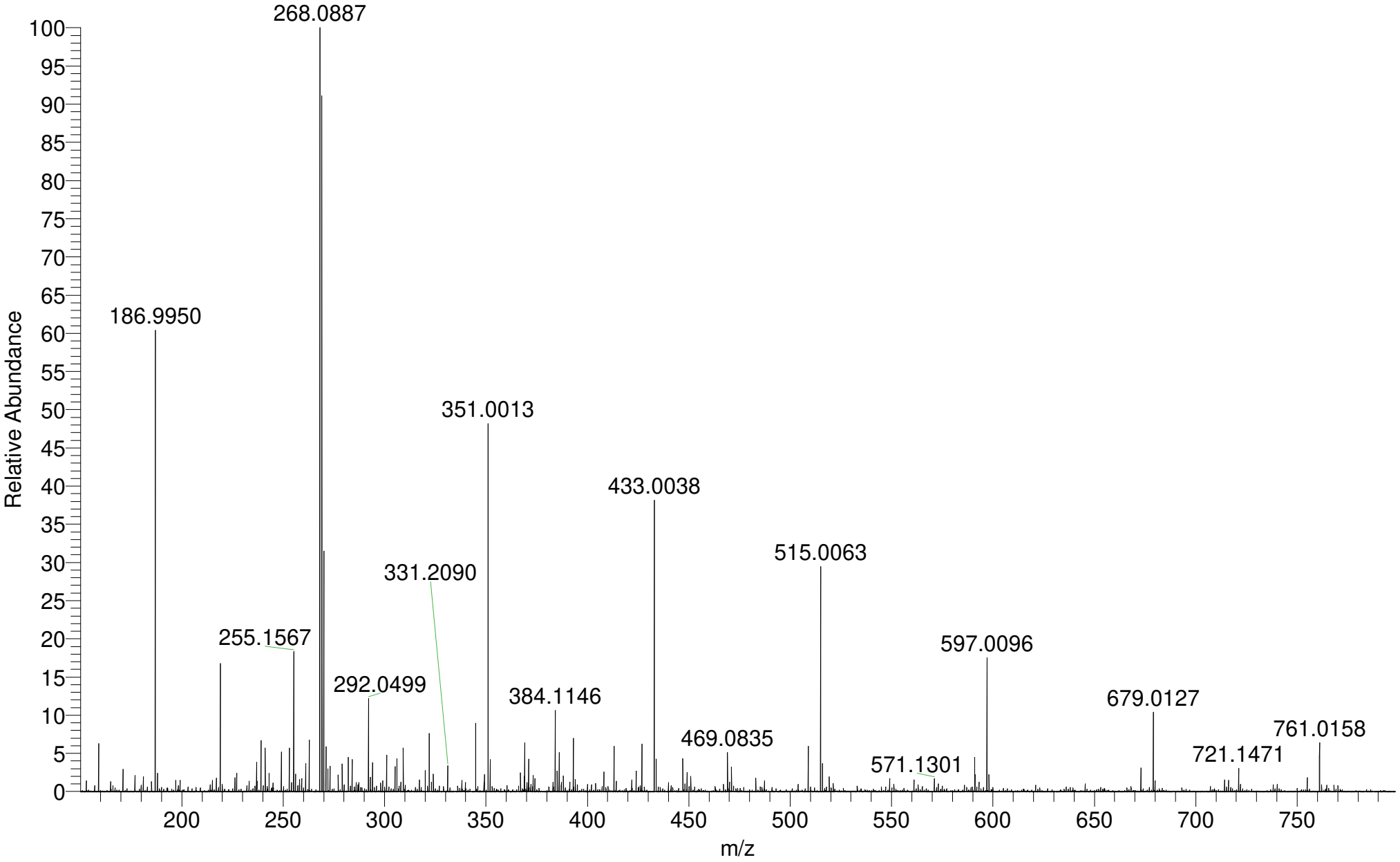
EM221 C17H14ClN
(DCM)/MeOH + 1% AcOH (conc)

EPSRC National Facility Swansea
LTQ Orbitrap XL

22/03/2019 09:40:00

HERLEE_EJCRF_51954_R4 #25-38 RT: 0.72-1.08 AV: 14 SM: 7G NL: 5.06E6
T: FTMS + p NSI Full ms [150.00-2000.00]

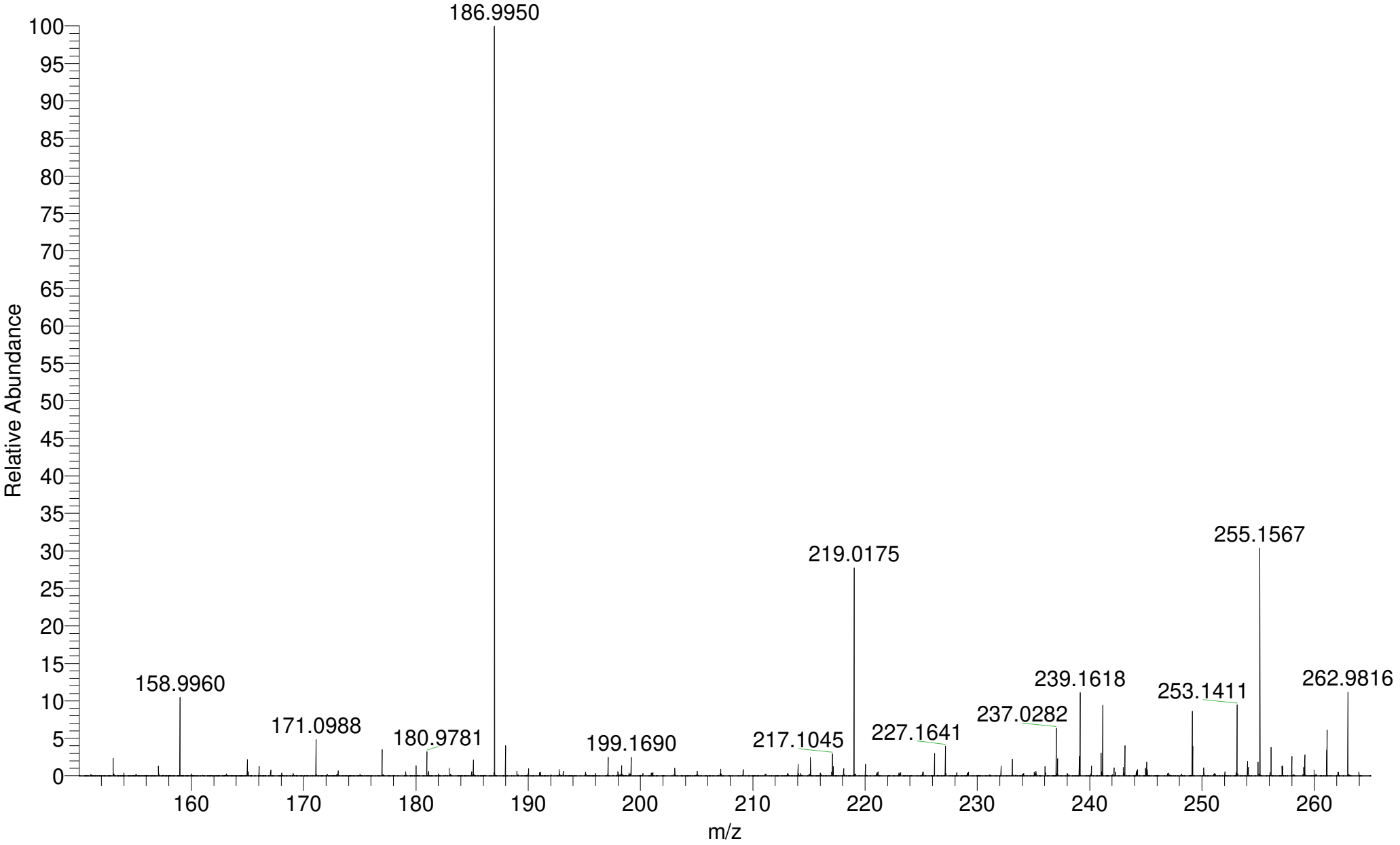


EM221 C17H14ClN
(DCM)/MeOH + 1% AcOH (conc)

EPSRC National Facility Swansea
LTQ Orbitrap XL

22/03/2019 09:40:00

HERLEE_EJCRF_51954_R4 #25-38 RT: 0.72-1.08 AV: 14 SM: 7G NL: 3.06E6
T: FTMS + p NSI Full ms [150.00-2000.00]

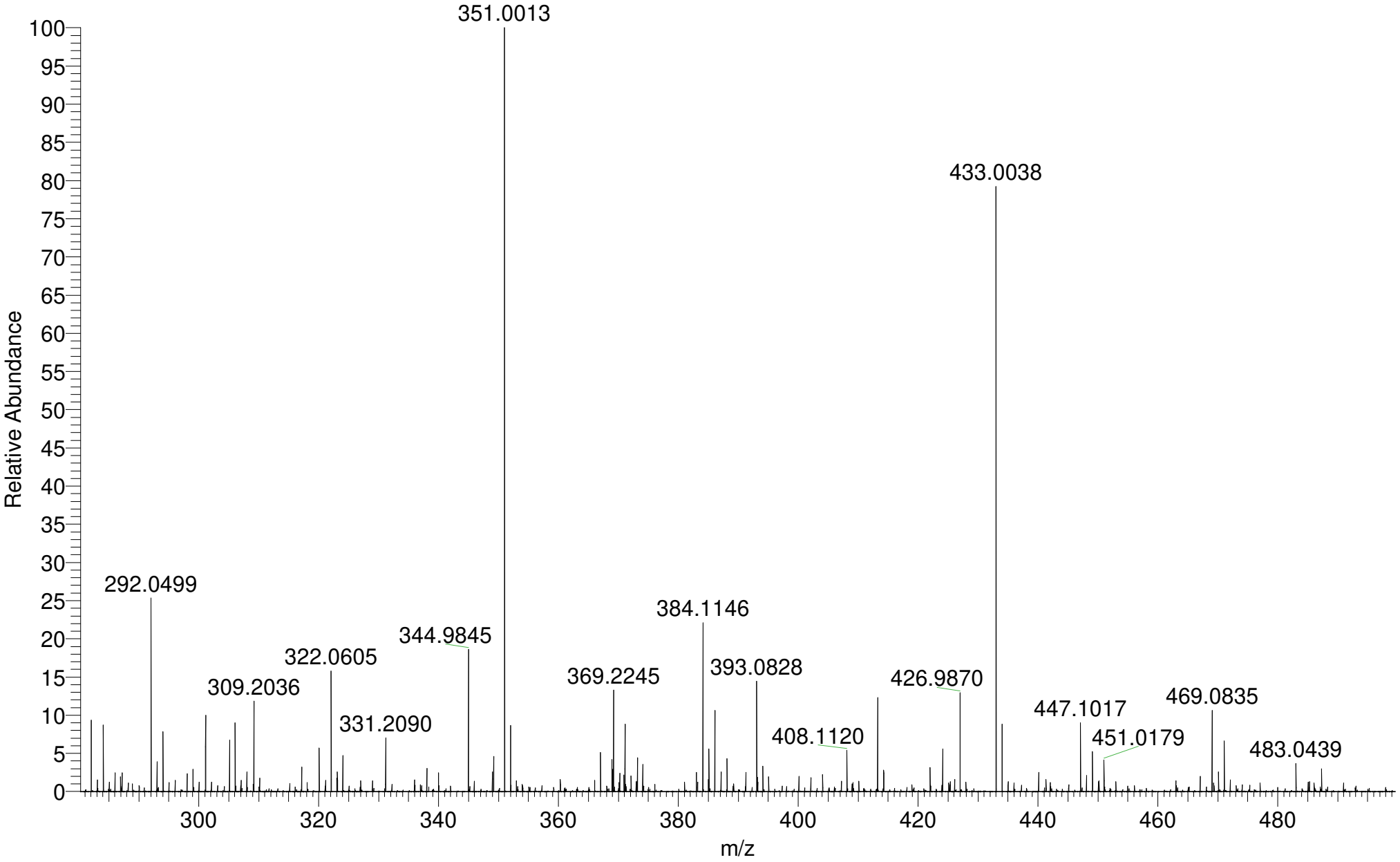


EM221 C17H14ClN
(DCM)/MeOH + 1% AcOH (conc)

EPSRC National Facility Swansea
LTQ Orbitrap XL

22/03/2019 09:40:00

HERLEE_EJCRF_51954_R4 #25-38 RT: 0.72-1.08 AV: 14 SM: 7G NL: 2.44E6
T: FTMS + p NSI Full ms [150.00-2000.00]

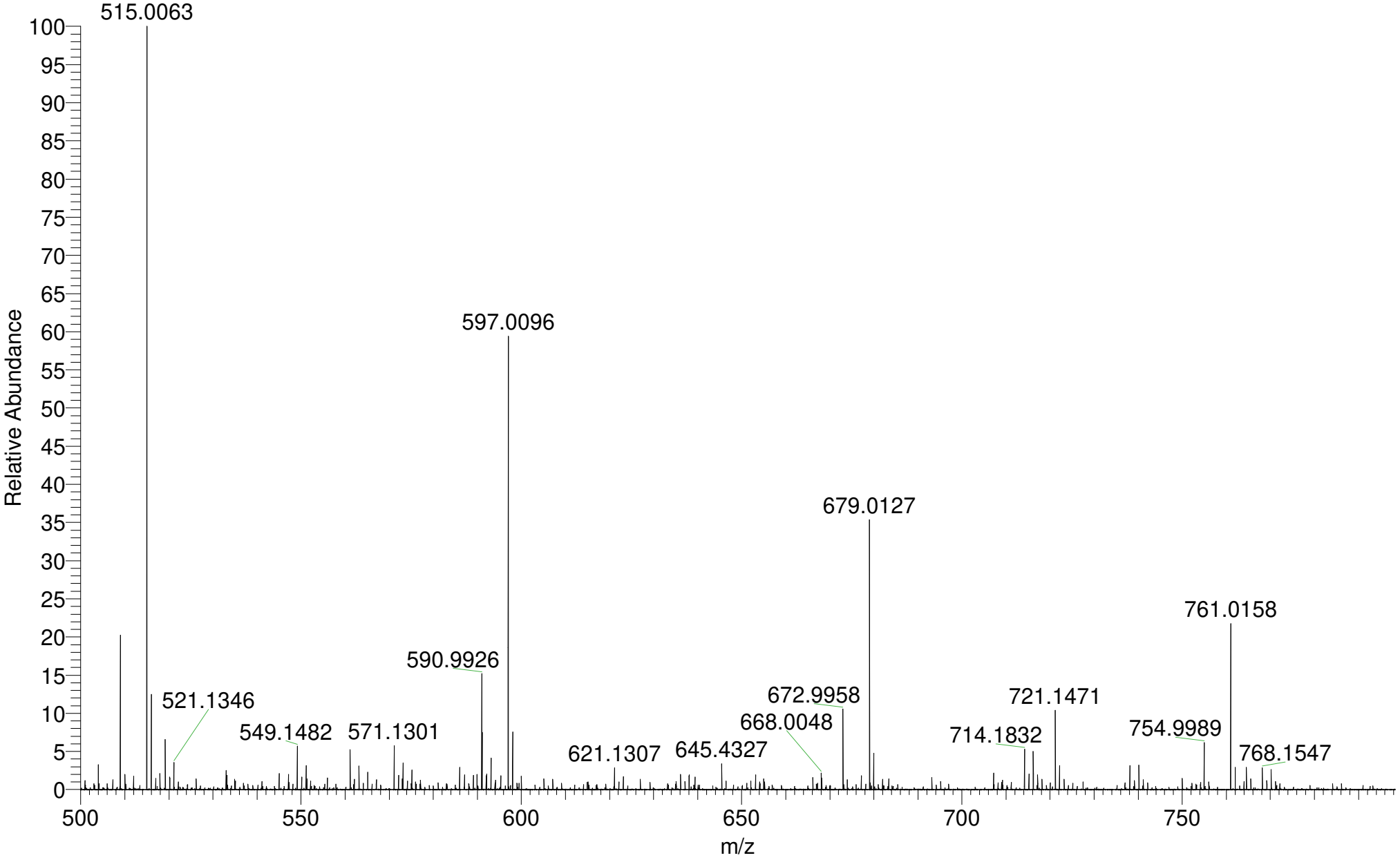


EM221 C17H14ClN
(DCM)/MeOH + 1% AcOH (conc)

EPSRC National Facility Swansea
LTQ Orbitrap XL

22/03/2019 09:40:00

HERLEE_EJCRF_51954_R4 #25-38 RT: 0.72-1.08 AV: 14 SM: 7G NL: 1.49E6
T: FTMS + p NSI Full ms [150.00-2000.00]

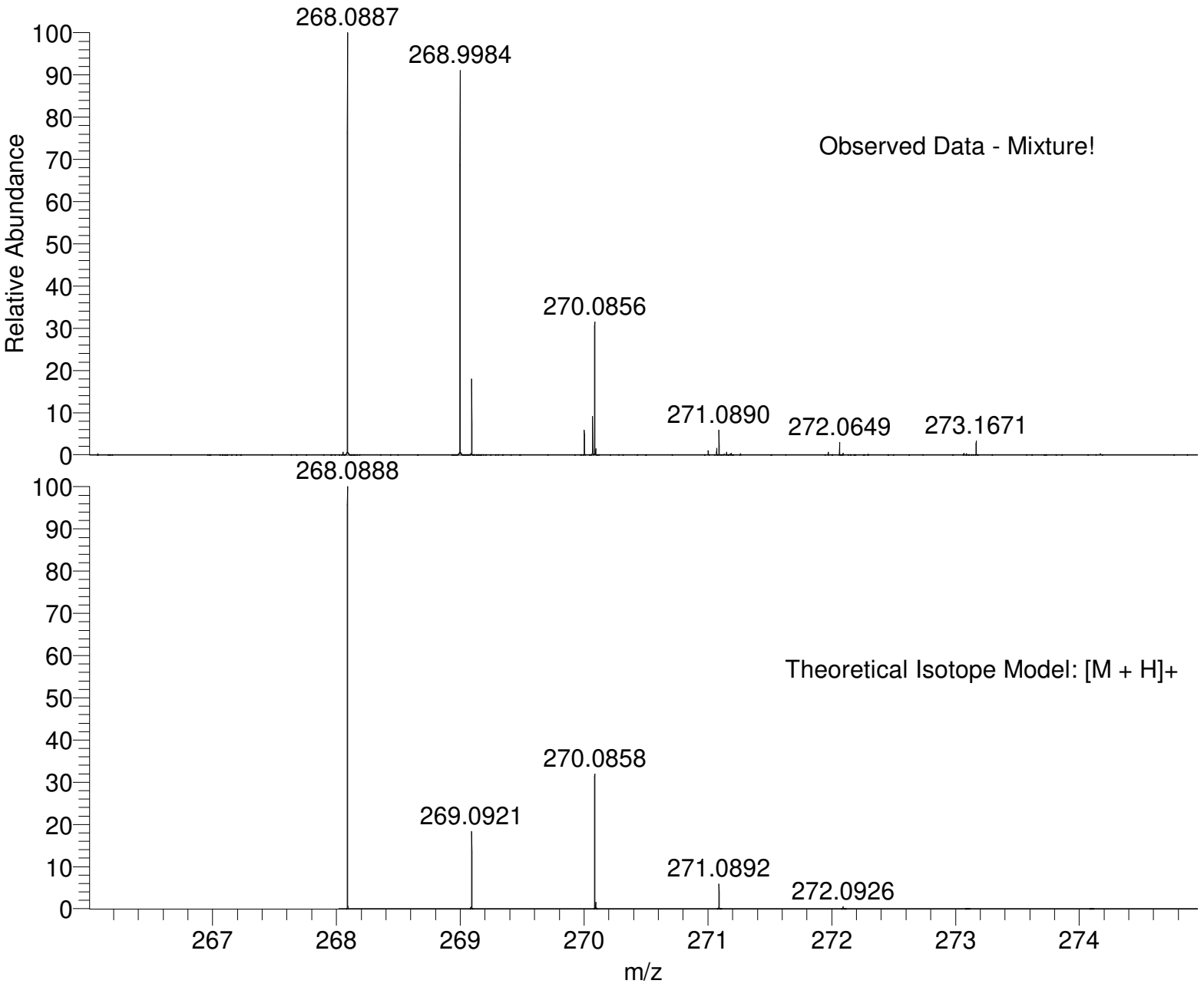


EM221 C17H14ClN
(DCM)/MeOH + 1% AcOH (conc)

EPSRC National Facility Swansea
LTQ Orbitrap XL

22/03/2019 09:40:00

SM: 7G



Isotope:	Min. .. Max.		
14 N	0....10		
16 O	0....10		
12 C	0....60		
1 H	0....80		
23 Na	0....0		
35 Cl	0....2		
Tolerance Window:	+- 5.00 ppm		
Db/Ring Equiv:	-30.. 100	N-Rule:	Do not use
Fits:	500	Charge:	1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
268.0887	268.0888	-0.2	10.5	$C_{17} H_{15} N_{1} Cl_{1}$
	268.0888	-0.3	2.5	$C_{6} H_{14} O_{7} N_{5}$
	268.0883	1.6	15.0	$C_{20} H_{12} O_{1}$
	268.0893	-2.1	-2.0	$C_{3} H_{17} O_{6} N_{6} Cl_{1}$
	268.0879	2.9	-7.0	$C_{2} H_{21} O_{10} N_{2} Cl_{1}$
	268.0879	2.9	-1.5	$C_{1} H_{15} O_{5} N_{9} Cl_{1}$
	268.0897	-3.9	-6.5	$H_{20} O_{5} N_{7} Cl_{2}$
	268.0898	-3.9	-12.0	$C_{1} H_{26} O_{10} Cl_{2}$
	268.0874	4.7	3.0	$C_{4} H_{12} O_{6} N_{8}$