

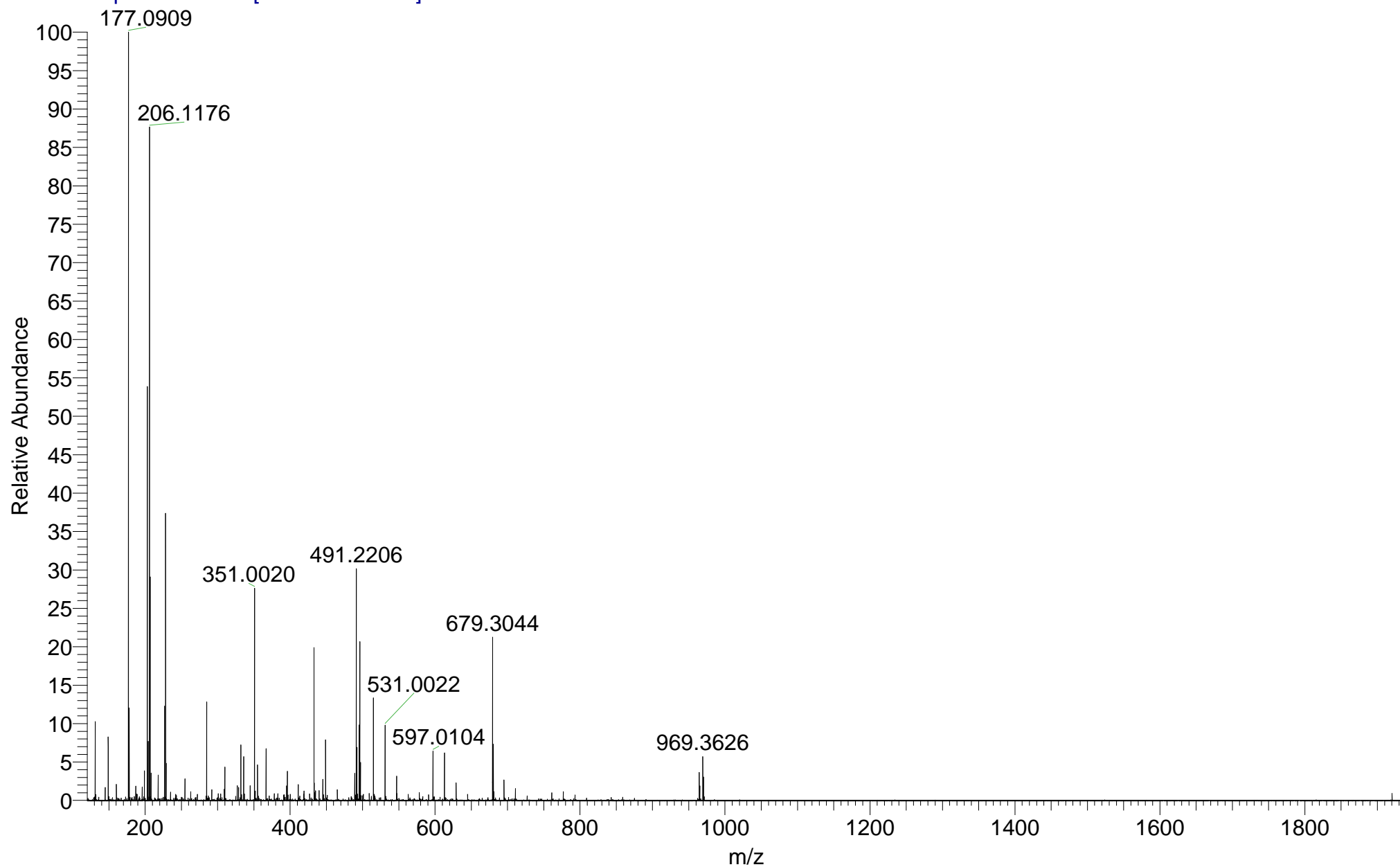
O:\IMPBUL\_TWKJT\_50432  
(DCM)/MeOH + NH4OAc  
AB5-548

EPSRC UK National MS Facility  
LTQ Orbitrap XL

C12H15NO2  
26/11/2018 08:13:42

IMPBUL\_TWKJT\_50432 #38-53 RT: 0.65-1.02 AV: 15 SM: 7G NL: 1.75E6

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



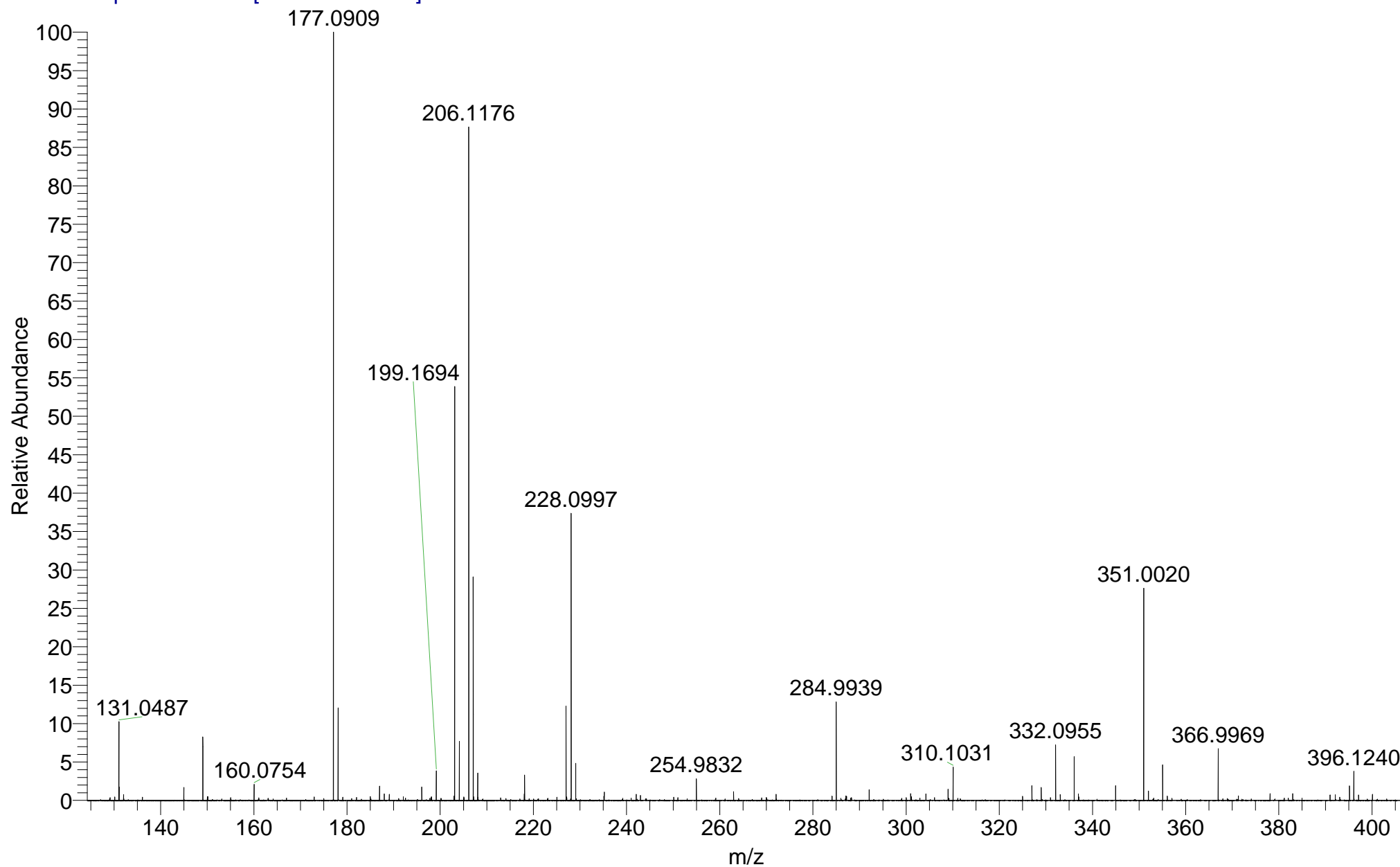
O:\IMPBUL\_TWKTJ\_50432  
(DCM)/MeOH + NH4OAc  
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26/11/2018 08:13:42

IMPBUL\_TWKTJ\_50432 #38-53 RT: 0.65-1.02 AV: 15 SM: 7G NL: 1.75E6

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

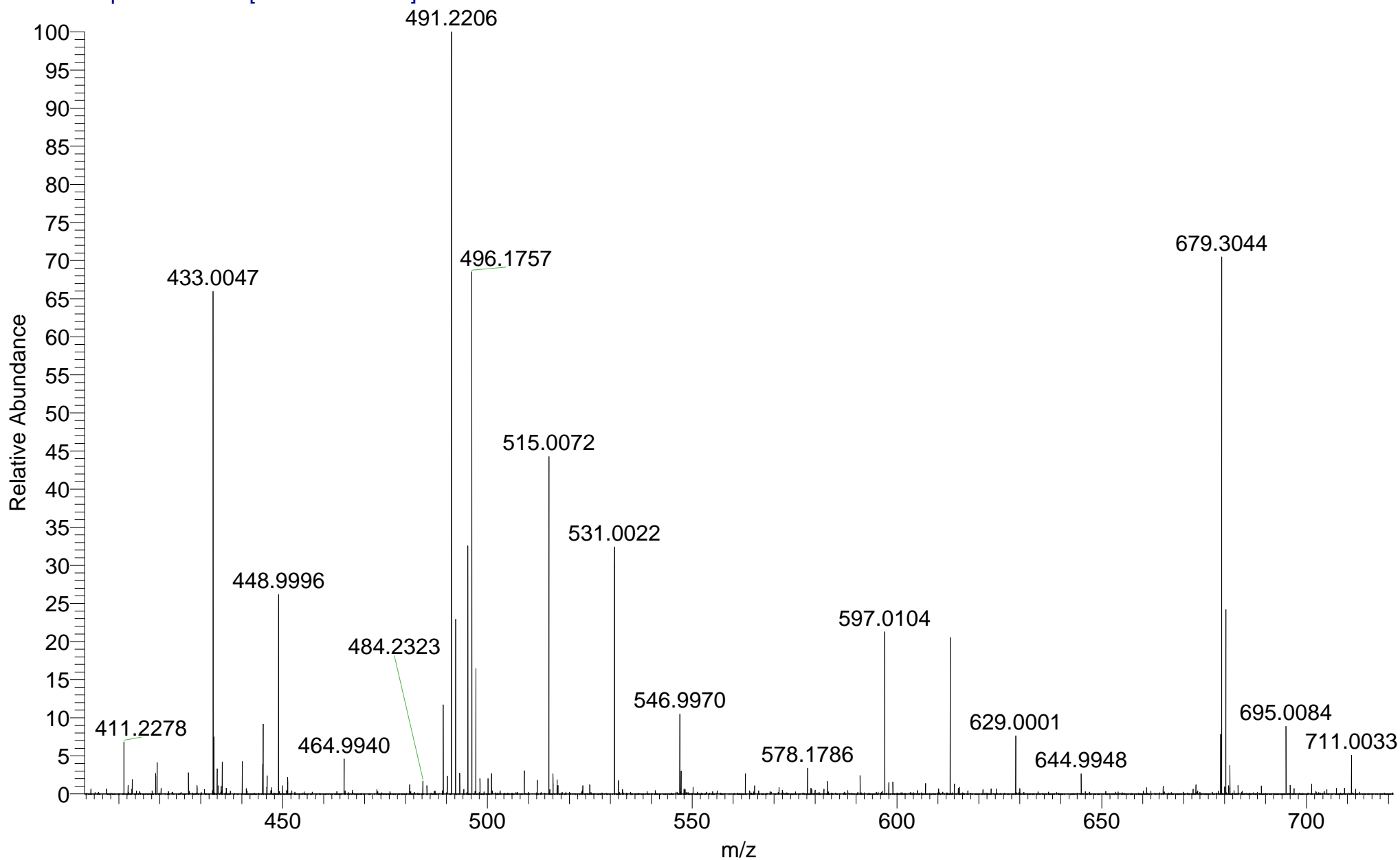


O:\IMPBUL\_TWKJT\_50432  
(DCM)/MeOH + NH4OAc  
AB5-548

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LTQ Orbitrap XL

C12H15NO2  
26/11/2018 08:13:42

IMPBUL\_TWKJT\_50432 #38-53 RT: 0.65-1.02 AV: 15 SM: 7G NL: 5.28E5  
T: FTMS + p NSI Full ms [120.00-1935.00]

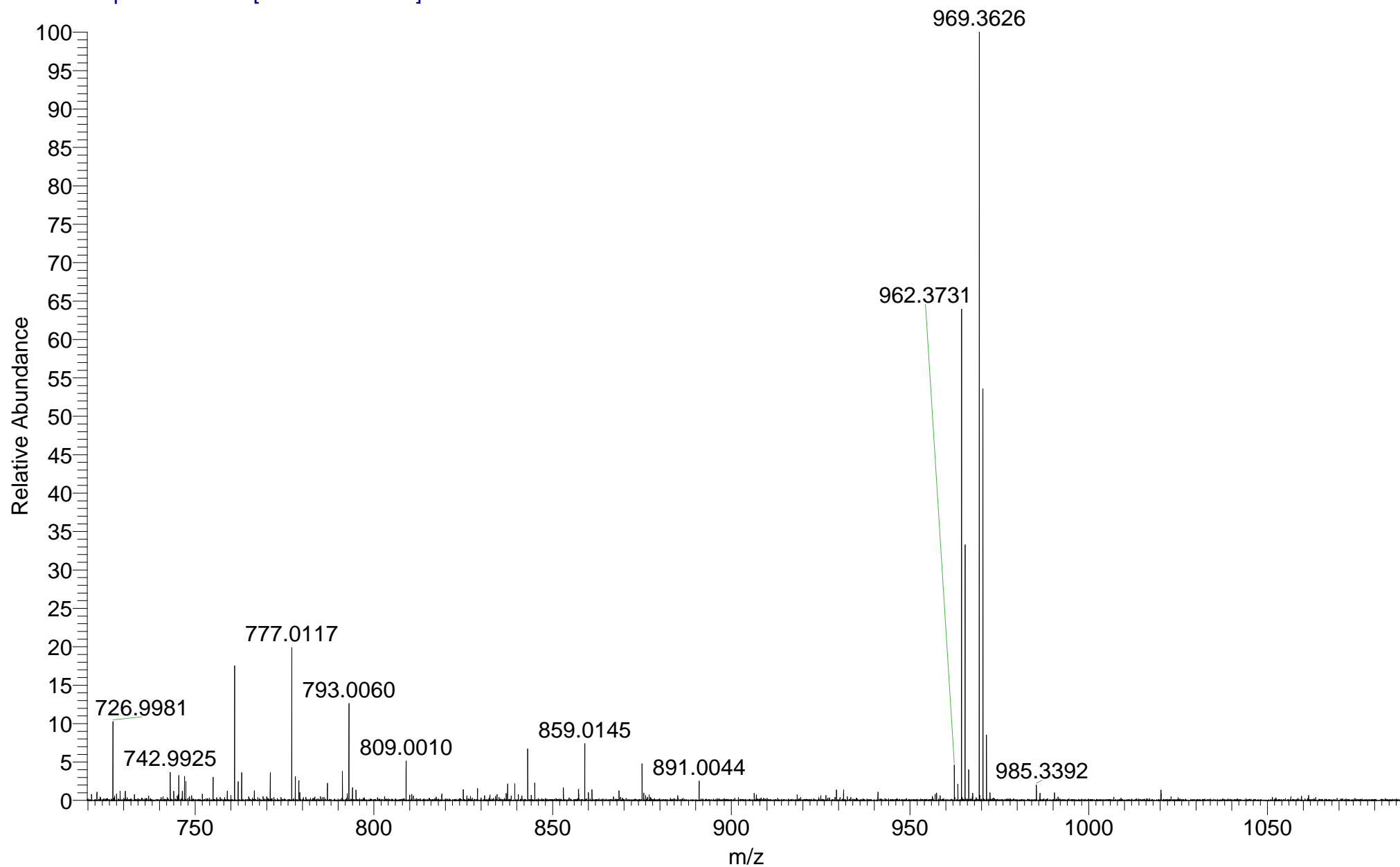


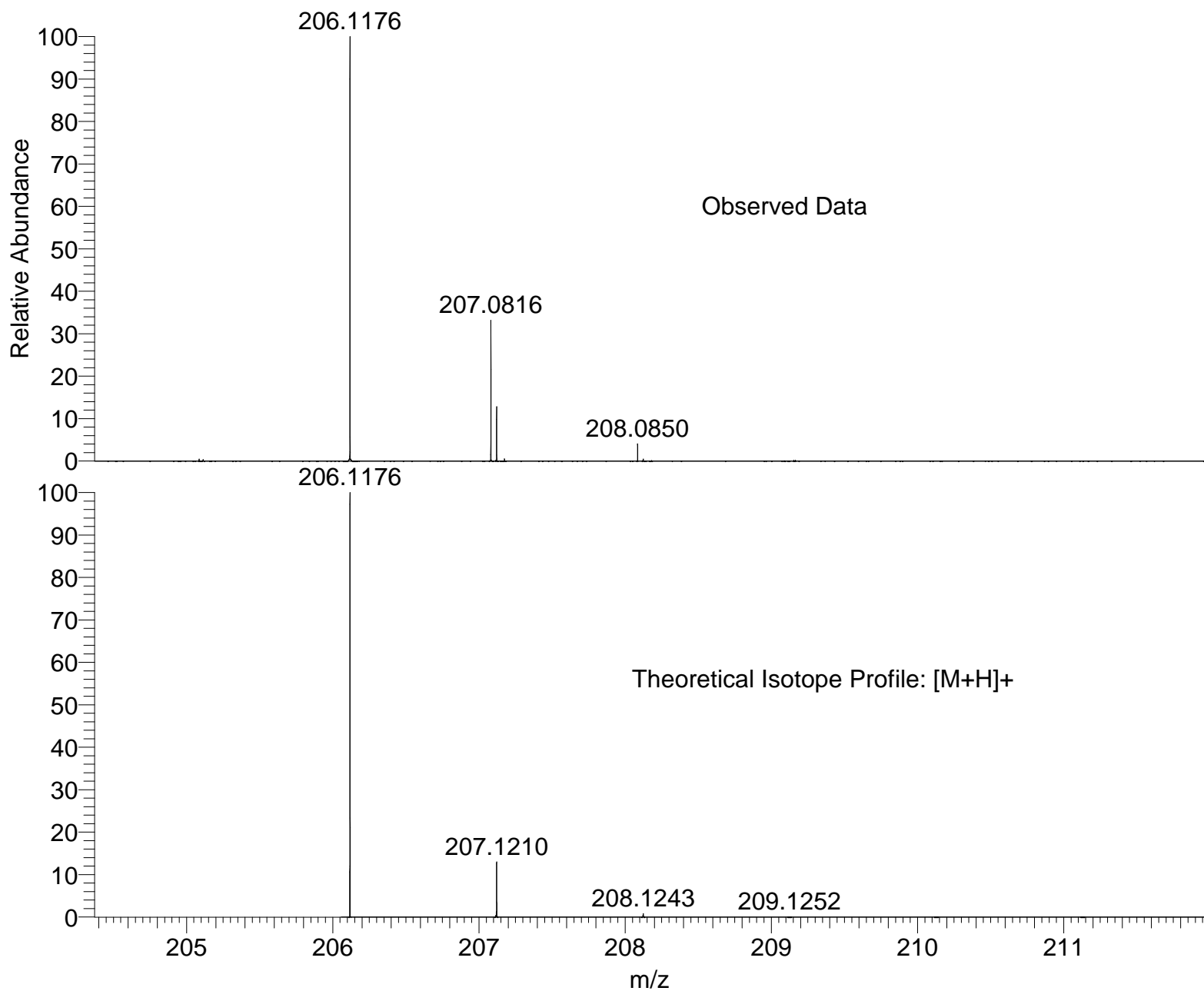
O:\IMPBUL\_TWKTJ\_50432  
(DCM)/MeOH + NH<sub>4</sub>OAc  
AB5-548

EPSRC UK National MS Facility  
LTQ Orbitrap XL

C<sub>12</sub>H<sub>15</sub>NO<sub>2</sub>  
26/11/2018 08:13:42

IMPBUL\_TWKTJ\_50432 #38-53 RT: 0.65-1.02 AV: 15 SM: 7G NL: 9.96E4  
T: FTMS + p NSI Full ms [120.00-1935.00]





NL:  
1.54E6  
IMPBUL\_TWKTJ\_50432#38-  
53 RT: 0.65-1.02 AV: 15 T:  
FTMS + p NSI Full ms  
[120.00-1935.00]

NL:  
2.04E4  
C<sub>12</sub>H<sub>15</sub>NO<sub>2</sub>H:  
C<sub>12</sub>H<sub>16</sub>N<sub>1</sub>O<sub>2</sub>  
p (gss, s /p:40) Chrg 1  
R: 100000 Res .Pwr . @FWHM

Isotope:                   Min. .. Max.  
 14 N                   0....15  
 16 O                   0....20  
 12 C                   0....80  
 1 H                   0....100  
 23 Na                  0....0  
 Tolerance Window:   +- 5.00 ppm  
 Db/Ring Equiv:       -10.. 500  
 Fits:                  300

N-Rule:   Do not use  
 Charge:   1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
206.1176	206.1176	0.2	5.5	C <sub>12</sub> H <sub>16</sub> O <sub>2</sub> N <sub>1</sub>