

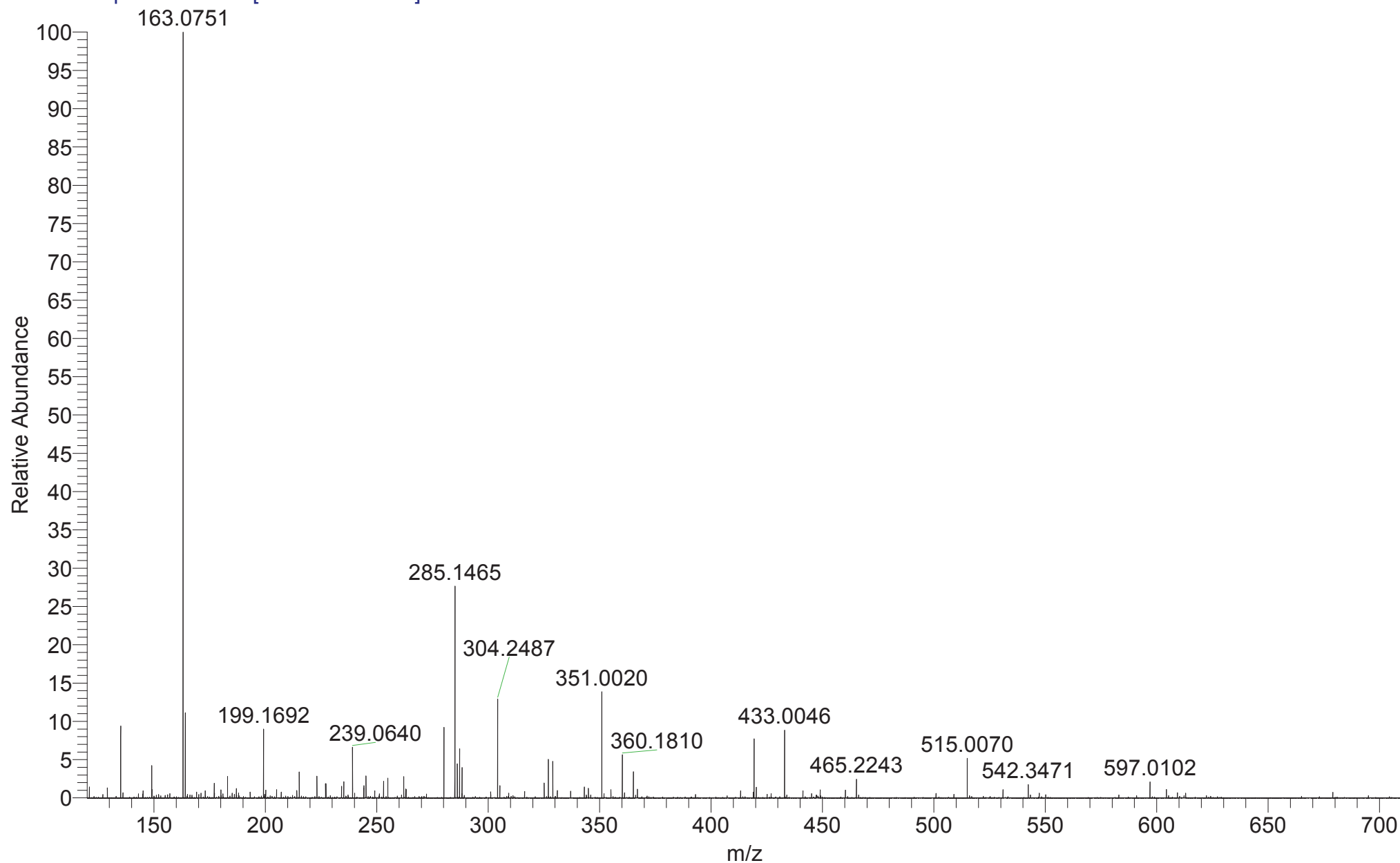
O:\IMPBUL\_CNR3U\_45526  
(DCM)/MeOH + NH<sub>4</sub>OAc  
JR-1-105-1

EPSRC UK National MS Facility  
LTQ Orbitrap XL

C16H22O3  
30/05/2018 11:07:45

IMPBUL\_CNR3U\_45526 #38-53 RT: 0.66-1.04 AV: 15 SM: 7G NL: 2.38E6

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

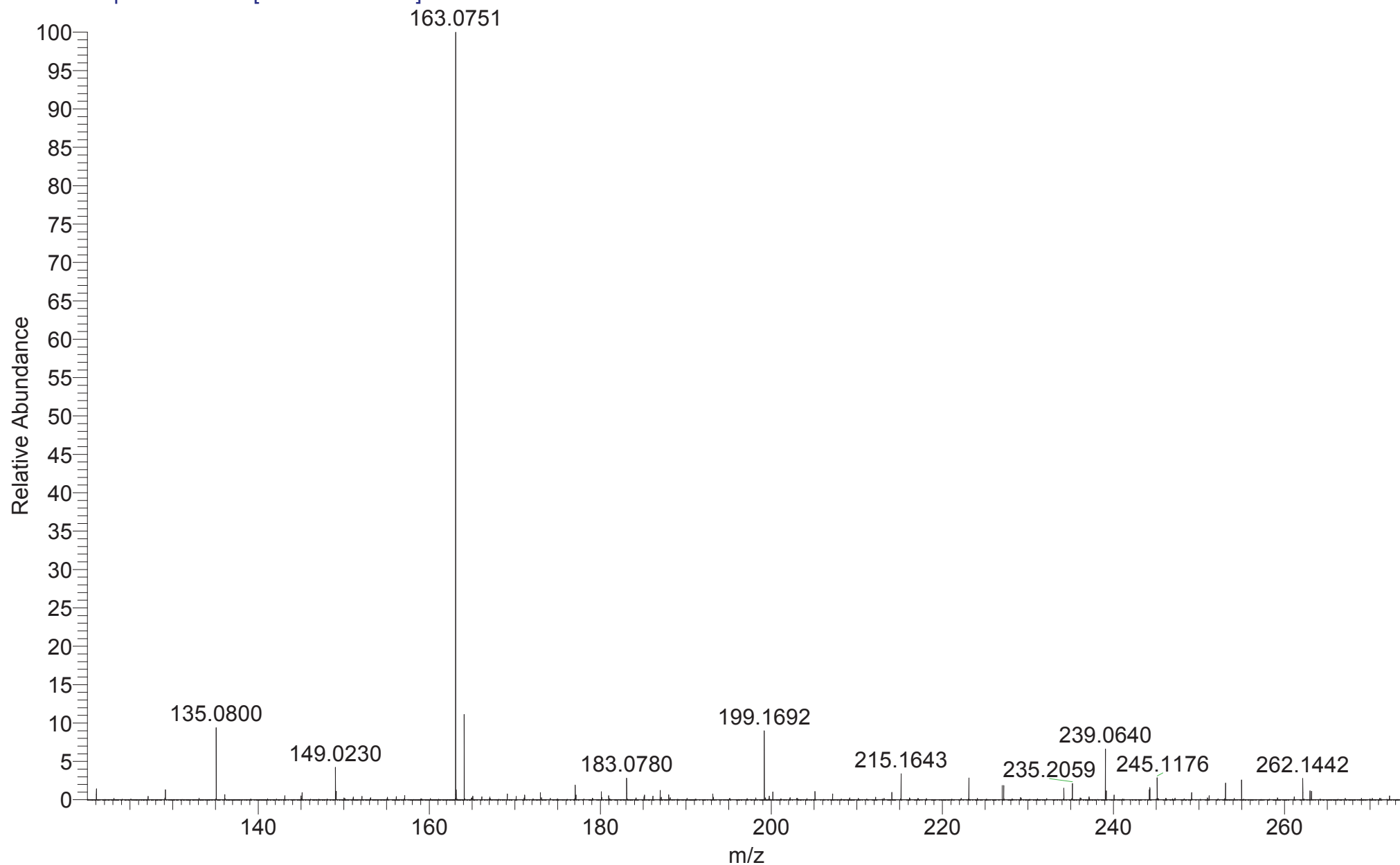


O:\IMPBUL\_CNR3U\_45526  
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IMPBUL\_CNR3U\_45526 #38-53 RT: 0.66-1.04 AV: 15 SM: 7G NL: 2.38E6  
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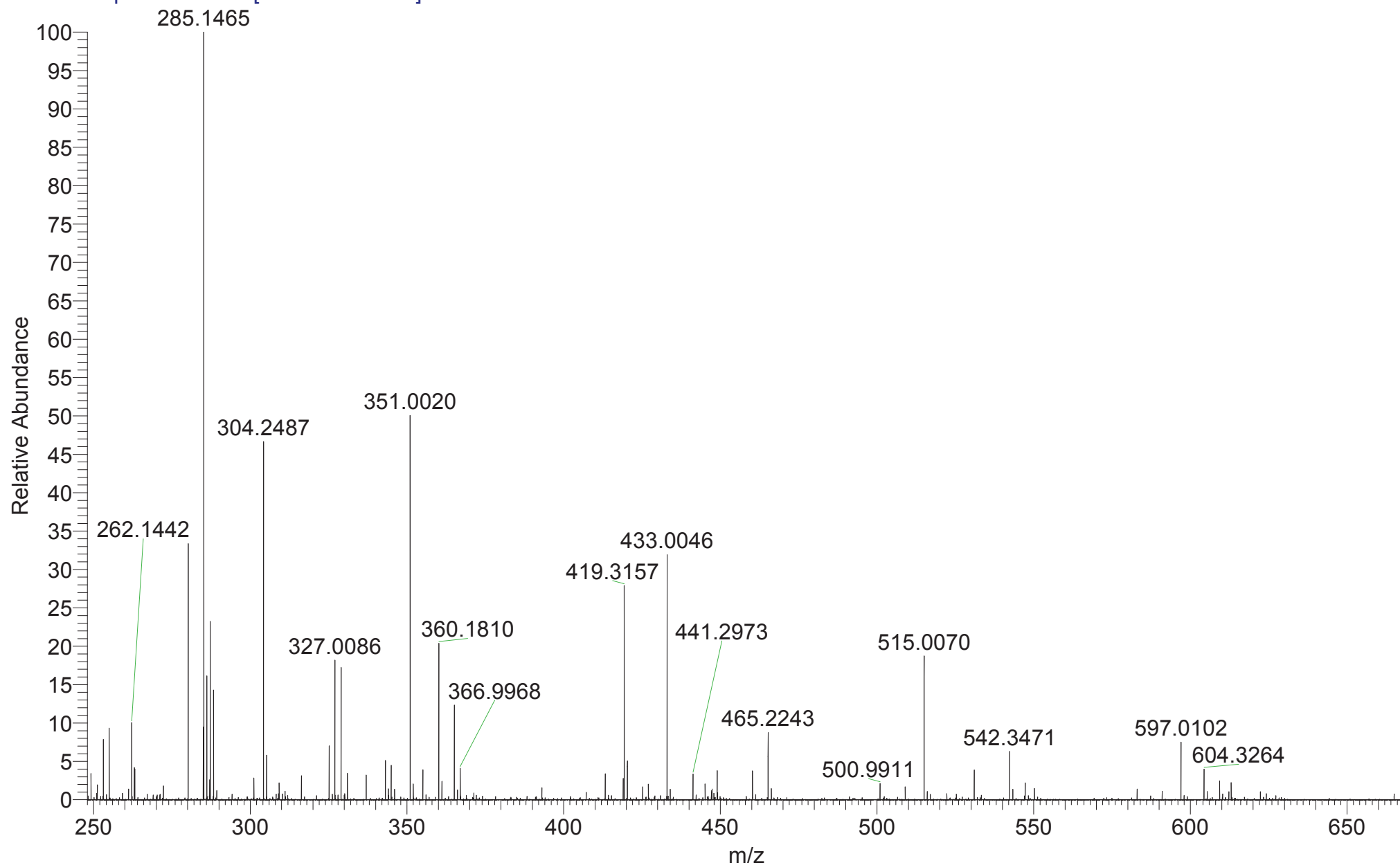
O:\IMPBUL\_CNR3U\_45526  
(DCM)/MeOH + NH4OAc  
JR-1-105-1

EPSRC UK National MS Facility  
LTQ Orbitrap XL

C16H22O3  
30/05/2018 11:07:45

IMPBUL\_CNR3U\_45526 #38-53 RT: 0.66-1.04 AV: 15 SM: 7G NL: 6.58E5

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



SM: 7G



NL:  
6.58E5  
IMPBUL\_CNR3U\_45526#38-  
53 RT: 0.66-1.04 AV: 15 T:  
FTMS + p NSI Full ms  
[120.00-1935.00]

NL:  
1.96E4  
C<sub>16</sub>H<sub>22</sub>O<sub>3</sub>Na:  
C<sub>16</sub>H<sub>22</sub>O<sub>3</sub>Na<sub>1</sub>  
p (gss, s /p:40) Chrg 1  
R: 100000 Res .Pwr . @FWHM

NL:  
1.95E4  
C<sub>16</sub>H<sub>22</sub>O<sub>3</sub>NH<sub>4</sub>:  
C<sub>16</sub>H<sub>26</sub>O<sub>3</sub>N<sub>1</sub>  
p (gss, s /p:40) Chrg 1  
R: 100000 Res .Pwr . @FWHM

Isotope:                   Min. .. Max.  
 14 N                      0....10  
 16 O                      0....20  
 12 C                      0....60  
 1 H                       0....80  
 23 Na                     0....0  
 Tolerance Window:       +- 10.00 ppm  
 Db/Ring Equiv:          -3.. 100  
 Fits:                     150

N-Rule:   Do not use  
 Charge:   1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
280.1912	280.1907	1.7	4.5	C <sub>16</sub> H <sub>26</sub> O <sub>3</sub> N <sub>1</sub>
	280.1926	-4.9	-3.0	C <sub>3</sub> H <sub>24</sub> O <sub>5</sub> N <sub>10</sub>
	280.1894	6.5	5.0	C <sub>14</sub> H <sub>24</sub> O <sub>2</sub> N <sub>4</sub>
	280.1934	-7.9	9.0	C <sub>19</sub> H <sub>24</sub> N <sub>2</sub>