

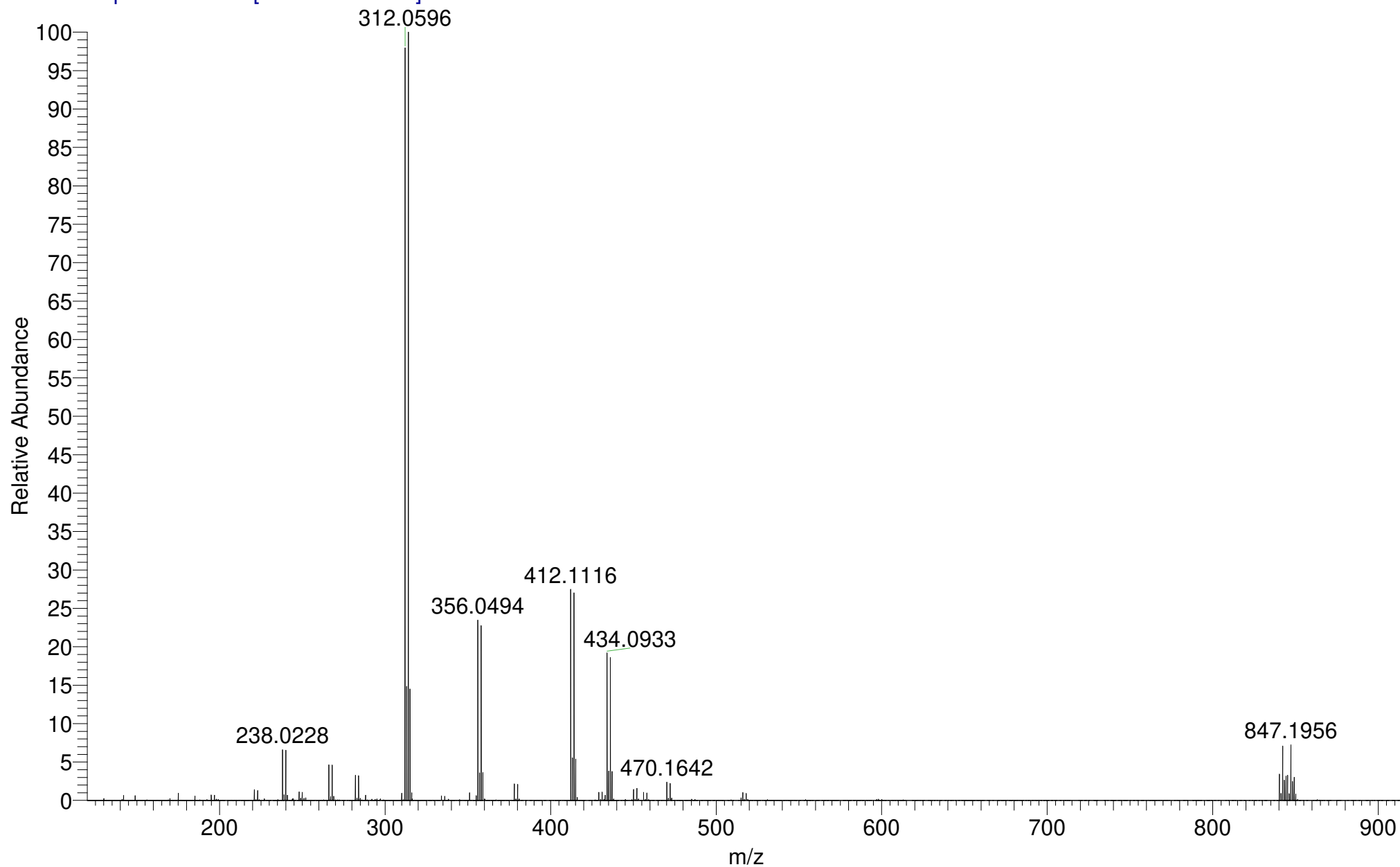
AB3-319  
(DCM)/MeOH + NH4OAc  
C19H26BrNO4

EPSRC National Facility Swansea  
LTQ Orbitrap XL

IMPBUL-AJB  
22/02/2018 17:04:08

IMPBUL\_CM47V\_42209 #33-40 RT: 0.74-1.02 AV: 6 SM: 7G NL: 2.44E7

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

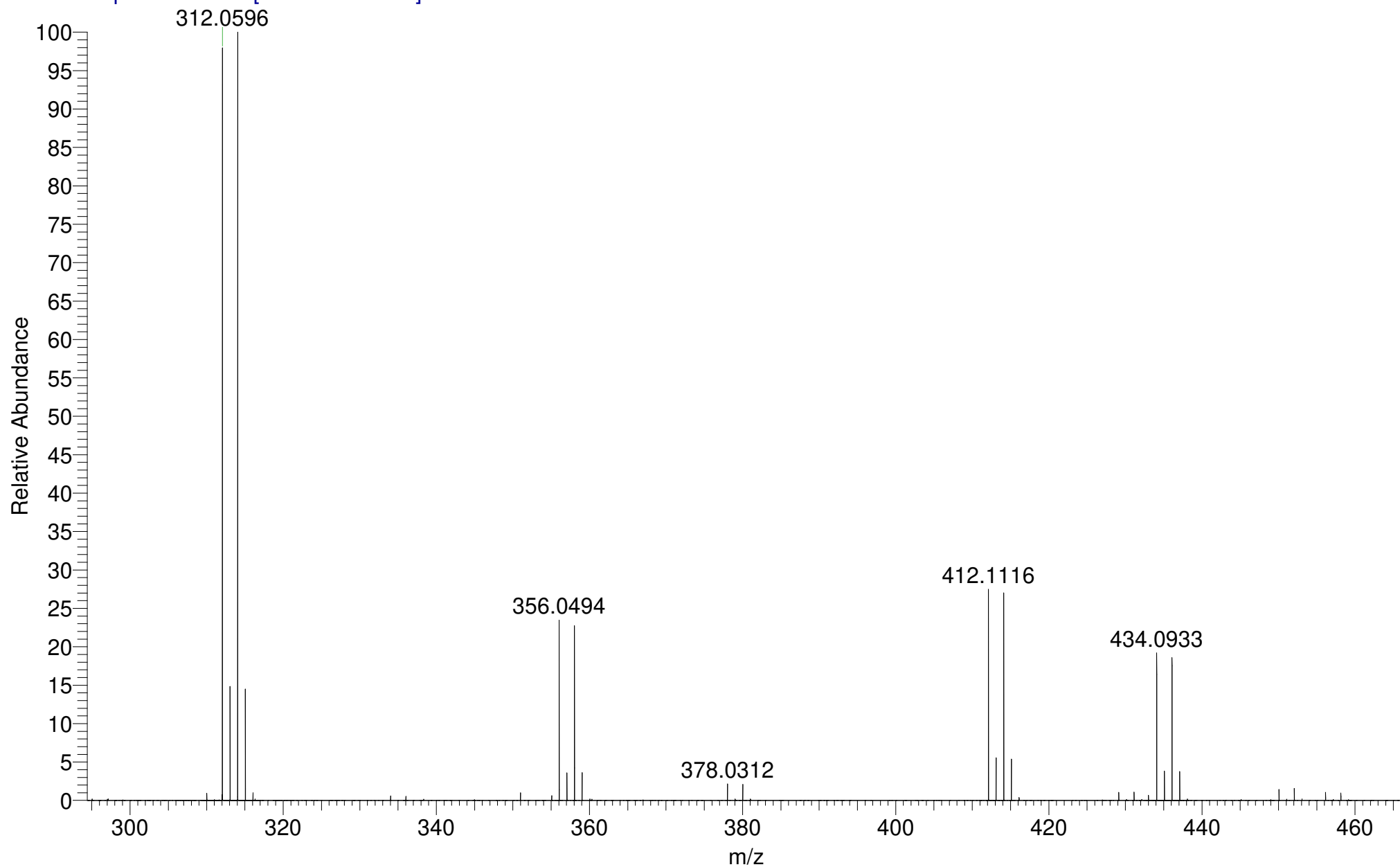


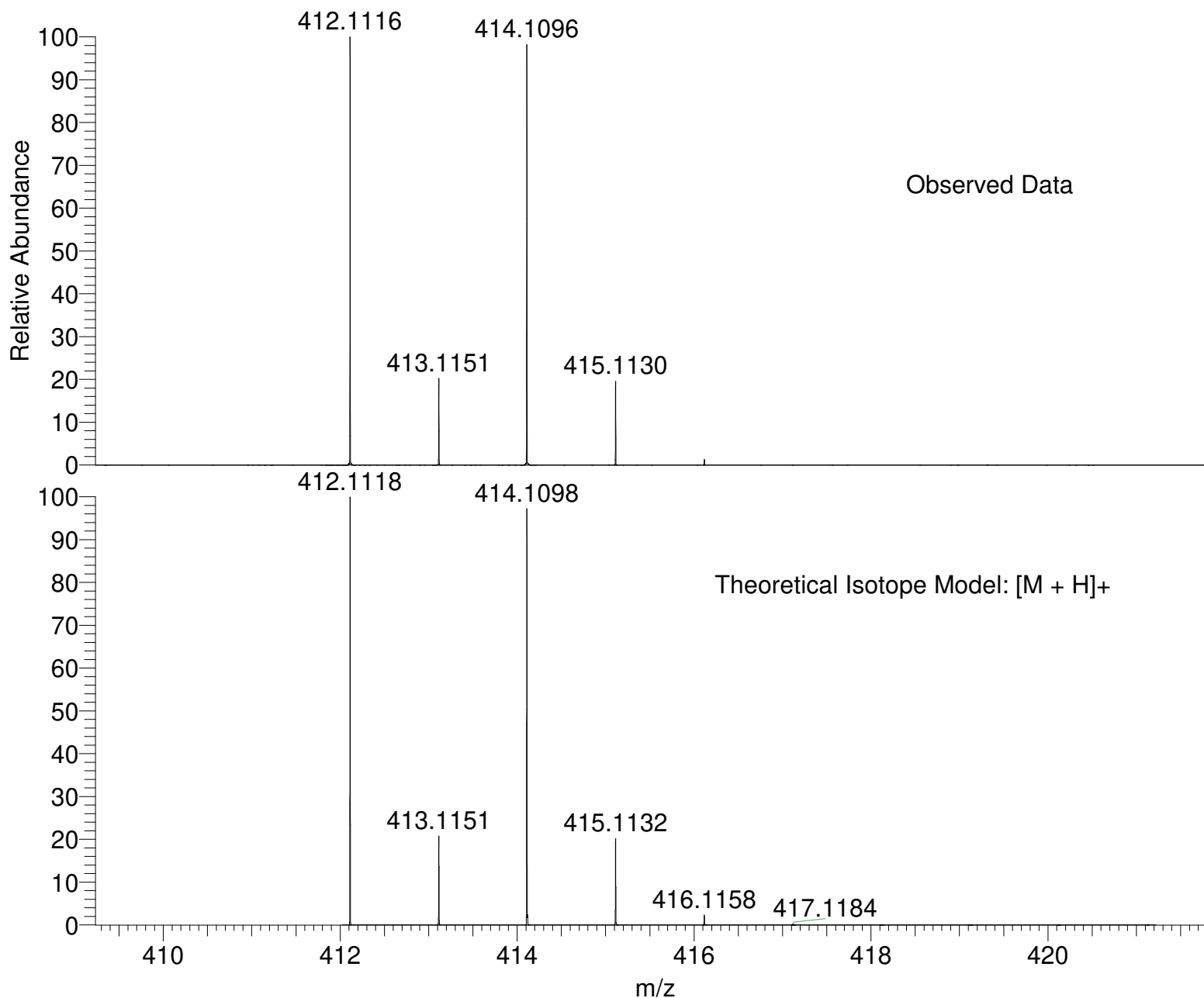
AB3-319  
(DCM)/MeOH + NH<sub>4</sub>OAc  
C<sub>19</sub>H<sub>26</sub>BrNO<sub>4</sub>

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LTQ Orbitrap XL

IMPBUL-AJB  
22/02/2018 17:04:08

IMPBUL\_CM47V\_42209 #33-40 RT: 0.74-1.02 AV: 6 SM: 7G NL: 2.44E7  
T: FTMS + p NSI Full ms [120.00-1935.00]





NL:  
6.70E6  
IMPBUL\_CM47V\_42209#33-  
40 RT: 0.74-1.02 AV: 6 T:  
FTMS + p NSI Full ms  
[120.00-1935.00]

NL:  
9.54E3  
C<sub>19</sub>H<sub>26</sub>BrNO<sub>4</sub>H:  
C<sub>19</sub>H<sub>27</sub>Br<sub>1</sub>N<sub>1</sub>O<sub>4</sub>  
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....90  
 23 Na                  0....0  
 79 Br                  0....5  
 Tolerance Window:   +- 5.00 ppm  
 Db/Ring Equiv:       -3.. 100  
 Fits:                  150

N-Rule:   Do not use  
 Charge:   1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
412.1116	412.1117	-0.4	2.0	C <sub>2</sub> H <sub>16</sub> O <sub>11</sub> N <sub>14</sub>
	412.1118	-0.5	6.5	C <sub>19</sub> H <sub>27</sub> O <sub>4</sub> N <sub>1</sub> Br <sub>1</sub>
	412.1112	0.9	9.0	C <sub>17</sub> H <sub>20</sub> O <sub>10</sub> N <sub>2</sub>
	412.1112	0.9	14.5	C <sub>16</sub> H <sub>14</sub> O <sub>5</sub> N <sub>9</sub>
	412.1121	-1.2	26.5	C <sub>32</sub> H <sub>14</sub> N <sub>1</sub>
	412.1123	-1.7	-0.5	C <sub>4</sub> H <sub>23</sub> O <sub>5</sub> N <sub>13</sub> Br <sub>1</sub>
	412.1126	-2.4	19.5	C <sub>17</sub> H <sub>10</sub> O <sub>1</sub> N <sub>13</sub>
	412.1126	-2.4	14.0	C <sub>18</sub> H <sub>16</sub> O <sub>6</sub> N <sub>6</sub>
	412.1105	2.8	7.0	C <sub>17</sub> H <sub>25</sub> O <sub>3</sub> N <sub>4</sub> Br <sub>1</sub>
	412.1104	2.9	-3.0	C <sub>1</sub> H <sub>20</sub> O <sub>15</sub> N <sub>10</sub>
	412.1131	-3.6	1.5	C <sub>4</sub> H <sub>18</sub> O <sub>12</sub> N <sub>11</sub>
	412.1131	-3.7	11.5	C <sub>20</sub> H <sub>23</sub> N <sub>5</sub> Br <sub>1</sub>
	412.1099	4.1	9.5	C <sub>15</sub> H <sub>18</sub> O <sub>9</sub> N <sub>5</sub>
	412.1099	4.1	15.0	C <sub>14</sub> H <sub>12</sub> O <sub>4</sub> N <sub>12</sub>
	412.1136	-5.0	-1.0	C <sub>6</sub> H <sub>25</sub> O <sub>6</sub> N <sub>10</sub> Br <sub>1</sub>