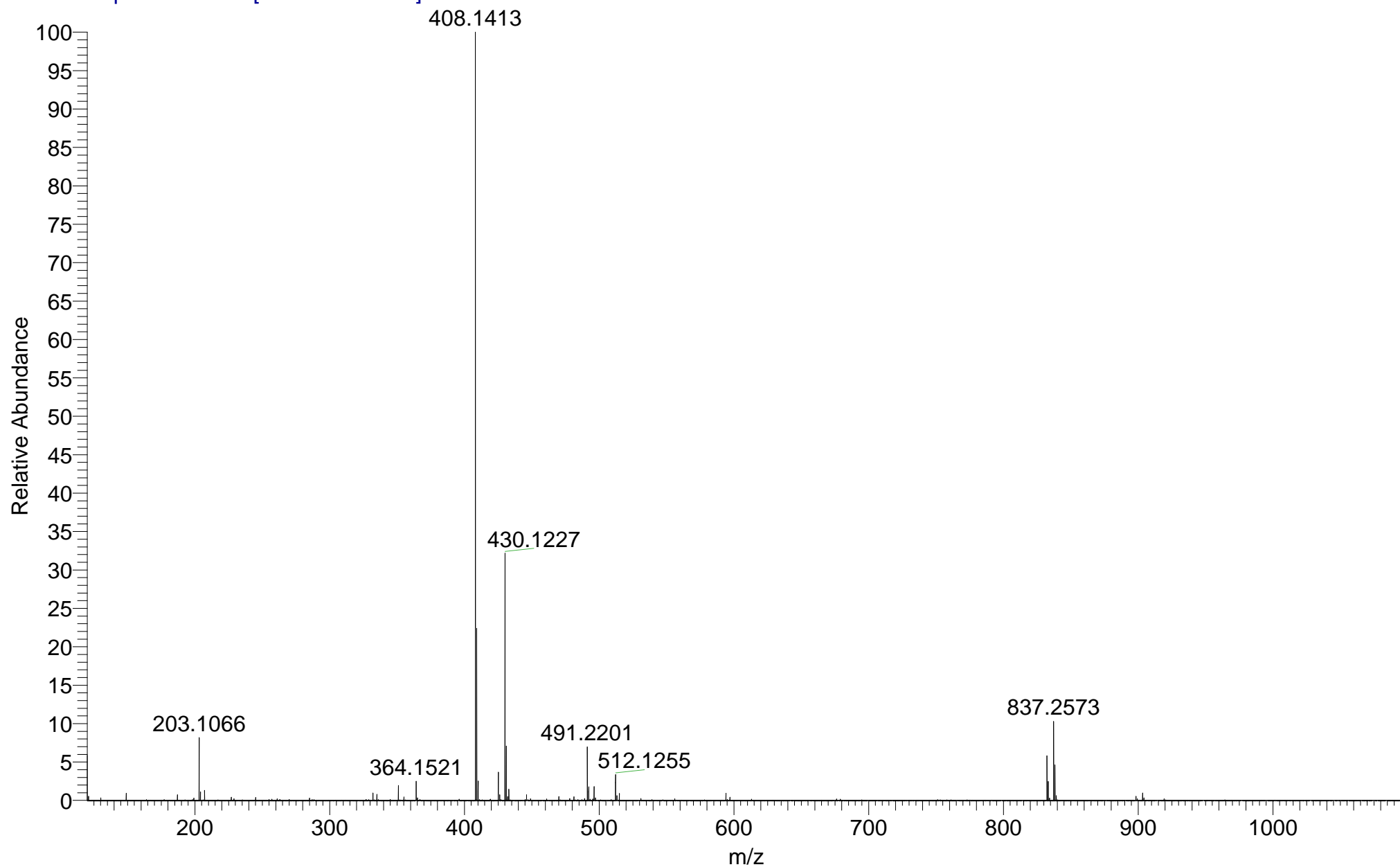


IMPBUL\_TVXP7\_50396 #37-52 RT: 0.65-1.05 AV: 16 SM: 7G NL: 1.65E7  
T: FTMS + p NSI Full ms [120.00-1935.00]



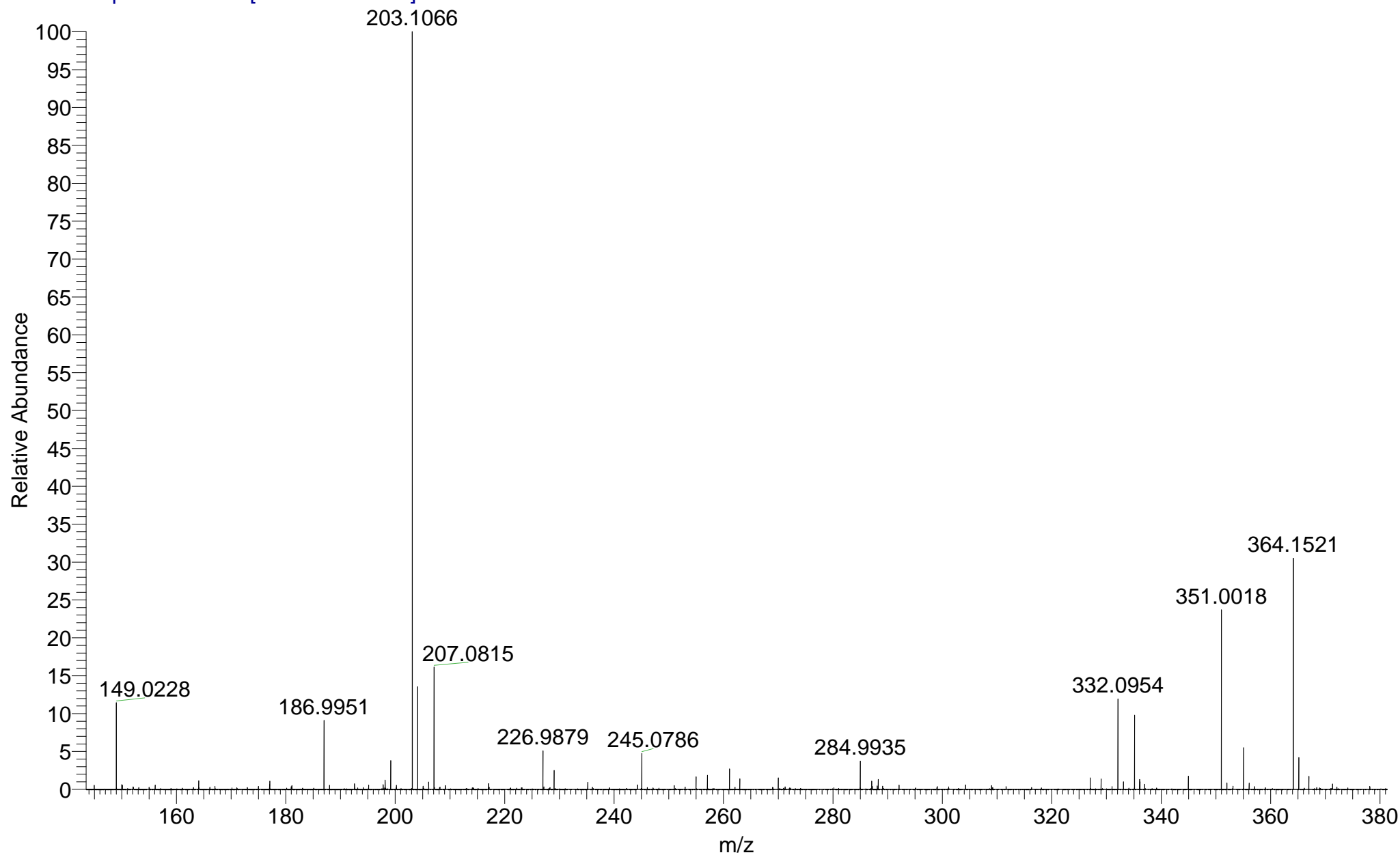
O:\IMPBUL\_TVXP7\_50396  
(DCM)/MeOH + NH4OAc  
AB5-539

EPSRC UK National MS Facility  
LTQ Orbitrap XL

C18H22F3NO4  
26/11/2018 08:16:33

IMPBUL\_TVXP7\_50396 #37-52 RT: 0.65-1.05 AV: 16 SM: 7G NL: 1.35E6

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



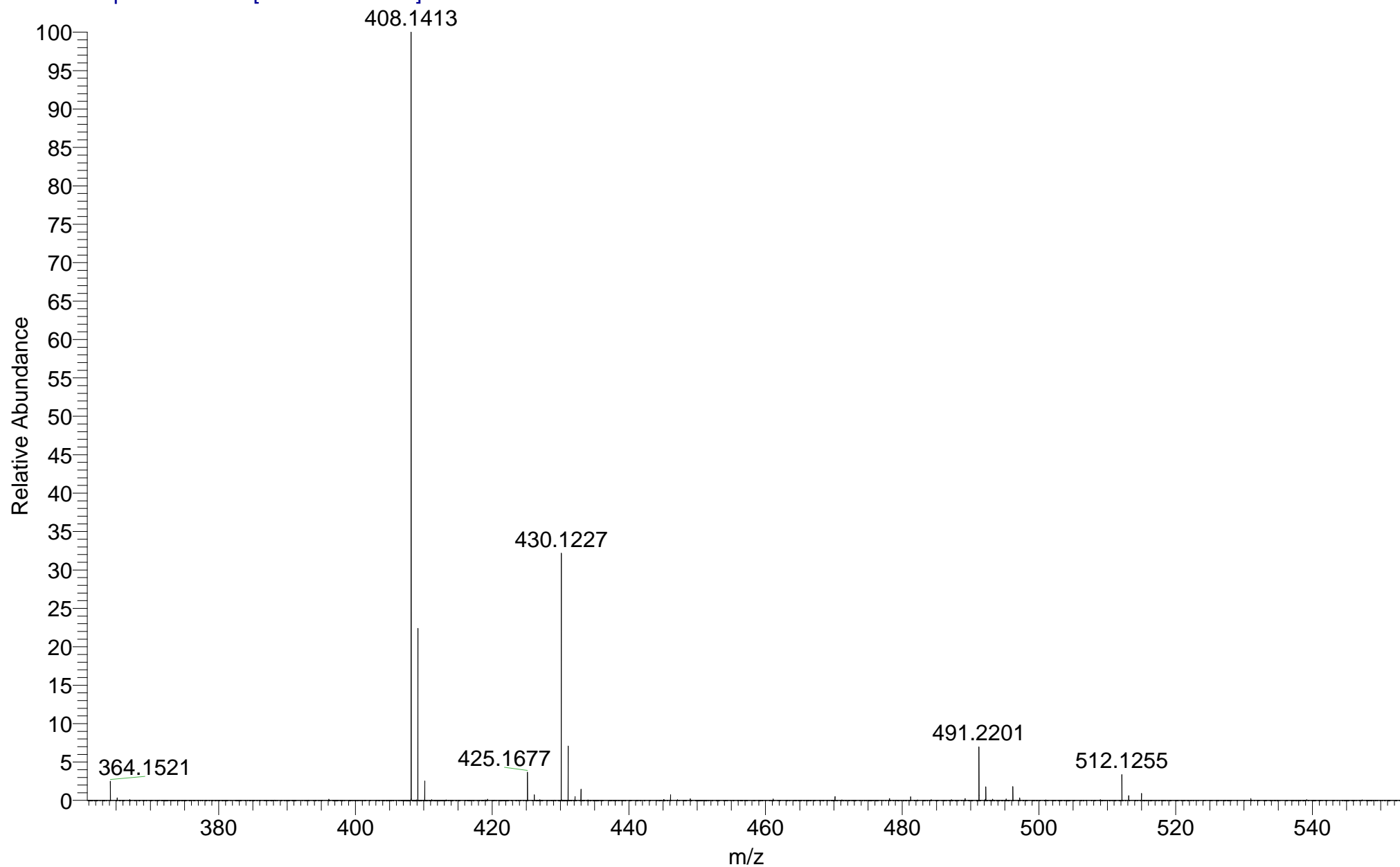
O:\IMPBUL\_TVXP7\_50396  
(DCM)/MeOH + NH4OAc  
AB5-539

EPSRC UK National MS Facility  
LTQ Orbitrap XL

C18H22F3NO4  
26/11/2018 08:16:33

IMPBUL\_TVXP7\_50396 #37-52 RT: 0.65-1.05 AV: 16 SM: 7G NL: 1.65E7

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

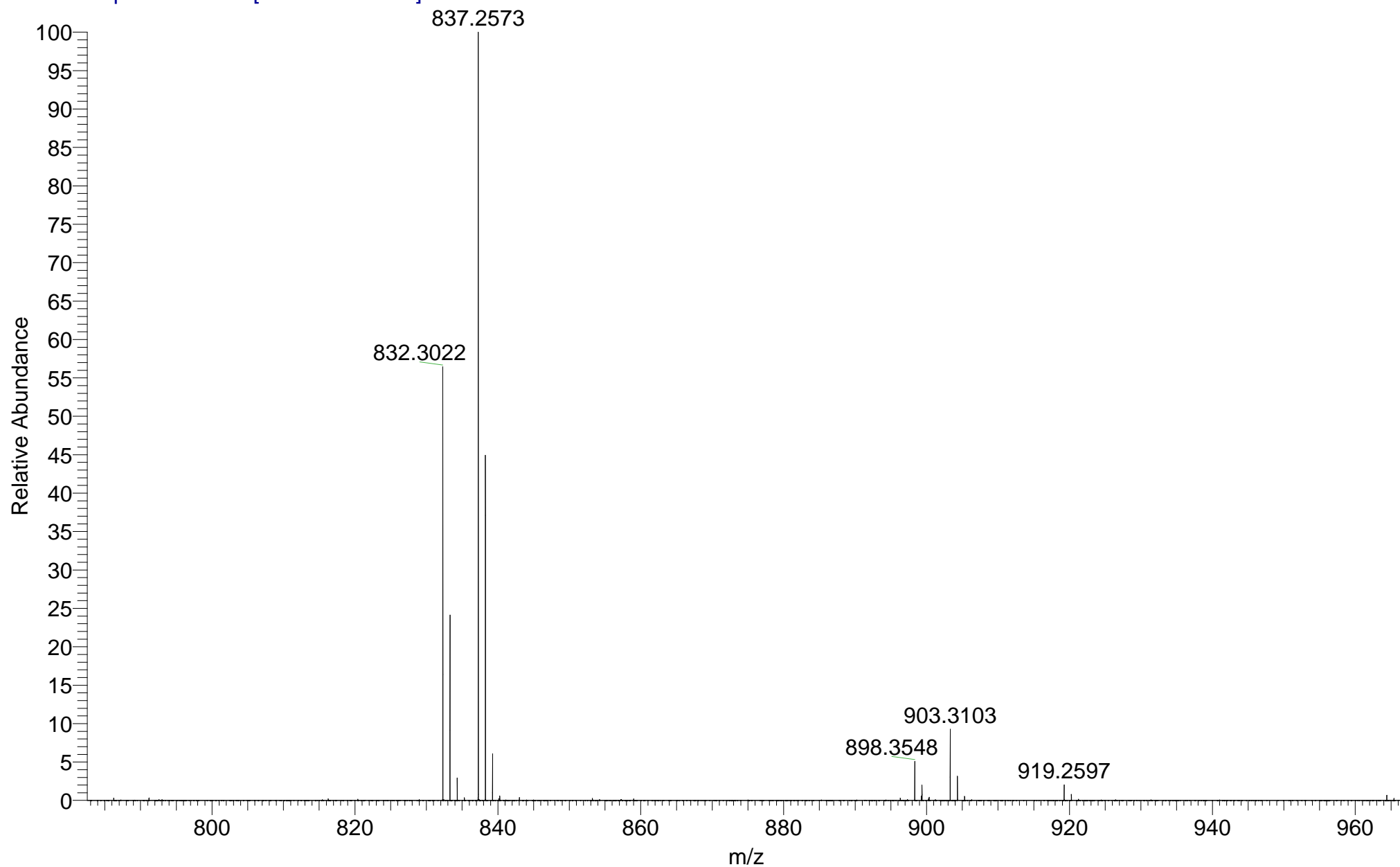


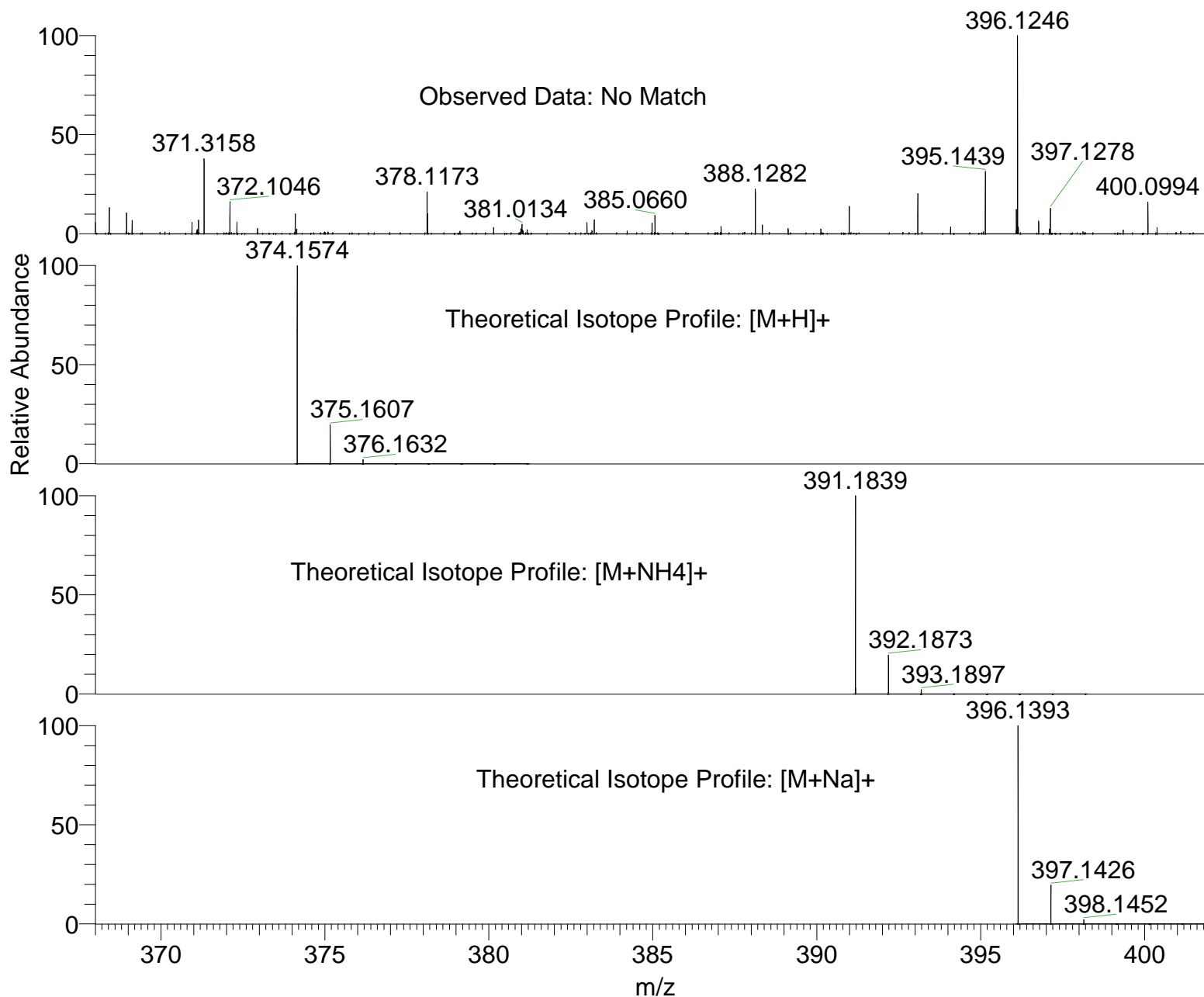
O:\IMPBUL\_TVXP7\_50396  
(DCM)/MeOH + NH4OAc  
AB5-539

EPSRC UK National MS Facility  
LTQ Orbitrap XL

C18H22F3NO4  
26/11/2018 08:16:33

IMPBUL\_TVXP7\_50396 #37-52 RT: 0.65-1.05 AV: 16 SM: 7G NL: 1.70E6  
T: FTMS + p NSI Full ms [120.00-1935.00]





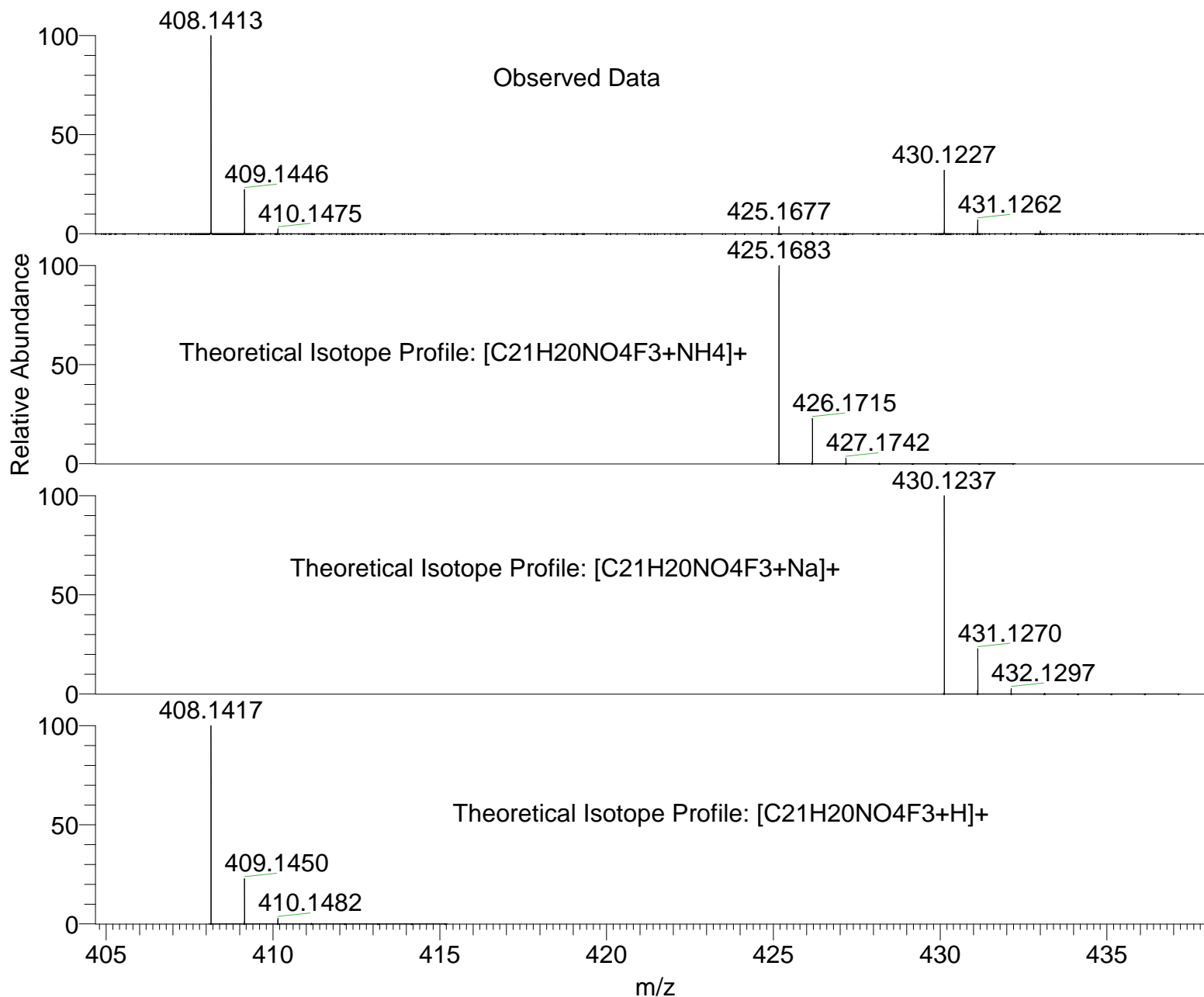
NL:  
2.49E4  
IMPBUL\_TVXP7\_50396#37-52  
RT: 0.65-1.05 AV: 16 T:  
FTMS + p NSI Full ms  
[120.00-1935.00]

NL:  
1.90E4  
C<sub>18</sub>H<sub>22</sub>F<sub>3</sub>NO<sub>4</sub>H:  
C<sub>18</sub>H<sub>23</sub>F<sub>3</sub>N<sub>1</sub>O<sub>4</sub>  
p (gss, s /p:40) Chrg 1  
R: 100000 Res .Pwr . @FWHM

NL:  
1.89E4  
C<sub>18</sub>H<sub>22</sub>F<sub>3</sub>NO<sub>4</sub>NH<sub>4</sub>:  
C<sub>18</sub>H<sub>26</sub>F<sub>3</sub>N<sub>2</sub>O<sub>4</sub>  
p (gss, s /p:40) Chrg 1  
R: 100000 Res .Pwr . @FWHM

NL:  
1.90E4  
C<sub>18</sub>H<sub>22</sub>F<sub>3</sub>NO<sub>4</sub>Na:  
C<sub>18</sub>H<sub>22</sub>F<sub>3</sub>N<sub>1</sub>O<sub>4</sub>Na<sub>1</sub>  
p (gss, s /p:40) Chrg 1  
R: 100000 Res .Pwr . @FWHM

SM: 7G



NL:  
1.65E7  
IMPBUL\_TVXP7\_50396#37-52  
RT: 0.65-1.05 AV: 16 T:  
FTMS + p NSI Full ms  
[120.00-1935.00]

NL:  
1.84E4  
C<sub>21</sub>H<sub>20</sub>NO<sub>4</sub>F<sub>3</sub>NH<sub>4</sub>:  
C<sub>21</sub>H<sub>24</sub>N<sub>2</sub>O<sub>4</sub>F<sub>3</sub>  
p (gss, s /p:40) Chrg 1  
R: 100000 Res .Pwr . @FWHM

NL:  
1.84E4  
C<sub>21</sub>H<sub>20</sub>NO<sub>4</sub>F<sub>3</sub>Na:  
C<sub>21</sub>H<sub>20</sub>N<sub>1</sub>O<sub>4</sub>F<sub>3</sub>Na<sub>1</sub>  
p (gss, s /p:40) Chrg 1  
R: 100000 Res .Pwr . @FWHM

NL:  
1.84E4  
C<sub>21</sub>H<sub>20</sub>NO<sub>4</sub>F<sub>3</sub>H:  
C<sub>21</sub>H<sub>21</sub>N<sub>1</sub>O<sub>4</sub>F<sub>3</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....1  
 19 F                   0....7  
 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
408.1413	408.1413	0.0	5.5	C <sub>15</sub> H <sub>23</sub> O <sub>9</sub> N <sub>3</sub> F <sub>1</sub>
	408.1413	-0.0	3.5	C <sub>11</sub> H <sub>19</sub> O <sub>4</sub> N <sub>7</sub> F <sub>5</sub>
	408.1413	0.1	11.0	C <sub>14</sub> H <sub>17</sub> O <sub>4</sub> N <sub>10</sub> F <sub>1</sub>
	408.1413	-0.1	-2.0	C <sub>12</sub> H <sub>25</sub> O <sub>9</sub> F <sub>5</sub>
	408.1411	0.4	-5.5	C <sub>7</sub> H <sub>24</sub> O <sub>9</sub> N <sub>3</sub> F <sub>6</sub>
	408.1415	-0.4	14.5	C <sub>19</sub> H <sub>18</sub> O <sub>4</sub> N <sub>7</sub>
	408.1411	0.4	0.0	C <sub>6</sub> H <sub>18</sub> O <sub>4</sub> N <sub>10</sub> F <sub>6</sub>
	408.1415	-0.5	9.0	C <sub>20</sub> H <sub>24</sub> O <sub>9</sub>
	408.1411	0.5	2.0	C <sub>10</sub> H <sub>22</sub> O <sub>9</sub> N <sub>6</sub> F <sub>2</sub>
	408.1415	-0.5	7.0	C <sub>16</sub> H <sub>20</sub> O <sub>4</sub> N <sub>4</sub> F <sub>4</sub>
	408.1411	0.5	7.5	C <sub>9</sub> H <sub>16</sub> O <sub>4</sub> N <sub>13</sub> F <sub>2</sub>
	408.1409	0.9	-9.0	C <sub>2</sub> H <sub>23</sub> O <sub>9</sub> N <sub>6</sub> F <sub>7</sub>
	408.1409	0.9	-3.5	C <sub>1</sub> H <sub>17</sub> O <sub>4</sub> N <sub>13</sub> F <sub>7</sub>
	408.1409	1.0	-7.0	C <sub>6</sub> H <sub>27</sub> O <sub>14</sub> N <sub>2</sub> F <sub>3</sub>
	408.1409	1.0	-1.5	C <sub>5</sub> H <sub>21</sub> O <sub>9</sub> N <sub>9</sub> F <sub>3</sub>
	408.1417	-1.0	10.5	C <sub>21</sub> H <sub>21</sub> O <sub>4</sub> N <sub>1</sub> F <sub>3</sub>
	408.1418	-1.2	-1.5	H <sub>19</sub> O <sub>10</sub> N <sub>15</sub> F <sub>1</sub>
	408.1418	-1.2	-7.0	C <sub>1</sub> H <sub>25</sub> O <sub>15</sub> N <sub>8</sub> F <sub>1</sub>
	408.1407	1.5	-5.0	H <sub>20</sub> O <sub>9</sub> N <sub>12</sub> F <sub>4</sub>
	408.1407	1.6	-8.5	C <sub>5</sub> H <sub>30</sub> O <sub>19</sub> N <sub>1</sub>
	408.1406	1.6	-3.0	C <sub>4</sub> H <sub>24</sub> O <sub>14</sub> N <sub>8</sub>
	408.1406	1.6	2.5	C <sub>3</sub> H <sub>18</sub> O <sub>9</sub> N <sub>15</sub>
	408.1420	-1.7	2.0	C <sub>5</sub> H <sub>20</sub> O <sub>10</sub> N <sub>12</sub>
	408.1420	-1.7	-3.5	C <sub>6</sub> H <sub>26</sub> O <sub>15</sub> N <sub>5</sub>
	408.1406	1.8	14.5	C <sub>24</sub> H <sub>20</sub> O <sub>3</sub> N <sub>1</sub> F <sub>2</sub>
	408.1420	-1.8	-5.5	C <sub>2</sub> H <sub>22</sub> O <sub>10</sub> N <sub>9</sub> F <sub>4</sub>
	408.1404	2.2	3.5	C <sub>16</sub> H <sub>21</sub> O <sub>3</sub> N <sub>1</sub> F <sub>7</sub>
	408.1422	-2.3	3.5	C <sub>6</sub> H <sub>17</sub> O <sub>5</sub> N <sub>13</sub> F <sub>3</sub>
	408.1404	2.3	11.0	C <sub>19</sub> H <sub>19</sub> O <sub>3</sub> N <sub>4</sub> F <sub>3</sub>
	408.1422	-2.3	-2.0	C <sub>7</sub> H <sub>23</sub> O <sub>10</sub> N <sub>6</sub> F <sub>3</sub>
	408.1423	-2.4	-4.0	C <sub>3</sub> H <sub>19</sub> O <sub>5</sub> N <sub>10</sub> F <sub>7</sub>

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
	408.1423	-2.4	-9.5	C <sub>4</sub> H <sub>25</sub> O <sub>10</sub> N <sub>3</sub> F <sub>7</sub>
	408.1402	2.7	2.0	C <sub>15</sub> H <sub>24</sub> O <sub>8</sub> F <sub>4</sub>
	408.1424	-2.7	7.0	C <sub>11</sub> H <sub>18</sub> O <sub>5</sub> N <sub>10</sub> F <sub>2</sub>
	408.1402	2.8	7.5	C <sub>14</sub> H <sub>18</sub> O <sub>3</sub> N <sub>7</sub> F <sub>4</sub>
	408.1424	-2.8	1.5	C <sub>12</sub> H <sub>24</sub> O <sub>10</sub> N <sub>3</sub> F <sub>2</sub>
	408.1425	-2.8	5.0	C <sub>7</sub> H <sub>14</sub> N <sub>14</sub> F <sub>6</sub>
	408.1401	2.8	9.5	C <sub>18</sub> H <sub>22</sub> O <sub>8</sub> N <sub>3</sub>
	408.1425	-2.8	-0.5	C <sub>8</sub> H <sub>20</sub> O <sub>5</sub> N <sub>7</sub> F <sub>6</sub>
	408.1401	2.9	15.0	C <sub>17</sub> H <sub>16</sub> O <sub>3</sub> N <sub>10</sub>
	408.1425	-2.9	-6.0	C <sub>9</sub> H <sub>26</sub> O <sub>10</sub> F <sub>6</sub>
	408.1426	-3.2	16.0	C <sub>15</sub> H <sub>13</sub> N <sub>14</sub> F <sub>1</sub>
	408.1400	3.2	-1.5	C <sub>10</sub> H <sub>23</sub> O <sub>8</sub> N <sub>3</sub> F <sub>5</sub>
	408.1426	-3.2	10.5	C <sub>16</sub> H <sub>19</sub> O <sub>5</sub> N <sub>7</sub> F <sub>1</sub>
	408.1400	3.2	4.0	C <sub>9</sub> H <sub>17</sub> O <sub>3</sub> N <sub>10</sub> F <sub>5</sub>
	408.1426	-3.3	5.0	C <sub>17</sub> H <sub>25</sub> O <sub>10</sub> F <sub>1</sub>
	408.1427	-3.3	8.5	C <sub>12</sub> H <sub>15</sub> N <sub>11</sub> F <sub>5</sub>
	408.1399	3.3	6.0	C <sub>13</sub> H <sub>21</sub> O <sub>8</sub> N <sub>6</sub> F <sub>1</sub>
	408.1427	-3.3	3.0	C <sub>13</sub> H <sub>21</sub> O <sub>5</sub> N <sub>4</sub> F <sub>5</sub>
	408.1399	3.3	11.5	C <sub>12</sub> H <sub>15</sub> O <sub>3</sub> N <sub>13</sub> F <sub>1</sub>
	408.1428	-3.7	19.5	C <sub>20</sub> H <sub>14</sub> N <sub>11</sub>
	408.1398	3.7	-5.0	C <sub>5</sub> H <sub>22</sub> O <sub>8</sub> N <sub>6</sub> F <sub>6</sub>
	408.1428	-3.7	14.0	C <sub>21</sub> H <sub>20</sub> O <sub>5</sub> N <sub>4</sub>
	408.1398	3.7	0.5	C <sub>4</sub> H <sub>16</sub> O <sub>3</sub> N <sub>13</sub> F <sub>6</sub>
	408.1397	3.8	-3.0	C <sub>9</sub> H <sub>26</sub> O <sub>13</sub> N <sub>2</sub> F <sub>2</sub>
	408.1429	-3.8	12.0	C <sub>17</sub> H <sub>16</sub> N <sub>8</sub> F <sub>4</sub>
	408.1397	3.8	2.5	C <sub>8</sub> H <sub>20</sub> O <sub>8</sub> N <sub>9</sub> F <sub>2</sub>
	408.1429	-3.8	6.5	C <sub>18</sub> H <sub>22</sub> O <sub>5</sub> N <sub>1</sub> F <sub>4</sub>
	408.1396	4.2	-8.5	H <sub>21</sub> O <sub>8</sub> N <sub>9</sub> F <sub>7</sub>
	408.1395	4.3	-6.5	C <sub>4</sub> H <sub>25</sub> O <sub>13</sub> N <sub>5</sub> F <sub>3</sub>
	408.1431	-4.3	15.5	C <sub>22</sub> H <sub>17</sub> N <sub>5</sub> F <sub>3</sub>
	408.1395	4.3	-1.0	C <sub>3</sub> H <sub>19</sub> O <sub>8</sub> N <sub>12</sub> F <sub>3</sub>
	408.1431	-4.4	8.0	C <sub>19</sub> H <sub>19</sub> N <sub>2</sub> F <sub>7</sub>
	408.1431	-4.5	-2.0	C <sub>2</sub> H <sub>21</sub> O <sub>11</sub> N <sub>12</sub> F <sub>1</sub>
	408.1431	-4.5	-7.5	C <sub>3</sub> H <sub>27</sub> O <sub>16</sub> N <sub>5</sub> F <sub>1</sub>
	408.1394	4.6	18.5	C <sub>27</sub> H <sub>19</sub> O <sub>2</sub> N <sub>1</sub> F <sub>1</sub>
	408.1433	-4.8	19.0	C <sub>27</sub> H <sub>18</sub> N <sub>2</sub> F <sub>2</sub>
	408.1393	4.9	-8.0	C <sub>3</sub> H <sub>28</sub> O <sub>18</sub> N <sub>4</sub>
	408.1393	4.9	-2.5	C <sub>2</sub> H <sub>22</sub> O <sub>13</sub> N <sub>11</sub>
	408.1393	5.0	7.5	C <sub>19</sub> H <sub>20</sub> O <sub>2</sub> N <sub>1</sub> F <sub>6</sub>
	408.1433	-5.0	1.5	C <sub>7</sub> H <sub>22</sub> O <sub>11</sub> N <sub>9</sub>
	408.1433	-5.0	-4.0	C <sub>8</sub> H <sub>28</sub> O <sub>16</sub> N <sub>2</sub>
430.1227	430.1227	-0.1	6.0	C <sub>8</sub> H <sub>16</sub> O <sub>7</sub> N <sub>12</sub> F <sub>2</sub>
	430.1228	-0.1	0.5	C <sub>9</sub> H <sub>22</sub> O <sub>12</sub> N <sub>5</sub> F <sub>2</sub>



Mass	Theoretical	Delta	RDB	Composition
Mass		[ppm]		
430.1226	0.1	25.5	C <sub>32</sub> H <sub>16</sub> O <sub>1</sub> N <sub>1</sub>	
430.1226	0.2	-5.0	H <sub>19</sub> O <sub>9</sub> N <sub>12</sub> F <sub>4</sub> Na <sub>1</sub>	
430.1228	-0.2	-1.5	C <sub>5</sub> H <sub>18</sub> O <sub>7</sub> N <sub>9</sub> F <sub>6</sub>	
430.1228	-0.2	-7.0	C <sub>6</sub> H <sub>24</sub> O <sub>12</sub> N <sub>2</sub> F <sub>6</sub>	
430.1226	0.2	-8.5	C <sub>5</sub> H <sub>29</sub> O <sub>19</sub> N <sub>1</sub> Na <sub>1</sub>	
430.1226	0.2	-3.0	C <sub>4</sub> H <sub>23</sub> O <sub>14</sub> N <sub>8</sub> Na <sub>1</sub>	
430.1226	0.3	-5.0	H <sub>17</sub> O <sub>7</sub> N <sub>12</sub> F <sub>7</sub>	
430.1226	0.3	2.5	C <sub>3</sub> H <sub>17</sub> O <sub>9</sub> N <sub>15</sub> Na <sub>1</sub>	
430.1228	-0.3	-1.5	C <sub>5</sub> H <sub>20</sub> O <sub>9</sub> N <sub>9</sub> F <sub>3</sub> Na <sub>1</sub>	
430.1228	-0.3	-7.0	C <sub>6</sub> H <sub>26</sub> O <sub>14</sub> N <sub>2</sub> F <sub>3</sub> Na <sub>1</sub>	
430.1226	0.3	-8.5	C <sub>5</sub> H <sub>27</sub> O <sub>17</sub> N <sub>1</sub> F <sub>3</sub>	
430.1226	0.3	-3.0	C <sub>4</sub> H <sub>21</sub> O <sub>12</sub> N <sub>8</sub> F <sub>3</sub>	
430.1225	0.4	2.5	C <sub>3</sub> H <sub>15</sub> O <sub>7</sub> N <sub>15</sub> F <sub>3</sub>	
430.1229	-0.4	-3.5	C <sub>1</sub> H <sub>16</sub> O <sub>4</sub> N <sub>13</sub> F <sub>7</sub> Na <sub>1</sub>	
430.1229	-0.4	-9.0	C <sub>2</sub> H <sub>22</sub> O <sub>9</sub> N <sub>6</sub> F <sub>7</sub> Na <sub>1</sub>	
430.1225	0.4	14.5	C <sub>24</sub> H <sub>19</sub> O <sub>3</sub> N <sub>1</sub> F <sub>2</sub> Na <sub>1</sub>	
430.1225	0.5	14.5	C <sub>24</sub> H <sub>17</sub> O <sub>1</sub> N <sub>1</sub> F <sub>5</sub>	
430.1229	-0.6	9.5	C <sub>13</sub> H <sub>17</sub> O <sub>7</sub> N <sub>9</sub> F <sub>1</sub>	
430.1230	-0.6	4.0	C <sub>14</sub> H <sub>23</sub> O <sub>12</sub> N <sub>2</sub> F <sub>1</sub>	
430.1224	0.6	22.0	C <sub>27</sub> H <sub>15</sub> O <sub>1</sub> N <sub>4</sub> F <sub>1</sub>	
430.1230	-0.7	7.5	C <sub>9</sub> H <sub>13</sub> O <sub>2</sub> N <sub>13</sub> F <sub>5</sub>	
430.1230	-0.7	2.0	C <sub>10</sub> H <sub>19</sub> O <sub>7</sub> N <sub>6</sub> F <sub>5</sub>	
430.1230	-0.8	7.5	C <sub>9</sub> H <sub>15</sub> O <sub>4</sub> N <sub>13</sub> F <sub>2</sub> Na <sub>1</sub>	
430.1230	-0.8	2.0	C <sub>10</sub> H <sub>21</sub> O <sub>9</sub> N <sub>6</sub> F <sub>2</sub> Na <sub>1</sub>	
430.1224	0.8	3.5	C <sub>16</sub> H <sub>20</sub> O <sub>3</sub> N <sub>1</sub> F <sub>7</sub> Na <sub>1</sub>	
430.1231	-0.8	0.0	C <sub>6</sub> H <sub>17</sub> O <sub>4</sub> N <sub>10</sub> F <sub>6</sub> Na <sub>1</sub>	
430.1231	-0.9	-5.5	C <sub>7</sub> H <sub>23</sub> O <sub>9</sub> N <sub>3</sub> F <sub>6</sub> Na <sub>1</sub>	
430.1223	0.9	11.0	C <sub>19</sub> H <sub>18</sub> O <sub>3</sub> N <sub>4</sub> F <sub>3</sub> Na <sub>1</sub>	
430.1223	0.9	-4.5	C <sub>3</sub> H <sub>24</sub> O <sub>17</sub> N <sub>7</sub>	
430.1223	0.9	1.0	C <sub>2</sub> H <sub>18</sub> O <sub>12</sub> N <sub>14</sub>	
430.1223	1.0	11.0	C <sub>19</sub> H <sub>16</sub> O <sub>1</sub> N <sub>4</sub> F <sub>6</sub>	
430.1231	-1.0	18.5	C <sub>17</sub> H <sub>12</sub> O <sub>2</sub> N <sub>13</sub>	
430.1231	-1.0	13.0	C <sub>18</sub> H <sub>18</sub> O <sub>7</sub> N <sub>6</sub>	
430.1222	1.1	13.0	C <sub>23</sub> H <sub>20</sub> O <sub>6</sub> F <sub>2</sub>	
430.1222	1.1	18.5	C <sub>22</sub> H <sub>14</sub> O <sub>1</sub> N <sub>7</sub> F <sub>2</sub>	
430.1232	-1.1	11.0	C <sub>14</sub> H <sub>14</sub> O <sub>2</sub> N <sub>10</sub> F <sub>4</sub>	
430.1232	-1.1	5.5	C <sub>15</sub> H <sub>20</sub> O <sub>7</sub> N <sub>3</sub> F <sub>4</sub>	
430.1232	-1.2	11.0	C <sub>14</sub> H <sub>16</sub> O <sub>4</sub> N <sub>10</sub> F <sub>1</sub> Na <sub>1</sub>	
430.1232	-1.2	5.5	C <sub>15</sub> H <sub>22</sub> O <sub>9</sub> N <sub>3</sub> F <sub>1</sub> Na <sub>1</sub>	
430.1233	-1.3	3.5	C <sub>11</sub> H <sub>18</sub> O <sub>4</sub> N <sub>7</sub> F <sub>5</sub> Na <sub>1</sub>	
430.1233	-1.3	-2.0	C <sub>12</sub> H <sub>24</sub> O <sub>9</sub> F <sub>5</sub> Na <sub>1</sub>	
430.1221	1.3	2.0	C <sub>15</sub> H <sub>23</sub> O <sub>8</sub> F <sub>4</sub> Na <sub>1</sub>	
430.1221	1.3	7.5	C <sub>14</sub> H <sub>17</sub> O <sub>3</sub> N <sub>7</sub> F <sub>4</sub> Na <sub>1</sub>	

Mass	Theoretical	Delta	RDB	Composition
Mass		[ppm]		
430.1221	1.4	2.0	C <sub>15</sub> H <sub>21</sub> O <sub>6</sub> F <sub>7</sub>	
430.1221	1.4	9.5	C <sub>18</sub> H <sub>21</sub> O <sub>8</sub> N <sub>3</sub> Na <sub>1</sub>	
430.1221	1.4	7.5	C <sub>14</sub> H <sub>15</sub> O <sub>1</sub> N <sub>7</sub> F <sub>7</sub>	
430.1221	1.4	15.0	C <sub>17</sub> H <sub>15</sub> O <sub>3</sub> N <sub>10</sub> Na <sub>1</sub>	
430.1220	1.5	9.5	C <sub>18</sub> H <sub>19</sub> O <sub>6</sub> N <sub>3</sub> F <sub>3</sub>	
430.1220	1.5	15.0	C <sub>17</sub> H <sub>13</sub> O <sub>1</sub> N <sub>10</sub> F <sub>3</sub>	
430.1234	-1.6	14.5	C <sub>19</sub> H <sub>15</sub> O <sub>2</sub> N <sub>7</sub> F <sub>3</sub>	
430.1234	-1.6	9.0	C <sub>20</sub> H <sub>21</sub> O <sub>7</sub> F <sub>3</sub>	
430.1234	-1.7	14.5	C <sub>19</sub> H <sub>17</sub> O <sub>4</sub> N <sub>7</sub> Na <sub>1</sub>	
430.1234	-1.7	7.0	C <sub>16</sub> H <sub>17</sub> O <sub>2</sub> N <sub>4</sub> F <sub>7</sub>	
430.1234	-1.7	9.0	C <sub>20</sub> H <sub>23</sub> O <sub>9</sub> Na <sub>1</sub>	
430.1235	-1.8	-8.5	H <sub>25</sub> O <sub>18</sub> N <sub>7</sub> F <sub>1</sub>	
430.1235	-1.8	7.0	C <sub>16</sub> H <sub>19</sub> O <sub>4</sub> N <sub>4</sub> F <sub>4</sub> Na <sub>1</sub>	
430.1219	1.8	-1.5	C <sub>10</sub> H <sub>22</sub> O <sub>8</sub> N <sub>3</sub> F <sub>5</sub> Na <sub>1</sub>	
430.1219	1.8	4.0	C <sub>9</sub> H <sub>16</sub> O <sub>3</sub> N <sub>10</sub> F <sub>5</sub> Na <sub>1</sub>	
430.1219	1.9	6.0	C <sub>13</sub> H <sub>20</sub> O <sub>8</sub> N <sub>6</sub> F <sub>1</sub> Na <sub>1</sub>	
430.1219	1.9	11.5	C <sub>12</sub> H <sub>14</sub> O <sub>3</sub> N <sub>13</sub> F <sub>1</sub> Na <sub>1</sub>	
430.1218	2.0	6.0	C <sub>13</sub> H <sub>18</sub> O <sub>6</sub> N <sub>6</sub> F <sub>4</sub>	
430.1218	2.0	11.5	C <sub>12</sub> H <sub>12</sub> O <sub>1</sub> N <sub>13</sub> F <sub>4</sub>	
430.1236	-2.1	18.0	C <sub>24</sub> H <sub>16</sub> O <sub>2</sub> N <sub>4</sub> F <sub>2</sub>	
430.1218	2.1	8.0	C <sub>17</sub> H <sub>22</sub> O <sub>11</sub> N <sub>2</sub>	
430.1218	2.1	13.5	C <sub>16</sub> H <sub>16</sub> O <sub>6</sub> N <sub>9</sub>	
430.1236	-2.1	10.5	C <sub>21</sub> H <sub>18</sub> O <sub>2</sub> N <sub>1</sub> F <sub>6</sub>	
430.1237	-2.2	0.5	C <sub>4</sub> H <sub>20</sub> O <sub>13</sub> N <sub>11</sub>	
430.1237	-2.2	-5.0	C <sub>5</sub> H <sub>26</sub> O <sub>18</sub> N <sub>4</sub>	
430.1237	-2.2	10.5	C <sub>21</sub> H <sub>20</sub> O <sub>4</sub> N <sub>1</sub> F <sub>3</sub> Na <sub>1</sub>	
430.1217	2.3	-5.0	C <sub>5</sub> H <sub>21</sub> O <sub>8</sub> N <sub>6</sub> F <sub>6</sub> Na <sub>1</sub>	
430.1217	2.3	0.5	C <sub>4</sub> H <sub>15</sub> O <sub>3</sub> N <sub>13</sub> F <sub>6</sub> Na <sub>1</sub>	
430.1237	-2.3	-1.5	H <sub>16</sub> O <sub>8</sub> N <sub>15</sub> F <sub>4</sub>	
430.1237	-2.3	-7.0	C <sub>1</sub> H <sub>22</sub> O <sub>13</sub> N <sub>8</sub> F <sub>4</sub>	
430.1217	2.3	-3.0	C <sub>9</sub> H <sub>25</sub> O <sub>13</sub> N <sub>2</sub> F <sub>2</sub> Na <sub>1</sub>	
430.1217	2.4	2.5	C <sub>8</sub> H <sub>19</sub> O <sub>8</sub> N <sub>9</sub> F <sub>2</sub> Na <sub>1</sub>	
430.1237	-2.4	-1.5	H <sub>18</sub> O <sub>10</sub> N <sub>15</sub> F <sub>1</sub> Na <sub>1</sub>	
430.1237	-2.4	-7.0	C <sub>1</sub> H <sub>24</sub> O <sub>15</sub> N <sub>8</sub> F <sub>1</sub> Na <sub>1</sub>	
430.1217	2.4	-3.0	C <sub>9</sub> H <sub>23</sub> O <sub>11</sub> N <sub>2</sub> F <sub>5</sub>	
430.1216	2.4	2.5	C <sub>8</sub> H <sub>17</sub> O <sub>6</sub> N <sub>9</sub> F <sub>5</sub>	
430.1238	-2.5	21.5	C <sub>29</sub> H <sub>17</sub> O <sub>2</sub> N <sub>1</sub> F <sub>1</sub>	
430.1216	2.5	4.5	C <sub>12</sub> H <sub>21</sub> O <sub>11</sub> N <sub>5</sub> F <sub>1</sub>	
430.1216	2.5	10.0	C <sub>11</sub> H <sub>15</sub> O <sub>6</sub> N <sub>12</sub> F <sub>1</sub>	
430.1215	2.7	-8.5	H <sub>20</sub> O <sub>8</sub> N <sub>9</sub> F <sub>7</sub> Na <sub>1</sub>	
430.1239	-2.8	2.0	C <sub>5</sub> H <sub>17</sub> O <sub>8</sub> N <sub>12</sub> F <sub>3</sub>	
430.1239	-2.8	-3.5	C <sub>6</sub> H <sub>23</sub> O <sub>13</sub> N <sub>5</sub> F <sub>3</sub>	
430.1215	2.8	-6.5	C <sub>4</sub> H <sub>24</sub> O <sub>13</sub> N <sub>5</sub> F <sub>3</sub> Na <sub>1</sub>	

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
430.1215	430.1215	2.8	-1.0	C <sub>3</sub> H <sub>18</sub> O <sub>8</sub> N <sub>12</sub> F <sub>3</sub> Na <sub>1</sub>
430.1239	430.1239	-2.9	2.0	C <sub>5</sub> H <sub>19</sub> O <sub>10</sub> N <sub>12</sub> Na <sub>1</sub>
430.1239	430.1239	-2.9	-5.5	C <sub>2</sub> H <sub>19</sub> O <sub>8</sub> N <sub>9</sub> F <sub>7</sub>
430.1239	430.1239	-2.9	-3.5	C <sub>6</sub> H <sub>25</sub> O <sub>15</sub> N <sub>5</sub> Na <sub>1</sub>
430.1215	430.1215	2.9	-6.5	C <sub>4</sub> H <sub>22</sub> O <sub>11</sub> N <sub>5</sub> F <sub>6</sub>
430.1214	430.1214	2.9	-1.0	C <sub>3</sub> H <sub>16</sub> O <sub>6</sub> N <sub>12</sub> F <sub>6</sub>
430.1240	430.1240	-3.0	-5.5	C <sub>2</sub> H <sub>21</sub> O <sub>10</sub> N <sub>9</sub> F <sub>4</sub> Na <sub>1</sub>
430.1214	430.1214	3.0	-4.5	C <sub>8</sub> H <sub>26</sub> O <sub>16</sub> N <sub>1</sub> F <sub>2</sub>
430.1214	430.1214	3.0	1.0	C <sub>7</sub> H <sub>20</sub> O <sub>11</sub> N <sub>8</sub> F <sub>2</sub>
430.1214	430.1214	3.0	6.5	C <sub>6</sub> H <sub>14</sub> O <sub>6</sub> N <sub>15</sub> F <sub>2</sub>
430.1214	430.1214	3.1	18.5	C <sub>27</sub> H <sub>18</sub> O <sub>2</sub> N <sub>1</sub> F <sub>1</sub> Na <sub>1</sub>
430.1213	430.1213	3.2	18.5	C <sub>27</sub> H <sub>16</sub> N <sub>1</sub> F <sub>4</sub>
430.1241	430.1241	-3.2	5.5	C <sub>10</sub> H <sub>18</sub> O <sub>8</sub> N <sub>9</sub> F <sub>2</sub>
430.1241	430.1241	-3.2	0.0	C <sub>11</sub> H <sub>24</sub> O <sub>13</sub> N <sub>2</sub> F <sub>2</sub>
430.1213	430.1213	3.3	26.0	C <sub>30</sub> H <sub>14</sub> N <sub>4</sub>
430.1241	430.1241	-3.3	3.5	C <sub>6</sub> H <sub>14</sub> O <sub>3</sub> N <sub>13</sub> F <sub>6</sub>
430.1241	430.1241	-3.3	-2.0	C <sub>7</sub> H <sub>20</sub> O <sub>8</sub> N <sub>6</sub> F <sub>6</sub>
430.1213	430.1213	3.4	-8.0	C <sub>3</sub> H <sub>27</sub> O <sub>18</sub> N <sub>4</sub> Na <sub>1</sub>
430.1213	430.1213	3.4	-2.5	C <sub>2</sub> H <sub>21</sub> O <sub>13</sub> N <sub>11</sub> Na <sub>1</sub>
430.1242	430.1242	-3.4	3.5	C <sub>6</sub> H <sub>16</sub> O <sub>5</sub> N <sub>13</sub> F <sub>3</sub> Na <sub>1</sub>
430.1242	430.1242	-3.4	-2.0	C <sub>7</sub> H <sub>22</sub> O <sub>10</sub> N <sub>6</sub> F <sub>3</sub> Na <sub>1</sub>
430.1212	430.1212	3.4	7.5	C <sub>19</sub> H <sub>19</sub> O <sub>2</sub> N <sub>1</sub> F <sub>6</sub> Na <sub>1</sub>
430.1212	430.1212	3.4	-8.0	C <sub>3</sub> H <sub>25</sub> O <sub>16</sub> N <sub>4</sub> F <sub>3</sub>
430.1212	430.1212	3.5	-2.5	C <sub>2</sub> H <sub>19</sub> O <sub>11</sub> N <sub>11</sub> F <sub>3</sub>
430.1242	430.1242	-3.5	-4.0	C <sub>3</sub> H <sub>18</sub> O <sub>5</sub> N <sub>10</sub> F <sub>7</sub> Na <sub>1</sub>
430.1242	430.1242	-3.5	-9.5	C <sub>4</sub> H <sub>24</sub> O <sub>10</sub> N <sub>3</sub> F <sub>7</sub> Na <sub>1</sub>
430.1212	430.1212	3.5	15.0	C <sub>22</sub> H <sub>17</sub> O <sub>2</sub> N <sub>4</sub> F <sub>2</sub> Na <sub>1</sub>
430.1211	430.1211	3.6	15.0	C <sub>22</sub> H <sub>15</sub> N <sub>4</sub> F <sub>5</sub>
430.1243	430.1243	-3.7	14.5	C <sub>14</sub> H <sub>13</sub> O <sub>3</sub> N <sub>13</sub> F <sub>1</sub>
430.1243	430.1243	-3.7	9.0	C <sub>15</sub> H <sub>19</sub> O <sub>8</sub> N <sub>6</sub> F <sub>1</sub>
430.1211	430.1211	3.7	17.0	C <sub>26</sub> H <sub>19</sub> O <sub>5</sub> F <sub>1</sub>
430.1211	430.1211	3.7	22.5	C <sub>25</sub> H <sub>13</sub> N <sub>7</sub> F <sub>1</sub>
430.1243	430.1243	-3.8	7.0	C <sub>11</sub> H <sub>15</sub> O <sub>3</sub> N <sub>10</sub> F <sub>5</sub>
430.1243	430.1243	-3.8	1.5	C <sub>12</sub> H <sub>21</sub> O <sub>8</sub> N <sub>3</sub> F <sub>5</sub>
430.1244	430.1244	-3.9	7.0	C <sub>11</sub> H <sub>17</sub> O <sub>5</sub> N <sub>10</sub> F <sub>2</sub> Na <sub>1</sub>
430.1244	430.1244	-3.9	1.5	C <sub>12</sub> H <sub>23</sub> O <sub>10</sub> N <sub>3</sub> F <sub>2</sub> Na <sub>1</sub>
430.1210	430.1210	3.9	4.0	C <sub>14</sub> H <sub>18</sub> O <sub>2</sub> N <sub>4</sub> F <sub>7</sub> Na <sub>1</sub>
430.1244	430.1244	-4.0	5.0	C <sub>7</sub> H <sub>13</sub> N <sub>14</sub> F <sub>6</sub> Na <sub>1</sub>
430.1244	430.1244	-4.0	-0.5	C <sub>8</sub> H <sub>19</sub> O <sub>5</sub> N <sub>7</sub> F <sub>6</sub> Na <sub>1</sub>
430.1244	430.1244	-4.0	-6.0	C <sub>9</sub> H <sub>25</sub> O <sub>10</sub> F <sub>6</sub> Na <sub>1</sub>
430.1210	430.1210	4.0	6.0	C <sub>18</sub> H <sub>22</sub> O <sub>7</sub> F <sub>3</sub> Na <sub>1</sub>
430.1210	430.1210	4.0	11.5	C <sub>17</sub> H <sub>16</sub> O <sub>2</sub> N <sub>7</sub> F <sub>3</sub> Na <sub>1</sub>
430.1210	430.1210	4.0	-4.0	C <sub>1</sub> H <sub>22</sub> O <sub>16</sub> N <sub>10</sub>

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
430.1209	4.1	6.0	C <sub>18</sub> H <sub>20</sub> O <sub>5</sub> F <sub>6</sub>	
430.1209	4.1	11.5	C <sub>17</sub> H <sub>14</sub> N <sub>7</sub> F <sub>6</sub>	
430.1245	-4.2	18.0	C <sub>19</sub> H <sub>14</sub> O <sub>3</sub> N <sub>10</sub>	
430.1245	-4.2	12.5	C <sub>20</sub> H <sub>20</sub> O <sub>8</sub> N <sub>3</sub>	
430.1209	4.2	13.5	C <sub>21</sub> H <sub>18</sub> O <sub>5</sub> N <sub>3</sub> F <sub>2</sub>	
430.1209	4.2	19.0	C <sub>20</sub> H <sub>12</sub> N <sub>10</sub> F <sub>2</sub>	
430.1245	-4.2	10.5	C <sub>16</sub> H <sub>16</sub> O <sub>3</sub> N <sub>7</sub> F <sub>4</sub>	
430.1245	-4.3	5.0	C <sub>17</sub> H <sub>22</sub> O <sub>8</sub> F <sub>4</sub>	
430.1246	-4.3	16.0	C <sub>15</sub> H <sub>12</sub> N <sub>14</sub> F <sub>1</sub> Na <sub>1</sub>	
430.1246	-4.3	10.5	C <sub>16</sub> H <sub>18</sub> O <sub>5</sub> N <sub>7</sub> F <sub>1</sub> Na <sub>1</sub>	
430.1246	-4.4	5.0	C <sub>17</sub> H <sub>24</sub> O <sub>10</sub> F <sub>1</sub> Na <sub>1</sub>	
430.1246	-4.4	8.5	C <sub>12</sub> H <sub>14</sub> N <sub>11</sub> F <sub>5</sub> Na <sub>1</sub>	
430.1246	-4.4	3.0	C <sub>13</sub> H <sub>20</sub> O <sub>5</sub> N <sub>4</sub> F <sub>5</sub> Na <sub>1</sub>	
430.1208	4.5	2.5	C <sub>13</sub> H <sub>21</sub> O <sub>7</sub> N <sub>3</sub> F <sub>4</sub> Na <sub>1</sub>	
430.1208	4.5	8.0	C <sub>12</sub> H <sub>15</sub> O <sub>2</sub> N <sub>10</sub> F <sub>4</sub> Na <sub>1</sub>	
430.1207	4.5	2.5	C <sub>13</sub> H <sub>19</sub> O <sub>5</sub> N <sub>3</sub> F <sub>7</sub>	
430.1207	4.5	10.0	C <sub>16</sub> H <sub>19</sub> O <sub>7</sub> N <sub>6</sub> Na <sub>1</sub>	
430.1207	4.6	8.0	C <sub>12</sub> H <sub>13</sub> N <sub>10</sub> F <sub>7</sub>	
430.1207	4.6	15.5	C <sub>15</sub> H <sub>13</sub> O <sub>2</sub> N <sub>13</sub> Na <sub>1</sub>	
430.1207	4.6	10.0	C <sub>16</sub> H <sub>17</sub> O <sub>5</sub> N <sub>6</sub> F <sub>3</sub>	
430.1207	4.7	15.5	C <sub>15</sub> H <sub>11</sub> N <sub>13</sub> F <sub>3</sub>	
430.1247	-4.7	14.0	C <sub>21</sub> H <sub>17</sub> O <sub>3</sub> N <sub>4</sub> F <sub>3</sub>	
430.1248	-4.8	19.5	C <sub>20</sub> H <sub>13</sub> N <sub>11</sub> Na <sub>1</sub>	
430.1248	-4.8	14.0	C <sub>21</sub> H <sub>19</sub> O <sub>5</sub> N <sub>4</sub> Na <sub>1</sub>	
430.1248	-4.8	6.5	C <sub>18</sub> H <sub>19</sub> O <sub>3</sub> N <sub>1</sub> F <sub>7</sub>	
430.1248	-4.9	-3.5	C <sub>1</sub> H <sub>21</sub> O <sub>14</sub> N <sub>11</sub> F <sub>1</sub>	
430.1248	-4.9	12.0	C <sub>17</sub> H <sub>15</sub> N <sub>8</sub> F <sub>4</sub> Na <sub>1</sub>	
430.1248	-4.9	-9.0	C <sub>2</sub> H <sub>27</sub> O <sub>19</sub> N <sub>4</sub> F <sub>1</sub>	
430.1248	-4.9	6.5	C <sub>18</sub> H <sub>21</sub> O <sub>5</sub> N <sub>1</sub> F <sub>4</sub> Na <sub>1</sub>	
430.1206	4.9	-1.0	C <sub>8</sub> H <sub>20</sub> O <sub>7</sub> N <sub>6</sub> F <sub>5</sub> Na <sub>1</sub>	
430.1206	4.9	4.5	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> N <sub>13</sub> F <sub>5</sub> Na <sub>1</sub>	