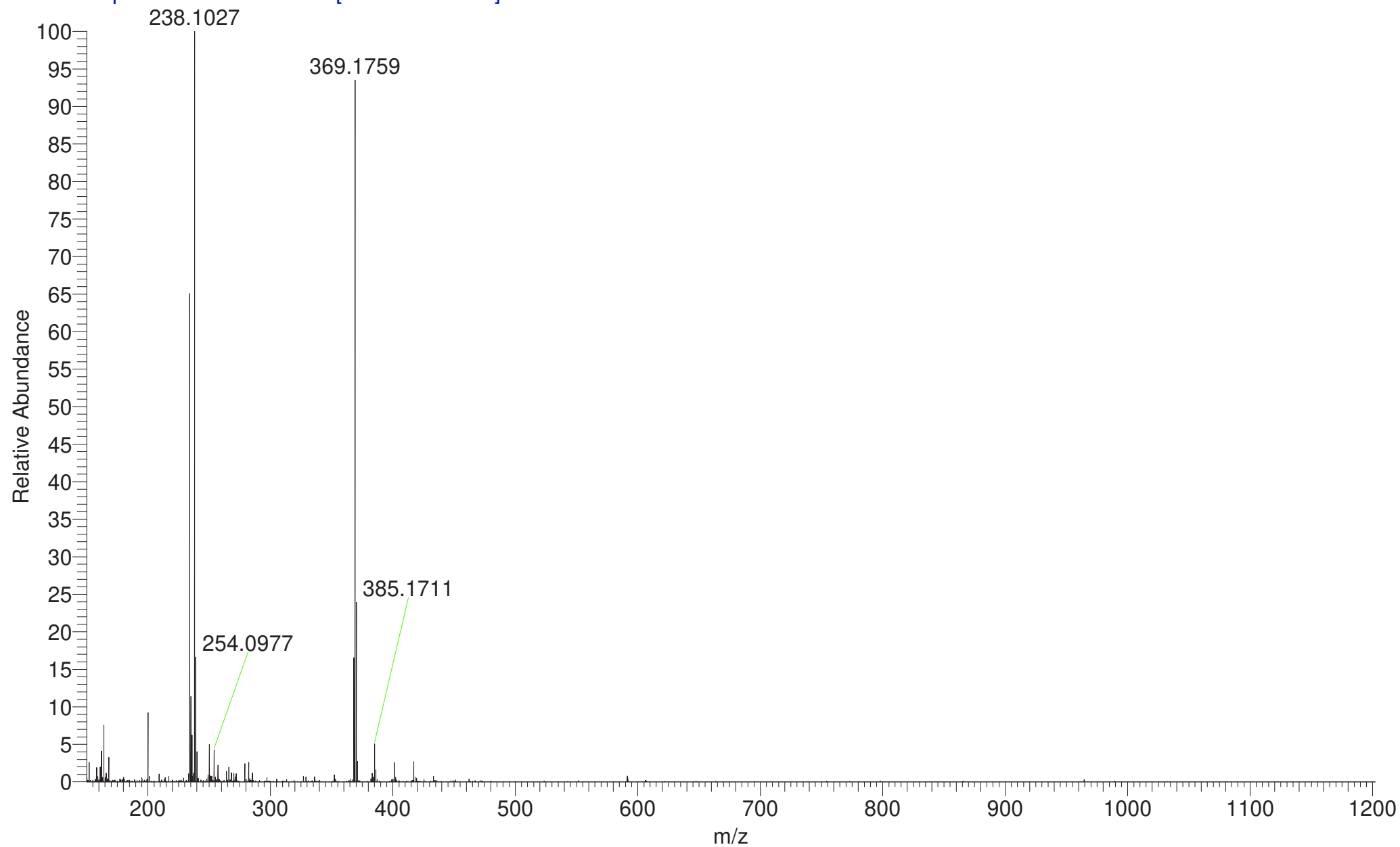
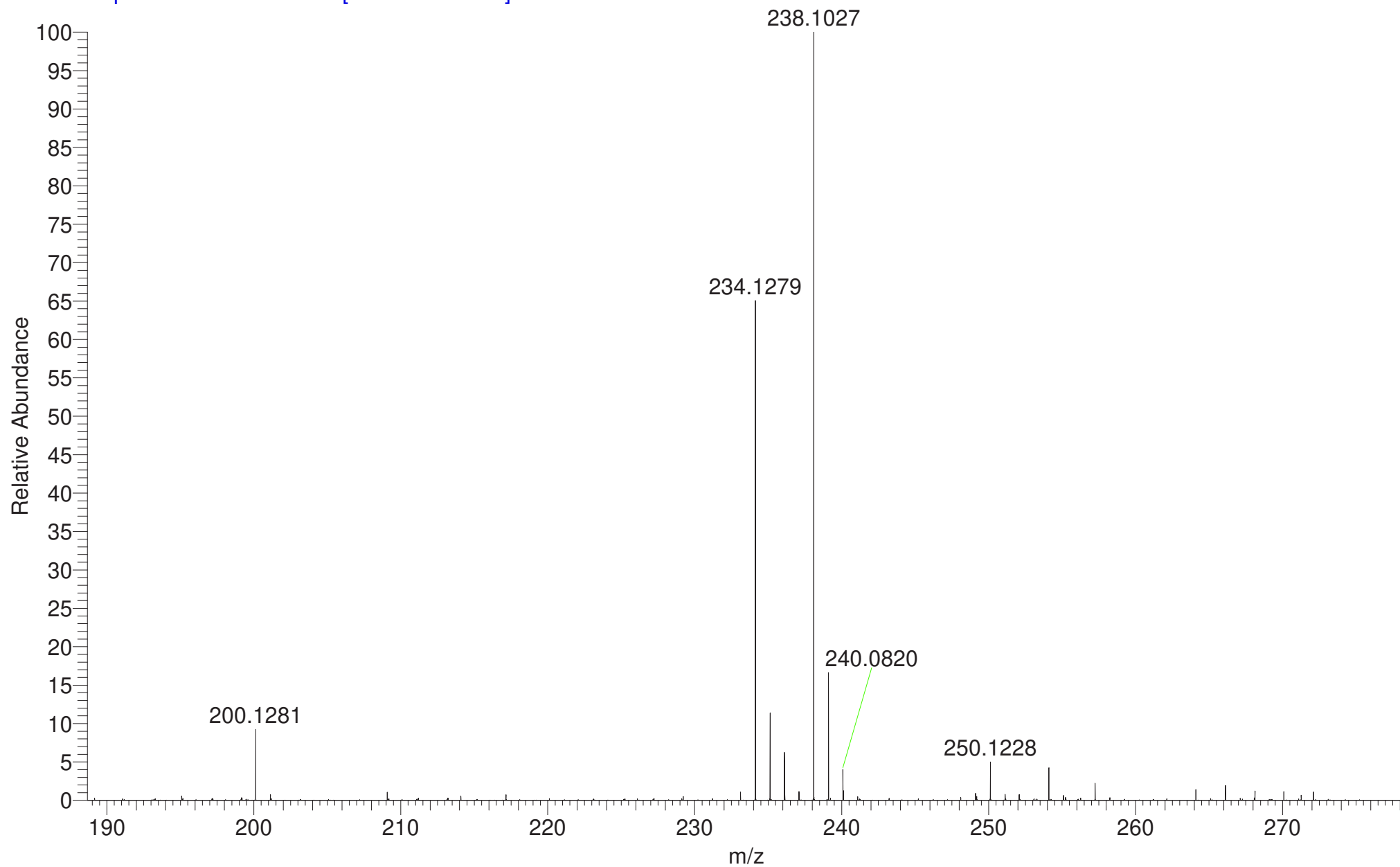


HERLEE\_EE7EF\_PA\_A #17-19 RT: 0.89-1.00 AV: 3 NL: 3.36E7  
T: FTMS + p APCI corona Full ms [150.00-1200.00]



HERLEE\_EE7EF\_PA\_A #17-19 RT: 0.89-1.00 AV: 3 NL: 3.36E7  
T: FTMS + p APCI corona Full ms [150.00-1200.00]

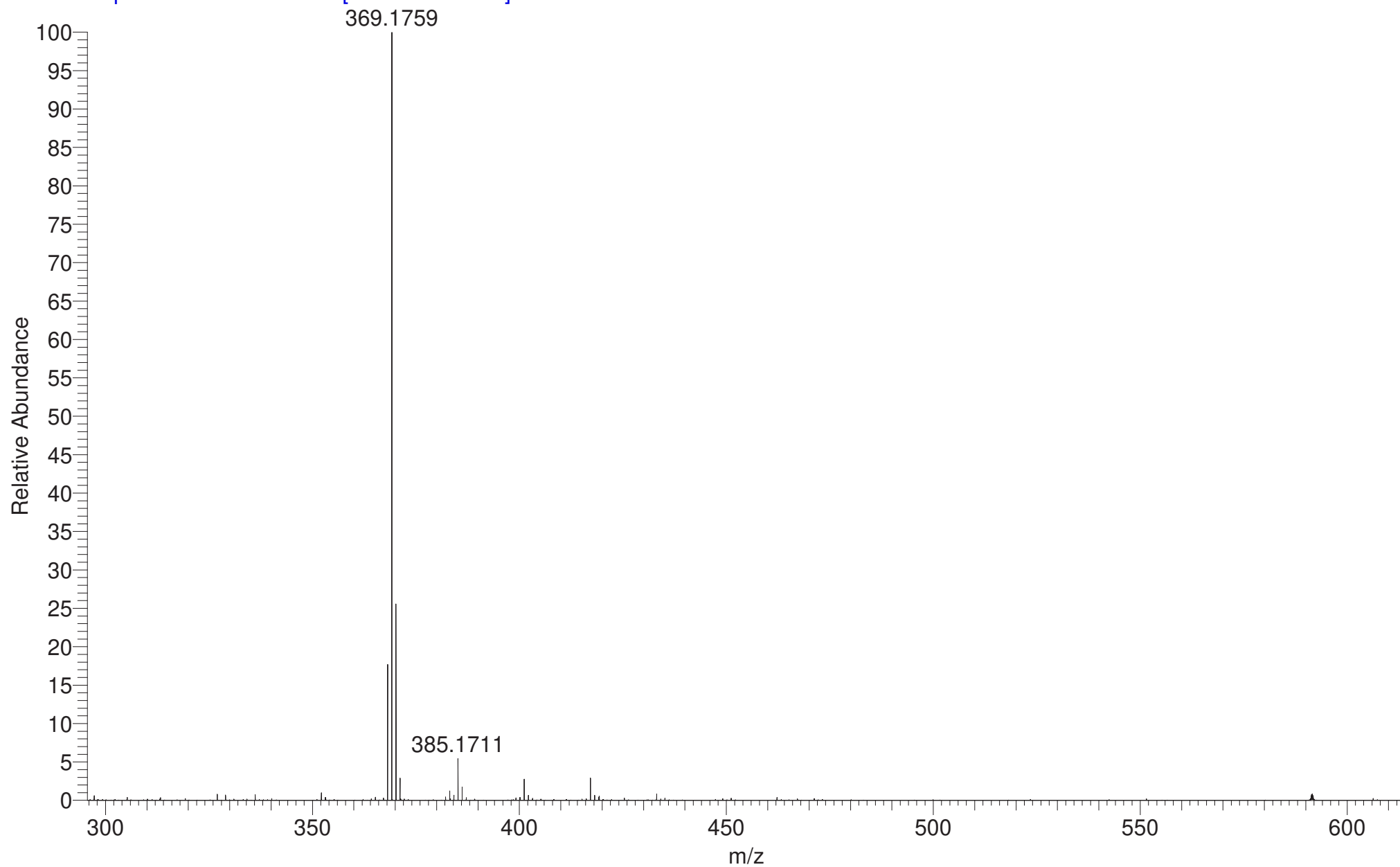


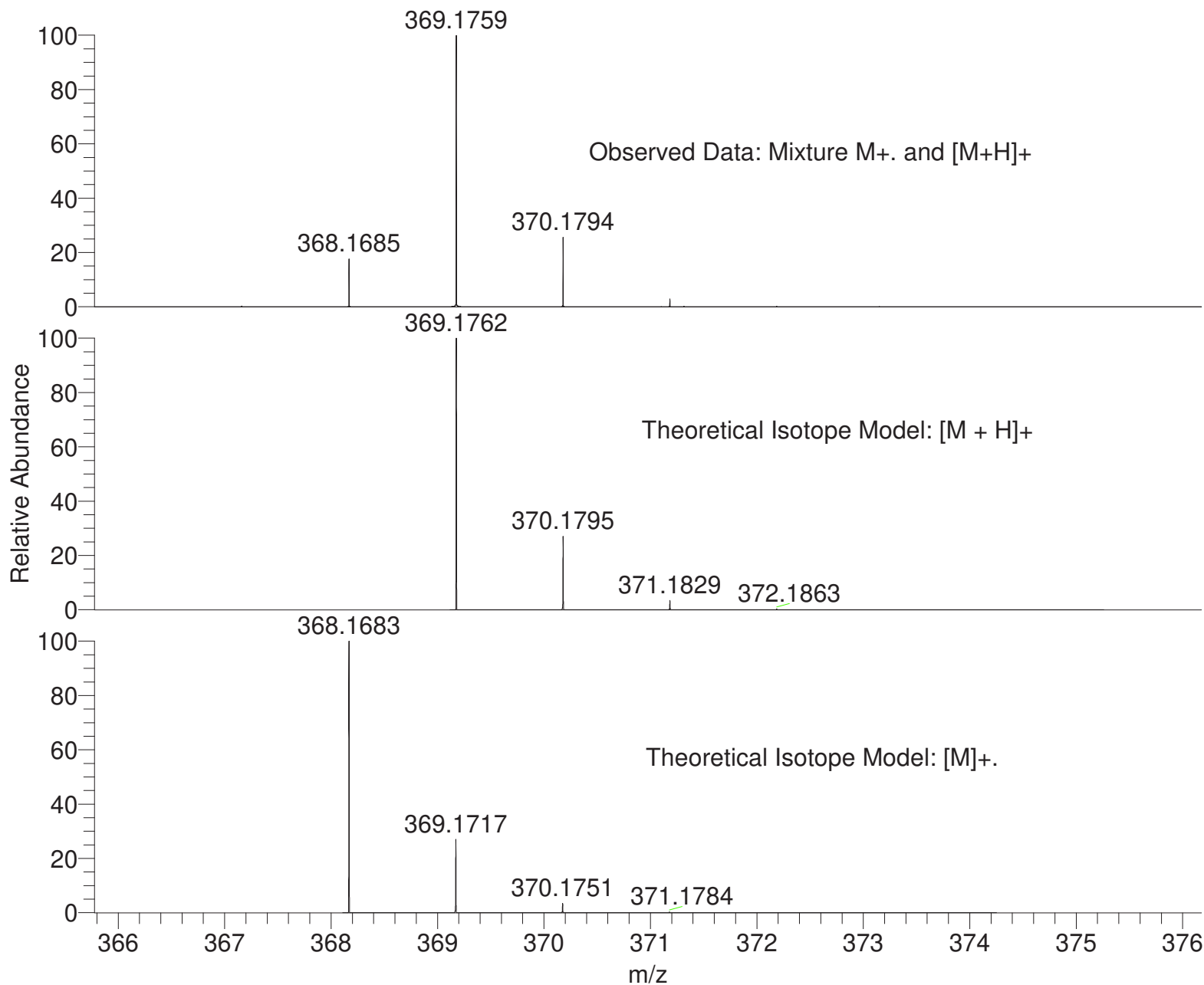
P:\HERLEE\_EE7EF\_PA\_A  
EM515 MW=368? C25H21FN2  
ASAP (SOLID)

National Mass Spectrometry Facility, Swansea  
LTQ Orbitrap XL

21/07/2020 15:15:28

HERLEE\_EE7EF\_PA\_A #17-19 RT: 0.89-1.00 AV: 3 NL: 3.14E7  
T: FTMS + p APCI corona Full ms [150.00-1200.00]





NL:  
3.14E7  
HERLEE\_EE7EF\_PA\_A#17-19  
RT: 0.89-1.00 AV: 3 T: FTMS  
+ p APCI corona Full ms  
[150.00-1200.00]

NL:  
1.78E4  
C<sub>25</sub> H<sub>21</sub> FN<sub>2</sub> H:  
C<sub>25</sub> H<sub>22</sub> F<sub>1</sub> N<sub>2</sub>  
p (gss, s /p:40) Chrg 1  
R: 100000 Res .Pwr . @FWHM

NL:  
1.78E4  
C<sub>25</sub> H<sub>21</sub> FN<sub>2</sub>:  
C<sub>25</sub> H<sub>21</sub> F<sub>1</sub> N<sub>2</sub>  
p (gss, s /p:40) Chrg 1  
R: 100000 Res .Pwr . @FWHM

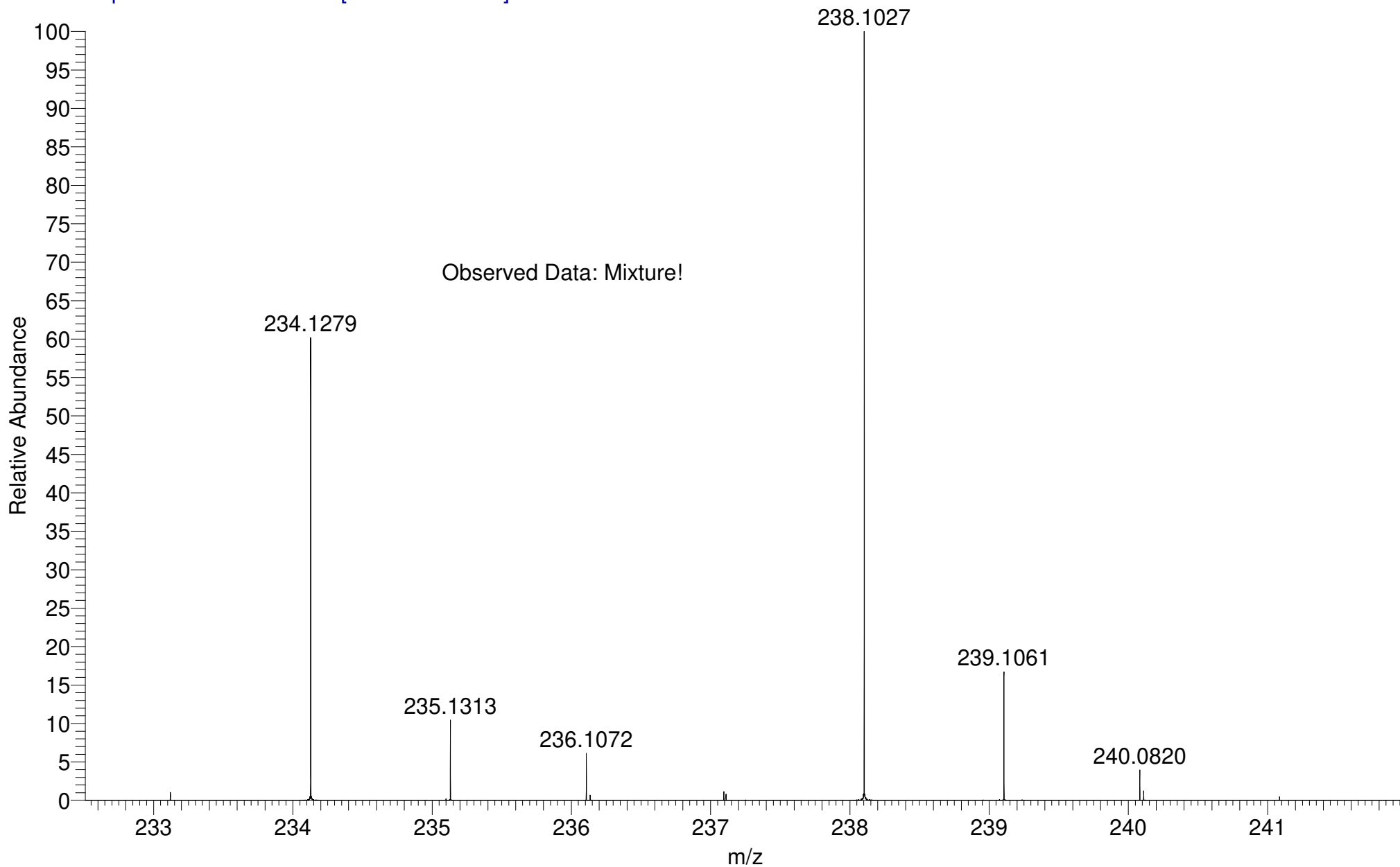
Isotope:                   Min. .. Max.  
 14 N                        0....15  
 16 O                        0....15  
 12 C                        0....80  
 1 H                         0....100  
 23 Na                      0....0  
 19 F                        0....4  
 Tolerance Window:       +- 5.00 ppm  
 Db/Ring Equiv:           -3.. 100  
 Fits:                      150

N-Rule:   Do not use  
 Charge:   1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
368.1685	368.1686	-0.4	0.0	C <sub>6</sub> H <sub>22</sub> O <sub>6</sub> N <sub>10</sub> F <sub>2</sub>
	368.1683	0.5	16.0	C <sub>25</sub> H <sub>21</sub> N <sub>2</sub> F <sub>1</sub>
	368.1688	-0.9	9.0	C <sub>10</sub> H <sub>17</sub> O <sub>1</sub> N <sub>14</sub> F <sub>1</sub>
	368.1688	-0.9	3.5	C <sub>11</sub> H <sub>23</sub> O <sub>6</sub> N <sub>7</sub> F <sub>1</sub>
	368.1688	-0.9	-2.0	C <sub>12</sub> H <sub>29</sub> O <sub>11</sub> F <sub>1</sub>
	368.1681	1.0	12.5	C <sub>20</sub> H <sub>20</sub> N <sub>5</sub> F <sub>2</sub>
	368.1690	-1.4	12.5	C <sub>15</sub> H <sub>18</sub> O <sub>1</sub> N <sub>11</sub>
	368.1690	-1.5	7.0	C <sub>16</sub> H <sub>24</sub> O <sub>6</sub> N <sub>4</sub>
	368.1679	1.5	3.5	C <sub>16</sub> H <sub>25</sub> O <sub>5</sub> N <sub>1</sub> F <sub>3</sub>
	368.1679	1.6	9.0	C <sub>15</sub> H <sub>19</sub> N <sub>8</sub> F <sub>3</sub>
	368.1691	-1.6	5.0	C <sub>12</sub> H <sub>20</sub> O <sub>1</sub> N <sub>8</sub> F <sub>4</sub>
	368.1691	-1.6	-0.5	C <sub>13</sub> H <sub>26</sub> O <sub>6</sub> N <sub>1</sub> F <sub>4</sub>
	368.1677	2.1	0.0	C <sub>11</sub> H <sub>24</sub> O <sub>5</sub> N <sub>4</sub> F <sub>4</sub>
	368.1677	2.1	5.5	C <sub>10</sub> H <sub>18</sub> N <sub>11</sub> F <sub>4</sub>
	368.1693	-2.1	8.5	C <sub>17</sub> H <sub>21</sub> O <sub>1</sub> N <sub>5</sub> F <sub>3</sub>
	368.1677	2.2	2.0	C <sub>15</sub> H <sub>28</sub> O <sub>10</sub>
	368.1677	2.2	7.5	C <sub>14</sub> H <sub>22</sub> O <sub>5</sub> N <sub>7</sub>
	368.1677	2.2	13.0	C <sub>13</sub> H <sub>16</sub> N <sub>14</sub>
	368.1695	-2.6	12.0	C <sub>22</sub> H <sub>22</sub> O <sub>1</sub> N <sub>2</sub> F <sub>2</sub>
	368.1675	2.7	-1.5	C <sub>10</sub> H <sub>27</sub> O <sub>10</sub> N <sub>3</sub> F <sub>1</sub>
	368.1675	2.7	4.0	C <sub>9</sub> H <sub>21</sub> O <sub>5</sub> N <sub>10</sub> F <sub>1</sub>
	368.1673	3.3	0.5	C <sub>4</sub> H <sub>20</sub> O <sub>5</sub> N <sub>13</sub> F <sub>2</sub>
	368.1700	-4.0	5.0	C <sub>7</sub> H <sub>18</sub> O <sub>2</sub> N <sub>14</sub> F <sub>2</sub>
	368.1700	-4.0	-0.5	C <sub>8</sub> H <sub>24</sub> O <sub>7</sub> N <sub>7</sub> F <sub>2</sub>
	368.1702	-4.5	8.5	C <sub>12</sub> H <sub>19</sub> O <sub>2</sub> N <sub>11</sub> F <sub>1</sub>
	368.1702	-4.6	3.0	C <sub>13</sub> H <sub>25</sub> O <sub>7</sub> N <sub>4</sub> F <sub>1</sub>
	368.1668	4.6	7.5	C <sub>19</sub> H <sub>24</sub> O <sub>4</sub> N <sub>1</sub> F <sub>2</sub>
369.1759	369.1760	-0.1	12.0	C <sub>20</sub> H <sub>21</sub> N <sub>5</sub> F <sub>2</sub>
	369.1758	0.4	3.0	C <sub>16</sub> H <sub>26</sub> O <sub>5</sub> N <sub>1</sub> F <sub>3</sub>
	369.1758	0.4	8.5	C <sub>15</sub> H <sub>20</sub> N <sub>8</sub> F <sub>3</sub>
	369.1762	-0.7	15.5	C <sub>25</sub> H <sub>22</sub> N <sub>2</sub> F <sub>1</sub>

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
369.1756	369.1756	0.9	-0.5	C <sub>11</sub> H <sub>25</sub> O <sub>5</sub> N <sub>4</sub> F <sub>4</sub>
369.1756	369.1756	0.9	5.0	C <sub>10</sub> H <sub>19</sub> N <sub>11</sub> F <sub>4</sub>
369.1755	369.1755	1.0	1.5	C <sub>15</sub> H <sub>29</sub> O <sub>10</sub>
369.1755	369.1755	1.0	7.0	C <sub>14</sub> H <sub>23</sub> O <sub>5</sub> N <sub>7</sub>
369.1755	369.1755	1.0	12.5	C <sub>13</sub> H <sub>17</sub> N <sub>14</sub>
369.1765	369.1765	-1.5	-0.5	C <sub>6</sub> H <sub>23</sub> O <sub>6</sub> N <sub>10</sub> F <sub>2</sub>
369.1753	369.1753	1.6	-2.0	C <sub>10</sub> H <sub>28</sub> O <sub>10</sub> N <sub>3</sub> F <sub>1</sub>
369.1753	369.1753	1.6	3.5	C <sub>9</sub> H <sub>22</sub> O <sub>5</sub> N <sub>10</sub> F <sub>1</sub>
369.1767	369.1767	-2.0	8.5	C <sub>10</sub> H <sub>18</sub> O <sub>1</sub> N <sub>14</sub> F <sub>1</sub>
369.1767	369.1767	-2.1	3.0	C <sub>11</sub> H <sub>24</sub> O <sub>6</sub> N <sub>7</sub> F <sub>1</sub>
369.1767	369.1767	-2.1	-2.5	C <sub>12</sub> H <sub>30</sub> O <sub>11</sub> F <sub>1</sub>
369.1751	369.1751	2.1	0.0	C <sub>4</sub> H <sub>21</sub> O <sub>5</sub> N <sub>13</sub> F <sub>2</sub>
369.1769	369.1769	-2.6	12.0	C <sub>15</sub> H <sub>19</sub> O <sub>1</sub> N <sub>11</sub>
369.1769	369.1769	-2.6	6.5	C <sub>16</sub> H <sub>25</sub> O <sub>6</sub> N <sub>4</sub>
369.1769	369.1769	-2.7	4.5	C <sub>12</sub> H <sub>21</sub> O <sub>1</sub> N <sub>8</sub> F <sub>4</sub>
369.1769	369.1769	-2.7	-1.0	C <sub>13</sub> H <sub>27</sub> O <sub>6</sub> N <sub>1</sub> F <sub>4</sub>
369.1771	369.1771	-3.2	8.0	C <sub>17</sub> H <sub>22</sub> O <sub>1</sub> N <sub>5</sub> F <sub>3</sub>
369.1746	369.1746	3.5	7.0	C <sub>19</sub> H <sub>25</sub> O <sub>4</sub> N <sub>1</sub> F <sub>2</sub>
369.1773	369.1773	-3.8	11.5	C <sub>22</sub> H <sub>23</sub> O <sub>1</sub> N <sub>2</sub> F <sub>2</sub>
369.1744	369.1744	4.0	3.5	C <sub>14</sub> H <sub>24</sub> O <sub>4</sub> N <sub>4</sub> F <sub>3</sub>
369.1742	369.1742	4.6	0.0	C <sub>9</sub> H <sub>23</sub> O <sub>4</sub> N <sub>7</sub> F <sub>4</sub>
369.1742	369.1742	4.7	2.0	C <sub>13</sub> H <sub>27</sub> O <sub>9</sub> N <sub>3</sub>
369.1742	369.1742	4.7	7.5	C <sub>12</sub> H <sub>21</sub> O <sub>4</sub> N <sub>10</sub>

HERLEE\_EE7EF\_PA\_A #17-19 RT: 0.89-1.00 AV: 3 SB: 11 0.00-0.56 NL: 3.33E7  
T: FTMS + p APCI corona Full ms [150.00-1200.00]



Isotope:                   Min. .. Max.  
 14 N                       0....15  
 16 O                       0....15  
 12 C                       0....80  
 1 H                        0....100  
 23 Na                      0....0  
 19 F                       0....4  
 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
<b>234.1279</b>	234.1277	0.7	10.5	C <sub>17</sub> H <sub>16</sub> N <sub>1</sub>
	234.1282	-1.4	3.5	C <sub>2</sub> H <sub>12</sub> O <sub>1</sub> N <sub>13</sub>
	234.1282	-1.4	-2.0	C <sub>3</sub> H <sub>18</sub> O <sub>6</sub> N <sub>6</sub>
	234.1275	1.6	7.0	C <sub>12</sub> H <sub>15</sub> N <sub>4</sub> F <sub>1</sub>
	234.1273	2.4	-2.0	C <sub>8</sub> H <sub>20</sub> O <sub>5</sub> F <sub>2</sub>
	234.1285	-2.4	-0.5	C <sub>4</sub> H <sub>15</sub> O <sub>1</sub> N <sub>7</sub> F <sub>3</sub>
	234.1273	2.4	3.5	C <sub>7</sub> H <sub>14</sub> N <sub>7</sub> F <sub>2</sub>
	234.1287	-3.3	3.0	C <sub>9</sub> H <sub>16</sub> O <sub>1</sub> N <sub>4</sub> F <sub>2</sub>
	234.1271	3.3	0.0	C <sub>2</sub> H <sub>13</sub> N <sub>10</sub> F <sub>3</sub>
	234.1289	-4.1	6.5	C <sub>14</sub> H <sub>17</sub> O <sub>1</sub> N <sub>1</sub> F <sub>1</sub>
	234.1269	4.3	-1.5	C <sub>1</sub> H <sub>16</sub> O <sub>5</sub> N <sub>9</sub>
<b>238.1027</b>	238.1027	0.2	10.5	C <sub>16</sub> H <sub>13</sub> N <sub>1</sub> F <sub>1</sub>
	238.1025	1.0	7.0	C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> F <sub>2</sub>
	238.1023	1.8	-2.0	C <sub>7</sub> H <sub>17</sub> O <sub>5</sub> F <sub>3</sub>
	238.1023	1.9	3.5	C <sub>6</sub> H <sub>11</sub> N <sub>7</sub> F <sub>3</sub>
	238.1032	-1.9	3.5	C <sub>1</sub> H <sub>9</sub> O <sub>1</sub> N <sub>13</sub> F <sub>1</sub>
	238.1032	-1.9	-2.0	C <sub>2</sub> H <sub>15</sub> O <sub>6</sub> N <sub>6</sub> F <sub>1</sub>
	238.1021	2.7	0.0	C <sub>1</sub> H <sub>10</sub> N <sub>10</sub> F <sub>4</sub>
	238.1034	-2.8	7.0	C <sub>6</sub> H <sub>10</sub> O <sub>1</sub> N <sub>10</sub>
	238.1034	-2.8	1.5	C <sub>7</sub> H <sub>16</sub> O <sub>6</sub> N <sub>3</sub>
	238.1020	2.9	2.0	C <sub>5</sub> H <sub>14</sub> O <sub>5</sub> N <sub>6</sub>
	238.1020	2.9	7.5	C <sub>4</sub> H <sub>8</sub> N <sub>13</sub>
	238.1034	-2.9	-0.5	C <sub>3</sub> H <sub>12</sub> O <sub>1</sub> N <sub>7</sub> F <sub>4</sub>
	238.1018	3.7	-1.5	H <sub>13</sub> O <sub>5</sub> N <sub>9</sub> F <sub>1</sub>
	238.1036	-3.8	3.0	C <sub>8</sub> H <sub>13</sub> O <sub>1</sub> N <sub>4</sub> F <sub>3</sub>
	238.1038	-4.6	6.5	C <sub>13</sub> H <sub>14</sub> O <sub>1</sub> N <sub>1</sub> F <sub>2</sub>