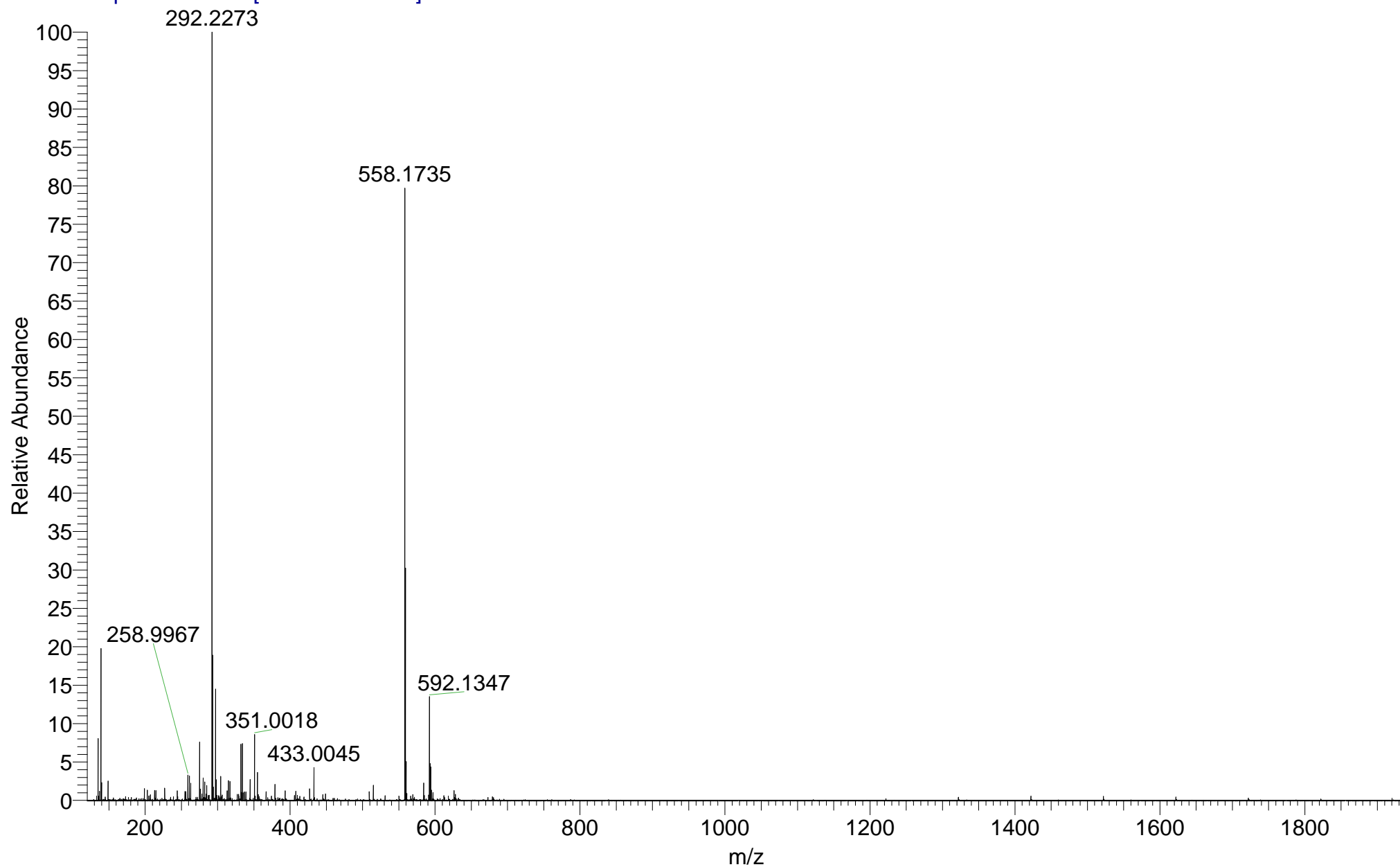


UEAFIL\_F7TFY\_56 #33-47 RT: 0.72-1.02 AV: 12 SM: 7G NL: 1.00E7

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

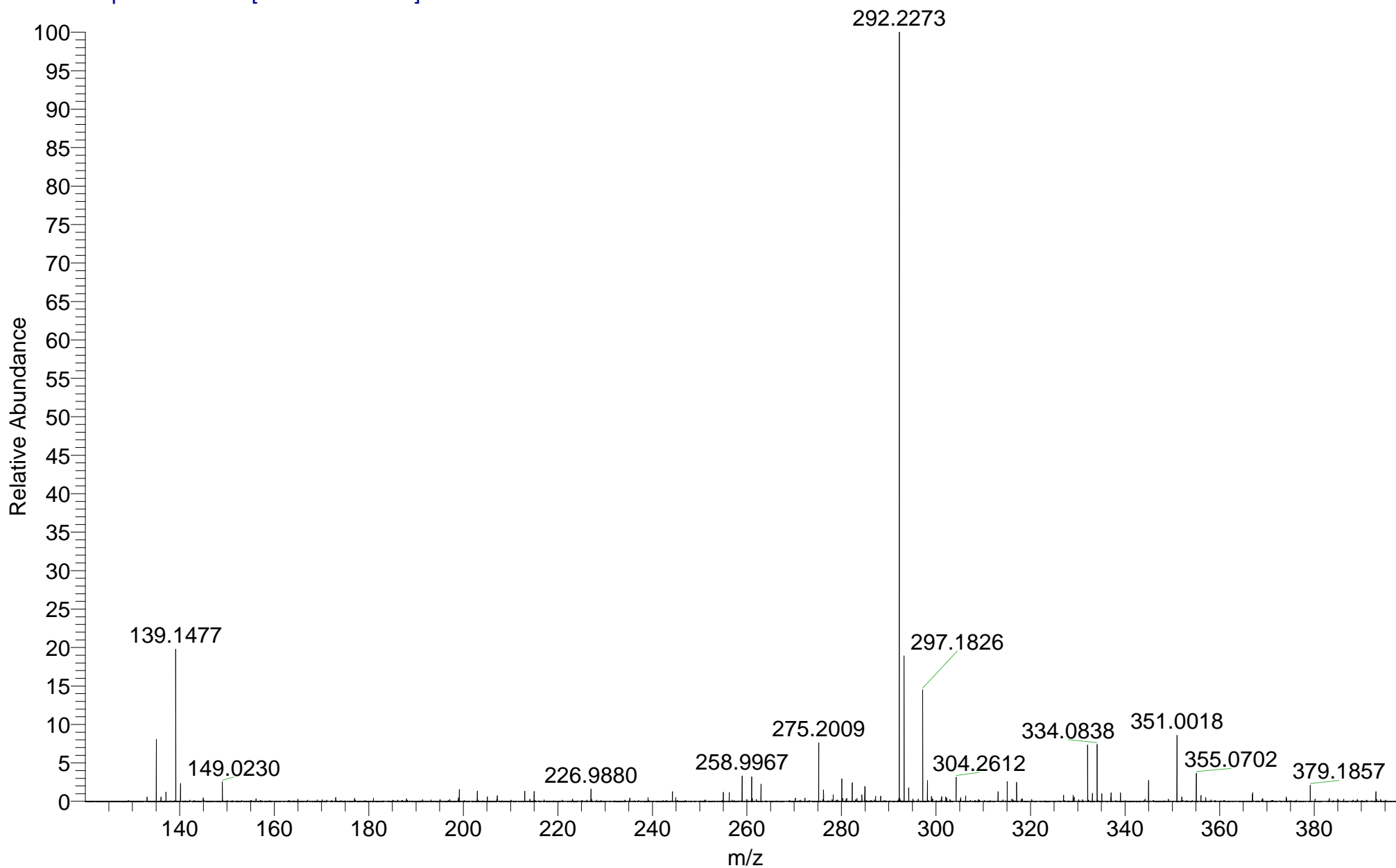


MAR26  
(DCM)/MeOH + NH<sub>4</sub>OAc  
C<sub>36</sub>H<sub>23</sub>N<sub>5</sub>S

EPSRC National Facility Swansea  
LTQ Orbitrap XL

UEAFIL  
16/05/2016 08:57:50

UEAFIL\_F7TFY\_56 #33-47 RT: 0.72-1.02 AV: 12 SM: 7G NL: 1.00E7  
T: FTMS + p NSI Full ms [120.00-1935.00]



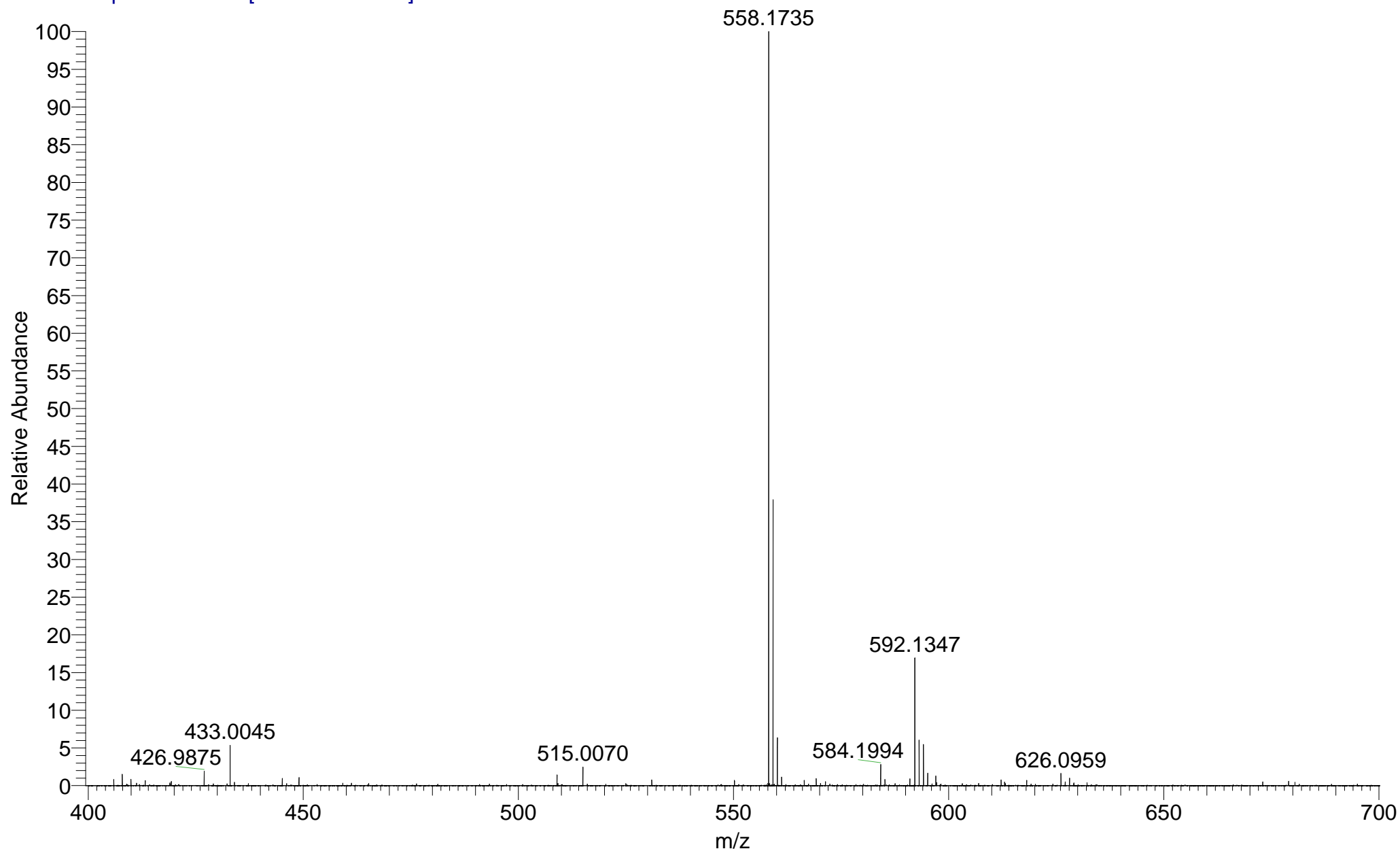
MAR26  
(DCM)/MeOH + NH<sub>4</sub>OAc  
C<sub>36</sub>H<sub>23</sub>N<sub>5</sub>S

EPSRC National Facility Swansea  
LTQ Orbitrap XL

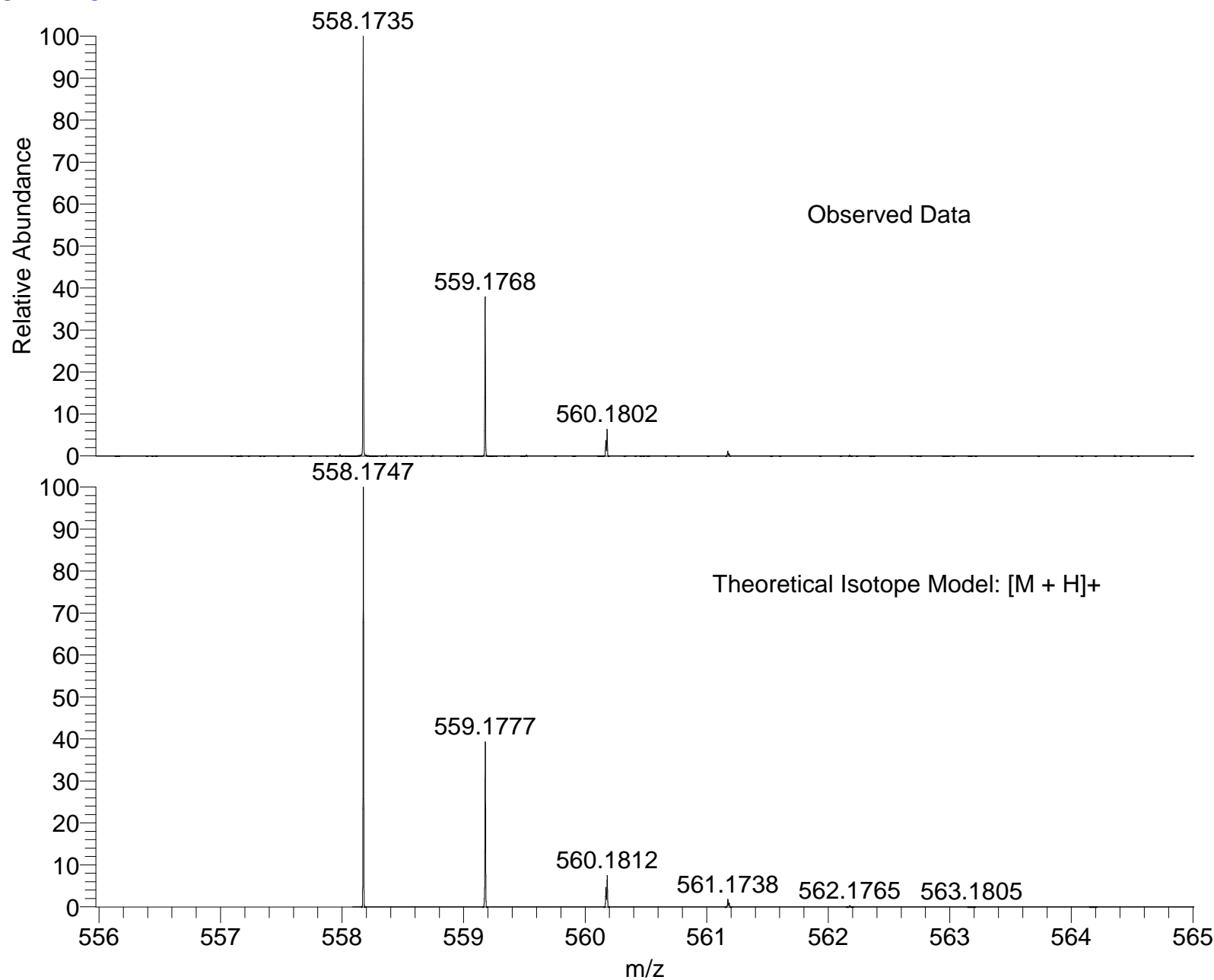
UEAFIL  
16/05/2016 08:57:50

UEAFIL\_F7TFY\_56 #33-47 RT: 0.72-1.02 AV: 12 SM: 7G NL: 7.97E6

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



SM: 7G



NL:  
7.97E6  
UEAFIL\_F7TFY\_56#33-47  
RT: 0.72-1.02 AV: 12 T: FTMS  
+ p NSI Full ms  
[120.00-1935.00]

NL:  
1.48E4  
C<sub>36</sub>H<sub>23</sub>N<sub>5</sub>SH:  
C<sub>36</sub>H<sub>24</sub>N<sub>5</sub>S<sub>1</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  
 32 S                   0....2  
 Tolerance Window:   +- 5.00 ppm  
 Db/Ring Equiv:       -3.. 100  
 Fits:                  700

N-Rule:   Do not use  
 Charge:   1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
558.1735	558.1734	0.3	22.5	C <sub>35</sub> H <sub>28</sub> O <sub>4</sub> N <sub>1</sub> S <sub>1</sub>
	558.1737	-0.3	7.0	C <sub>13</sub> H <sub>26</sub> O <sub>13</sub> N <sub>12</sub>
	558.1732	0.5	1.0	C <sub>13</sub> H <sub>34</sub> O <sub>12</sub> N <sub>8</sub> S <sub>2</sub>
	558.1732	0.5	6.5	C <sub>12</sub> H <sub>28</sub> O <sub>7</sub> N <sub>15</sub> S <sub>2</sub>
	558.1732	0.6	14.0	C <sub>28</sub> H <sub>30</sub> O <sub>12</sub>
	558.1732	0.6	19.5	C <sub>27</sub> H <sub>24</sub> O <sub>7</sub> N <sub>7</sub>
	558.1732	0.6	25.0	C <sub>26</sub> H <sub>18</sub> O <sub>2</sub> N <sub>14</sub>
	558.1739	-0.6	15.5	C <sub>20</sub> H <sub>24</sub> O <sub>5</sub> N <sub>13</sub> S <sub>1</sub>
	558.1739	-0.7	10.0	C <sub>21</sub> H <sub>30</sub> O <sub>10</sub> N <sub>6</sub> S <sub>1</sub>
	558.1730	0.8	-2.0	C <sub>5</sub> H <sub>30</sub> O <sub>15</sub> N <sub>14</sub> S <sub>1</sub>
	558.1740	-1.0	18.5	C <sub>28</sub> H <sub>28</sub> O <sub>2</sub> N <sub>7</sub> S <sub>2</sub>
	558.1740	-1.0	13.0	C <sub>29</sub> H <sub>34</sub> O <sub>7</sub> S <sub>2</sub>
	558.1727	1.4	13.5	C <sub>27</sub> H <sub>32</sub> O <sub>6</sub> N <sub>3</sub> S <sub>2</sub>
	558.1727	1.4	19.0	C <sub>26</sub> H <sub>26</sub> O <sub>1</sub> N <sub>10</sub> S <sub>2</sub>
	558.1727	1.5	32.0	C <sub>41</sub> H <sub>22</sub> O <sub>1</sub> N <sub>2</sub> S <sub>1</sub>
	558.1725	1.7	5.0	C <sub>20</sub> H <sub>34</sub> O <sub>14</sub> N <sub>2</sub> S <sub>1</sub>
	558.1725	1.8	10.5	C <sub>19</sub> H <sub>28</sub> O <sub>9</sub> N <sub>9</sub> S <sub>1</sub>
	558.1745	-1.8	24.5	C <sub>28</sub> H <sub>20</sub> O <sub>3</sub> N <sub>11</sub>
	558.1745	-1.8	19.0	C <sub>29</sub> H <sub>26</sub> O <sub>8</sub> N <sub>4</sub>
	558.1745	-1.9	6.0	C <sub>14</sub> H <sub>30</sub> O <sub>8</sub> N <sub>12</sub> S <sub>2</sub>
	558.1746	-1.9	0.5	C <sub>15</sub> H <sub>36</sub> O <sub>13</sub> N <sub>5</sub> S <sub>2</sub>
	558.1723	2.1	7.5	C <sub>11</sub> H <sub>24</sub> O <sub>12</sub> N <sub>15</sub>
	558.1747	-2.1	27.5	C <sub>36</sub> H <sub>24</sub> N <sub>5</sub> S <sub>1</sub>
	558.1720	2.7	23.0	C <sub>33</sub> H <sub>26</sub> O <sub>3</sub> N <sub>4</sub> S <sub>1</sub>
	558.1750	-2.7	6.5	C <sub>15</sub> H <sub>28</sub> O <sub>14</sub> N <sub>9</sub>
	558.1719	2.9	1.5	C <sub>11</sub> H <sub>32</sub> O <sub>11</sub> N <sub>11</sub> S <sub>2</sub>
	558.1718	3.0	14.5	C <sub>26</sub> H <sub>28</sub> O <sub>11</sub> N <sub>3</sub>
	558.1718	3.0	20.0	C <sub>25</sub> H <sub>22</sub> O <sub>6</sub> N <sub>10</sub>
	558.1752	-3.0	15.0	C <sub>22</sub> H <sub>26</sub> O <sub>6</sub> N <sub>10</sub> S <sub>1</sub>
	558.1752	-3.1	9.5	C <sub>23</sub> H <sub>32</sub> O <sub>11</sub> N <sub>3</sub> S <sub>1</sub>
	558.1754	-3.4	18.0	C <sub>30</sub> H <sub>30</sub> O <sub>3</sub> N <sub>4</sub> S <sub>2</sub>

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
	558.1714	3.8	14.0	C <sub>25</sub> H <sub>30</sub> O <sub>5</sub> N <sub>6</sub> S <sub>2</sub>
	558.1714	3.8	19.5	C <sub>24</sub> H <sub>24</sub> N <sub>13</sub> S <sub>2</sub>
	558.1713	3.9	32.5	C <sub>39</sub> H <sub>20</sub> N <sub>5</sub>
	558.1757	-4.0	2.5	C <sub>8</sub> H <sub>28</sub> O <sub>12</sub> N <sub>15</sub> S <sub>1</sub>
	558.1712	4.2	5.5	C <sub>18</sub> H <sub>32</sub> O <sub>13</sub> N <sub>5</sub> S <sub>1</sub>
	558.1712	4.2	11.0	C <sub>17</sub> H <sub>26</sub> O <sub>8</sub> N <sub>12</sub> S <sub>1</sub>
	558.1759	-4.2	24.0	C <sub>30</sub> H <sub>22</sub> O <sub>4</sub> N <sub>8</sub>
	558.1759	-4.2	18.5	C <sub>31</sub> H <sub>28</sub> O <sub>9</sub> N <sub>1</sub>
	558.1759	-4.3	5.5	C <sub>16</sub> H <sub>32</sub> O <sub>9</sub> N <sub>9</sub> S <sub>2</sub>
	558.1759	-4.3	0.0	C <sub>17</sub> H <sub>38</sub> O <sub>14</sub> N <sub>2</sub> S <sub>2</sub>
	558.1760	-4.5	27.0	C <sub>38</sub> H <sub>26</sub> O <sub>1</sub> N <sub>2</sub> S <sub>1</sub>