

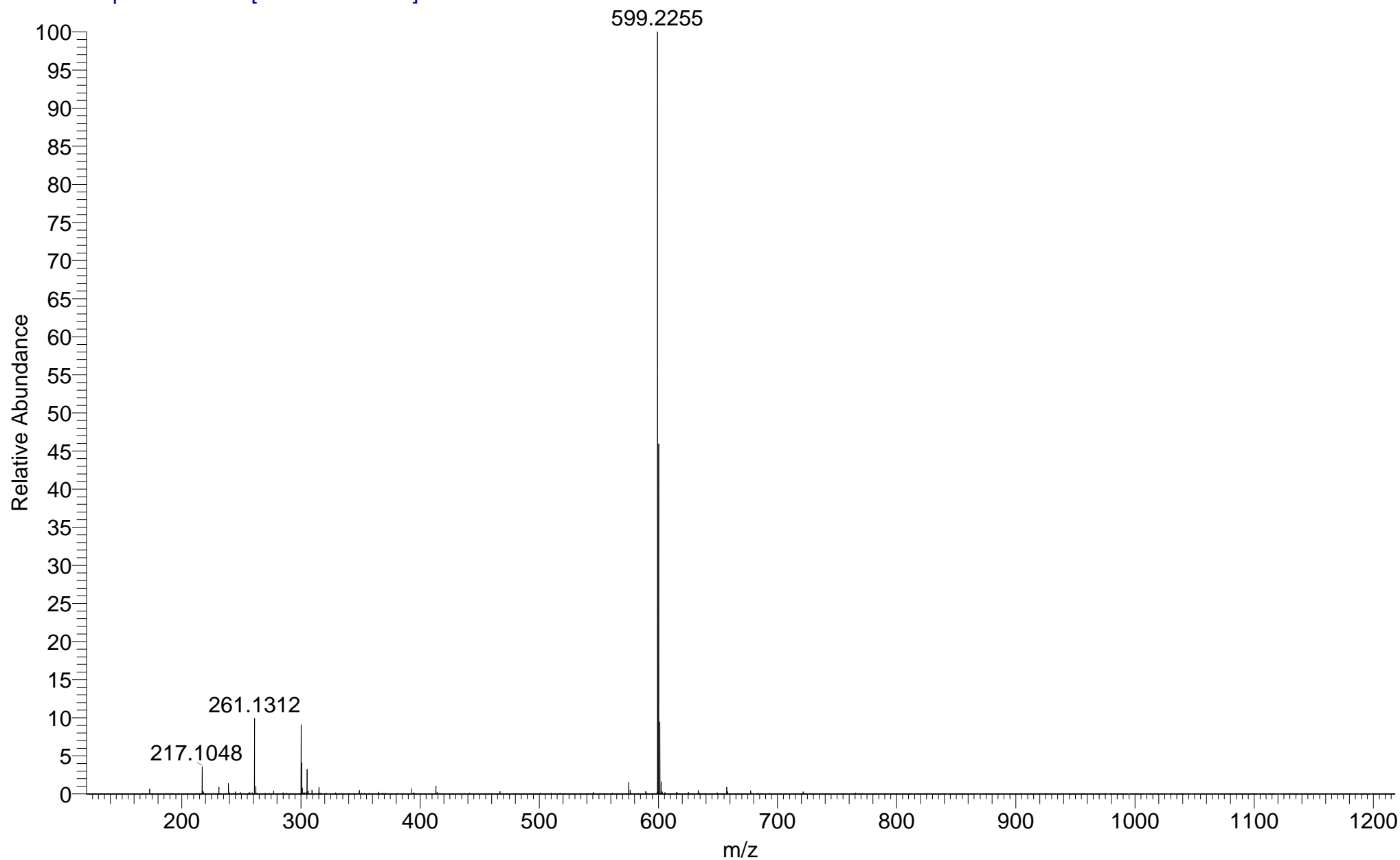
MAR-58  
(MeCN)/(MeOH)  
C40H31F6N4PS

EPSRC National Facility Swansea  
LTQ Orbitrap XL

UEAFIL  
10/25/16 14:26:50

UEAFIL\_4PCUZ\_95 #9-16 RT: 0.20-0.53 AV: 7 SM: 7G NL: 3.42E7

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



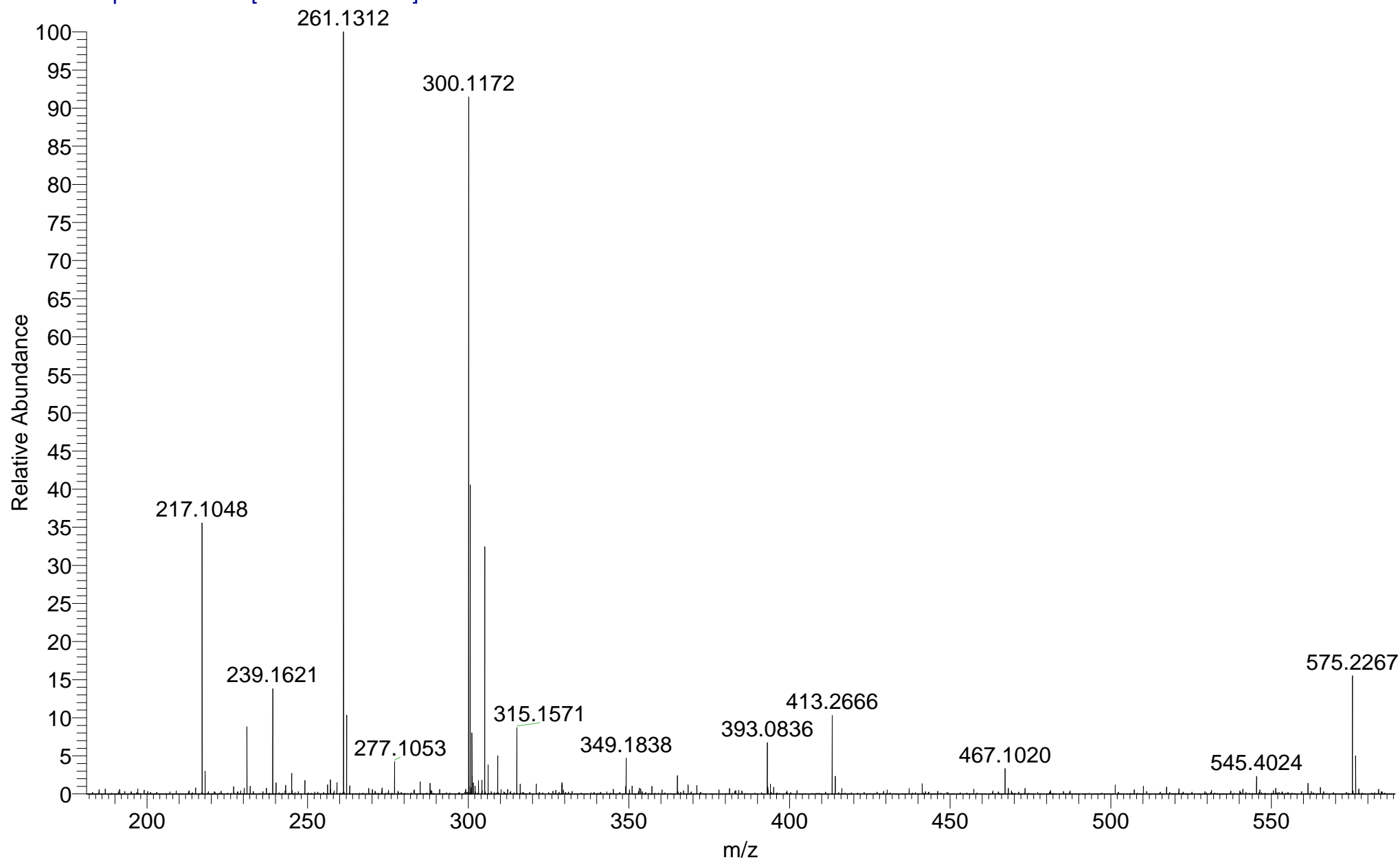
MAR-58  
(MeCN)/(MeOH)  
C40H31F6N4PS

EPSRC National Facility Swansea  
LTQ Orbitrap XL

UEAFIL  
10/25/16 14:26:50

UEAFIL\_4PCUZ\_95 #9-16 RT: 0.20-0.53 AV: 7 SM: 7G NL: 3.39E6

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



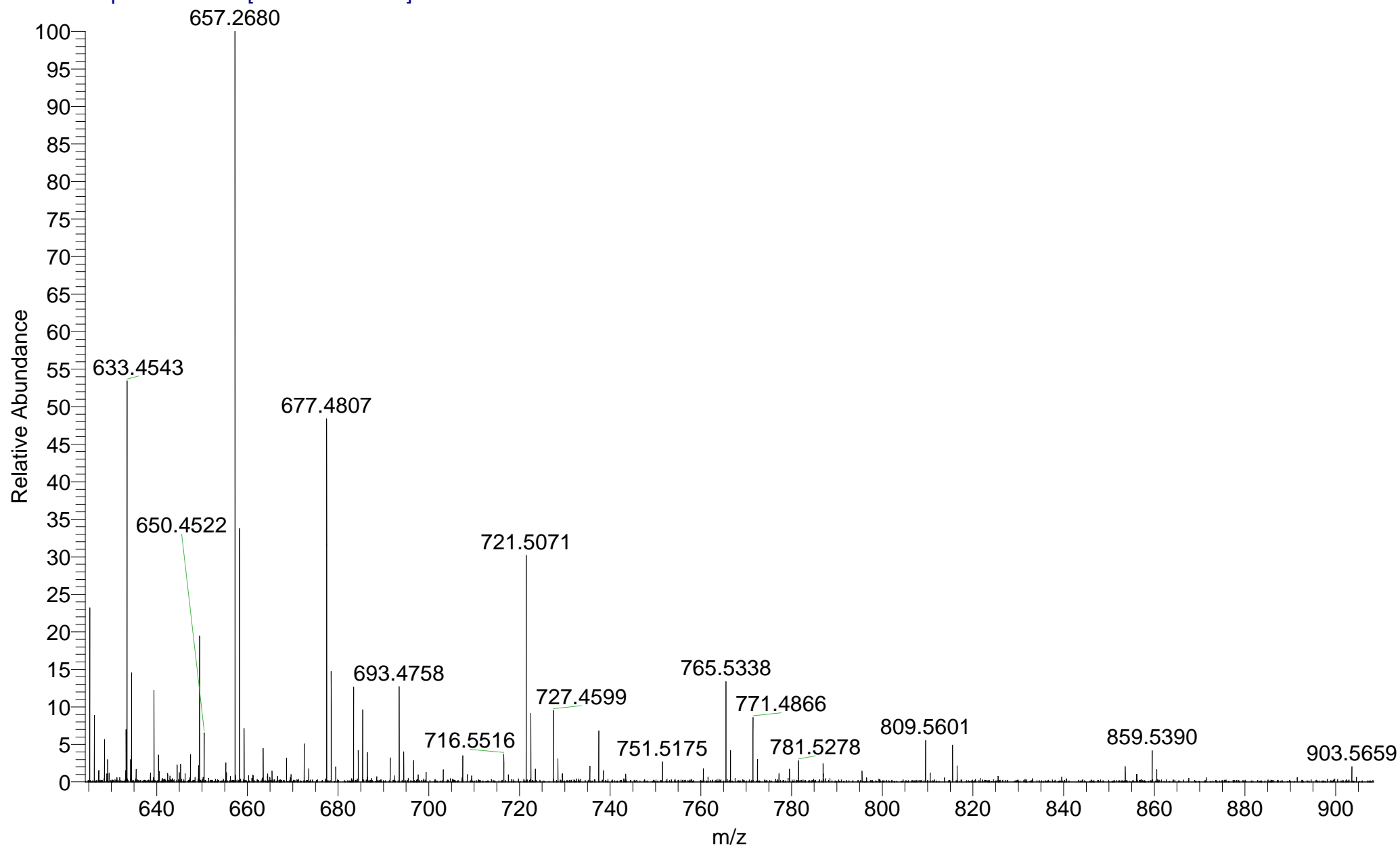
MAR-58  
(MeCN)/(MeOH)  
C40H31F6N4PS

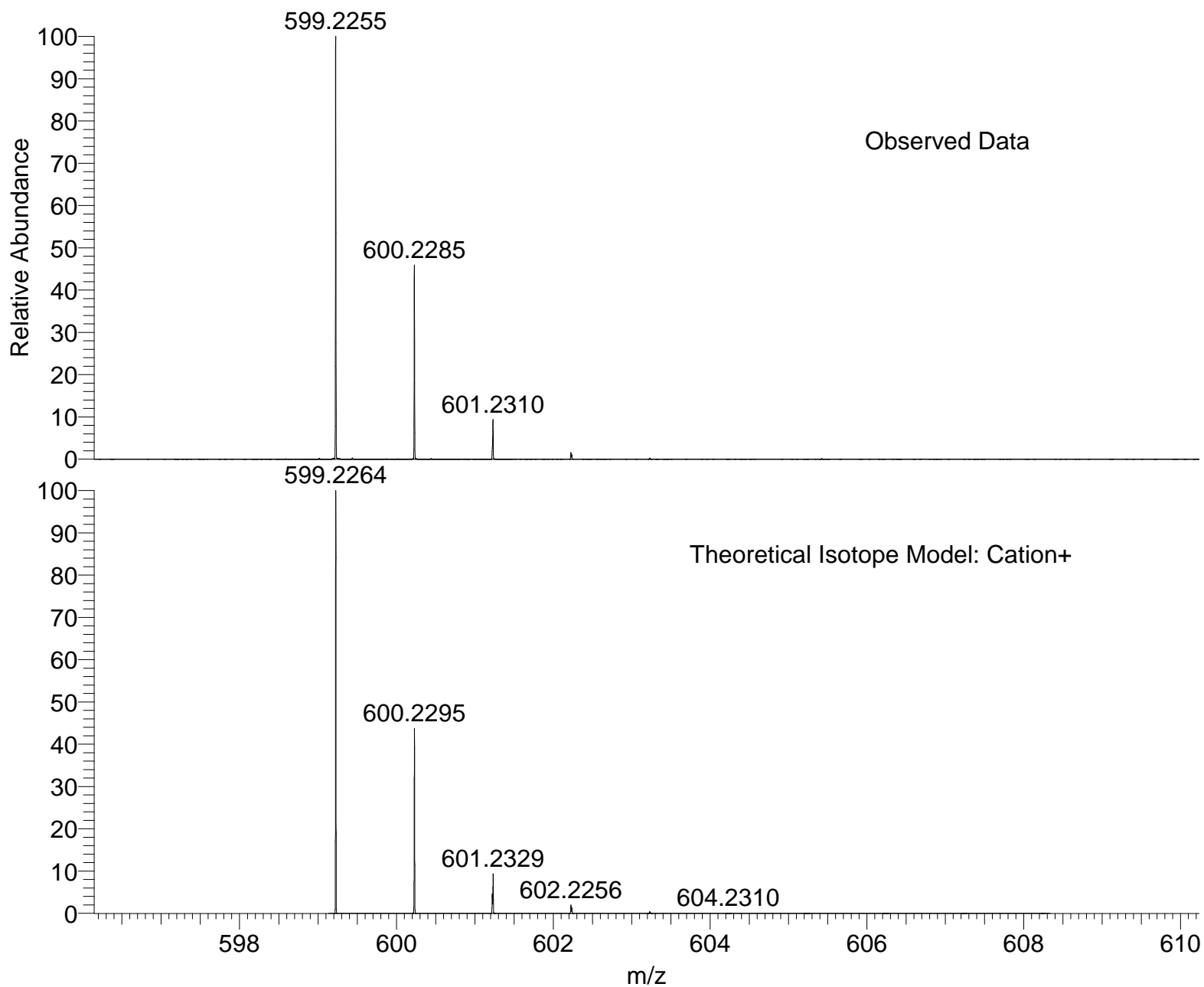
EPSRC National Facility Swansea  
LTQ Orbitrap XL

UEAFIL  
10/25/16 14:26:50

UEAFIL\_4PCUZ\_95 #9-16 RT: 0.20-0.53 AV: 7 SM: 7G NL: 3.00E5

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





NL:  
3.42E7  
UEAFIL\_4PCUZ\_95#9-16 RT:  
0.20-0.53 AV: 7 T: FTMS + p  
NSI Full ms [120.00-1935.00]

NL:  
1.42E4  
C<sub>40</sub> H<sub>31</sub> N<sub>4</sub> S:  
C<sub>40</sub> H<sub>31</sub> N<sub>4</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....50  
 1 H 0....70  
 23 Na 0....0  
 32 S 0....5  
 Tolerance Window: +- 5.00 ppm  
 Db/Ring Equiv: -3.. 100  
 Fits: 100

N-Rule: Do not use  
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
599.2255	599.2256	-0.1	15.5	C <sub>24</sub> H <sub>31</sub> O <sub>5</sub> N <sub>12</sub> S <sub>1</sub>
	599.2256	-0.1	10.0	C <sub>25</sub> H <sub>37</sub> O <sub>10</sub> N <sub>5</sub> S <sub>1</sub>
	599.2256	-0.2	-3.0	C <sub>10</sub> H <sub>41</sub> O <sub>10</sub> N <sub>13</sub> S <sub>3</sub>
	599.2254	0.2	7.0	C <sub>17</sub> H <sub>33</sub> O <sub>13</sub> N <sub>11</sub>
	599.2253	0.4	12.5	C <sub>32</sub> H <sub>43</sub> O <sub>1</sub> N <sub>2</sub> S <sub>4</sub>
	599.2257	-0.4	18.5	C <sub>32</sub> H <sub>35</sub> O <sub>2</sub> N <sub>6</sub> S <sub>2</sub>
	599.2258	-0.5	5.5	C <sub>17</sub> H <sub>39</sub> O <sub>2</sub> N <sub>14</sub> S <sub>4</sub>
	599.2258	-0.5	0.0	C <sub>18</sub> H <sub>45</sub> O <sub>7</sub> N <sub>7</sub> S <sub>4</sub>
	599.2251	0.7	4.0	C <sub>25</sub> H <sub>45</sub> O <sub>9</sub> N <sub>1</sub> S <sub>3</sub>
	599.2251	0.7	9.5	C <sub>24</sub> H <sub>39</sub> O <sub>4</sub> N <sub>8</sub> S <sub>3</sub>
	599.2251	0.7	22.5	C <sub>39</sub> H <sub>35</sub> O <sub>4</sub> S <sub>1</sub>
	599.2260	-0.8	3.0	C <sub>26</sub> H <sub>49</sub> O <sub>4</sub> N <sub>1</sub> S <sub>5</sub>
	599.2249	1.0	1.0	C <sub>17</sub> H <sub>41</sub> O <sub>12</sub> N <sub>7</sub> S <sub>2</sub>
	599.2249	1.0	6.5	C <sub>16</sub> H <sub>35</sub> O <sub>7</sub> N <sub>14</sub> S <sub>2</sub>
	599.2249	1.0	19.5	C <sub>31</sub> H <sub>31</sub> O <sub>7</sub> N <sub>6</sub>
	599.2249	1.1	25.0	C <sub>30</sub> H <sub>25</sub> O <sub>2</sub> N <sub>13</sub>
	599.2262	-1.2	24.5	C <sub>32</sub> H <sub>27</sub> O <sub>3</sub> N <sub>10</sub>
	599.2262	-1.2	19.0	C <sub>33</sub> H <sub>33</sub> O <sub>8</sub> N <sub>3</sub>
	599.2262	-1.3	6.0	C <sub>18</sub> H <sub>37</sub> O <sub>8</sub> N <sub>11</sub> S <sub>2</sub>
	599.2263	-1.3	0.5	C <sub>19</sub> H <sub>43</sub> O <sub>13</sub> N <sub>4</sub> S <sub>2</sub>
	599.2247	1.3	-2.0	C <sub>9</sub> H <sub>37</sub> O <sub>15</sub> N <sub>13</sub> S <sub>1</sub>
	599.2246	1.5	3.5	C <sub>24</sub> H <sub>47</sub> O <sub>3</sub> N <sub>4</sub> S <sub>5</sub>
	599.2264	-1.5	27.5	C <sub>40</sub> H <sub>31</sub> N <sub>4</sub> S <sub>1</sub>
	599.2264	-1.5	14.5	C <sub>25</sub> H <sub>35</sub> N <sub>12</sub> S <sub>3</sub>
	599.2264	-1.6	9.0	C <sub>26</sub> H <sub>41</sub> O <sub>5</sub> N <sub>5</sub> S <sub>3</sub>
	599.2244	1.8	0.5	C <sub>16</sub> H <sub>43</sub> O <sub>6</sub> N <sub>10</sub> S <sub>4</sub>
	599.2244	1.8	13.5	C <sub>31</sub> H <sub>39</sub> O <sub>6</sub> N <sub>2</sub> S <sub>2</sub>
	599.2244	1.8	19.0	C <sub>30</sub> H <sub>33</sub> O <sub>1</sub> N <sub>9</sub> S <sub>2</sub>
	599.2244	1.9	32.0	C <sub>45</sub> H <sub>29</sub> O <sub>1</sub> N <sub>1</sub>
	599.2267	-2.0	12.0	C <sub>18</sub> H <sub>29</sub> O <sub>9</sub> N <sub>15</sub>
	599.2267	-2.0	6.5	C <sub>19</sub> H <sub>35</sub> O <sub>14</sub> N <sub>8</sub>

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
599.2242	2.1	5.0	C <sub>24</sub> H <sub>41</sub> O <sub>14</sub> N <sub>1</sub> S <sub>1</sub>	
599.2242	2.1	10.5	C <sub>23</sub> H <sub>35</sub> O <sub>9</sub> N <sub>8</sub> S <sub>1</sub>	
599.2242	2.1	16.0	C <sub>22</sub> H <sub>29</sub> O <sub>4</sub> N <sub>15</sub> S <sub>1</sub>	
599.2269	-2.3	15.0	C <sub>26</sub> H <sub>33</sub> O <sub>6</sub> N <sub>9</sub> S <sub>1</sub>	
599.2269	-2.3	9.5	C <sub>27</sub> H <sub>39</sub> O <sub>11</sub> N <sub>2</sub> S <sub>1</sub>	
599.2240	2.4	7.5	C <sub>15</sub> H <sub>31</sub> O <sub>12</sub> N <sub>14</sub>	
599.2239	2.6	13.0	C <sub>30</sub> H <sub>41</sub> N <sub>5</sub> S <sub>4</sub>	
599.2271	-2.6	18.0	C <sub>34</sub> H <sub>37</sub> O <sub>3</sub> N <sub>3</sub> S <sub>2</sub>	
599.2271	-2.7	5.0	C <sub>19</sub> H <sub>41</sub> O <sub>3</sub> N <sub>11</sub> S <sub>4</sub>	
599.2271	-2.7	-0.5	C <sub>20</sub> H <sub>47</sub> O <sub>8</sub> N <sub>4</sub> S <sub>4</sub>	
599.2238	2.9	4.5	C <sub>23</sub> H <sub>43</sub> O <sub>8</sub> N <sub>4</sub> S <sub>3</sub>	
599.2237	2.9	10.0	C <sub>22</sub> H <sub>37</sub> O <sub>3</sub> N <sub>11</sub> S <sub>3</sub>	
599.2237	3.0	23.0	C <sub>37</sub> H <sub>33</sub> O <sub>3</sub> N <sub>3</sub> S <sub>1</sub>	
599.2273	-3.0	8.0	C <sub>27</sub> H <sub>45</sub> N <sub>5</sub> S <sub>5</sub>	
599.2274	-3.2	2.5	C <sub>12</sub> H <sub>35</sub> O <sub>12</sub> N <sub>14</sub> S <sub>1</sub>	
599.2236	3.2	1.5	C <sub>15</sub> H <sub>39</sub> O <sub>11</sub> N <sub>10</sub> S <sub>2</sub>	
599.2235	3.3	14.5	C <sub>30</sub> H <sub>35</sub> O <sub>11</sub> N <sub>2</sub>	
599.2235	3.3	20.0	C <sub>29</sub> H <sub>29</sub> O <sub>6</sub> N <sub>9</sub>	
599.2276	-3.4	24.0	C <sub>34</sub> H <sub>29</sub> O <sub>4</sub> N <sub>7</sub>	
599.2276	-3.4	18.5	C <sub>35</sub> H <sub>35</sub> O <sub>9</sub>	
599.2276	-3.5	11.0	C <sub>19</sub> H <sub>33</sub> O <sub>4</sub> N <sub>15</sub> S <sub>2</sub>	
599.2276	-3.5	5.5	C <sub>20</sub> H <sub>39</sub> O <sub>9</sub> N <sub>8</sub> S <sub>2</sub>	
599.2276	-3.5	0.0	C <sub>21</sub> H <sub>45</sub> O <sub>14</sub> N <sub>1</sub> S <sub>2</sub>	
599.2233	3.7	-1.5	C <sub>23</sub> H <sub>51</sub> O <sub>7</sub> S <sub>5</sub>	
599.2233	3.7	4.0	C <sub>22</sub> H <sub>45</sub> O <sub>2</sub> N <sub>7</sub> S <sub>5</sub>	
599.2277	-3.7	27.0	C <sub>42</sub> H <sub>33</sub> O <sub>1</sub> N <sub>1</sub> S <sub>1</sub>	
599.2278	-3.8	14.0	C <sub>27</sub> H <sub>37</sub> O <sub>1</sub> N <sub>9</sub> S <sub>3</sub>	
599.2278	-3.8	8.5	C <sub>28</sub> H <sub>43</sub> O <sub>6</sub> N <sub>2</sub> S <sub>3</sub>	
599.2231	4.0	1.0	C <sub>14</sub> H <sub>41</sub> O <sub>5</sub> N <sub>13</sub> S <sub>4</sub>	
599.2231	4.1	14.0	C <sub>29</sub> H <sub>37</sub> O <sub>5</sub> N <sub>5</sub> S <sub>2</sub>	
599.2231	4.1	19.5	C <sub>28</sub> H <sub>31</sub> N <sub>12</sub> S <sub>2</sub>	
599.2230	4.1	32.5	C <sub>43</sub> H <sub>27</sub> N <sub>4</sub>	
599.2281	-4.3	11.5	C <sub>20</sub> H <sub>31</sub> O <sub>10</sub> N <sub>12</sub>	
599.2281	-4.3	6.0	C <sub>21</sub> H <sub>37</sub> O <sub>15</sub> N <sub>5</sub>	
599.2229	4.4	5.5	C <sub>22</sub> H <sub>39</sub> O <sub>13</sub> N <sub>4</sub> S <sub>1</sub>	
599.2229	4.4	11.0	C <sub>21</sub> H <sub>33</sub> O <sub>8</sub> N <sub>11</sub> S <sub>1</sub>	
599.2282	-4.6	20.0	C <sub>27</sub> H <sub>29</sub> O <sub>2</sub> N <sub>13</sub> S <sub>1</sub>	
599.2282	-4.6	14.5	C <sub>28</sub> H <sub>35</sub> O <sub>7</sub> N <sub>6</sub> S <sub>1</sub>	
599.2283	-4.6	1.5	C <sub>13</sub> H <sub>39</sub> O <sub>7</sub> N <sub>14</sub> S <sub>3</sub>	
599.2226	4.9	8.0	C <sub>29</sub> H <sub>45</sub> O <sub>4</sub> N <sub>1</sub> S <sub>4</sub>	
599.2284	-4.9	17.5	C <sub>36</sub> H <sub>39</sub> O <sub>4</sub> S <sub>2</sub>	
599.2285	-4.9	4.5	C <sub>21</sub> H <sub>43</sub> O <sub>4</sub> N <sub>8</sub> S <sub>4</sub>	
599.2285	-5.0	-1.0	C <sub>22</sub> H <sub>49</sub> O <sub>9</sub> N <sub>1</sub> S <sub>4</sub>	