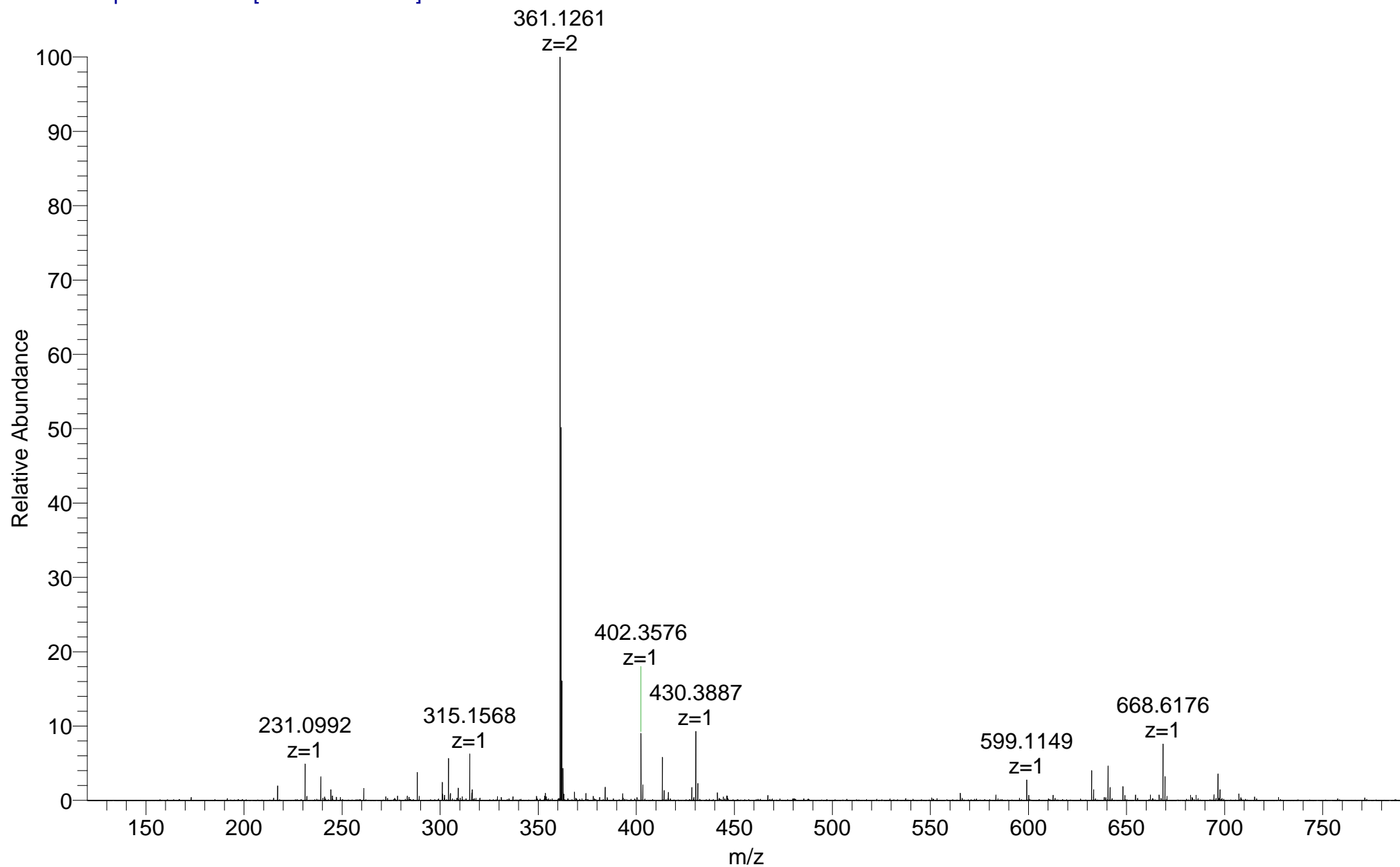


MAR-57  
(MeCN)/(MeOH)  
C47H38F12N4P2S2

EPSRC National Facility Swansea  
LTQ Orbitrap XL

UEAFIL  
10/25/16 14:29:45

UEAFIL\_BRPZT\_96 #20-28 RT: 0.67-1.05 AV: 8 SM: 7G NL: 1.67E6  
T: FTMS + p NSI Full ms [120.00-1935.00]



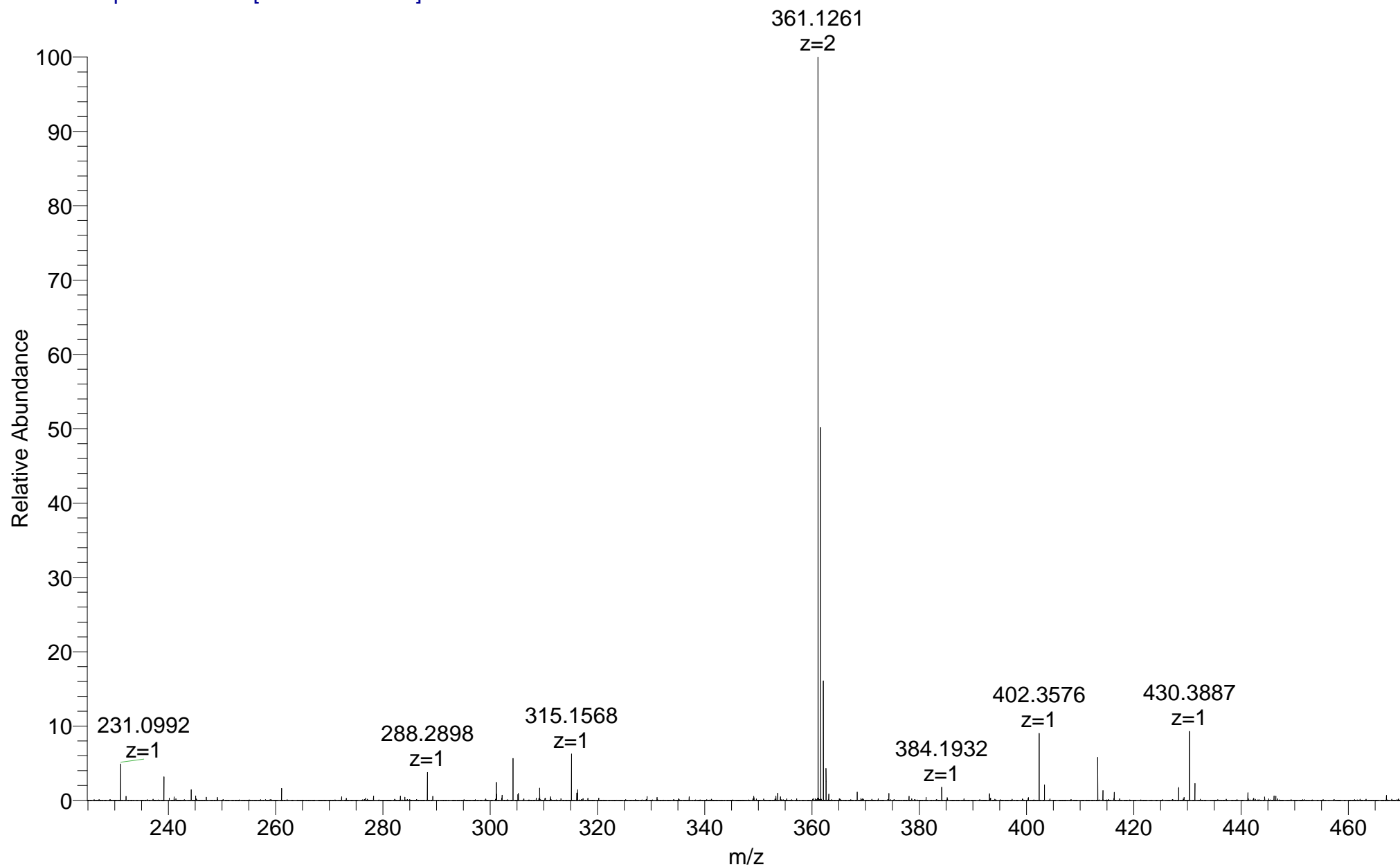
MAR-57  
(MeCN)/(MeOH)  
C47H38F12N4P2S2

EPSRC National Facility Swansea  
LTQ Orbitrap XL

UEAFIL  
10/25/16 14:29:45

UEAFIL\_BRPZT\_96 #20-28 RT: 0.67-1.05 AV: 8 SM: 7G NL: 1.67E6

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

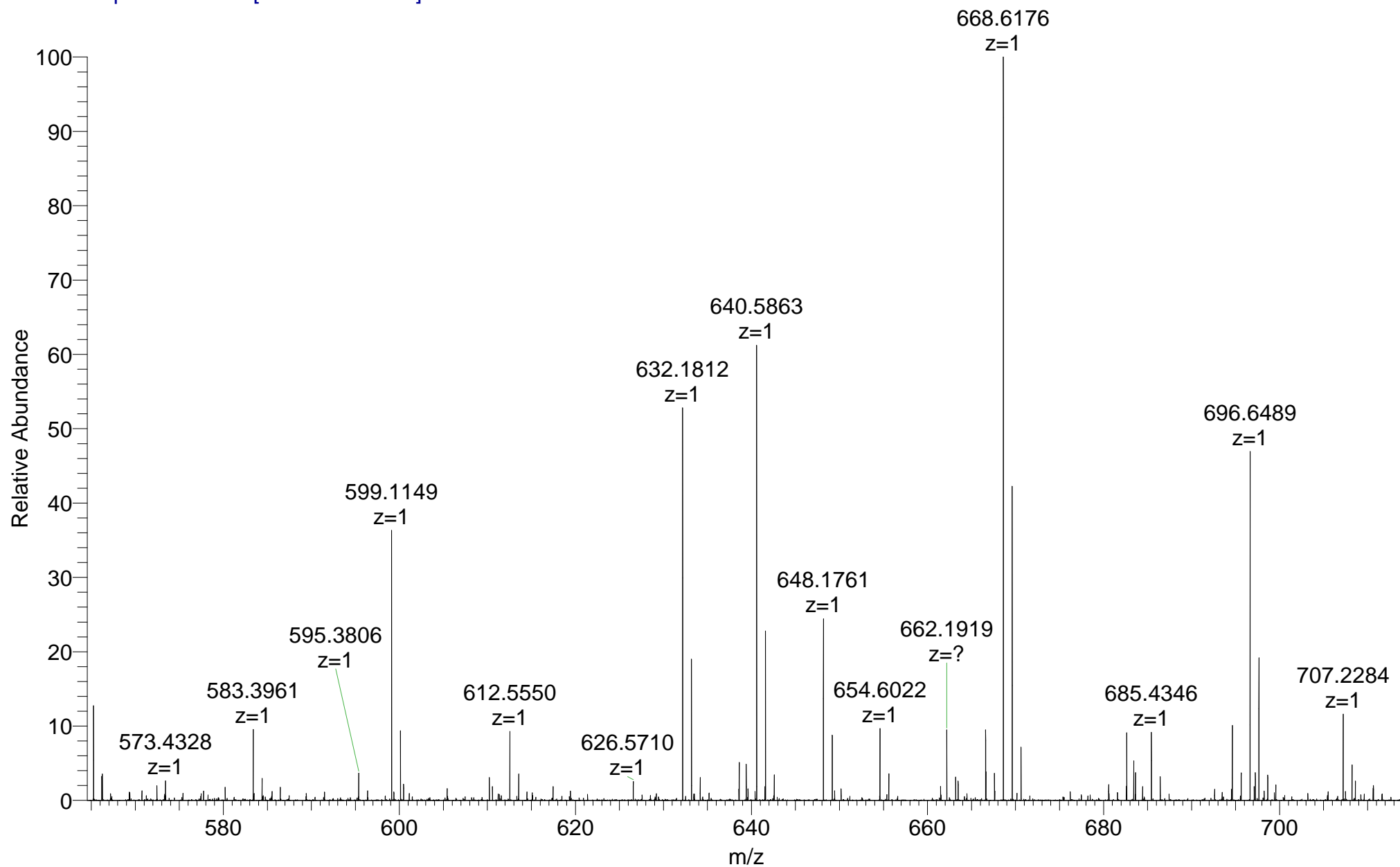


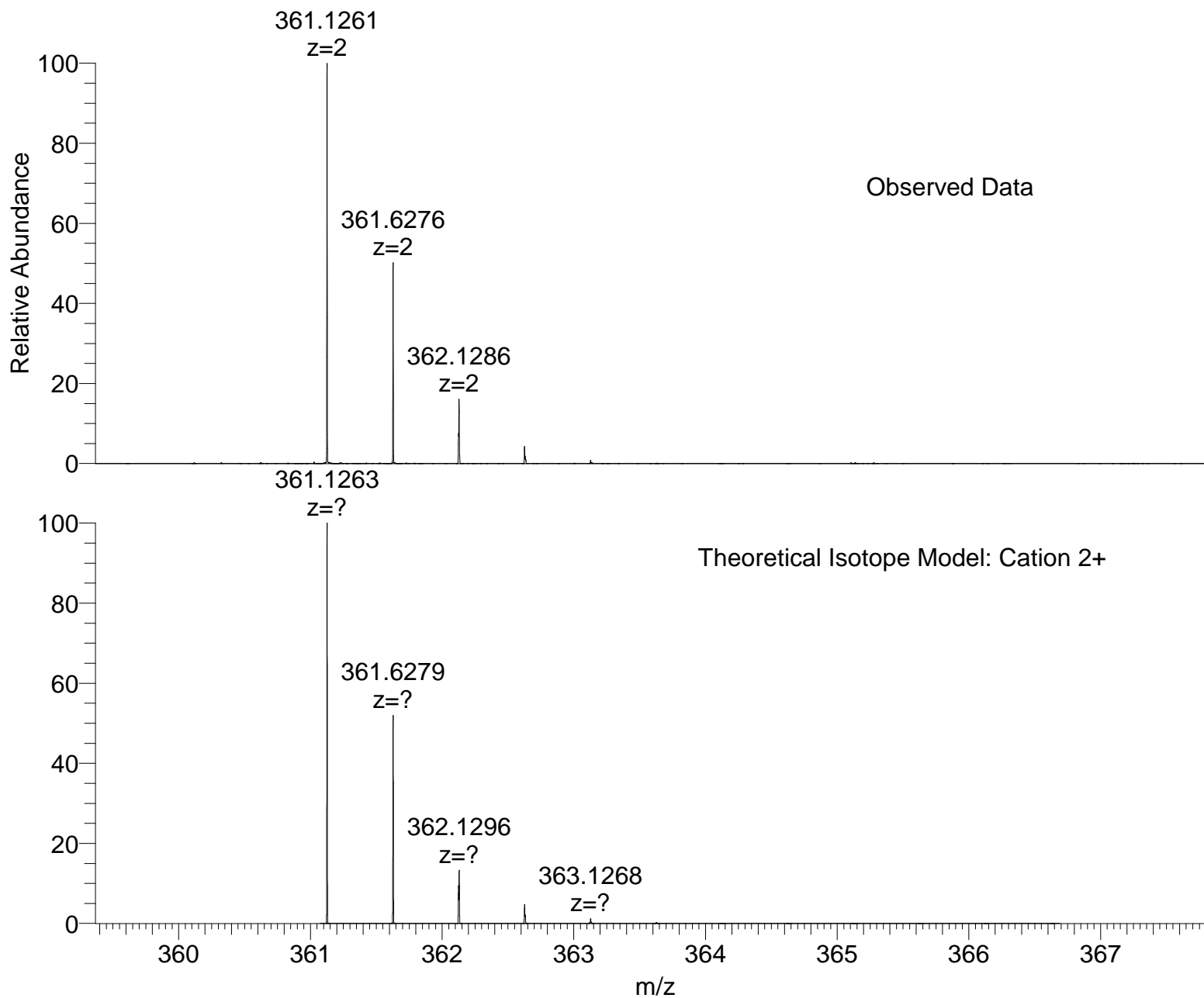
MAR-57  
(MeCN)/(MeOH)  
C47H38F12N4P2S2

EPSRC National Facility Swansea  
LTQ Orbitrap XL

UEAFIL  
10/25/16 14:29:45

UEAFIL\_BRPZT\_96 #20-28 RT: 0.67-1.05 AV: 8 SM: 7G NL: 1.27E5  
T: FTMS + p NSI Full ms [120.00-1935.00]





NL:  
1.67E6  
UEAFIL\_BRPZT\_96#20-28  
RT: 0.67-1.05 AV: 8 T: FTMS  
+ p NSI Full ms  
[120.00-1935.00]

NL:  
1.25E4  
C<sub>47</sub> H<sub>38</sub> N<sub>4</sub> S<sub>2</sub>:  
C<sub>47</sub> H<sub>38</sub> N<sub>4</sub> S<sub>2</sub>  
p (gss, s /p:40) Chrg 2  
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: 2

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
361.1261	361.1260	0.2	-2.0	C <sub>26</sub> H <sub>58</sub> O <sub>12</sub> S <sub>5</sub>
	361.1260	0.2	3.5	C <sub>25</sub> H <sub>52</sub> O <sub>7</sub> N <sub>7</sub> S <sub>5</sub>
	361.1260	0.2	9.0	C <sub>24</sub> H <sub>46</sub> O <sub>2</sub> N <sub>14</sub> S <sub>5</sub>
	361.1262	-0.2	19.5	C <sub>32</sub> H <sub>36</sub> O <sub>11</sub> N <sub>9</sub>
	361.1260	0.2	22.0	C <sub>39</sub> H <sub>42</sub> O <sub>2</sub> N <sub>6</sub> S <sub>3</sub>
	361.1259	0.4	0.5	C <sub>17</sub> H <sub>48</sub> O <sub>10</sub> N <sub>13</sub> S <sub>4</sub>
	361.1263	-0.4	28.0	C <sub>39</sub> H <sub>34</sub> O <sub>3</sub> N <sub>10</sub> S <sub>1</sub>
	361.1263	-0.4	22.5	C <sub>40</sub> H <sub>40</sub> O <sub>8</sub> N <sub>3</sub> S <sub>1</sub>
	361.1259	0.5	13.5	C <sub>32</sub> H <sub>44</sub> O <sub>10</sub> N <sub>5</sub> S <sub>2</sub>
	361.1259	0.5	19.0	C <sub>31</sub> H <sub>38</sub> O <sub>5</sub> N <sub>12</sub> S <sub>2</sub>
	361.1263	-0.5	9.5	C <sub>25</sub> H <sub>44</sub> O <sub>8</sub> N <sub>11</sub> S <sub>3</sub>
	361.1263	-0.5	4.0	C <sub>26</sub> H <sub>50</sub> O <sub>13</sub> N <sub>4</sub> S <sub>3</sub>
	361.1259	0.5	32.0	C <sub>46</sub> H <sub>34</sub> O <sub>5</sub> N <sub>4</sub>
	361.1259	0.5	37.5	C <sub>45</sub> H <sub>28</sub> N <sub>11</sub>
	361.1263	-0.7	31.0	C <sub>47</sub> H <sub>38</sub> N <sub>4</sub> S <sub>2</sub>
	361.1258	0.7	10.5	C <sub>24</sub> H <sub>40</sub> O <sub>13</sub> N <sub>11</sub> S <sub>1</sub>
	361.1264	-0.7	18.0	C <sub>32</sub> H <sub>42</sub> N <sub>12</sub> S <sub>4</sub>
	361.1264	-0.7	12.5	C <sub>33</sub> H <sub>48</sub> O <sub>5</sub> N <sub>5</sub> S <sub>4</sub>
	361.1258	0.9	16.0	C <sub>39</sub> H <sub>50</sub> O <sub>1</sub> N <sub>2</sub> S <sub>5</sub>
	361.1257	1.1	7.5	C <sub>32</sub> H <sub>52</sub> O <sub>9</sub> N <sub>1</sub> S <sub>4</sub>
	361.1257	1.1	13.0	C <sub>31</sub> H <sub>46</sub> O <sub>4</sub> N <sub>8</sub> S <sub>4</sub>
	361.1265	-1.1	15.5	C <sub>25</sub> H <sub>36</sub> O <sub>9</sub> N <sub>15</sub> S <sub>1</sub>
	361.1265	-1.1	10.0	C <sub>26</sub> H <sub>42</sub> O <sub>14</sub> N <sub>8</sub> S <sub>1</sub>
	361.1257	1.2	26.0	C <sub>46</sub> H <sub>42</sub> O <sub>4</sub> S <sub>2</sub>
	361.1266	-1.3	37.0	C <sub>47</sub> H <sub>30</sub> O <sub>1</sub> N <sub>8</sub>
	361.1266	-1.3	31.5	C <sub>48</sub> H <sub>36</sub> O <sub>6</sub> N <sub>1</sub>
	361.1256	1.4	4.5	C <sub>24</sub> H <sub>48</sub> O <sub>12</sub> N <sub>7</sub> S <sub>3</sub>
	361.1256	1.4	10.0	C <sub>23</sub> H <sub>42</sub> O <sub>7</sub> N <sub>14</sub> S <sub>3</sub>
	361.1266	-1.4	18.5	C <sub>33</sub> H <sub>40</sub> O <sub>6</sub> N <sub>9</sub> S <sub>2</sub>
	361.1266	-1.4	13.0	C <sub>34</sub> H <sub>46</sub> O <sub>11</sub> N <sub>2</sub> S <sub>2</sub>
	361.1256	1.4	23.0	C <sub>38</sub> H <sub>38</sub> O <sub>7</sub> N <sub>6</sub> S <sub>1</sub>

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
	361.1256	1.4	28.5	C <sub>37</sub> H <sub>32</sub> O <sub>2</sub> N <sub>13</sub> S <sub>1</sub>
	361.1266	-1.4	0.0	C <sub>19</sub> H <sub>50</sub> O <sub>11</sub> N <sub>10</sub> S <sub>4</sub>
	361.1255	1.6	1.5	C <sub>16</sub> H <sub>44</sub> O <sub>15</sub> N <sub>13</sub> S <sub>2</sub>
	361.1267	-1.6	21.5	C <sub>41</sub> H <sub>44</sub> O <sub>3</sub> N <sub>3</sub> S <sub>3</sub>
	361.1255	1.7	14.5	C <sub>31</sub> H <sub>40</sub> O <sub>15</sub> N <sub>5</sub>
	361.1255	1.7	20.0	C <sub>30</sub> H <sub>34</sub> O <sub>10</sub> N <sub>12</sub>
	361.1267	-1.7	8.5	C <sub>26</sub> H <sub>48</sub> O <sub>3</sub> N <sub>11</sub> S <sub>5</sub>
	361.1267	-1.7	3.0	C <sub>27</sub> H <sub>54</sub> O <sub>8</sub> N <sub>4</sub> S <sub>5</sub>
	361.1254	2.0	-1.5	C <sub>24</sub> H <sub>56</sub> O <sub>11</sub> N <sub>3</sub> S <sub>5</sub>
	361.1254	2.0	4.0	C <sub>23</sub> H <sub>50</sub> O <sub>6</sub> N <sub>10</sub> S <sub>5</sub>
	361.1268	-2.0	24.5	C <sub>33</sub> H <sub>32</sub> O <sub>7</sub> N <sub>13</sub>
	361.1268	-2.0	19.0	C <sub>34</sub> H <sub>38</sub> O <sub>12</sub> N <sub>6</sub>
	361.1254	2.1	17.0	C <sub>38</sub> H <sub>46</sub> O <sub>6</sub> N <sub>2</sub> S <sub>3</sub>
	361.1253	2.1	22.5	C <sub>37</sub> H <sub>40</sub> O <sub>1</sub> N <sub>9</sub> S <sub>3</sub>
	361.1269	-2.1	6.0	C <sub>19</sub> H <sub>42</sub> O <sub>12</sub> N <sub>14</sub> S <sub>2</sub>
	361.1269	-2.3	27.5	C <sub>41</sub> H <sub>36</sub> O <sub>4</sub> N <sub>7</sub> S <sub>1</sub>
	361.1269	-2.3	22.0	C <sub>42</sub> H <sub>42</sub> O <sub>9</sub> S <sub>1</sub>
	361.1253	2.3	8.5	C <sub>31</sub> H <sub>48</sub> O <sub>14</sub> N <sub>1</sub> S <sub>2</sub>
	361.1253	2.3	14.0	C <sub>30</sub> H <sub>42</sub> O <sub>9</sub> N <sub>8</sub> S <sub>2</sub>
	361.1269	-2.3	14.5	C <sub>26</sub> H <sub>40</sub> O <sub>4</sub> N <sub>15</sub> S <sub>3</sub>
	361.1253	2.3	19.5	C <sub>29</sub> H <sub>36</sub> O <sub>4</sub> N <sub>15</sub> S <sub>2</sub>
	361.1269	-2.3	9.0	C <sub>27</sub> H <sub>46</sub> O <sub>9</sub> N <sub>8</sub> S <sub>3</sub>
	361.1269	-2.3	3.5	C <sub>28</sub> H <sub>52</sub> O <sub>14</sub> N <sub>1</sub> S <sub>3</sub>
	361.1252	2.4	27.0	C <sub>45</sub> H <sub>38</sub> O <sub>9</sub>
	361.1252	2.4	32.5	C <sub>44</sub> H <sub>32</sub> O <sub>4</sub> N <sub>7</sub>
	361.1270	-2.5	30.5	C <sub>49</sub> H <sub>40</sub> O <sub>1</sub> N <sub>1</sub> S <sub>2</sub>
	361.1252	2.6	11.0	C <sub>22</sub> H <sub>38</sub> O <sub>12</sub> N <sub>14</sub> S <sub>1</sub>
	361.1270	-2.6	17.5	C <sub>34</sub> H <sub>44</sub> O <sub>1</sub> N <sub>9</sub> S <sub>4</sub>
	361.1270	-2.6	12.0	C <sub>35</sub> H <sub>50</sub> O <sub>6</sub> N <sub>2</sub> S <sub>4</sub>
	361.1251	2.7	16.5	C <sub>37</sub> H <sub>48</sub> N <sub>5</sub> S <sub>5</sub>
	361.1250	3.0	8.0	C <sub>30</sub> H <sub>50</sub> O <sub>8</sub> N <sub>4</sub> S <sub>4</sub>
	361.1250	3.0	13.5	C <sub>29</sub> H <sub>44</sub> O <sub>3</sub> N <sub>11</sub> S <sub>4</sub>
	361.1272	-3.0	15.0	C <sub>27</sub> H <sub>38</sub> O <sub>10</sub> N <sub>12</sub> S <sub>1</sub>
	361.1272	-3.0	9.5	C <sub>28</sub> H <sub>44</sub> O <sub>15</sub> N <sub>5</sub> S <sub>1</sub>
	361.1250	3.0	26.5	C <sub>44</sub> H <sub>40</sub> O <sub>3</sub> N <sub>3</sub> S <sub>2</sub>
	361.1273	-3.2	36.5	C <sub>49</sub> H <sub>32</sub> O <sub>2</sub> N <sub>5</sub>
	361.1249	3.2	5.0	C <sub>22</sub> H <sub>46</sub> O <sub>11</sub> N <sub>10</sub> S <sub>3</sub>
	361.1273	-3.2	23.5	C <sub>34</sub> H <sub>36</sub> O <sub>2</sub> N <sub>13</sub> S <sub>2</sub>
	361.1273	-3.2	18.0	C <sub>35</sub> H <sub>42</sub> O <sub>7</sub> N <sub>6</sub> S <sub>2</sub>
	361.1249	3.3	18.0	C <sub>37</sub> H <sub>42</sub> O <sub>11</sub> N <sub>2</sub> S <sub>1</sub>
	361.1249	3.3	23.5	C <sub>36</sub> H <sub>36</sub> O <sub>6</sub> N <sub>9</sub> S <sub>1</sub>
	361.1273	-3.3	5.0	C <sub>20</sub> H <sub>46</sub> O <sub>7</sub> N <sub>14</sub> S <sub>4</sub>
	361.1273	-3.3	-0.5	C <sub>21</sub> H <sub>52</sub> O <sub>12</sub> N <sub>7</sub> S <sub>4</sub>

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
361.1274	361.1274	-3.5	21.0	C <sub>43</sub> H <sub>46</sub> O <sub>4</sub> S <sub>3</sub>
361.1248	361.1248	3.5	15.0	C <sub>29</sub> H <sub>38</sub> O <sub>14</sub> N <sub>8</sub>
361.1248	361.1248	3.5	20.5	C <sub>28</sub> H <sub>32</sub> O <sub>9</sub> N <sub>15</sub>
361.1274	361.1274	-3.5	8.0	C <sub>28</sub> H <sub>50</sub> O <sub>4</sub> N <sub>8</sub> S <sub>5</sub>
361.1274	361.1274	-3.5	2.5	C <sub>29</sub> H <sub>56</sub> O <sub>9</sub> N <sub>1</sub> S <sub>5</sub>
361.1247	361.1247	3.9	-1.0	C <sub>22</sub> H <sub>54</sub> O <sub>10</sub> N <sub>6</sub> S <sub>5</sub>
361.1247	361.1247	3.9	4.5	C <sub>21</sub> H <sub>48</sub> O <sub>5</sub> N <sub>13</sub> S <sub>5</sub>
361.1275	361.1275	-3.9	24.0	C <sub>35</sub> H <sub>34</sub> O <sub>8</sub> N <sub>10</sub>
361.1275	361.1275	-3.9	18.5	C <sub>36</sub> H <sub>40</sub> O <sub>13</sub> N <sub>3</sub>
361.1247	361.1247	3.9	17.5	C <sub>36</sub> H <sub>44</sub> O <sub>5</sub> N <sub>5</sub> S <sub>3</sub>
361.1247	361.1247	3.9	23.0	C <sub>35</sub> H <sub>38</sub> N <sub>12</sub> S <sub>3</sub>
361.1275	361.1275	-3.9	5.5	C <sub>21</sub> H <sub>44</sub> O <sub>13</sub> N <sub>11</sub> S <sub>2</sub>
361.1247	361.1247	4.0	36.0	C <sub>50</sub> H <sub>34</sub> N <sub>4</sub> S <sub>1</sub>
361.1276	361.1276	-4.1	32.5	C <sub>42</sub> H <sub>32</sub> N <sub>11</sub> S <sub>1</sub>
361.1276	361.1276	-4.1	27.0	C <sub>43</sub> H <sub>38</sub> O <sub>5</sub> N <sub>4</sub> S <sub>1</sub>
361.1246	361.1246	4.2	9.0	C <sub>29</sub> H <sub>46</sub> O <sub>13</sub> N <sub>4</sub> S <sub>2</sub>
361.1246	361.1246	4.2	14.5	C <sub>28</sub> H <sub>40</sub> O <sub>8</sub> N <sub>11</sub> S <sub>2</sub>
361.1276	361.1276	-4.2	14.0	C <sub>28</sub> H <sub>42</sub> O <sub>5</sub> N <sub>12</sub> S <sub>3</sub>
361.1276	361.1276	-4.2	8.5	C <sub>29</sub> H <sub>48</sub> O <sub>10</sub> N <sub>5</sub> S <sub>3</sub>
361.1246	361.1246	4.2	27.5	C <sub>43</sub> H <sub>36</sub> O <sub>8</sub> N <sub>3</sub>
361.1246	361.1246	4.2	33.0	C <sub>42</sub> H <sub>30</sub> O <sub>3</sub> N <sub>10</sub>
361.1277	361.1277	-4.4	17.0	C <sub>36</sub> H <sub>46</sub> O <sub>2</sub> N <sub>6</sub> S <sub>4</sub>
361.1244	361.1244	4.6	11.5	C <sub>36</sub> H <sub>52</sub> O <sub>4</sub> N <sub>1</sub> S <sub>5</sub>
361.1278	361.1278	-4.6	11.5	C <sub>21</sub> H <sub>36</sub> O <sub>14</sub> N <sub>15</sub>
361.1244	361.1244	4.8	3.0	C <sub>29</sub> H <sub>54</sub> O <sub>12</sub> S <sub>4</sub>
361.1244	361.1244	4.8	8.5	C <sub>28</sub> H <sub>48</sub> O <sub>7</sub> N <sub>7</sub> S <sub>4</sub>