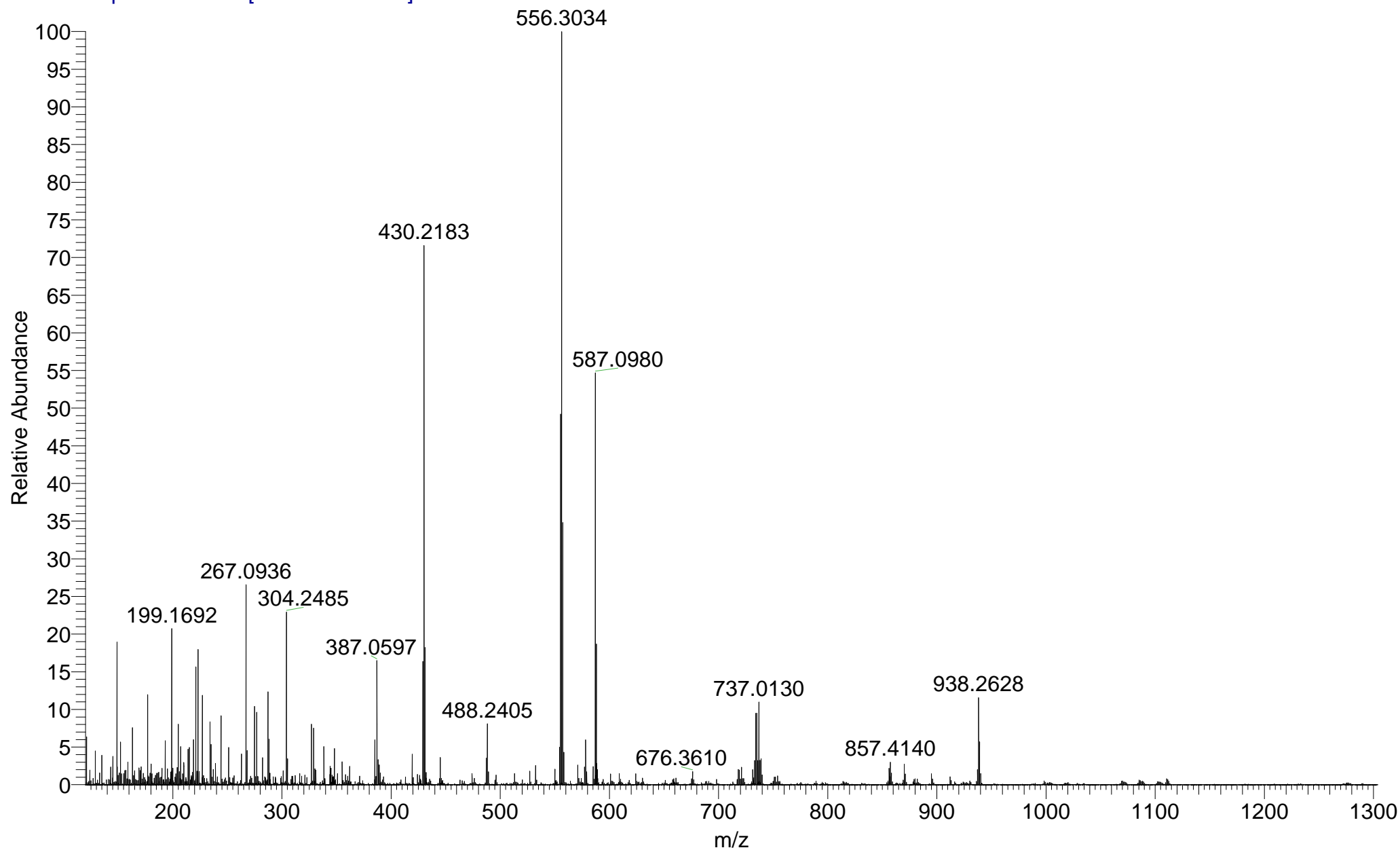


MLO42  
(DCM)/MeOH + NH4OAc  
C32H39B2NO6

EPSRC National Facility Swansea  
LTQ Orbitrap XL

BATJAM-AS  
07/12/2016 13:02:52

BATJAM\_7L3KJ\_104 #22-28 RT: 0.74-1.02 AV: 6 SM: 7G NL: 1.90E6  
T: FTMS + p NSI Full ms [120.00-1935.00]



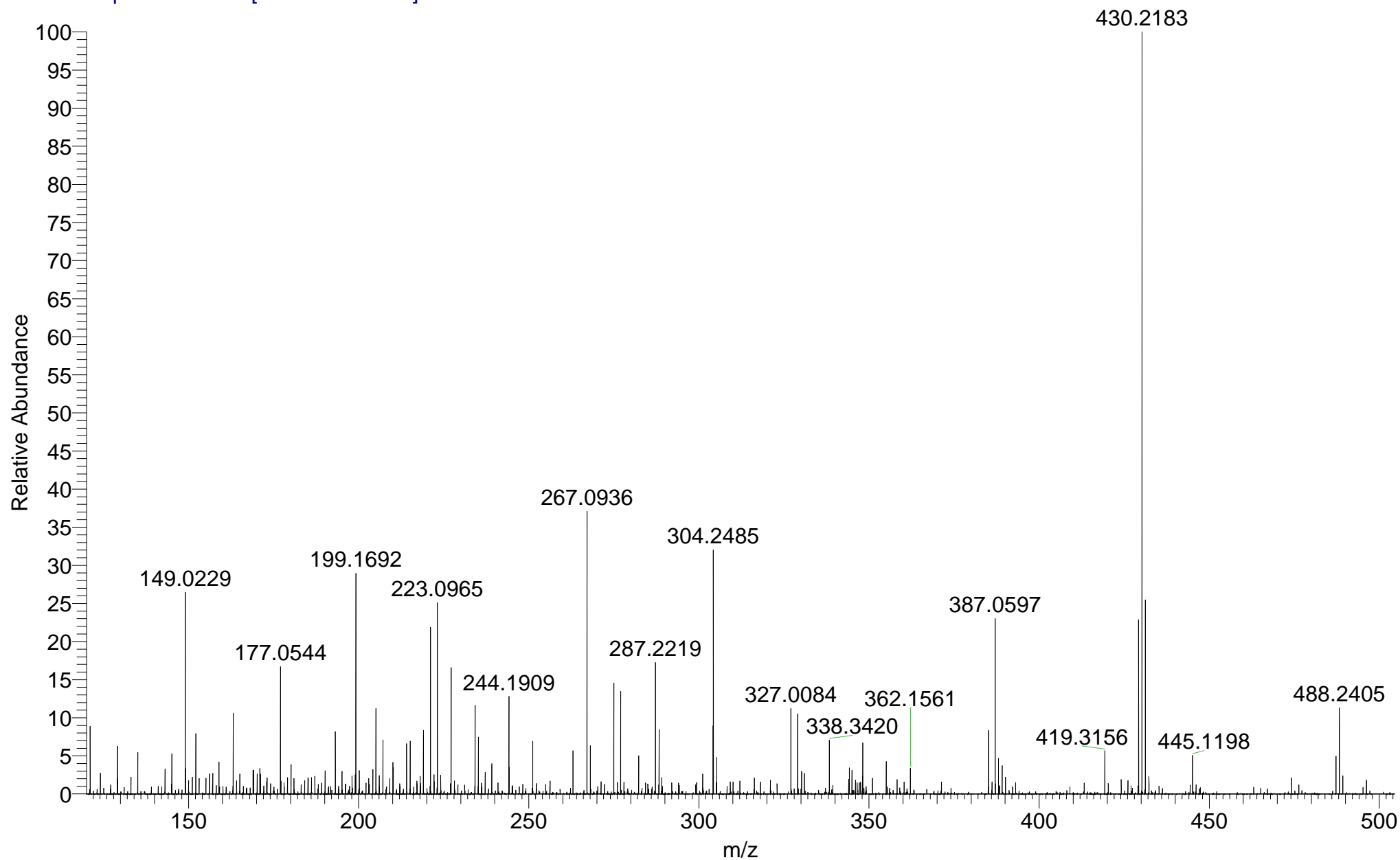
MLO42  
(DCM)/MeOH + NH<sub>4</sub>OAc  
C<sub>32</sub>H<sub>39</sub>B<sub>2</sub>NO<sub>6</sub>

EPSRC National Facility Swansea  
LTQ Orbitrap XL

BATJAM-AS  
07/12/2016 13:02:52

BATJAM\_7L3KJ\_104 #22-28 RT: 0.74-1.02 AV: 6 SM: 7G NL: 1.36E6

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



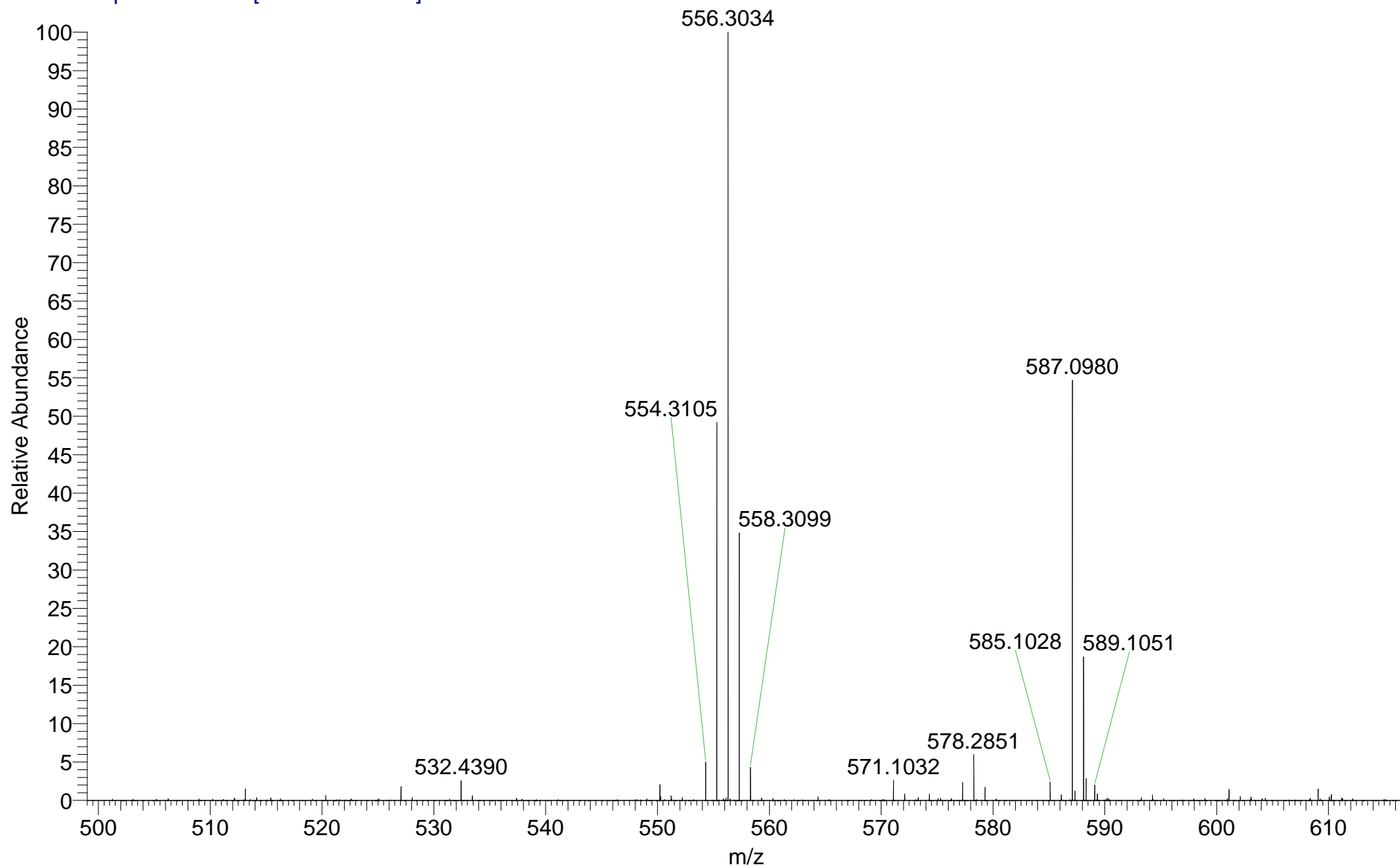
MLO42  
(DCM)/MeOH + NH<sub>4</sub>OAc  
C<sub>32</sub>H<sub>39</sub>B<sub>2</sub>NO<sub>6</sub>

EPSRC National Facility Swansea  
LTQ Orbitrap XL

BATJAM-AS  
07/12/2016 13:02:52

BATJAM\_7L3KJ\_104 #22-28 RT: 0.74-1.02 AV: 6 SM: 7G NL: 1.90E6

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



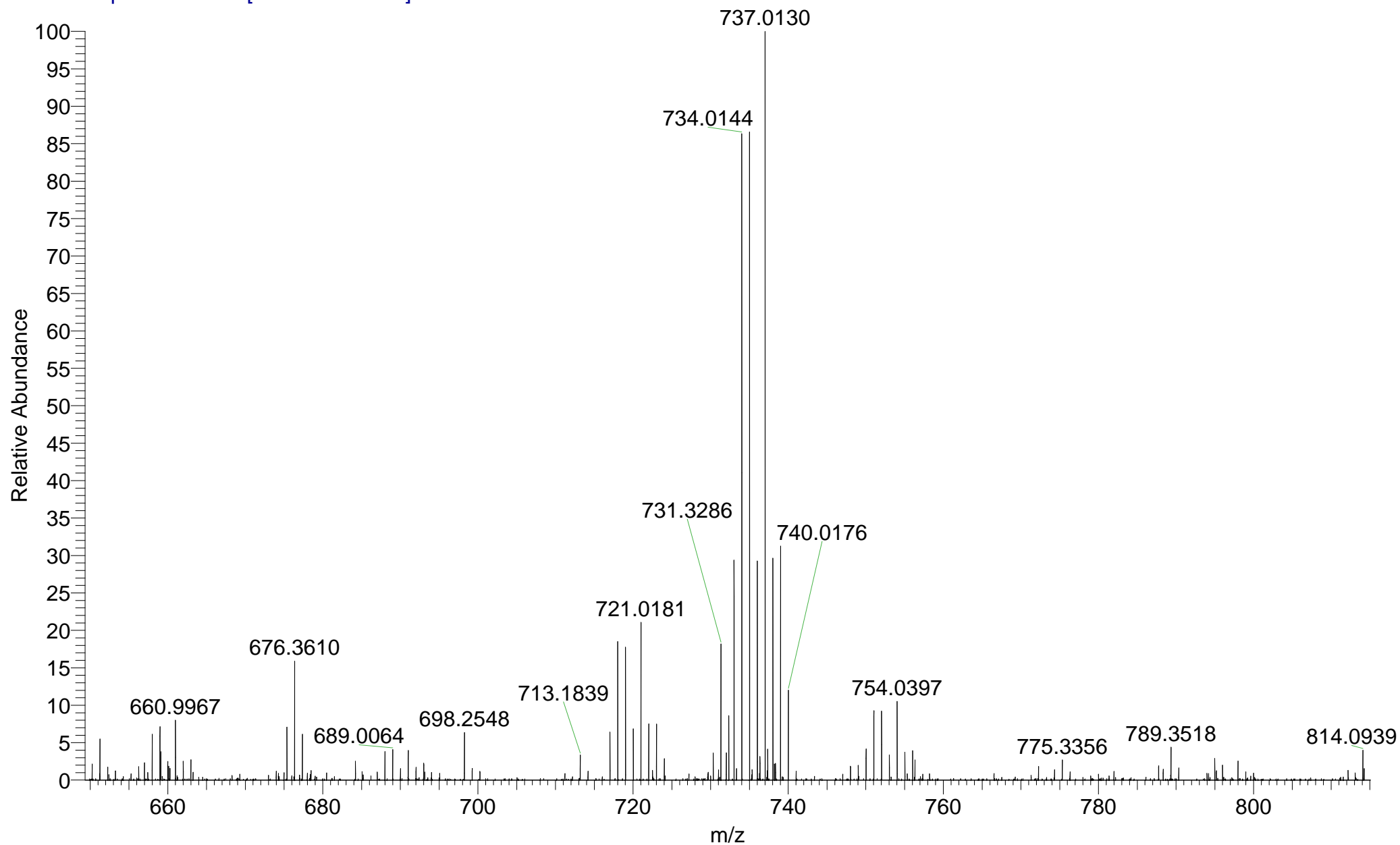
MLO42  
(DCM)/MeOH + NH4OAc  
C32H39B2NO6

EPSRC National Facility Swansea  
LTQ Orbitrap XL

BATJAM-AS  
07/12/2016 13:02:52

BATJAM\_7L3KJ\_104 #22-28 RT: 0.74-1.02 AV: 6 SM: 7G NL: 2.08E5

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



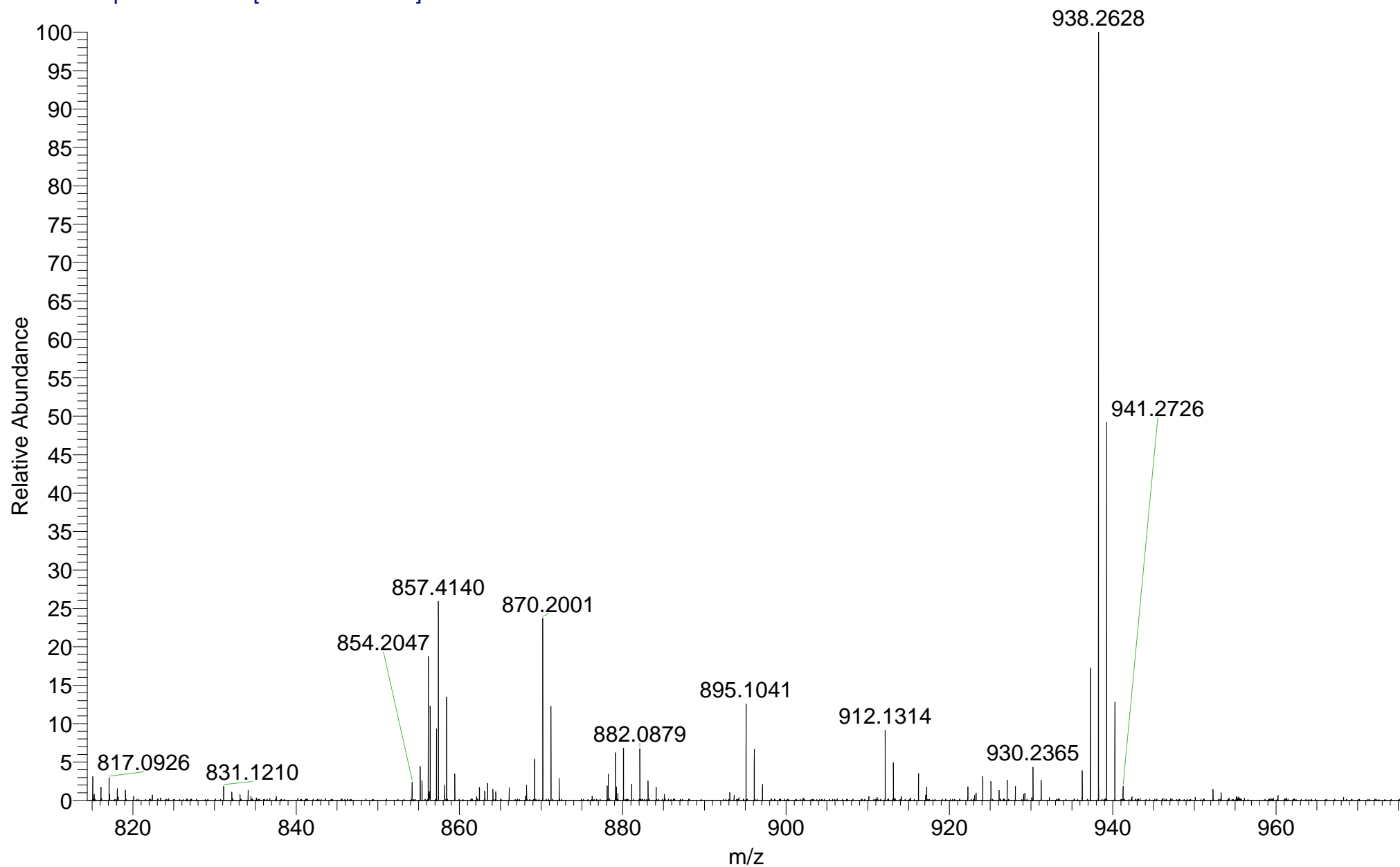
MLO42  
(DCM)/MeOH + NH<sub>4</sub>OAc  
C<sub>32</sub>H<sub>39</sub>B<sub>2</sub>NO<sub>6</sub>

EPSRC National Facility Swansea  
LTQ Orbitrap XL

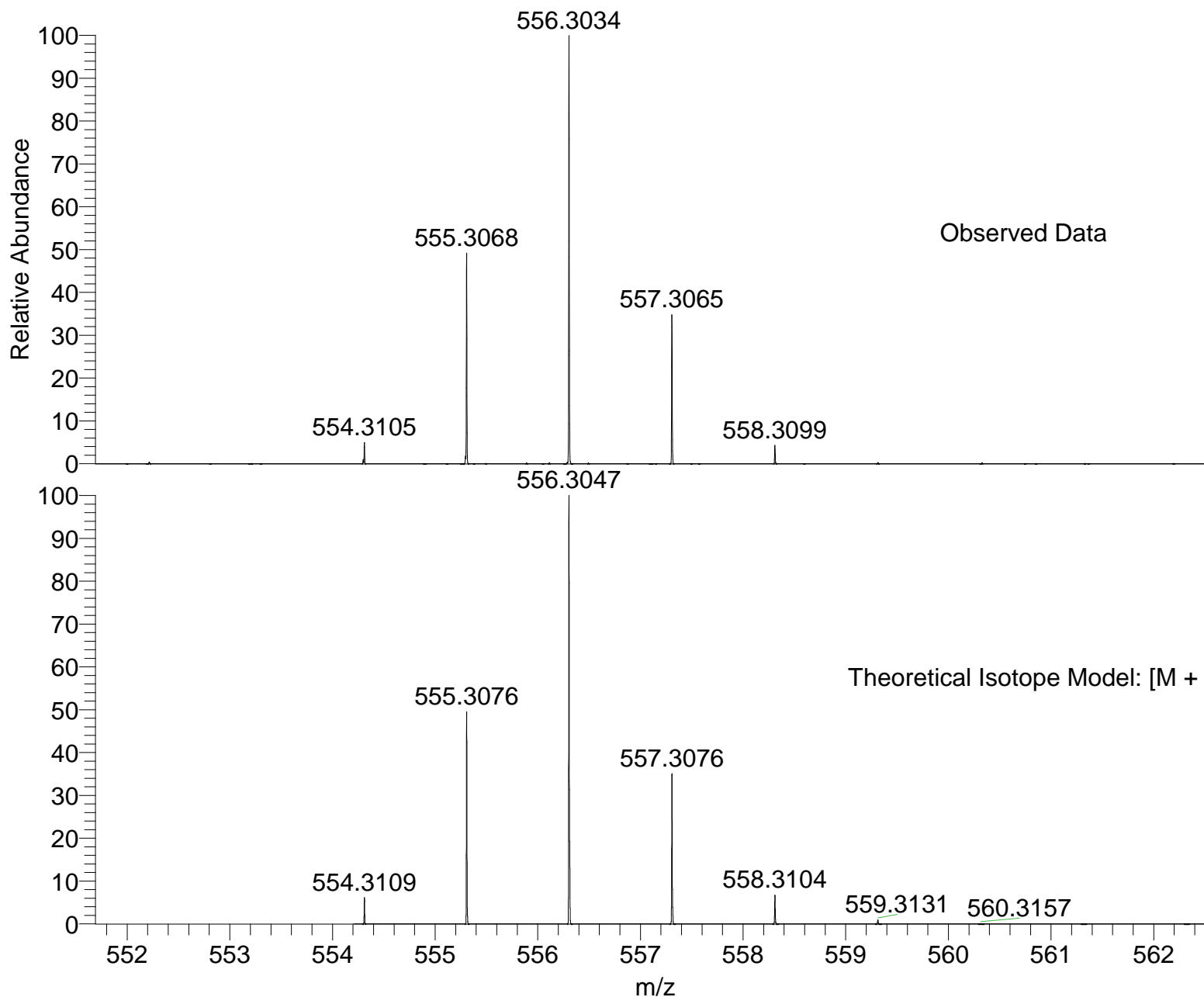
BATJAM-AS  
07/12/2016 13:02:52

BATJAM\_7L3KJ\_104 #22-28 RT: 0.74-1.02 AV: 6 SM: 7G NL: 2.19E5

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



SM: 7G



NL:  
1.90E6  
BATJAM\_7L3KJ\_104#22-28  
RT: 0.74-1.02 AV: 6 T: FTMS  
+ p NSI Full ms  
[120.00-1935.00]

NL:  
1.05E4  
C<sub>32</sub>H<sub>39</sub>B<sub>2</sub>NO<sub>6</sub>H:  
C<sub>32</sub>H<sub>40</sub>B<sub>2</sub>N<sub>1</sub>O<sub>6</sub>  
p (gss, s /p:40) Chrg 1  
R: 100000 Res .Pwr . @FWHM

Isotope: Min. .. Max.  
 14 N 0....10  
 16 O 0....15  
 12 C 0....50  
 1 H 0....60  
 23 Na 0....0  
 10 B 0....4  
 Tolerance Window: +- 5.00 ppm  
 Db/Ring Equiv: -3.. 100  
 Fits: 300

N-Rule: Do not use  
 Charge: 1

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
554.3105	554.3105	-0.1	21.0	C <sub>31</sub> H <sub>30</sub> N <sub>8</sub> <sup>10</sup> B <sub>4</sub>
	554.3105	-0.1	15.5	C <sub>32</sub> H <sub>36</sub> O <sub>5</sub> N <sub>1</sub> <sup>10</sup> B <sub>4</sub>
	554.3104	0.2	-0.5	C <sub>16</sub> H <sub>44</sub> O <sub>12</sub> N <sub>9</sub>
	554.3106	-0.3	6.5	C <sub>24</sub> H <sub>42</sub> O <sub>9</sub> N <sub>5</sub> <sup>10</sup> B <sub>1</sub>
	554.3103	0.4	8.5	C <sub>24</sub> H <sub>38</sub> O <sub>8</sub> N <sub>5</sub> <sup>10</sup> B <sub>3</sub>
	554.3101	0.7	19.0	C <sub>38</sub> H <sub>40</sub> O <sub>3</sub> <sup>10</sup> B <sub>1</sub>
	554.3109	-0.7	19.0	C <sub>31</sub> H <sub>34</sub> O <sub>1</sub> N <sub>8</sub> <sup>10</sup> B <sub>2</sub>
	554.3109	-0.7	13.5	C <sub>32</sub> H <sub>40</sub> O <sub>6</sub> N <sub>1</sub> <sup>10</sup> B <sub>2</sub>
	554.3101	0.8	1.5	C <sub>16</sub> H <sub>40</sub> O <sub>11</sub> N <sub>9</sub> <sup>10</sup> B <sub>2</sub>
	554.3111	-1.0	3.0	C <sub>18</sub> H <sub>38</sub> O <sub>11</sub> N <sub>6</sub> <sup>10</sup> B <sub>4</sub>
	554.3099	1.1	12.0	C <sub>30</sub> H <sub>42</sub> O <sub>6</sub> N <sub>4</sub>
	554.3098	1.3	21.0	C <sub>38</sub> H <sub>36</sub> O <sub>2</sub> <sup>10</sup> B <sub>3</sub>
	554.3112	-1.3	17.0	C <sub>31</sub> H <sub>38</sub> O <sub>2</sub> N <sub>8</sub>
	554.3112	-1.3	11.5	C <sub>32</sub> H <sub>44</sub> O <sub>7</sub> N <sub>1</sub>
	554.3097	1.4	-2.0	C <sub>17</sub> H <sub>42</sub> O <sub>15</sub> N <sub>2</sub> <sup>10</sup> B <sub>4</sub>
	554.3097	1.4	3.5	C <sub>16</sub> H <sub>36</sub> O <sub>10</sub> N <sub>9</sub> <sup>10</sup> B <sub>4</sub>
	554.3114	-1.6	1.0	C <sub>18</sub> H <sub>42</sub> O <sub>12</sub> N <sub>6</sub> <sup>10</sup> B <sub>2</sub>
	554.3095	1.7	14.0	C <sub>30</sub> H <sub>38</sub> O <sub>5</sub> N <sub>4</sub> <sup>10</sup> B <sub>2</sub>
	554.3116	-2.1	13.5	C <sub>25</sub> H <sub>34</sub> O <sub>4</sub> N <sub>9</sub> <sup>10</sup> B <sub>3</sub>
	554.3116	-2.1	8.0	C <sub>26</sub> H <sub>40</sub> O <sub>9</sub> N <sub>2</sub> <sup>10</sup> B <sub>3</sub>
	554.3093	2.2	1.5	C <sub>23</sub> H <sub>46</sub> O <sub>13</sub> N <sub>1</sub> <sup>10</sup> B <sub>1</sub>
	554.3093	2.2	7.0	C <sub>22</sub> H <sub>40</sub> O <sub>8</sub> N <sub>9</sub> <sup>10</sup> B <sub>1</sub>
	554.3117	-2.2	-1.0	C <sub>18</sub> H <sub>46</sub> O <sub>13</sub> N <sub>6</sub>
	554.3092	2.3	16.0	C <sub>30</sub> H <sub>34</sub> O <sub>4</sub> N <sub>4</sub> <sup>10</sup> B <sub>4</sub>
	554.3119	-2.5	20.5	C <sub>33</sub> H <sub>32</sub> O <sub>1</sub> N <sub>5</sub> <sup>10</sup> B <sub>4</sub>
	554.3120	-2.7	11.5	C <sub>25</sub> H <sub>38</sub> O <sub>5</sub> N <sub>9</sub> <sup>10</sup> B <sub>1</sub>
	554.3120	-2.7	6.0	C <sub>25</sub> H <sub>38</sub> O <sub>10</sub> N <sub>2</sub> <sup>10</sup> B <sub>1</sub>
	554.3090	2.8	3.5	C <sub>23</sub> H <sub>42</sub> O <sub>12</sub> N <sub>1</sub> <sup>10</sup> B <sub>3</sub>
	554.3090	2.8	9.0	C <sub>22</sub> H <sub>36</sub> O <sub>7</sub> N <sub>8</sub> <sup>10</sup> B <sub>3</sub>
	554.3088	3.1	19.5	C <sub>36</sub> H <sub>38</sub> O <sub>2</sub> N <sub>3</sub> <sup>10</sup> B <sub>1</sub>
	554.3122	-3.1	18.5	C <sub>33</sub> H <sub>36</sub> O <sub>2</sub> N <sub>5</sub> <sup>10</sup> B <sub>2</sub>

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
	554.3124	-3.4	8.0	C <sub>19</sub> H <sub>34</sub> O <sub>7</sub> N <sub>10</sub> <sup>10</sup> B <sub>4</sub>
	554.3124	-3.4	2.5	C <sub>20</sub> H <sub>40</sub> O <sub>12</sub> N <sub>3</sub> <sup>10</sup> B <sub>4</sub>
	554.3085	3.5	7.0	C <sub>29</sub> H <sub>46</sub> O <sub>10</sub>
	554.3085	3.5	12.5	C <sub>28</sub> H <sub>40</sub> O <sub>5</sub> N <sub>7</sub>
	554.3085	3.7	21.5	C <sub>36</sub> H <sub>34</sub> O <sub>1</sub> N <sub>3</sub> <sup>10</sup> B <sub>3</sub>
	554.3126	-3.7	16.5	C <sub>33</sub> H <sub>40</sub> O <sub>3</sub> N <sub>5</sub>
	554.3084	3.8	-1.5	C <sub>15</sub> H <sub>40</sub> O <sub>14</sub> N <sub>5</sub> <sup>10</sup> B <sub>4</sub>
	554.3127	-4.0	6.0	C <sub>19</sub> H <sub>38</sub> O <sub>8</sub> N <sub>10</sub> <sup>10</sup> B <sub>2</sub>
	554.3127	-4.0	0.5	C <sub>20</sub> H <sub>44</sub> O <sub>13</sub> N <sub>3</sub> <sup>10</sup> B <sub>2</sub>
	554.3082	4.1	9.0	C <sub>29</sub> H <sub>42</sub> O <sub>9</sub> <sup>10</sup> B <sub>2</sub>
	554.3082	4.1	14.5	C <sub>28</sub> H <sub>36</sub> O <sub>4</sub> N <sub>7</sub> <sup>10</sup> B <sub>2</sub>
	554.3128	-4.2	23.5	C <sub>41</sub> H <sub>38</sub> N <sub>1</sub> <sup>10</sup> B <sub>1</sub>
	554.3130	-4.5	13.0	C <sub>27</sub> H <sub>36</sub> O <sub>5</sub> N <sub>6</sub> <sup>10</sup> B <sub>3</sub>
	554.3080	4.6	2.0	C <sub>21</sub> H <sub>44</sub> O <sub>12</sub> N <sub>4</sub> <sup>10</sup> B <sub>1</sub>
	554.3131	-4.6	4.0	C <sub>19</sub> H <sub>42</sub> O <sub>9</sub> N <sub>10</sub>
	554.3131	-4.7	-1.5	C <sub>20</sub> H <sub>48</sub> O <sub>14</sub> N <sub>3</sub>
	554.3079	4.7	11.0	C <sub>29</sub> H <sub>38</sub> O <sub>8</sub> <sup>10</sup> B <sub>4</sub>
	554.3079	4.8	16.5	C <sub>28</sub> H <sub>32</sub> O <sub>3</sub> N <sub>7</sub> <sup>10</sup> B <sub>4</sub>
	554.3132	-4.9	20.0	C <sub>35</sub> H <sub>34</sub> O <sub>2</sub> N <sub>2</sub> <sup>10</sup> B <sub>4</sub>



Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
------	---------------------	----------------	-----	-------------

Mass	Theoretical Mass	Delta [ppm]	RDB	Composition
------	---------------------	----------------	-----	-------------