Worklist: 1751

6/8/2017

LAB CASE	ITEM	TASK ID	DESCRIPTION
C2017-0747	1	86712	AM 3 Urine Carboxy-THC
C2017-1005	3	86709	AM 3 Urine Carboxy-THC
C2017-1006	1	86710	AM 3 Urine Carboxy-THC
C2017-1021	1	86711	AM 3 Urine Carboxy-THC

1

2.4.4 Carboxy-THC
QC Calculations

Run Date: **6/6/2017**

Case Calculations:

Lab Case #: *BRC3*

EIC Ion 371 Corr. Area:	67217	
EIC Ion 473 Corr. Area:	32106	473:371 Ratio: **0.478**
EIC Ion 488 Corr. Area:	23792	488:371 Ratio: **0.354**

Quality Contol Calculations:

Retention Time acceptable range: 4.553 to 4.753

	1st ctrl	2nd ctrl
EIC Ion 371 Corr. Area:	289639	315415
EIC Ion 473 Corr. Area:	134797	147856
EIC Ion 488 Corr. Area:	87658	92066

Approximate minimum corrected area of 371 ion: ~ **57928**

Ratio of 473:371

1st ctrl **0.465** 2nd ctrl **0.469** avg. 0.467
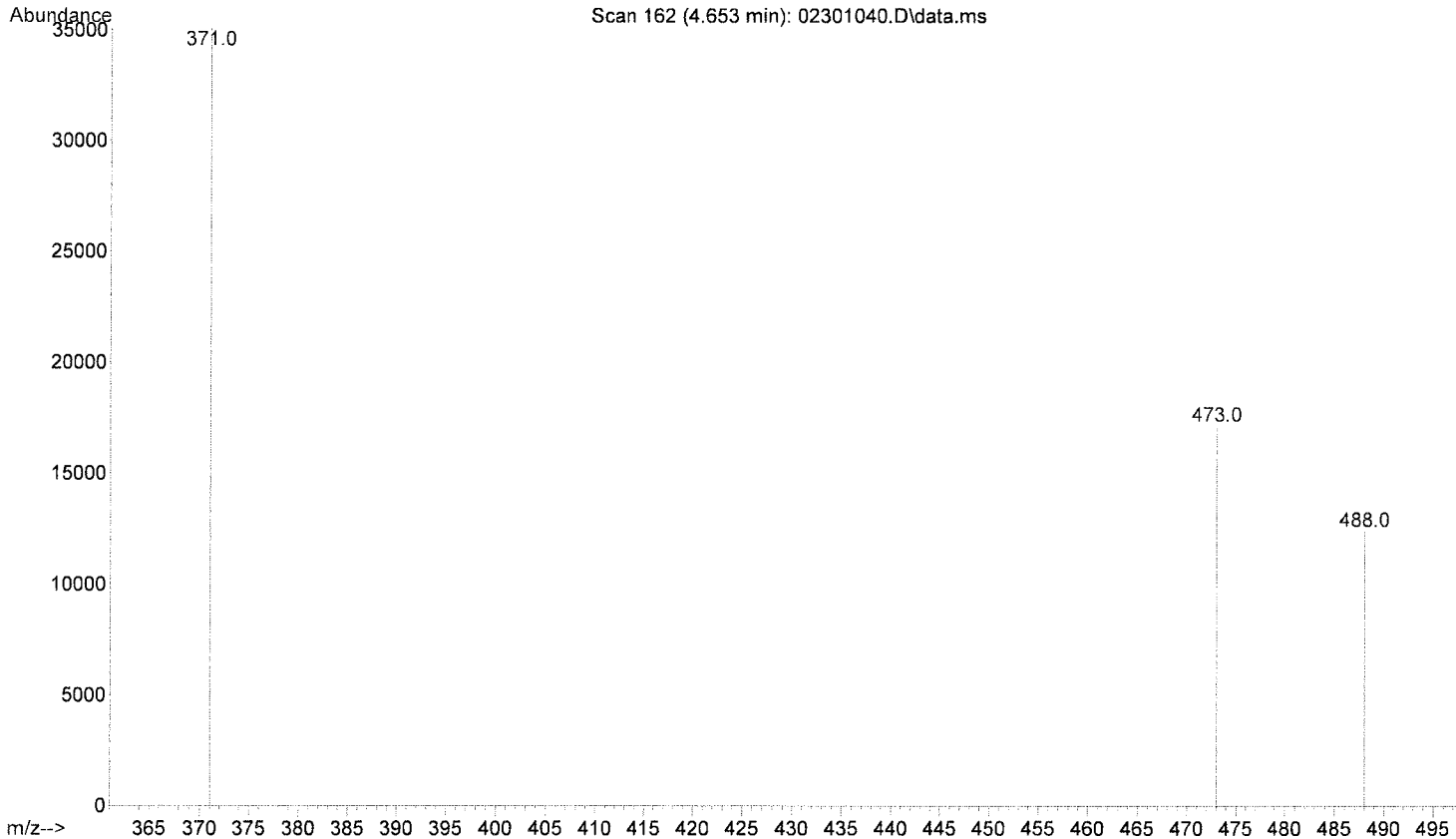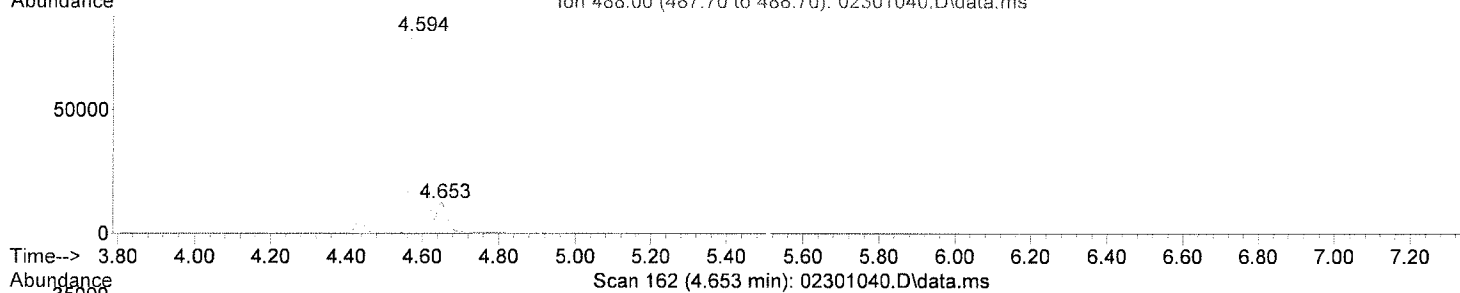
Accepted Range
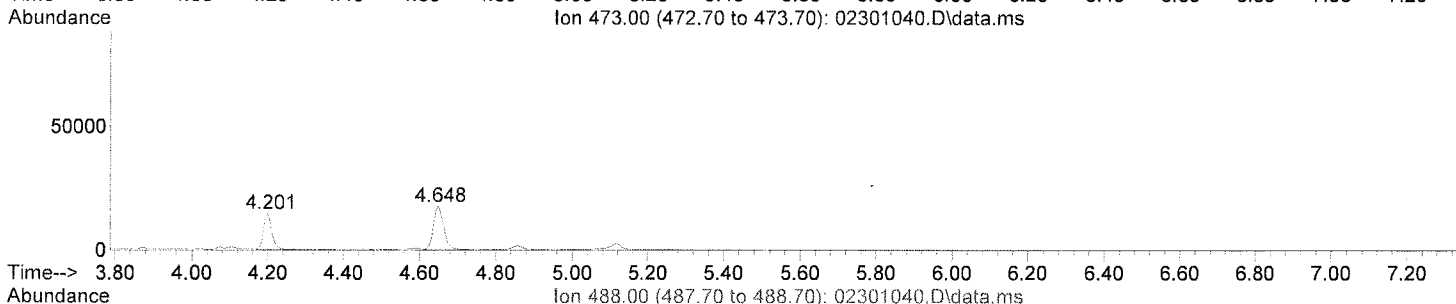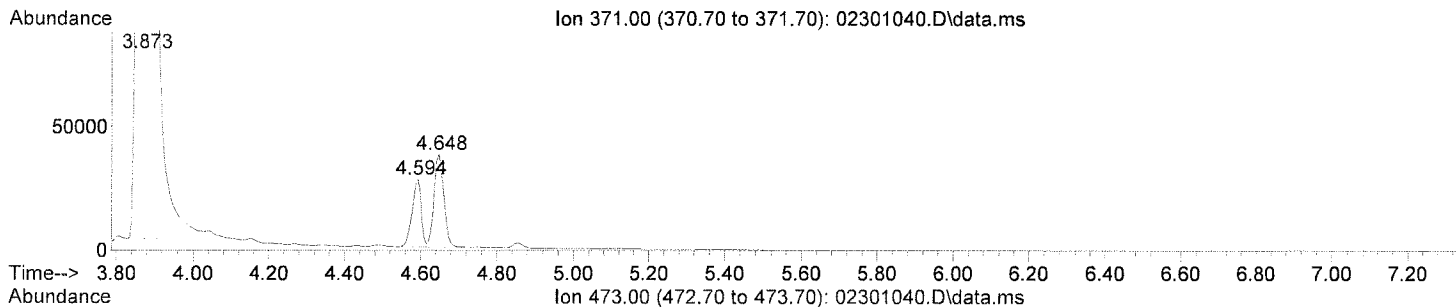(+/- 20%)   **0.374** - **0.560**

Ratio of 488:371

1st ctrl **0.303** 2nd ctrl **0.292** avg 0.297

Accepted Range
(+/- 20%):   **0.238** - **0.357**

Carboxy-calculation sheet
Revision 0 effective date 10/23/13
Issuing authority: Quality Manager

File   :I:\Instrument Data\CDA\5977 TOX GCMS CdA\2017\6-6-2017\02301
...   040.D
Operator   : Instrument 65198
Instrument :   Instrument # 65198- Tox Cd'A
Acquired   : 06 Jun 2017 23:10   using AcqMethod cthc 101415.M
Sample Name: brc3 control
Misc Info   : lot 68440; am 3

Abundance   Ion 371.00 (370.70 to 371.70): 02301040.D\data.ms

3.873

50000
                                        4.648
                                  4.594

0
Time--> 3.80 4.00 4.20 4.40 4.60 4.80 5.00 5.20 5.40 5.60 5.80 6.00 6.20 6.40 6.60 6.80 7.00 7.20
Abundance   Ion 473.00 (472.70 to 473.70): 02301040.D\data.ms

50000

              4.201   4.648

0
Time--> 3.80 4.00 4.20 4.40 4.60 4.80 5.00 5.20 5.40 5.60 5.80 6.00 6.20 6.40 6.60 6.80 7.00 7.20
Abundance   Ion 488.00 (487.70 to 488.70): 02301040.D\data.ms
              4.594

50000

              4.653

0
Time--> 3.80 4.00 4.20 4.40 4.60 4.80 5.00 5.20 5.40 5.60 5.80 6.00 6.20 6.40 6.60 6.80 7.00 7.20
Abundance   Scan 162 (4.653 min): 02301040.D\data.ms
35000
        371.0

30000

25000

20000
                                                                            473.0

15000
                                                                                  488.0

10000

5000

0
m/z-->   365 370 375 380 385 390 395 400 405 410 415 420 425 430 435 440 445 450 455 460 465 470 475 480 485 490 495

```
Data Path : I:\Instrument Data\CDA\5977 TOX GCMS CdA\2017\6-6-2017\
Data File : 02301040.D
Acq On    : 06 Jun 2017  23:10
Operator  : Instrument 65198
Sample    : brc3 control
Misc      : lot 68440;  am 3
ALS Vial  : 23    Sample Multiplier: 1


Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON                        Filtering: 5
Sampling  : 1                          Min Area: 15000 Area counts
Start Thrs: 0.2                        Max Peaks: 100
Stop Thrs : 0                          Peak Location: TOP


If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5


Method    : C:\msdchem\1\METHODS\DEFAULT.M
Title     :


Signal      : EIC Ion 371.00 (370.70 to 371.70): 02301040.D\data.ms
```

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.873	9	17	46	rBV	7255015	9265731	100.00%	98.817%
2	4.594	142	151	155	rBV	27295	43728	0.47%	0.466%
3	4.648	155	161	176	rVB	37502	67217	0.73%	0.717%

```
              Sum of corrected areas:     9376676
Signal      : EIC Ion 473.00 (472.70 to 473.70): 02301040.D\data.ms
```

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.201	72	78	97	rVB	14413	21094	65.70%	39.650%
2	4.648	154	161	178	rVB	17340	32106	100.00%	60.350%

```
              Sum of corrected areas:     53200
Signal      : EIC Ion 488.00 (487.70 to 488.70): 02301040.D\data.ms
```
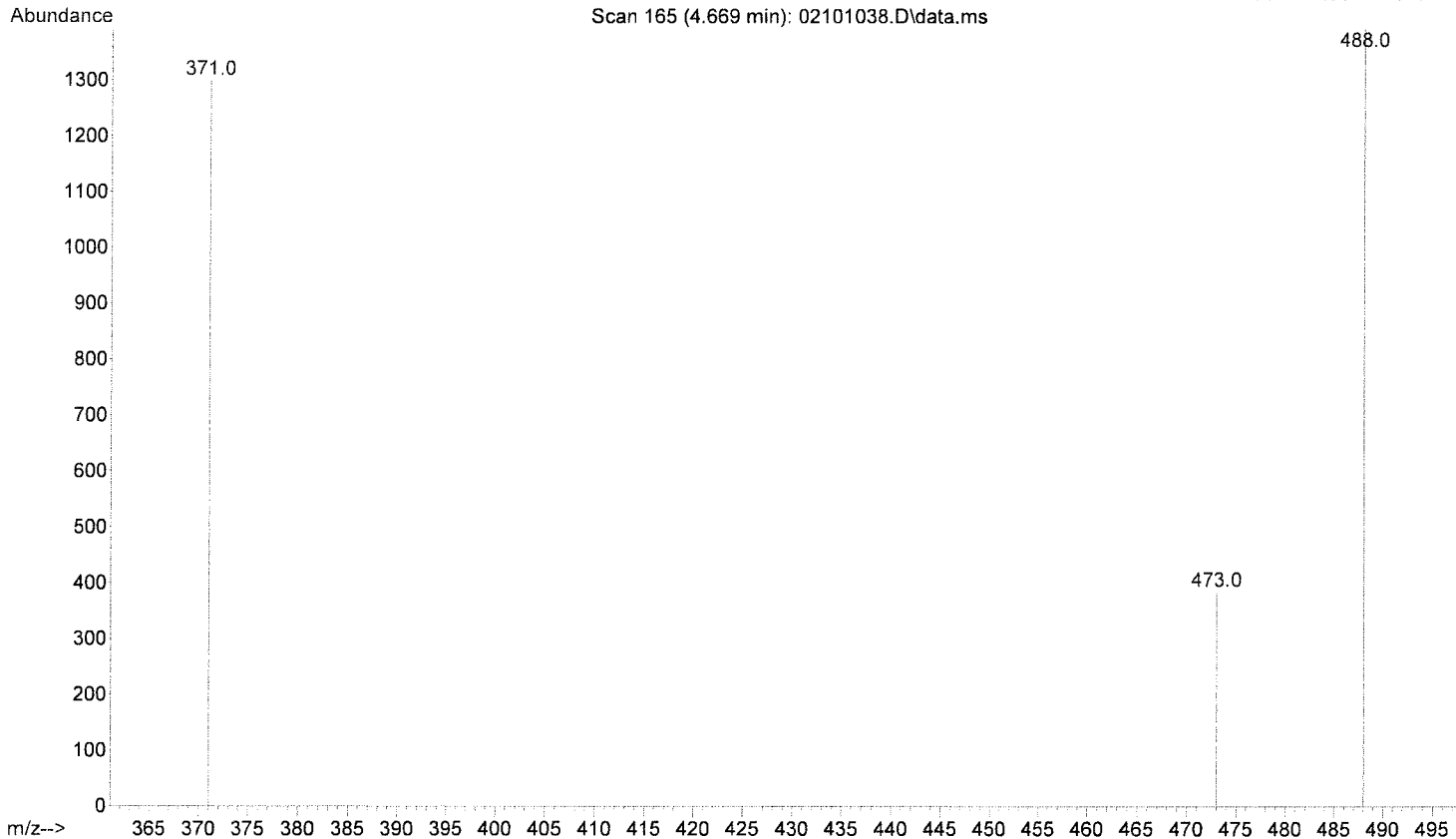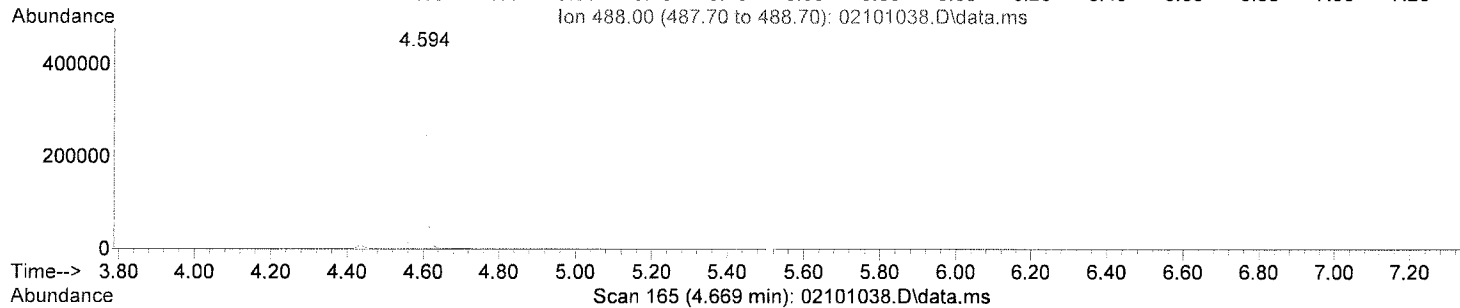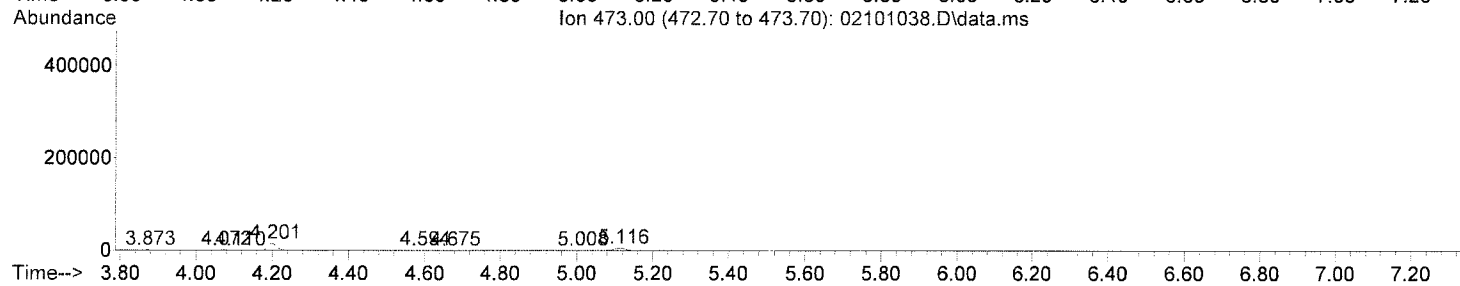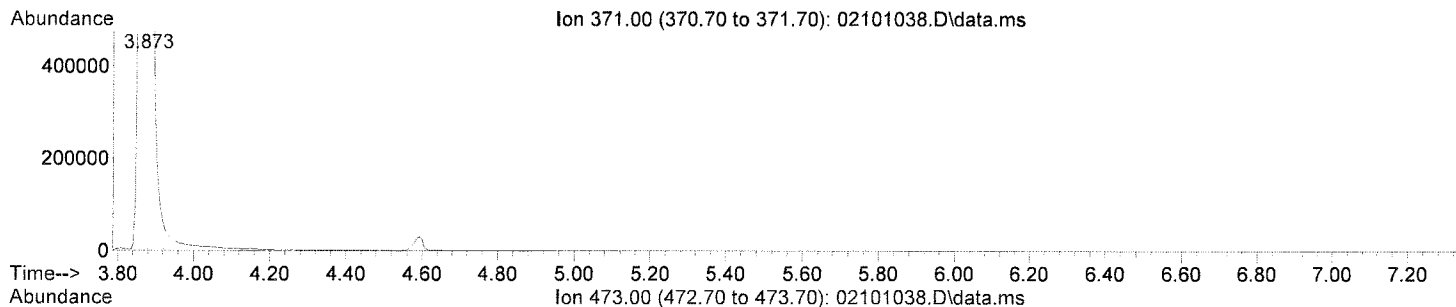
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.594	140	151	158	rBV	520114	846909	100.00%	97.267%
2	4.653	158	162	195	rVB2	12112	23792	2.81%	2.733%

```
              Sum of corrected areas:     870701

DEFAULT.M Thu Jun 08 11:36:57 2017
```

Ion 371.00 (370.70 to 371.70): 02101038.D\data.ms

Ion 473.00 (472.70 to 473.70): 02101038.D\data.ms

Ion 488.00 (487.70 to 488.70): 02101038.D\data.ms

Scan 165 (4.669 min): 02101038.D\data.ms

```
Data Path : I:\Instrument Data\CDA\5977 TOX GCMS CdA\2017\6-6-2017\
Data File : 02101038.D
Acq On    : 06 Jun 2017  22:52
Operator  : Instrument 65198
Sample    : negative control
Misc      : lot 42617;  am 3
ALS Vial  : 21   Sample Multiplier: 1


Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON                    Filtering: 5
Sampling  : 1                     Min Area: 2 % of largest Peak
Start Thrs: 0.2                   Max Peaks: 100
Stop Thrs : 0                     Peak Location: TOP


If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5


Method    : C:\msdchem\1\METHODS\DEFAULT.M
Title     :


Signal    : EIC Ion 371.00 (370.70 to 371.70): 02101038.D\data.ms
```

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.873	9	17	65	rBV	7564653	10049540	100.00%	100.000%

```
                 Sum of corrected areas:     10049540
    Signal    : EIC Ion 473.00 (472.70 to 473.70): 02101038.D\data.ms
```

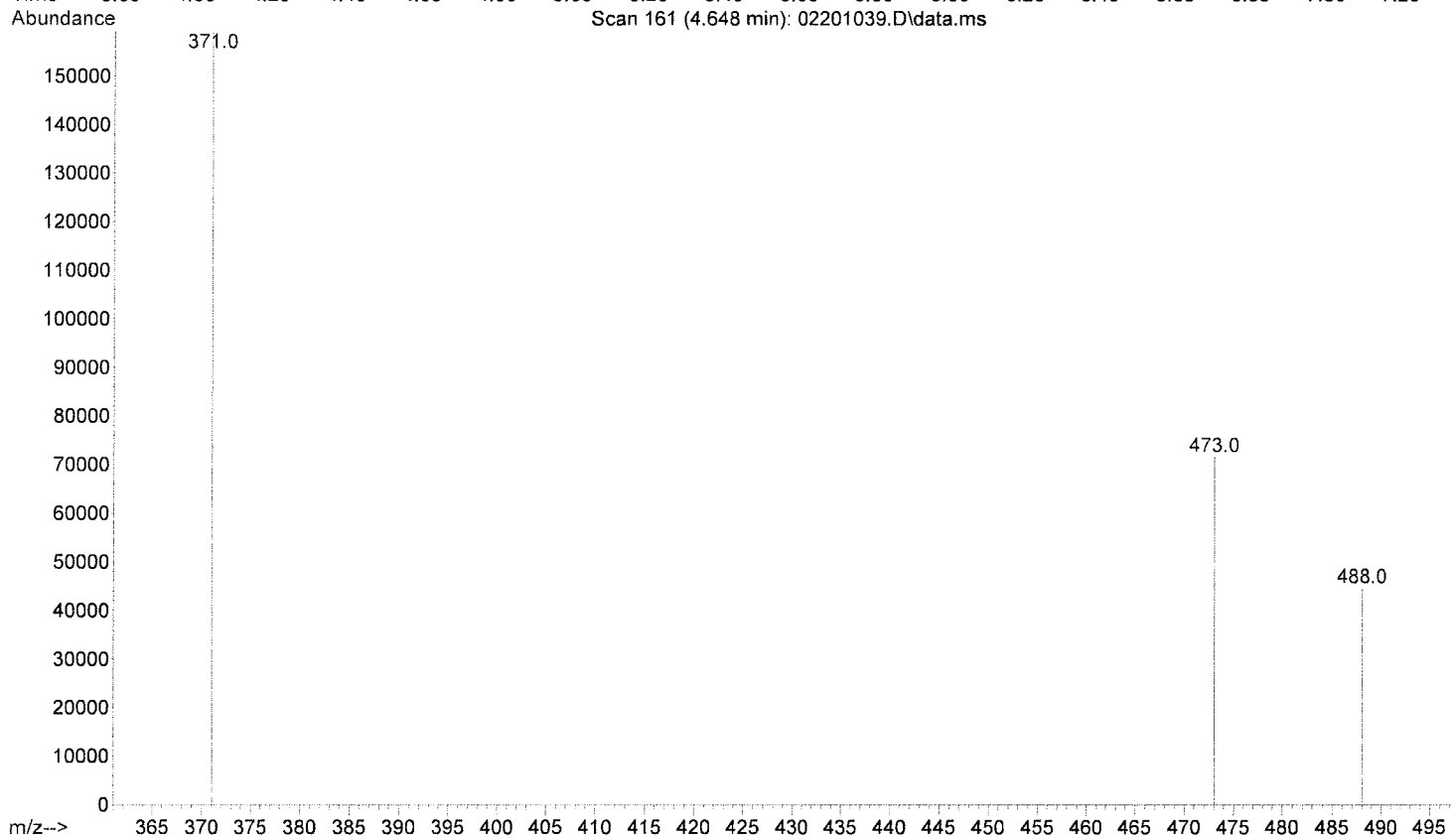| peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.873	12	17	27	rVB	612	767	3.47%	2.028%
2	4.072	48	54	58	rBV	835	1174	5.30%	3.104%
3	4.110	58	61	68	rVV2	451	710	3.21%	1.877%
4	4.201	71	78	97	rVB	15062	22131	100.00%	58.504%
5	4.594	144	151	156	rVB	538	866	3.91%	2.289%
6	4.675	159	166	176	rVB	349	627	2.83%	1.658%
7	5.008	221	228	233	rBV2	208	443	2.00%	1.171%
8	5.116	234	248	280	rVB	5055	11110	50.20%	29.370%

```
                 Sum of corrected areas:       37828
    Signal    : EIC Ion 488.00 (487.70 to 488.70): 02101038.D\data.ms
```
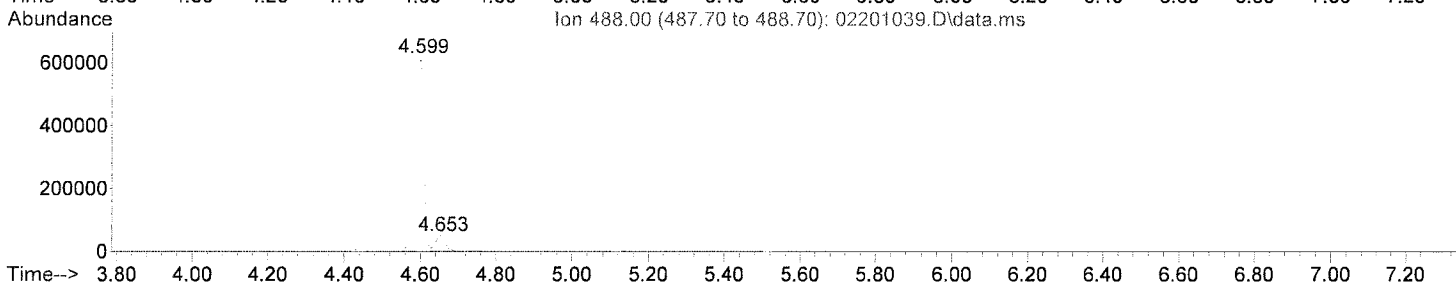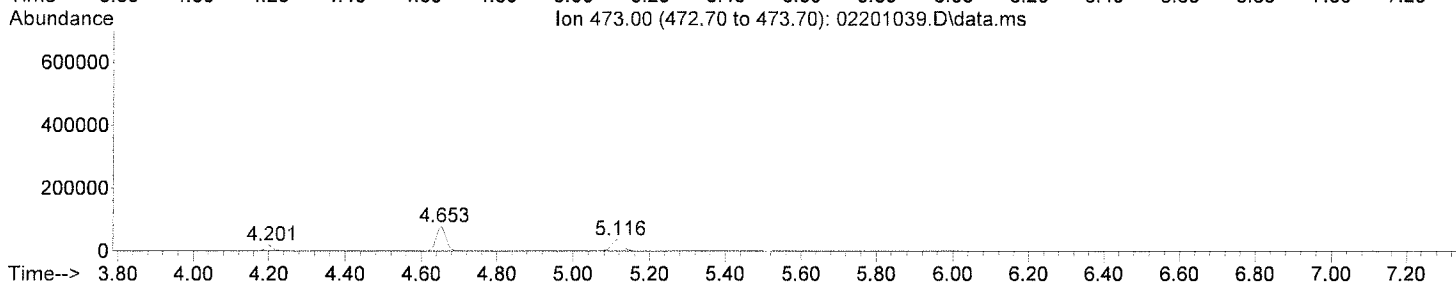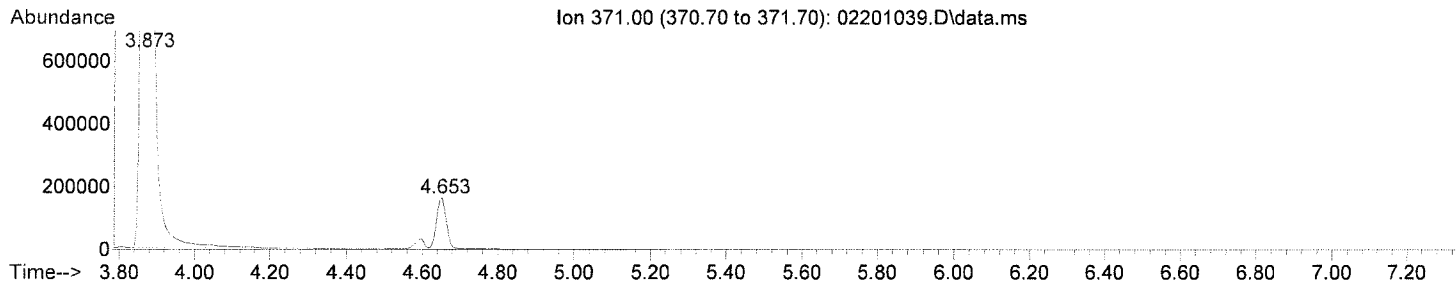
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.594	140	151	206	rBV	563534	931500	100.00%	100.000%

```
                 Sum of corrected areas:      931500
```

DEFAULT.M Thu Jun 08 11:24:17 2017

Ion 371.00 (370.70 to 371.70): 02201039.D\data.ms

Ion 473.00 (472.70 to 473.70): 02201039.D\data.ms

Ion 488.00 (487.70 to 488.70): 02201039.D\data.ms

Scan 161 (4.648 min): 02201039.D\data.ms

```
Data Path : I:\Instrument Data\CDA\5977 TOX GCMS CdA\2017\6-6-2017\
Data File : 02201039.D
Acq On    : 06 Jun 2017  23:01
Operator  : Instrument 65198
Sample    : positive control
Misc      : FE03121501 in neg lot 42617;   am 3
ALS Vial  : 22    Sample Multiplier: 1


Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON                        Filtering: 5
Sampling  : 1                          Min Area: 2 % of largest Peak
Start Thrs: 0.2                       Max Peaks: 100
Stop Thrs : 0                      Peak Location: TOP


If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5


Method    : C:\msdchem\1\METHODS\DEFAULT.M
Title     :


Signal    : EIC Ion 371.00 (370.70 to 371.70): 02201039.D\data.ms

peak  R.T.  first  max last  PK   peak     corr.    corr.    % of
 #    min   scan  scan scan  TY  height    area     % max.   total
---  -----  ----- ---- ---- ---  -------  -------  -------  -------
 1   3.873      9   17   46 rBV  8330639 10968563 100.00%  97.427%
 2   4.653    155  162  184 rVB   161415   289639   2.64%   2.573%


               Sum of corrected areas:    11258202
Signal    : EIC Ion 473.00 (472.70 to 473.70): 02201039.D\data.ms

peak  R.T.  first  max last  PK   peak     corr.    corr.    % of
 #    min   scan  scan scan  TY  height    area     % max.   total
---  -----  ----- ---- ---- ---  -------  -------  -------  -------
 1   4.201     68   78   98 rVB    17252    25197  18.69%  10.979%
 2   4.653    154  162  181 rVB    76950   134797 100.00%  58.736%
 3   5.116    236  248  281 rVB    34992    69504  51.56%  30.285%


               Sum of corrected areas:     229498
Signal    : EIC Ion 488.00 (487.70 to 488.70): 02201039.D\data.ms

peak  R.T.  first  max last  PK   peak     corr.    corr.    % of
 #    min   scan  scan scan  TY  height    area     % max.   total
---  -----  ----- ---- ---- ---  -------  -------  -------  -------
 1   4.599    140  152  157 rBV   615240   993875 100.00%  91.895%
 2   4.653    157  162  172 rVB    48560    87658   8.82%   8.105%


               Sum of corrected areas:    1081533

DEFAULT.M Thu Jun 08 11:25:24 2017
```
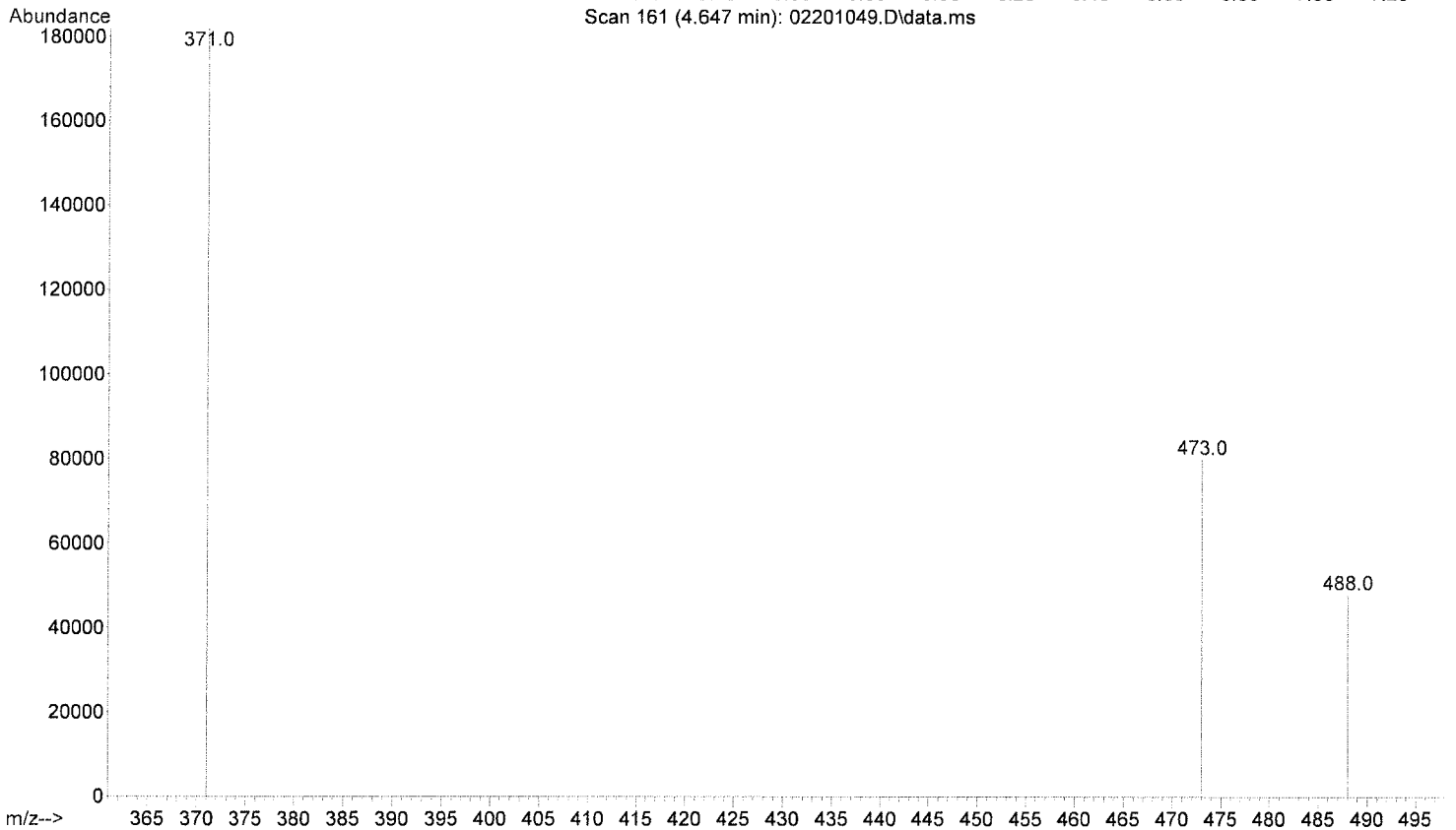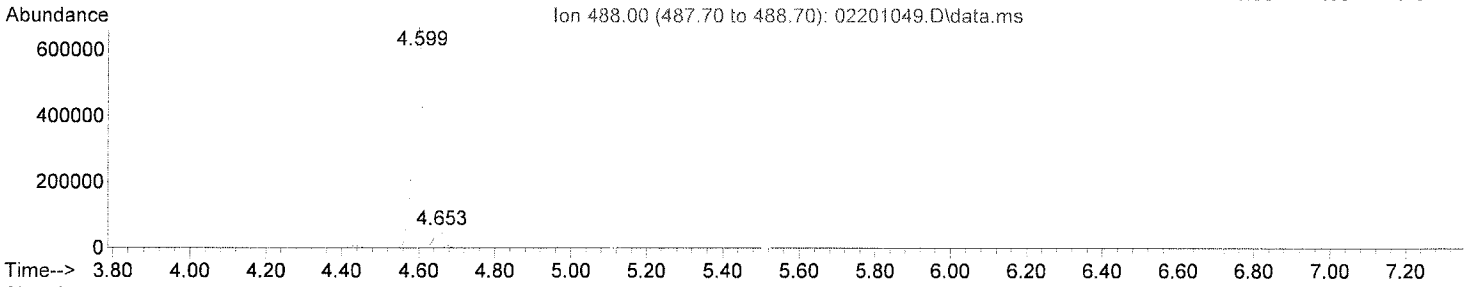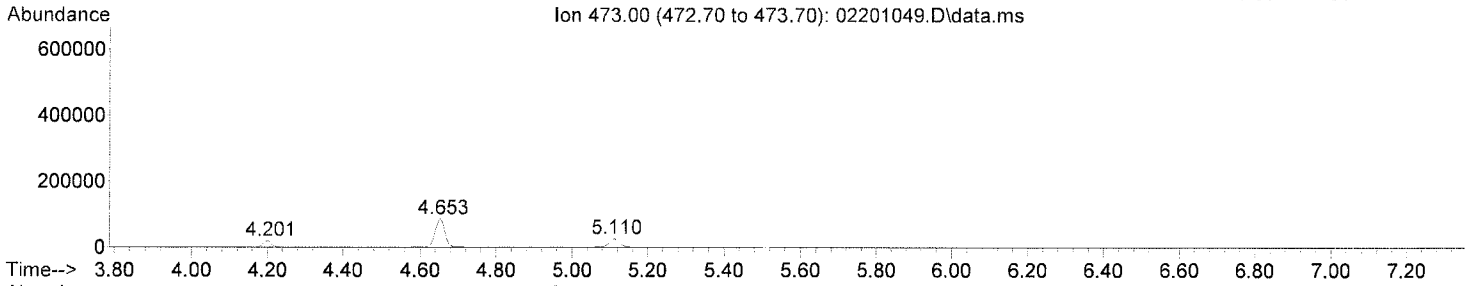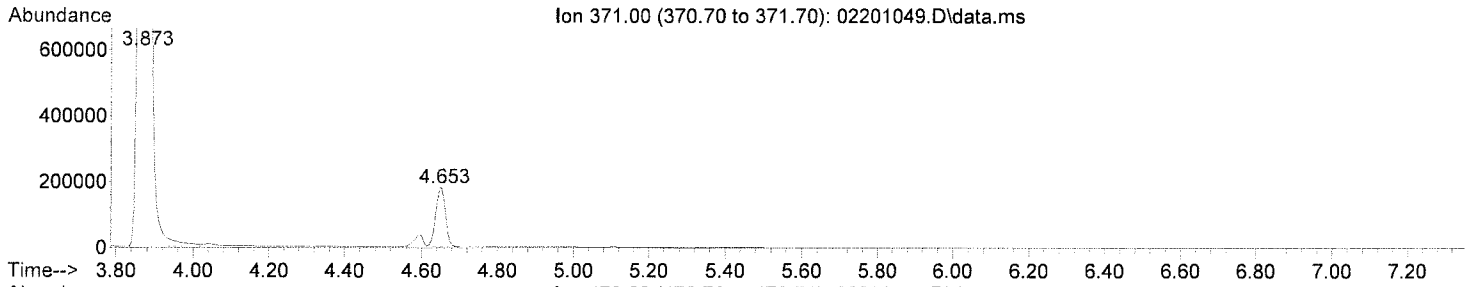
File   :I:\Instrument Data\CDA\5977 TOX GCMS CdA\2017\6-6-2017\02201
...   049.D
Operator   : Instrument 65198
Instrument :   Instrument # 65198- Tox Cd'A
Acquired   : 07 Jun 2017   00:34   using AcqMethod cthc 101415.M
Sample Name: positive control
Misc Info : FE03121501 in neg lot 42617;   am 3

```
Data Path : I:\Instrument Data\CDA\5977 TOX GCMS CdA\2017\6-6-2017\
Data File : 02201049.D
Acq On    : 07 Jun 2017  00:34
Operator  : Instrument 65198
Sample    : positive control
Misc      : FE03121501 in neg lot 42617;   am 3
ALS Vial  : 22    Sample Multiplier: 1


Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON                        Filtering: 5
Sampling  : 1                          Min Area: 2 % of largest Peak
Start Thrs: 0.2                        Max Peaks: 100
Stop Thrs : 0                          Peak Location: TOP


If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5


Method    : C:\msdchem\1\METHODS\DEFAULT.M
Title     :


Signal    : EIC Ion 371.00 (370.70 to 371.70): 02201049.D\data.ms
```

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.873	8	17	44	rBV	8384628	11538546	100.00%	97.339%
2	4.653	155	162	184	rVB	178809	315415	2.73%	2.661%

```
             Sum of corrected areas:     11853961
Signal    : EIC Ion 473.00 (472.70 to 473.70): 02201049.D\data.ms
```

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.201	68	78	90	rBV	19568	27497	18.60%	12.232%
2	4.653	154	162	178	rVB	85937	147856	100.00%	65.774%
3	5.110	237	247	259	rVB	25854	49442	33.44%	21.994%

```
             Sum of corrected areas:      224795
Signal    : EIC Ion 488.00 (487.70 to 488.70): 02201049.D\data.ms
```

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.599	139	152	157	rBV	676351	1077001	100.00%	92.125%
2	4.653	157	162	171	rVB	53882	92066	8.55%	7.875%

```
             Sum of corrected areas:     1169067

DEFAULT.M Thu Jun 08 11:26:39 2017
```