



## LC-MS Conditions for Samples # 1 to 60

All samples were run on a Surveyor HPLC-Thermo Finnigan LCQ DECA ion trap mass spectrometer system (Thermo Finnigan, San Jose, CA, USA) in ESI positive mode using a Luna C18(2), 20 x 2.00 mm column (Phenomenex, Torrance, CA, USA). The mobile phase and gradient were as follows -

Aqueous phase= 1% Solution A, 0.03% Trifluoroacetic acid in Water  
Organic phase= 1% Solution A, 0.03% Trifluoroacetic acid in Methanol  
(Solution A= 2mM Ammonium Acetate in 2-Propanol:Water 90:10)

5% Organic phase 0 - 0.2 min, 5 - 100% Org. 0.2 - 2.5 min, 100% Org. 2.5 - 3.5 min, 100 - 5% Org. 3.5 - 3.6 min, 5% Org. 3.6 - 5.0 min.

The delay time between the HPLC trace and the MS TIC is about 0.07 min. Flow rate= 300 $\mu$ L/min.

The samples were prepared by taking 5  $\mu$ l sample at 10mM in DMSO and adding 2 mL of 2mM Ammonium acetate in 50:50 Methanol:Water. All samples were filtered using 0.45  $\mu$ m PTFE syringe filters (Canadian Life Science, Peterborough, ON, Canada).

The mass spectrometer parameters were as follows-

Sheath Gas Flow Rate(arb) :	50
Aux Gas Flow Rate(arb):	10
Spray Voltage (kV):	1.5
Capillary Temp ( $^{\circ}$ C):	235
Capillary Voltage (V):	10.00
Tube Lens offset (V):	-10.00

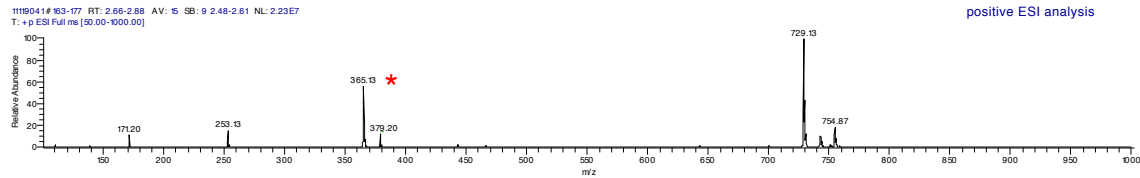
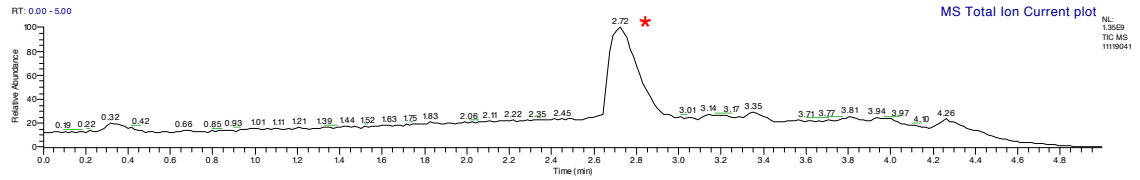
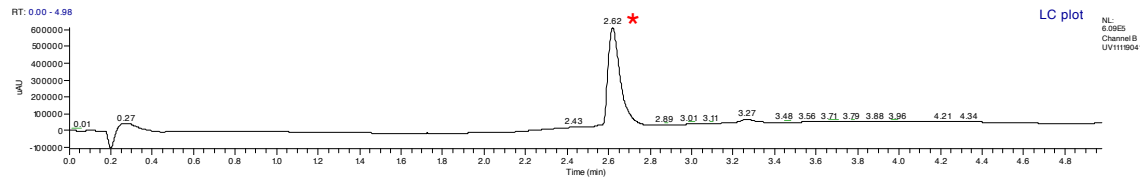
Prepared by:

Karen Robinson, B.Sc  
Mass Spectrometry Analyst

### Sample 1:

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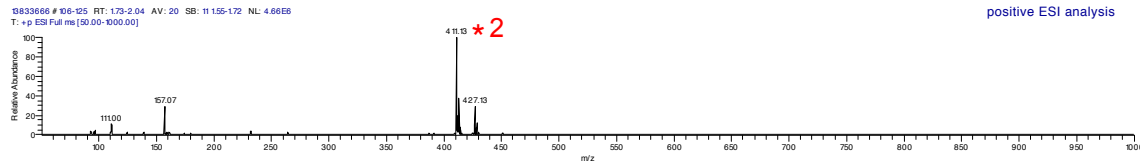
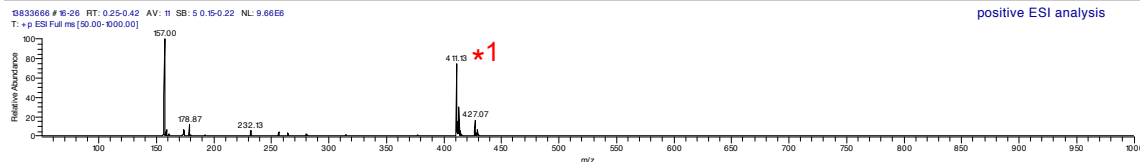
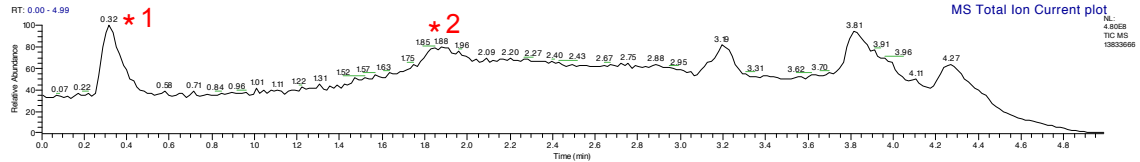
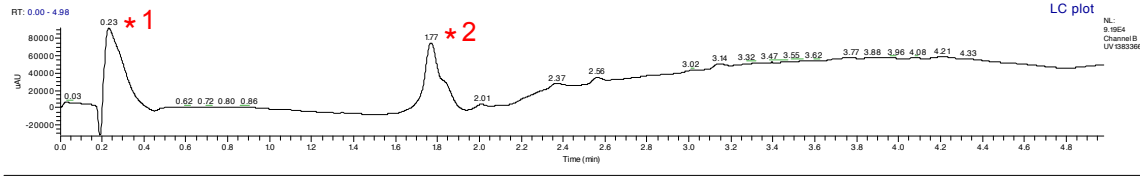
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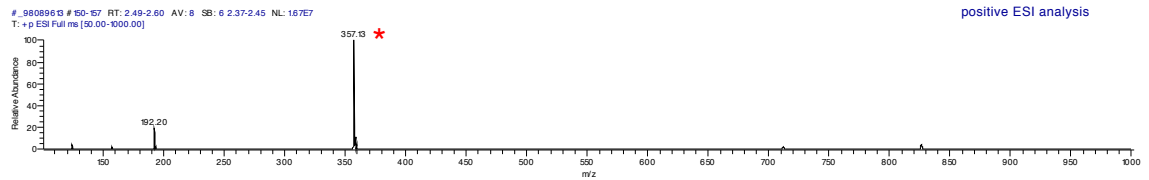
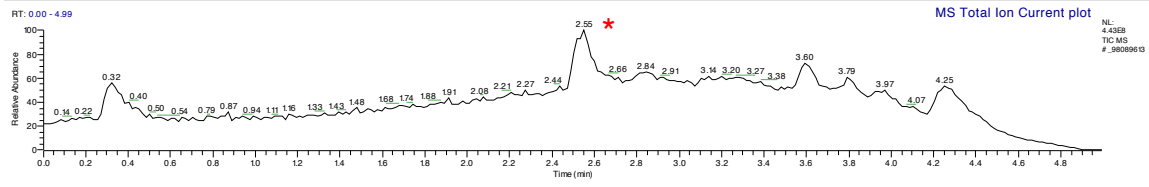
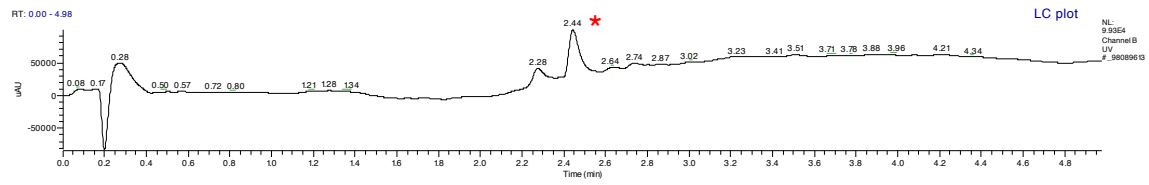
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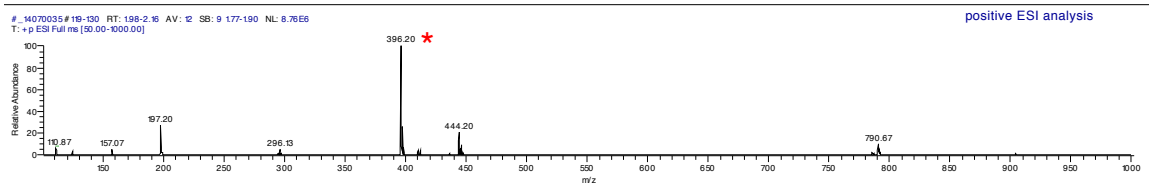
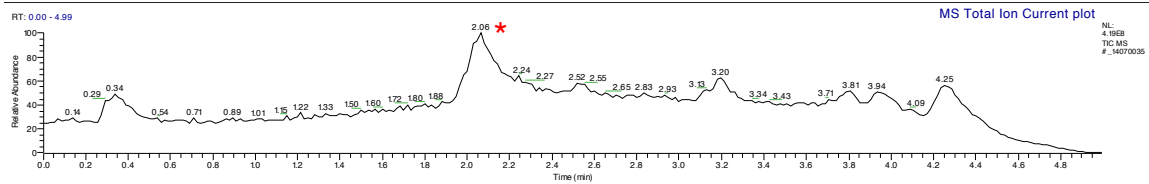
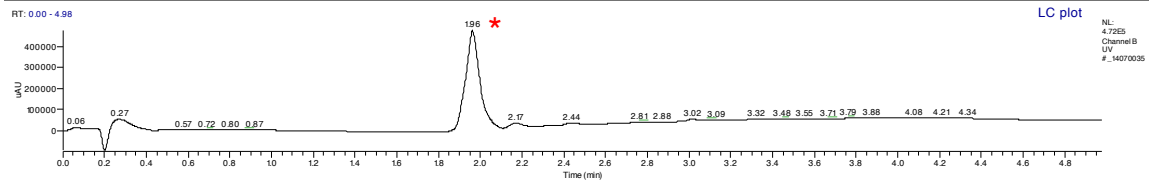
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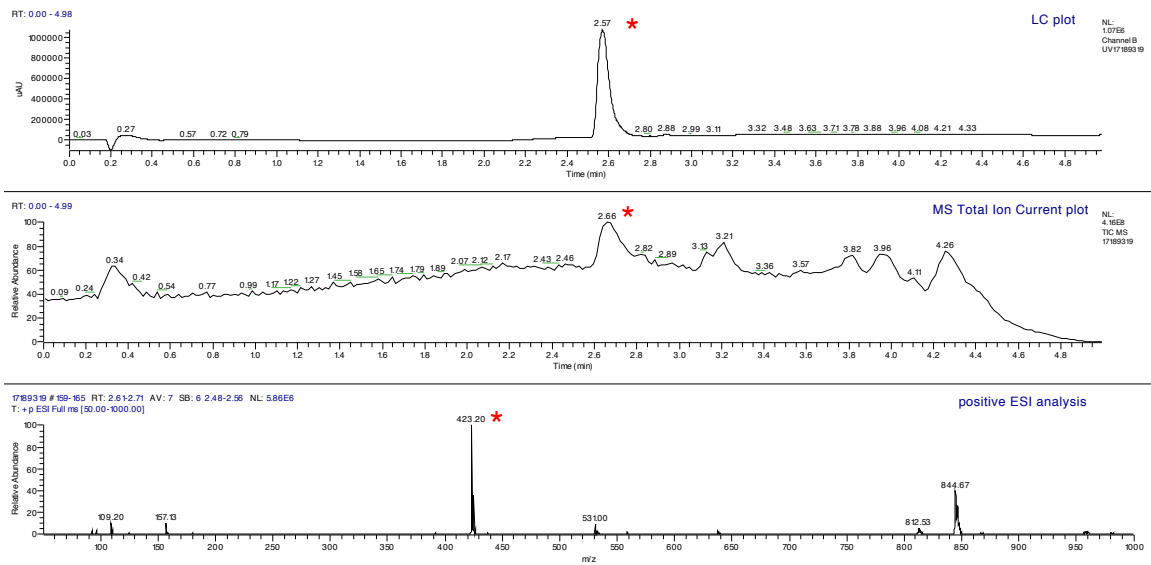
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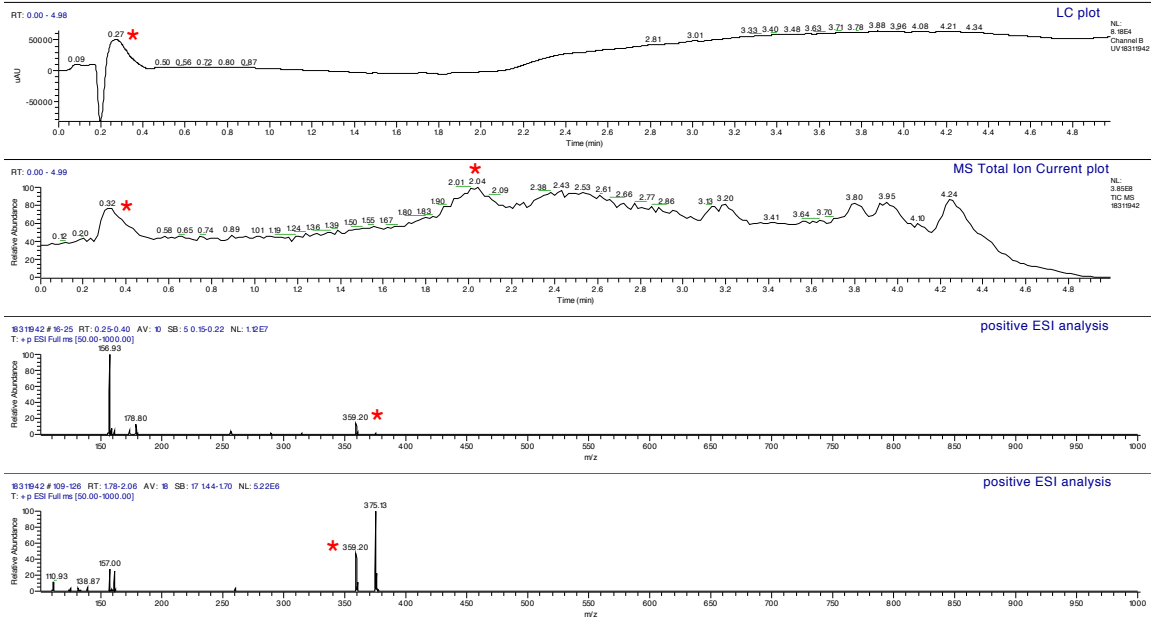
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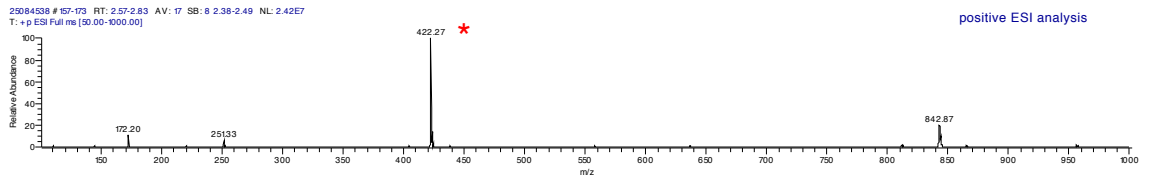
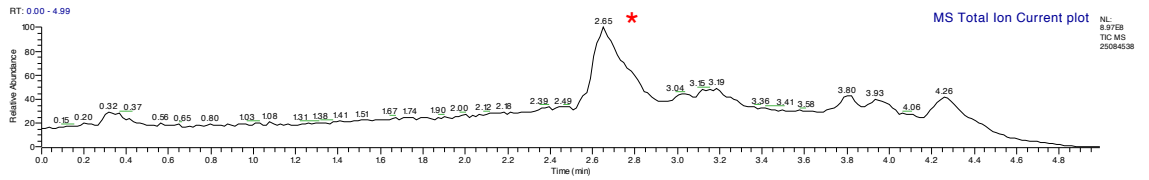
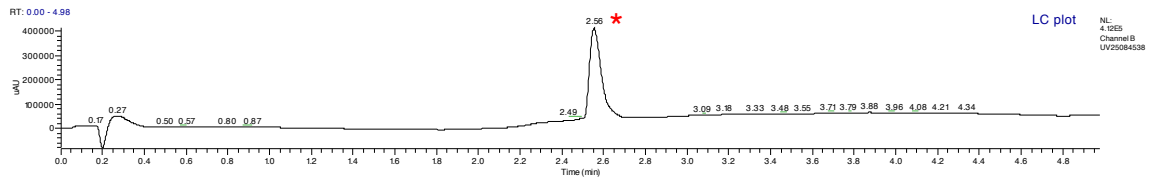
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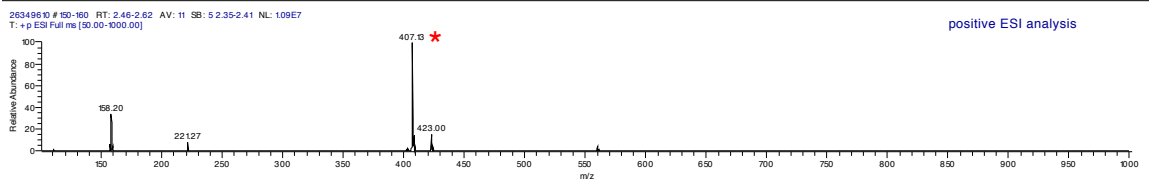
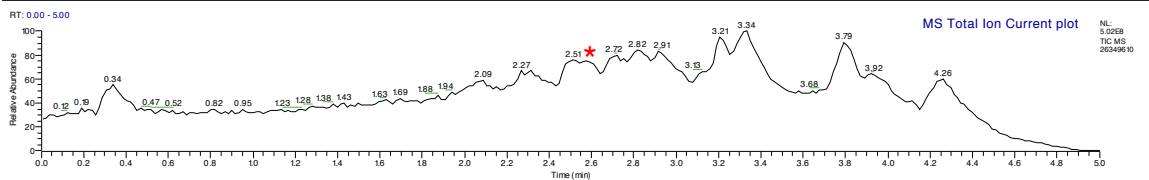
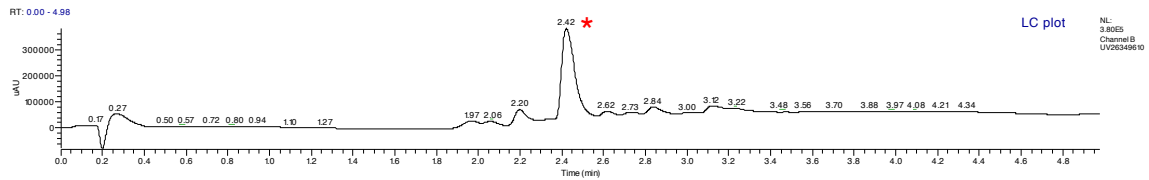
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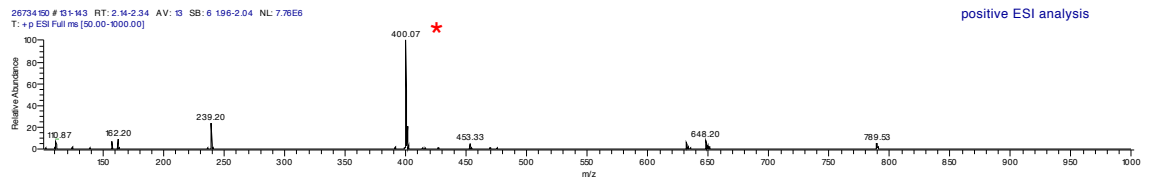
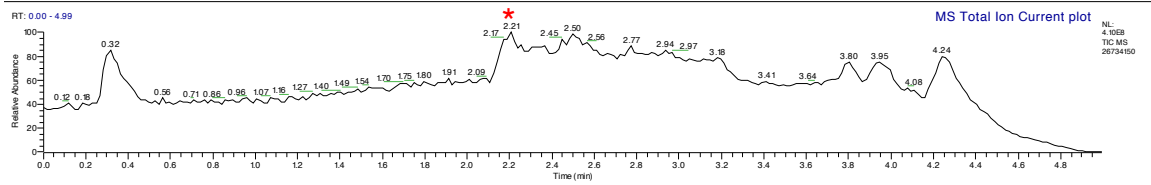
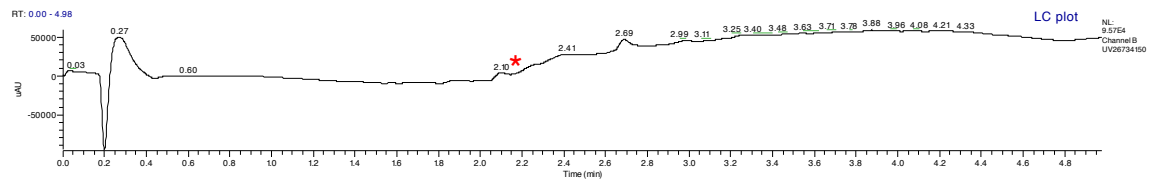
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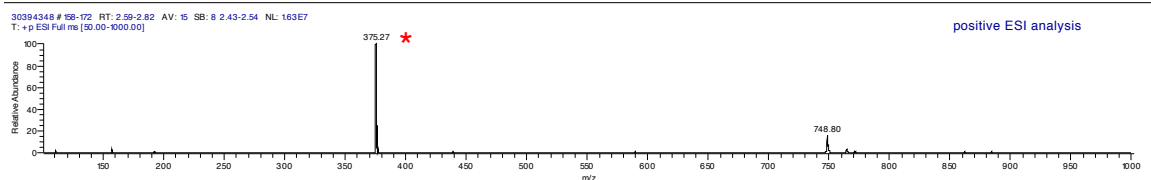
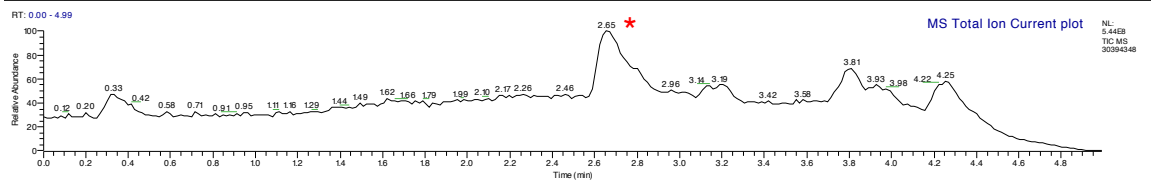
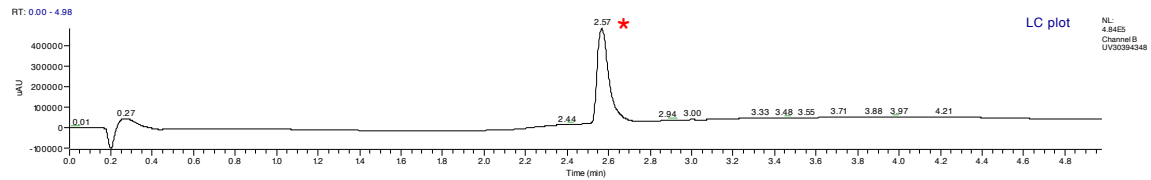
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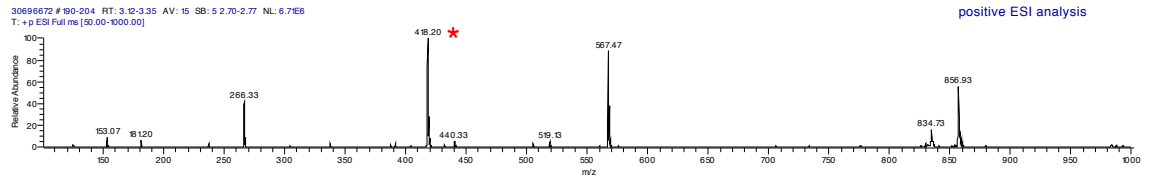
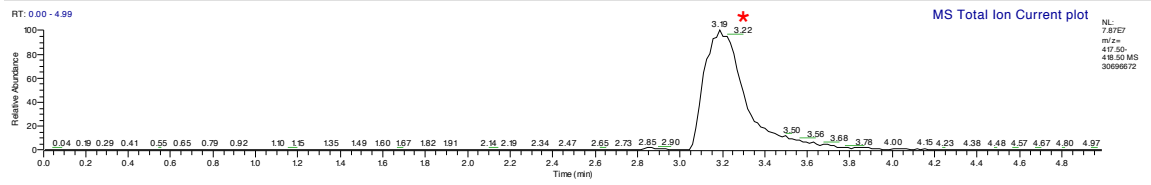
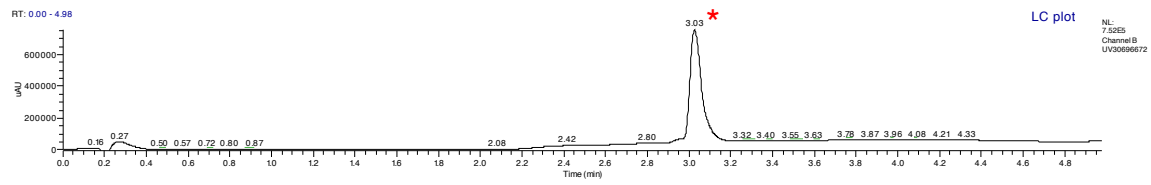
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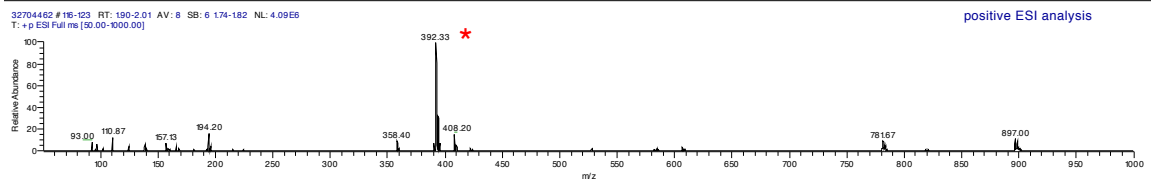
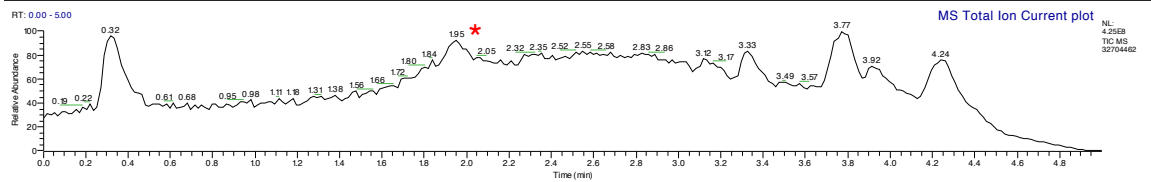
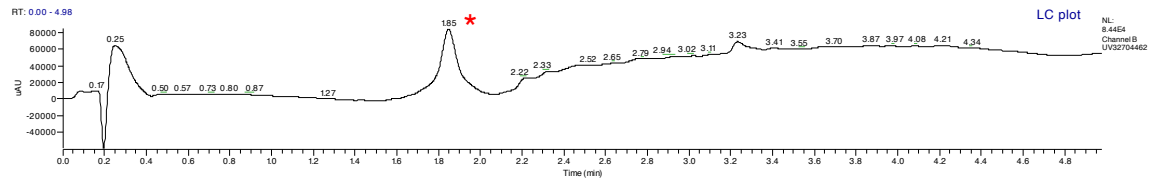
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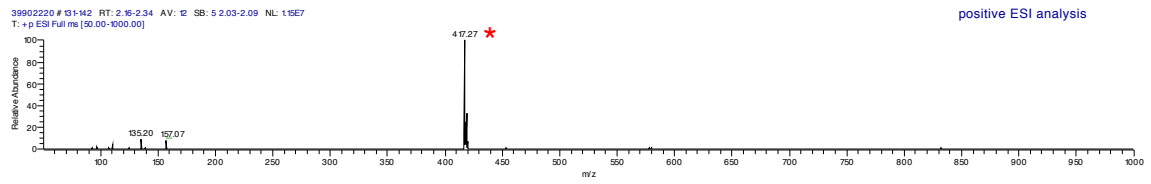
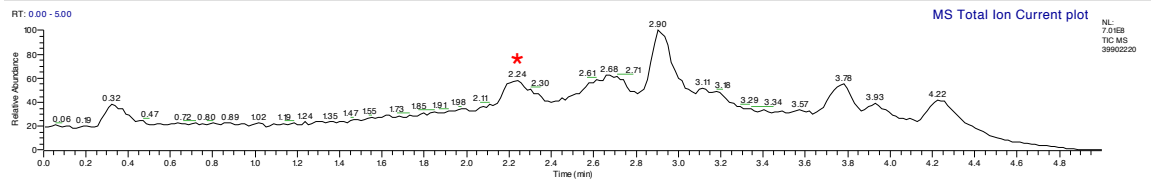
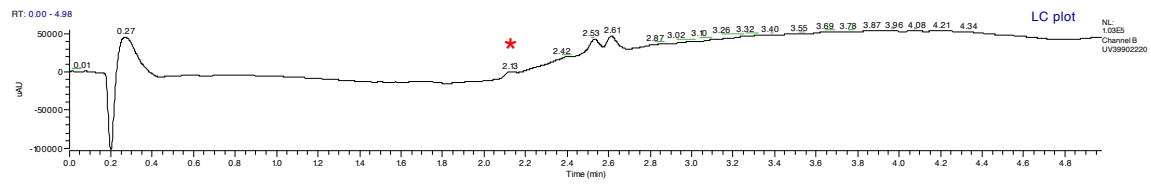
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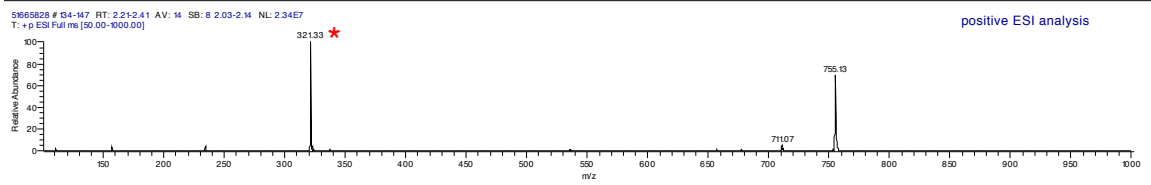
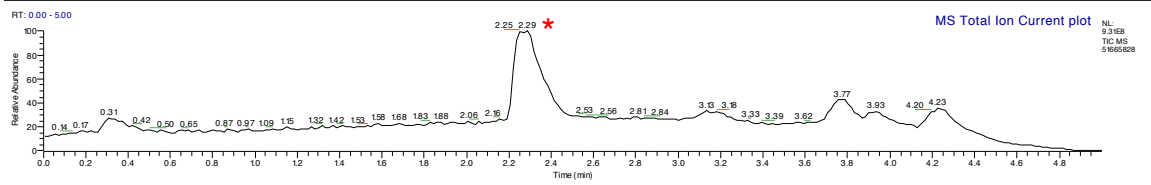
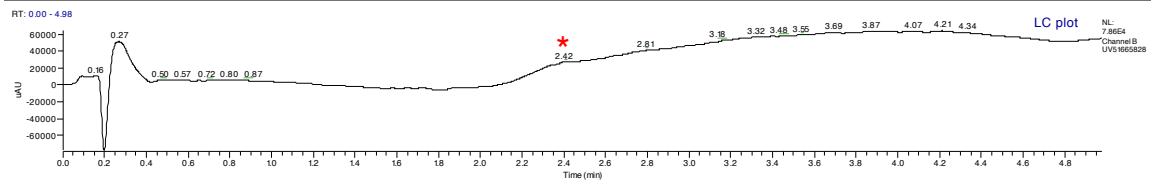
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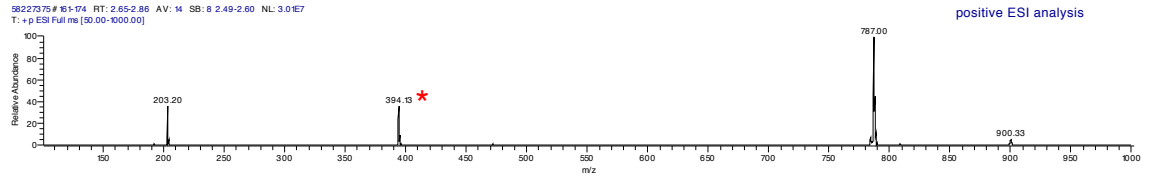
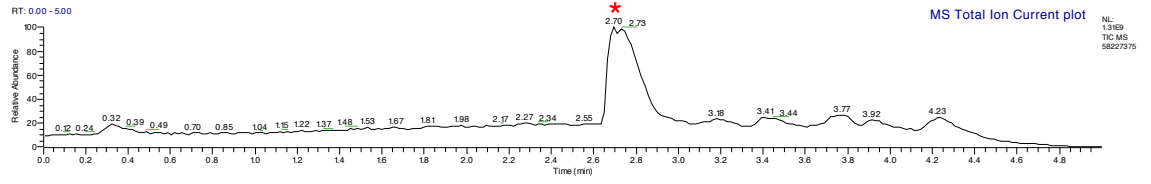
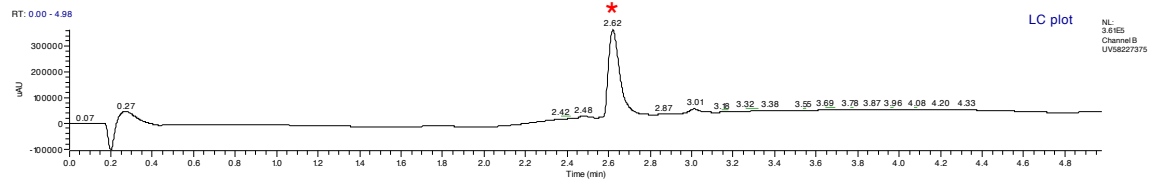




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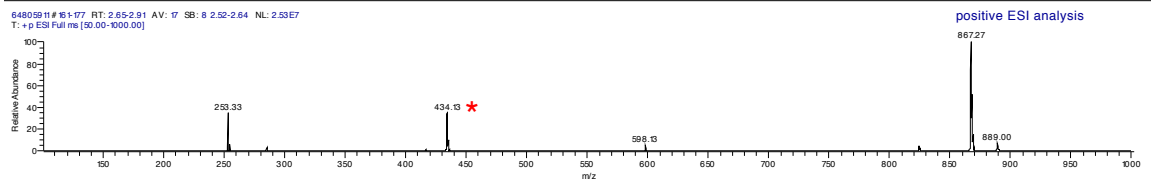
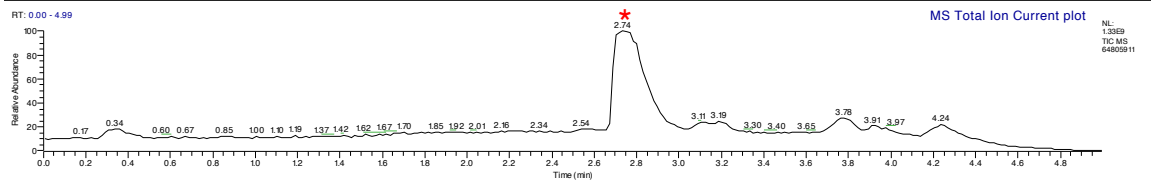
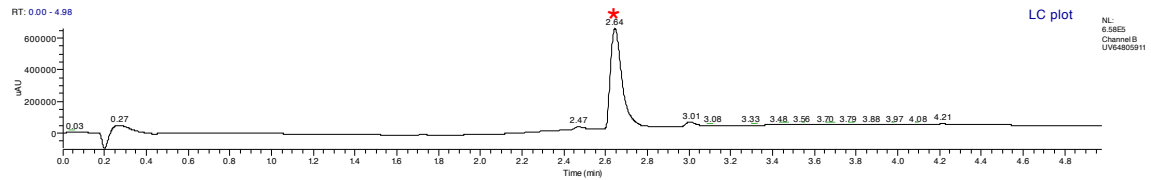
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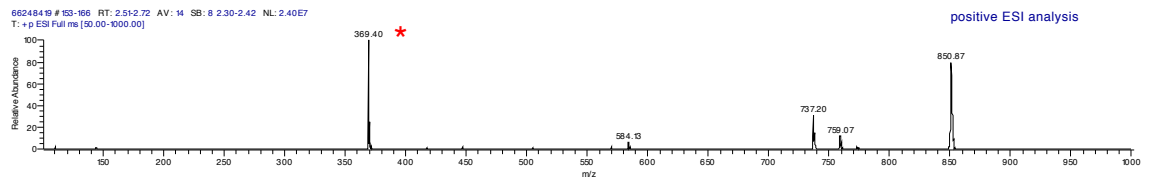
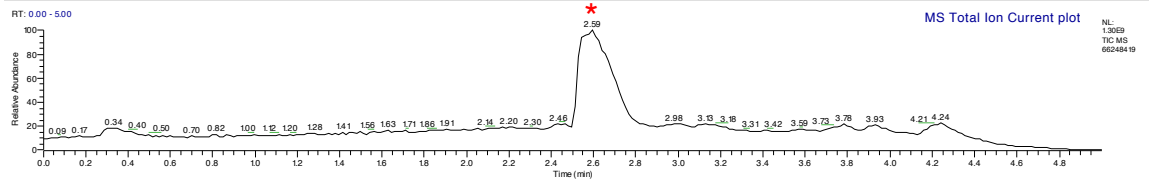
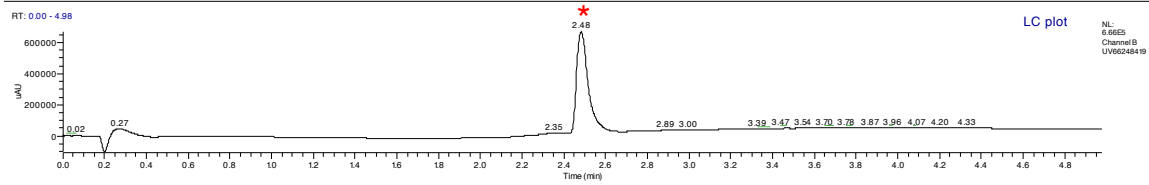
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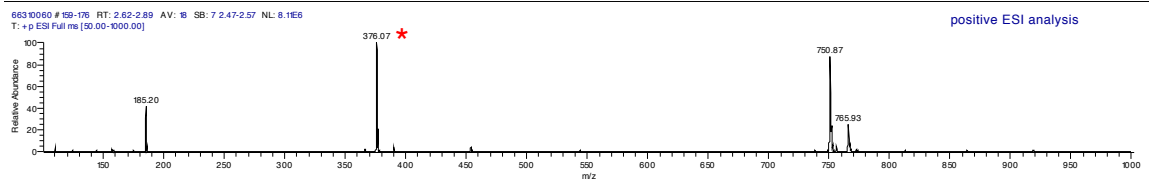
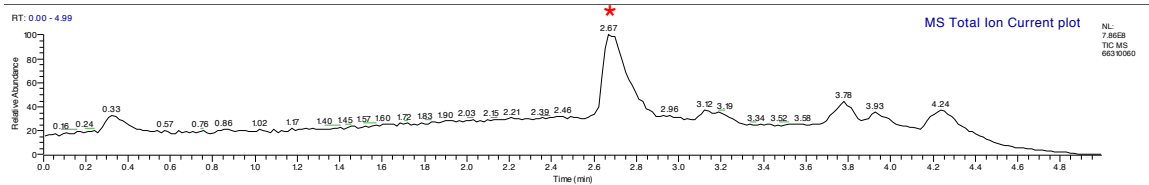
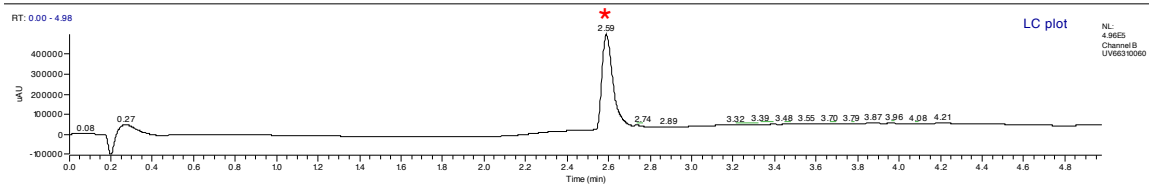
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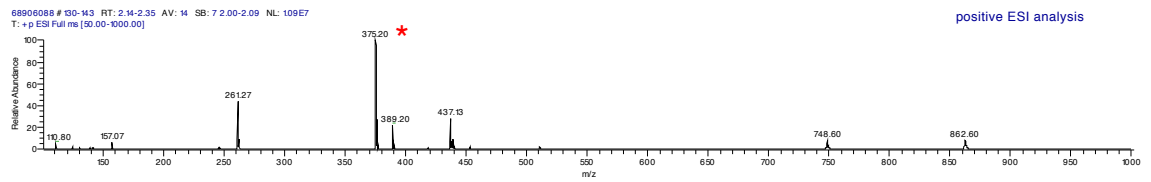
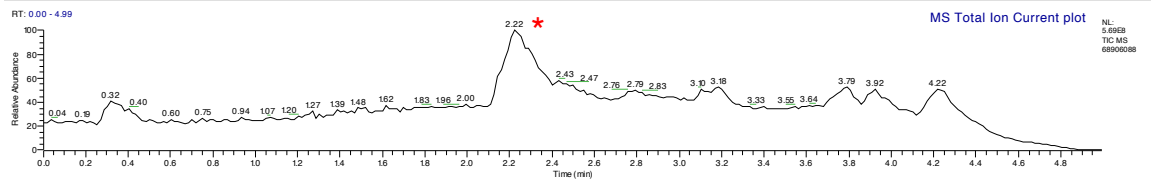
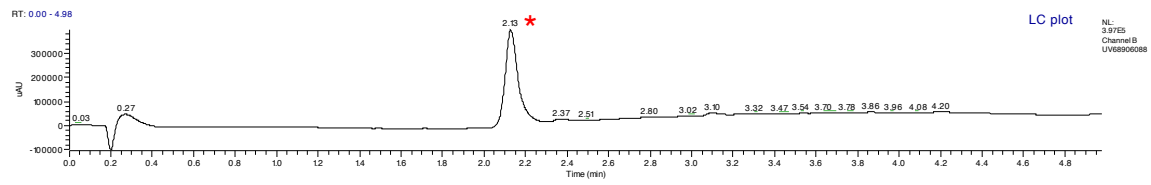
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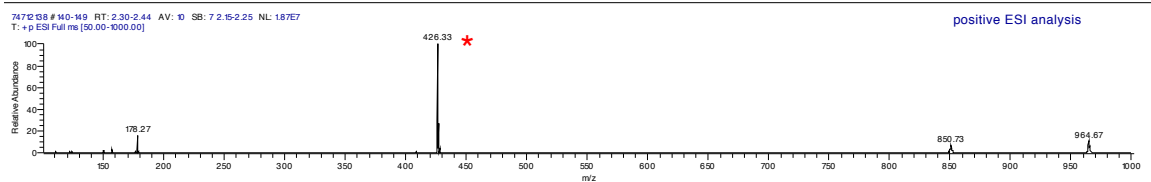
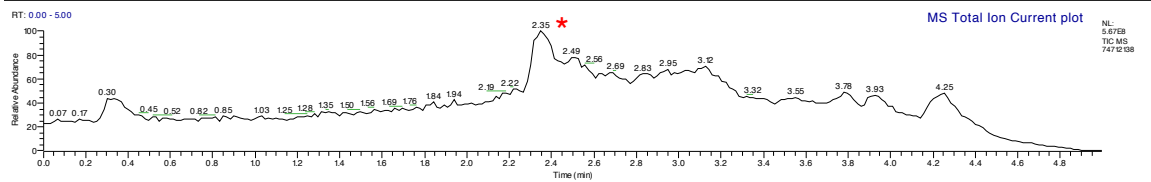
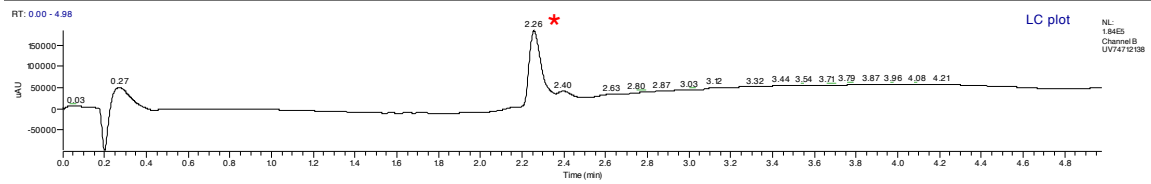
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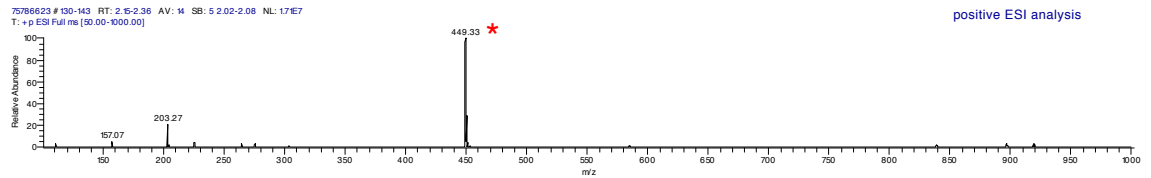
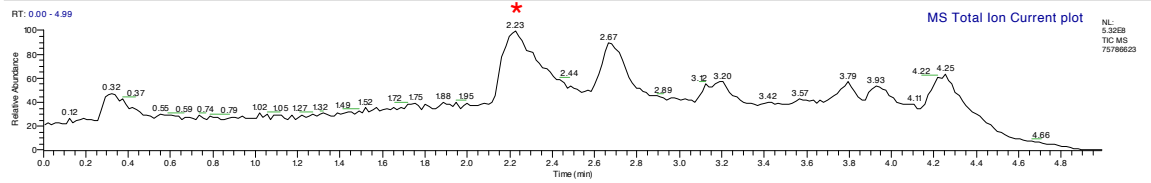
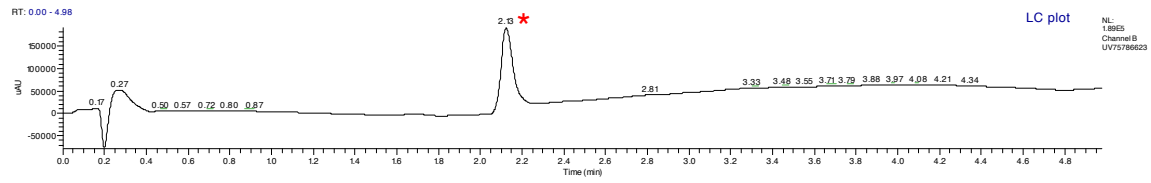
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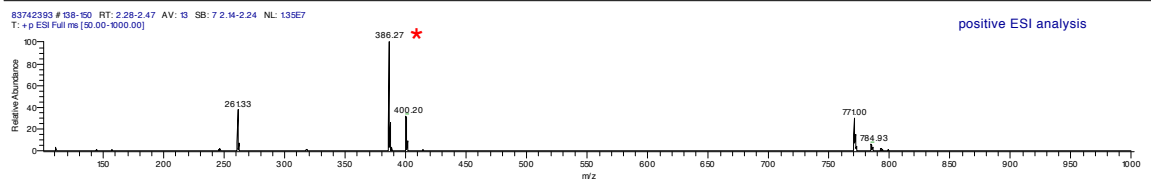
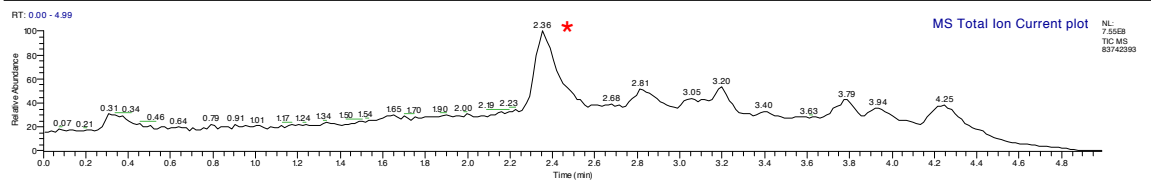
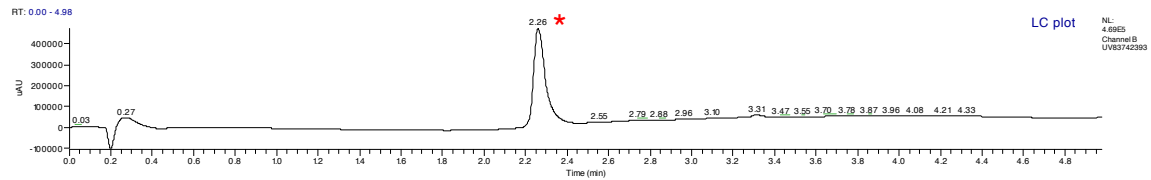
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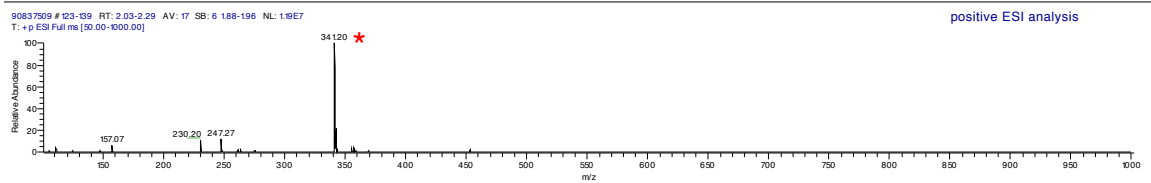
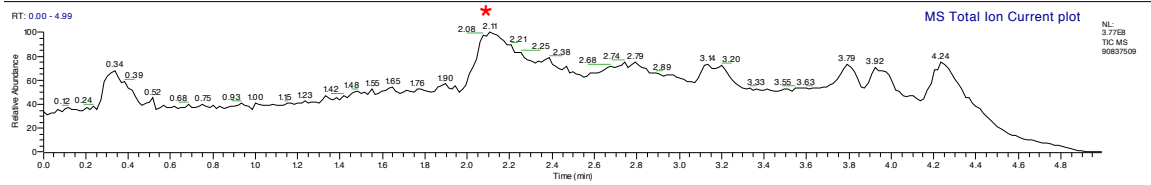
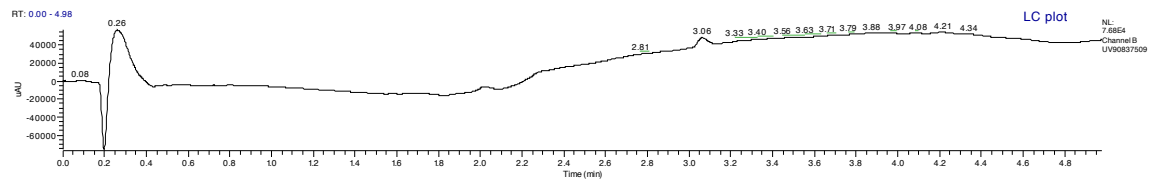
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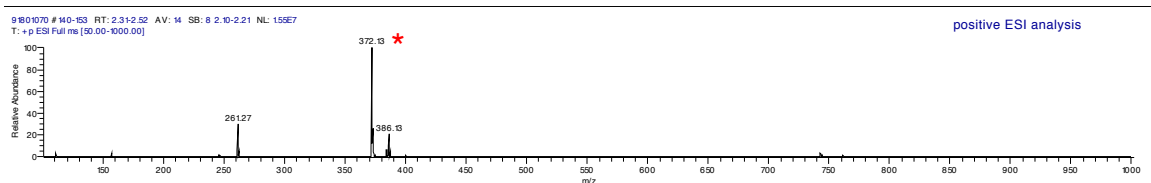
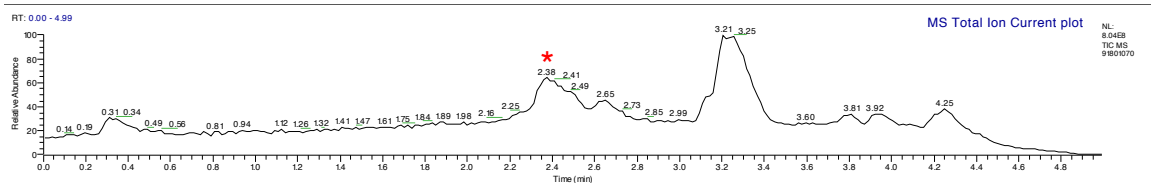
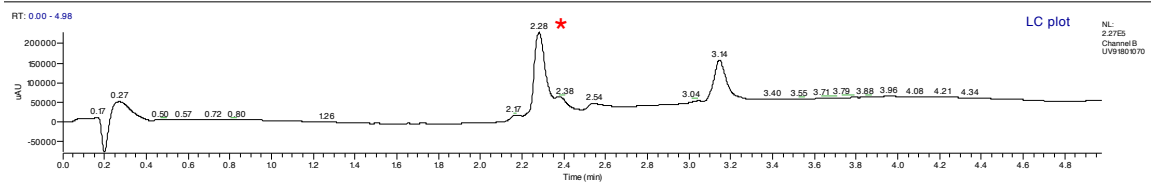
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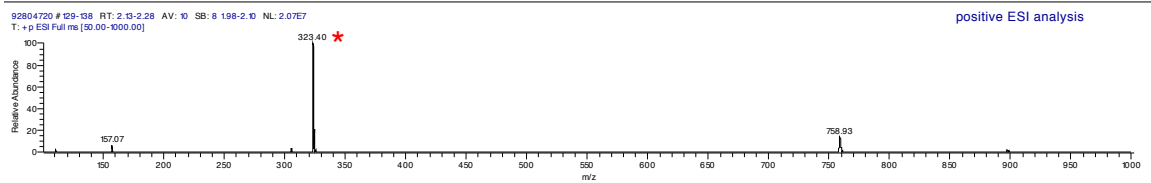
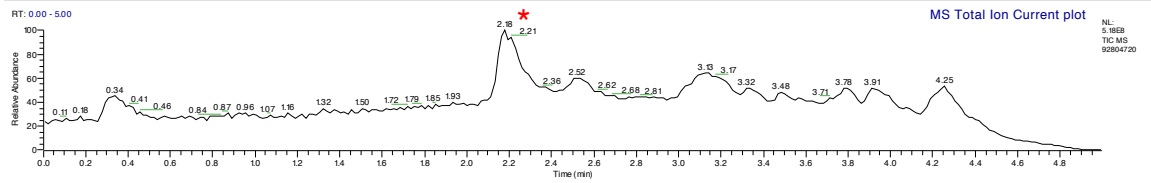
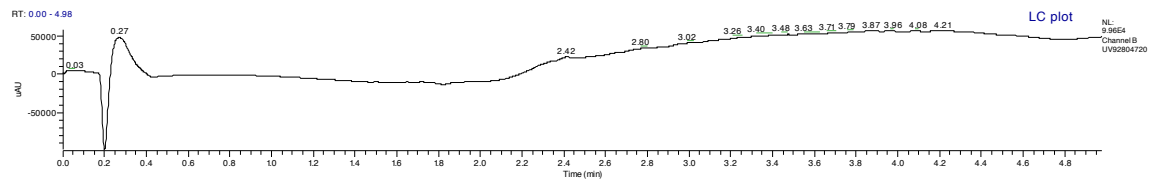
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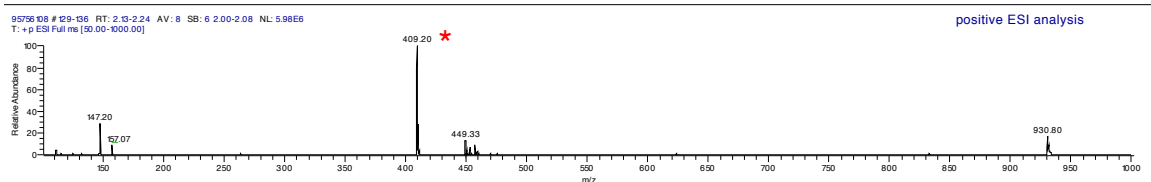
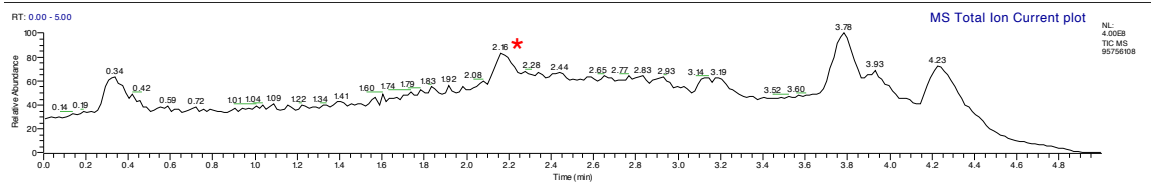
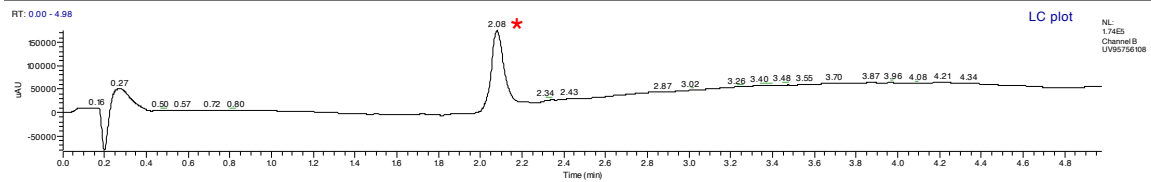
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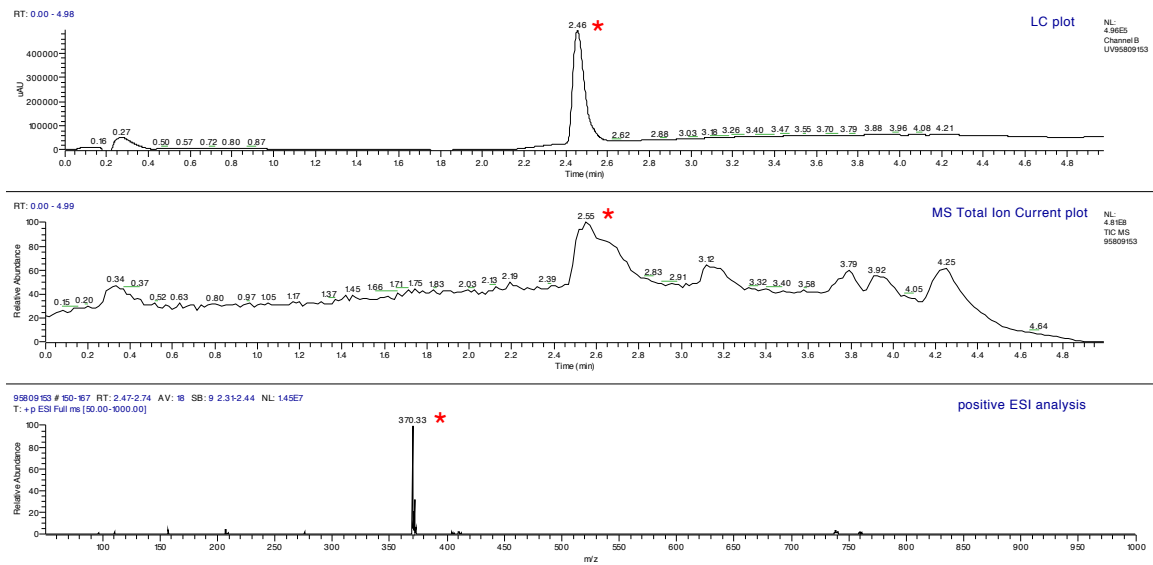
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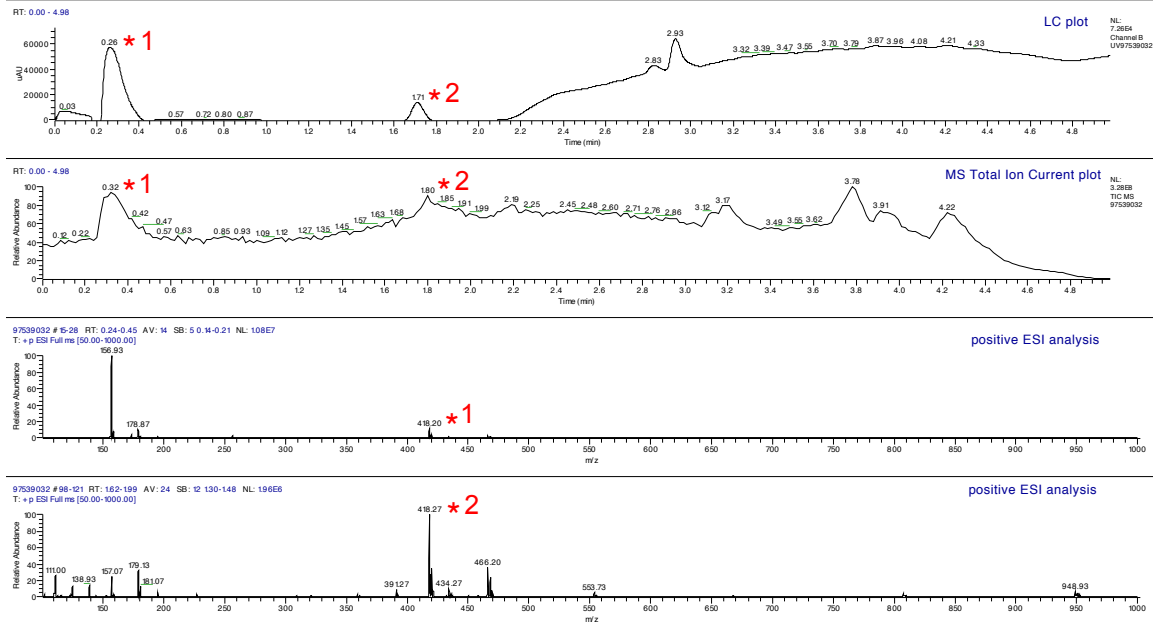
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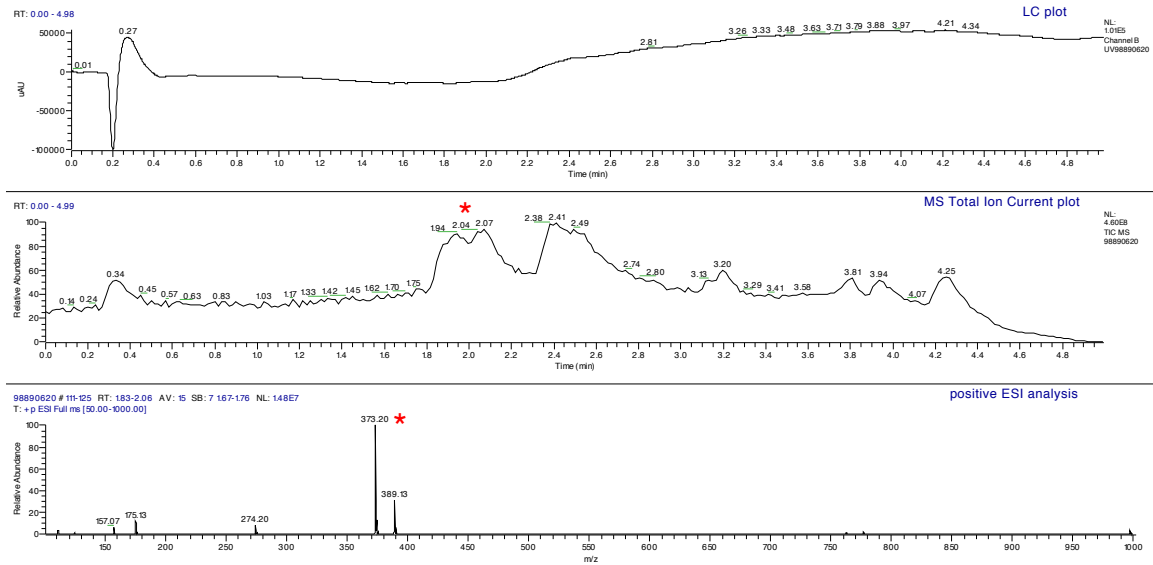
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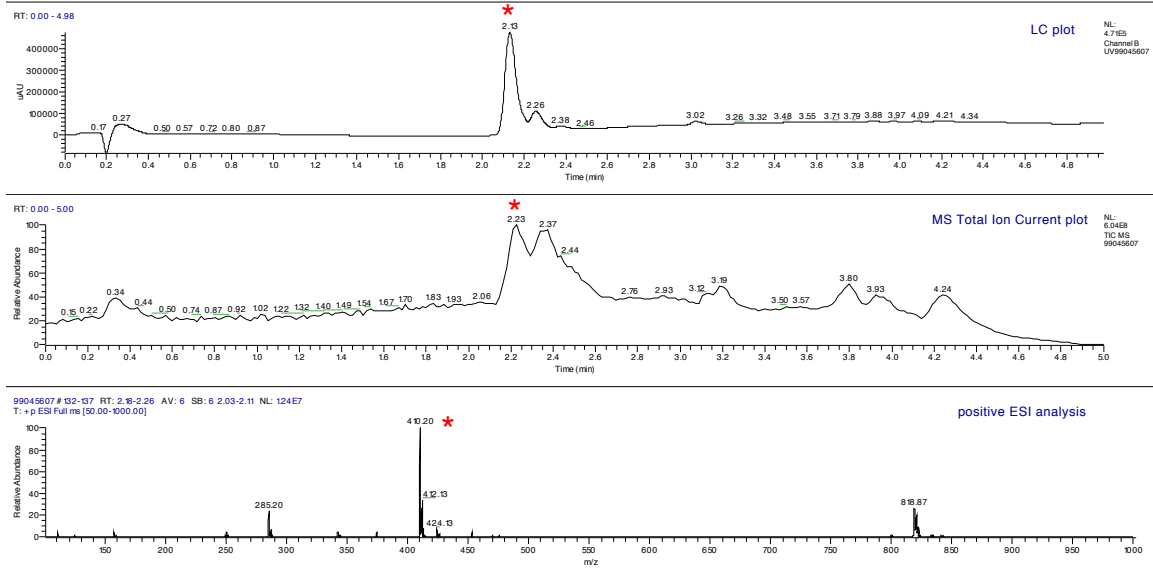
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### Sample 30:

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4/17/2009 9:23:02 PM

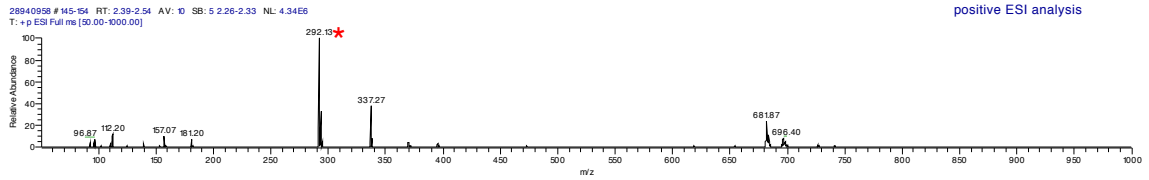
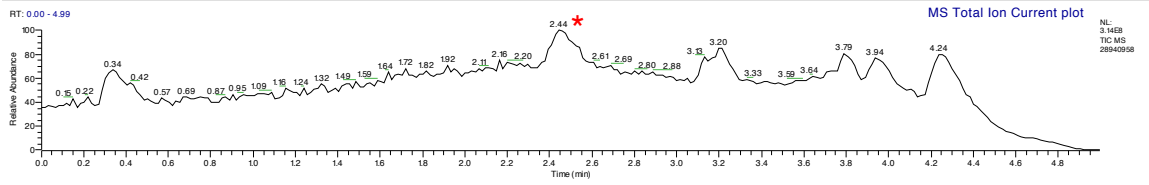
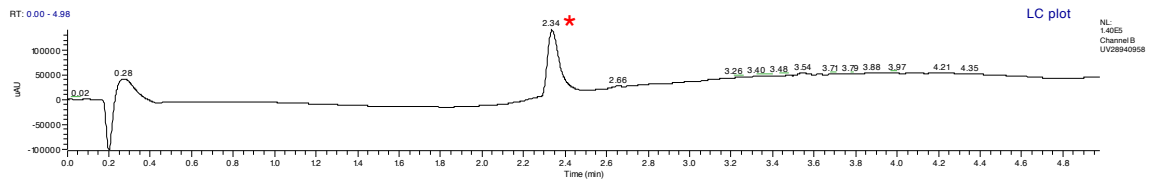




### Sample 31:

C:\Dalton\data\041709\28940958

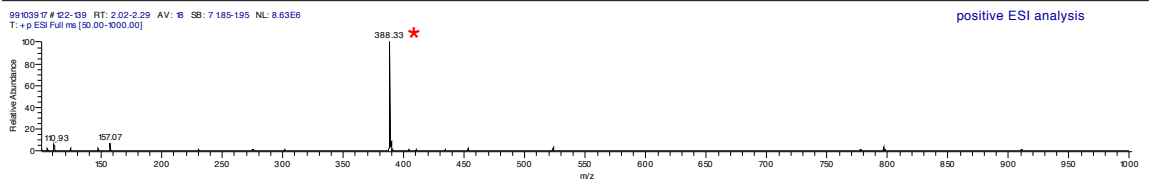
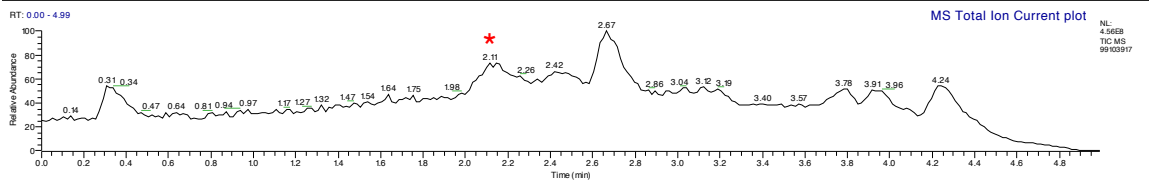
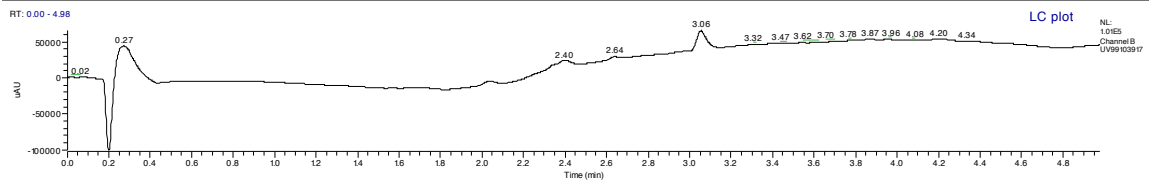
4/17/2009 9:40:04 PM



### Sample 32:

C:\Dalton\data\041709\99103917

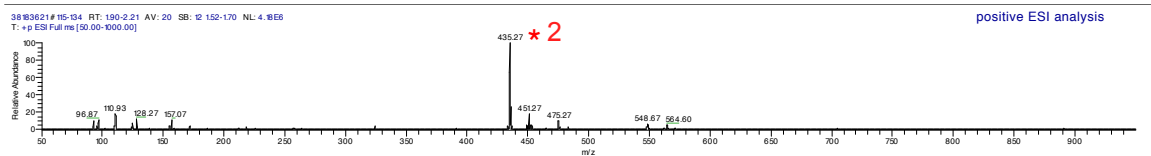
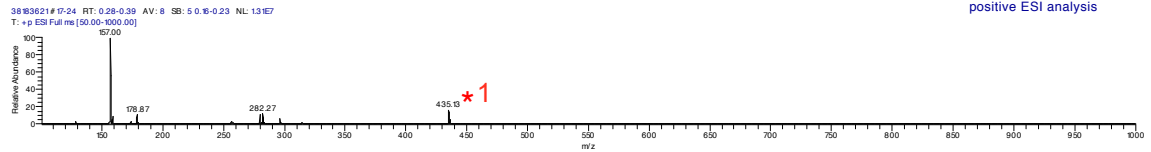
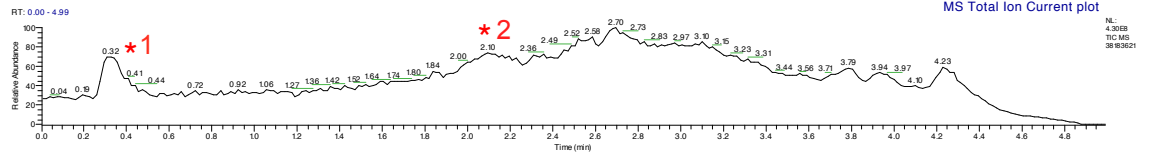
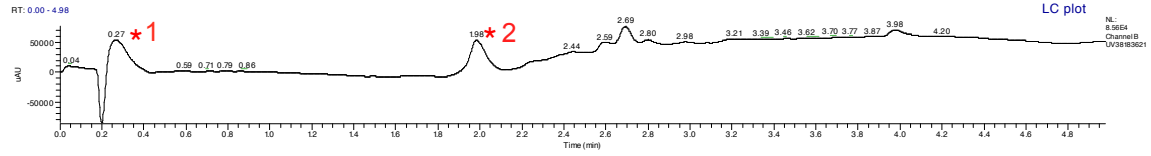
4/17/2009 9:45:49 PM



### Sample 33:

C:\Dalton\data\041709\38183621

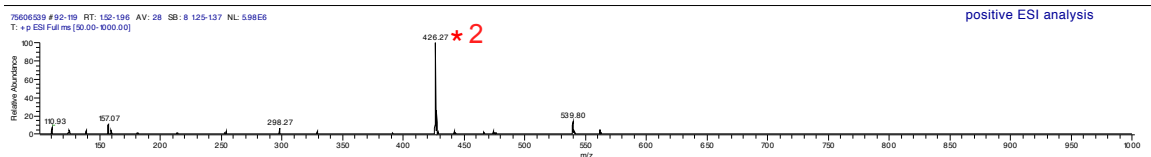
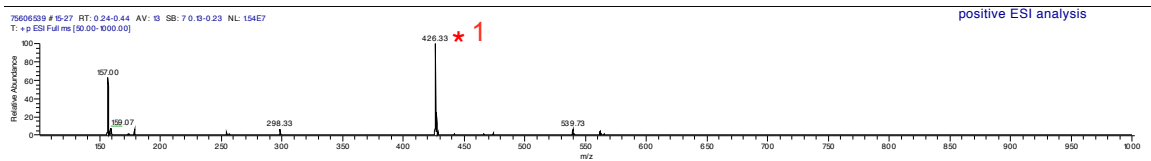
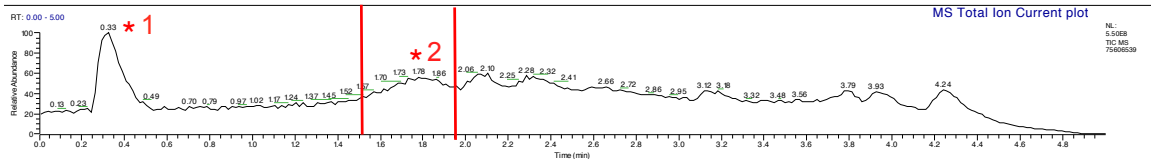
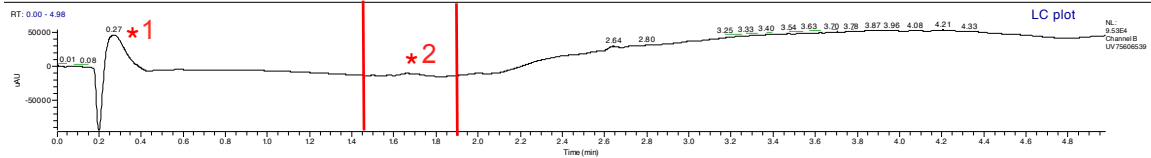
4/17/2009 9:51:35 PM



### Sample 34:

C:\Dalton\data\041709\75606539

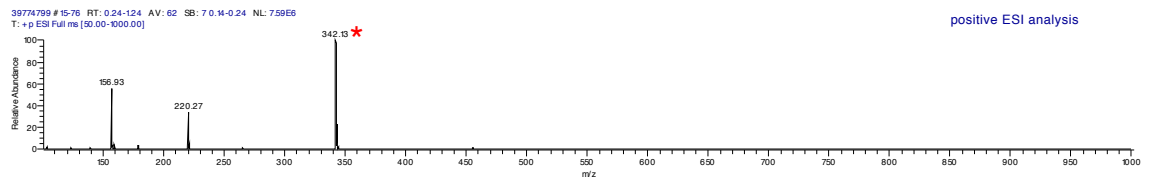
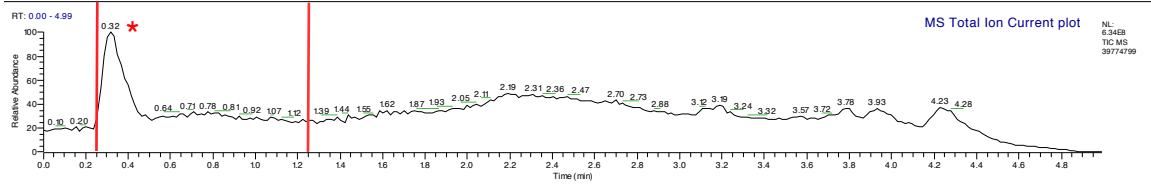
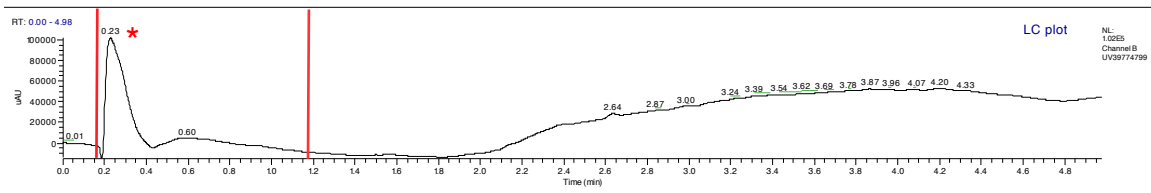
4/17/2009 9:57:22 PM



### Sample 35:

C:\Dalton\data\041709\39774799

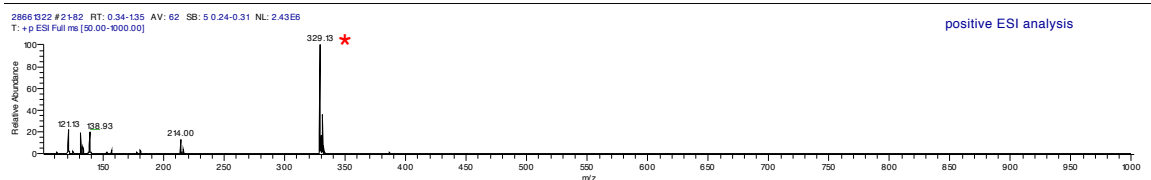
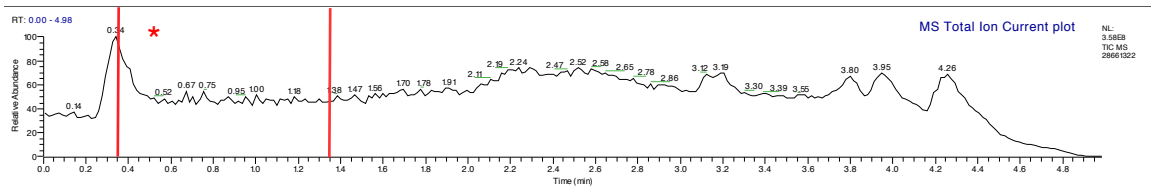
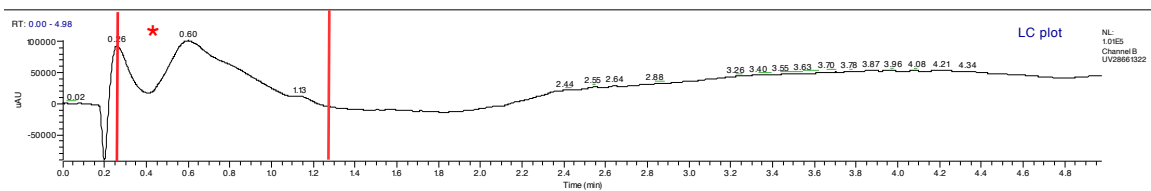
4/17/2009 10:03:08 PM



### Sample 36:

C:\Dalton\data\041709\28661322

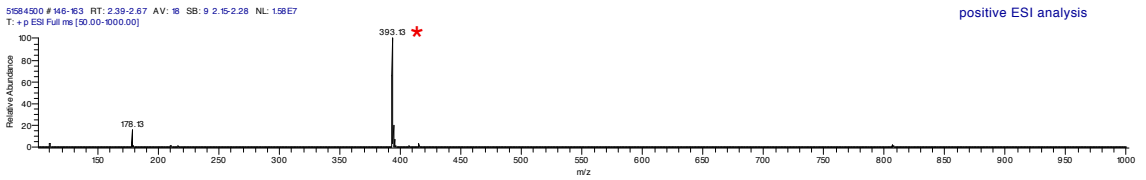
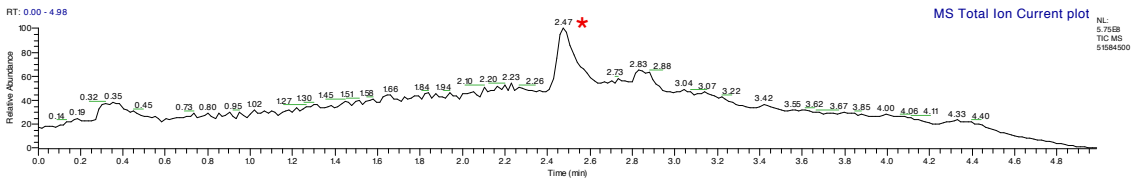
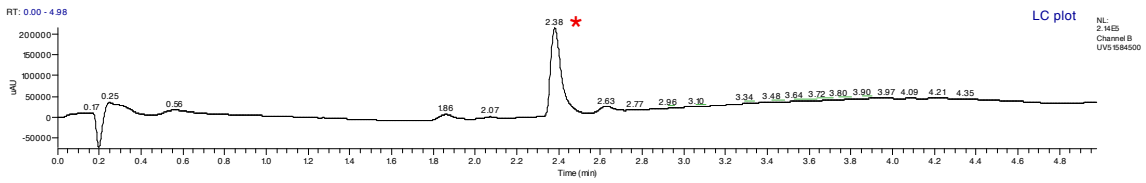
4/17/2009 10:08:55 PM



### Sample 37:

C:\Dalton\data\050509\51584500

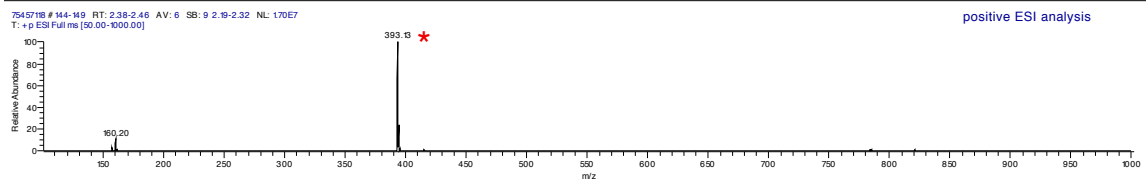
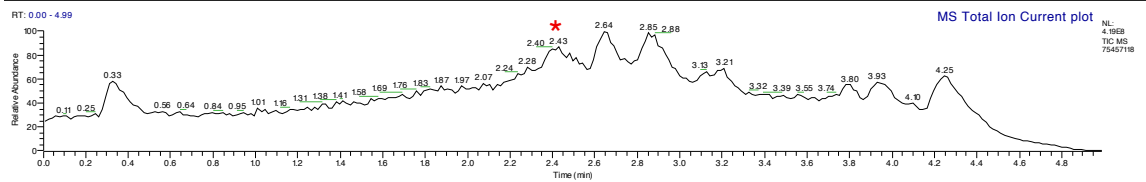
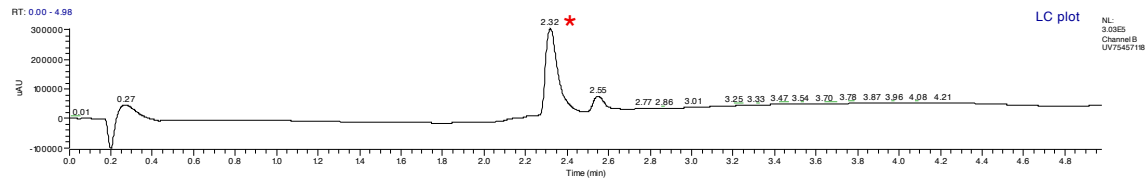
5/5/2009 11:07:46 AM



### Sample 38:

C:\Dalton\data\041709\75457118

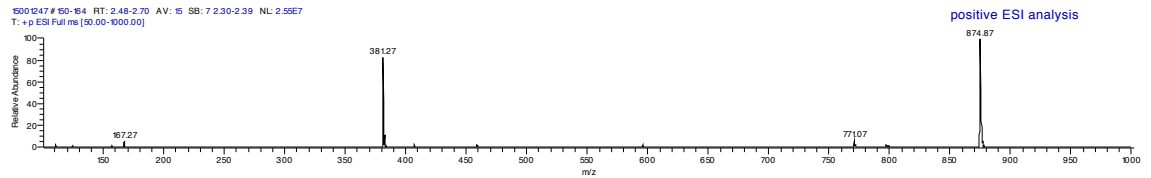
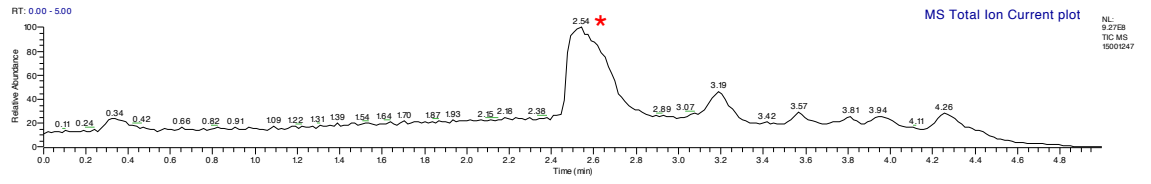
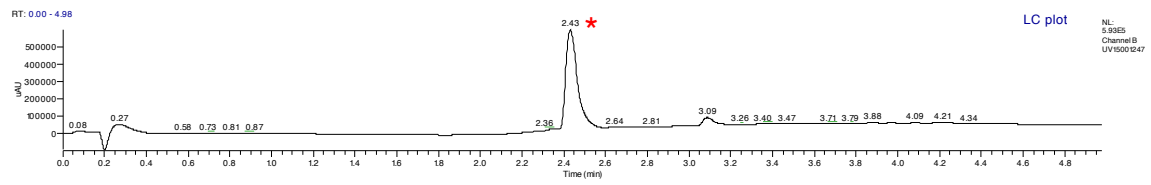
4/17/2009 10:20:26 PM



### Sample 39

C:\Dalton\data\041709\15001247

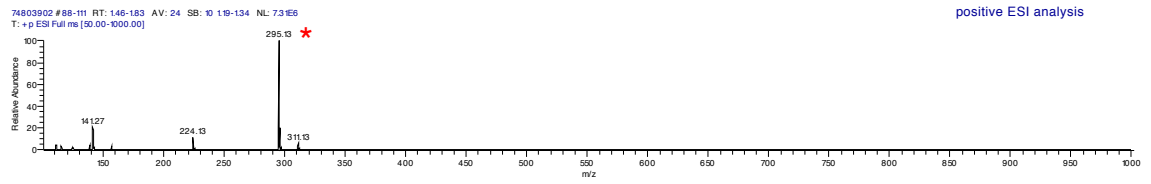
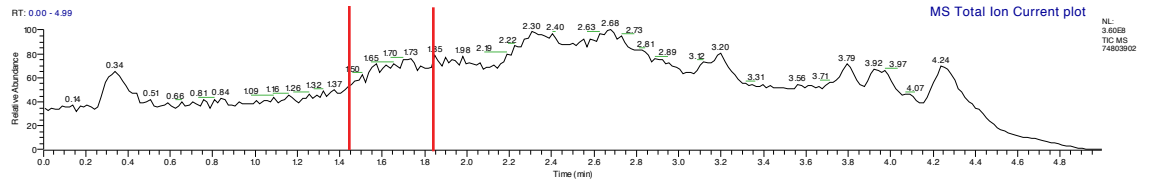
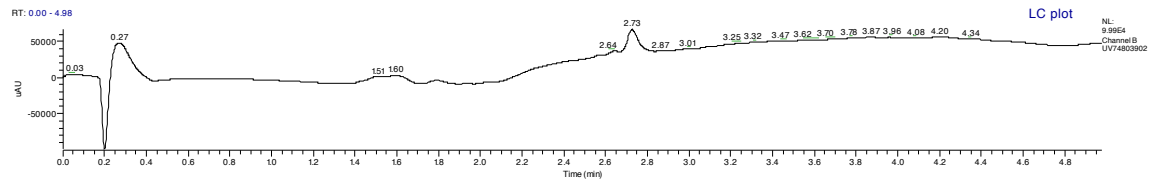
4/17/2009 10:26:12 PM



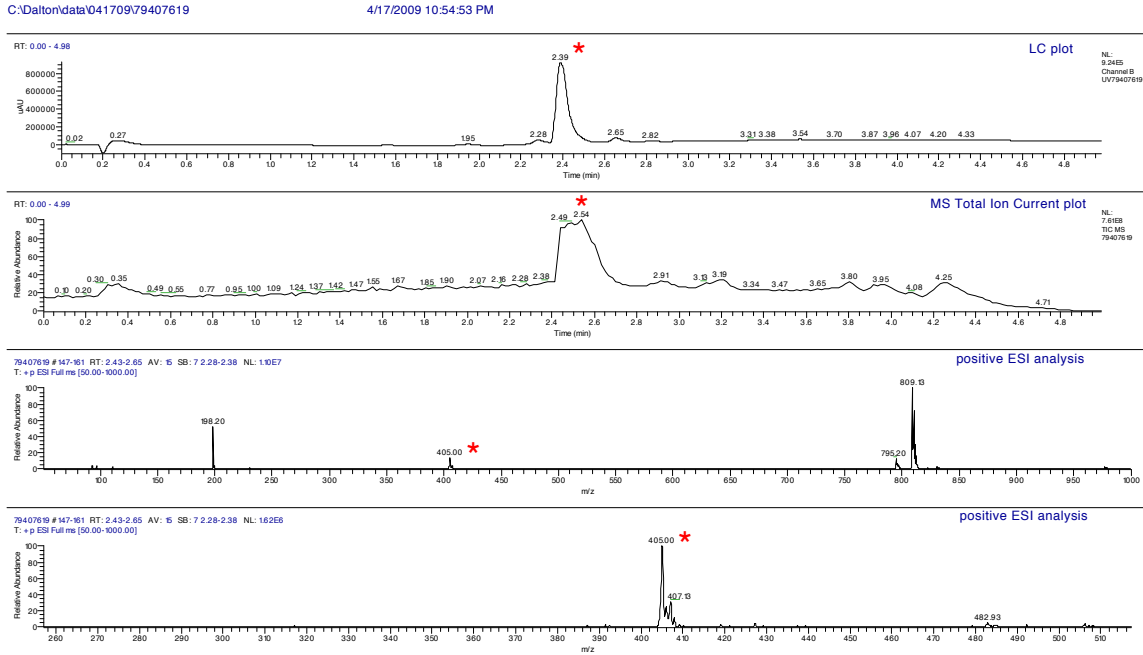
### Sample 40

C:\Dalton\data\041709\74803902

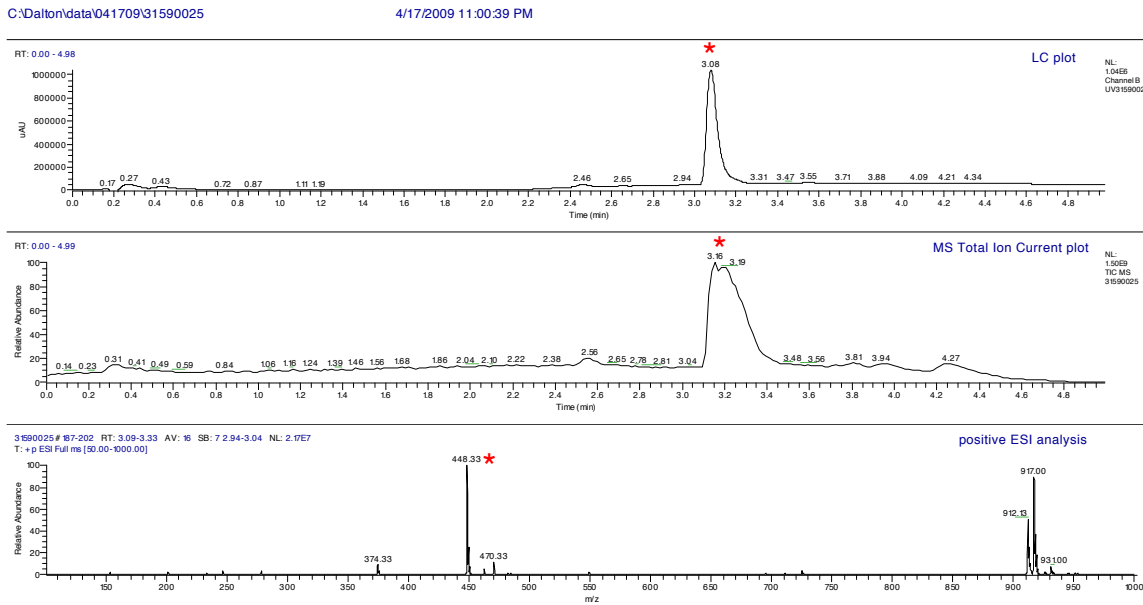
4/17/2009 10:31:57 PM



### Sample 41:



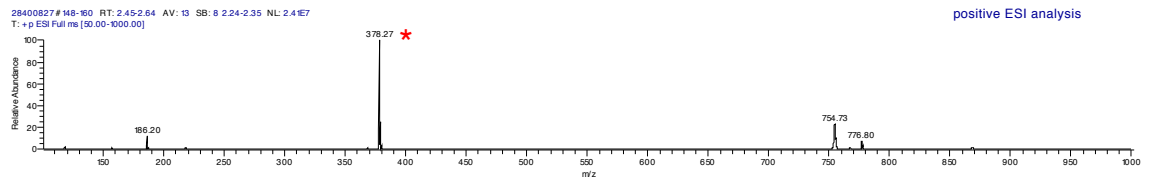
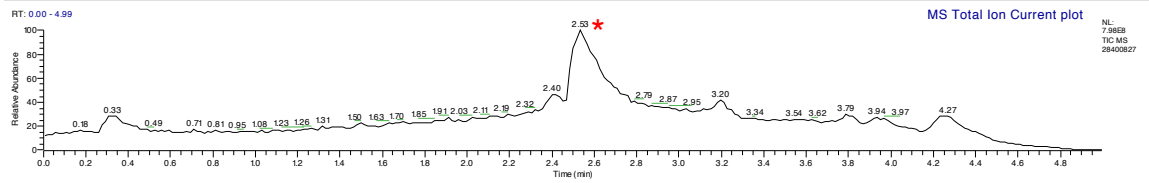
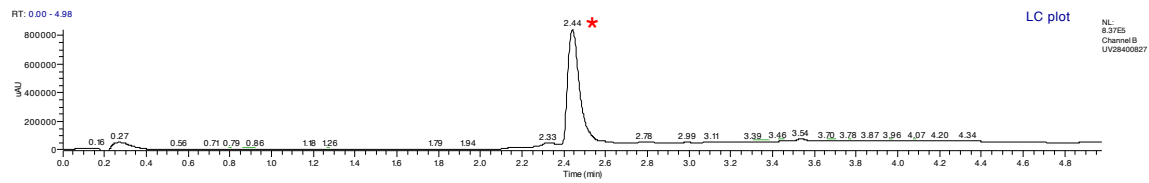
### Sample 42:



### Sample 43:

C:\Dalton\data\041709\28400827

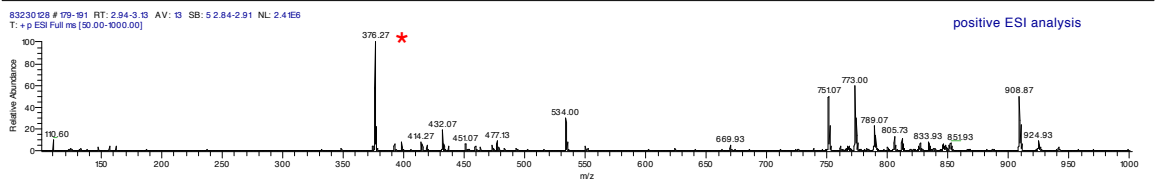
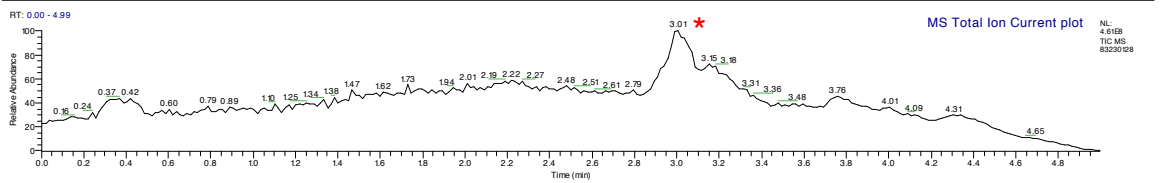
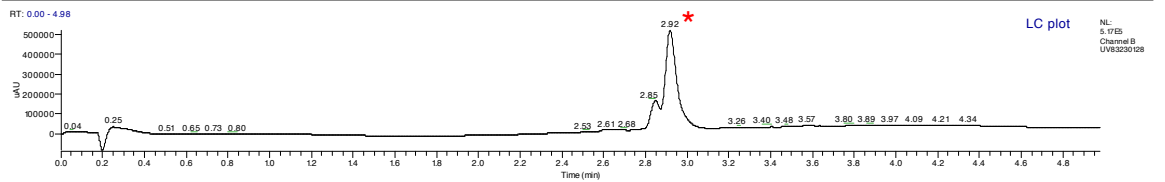
4/17/2009 11:06:19 PM



### Sample 44:

C:\Dalton\data\050509\83230128

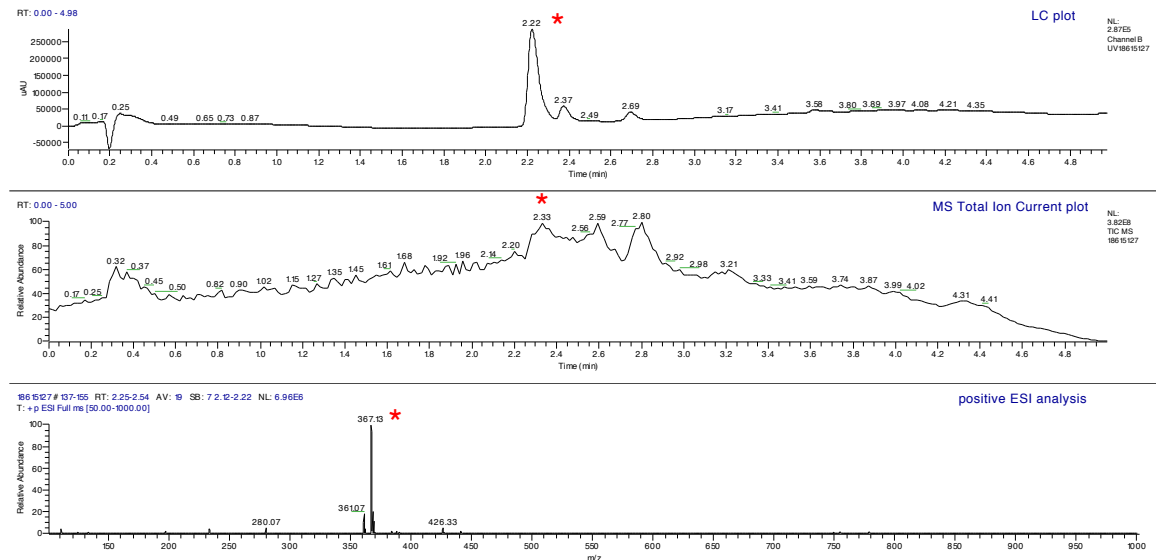
5/5/2009 11:19:07 AM



### Sample 45:

C:\Dalton\data\050509\18615127

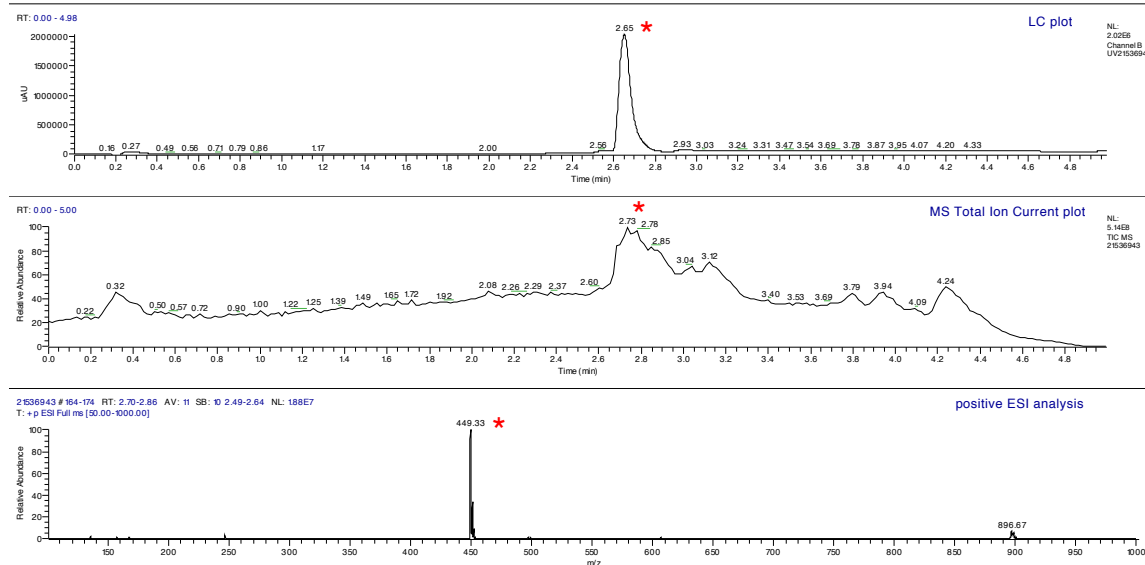
5/5/2009 11:30:32 AM



### Sample 46:

C:\Dalton\data\041709\21536943

4/17/2009 11:23:30 PM

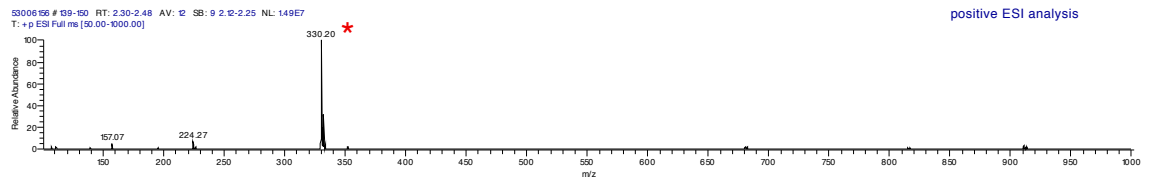
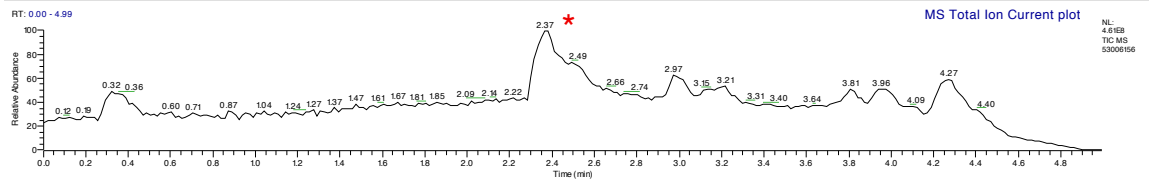
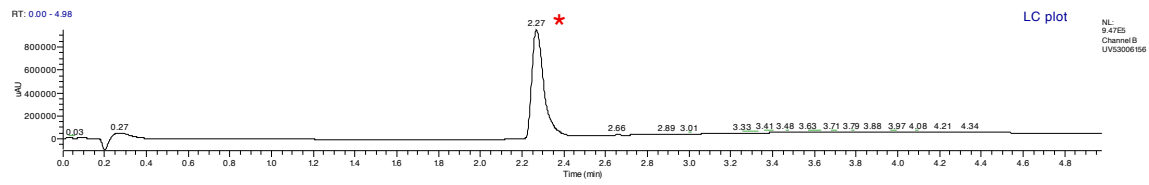




### Sample 47:

C:\Dalton\data\041709\53006156

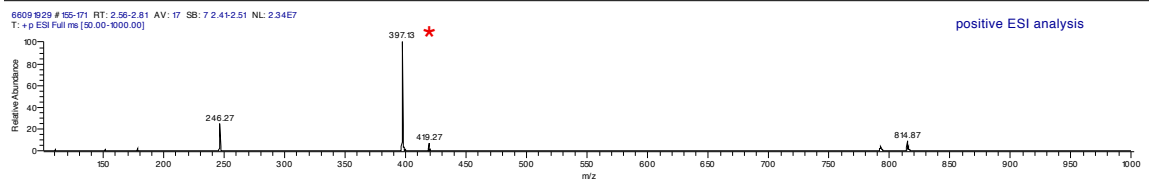
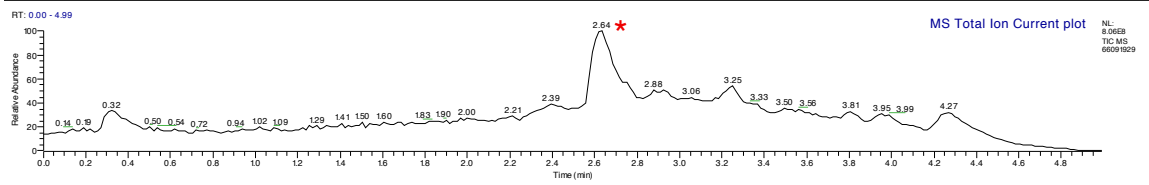
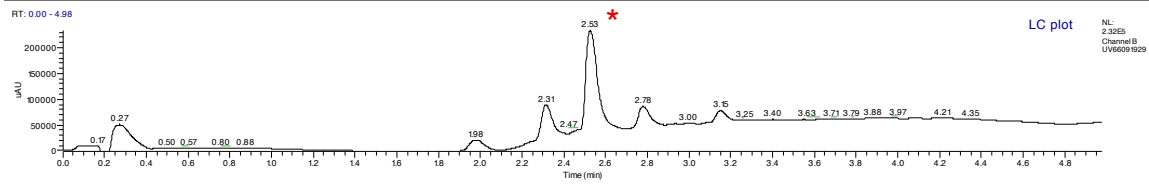
4/17/2009 11:29:10 PM



### Sample 48:

C:\Dalton\data\041709\66091929

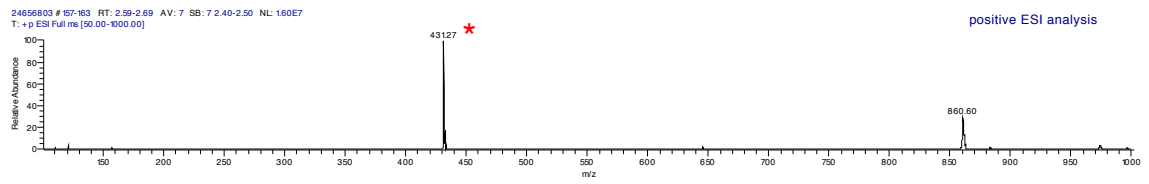
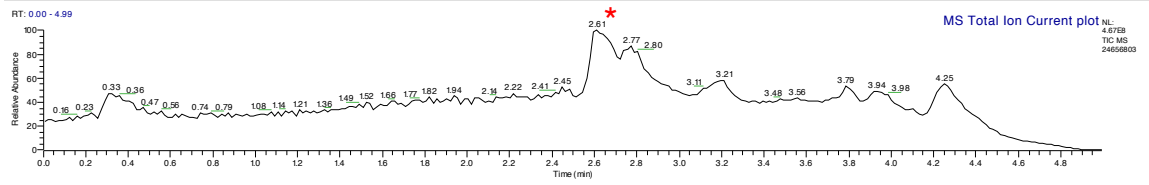
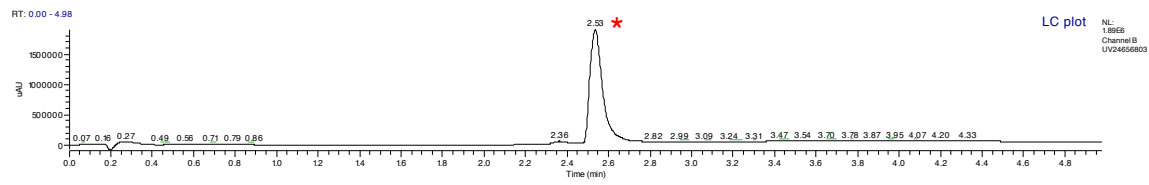
4/17/2009 11:34:55 PM



Sample 49:

C:\Dalton\data\041709\24656803

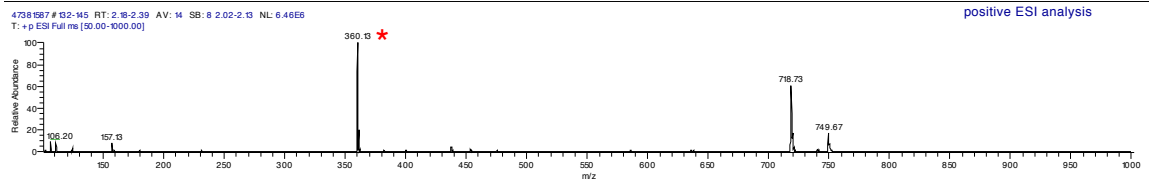
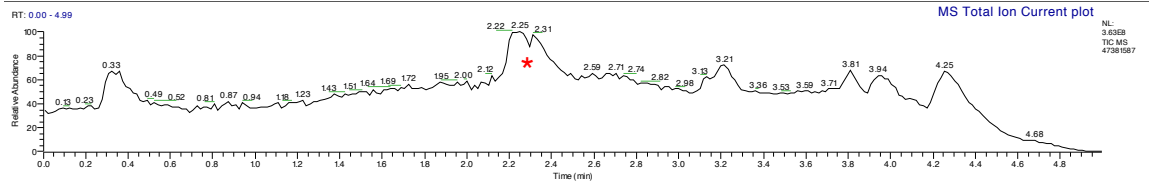
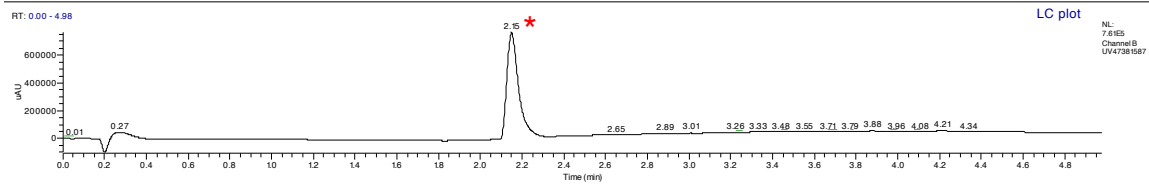
4/17/2009 11:40:35 PM



Sample 50:

C:\Dalton\data\041709\47381587

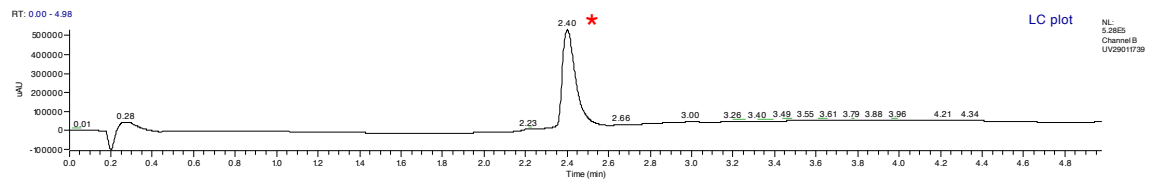
4/17/2009 11:46:17 PM



Sample 51:

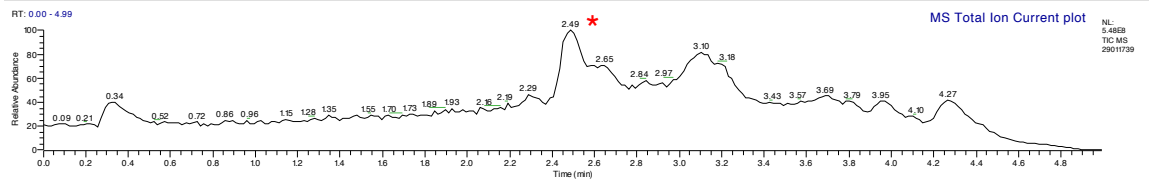
C:\Dalton\data\041709\29011739

4/18/2009 12:03:33 AM



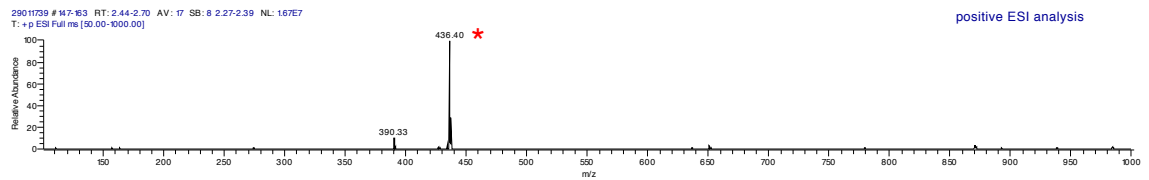
LC plot

NL: 3-565  
Channel B  
UV29011739



MS Total Ion Current plot

NL: 3-565  
TIC-MS  
29011739



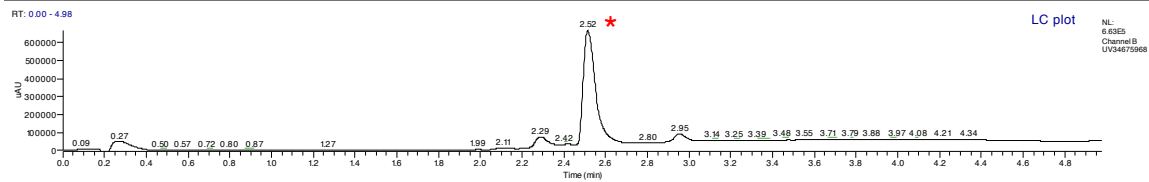
positive ESI analysis

29011739 # 117-63 RT: 2.44-2.70 AV: 17 SB: 8 2.27-2.39 NL: 167E7  
T: +p ESI Full ms [50.00-1000.00]

Sample 52:

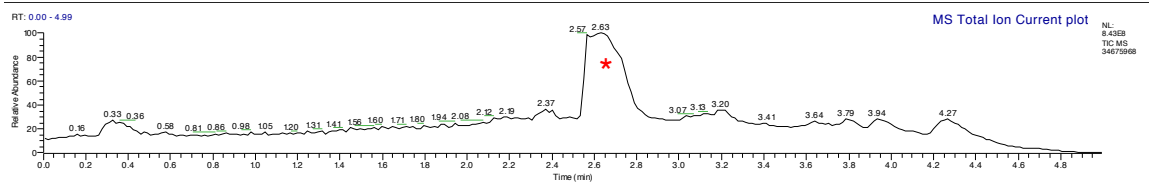
C:\Dalton\data\041709\34675968

4/18/2009 12:09:18 AM



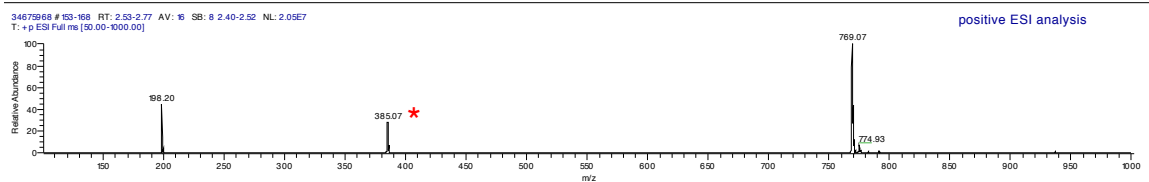
LC plot

NL: 8-4305  
Channel B  
UV34675968



MS Total Ion Current plot

NL: 8-4305  
TIC-MS  
34675968



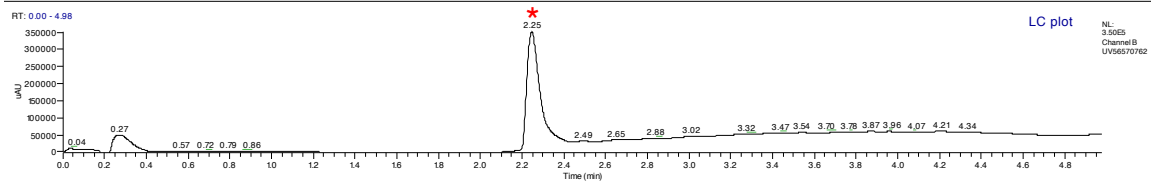
positive ESI analysis

34675968 # 153-168 RT: 2.53-2.77 AV: 16 SB: 8 2.40-2.52 NL: 2.05E7  
T: +p ESI Full ms [50.00-1000.00]

### Sample 53

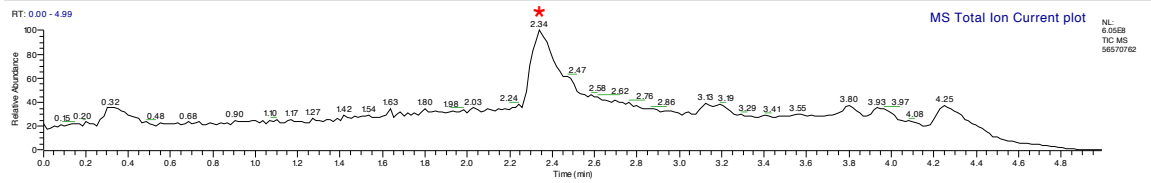
C:\Dalton\data\041709\56570762

4/18/2009 12:14:58 AM



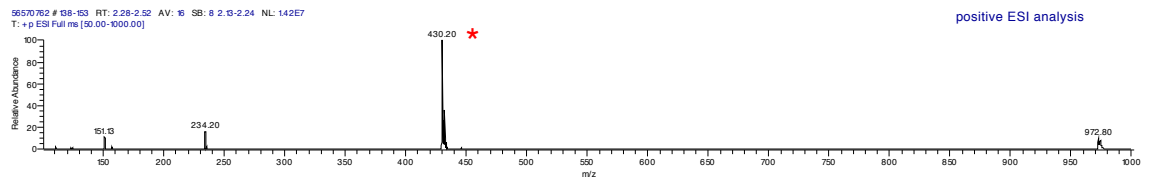
LC plot

NL: 3.565  
Channel B  
UV56570762



MS Total Ion Current plot

NL: 4.558  
TIC-MS  
56570762

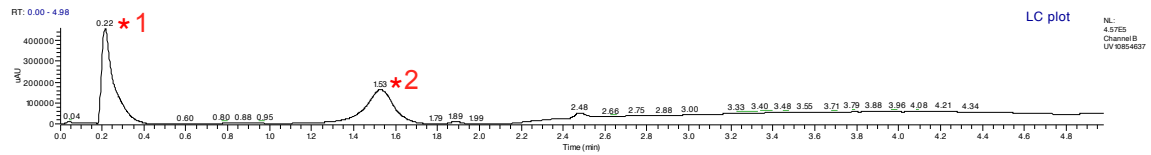


positive ESI analysis

### Sample 54

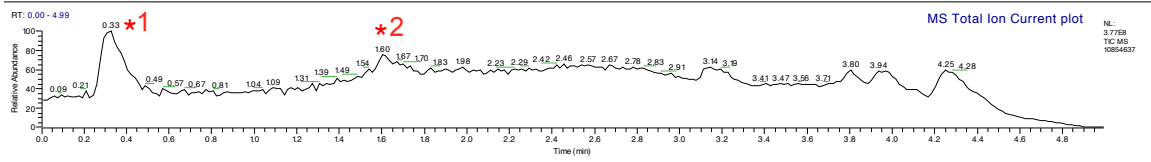
C:\Dalton\data\041709\10854637

4/18/2009 12:20:44 AM



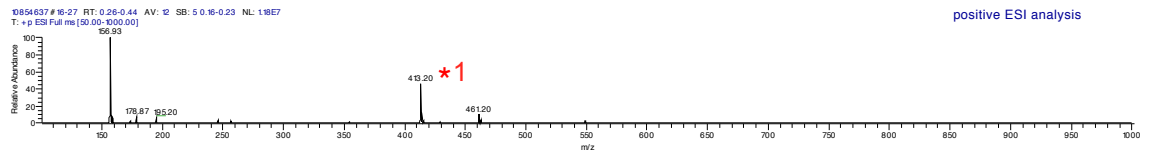
LC plot

NL: 4.575  
Channel B  
UV 10854637

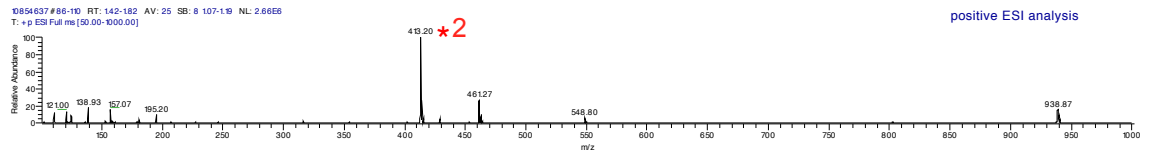


MS Total Ion Current plot

NL: 3.778  
TIC-MS  
10854637



positive ESI analysis

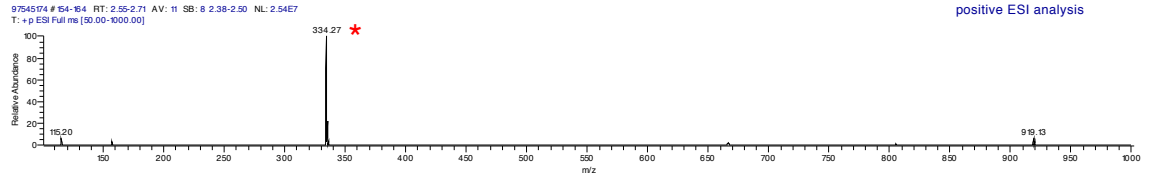
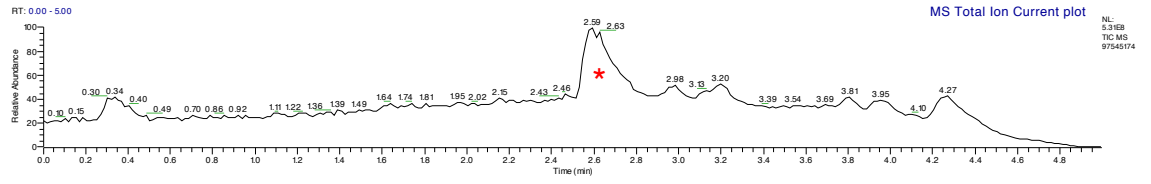
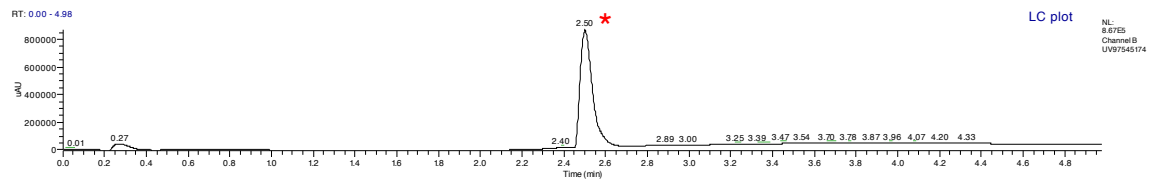


positive ESI analysis

### Sample 55:

C:\Dalton\data\041709\97545174

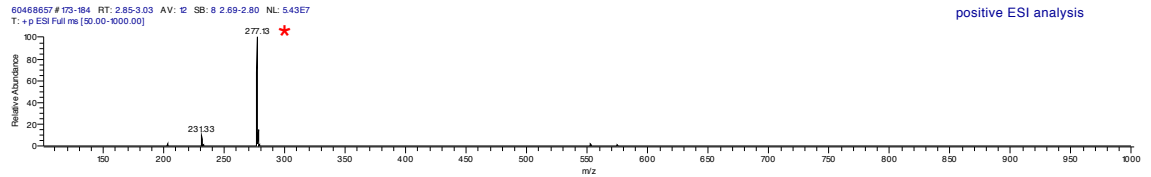
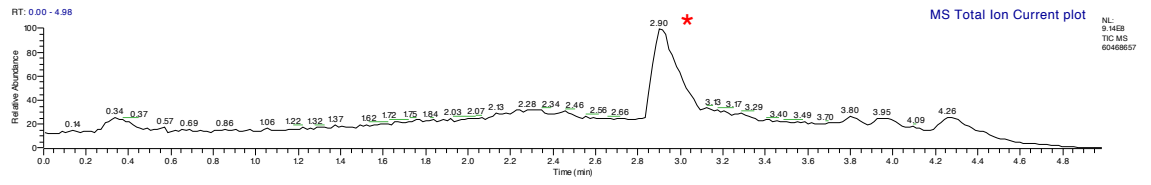
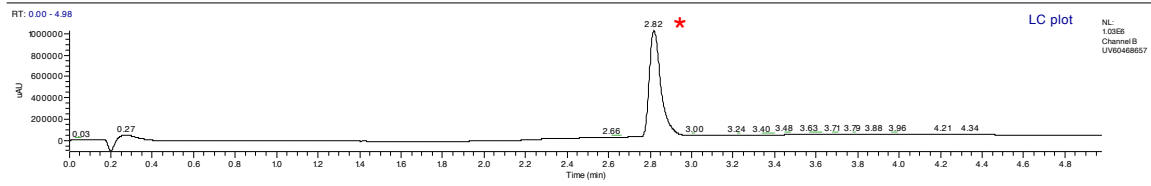
4/18/2009 12:26:29 AM



### Sample 56:

C:\Dalton\data\041709\60468657

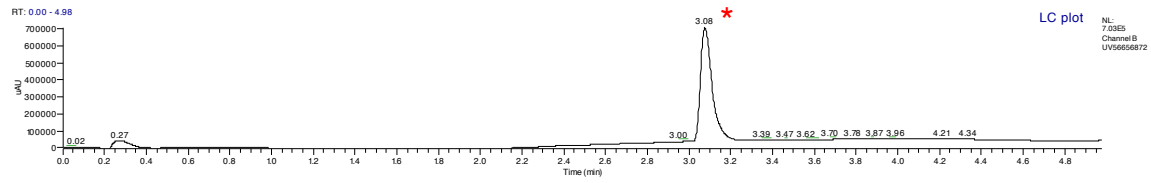
4/18/2009 12:32:15 AM



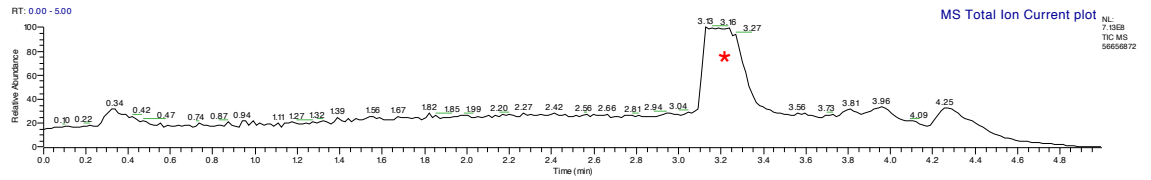
### Sample 57:

C:\Dalton\data\041709\56656872

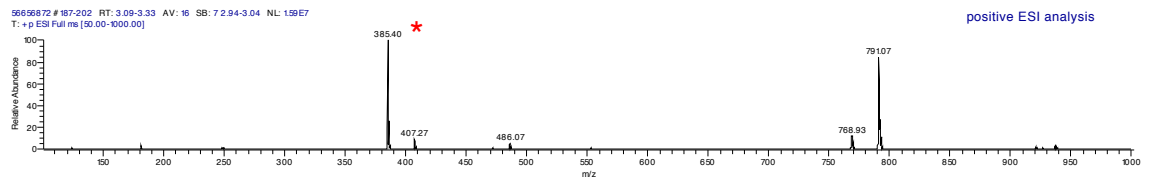
4/18/2009 12:38:00 AM



LC plot  
NL: 7.565  
Channel B  
UV56656872



MS Total Ion Current plot  
NL: 7.565  
TIC MS  
56656872

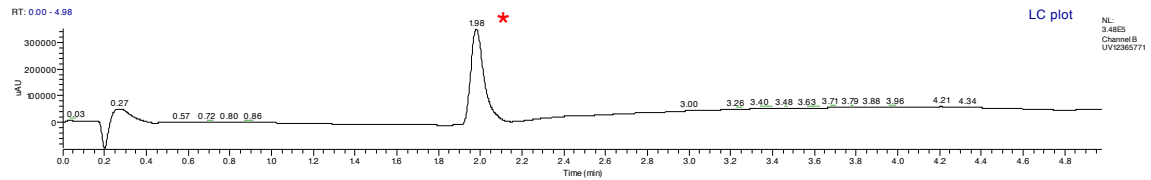


positive ESI analysis

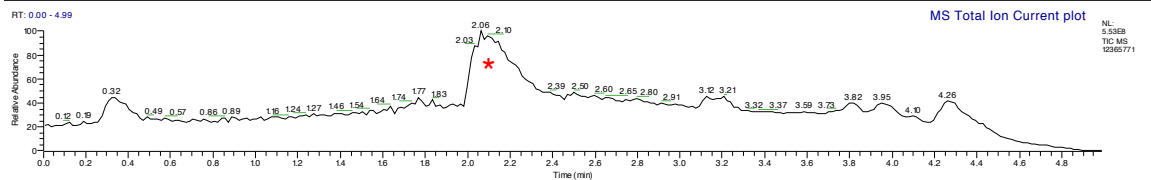
### Sample 58:

C:\Dalton\data\041709\12365771

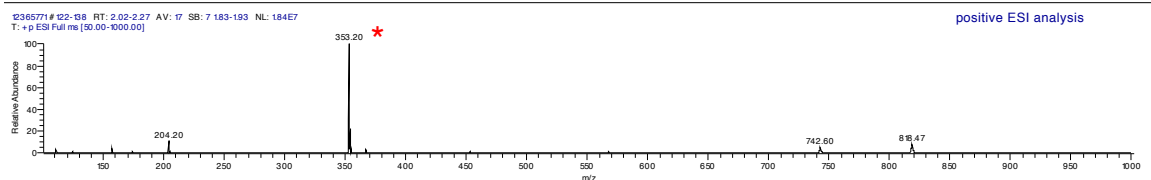
4/18/2009 12:43:46 AM



LC plot  
NL: 3.483  
Channel B  
UV12365771



MS Total Ion Current plot  
NL: 3.533  
TIC MS  
12365771

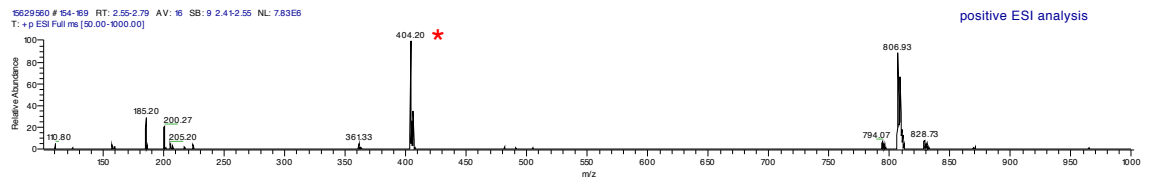
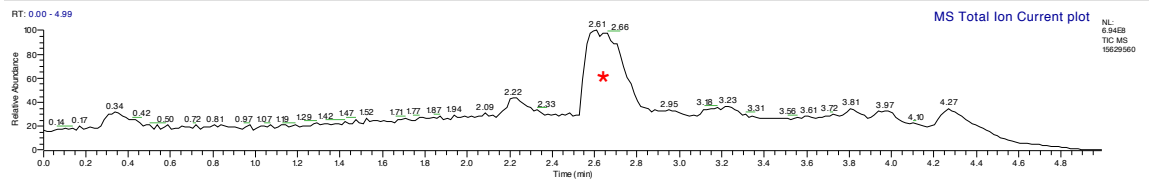
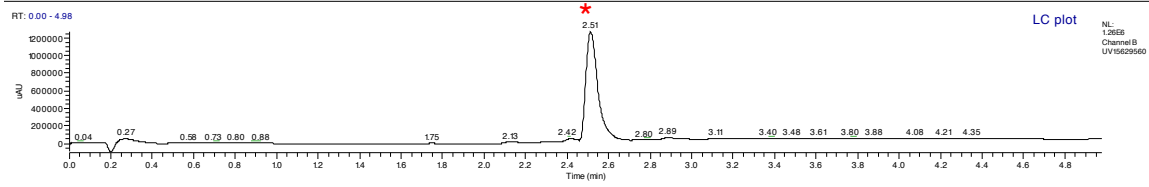


positive ESI analysis

### Sample 59

C:\Dalton\data\041709\15629560

4/18/2009 12:49:30 AM



### Sample 60

C:\Dalton\data\041709\99405798

4/18/2009 12:55:15 AM

