

This is a special file, named RPTHEAD.TXT, in the directory of a method which allows you to customize the report header page.
It can be used to identify the laboratory which uses the method.

This file is printed on the first page with the report styles:

Header+Short, GLP+Short, GLP+Detail, Short+Spec, Detail+Spec, Full

```

      XXXX  XXX
    XX  XX  XX
  XX      XX      XXXXX  XXX XX
  XX      XX XXX  XX      X  XX X XX
  XX      X  XXX XX  XXXXXXXX  XX X XX
    XX  XX  XX  XX  XX      XX  XX
      XXXX  XXX  XXX  XXXXX  XXX  XXX

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  XXXXXX      X      X      XX
XX  X  XX      XX
XX      XXXXX  XXXXX  XXXXX  XXX      XXXX  XX XXX
  XXXXX  XX      X  XX      XX  XX  XX  XX  XXX XX
      XX  XX      XXXXXX  XX      XX  XX  XX  XX
X  XX  XX XX  X  XX  XX XX  XX  XX  XX  XX  XX
XXXXXX      XXX  XXXXX X  XXX  XXXX  XXXX  XX  XX

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                                X
  XX XXX  XXXXX  XX XXX  XXXX  XX XXX  XXXXX
  XXX XX  XX  X  XX  XX  XX  XX  XXX XX  XX
  XX      XXXXXXXX  XX  XX  XX  XX  XX
  XX      XX      XXXXX  XX  XX  XX  XX  XX  XX
XXXX      XXXXX  XX      XXXX  XXXX      XXX
                XXXX

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  XXX      XXX
  XX      XX
  XX      XXXXX  XXXXX  XX  XXXXX  XX XXX
  XX XXX  XX  X      X  XXXXX  XX  X  XXX XX
  XXX XX  XXXXXXXX  XXXXXXXX  XX  XX  XXXXXXXX  XX
  XX  XX  XX      X  XX  XX  XX  XX      XX
  XXX  XXX  XXXXX  XXXXX X  XXXX X  XXXXX  XXXX

```

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  X      XXX      X
  XX      XX      XX
XXXXX  XXXXX  XXX XX  XX XXX  XX  XXXXX  XXXXX  XXXXX
XX  XX  X  XX X XX  XX  XX  XX      X  XX  XX  X
XX  XXXXXXXX  XX X XX  XX  XX  XX  XXXXXXXX  XX  XXXXXXXX
XX XX  XX      XX  XX  XXXXX  XX  X  XX  XX  XX  XX
  XXX  XXXXX  XXX  XXX  XX      XXXX  XXXXX X  XXX  XXXXX
                XXXX

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Sample Name: Blank

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=====
Acq. Operator   : user                      Seq. Line :    1
Sample Operator : user
Acq. Instrument : SFC LCMS                  Location  :    1
Injection Date  : 11/08/2023 02:07:52      Inj       :    1
                                           Inj Volume: 0.200 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 2.000 µl
Sequence File   : D:\Data\2023\Yunfei_R0AR\2023-08-10_MBAAd_Calib_2uL 2023-08-11 02-05-23\2023
                  -08-10_MBAAd_Calib_2uL.S
Method          : D:\Data\2023\Yunfei_R0AR\2023-08-10_MBAAd_Calib_2uL 2023-08-11 02-05-23\C0L1
                  _5NH4FA_MECN_5T095_1MIN_100-600MS_POS.M (Sequence Method)
Last changed    : 24/07/2023 15:04:14 by administrator
=====

```

Module	Type	Firmware rev.	Serial number
Column Comp.	G7116A	D.07.23 [0009]	DEAED08985
Make Up Pump 2	G7110B	D.07.23 [0009]	DEAEH00761
Valve 3	G1170A	D.07.23 [0009]	DEBAD03734
Multi sampler 4	G4767A	D.07.24 [0001]	DEAFD00218
LC Pump 5	PumpValveCluster		
Pump 5	G7111B	D.07.24 [0001]	DEAEW03495
SFC Binary Pump 6	G4782A	D.07.23 [0009]	DEAGN00153
DAD 7	G7115A	D.07.23 [0009]	DEAC605436
SFC 8	G4301A	A.03.09 [0005]	SG18067002
ELSD 9	G4260B		GB23230008
Agilent G6125B MSD	G6125B	3.02.50	SG1823N002

Software Revision: Rev. C.01.09 [161] Copyright © Agilent Technologies

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                        Column(s)
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Column Description : Raptor C18
Serial #           : 288
Product#           : 9304A52      Batch# : 220519B
Diameter           : 2.1 mm       Length : 50.0 mm
Particle size      : 2.7 µm       Void volume : 0.10 ml
# Injections       : 431
Maximum Pressure   : 600.0 bar     Maximum pH : 8.0
Minimum pH         : 2.0
Maximum Temperature: 60.0 °C
Comment            : New 2023-08-03
=====

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Instrument Conditions	At Start	At Stop
Column Temp. (left)	39.9	40.0 °C
Column Temp. (right)	32.4	32.4 °C
Pressure	0.0	0.0 bar
Flow	0.000	0.000 ml/min

Detector Lamp Burn Times:	Current On-Time	Accumulated On-Time
DAD 1, UV Lamp	0.02	849.1 h
DAD 1, Visible Lamp	0.00	331.2 h

```

Solvent Description :
PMP1, Solvent A     :
PMP2, Solvent A     :

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Sample Name: Blank

PMP2, Solvent A :
 PMP2, Solvent B :
 PMP2, Solvent B :

=====

MSD parameters
 Tune file name : C:\Users\Public\Documents\ChemStation\1\MStune\6125BTUN\atunes. tun
 (Wed Aug 2 16:39:21 2023)
 Ionization mode : ES-API

MSD Instrument Conditions	At Start	At Stop
Quad Temp	100	100 C
Gas Temp	348	350 C
RoughVac	2	2 Torr
HighVac	5.1E-009	5.1E-009 Torr
CapCur	657	654 nA
ChamCur	8.6E-001	1.2E-001 µA
DryingGas	12	12 l/min
Neb Pres	35	35 psi g
Turbo1Spd	100	100 %
Turbo1Pwr	127	138 W
RF Drive	2	15 %
Qd TpDrv	16	16 %
Gas TpDrv	35	35 %
Neb PrDrv	50	49 %
Gas FI Drv	61	61 %

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MSD tuning (calibration) parameters
 Ionization polarity : Positive
 Skim1 : 30 V
 Skim2 :
 Ion Energy : 5.0 V
 Lens1 : 3.2 V
 Lens2 :
 Iris : -400 V
 HED : 10000 V
 Width Gain : -186
 Width Offset : Variable

Mass	Value
118.08	-24
622.03	-29
922.01	-22
1521.97	-24

Mass	Value
118.08	0.752
622.03	0.846
922.01	0.836
1521.97	0.752

Quad DC : 0.00 V
 Octopole Peak : 650 V
 Octopole Knee :

Sample Name: Blank

```

Lens2DC          :      Variabl e
                  Mass           :      Val ue
                  -----
                  50.00          :      0.5
                  100.00         :      1.0
                  350.00         :      2.0
                  1000.00        :      4.0
                  2000.00        :      6.0
                  -----

L2RFEn           :      1
L2RFPh           :      162
L2RFAMP          :      Variabl e
                  Mass           :      Val ue
                  -----
                  118.08         :      51
                  622.03         :      95
                  922.01         :      105
                  1521.97        :      145
                  -----

Mass Filter      :      Gaussi an
Time Filter      :      Gaussi an
Time Filter Width :      0.030

Ionization polarity :      Negative
Skim1            :      35 V
Skim2            :
Ion Energy       :      5.0 V
Lens1            :      -3.4 V
Lens2            :
Iris             :      400 V
HED              :      10000 V
Width Gain       :      -187
Width Offset     :      Variabl e
                  Mass           :      Val ue
                  -----
                  112.99         :      -32
                  601.98         :      -76
                  1033.99        :      -74
                  1633.95        :      -32
                  -----

Mass Gain        :      -12.85
Mass Offset      :      Variabl e
                  Mass           :      Val ue
                  -----
                  112.99         :      0.774
                  601.98         :      0.868
                  1033.99        :      0.840
                  1633.95        :      0.774
                  -----

Quad DC          :      0.00 V
Octopole Peak    :      650 V
Octopole Knee    :
Lens2DC          :      Variabl e
                  Mass           :      Val ue
                  -----
                  50.00          :      0.5
                  100.00         :      1.0

```

Sample Name: Bl ank

350.00 : 2.0
1000.00 : 4.0
2000.00 : 6.0

L2RFEn : 1
L2RFPh : 162
L2RFamp : Vari able

Mass : Value

112.99 : 70
601.98 : 110
1033.99 : 130
1633.95 : 150

Mass Filter : Gaussi an
Time Filter : Gaussi an
Time Filter Width : 0.030

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Run Logbook

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11 Aug 23 02:15 AM

Logbook File: D:\Data\20...i_ROAR\2023-08-10_MBAAd_Cal i b_2uL 2023-08-11 02-05-23\001-1-Bl ank.D\RUN.LOG

Module	# Event Message	Date Time
Method	Method started: line# 1 at location '1' inj> # 1	11/08/2023 02:05:30
CP Macro	PreRun macro: 'LAMPALL ON'	11/08/2023 02:05:31
Method	Instrument running sample from location 1	11/08/2023 02:05:31
G4260B	G4260B: ELSD - Switch On	11/08/2023 02:05:32
G7115A	G7115A: DEAC605436 - Lamp ignition	11/08/2023 02:05:32
G7116A	G7116A: DEAED08985 - Thermostat on	11/08/2023 02:05:32
G7110B	G7110B: DEAEH00761 - Pump on	11/08/2023 02:05:32
G4782A	G4782A: DEAGN00153 - Pump on	11/08/2023 02:05:33
PumpVal ve	G7111B: DEAEW03495 - Pump on	11/08/2023 02:05:33
G4260B	G4260B: ELSD - Autozero	11/08/2023 02:06:04
G7115A	G7115A: DEAC605436 - Lamp: retry ignition	11/08/2023 02:06:07
G7115A	G7115A: DEAC605436 - Detector: Prepare	11/08/2023 02:06:33
G7115A	G7115A: DEAC605436 - Lamp on	11/08/2023 02:06:33
G7115A	G7115A: DEAC605436 - Detector: Idle	11/08/2023 02:06:49
G7115A	G7115A: DEAC605436 - Detector: Prepare	11/08/2023 02:07:15
G7115A	G7115A: DEAC605436 - Detector: Idle	11/08/2023 02:07:31
G4767A	G4767A: DEAFD00218 - Draw command finished	11/08/2023 02:07:40
G4767A	G4767A: DEAFD00218 - Sampler wash is active	11/08/2023 02:07:41
G4767A	G4767A: DEAFD00218 - Sampler wash is idle	11/08/2023 02:07:48
G4767A	G4767A: DEAFD00218 - Sample preparation time: > 17 sec	11/08/2023 02:07:48
PumpVal ve	G7111B: DEAEW03495 - Run	11/08/2023 02:07:50
PumpVal ve	G7111B: DEAEW03495 - Postrun	11/08/2023 02:12:27
PumpVal ve	G1170A: DEBAD03715 - Postrun	11/08/2023 02:12:27
G1170A	G1170A: DEBAD03734 - Postrun	11/08/2023 02:12:28
G7116A	G7116A: DEAED08985 - Postrun	11/08/2023 02:12:29
Method	Saving Method COL1_5NH4FA_MECN_5T095_1MIN_10> 0-600MS_POS.M	11/08/2023 02:14:48
Method	Instrument run completed	11/08/2023 02:15:23

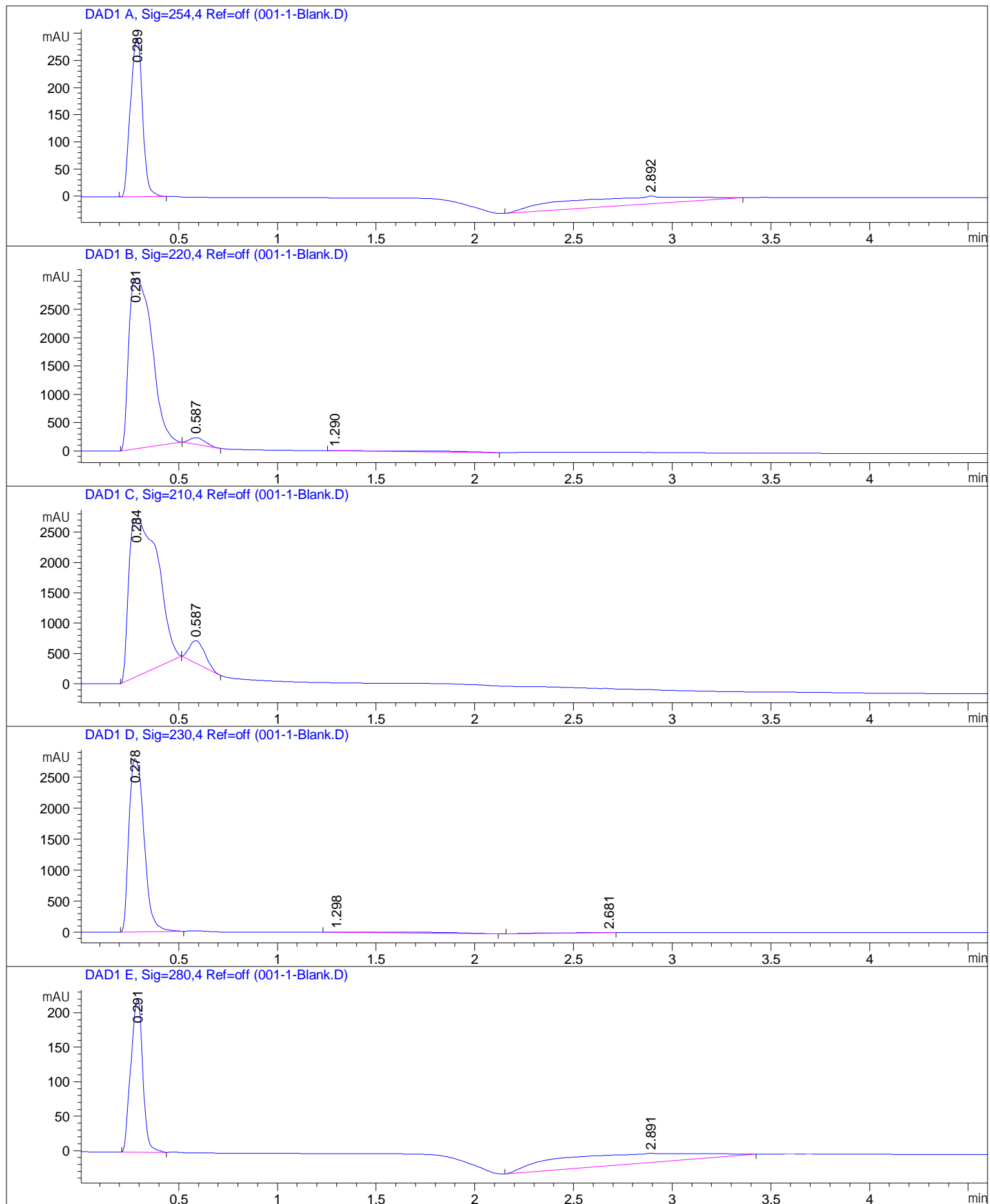
Sample Name: Blank

CP Macro Analyzing rawdata 001-1-Blank.D

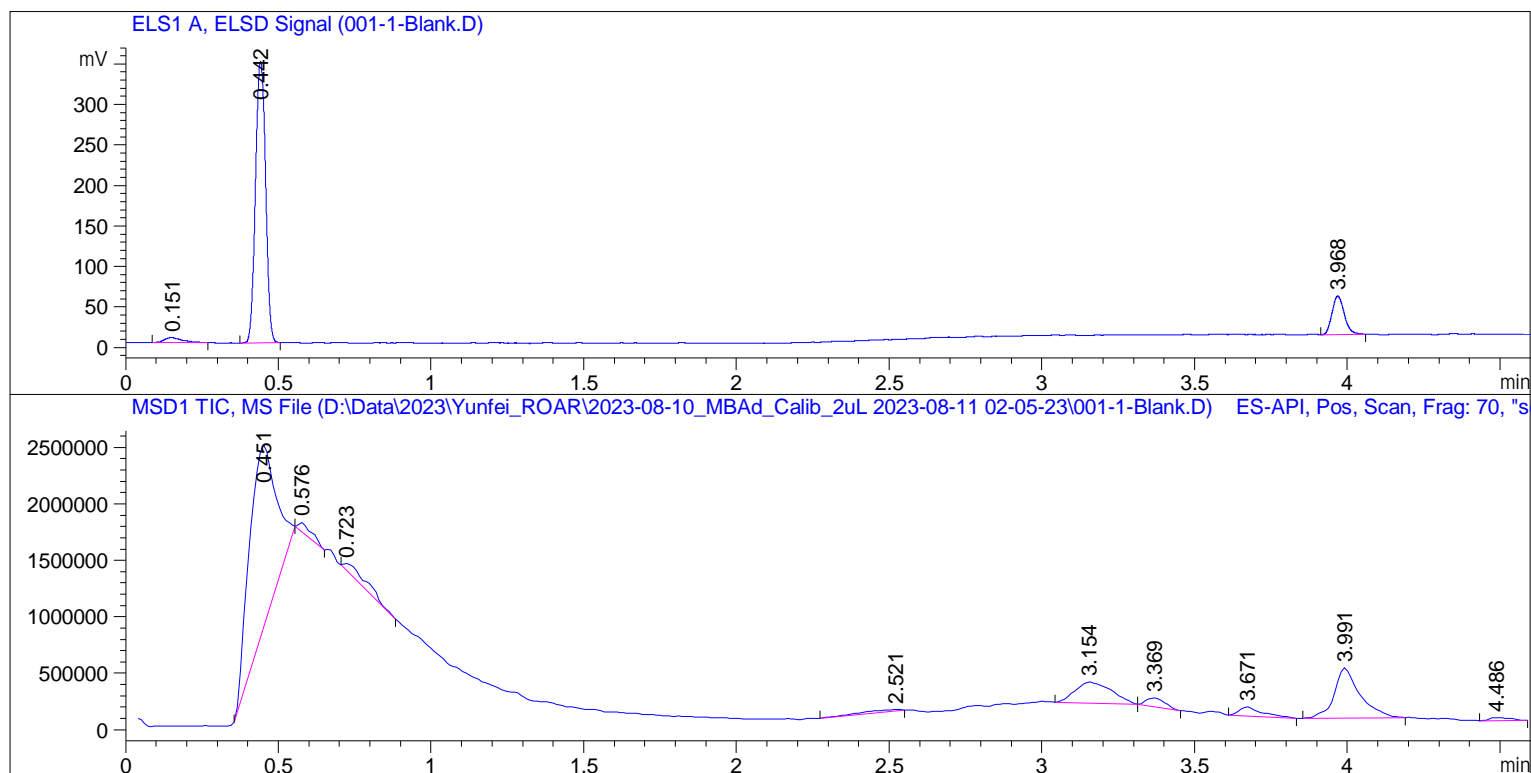
11/08/2023 02:15:24

Method Saving Method DA.M

11/08/2023 02:15:26



Sample Name: Blank



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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254, 4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.289	BB	0.0673	1245.71301	294.60901	63.4371
2	2.892	BB	0.5994	717.98425	14.26146	36.5629

Totals : 1963.69727 308.87047

Signal 2: DAD1 B, Sig=220, 4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.281	BB	0.1171	2.45842e4	3015.30420	95.7784
2	0.587	BB	0.0878	653.26465	119.37508	2.5451
3	1.290	BB	2.9171	430.31705	1.72933	1.6765

Totals : 2.56678e4 3136.40861

Signal 3: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.284	BB	0.1396	2.63250e4	2610.61768	92.8255
2	0.587	BB	0.0903	2034.65283	369.16519	7.1745

Totals : 2.83597e4 2979.78287

Signal 4: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.278	BB	0.0858	1.48357e4	2801.60132	96.2372
2	1.298	BB	1.7652	436.46881	2.91108	2.8313
3	2.681	BB	1.0300	143.59474	1.64571	0.9315

Totals : 1.54157e4 2806.15811

Signal 5: DAD1 E, Sig=280,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.291	BB	0.0647	931.65778	223.05247	53.9390
2	2.891	BB	0.7048	795.58496	13.39841	46.0610

Totals : 1727.24274 236.45089

Signal 6: ELS1 A, ELSD Signal

Peak #	RetTime [min]	Type	Width [min]	Area [mV*s]	Height [mV]	Area %
1	0.151	BB	0.0511	25.39200	6.49831	2.6572
2	0.442	BB	0.0369	798.17480	346.78381	83.5269
3	3.968	BB	0.0435	132.02295	47.35556	13.8159

Totals : 955.58975 400.63769

Signal 7: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.451	BB	0.0965	9.93788e6	1.62904e6	62.4405
2	0.576	BB	0.0481	2.64338e5	7.98892e4	1.6609
3	0.723	BB	0.1102	5.11214e5	5.74161e4	3.2120
4	2.521	BB	0.1668	1.88173e5	1.49746e4	1.1823
5	3.154	BB	0.1061	1.53656e6	1.85614e5	9.6543
6	3.369	BB	0.0729	3.19811e5	7.83509e4	2.0094
7	3.671	BB	0.0737	4.15498e5	7.93402e4	2.6106
8	3.991	BB	0.0843	2.60728e6	4.44003e5	16.3818
9	4.486	BBA	0.0683	1.35003e5	2.67866e4	0.8482

Totals : 1.59158e7 2.59542e6

Summed Peaks Report

Signal 1: DAD1 A, Sig=254, 4 Ref=off
Empty table.

Signal 2: DAD1 B, Sig=220, 4 Ref=off
Empty table.

Signal 3: DAD1 C, Sig=210, 4 Ref=off
Empty table.

Signal 4: DAD1 D, Sig=230, 4 Ref=off
Empty table.

Signal 5: DAD1 E, Sig=280, 4 Ref=off
Empty table.

Signal 6: ELS1 A, ELSD Signal
Empty table.

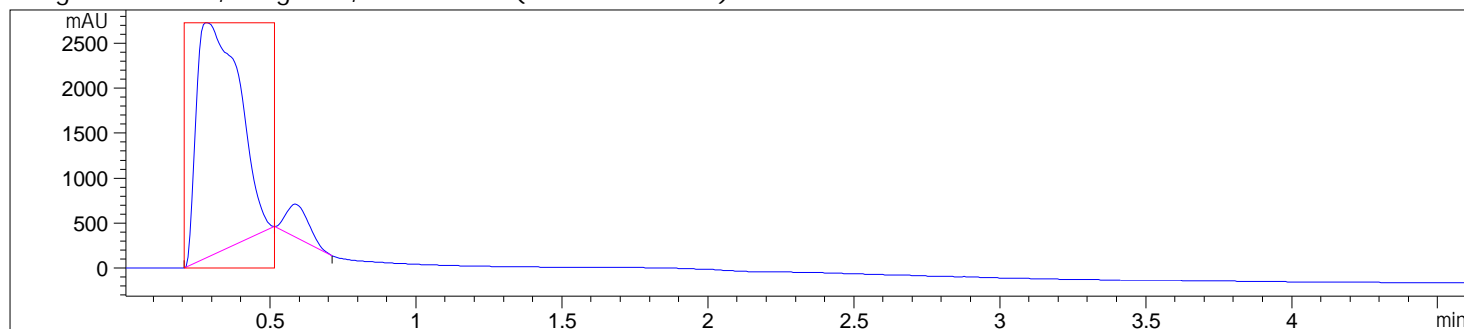
Signal 7: MSD1 TIC, MS File
Empty table.

Final Summed Peaks Report

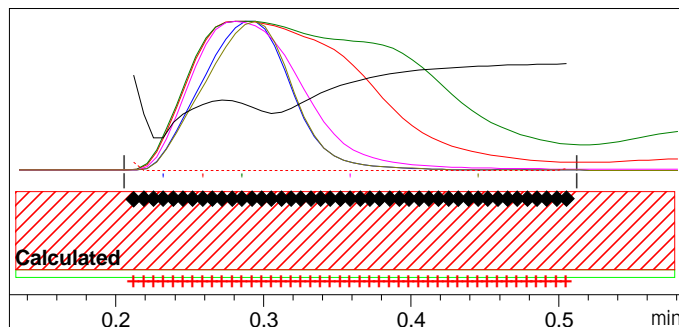
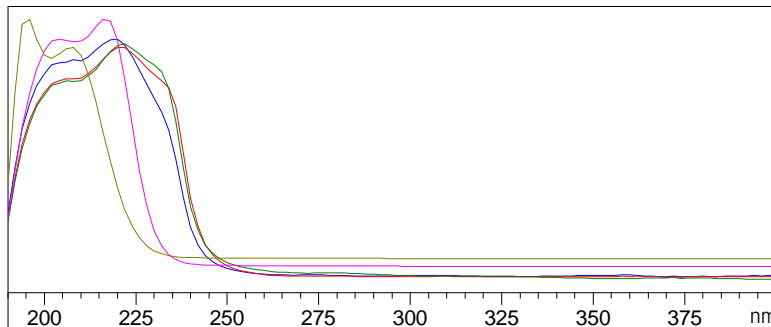
Signal 1: DAD1 A, Sig=254, 4 Ref=off
Signal 2: DAD1 B, Sig=220, 4 Ref=off
Signal 3: DAD1 C, Sig=210, 4 Ref=off
Signal 4: DAD1 D, Sig=230, 4 Ref=off
Signal 5: DAD1 E, Sig=280, 4 Ref=off
Signal 6: ELS1 A, ELSD Signal

Signal 7: MSD1 TIC, MS File

Signal DAD1 C, Sig=210, 4 Ref=off (001-1-Bl ank.D)



Peak : 2 at 0.284 min Name : ?



-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 822.405 (45 of 45 spectra exceed the calculated threshold limit.)

Threshold : 999.991 (Calculated with 45 of 45 spectra)

Reference : Peak start and end spectra (integrated) (0.205 / 0.512)

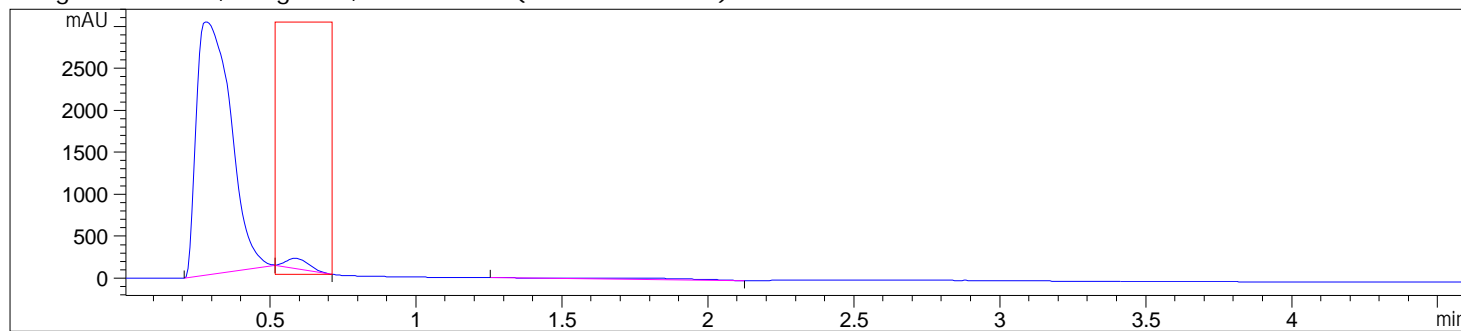
Spectra : 5 (Selection automatic, 5)

Noise Threshold : 0.053 (12 spectra, St.Dev 0.0274 + 3 * 0.0085)

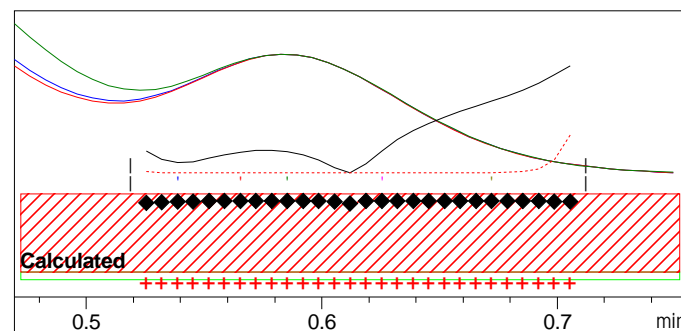
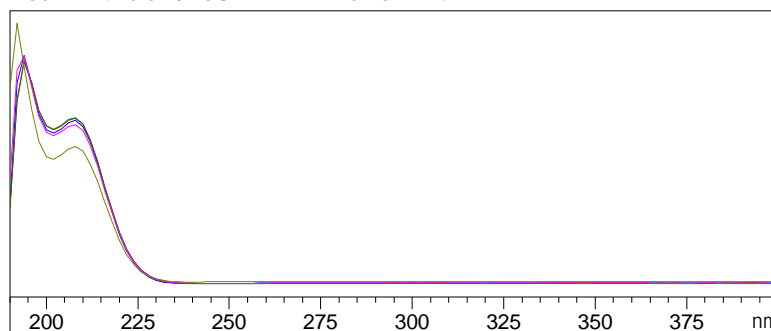
Warning : Spectral absorbances > 1000 mAU (see help for more information)

Sample Name: Blank

Signal DAD1 B, Sig=220, 4 Ref=off (001-1-Blank.D)



Peak : 4 at 0.587 min Name : ?



-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 929.102 (28 of 28 spectra exceed the calculated threshold limit.)

Threshold : 999.742 (Calculated with 28 of 28 spectra)

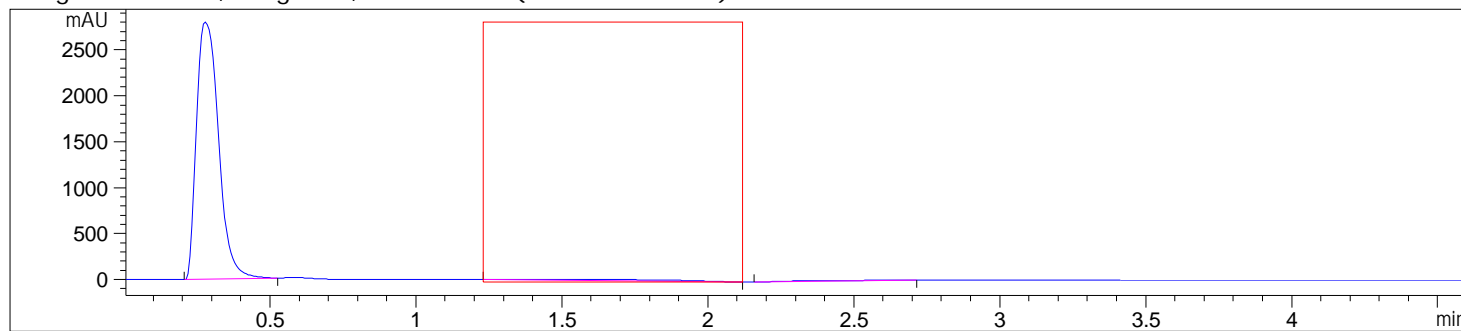
Reference : Peak start and end spectra (integrated) (0.519 / 0.712)

Spectra : 5 (Selection automatic, 5)

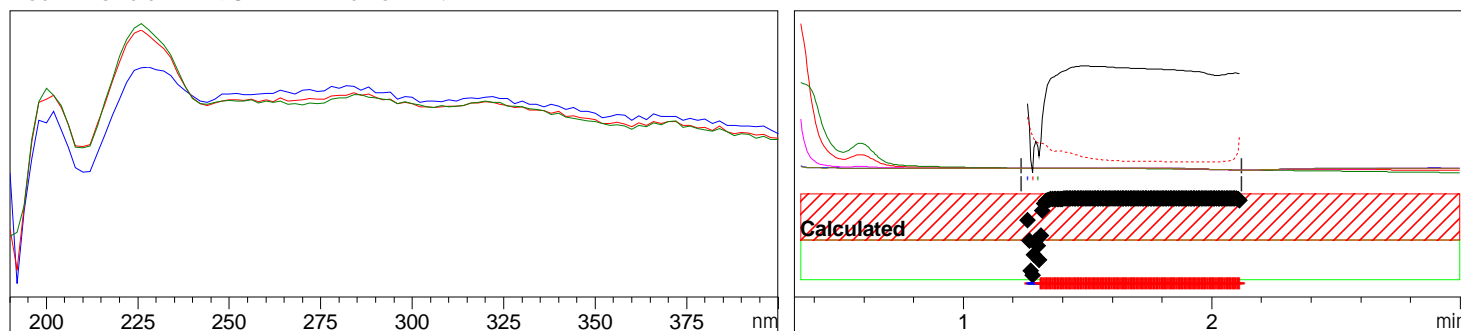
Noise Threshold: 0.053 (12 spectra, St.Dev 0.0274 + 3 * 0.0085)

Sample Name: Blank

Signal DAD1 D, Sig=230, 4 Ref=off (001-1-Blank.D)



Peak : 6 at 1.298 min Name : ?



-> The purity factor exceeds the calculated threshold limit. <-

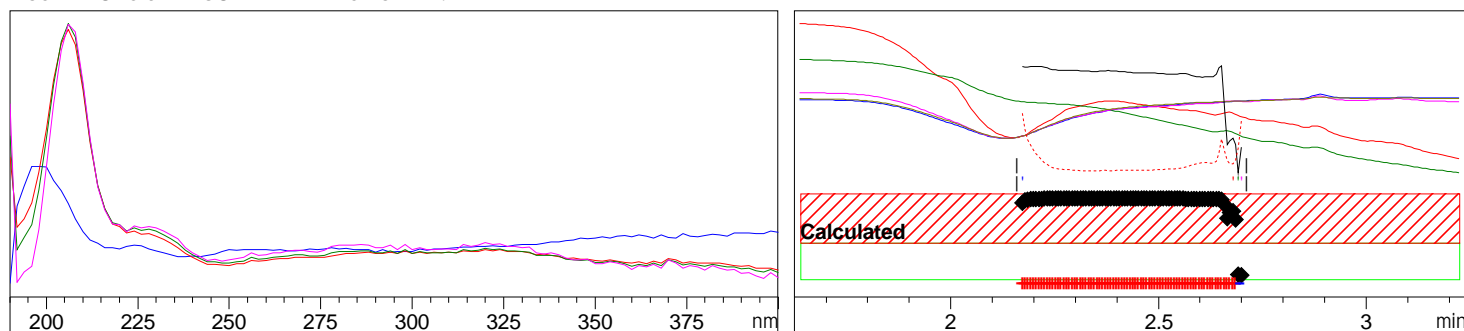
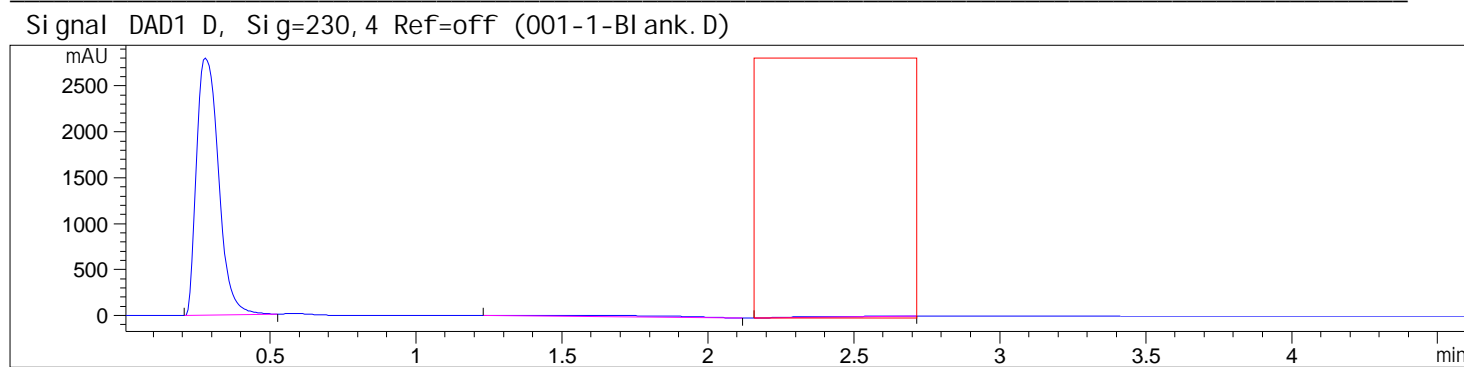
Purity factor : 191.551 (121 of 129 spectra exceed the calculated threshold limit.)

Threshold : 987.482 (Calculated with 121 of 129 spectra)

Reference : Peak start and end spectra (integrated) (1.232 / 2.119)

Spectra : 3 (Selection automatic, 5)

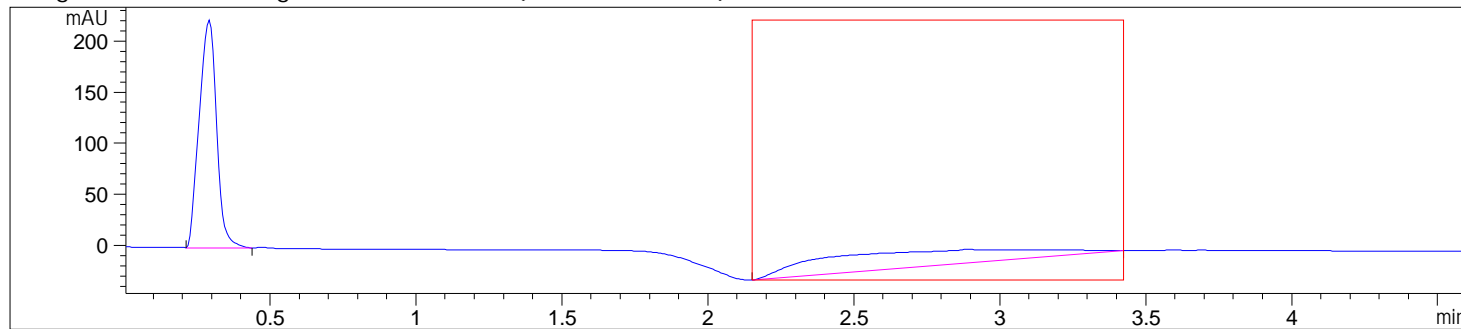
Noise Threshold : 0.053 (12 spectra, St.Dev 0.0274 + 3 * 0.0085)



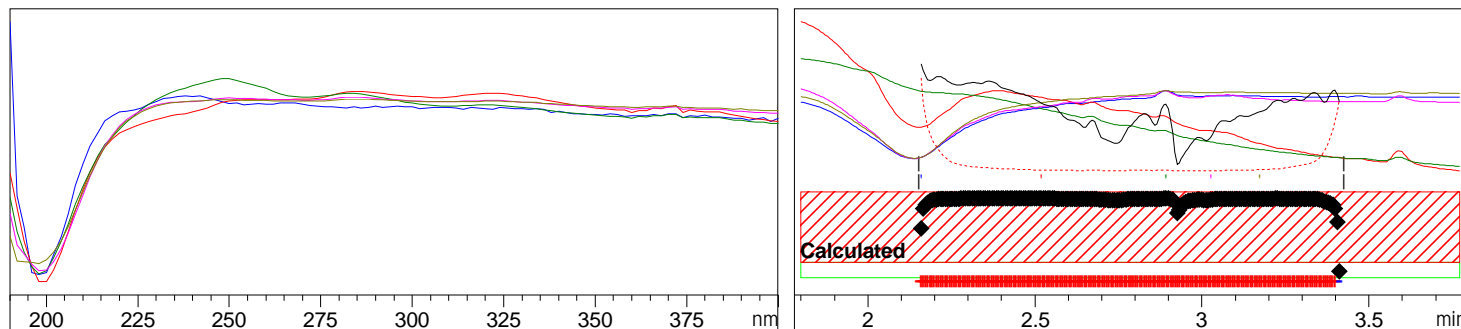
-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 365.819 (78 of 80 spectra exceed the calculated threshold limit.)
Threshold : 990.586 (Calculated with 78 of 80 spectra)
Reference : Peak start and end spectra (integrated) (2.159 / 2.712)
Spectra : 4 (Selection automatic, 5)
Noise Threshold: 0.053 (12 spectra, St.Dev 0.0274 + 3 * 0.0085)

Signal DAD1 E, Sig=280, 4 Ref=off (001-1-Blank.D)



Peak : 9 at 2.891 min Name : ?



-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 968.440 (188 of 189 spectra exceed the calculated threshold limit.)

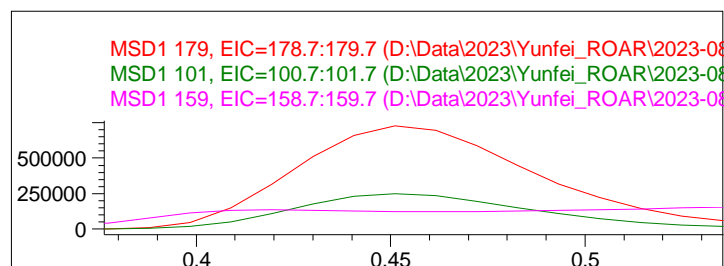
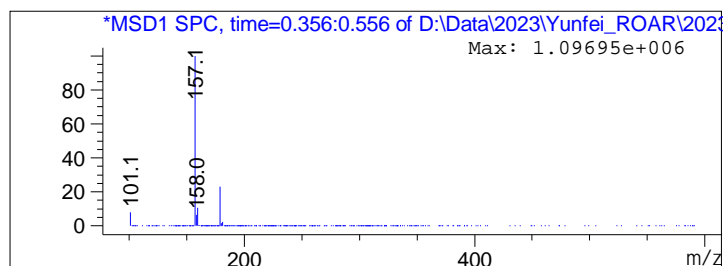
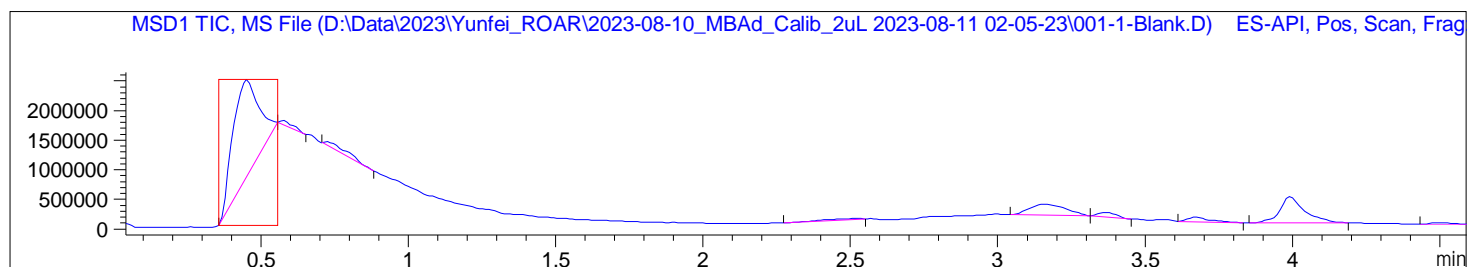
Threshold : 998.833 (Calculated with 188 of 189 spectra)

Reference : Peak start and end spectra (integrated) (2.152 / 3.425)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.053 (12 spectra, St.Dev 0.0274 + 3 * 0.0085)

Sample Name: Blank

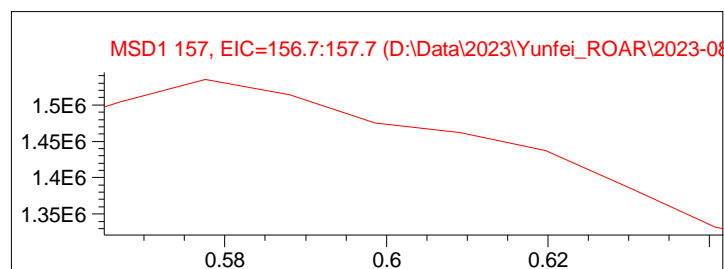
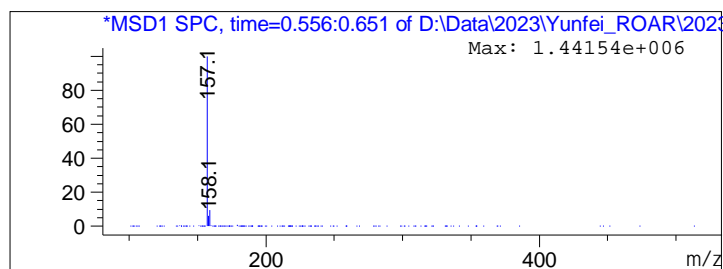
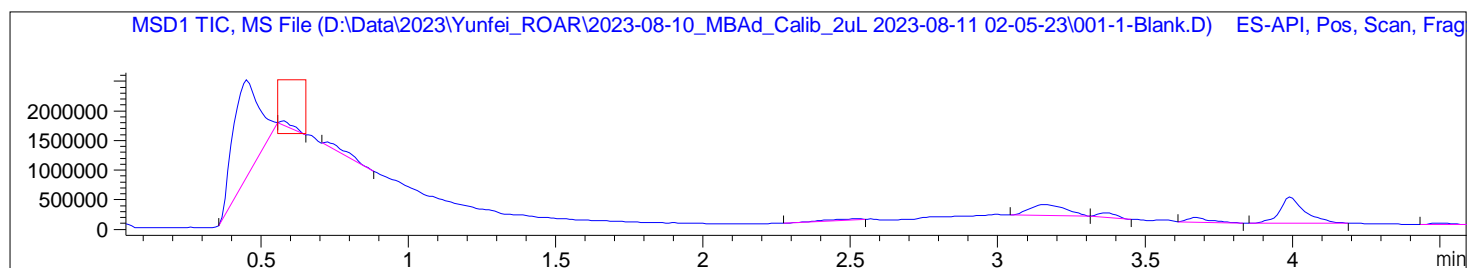


Peak #1 at 0.451 min (0.356 to 0.555 min)

-> The analysis found 2 components, indicating an impure peak. <-

Component 1: Peak at Scan 40.1. Top ions are 179 101

Component 2: Peak at Scan 48.8. Top ions are 159

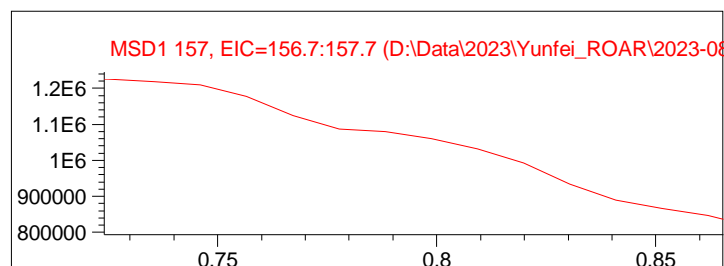
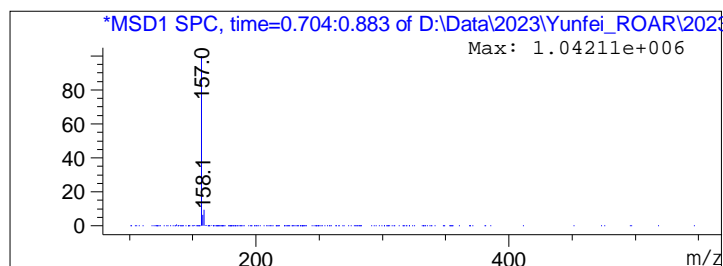
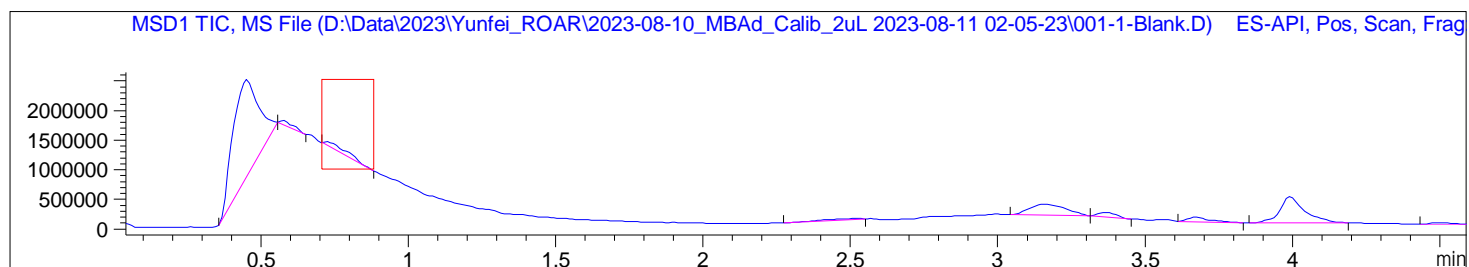


Peak #2 at 0.576 min (0.555 to 0.651 min)

-> The analysis found only one component, indicating a pure peak. <-

Component 1: Peak at Scan 52.1. Top ions are 157

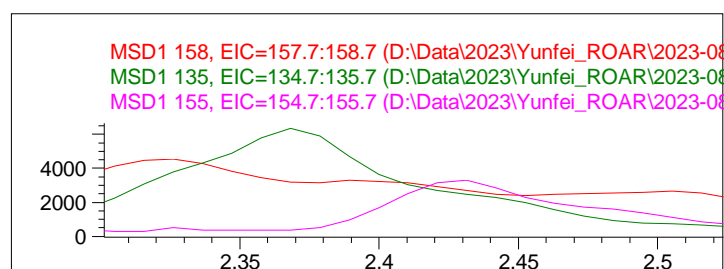
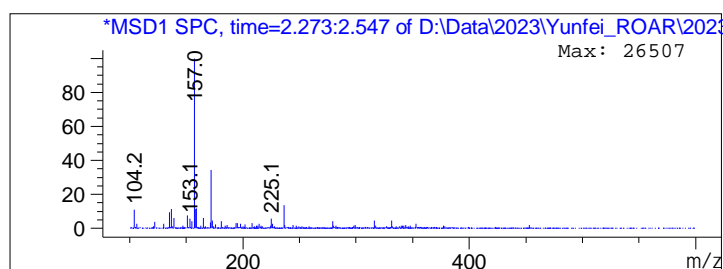
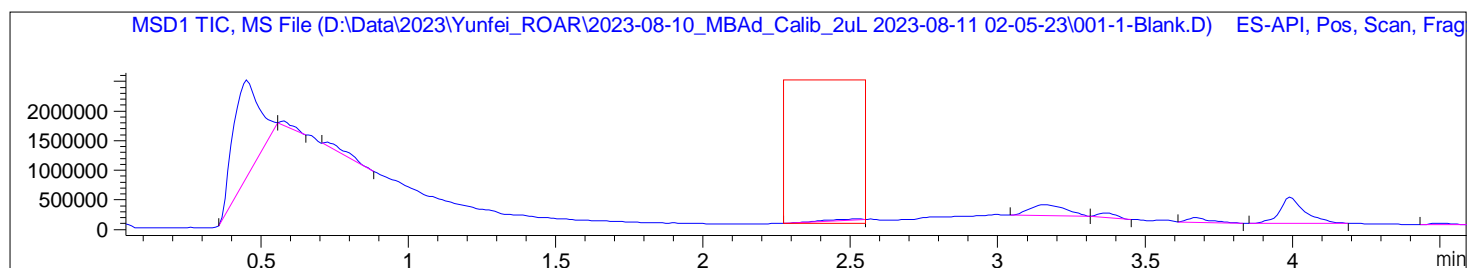
Sample Name: Blank



Peak #3 at 0.723 min (0.706 to 0.883 min)

-> The analysis found only one component, indicating a pure peak. <-

Component 1: Peak at Scan 66.2. Top ions are 157



Peak #4 at 2.521 min (2.273 to 2.551 min)

-> The analysis found 5 components, indicating an impure peak. <-

Component 1: Peak at Scan 217.8. Top ions are 158

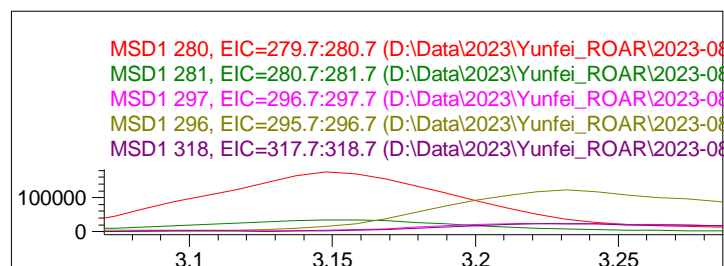
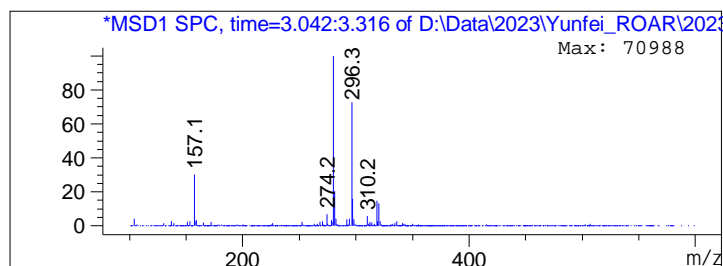
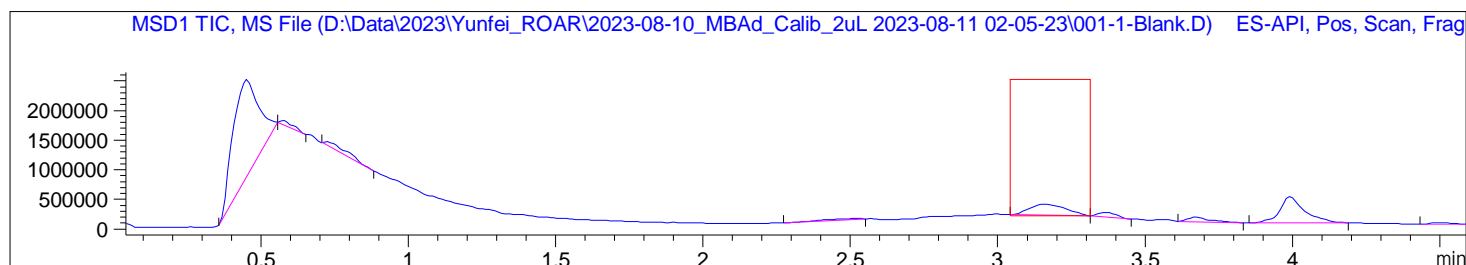
Component 2: Peak at Scan 222.1. Top ions are 135

Component 3: Peak at Scan 227.7. Top ions are 155

Component 4: Peak at Scan 228.4. Top ions are 172

Component 5: Peak at Scan 236.2. Top ions are 236

Sample Name: Blank



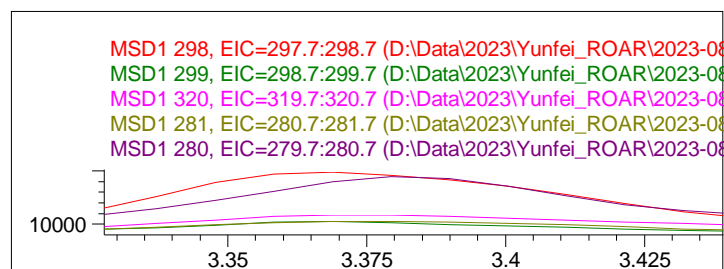
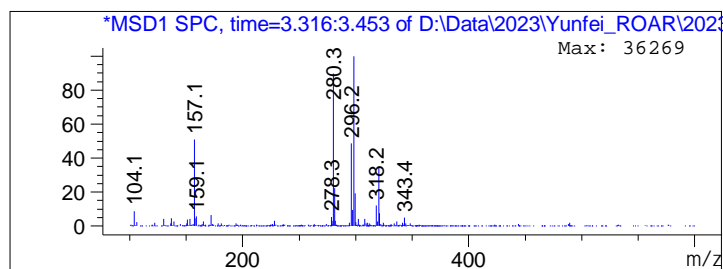
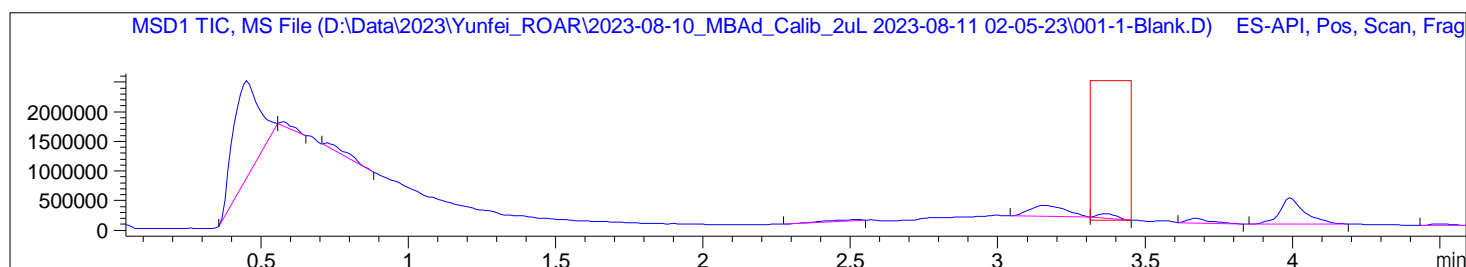
Peak #5 at 3.154 min (3.043 to 3.314 min)

-> The analysis found 3 components, indicating an impure peak. <-

Component 1: Peak at Scan 296.2. Top ions are 280 281 320

Component 2: Peak at Scan 303.3. Top ions are 297

Component 3: Peak at Scan 304.0. Top ions are 296 318



Peak #6 at 3.369 min (3.314 to 3.453 min)

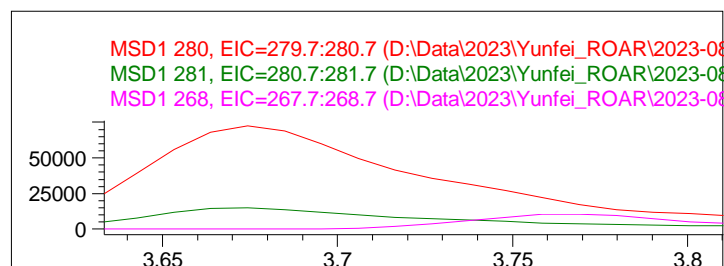
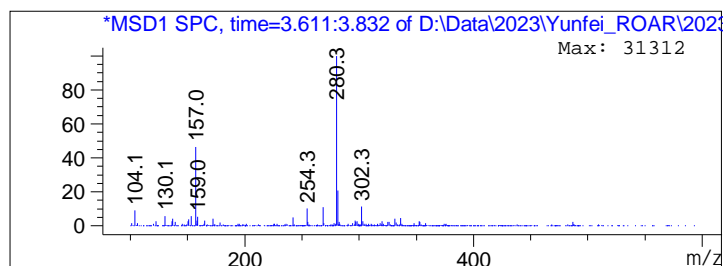
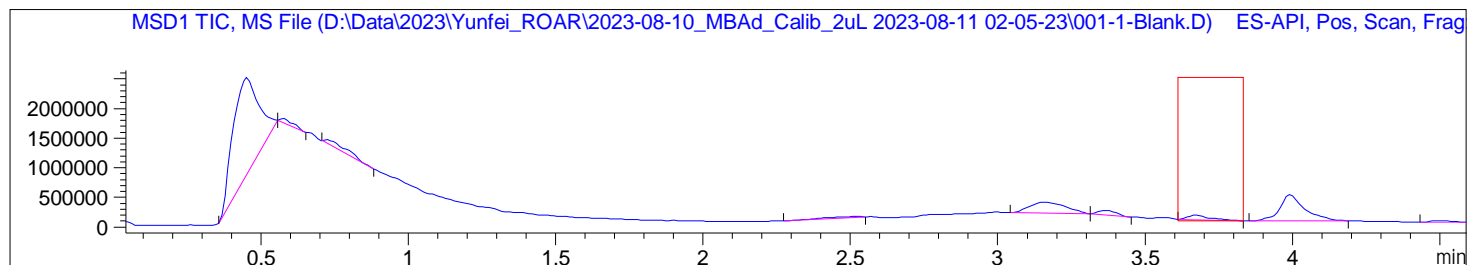
-> The analysis found 3 components, indicating an impure peak. <-

Component 1: Peak at Scan 316.9. Top ions are 298 299

Component 2: Peak at Scan 317.6. Top ions are 320 281

Component 3: Peak at Scan 318.3. Top ions are 280

Sample Name: Blank

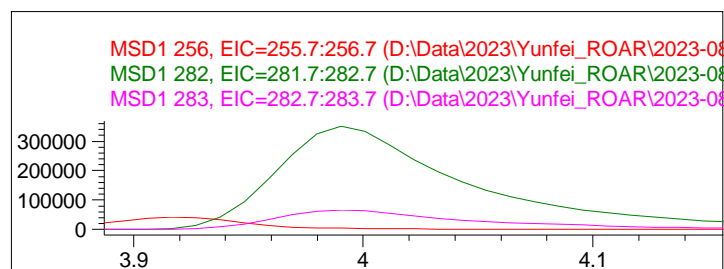
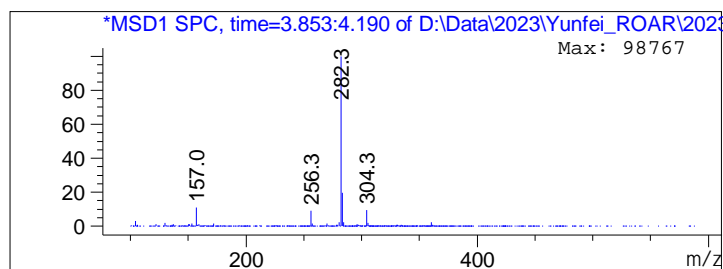
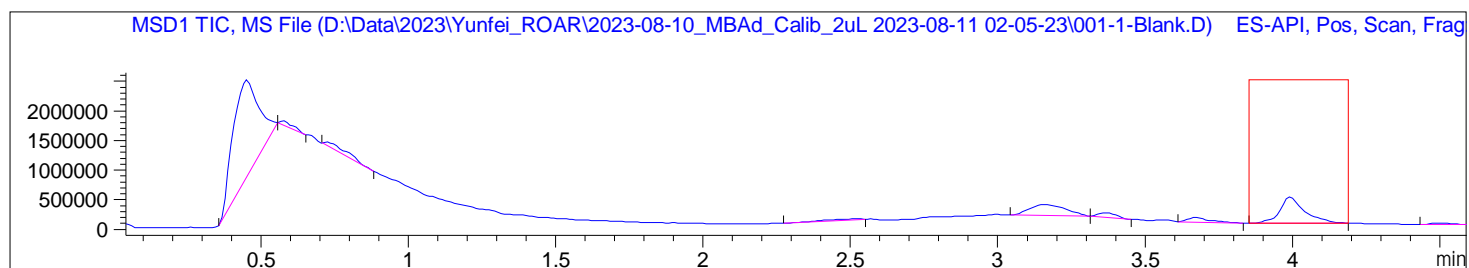


Peak #7 at 3.671 min (3.611 to 3.832 min)

-> The analysis found 2 components, indicating an impure peak. <-

Component 1: Peak at Scan 345.9. Top ions are 280 281

Component 2: Peak at Scan 354.8. Top ions are 268



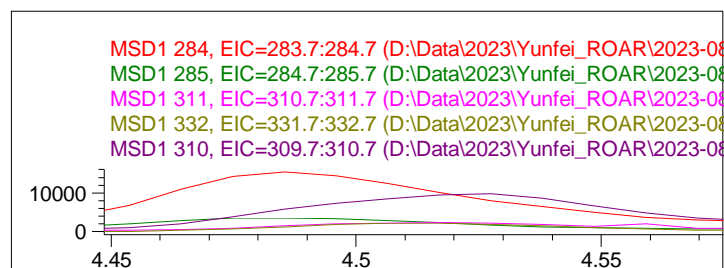
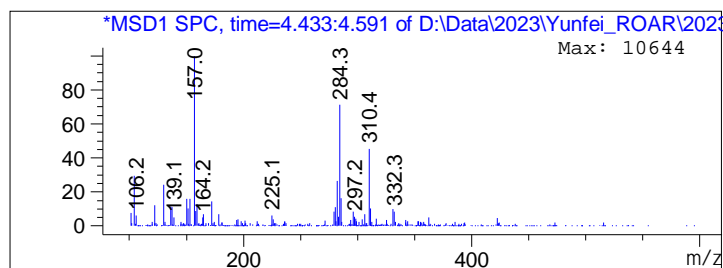
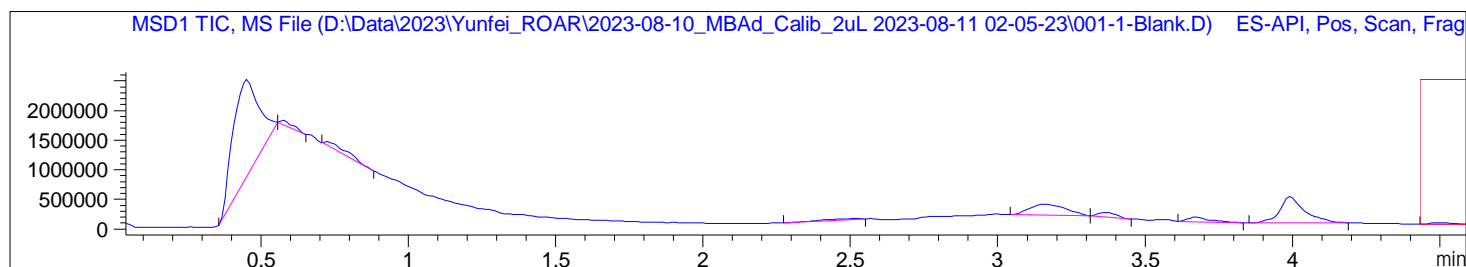
Peak #8 at 3.991 min (3.853 to 4.190 min)

-> The analysis found 2 components, indicating an impure peak. <-

Component 1: Peak at Scan 369.2. Top ions are 256

Component 2: Peak at Scan 376.1. Top ions are 282 283

Sample Name: Blank



Peak #9 at 4.486 min (4.433 to 4.591 min)

-> The analysis found 3 components, indicating an impure peak. <-

Component 1: Peak at Scan 422.9. Top ions are 284 285 306

Component 2: Peak at Scan 425.8. Top ions are 311 332

Component 3: Peak at Scan 426.7. Top ions are 310

*** End of Report ***