

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  XXXXXXX  XX X XX
    XX XX  XX XX  XX      XX   XX
      XXXX  XXX  XXX  XXXXX  XXX  XXX

```

```

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

```

```

                                X
  XX XXX  XXXXX  XX XXX  XXXX  XX XXX  XXXXX
  XXX XX  XX    X  XX  XX  XX  XX  XXX XX  XX
  XX      XXXXXXX  XX  XX  XX  XX  XX      XX
  XX      XX      XXXXX  XX  XX  XX      XX XX
XXXX      XXXXX  XX      XXXX  XXXX      XXX
                XXXX

```

```

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

```

```

  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  XXXXXXX  XX X XX  XX  XX  XX  XXXXXXX  XX  XXXXXXX
XX XX  XX      XX  XX  XXXXX  XX  X  XX  XX XX  XX
  XXX  XXXXX  XXX  XXX  XX      XXXX  XXXXX X  XXX  XXXXX
                XXXX

```

```
=====
Acq. Operator   : user                               Seq. Line :    4
Sample Operator : user
Acq. Instrument : SFC LCMS                           Location  :   D2F-E3
Injection Date  : 11/08/2023 02:32:32                 Inj       :    1
                                                    Inj Volume : 0.200 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 2.000 µl
Acq. Method     : D:\Data\2023\Yunfei_R0AR\2023-08-10_MBAAd_Calib_2uL 2023-08-11 02-05-23\COL1
                  _5NH4FA_MECN_5T095_1MIN_100-600MS_POS.M
Last changed    : 24/07/2023 15:04:14 by administrator
Analysis Method : D:\Data\2023\Yunfei_R0AR\2023-08-10 baseline corrected\2023-08-11 02-05-23_
                  MBAAd_Calib_2uL\COL1_5NH4FA_MECN_5T095_1MIN_100-600MS_POS.M (Sequence Method
                  )
Last changed    : 24/07/2023 15:04:14 by administrator
Additional Info : Peak(s) manually integrated
=====
```

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
Multisampler 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

=====

Column(s)

=====

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 : 434

Maximum Pressure : 600.0 bar Maximum pH : 8.0

Minimum pH : 2.0

Maximum Temperature: 60.0 °C

Comment : New 2023-08-03

```
=====
Instrument Conditions      :      At Start          At Stop
Column Temp. (left)      :          40.0            40.0   °C
Column Temp. (right)     :          32.4            32.4   °C
Pressure                  :           0.0            0.0   bar
Flow                      :           0.000          0.000 ml /mi n
```

```
Detector Lamp Burn Times: Current On-Time  Accumulated On-Time
DAD 1, UV Lamp           :           0.43            849.5   h
DAD 1, Visible Lamp      :           0.00            331.2   h
```

```
Solvent Description      :
PMP1, Solvent A          :
PMP2, Solvent A          :
PMP2, Solvent A          :
PMP2, Solvent B          :
PMP2, Solvent B          :
```

=====

MSD parameters

```
Tune file name           :      C:\Users\Publ i c\Documents\ChemStati on\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                  :           350            350 C
RoughVac                  :           2              2 Torr
Hi ghVac                  :      5. 2E-009          5. 2E-009 Torr
CapCur                   :           5              655 nA
ChamCur                  :      8. 0E-002          1. 3E-001 µA
Dryi ngGas                :           12            12 l /mi n
Neb Pres                  :           35            35 psi g
Turbo1Spd                :           100            100 %
Turbo1Pwr                :           127            127 W
RF Drive                  :           1              15 %
Qd TpDrv                 :           16            16 %
Gas TpDrv                :           35            35 %
Neb PrDrv                :           50            50 %
Gas FI Drv               :           61            61 %
```

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MSD tuning (calibration) parameters

```
Ionization polarity      :      Posi tive
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             :      Vari abl e
Mass                     :      Value
-----
118.08                   :      -24
622.03                   :      -29
```

922.01 : -22
1521.97 : -24

Mass Gain : -12.80
Mass Offset : Variabl e
Mass : Val ue

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 :
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
L2RF Amp : 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 polari ty : Negati ve
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 : Vari able

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 : Vari able

Mass	:	Val ue

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

=====
=====
Run Logbook
=====

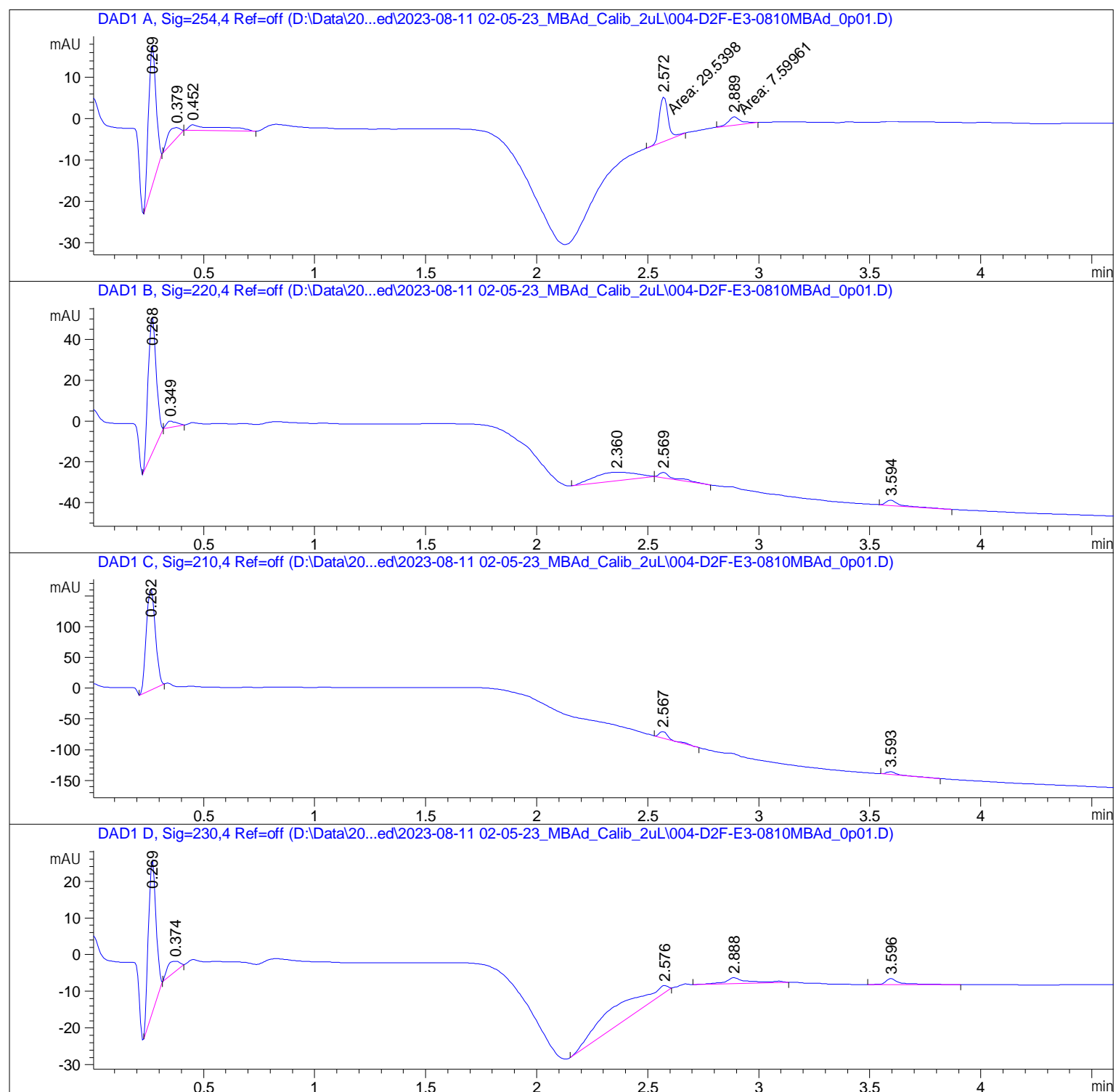
11 Aug 23 12:16 PM

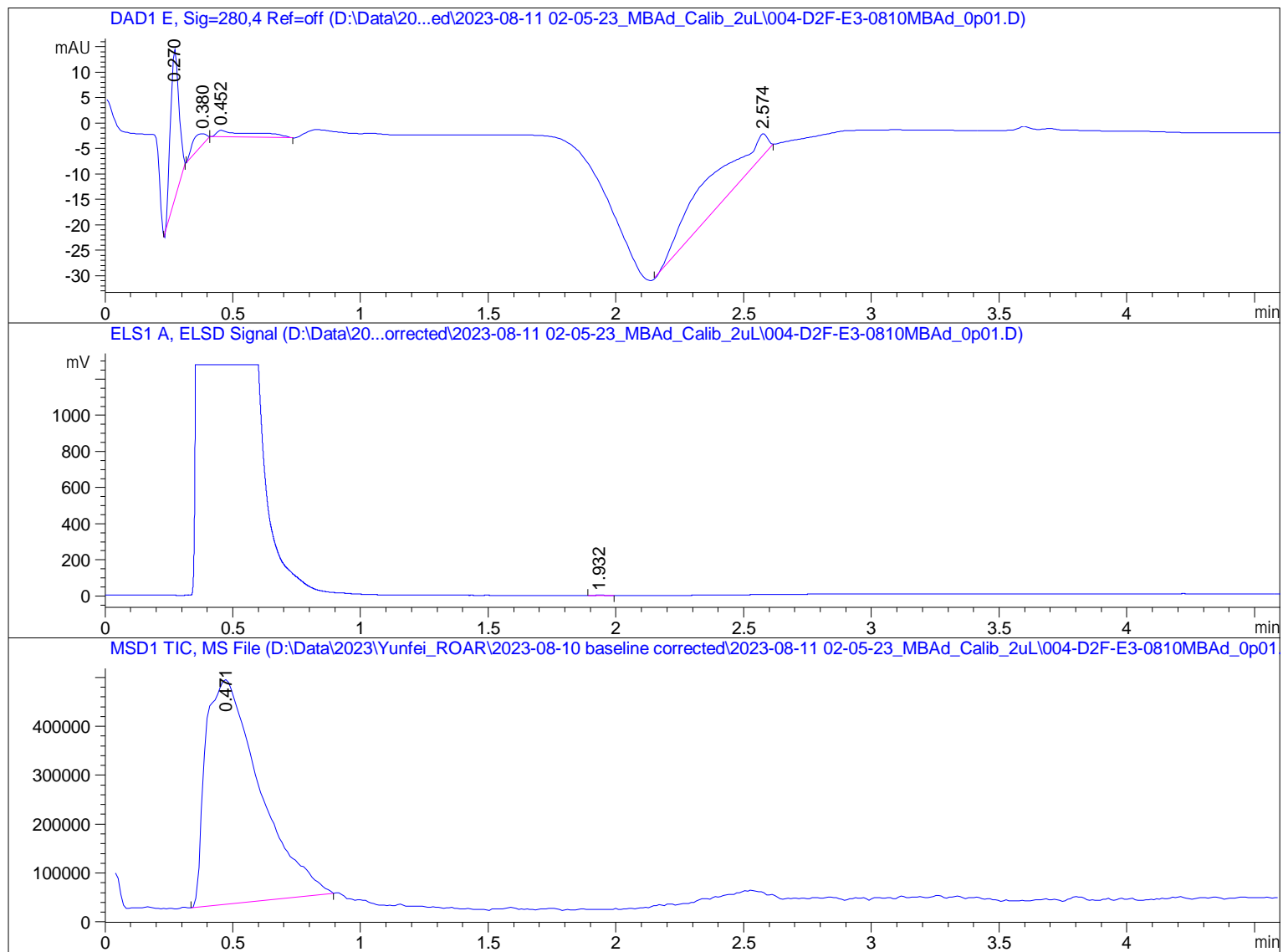
Logbook File: D:\Data\20...cted\2023-08-11 02-05-23_MBAAd_Cal i b_2uL\004-D2F-E3-0810MBAAd_Op01. D\RUN. LOG

Module	# Event Message	Date Time
-----	-----	-----
Method	Method started: line# 4 at location 'D2F-E3>' ' inj# 1	11/08/2023 02:31:45
CP Macro	PreRun macro: 'LAMPALL ON'	11/08/2023 02:31:46
G4260B	G4260B: ELSD - Autozero	11/08/2023 02:31:47
G4260B	G4260B: ELSD - AI ready switched on	11/08/2023 02:31:47
Method	Instrument running sample from location D2F->E3	11/08/2023 02:31:47
G7115A	G7115A: DEAC605436 - Detector: Prepare	11/08/2023 02:31:58
G7115A	G7115A: DEAC605436 - Detector: Idle	11/08/2023 02:32:15
G4767A	G4767A: DEAFD00218 - Draw command finished	11/08/2023 02:32:22
G4767A	G4767A: DEAFD00218 - Sampler wash is active	11/08/2023 02:32:23
G4767A	G4767A: DEAFD00218 - Sampler wash is idle	11/08/2023 02:32:29
G4767A	G4767A: DEAFD00218 - Sample preparation time: >15 sec	11/08/2023 02:32:29
PumpVal ve	G7111B: DEAEW03495 - Run	11/08/2023 02:32:31

Sample Name: 0810MBAAd_0p01

PumpVal ve	G7111B: DEAEW03495 - Postrun	11/08/2023 02: 37: 07
G4767A	G4767A: DEAFD00218 - Postrun	11/08/2023 02: 37: 08
G7110B	G7110B: DEAEH00761 - Postrun	11/08/2023 02: 37: 10
PumpVal ve	G1170A: DEBAD03715 - Postrun	11/08/2023 02: 37: 10
G4782A	G4782A: DEAGN00153 - Postrun	11/08/2023 02: 37: 11
G7116A	G7116A: DEAED08985 - Postrun	11/08/2023 02: 37: 11
G1170A	G1170A: DEBAD03734 - Postrun	11/08/2023 02: 37: 12
Method	Saving Method COL1_5NH4FA_MECN_5T095_1MIN_10> 0-600MS_POS.M	11/08/2023 02: 39: 52
Method	Instrument run completed	11/08/2023 02: 39: 53
CP Macro	Analyzing rawdata 004-D2F-E3-0810MBAAd_0p01.D	11/08/2023 02: 39: 54
Method	Saving Method DA.M	11/08/2023 02: 39: 55
Method	Method completed	11/08/2023 02: 40: 04





Area Percent Report

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	0.269	BB	0.0353	79.35354	33.93908	55.5756
2	0.379	BB	0.0770	12.18989	2.49404	8.5372
3	0.452	BB	0.1281	14.10198	1.39256	9.8764
4	2.572	MM	0.0455	29.53979	10.81267	20.6883
5	2.889	MM	0.0633	7.59961	2.00049	5.3224

Totals : 142.78481 50.63884

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.268	BB	0.0414	168.99480	66.97280	66.5638
2	0.349	BB	0.0460	9.53409	3.09092	3.7553
3	2.360	BB	0.2226	54.26328	4.09401	21.3733
4	2.569	BB	0.0651	11.59585	2.54567	4.5674
5	3.594	BBA	0.0552	9.49595	2.56427	3.7403
Totals :				253.88397	79.26768	

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.262	BB	0.0453	471.17661	165.24762	90.9265
2	2.567	BB	0.0476	31.65636	10.38630	6.1090
3	3.593	BBA	0.0511	15.36203	4.58461	2.9645
Totals :				518.19500	180.21853	

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.269	BB	0.0378	99.44431	41.77128	45.5008
2	0.374	BB	0.0725	12.00034	2.66897	5.4908
3	2.576	BB	0.5631	87.97594	1.86243	40.2535
4	2.888	BB	0.0951	11.74362	1.64934	5.3733
5	3.596	BB	0.0647	7.39077	1.63627	3.3817
Totals :				218.55498	49.58829	

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.270	BB	0.0373	70.24749	29.99230	30.6352
2	0.380	BB	0.0767	11.13358	2.29002	4.8554
3	0.452	BB	0.1292	13.32950	1.30424	5.8130
4	2.574	BB	0.3736	134.59264	4.34214	58.6964
Totals :				229.30320	37.92869	

Signal 6: ELS1 A, ELSD Signal

Peak #	RetTime [min]	Type	Width [min]	Area [mV*s]	Height [mV]	Area %
1	1.932	BB	0.0365	5.07346	1.84997	100.0000

Totals : 5.07346 1.84997

Signal 7: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.471	BB	0.1866	6.72901e6	4.59571e5	100.0000

Totals : 6.72901e6 4.59571e5

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.

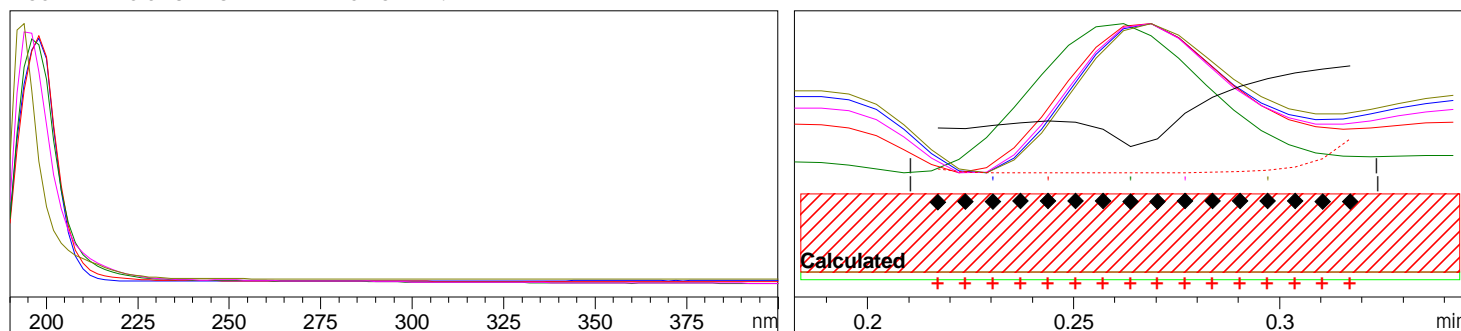
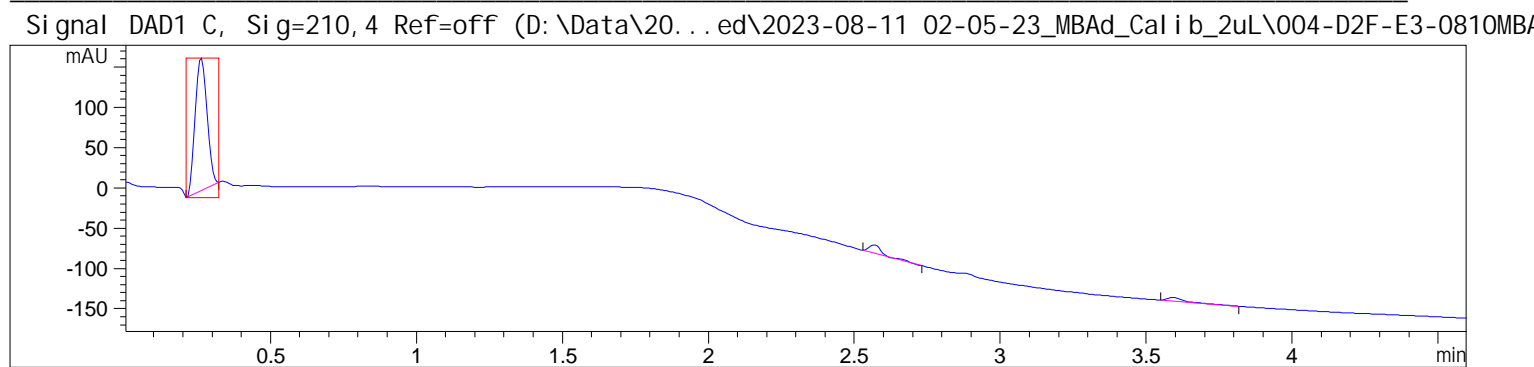
Signal 6: ELS1 A, ELSD Signal
Empty table.

Signal 7: MSD1 TIC, MS File
Empty table.

Final Summed Peaks Report

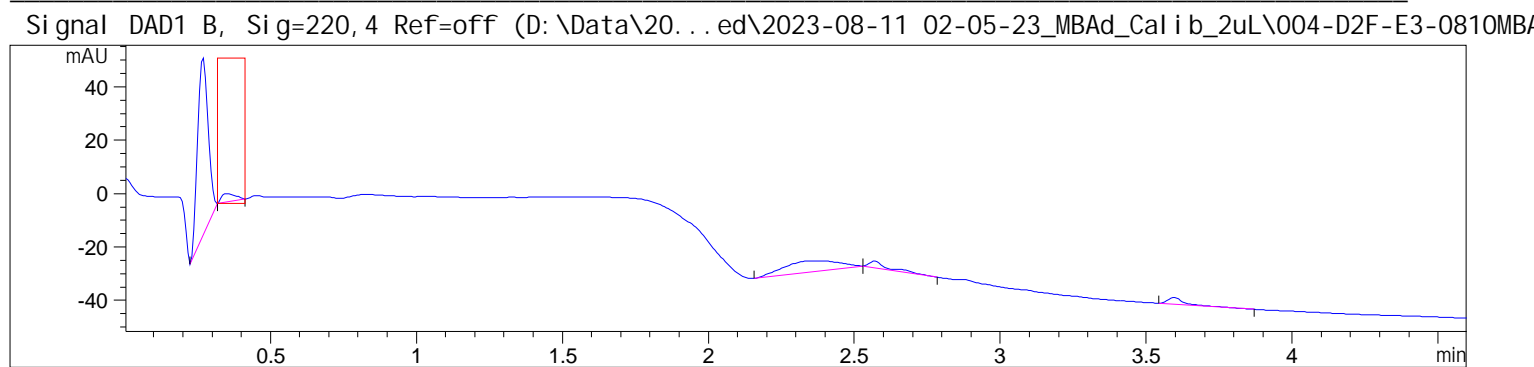
Signal 1: DAD1 A, Sig=254, 4 Ref=off

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

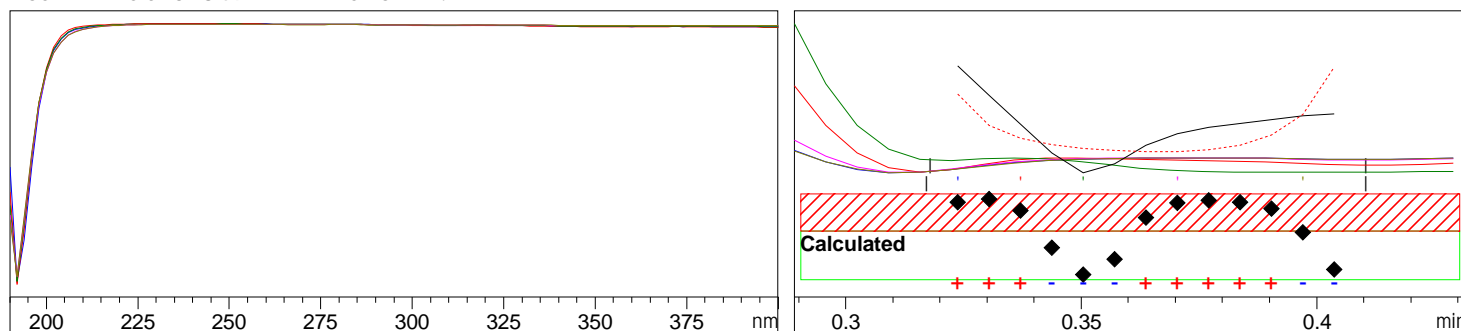


-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 889.350 (16 of 16 spectra exceed the calculated threshold limit.)
Threshold : 999.657 (Calculated with 16 of 16 spectra)
Reference : Peak start and end spectra (integrated) (0.210 / 0.324)
Spectra : 5 (Selection automatic, 5)
Noise Threshold : 0.623 (12 spectra, St.Dev 0.2559 + 3 * 0.1225)
Warning : Spectral absorbances > 1000 mAU (see help for more information)



Peak : 2 at 0.349 min Name : ?



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

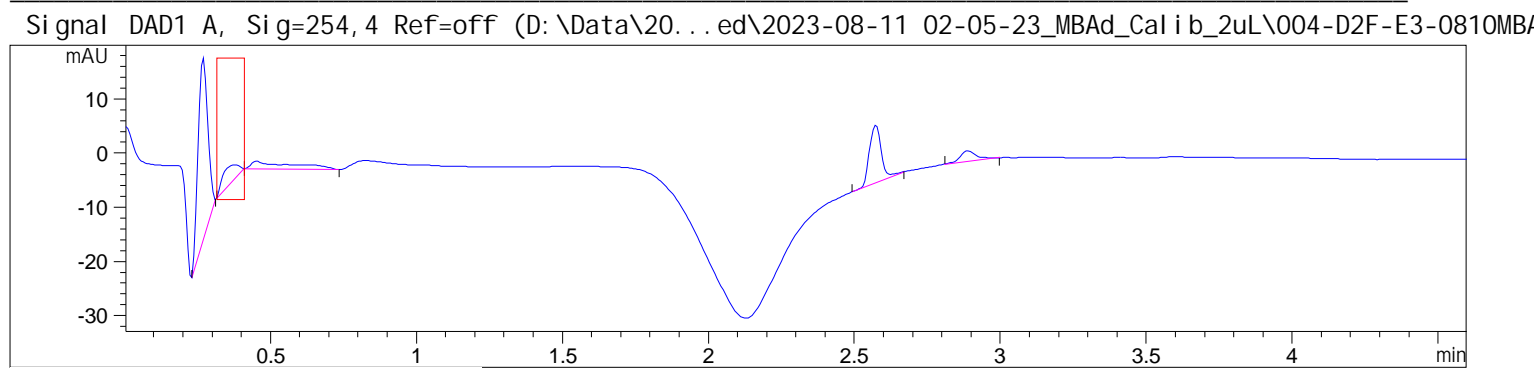
Purity factor : 996.867 (8 of 13 spectra exceed the calculated threshold limit.)

Threshold : 998.581 (Calculated with 8 of 13 spectra)

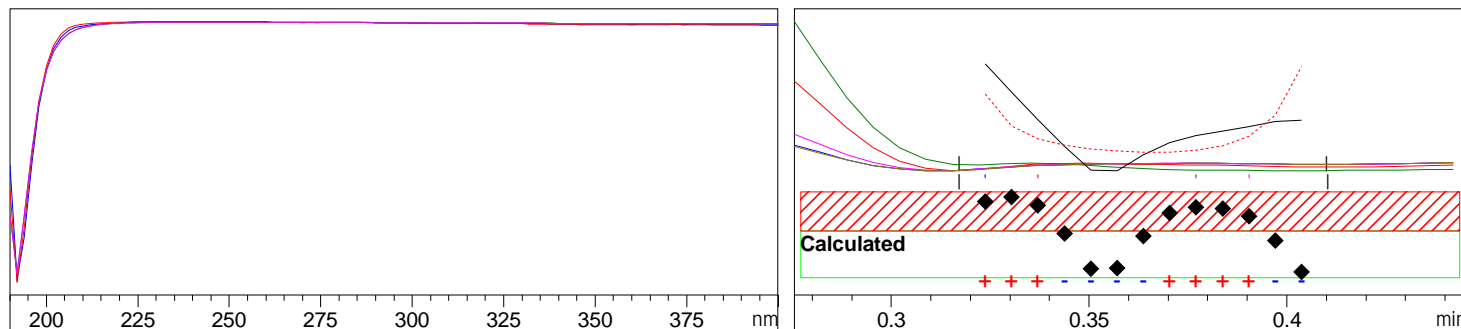
Reference : Peak start and end spectra (integrated) (0.317 / 0.410)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.623 (12 spectra, St.Dev 0.2559 + 3 * 0.1225)

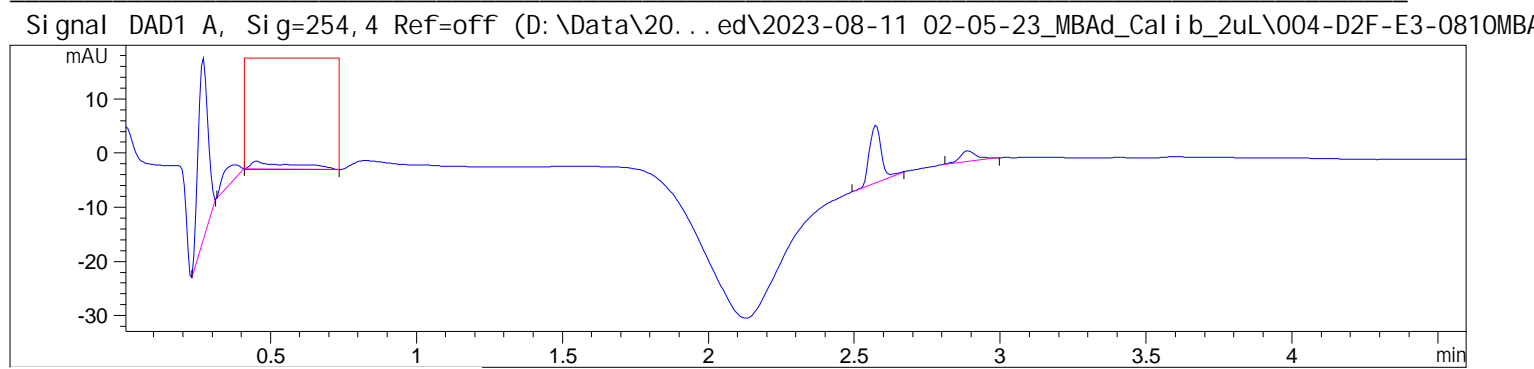


Peak : 3 at 0.379 min Name : ?

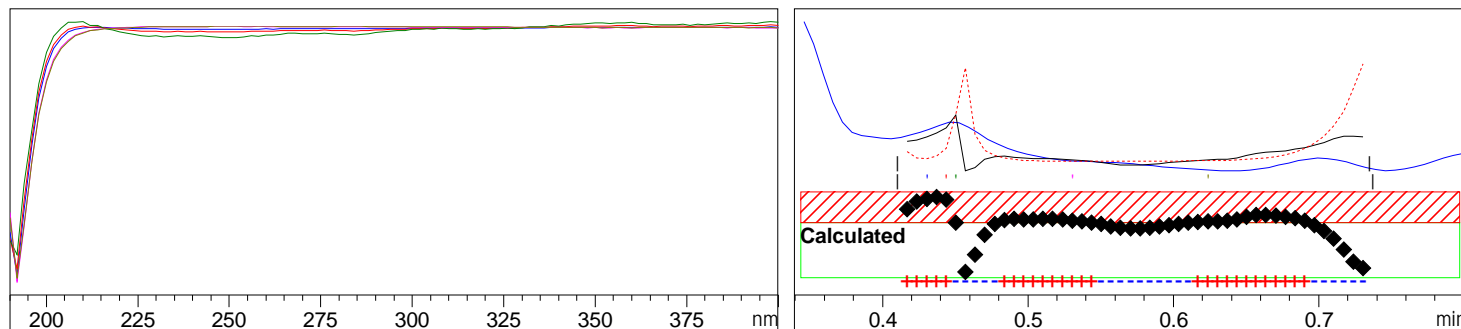


-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 996.504 (7 of 13 spectra exceed the calculated threshold limit.)
Threshold : 998.396 (Calculated with 7 of 13 spectra)
Reference : Peak start and end spectra (integrated) (0.317 / 0.410)
Spectra : 4 (Selection automatic, 5)
Noise Threshold: 0.623 (12 spectra, St.Dev 0.2559 + 3 * 0.1225)



Peak : 4 at 0.452 min Name : ?



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

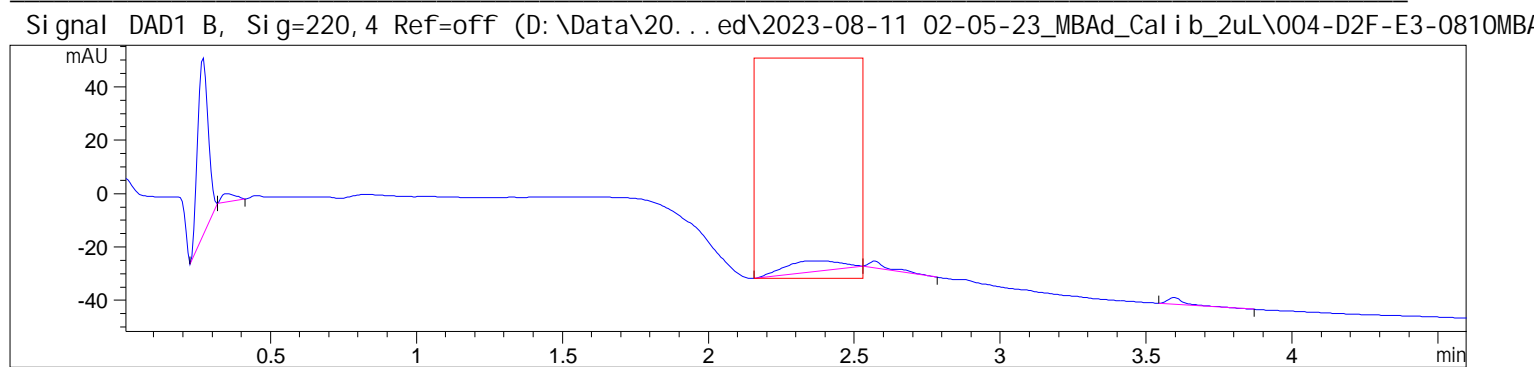
Purity factor : 916.460 (27 of 48 spectra exceed the calculated threshold limit.)

Threshold : 930.523 (Calculated with 27 of 48 spectra)

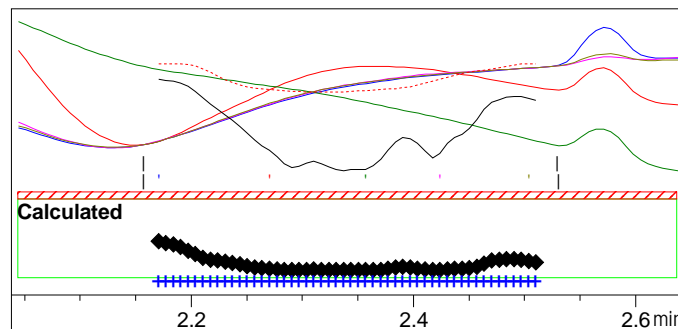
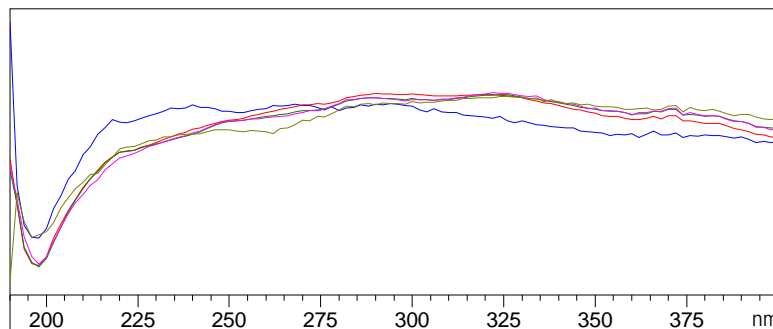
Reference : Peak start and end spectra (integrated) (0.410 / 0.737)

Spectra : 5 (Selection automatic, 5)

Noise Threshold : 0.623 (12 spectra, St.Dev 0.2559 + 3 * 0.1225)

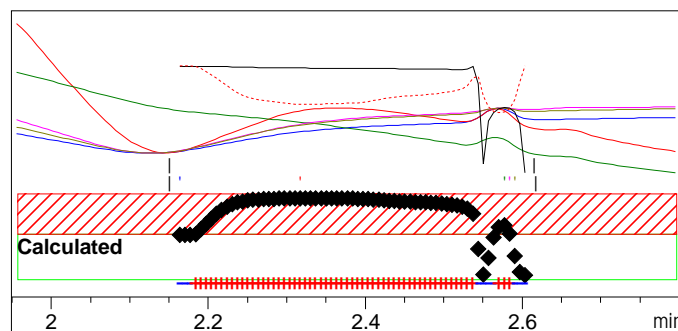
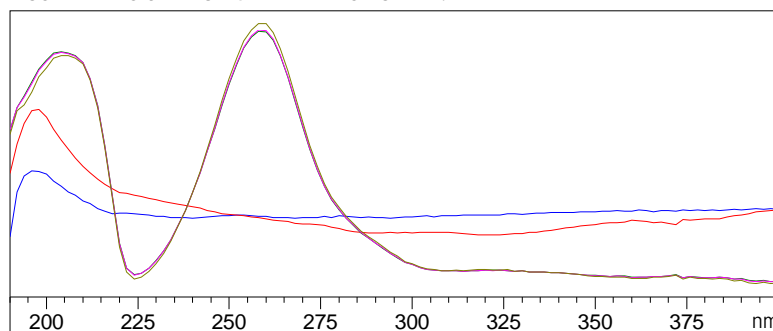
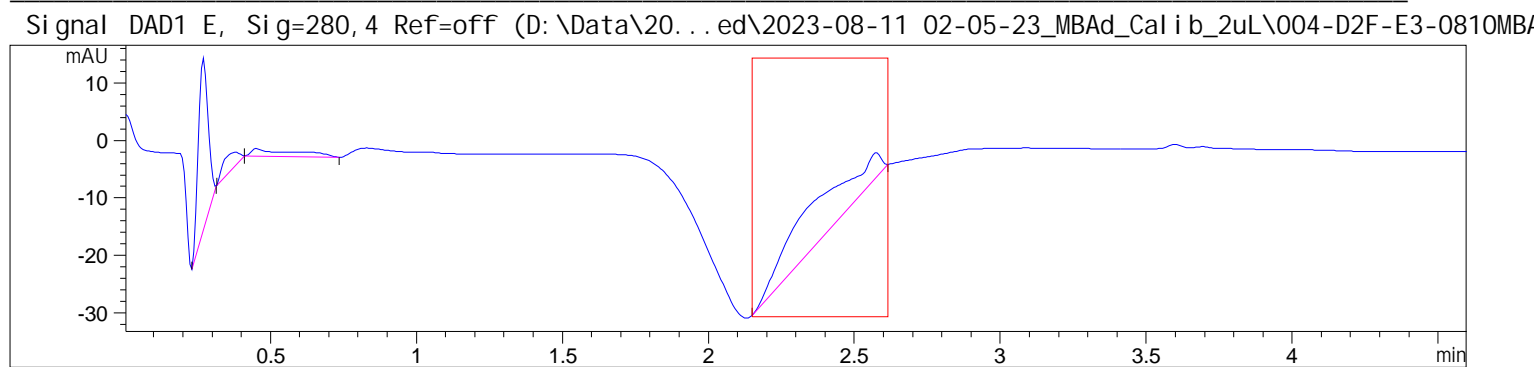


Peak : 6 at 2.360 min Name : ?



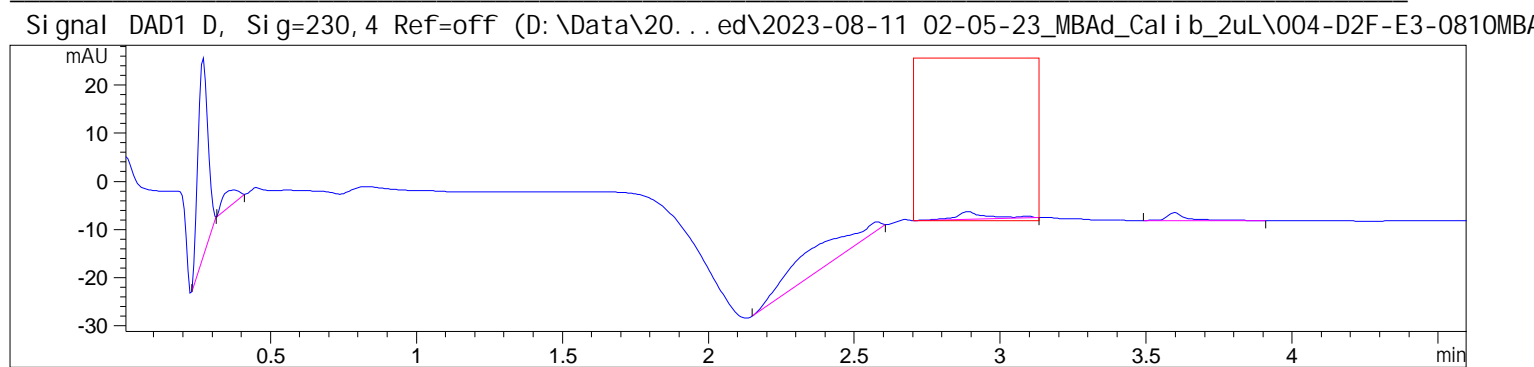
-> The purity factor is within the calculated threshold limit. <-

Purity factor : 929.635 (52 of 52 spectra are within the calculated threshold limit.)
Threshold : 514.361 (Calculated with 52 of 52 spectra)
Reference : Peak start and end spectra (integrated) (2.157 / 2.530)
Spectra : 5 (Selection automatic, 5)
Noise Threshold: 0.623 (12 spectra, St.Dev 0.2559 + 3 * 0.1225)

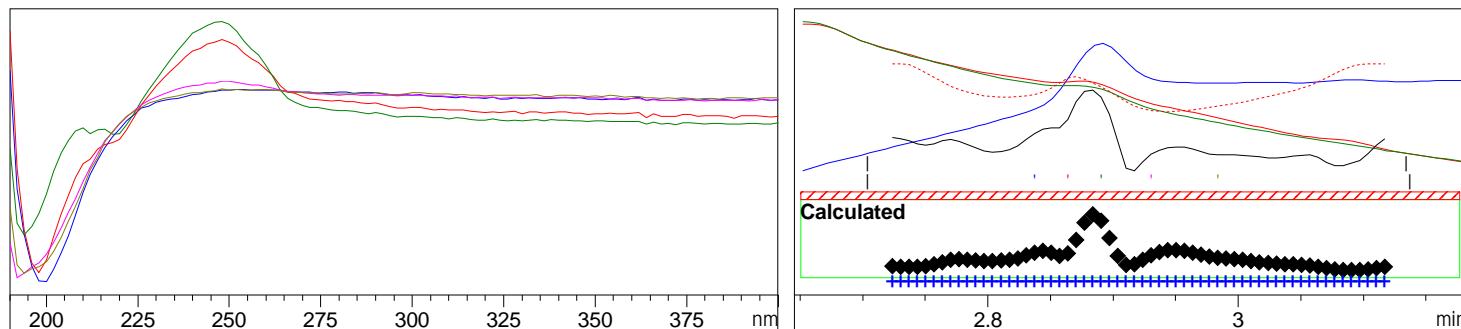


-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 148.153 (57 of 67 spectra exceed the calculated threshold limit.)
Threshold : 786.313 (Calculated with 57 of 67 spectra)
Reference : Peak start and end spectra (integrated) (2.150 / 2.617)
Spectra : 5 (Selection automatic, 5)
Noise Threshold: 0.623 (12 spectra, St.Dev 0.2559 + 3 * 0.1225)



Peak : 8 at 2.888 min Name : ?



-> The purity factor is within the calculated threshold limit. <-

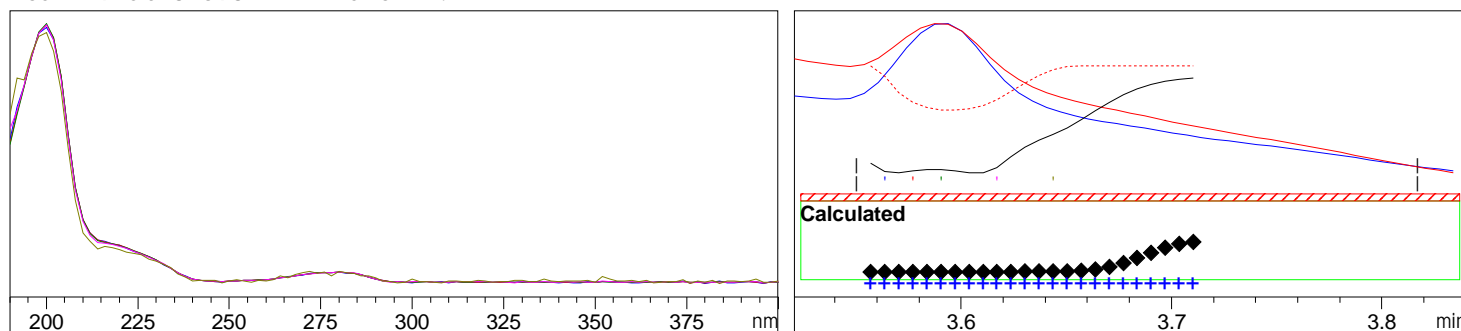
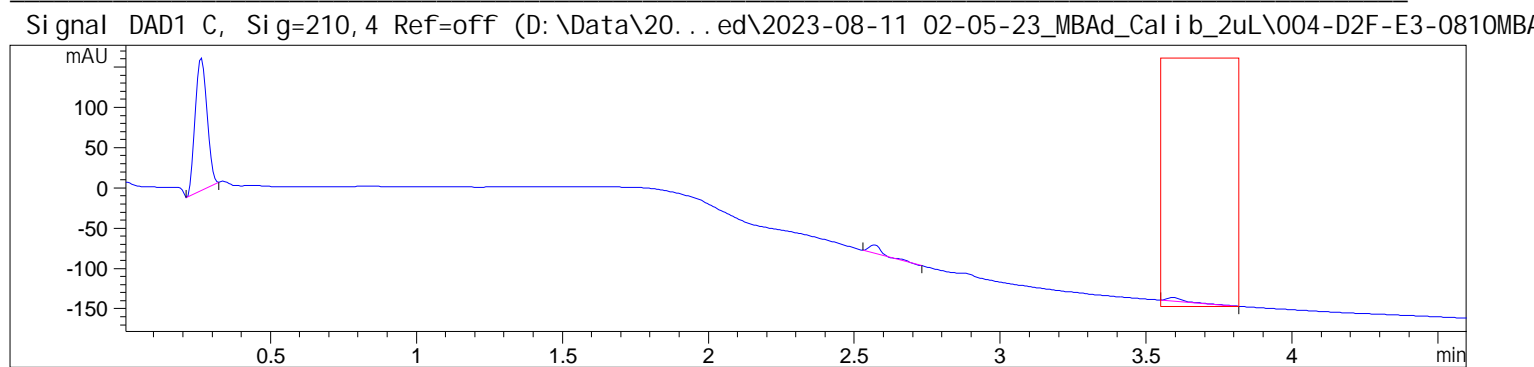
Purity factor : 909.265 (60 of 60 spectra are within the calculated threshold limit.)

Threshold : 503.937 (Calculated with 60 of 60 spectra)

Reference : Peak start and end spectra (integrated) (2.704 / 3.137)

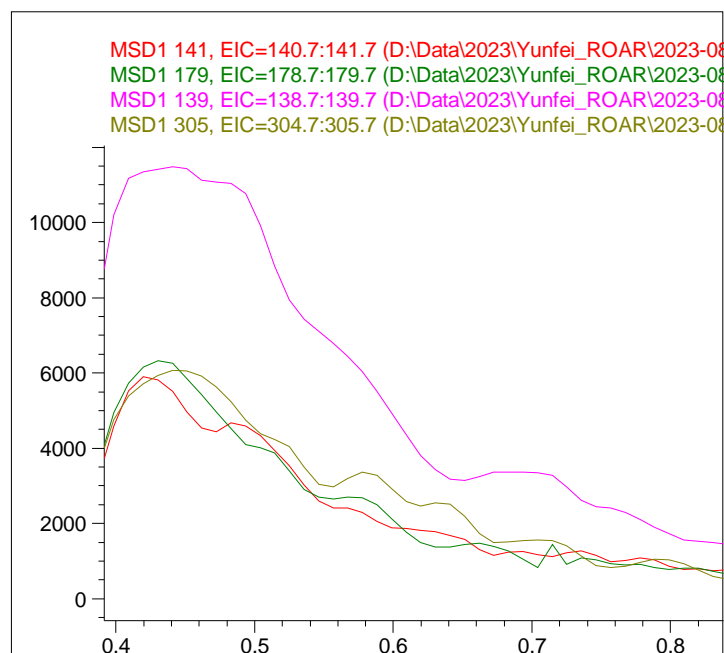
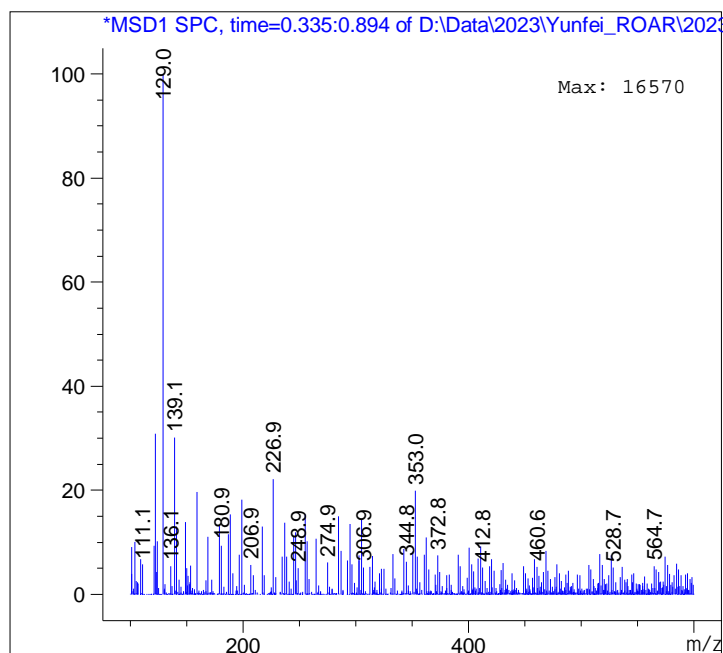
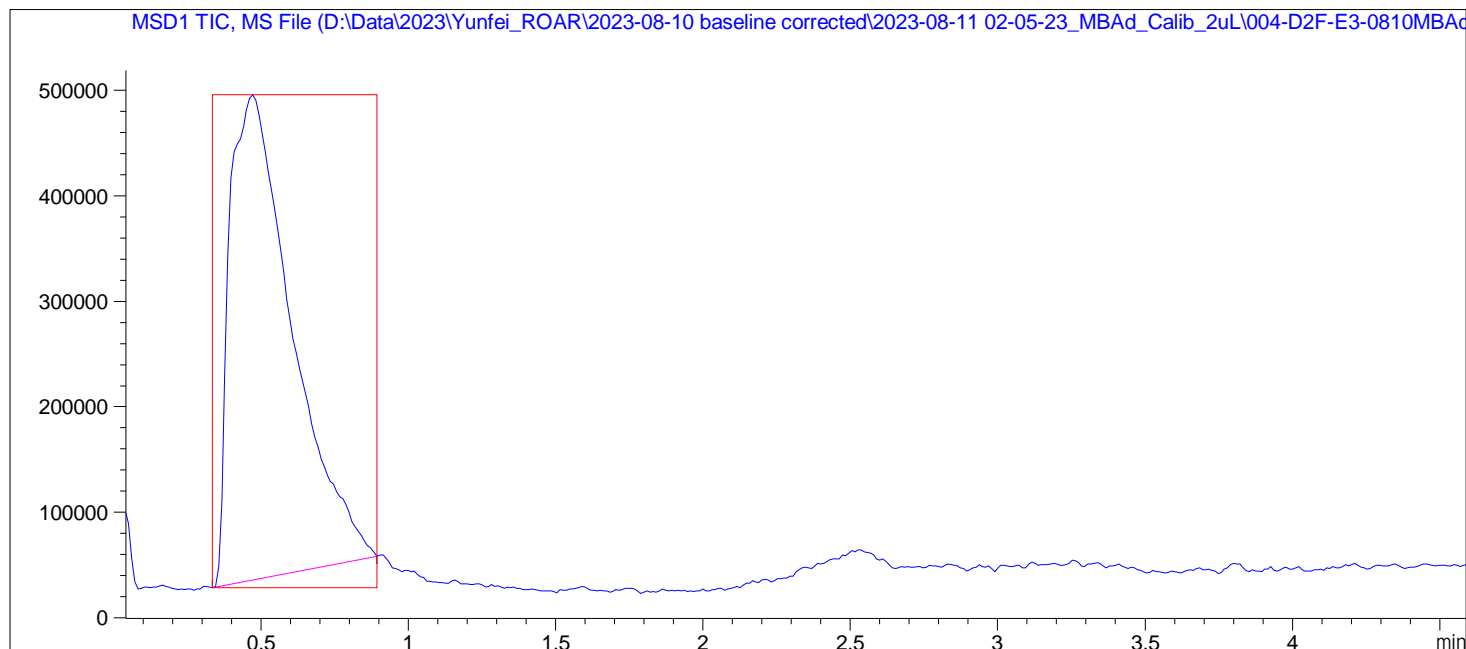
Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.623 (12 spectra, St.Dev 0.2559 + 3 * 0.1225)



-> The purity factor is within the calculated threshold limit. <-

Purity factor : 918.718 (24 of 24 spectra are within the calculated threshold limit.)
Threshold : 423.201 (Calculated with 24 of 24 spectra)
Reference : Peak start and end spectra (integrated) (3.550 / 3.817)
Spectra : 5 (Selection automatic, 5)
Noise Threshold: 0.623 (12 spectra, St.Dev 0.2559 + 3 * 0.1225)



Peak #1 at 0.471 min (0.335 to 0.894 min)

-> The analysis found 8 components, indicating an impure peak. <-

Component 1: Peak at Scan 37.3. Top ions are 141
Component 2: Peak at Scan 38.2. Top ions are 179
Component 3: Peak at Scan 39.2. Top ions are 139 305
Component 4: Peak at Scan 39.9. Top ions are 129
Component 5: Peak at Scan 40.7. Top ions are 122
Component 6: Peak at Scan 42.9. Top ions are 101 189
Component 7: Peak at Scan 43.6. Top ions are 255
Component 8: Peak at Scan 49.8. Top ions are 199

*** End of Report ***