

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
  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
```

Sample Name: 0810MBAAd\_Op05

```
=====
Acq. Operator   : user                      Seq. Line :    5
Sample Operator : user
Acq. Instrument : SFC LCMS                  Location  :   D2F-E4
Injection Date  : 11/08/2023 02:41:06       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\C0L1
                  _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\C0L1_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       : 435
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	Accumul ated On-Time
DAD 1, UV Lamp	: 0.58	849.6 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	:	5.3E-009	5.3E-009 Torr
CapCur	:	5	656 nA
ChamCur	:	8.0E-002	1.5E-001 µA
Dryi ngGas	:	12	12 l /mi n
Neb Pres	:	35	35 psi g
Turbo1Spd	:	100	100 %
Turbo1Pwr	:	127	129 W
RF Drive	:	1	15 %
Qd TpDrv	:	16	16 %
Gas TpDrv	:	35	36 %
Neb PrDrv	:	50	49 %
Gas FI Drv	:	61	61 %

=====

#### MSD tuning (calibration) parameters

Ionization polari ty	:	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

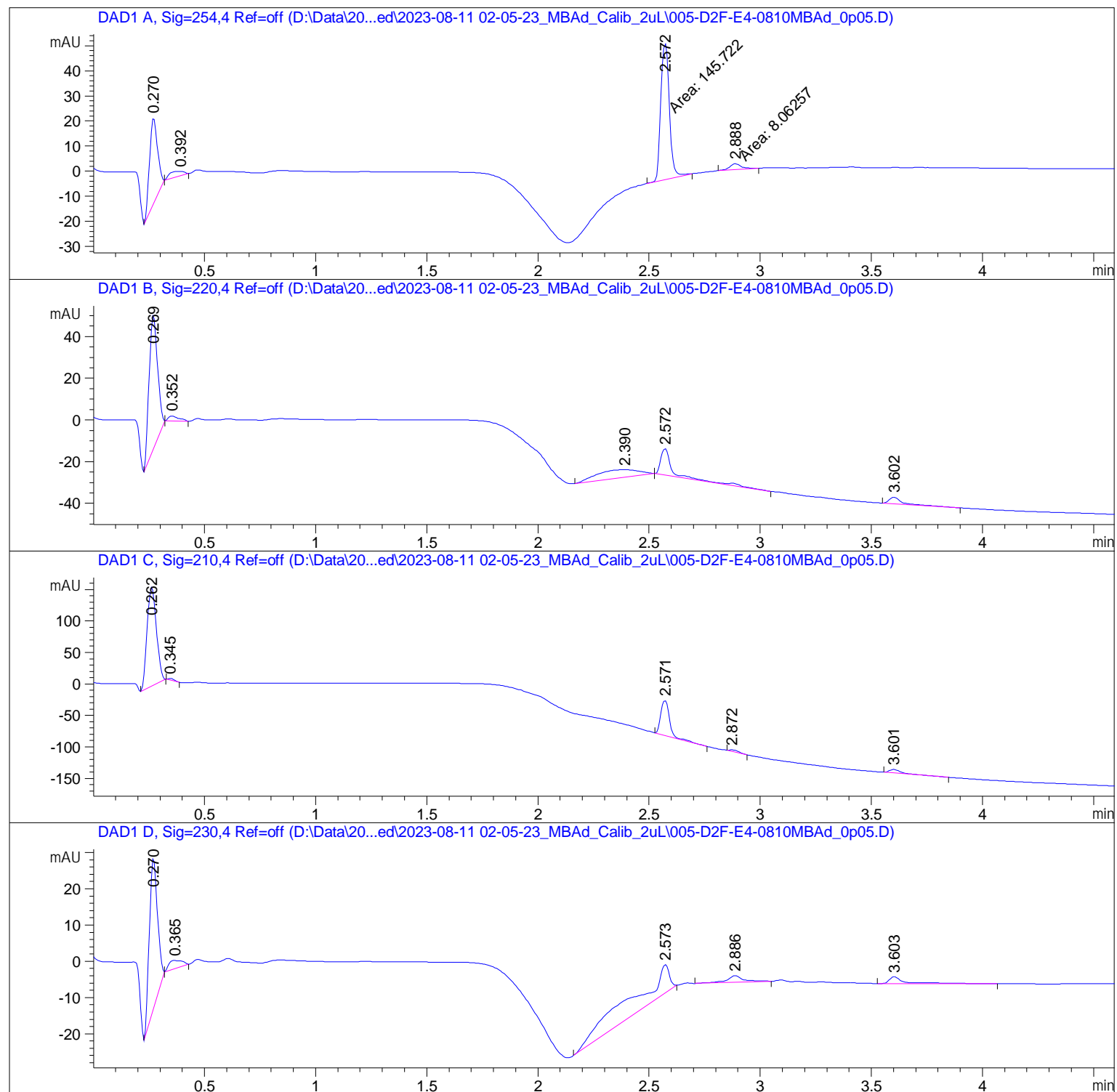
=====  
=====  
Run Logbook  
=====

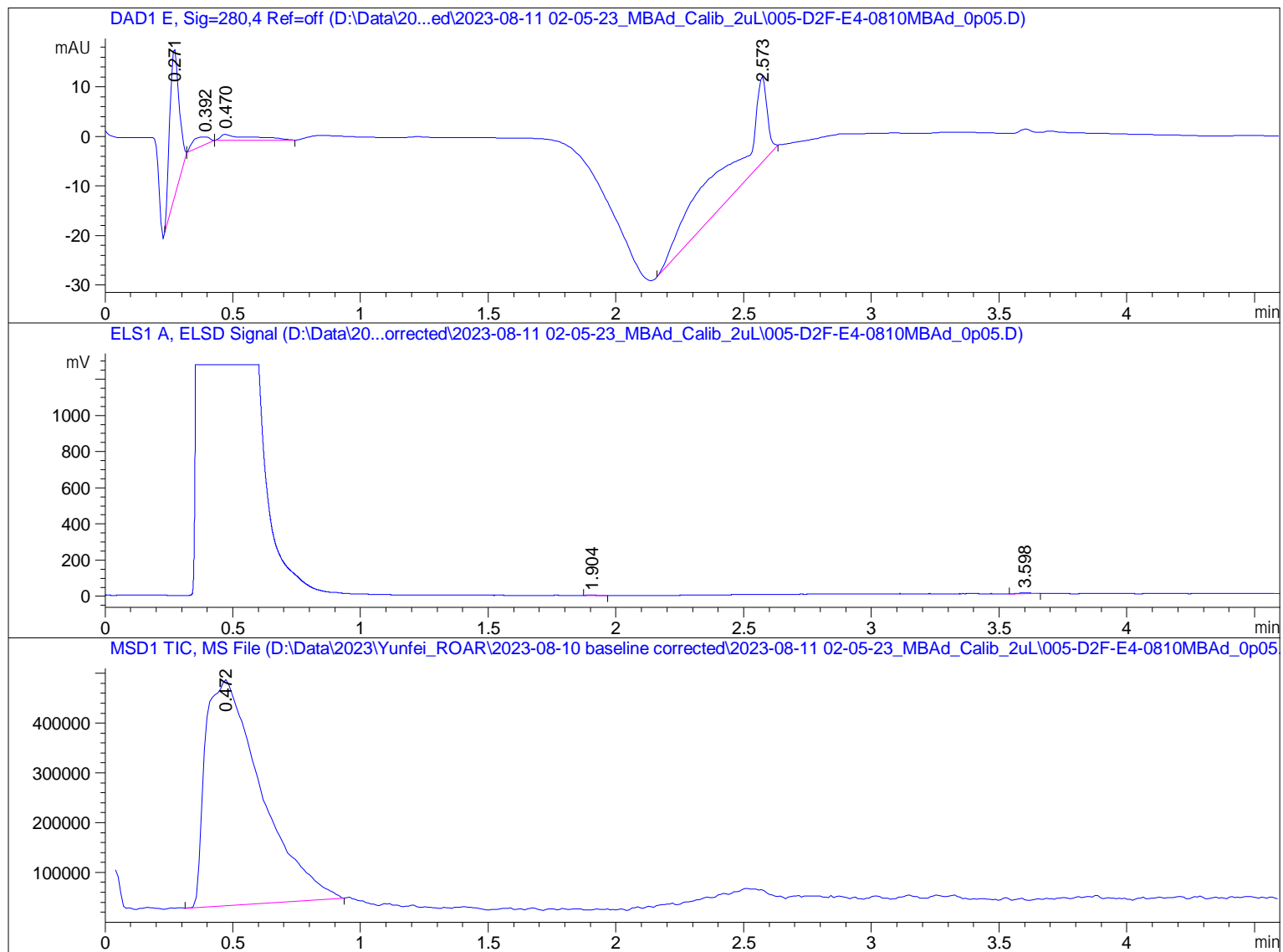
11 Aug 23 12:16 PM  
Logbook File: D:\Data\20...cted\2023-08-11 02-05-23\_MBAd\_Cal i b\_2uL\005-D2F-E4-0810MBAd\_Op05. D\RUN. LOG

Module	# Event Message	Date Time
-----		
Method	Method started: line# 5 at location 'D2F-E4>' ' inj# 1	11/08/2023 02:40:06
CP Macro	PreRun macro: 'LAMPALL ON'	11/08/2023 02:40:07
G4260B	G4260B: ELSD - Autozero	11/08/2023 02:40:07
G4260B	G4260B: ELSD - Al ready swi tched on	11/08/2023 02:40:07
Method	Instrument running sample from location D2F->E4	11/08/2023 02:40:08
G7115A	G7115A: DEAC605436 - Detector: Prepare	11/08/2023 02:40:24
G7115A	G7115A: DEAC605436 - Detector: Idle	11/08/2023 02:40:40
G4767A	G4767A: DEAFD00218 - Draw command finished	11/08/2023 02:40:56
G4767A	G4767A: DEAFD00218 - Sampler wash is active	11/08/2023 02:40:57
G4767A	G4767A: DEAFD00218 - Sampler wash is idle	11/08/2023 02:41:04
G4767A	G4767A: DEAFD00218 - Sample preparation time: >24 sec	11/08/2023 02:41:04
PumpVal ve	G7111B: DEAEW03495 - Run	11/08/2023 02:41:06

Sample Name: 0810MBAAd\_Op05

PumpVal ve	G7111B: DEAEW03495 - Postrun	11/08/2023 02: 45: 42
G4767A	G4767A: DEAFD00218 - Postrun	11/08/2023 02: 45: 42
G7110B	G7110B: DEAEH00761 - Postrun	11/08/2023 02: 45: 43
PumpVal ve	G1170A: DEBAD03715 - Postrun	11/08/2023 02: 45: 43
G4782A	G4782A: DEAGN00153 - Postrun	11/08/2023 02: 45: 44
G1170A	G1170A: DEBAD03734 - Postrun	11/08/2023 02: 45: 44
Method	Saving Method COL1_5NH4FA_MECN_5T095_1MIN_10> 0-600MS_POS.M	11/08/2023 02: 47: 50
Method	Instrument run completed	11/08/2023 02: 47: 51
CP Macro	Analyzing rawdata 005-D2F-E4-0810MBAAd_Op05.D	11/08/2023 02: 47: 52
Method	Saving Method DA.M	11/08/2023 02: 47: 53
Method	Method completed	11/08/2023 02: 48: 01





# 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	0.270	BB	0.0391	85.77565	34.39181	34.4685
2	0.392	BB	0.0888	9.29189	1.67225	3.7339
3	2.572	MM	0.0446	145.72212	54.47105	58.5577
4	2.888	MM	0.0584	8.06257	2.30040	3.2399

Totals : 248.85223 92.83551

Sample Name: 0810MBAAd\_Op05

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.269	BB	0.0408	170.56299	64.50861	59.6210
2	0.352	BB	0.0490	7.41141	2.33626	2.5907
3	2.390	BB	0.1832	51.20403	3.61549	17.8986
4	2.572	BB	0.0537	44.88852	12.57296	15.6910
5	3.602	BBA	0.0590	12.01158	3.11173	4.1987

Totals : 286.07852 86.14506

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	0.0482	461.83667	157.47659	71.6210
2	0.345	BB	0.0329	5.58987	2.85254	0.8669
3	2.571	BB	0.0437	150.36545	55.42520	23.3185
4	2.872	BB	0.0495	6.73022	2.09349	1.0437
5	3.601	BBA	0.0553	20.31154	5.73801	3.1499

Totals : 644.83375 223.58582

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.270	BB	0.0397	106.61059	41.93422	43.8808
2	0.365	BB	0.0621	9.21411	2.23665	3.7925
3	2.573	BB	0.1738	108.19279	7.80238	44.5321
4	2.886	BB	0.0725	9.54083	1.84022	3.9270
5	3.603	BB	0.0713	9.39655	1.91416	3.8676

Totals : 242.95487 55.72763

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.271	BB	0.0393	75.83539	30.21096	27.6265
2	0.392	BB	0.0873	8.39694	1.54688	3.0590
3	0.470	BB	0.1039	10.25817	1.27510	3.7370
4	2.573	BB	0.1335	180.01231	17.28116	65.5776

Totals : 274.50281 50.31410



Signal 6: ELS1 A, ELSD Signal

Peak #	RetTime [min]	Type	Width [min]	Area [mV*s]	Height [mV]	Area %
1	1.904	BB	0.0369	4.75225	2.10105	24.5265
2	3.598	BB	0.0468	14.62377	4.63819	75.4735

Totals : 19.37602 6.73924

Signal 7: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.472	BB	0.1892	6.87590e6	4.54272e5	100.0000

Totals : 6.87590e6 4.54272e5

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.

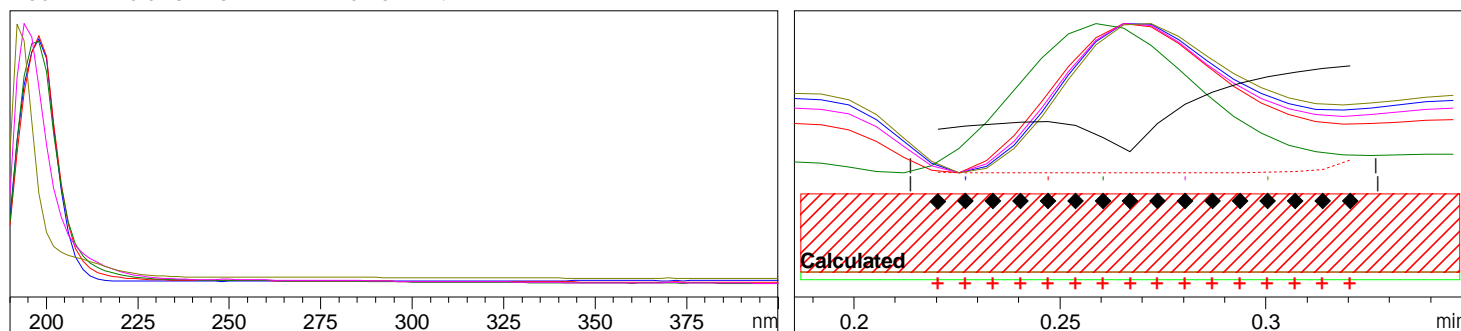
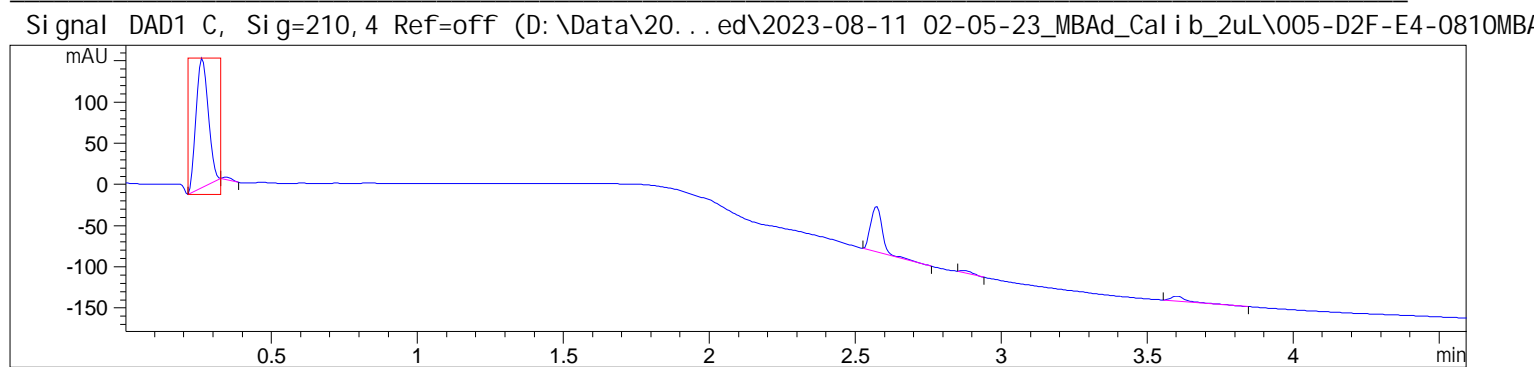
Signal 6: ELS1 A, ELSD Signal  
Empty table.

Signal 7: MSD1 TIC, MS File  
Empty table.

Final Summed Peaks Report

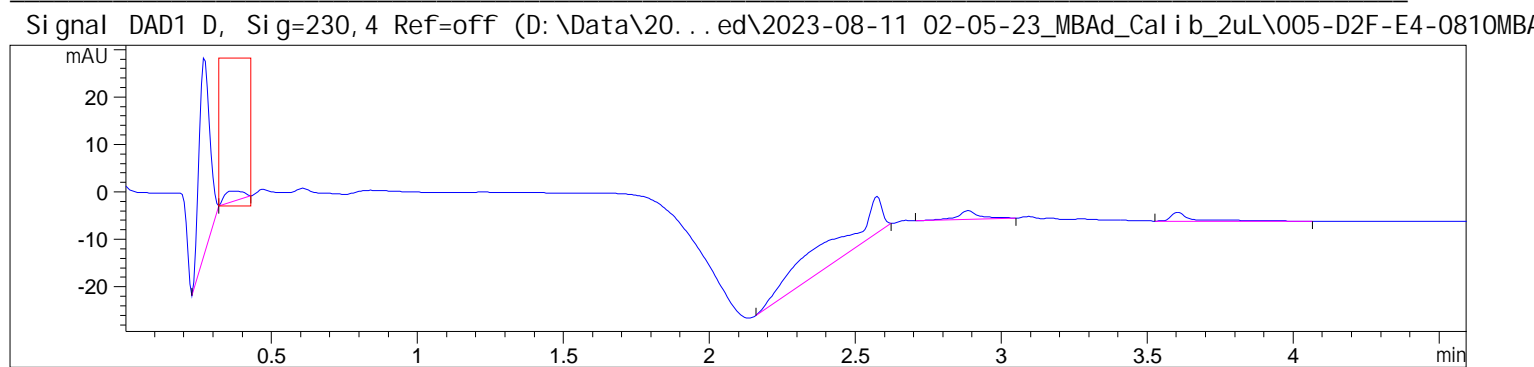
Signal 1: DAD1 A, Sig=254,4 Ref=off

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

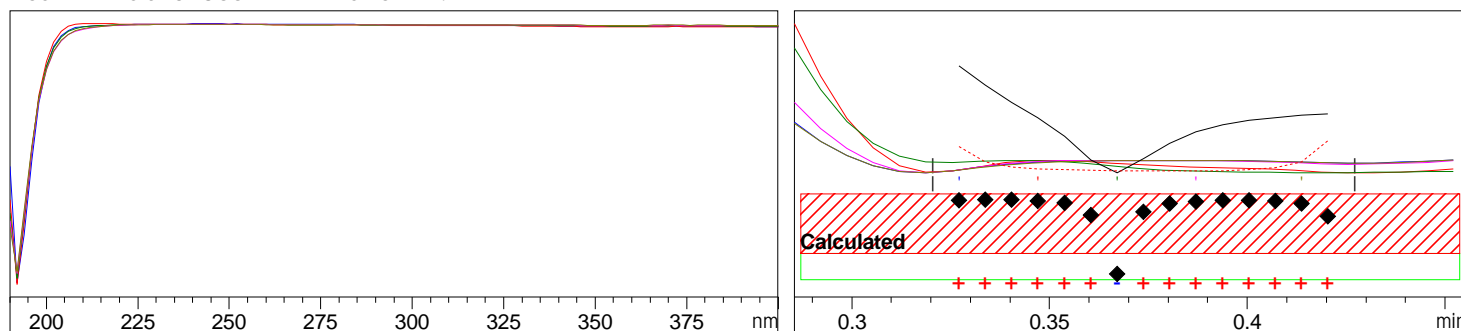


-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 843.255 (16 of 16 spectra exceed the calculated threshold limit.)  
Threshold : 999.942 (Calculated with 16 of 16 spectra)  
Reference : Peak start and end spectra (integrated) (0.214 / 0.327)  
Spectra : 5 (Selection automatic, 5)  
Noise Threshold : 0.200 (12 spectra, St.Dev 0.0725 + 3 \* 0.0427)  
Warning : Spectral absorbances > 1000 mAU (see help for more information)



Peak : 2 at 0.365 min Name : ?



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

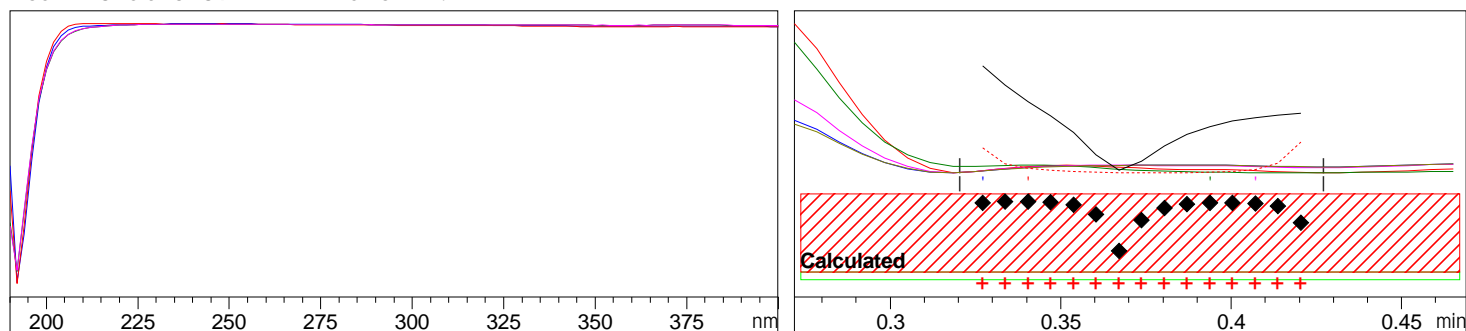
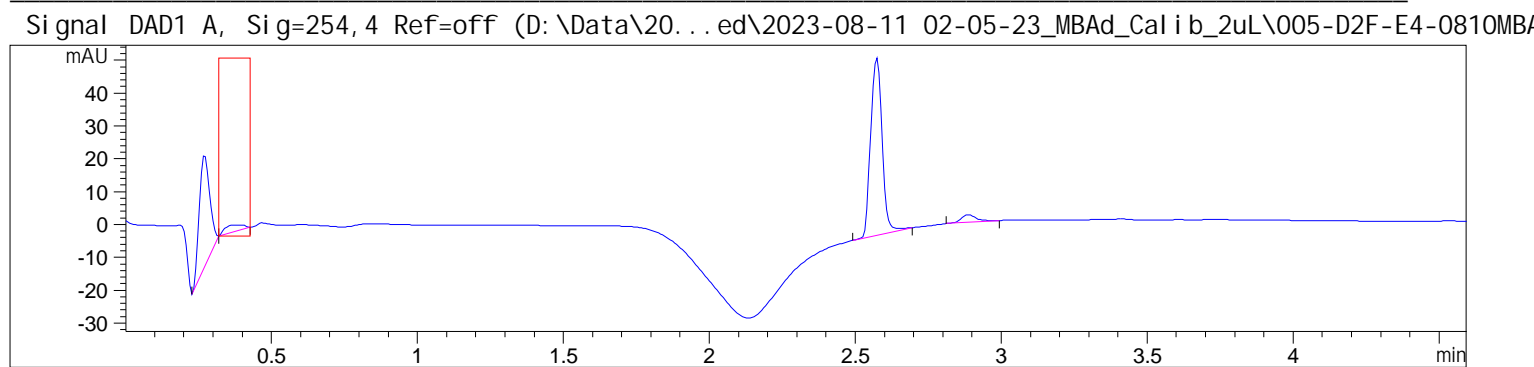
Purity factor : 996.457 (14 of 15 spectra exceed the calculated threshold limit.)

Threshold : 999.740 (Calculated with 14 of 15 spectra)

Reference : Peak start and end spectra (integrated) (0.320 / 0.427)

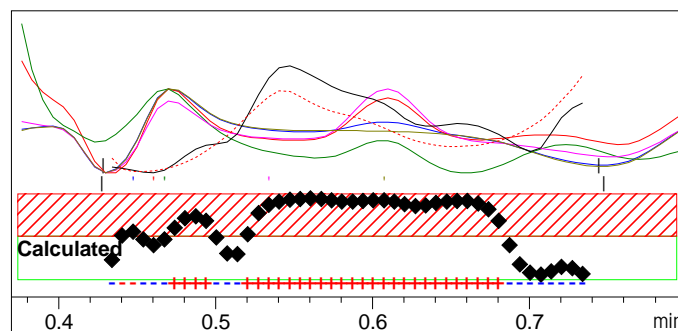
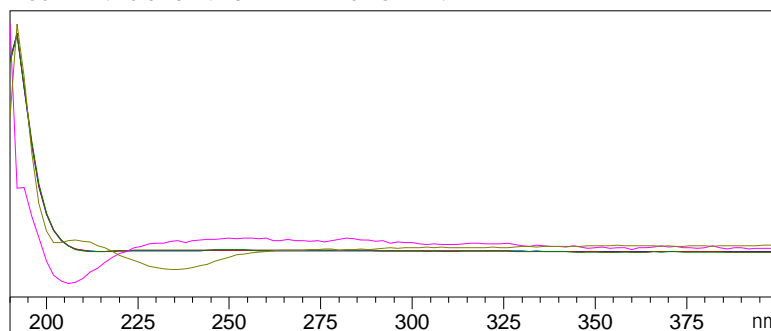
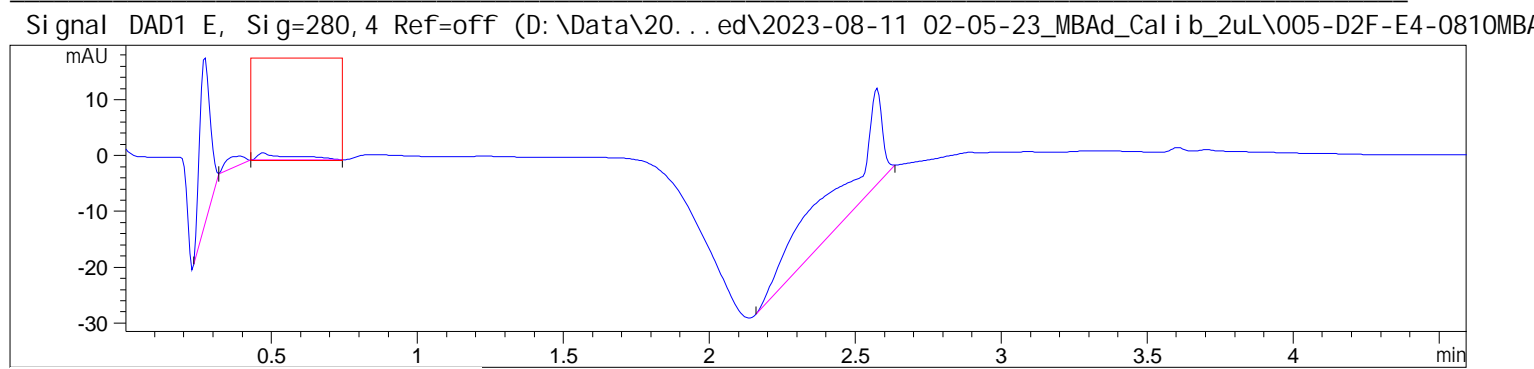
Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.200 (12 spectra, St.Dev 0.0725 + 3 \* 0.0427)



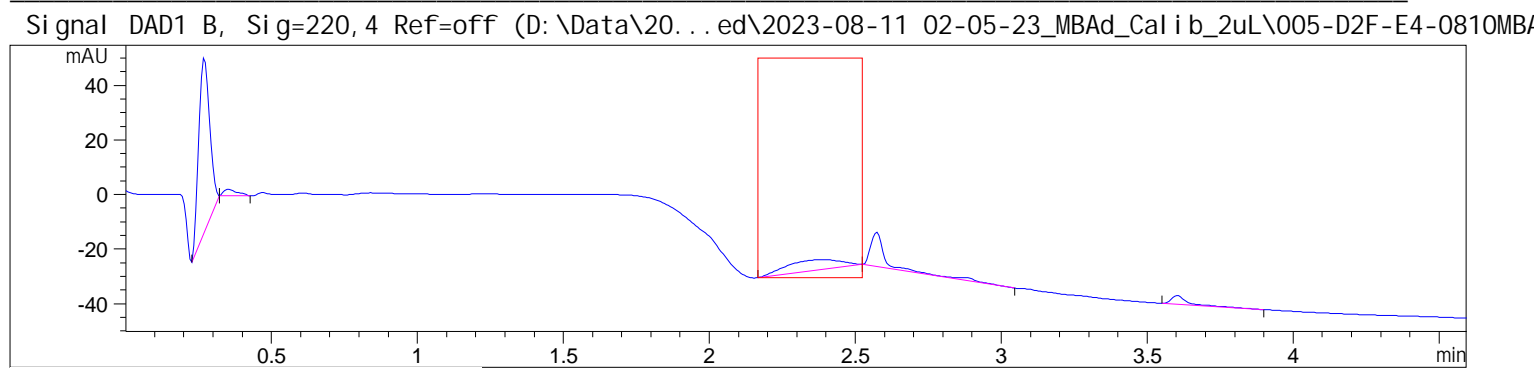
-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 996.665 (15 of 15 spectra exceed the calculated threshold limit.)  
Threshold : 999.738 (Calculated with 15 of 15 spectra)  
Reference : Peak start and end spectra (integrated) (0.320 / 0.427)  
Spectra : 4 (Selection automatic, 5)  
Noise Threshold: 0.200 (12 spectra, St.Dev 0.0725 + 3 \* 0.0427)

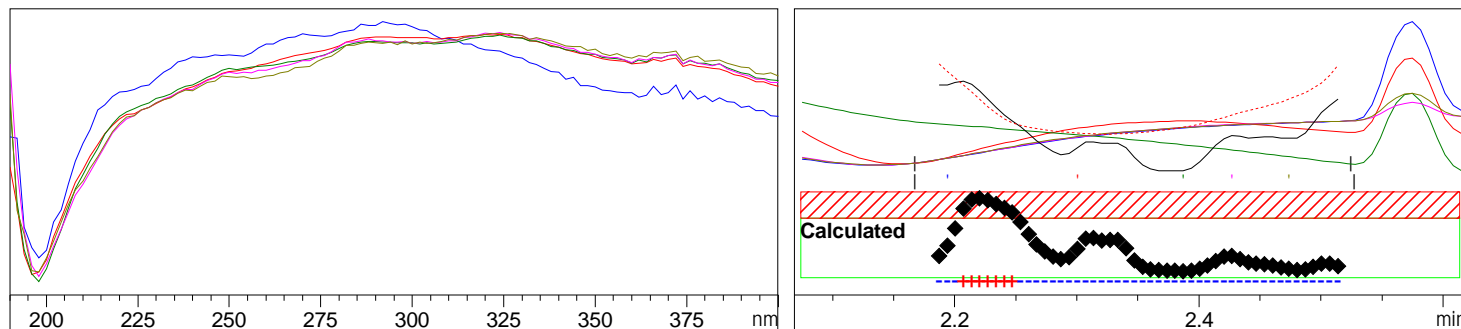


-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 808.747 (29 of 46 spectra exceed the calculated threshold limit.)  
Threshold : 956.225 (Calculated with 29 of 46 spectra)  
Reference : Peak start and end spectra (integrated) (0.427 / 0.747)  
Spectra : 5 (Selection automatic, 5)  
Noise Threshold: 0.200 (12 spectra, St.Dev 0.0725 + 3 \* 0.0427)



Peak : 6 at 2.390 min Name : ?



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

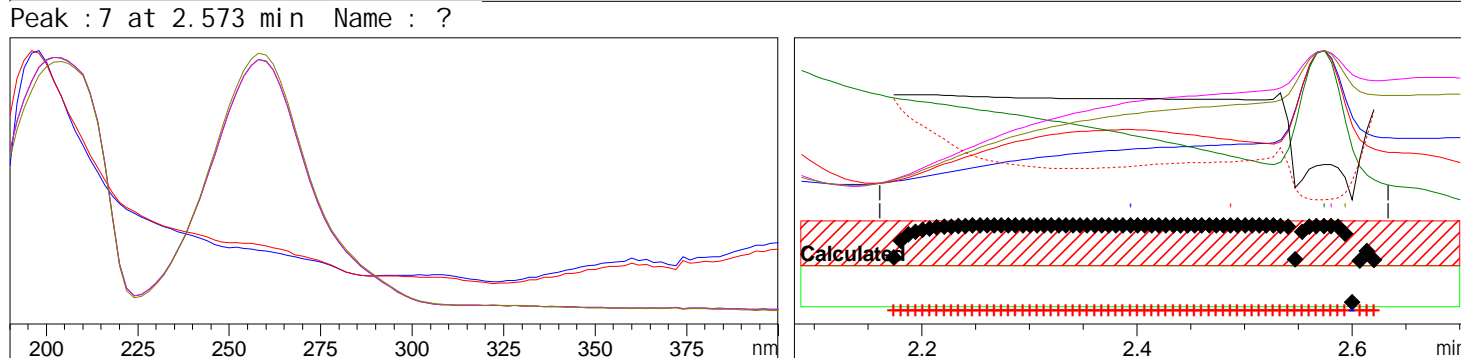
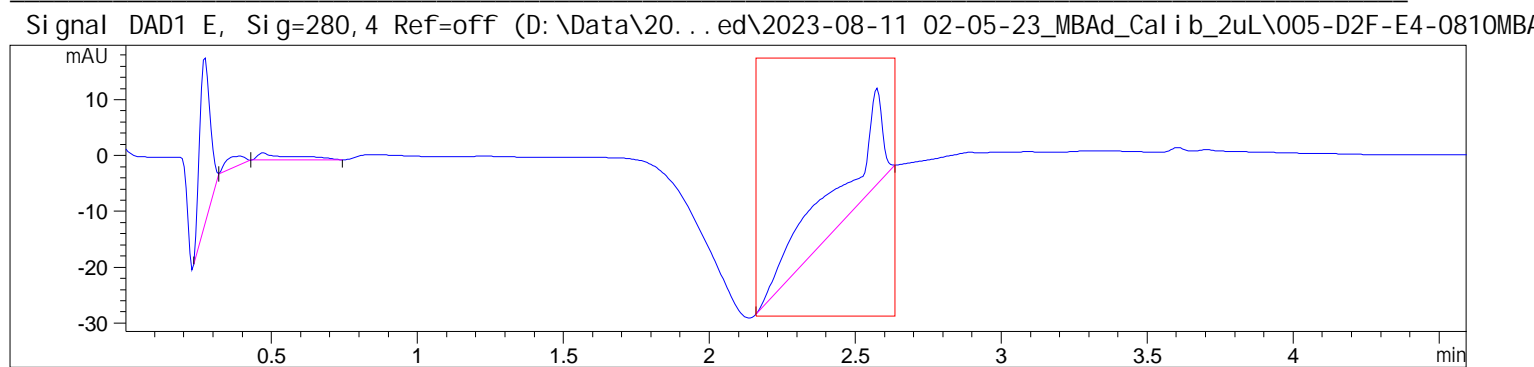
Purity factor : 886.698 (7 of 50 spectra exceed the calculated threshold limit.)

Threshold : 915.131 (Calculated with 7 of 50 spectra)

Reference : Peak start and end spectra (integrated) (2.167 / 2.527)

Spectra : 5 (Selection automatic, 5)

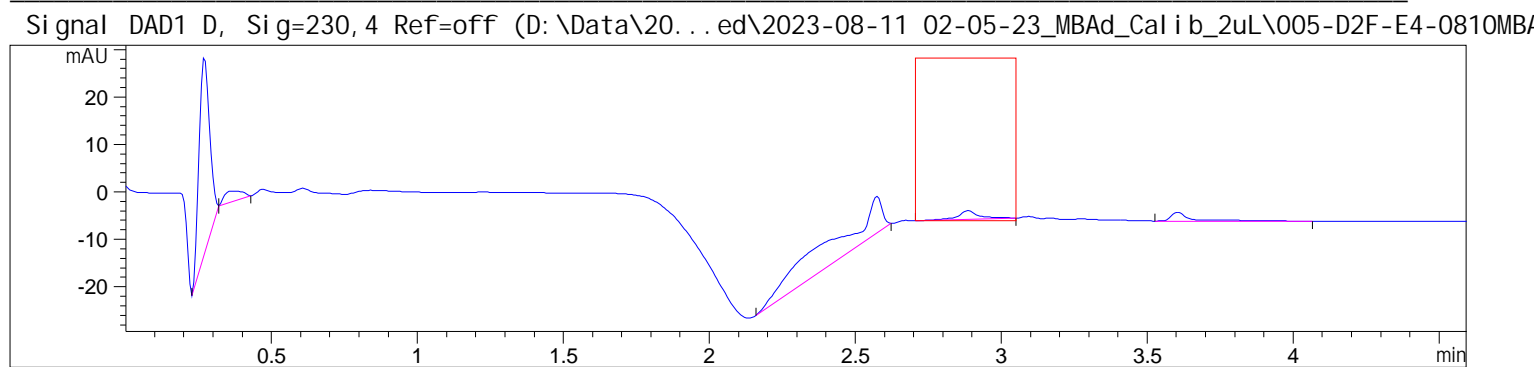
Noise Threshold: 0.200 (12 spectra, St.Dev 0.0725 + 3 \* 0.0427)



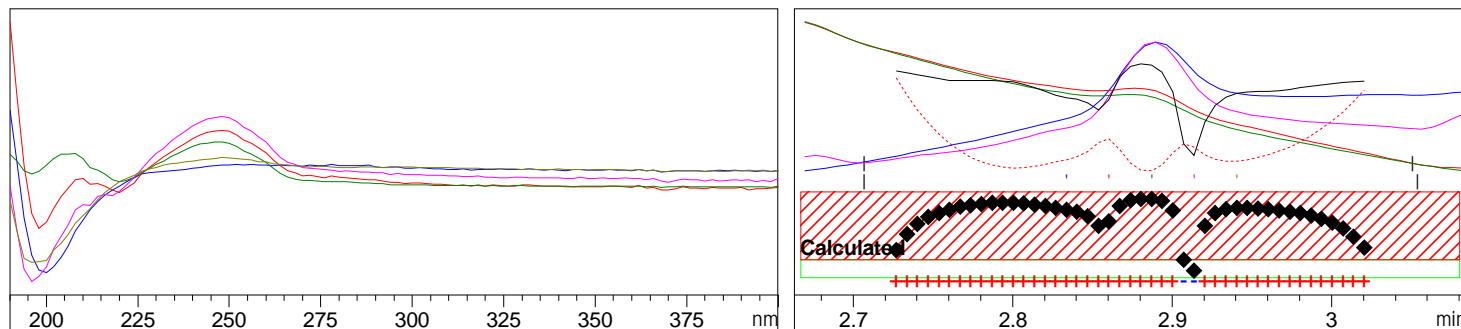
-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 437.318 (67 of 68 spectra exceed the calculated threshold limit.)  
Threshold : 965.628 (Calculated with 67 of 68 spectra)  
Reference : Peak start and end spectra (integrated) (2.160 / 2.634)  
Spectra : 5 (Selection automatic, 5)  
Noise Threshold: 0.200 (12 spectra, St.Dev 0.0725 + 3 \* 0.0427)





Peak : 8 at 2.886 min Name : ?



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

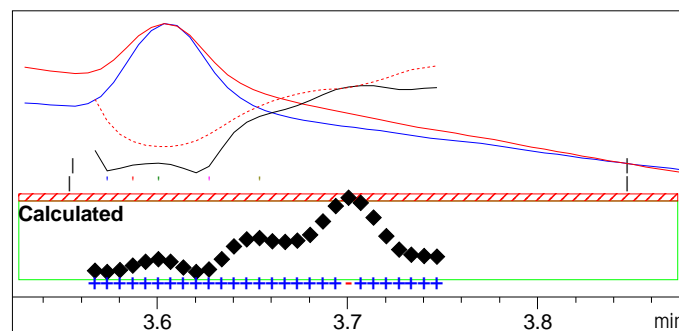
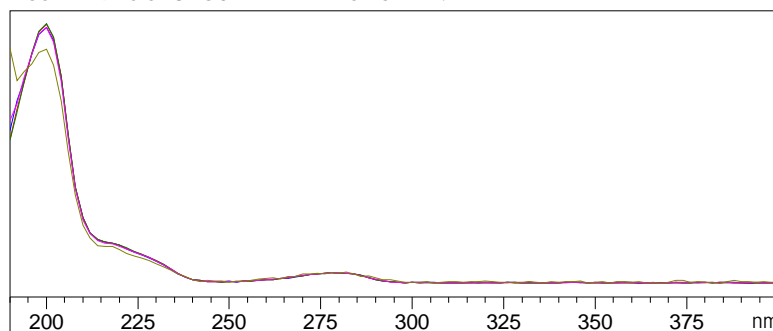
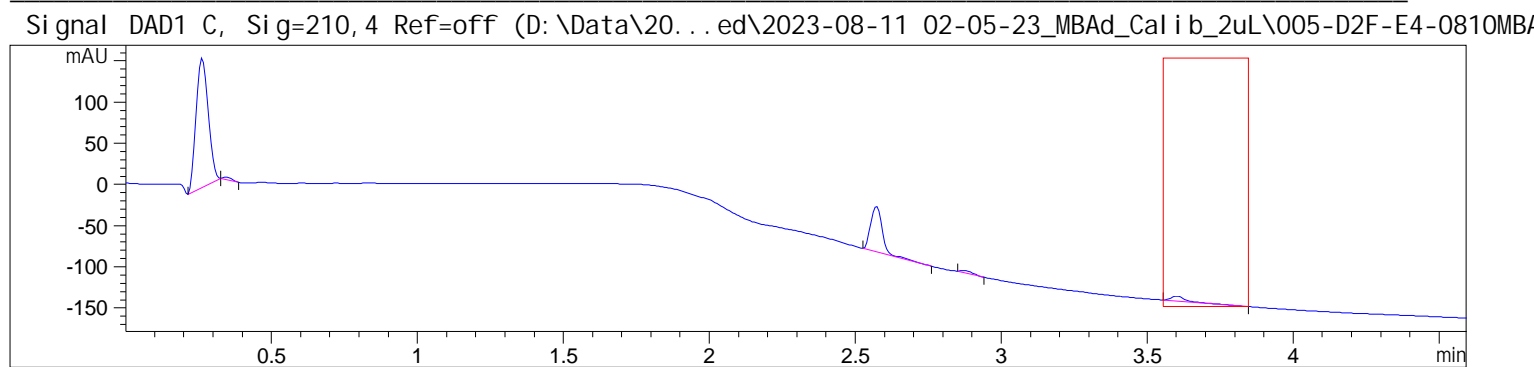
Purity factor : 460.382 (43 of 45 spectra exceed the calculated threshold limit.)

Threshold : 828.659 (Calculated with 43 of 45 spectra)

Reference : Peak start and end spectra (integrated) (2.707 / 3.054)

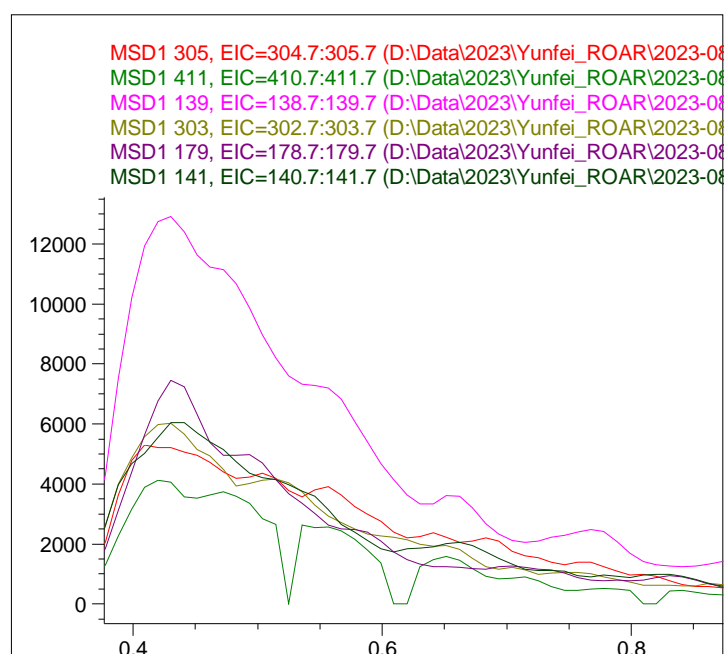
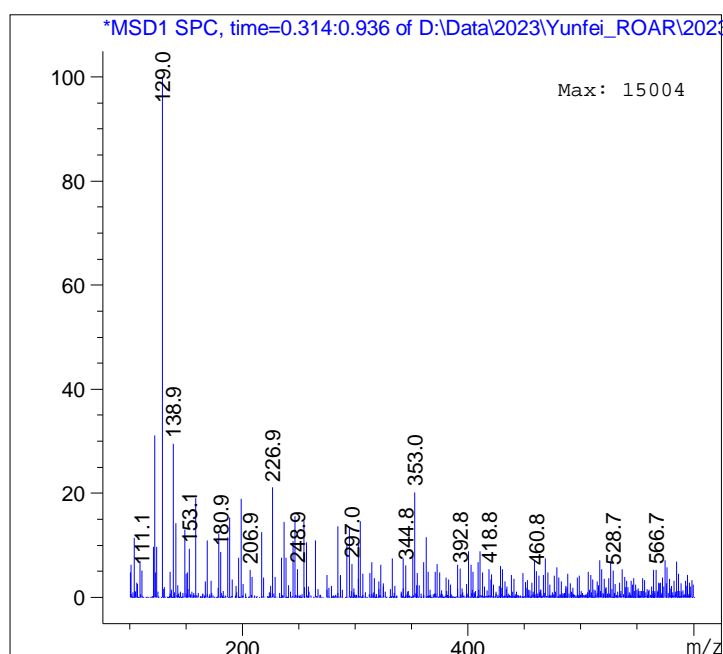
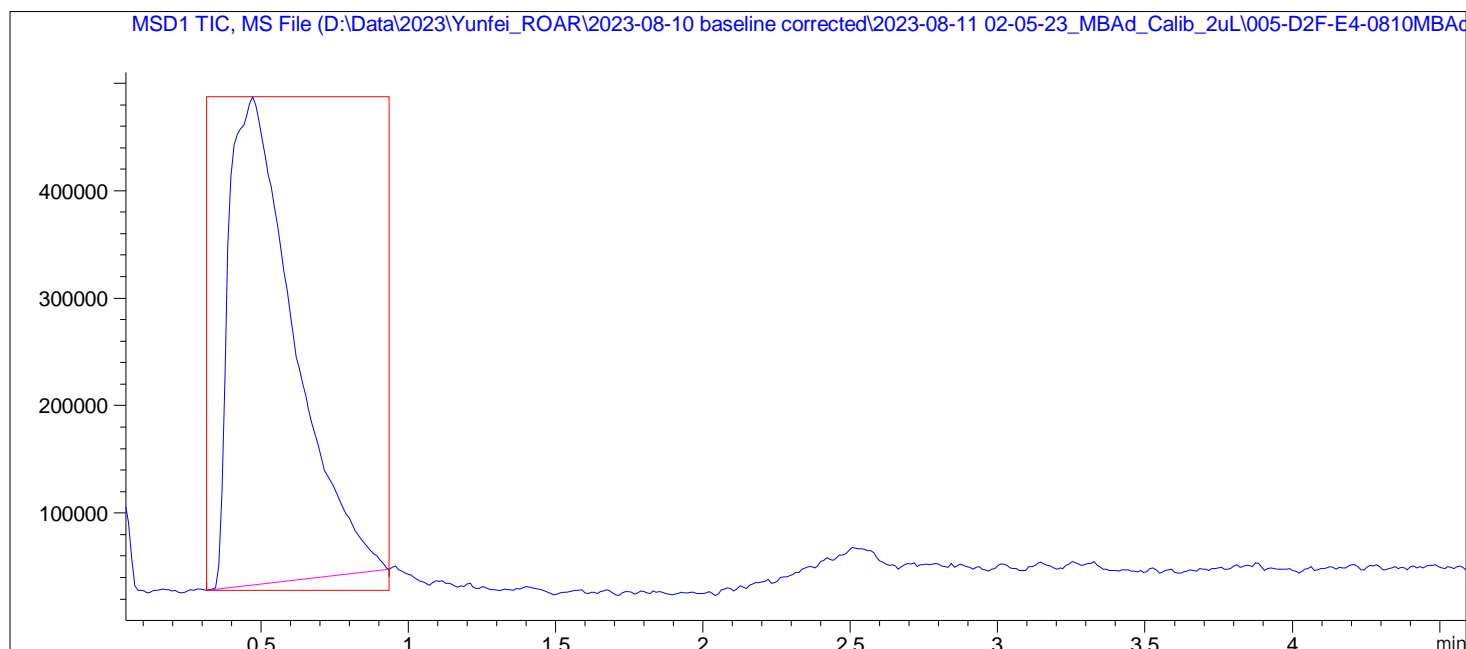
Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.200 (12 spectra, St.Dev 0.0725 + 3 \* 0.0427)



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

Purity factor : 925.540 (27 of 28 spectra are within the calculated threshold limit.)  
Threshold : 812.726 (Calculated with 27 of 28 spectra)  
Reference : Peak start and end spectra (integrated) (3.554 / 3.847)  
Spectra : 5 (Selection automatic, 5)  
Noise Threshold: 0.200 (12 spectra, St.Dev 0.0725 + 3 \* 0.0427)



Peak #1 at 0.472 min ( 0.314 to 0.936 min)

-> The analysis found 10 components, indicating an impure peak. <-

Component 1: Peak at Scan 36.4. Top ions are 305 411  
Component 2: Peak at Scan 37.6. Top ions are 139 303 245  
Component 3: Peak at Scan 38.5. Top ions are 179 141 187  
Component 4: Peak at Scan 39.6. Top ions are 122 247 285  
Component 5: Peak at Scan 41.6. Top ions are 129 189 149  
Component 6: Peak at Scan 42.4. Top ions are 101 255 169  
Component 7: Peak at Scan 44.4. Top ions are 575 353  
Component 8: Peak at Scan 46.7. Top ions are 227  
Component 9: Peak at Scan 49.4. Top ions are 199  
Component 10: Peak at Scan 51.3. Top ions are 159

\*\*\* End of Report \*\*\*