

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  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
```

Sample Name: 0810MBAAd_Op5

```
=====
Acq. Operator   : user                               Seq. Line :    7
Sample Operator : user
Acq. Instrument : SFC LCMS                           Location  :   D2F-E6
Injection Date  : 11/08/2023 02:56:40                 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       : 437
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/min
=====
```

```
Detector Lamp Burn Times: Current On-Time   Accumulated On-Time
DAD 1, UV Lamp           :          0.84            849.9   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\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                   :          350            350 C
RoughVac                   :          2              2 Torr
HighVac                   :      5.3E-009        5.3E-009 Torr
CapCur                    :          5              656 nA
ChamCur                   :      1.1E-001        1.6E-001 µA
DryingGas                  :          12            12 l/min
Neb Pres                   :          35            35 psi g
Turbo1Spd                  :          100           100 %
Turbo1Pwr                  :          126           127 W
RF Drive                   :          1              15 %
Qd TpDrv                   :          16            16 %
Gas TpDrv                   :          35            35 %
Neb PrDrv                  :          50            49 %
Gas FI Drv                 :          61            61 %
=====
```

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
=====
```

Sample Name: 0810MBAd_Op5

922.01	:	-22
1521.97	:	-24

Mass Gain	:	-12.80
Mass Offset	:	Variable

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	:	
Lens2DC	:	Variable

Mass	:	Value
------	---	-------

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	:	Variable

Mass	:	Value
------	---	-------

118.08	:	51
622.03	:	95
922.01	:	105
1521.97	:	145

Mass Filter	:	Gaussian
Time Filter	:	Gaussian
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	:	Variable

Mass	:	Value
------	---	-------

112.99	:	-32
601.98	:	-76
1033.99	:	-74
1633.95	:	-32

Mass Gain	:	-12.85
Mass Offset	:	Variable

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 abl 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 : Vari abl e

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
=====

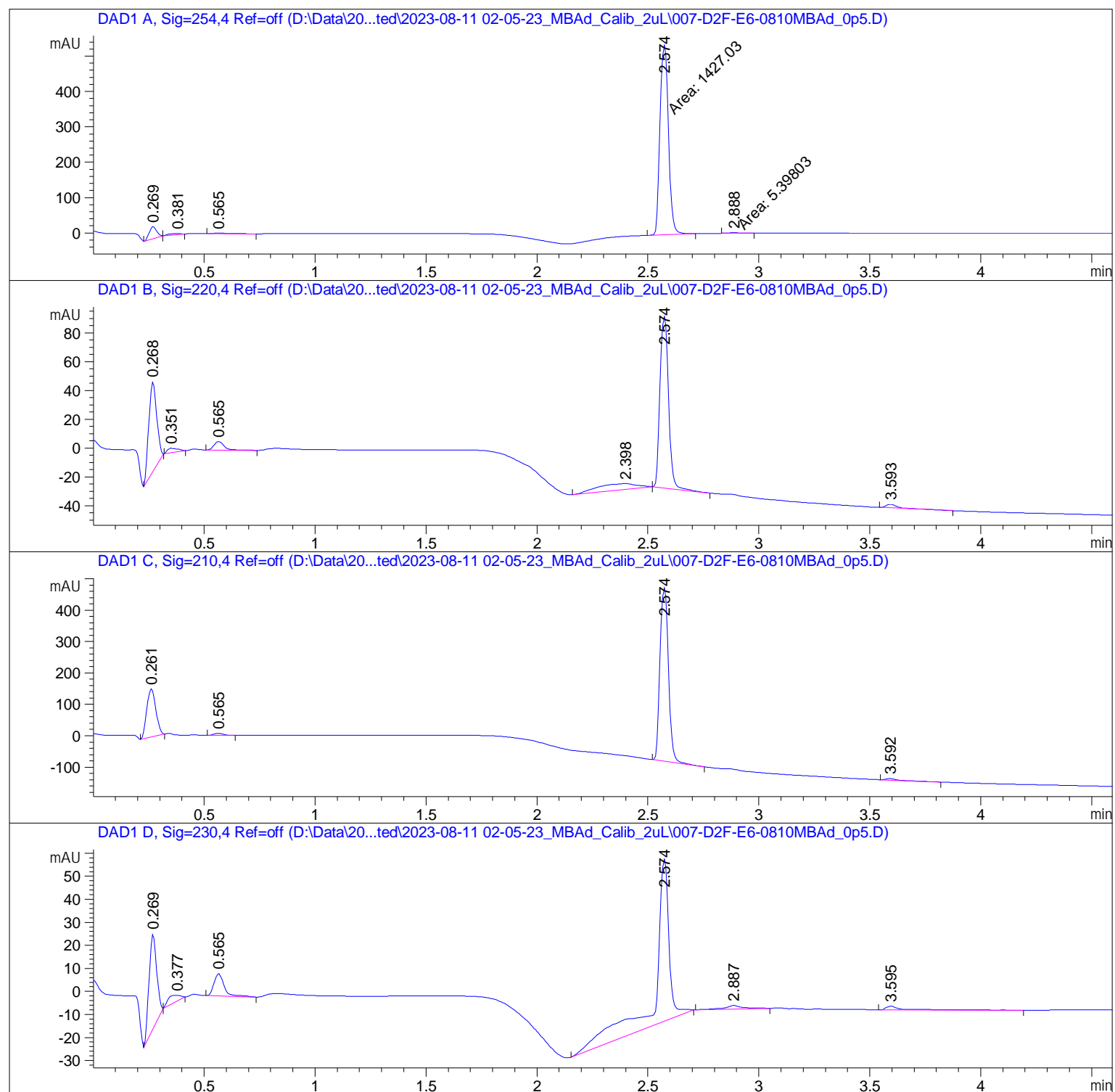
11 Aug 23 12:17 PM
Logbook File: D:\Data\20...ected\2023-08-11 02-05-23_MBAAd_Cal i b_2uL\007-D2F-E6-0810MBAAd_Op5. D\RUN. LOG

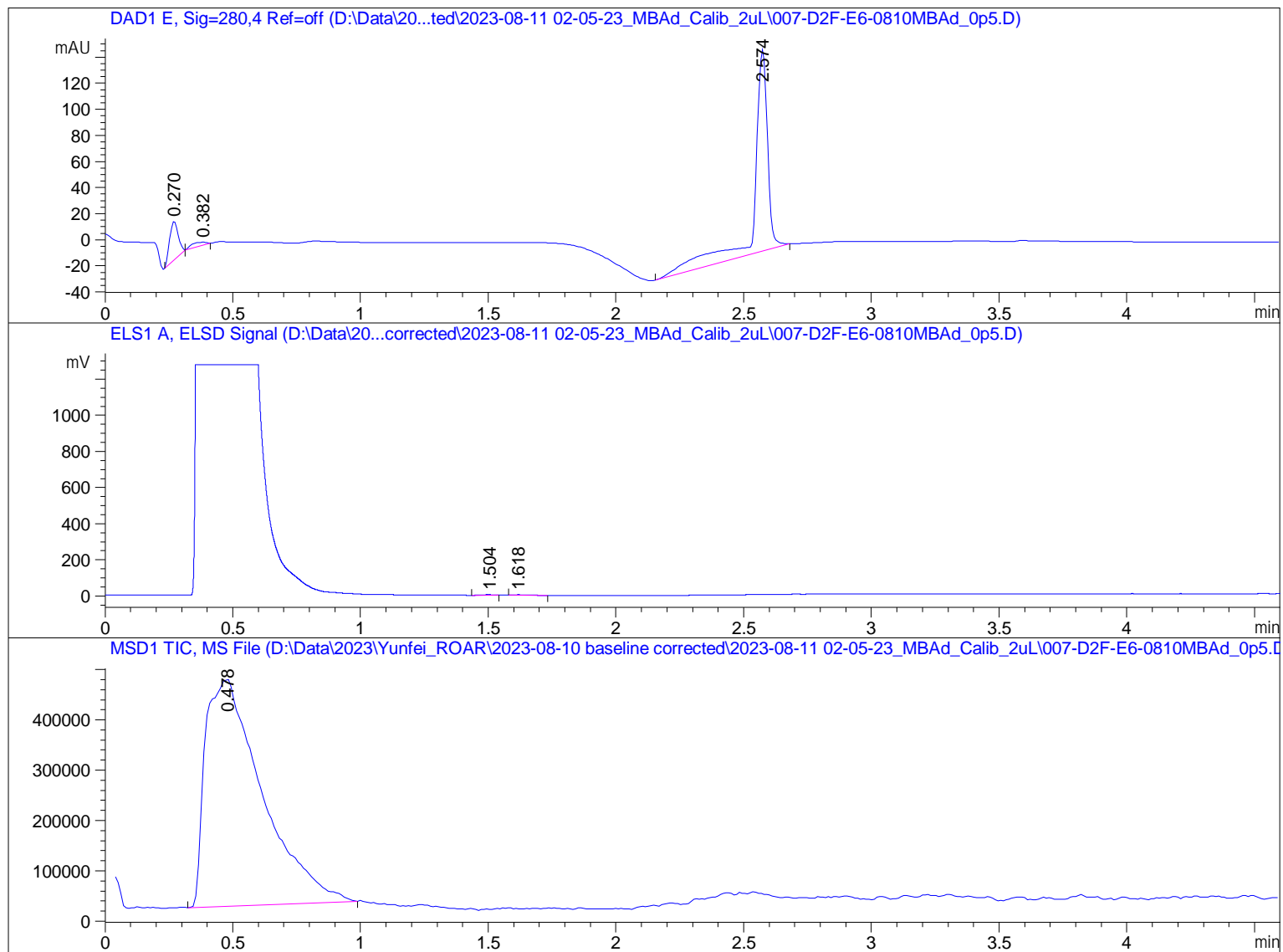
Module	# Event Message	Date Time

Method	Method started: line# 7 at location 'D2F-E6> ' inj# 1	11/08/2023 02:55:48
CP Macro	PreRun macro: 'LAMPALL ON'	11/08/2023 02:55:55
G4260B	G4260B: ELSD - Autozero	11/08/2023 02:55:55
G4260B	G4260B: ELSD - Al ready swit ched on	11/08/2023 02:55:56
Method	Instrument running sample from location D2F-> E6	11/08/2023 02:55:56
G7115A	G7115A: DEAC605436 - Detector: Prepare	11/08/2023 02:56:07
G7115A	G7115A: DEAC605436 - Detector: Idle	11/08/2023 02:56:23
G4767A	G4767A: DEAFD00218 - Draw command finished	11/08/2023 02:56:30
G4767A	G4767A: DEAFD00218 - Sampler wash is active	11/08/2023 02:56:31
G4767A	G4767A: DEAFD00218 - Sampler wash is idle	11/08/2023 02:56:38
G4767A	G4767A: DEAFD00218 - Sample preparation time: > 15 sec	11/08/2023 02:56:38
PumpVal ve	G7111B: DEAEW03495 - Run	11/08/2023 02:56:40

Sample Name: 0810MBAAd_Op5

PumpVal ve	G7111B: DEAEW03495 - Postrun	11/08/2023 03:01:16
G4767A	G4767A: DEAFD00218 - Postrun	11/08/2023 03:01:17
G7110B	G7110B: DEAEH00761 - Postrun	11/08/2023 03:01:17
PumpVal ve	G1170A: DEBAD03715 - Postrun	11/08/2023 03:01:18
G4782A	G4782A: DEAGN00153 - Postrun	11/08/2023 03:01:18
G1170A	G1170A: DEBAD03734 - Postrun	11/08/2023 03:01:19
Method	Saving Method COL1_5NH4FA_MECN_5T095_1MIN_10> 0-600MS_POS.M	11/08/2023 03:03:31
Method	Instrument run completed	11/08/2023 03:03:32
CP Macro	Analyzing rawdata 007-D2F-E6-0810MBAAd_Op5.D	11/08/2023 03:03:32
Method	Saving Method DA.M	11/08/2023 03:03:34
Method	Method completed	11/08/2023 03:03:41





=====
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	0.0372	79.14350	33.89087	5.1629
2	0.381	BB	0.0797	12.26610	2.39772	0.8002
3	0.565	BB	0.0618	9.09900	2.13232	0.5936
4	2.574	MM	0.0442	1427.03235	538.05249	93.0913
5	2.888	MM	0.0533	5.39803	1.68893	0.3521

Totals : 1532.93898 578.16233

Sample Name: 0810MBAAd_Op5

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	0.0392	156.10817	62.42230	27.4045
2	0.351	BB	0.0475	9.91421	3.08829	1.7404
3	0.565	BB	0.0499	19.26789	5.93837	3.3824
4	2.398	BB	0.1688	54.51808	4.10799	9.5705
5	2.574	BB	0.0435	320.70331	118.94065	56.2988
6	3.593	BBA	0.0542	9.13305	2.52235	1.6033

Totals : 569.64471 197.01995

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.261	BB	0.0471	436.45480	153.98508	22.5271
2	0.565	BB	0.0452	17.50126	6.15902	0.9033
3	2.574	BB	0.0430	1468.51978	552.17963	75.7960
4	3.592	BBA	0.0496	14.98684	4.65197	0.7735

Totals : 1937.46268 716.97570

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	98.17656	41.20560	20.8264
2	0.377	BB	0.0759	11.94634	2.49539	2.5342
3	0.565	BB	0.0491	30.67048	9.64670	6.5062
4	2.574	BB	0.0642	314.27600	70.23571	66.6680
5	2.887	BB	0.0774	8.69304	1.55192	1.8441
6	3.595	BB	0.0688	7.64236	1.57057	1.6212

Totals : 471.40479 126.70591

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	0.0372	69.62183	29.86359	10.6729
2	0.382	BB	0.0788	11.03713	2.18966	1.6920
3	2.574	BB	0.0552	571.66327	154.29079	87.6351

Totals : 652.32223 186.34403

Signal 6: ELS1 A, ELSD Signal

Peak #	RetTime [min]	Type	Width [min]	Area [mV*s]	Height [mV]	Area %
1	1.504	BB	0.0385	9.59284	3.14930	45.3065
2	1.618	BB	0.0549	11.58036	3.04297	54.6935

Totals : 21.17321 6.19227

Signal 7: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.478	BB	0.1918	6.93565e6	4.51699e5	100.0000

Totals : 6.93565e6 4.51699e5

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.

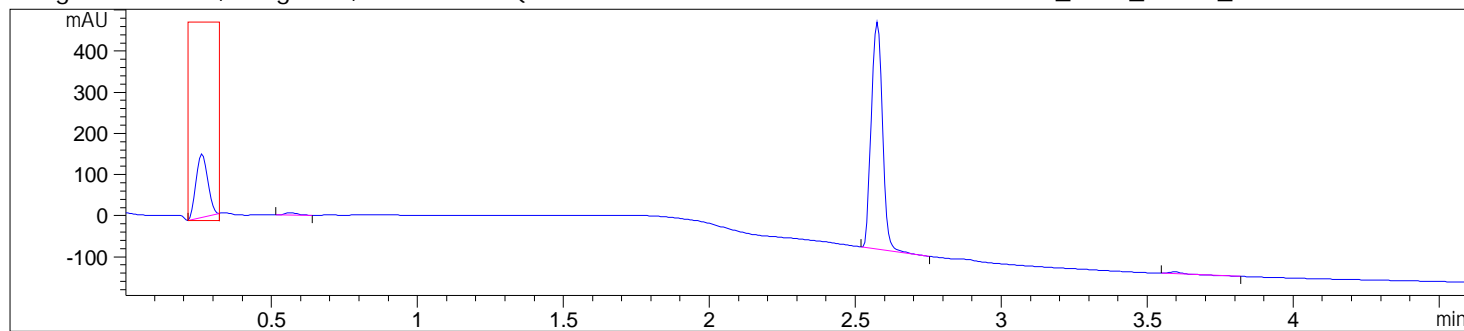
Final Summed Peaks Report

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

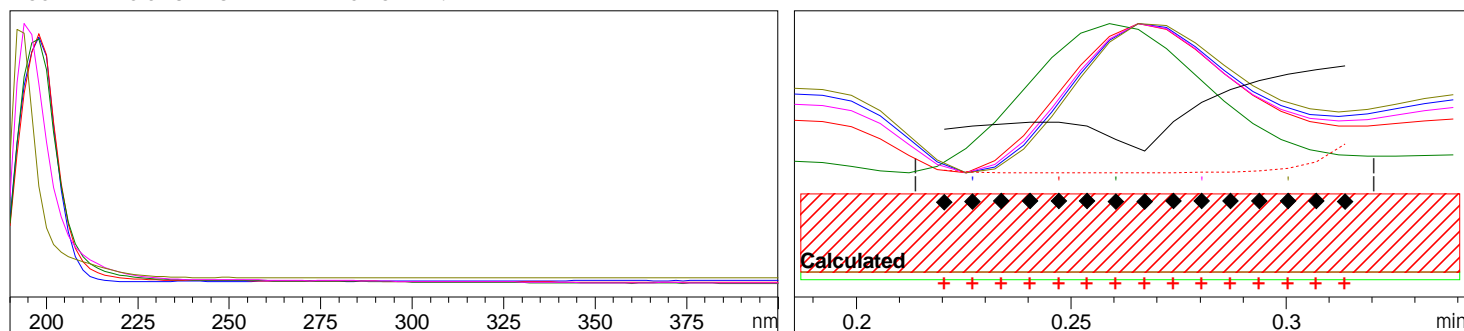
Signal 2: DAD1 B, Sig=220, 4 Ref=off
Signal 3: DAD1 C, Sig=210, 4 Ref=off
Signal 4: DAD1 D, Sig=230, 4 Ref=off
Signal 5: DAD1 E, Sig=280, 4 Ref=off
Signal 6: ELS1 A, ELSD Signal
Signal 7: MSD1 TIC, MS File

Sample Name: 0810MBAAd_Op5

Signal DAD1 C, Sig=210, 4 Ref=off (D:\Data\20...ted\2023-08-11 02-05-23_MBAAd_Cal i b_2uL\007-D2F-E6-0810MBAAd_Op5.D)



Peak : 1 at 0.261 min Name : ?



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

Purity factor : 884.126 (15 of 15 spectra exceed the calculated threshold limit.)

Threshold : 999.739 (Calculated with 15 of 15 spectra)

Reference : Peak start and end spectra (integrated) (0.214 / 0.320)

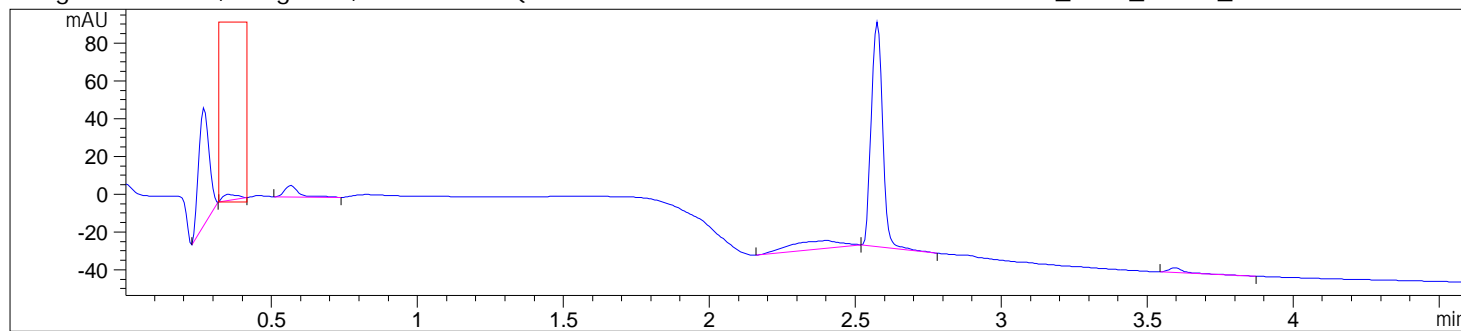
Spectra : 5 (Selection automatic, 5)

Noise Threshold : 0.576 (12 spectra, St.Dev 0.2465 + 3 * 0.11)

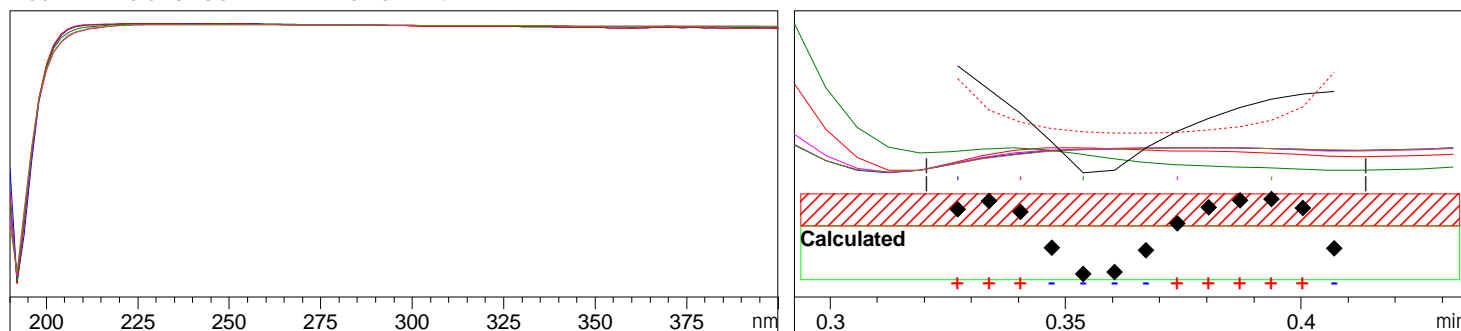
Warning : Spectral absorbances > 1000 mAU (see help for more information)

Sample Name: 0810MBAAd_Op5

Signal DAD1 B, Sig=220, 4 Ref=off (D:\Data\20...ted\2023-08-11 02-05-23_MBAAd_Cal i b_2uL\007-D2F-E6-0810MBAAd_Op5.D)



Peak : 2 at 0.351 min Name : ?



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

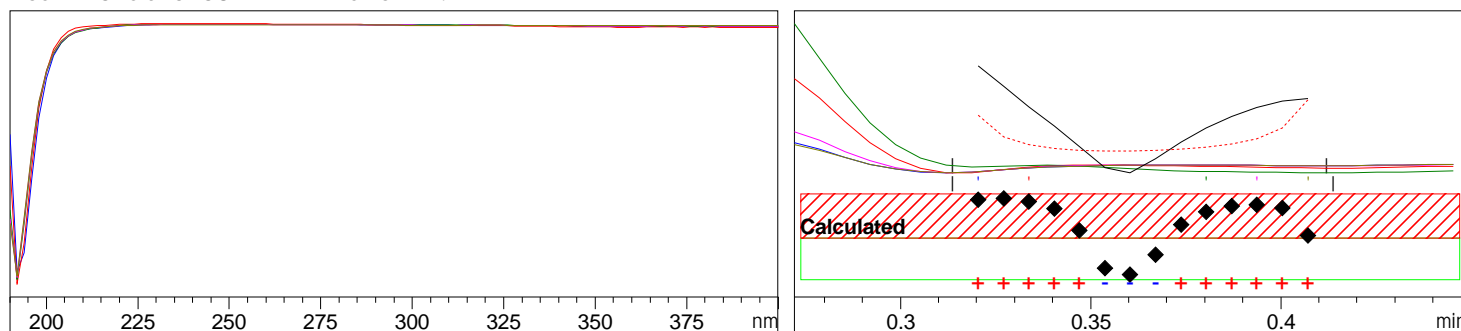
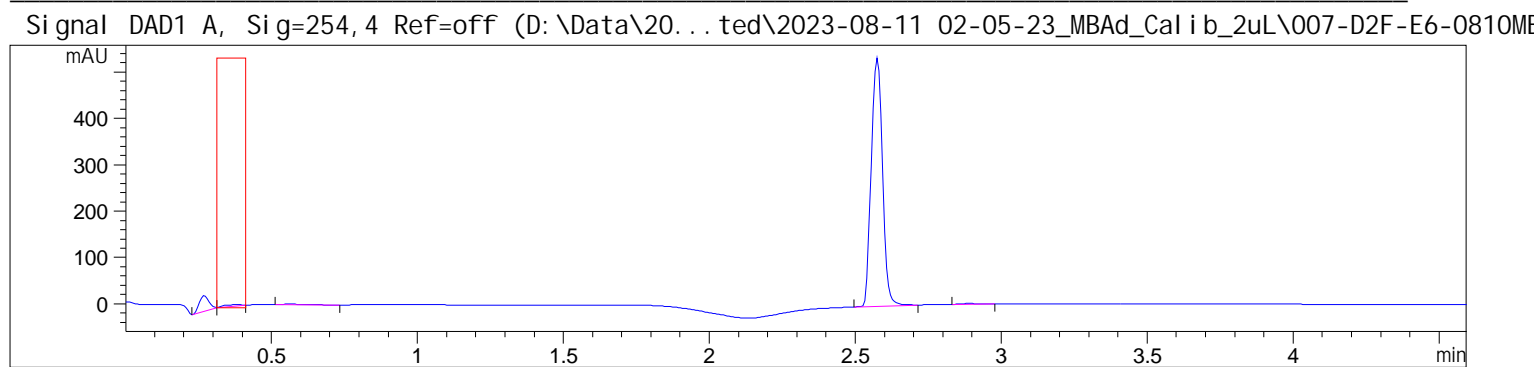
Purity factor : 995.439 (8 of 13 spectra exceed the calculated threshold limit.)

Threshold : 997.144 (Calculated with 8 of 13 spectra)

Reference : Peak start and end spectra (integrated) (0.320 / 0.414)

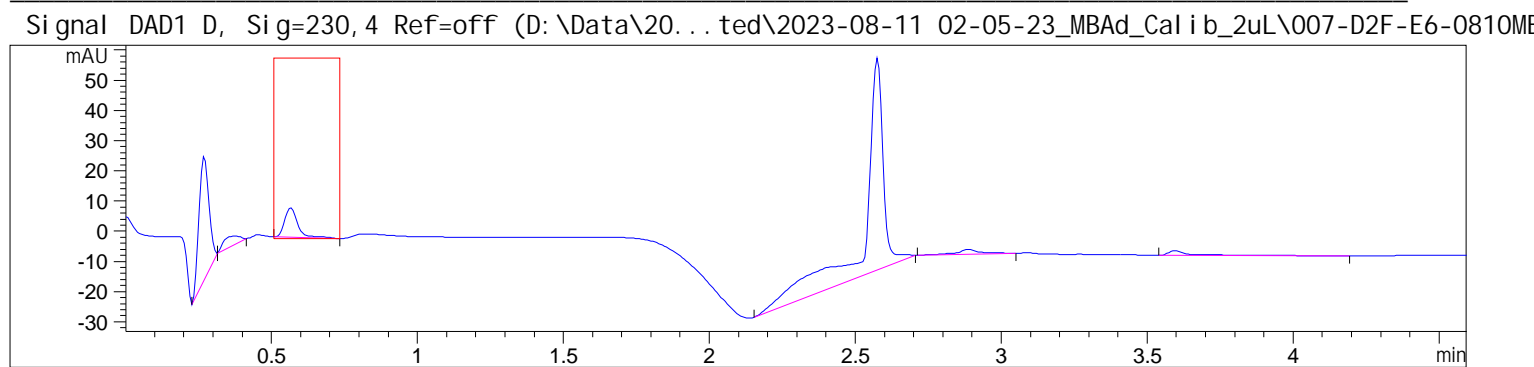
Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.576 (12 spectra, St.Dev 0.2465 + 3 * 0.11)

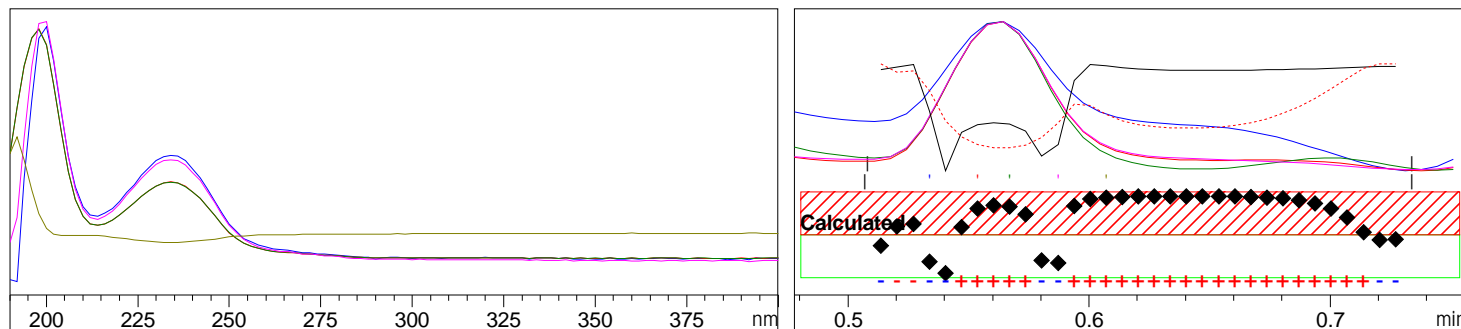


-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 992.437 (11 of 14 spectra exceed the calculated threshold limit.)
Threshold : 997.637 (Calculated with 11 of 14 spectra)
Reference : Peak start and end spectra (integrated) (0.314 / 0.414)
Spectra : 5 (Selection automatic, 5)
Noise Threshold: 0.576 (12 spectra, St.Dev 0.2465 + 3 * 0.11)



Peak : 5 at 0.565 min Name : ?



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

Purity factor : 377.756 (24 of 33 spectra exceed the calculated threshold limit.)

Threshold : 881.425 (Calculated with 24 of 33 spectra)

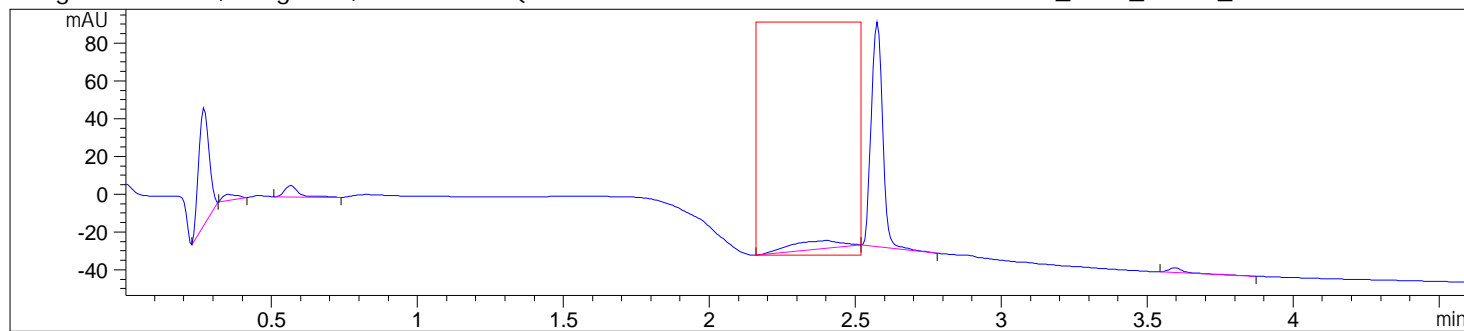
Reference : Peak start and end spectra (integrated) (0.507 / 0.734)

Spectra : 5 (Selection automatic, 5)

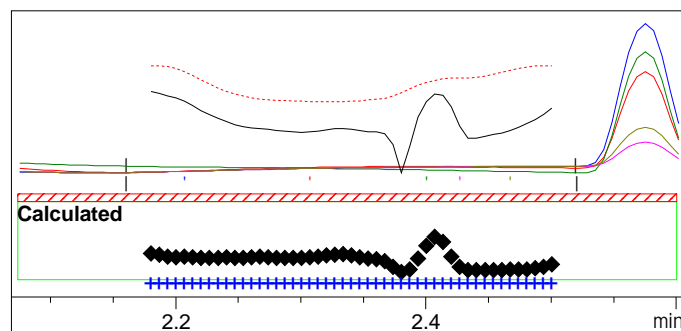
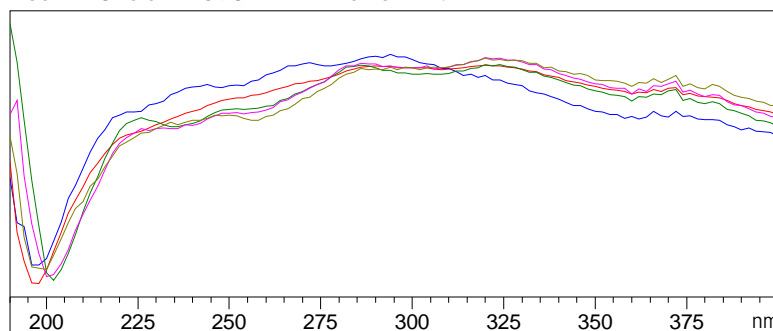
Noise Threshold: 0.576 (12 spectra, St.Dev 0.2465 + 3 * 0.11)

Sample Name: 0810MBAd_Op5

Signal DAD1 B, Sig=220, 4 Ref=off (D:\Data\20...ted\2023-08-11 02-05-23_MBAd_Cal i b_2uL\007-D2F-E6-0810MBAd_Op5.D)



Peak : 8 at 2.398 min Name : ?



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

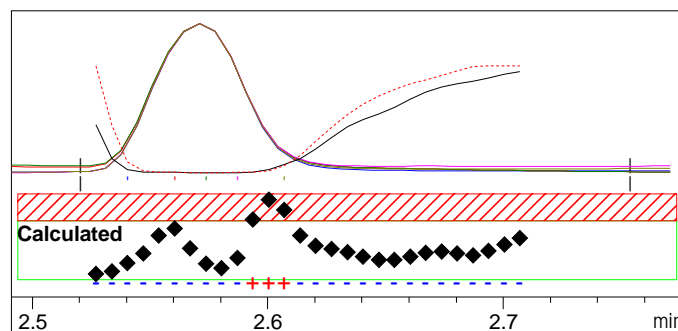
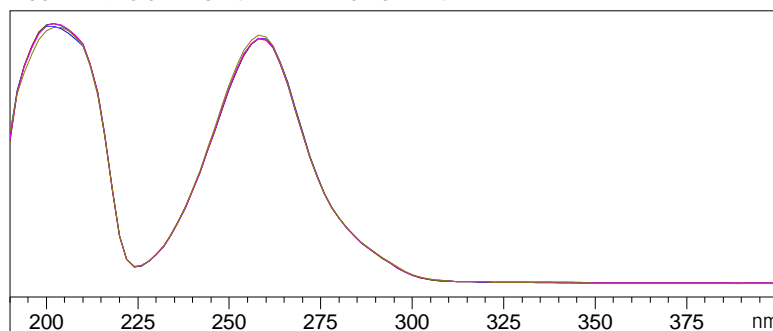
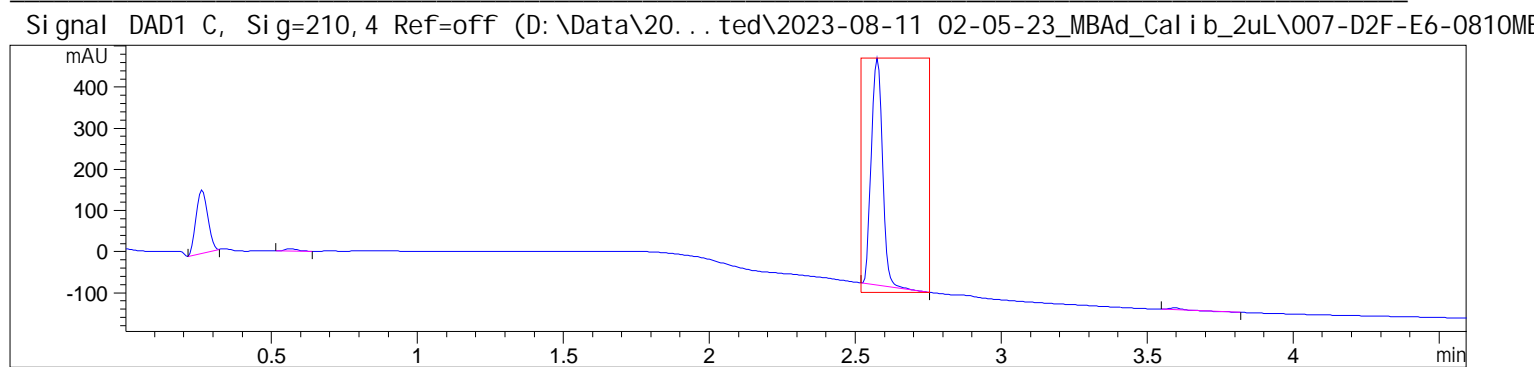
Purity factor : 919.676 (49 of 49 spectra are within the calculated threshold limit.)

Threshold : 533.304 (Calculated with 49 of 49 spectra)

Reference : Peak start and end spectra (integrated) (2.160 / 2.520)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.576 (12 spectra, St.Dev 0.2465 + 3 * 0.11)

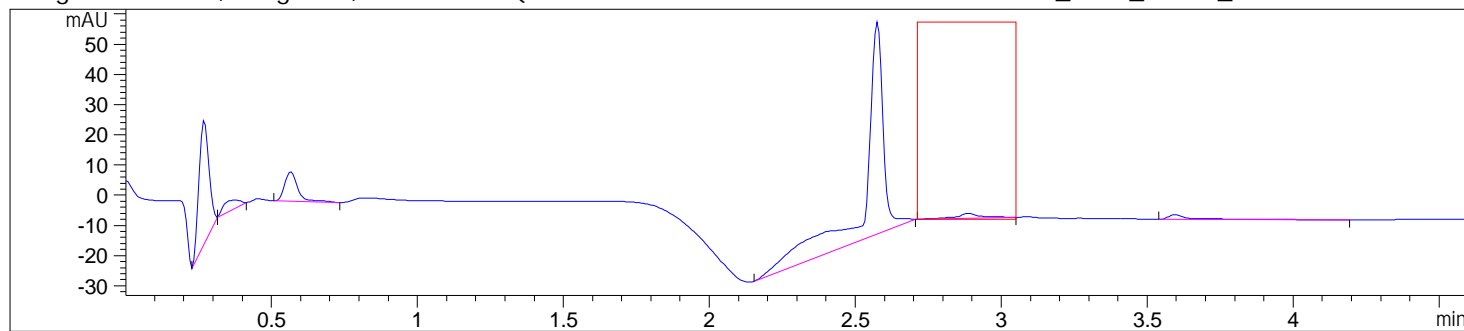


-> The purity factor exceeds the calculated threshold limit. <-

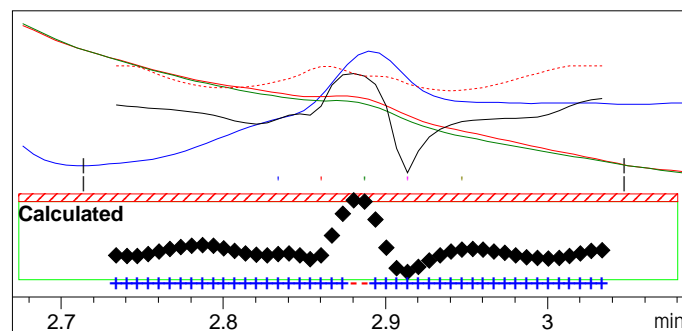
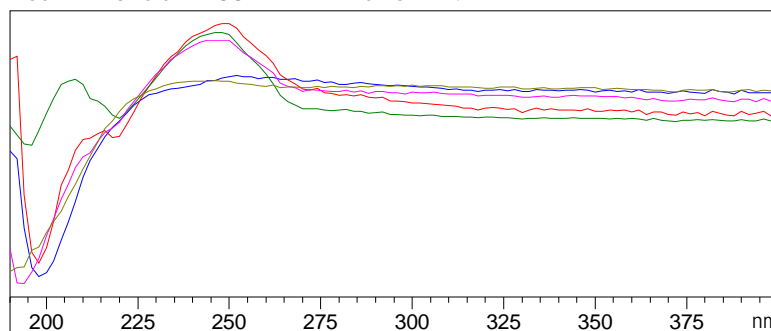
Purity factor : 999.806 (3 of 28 spectra exceed the calculated threshold limit.)
Threshold : 999.853 (Calculated with 3 of 28 spectra)
Reference : Peak start and end spectra (integrated) (2.520 / 2.754)
Spectra : 5 (Selection automatic, 5)
Noise Threshold: 0.576 (12 spectra, St.Dev 0.2465 + 3 * 0.11)

Sample Name: 0810MBAd_Op5

Signal DAD1 D, Sig=230, 4 Ref=off (D:\Data\20...ted\2023-08-11 02-05-23_MBAd_Cal i b_2uL\007-D2F-E6-0810MBAd_Op5.D)



Peak : 10 at 2.887 min Name : ?



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

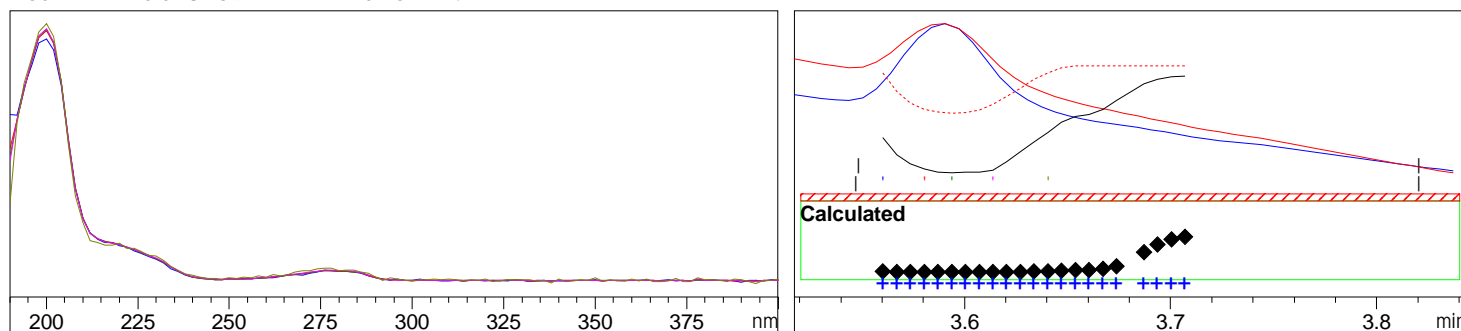
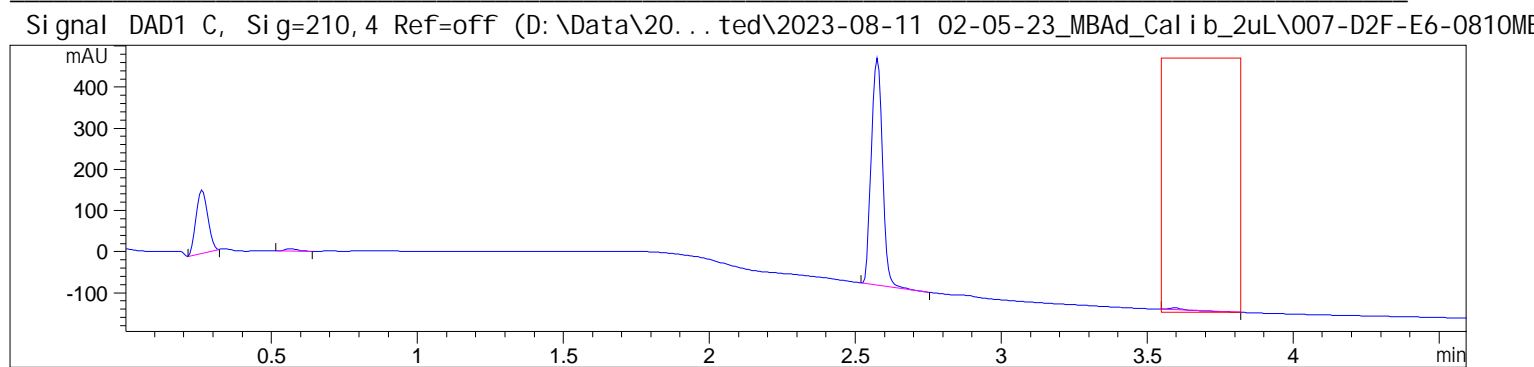
Purity factor : 773.255 (44 of 46 spectra are within the calculated threshold limit.)

Threshold : 300.463 (Calculated with 44 of 46 spectra)

Reference : Peak start and end spectra (integrated) (2.714 / 3.047)

Spectra : 5 (Selection automatic, 5)

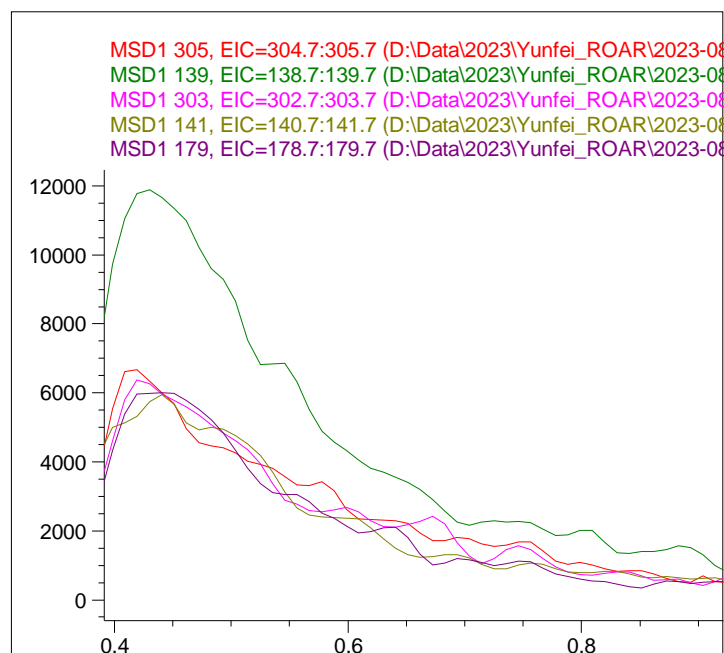
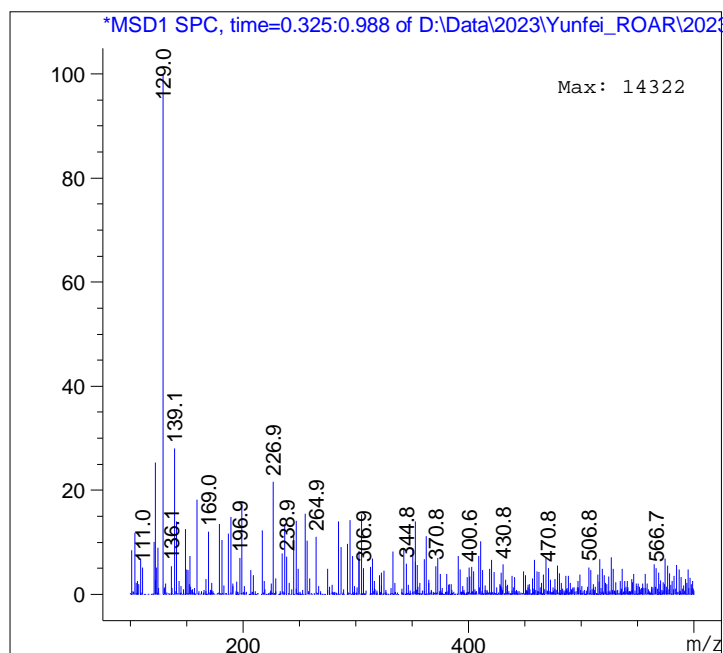
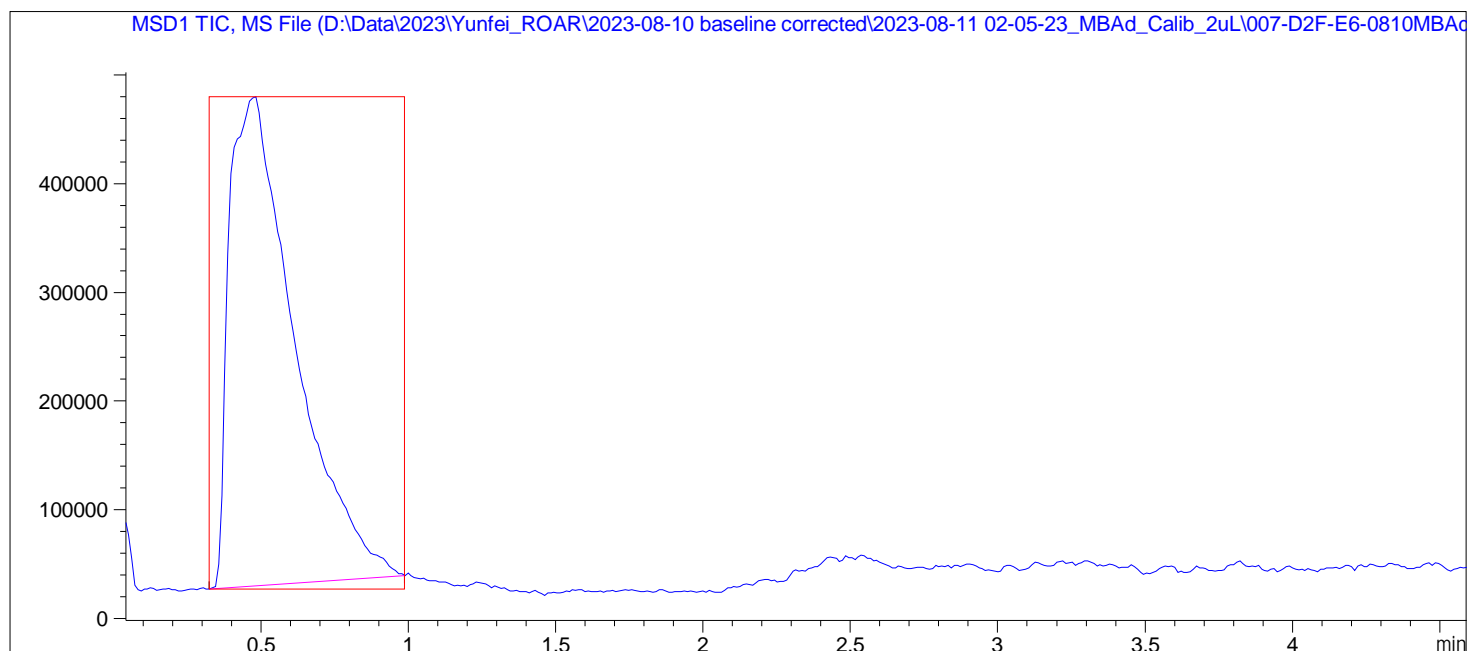
Noise Threshold: 0.576 (12 spectra, St.Dev 0.2465 + 3 * 0.11)



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

Purity factor : 915.085 (22 of 22 spectra are within the calculated threshold limit.)
Threshold : 484.604 (Calculated with 22 of 22 spectra)
Reference : Peak start and end spectra (integrated) (3.547 / 3.820)
Spectra : 5 (Selection automatic, 5)
Noise Threshold: 0.576 (12 spectra, St.Dev 0.2465 + 3 * 0.11)

Sample Name: 0810MBAAd_Op5



Peak #1 at 0.478 min (0.325 to 0.988 min)

-> The analysis found 7 components, indicating an impure peak. <-

Component 1: Peak at Scan 36.6. Top ions are 305

Component 2: Peak at Scan 37.6. Top ions are 139 303

Component 3: Peak at Scan 38.9. Top ions are 141 179

Component 4: Peak at Scan 41.0. Top ions are 129 189

Component 5: Peak at Scan 42.8. Top ions are 255

Component 6: Peak at Scan 43.6. Top ions are 122

Component 7: Peak at Scan 47.1. Top ions are 199

*** End of Report ***