

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

```

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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

```

```

                                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      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  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: unusedMBA20

```

=====
Acq. Operator   : user                      Seq. Line :    5
Sample Operator : user
Acq. Instrument : SFC LCMS                  Location  :   D2F-F4
Injection Date  : 07/09/2023 15:51:41      Inj       :    1
                                           Inj Volume: 0.200 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 2.000 µl
Method          : D:\Data\2023\Yunfei_ROAR\2023-09-07_newSTEMPO_0p9VProduct_re 2023-09-07 15-
                  17-08\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       : 941
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)	32.3	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	0.57	944.1 h
DAD 1, Visible Lamp	0.00	352.8 h

```

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

```

Sample Name: unusedMBA20

PMP2, Solvent B :  
PMP2, Solvent B :

## =====

## MSD parameters

Tune file name : C:\Users\Public\Documents\ChemStation\1\MStune\6125BTUN\atunes. tun  
(Tue Aug 22 12:21:28 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	6.8E-009	6.7E-009 Torr
CapCur	5	645 nA
ChamCur	9.0E-002	6.4E-001 µA
DryingGas	12	12 l/min
Neb Pres	35	35 psig
Turbo1Spd	100	100 %
Turbo1Pwr	128	127 W
RF Drive	1	15 %
Qd TpDrv	17	17 %
Gas TpDrv	35	35 %
Neb PrDrv	50	50 %
Gas FIDrv	62	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 : -185  
Width Offset : Variable

Mass	Value
------	-------

118.08	-24
622.03	-50
922.01	-31
1521.97	-24

Mass Gain : -12.80  
Mass Offset : Variable

Mass	Value
------	-------

118.08	0.758
622.03	0.862
922.01	0.824
1521.97	0.758

Quad DC : 0.00 V  
Octopole Peak : 650 V  
Octopole Knee :  
Lens2DC : Variable

Sample Name: unusedMBA20

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 : 144  
 L2RFamp : Variable

Mass	:	Value
118.08	:	57
622.03	:	100
922.01	:	95
1521.97	:	120

Mass Filter : Gaussian  
 Time Filter : Gaussian  
 Time Filter Width : 0.030

Ionization polarity : Negative  
 Skim1 : 35 V  
 Skim2 :  
 Ion Energy : 5.0 V  
 Lens1 : -3.6 V  
 Lens2 :  
 Iris : 400 V  
 HED : 10000 V  
 Width Gain : -186  
 Width Offset : Variable

Mass	:	Value
112.99	:	-39
601.98	:	-64
1033.99	:	-84
1633.95	:	-39

Mass Gain : -12.80  
 Mass Offset : Variable

Mass	:	Value
112.99	:	0.786
601.98	:	0.872
1033.99	:	0.878
1633.95	:	0.786

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      :   Vari able
Mass         :    Val ue
-----
112.99       :    72
601.98       :   110
1033.99      :   135
1633.95      :   150
-----

```

```

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

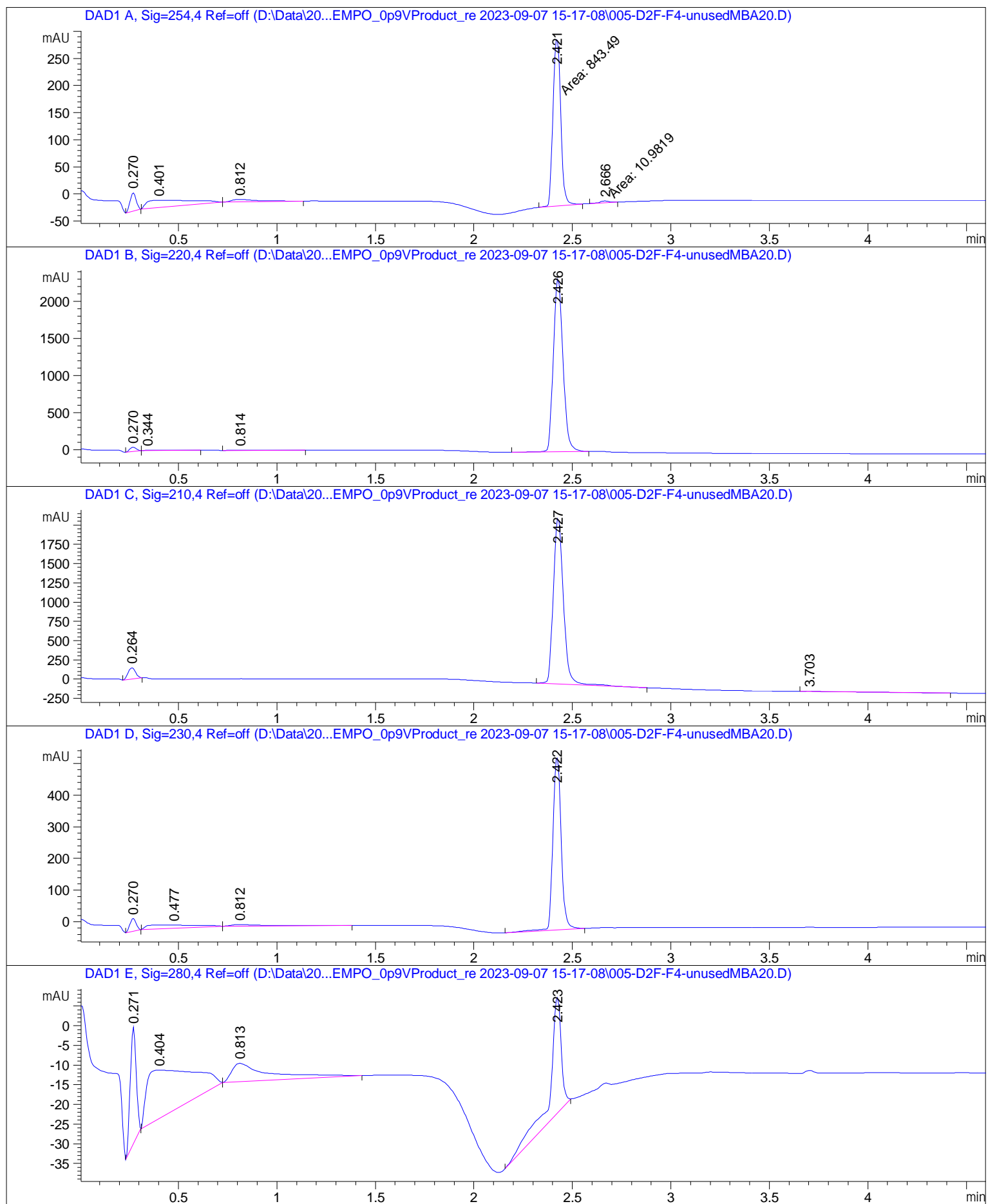
```

Run Logbook

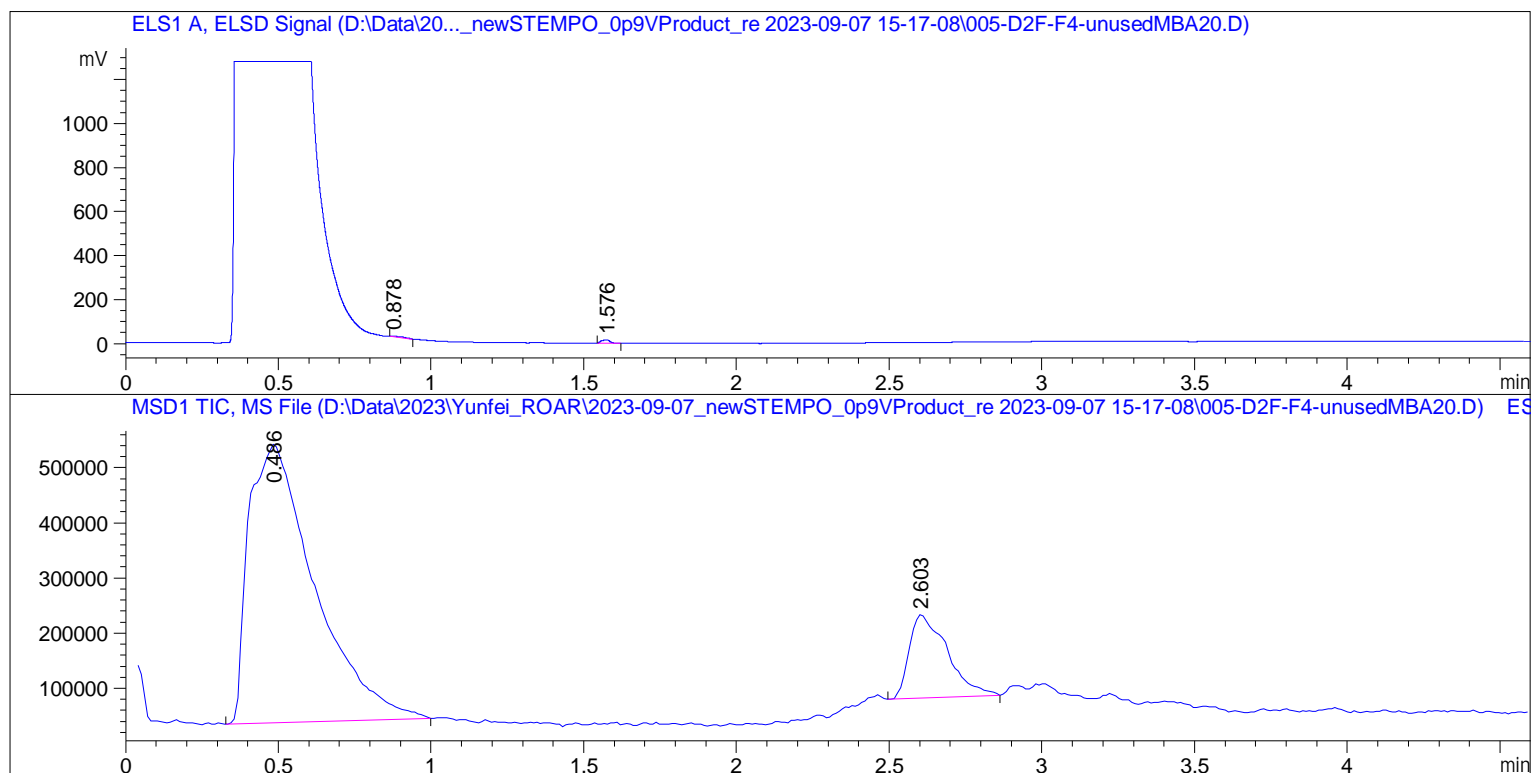
18 Sep 23 11:22 AM  
Logbook File: D:\Data\20...STEMPO\_0p9VProduct\_re 2023-09-07 15-17-08\005-D2F-F4-unusedMBA20.D\RUN.LOG

Module	# Event Message	Date Time
Method	Method started: line# 5 at location 'D2F-F4> ' inj# 1	07/09/2023 15:50:56
CP Macro	PreRun macro: 'LAMPALL ON'	07/09/2023 15:50:57
G4260B	G4260B: ELSD - Autozero	07/09/2023 15:50:57
G4260B	G4260B: ELSD - Al ready switched on	07/09/2023 15:50:57
Method	Instrument running sample from location D2F-> F4	07/09/2023 15:50:58
G7115A	G7115A: DEAC605436 - Detector: Prepare	07/09/2023 15:51:08
G7115A	G7115A: DEAC605436 - Detector: Idle	07/09/2023 15:51:24
G4767A	G4767A: DEAFD00218 - Draw command finished	07/09/2023 15:51:31
G4767A	G4767A: DEAFD00218 - Sampler wash is active	07/09/2023 15:51:33
G4767A	G4767A: DEAFD00218 - Sampler wash is idle	07/09/2023 15:51:39
G4767A	G4767A: DEAFD00218 - Sample preparation time: > 15 sec	07/09/2023 15:51:39
PumpVal ve	G7111B: DEAEW03495 - Run	07/09/2023 15:51:41
PumpVal ve	G7111B: DEAEW03495 - Postrun	07/09/2023 15:56:17
G4767A	G4767A: DEAFD00218 - Postrun	07/09/2023 15:56:17
G7110B	G7110B: DEAEH00761 - Postrun	07/09/2023 15:56:18
PumpVal ve	G1170A: DEBAD03715 - Postrun	07/09/2023 15:56:19
G4782A	G4782A: DEAGN00153 - Postrun	07/09/2023 15:56:19
G1170A	G1170A: DEBAD03734 - Postrun	07/09/2023 15:56:19
Method	Saving Method COL1_5NH4FA_MECN_5TO95_1MIN_10> 0-600MS_POS.M	07/09/2023 15:58:25
Method	Instrument run completed	07/09/2023 15:58:26
CP Macro	Analyzing rawdata 005-D2F-F4-unusedMBA20.D	07/09/2023 15:58:26
Method	Saving Method DA.M	07/09/2023 15:58:28
Method	Method completed	07/09/2023 15:58:34

Sample Name: unusedMBA20



Sample Name: unusedMBA20



=====  
 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	0.0348	72.29606	33.94904	6.1494
2	0.401	BB	0.2153	204.97348	13.19069	17.4347
3	0.812	BB	0.1360	43.91967	4.74521	3.7357
4	2.421	MM	0.0451	843.48981	311.64563	71.7460
5	2.666	MM	0.0521	10.98193	3.51344	0.9341

Totals : 1175.66095 367.04400

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.270	BB	0.0366	135.84854	59.65034	1.6633
2	0.344	BB	0.1061	67.80515	8.06167	0.8302
3	0.814	BB	0.1391	43.28179	4.54339	0.5299
4	2.426	BB	0.0536	7920.49512	2336.42896	96.9766

Sample Name: unusedMBA20

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
----- ----- ----- ----- ----- ----- -----						
Totals :				8167.43060	2408.68436	

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
----- ----- ----- ----- ----- ----- -----						
1	0.264	BB	0.0426	389.02087	148.21906	4.8273
2	2.427	BB	0.0573	7624.31445	2153.88672	94.6084
3	3.703	BBA	0.0988	45.47953	6.11632	0.5643
----- ----- ----- ----- ----- ----- -----						
Totals :				8058.81486	2308.22210	

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	0.0354	89.02857	40.93458	4.6161
2	0.477	BB	0.2338	187.02251	9.83625	9.6970
3	0.812	BB	0.1695	59.99279	4.87617	3.1106
4	2.422	BB	0.0458	1592.62305	549.20776	82.5764
----- ----- ----- ----- ----- ----- -----						
Totals :				1928.66692	604.85477	

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	0.0347	62.61810	29.62425	14.5234
2	0.404	BB	0.2137	191.27625	12.28039	44.3638
3	0.813	BB	0.1791	59.89372	4.62568	13.8915
4	2.423	BB	0.0584	117.36610	29.48024	27.2214
----- ----- ----- ----- ----- ----- -----						
Totals :				431.15416	76.01056	

Signal 6: ELS1 A, ELSD Signal

Peak #	RetTime [min]	Type	Width [min]	Area [mV*s]	Height [mV]	Area %
----- ----- ----- ----- ----- ----- -----						
1	0.878	BB	0.0574	11.27327	2.53340	28.3069
2	1.576	BB	0.0340	28.55192	13.89025	71.6931
----- ----- ----- ----- ----- ----- -----						
Totals :				39.82518	16.42365	



Signal 7: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.486	BB	0.1934	7.54676e6	5.04602e5	85.2151
2	2.603	BB	0.1197	1.30937e6	1.51616e5	14.7849

Totals : 8.85613e6 6.56218e5

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.

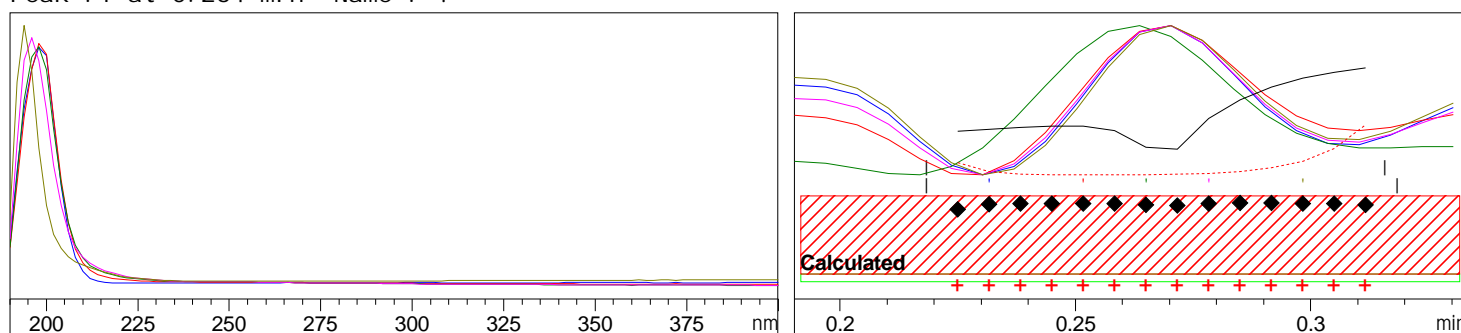
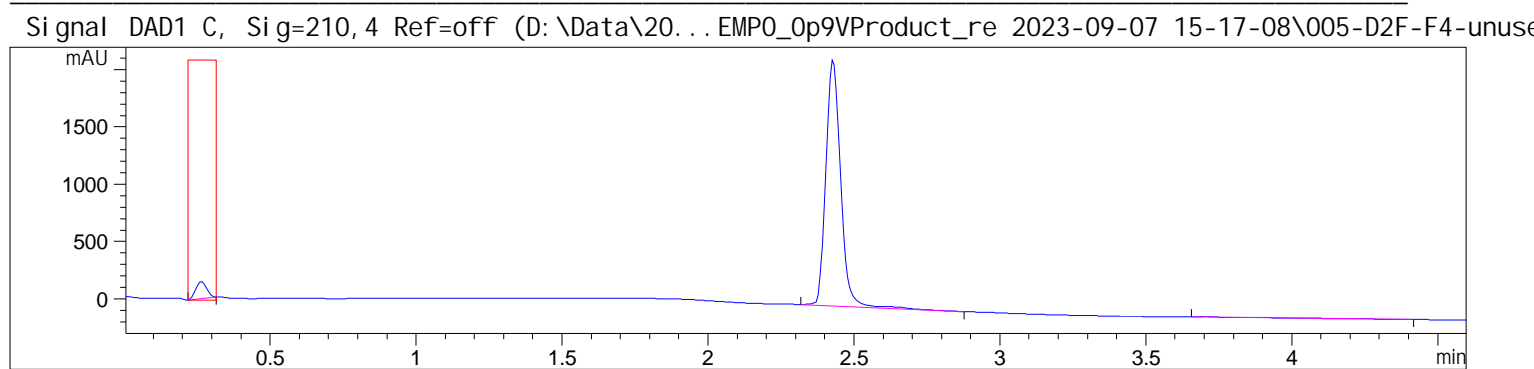
Signal 6: ELS1 A, ELSD Signal  
Empty table.

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: unusedMBA20



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

Purity factor : 905.543 (14 of 14 spectra exceed the calculated threshold limit.)

Threshold : 998.753 (Calculated with 14 of 14 spectra)

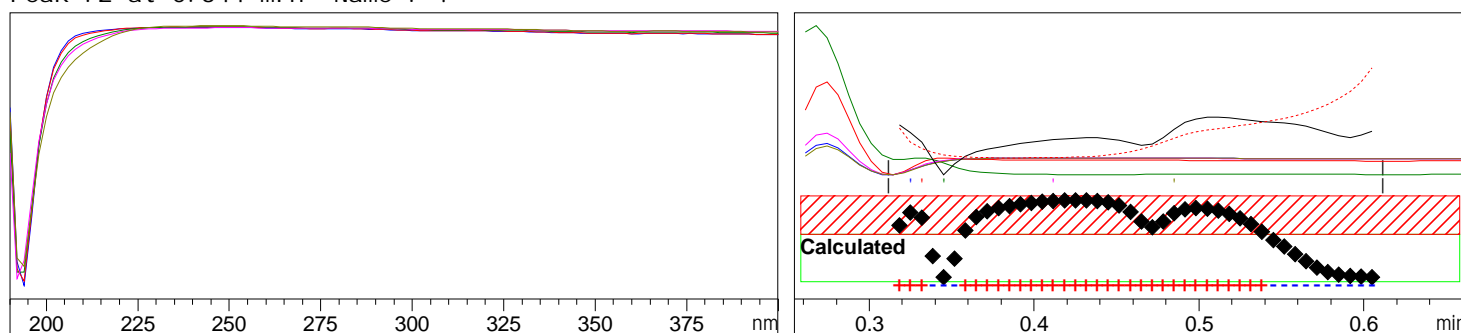
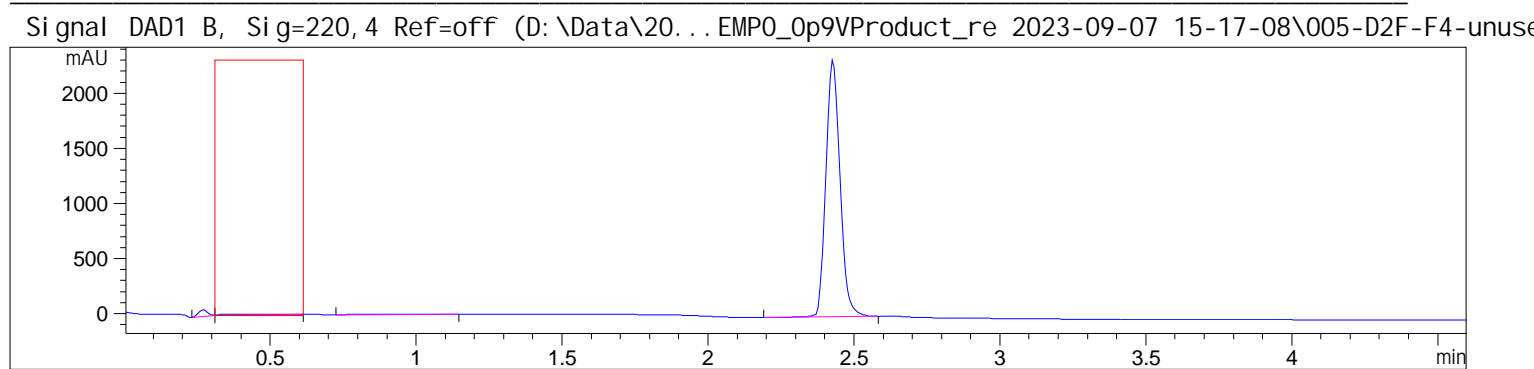
Reference : Peak start and end spectra (integrated) (0.218 / 0.318)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 1.425 (12 spectra, St.Dev 0.5947 + 3 \* 0.2766)

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

Sample Name: unusedMBA20



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

Purity factor : 989.142 (31 of 44 spectra exceed the calculated threshold limit.)

Threshold : 994.462 (Calculated with 31 of 44 spectra)

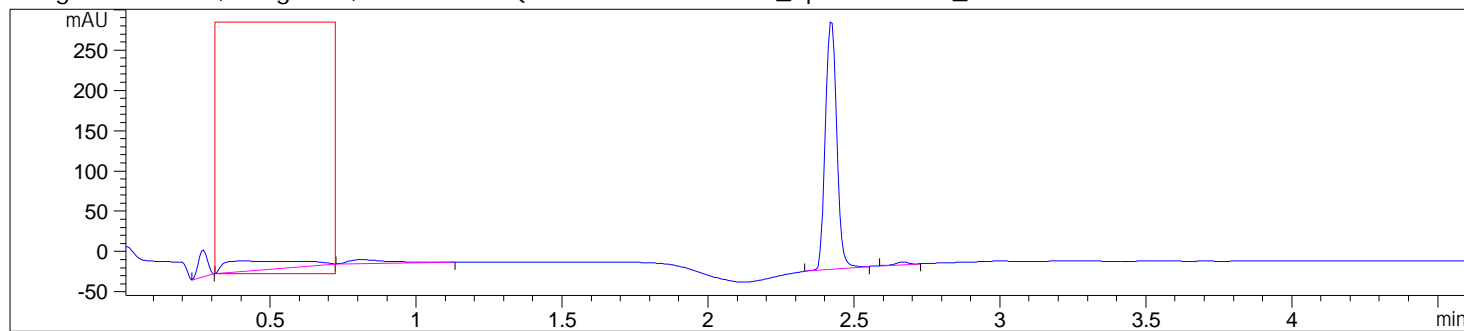
Reference : Peak start and end spectra (integrated) (0.312 / 0.612)

Spectra : 5 (Selection automatic, 5)

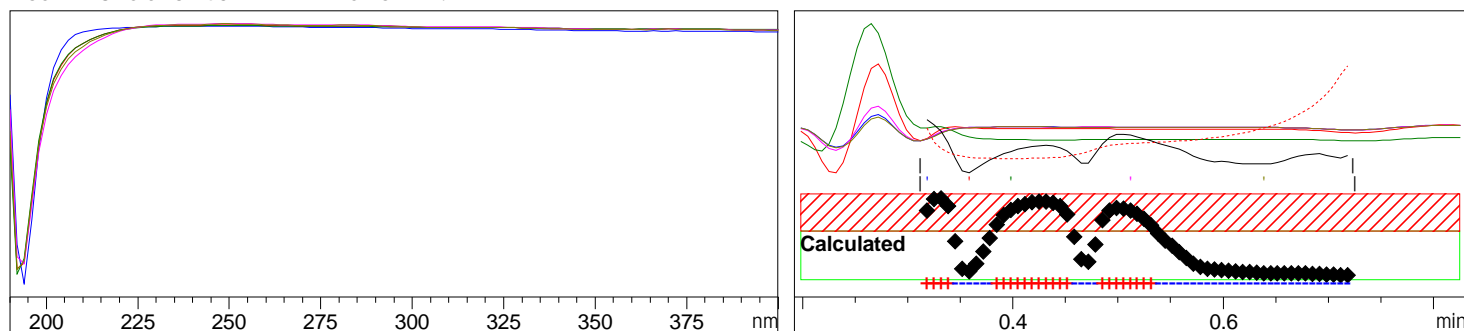
Noise Threshold: 1.425 (12 spectra, St.Dev 0.5947 + 3 \* 0.2766)

Sample Name: unusedMBA20

Signal DAD1 A, Sig=254, 4 Ref=off (D:\Data\20...EMP0\_0p9VProduct\_re 2023-09-07 15-17-08\005-D2F-F4-unusedMBA20.D)



Peak : 3 at 0.401 min Name : ?



-&gt; The purity factor exceeds the calculated threshold limit. &lt;-

Purity factor : 994.029 (23 of 61 spectra exceed the calculated threshold limit.)

Threshold : 997.114 (Calculated with 23 of 61 spectra)

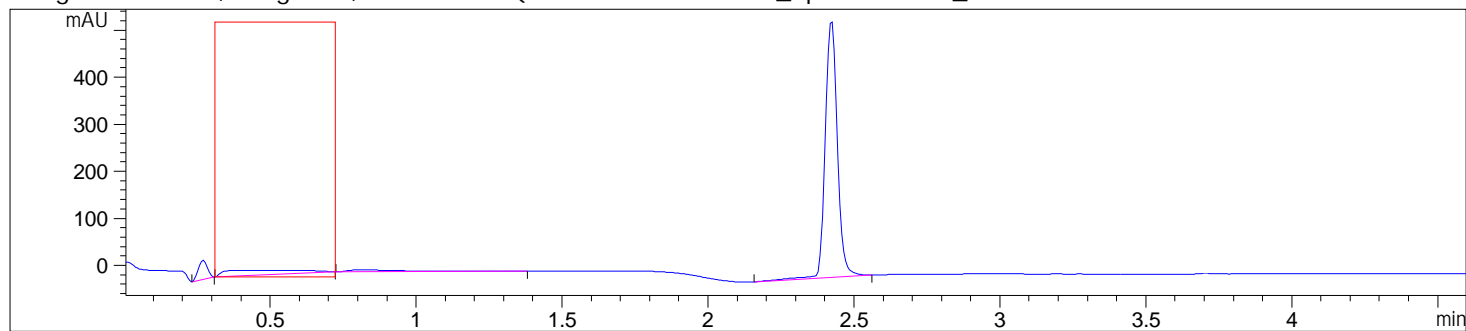
Reference : Peak start and end spectra (integrated) (0.312 / 0.725)

Spectra : 5 (Selection automatic, 5)

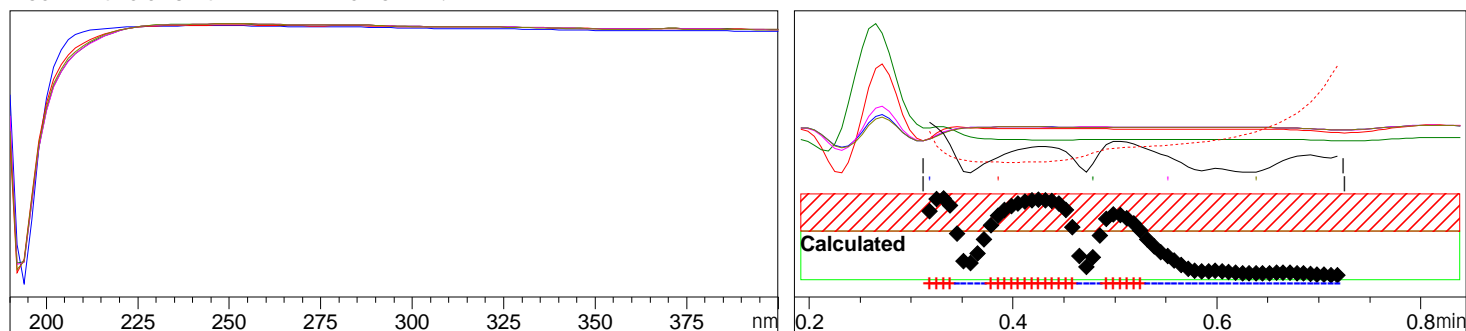
Noise Threshold: 1.425 (12 spectra, St.Dev 0.5947 + 3 \* 0.2766)

Sample Name: unusedMBA20

Signal DAD1 D, Sig=230, 4 Ref=off (D:\Data\20...EMP0\_0p9VProduct\_re 2023-09-07 15-17-08\005-D2F-F4-unusedMBA20.D)



Peak : 4 at 0.477 min Name : ?



-&gt; The purity factor exceeds the calculated threshold limit. &lt;-

Purity factor : 994.191 (23 of 61 spectra exceed the calculated threshold limit.)

Threshold : 997.173 (Calculated with 23 of 61 spectra)

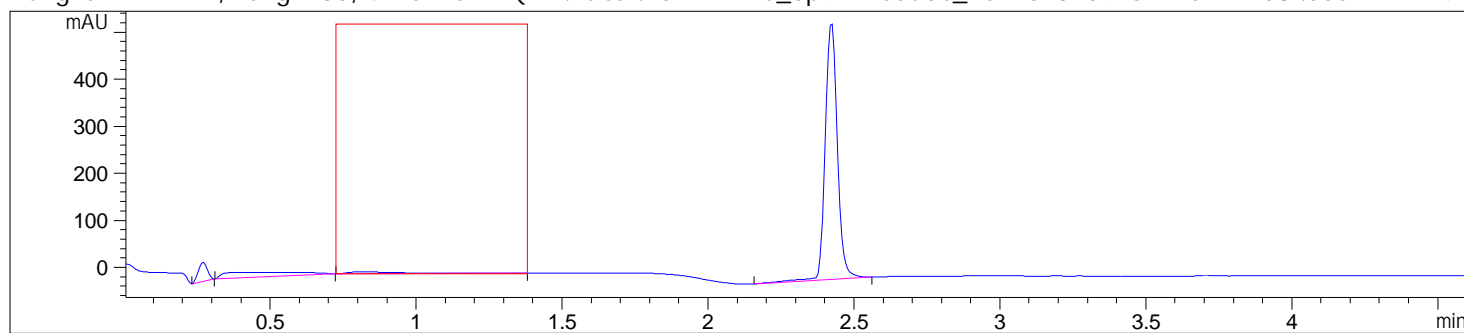
Reference : Peak start and end spectra (integrated) (0.312 / 0.725)

Spectra : 5 (Selection automatic, 5)

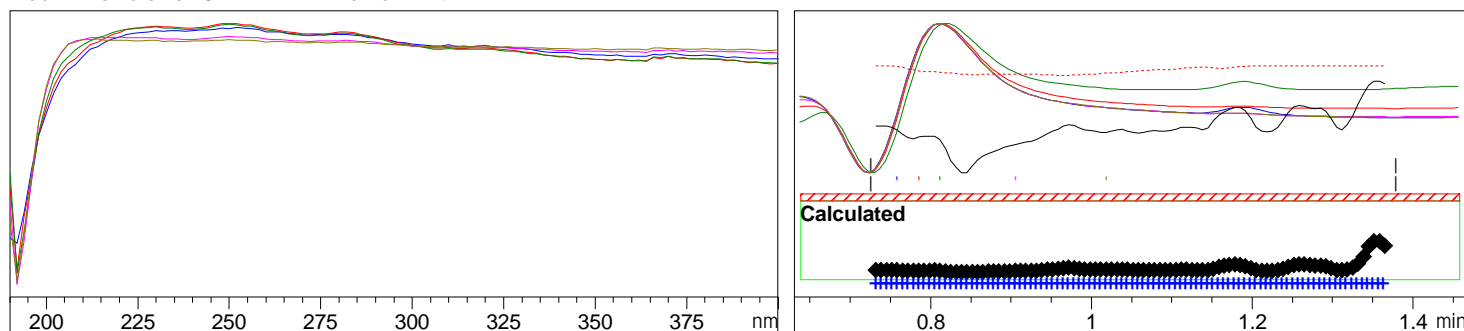
Noise Threshold: 1.425 (12 spectra, St.Dev 0.5947 + 3 \* 0.2766)

Sample Name: unusedMBA20

Signal DAD1 D, Sig=230, 4 Ref=off (D:\Data\20...EMP0\_0p9VProduct\_re 2023-09-07 15-17-08\005-D2F-F4-unusedMBA20.D)



Peak : 5 at 0.812 min Name : ?



-&gt; The purity factor is within the calculated threshold limit. &lt;-

Purity factor : 943.959 (96 of 96 spectra are within the calculated threshold limit.)

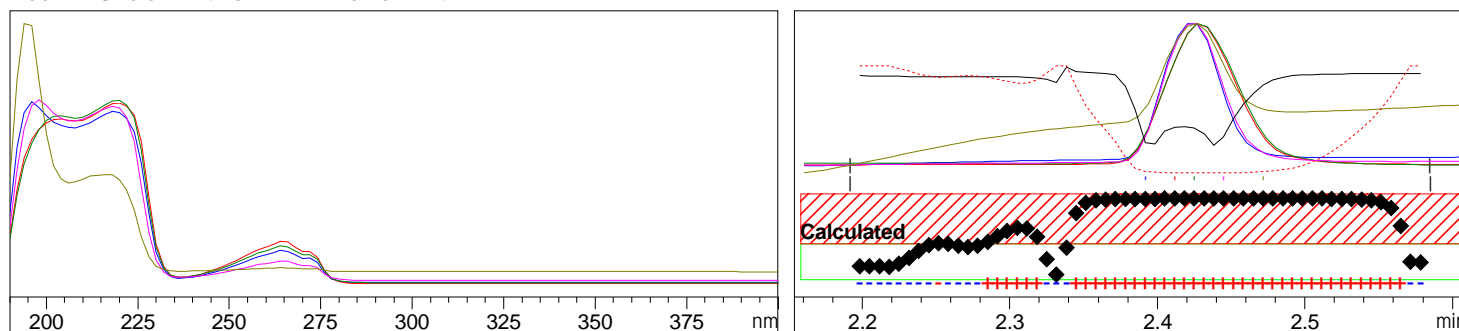
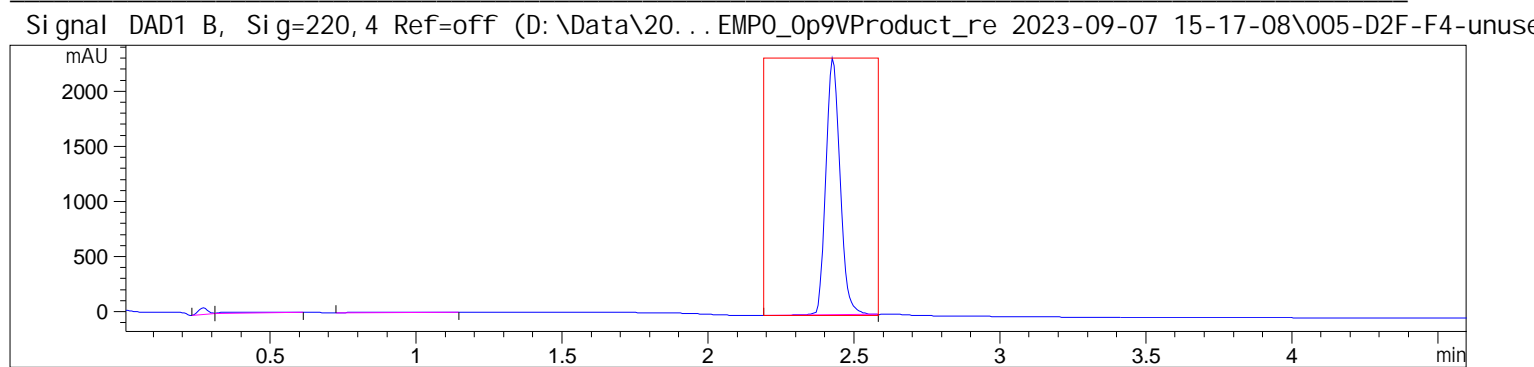
Threshold : 172.814 (Calculated with 96 of 96 spectra)

Reference : Peak start and end spectra (integrated) (0.725 / 1.378)

Spectra : 5 (Selection automatic, 5)

Noise Threshold : 1.425 (12 spectra, St.Dev 0.5947 + 3 \* 0.2766)

Warning : Calculated Noise Level &gt; 1.00 (see information in threshold calculation)

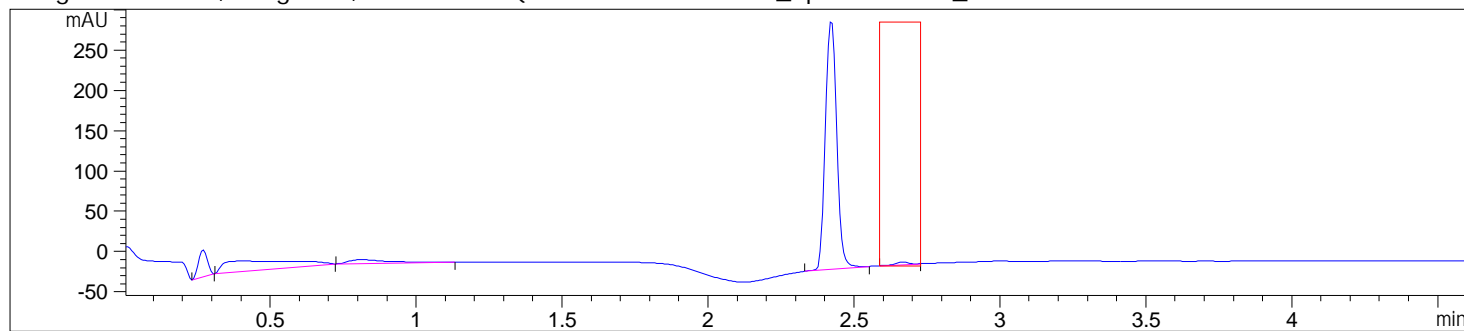


-> The purity factor exceeds the calculated threshold limit. <-

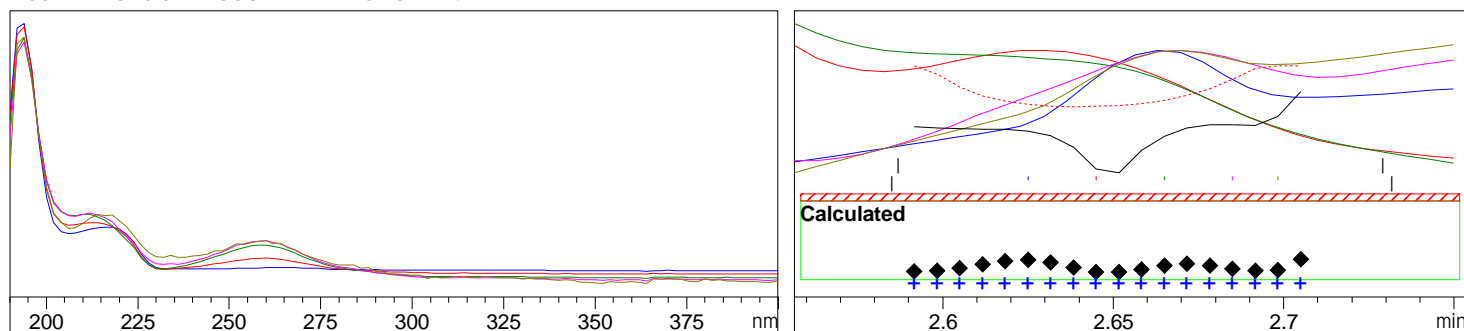
Purity factor : 641.399 (40 of 58 spectra exceed the calculated threshold limit.)  
Threshold : 923.503 (Calculated with 40 of 58 spectra)  
Reference : Peak start and end spectra (integrated) (2.192 / 2.585)  
Spectra : 5 (Selection automatic, 5)  
Noise Threshold: 1.425 (12 spectra, St.Dev 0.5947 + 3 \* 0.2766)  
Warning : Spectral absorbances > 1000 mAU (see help for more information)

Sample Name: unusedMBA20

Signal DAD1 A, Sig=254, 4 Ref=off (D:\Data\20...EMP0\_Op9VProduct\_re 2023-09-07 15-17-08\005-D2F-F4-unusedMBA20.D)



Peak : 10 at 2.666 min Name : ?



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

Purity factor : 974.630 (18 of 18 spectra are within the calculated threshold limit.)

Threshold : 642.770 (Calculated with 18 of 18 spectra)

Reference : Peak start and end spectra (integrated) (2.585 / 2.732)

Spectra : 5 (Selection automatic, 5)

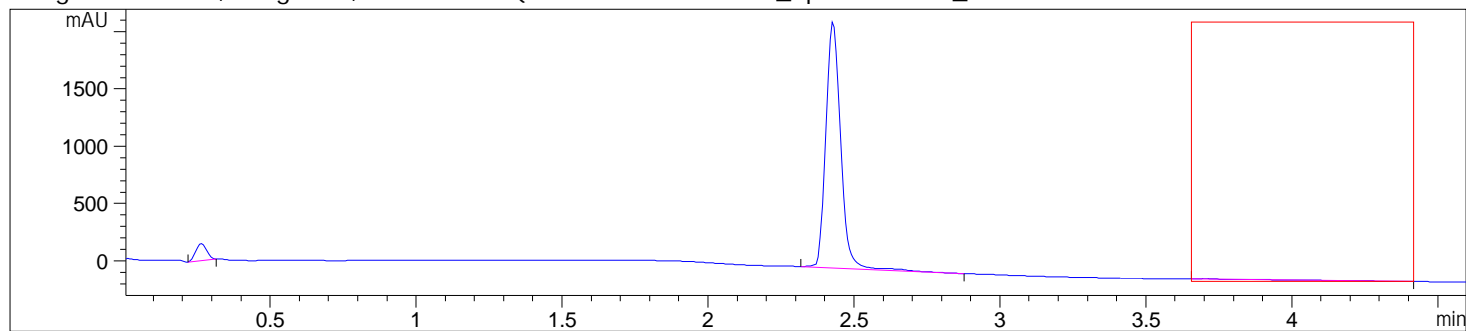
Noise Threshold : 1.425 (12 spectra, St.Dev 0.5947 + 3 \* 0.2766)

Warning : Calculated Noise Level > 1.00 (see information in threshold calculation)

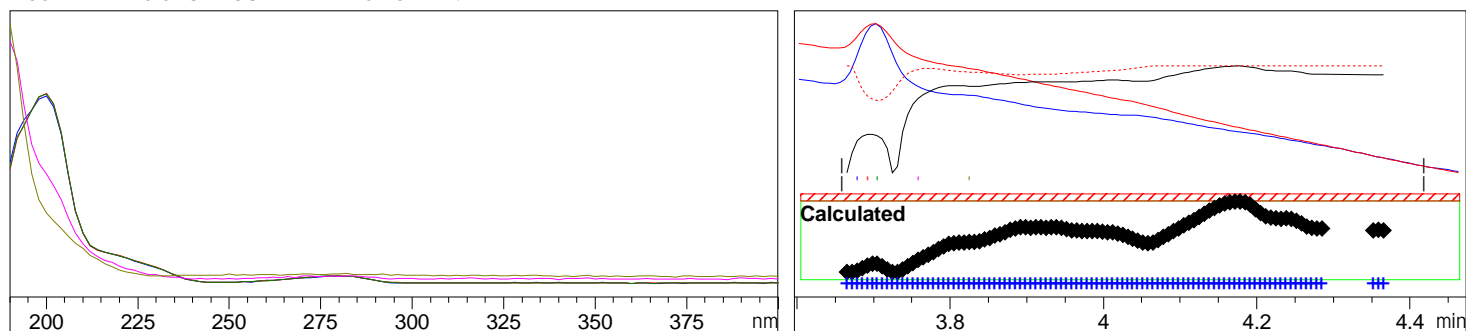


Sample Name: unusedMBA20

Signal DAD1 C, Sig=210, 4 Ref=off (D:\Data\20...EMP0\_Op9VProduct\_re 2023-09-07 15-17-08\005-D2F-F4-unusedMBA20.D)



Peak : 11 at 3.703 min Name : ?



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

Purity factor : 546.639 (97 of 97 spectra are within the calculated threshold limit.)

Threshold : 215.790 (Calculated with 97 of 97 spectra)

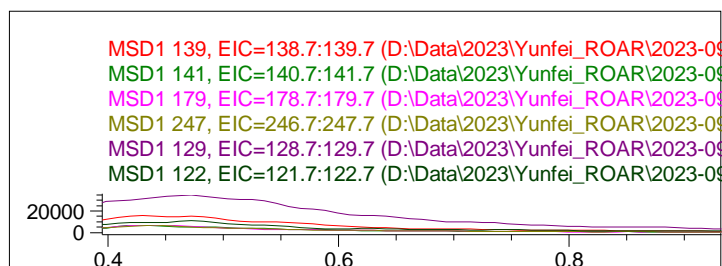
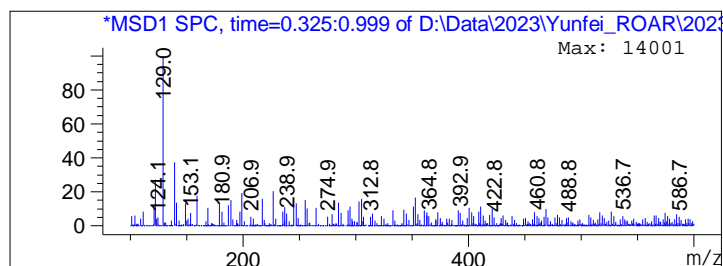
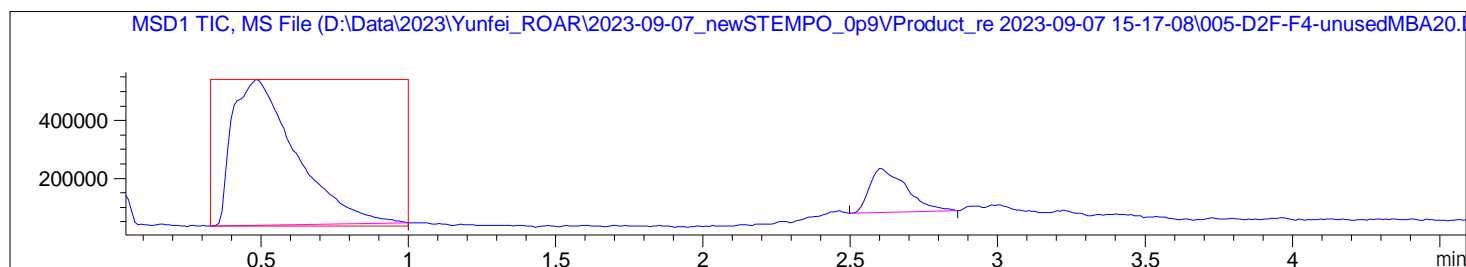
Reference : Peak start and end spectra (integrated) (3.658 / 4.418)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 1.425 (12 spectra, St.Dev 0.5947 + 3 \* 0.2766)

Warning : Calculated Noise Level > 1.00 (see information in threshold calculation)

Sample Name: unusedMBA20



Peak #1 at 0.486 min ( 0.328 to 0.999 min)

-&gt; The analysis found 6 components, indicating an impure peak. &lt;-

Component 1: Peak at Scan 37.9. Top ions are 139 141 305

Component 2: Peak at Scan 39.1. Top ions are 179 247

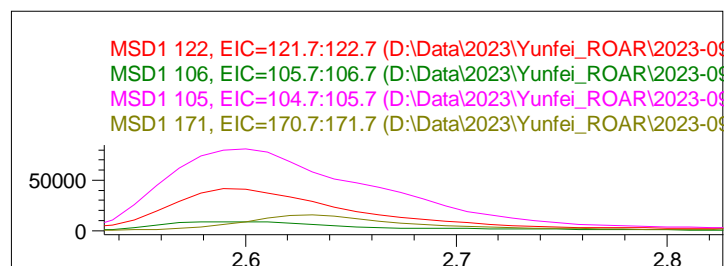
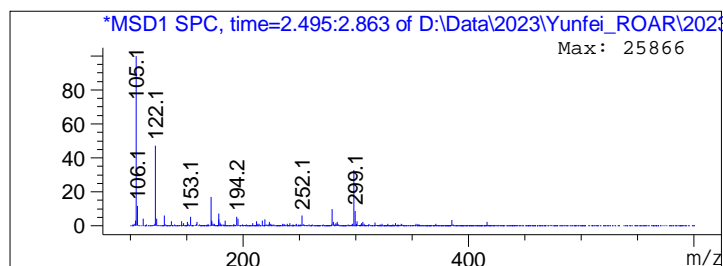
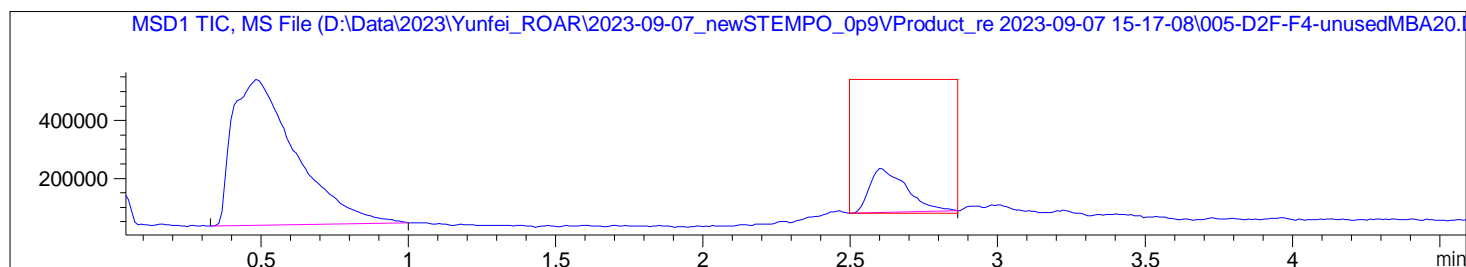
Component 3: Peak at Scan 41.9. Top ions are 129 122

Component 4: Peak at Scan 43.4. Top ions are 189

Component 5: Peak at Scan 45.3. Top ions are 255

Component 6: Peak at Scan 46.8. Top ions are 199

Sample Name: unusedMBA20



Peak #2 at 2.603 min ( 2.496 to 2.863 min)

-&gt; The analysis found 5 components, indicating an impure peak. &lt;-

Component 1: Peak at Scan 243.1. Top ions are 122 106

Component 2: Peak at Scan 243.8. Top ions are 105

Component 3: Peak at Scan 246.8. Top ions are 171

Component 4: Peak at Scan 248.3. Top ions are 178

Component 5: Peak at Scan 251.8. Top ions are 298

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