

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

```

```

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

```

Sample Name: freshC03

```
=====
Acq. Operator   : user                      Seq. Line :    2
Sample Operator : user
Acq. Instrument : SFC LCMS                  Location  :   D2F-E1
Injection Date  : 11/08/2023 02:16:56       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       : 432
Maximum Pressure   : 600.0 bar     Maximum pH : 8.0
Minimum pH         : 2.0
Maximum Temperature: 60.0 °C
Comment            : New 2023-08-03
```

Sample Name: freshC03

```

=====
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           :          0.17          849.2   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
HighVac                   :      5.1E-009      5.2E-009 Torr
CapCur                   :           5          660 nA
ChamCur                  :      8.0E-002      5.6E-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          49 %
Gas FI Drv               :           62          61 %

```

## 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

```

Sample Name: freshC03

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
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 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

Sample Name: freshC03

Mass	:	Value
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 : 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
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 12:13 PM

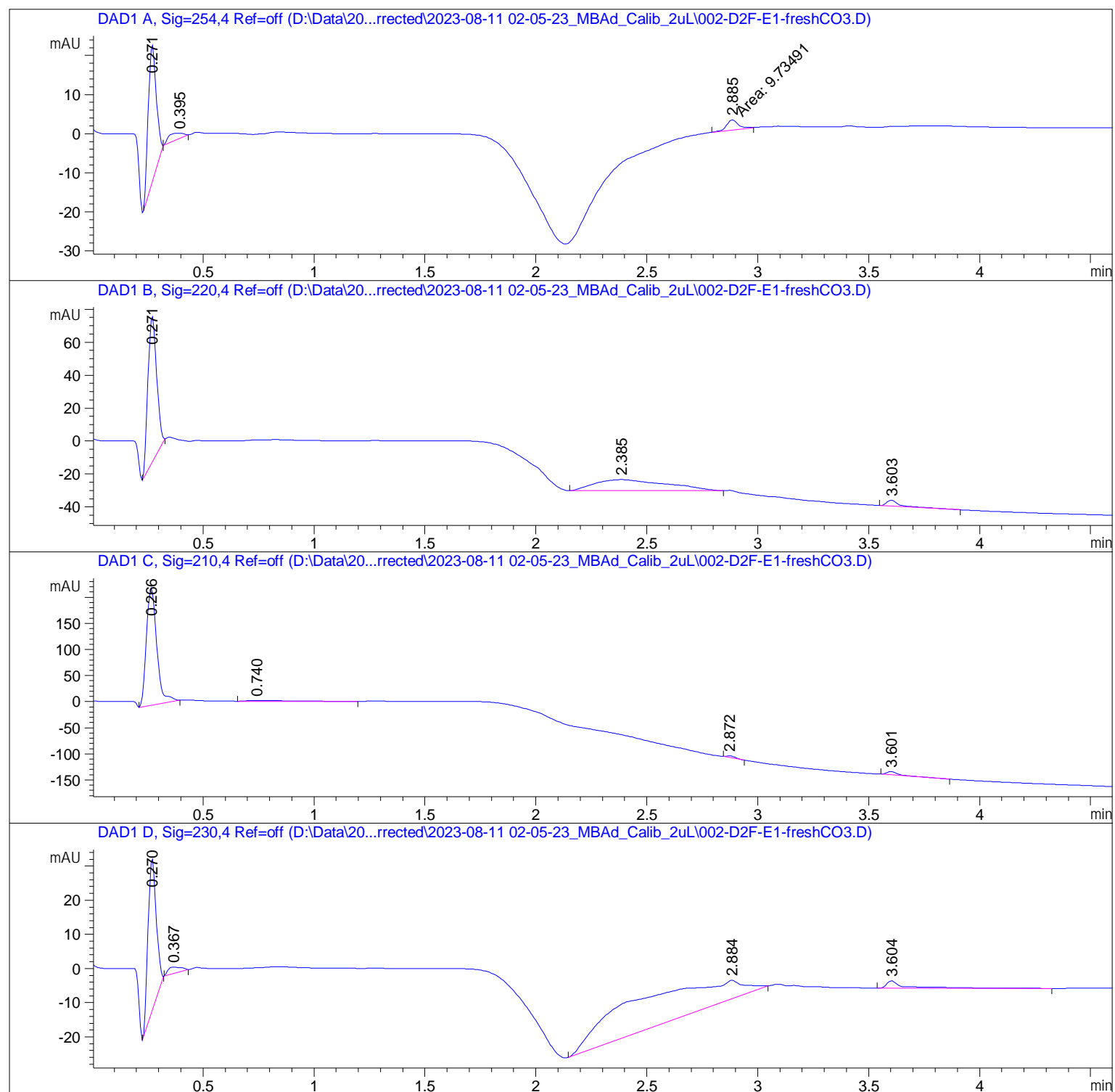
Logbook File: D:\Data\20... corrected\2023-08-11 02-05-23\_MBAAd\_Cal i b\_2uL\002-D2F-E1-freshC03.D\RUN.LOG

Module	# Event Message	Date Time
Method	Method started: line# 2 at location 'D2F-E1> ' inj# 1	11/08/2023 02:15:44
CP Macro	PreRun macro: 'LAMPALL ON'	11/08/2023 02:15:44
G4260B	G4260B: ELSD - Autozero	11/08/2023 02:15:45
G4260B	G4260B: ELSD - Al ready switched on	11/08/2023 02:15:46
Method	Instrument running sample from location D2F-> E1	11/08/2023 02:15:46
G7115A	G7115A: DEAC605436 - Detector: Prepare	11/08/2023 02:16:14
G7115A	G7115A: DEAC605436 - Detector: Idle	11/08/2023 02:16:30
G4767A	G4767A: DEAFD00218 - Draw command finished	11/08/2023 02:16:47
G4767A	G4767A: DEAFD00218 - Sampler wash is active	11/08/2023 02:16:48
G4767A	G4767A: DEAFD00218 - Sampler wash is idle	11/08/2023 02:16:54
G4767A	G4767A: DEAFD00218 - Sample preparation time: > 25 sec	11/08/2023 02:16:54
PumpVal ve	G7111B: DEAEW03495 - Run	11/08/2023 02:16:56

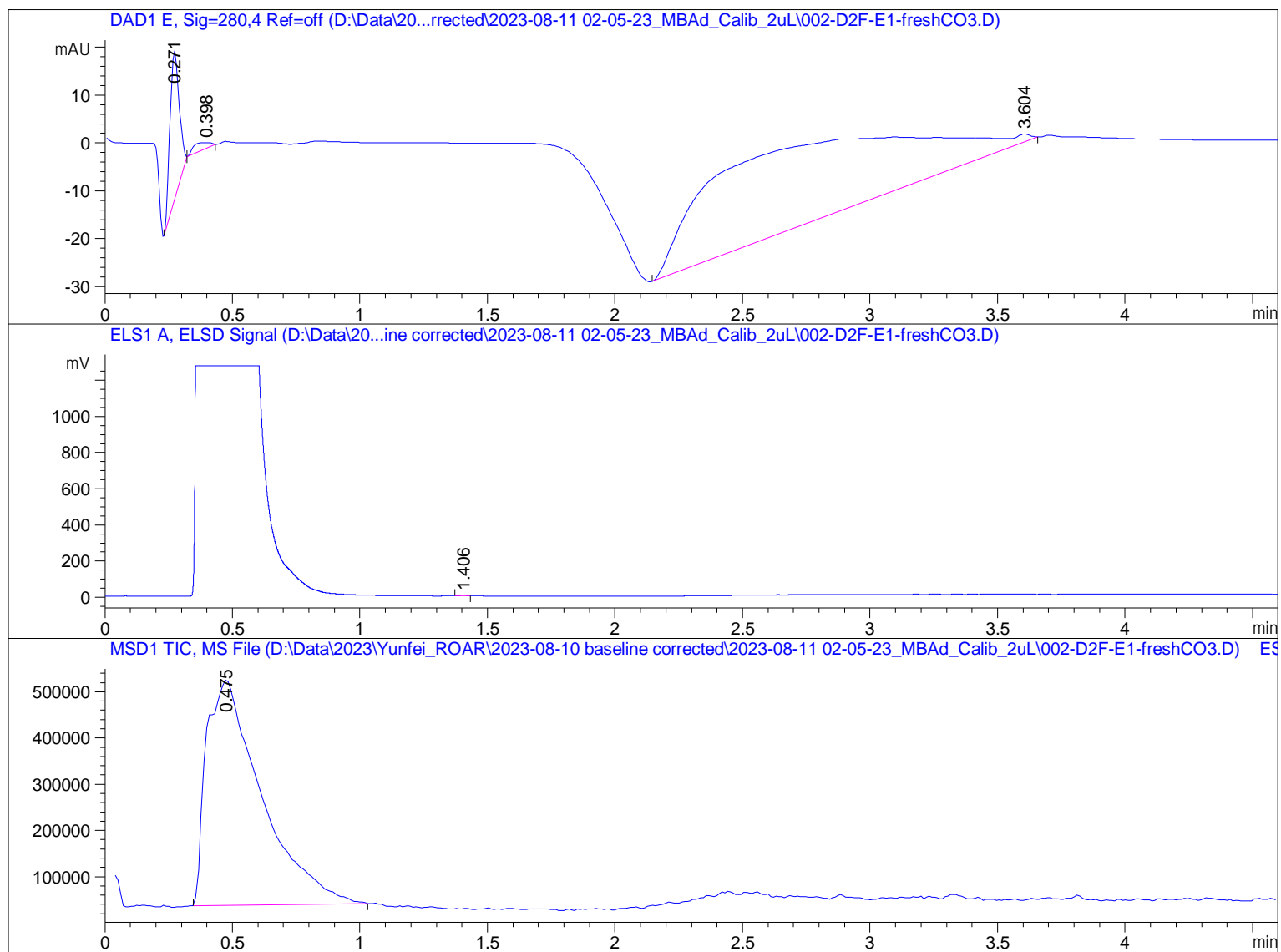
Sample Name: freshCO3

PumpValve	G7111B: DEAEW03495 - Postrun	11/08/2023 02: 21: 32
PumpValve	G1170A: DEBAD03715 - Postrun	11/08/2023 02: 21: 33
G4767A	G4767A: DEAFD00218 - Postrun	11/08/2023 02: 21: 33
G1170A	G1170A: DEBAD03734 - Postrun	11/08/2023 02: 21: 34
G4782A	G4782A: DEAGN00153 - Postrun	11/08/2023 02: 21: 34
Method	Saving Method COL1_5NH4FA_MECN_5T095_1MIN_10> 0-600MS_POS.M	11/08/2023 02: 23: 42
Method	Instrument run completed	11/08/2023 02: 23: 43
CP Macro	Analyzing rawdata 002-D2F-E1-freshCO3.D	11/08/2023 02: 23: 43
Method	Saving Method DA.M	11/08/2023 02: 23: 45
Method	Method completed	11/08/2023 02: 23: 52

=====



Sample Name: freshCO3

=====  
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	0.271	BB	0.0395	88.65765	35.10416	83.2566
2	0.395	BB	0.0943	8.09470	1.34377	7.6016
3	2.885	MM	0.0603	9.73491	2.68954	9.1419

Totals : 106.48727 39.13747

Sample Name: freshC03

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.271	BB	0.0440	242.52191	88.46867	59.2865
2	2.385	BB	0.3243	152.67987	6.73887	37.3239
3	3.603	BBA	0.0581	13.86592	3.51014	3.3896

Totals : 409.06771 98.71769

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.266	BB	0.0521	735.31177	224.94415	93.5762
2	0.740	BB	0.1409	18.44635	1.80934	2.3475
3	2.872	BB	0.0476	8.77123	2.87725	1.1162
4	3.601	BBA	0.0539	23.26021	6.47670	2.9601

Totals : 785.78955 236.10744

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	0.0399	113.86191	44.50167	24.3382
2	0.367	BB	0.0623	7.76305	1.87645	1.6594
3	2.884	BB	0.7373	333.49017	5.36400	71.2842
4	3.604	BB	0.0807	12.71667	2.16072	2.7182

Totals : 467.83180 53.90283

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	0.0416	79.34656	31.25973	7.3441
2	0.398	BB	0.0993	7.28664	1.15971	0.6744
3	3.604	BB	6.7223	993.77637	1.72780	91.9814

Totals : 1080.40956 34.14723



Signal 6: ELS1 A, ELSD Signal

Peak #	RetTime [min]	Type	Width [min]	Area [mV*s]	Height [mV]	Area %
1	1.406	BB	0.0334	6.79809	3.46924	100.0000

Totals : 6.79809 3.46924

Signal 7: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.475	BB	0.2001	7.31858e6	4.88382e5	100.0000

Totals : 7.31858e6 4.88382e5

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.

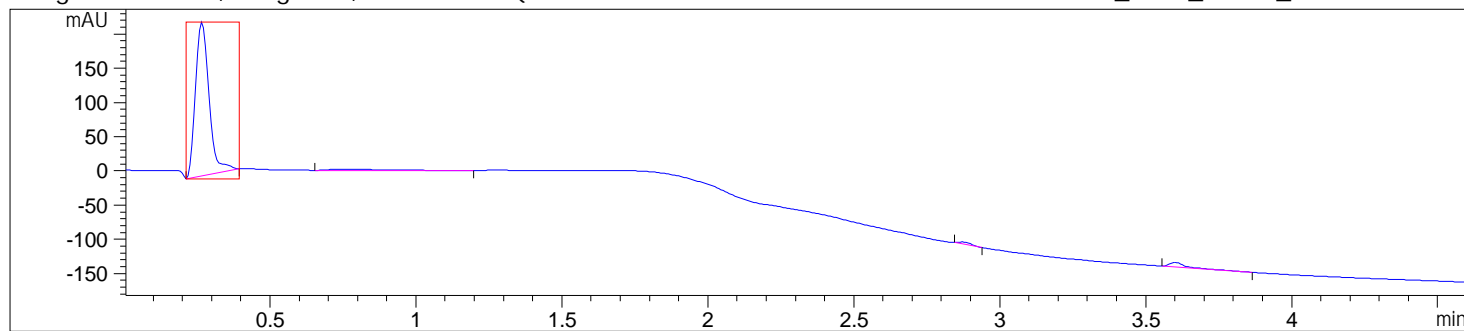
Final Summed Peaks Report

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

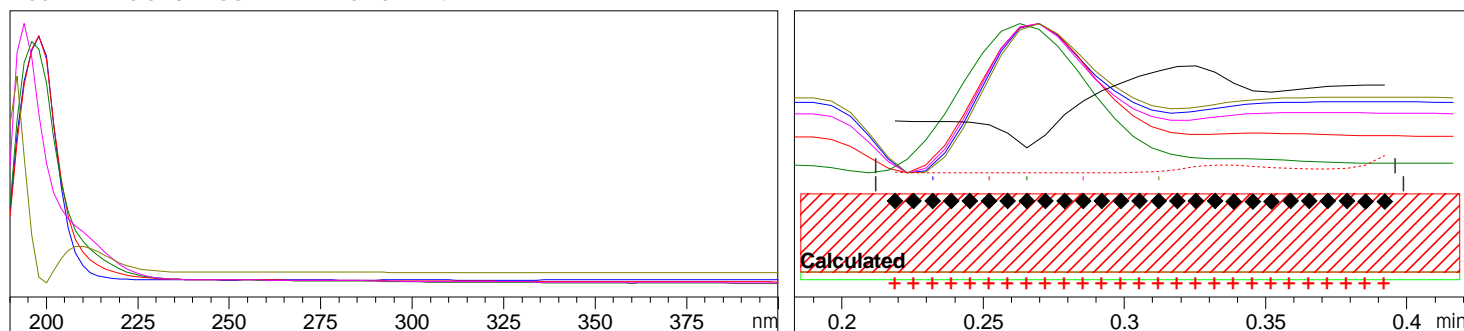
Signal 2: DAD1 B, Sig=220, 4 Ref=off  
Signal 3: DAD1 C, Sig=210, 4 Ref=off  
Signal 4: DAD1 D, Sig=230, 4 Ref=off  
Signal 5: DAD1 E, Sig=280, 4 Ref=off  
Signal 6: ELS1 A, ELSD Signal  
Signal 7: MSD1 TIC, MS File

Sample Name: freshC03

Signal DAD1 C, Sig=210, 4 Ref=off (D:\Data\20... rrected\2023-08-11 02-05-23\_MBAd\_Cal i b\_2uL\002-D2F-E1-fr



Peak : 1 at 0.266 min Name : ?



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

Purity factor : 763.495 (27 of 27 spectra exceed the calculated threshold limit.)

Threshold : 999.848 (Calculated with 27 of 27 spectra)

Reference : Peak start and end spectra (integrated) (0.212 / 0.399)

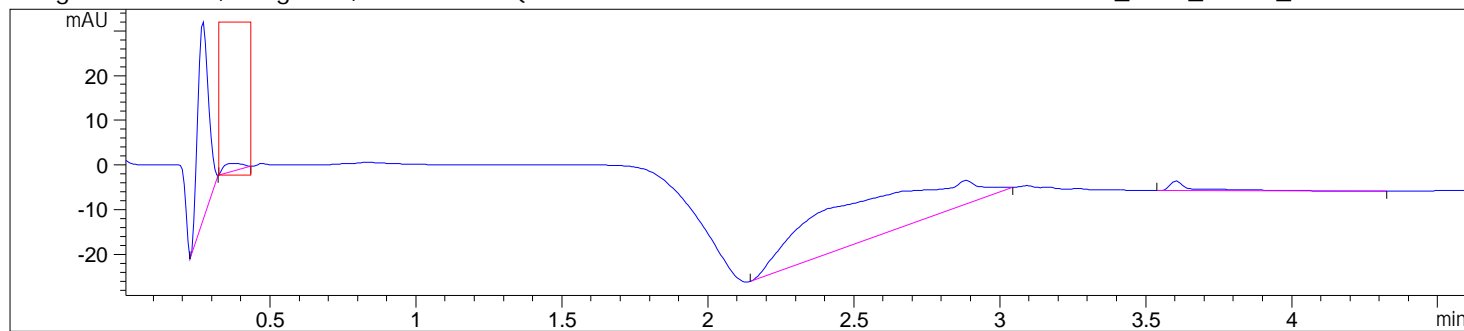
Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.222 (12 spectra, St.Dev 0.0886 + 3 \* 0.0444)

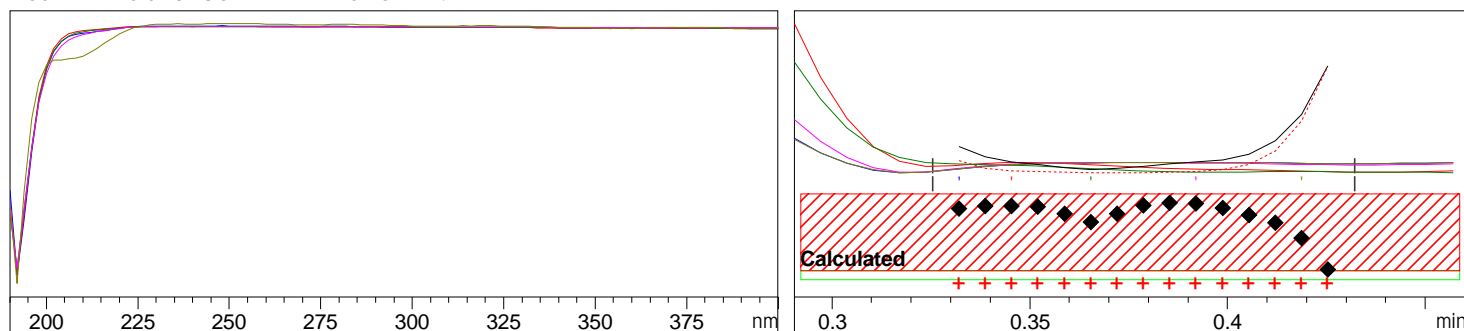
Warning : Spectral absorbances &gt; 1000 mAU (see help for more information)

Sample Name: freshC03

Signal DAD1 D, Sig=230,4 Ref=off (D:\Data\20...rrected\2023-08-11 02-05-23\_MBAAd\_Cal i b\_2uL\002-D2F-E1-fr



Peak : 2 at 0.367 min Name : ?



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

Purity factor : 930.552 (15 of 15 spectra exceed the calculated threshold limit.)

Threshold : 933.431 (Calculated with 15 of 15 spectra)

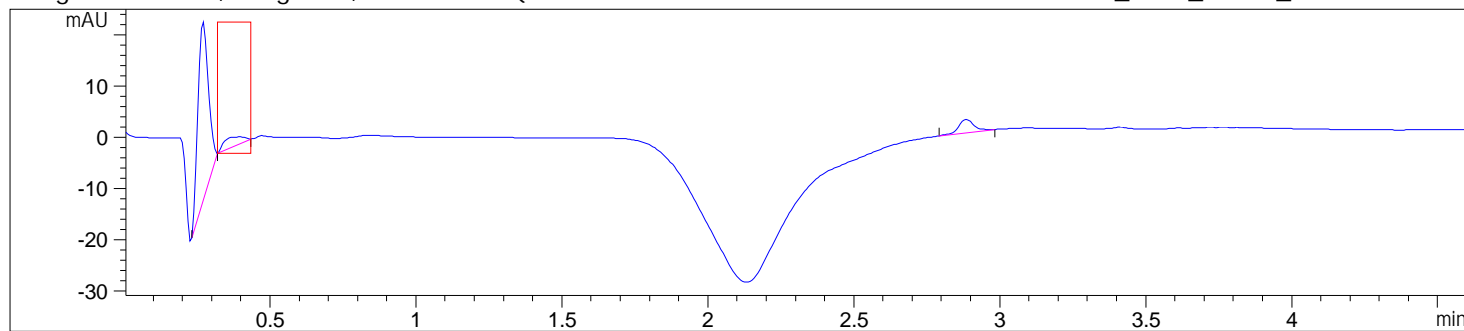
Reference : Peak start and end spectra (integrated) (0.325 / 0.432)

Spectra : 5 (Selection automatic, 5)

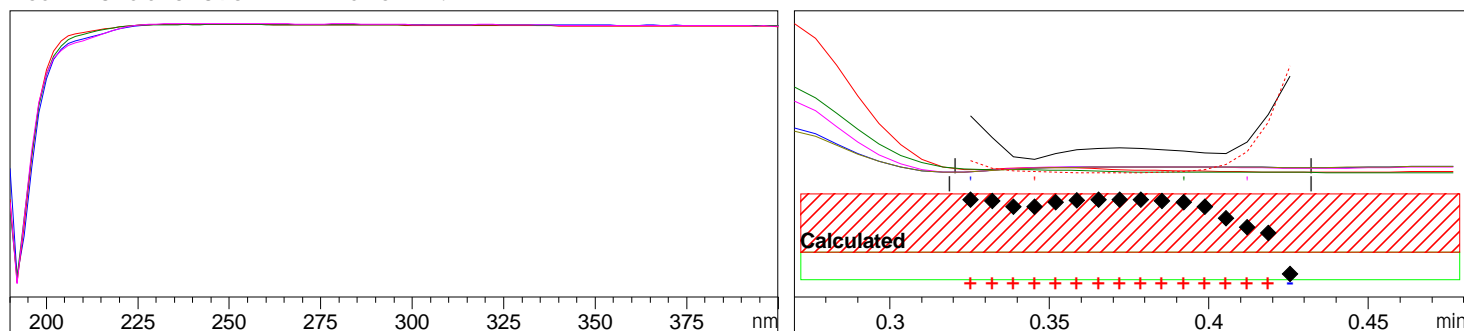
Noise Threshold: 0.222 (12 spectra, St.Dev 0.0886 + 3 \* 0.0444)

Sample Name: freshC03

Signal DAD1 A, Sig=254, 4 Ref=off (D:\Data\20... rrected\2023-08-11 02-05-23\_MBAd\_Cal i b\_2uL\002-D2F-E1-fr



Peak : 3 at 0.395 min Name : ?



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

Purity factor : 997.477 (15 of 16 spectra exceed the calculated threshold limit.)

Threshold : 999.309 (Calculated with 15 of 16 spectra)

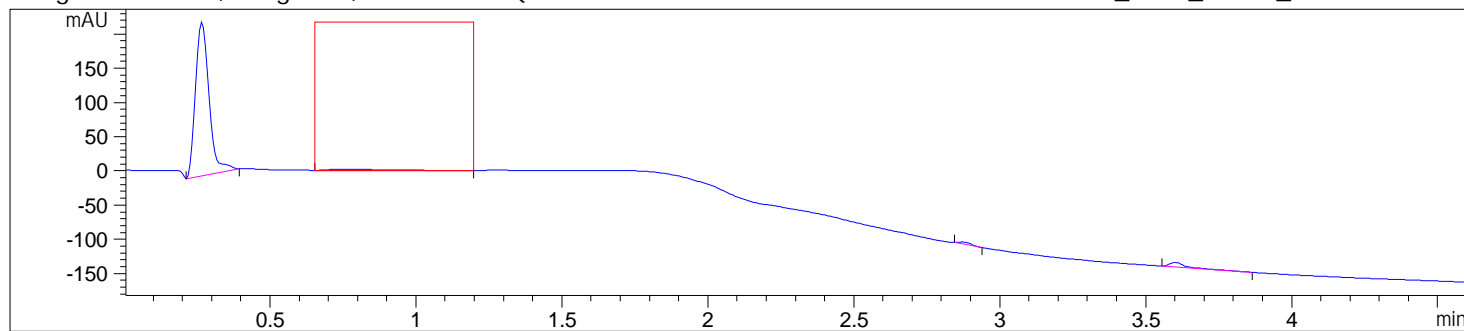
Reference : Peak start and end spectra (integrated) (0.319 / 0.432)

Spectra : 4 (Selection automatic, 5)

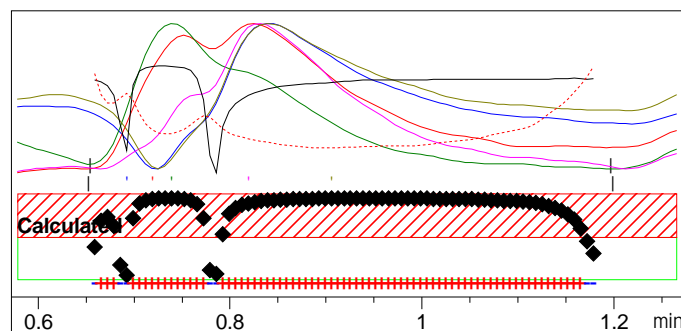
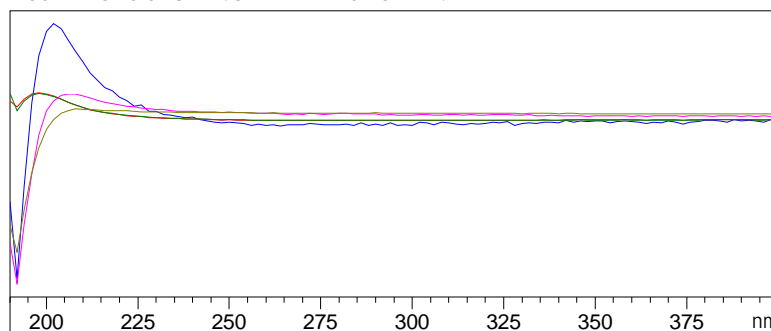
Noise Threshold: 0.222 (12 spectra, St.Dev 0.0886 + 3 \* 0.0444)

Sample Name: freshC03

Signal DAD1 C, Sig=210, 4 Ref=off (D:\Data\20... rrected\2023-08-11 02-05-23\_MBAAd\_Cal i b\_2uL\002-D2F-E1-fr



Peak : 5 at 0.740 min Name : ?



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

Purity factor : 443.681 (72 of 79 spectra exceed the calculated threshold limit.)

Threshold : 908.862 (Calculated with 72 of 79 spectra)

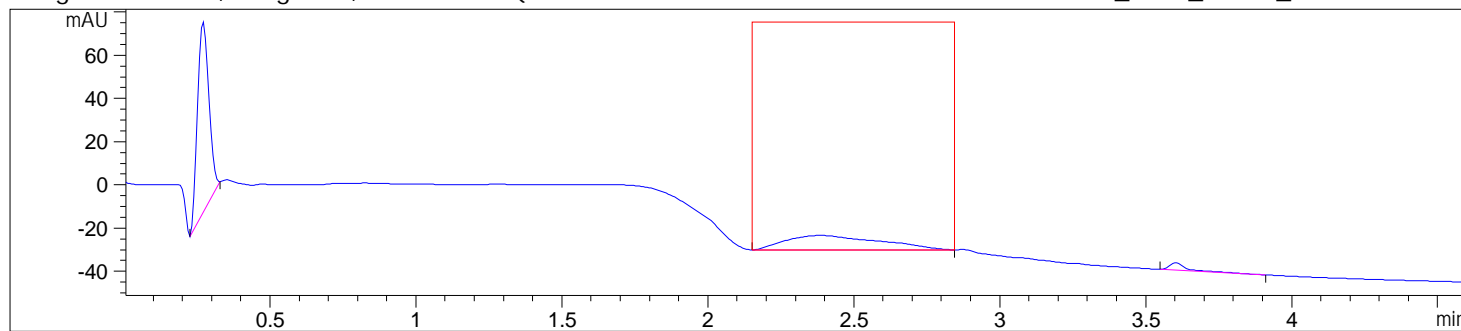
Reference : Peak start and end spectra (integrated) (0.652 / 1.199)

Spectra : 5 (Selection automatic, 5)

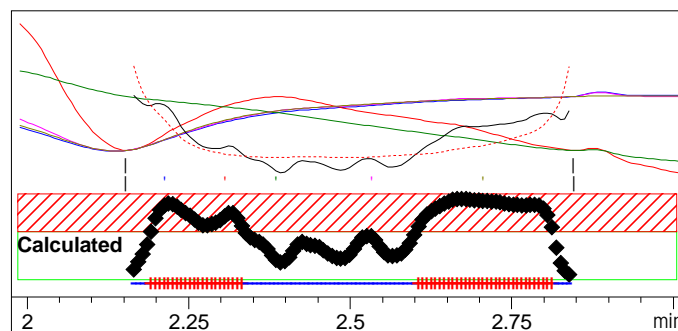
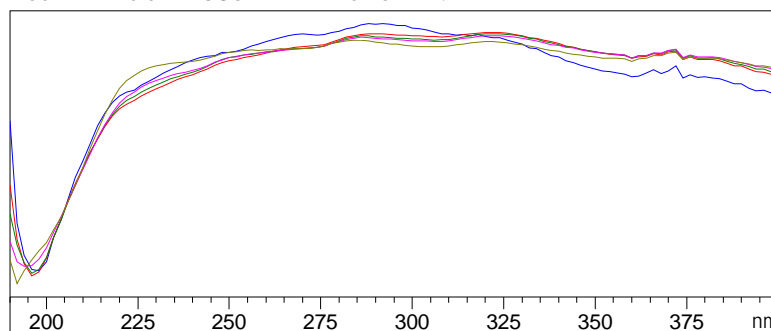
Noise Threshold: 0.222 (12 spectra, St.Dev 0.0886 + 3 \* 0.0444)

Sample Name: freshC03

Signal DAD1 B, Sig=220, 4 Ref=off (D:\Data\20... rrected\2023-08-11 02-05-23\_MBAAd\_Cal i b\_2uL\002-D2F-E1-fr



Peak : 7 at 2.385 min Name : ?



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

Purity factor : 977.117 (54 of 102 spectra exceed the calculated threshold limit.)

Threshold : 988.169 (Calculated with 54 of 102 spectra)

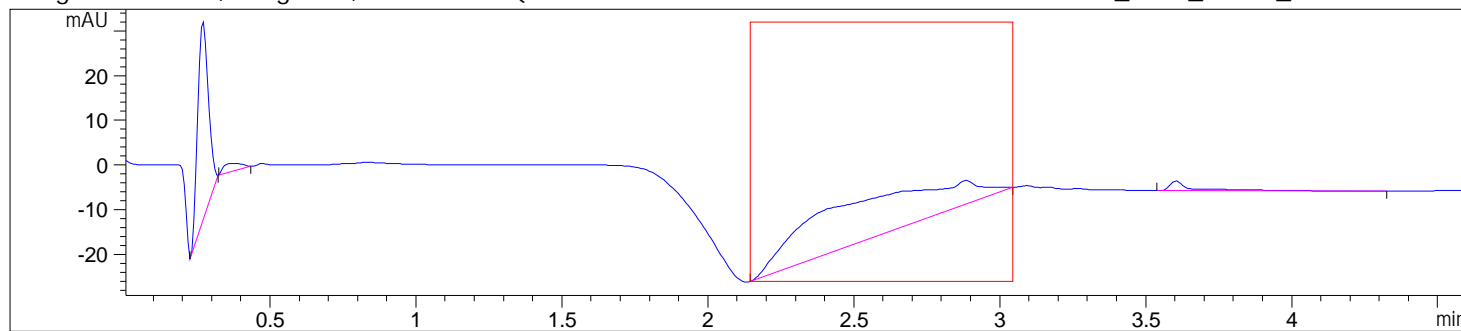
Reference : Peak start and end spectra (integrated) (2.152 / 2.845)

Spectra : 5 (Selection automatic, 5)

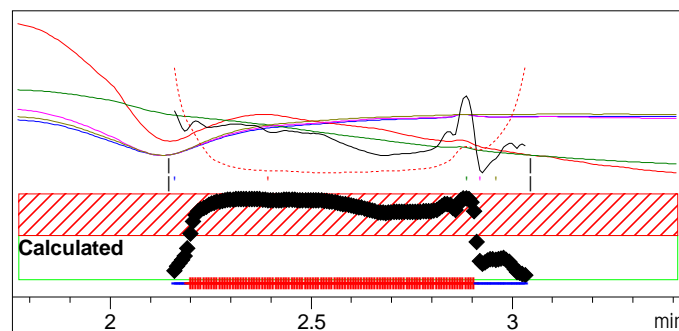
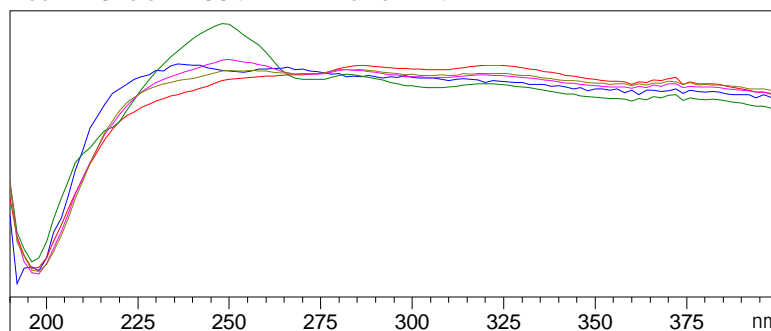
Noise Threshold: 0.222 (12 spectra, St.Dev 0.0886 + 3 \* 0.0444)

Sample Name: freshC03

Signal DAD1 D, Sig=230, 4 Ref=off (D:\Data\20... rrected\2023-08-11 02-05-23\_MBAAd\_Cal i b\_2uL\002-D2F-E1-fr



Peak : 8 at 2.884 min Name : ?



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

Purity factor : 978.758 (107 of 132 spectra exceed the calculated threshold limit.)

Threshold : 995.341 (Calculated with 107 of 132 spectra)

Reference : Peak start and end spectra (integrated) (2.145 / 3.045)

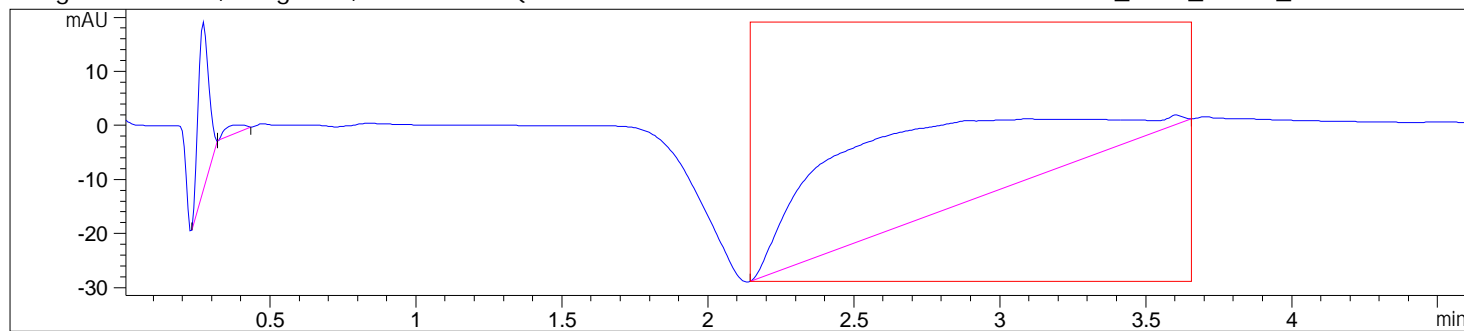
Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.222 (12 spectra, St.Dev 0.0886 + 3 \* 0.0444)

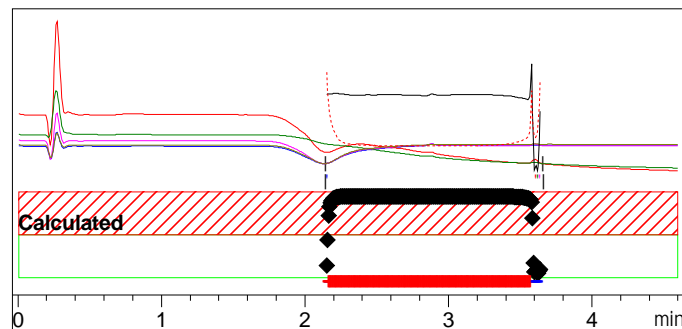
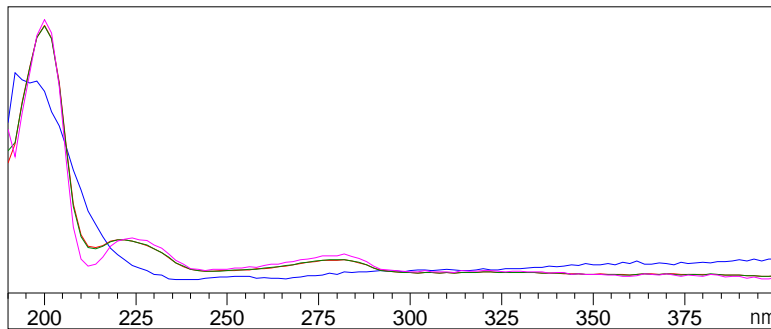


Sample Name: freshC03

Signal DAD1 E, Sig=280, 4 Ref=off (D:\Data\20... rrected\2023-08-11 02-05-23\_MBAAd\_Cal i b\_2uL\002-D2F-E1-fr



Peak : 9 at 3.604 min Name : ?



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

Purity factor : 858.858 (214 of 224 spectra exceed the calculated threshold limit.)

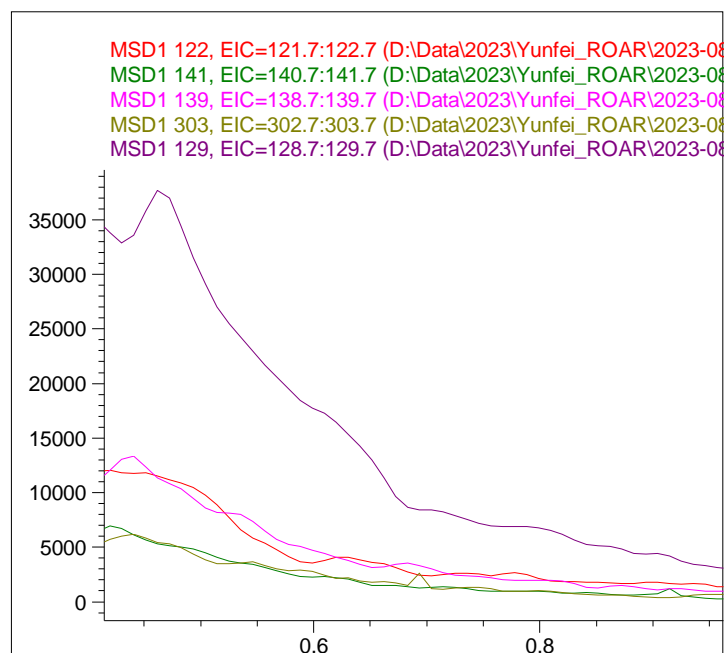
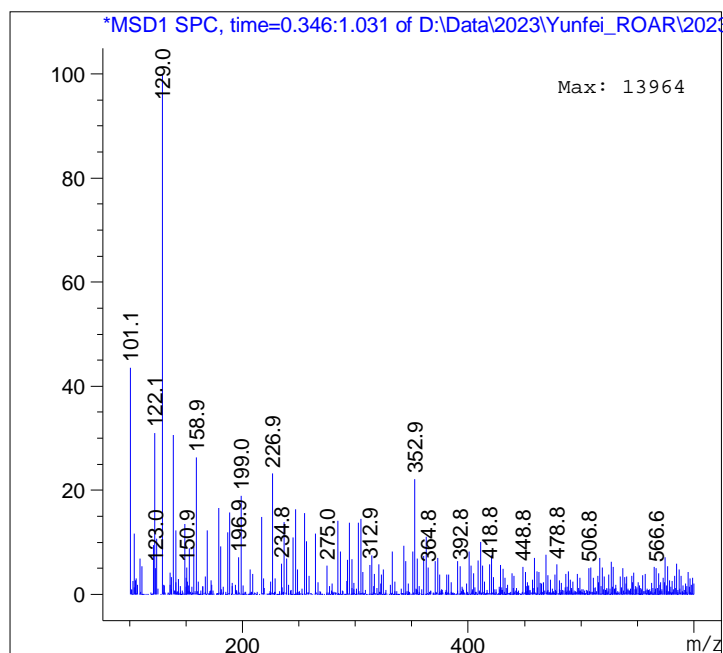
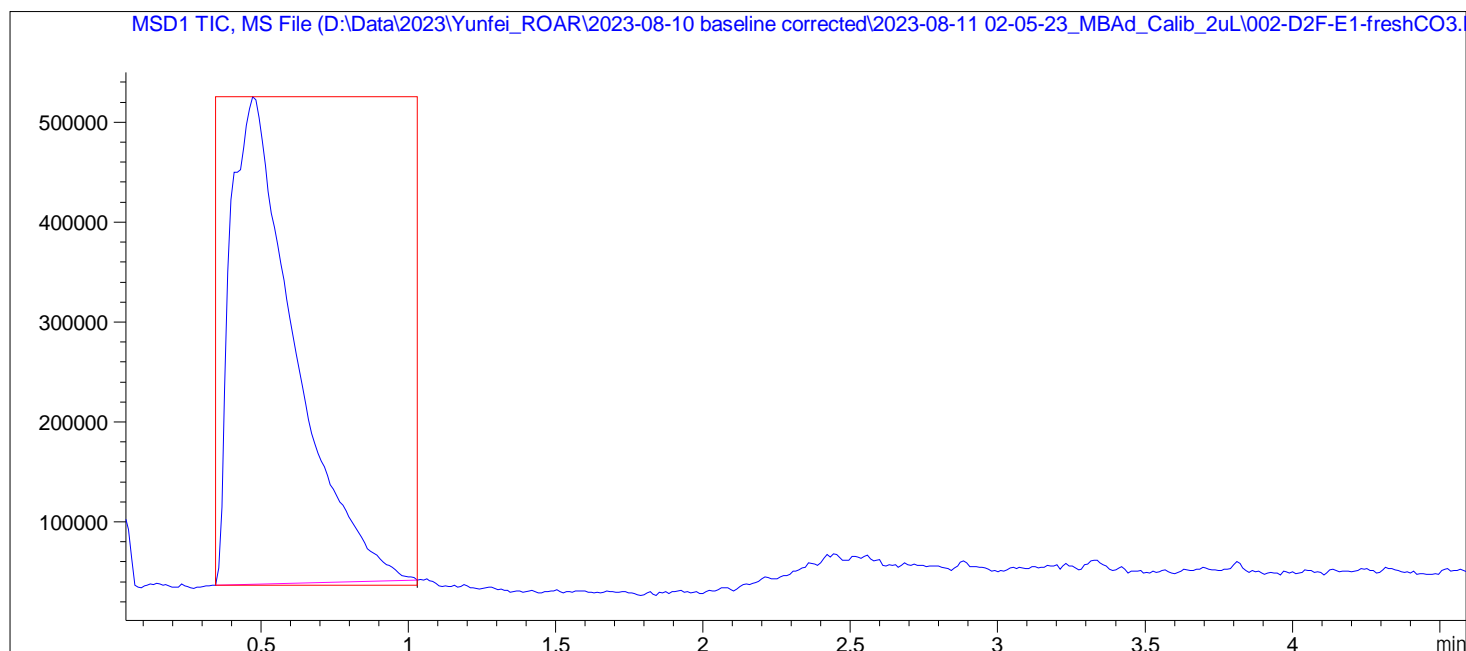
Threshold : 992.762 (Calculated with 214 of 224 spectra)

Reference : Peak start and end spectra (integrated) (2.145 / 3.659)

Spectra : 4 (Selection automatic, 5)

Noise Threshold: 0.222 (12 spectra, St.Dev 0.0886 + 3 \* 0.0444)

Sample Name: freshC03



Peak #1 at 0.475 min ( 0.346 to 1.031 min)

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

Component 1: Peak at Scan 37.2. Top ions are 122 141 179

Component 2: Peak at Scan 38.8. Top ions are 139 303

Component 3: Peak at Scan 41.2. Top ions are 129

Component 4: Peak at Scan 42.0. Top ions are 189

Component 5: Peak at Scan 42.7. Top ions are 101

Component 6: Peak at Scan 47.5. Top ions are 159 199

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