

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

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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
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  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: freshC03pH8_3

```
=====
Acq. Operator   : user                      Seq. Line :    6
Sample Operator : user
Acq. Instrument : SFC LCMS                  Location  :   D2F-F1
Injection Date  : 07/09/2023 15:59:21      Inj       :    1
                                           Inj Volume: 0.200 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 2.000 µl
Sequence File   : D:\Data\2023\Yunfei_R0AR\2023-09-07_newSTEMPO_0p9VProduct_re 2023-09-07 15-
                  17-08\2023-09-07_newSTEMPO_0p9VProduct_re.S
Method          : D:\Data\2023\Yunfei_R0AR\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
=====
```

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
Multi sampler 4	G4767A	D.07.24 [0001]	DEAFD00218
LC Pump 5	PumpVal veCl uster		
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       : 942
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	0.70	944.2 h
DAD 1, Visible Lamp	0.00	352.8 h

Solvent Description :

PMP1, Solvent A :

PMP2, Solvent A :

Sample Name: freshC03pH8_3

PMP2, Solvent A :
 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	6.7E-009	6.6E-009 Torr
CapCur	5	640 nA
ChamCur	8.0E-002	1.1E-001 µA
DryingGas	12	12 l/min
Neb Pres	35	35 psi g
Turbo1Spd	100	100 %
Turbo1Pwr	127	128 W
RF Drive	1	15 %
Qd TpDrv	17	17 %
Gas TpDrv	35	35 %
Neb PrDrv	50	50 %
Gas FI Drv	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          :  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          :  144
L2RFAmp         :  Variabl e
                  :  Mass           :  Val ue
                  :  -----
                  :  118.08         :  57
                  :  622.03         :  100
                  :  922.01         :  95
                  :  1521.97        :  120
                  :  -----

```

```

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

```

```

Ioni zati on pol ari ty :  Negati ve
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      :  Variabl e

```

```

                  :  Mass           :  Val ue
                  :  -----
                  :  112.99         :  -39
                  :  601.98         :  -64
                  :  1033.99        :  -84
                  :  1633.95        :  -39
                  :  -----

```

```

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

Mass : Value

112.99 : 72
601.98 : 110
1033.99 : 135
1633.95 : 150

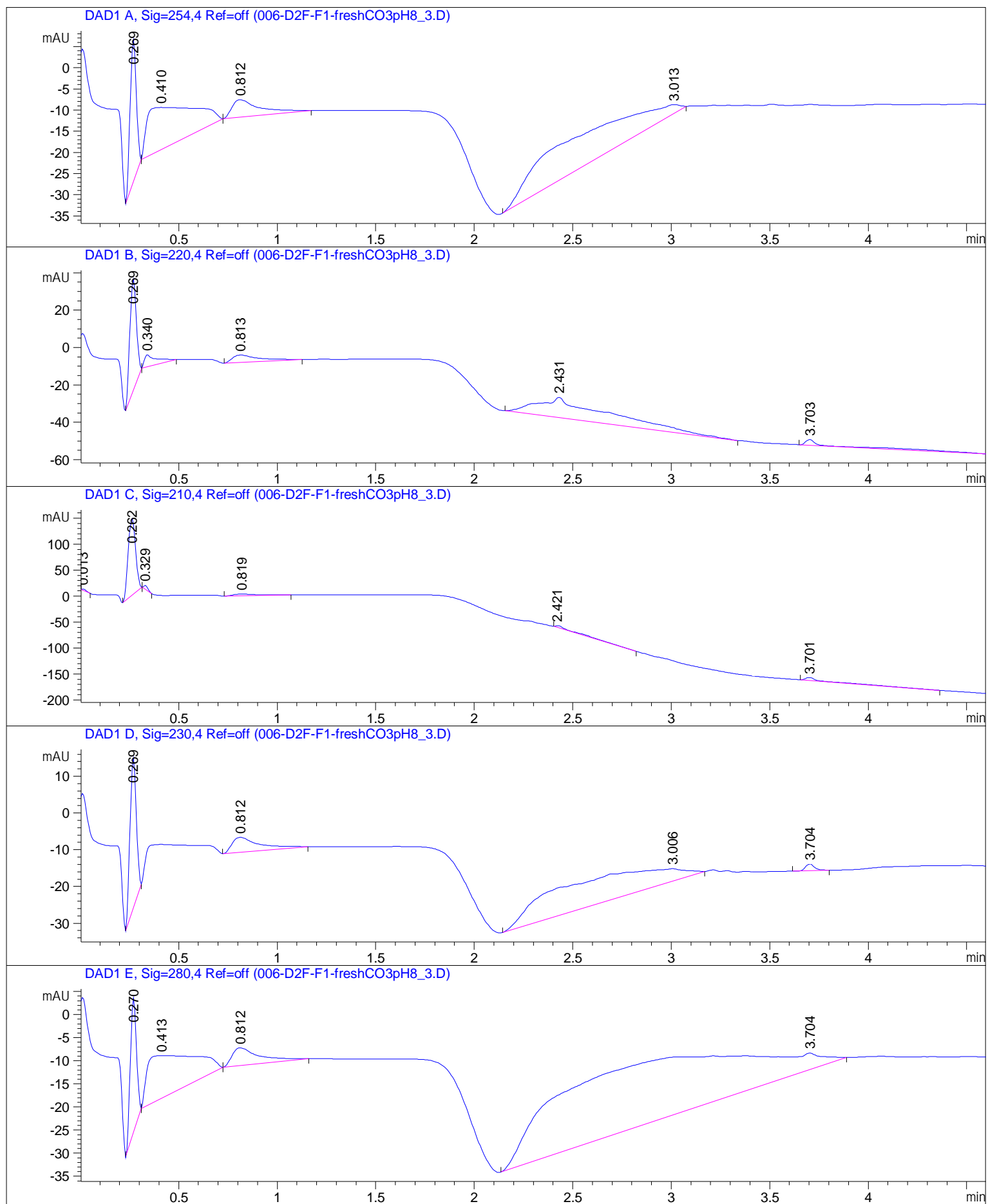
Mass Filter : Gaussi an
Time Filter : Gaussi an
Time Filter Width : 0.030

Run Logbook

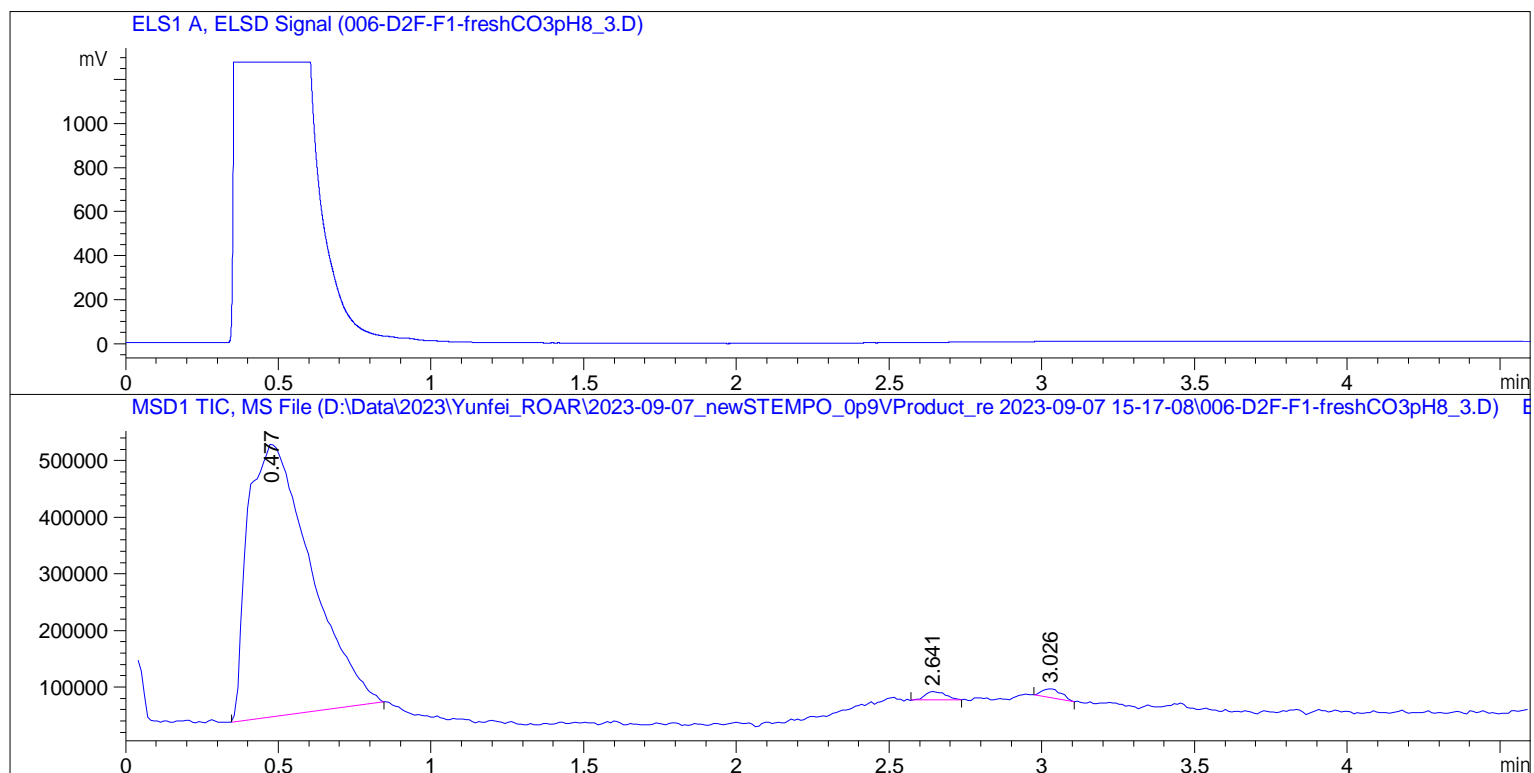
7 Sep 23 04:06 PM

Logbook File: D:\Data\20...EMP0_0p9VProduct_re 2023-09-07 15-17-08\006-D2F-F1-freshC03pH8_3.D\RUN.LOG

Module	# Event Message	Date Time
Method	Method started: line# 6 at location 'D2F-F1> ' inj# 1	07/09/2023 15:58:35
CP Macro	PreRun macro: 'LAMPALL ON'	07/09/2023 15:58:36
G4260B	G4260B: ELSD - Autozero	07/09/2023 15:58:37
G4260B	G4260B: ELSD - Already switched on	07/09/2023 15:58:37
Method	Instrument running sample from location D2F-> F1	07/09/2023 15:58:37
G7115A	G7115A: DEAC605436 - Detector: Prepare	07/09/2023 15:58:48
G7115A	G7115A: DEAC605436 - Detector: Idle	07/09/2023 15:59:04
G4767A	G4767A: DEAFD00218 - Draw command finished	07/09/2023 15:59:11
G4767A	G4767A: DEAFD00218 - Sampler wash is active	07/09/2023 15:59:12
G4767A	G4767A: DEAFD00218 - Sampler wash is idle	07/09/2023 15:59:19
G4767A	G4767A: DEAFD00218 - Sample preparation time: > 15 sec	07/09/2023 15:59:19
G4767A	G4767A: DEAFD00218 - Run	07/09/2023 15:59:21
PumpVal ve	G7111B: DEAEW03495 - Postrun	07/09/2023 16:03:57
G4767A	G4767A: DEAFD00218 - Postrun	07/09/2023 16:03:57
PumpVal ve	G1170A: DEBAD03715 - Postrun	07/09/2023 16:03:58
G7110B	G7110B: DEAEH00761 - Postrun	07/09/2023 16:03:58
G7116A	G7116A: DEAEH00761 - Postrun	07/09/2023 16:03:58
G4782A	G4782A: DEAGN00153 - Postrun	07/09/2023 16:03:59
Method	Saving Method COL1_5NH4FA_MECN_5T095_1MIN_10> 0-600MS_POS.M	07/09/2023 16:06:10
Method	Instrument run completed	07/09/2023 16:06:32
CP Macro	Analyzing rawdata 006-D2F-F1-freshC03pH8_3.D	07/09/2023 16:06:32
Method	Saving Method DA.M	07/09/2023 16:06:35



Sample Name: freshCO3pH8_3



=====
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	0.0356	73.69030	33.59963	12.8755
2	0.410	BB	0.2193	161.67467	9.96510	28.2484
3	0.812	BB	0.1399	40.38671	4.13657	7.0565
4	3.013	BB	1.6770	296.58014	2.08811	51.8196

Totals : 572.33182 49.78941

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	0.0370	137.70018	59.49975	26.9752
2	0.340	BB	0.0596	27.18277	6.38762	5.3250
3	0.813	BB	0.1329	35.45065	3.87040	6.9447
4	2.431	BB	0.3164	282.54642	10.82770	55.3502
5	3.703	BBA	0.1192	27.59000	3.00158	5.4048

Sample Name: freshC03pH8_3

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
----- ----- ----- ----- ----- ----- -----						
Totals :				510.47001	83.58706	

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
----- ----- ----- ----- ----- ----- -----						
1	0.013	BB	0.0291	5.17502	2.95984	1.0690
2	0.262	BB	0.0427	390.22940	148.12424	80.6107
3	0.329	BB	0.0261	10.69272	6.90884	2.2088
4	0.819	BB	0.1252	27.60553	3.24598	5.7025
5	2.421	BB	0.0998	20.94898	2.78385	4.3275
6	3.701	BBA	0.0732	29.43977	5.60781	6.0814
----- ----- ----- ----- ----- ----- -----						
Totals :				484.09142	169.63055	

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	0.0361	91.57137	40.90756	20.8498
2	0.812	BB	0.1364	38.44740	4.06131	8.7540
3	3.006	BB	1.0592	303.40964	3.38020	69.0830
4	3.704	BB	0.0484	5.76736	1.84939	1.3132
----- ----- ----- ----- ----- ----- -----						
Totals :				439.19577	50.19845	

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	0.0354	63.37006	29.15797	5.3549
2	0.413	BB	0.2217	150.18462	9.23424	12.6910
3	0.812	BB	0.1382	36.87744	3.83305	3.1162
4	3.704	BB	3.0280	932.96008	3.60897	78.8378
----- ----- ----- ----- ----- ----- -----						
Totals :				1183.39219	45.83423	

Signal 6: ELS1 A, ELSD Signal

Signal 7: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.477	BB	0.1853	6.87681e6	4.82418e5	98.0798
2	2.641	BB	0.0594	6.79466e4	1.49313e4	0.9691
3	3.026	BB	0.0701	6.66848e4	1.52215e4	0.9511

Totals : 7.01144e6 5.12571e5

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.

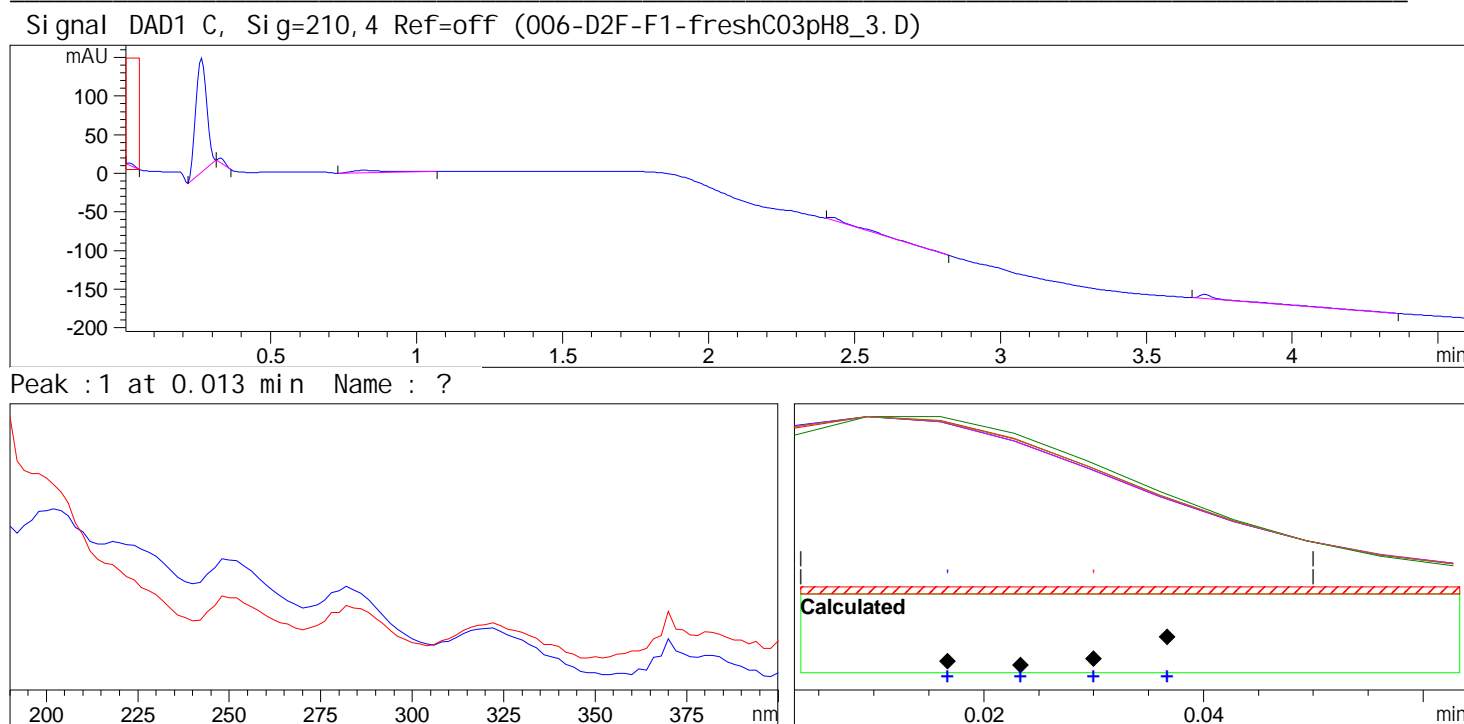
Signal 5: DAD1 E, Sig=280, 4 Ref=off
Empty table.

Signal 6: ELS1 A, ELSD Signal
Empty table.

Signal 7: MSD1 TIC, MS File
Empty table.

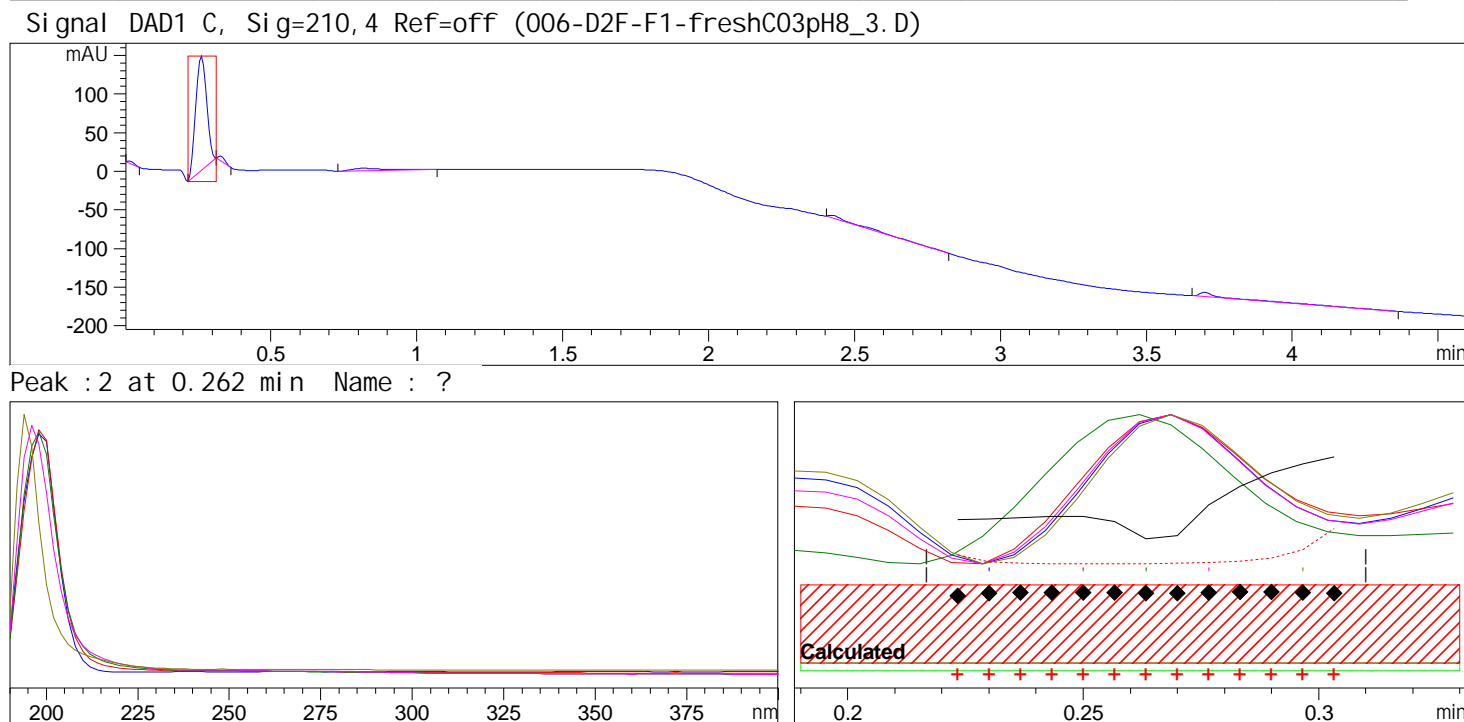
Final Summed Peaks Report

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



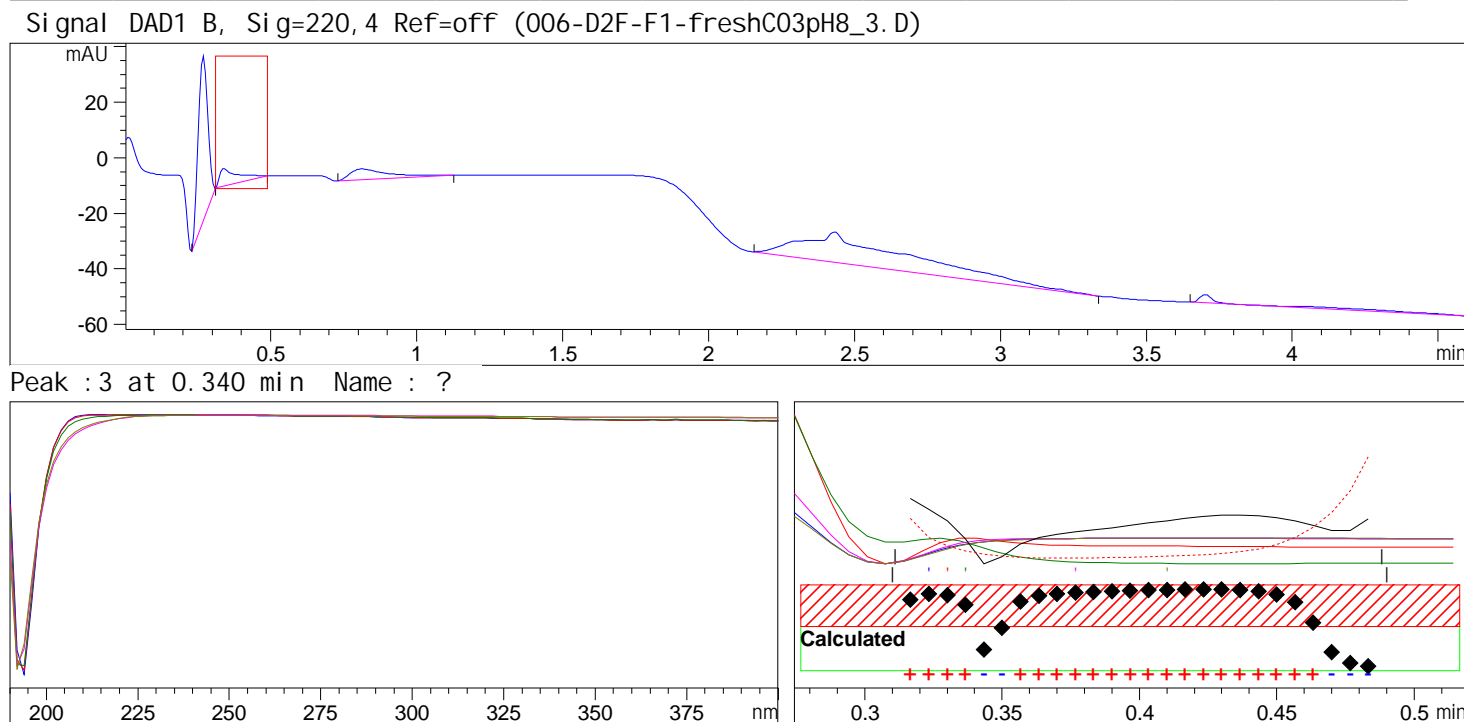
-> The purity factor is within the calculated threshold limit. <-

Purity factor : 863.753 (4 of 4 spectra are within the calculated threshold limit.)
Threshold : 0.000 (Calculated with 4 of 4 spectra)
Reference : Peak start and end spectra (integrated) (0.003 / 0.050)
Spectra : 2 (Selection automatic, 5)
Noise Threshold: 1.084 (12 spectra, St.Dev 0.4826 + 3 * 0.2004)
Warning : Calculated Noise Level > 1.00 (see information in threshold calculation)



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

Purity factor : 938.895 (13 of 13 spectra exceed the calculated threshold limit.)
Threshold : 999.549 (Calculated with 13 of 13 spectra)
Reference : Peak start and end spectra (integrated) (0.217 / 0.310)
Spectra : 5 (Selection automatic, 5)
Noise Threshold: 1.084 (12 spectra, St.Dev 0.4826 + 3 * 0.2004)
Warning : Spectral absorbances > 1000 mAU (see help for more information)



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

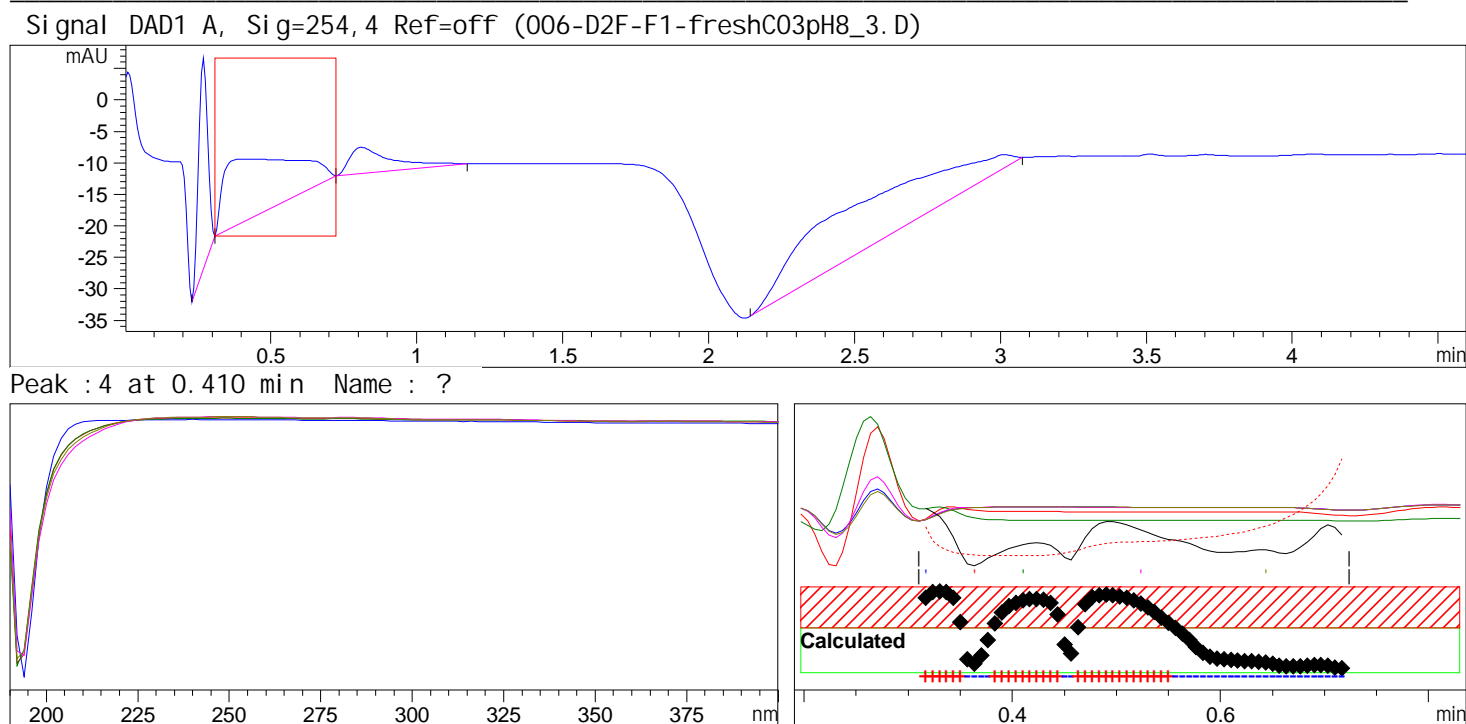
Purity factor : 991.738 (21 of 26 spectra exceed the calculated threshold limit.)

Threshold : 998.046 (Calculated with 21 of 26 spectra)

Reference : Peak start and end spectra (integrated) (0.310 / 0.490)

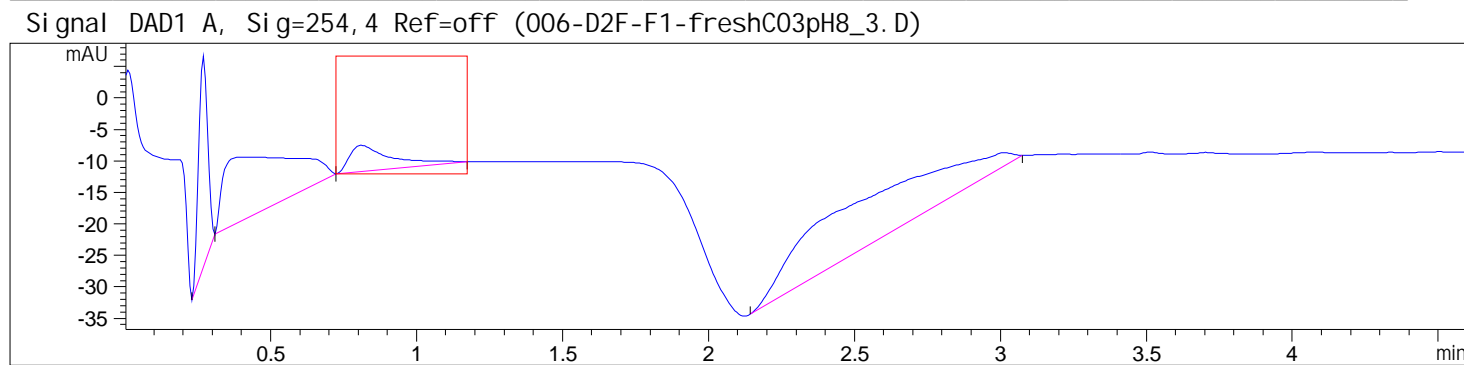
Spectra : 5 (Selection automatic, 5)

Noise Threshold: 1.084 (12 spectra, St.Dev 0.4826 + 3 * 0.2004)

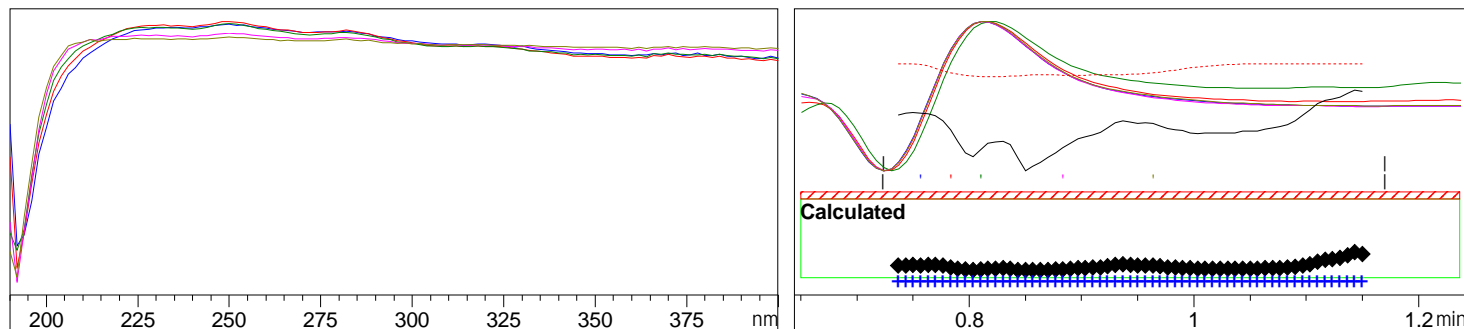


-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 993.426 (30 of 61 spectra exceed the calculated threshold limit.)
Threshold : 998.193 (Calculated with 30 of 61 spectra)
Reference : Peak start and end spectra (integrated) (0.310 / 0.723)
Spectra : 5 (Selection automatic, 5)
Noise Threshold: 1.084 (12 spectra, St.Dev 0.4826 + 3 * 0.2004)



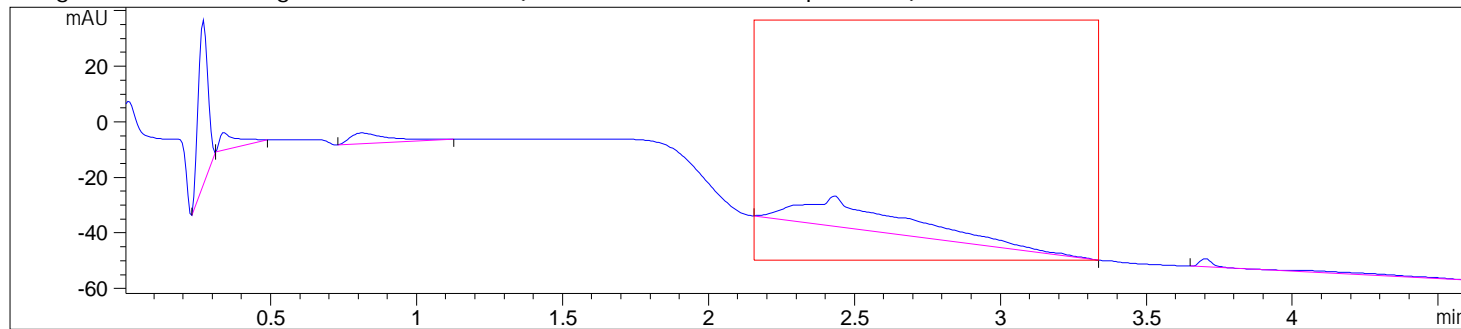
Peak : 6 at 0.812 min Name : ?



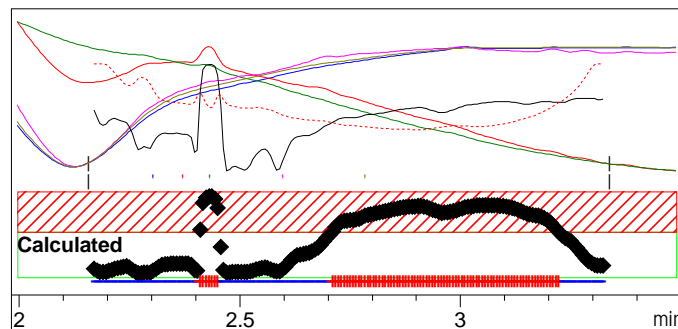
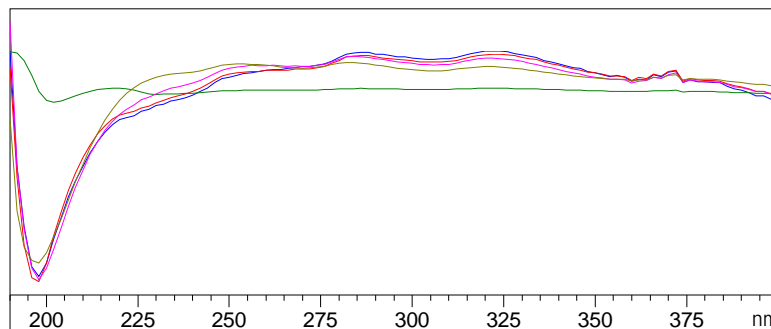
-> The purity factor is within the calculated threshold limit. <-

Purity factor : 949.746 (63 of 63 spectra are within the calculated threshold limit.)
Threshold : 230.260 (Calculated with 63 of 63 spectra)
Reference : Peak start and end spectra (integrated) (0.723 / 1.170)
Spectra : 5 (Selection automatic, 5)
Noise Threshold: 1.084 (12 spectra, St.Dev 0.4826 + 3 * 0.2004)
Warning : Calculated Noise Level > 1.00 (see information in threshold calculation)

Signal DAD1 B, Sig=220, 4 Ref=off (006-D2F-F1-freshC03pH8_3.D)



Peak : 7 at 2.431 min Name : ?



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

Purity factor : 788.596 (85 of 174 spectra exceed the calculated threshold limit.)

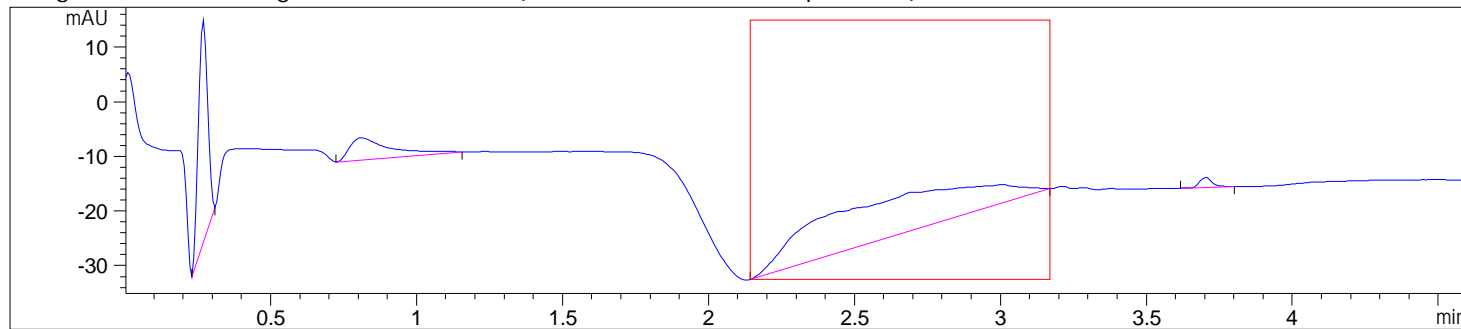
Threshold : 905.308 (Calculated with 85 of 174 spectra)

Reference : Peak start and end spectra (integrated) (2.157 / 3.337)

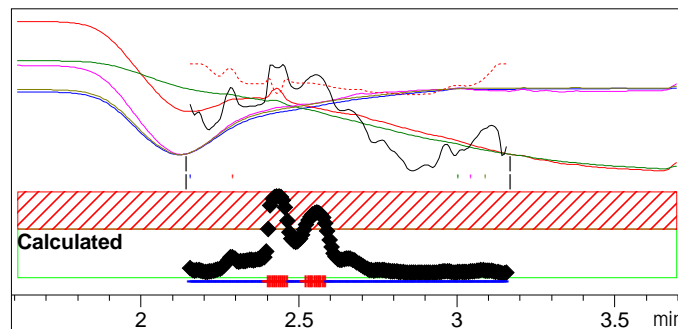
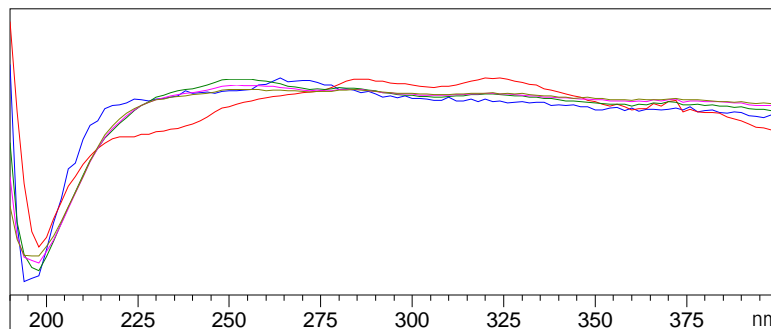
Spectra : 5 (Selection automatic, 5)

Noise Threshold: 1.084 (12 spectra, St.Dev 0.4826 + 3 * 0.2004)

Signal DAD1 D, Sig=230, 4 Ref=off (006-D2F-F1-freshC03pH8_3.D)



Peak : 9 at 3.006 min Name : ?



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

Purity factor : 342.605 (20 of 151 spectra exceed the calculated threshold limit.)

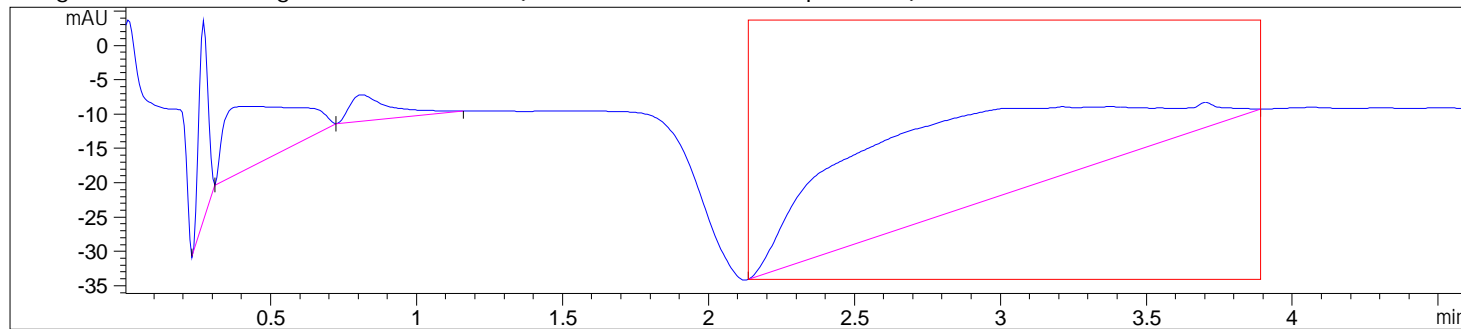
Threshold : 657.351 (Calculated with 20 of 151 spectra)

Reference : Peak start and end spectra (integrated) (2.143 / 3.170)

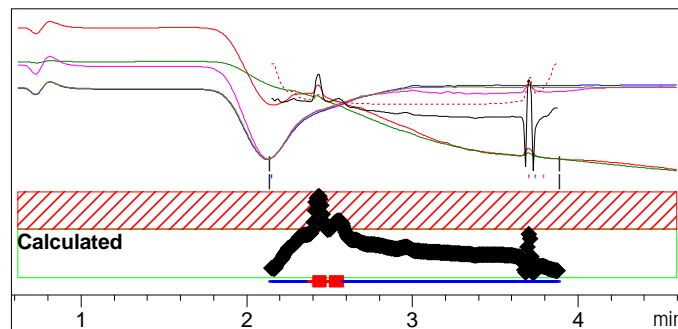
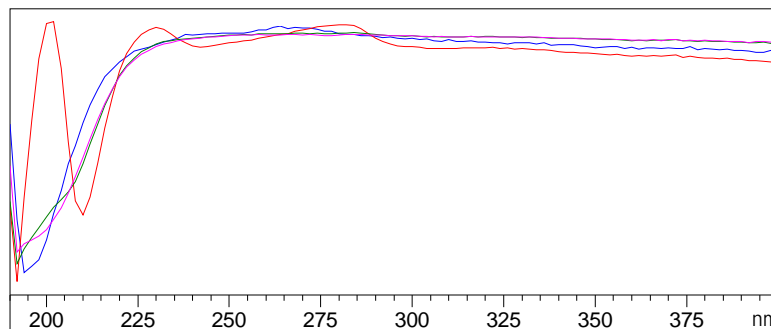
Spectra : 5 (Selection automatic, 5)

Noise Threshold: 1.084 (12 spectra, St.Dev 0.4826 + 3 * 0.2004)

Signal DAD1 E, Sig=280, 4 Ref=off (006-D2F-F1-freshC03pH8_3.D)



Peak : 10 at 3.704 min Name : ?



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

Purity factor : 817.183 (25 of 260 spectra exceed the calculated threshold limit.)

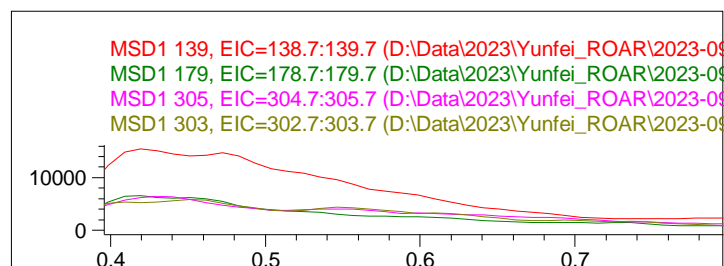
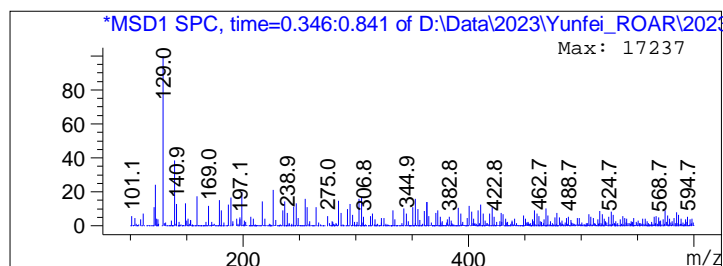
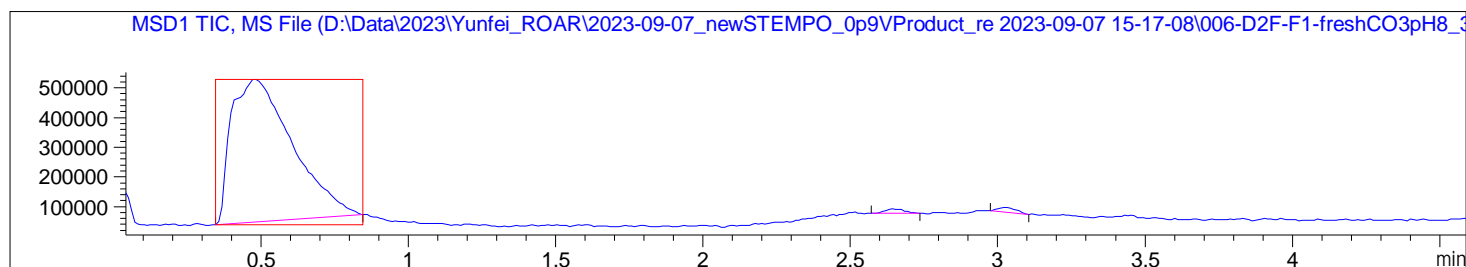
Threshold : 897.055 (Calculated with 25 of 260 spectra)

Reference : Peak start and end spectra (integrated) (2.137 / 3.890)

Spectra : 4 (Selection automatic, 5)

Noise Threshold: 1.084 (12 spectra, St.Dev 0.4826 + 3 * 0.2004)

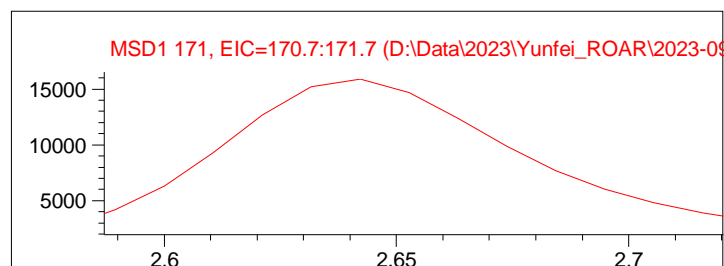
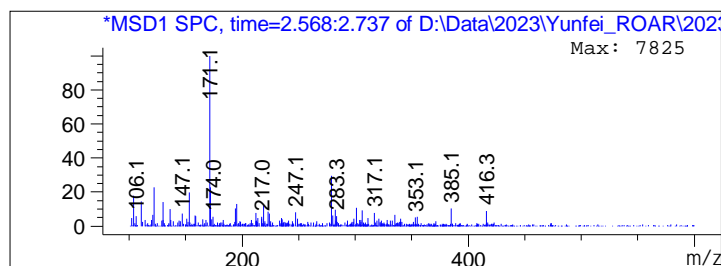
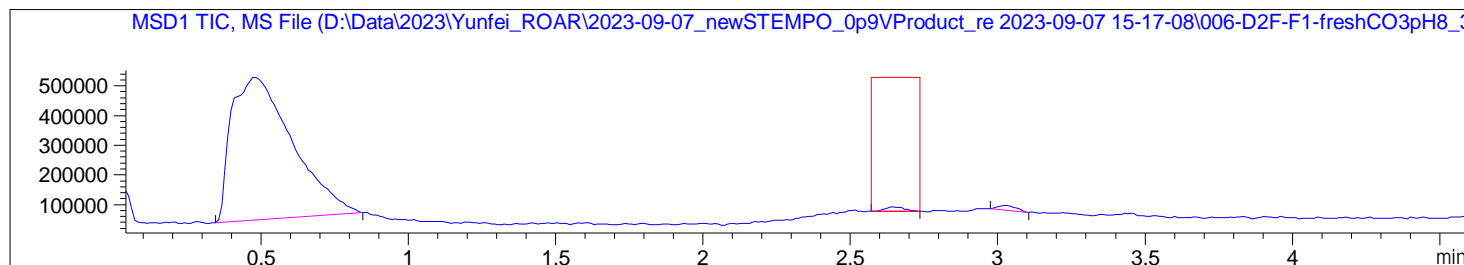
Sample Name: freshCO3pH8_3



Peak #1 at 0.477 min (0.346 to 0.845 min)

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

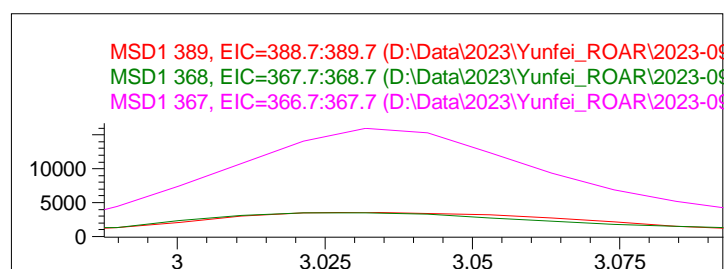
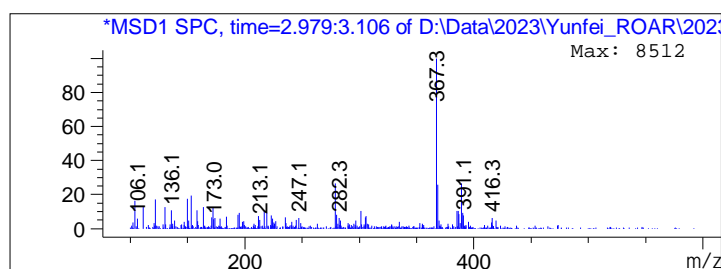
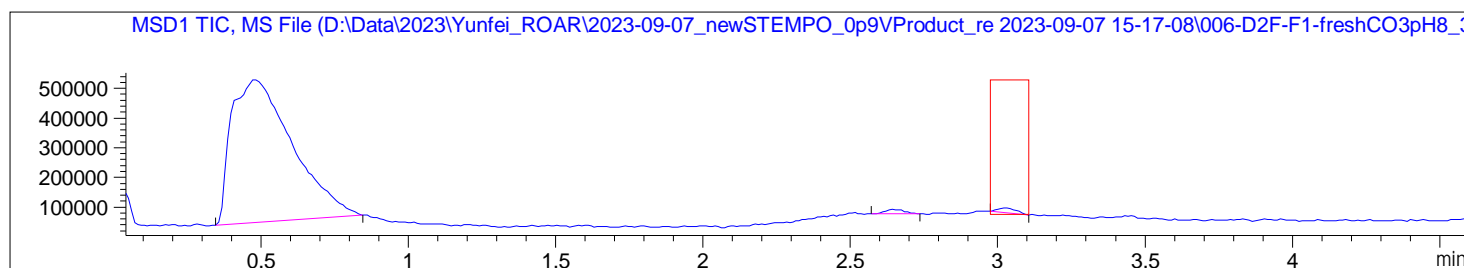
Component 1: Peak at Scan 36.9. Top ions are 139 179
Component 2: Peak at Scan 38.2. Top ions are 305
Component 3: Peak at Scan 40.2. Top ions are 303
Component 4: Peak at Scan 42.0. Top ions are 189
Component 5: Peak at Scan 42.8. Top ions are 129 122
Component 6: Peak at Scan 45.6. Top ions are 199 255
Component 7: Peak at Scan 49.2. Top ions are 227



Peak #2 at 2.641 min (2.570 to 2.737 min)

-> The analysis found only one component, indicating a pure peak. <-

Component 1: Peak at Scan 247.9. Top ions are 171



Peak #3 at 3.026 min (2.974 to 3.106 min)

-> The analysis found 2 components, indicating an impure peak. <-

Component 1: Peak at Scan 284.5. Top ions are 389 368 390

Component 2: Peak at Scan 285.2. Top ions are 367

*** End of Report ***