

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

```

```

                                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: noCata\_0p4V

```

=====
Acq. Operator   : user                      Seq. Line :    8
Sample Operator : user
Acq. Instrument : SFC LCMS                  Location  :   D2F-F6
Injection Date  : 07/09/2023 16:15:43      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       : 944
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	32.5 °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	0.97	944.5 h
DAD 1, Visible Lamp	0.00	352.8 h

```

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

```

Sample Name: noCata\_Op4V

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	6.4E-009	6.4E-009 Torr
CapCur	646	639 nA
ChamCur	9.5E-001	1.3E-001 µA
DryingGas	12	12 l/min
Neb Pres	35	35 psig
Turbo1Spd	100	100 %
Turbo1Pwr	127	127 W
RF Drive	2	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: noCata\_Op4V

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

Sample Name: noCata\_Op4V

1000.00 : 4.0  
2000.00 : 6.0

```

-----
L2RFEn      : 1
L2RFPh      : 162
L2RFAmp     : Variable
Mass        : Value
-----
112.99      : 72
601.98      : 110
1033.99     : 135
1633.95     : 150
-----
Mass Filter  : Gaussian
Time Filter  : Gaussian
Time Filter Width : 0.030

```

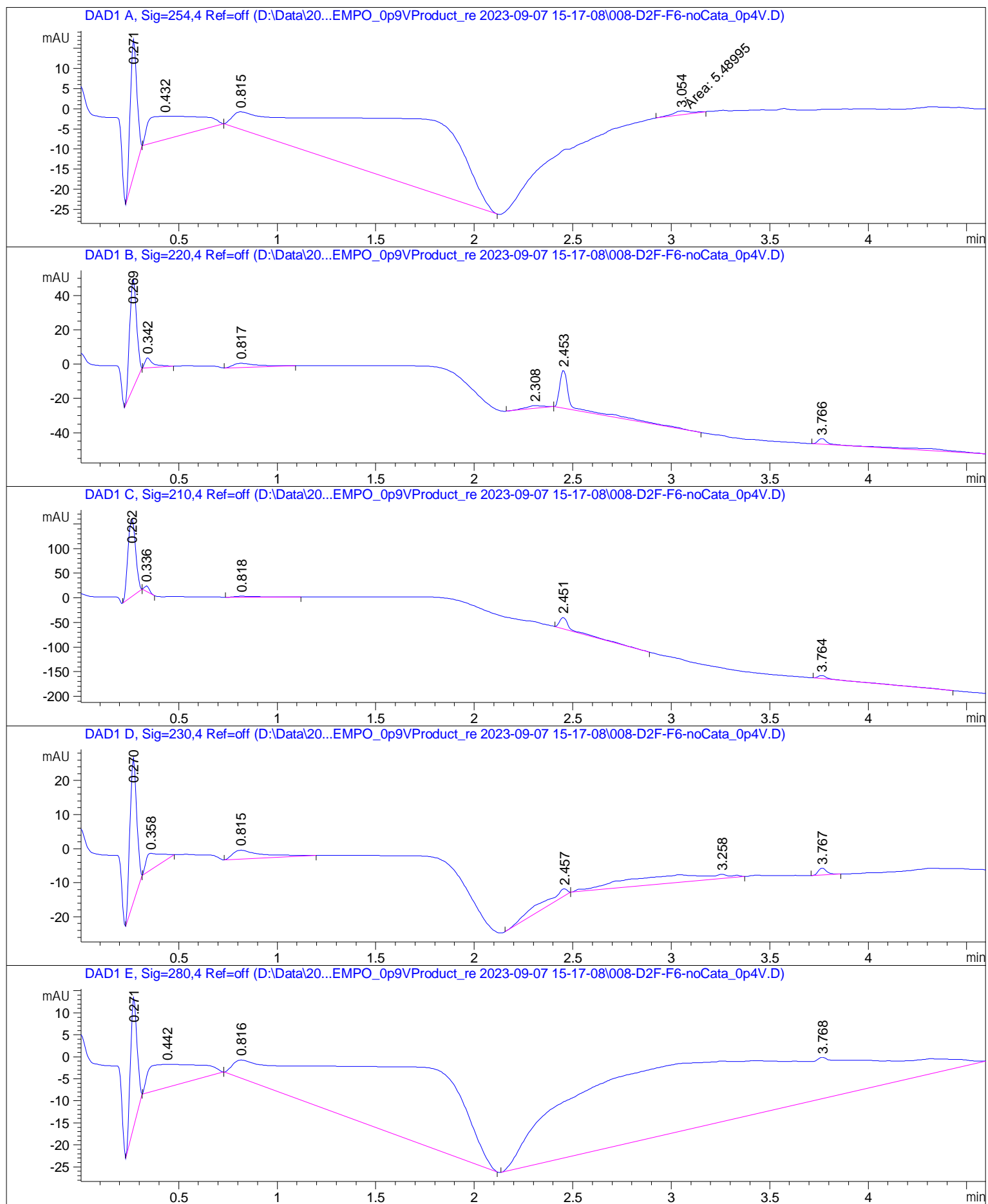
=====  
=====  
Run Logbook  
=====

18 Sep 23 11:23 AM

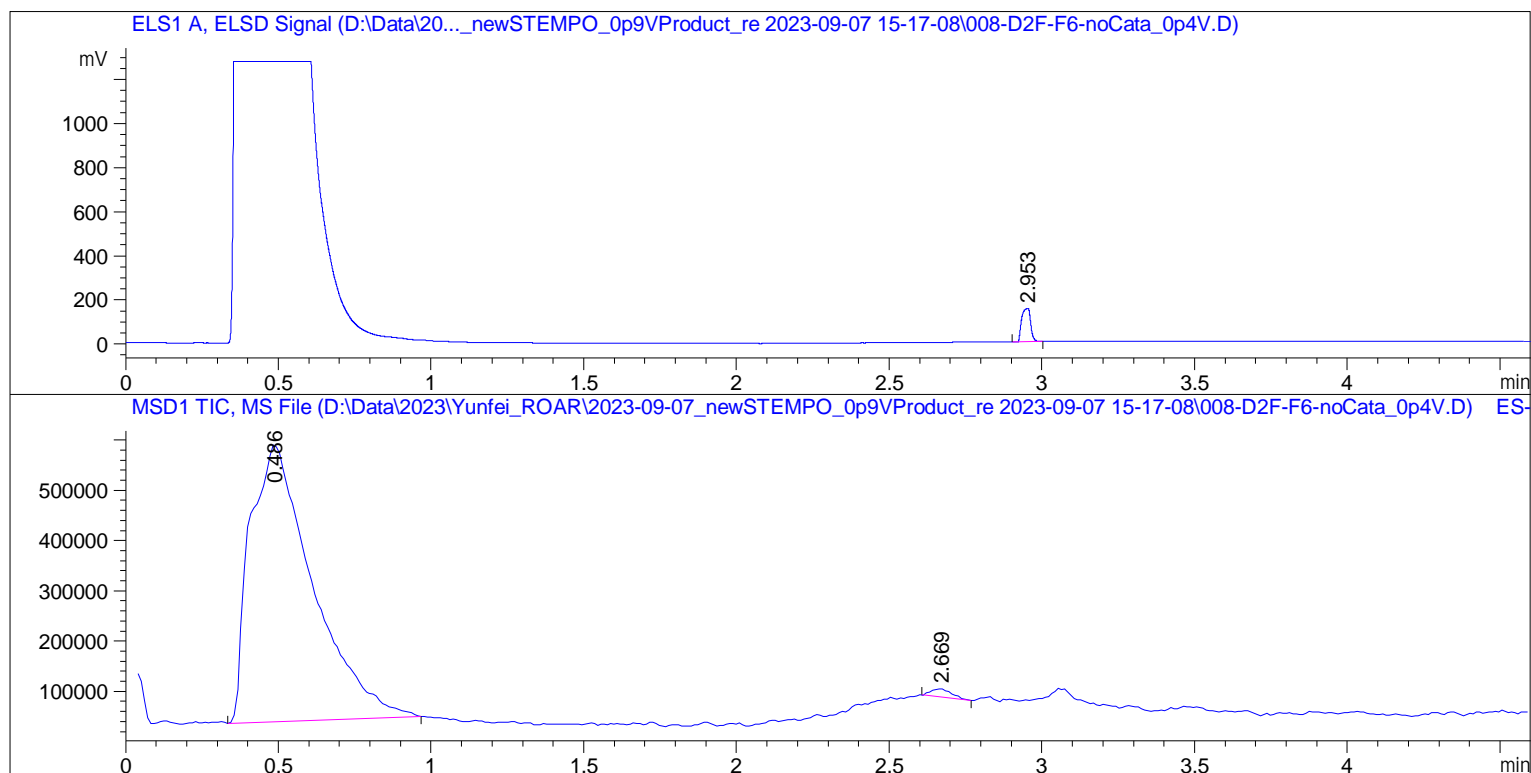
Logbook File: D:\Data\20...STEMPO\_Op9VProduct\_re 2023-09-07 15-17-08\008-D2F-F6-noCata\_Op4V.D\RUN.LOG

Module	# Event Message	Date Time
Method	Method started: line# 8 at location 'D2F-F6>' ' inj# 1	07/09/2023 16:14:54
CP Macro	PreRun macro: 'LAMPALL ON'	07/09/2023 16:14:55
G4260B	G4260B: ELSD - Autozero	07/09/2023 16:14:55
G4260B	G4260B: ELSD - Already switched on	07/09/2023 16:14:56
Method	Instrument running sample from location D2F->F6	07/09/2023 16:14:56
G7115A	G7115A: DEAC605436 - Detector: Prepare	07/09/2023 16:15:07
G7115A	G7115A: DEAC605436 - Detector: Idle	07/09/2023 16:15:23
G4767A	G4767A: DEAFD00218 - Draw command finished	07/09/2023 16:15:30
G4767A	G4767A: DEAFD00218 - Sampler wash is active	07/09/2023 16:15:32
G4767A	G4767A: DEAFD00218 - Sampler wash is idle	07/09/2023 16:15:38
G4767A	G4767A: DEAFD00218 - Sample preparation time: >15 sec	07/09/2023 16:15:42
PumpVal ve	G7111B: DEAEW03495 - Run	07/09/2023 16:15:43
PumpVal ve	G7111B: DEAEW03495 - Postrun	07/09/2023 16:20:16
G4767A	G4767A: DEAFD00218 - Postrun	07/09/2023 16:20:16
PumpVal ve	G1170A: DEBAD03715 - Postrun	07/09/2023 16:20:17
G7110B	G7110B: DEAEH00761 - Postrun	07/09/2023 16:20:17
G7116A	G7116A: DEAEH00761 - Postrun	07/09/2023 16:20:18
G4782A	G4782A: DEAGN00153 - Postrun	07/09/2023 16:20:18
Method	Saving Method COL1_5NH4FA_MECN_5TO95_1MIN_10>0-600MS_POS.M	07/09/2023 16:22:24
Method	Instrument run completed	07/09/2023 16:22:25
CP Macro	Analyzing rawdata 008-D2F-F6-noCata_Op4V.D	07/09/2023 16:22:25
Method	Saving Method DA.M	07/09/2023 16:22:27
Method	Method completed	07/09/2023 16:22:34

=====



Sample Name: noCata\_Op4V



=====  
 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	0.0373	79.57262	33.95910	7.7316
2	0.432	BB	0.2360	98.06761	5.72192	9.5287
3	0.815	BB	2.3022	846.05048	4.33260	82.2062
4	3.054	MM	0.0993	5.48995	9.21269e-1	0.5334

Totals : 1029.18066 44.93488

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	0.0404	155.07262	63.60394	47.2926
2	0.342	BB	0.0410	16.24057	5.74410	4.9529
3	0.817	BB	0.1271	20.56193	2.37320	6.2708
4	2.308	BB	0.0865	10.56955	1.70189	3.2234
5	2.453	BB	0.0593	89.66640	22.10009	27.3456

Sample Name: noCata\_Op4V

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
6	3.766	BBA	0.1360	35.78941	3.36615	10.9147

Totals : 327.90048 98.88937

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	0.0437	432.04080	159.07706	73.3233
2	0.336	BB	0.0288	19.81764	11.09176	3.3633
3	0.818	BB	0.1271	17.50539	1.98117	2.9709
4	2.451	BB	0.0539	82.34377	22.90545	13.9749
5	3.764	BBA	0.0845	37.51983	6.20731	6.3676

Totals : 589.22744 201.26274

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	0.0378	101.06351	42.38055	38.0397
2	0.358	BB	0.0732	25.70286	4.90363	9.6744
3	0.815	BB	0.1422	26.21678	2.58687	9.8678
4	2.457	BB	0.1683	29.01513	2.16553	10.9211
5	3.258	BB	0.7596	77.80743	1.21420	29.2862
6	3.767	BB	0.0466	5.87361	1.97826	2.2108

Totals : 265.67931 55.22904

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	0.0372	68.74922	29.49118	2.8272
2	0.442	BB	0.2435	91.00340	5.21847	3.7423
3	0.816	BB	2.4085	849.22217	4.15500	34.9226
4	3.768	BBA	1.7785	1422.75281	9.39617	58.5079

Totals : 2431.72759 48.26082



Signal 6: ELS1 A, ELSD Signal

Peak #	RetTime [min]	Type	Width [min]	Area [mV*s]	Height [mV]	Area %
1	2.953	BB	0.0336	303.88266	150.49565	100.0000

Totals : 303.88266 150.49565

Signal 7: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.486	BB	0.1790	7.88107e6	5.52841e5	99.0706
2	2.669	BB	0.0661	7.39336e4	1.61294e4	0.9294

Totals : 7.95501e6 5.68970e5

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.

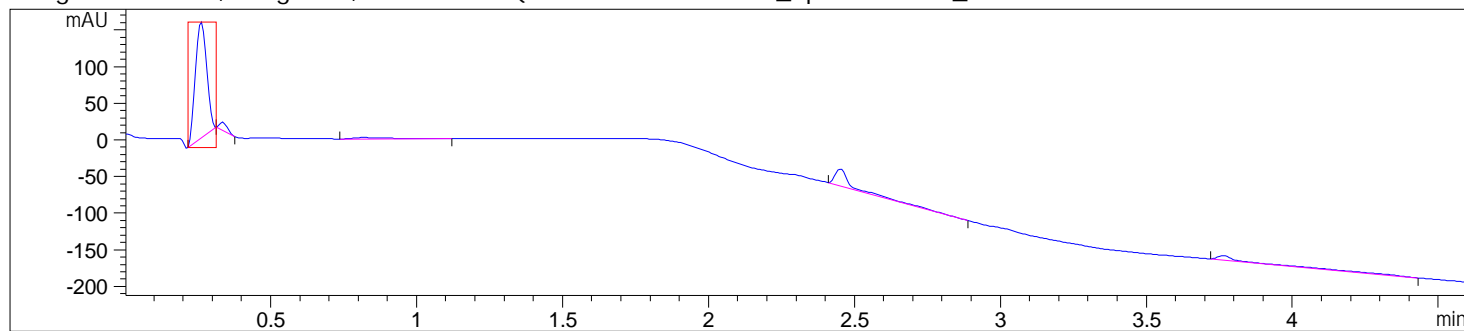
Final Summed Peaks Report

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

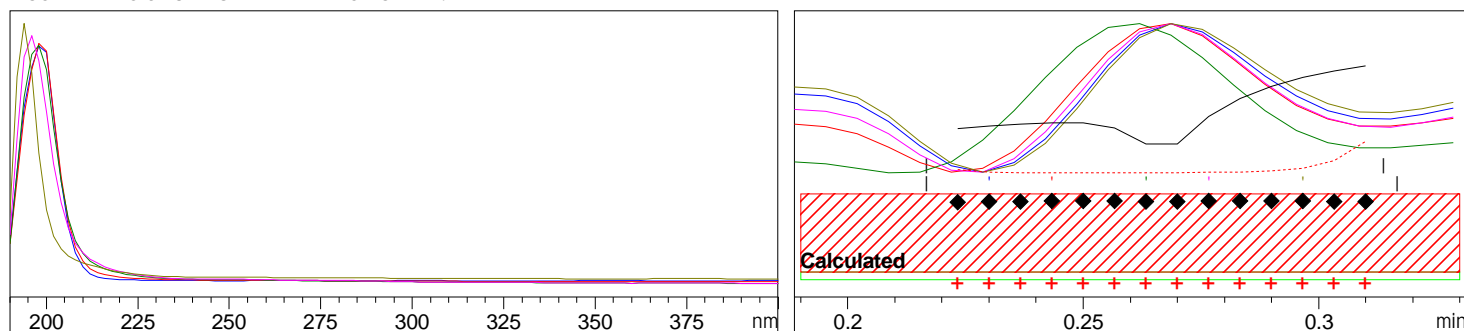
Signal 2: DAD1 B, Sig=220, 4 Ref=off  
Signal 3: DAD1 C, Sig=210, 4 Ref=off  
Signal 4: DAD1 D, Sig=230, 4 Ref=off  
Signal 5: DAD1 E, Sig=280, 4 Ref=off  
Signal 6: ELS1 A, ELSD Signal  
Signal 7: MSD1 TIC, MS File

Sample Name: noCata\_Op4V

Signal DAD1 C, Sig=210, 4 Ref=off (D:\Data\20...EMP0\_Op9VProduct\_re 2023-09-07 15-17-08\008-D2F-F6-noCat



Peak : 1 at 0.262 min Name : ?



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

Purity factor : 893.892 (14 of 14 spectra exceed the calculated threshold limit.)

Threshold : 999.667 (Calculated with 14 of 14 spectra)

Reference : Peak start and end spectra (integrated) (0.217 / 0.317)

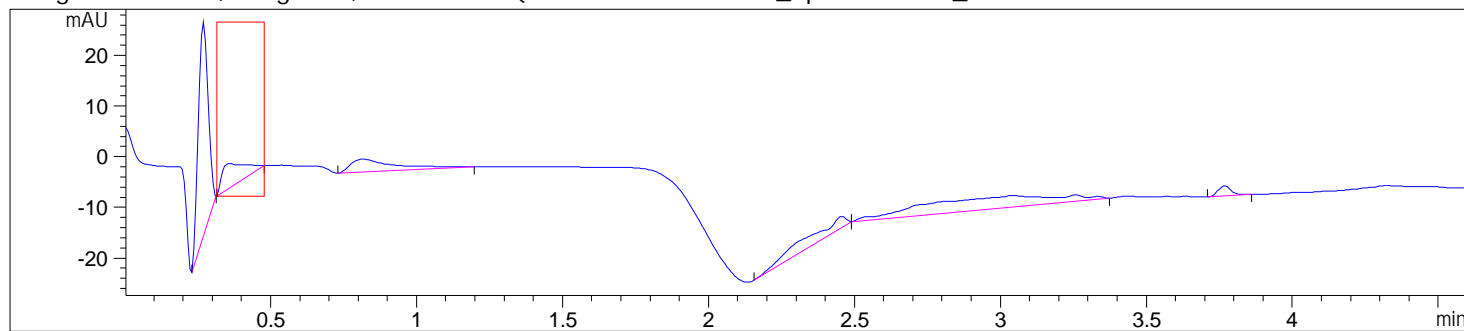
Spectra : 5 (Selection automatic, 5)

Noise Threshold : 0.666 (12 spectra, St.Dev 0.3207 + 3 \* 0.1152)

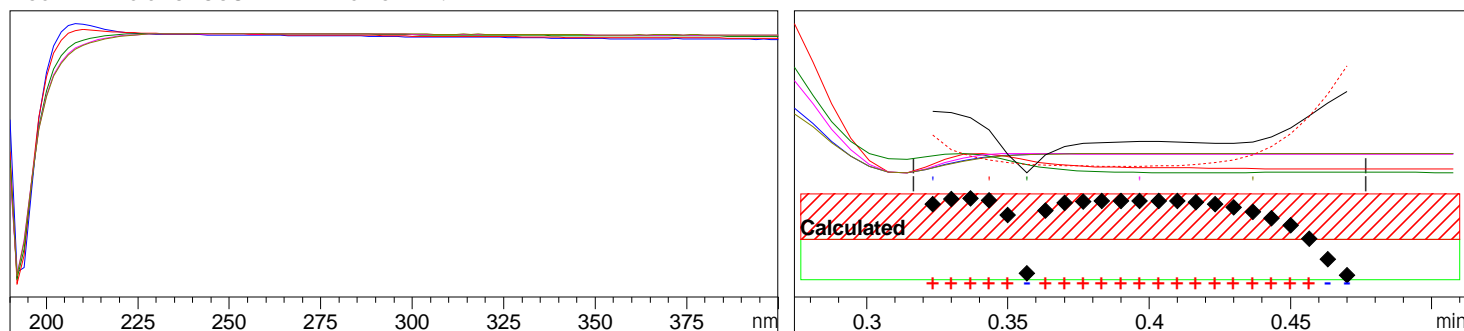
Warning : Spectral absorbances &gt; 1000 mAU (see help for more information)

Sample Name: noCata\_Op4V

Signal DAD1 D, Sig=230, 4 Ref=off (D:\Data\20...EMP0\_Op9VProduct\_re 2023-09-07 15-17-08\008-D2F-F6-noCat



Peak : 2 at 0.358 min Name : ?



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

Purity factor : 990.414 (20 of 23 spectra exceed the calculated threshold limit.)

Threshold : 997.177 (Calculated with 20 of 23 spectra)

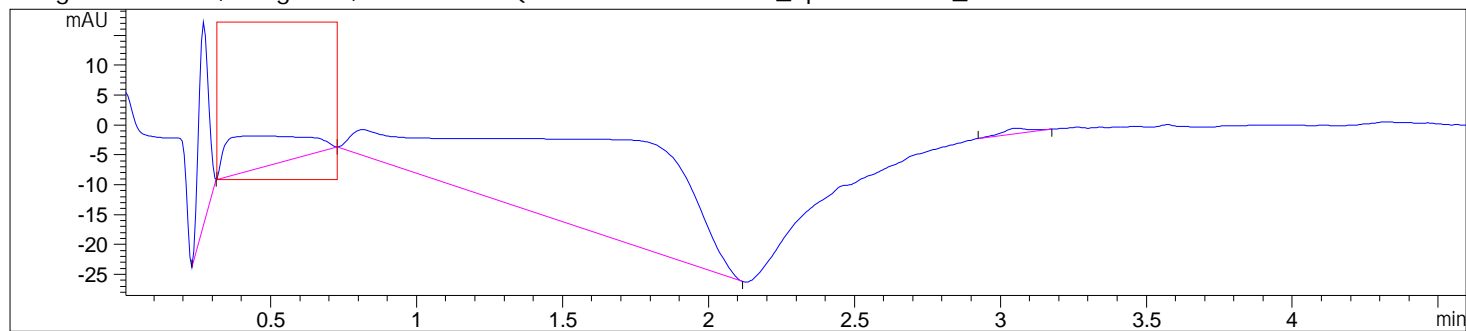
Reference : Peak start and end spectra (integrated) (0.317 / 0.477)

Spectra : 5 (Selection automatic, 5)

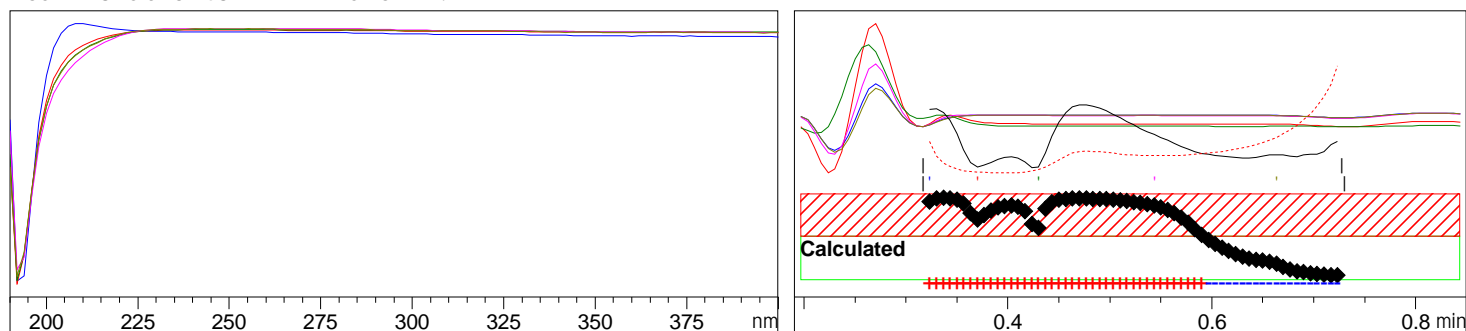
Noise Threshold: 0.666 (12 spectra, St.Dev 0.3207 + 3 \* 0.1152)

Sample Name: noCata\_Op4V

Signal DAD1 A, Sig=254, 4 Ref=off (D:\Data\20...EMP0\_Op9VProduct\_re 2023-09-07 15-17-08\008-D2F-F6-noCat



Peak : 3 at 0.432 min Name : ?



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

Purity factor : 979.945 (41 of 61 spectra exceed the calculated threshold limit.)

Threshold : 998.134 (Calculated with 41 of 61 spectra)

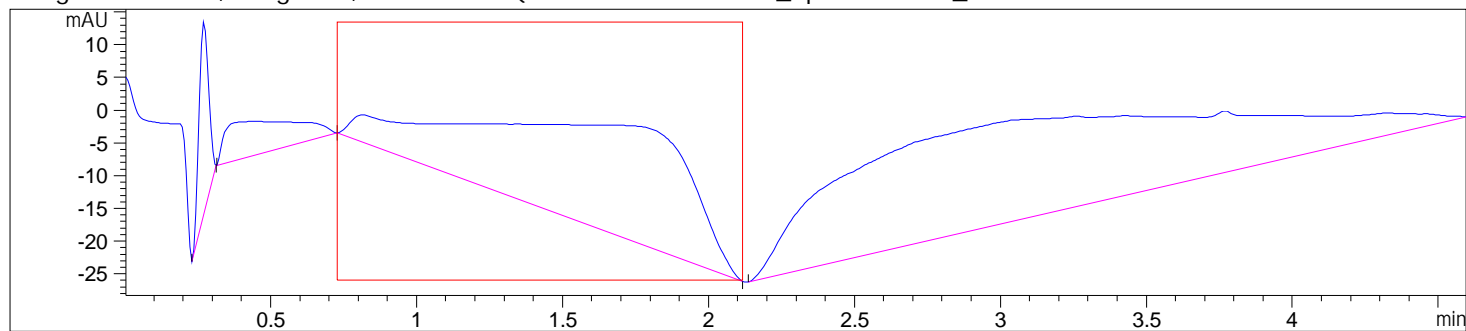
Reference : Peak start and end spectra (integrated) (0.317 / 0.730)

Spectra : 5 (Selection automatic, 5)

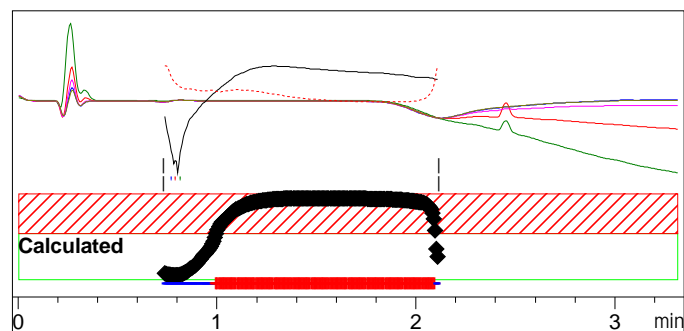
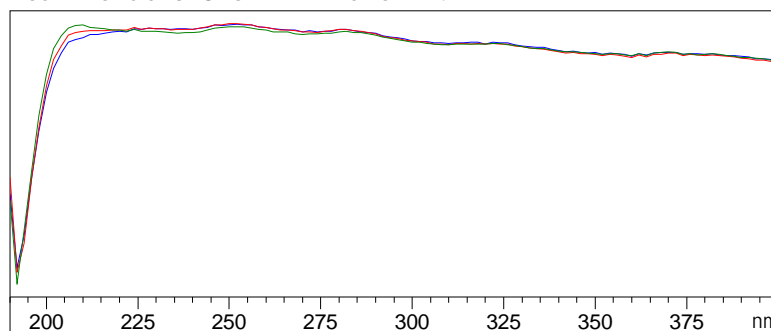
Noise Threshold: 0.666 (12 spectra, St.Dev 0.3207 + 3 \* 0.1152)

Sample Name: noCata\_0p4V

Signal DAD1 E, Sig=280, 4 Ref=off (D:\Data\20...EMP0\_0p9VProduct\_re 2023-09-07 15-17-08\008-D2F-F6-noCat



Peak : 5 at 0.816 min Name : ?



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

Purity factor : 290.105 (166 of 207 spectra exceed the calculated threshold limit.)

Threshold : 845.901 (Calculated with 166 of 207 spectra)

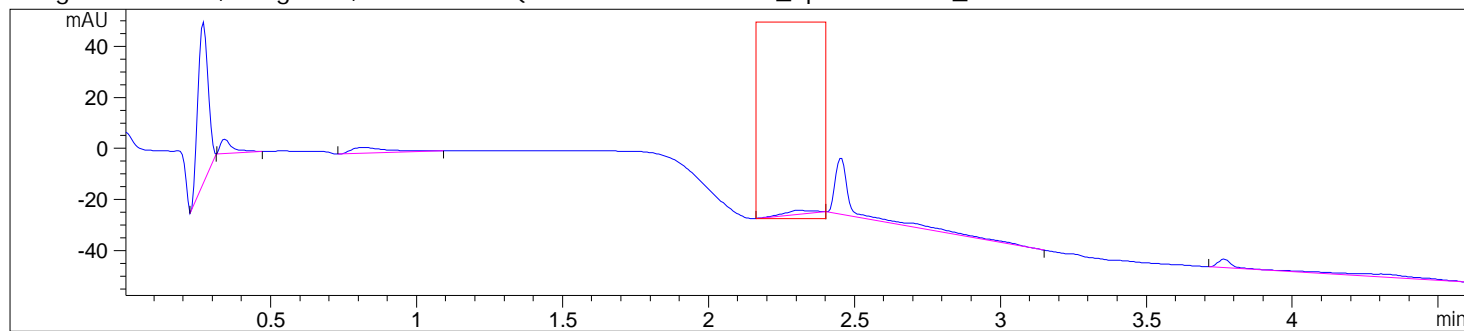
Reference : Peak start and end spectra (integrated) (0.730 / 2.117)

Spectra : 3 (Selection automatic, 5)

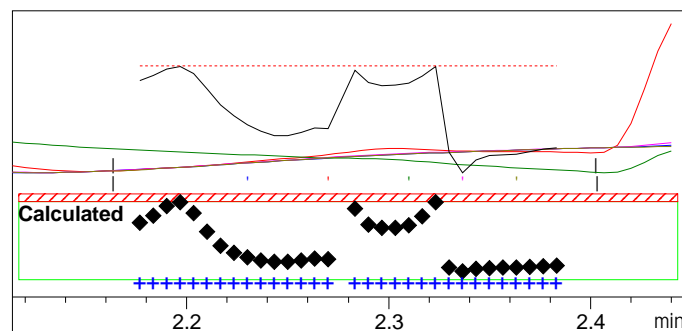
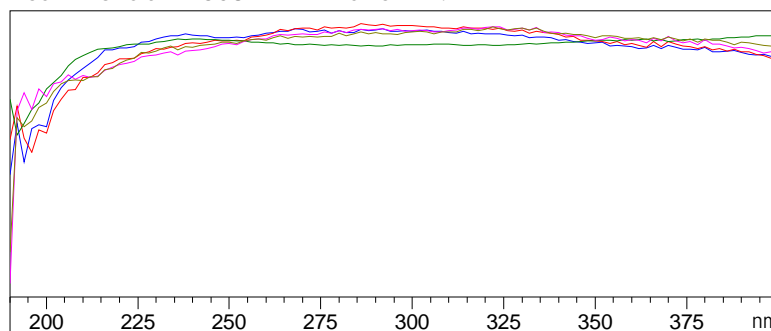
Noise Threshold: 0.666 (12 spectra, St.Dev 0.3207 + 3 \* 0.1152)

Sample Name: noCata\_0p4V

Signal DAD1 B, Sig=220, 4 Ref=off (D:\Data\20...EMP0\_0p9VProduct\_re 2023-09-07 15-17-08\008-D2F-F6-noCat



Peak : 6 at 2.308 min Name : ?



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

Purity factor : 538.018 (31 of 31 spectra are within the calculated threshold limit.)

Threshold : 0.000 (Calculated with 31 of 31 spectra)

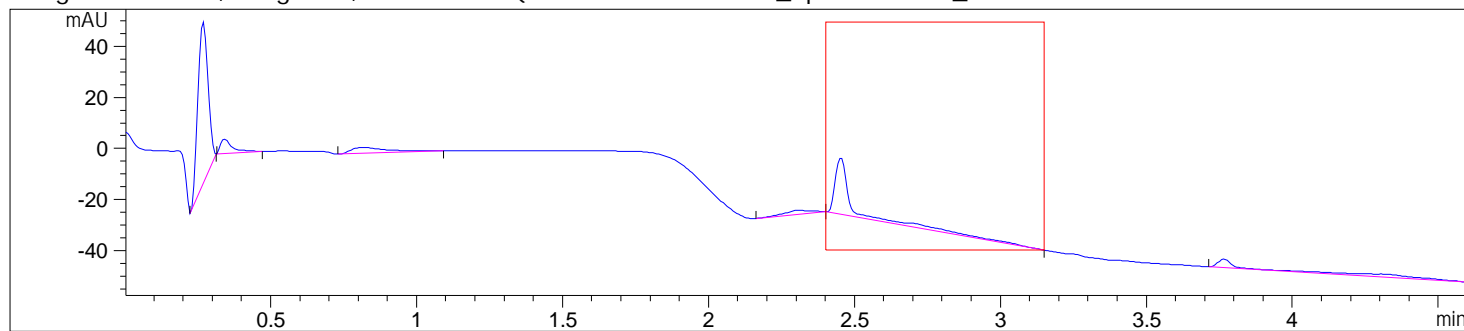
Reference : Peak start and end spectra (integrated) (2.163 / 2.403)

Spectra : 5 (Selection automatic, 5)

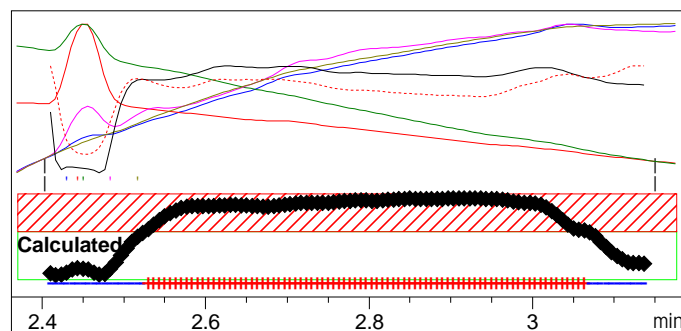
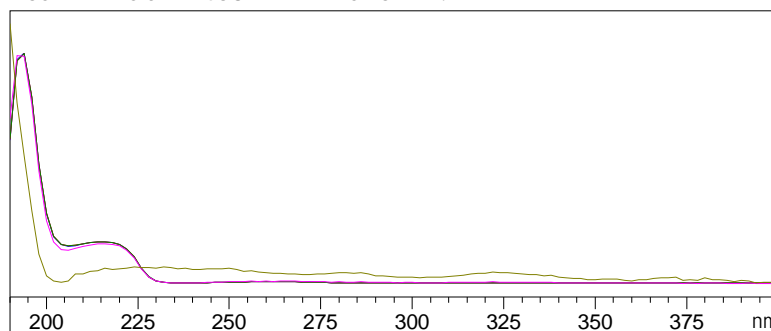
Noise Threshold: 0.666 (12 spectra, St.Dev 0.3207 + 3 \* 0.1152)

Sample Name: noCata\_0p4V

Signal DAD1 B, Sig=220, 4 Ref=off (D:\Data\20...EMP0\_0p9VProduct\_re 2023-09-07 15-17-08\008-D2F-F6-noCat



Peak : 7 at 2.453 min Name : ?



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

Purity factor : 321.107 (81 of 110 spectra exceed the calculated threshold limit.)

Threshold : 734.233 (Calculated with 81 of 110 spectra)

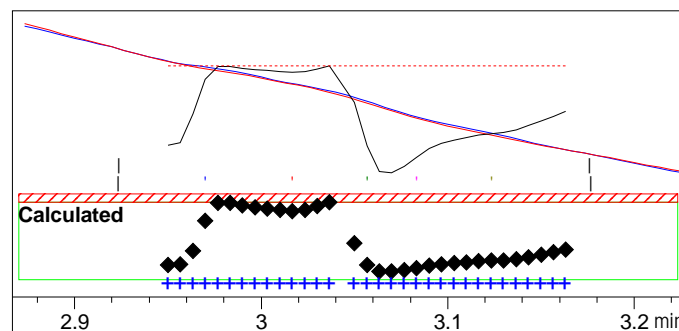
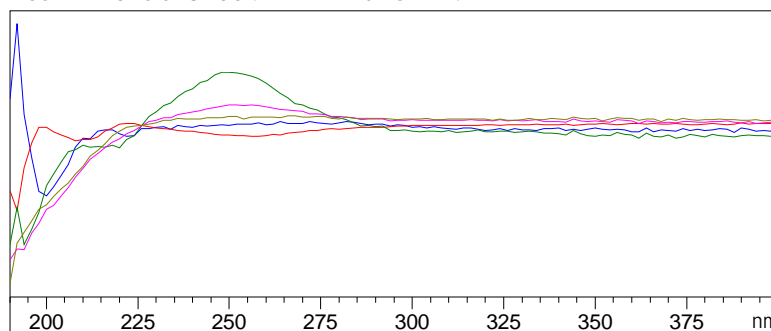
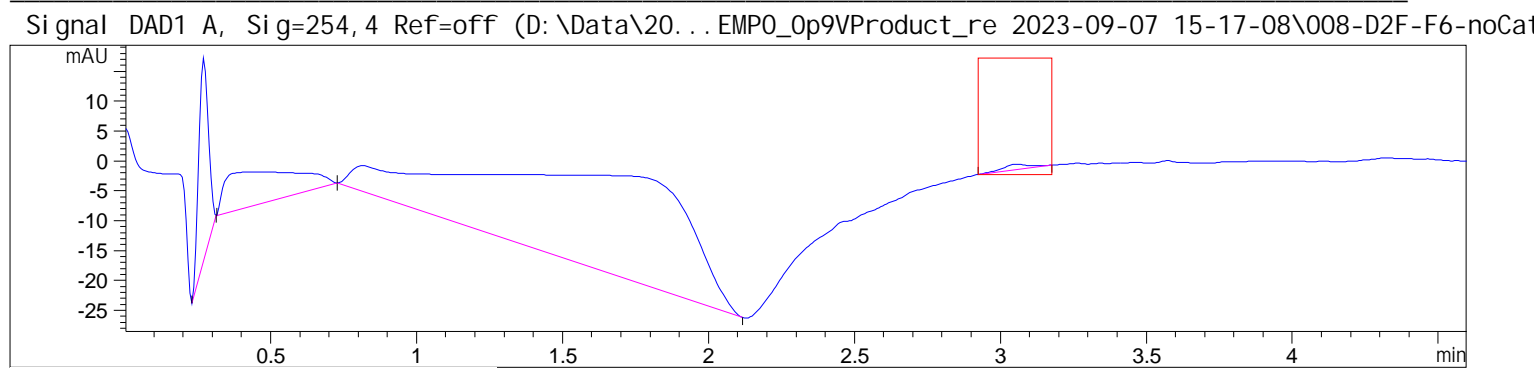
Reference : Peak start and end spectra (integrated) (2.403 / 3.150)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.666 (12 spectra, St.Dev 0.3207 + 3 \* 0.1152)



Sample Name: noCata\_0p4V



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

Purity factor : 520.634 (32 of 32 spectra are within the calculated threshold limit.)

Threshold : 0.000 (Calculated with 32 of 32 spectra)

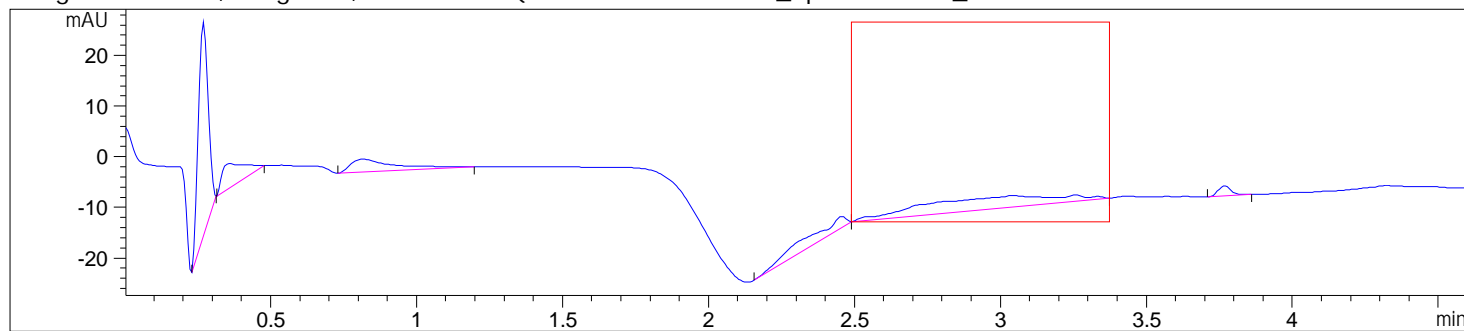
Reference : Peak start and end spectra (integrated) (2.923 / 3.177)

Spectra : 5 (Selection automatic, 5)

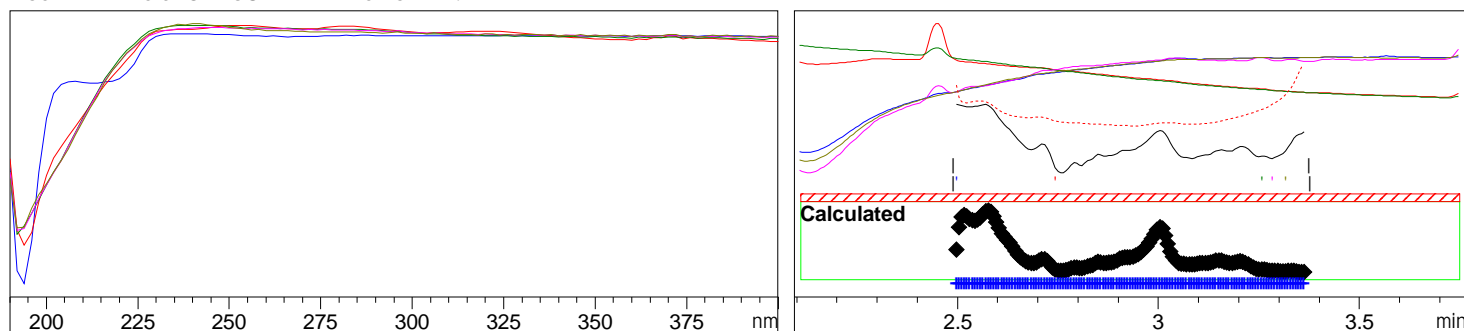
Noise Threshold : 0.666 (12 spectra, St.Dev 0.3207 + 3 \* 0.1152)

Sample Name: noCata\_Op4V

Signal DAD1 D, Sig=230, 4 Ref=off (D:\Data\20...EMP0\_Op9VProduct\_re 2023-09-07 15-17-08\008-D2F-F6-noCat



Peak : 11 at 3.258 min Name : ?



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

Purity factor : 980.153 (131 of 131 spectra are within the calculated threshold limit.)

Threshold : 911.447 (Calculated with 131 of 131 spectra)

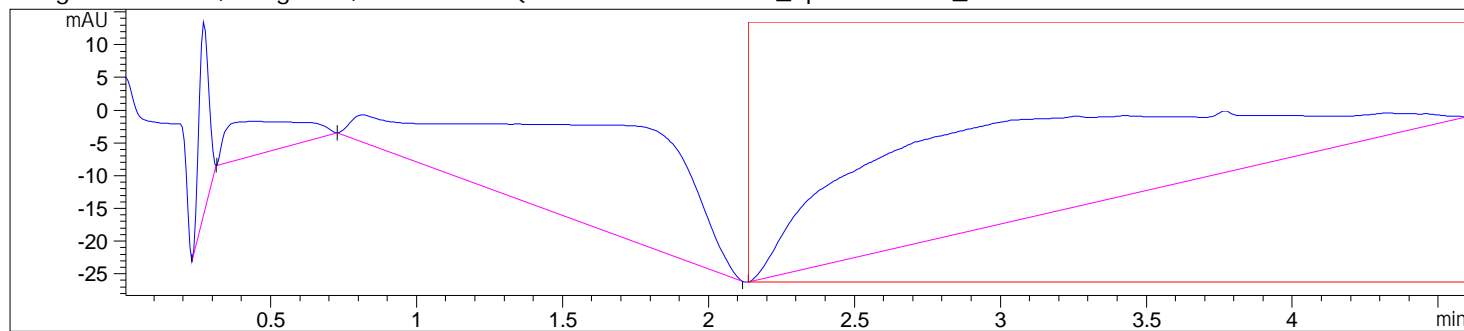
Reference : Peak start and end spectra (integrated) (2.490 / 3.377)

Spectra : 5 (Selection automatic, 5)

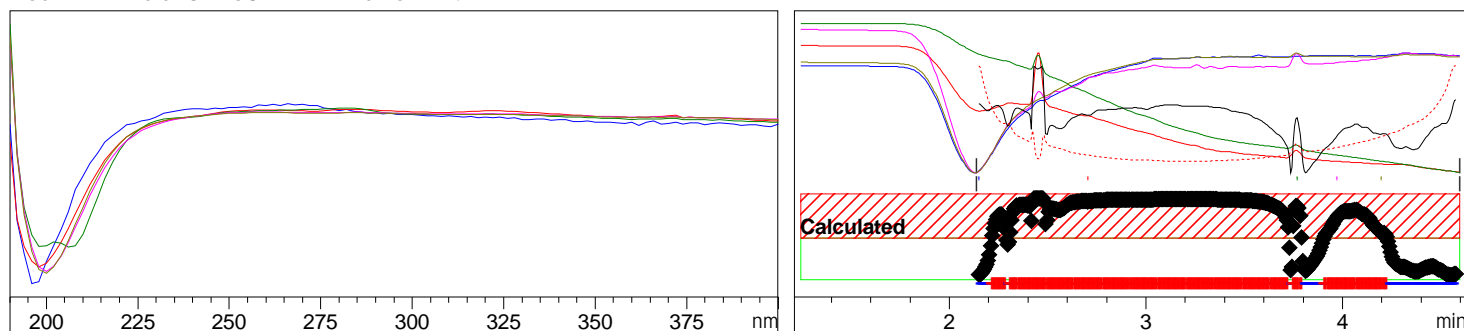
Noise Threshold: 0.666 (12 spectra, St.Dev 0.3207 + 3 \* 0.1152)

Sample Name: noCata\_Op4V

Signal DAD1 E, Sig=280, 4 Ref=off (D:\Data\20...EMP0\_Op9VProduct\_re 2023-09-07 15-17-08\008-D2F-F6-noCat



Peak : 12 at 3.768 min Name : ?



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

Purity factor : 921.125 (279 of 365 spectra exceed the calculated threshold limit.)

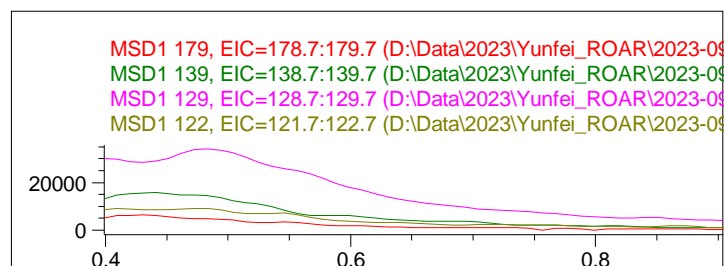
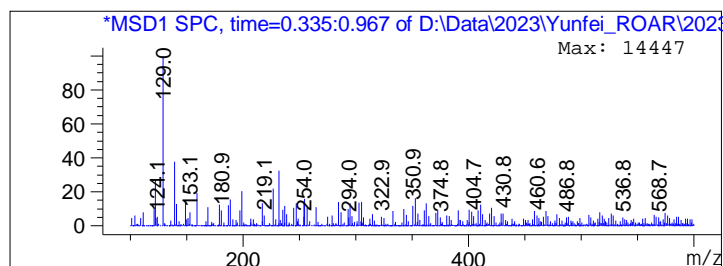
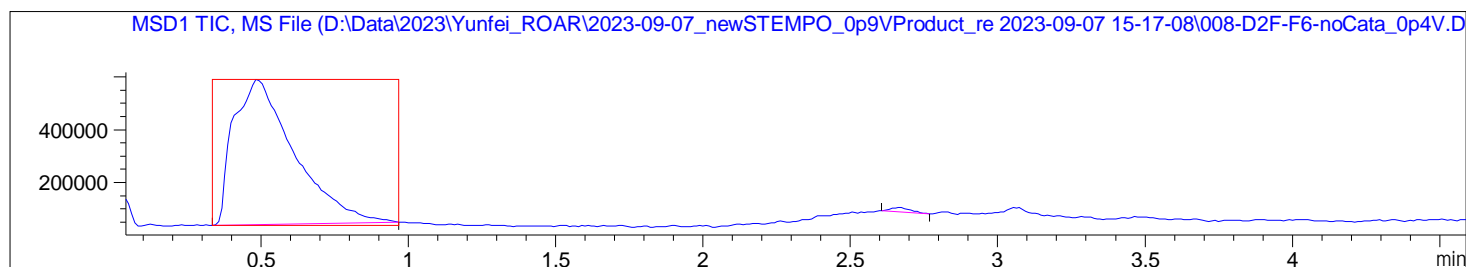
Threshold : 992.996 (Calculated with 279 of 365 spectra)

Reference : Peak start and end spectra (integrated) (2.137 / 4.597)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.666 (12 spectra, St.Dev 0.3207 + 3 \* 0.1152)

Sample Name: noCata\_0p4V

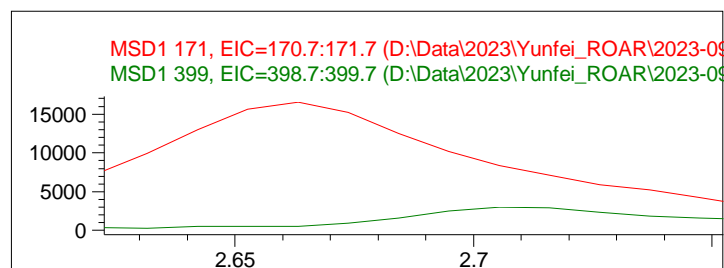
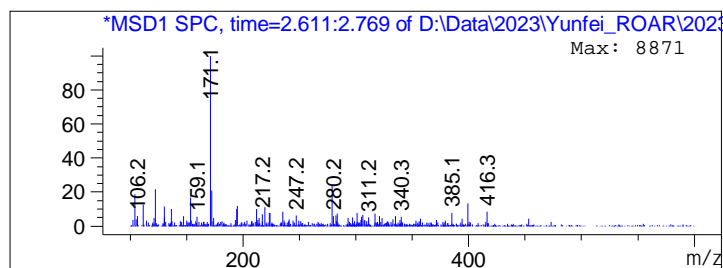
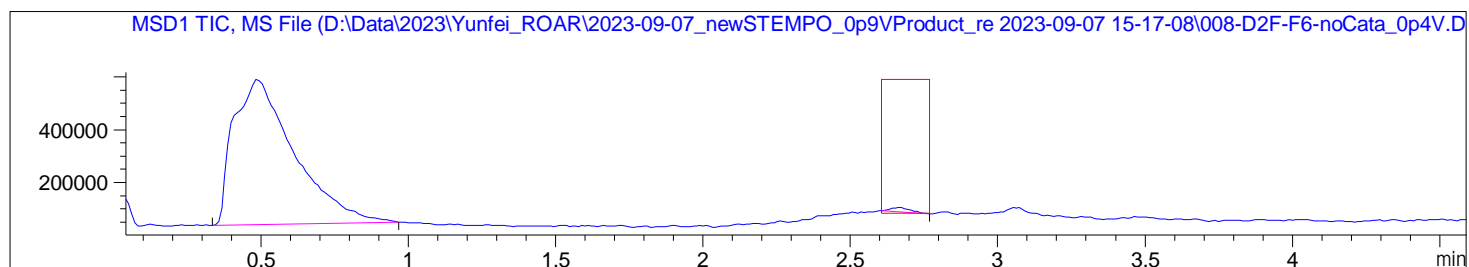


Peak #1 at 0.486 min ( 0.335 to 0.967 min)

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

Component 1: Peak at Scan 38.0. Top ions are 179  
Component 2: Peak at Scan 38.8. Top ions are 139  
Component 3: Peak at Scan 42.5. Top ions are 129 122 411  
Component 4: Peak at Scan 43.5. Top ions are 255 189  
Component 5: Peak at Scan 44.6. Top ions are 232 254  
Component 6: Peak at Scan 47.6. Top ions are 199

Sample Name: noCata\_0p4V



Peak #2 at 2.669 min ( 2.606 to 2.769 min)

-&gt; The analysis found 2 components, indicating an impure peak. &lt;-

Component 1: Peak at Scan 249.9. Top ions are 171

Component 2: Peak at Scan 254.3. Top ions are 399

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