

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

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      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

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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  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      XXXXXXXX  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  XXXXXXXX  XXXXXXXX  XX  XX  XXXXXXXX  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
XXXXXX  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: noCata_0p9V

```

=====
Acq. Operator   : user                      Seq. Line :    7
Sample Operator : user
Acq. Instrument : SFC LCMS                  Location  :   D2F-F5
Injection Date  : 07/09/2023 16:07:43      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       : 943
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	0.83	944.4 h
DAD 1, Visible Lamp	0.00	352.8 h

```

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

```

Sample Name: noCata_Op9V

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	6.6E-009	6.5E-009 Torr
CapCur	646	639 nA
ChamCur	9.6E-001	1.7E-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

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 : Variabl e

Mass	:	Value

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

Ionization polari ty : 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 : Variabl e

Mass	:	Value

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

Mass Gain : -12.80
Mass Offset : Variabl e

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 : Variabl e

Mass	:	Value

50.00	:	0.5
100.00	:	1.0
350.00	:	2.0

Sample Name: noCata_Op9V

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

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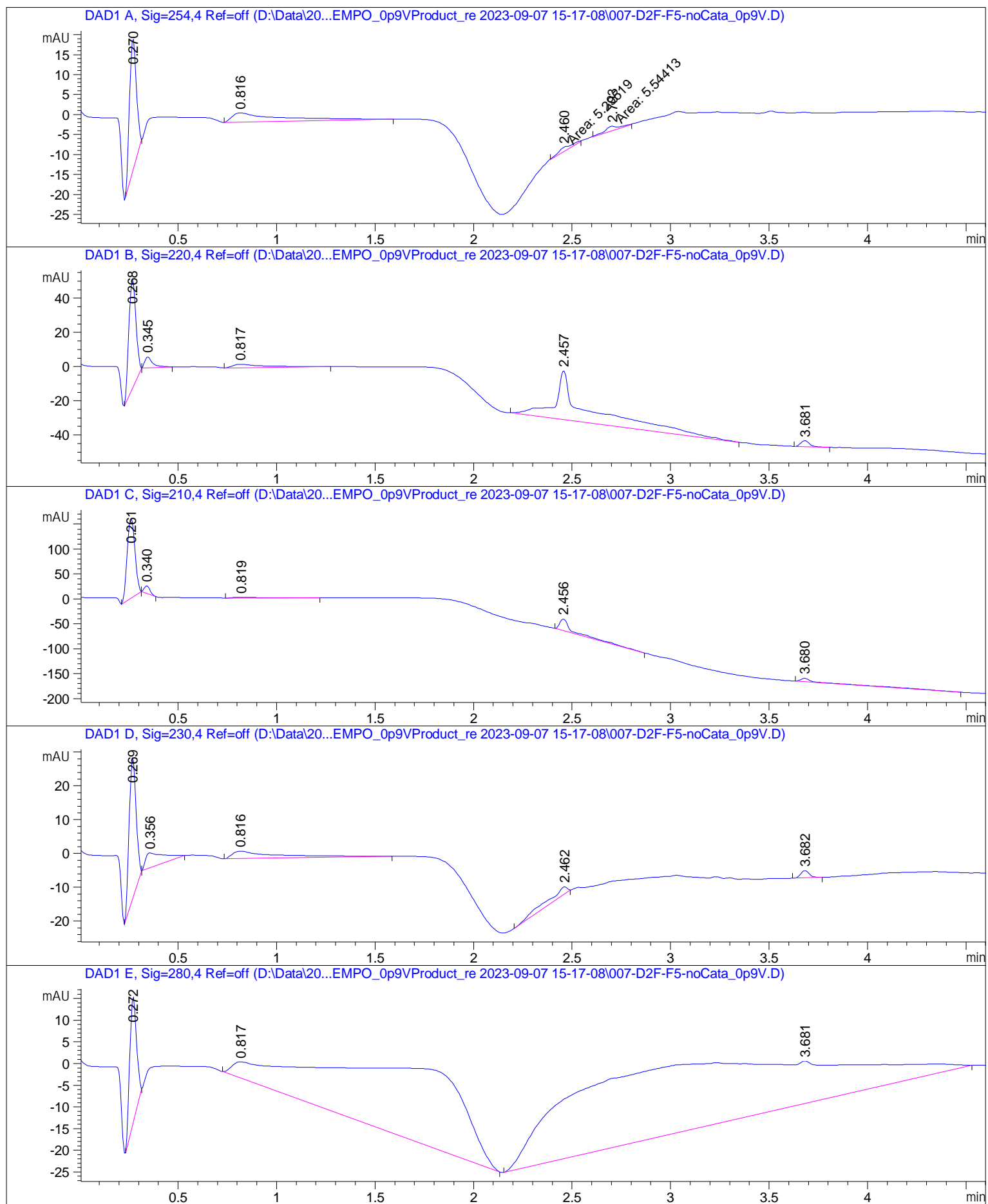
18 Sep 23 11:23 AM

Logbook File: D:\Data\20...STEMPO_Op9VProduct_re 2023-09-07 15-17-08\007-D2F-F5-noCata_Op9V.D\RUN.LOG

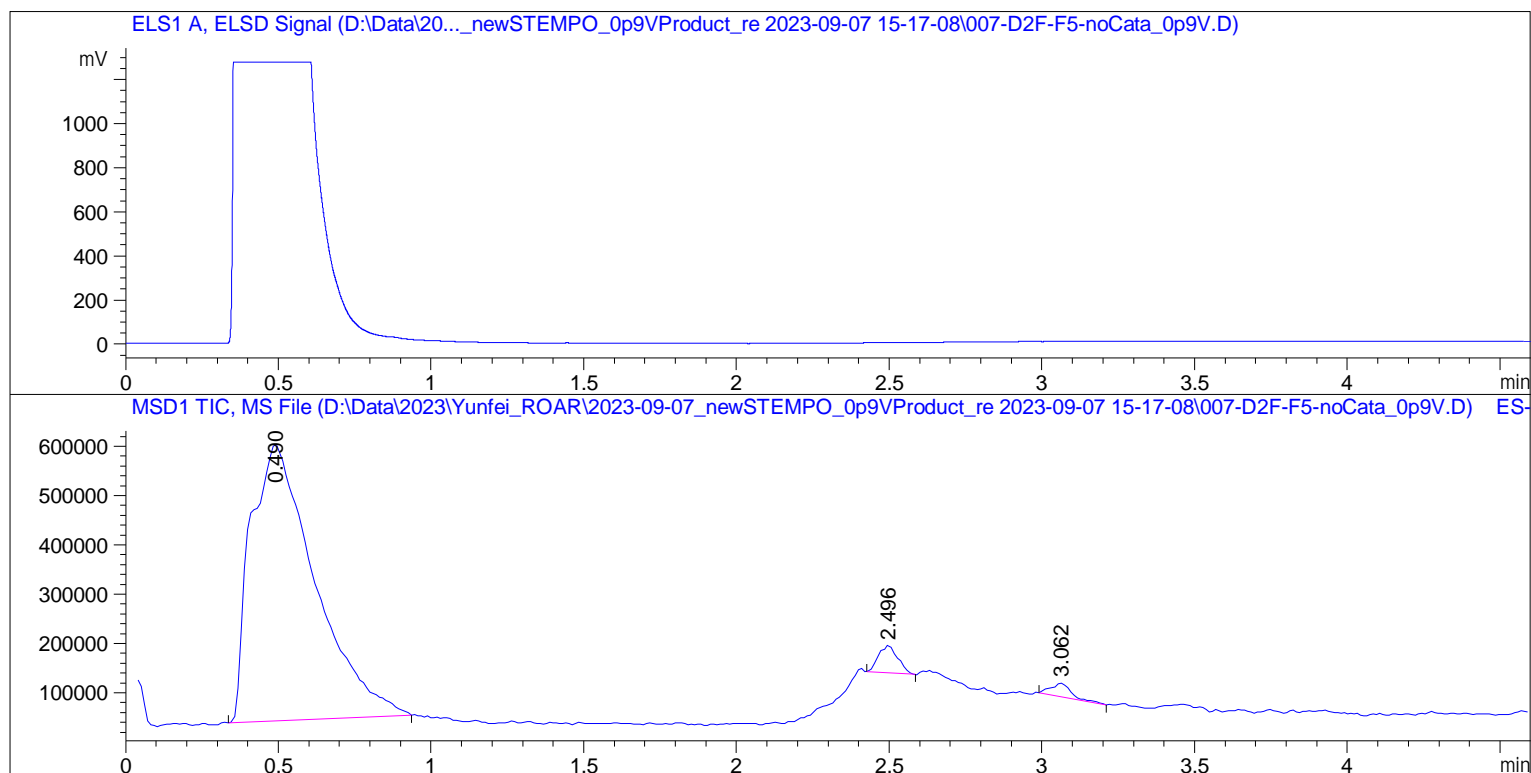
Module	# Event Message	Date Time
Method	Method started: line# 7 at location 'D2F-F5> ' inj# 1	07/09/2023 16:06:46
CP Macro	PreRun macro: 'LAMPALL ON'	07/09/2023 16:06:47
G4260B	G4260B: ELSD - Autozero	07/09/2023 16:06:48
G4260B	G4260B: ELSD - Already switched on	07/09/2023 16:06:48
Method	Instrument running sample from location D2F-> F5	07/09/2023 16:06:48
G7115A	G7115A: DEAC605436 - Detector: Prepare	07/09/2023 16:06:59
G7115A	G7115A: DEAC605436 - Detector: Idle	07/09/2023 16:07:15
G4767A	G4767A: DEAFD00218 - Draw command finished	07/09/2023 16:07:30
G4767A	G4767A: DEAFD00218 - Sampler wash is active	07/09/2023 16:07:34
G4767A	G4767A: DEAFD00218 - Sampler wash is idle	07/09/2023 16:07:38
G4767A	G4767A: DEAFD00218 - Sample preparation time: > 24 sec	07/09/2023 16:07:43
PumpValve	G7111B: DEAEW03495 - Run	07/09/2023 16:07:43
G4767A	G4767A: DEAFD00218 - Postrun	07/09/2023 16:12:16
G7110B	G7110B: DEAEH00761 - Postrun	07/09/2023 16:12:17
PumpValve	G1170A: DEBAD03715 - Postrun	07/09/2023 16:12:18
G4782A	G4782A: DEAGN00153 - Postrun	07/09/2023 16:12:18
G7116A	G7116A: DEAE08985 - Postrun	07/09/2023 16:12:19
Method	Saving Method COL1_5NH4FA_MECN_5T095_1MIN_10> 0-600MS_POS.M	07/09/2023 16:14:38
Method	Instrument run completed	07/09/2023 16:14:40
CP Macro	Analyzing rawdata 007-D2F-F5-noCata_Op9V.D	07/09/2023 16:14:41
Method	Saving Method DA.M	07/09/2023 16:14:44
Method	Method completed	07/09/2023 16:14:52

=====

Sample Name: noCata_0p9V



Sample Name: noCata_0p9V



=====
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	0.0380	79.81847	33.23786	62.1386
2	0.816	BB	0.2151	37.79449	2.30789	29.4230
3	2.460	MM	0.0810	5.29519	1.08889	4.1223
4	2.703	MM	0.0760	5.54413	1.21583	4.3161

Totals : 128.45229 37.85047

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	160.30167	64.08332	29.1013
2	0.345	BB	0.0404	17.85943	6.42471	3.2422
3	0.817	BB	0.1596	23.61394	2.03242	4.2869
4	2.457	BB	0.1502	338.14774	28.54725	61.3877
5	3.681	BB	0.0496	10.91708	3.57496	1.9819

Sample Name: noCata_Op9V

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
Total s :				550.83985	104.66267	

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	0.0462	443.59036	160.65456	69.7332
2	0.340	BB	0.0339	30.84786	15.06428	4.8493
3	0.819	BB	0.1444	16.23838	1.59992	2.5527
4	2.456	BB	0.0601	96.41304	23.37888	15.1563
5	3.680	BBA	0.0976	49.03543	6.84298	7.7085
Total s :				636.12508	207.54061	

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	0.0385	102.62906	42.06338	53.2880
2	0.356	BB	0.0850	27.83744	4.44603	14.4540
3	0.816	BB	0.2138	35.62880	2.21381	18.4995
4	2.462	BB	0.1245	20.11607	2.08642	10.4448
5	3.682	BB	0.0465	6.38185	2.15799	3.3136
Total s :				192.59321	52.96762	

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.272	BB	0.0401	69.95925	29.06763	3.0456
2	0.817	BB	2.6559	838.77026	3.71807	36.5148
3	3.681	BBA	1.6586	1388.34106	9.84907	60.4396
Total s :				2297.07058	42.63477	

Signal 6: ELS1 A, ELSD Signal

Signal 7: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.490	BB	0.1896	8.20503e6	5.60842e5	95.7614
2	2.496	BB	0.0624	2.35489e5	5.52316e4	2.7484
3	3.062	BB	0.0651	1.27679e5	2.84148e4	1.4902

Totals : 8.56820e6 6.44489e5

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.

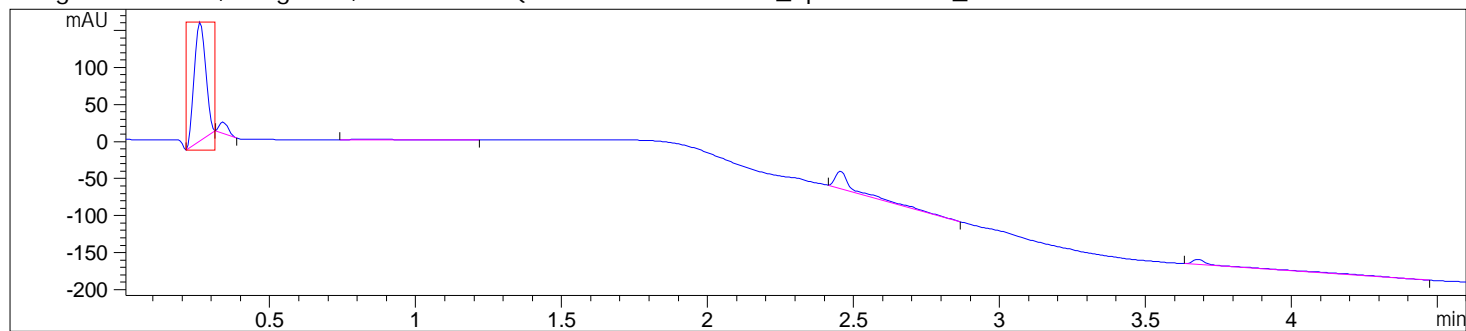
Signal 7: MSD1 TIC, MS File
Empty table.

Final Summed Peaks Report

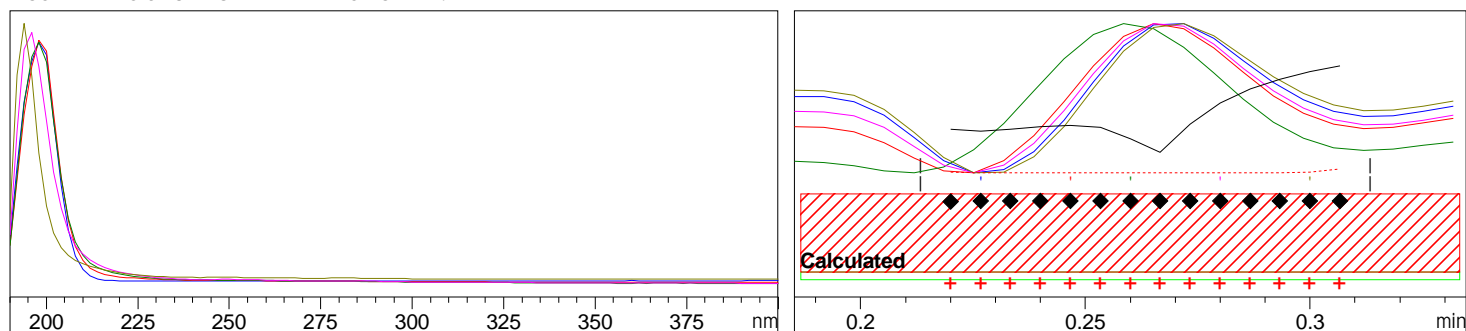
Signal 1: DAD1 A, Sig=254, 4 Ref=off
Signal 2: DAD1 B, Sig=220, 4 Ref=off
Signal 3: DAD1 C, Sig=210, 4 Ref=off
Signal 4: DAD1 D, Sig=230, 4 Ref=off
Signal 5: DAD1 E, Sig=280, 4 Ref=off
Signal 6: ELS1 A, ELSD Signal
Signal 7: MSD1 TIC, MS File

Sample Name: noCata_Op9V

Signal DAD1 C, Sig=210, 4 Ref=off (D:\Data\20...EMP0_Op9VProduct_re 2023-09-07 15-17-08\007-D2F-F5-noCat



Peak : 1 at 0.261 min Name : ?



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

Purity factor : 928.993 (14 of 14 spectra exceed the calculated threshold limit.)

Threshold : 999.986 (Calculated with 14 of 14 spectra)

Reference : Peak start and end spectra (integrated) (0.213 / 0.313)

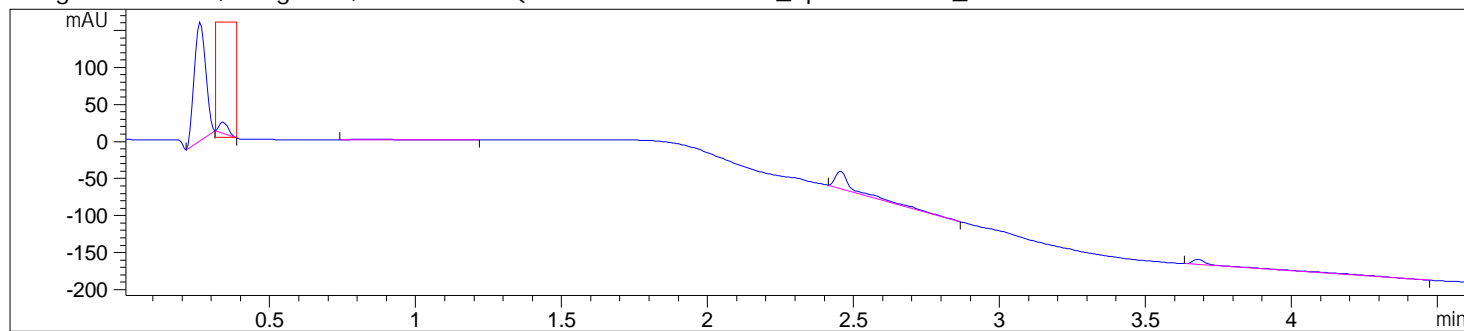
Spectra : 5 (Selection automatic, 5)

Noise Threshold : 0.170 (12 spectra, St.Dev 0.0828 + 3 * 0.0289)

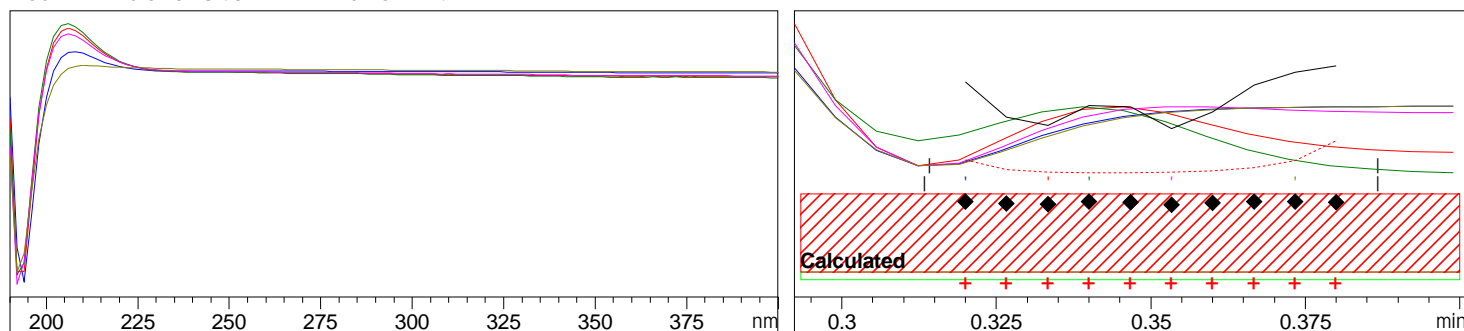
Warning : Spectral absorbances > 1000 mAU (see help for more information)

Sample Name: noCata_Op9V

Signal DAD1 C, Sig=210, 4 Ref=off (D:\Data\20...EMP0_Op9VProduct_re 2023-09-07 15-17-08\007-D2F-F5-noCat



Peak : 2 at 0.340 min Name : ?



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

Purity factor : 965.772 (10 of 10 spectra exceed the calculated threshold limit.)

Threshold : 999.226 (Calculated with 10 of 10 spectra)

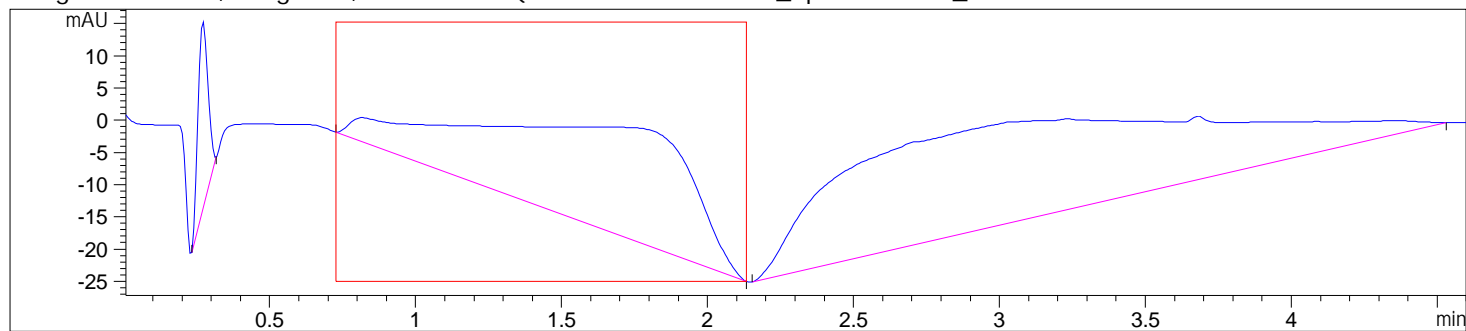
Reference : Peak start and end spectra (integrated) (0.313 / 0.387)

Spectra : 5 (Selection automatic, 5)

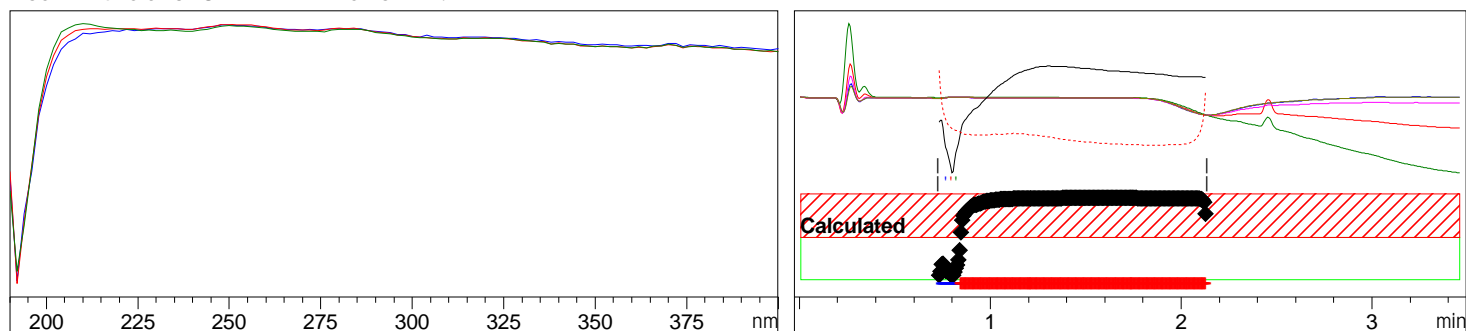
Noise Threshold: 0.170 (12 spectra, St.Dev 0.0828 + 3 * 0.0289)

Sample Name: noCata_0p9V

Signal DAD1 E, Sig=280, 4 Ref=off (D:\Data\20...EMP0_0p9VProduct_re 2023-09-07 15-17-08\007-D2F-F5-noCat



Peak : 4 at 0.817 min Name : ?



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

Purity factor : 383.651 (193 of 210 spectra exceed the calculated threshold limit.)

Threshold : 989.599 (Calculated with 193 of 210 spectra)

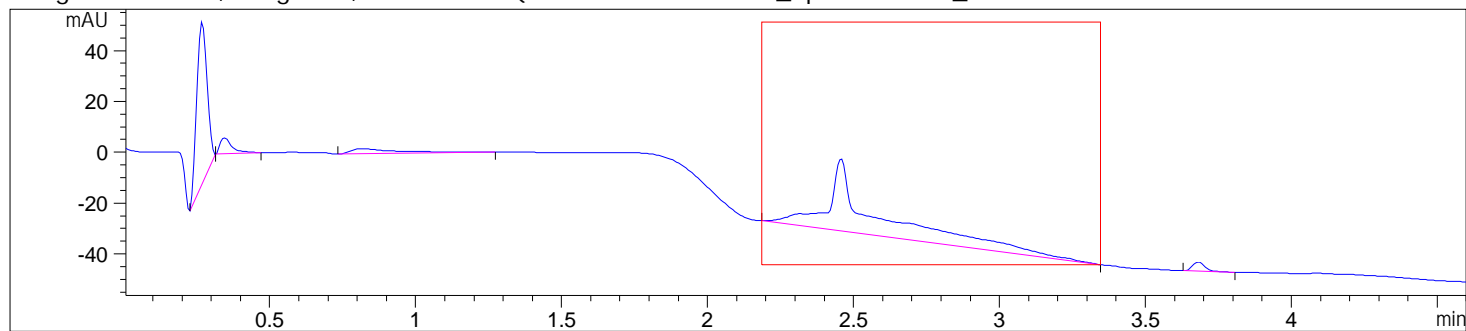
Reference : Peak start and end spectra (integrated) (0.727 / 2.133)

Spectra : 3 (Selection automatic, 5)

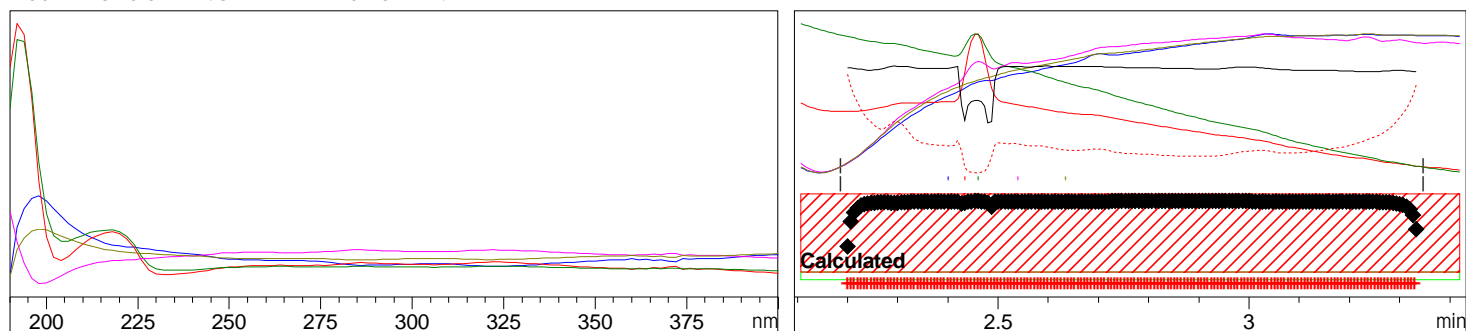
Noise Threshold: 0.170 (12 spectra, St.Dev 0.0828 + 3 * 0.0289)

Sample Name: noCata_Op9V

Signal DAD1 B, Sig=220, 4 Ref=off (D:\Data\20...EMP0_Op9VProduct_re 2023-09-07 15-17-08\007-D2F-F5-noCat



Peak : 5 at 2.457 min Name : ?



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

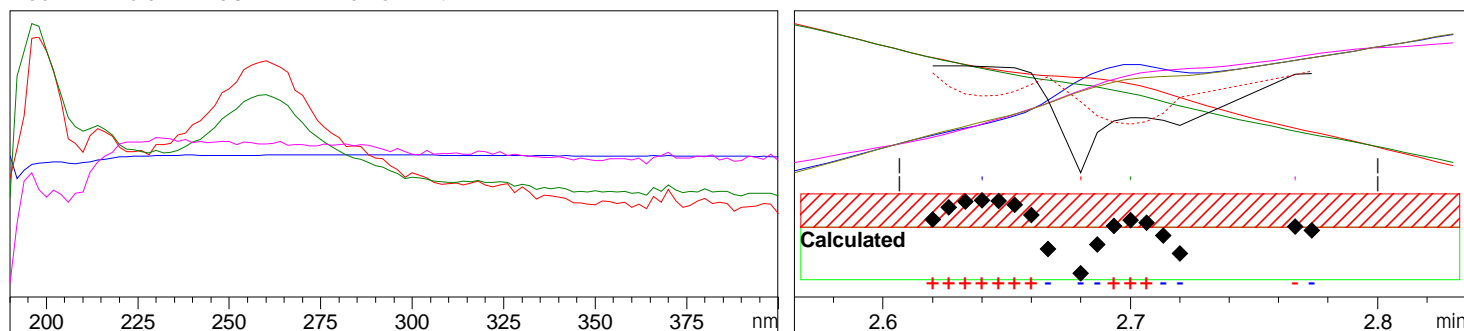
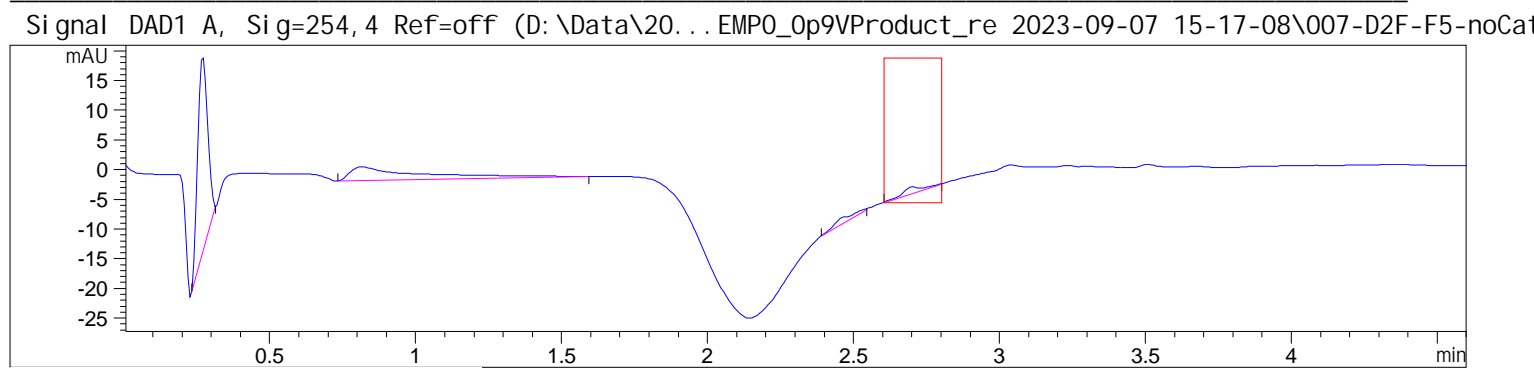
Purity factor : 189.892 (171 of 171 spectra exceed the calculated threshold limit.)

Threshold : 985.172 (Calculated with 171 of 171 spectra)

Reference : Peak start and end spectra (integrated) (2.187 / 3.347)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.170 (12 spectra, St.Dev 0.0828 + 3 * 0.0289)

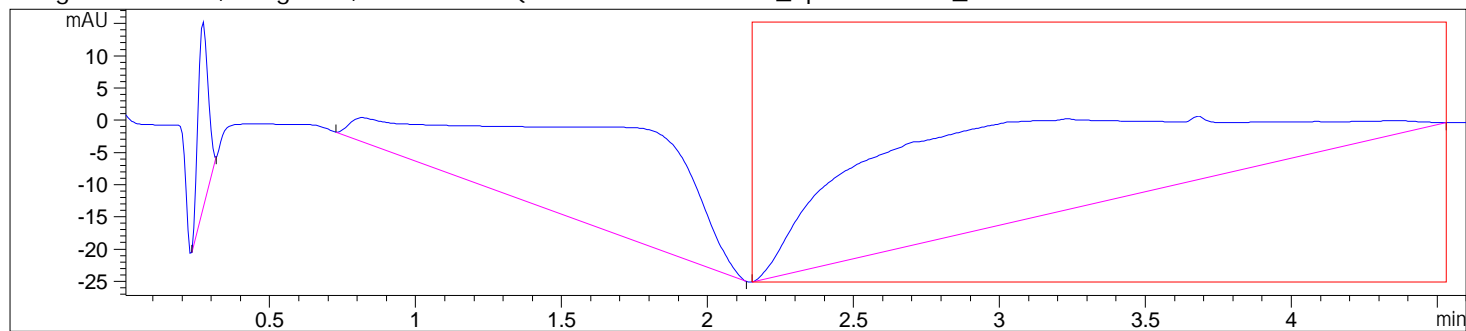


-> The purity factor exceeds the calculated threshold limit. <-

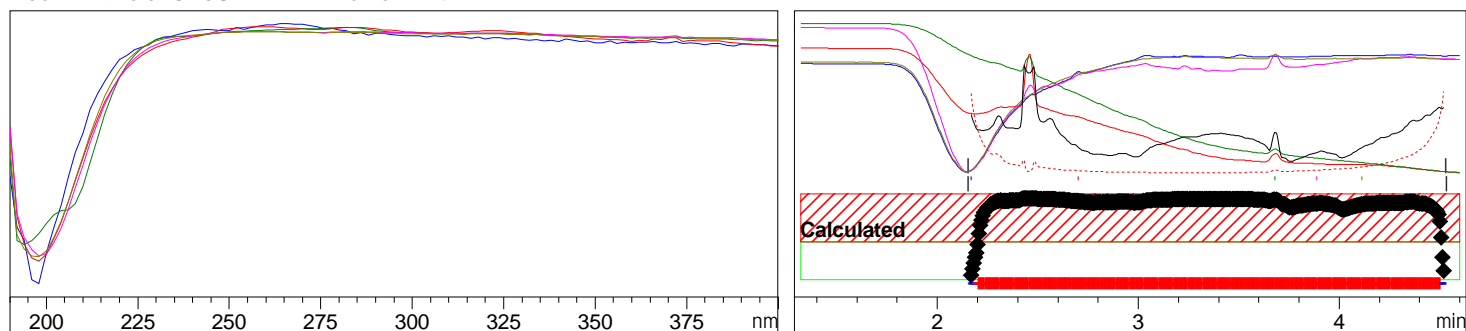
Purity factor : 211.079 (10 of 17 spectra exceed the calculated threshold limit.)
Threshold : 444.739 (Calculated with 10 of 17 spectra)
Reference : Peak start and end spectra (integrated) (2.607 / 2.800)
Spectra : 4 (Selection automatic, 5)
Noise Threshold: 0.170 (12 spectra, St.Dev 0.0828 + 3 * 0.0289)

Sample Name: noCata_Op9V

Signal DAD1 E, Sig=280, 4 Ref=off (D:\Data\20...EMP0_Op9VProduct_re 2023-09-07 15-17-08\007-D2F-F5-noCat



Peak : 9 at 3.681 min Name : ?



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

Purity factor : 971.922 (346 of 354 spectra exceed the calculated threshold limit.)

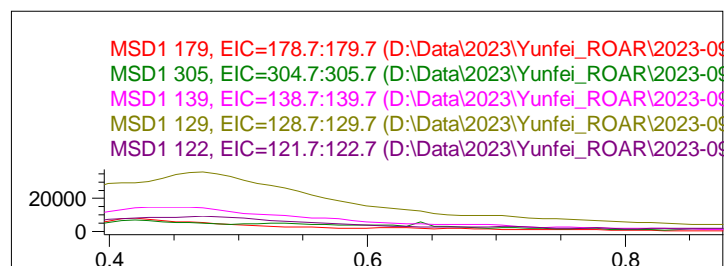
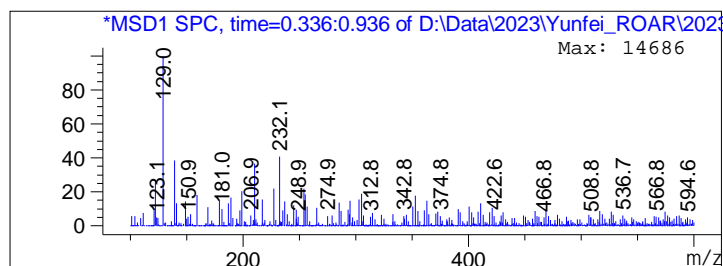
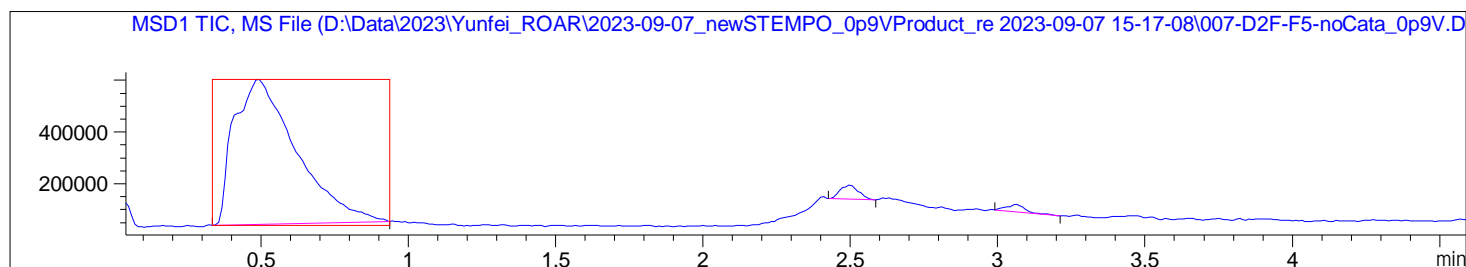
Threshold : 999.021 (Calculated with 346 of 354 spectra)

Reference : Peak start and end spectra (integrated) (2.153 / 4.533)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.170 (12 spectra, St.Dev 0.0828 + 3 * 0.0289)

Sample Name: noCata_Op9V

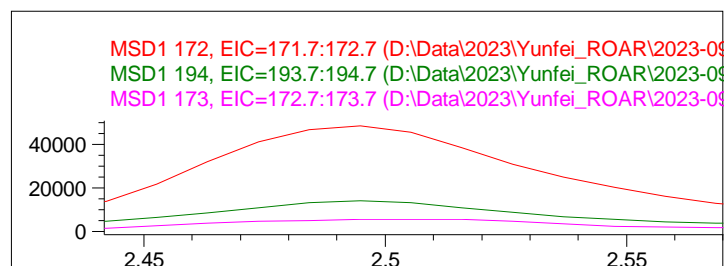
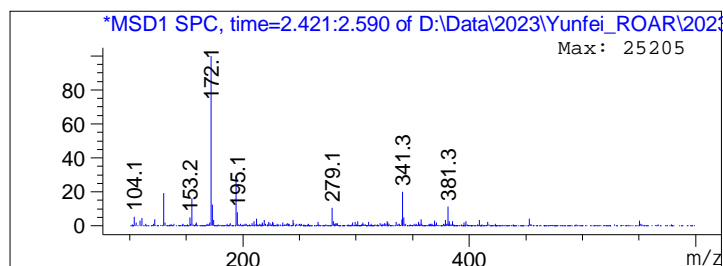
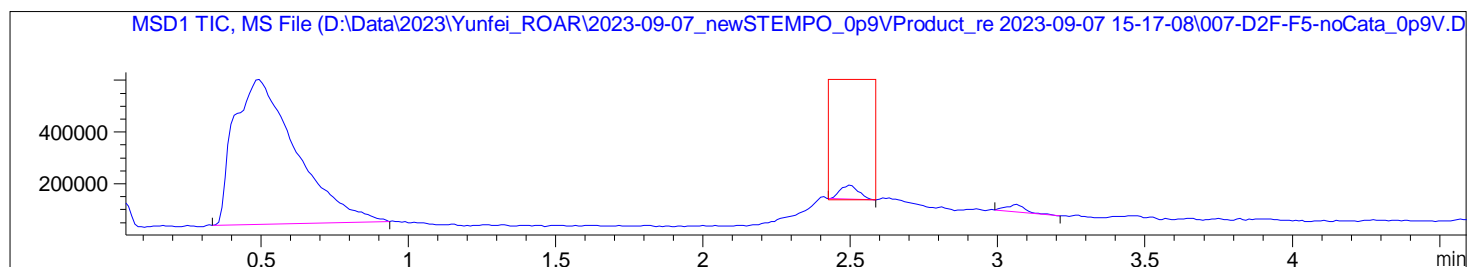


Peak #1 at 0.490 min (0.336 to 0.936 min)

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

Component 1: Peak at Scan 36.9. Top ions are 179 305
Component 2: Peak at Scan 38.6. Top ions are 139
Component 3: Peak at Scan 41.8. Top ions are 129 122
Component 4: Peak at Scan 43.3. Top ions are 255
Component 5: Peak at Scan 44.7. Top ions are 232 254
Component 6: Peak at Scan 47.2. Top ions are 199
Component 7: Peak at Scan 51.1. Top ions are 210

Sample Name: noCata_0p9V

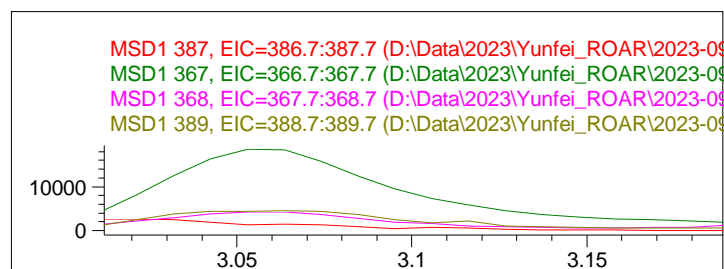
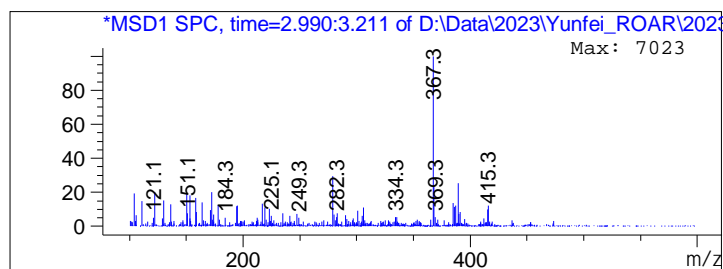
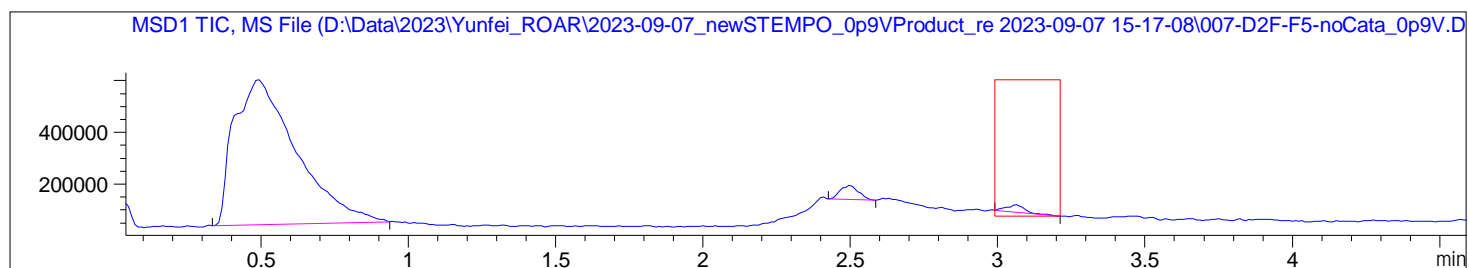


Peak #2 at 2.496 min (2.426 to 2.586 min)

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

Component 1: Peak at Scan 233.8. Top ions are 172 194 155

Component 2: Peak at Scan 235.1. Top ions are 173



Peak #3 at 3.062 min (2.990 to 3.211 min)

-> The analysis found 5 components, indicating an impure peak. <-

Component 1: Peak at Scan 283.9. Top ions are 387

Component 2: Peak at Scan 287.4. Top ions are 367 368

Component 3: Peak at Scan 288.1. Top ions are 389

Component 4: Peak at Scan 288.9. Top ions are 412

Component 5: Peak at Scan 296.2. Top ions are 415

*** End of Report ***