

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  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  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      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

```

```

  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  XXXX  XX      X  XX      XX XX  XX
  XXX      XXXXX  XXX  XXX  XX      XXXX  XXXXX X      XXX      XXXXX
                XXXX

```

Sample Name: Cata_0p9V

```

=====
Acq. Operator   : user                      Seq. Line :    3
Sample Operator : user
Acq. Instrument : SFC LCMS                 Location  :   D2F-F2
Injection Date  : 07/09/2023 15:35:53      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

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Column(s)

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```

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       : 939
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	32.3 °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	0.30	943.8 h
DAD 1, Visible Lamp	0.00	352.8 h

```

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

```

Sample Name: Cata_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	6.7E-009	6.7E-009 Torr
CapCur	5	639 nA
ChamCur	1.1E-001	1.3E-001 µA
DryingGas	12	12 l/min
Neb Pres	35	35 psig
Turbo1Spd	100	100 %
Turbo1Pwr	126	127 W
RF Drive	1	15 %
Qd TpDrv	16	16 %
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: Cata_Op9V

Mass	:	Value

50.00	:	0.5
100.00	:	1.0
350.00	:	2.0
1000.00	:	4.0
2000.00	:	6.0

Mass	:	Value

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

L2RFEn : 1

L2RFPh : 144

L2RFAmp : Variabl e

Sample Name: Cata_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

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Run Logbook

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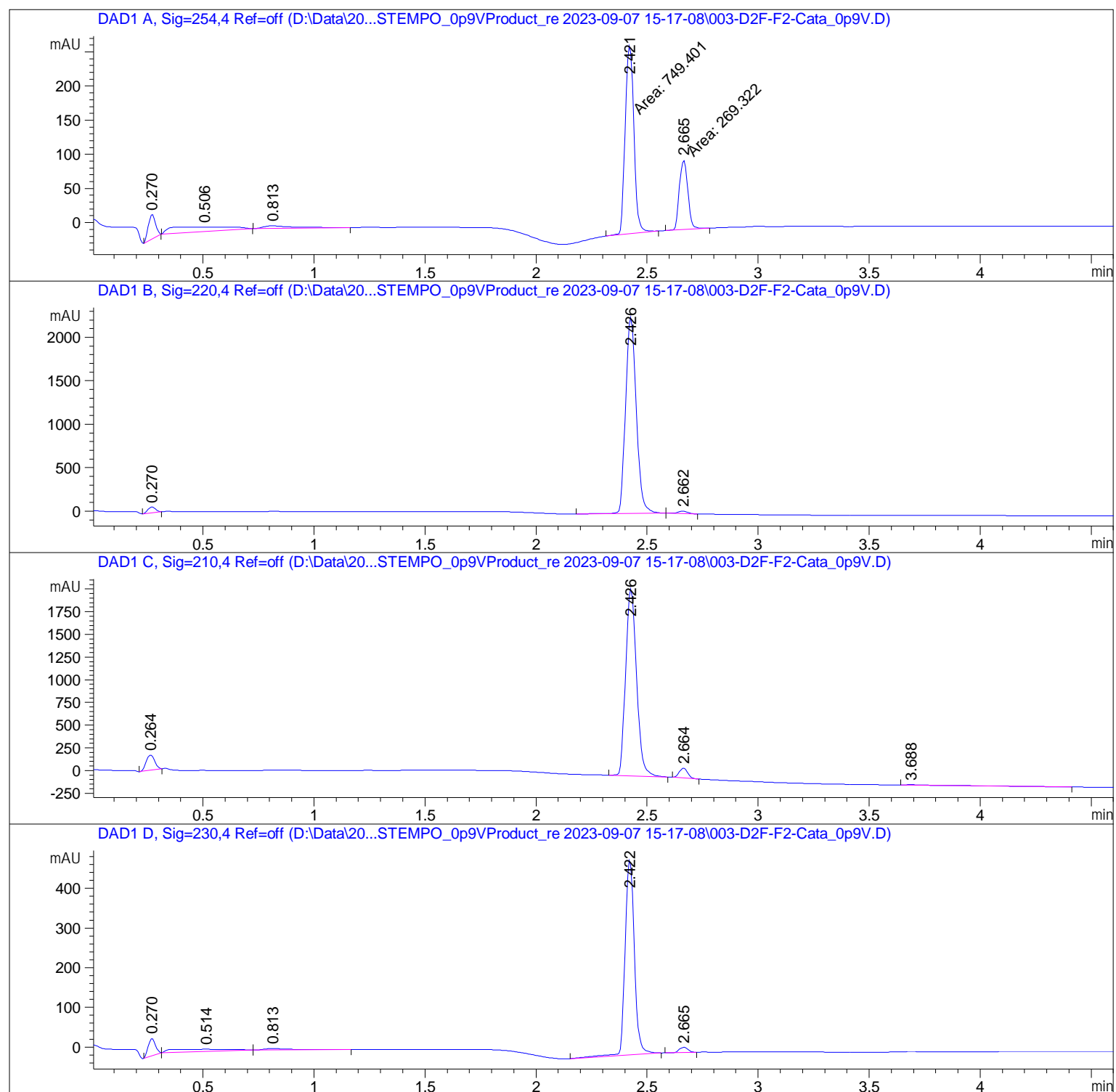
18 Sep 23 11:16 AM

Logbook File: D:\Data\20...ewSTEMPO_Op9VProduct_re 2023-09-07 15-17-08\003-D2F-F2-Cata_Op9V.D\RUN.LOG

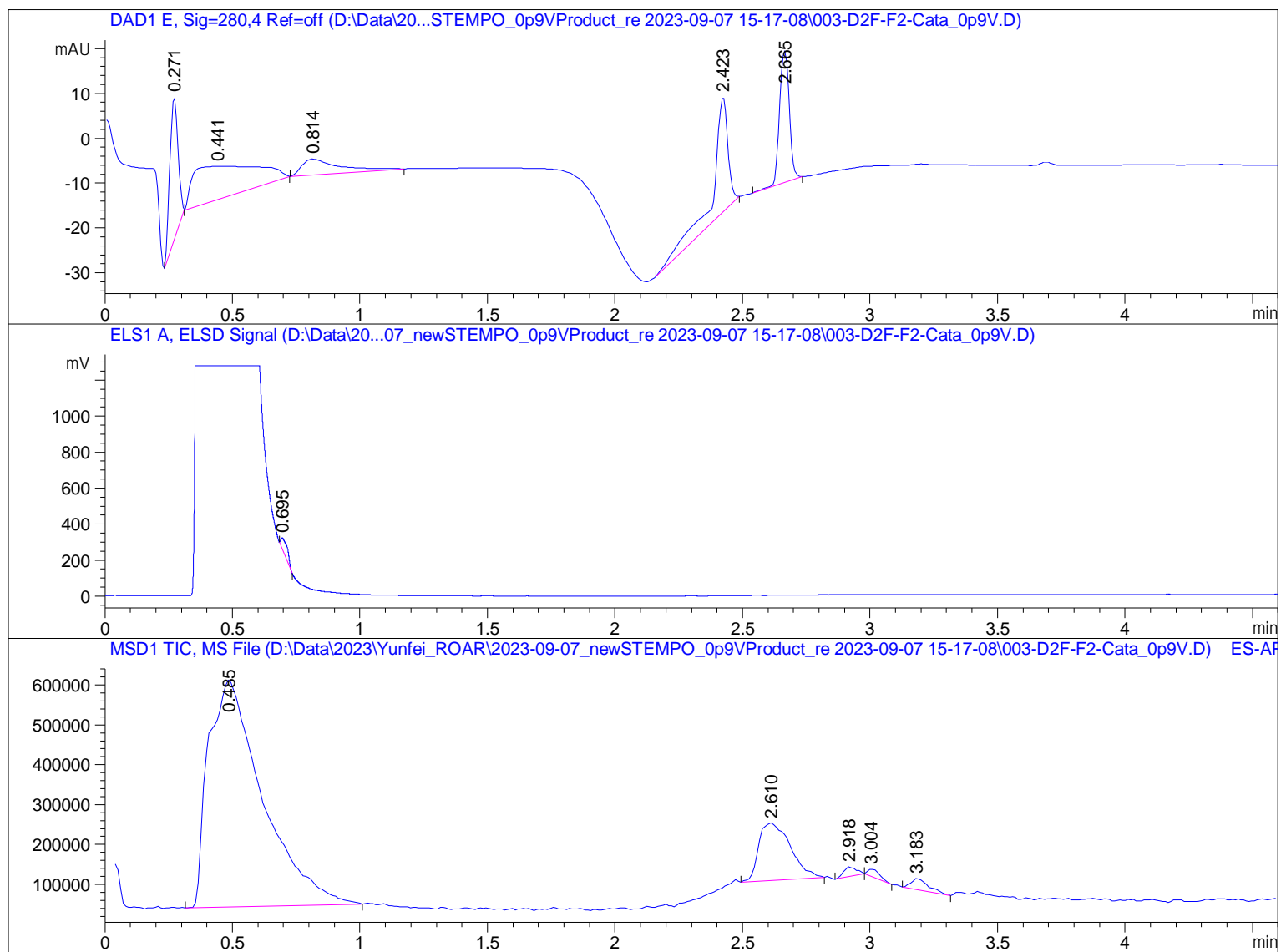
Module	# Event Message	Date Time
Method	Method started: line# 3 at location 'D2F-F2>' 'inj# 1'	07/09/2023 15:35:07
CP Macro	PreRun macro: 'LAMPALL ON'	07/09/2023 15:35:08
G4260B	G4260B: ELSD - Autozero	07/09/2023 15:35:08
G4260B	G4260B: ELSD - Already switched on	07/09/2023 15:35:09
Method	Instrument running sample from location D2F->F2	07/09/2023 15:35:09
G7115A	G7115A: DEAC605436 - Detector: Prepare	07/09/2023 15:35:20
G7115A	G7115A: DEAC605436 - Detector: Idle	07/09/2023 15:35:36
G4767A	G4767A: DEAFD00218 - Draw command finished	07/09/2023 15:35:43
G4767A	G4767A: DEAFD00218 - Sampler wash is active	07/09/2023 15:35:45
CP Comman	Queued item New changed state to Editing.	07/09/2023 15:35:48
G4767A	G4767A: DEAFD00218 - Sampler wash is idle	07/09/2023 15:35:51
G4767A	G4767A: DEAFD00218 - Sample preparation time: >15 sec	07/09/2023 15:35:51
PumpVal ve	G7111B: DEAEW03495 - Run	07/09/2023 15:35:53
CP Comman	Queued item New changed state to Pending.	07/09/2023 15:36:02
CP Comman	Queued item New changed state to Editing.	07/09/2023 15:36:11
CP Comman	Queued item New changed state to Pending.	07/09/2023 15:37:36
CP Comman	Queued item New changed state to Editing.	07/09/2023 15:38:02
CP Comman	Queued item New changed state to Pending.	07/09/2023 15:38:41
CP Comman	Queued item New changed state to Editing.	07/09/2023 15:39:51
CP Comman	Queued item New changed state to Pending.	07/09/2023 15:39:57
PumpVal ve	G7111B: DEAEW03495 - Postrun	07/09/2023 15:40:29
G4767A	G4767A: DEAFD00218 - Postrun	07/09/2023 15:40:29
PumpVal ve	G1170A: DEBAD03715 - Postrun	07/09/2023 15:40:30
G1170A	G1170A: DEBAD03734 - Postrun	07/09/2023 15:40:30
G7110B	G7110B: DEAEH00761 - Postrun	07/09/2023 15:40:31
G7116A	G7116A: DEAEH00895 - Postrun	07/09/2023 15:40:31
CP Comman	Queued item New changed state to Editing.	07/09/2023 15:40:56
CP Comman	Queued item New changed state to Pending.	07/09/2023 15:41:13

Sample Name: Cata_Op9V

CP Comman	Queued item New changed state to Editing.	07/09/2023 15:41:21
CP Comman	Queued item New changed state to Pending.	07/09/2023 15:41:23
Method	Saving Method COL1_5NH4FA_MECN_5T095_1MIN_10> 0-600MS_POS.M	07/09/2023 15:42:52
Method	Instrument run completed	07/09/2023 15:42:53
CP Macro	Analyzing rawdata 003-D2F-F2-Cata_Op9V.D	07/09/2023 15:42:53
Method	Saving Method DA.M	07/09/2023 15:42:55
Method	Method completed	07/09/2023 15:43:13



Sample Name: Cata_Op9V



=====
Area Percent Report
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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	0.0362	80.66556	35.86408	6.3420
2	0.506	BB	0.2534	136.19151	6.58218	10.7075
3	0.813	BB	0.1399	36.34143	3.72348	2.8572
4	2.421	MM	0.0451	749.40082	277.04837	58.9188
5	2.665	MM	0.0440	269.32236	102.12186	21.1744

Totals : 1271.92168 425.33998

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	0.0380	166.49977	69.46296	2.1471
2	2.426	BB	0.0528	7506.16895	2257.50708	96.7977
3	2.662	BB	0.0473	81.82138	27.06083	1.0551

Totals : 7754.49010 2354.03087

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	0.0435	447.93573	166.08377	5.7578
2	2.426	BB	0.0537	7010.09033	2061.97412	90.1076
3	2.664	BB	0.0424	273.96710	105.25428	3.5216
4	3.688	BBA	0.1072	47.69749	5.84820	0.6131

Totals : 7779.69065 2339.16037

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	0.0365	99.38764	43.69226	5.7916
2	0.514	BB	0.2553	118.35972	5.72353	6.8972
3	0.813	BB	0.1401	35.33907	3.61258	2.0593
4	2.422	BB	0.0458	1428.23364	492.61130	83.2275
5	2.665	BB	0.0432	34.74028	12.98121	2.0244

Totals : 1716.06036 558.62088

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	0.0363	72.06925	31.95687	17.3078
2	0.441	BB	0.2406	128.34706	7.39005	30.8232
3	0.814	BB	0.1421	34.87975	3.50487	8.3766
4	2.423	BB	0.0591	103.48608	25.63040	24.8527
5	2.665	BB	0.0429	77.61486	29.30306	18.6396

Totals : 416.39701 97.78524

Signal 6: ELS1 A, ELSD Signal

Peak #	RetTime [min]	Type	Width [min]	Area [mV*s]	Height [mV]	Area %
1	0.695	BB	0.0324	147.28409	62.78167	100.0000

Totals : 147.28409 62.78167

Signal 7: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.485	BB	0.1836	8.34385e6	5.69364e5	84.6463
2	2.610	BB	0.1214	1.23454e6	1.45011e5	12.5241
3	2.918	BB	0.0485	8.34738e4	2.49644e4	0.8468
4	3.004	BB	0.0573	6.04448e4	1.75923e4	0.6132
5	3.183	BB	0.0823	1.35008e5	2.76344e4	1.3696

Totals : 9.85731e6 7.84566e5

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.

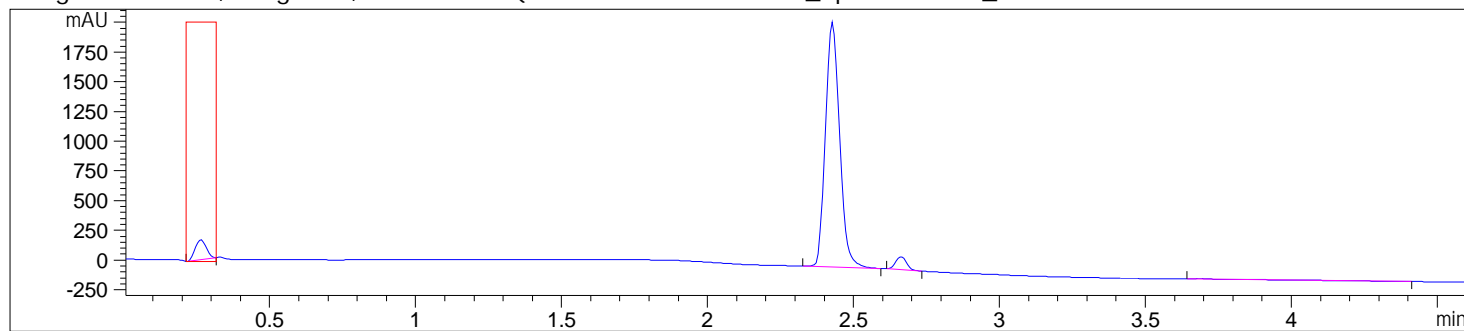
Signal 7: MSD1 TIC, MS File
Empty table.

Final Summed Peaks Report

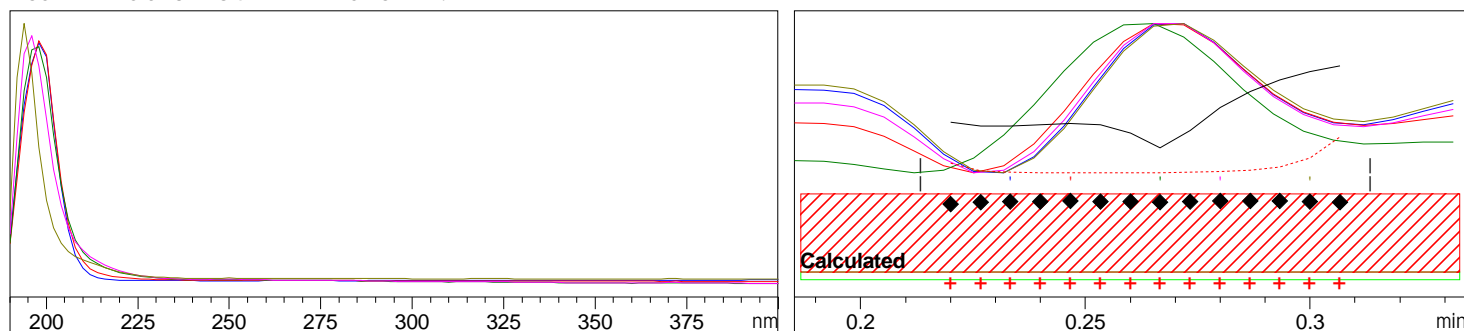
Signal 1: DAD1 A, Sig=254, 4 Ref=off
Signal 2: DAD1 B, Sig=220, 4 Ref=off
Signal 3: DAD1 C, Sig=210, 4 Ref=off
Signal 4: DAD1 D, Sig=230, 4 Ref=off
Signal 5: DAD1 E, Sig=280, 4 Ref=off
Signal 6: ELS1 A, ELSD Signal
Signal 7: MSD1 TIC, MS File

Sample Name: Cata_Op9V

Signal DAD1 C, Sig=210, 4 Ref=off (D:\Data\20...STEMPO_Op9VProduct_re 2023-09-07 15-17-08\003-D2F-F2-Cat



Peak : 1 at 0.264 min Name : ?



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

Purity factor : 938.690 (14 of 14 spectra exceed the calculated threshold limit.)

Threshold : 999.577 (Calculated with 14 of 14 spectra)

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

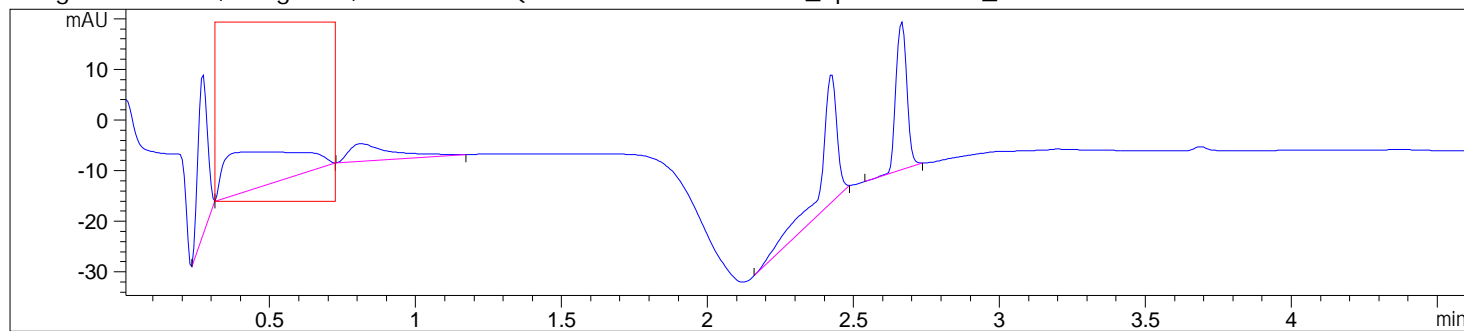
Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.983 (12 spectra, St.Dev 0.4105 + 3 * 0.1909)

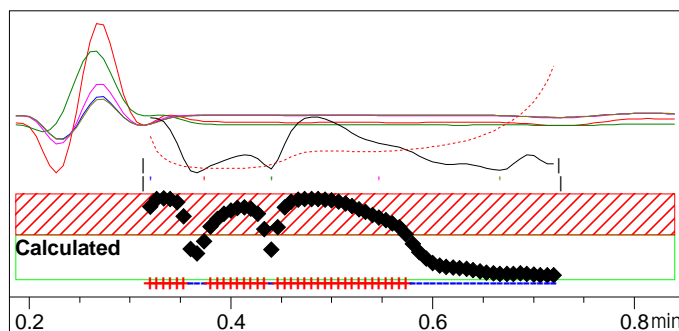
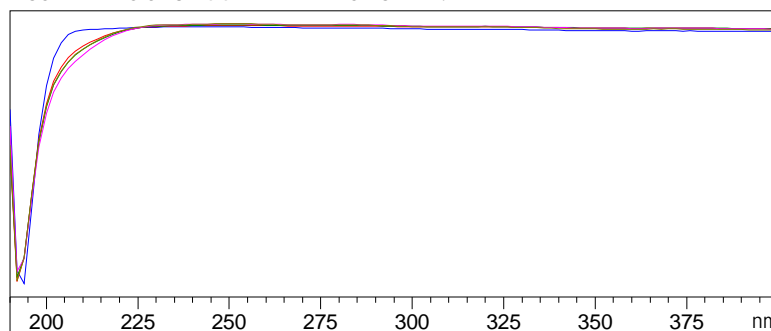
Warning : Spectral absorbances > 1000 mAU (see help for more information)

Sample Name: Cata_Op9V

Signal DAD1 E, Sig=280, 4 Ref=off (D:\Data\20...STEMPO_Op9VProduct_re 2023-09-07 15-17-08\003-D2F-F2-Cat



Peak : 2 at 0.441 min Name : ?



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

Purity factor : 987.624 (35 of 61 spectra exceed the calculated threshold limit.)

Threshold : 997.478 (Calculated with 35 of 61 spectra)

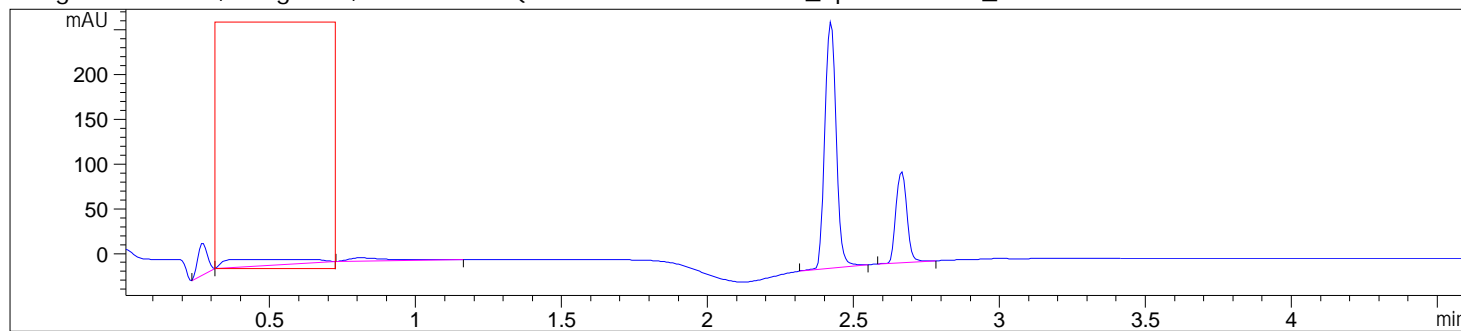
Reference : Peak start and end spectra (integrated) (0.313 / 0.727)

Spectra : 5 (Selection automatic, 5)

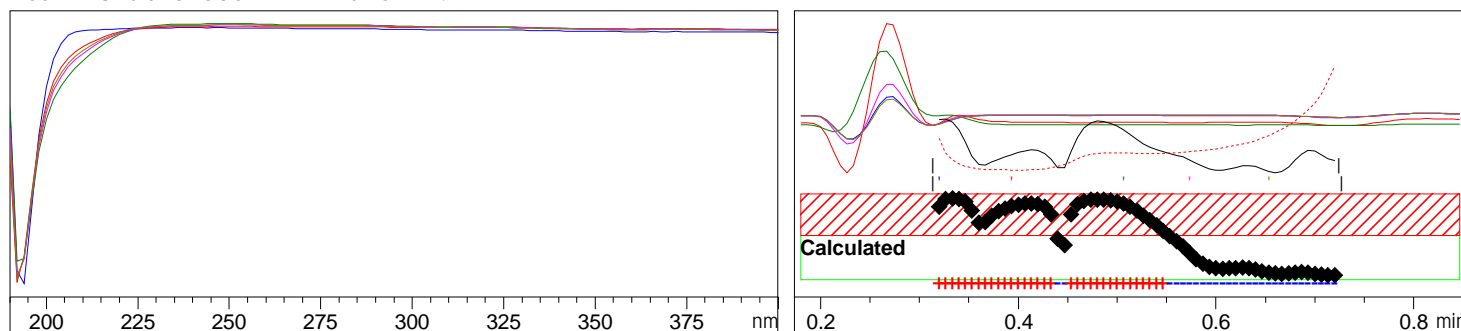
Noise Threshold: 0.983 (12 spectra, St.Dev 0.4105 + 3 * 0.1909)

Sample Name: Cata_Op9V

Signal DAD1 A, Sig=254, 4 Ref=off (D:\Data\20...STEMPO_Op9VProduct_re 2023-09-07 15-17-08\003-D2F-F2-Cat



Peak : 3 at 0.506 min Name : ?



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

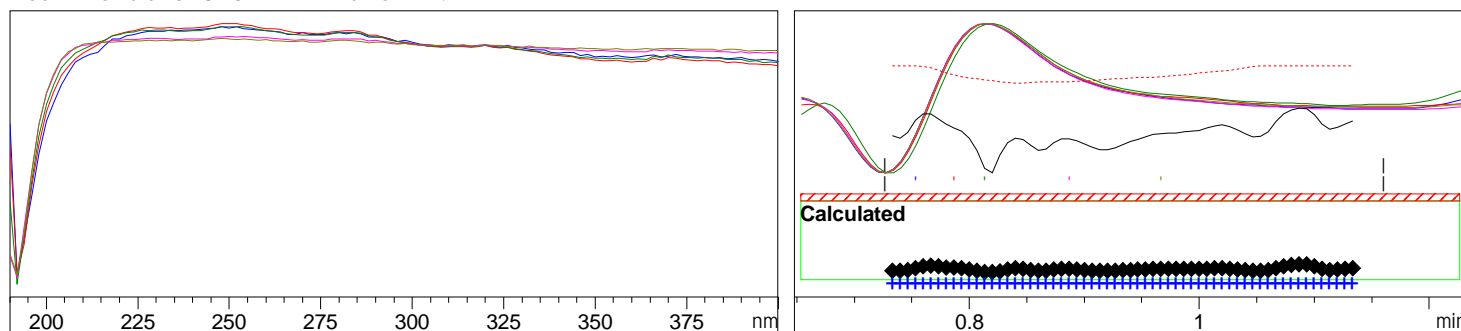
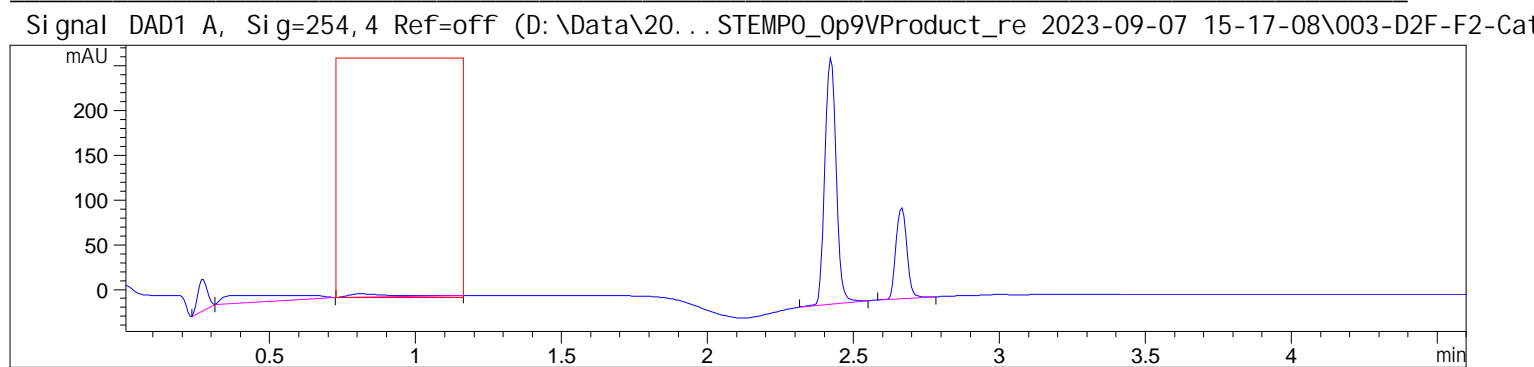
Purity factor : 988.396 (33 of 61 spectra exceed the calculated threshold limit.)

Threshold : 997.603 (Calculated with 33 of 61 spectra)

Reference : Peak start and end spectra (integrated) (0.313 / 0.727)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.983 (12 spectra, St.Dev 0.4105 + 3 * 0.1909)

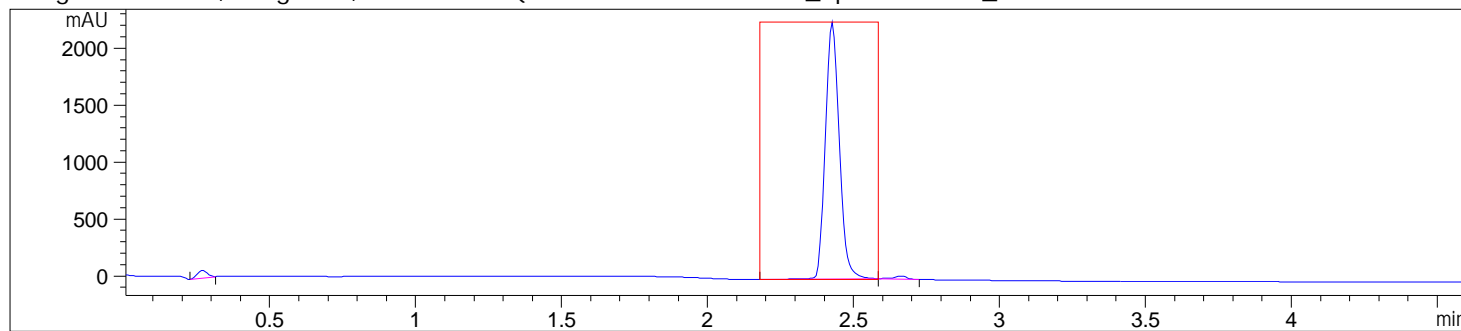


-> The purity factor is within the calculated threshold limit. <-

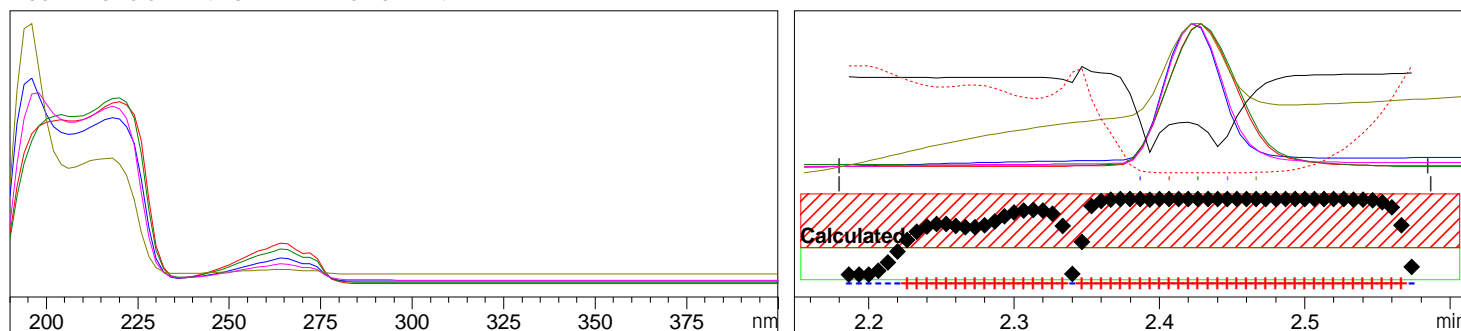
Purity factor : 959.834 (61 of 61 spectra are within the calculated threshold limit.)
Threshold : 284.824 (Calculated with 61 of 61 spectra)
Reference : Peak start and end spectra (integrated) (0.727 / 1.160)
Spectra : 5 (Selection automatic, 5)
Noise Threshold: 0.983 (12 spectra, St.Dev 0.4105 + 3 * 0.1909)

Sample Name: Cata_Op9V

Signal DAD1 B, Sig=220, 4 Ref=off (D:\Data\20...STEMPO_Op9VProduct_re 2023-09-07 15-17-08\003-D2F-F2-Cat



Peak : 6 at 2.426 min Name : ?



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

Purity factor : 624.040 (51 of 59 spectra exceed the calculated threshold limit.)

Threshold : 902.532 (Calculated with 51 of 59 spectra)

Reference : Peak start and end spectra (integrated) (2.180 / 2.587)

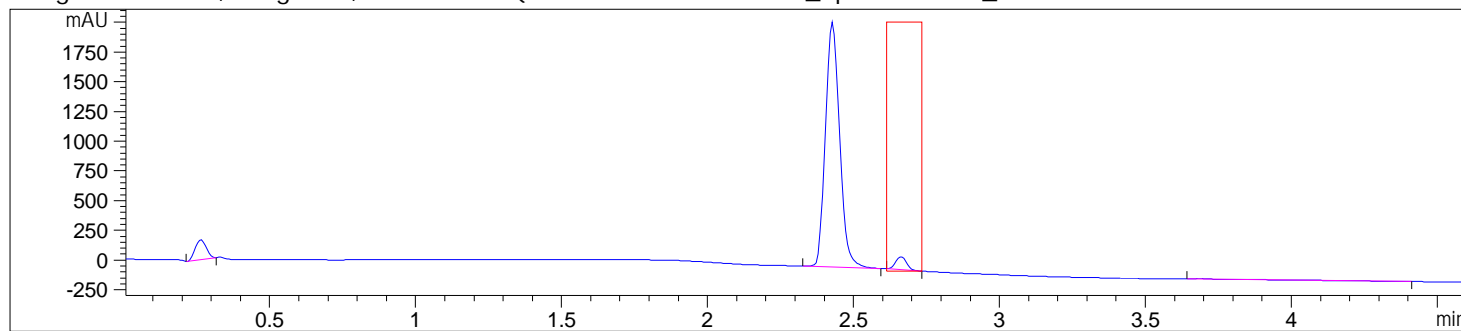
Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.983 (12 spectra, St.Dev 0.4105 + 3 * 0.1909)

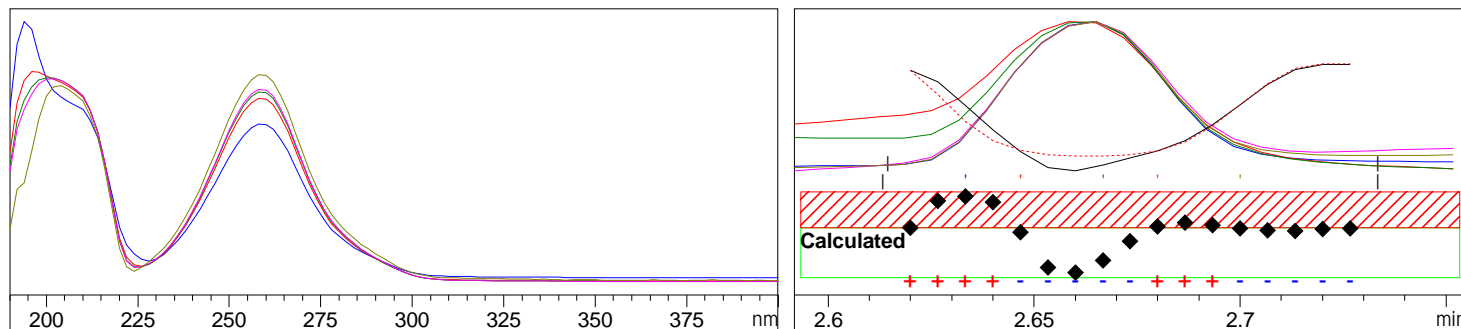
Warning : Spectral absorbances > 1000 mAU (see help for more information)

Sample Name: Cata_Op9V

Signal DAD1 C, Sig=210, 4 Ref=off (D:\Data\20...STEMPO_Op9VProduct_re 2023-09-07 15-17-08\003-D2F-F2-Cat



Peak : 8 at 2.664 min Name : ?



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

Purity factor : 856.685 (7 of 17 spectra exceed the calculated threshold limit.)

Threshold : 887.400 (Calculated with 7 of 17 spectra)

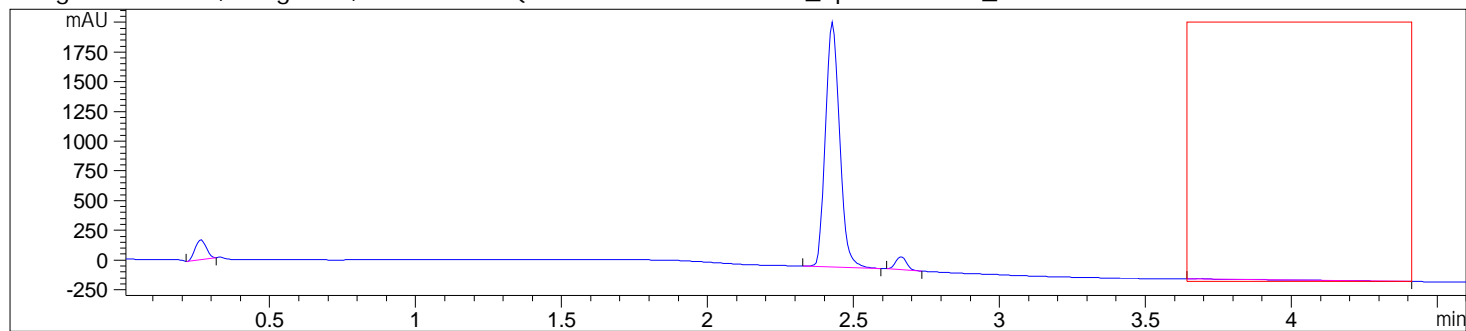
Reference : Peak start and end spectra (integrated) (2.613 / 2.733)

Spectra : 5 (Selection automatic, 5)

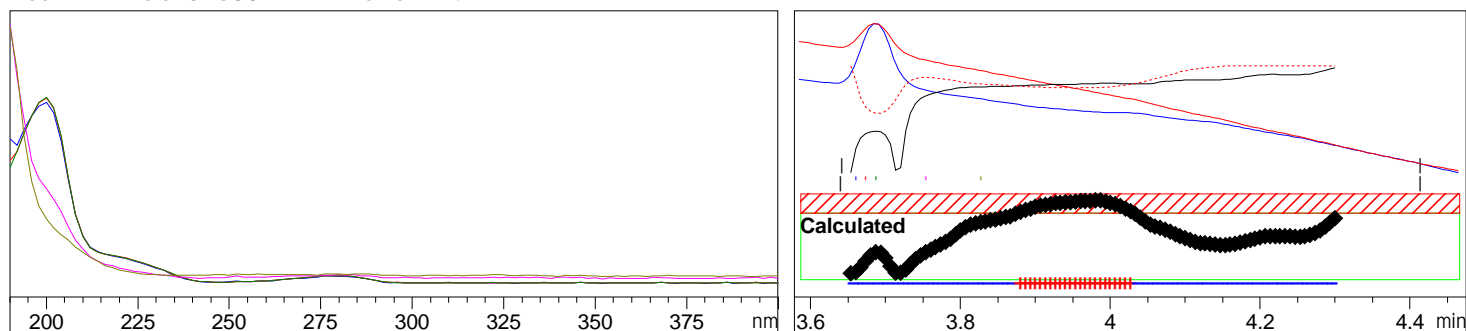
Noise Threshold: 0.983 (12 spectra, St.Dev 0.4105 + 3 * 0.1909)

Sample Name: Cata_Op9V

Signal DAD1 C, Sig=210, 4 Ref=off (D:\Data\20...STEMPO_Op9VProduct_re 2023-09-07 15-17-08\003-D2F-F2-Cat



Peak : 12 at 3.688 min Name : ?



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

Purity factor : 645.005 (23 of 98 spectra exceed the calculated threshold limit.)

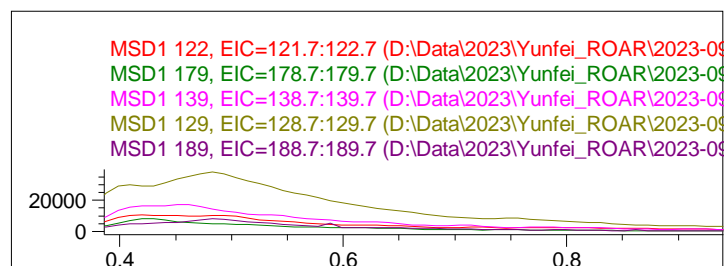
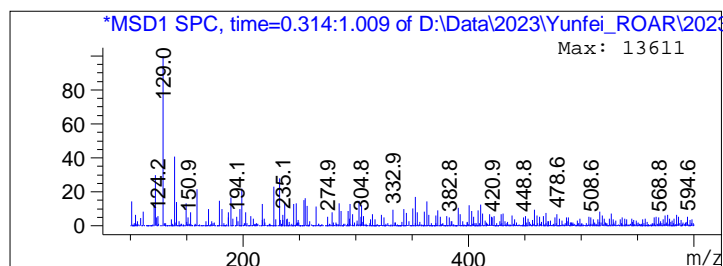
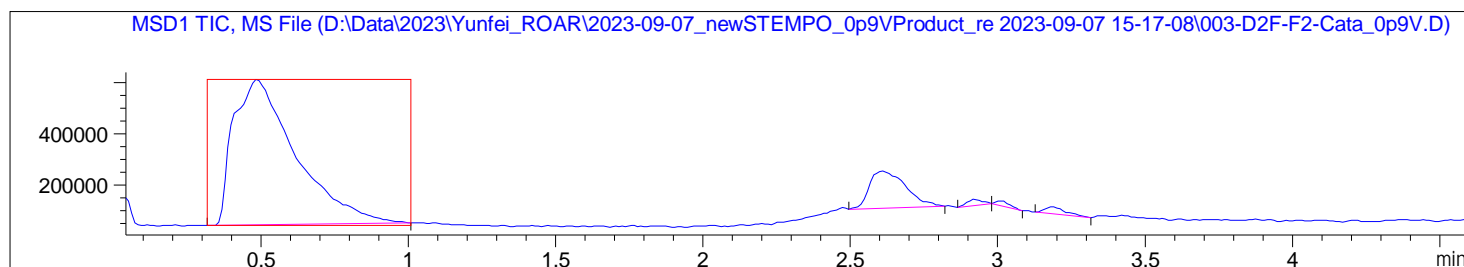
Threshold : 697.430 (Calculated with 23 of 98 spectra)

Reference : Peak start and end spectra (integrated) (3.640 / 4.413)

Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.983 (12 spectra, St.Dev 0.4105 + 3 * 0.1909)

Sample Name: Cata_Op9V

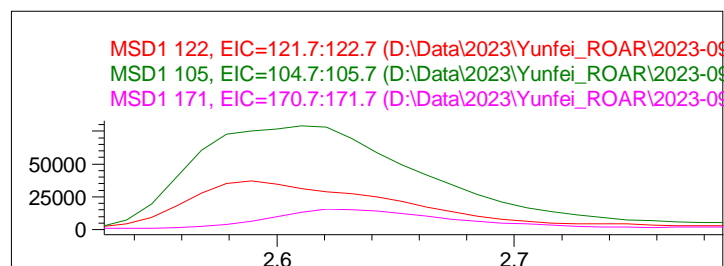
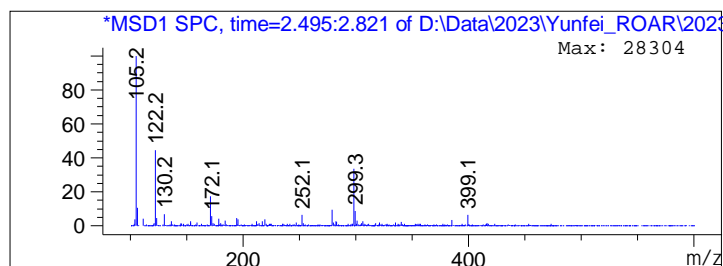
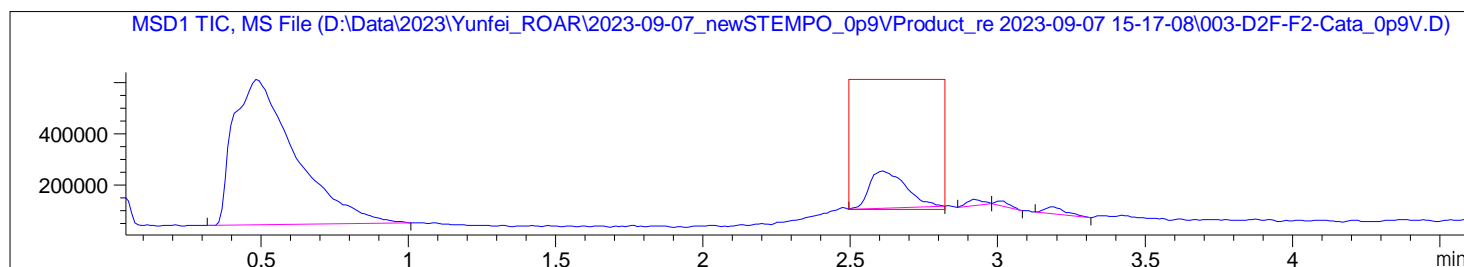


Peak #1 at 0.485 min (0.316 to 1.009 min)

-> The analysis found 6 components, indicating an impure peak. <-

Component 1: Peak at Scan 37.4. Top ions are 122 179
Component 2: Peak at Scan 40.5. Top ions are 139
Component 3: Peak at Scan 42.9. Top ions are 129 189 101
Component 4: Peak at Scan 44.1. Top ions are 232 254
Component 5: Peak at Scan 50.0. Top ions are 227
Component 6: Peak at Scan 73.9. Top ions are 202

Sample Name: Cata_Op9V



Peak #2 at 2.610 min (2.495 to 2.820 min)

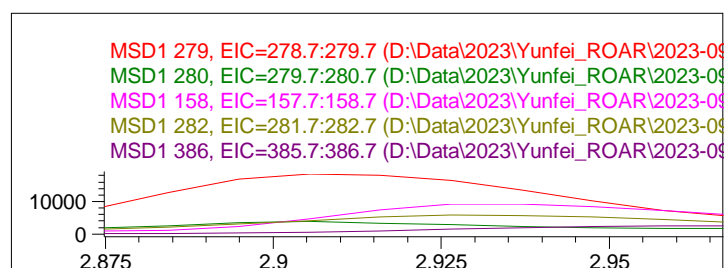
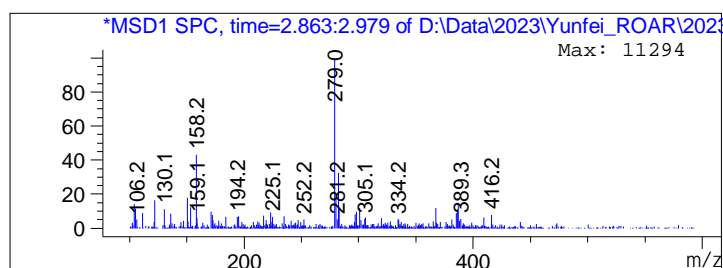
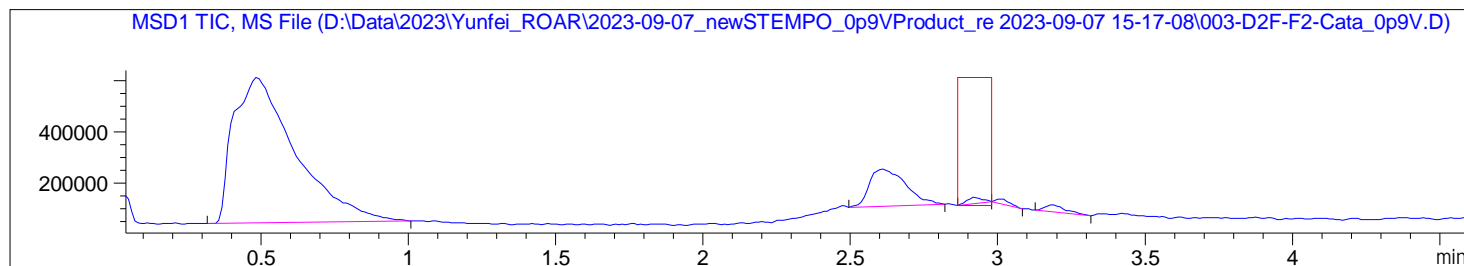
-> The analysis found 4 components, indicating an impure peak. <-

Component 1: Peak at Scan 243.0. Top ions are 122

Component 2: Peak at Scan 245.2. Top ions are 105

Component 3: Peak at Scan 246.5. Top ions are 171

Component 4: Peak at Scan 251.4. Top ions are 298



Peak #3 at 2.918 min (2.863 to 2.978 min)

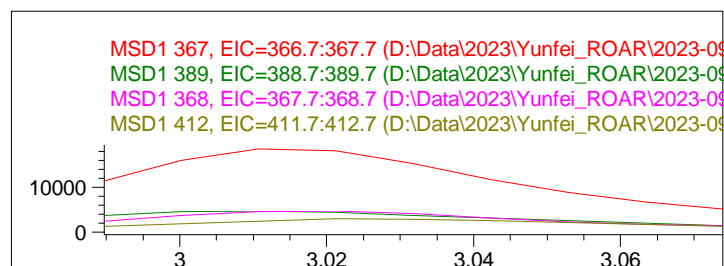
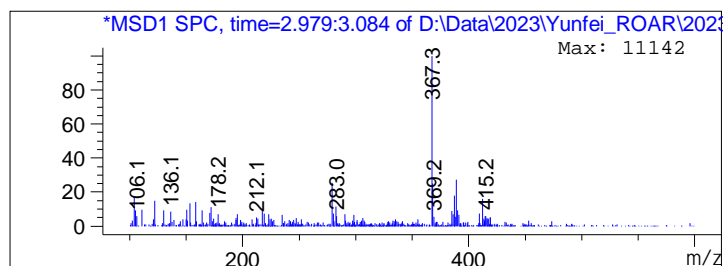
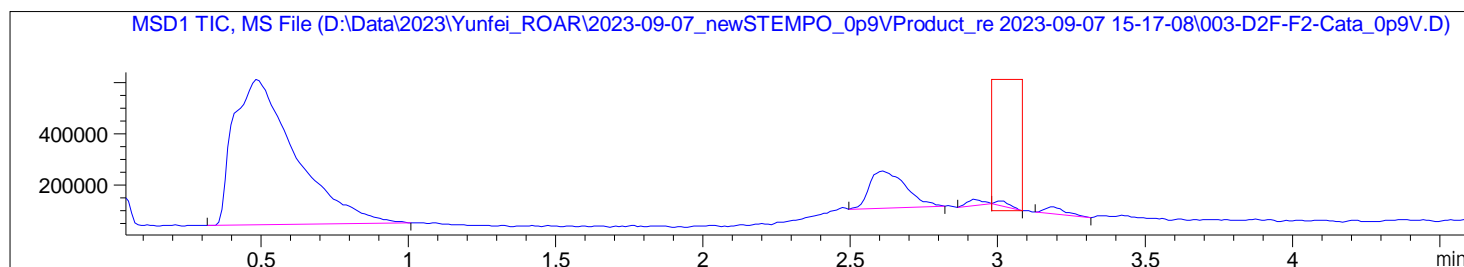
-> The analysis found 3 components, indicating an impure peak. <-

Component 1: Peak at Scan 273.2. Top ions are 279 280

Component 2: Peak at Scan 275.4. Top ions are 158 282

Component 3: Peak at Scan 278.3. Top ions are 386

Sample Name: Cata_Op9V



Peak #4 at 3.004 min (2.979 to 3.084 min)

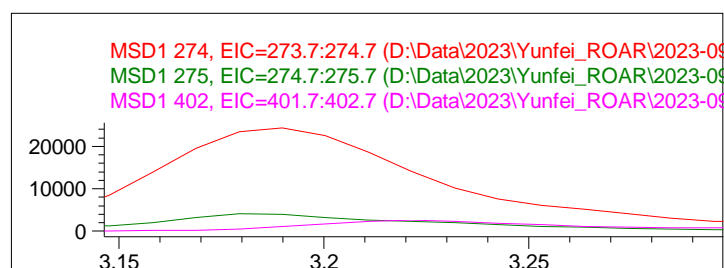
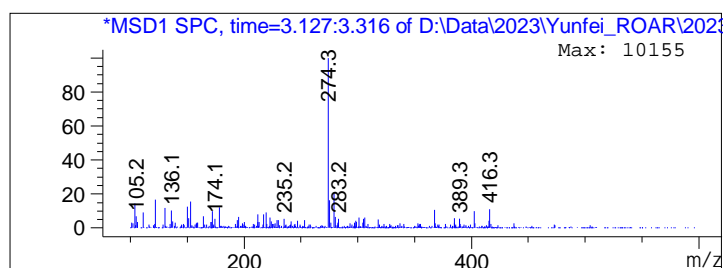
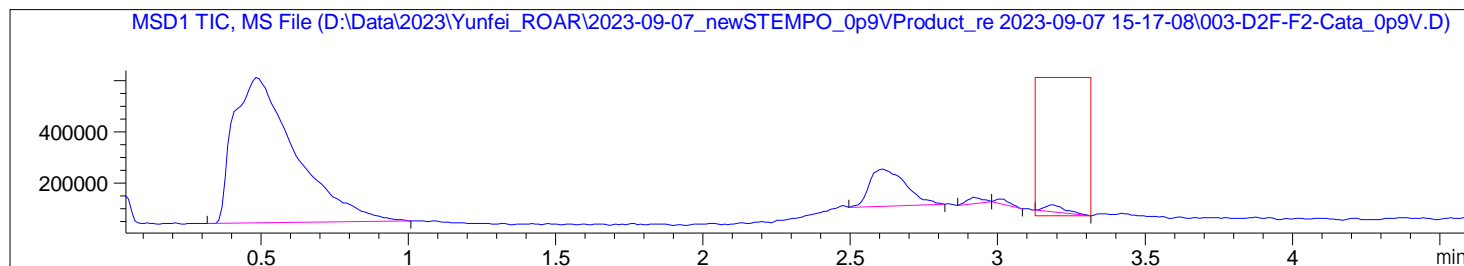
-> The analysis found 4 components, indicating an impure peak. <-

Component 1: Peak at Scan 283.1. Top ions are 367 389

Component 2: Peak at Scan 283.7. Top ions are 368

Component 3: Peak at Scan 284.4. Top ions are 412

Component 4: Peak at Scan 286.2. Top ions are 414



Peak #5 at 3.183 min (3.127 to 3.316 min)

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

Component 1: Peak at Scan 299.6. Top ions are 274 275

Component 2: Peak at Scan 302.9. Top ions are 402

*** End of Report ***