

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

```

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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
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: freshC03pH8\_1

```

=====
Acq. Operator   : user                      Seq. Line :    2
Sample Operator : user
Acq. Instrument : SFC LCMS                  Location  :   D2F-F1
Injection Date  : 07/09/2023 15:28:07      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)

=====

```

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       : 938
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	0.17	943.7 h
DAD 1, Visible Lamp	0.00	352.8 h

```

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

```

Sample Name: freshC03pH8\_1

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	8.0E-002	1.1E-001 µA
DryingGas	12	12 l/min
Neb Pres	35	35 psig
Turbo1Spd	100	100 %
Turbo1Pwr	127	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

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

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

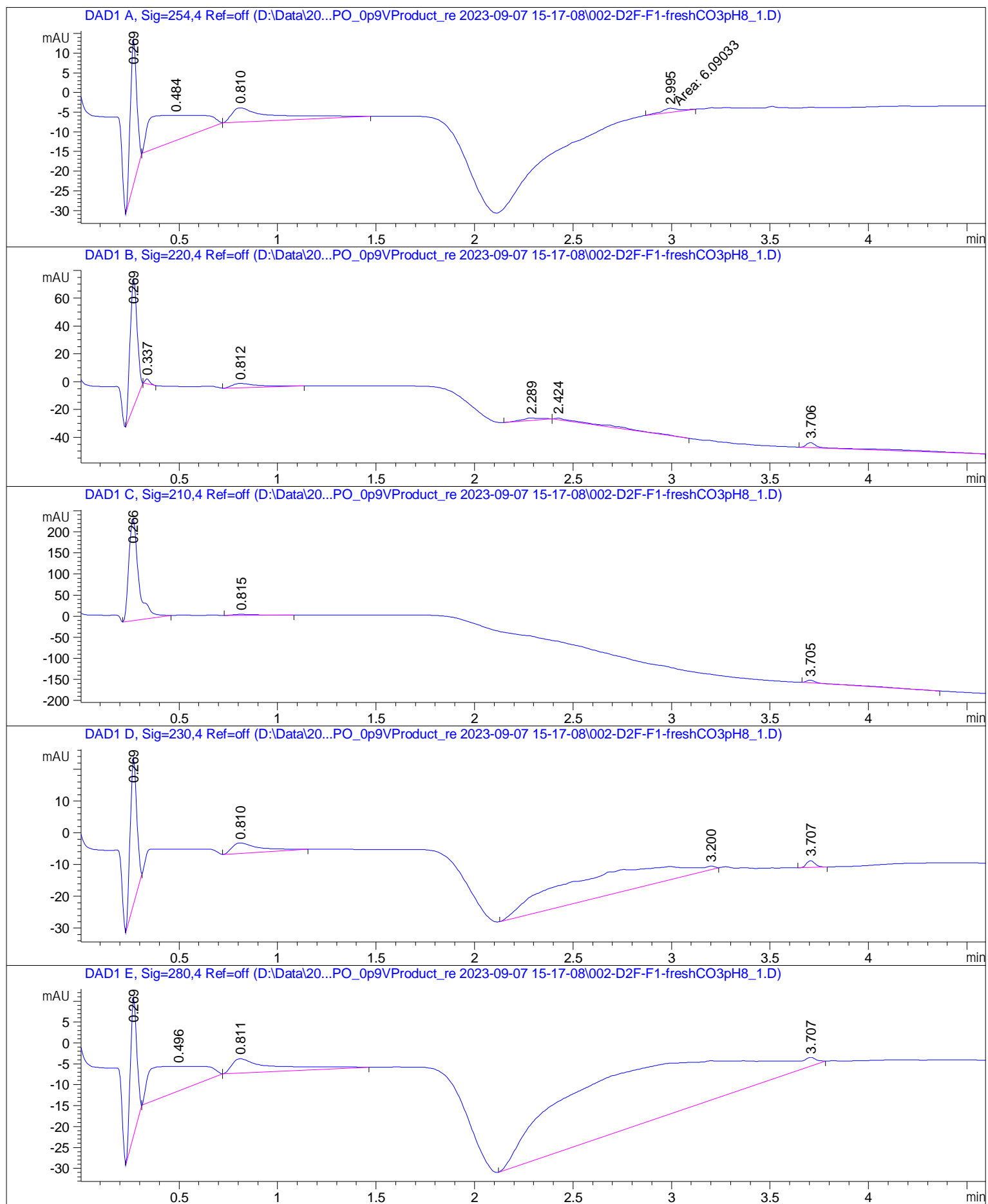
```

Run Logbook

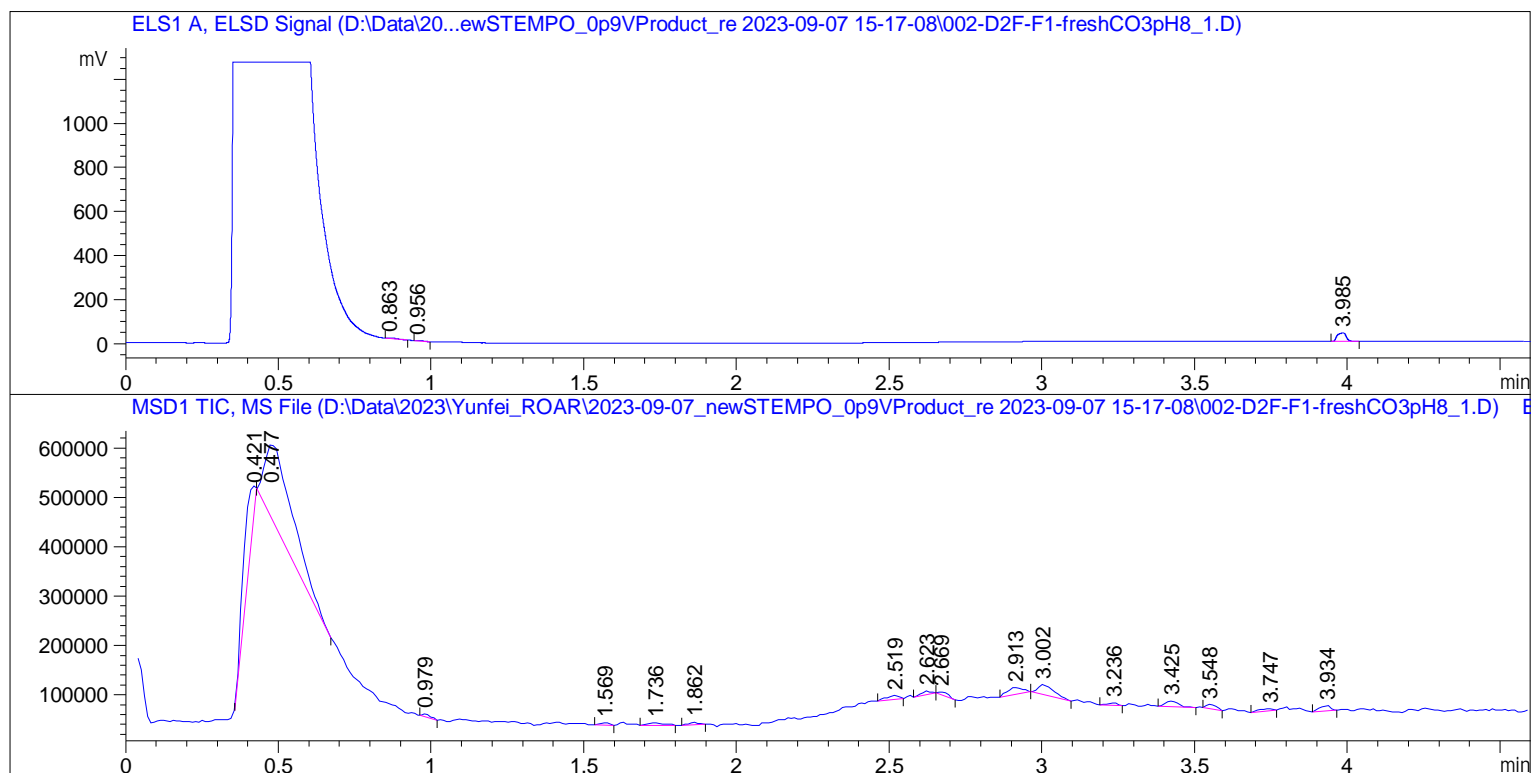
18 Sep 23 11:15 AM

Logbook File: D:\Data\20...EMPO\_0p9VProduct\_re 2023-09-07 15-17-08\002-D2F-F1-freshC03pH8\_1.D\RUN.LOG

Module	# Event Message	Date Time
Method	Method started: line# 2 at location 'D2F-F1>' ' inj # 1	07/09/2023 15:27:12
CP Macro	PreRun macro: 'LAMPALL ON'	07/09/2023 15:27:13
G4260B	G4260B: ELSD - Autozero	07/09/2023 15:27:14
G4260B	G4260B: ELSD - Al ready switched on	07/09/2023 15:27:14
Method	Instrument running sample from location D2F-> F1	07/09/2023 15:27:14
G7115A	G7115A: DEAC605436 - Detector: Prepare	07/09/2023 15:27:25
G7115A	G7115A: DEAC605436 - Detector: Idle	07/09/2023 15:27:41
G4767A	G4767A: DEAFD00218 - Draw command finished	07/09/2023 15:27:58
G4767A	G4767A: DEAFD00218 - Sampler wash is active	07/09/2023 15:27:59
G4767A	G4767A: DEAFD00218 - Sampler wash is idle	07/09/2023 15:28:05
G4767A	G4767A: DEAFD00218 - Sample preparation time: > 24 sec	07/09/2023 15:28:05
PumpVal ve	G7111B: DEAEW03495 - Run	07/09/2023 15:28:07
PumpVal ve	G7111B: DEAEW03495 - Postrun	07/09/2023 15:32:43
G4767A	G4767A: DEAFD00218 - Postrun	07/09/2023 15:32:44
PumpVal ve	G1170A: DEBAD03715 - Postrun	07/09/2023 15:32:44
G1170A	G1170A: DEBAD03734 - Postrun	07/09/2023 15:32:45
G4782A	G4782A: DEAGN00153 - Postrun	07/09/2023 15:32:45
G7110B	G7110B: DEAEH00761 - Postrun	07/09/2023 15:32:45
G7116A	G7116A: DEAEH00895 - Postrun	07/09/2023 15:32:46
Method	Saving Method COL1_5NH4FA_MECN_5T095_1MIN_10> 0-600MS_POS.M	07/09/2023 15:34:51
Method	Instrument run completed	07/09/2023 15:34:52
CP Macro	Analyzing rawdata 002-D2F-F1-freshC03pH8_1.D	07/09/2023 15:34:52
Method	Saving Method DA.M	07/09/2023 15:34:54
Method	Method completed	07/09/2023 15:35:06



Sample Name: freshCO3pH8\_1



=====  
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	0.0363	83.22035	36.87815	31.3903
2	0.484	BB	0.2400	124.42250	6.36617	46.9315
3	0.810	BB	0.1926	51.38168	3.59887	19.3809
4	2.995	MM	0.0964	6.09033	1.05242	2.2972

Totals : 265.11486 47.89562

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	0.0389	228.23611	91.99763	69.3485
2	0.337	BB	0.0273	5.94732	3.59642	1.8071
3	0.812	BB	0.1345	28.45421	3.05903	8.6457
4	2.289	BB	0.0894	11.77590	1.82186	3.5781
5	2.424	BB	0.2790	23.99381	1.05641	7.2904

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
6	3.706	BBA	0.1101	30.70739	3.65192	9.3303

Totals : 329.11475 105.18327

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	0.0524	845.48145	244.19980	93.3795
2	0.815	BB	0.1273	21.08284	2.47752	2.3285
3	3.705	BBA	0.0800	38.86070	6.66450	4.2920

Totals : 905.42499 253.34181

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	0.0369	105.71169	45.90547	23.1533
2	0.810	BB	0.1374	31.38926	3.28784	6.8750
3	3.200	BB	3.4959	313.16974	1.04872	68.5915
4	3.707	BB	0.0460	6.30122	2.16085	1.3801

Totals : 456.57190 52.40288

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.269	BB	0.0364	74.79455	33.10353	6.7113
2	0.496	BB	0.2472	118.53276	5.87919	10.6359
3	0.811	BB	0.1952	48.93298	3.41371	4.3907
4	3.707	BB	4.8526	872.20386	2.10215	78.2622

Totals : 1114.46415 44.49858

Signal 6: ELS1 A, ELSD Signal

Peak #	RetTime [min]	Type	Width [min]	Area [mV*s]	Height [mV]	Area %
1	0.863	BB	0.0341	5.53911	2.11425	6.6706
2	0.956	BB	0.0287	3.46343	1.78228	4.1709



Sample Name: freshC03pH8\_1

Peak #	RetTime [min]	Type	Width [min]	Area [mV*s]	Height [mV]	Area %
3	3.985	BB	0.0335	74.03541	36.68142	89.1585

Totals :                                      83.03795    40.57795

Signal 7: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.421	BB	0.0938	3.29168e5	4.87971e4	19.6970
2	0.477	BB	0.0975	1.01559e6	1.50953e5	60.7716
3	0.979	BB	0.0359	1.07122e4	4971.00781	0.6410
4	1.569	BB	0.0423	1.25348e4	5581.93115	0.7501
5	1.736	BB	0.0567	2.05227e4	5066.68018	1.2281
6	1.862	BB	0.0354	1.09839e4	5617.96191	0.6573
7	2.519	BB	0.0516	2.16694e4	7742.08984	1.2967
8	2.623	BB	0.0346	1.49646e4	6951.84668	0.8955
9	2.669	BB	0.0459	1.29375e4	4539.81641	0.7742
10	2.913	BB	0.0496	4.59956e4	1.33854e4	2.7523
11	3.002	BB	0.0567	7.11826e4	2.02983e4	4.2595
12	3.236	BB	0.0407	1.02282e4	4788.66748	0.6120
13	3.425	BB	0.0552	3.32230e4	1.07091e4	1.9880
14	3.548	BB	0.0465	2.14972e4	8387.64648	1.2864
15	3.747	BB	0.0473	1.33409e4	4071.89600	0.7983
16	3.934	BB	0.0409	2.66084e4	1.09928e4	1.5922

Totals :                                      1.67116e6    3.12855e5

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Summed Peaks Report

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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.

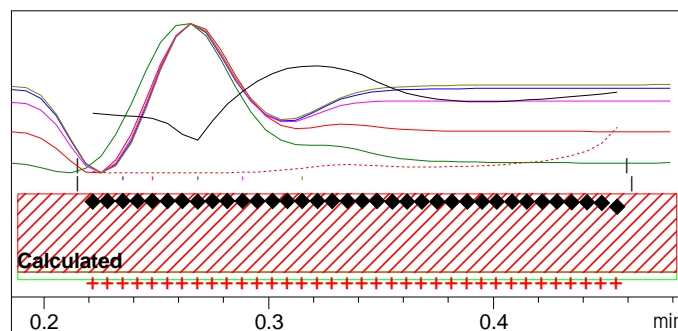
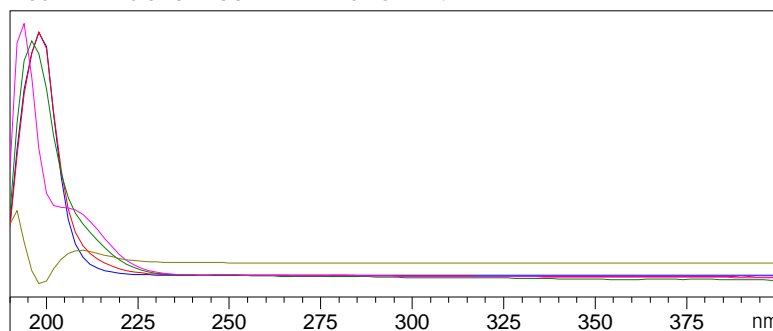
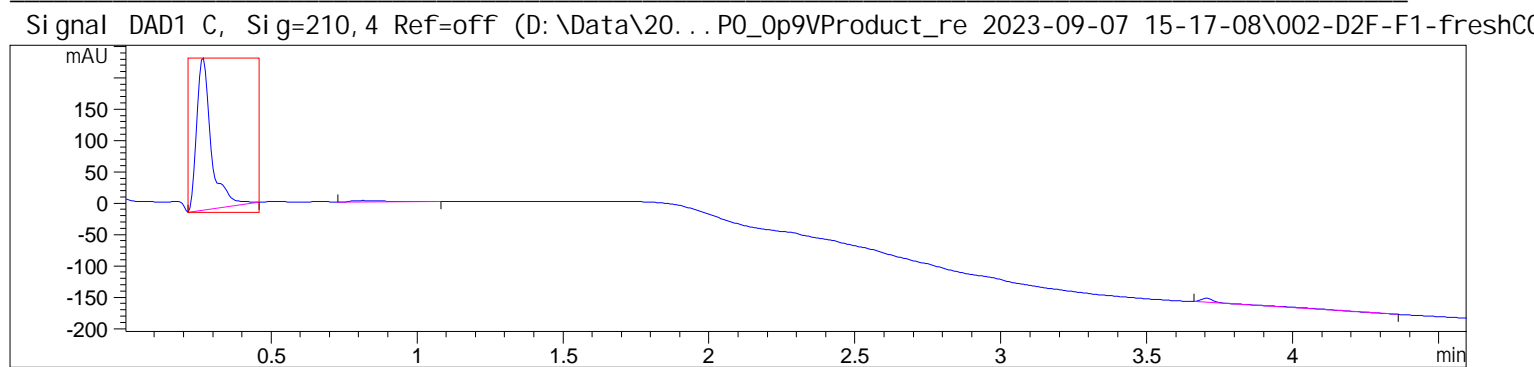
Signal 7: MSD1 TIC, MS File  
Empty table.

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Final Summed Peaks Report

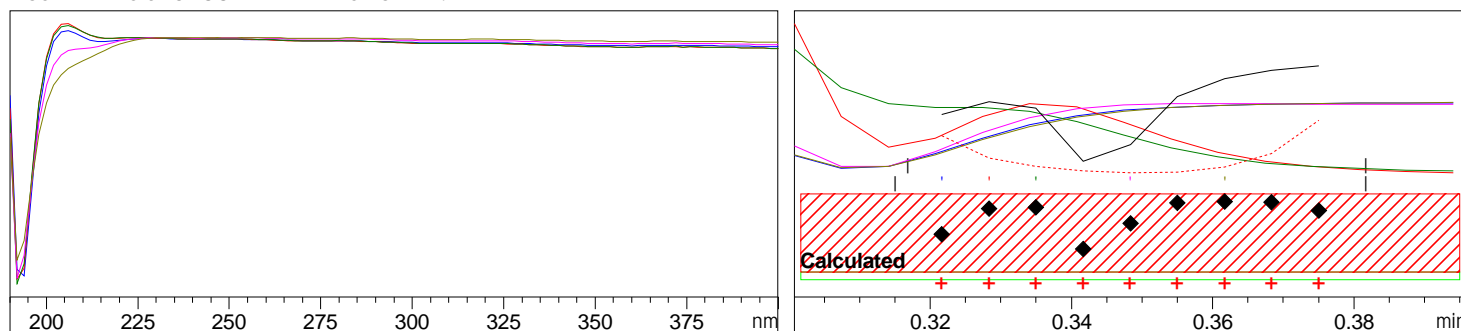
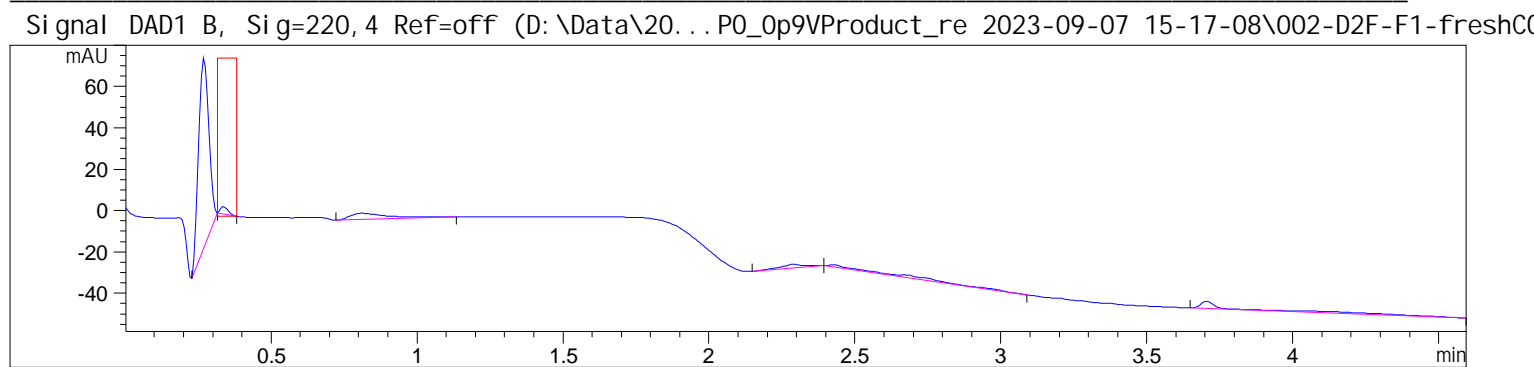
=====

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



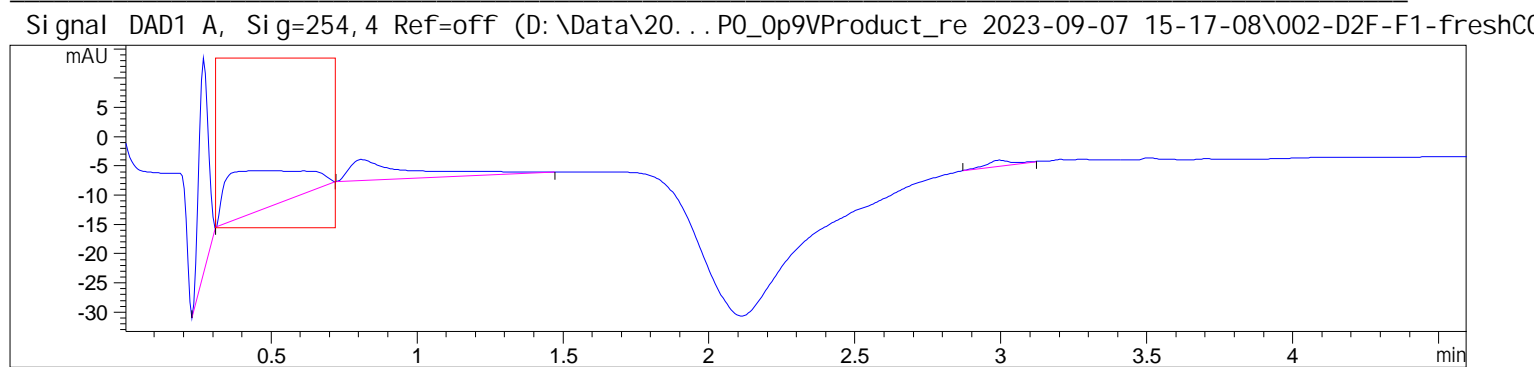
-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 765.384 (36 of 36 spectra exceed the calculated threshold limit.)  
Threshold : 999.280 (Calculated with 36 of 36 spectra)  
Reference : Peak start and end spectra (integrated) (0.215 / 0.462)  
Spectra : 5 (Selection automatic, 5)  
Noise Threshold : 0.374 (12 spectra, St.Dev 0.1702 + 3 \* 0.068)  
Warning : Spectral absorbances > 1000 mAU (see help for more information)

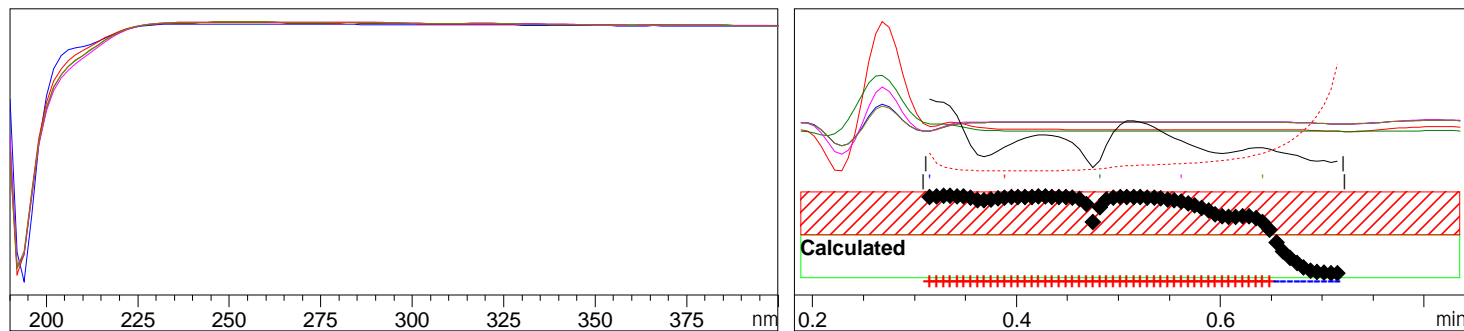


-> The purity factor exceeds the calculated threshold limit. <-

Purity factor : 970.453 (9 of 9 spectra exceed the calculated threshold limit.)  
Threshold : 996.038 (Calculated with 9 of 9 spectra)  
Reference : Peak start and end spectra (integrated) (0.315 / 0.382)  
Spectra : 5 (Selection automatic, 5)  
Noise Threshold: 0.374 (12 spectra, St.Dev 0.1702 + 3 \* 0.068)



Peak : 4 at 0.484 min Name : ?



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

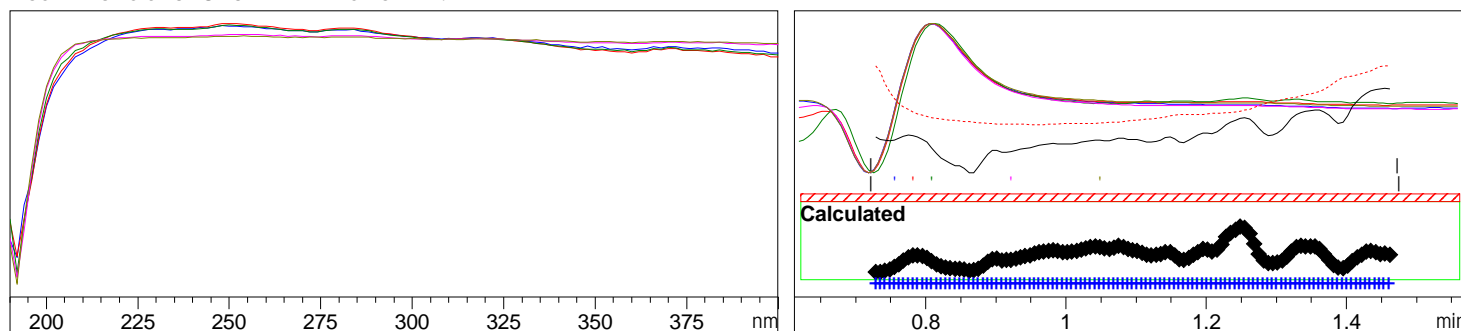
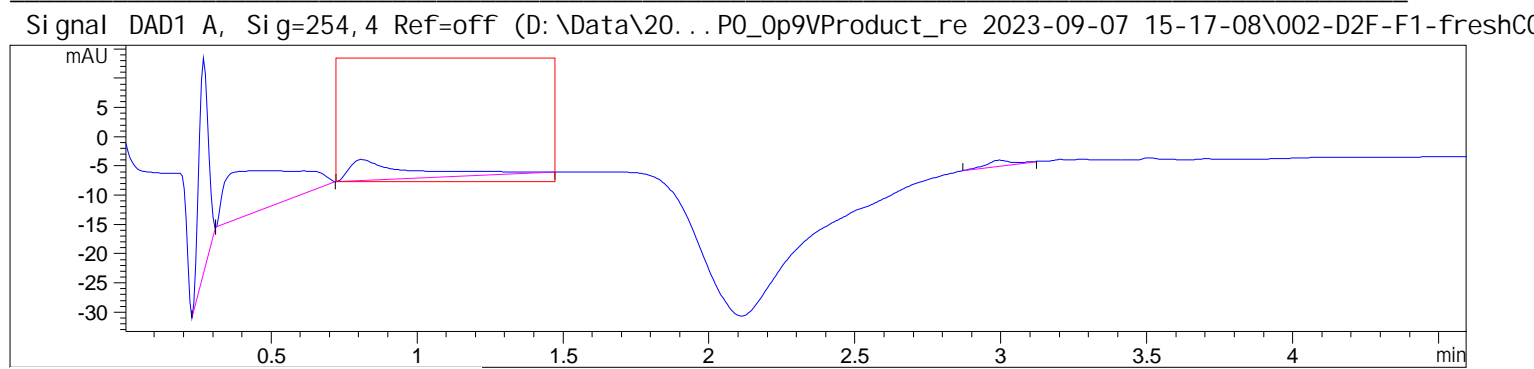
Purity factor : 995.747 (51 of 61 spectra exceed the calculated threshold limit.)

Threshold : 999.694 (Calculated with 51 of 61 spectra)

Reference : Peak start and end spectra (integrated) (0.308 / 0.722)

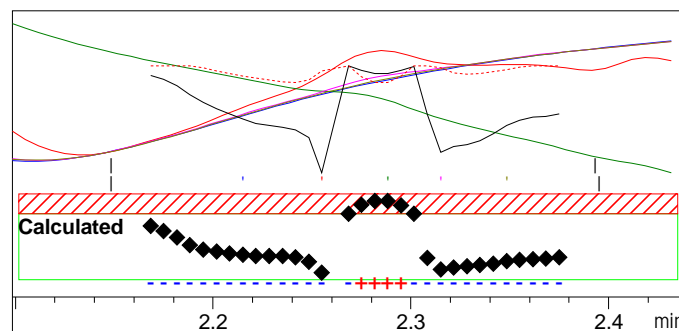
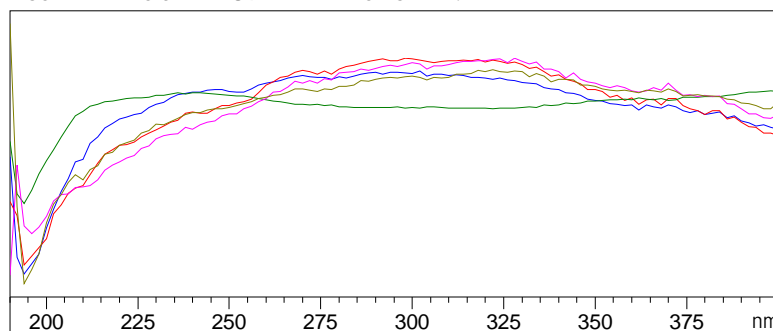
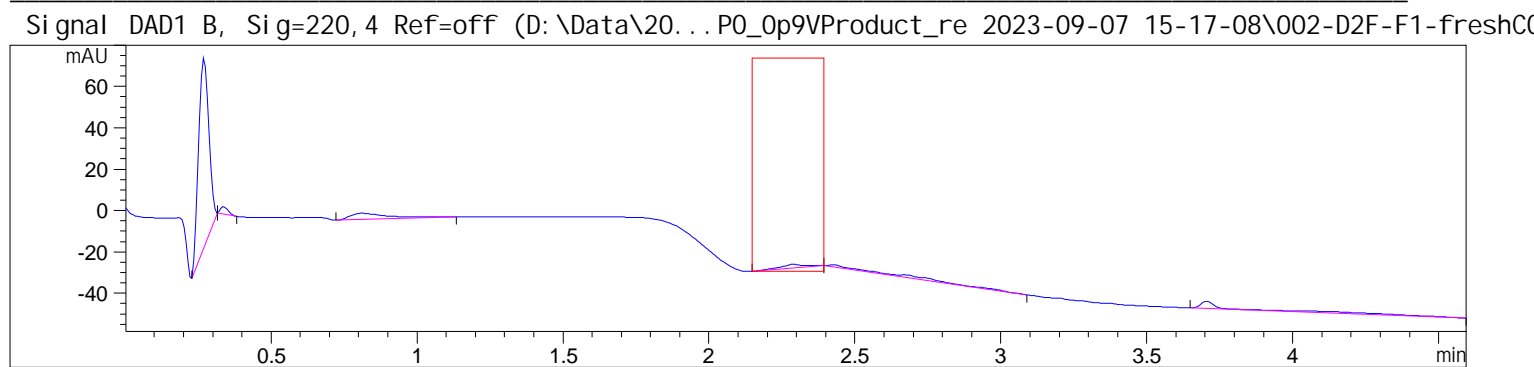
Spectra : 5 (Selection automatic, 5)

Noise Threshold: 0.374 (12 spectra, St.Dev 0.1702 + 3 \* 0.068)



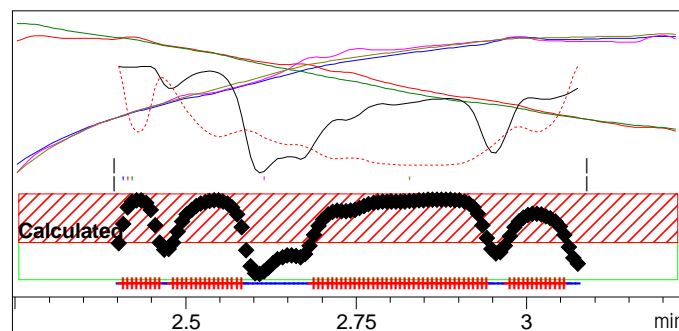
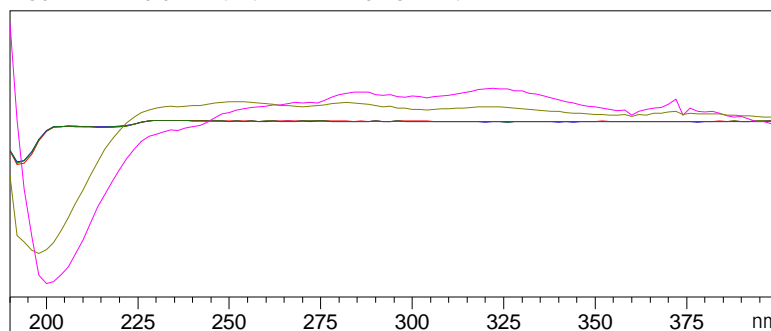
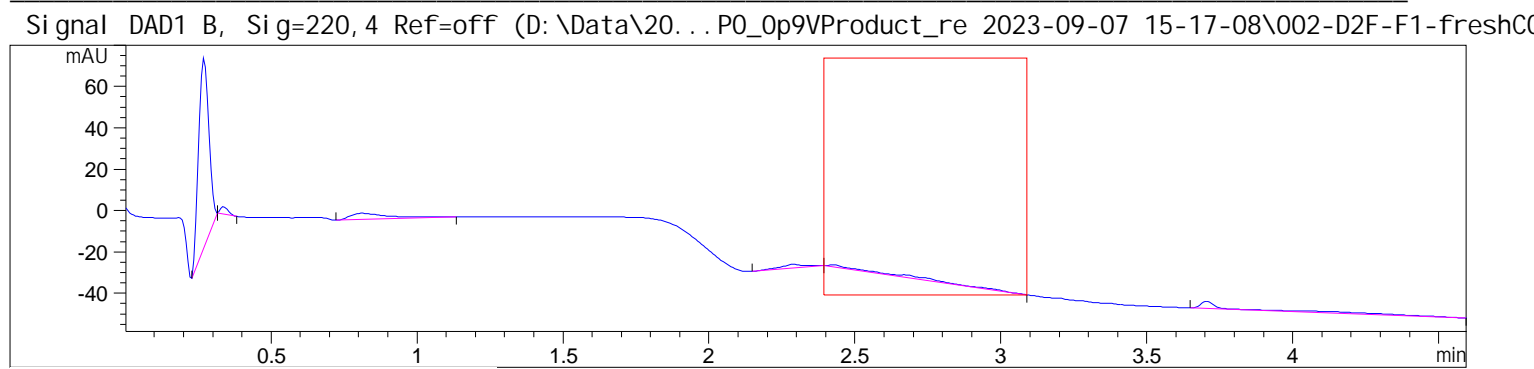
-> The purity factor is within the calculated threshold limit. <-

Purity factor : 964.030 (111 of 111 spectra are within the calculated threshold limit.)  
Threshold : 837.531 (Calculated with 111 of 111 spectra)  
Reference : Peak start and end spectra (integrated) (0.722 / 1.475)  
Spectra : 5 (Selection automatic, 5)  
Noise Threshold: 0.374 (12 spectra, St.Dev 0.1702 + 3 \* 0.068)



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

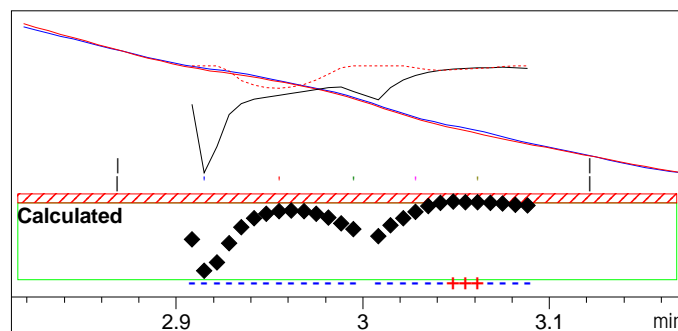
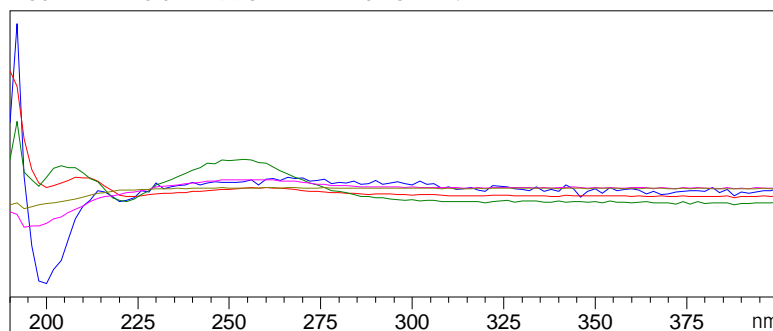
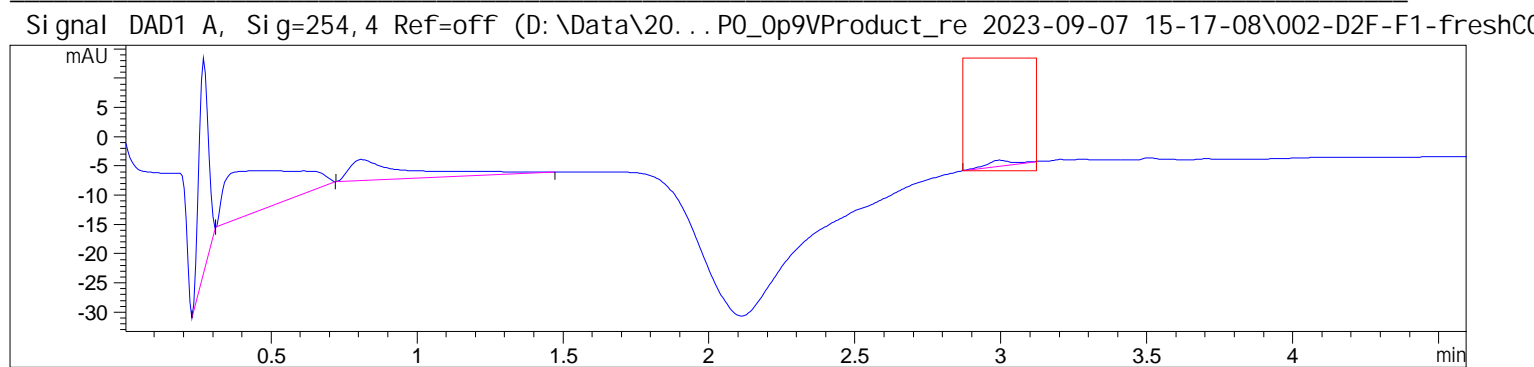
Purity factor : 123.804 (4 of 31 spectra exceed the calculated threshold limit.)  
Threshold : 263.961 (Calculated with 4 of 31 spectra)  
Reference : Peak start and end spectra (integrated) (2.148 / 2.395)  
Spectra : 5 (Selection automatic, 5)  
Noise Threshold: 0.374 (12 spectra, St.Dev 0.1702 + 3 \* 0.068)



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

Purity factor : 451.635 (77 of 102 spectra exceed the calculated threshold limit.)  
Threshold : 764.524 (Calculated with 77 of 102 spectra)  
Reference : Peak start and end spectra (integrated) (2.395 / 3.088)  
Spectra : 5 (Selection automatic, 5)  
Noise Threshold: 0.374 (12 spectra, St.Dev 0.1702 + 3 \* 0.068)



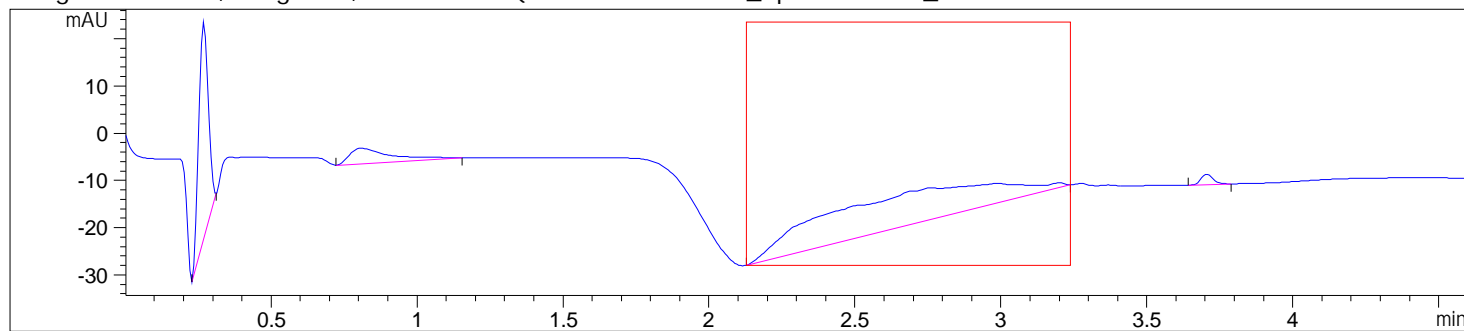


-> The purity factor exceeds the calculated threshold limit. <-

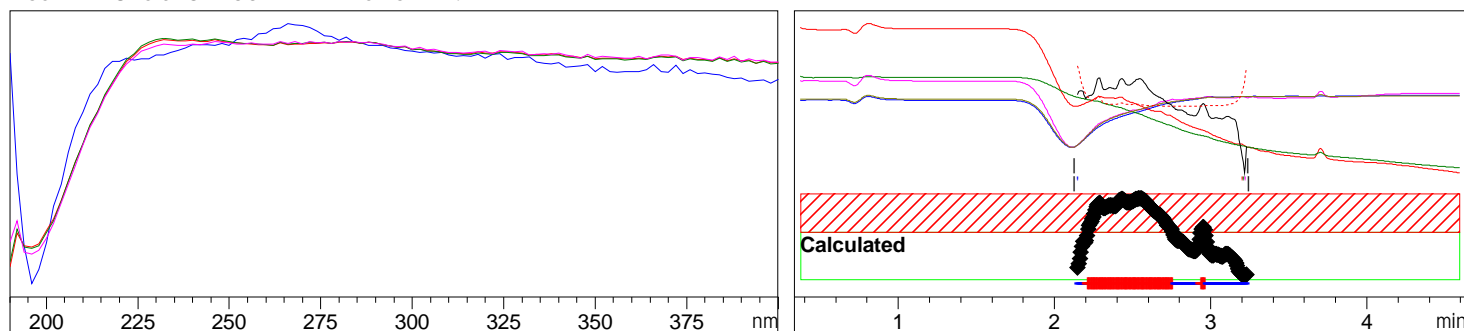
Purity factor : 34.399 (3 of 27 spectra exceed the calculated threshold limit.)  
Threshold : 42.439 (Calculated with 3 of 27 spectra)  
Reference : Peak start and end spectra (integrated) (2.868 / 3.122)  
Spectra : 5 (Selection automatic, 5)  
Noise Threshold : 0.374 (12 spectra, St.Dev 0.1702 + 3 \* 0.068)

Sample Name: freshC03pH8\_1

Signal DAD1 D, Sig=230, 4 Ref=off (D:\Data\20...P0\_0p9VProduct\_re 2023-09-07 15-17-08\002-D2F-F1-freshC03pH8\_1.D)



Peak : 18 at 3.200 min Name : ?



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

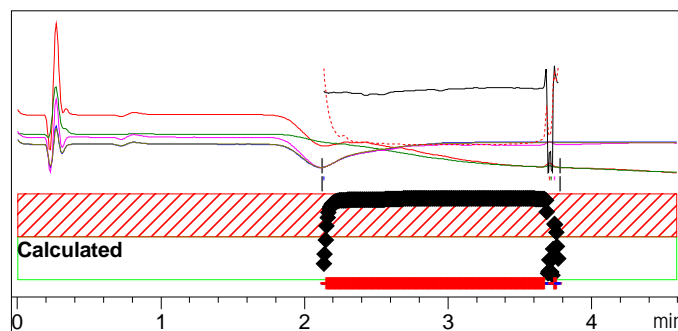
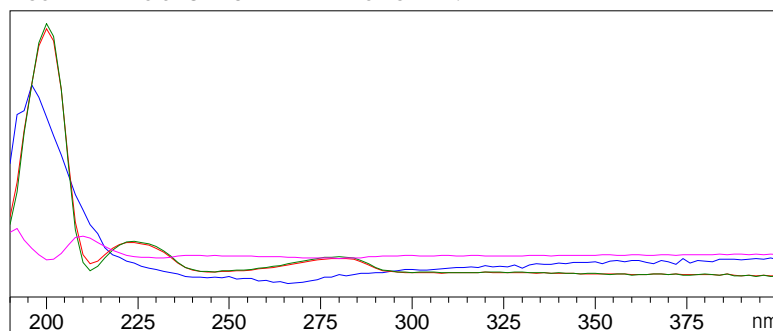
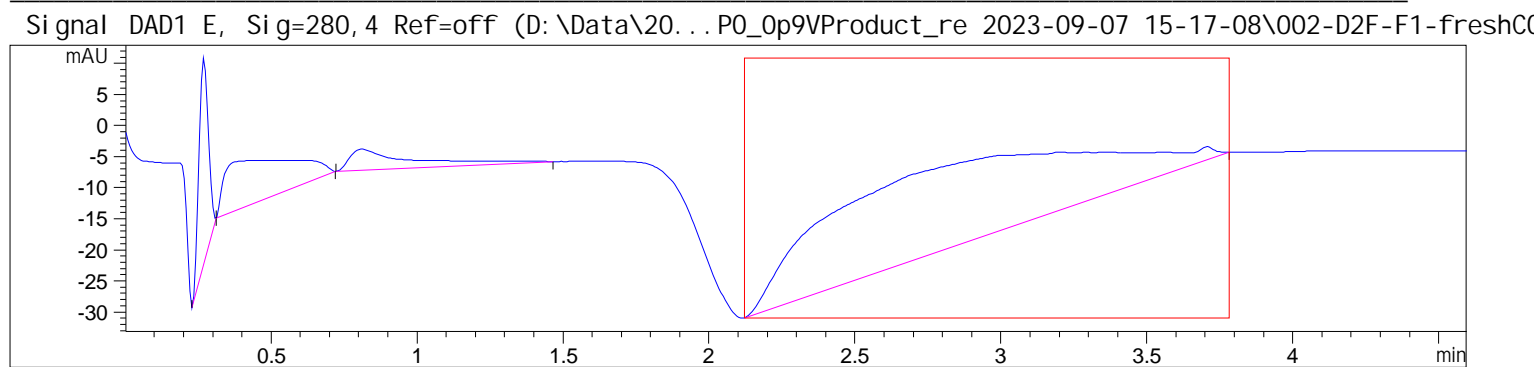
Purity factor : 727.082 (86 of 163 spectra exceed the calculated threshold limit.)

Threshold : 896.351 (Calculated with 86 of 163 spectra)

Reference : Peak start and end spectra (integrated) (2.128 / 3.242)

Spectra : 4 (Selection automatic, 5)

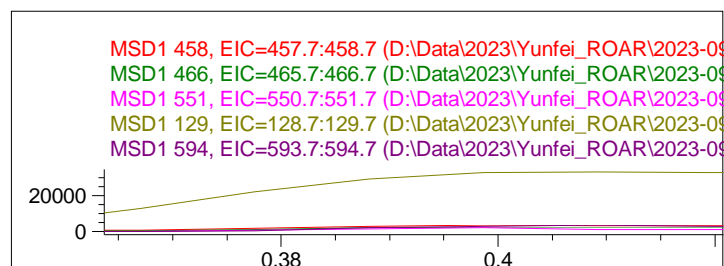
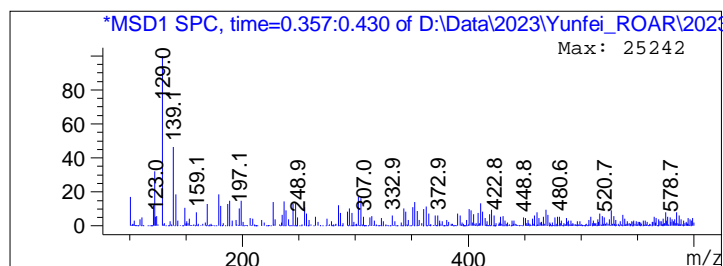
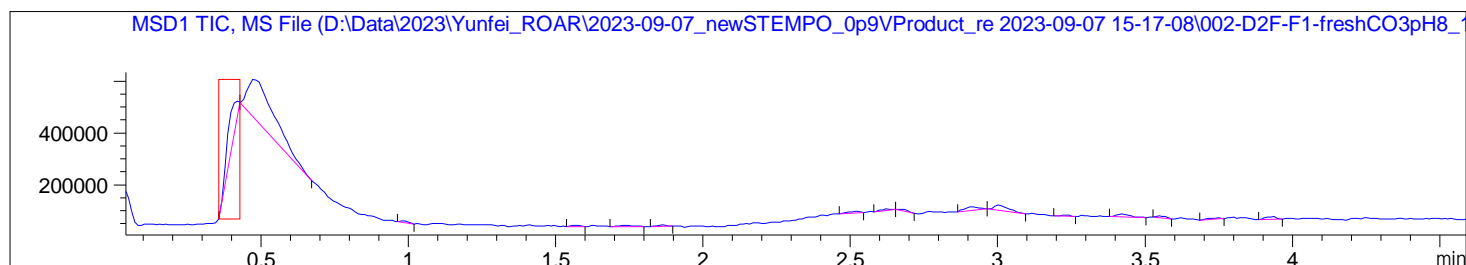
Noise Threshold: 0.374 (12 spectra, St.Dev 0.1702 + 3 \* 0.068)



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

Purity factor : 682.541 (234 of 246 spectra exceed the calculated threshold limit.)  
Threshold : 965.993 (Calculated with 234 of 246 spectra)  
Reference : Peak start and end spectra (integrated) (2.122 / 3.782)  
Spectra : 4 (Selection automatic, 5)  
Noise Threshold: 0.374 (12 spectra, St.Dev 0.1702 + 3 \* 0.068)

Sample Name: freshCO3pH8\_1



Peak #1 at 0.421 min ( 0.357 to 0.428 min)

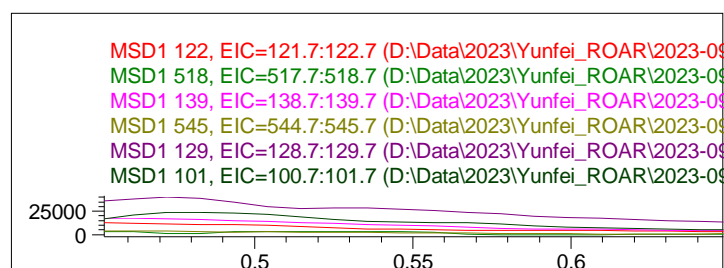
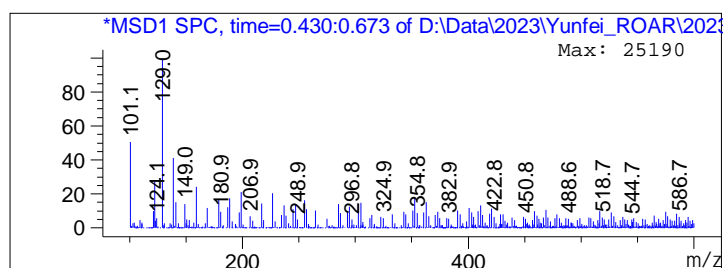
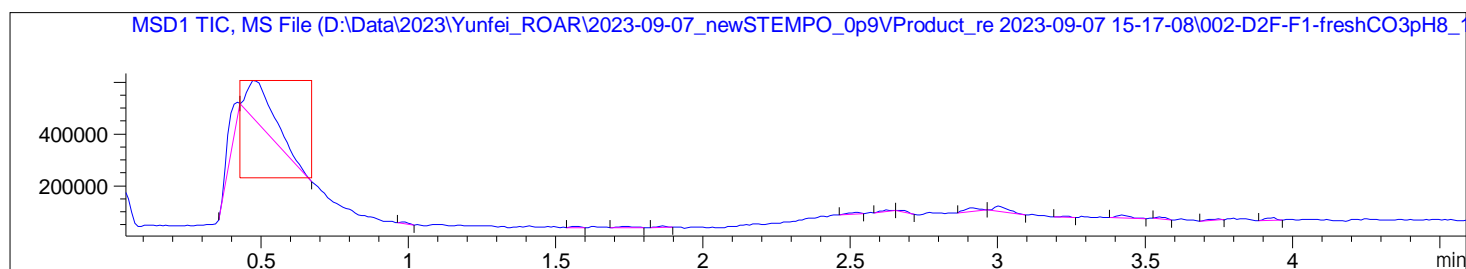
-&gt; The analysis found 4 components, indicating an impure peak. &lt;-

Component 1: Peak at Scan 33.0. Top ions are 458

Component 2: Peak at Scan 34.5. Top ions are 466 551 515

Component 3: Peak at Scan 35.8. Top ions are 129 594 573

Component 4: Peak at Scan 36.9. Top ions are 139 179 303



Peak #2 at 0.477 min ( 0.428 to 0.673 min)

-&gt; The analysis found 9 components, indicating an impure peak. &lt;-

Component 1: Peak at Scan 39.8. Top ions are 122 518 580

Component 2: Peak at Scan 41.4. Top ions are 139 545 540

Component 3: Peak at Scan 42.6. Top ions are 129 101 189

Component 4: Peak at Scan 43.8. Top ions are 564 577 149

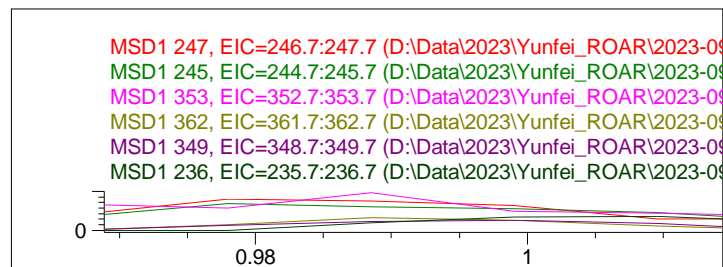
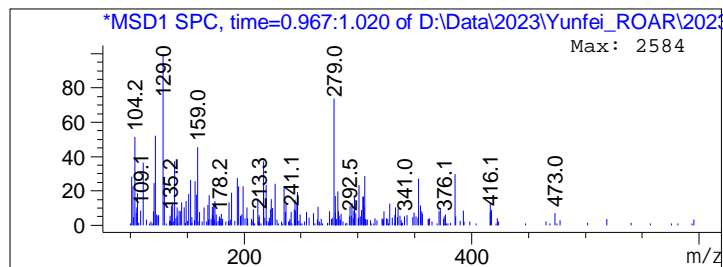
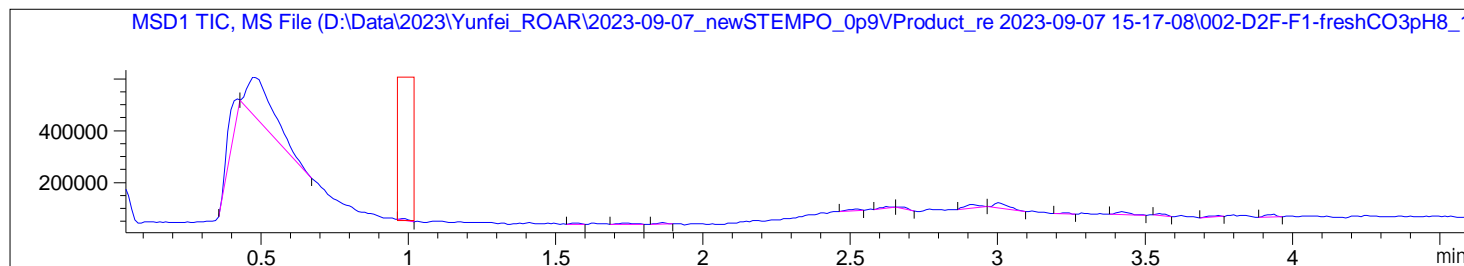
Component 5: Peak at Scan 45.1. Top ions are 217 199 555

Component 6: Peak at Scan 46.4. Top ions are 535 255 430

Component 7: Peak at Scan 48.0. Top ions are 159 227 489

Component 8: Peak at Scan 49.4. Top ions are 536 265 599

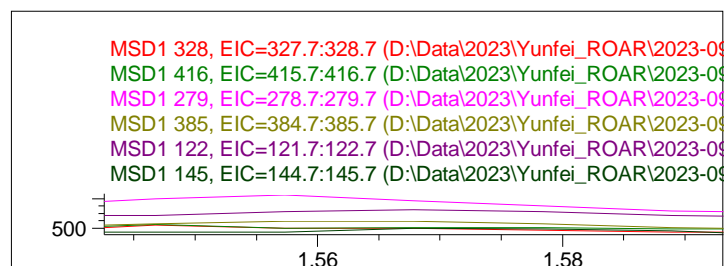
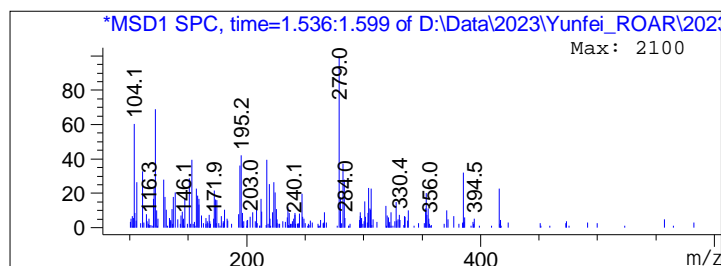
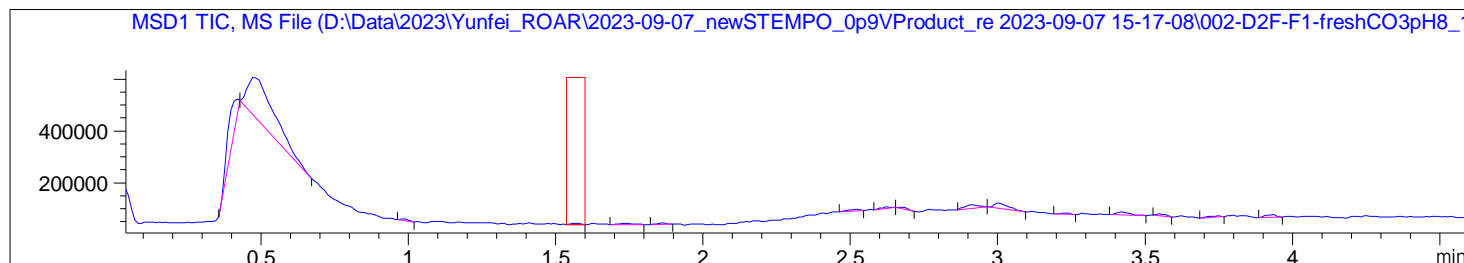
Component 9: Peak at Scan 51.0. Top ions are 428



Peak #3 at 0.979 min ( 0.963 to 1.020 min)

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

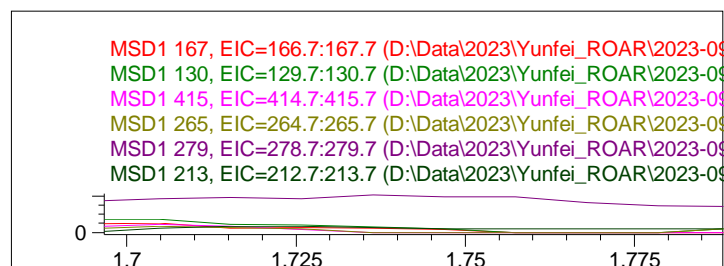
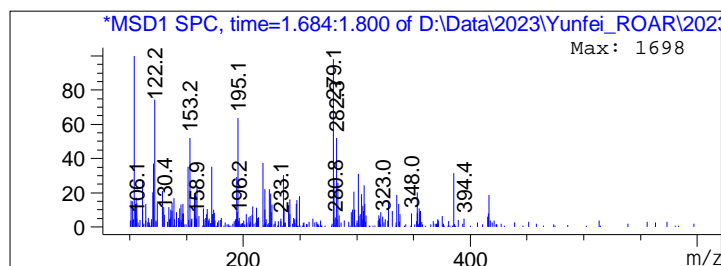
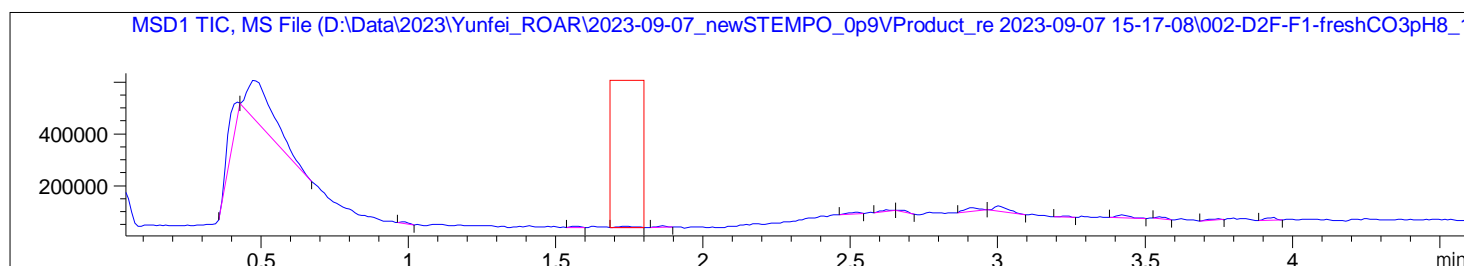
Component 1: Peak at Scan 89.9. Top ions are 247 245 305  
Component 2: Peak at Scan 91.1. Top ions are 353 362 240  
Component 3: Peak at Scan 92.1. Top ions are 349 236 351  
Component 4: Peak at Scan 93.1. Top ions are 135 385 123



Peak #4 at 1.569 min ( 1.536 to 1.599 min)

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

Component 1:	Peak at Scan 144.0.	Top ions are	328 416 180
Component 2:	Peak at Scan 145.0.	Top ions are	279 385 304
Component 3:	Peak at Scan 146.0.	Top ions are	122 145 161
Component 4:	Peak at Scan 146.9.	Top ions are	330 338 557
Component 5:	Peak at Scan 147.9.	Top ions are	335 322 354



Peak #5 at 1.736 min ( 1.685 to 1.800 min)

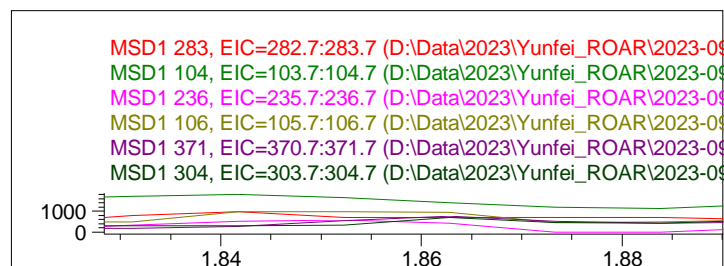
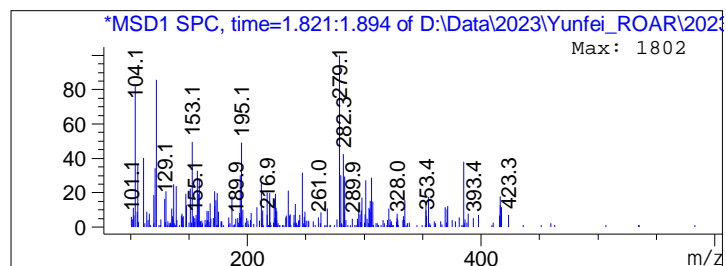
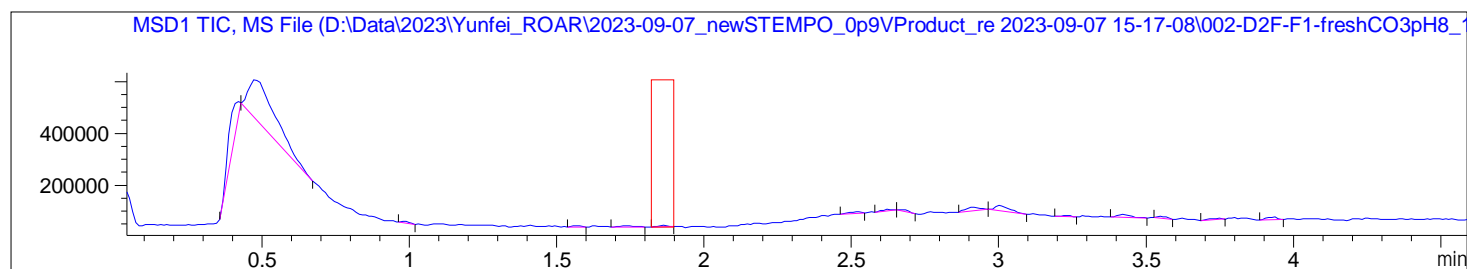
-> The analysis found 10 components, indicating an impure peak. <-

Component 1:	Peak at Scan 158.2.	Top ions are	167 130 102
Component 2:	Peak at Scan 159.1.	Top ions are	415 265 300
Component 3:	Peak at Scan 160.0.	Top ions are	279 213 513
Component 4:	Peak at Scan 161.0.	Top ions are	145 101 253
Component 5:	Peak at Scan 162.2.	Top ions are	172 337 194
Component 6:	Peak at Scan 163.3.	Top ions are	195 134 228
Component 7:	Peak at Scan 164.1.	Top ions are	305 246 335
Component 8:	Peak at Scan 165.3.	Top ions are	122 157 114

Sample Name: freshCO3pH8\_1

Component 9: Peak at Scan 166.3. Top ions are 236 225 104

Component 10: Peak at Scan 167.1. Top ions are 147 319 321



Peak #6 at 1.862 min ( 1.821 to 1.898 min)

-&gt; The analysis found 5 components, indicating an impure peak. &lt;-

Component 1: Peak at Scan 171.5. Top ions are 283 104 355

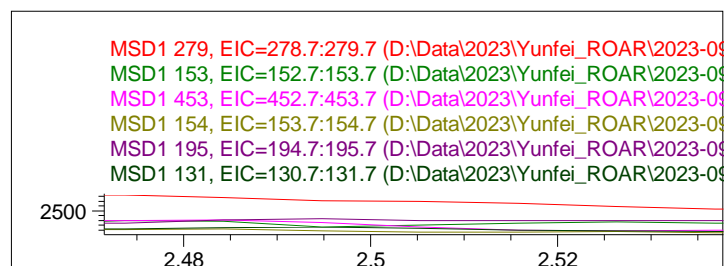
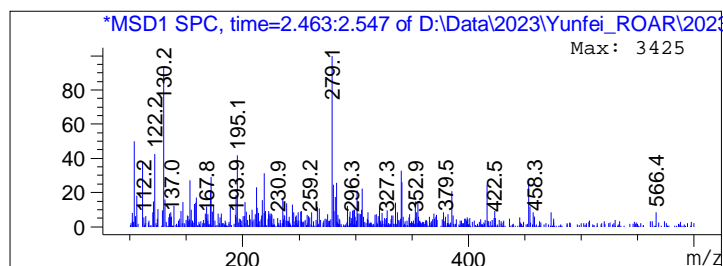
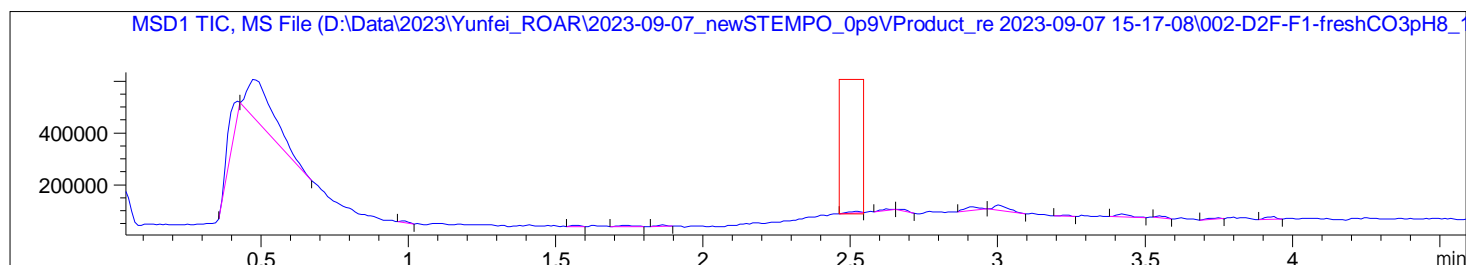
Component 2: Peak at Scan 172.8. Top ions are 236 106 196

Component 3: Peak at Scan 174.0. Top ions are 371 304 297

Component 4: Peak at Scan 174.8. Top ions are 212 158 102

Component 5: Peak at Scan 175.9. Top ions are 416 122 114

Sample Name: freshCO3pH8\_1



Peak #7 at 2.519 min ( 2.463 to 2.546 min)

-&gt; The analysis found 7 components, indicating an impure peak. &lt;-

Component 1: Peak at Scan 232.1. Top ions are 279 153 225

Component 2: Peak at Scan 233.1. Top ions are 453 154 283

Component 3: Peak at Scan 234.2. Top ions are 195 131 421

Component 4: Peak at Scan 235.2. Top ions are 341 105 293

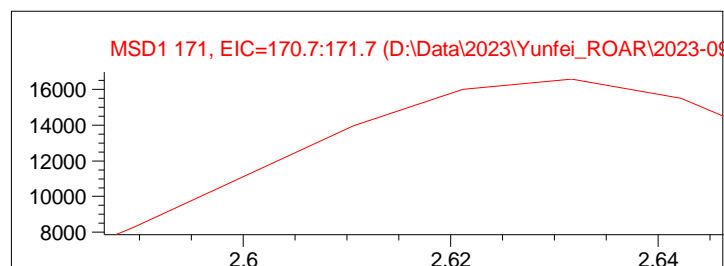
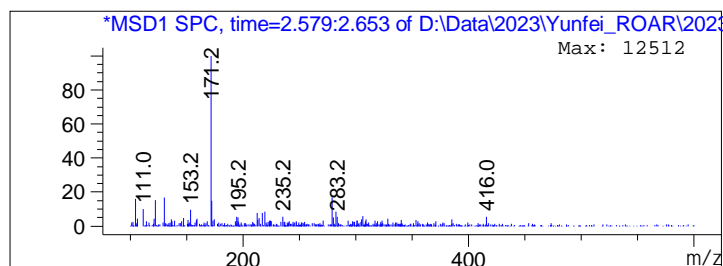
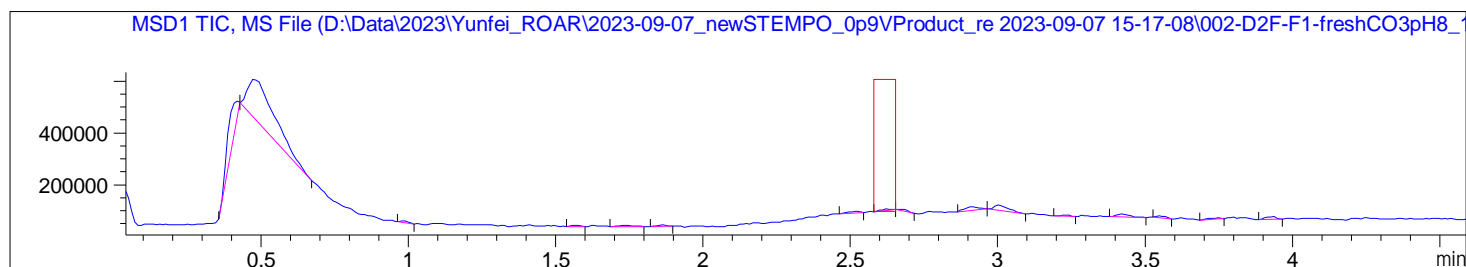
Component 5: Peak at Scan 236.4. Top ions are 340 423 219

Component 6: Peak at Scan 237.6. Top ions are 355 227 144

Component 7: Peak at Scan 238.4. Top ions are 306 412 405



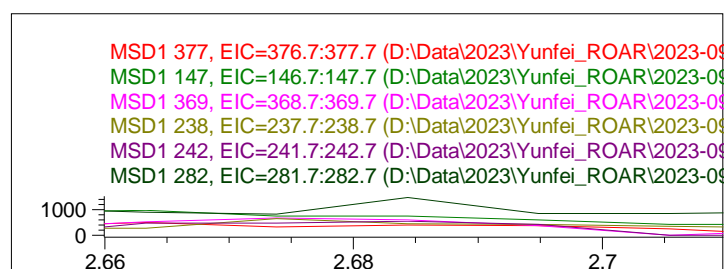
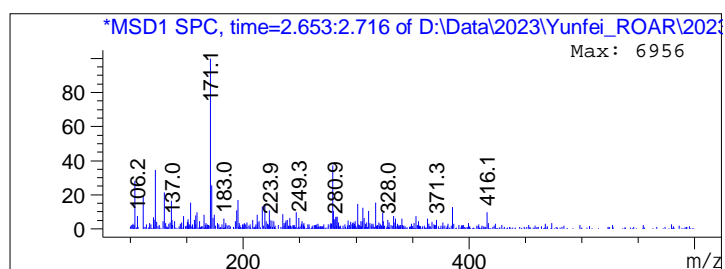
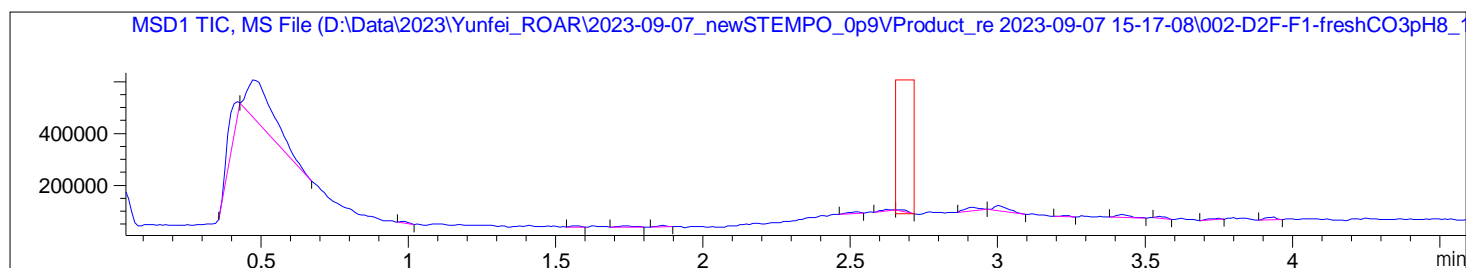
Sample Name: freshCO3pH8\_1



Peak #8 at 2.623 min ( 2.579 to 2.654 min)

-&gt; The analysis found only one component, indicating a pure peak. &lt;-

Component 1: Peak at Scan 246.9. Top ions are 171



Peak #9 at 2.669 min ( 2.654 to 2.716 min)

-&gt; The analysis found 5 components, indicating an impure peak. &lt;-

Component 1: Peak at Scan 250.1. Top ions are 377 147 281

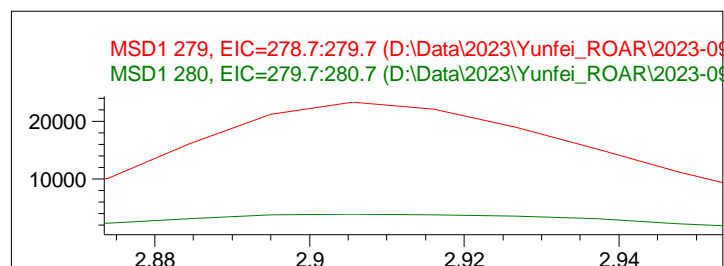
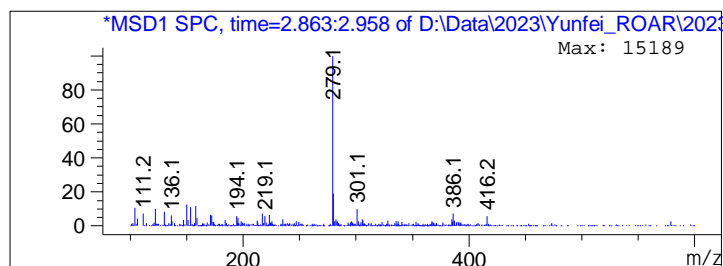
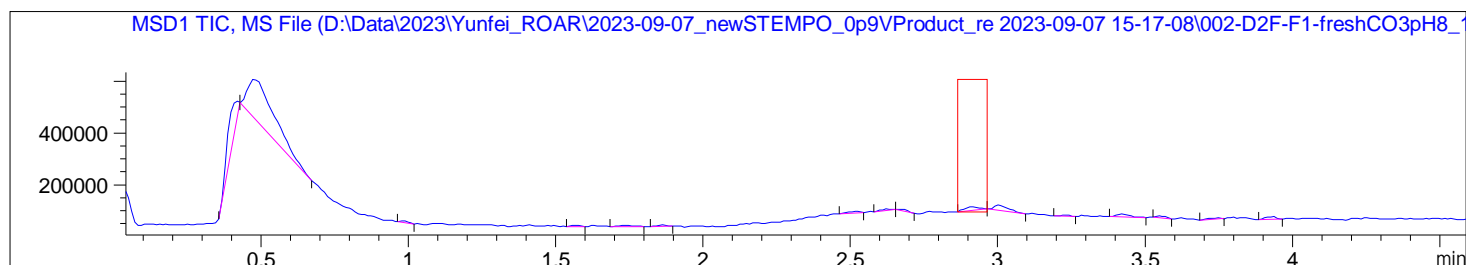
Component 2: Peak at Scan 251.2. Top ions are 369 238 237

Component 3: Peak at Scan 252.1. Top ions are 242 282 399

Component 4: Peak at Scan 253.1. Top ions are 355 301 266

Component 5: Peak at Scan 254.0. Top ions are 150 324 484

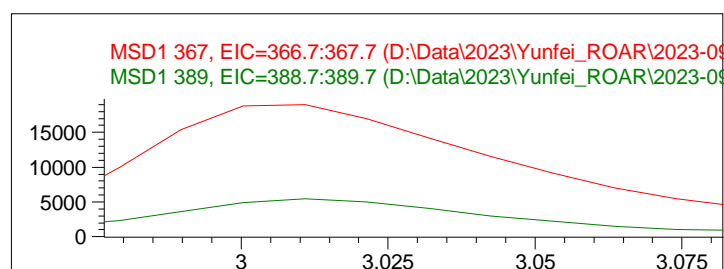
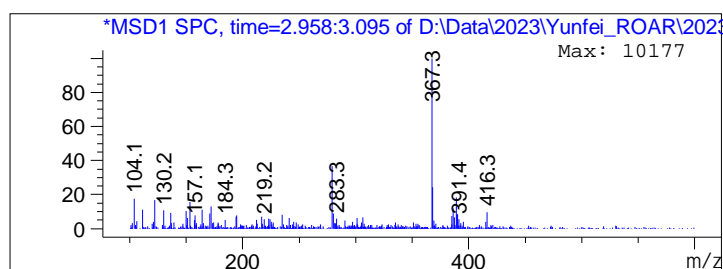
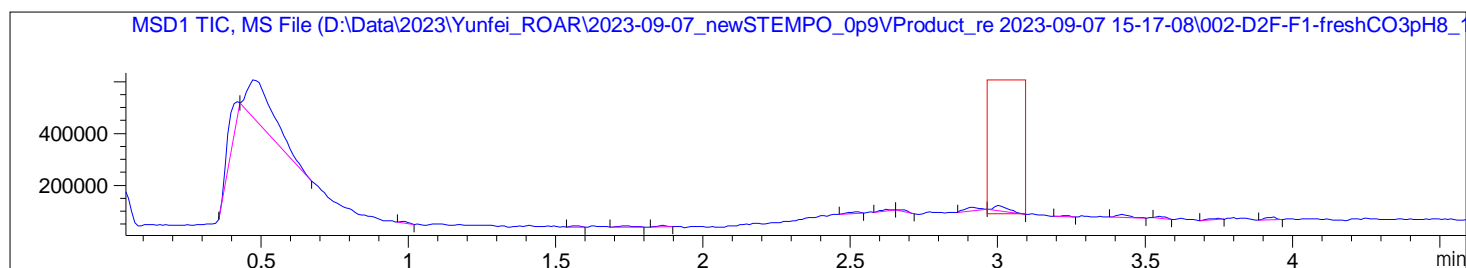
Sample Name: freshCO3pH8\_1



Peak #10 at 2.913 min ( 2.863 to 2.963 min)

-&gt; The analysis found only one component, indicating a pure peak. &lt;-

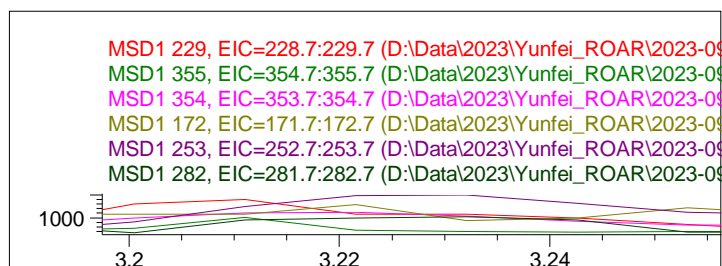
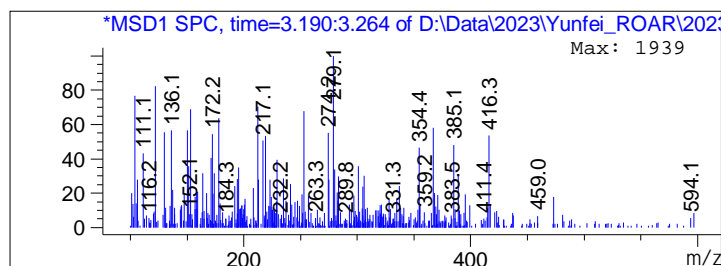
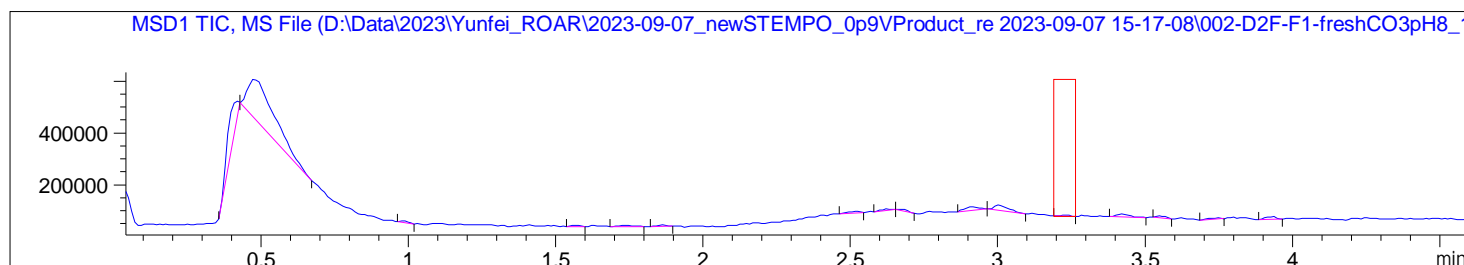
Component 1: Peak at Scan 273.1. Top ions are 279 280



Peak #11 at 3.002 min ( 2.963 to 3.095 min)

-&gt; The analysis found only one component, indicating a pure peak. &lt;-

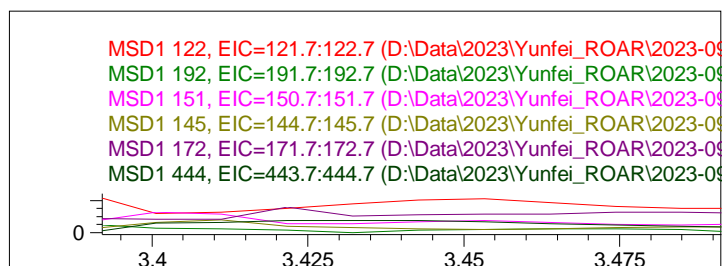
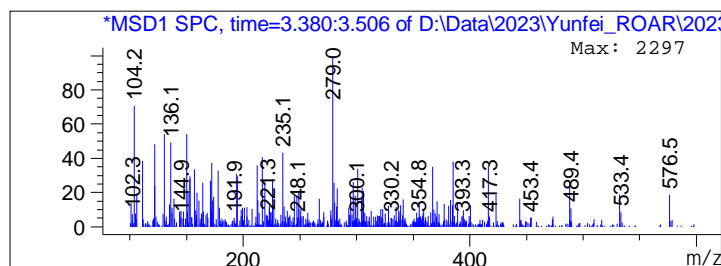
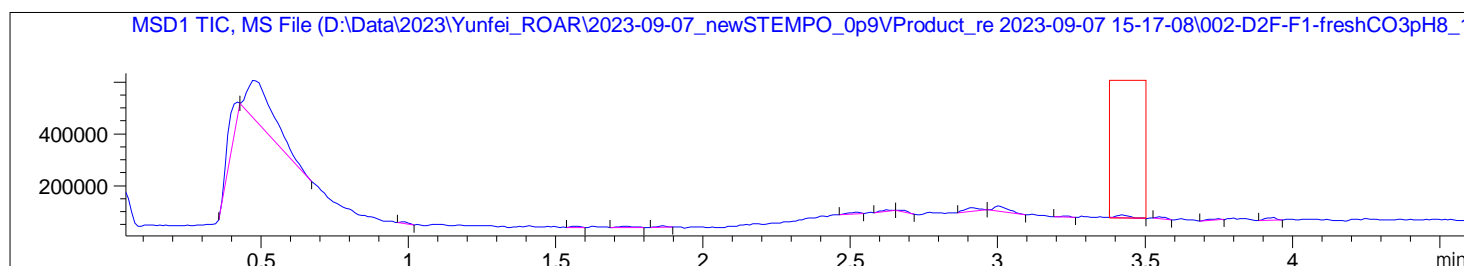
Component 1: Peak at Scan 282.8. Top ions are 367 389 368



Peak #12 at 3.236 min ( 3.190 to 3.264 min)

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

Component 1: Peak at Scan 301.4. Top ions are 229 355 301  
Component 2: Peak at Scan 302.8. Top ions are 354 172 375  
Component 3: Peak at Scan 303.9. Top ions are 253 282 596  
Component 4: Peak at Scan 305.0. Top ions are 283 200 309  
Component 5: Peak at Scan 306.1. Top ions are 145 212 159

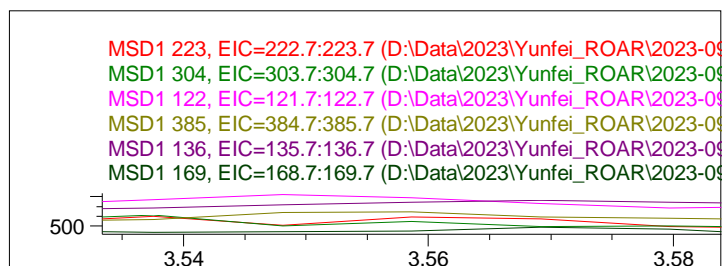
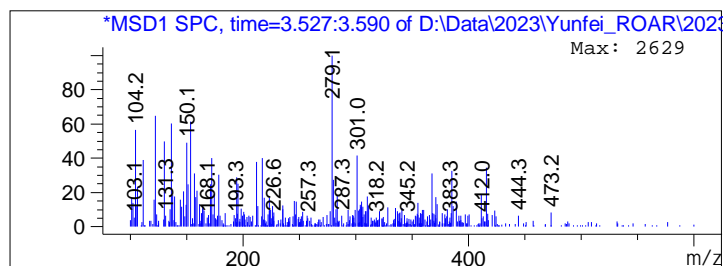
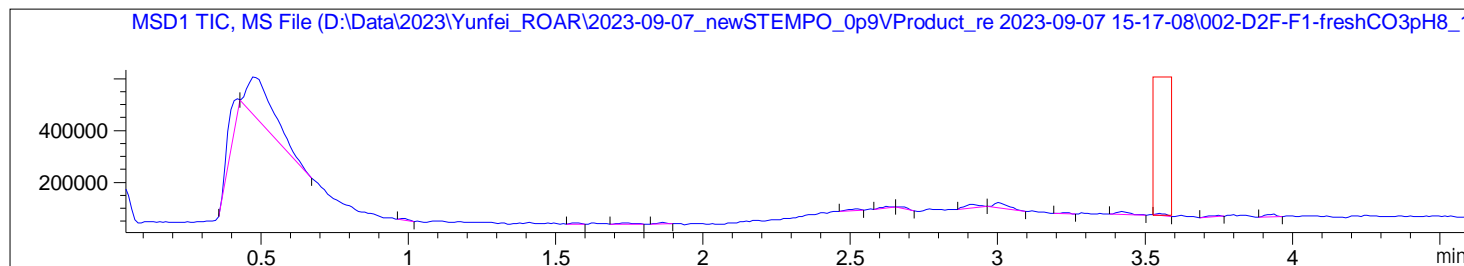


Peak #13 at 3.425 min ( 3.380 to 3.504 min)

-> The analysis found 9 components, indicating an impure peak. <-

Component 1: Peak at Scan 319.1. Top ions are 122 192 322  
Component 2: Peak at Scan 320.4. Top ions are 151 145 178  
Component 3: Peak at Scan 321.8. Top ions are 172 444 488  
Component 4: Peak at Scan 323.1. Top ions are 203 400 357  
Component 5: Peak at Scan 324.2. Top ions are 489 161 277  
Component 6: Peak at Scan 325.5. Top ions are 104 351 368  
Component 7: Peak at Scan 326.9. Top ions are 299 358 297  
Component 8: Peak at Scan 328.0. Top ions are 280 317 281

Component 9: Peak at Scan 329.1. Top ions are 241 269 416



Peak #14 at 3.548 min ( 3.527 to 3.590 min)

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

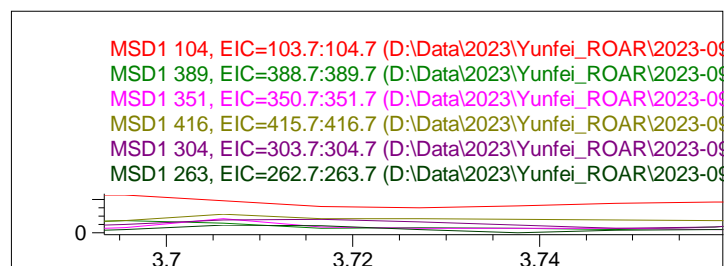
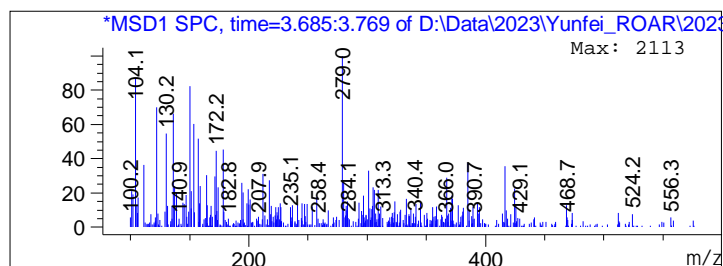
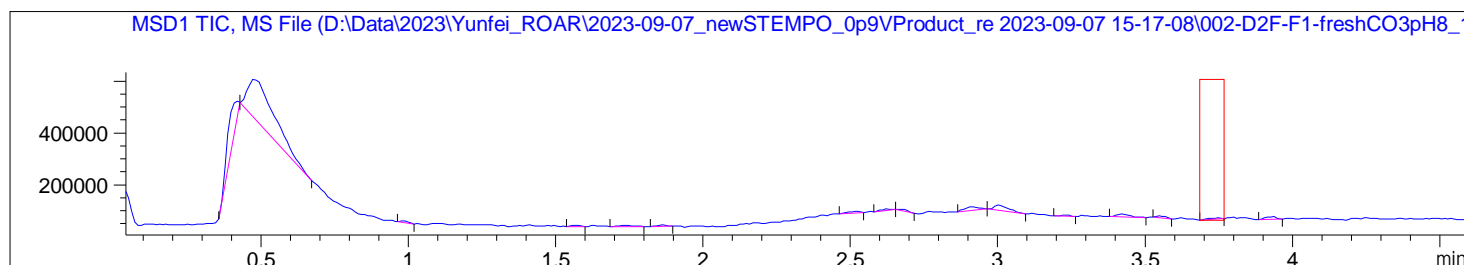
Component 1: Peak at Scan 333.1. Top ions are 223 304 301

Component 2: Peak at Scan 334.5. Top ions are 122 385 195

Component 3: Peak at Scan 335.8. Top ions are 136 169 235

Component 4: Peak at Scan 337.0. Top ions are 164 371 121

Sample Name: freshCO3pH8\_1



Peak #15 at 3.747 min ( 3.685 to 3.768 min)

-&gt; The analysis found 7 components, indicating an impure peak. &lt;-

Component 1: Peak at Scan 348.0. Top ions are 104 389 247

Component 2: Peak at Scan 349.1. Top ions are 351 416 371

Component 3: Peak at Scan 350.1. Top ions are 304 263 167

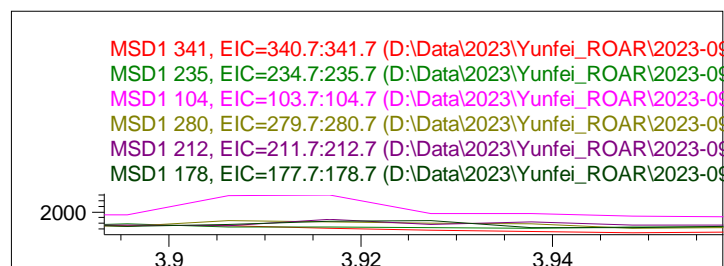
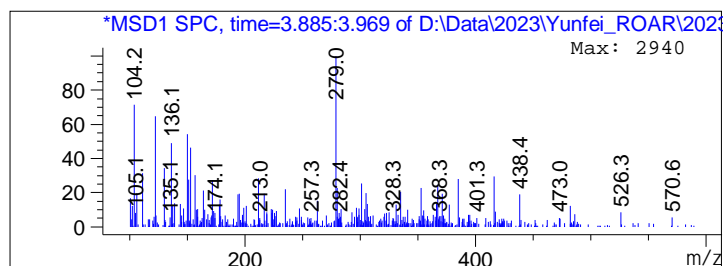
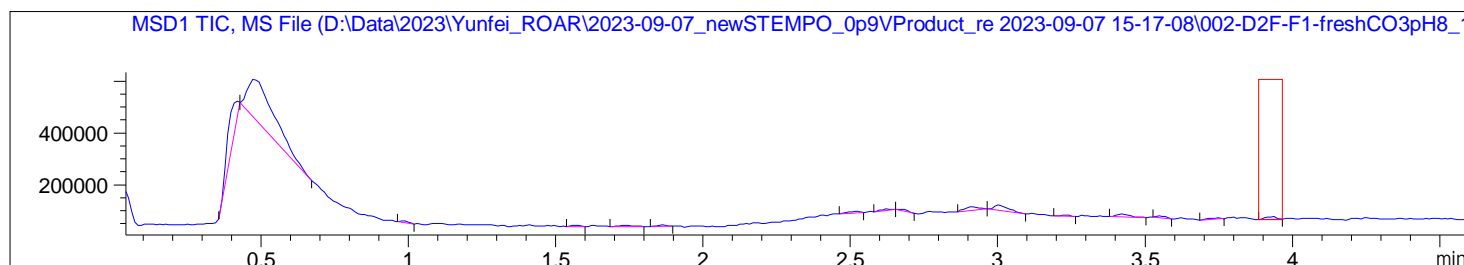
Component 4: Peak at Scan 351.2. Top ions are 172 345 301

Component 5: Peak at Scan 352.3. Top ions are 227 135 281

Component 6: Peak at Scan 353.2. Top ions are 199 150 308

Component 7: Peak at Scan 354.1. Top ions are 157 363 425

Sample Name: freshCO3pH8\_1



Peak #16 at 3.934 min ( 3.885 to 3.966 min)

-&gt; The analysis found 7 components, indicating an impure peak. &lt;-

Component 1: Peak at Scan 367.1. Top ions are 341 235 298  
Component 2: Peak at Scan 368.3. Top ions are 104 280 301  
Component 3: Peak at Scan 369.2. Top ions are 212 178 355  
Component 4: Peak at Scan 370.1. Top ions are 194 452 307  
Component 5: Peak at Scan 371.1. Top ions are 367 439 488  
Component 6: Peak at Scan 372.1. Top ions are 217 153 137  
Component 7: Peak at Scan 373.1. Top ions are 371 150 417

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