

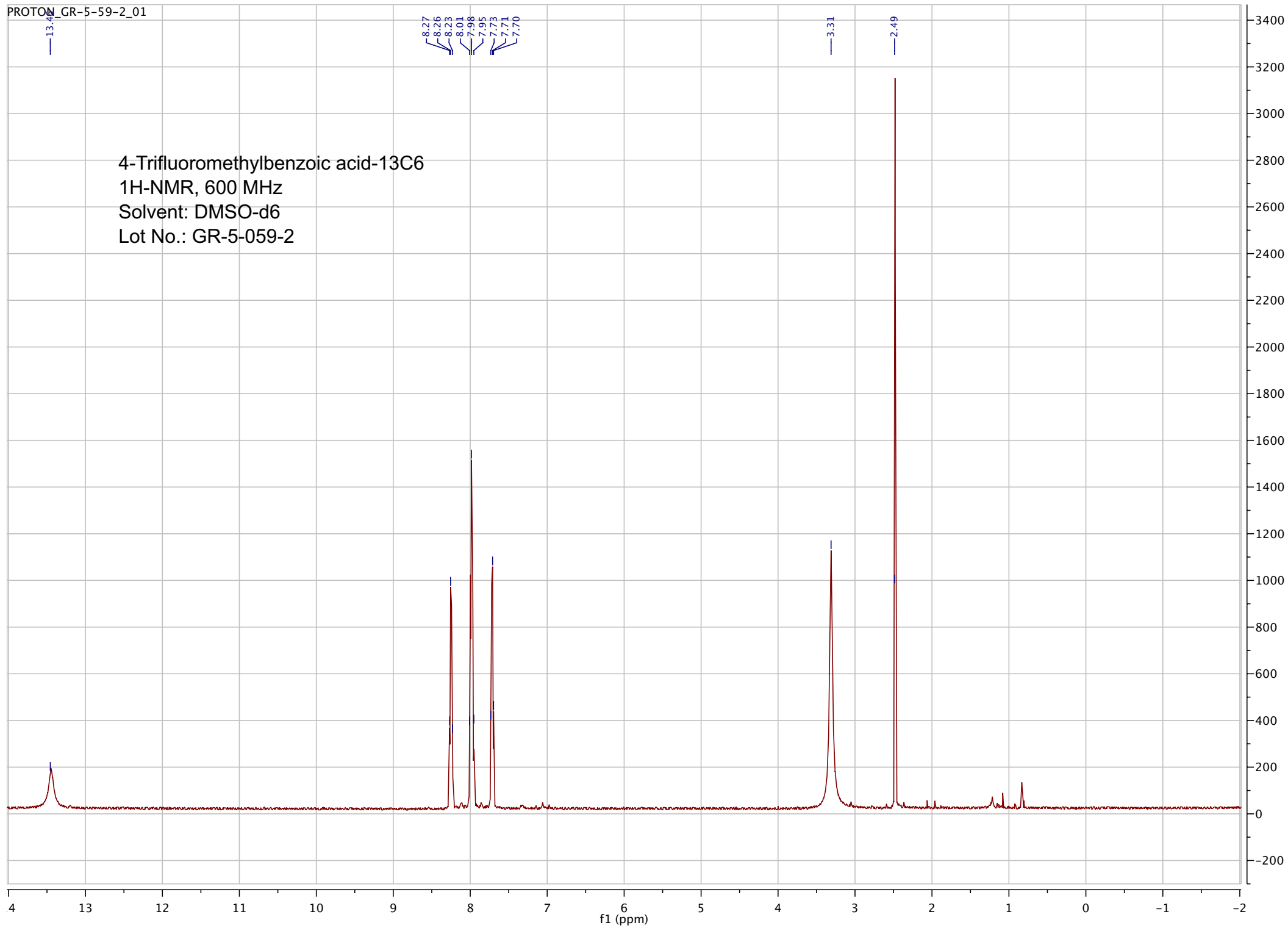
Name:	4-(Trifluoromethyl)benzoic acid- ¹³ C ₆
Lot#:	GR-5-059-2
Test Date:	12/17/2024 (re-test date: 12/17/2029)
CAS No.:	455-24-3 (unlabeled)
MF:	C ₂ ¹³ C ₆ H ₅ F ₃ O ₂
MW:	196.12
Appearance:	Beige Solid
Purity:	98.3% by HPLC (average of two sample preparations); 99% atom ¹³ C
¹H-NMR:	Conforms
MS-ESI (-)	Conforms (shows peak at m/z = 195.04 [M-H] ⁻)
Storage	Store at 0-5°C in a dry place away from direct sunlight

Approved by:

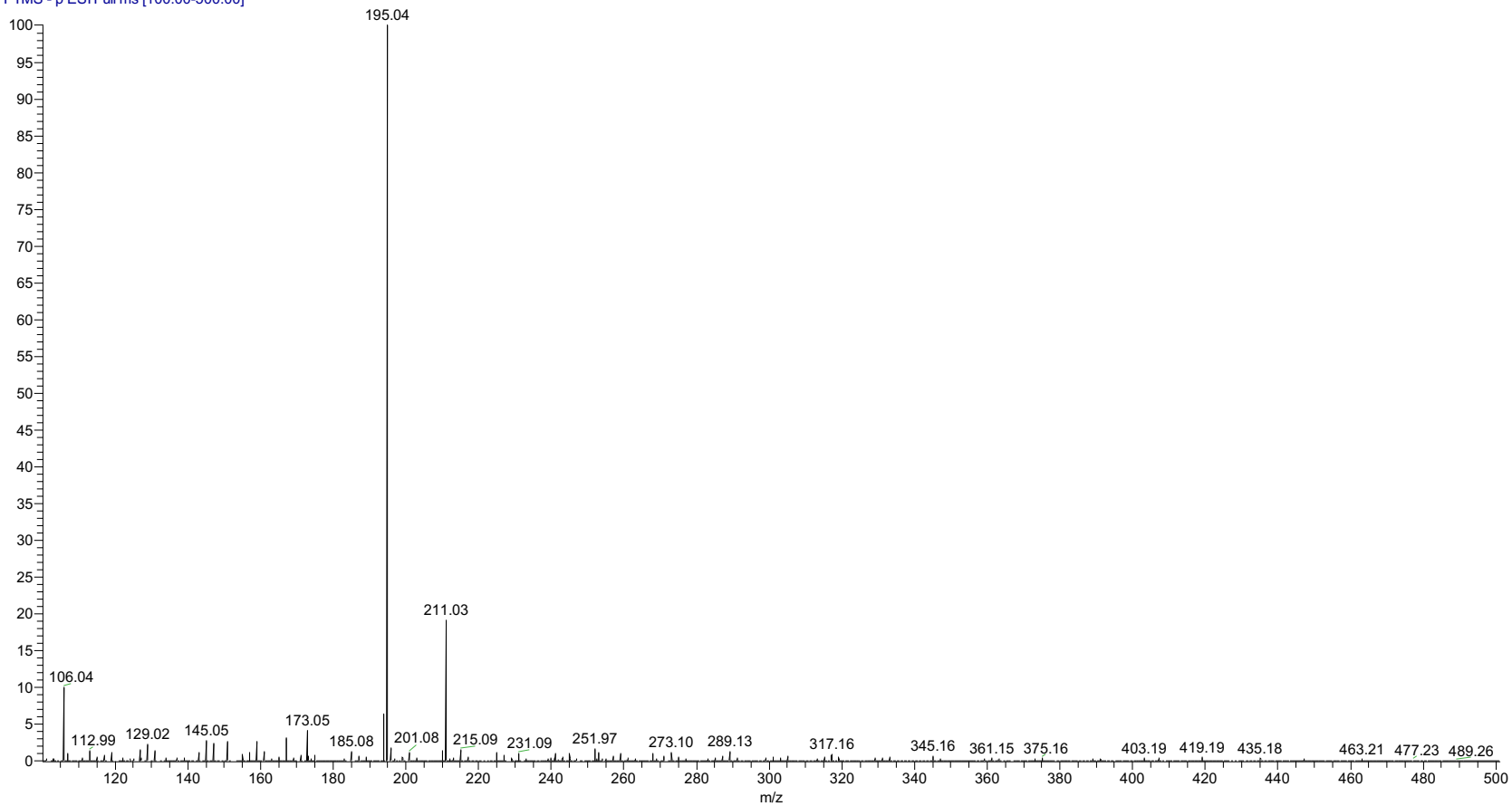
Date: 12/17/2024

Viorica Rusu, QC/QA Manager

4-Trifluoromethylbenzoic acid- $^{13}\text{C}_6$
1H-NMR, 600 MHz
Solvent: DMSO- d_6
Lot No.: GR-5-059-2

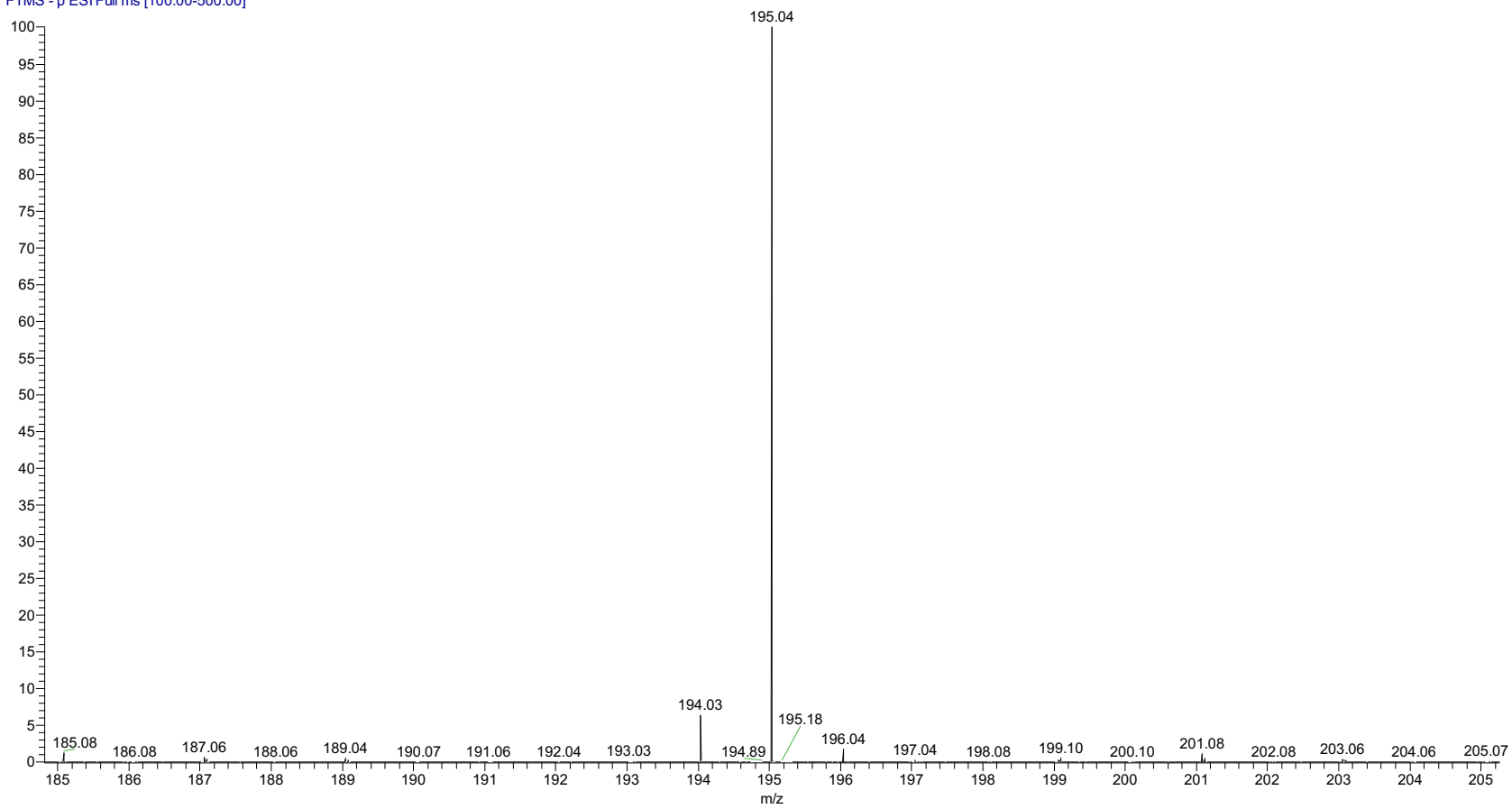


pp_2022_076_GR_05_059_2_1#521-525 RT: 2.35-2.36 AV: 5 NL: 1
T: FTMS - p ESI Full ms [100.00-500.00]



ESI-MS spectrum for sample GR-5-059-2. Shows monoisotopic [M-H]⁻ mass.

pp_2022_076_GR_05_059_2_1#521-525 RT: 2.35-2.36 AV: 5 NL: 1
T: FTMS -p ESI Full ms [100.00-500.00]



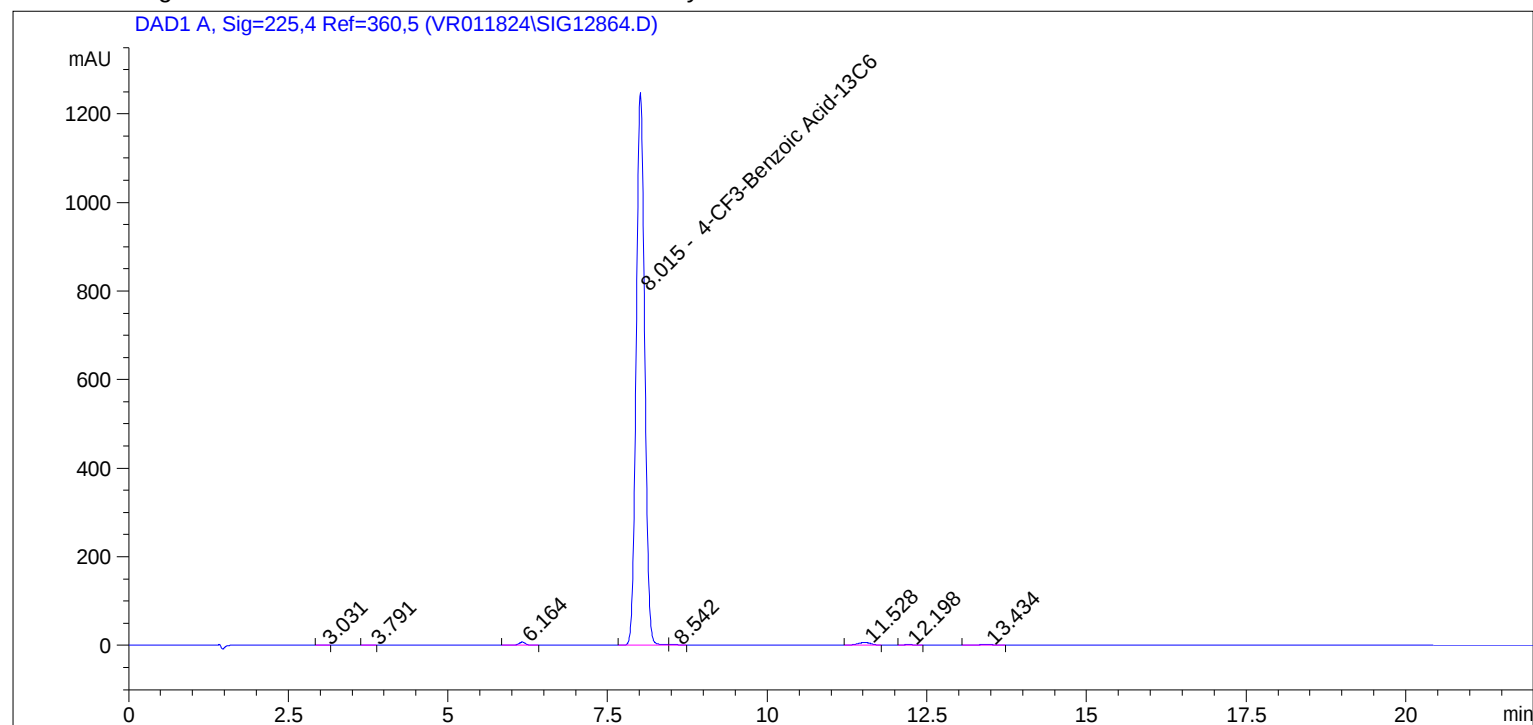
Expansion of above. Peak list below with intensity and relative intensity.

Sample Name: GR-5-059-2, spl-2

=====

Acq. Operator :
Acq. Instrument : Instrument 1 Location : Vial 96
Injection Date : 12/10/2024 4:37:07 PM Inj Volume : 10.0 µl

Acq. Method : C:\CHEM32\1\METHODS\VR121024_059.M
Last changed : 12/10/2024 4:36:04 PM
Analysis Method : C:\CHEM32\1\METHODS\VR121724_059PM.M
Last changed : 12/17/2024 11:37:36 AM by vrusu



=====

Area Percent Report

=====

Sorted By : Signal
Calib. Data Modified : 12/17/2024 11:36:50 AM
Multiplier: : 1.603e3
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=225,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	3.031	BB	0.0750	4.09117	0.0352	?
2	3.791	BB	0.0894	3.87430	0.0333	?
3	6.164	BB	0.1139	52.93713	0.4552	?
4	8.015	BV	0.1429	1.14377e4	98.3602	4-CF3-Benzoic Acid-13C6
5	8.542	VB	0.1285	8.42460	0.0724	?
6	11.528	BB	0.2254	86.61156	0.7448	?
7	12.198	BB	0.1596	12.10938	0.1041	?
8	13.434	BB	0.2123	22.63641	0.1947	?

Totals : 1.16283e4

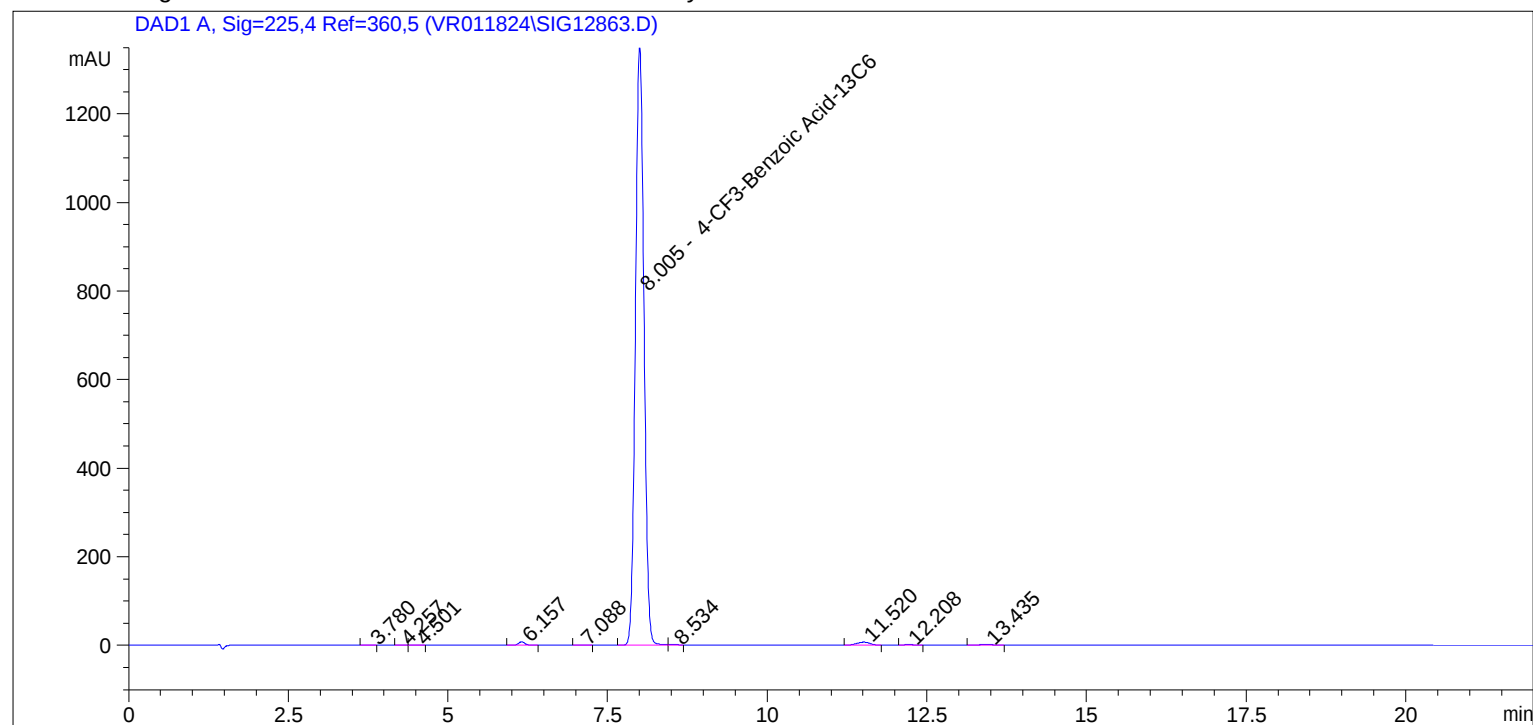
Sample Name: GR-5-059-2, spl-2

=====

*** End of Report ***

Sample Name: GR-5-059-2

```
=====
Acq. Operator   :
Acq. Instrument : Instrument 1                Location : Vial 95
Injection Date  : 12/10/2024 4:12:48 PM
                                           Inj Volume : 10.0 µl
Acq. Method     : C:\CHEM32\1\METHODS\VR121024_059.M
Last changed    : 12/10/2024 4:11:46 PM
Analysis Method : C:\CHEM32\1\METHODS\VR121724_059PM.M
Last changed    : 12/17/2024 11:37:36 AM by vrusu
=====
```



```
=====
                        Area Percent Report
=====
```

```
Sorted By           :      Signal
Calib. Data Modified :      12/17/2024 11:36:50 AM
Multiplier:         :      1.603e3
Dilution:           :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 A, Sig=225,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	3.780	BB	0.0823	4.18835	0.0329	?
2	4.257	BB	0.0853	3.79824	0.0298	?
3	4.501	BB	0.1093	4.94862	0.0389	?
4	6.157	BB	0.1085	55.47342	0.4358	?
5	7.088	BB	0.1101	4.71666	0.0371	?
6	8.005	BV	0.1437	1.25137e4	98.3138	4-CF3-Benzoic Acid-13C6
7	8.534	VB	0.1386	10.63222	0.0835	?
8	11.520	BB	0.2249	95.15305	0.7476	?
9	12.208	BB	0.1512	11.93867	0.0938	?
10	13.435	BB	0.1865	23.78102	0.1868	?

Sample Name: GR-5-059-2

Totals : 1.27284e4

=====

*** End of Report ***