

## Supplementary Materials

### Novel Disulfiram Derivatives as Aldh1a1-Selective Inhibitors

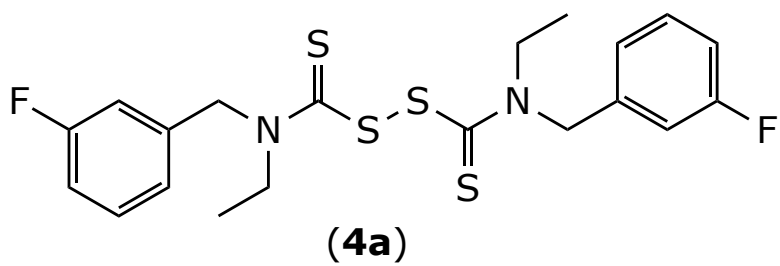
Ziad Omran<sup>1,2</sup>

<sup>1</sup> Department of Pharmaceutical Sciences, Pharmacy Program, Batterjee Medical College, Jeddah 21442, Saudi Arabia; [ziad.omran@bmc.edu.sa](mailto:ziad.omran@bmc.edu.sa)

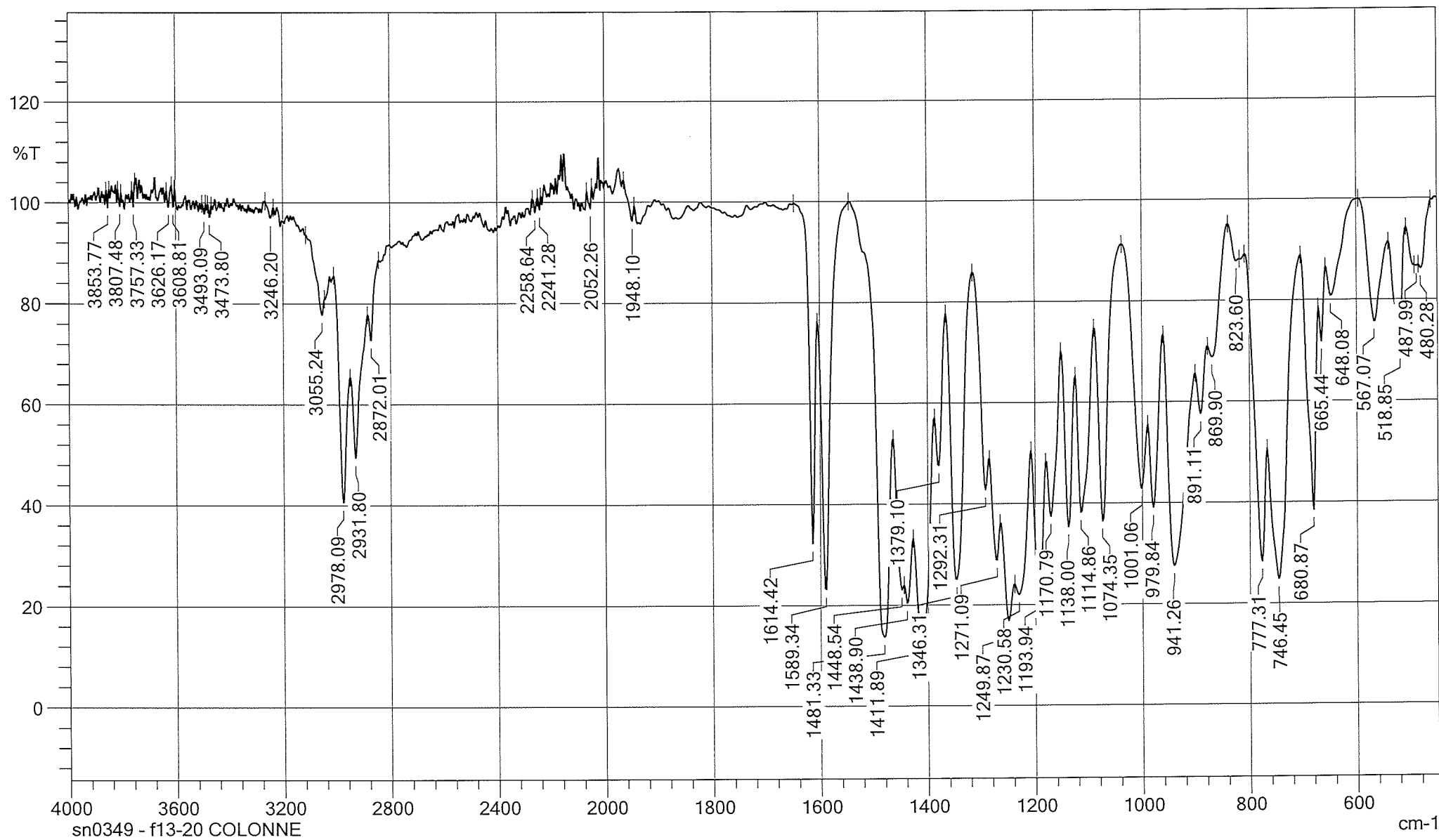
<sup>2</sup> College of Pharmacy, Umm Al-Qura University, Makkah 21955, Saudi Arabia

#### Table of Contents

Analytical data for compound <b>4a</b>	Page 2
Analytical data for compound <b>4b</b>	Page 9
Analytical data for compound <b>4c</b>	Page 16
Analytical data for compound <b>4d</b>	Page 24
Analytical data for compound <b>4e</b>	Page 31
Analytical data for compound <b>4f</b>	Page 38
Analytical data for compound <b>4g</b>	Page 45
Analytical data for compound <b>4h</b>	Page 52
Analytical data for compound <b>4i</b>	Page 59



Chemical Formula:  $\text{C}_{20}\text{H}_{22}\text{F}_2\text{N}_2\text{S}_4$   
Exact Mass: 456.0634



## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 14.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

536 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

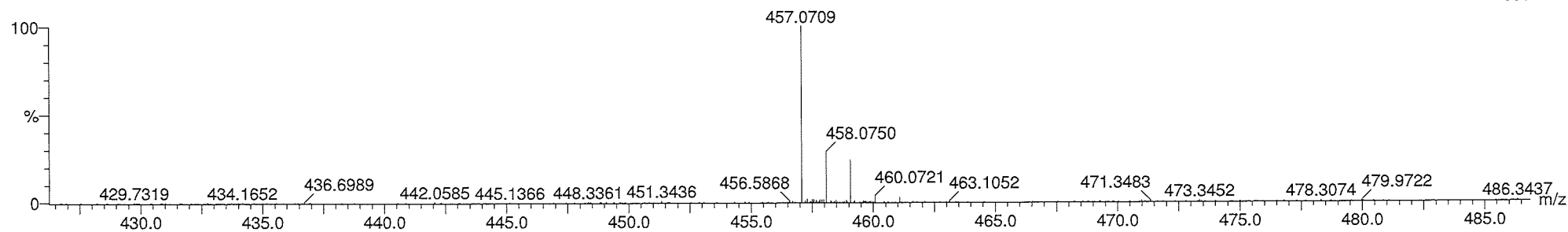
C: 0-500 H: 0-1000 N: 0-5 F: 1-3 S: 0-6

01-Jun-2021

2106005 567 (3.443) Cm (567:570-(535:540+596:601))

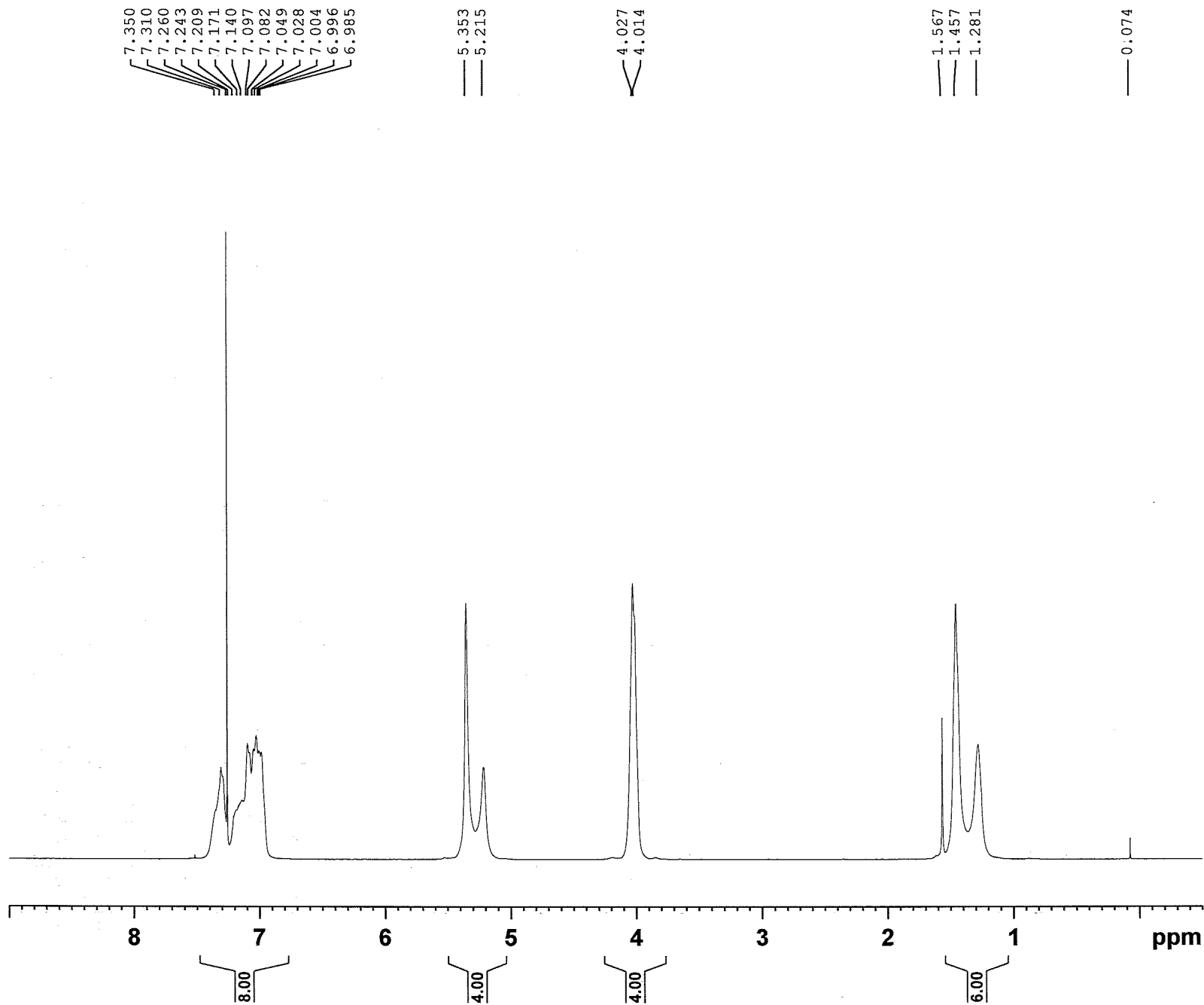
SN0349

2:12

1: TOF MS ES+  
1.68e+003

Minimum: 0.0  
Maximum: 5.0 5.0 14.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
457.0709	457.0712	-0.3	-0.7	9.5	153.0	0.0	C20 H23 N2 F2 S4

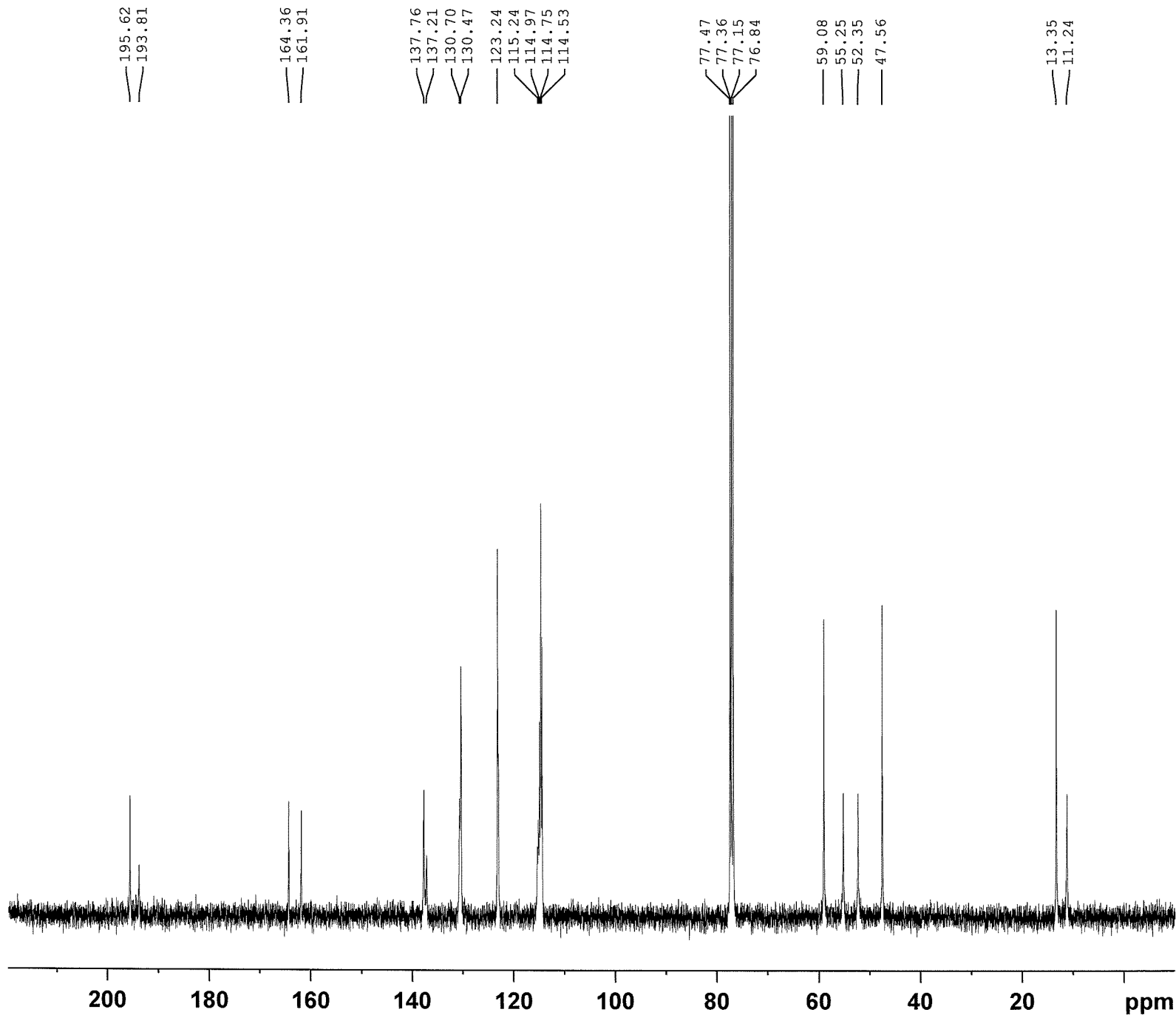


Current Data Parameters  
 NAME SN0349-L1  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210519  
 Time\_ 11.17  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 7978.724 Hz  
 FIDRES 0.243491 Hz  
 AQ 2.0534613 sec  
 RG 69.13  
 DW 62.667 usec  
 DE 6.50 usec  
 TE 296.2 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 399.7524686 MHz  
 NUC1 1H  
 P1 9.00 usec  
 PLW1 19.20000076 W

F2 - Processing parameters  
 SI 65536  
 SF 399.7500096 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME SN0349-LOT1  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210520  
 Time\_ 0.01  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 2048  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 199.3  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.5272687 MHz  
 NUC1 13C  
 P1 8.60 usec  
 PLW1 87.00000000 W

===== CHANNEL f2 =====  
 SFO2 399.7515990 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 19.20000076 W  
 PLW12 0.20000000 W  
 PLW13 0.15552001 W

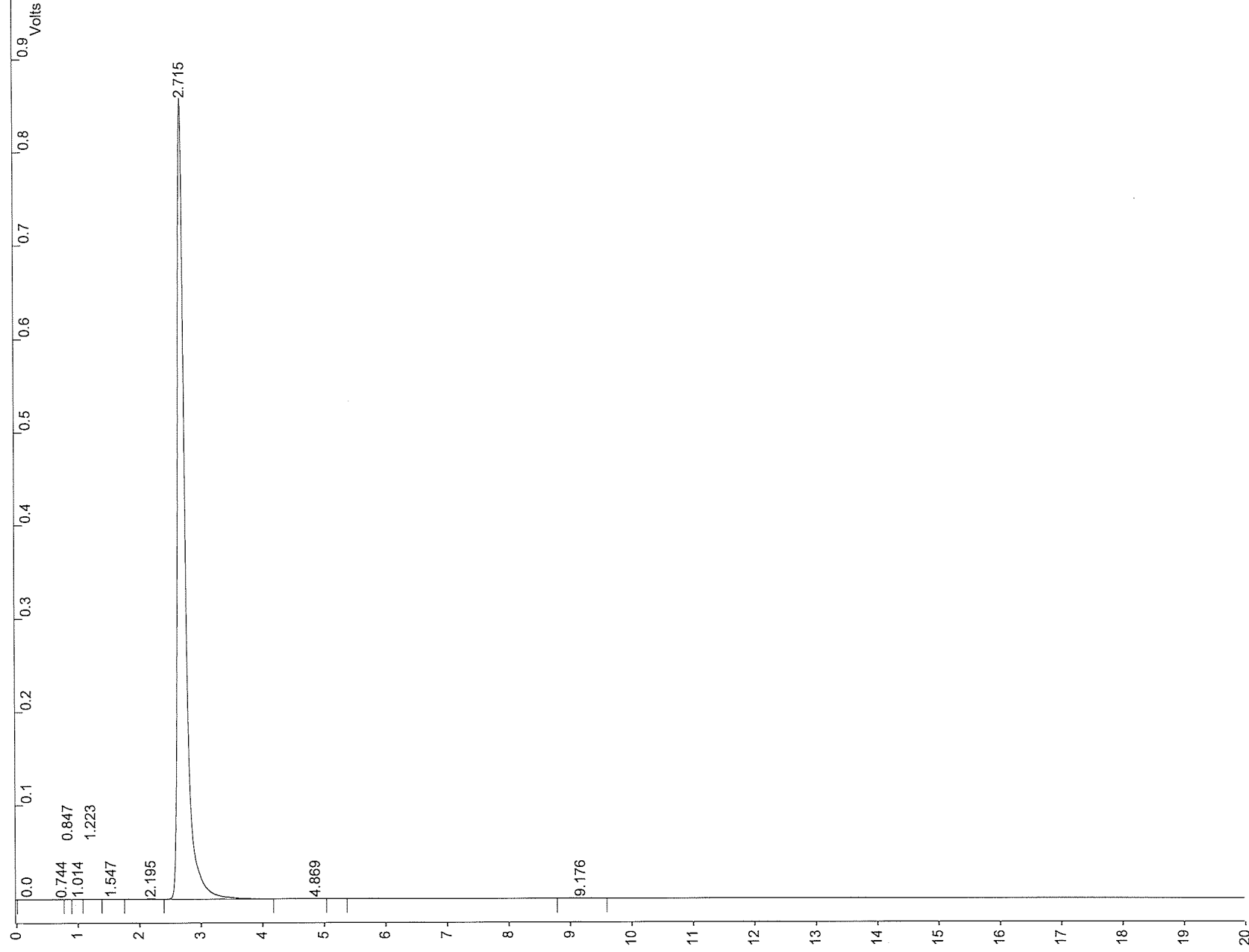
F2 - Processing parameters  
 SI 32768  
 SF 100.5172094 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

Title :  
Run File : C:\Users\DG\Documents\SYNTHENOVA\Mode opératoire\SN0346-49 421-26\thiuram HPLC\HPLC ok\SN0349-L1.run  
Method File : C:\star\startup1.mth  
Sample ID : SN0349-L1

Injection Date: 21/05/2021 14:56      Calculation Date: 21/05/2021 15:16

Operator : dg      Detector Type: 0800 (1 Volt)  
Workstation: HDD      Bus Address : 81  
Instrument : Instrument #1      Sample Rate : 10.00 Hz  
Channel : 2 = 2 1      Run Time : 20.002 min

Chart Speed = 1.08 cm/min      Attenuation = 4057      Zero Offset = 2%  
Start Time = 0.000 min      End Time = 20.002 min      Min / Tick = 1.00



Injection Date: 21/05/2021 14:56Calculation Date: 21/05/2021 15:16

Operator : dGDetector Type: 0800 (1 Volt)Workstation: HDDBus Address : 81Instrument : Instrument #1Sample Rate : 10.00 HzChannel : 2 = 2 1Run Time : 20.002 min

Run Mode : Analysis

Peak Measurement: Peak Area

Calculation Type: Percent

Peak No.	Peak Name	Result ( )	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		0.0288	0.744	0.000	2116	BV	10.2	
2		0.0147	0.847	0.000	1083	VV	6.1	
3		0.0201	1.014	0.000	1480	VV	6.8	
4		0.0350	1.223	0.000	2573	VV	13.4	
5		0.0512	1.547	0.000	3761	VV	12.3	
6		0.0811	2.195	0.000	5960	VV	7.8	
7		99.6518	2.715	0.000	7321431	VP	7.2	
8		0.0470	4.869	0.000	3456	PV	0.0	
9		0.0701	9.176	0.000	5152	BB	18.9	
Totals:		99.9998		0.000	7347012			

Total Unidentified Counts : 7347011 counts

Detected Peaks: 10Rejected Peaks: 1Identified Peaks: 0

Multiplier: 1Divisor: 1Unidentified Peak Factor: 1

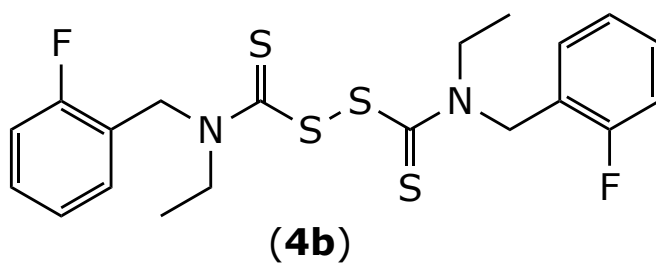
Baseline Offset: -152 microVoltsLSB: 1 microVolts

Noise (used): 29 microVolts - monitored before this run

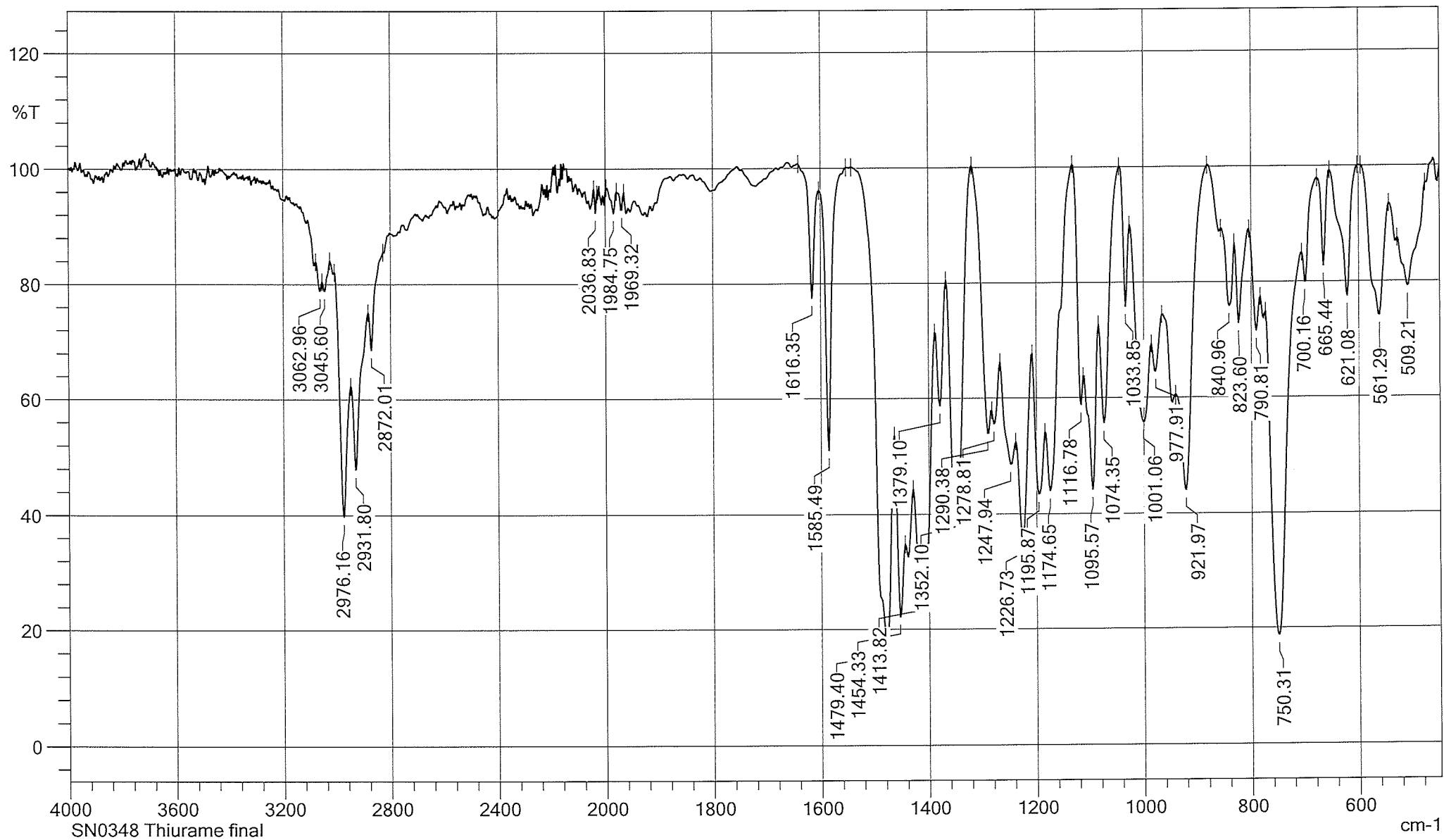
Manual injection

\*\*\*\*\*





Chemical Formula:  $\text{C}_{20}\text{H}_{22}\text{F}_2\text{N}_2\text{S}_4$   
Exact Mass: 456.0634



## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = 0.0, max = 14.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

536 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

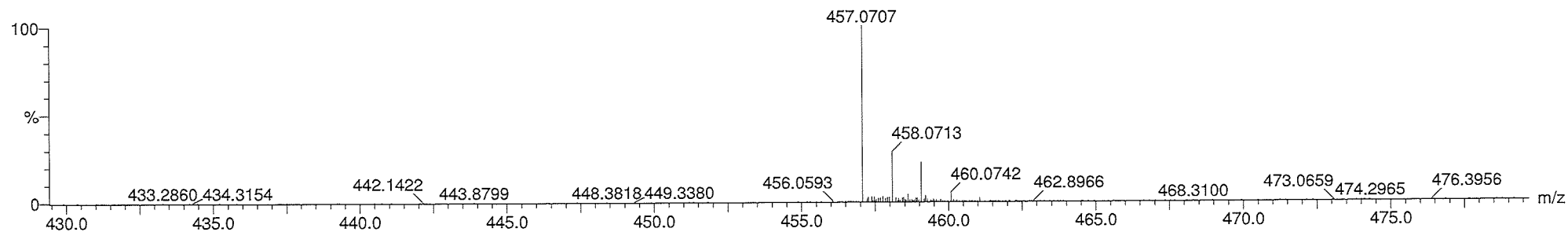
C: 0-500 H: 0-1000 N: 0-5 F: 1-3 S: 0-6

01-Jun-2021

2106004 579 (3.501) Cm (578:581-(549:553+622:627))

SN0348

2:11

1: TOF MS ES+  
1.04e+004

Minimum: 0.0  
Maximum: 5.0 10.0 14.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
457.0707	457.0712	-0.5	-1.1	9.5	434.3	0.0	C20 H23 N2 F2 S4
	457.0746	-3.9	-8.5	4.5	439.7	5.3	C17 H27 N2 F2 S5

7.519  
7.402  
7.258  
7.191  
7.090

5.411  
5.279

4.041

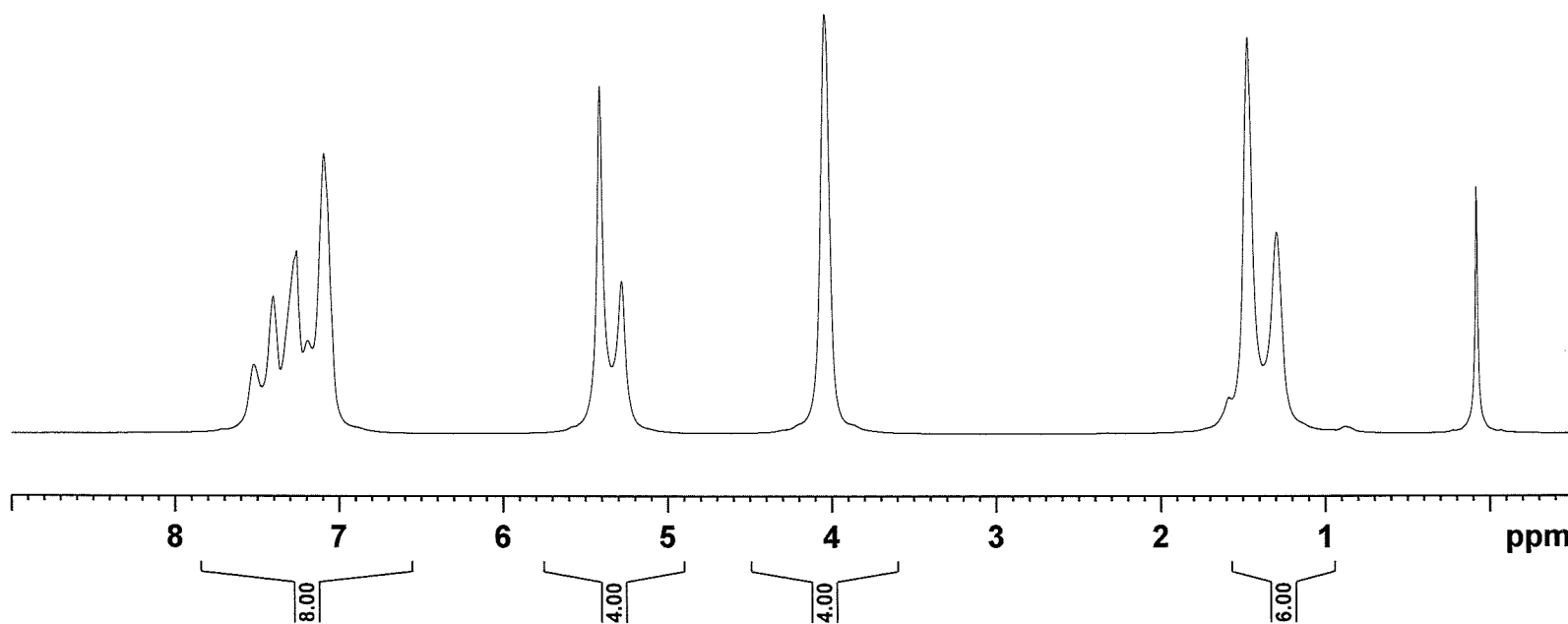
1.585  
1.468  
1.292

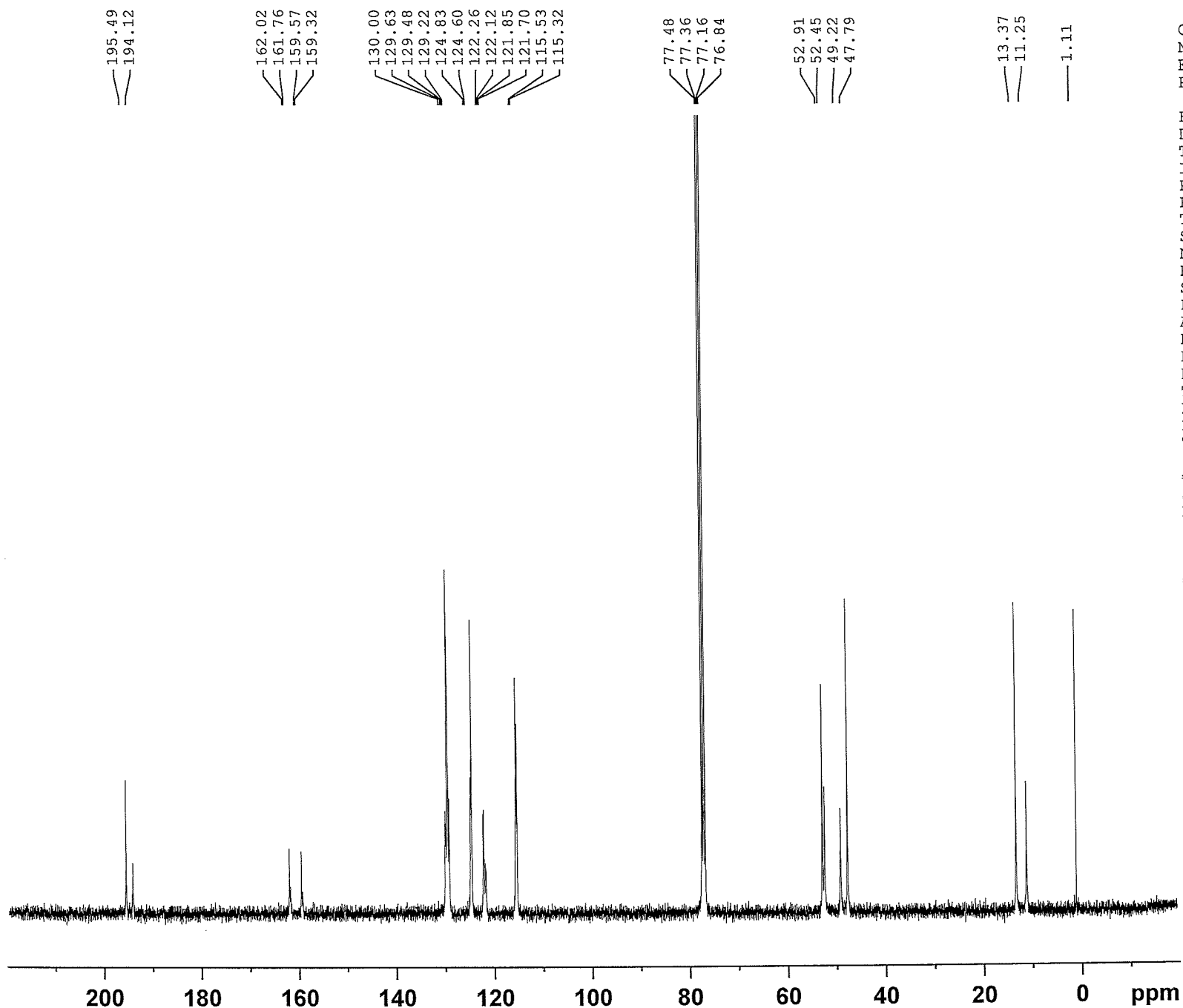
Current Data Parameters  
NAME SN0348-LOT1  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date 20210506  
Time 18.19  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 7978.724 Hz  
FIDRES 0.243491 Hz  
AQ 2.0534613 sec  
RG 30.7  
DW 62.667 usec  
DE 6.50 usec  
TE 296.2 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SF01 399.7524686 MHz  
NUC1 1H  
P1 9.00 usec  
PLW1 19.20000076 W

F2 - Processing parameters  
SI 65536  
SF 399.7500108 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
 NAME SN0348LOT1  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20210508  
 Time 15.13  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 2048  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 199.3  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.5272687 MHz  
 NUC1 13C  
 P1 8.60 usec  
 PLW1 87.00000000 W

===== CHANNEL f2 =====  
 SFO2 399.7515990 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 19.20000076 W  
 PLW12 0.20000000 W  
 PLW13 0.15552001 W

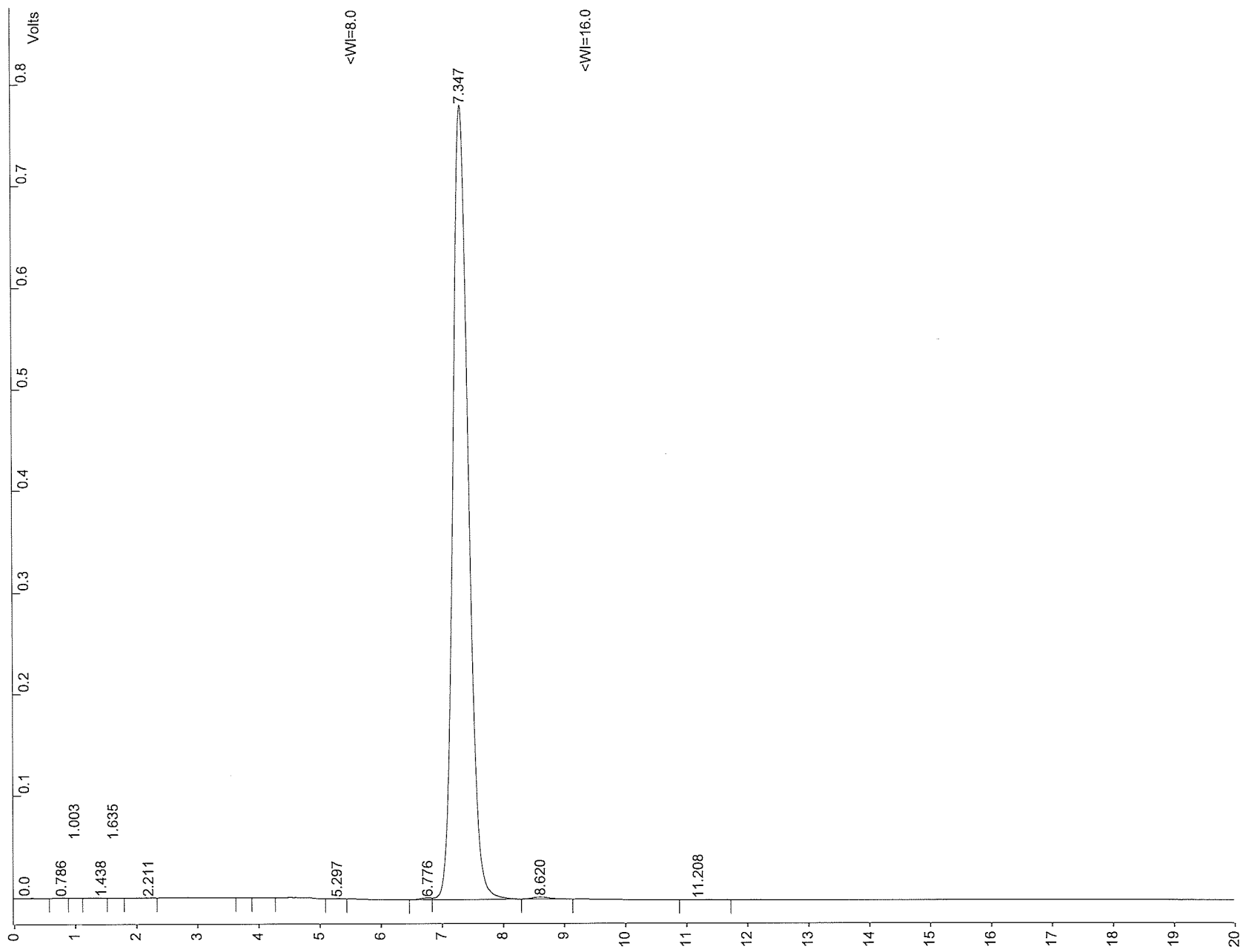
F2 - Processing parameters  
 SI 32768  
 SF 100.5172122 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

Title :  
Run File : C:\Users\DG\Documents\SYNTHENOVA\Mode opératoire\SN0346-49 421-26\thiuram HPLC\HPLC ok\SN0348-L1.run  
Method File : C:\star\startup1.mth  
Sample ID : SN0348-L1

Injection Date: 12/05/2021 16:02      Calculation Date: 12/05/2021 16:22

Operator : dG      Detector Type: 0800 (1 Volt)  
Workstation: HDD      Bus Address : 81  
Instrument : Instrument #1      Sample Rate : 10.00 Hz  
Channel : 2 = 2 1      Run Time : 20.002 min

Chart Speed = 1.08 cm/min      Attenuation = 3698      Zero Offset = 2%  
Start Time = 0.000 min      End Time = 20.002 min      Min / Tick = 1.00



<Wt=8.0

<Wt=16.0

Title :  
Run File : C:\Users\DG\Documents\SYNTHENOVA\Mode opératoire\SN0346-49 421-26\thiuram HPLC\HPLC ok\SN0348-L1.run  
Method File : C:\star\startup1.mth  
Sample ID : SN0348-L1

Injection Date: 12/05/2021 16:02      Calculation Date: 12/05/2021 16:22

Operator : dG                      Detector Type: 0800 (1 Volt)  
Workstation: HDD                  Bus Address : 81  
Instrument : Instrument #1        Sample Rate : 10.00 Hz  
Channel : 2 = 2 1                Run Time : 20.002 min

Run Mode : Analysis  
Peak Measurement: Peak Area  
Calculation Type: Percent

Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		0.0236	0.786	0.000	3277	BV	8.3	
2		0.0127	1.003	0.000	1761	VP	9.8	
3		0.0205	1.438	0.000	2838	PV	20.8	
4		0.0123	1.635	0.000	1713	VV	15.1	
5		0.0096	2.211	0.000	1332	VB	29.0	
6		0.0232	5.297	0.000	3214	BB	7.9	
7		0.1443	6.776	0.000	20032	BV	14.6	
8		99.4616	7.347	0.000	13805326	VB	16.1	
9		0.2707	8.620	0.000	37575	TS	0.0	
10		0.0216	11.208	0.000	2993	BB	19.8	
Totals:		100.0001		0.000	13880061			

Total Unidentified Counts : 13880062 counts

Detected Peaks: 12                  Rejected Peaks: 2                  Identified Peaks: 0

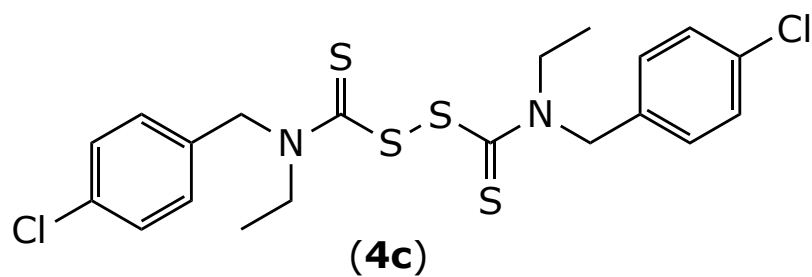
Multiplier: 1                  Divisor: 1                  Unidentified Peak Factor: 1

Baseline Offset: -24 microVolts                  LSB: 1 microVolts

Noise (used): 31 microVolts - monitored before this run

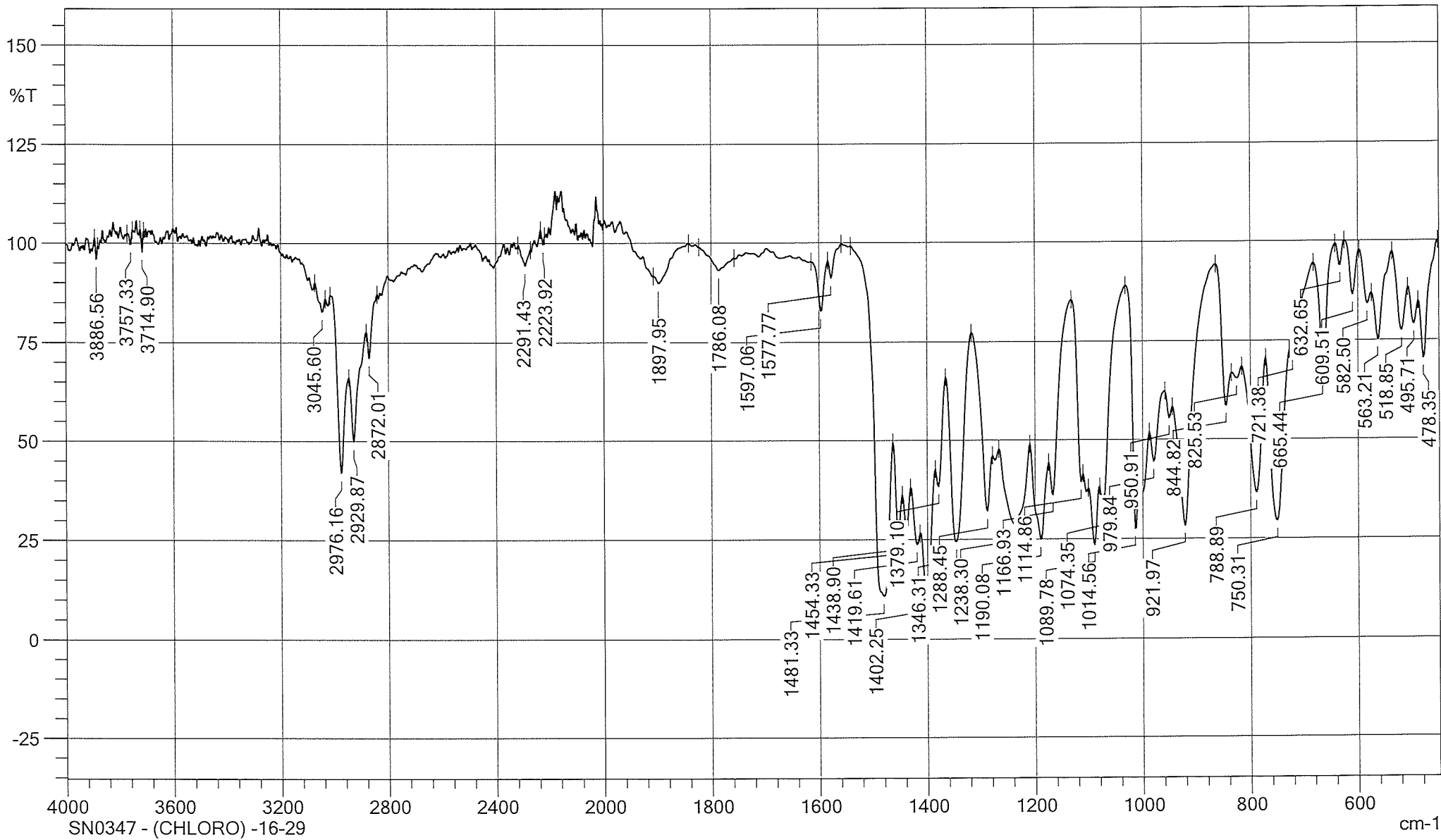
Manual injection

\*\*\*\*\*



Chemical Formula:  $\text{C}_{20}\text{H}_{22}\text{Cl}_2\text{N}_2\text{S}_4$   
Exact Mass: 488.0043





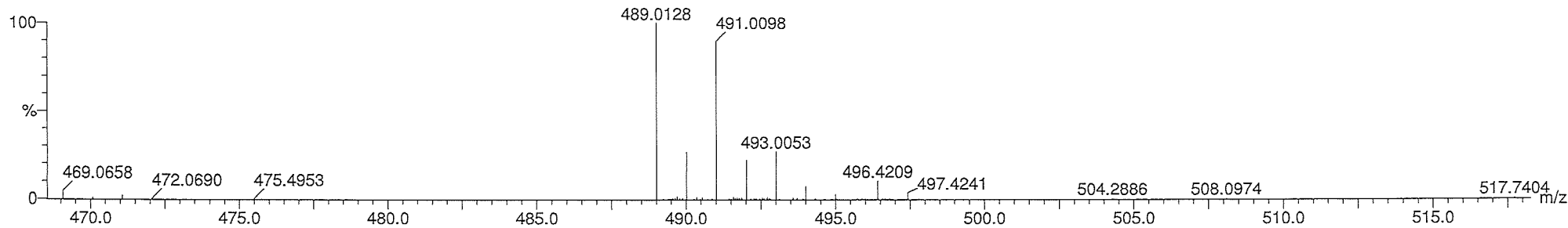
Multiple Mass Analysis: 3 mass(es) processed  
Tolerance = 10.0 PPM / DBE: min = 0.0, max = 14.0  
Element prediction: Off  
Number of isotope peaks used for i-FIT = 4  
  
Monoisotopic Mass, Even Electron Ions  
4839 formula(e) evaluated with 27 results within limits (up to 50 best isotopic matches for each mass)  
Elements Used:  
C: 0-500 H: 0-1000 N: 0-5 S: 0-6 35Cl: 0-2 37Cl: 0-2

01-Jun-2021  
2106003 619 (3.767) Cm (617:622-(576:598+677:700))

SN0347

2:10

1: TOF MS ES+  
6.65e+003



Minimum: 26.70 0.0  
Maximum: 100.00 5.0 10.0 14.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
489.0128	100.00	489.0137	-0.9	-1.8	9.5	167.6	1.1	C18 H22 N4 S5 35Cl
		489.0121	0.7	1.4	9.5	167.6	1.1	C20 H23 N2 S4 35Cl2
		489.0155	-2.7	-5.5	4.5	168.4	1.9	C17 H27 N2 S5 35Cl2
		489.0170	-4.2	-8.6	4.5	169.3	2.7	C15 H26 N4 S6 35Cl
		489.0136	-0.8	-1.6	11.5	169.6	3.0	C20 H20 N4 S2 35Cl 37Cl2
		489.0154	-2.6	-5.3	6.5	170.1	3.6	C19 H25 N2 S2 35Cl2 37Cl2
		489.0170	-4.2	-8.6	6.5	170.3	3.8	C17 H24 N4 S3 35Cl 37Cl2
		489.0121	0.7	1.4	11.5	172.8	6.3	C22 H21 N2 S 35Cl2 37Cl2
		491.0098	-4.3	-8.8	4.5	124.7	0.3	C15 H26 N4 S6 37Cl
		491.0107	-0.9	-1.8	9.5	126.3	1.9	C18 H22 N4 S5 37Cl
		491.0125	-2.7	-5.5	4.5	127.2	2.8	C17 H27 N2 S5 35Cl 37Cl
		491.0124	-2.6	-5.3	12.5	127.3	2.9	C23 H23 S6
491.0098	89.42	491.0060	3.8	7.7	4.5	128.5	4.1	C15 H25 N4 S5 35Cl2
		491.0110	-1.2	-2.4	4.5	129.5	5.1	C19 H28 S4 35Cl2 37Cl
		491.0092	0.6	1.2	9.5	129.5	5.1	C20 H23 N2 S4 35Cl 37Cl
		491.0093	0.5	1.0	1.5	131.6	7.2	C14 H27 N4 S3 35Cl2 37Cl2
		491.0076	2.2	4.5	9.5	132.6	8.2	C22 H24 S3 35Cl2 37Cl
		491.0059	3.9	7.9	6.5	135.0	10.6	C17 H23 N4 S2 35Cl2 37Cl2
		493.0047	0.6	1.2	9.5	64.6	0.5	C22 H24 S3 35Cl 37Cl2
		493.0062	-0.9	-1.8	9.5	65.8	1.7	C20 H23 N2 S4 37Cl2
		493.0080	-2.7	-5.5	4.5	66.7	2.6	C19 H28 S4 35Cl 37Cl2
		493.0047	0.6	1.2	7.5	67.3	3.2	C20 H26 S6 35Cl
		493.0030	2.3	4.7	4.5	67.7	3.6	C15 H25 N4 S5 35Cl 37Cl
		493.0015	3.8	7.7	4.5	68.1	4.0	C17 H26 N2 S4 35Cl2 37Cl
493.0053	26.71	493.0029	2.4	4.9	12.5	68.6	4.5	C21 H21 N2 S6

Multiple Mass Analysis: 3 mass(es) processed

Tolerance = 10.0 PPM / DBE: min = 0.0, max = 14.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

4839 formula(e) evaluated with 27 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-500 H: 0-1000 N: 0-5 S: 0-6 35Cl: 0-2 37Cl: 0-2

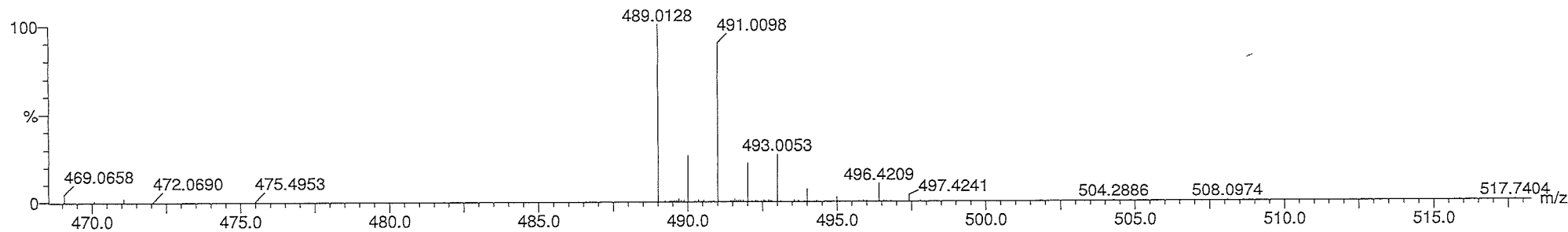
01-Jun-2021

2106003 619 (3.767) Cm (617:622-(576:598+677:700))

SN0347

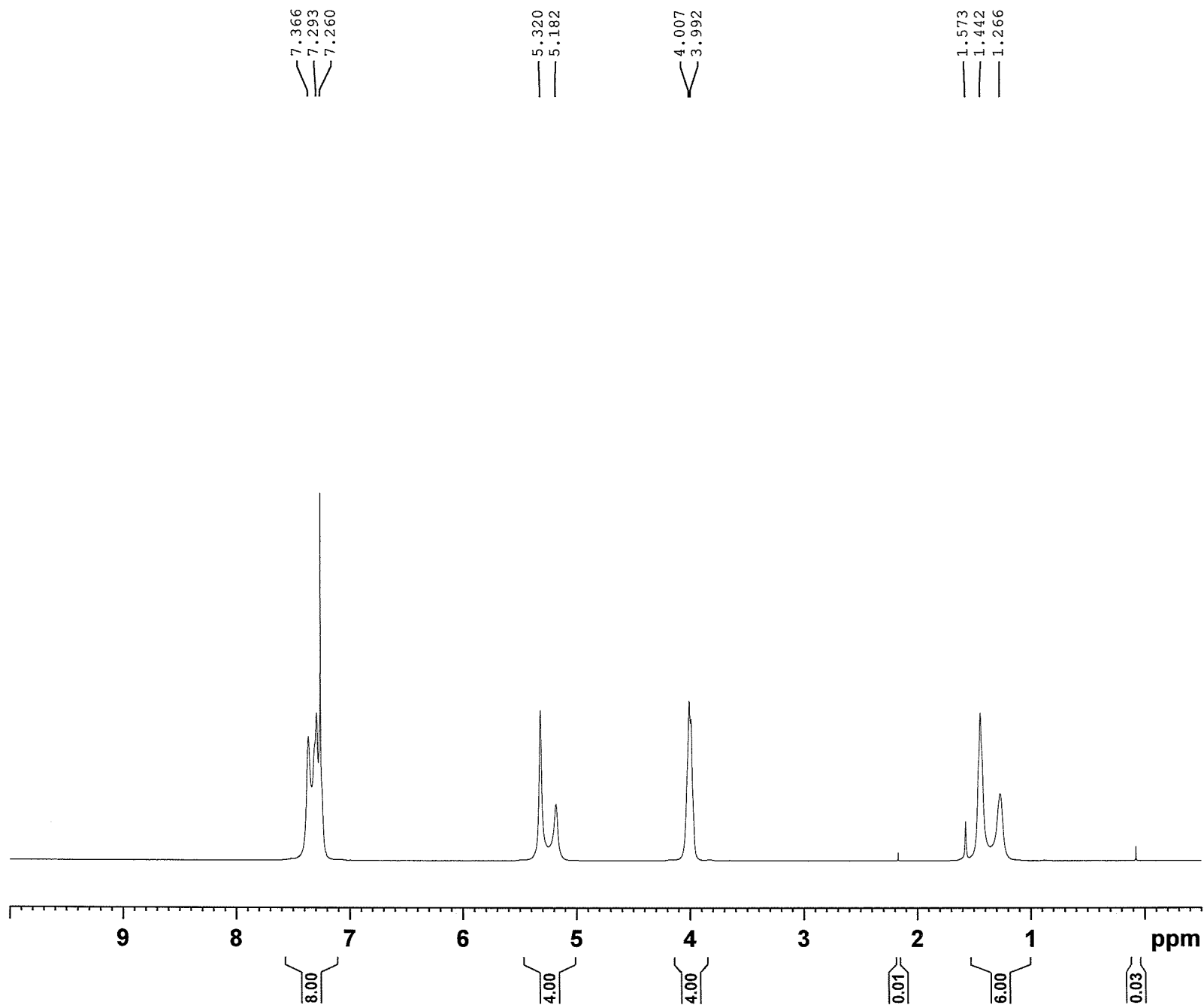
2:10

1: TOF MS ES+  
6.65e+003



Minimum: 26.70 0.0  
Maximum: 100.00 5.0 10.0 14.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
		493.0014	3.9	7.9	12.5	69.5	5.4	C23 H22 S5 35Cl

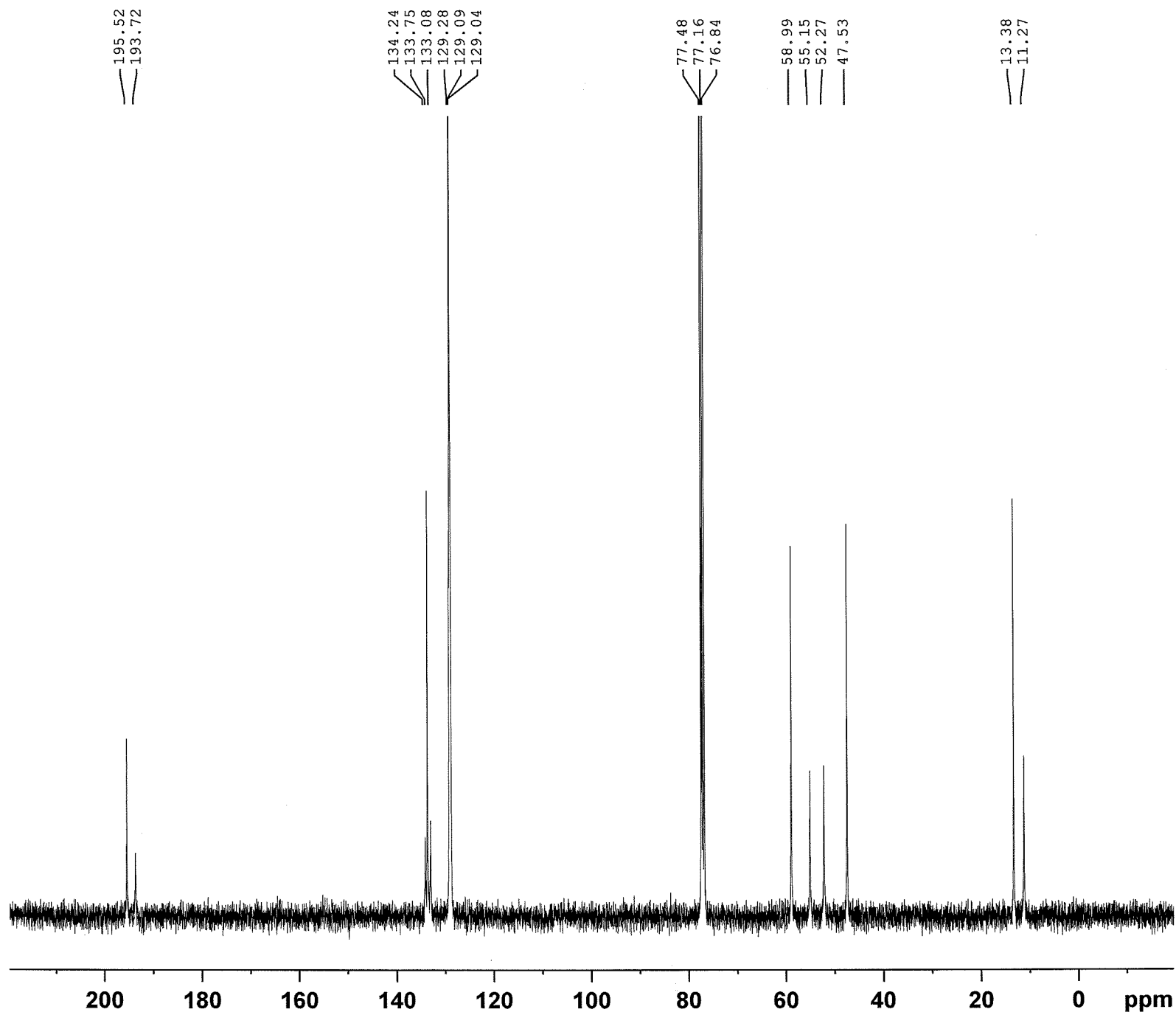


Current Data Parameters  
NAME SN0347-L1  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210519  
Time 10.53  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 7978.724 Hz  
FIDRES 0.243491 Hz  
AQ 2.0534613 sec  
RG 69.13  
DW 62.667 usec  
DE 6.50 usec  
TE 296.2 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 399.7524686 MHz  
NUC1 1H  
P1 9.00 usec  
PLW1 19.20000076 W

F2 - Processing parameters  
SI 65536  
SF 399.7500098 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Current Data Parameters  
NAME SN0347-LOT1  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210521  
Time\_ 0.24  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 2048  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 199.3  
DW 20.800 usec  
DE 6.50 usec  
TE 295.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 100.5272687 MHz  
NUC1 13C  
P1 8.60 usec  
PLW1 87.00000000 W

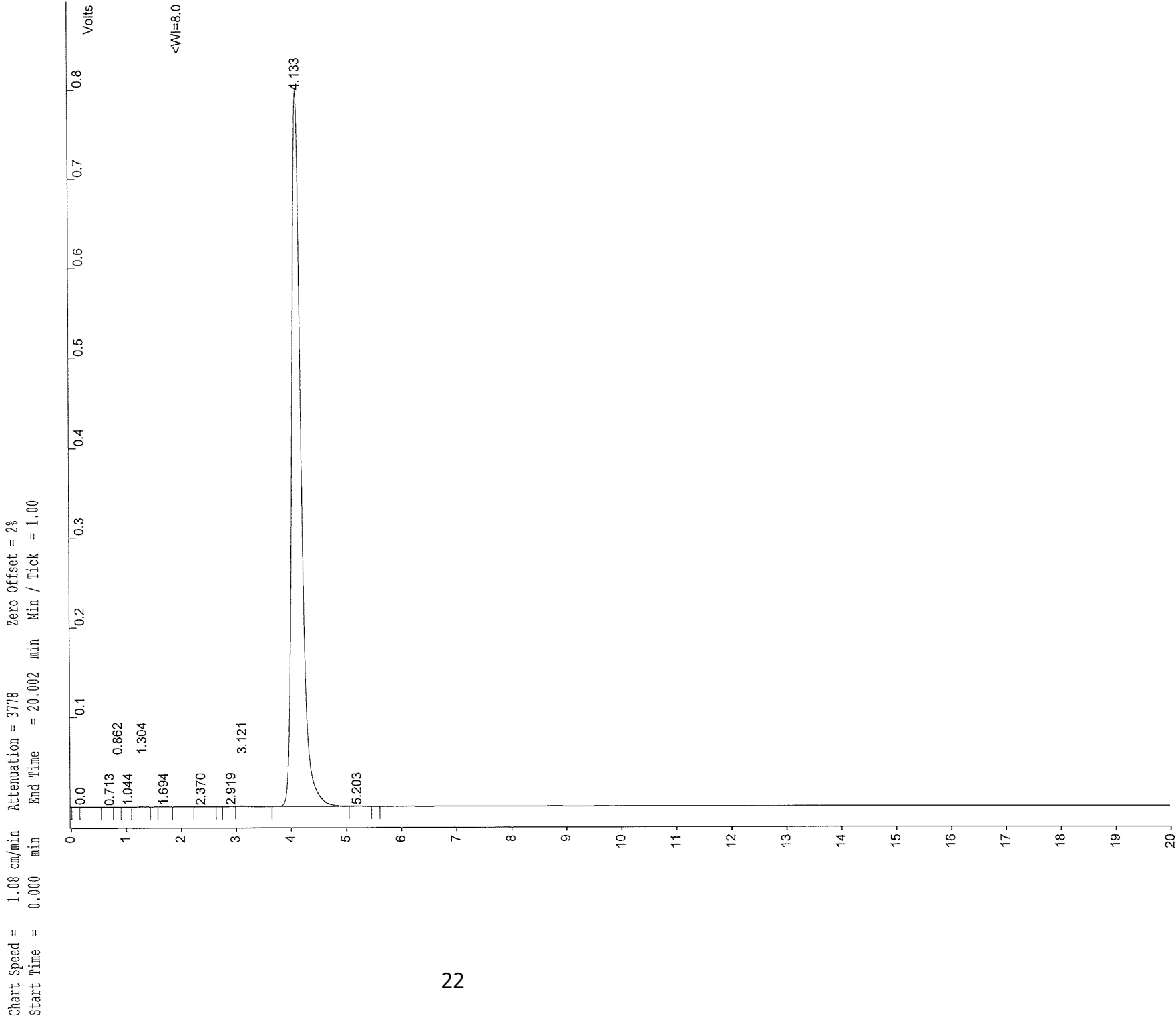
===== CHANNEL f2 =====  
SFO2 399.7515990 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 19.20000076 W  
PLW12 0.20000000 W  
PLW13 0.15552001 W

F2 - Processing parameters  
SI 32768  
SF 100.5172106 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Title :  
Run File : C:\Users\DG\Documents\SYNTHENOVA\Mode opératoire\SN0346-49 421-26\thiuram HPLC\HPLC ok\SN0347-L1.run  
Method File : C:\STAR\STARTUP1.MTH  
Sample ID : SN0347-L1

Injection Date: 21/05/2021 14:17      Calculation Date: 21/05/2021 14:37

Operator : dG      Detector Type: 0800 (1 Volt)  
Workstation: HDD      Bus Address : 81  
Instrument : Instrument #1      Sample Rate : 10.00 Hz  
Channel : 2 = 2 1      Run Time : 20.002 min



Title :  
Run File : C:\Users\DG\Documents\SYNTHENOVA\Mode opératoire\SN0346-49 421-26\thiuram HPLC\HPLC ok\SN0347-L1.run  
Method File : C:\STAR\STARTUP1.MTH  
Sample ID : SN0347-L1

Injection Date: 21/05/2021 14:17      Calculation Date: 21/05/2021 14:37

Operator : dG                      Detector Type: 0800 (1 Volt)  
Workstation: HDD                  Bus Address : 81  
Instrument : Instrument #1        Sample Rate : 10.00 Hz  
Channel : 2 = 2 1                Run Time : 20.002 min

Run Mode : Analysis  
Peak Measurement: Peak Area  
Calculation Type: Percent

Peak No.	Peak Name	Result ( )	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		0.0110	0.713	0.000	1018	BV	7.6	
2		0.0123	0.862	0.000	1138	VP	3.2	
3		0.0166	1.044	0.000	1539	PV	5.4	
4		0.0328	1.304	0.000	3048	VV	5.5	
5		0.0236	1.694	0.000	2195	VB	5.0	
6		0.0290	2.370	0.000	2697	BB	6.1	
7		0.0539	2.919	0.000	5010	BV	6.8	
8		0.1185	3.121	0.000	11007	VP	8.2	
9		99.6787	4.133	0.000	9260407	PB	10.2	
10		0.0236	5.203	0.000	2195	TS	0.0	
Totals:		100.0000		0.000	9290254			

Total Unidentified Counts : 9290255 counts

Detected Peaks: 12                  Rejected Peaks: 2                  Identified Peaks: 0

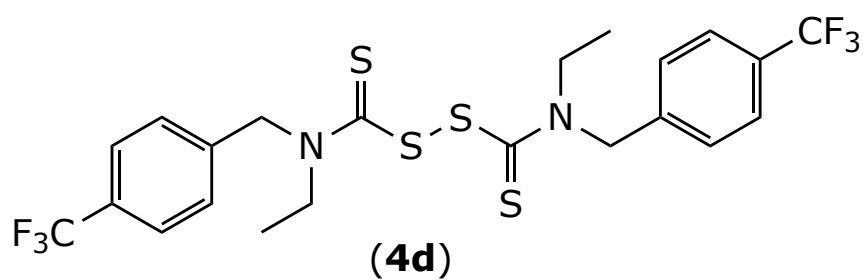
Multiplier: 1                  Divisor: 1                  Unidentified Peak Factor: 1

Baseline Offset: -160 microVolts                  LSB: 1 microVolts

Noise (used): 37 microVolts - monitored before this run

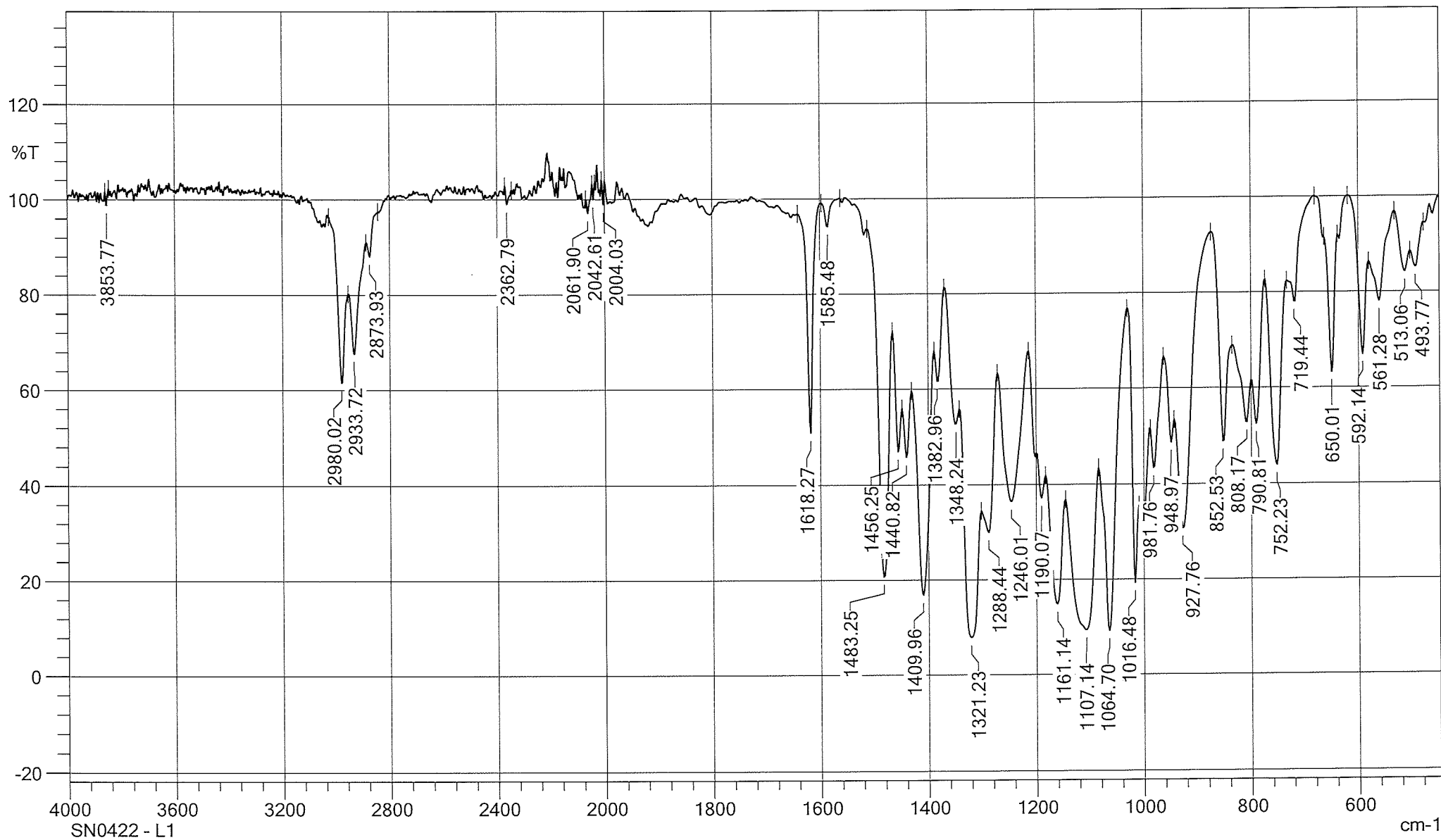
Manual injection

\*\*\*\*\*



Chemical Formula: C<sub>22</sub>H<sub>22</sub>F<sub>6</sub>N<sub>2</sub>S<sub>4</sub>  
Exact Mass: 556.0570





Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 14.0  
Element prediction: Off  
Number of isotope peaks used for i-FIT = 4

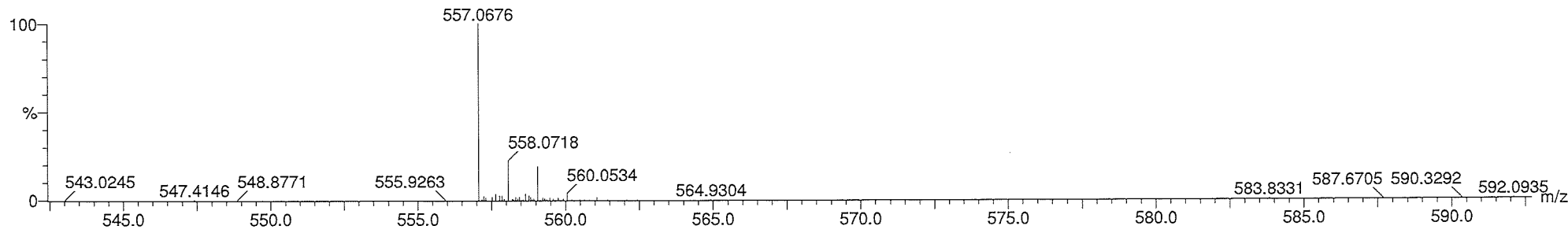
Monoisotopic Mass, Even Electron Ions  
522 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)  
Elements Used:  
C: 0-500 H: 0-1000 N: 0-3 S: 0-6 F: 4-7

01-Jun-2021  
2106007 612 (3.714) Cm (612:613-(594:595+648:663))

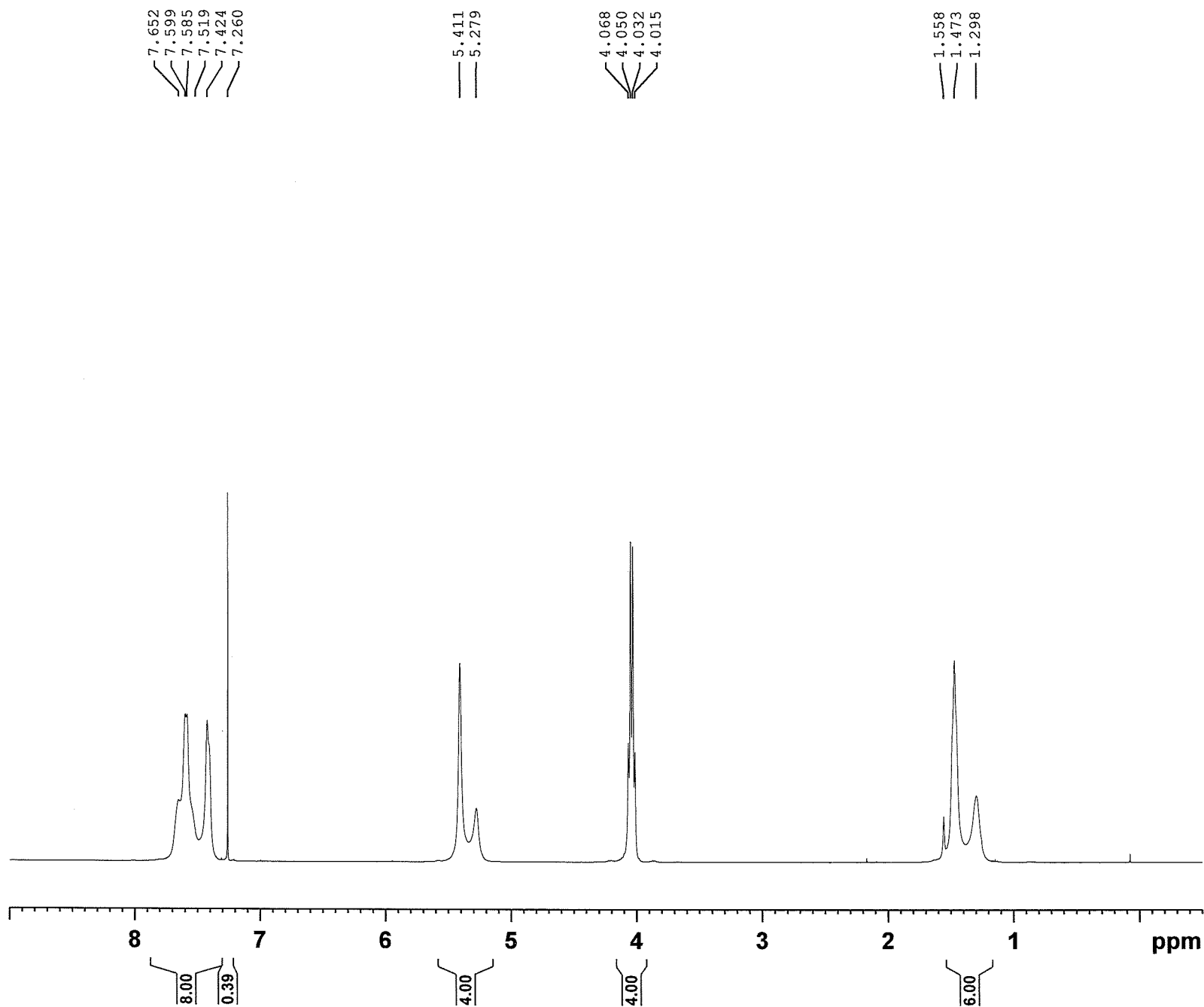
SN0422

2:14

1: TOF MS ES+  
8.37e+003



Minimum:				0.0						
Maximum:		5.0	5.0	14.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula			
557.0676	557.0648	2.8	5.0	9.5	248.5	0.4	C22	H23	N2	S4 F6
	557.0682	-0.6	-1.1	4.5	249.3	1.2	C19	H27	N2	S5 F6

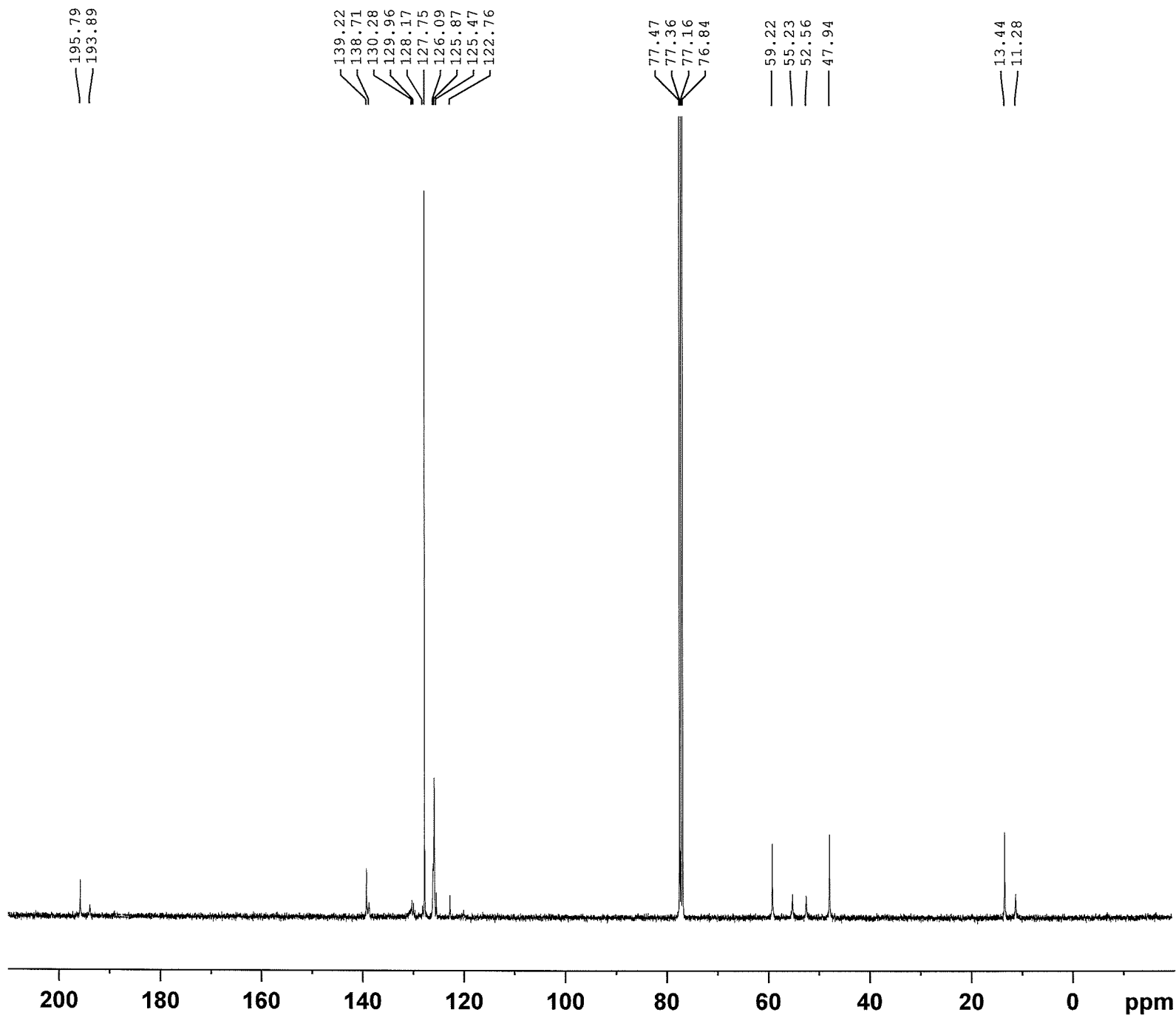


Current Data Parameters  
 NAME SN0422-L1  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20210526  
 Time 18.01  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 7978.724 Hz  
 FIDRES 0.243491 Hz  
 AQ 2.0534613 sec  
 RG 79.2  
 DW 62.667 usec  
 DE 6.50 usec  
 TE 296.2 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 399.7524686 MHz  
 NUC1 1H  
 P1 9.00 usec  
 PLW1 19.20000076 W

F2 - Processing parameters  
 SI 65536  
 SF 399.7500098 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME SN0422-lot1  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20210527  
 Time 23.18  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 2048  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 199.3  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.5272687 MHz  
 NUC1 13C  
 P1 8.60 usec  
 PLW1 87.00000000 W

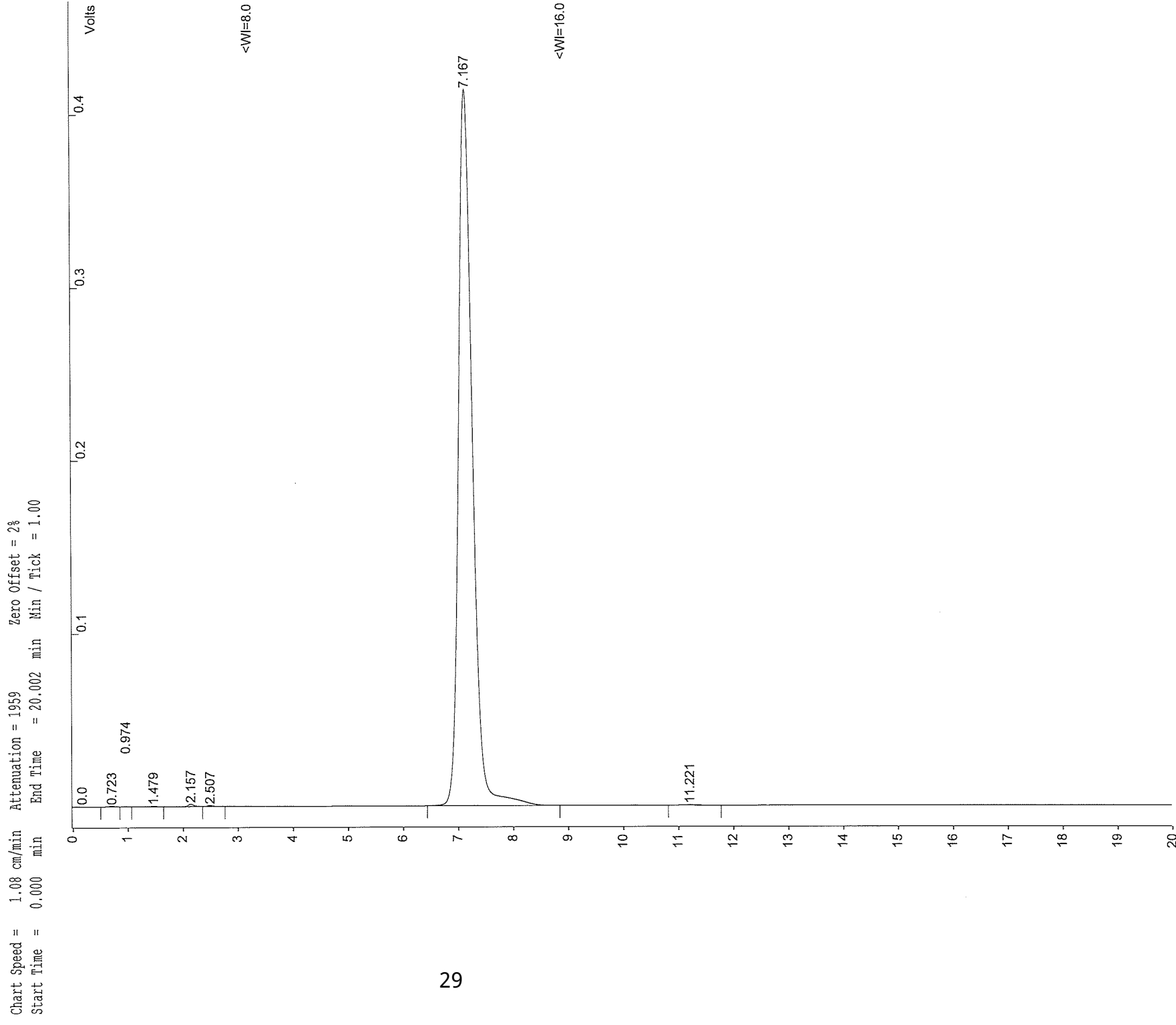
===== CHANNEL f2 =====  
 SFO2 399.7515990 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 19.20000076 W  
 PLW12 0.20000000 W  
 PLW13 0.15552001 W

F2 - Processing parameters  
 SI 32768  
 SF 100.5172078 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

Title :  
Run File : C:\Users\DG\Documents\SYNTHENOVA\Mode opératoire\SN0346-49 421-26\thiuram HPLC\HPLC ok\SN0422-L1.run  
Method File : C:\star\startup1.mth  
Sample ID : SN0422-L1

Injection Date: 26/05/2021 15:42      Calculation Date: 26/05/2021 16:02

Operator : dG      Detector Type: 0800 (1 Volt)  
Workstation: HDD      Bus Address : 81  
Instrument : Instrument #1      Sample Rate : 10.00 Hz  
Channel : 2 = 2 1      Run Time : 20.002 min



Print Date: Thu May 27 11:30:46 2021                      Page 1 of 1

Title :  
Run File : C:\Users\DG\Documents\SYNTHENOVA\Mode opératoire\SN0346-49 421-26\thiuram HPLC\HPLC ok\SN0422-L1.run  
Method File : C:\star\startup1.mth  
Sample ID : SN0422-L1

Injection Date: 26/05/2021 15:42      Calculation Date: 26/05/2021 16:02

Operator : dG                      Detector Type: 0800 (1 Volt)  
Workstation: HDD                      Bus Address : 81  
Instrument : Instrument #1              Sample Rate : 10.00 Hz  
Channel : 2 = 2 1                      Run Time : 20.002 min

Run Mode : Analysis  
Peak Measurement: Peak Area  
Calculation Type: Percent

Peak No.	Peak Name	Result ( )	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		0.0483	0.723	0.000	3523	BP	8.8	
2		0.0212	0.974	0.000	1544	PP	6.6	
3		0.0646	1.479	0.000	4706	PV	7.3	
4		0.1678	2.157	0.000	12235	VV	6.4	
5		0.0671	2.507	0.000	4893	VB	7.3	
6		99.5413	7.167	0.000	7257482	BB	15.6	
7		0.0897	11.221	0.000	6539	BB	22.8	
Totals:		100.0000		0.000	7290922			

Total Unidentified Counts :      7290923 counts

Detected Peaks: 7                      Rejected Peaks: 0                      Identified Peaks: 0

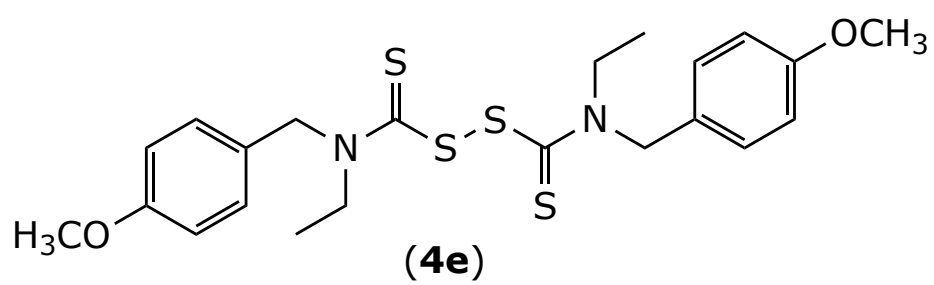
Multiplier: 1                      Divisor: 1                      Unidentified Peak Factor: 1

Baseline Offset: -12 microVolts                      LSB:      1 microVolts

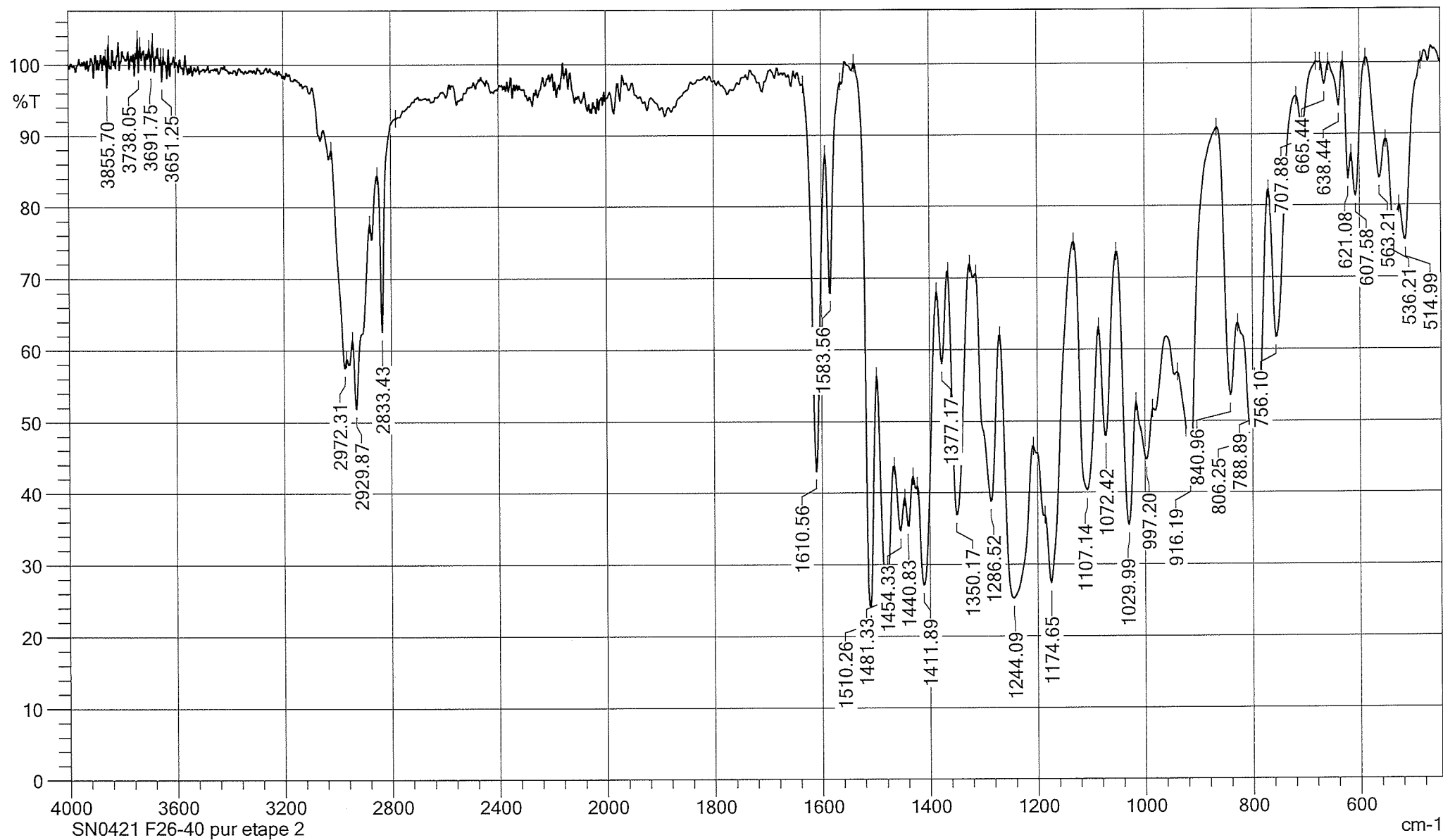
Noise (used): 68 microVolts - monitored before this run

Manual injection

\*\*\*\*\*



Chemical Formula: C<sub>22</sub>H<sub>28</sub>N<sub>2</sub>O<sub>2</sub>S<sub>4</sub>  
Exact Mass: 480.1034





## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 14.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

560 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

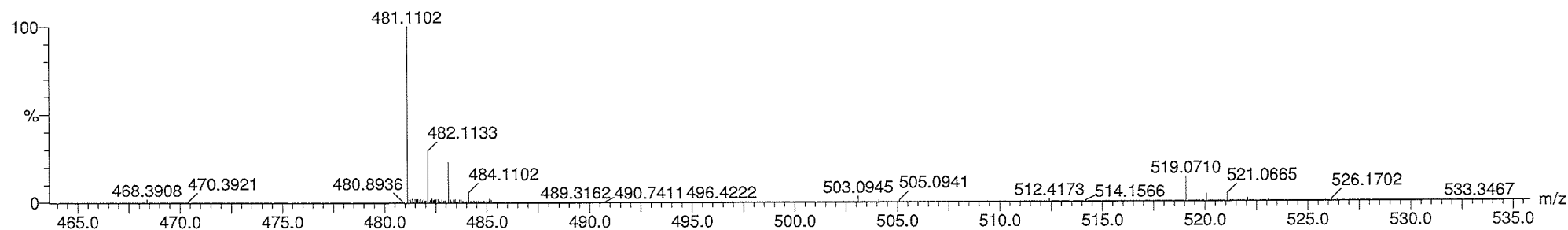
C: 0-500 H: 0-1000 N: 0-3 O: 0-3 S: 0-6

SN0421

2:13

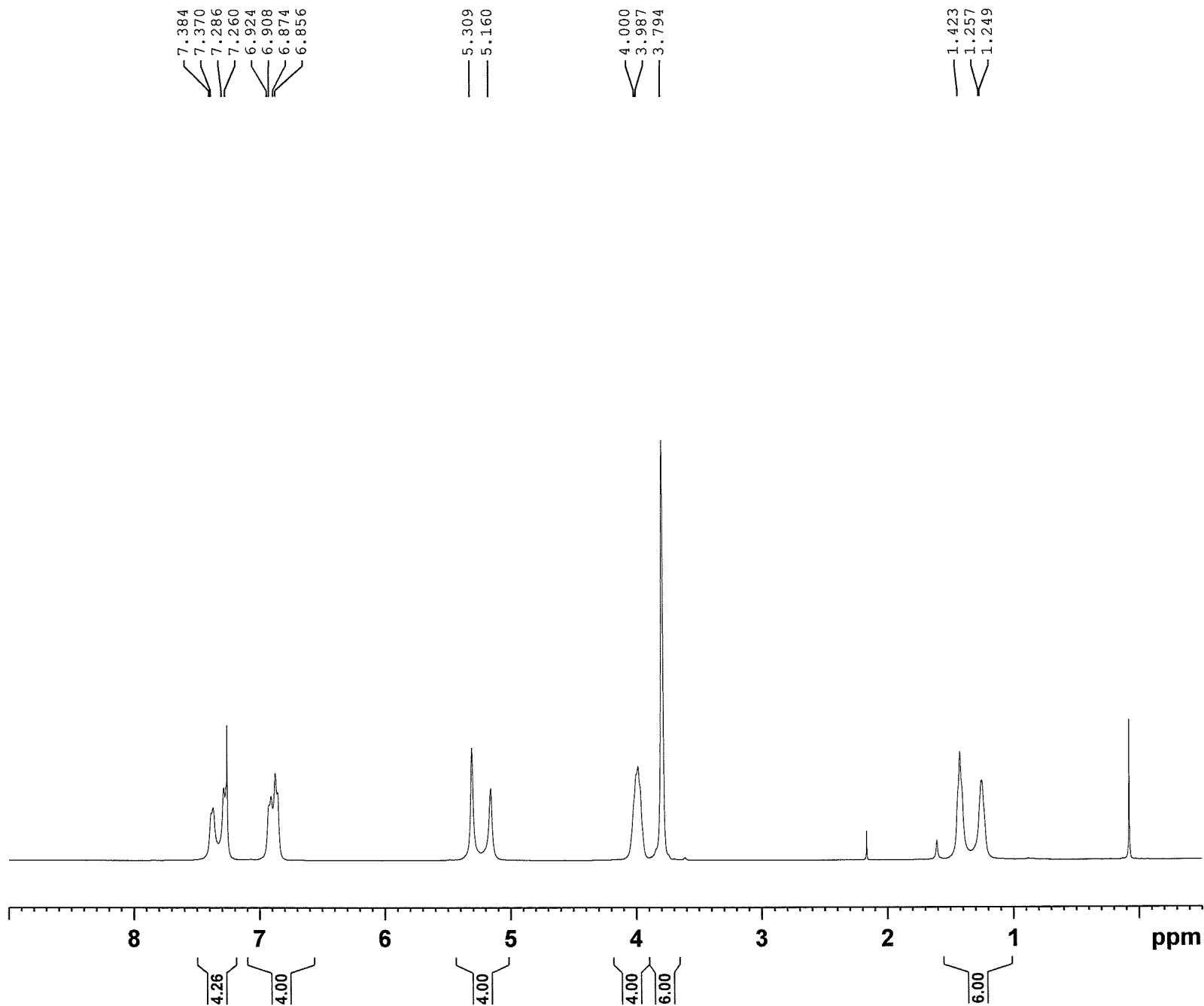
01-Jun-2021

2106006 554 (3.365) Cm (552:557)

1: TOF MS ES+  
5.62e+004

Minimum: 0.0  
Maximum: 5.0 5.0 14.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
481.1102	481.1112	-1.0	-2.1	9.5	690.6	0.0	C22 H29 N2 O2 S4

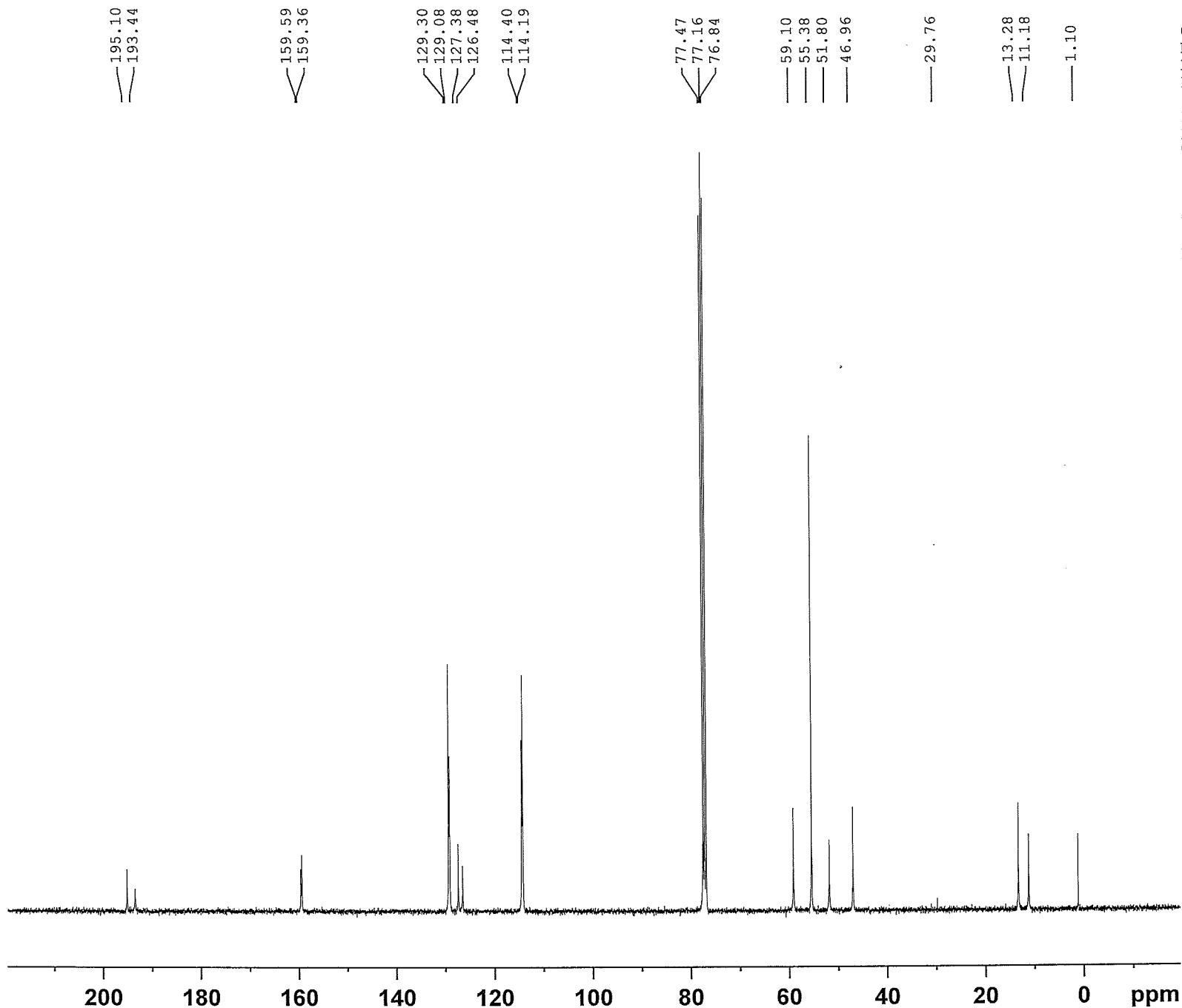


Current Data Parameters  
NAME SN0421  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210427  
Time 17.55  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 7978.724 Hz  
FIDRES 0.243491 Hz  
AQ 2.0534613 sec  
RG 30.7  
DW 62.667 usec  
DE 6.50 usec  
TE 296.2 K  
D1 2.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SF01 399.7524686 MHz  
NUC1 1H  
P1 9.00 usec  
PLW1 19.20000076 W

F2 - Processing parameters  
SI 65536  
SF 399.7500098 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



35

Current Data Parameters  
NAME SN0421-L1  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210501  
Time\_ 20.34  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 2048  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 199.3  
DW 20.800 usec  
DE 6.50 usec  
TE 295.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 100.5272687 MHz  
NUC1 13C  
P1 8.60 usec  
PLW1 87.00000000 W

===== CHANNEL f2 =====  
SFO2 399.7515990 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 19.20000076 W  
PLW12 0.20000000 W  
PLW13 0.15552001 W

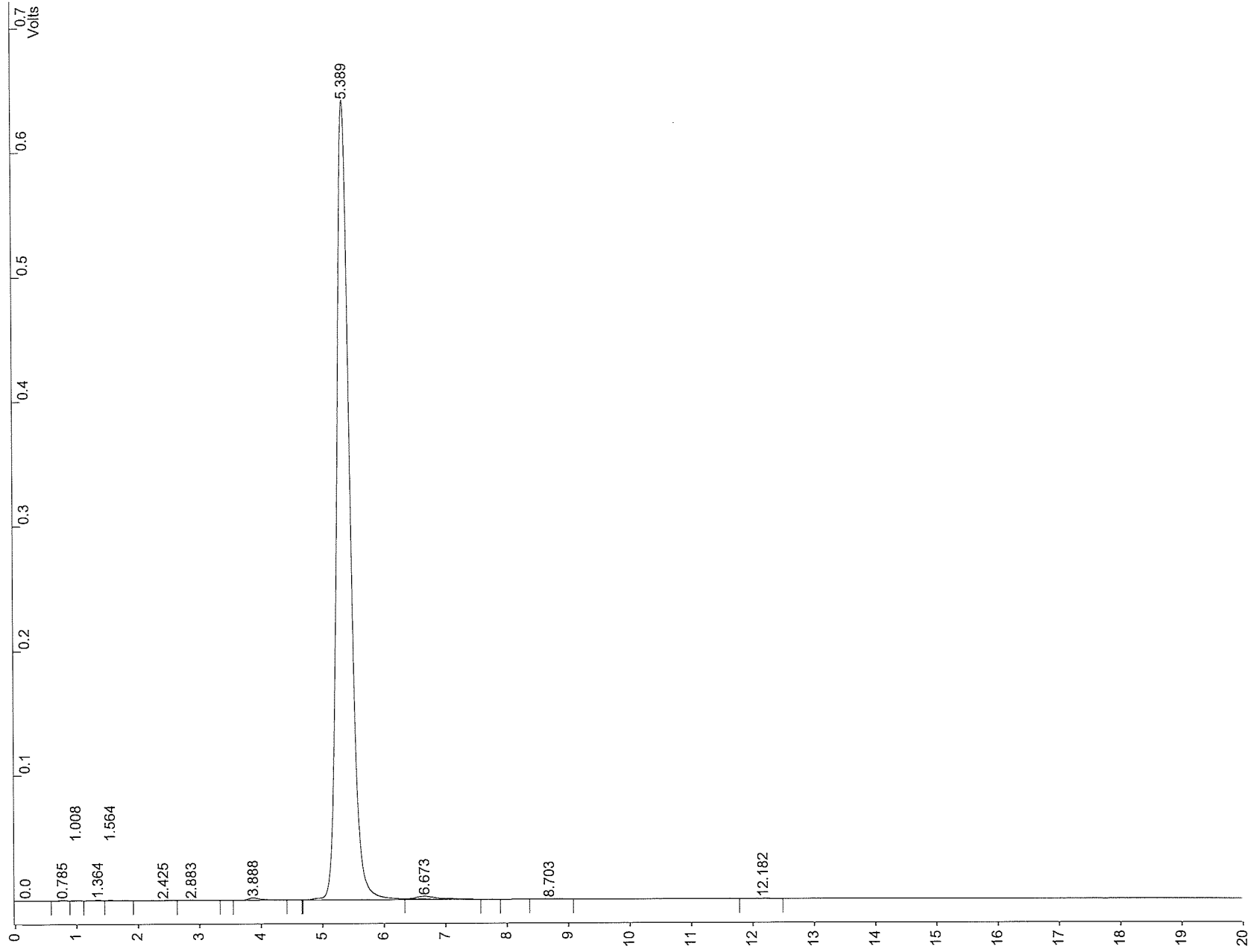
F2 - Processing parameters  
SI 32768  
SF 100.5172136 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Title :  
Run File : C:\Users\DG\Documents\SYNTHENOVA\Mode opératoire\SN0346-49 421-26\thiuram HPLC\HPLC ok\SN0421-L1.run  
Method File : C:\star\startup1.mth  
Sample ID : SN0421-L1

Injection Date: 12/05/2021 17:16      Calculation Date: 12/05/2021 17:36

Operator : dG      Detector Type: 0800 (1 Volt)  
Workstation: HDD      Bus Address : 81  
Instrument : Instrument #1      Sample Rate : 10.00 Hz  
Channel : 2 = 2 1      Run Time : 20.002 min

Chart Speed = 1.08 cm/min      Attenuation = 3035      Zero Offset = 2%  
Start Time = 0.000 min      End Time = 20.002 min      Min / Tick = 1.00



Run Mode : Analysis  
Peak Measurement: Peak Area  
Calculation Type: Percent

Peak No.	Peak Name	Result ( )	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		0.0469	0.785	0.000	4502	BV	7.8	
2		0.0185	1.008	0.000	1772	VV	10.3	
3		0.0628	1.364	0.000	6027	VV	7.0	
4		0.0660	1.564	0.000	6334	VV	7.5	
5		0.0466	2.425	0.000	4470	VV	0.0	
6		0.0438	2.883	0.000	4201	VB	10.1	
7		0.3073	3.888	0.000	29472	BB	11.2	
8		98.7962	5.389	0.000	9475442	VB	13.2	
9		0.5346	6.673	0.000	51273	TS	0.0	
10		0.0537	8.703	0.000	5148	BB	15.3	
11		0.0235	12.182	0.000	2256	BB	0.0	
Totals:		99.9999		0.000	9590897			

Total Unidentified Counts : 9590898 counts

Detected Peaks: 12      Rejected Peaks: 1      Identified Peaks: 0

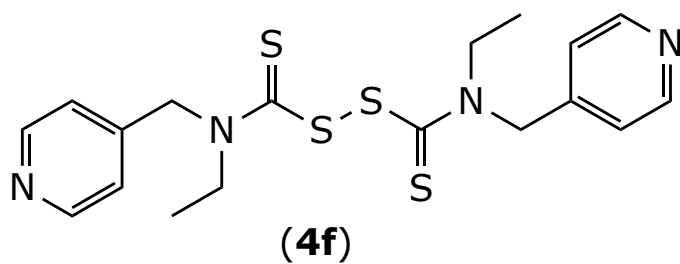
Multiplier: 1      Divisor: 1      Unidentified Peak Factor: 1

Baseline Offset: -38 microVolts      LSB: 1 microVolts

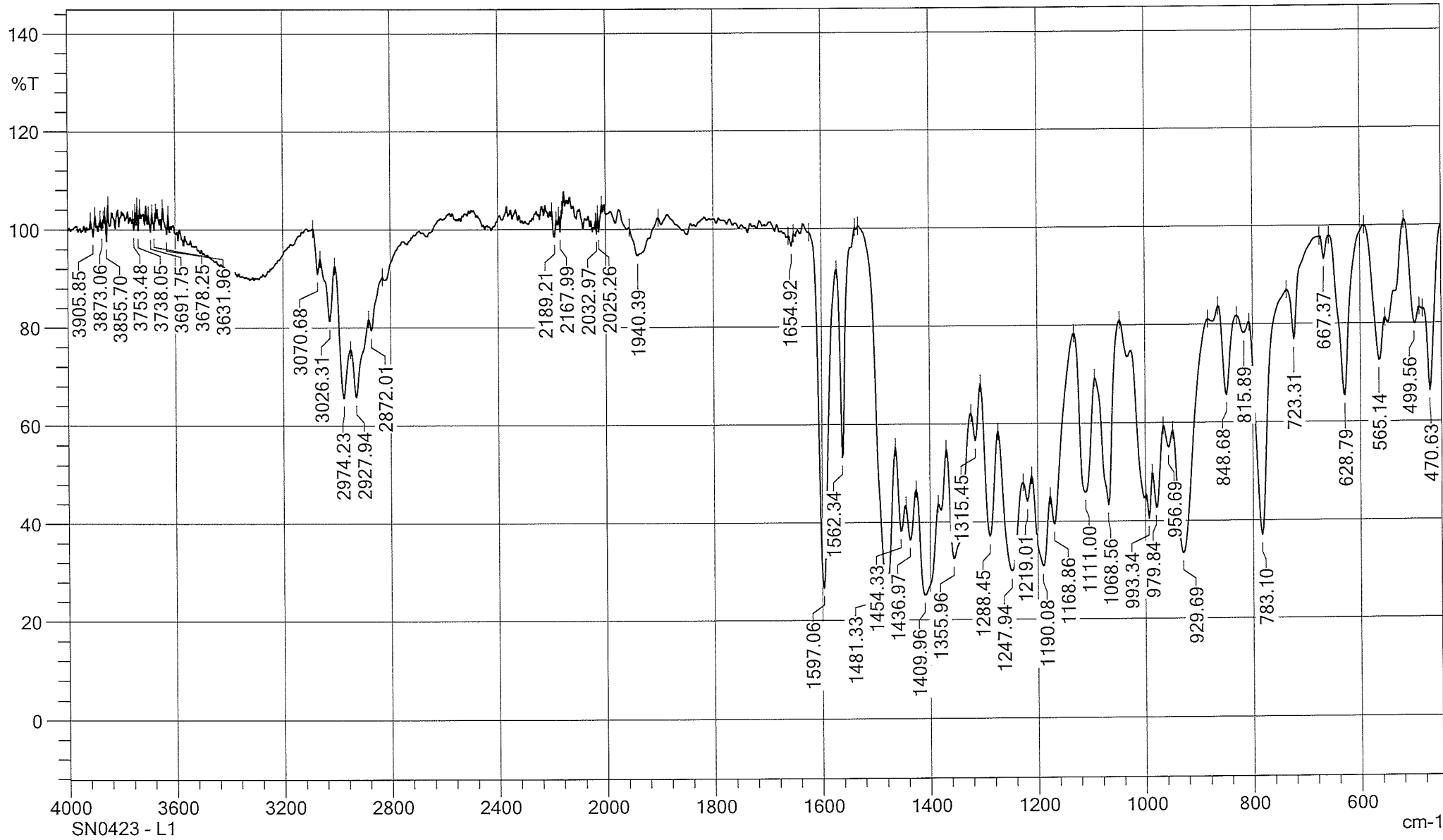
Noise (used): 34 microVolts - monitored before this run

Manual injection

\*\*\*\*\*



Chemical Formula: C<sub>18</sub>H<sub>22</sub>N<sub>4</sub>S<sub>4</sub>  
Exact Mass: 422.0727



## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 14.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

189 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

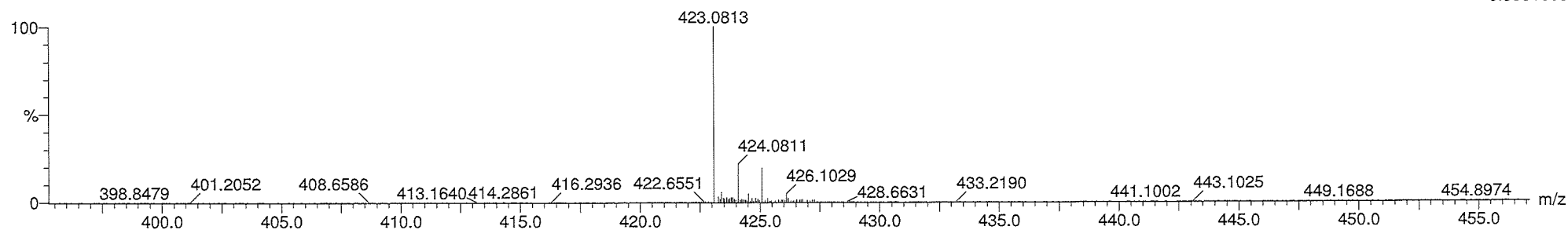
C: 0-500 H: 0-1000 N: 0-5 S: 0-6

01-Jun-2021

2106008 360 (2.176) Cm (360-(343+391))

SN0423

2:15

1: TOF MS ES+  
6.39e+003

Minimum: 0.0  
Maximum: 5.0 5.0 14.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
423.0813	423.0806	0.7	1.7	9.5	357.3	0.0	C18 H23 N4 S4



8.578  
8.512  
7.280  
7.279  
7.278  
7.276  
7.275  
7.274  
7.273  
7.271  
7.270  
7.269  
7.260  
7.234  
7.233  
7.228  
7.213  
7.148

5.291  
5.175

4.035  
4.017  
3.999  
3.981

2.510

1.432  
1.293  
1.263  
1.247  
1.212

Current Data Parameters  
NAME SN0423-L1  
EXPNO 10  
PROCNO 1

# F2 - Acquisition Parameters

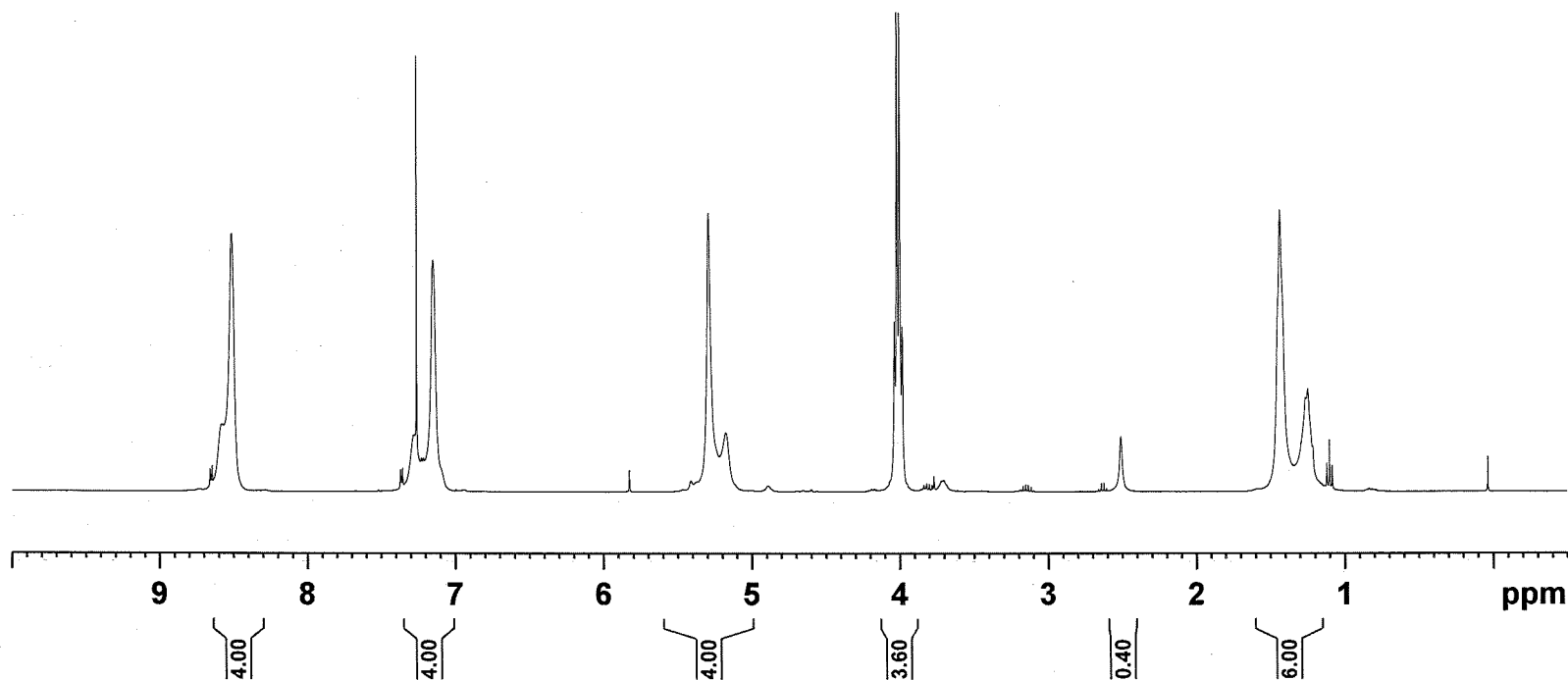
Date\_ 20210520  
Time\_ 17.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 7978.724 Hz  
FIDRES 0.243491 Hz  
AQ 2.0534613 sec  
RG 30.7  
DW 62.667 usec  
DE 6.50 usec  
TE 296.2 K  
D1 1.00000000 sec  
TD0 1

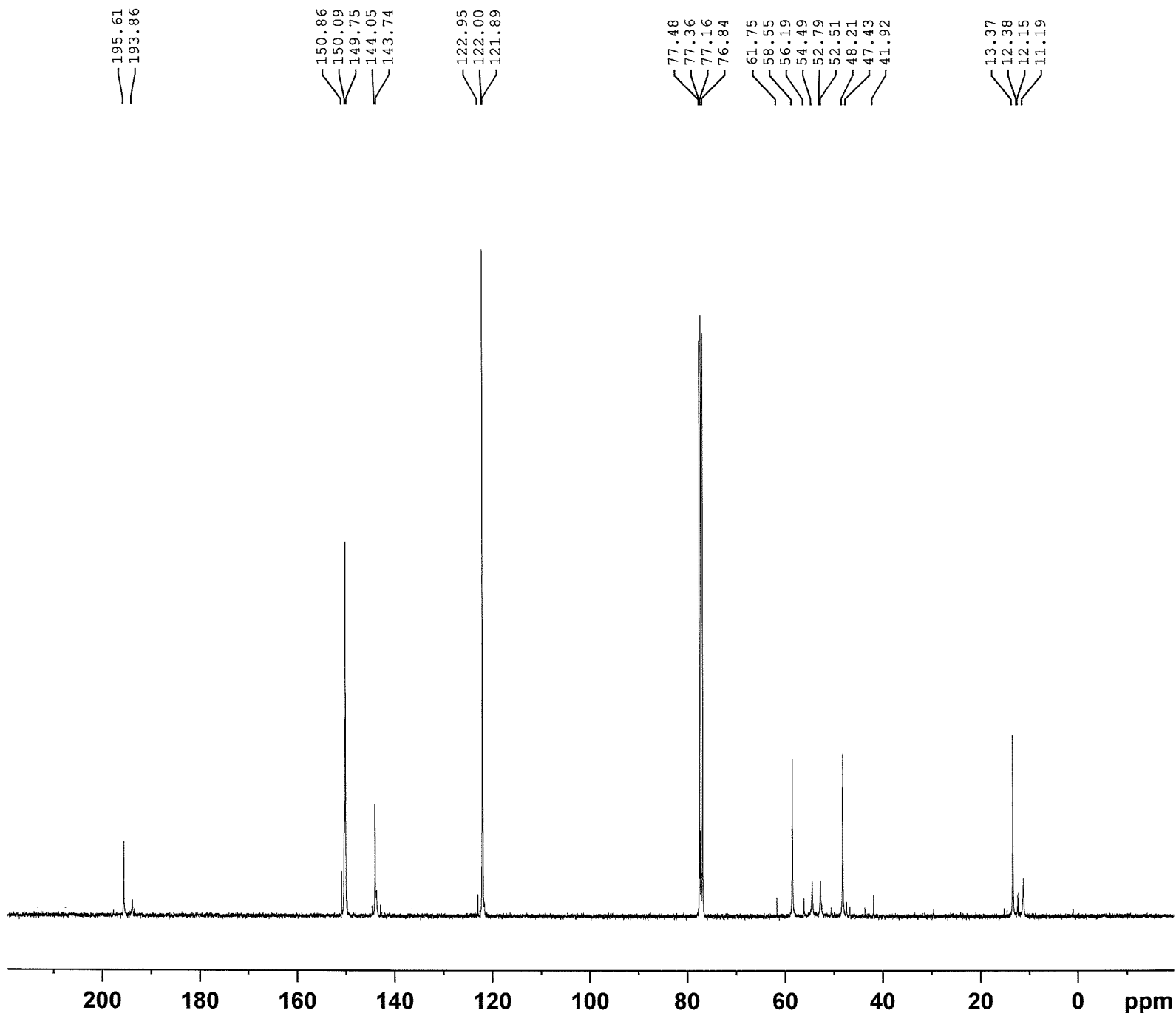
# ===== CHANNEL f1 =====

SFO1 399.7524686 MHz  
NUC1 1H  
P1 9.00 usec  
PLW1 19.20000076 W

# F2 - Processing parameters

SI 65536  
SF 399.7500100 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
 NAME SN0423-LOT1  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210523  
 Time\_ 9.02  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 2048  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 199.3  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.5272687 MHz  
 NUC1 13C  
 P1 8.60 usec  
 PLW1 87.00000000 W

===== CHANNEL f2 =====  
 SFO2 399.7515990 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 19.20000076 W  
 PLW12 0.20000000 W  
 PLW13 0.15552001 W

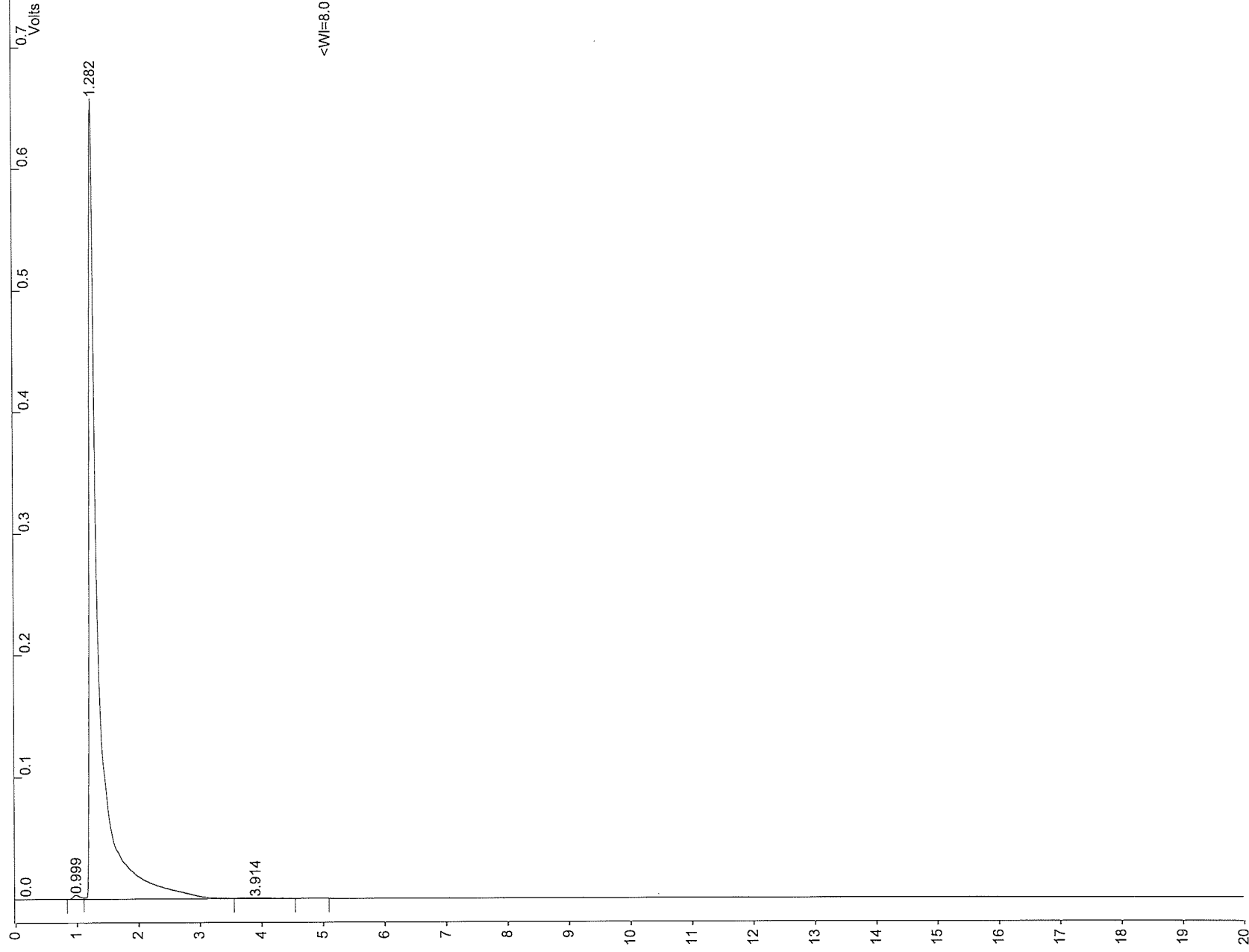
F2 - Processing parameters  
 SI 32768  
 SF 100.5172217 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

Title :  
Run File : C:\Users\DG\Documents\SYNTHENOVA\Mode opératoire\SN0346-49 421-26\thiuram HPLC\HPLC ok\SN0423-L1.run  
Method File : C:\star\startup1.mth  
Sample ID : SN0423-L1

Injection Date: 27/05/2021 10:55      Calculation Date: 27/05/2021 11:15

Operator : DG      Detector Type: 0800 (1 Volt)  
Workstation: HDD      Bus Address : 81  
Instrument : Instrument #1      Sample Rate : 10.00 Hz  
Channel : 2 = 2 1      Run Time : 20.002 min

Chart Speed = 1.08 cm/min      Attenuation = 3112      Zero Offset = 2%  
Start Time = 0.000 min      End Time = 20.002 min      Min / Tick = 1.00



<W=8.0

Title :  
Run File : C:\Users\DG\Documents\SYNTHENOVA\Mode opératoire\SN0346-49 421-26\thiuram HPLC\HPLC ok\SN0423-L1.run  
Method File : C:\star\startup1.mth  
Sample ID : SN0423-L1

Injection Date: 27/05/2021 10:55      Calculation Date: 27/05/2021 11:15

Operator : DG                      Detector Type: 0800 (1 Volt)  
Workstation: HDD                  Bus Address : 81  
Instrument : Instrument #1        Sample Rate : 10.00 Hz  
Channel : 2 = 2 1                Run Time : 20.002 min

Run Mode : Analysis  
Peak Measurement: Peak Area  
Calculation Type: Percent

Peak No.	Peak Name	Result ( )	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		0.3955	0.999	0.000	26791	BV	7.7	
2		99.4729	1.282	0.000	6738153	VB	6.2	
3		0.1316	3.914	0.000	8912	TS	0.0	
Totals:		100.0000		0.000	6773856			

Total Unidentified Counts : 6773856 counts

Detected Peaks: 3                  Rejected Peaks: 0                  Identified Peaks: 0

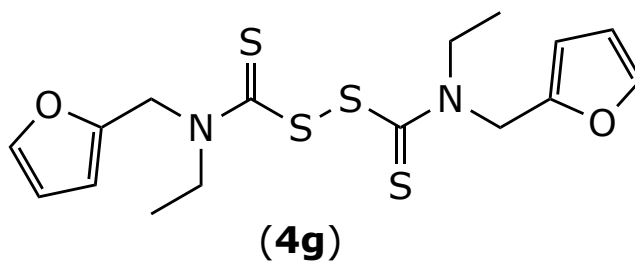
Multiplier: 1                  Divisor: 1                  Unidentified Peak Factor: 1

Baseline Offset: 4 microVolts                  LSB: 1 microVolts

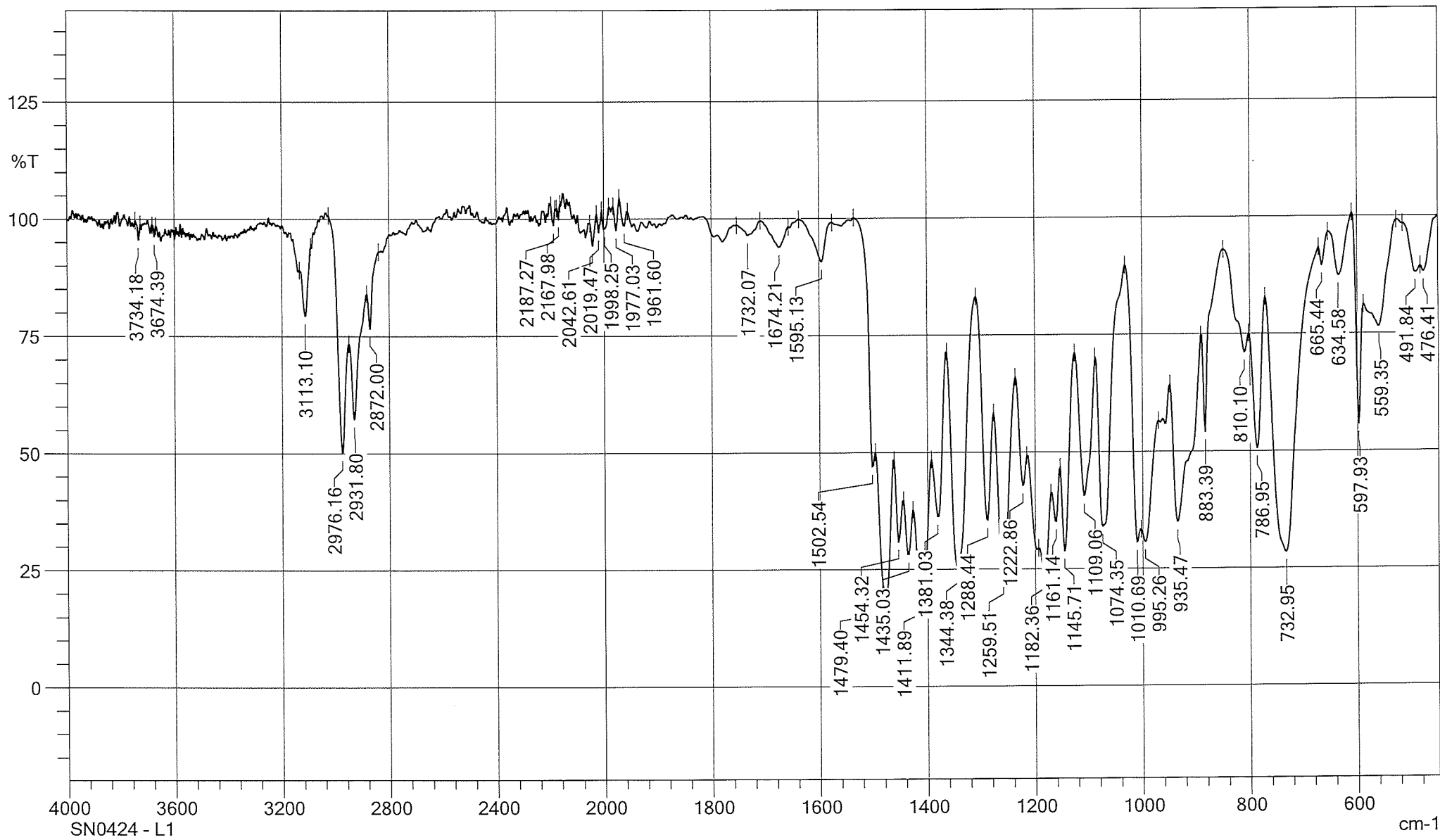
Noise (used): 35 microVolts - monitored before this run

Manual injection

\*\*\*\*\*



Chemical Formula:  $\text{C}_{16}\text{H}_{20}\text{N}_2\text{O}_2\text{S}_4$   
Exact Mass: 400.0408



## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 14.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

662 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

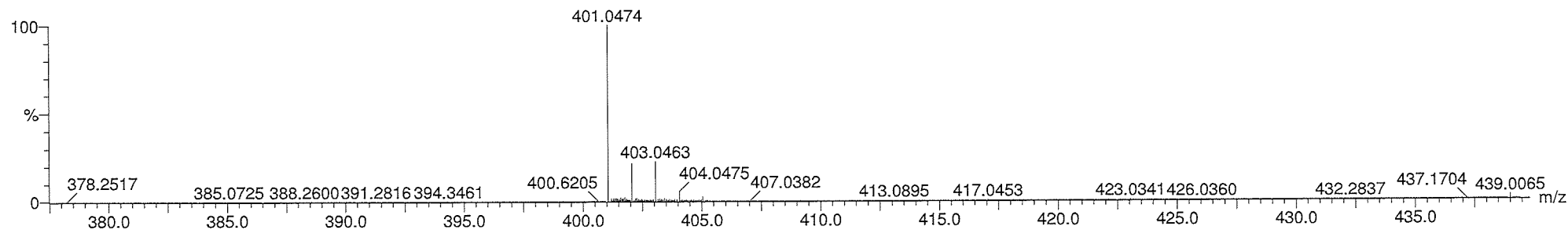
C: 0-500 H: 0-1000 N: 0-5 O: 0-3 S: 0-6

SN0424

2:16

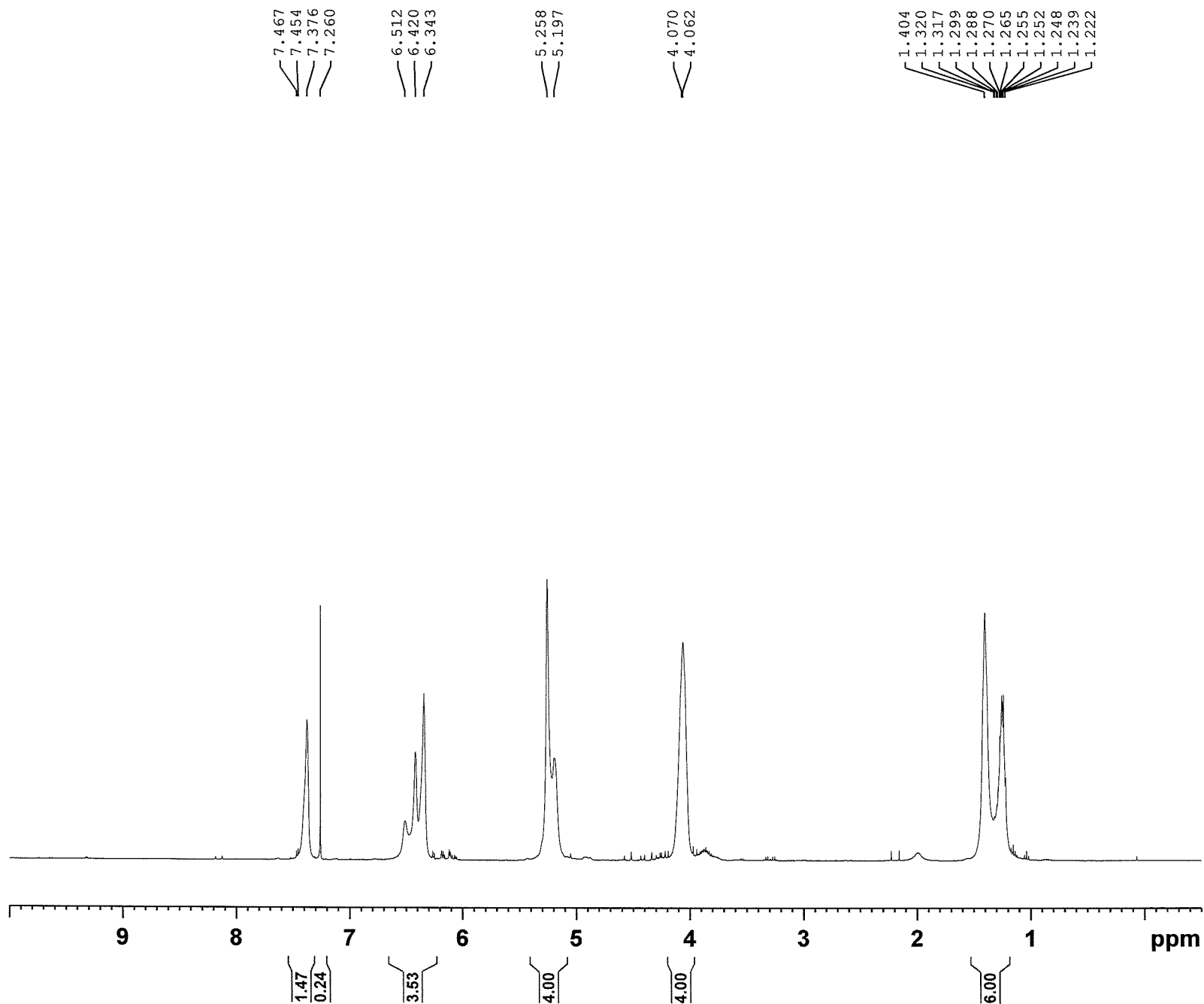
01-Jun-2021

2106009 510 (3.078) Cm (508:513)

1: TOF MS ES+  
7.96e+004

Minimum: 0.0  
Maximum: 5.0 5.0 14.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
401.0474	401.0486	-1.2	-3.0	7.5	866.2	0.0	C16 H21 N2 O2 S4



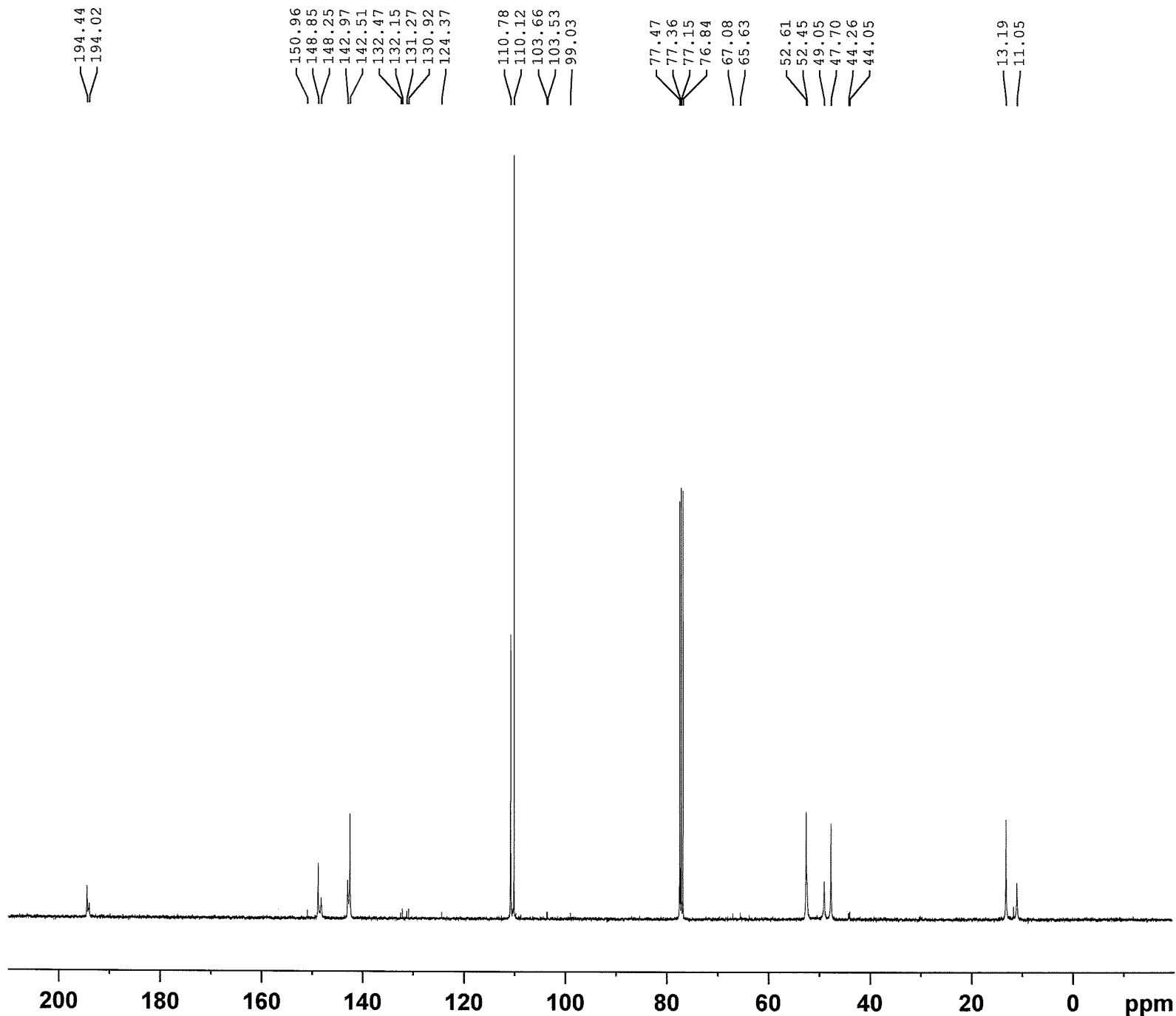
Current Data Parameters  
 NAME SN0424LOT1  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210523  
 Time 5.00  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 7978.724 Hz  
 FIDRES 0.243491 Hz  
 AQ 2.0534613 sec  
 RG 30.7  
 DW 62.667 usec  
 DE 6.50 usec  
 TE 296.2 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SF01 399.7524686 MHz  
 NUC1 1H  
 P1 9.00 usec  
 PLW1 19.20000076 W

F2 - Processing parameters  
 SI 65536  
 SF 399.7500098 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





Current Data Parameters  
 NAME SN0424LOT1  
 EXPNO 11  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210523  
 Time\_ 7.00  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 2048  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 199.3  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.5272687 MHz  
 NUC1 13C  
 P1 8.60 usec  
 PLW1 87.00000000 W

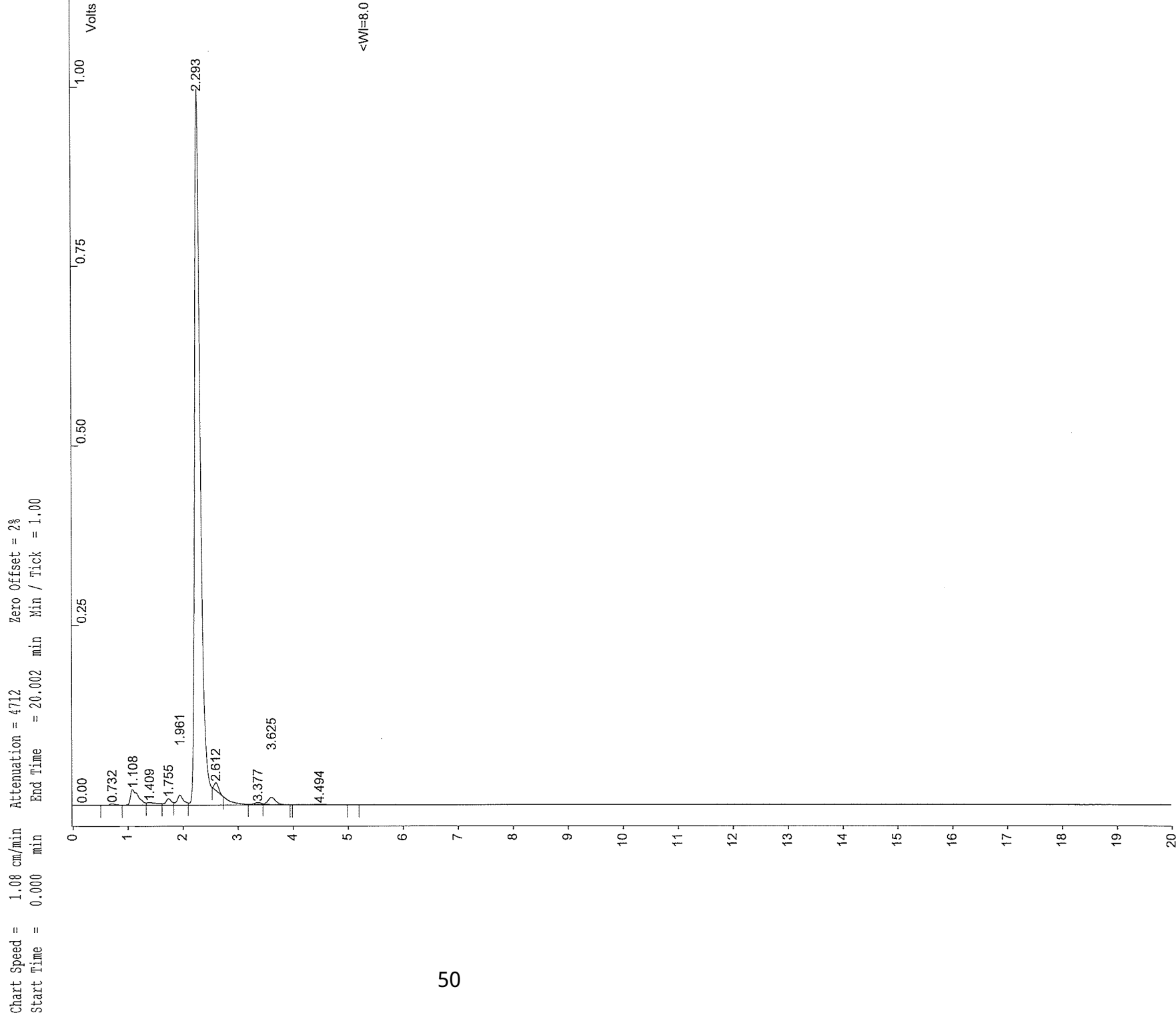
===== CHANNEL f2 =====  
 SFO2 399.7515990 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 19.20000076 W  
 PLW12 0.20000000 W  
 PLW13 0.15552001 W

F2 - Processing parameters  
 SI 32768  
 SF 100.5172175 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

Title :  
Run File : C:\Users\DG\Documents\SYNTHENOVA\Mode opératoire\SN0346-49 421-26\thiuram HPLC\HPLC ok\SN0424-L1.run  
Method File : C:\star\startup1.mth  
Sample ID : SN0424-L1

Injection Date: 21/05/2021 16:11      Calculation Date: 21/05/2021 16:31

Operator : dG      Detector Type: 0800 (1 Volt)  
Workstation: HDD      Bus Address : 81  
Instrument : Instrument #1      Sample Rate : 10.00 Hz  
Channel : 2 = 2 1      Run Time : 20.002 min



Title :  
Run File : C:\Users\DG\Documents\SYNTHENOVA\Mode opératoire\SN0346-49 421-26\thiuram HPLC\HPLC ok\SN0424-L1.run  
Method File : C:\star\startup1.mth  
Sample ID : SN0424-L1

Injection Date: 21/05/2021 16:11      Calculation Date: 21/05/2021 16:31

Operator : dG      Detector Type: 0800 (1 Volt)  
Workstation: HDD      Bus Address : 81  
Instrument : Instrument #1      Sample Rate : 10.00 Hz  
Channel : 2 = 2 1      Run Time : 20.002 min

Run Mode : Analysis  
Peak Measurement: Peak Area  
Calculation Type: Percent

Peak No.	Peak Name	Result ( )	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		0.1945	0.732	0.000	16025	BV	6.9	
2		2.7035	1.108	0.000	222712	VV	9.3	
3		0.6027	1.409	0.000	49648	VV	0.0	
4		0.8249	1.755	0.000	67959	VV	6.8	
5		1.3568	1.961	0.000	111774	VV	6.8	
6		91.9821	2.293	0.000	7577512	VB	6.4	
7		0.6958	2.612	0.000	57322	TS	0.0	
8		0.2441	3.377	0.000	20110	TF	0.0	
9		1.1896	3.625	0.000	97998	TF	0.0	
10		0.2060	4.494	0.000	16973	TS	0.0	
Totals:		100.0000		0.000	8238033			

Total Unidentified Counts : 8238033 counts

Detected Peaks: 10      Rejected Peaks: 0      Identified Peaks: 0

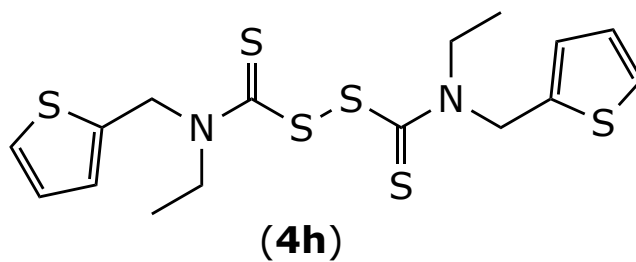
Multiplier: 1      Divisor: 1      Unidentified Peak Factor: 1

Baseline Offset: -43 microVolts      LSB: 1 microVolts

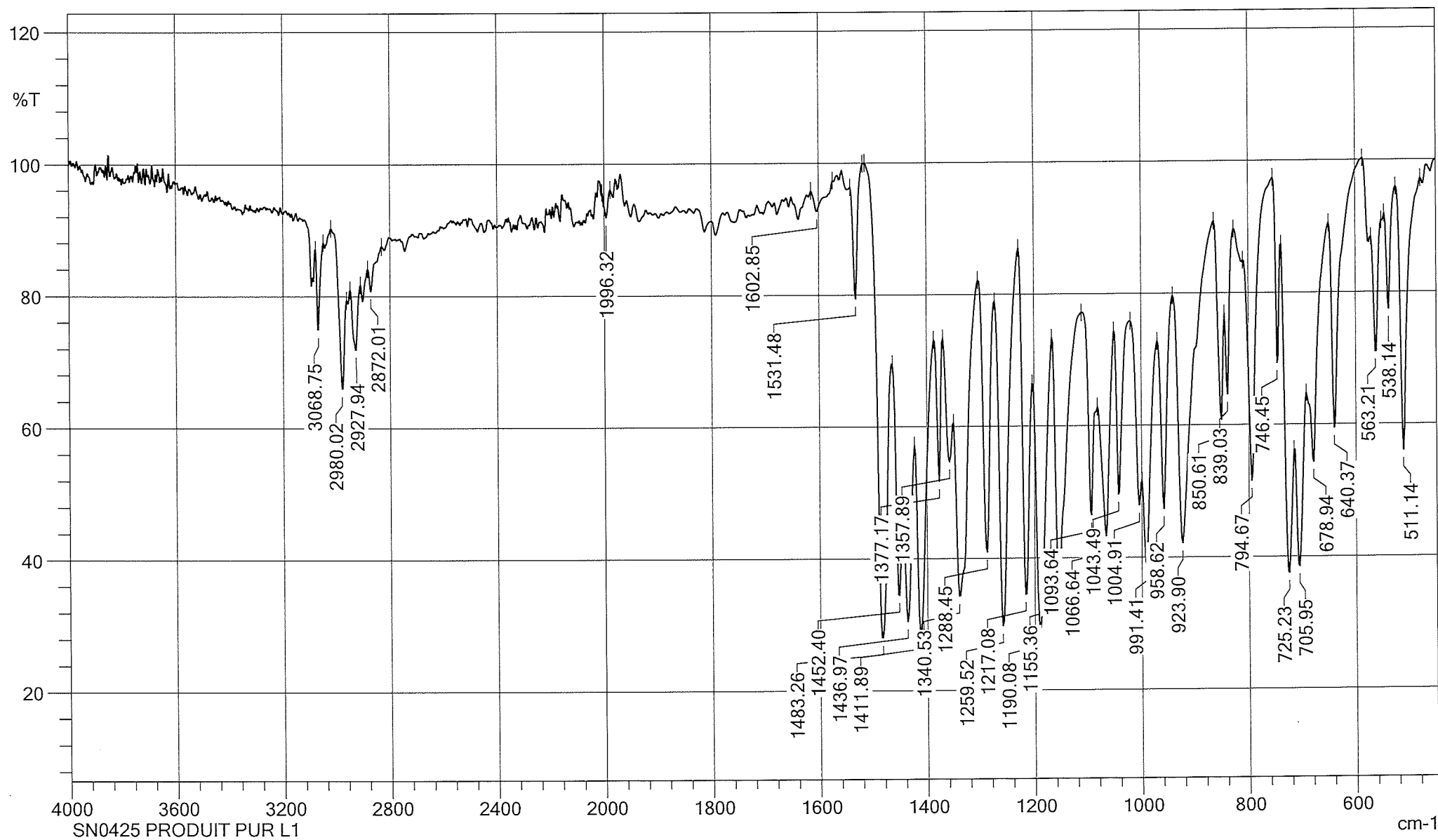
Noise (used): 26 microVolts - monitored before this run

Manual injection

\*\*\*\*\*



Chemical Formula: C<sub>16</sub>H<sub>20</sub>N<sub>2</sub>S<sub>6</sub>  
Exact Mass: 431.9951



## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 14.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

194 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

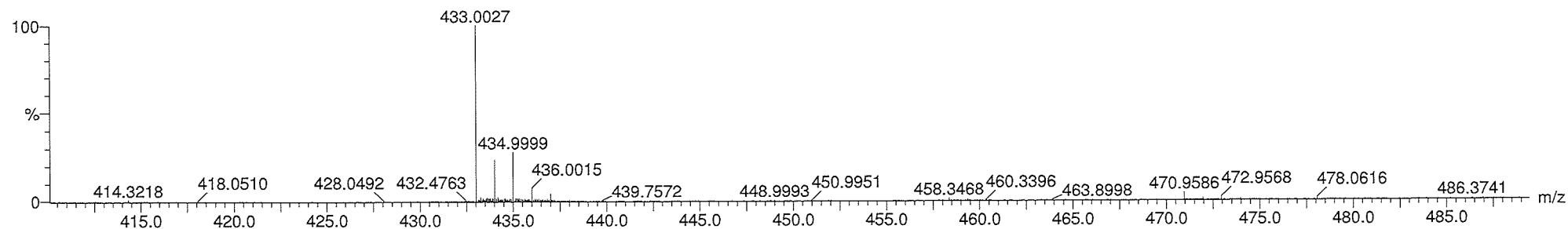
C: 0-500 H: 0-1000 N: 0-5 S: 0-6

SN0425

2:17

01-Jun-2021

2106010 540 (3.282) Cm (537:543-(506:514+567:578))

1: TOF MS ES+  
4.10e+004

Minimum: 0.0  
Maximum: 5.0 5.0 14.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
433.0027	433.0029	-0.2	-0.5	7.5	714.7	0.0	C16 H21 N2 S6

— 7.260  
— 7.107  
— 6.966

— 5.427

— 4.034

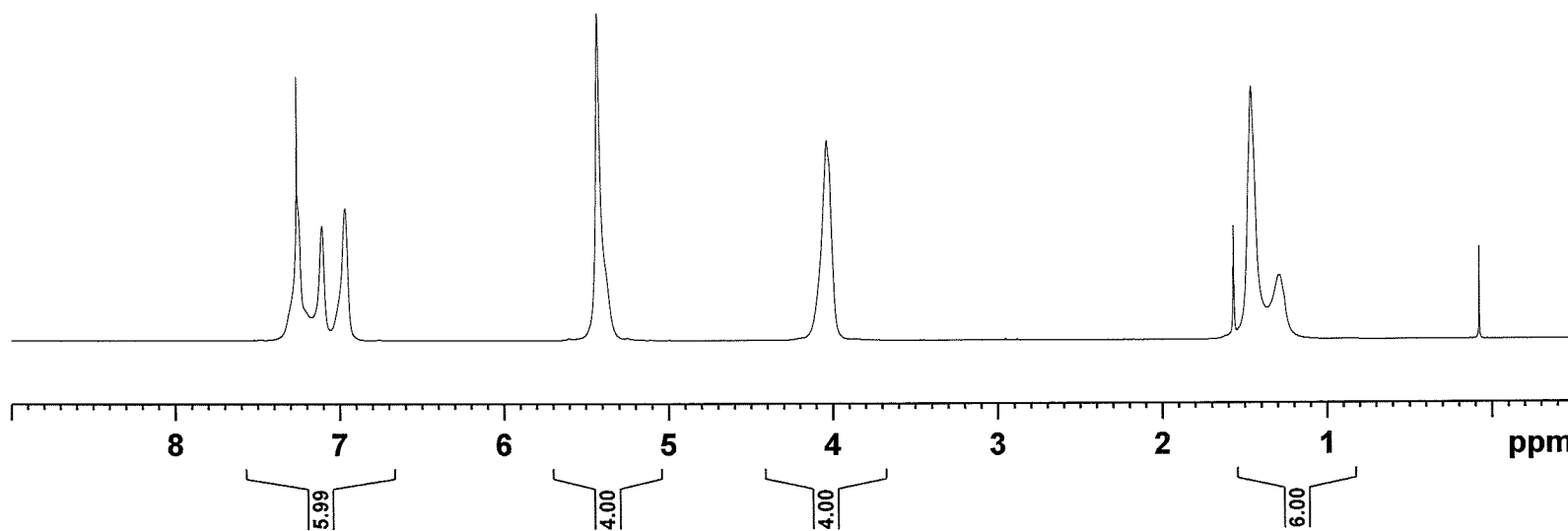
— 1.457  
— 1.288

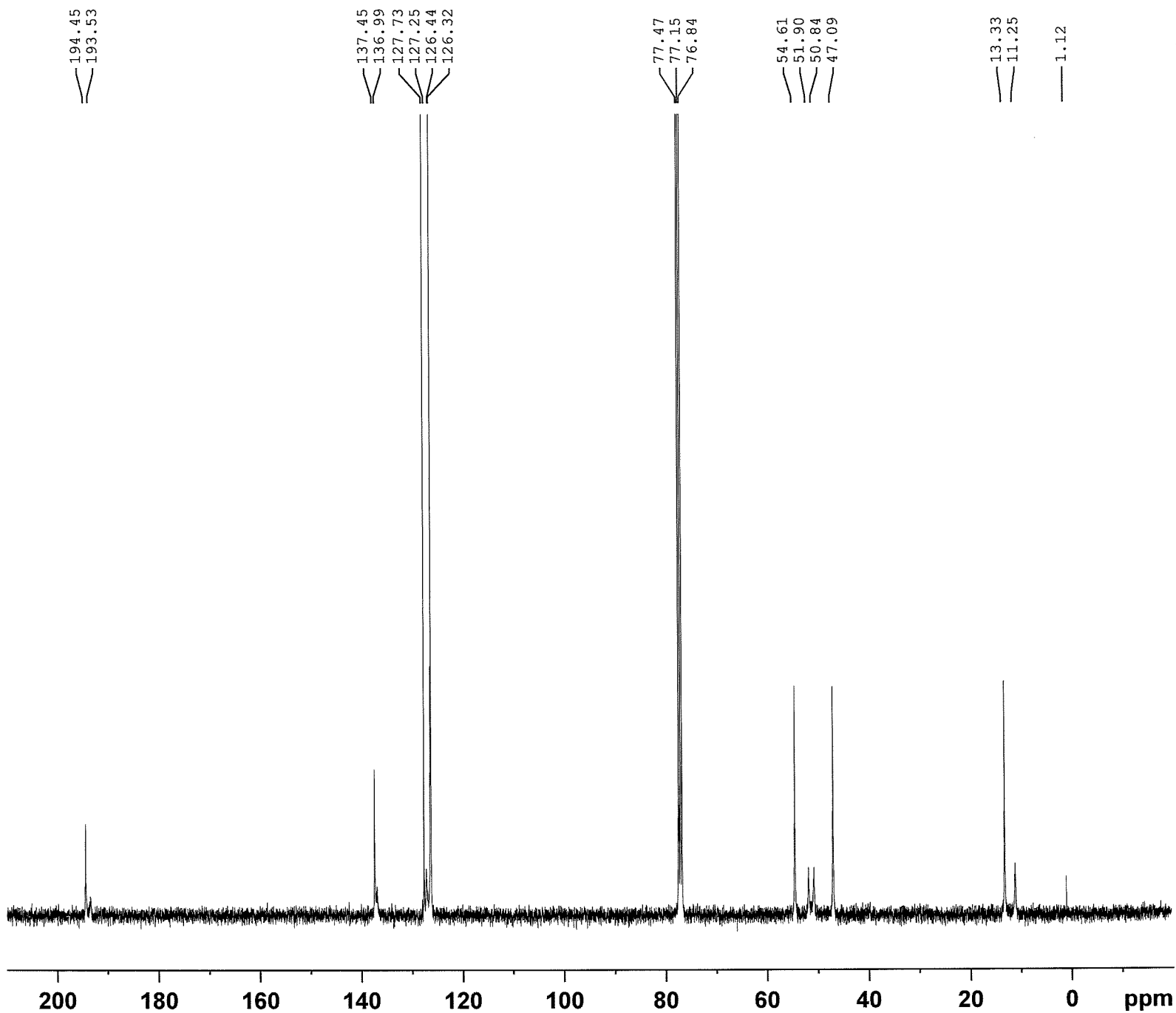
Current Data Parameters  
NAME SN0425LOT1  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210510  
Time\_ 14.43  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 7978.724 Hz  
FIDRES 0.243491 Hz  
AQ 2.0534613 sec  
RG 69.13  
DW 62.667 usec  
DE 6.50 usec  
TE 296.2 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 399.7524686 MHz  
NUC1 1H  
P1 9.00 usec  
PLW1 19.20000076 W

F2 - Processing parameters  
SI 65536  
SF 399.7500097 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





56

Current Data Parameters  
NAME SN0425-FINAL  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210511  
Time\_ 5.00  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 2048  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 199.3  
DW 20.800 usec  
DE 6.50 usec  
TE 295.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 100.5272687 MHz  
NUC1 13C  
P1 8.60 usec  
PLW1 87.00000000 W

===== CHANNEL f2 =====  
SFO2 399.7515990 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 19.20000076 W  
PLW12 0.20000000 W  
PLW13 0.15552001 W

F2 - Processing parameters  
SI 32768  
SF 100.5172114 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

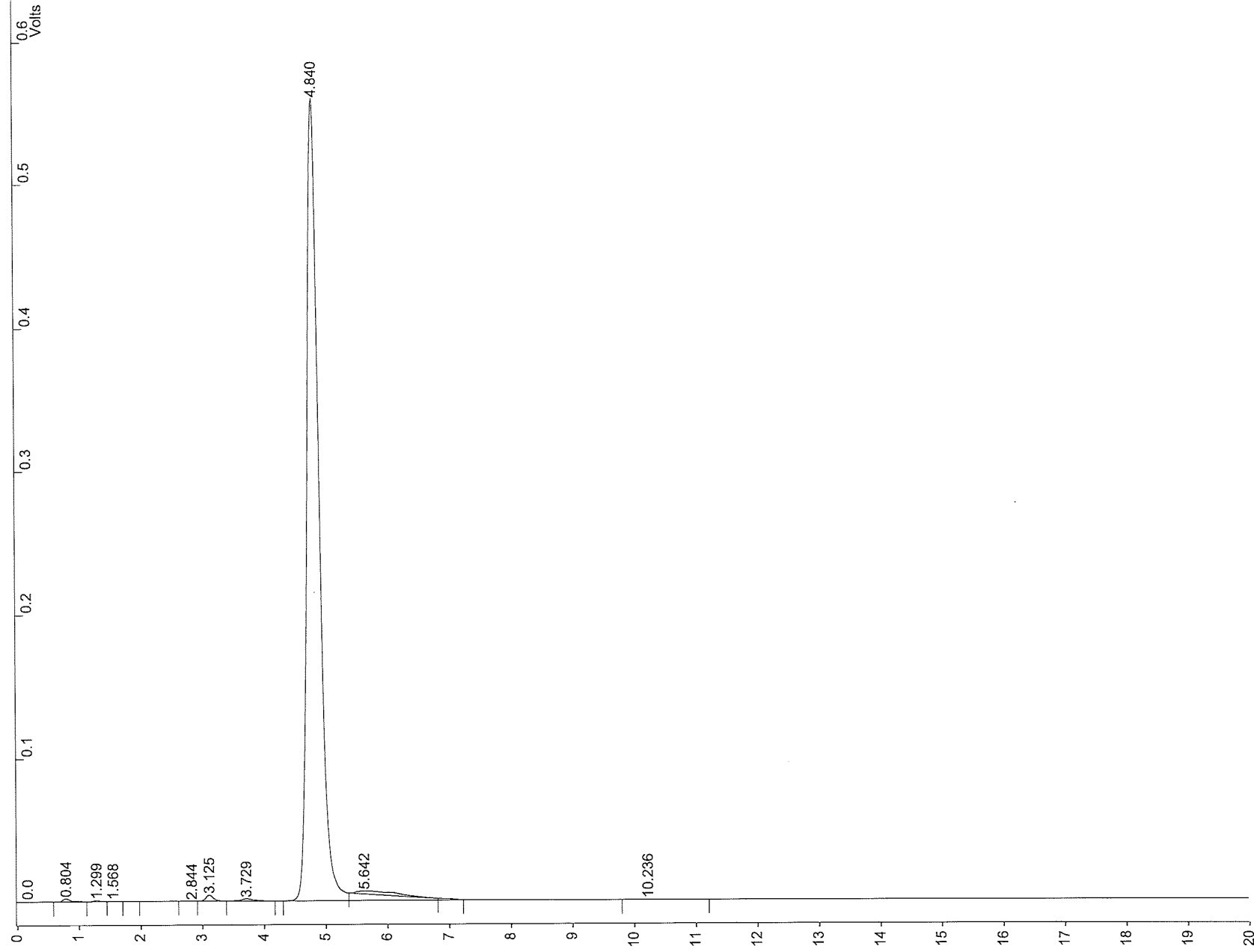


Title :  
Run File : C:\Users\DG\Documents\SYNTHENOVA\Mode opératoire\SN0346-49 421-26\thiuram HPLC\HPLC ok\SN0425-I1.run  
Method File : C:\star\startup1.mth  
Sample ID : SN0425-I1

Injection Date: 12/05/2021 16:53      Calculation Date: 12/05/2021 17:13

Operator : dG      Detector Type: 0800 (1 Volt)  
Workstation: HDD      Bus Address : 81  
Instrument : Instrument #1      Sample Rate : 10.00 Hz  
Channel : 2 = 2 1      Run Time : 20.002 min

Chart Speed = 1.08 cm/min      Attenuation = 2647      Zero Offset = 2%  
Start Time = 0.000 min      End Time = 20.002 min      Min / Tick = 1.00



Title :  
Run File : C:\Users\DG\Documents\SYNTHENOVA\Mode opératoire\SN0346-49 421-26\thiuram HPLC\HPLC ok\SN0425-L1.run  
Method File : C:\star\startup1.mth  
Sample ID : SN0425-L1

Injection Date: 12/05/2021 16:53      Calculation Date: 12/05/2021 17:13

Operator : dG      Detector Type: 0800 (1 Volt)  
Workstation: HDD      Bus Address : 81  
Instrument : Instrument #1      Sample Rate : 10.00 Hz  
Channel : 2 = 2 1      Run Time : 20.002 min

Run Mode : Analysis  
Peak Measurement: Peak Area  
Calculation Type: Percent

Peak No.	Peak Name	Result ( )	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		0.2273	0.804	0.000	18378	BP	7.0	
2		0.0788	1.299	0.000	6368	PV	8.3	
3		0.0339	1.568	0.000	2744	VV	8.8	
4		0.0160	2.844	0.000	1292	BV	10.3	
5		0.4527	3.125	0.000	36597	VV	7.7	
6		0.2954	3.729	0.000	23887	VB	11.1	
7		97.5228	4.840	0.000	7884557	BB	12.2	
8		1.2970	5.642	0.000	104861	TS	0.0	
9		0.0761	10.236	0.000	6154	BB	0.0	
Totals:		100.0000		0.000	8084838			

Total Unidentified Counts : 8084837 counts

Detected Peaks: 10      Rejected Peaks: 1      Identified Peaks: 0

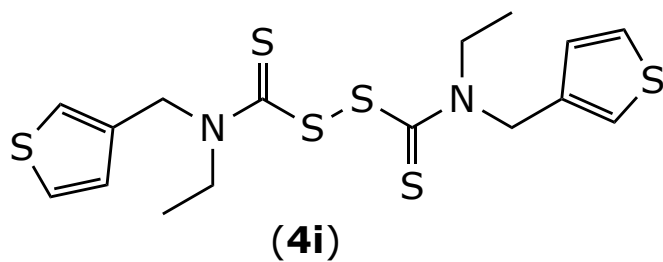
Multiplier: 1      Divisor: 1      Unidentified Peak Factor: 1

Baseline Offset: -33 microVolts      LSB: 1 microVolts

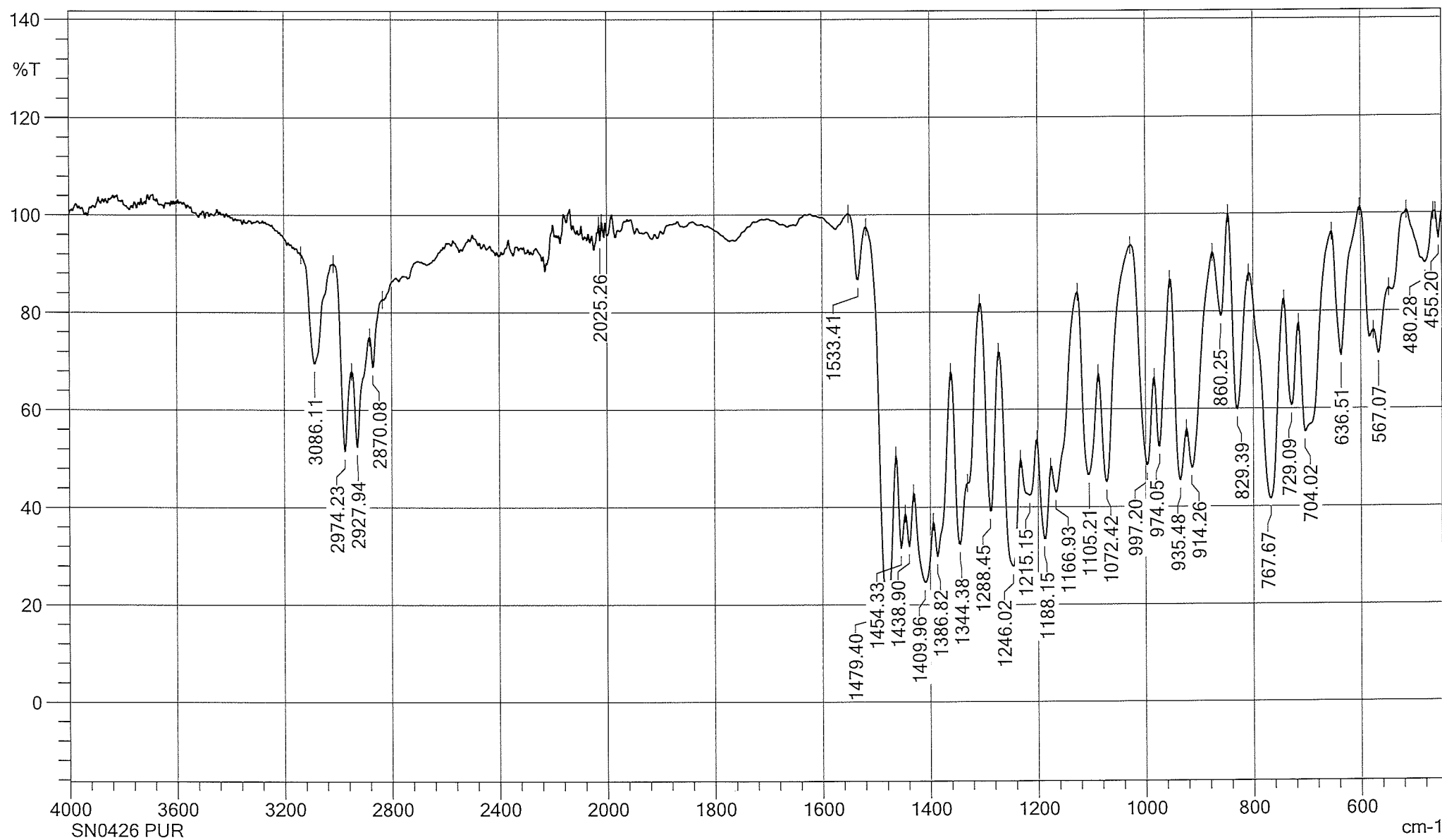
Noise (used): 28 microVolts - monitored before this run

Manual injection

\*\*\*\*\*



Chemical Formula: C<sub>16</sub>H<sub>20</sub>N<sub>2</sub>S<sub>6</sub>  
Exact Mass: 431.9951



## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 14.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

194 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

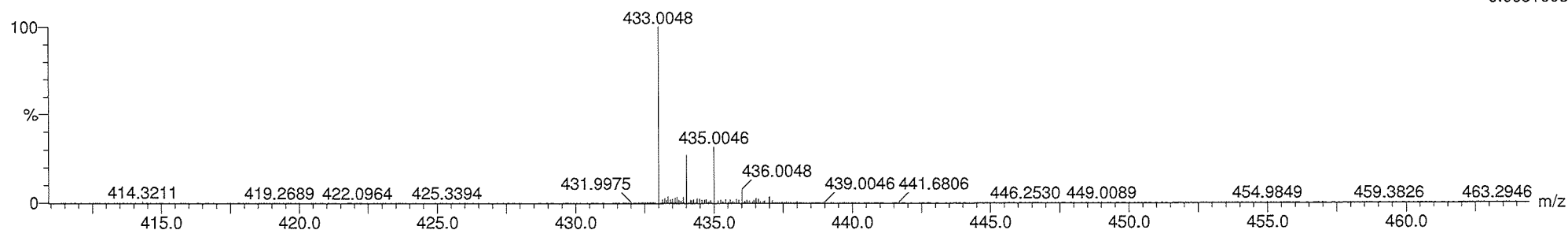
C: 0-500 H: 0-1000 N: 0-5 S: 0-6

01-Jun-2021

2106011 546 (3.304) Cm (543:546-(533:536+574:575))

SN0426

2:18

1: TOF MS ES+  
9.06e+003

Minimum: 0.0  
Maximum: 5.0 5.0 14.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
433.0048	433.0029	1.9	4.4	7.5	432.0	0.0	C16 H21 N2 S6

7.367  
7.260  
7.130

5.324  
5.194

4.021

1.431  
1.259

Current Data Parameters  
NAME SN0426-L1  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters

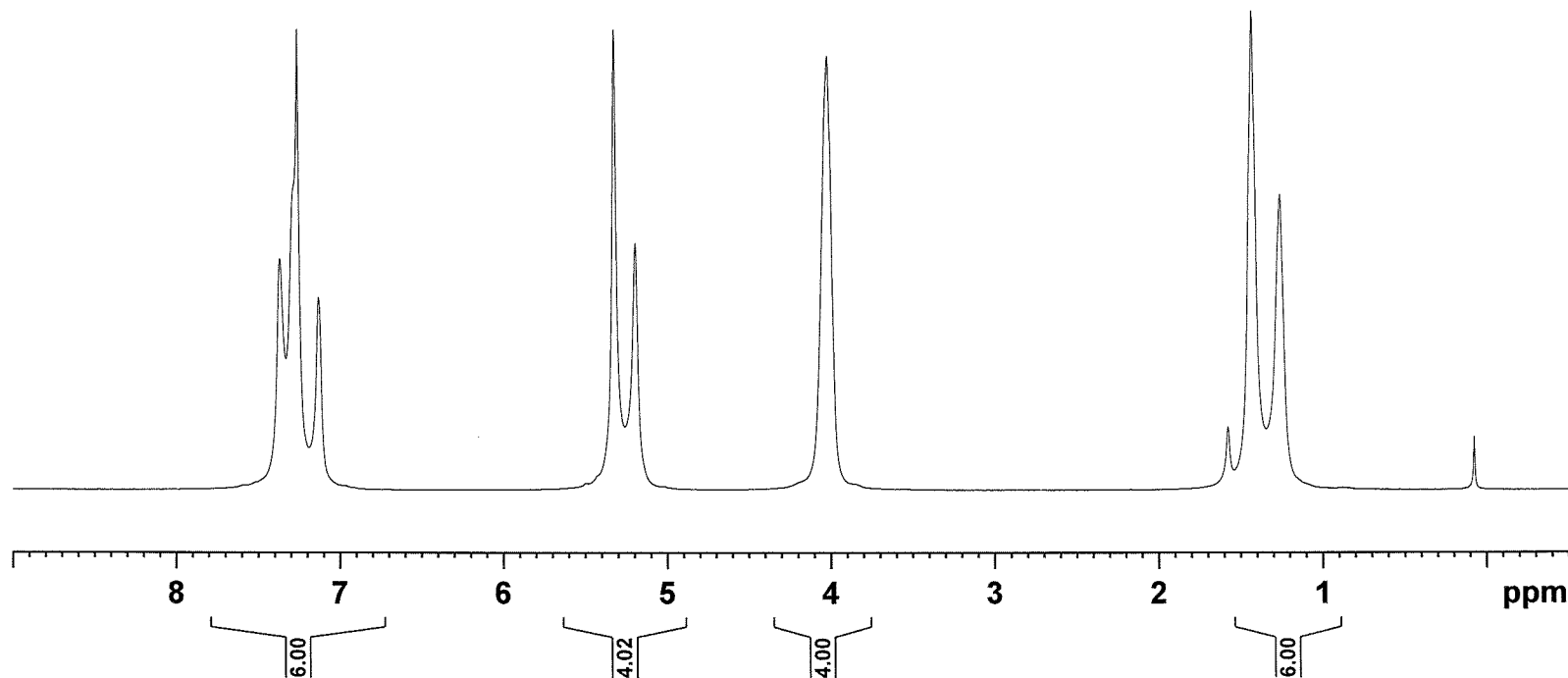
Date\_ 20210429  
Time 14.51  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 7978.724 Hz  
FIDRES 0.243491 Hz  
AQ 2.0534613 sec  
RG 61.21  
DW 62.667 usec  
DE 6.50 usec  
TE 296.2 K  
D1 2.00000000 sec  
TD0 1

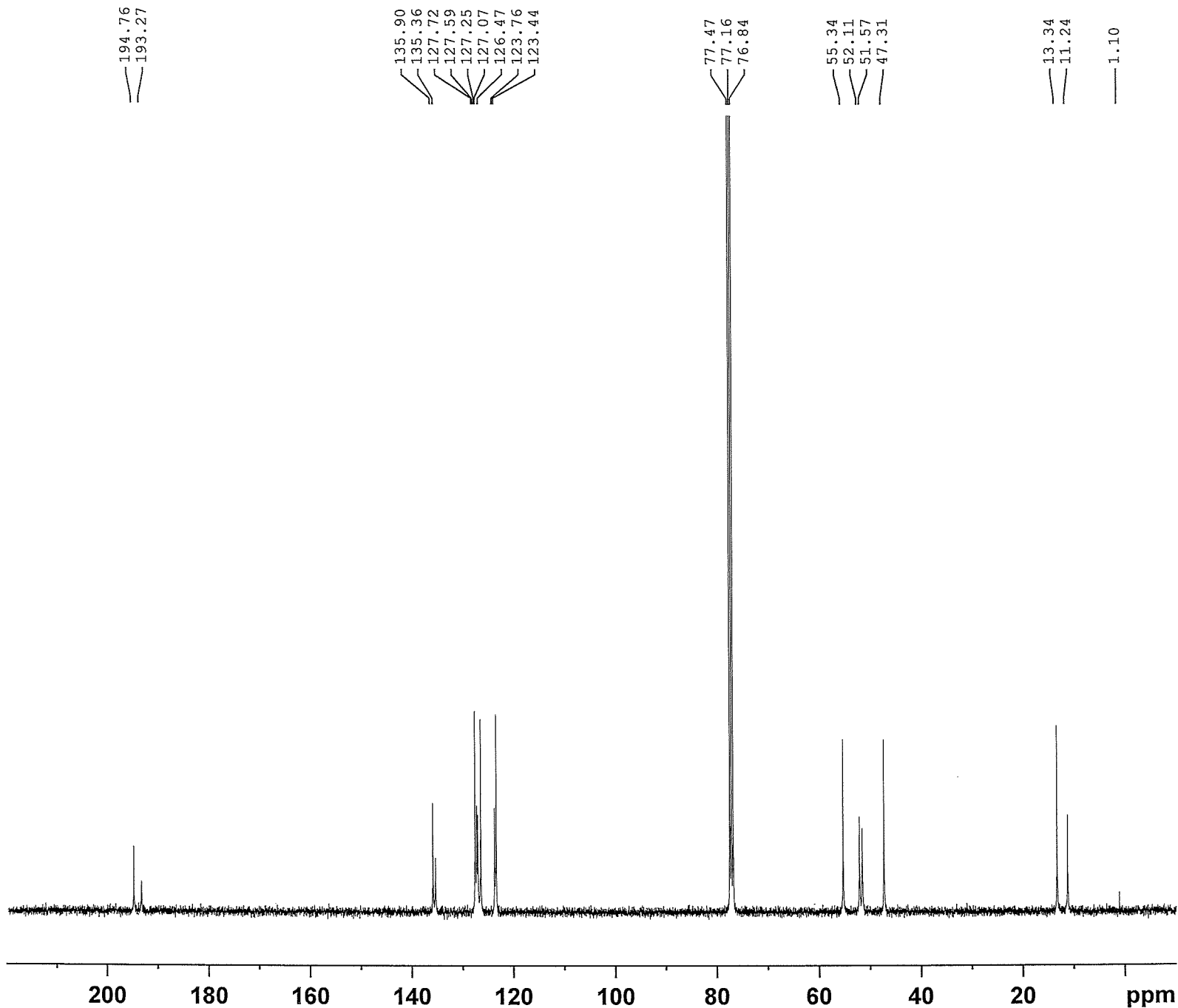
===== CHANNEL f1 =====

SFO1 399.7524686 MHz  
NUC1 1H  
P1 9.00 usec  
PLW1 19.20000076 W

F2 - Processing parameters

SI 65536  
SF 399.7500100 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
NAME SN042611  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20210501  
Time\_ 22.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 2048  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 199.3  
DW 20.800 usec  
DE 6.50 usec  
TE 295.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====

SFO1 100.5272687 MHz  
NUC1 13C  
P1 8.60 usec  
PLW1 87.00000000 W

===== CHANNEL f2 =====

SFO2 399.7515990 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 19.20000076 W  
PLW12 0.20000000 W  
PLW13 0.15552001 W

F2 - Processing parameters

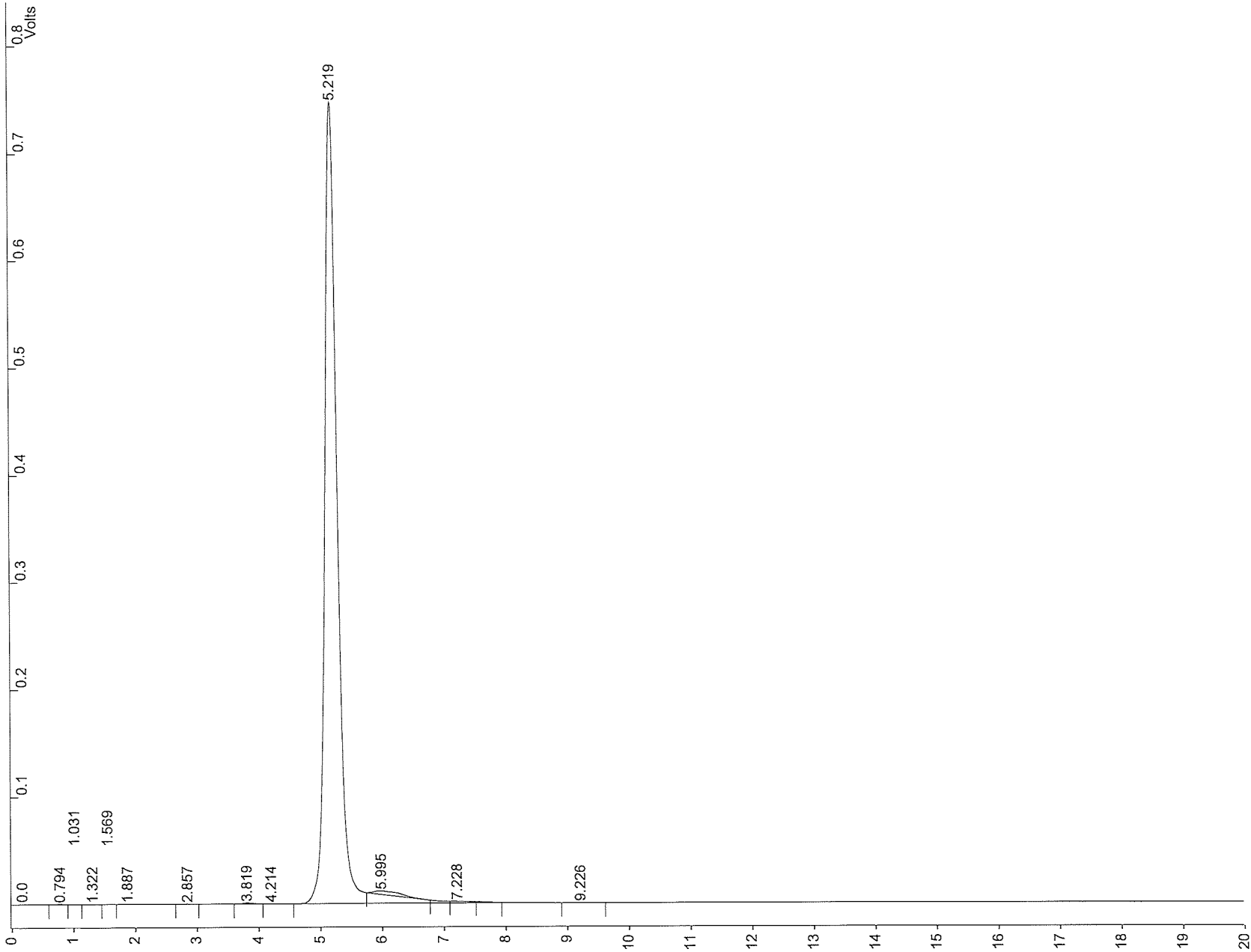
SI 32768  
SF 100.5172130 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Title :  
Run File : C:\Users\DG\Documents\SYNTHENOVA\Mode opératoire\SN0346-49 421-26\thiuram HPLC\HPLC ok\SN0426-L1.run  
Method File : C:\star\startupl.mth  
Sample ID : SN0426-L1

Injection Date: 12/05/2021 15:31      Calculation Date: 12/05/2021 15:51

Operator : DG      Detector Type: 0800 (1 Volt)  
Workstation: HDD      Bus Address : 81  
Instrument : Instrument #1      Sample Rate : 10.00 Hz  
Channel : 2 = 2 1      Run Time : 20.002 min

Chart Speed = 1.08 cm/min      Attenuation = 3539      Zero Offset = 2%  
Start Time = 0.000 min      End Time = 20.002 min      Min / Tick = 1.00





Title :  
Run File : C:\Users\DG\Documents\SYNTHENOVA\Mode opératoire\SN0346-49 421-26\thiuram HPLC\HPLC ok\SN0426-L1.run  
Method File : C:\star\startup1.mth  
Sample ID : SN0426-L1

Injection Date: 12/05/2021 15:31      Calculation Date: 12/05/2021 15:51

Operator : DG                      Detector Type: 0800 (1 Volt)  
Workstation: HDD                  Bus Address : 81  
Instrument : Instrument #1        Sample Rate : 10.00 Hz  
Channel : 2 = 2 1                Run Time : 20.002 min

Run Mode : Analysis  
Peak Measurement: Peak Area  
Calculation Type: Percent

Peak No.	Peak Name	Result ( )	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		0.0356	0.794	0.000	3907	BV	7.3	
2		0.0138	1.031	0.000	1518	VP	7.8	
3		0.0194	1.322	0.000	2129	PV	10.8	
4		0.0145	1.569	0.000	1591	VV	7.3	
5		0.0451	1.887	0.000	4947	VP	6.8	
6		0.0112	2.857	0.000	1226	PB	8.3	
7		0.1067	3.819	0.000	11693	BV	10.9	
8		0.0271	4.214	0.000	2969	VP	11.6	
9		98.7029	5.219	0.000	10818486	PB	12.2	
10		0.9584	5.995	0.000	105049	TS	0.0	
11		0.0240	7.228	0.000	2631	TS	0.0	
12		0.0411	9.226	0.000	4510	BB	16.1	
Totals:		99.9998		0.000	10960656			

Total Unidentified Counts : 10960656 counts

Detected Peaks: 12                  Rejected Peaks: 0                  Identified Peaks: 0

Multiplier: 1                  Divisor: 1                  Unidentified Peak Factor: 1

Baseline Offset: -37 microVolts                  LSB: 1 microVolts

Noise (used): 31 microVolts - monitored before this run

Manual injection

\*\*\*\*\*