

Supplementary Information

Evaluation of Substituted *N*-Aryl Maleimide and Acrylamides for Bioconjugation

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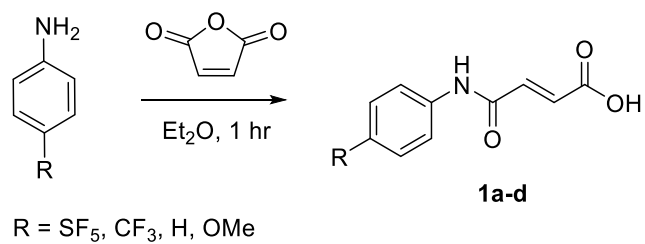


Table S1: Yields obtained of *N*-aryl maleamic acids.

Compound	R	Yield (%)
1a	SF ₅	93
1b	CF ₃	92
1c	H	87
1d	OMe	95

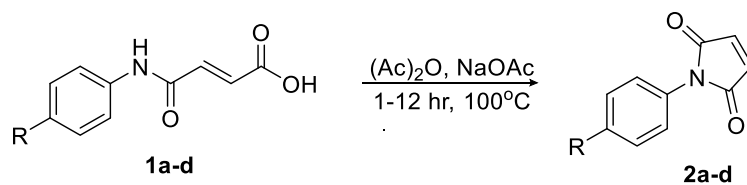


Table S2: Cyclisation of *N*-aryl maleamic acid derivatives into corresponding *N*-aryl maleimides using acetic anhydride, sodium acetate, 100°C 1-12 hr.

Compound	R	Yield (%)
2a	SF ₅	84
2b	CF ₃	88
2c	H	79
2d	OMe	93

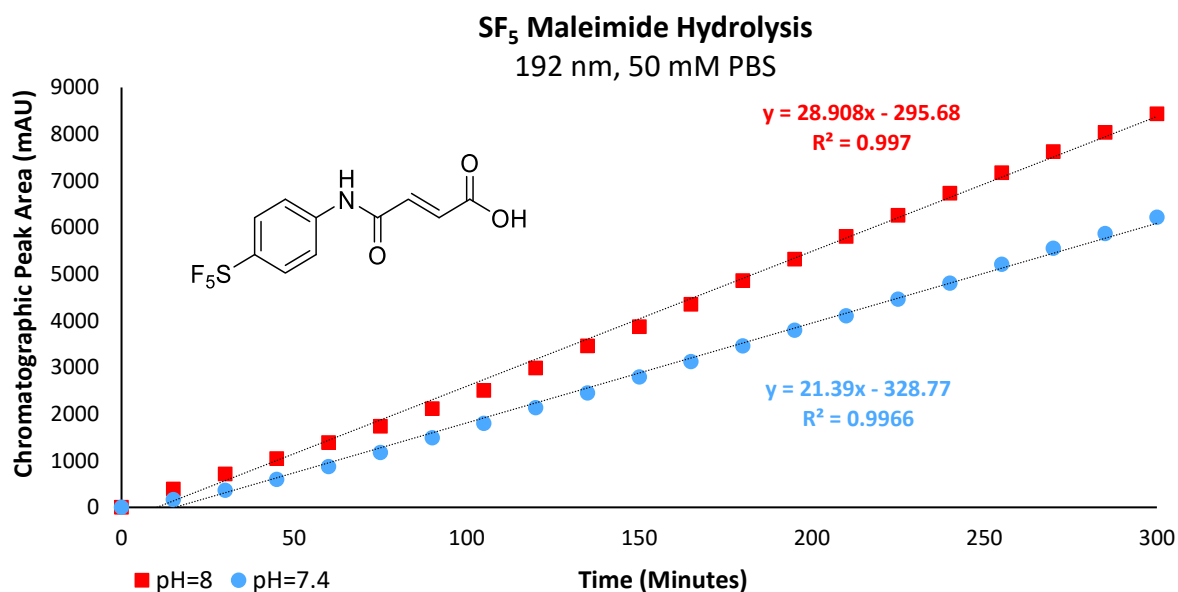


Figure S1: Graph plotting chromatographic peak area of the peak corresponding to the -SF₅ maleamic acid (**1a**) over time.

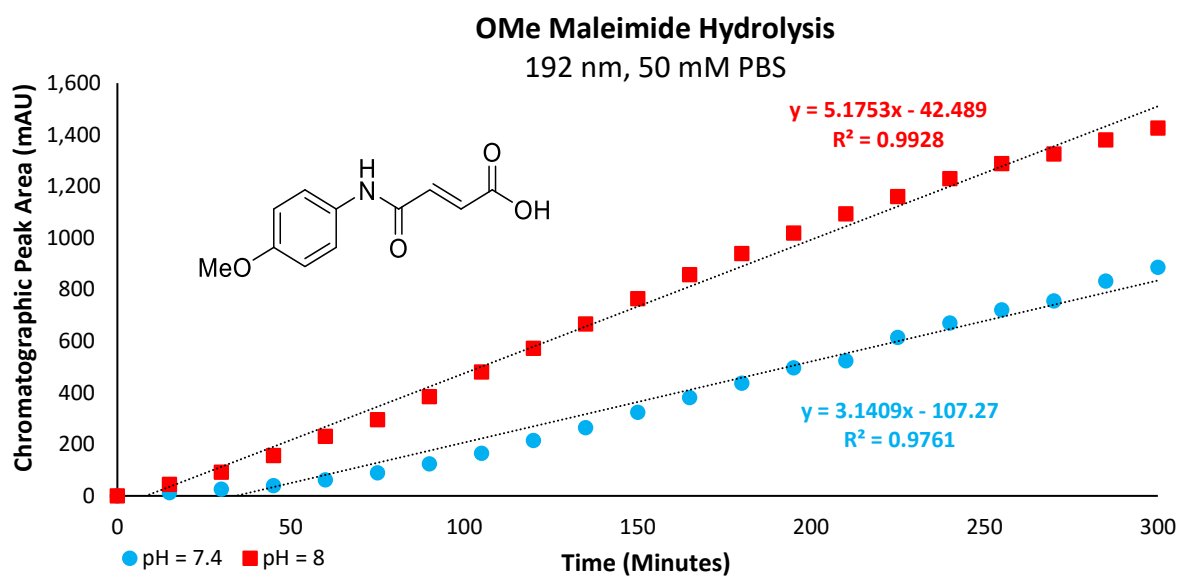


Figure S2: Graph plotting chromatographic peak area of the peak corresponding to the -OMe maleamic acid (**1d**) over time.

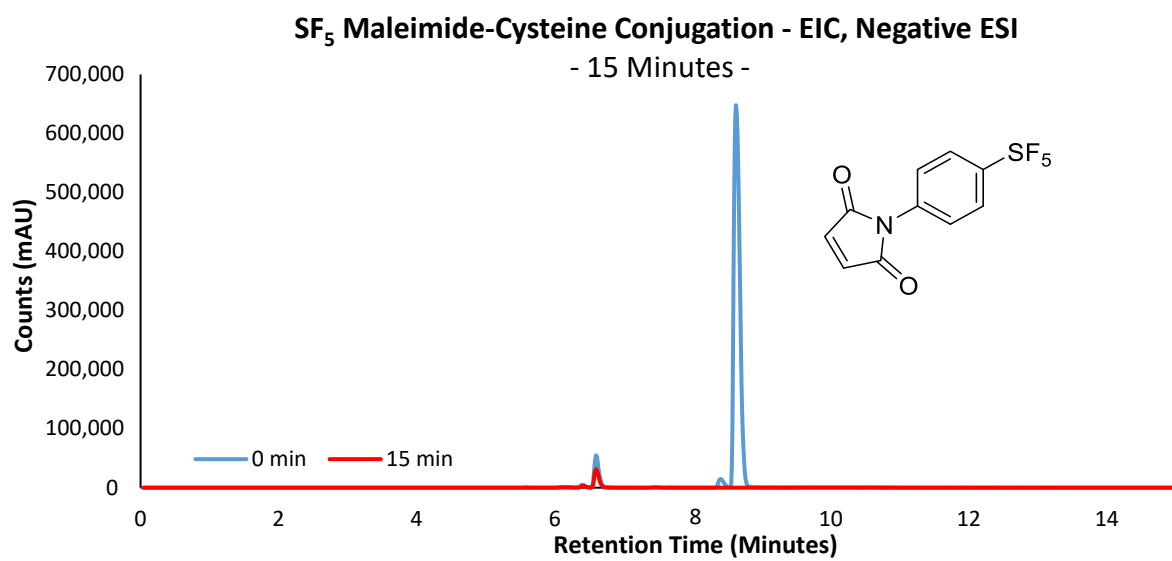


Figure S3: Extracted ion chromatogram showing the disappearance of the signal corresponding to -SF₅ maleimide within 15 minutes from the initial injection.

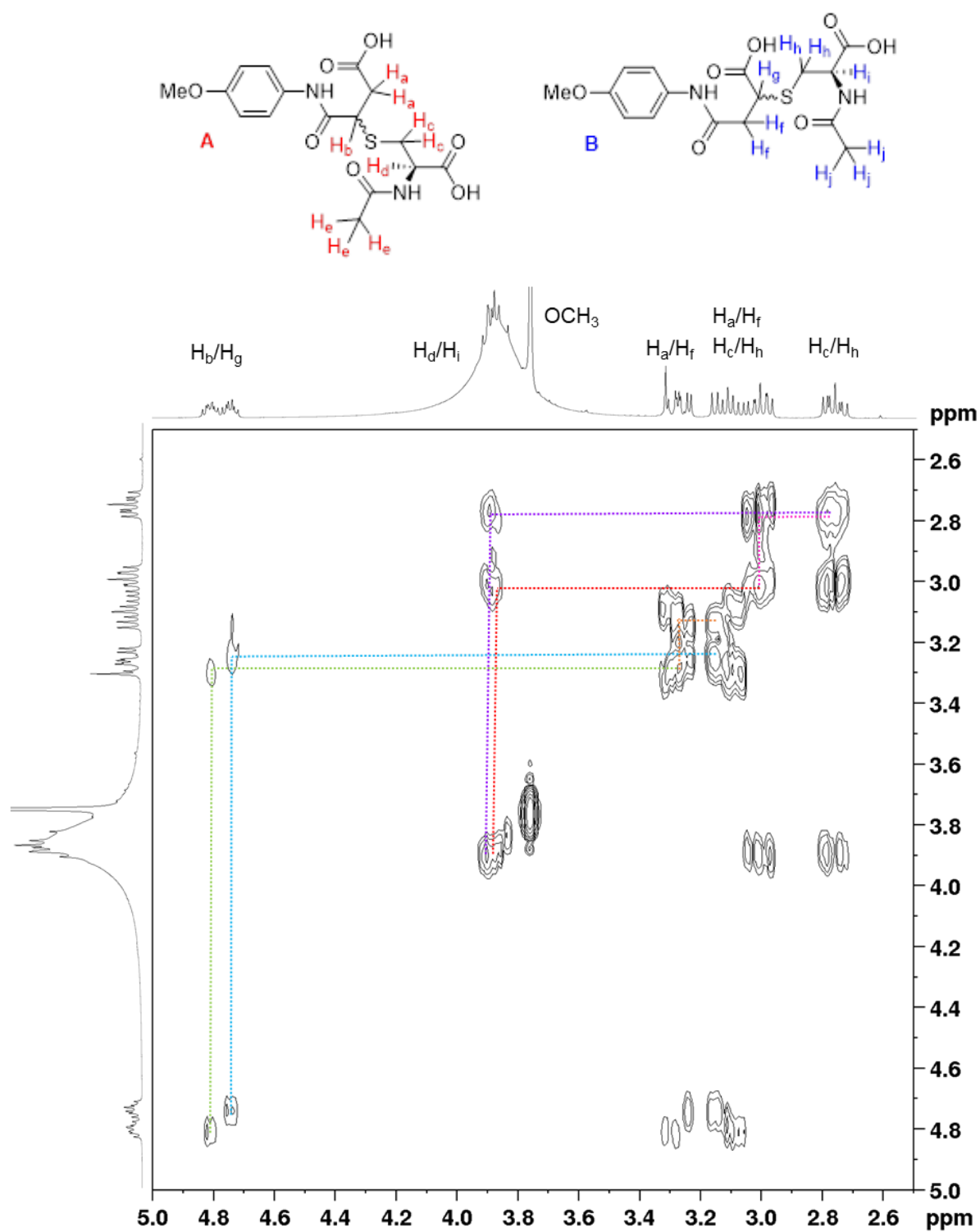


Figure S4: ^1H -NMR COSY of the -OMe regioisomeric mixture (4d).

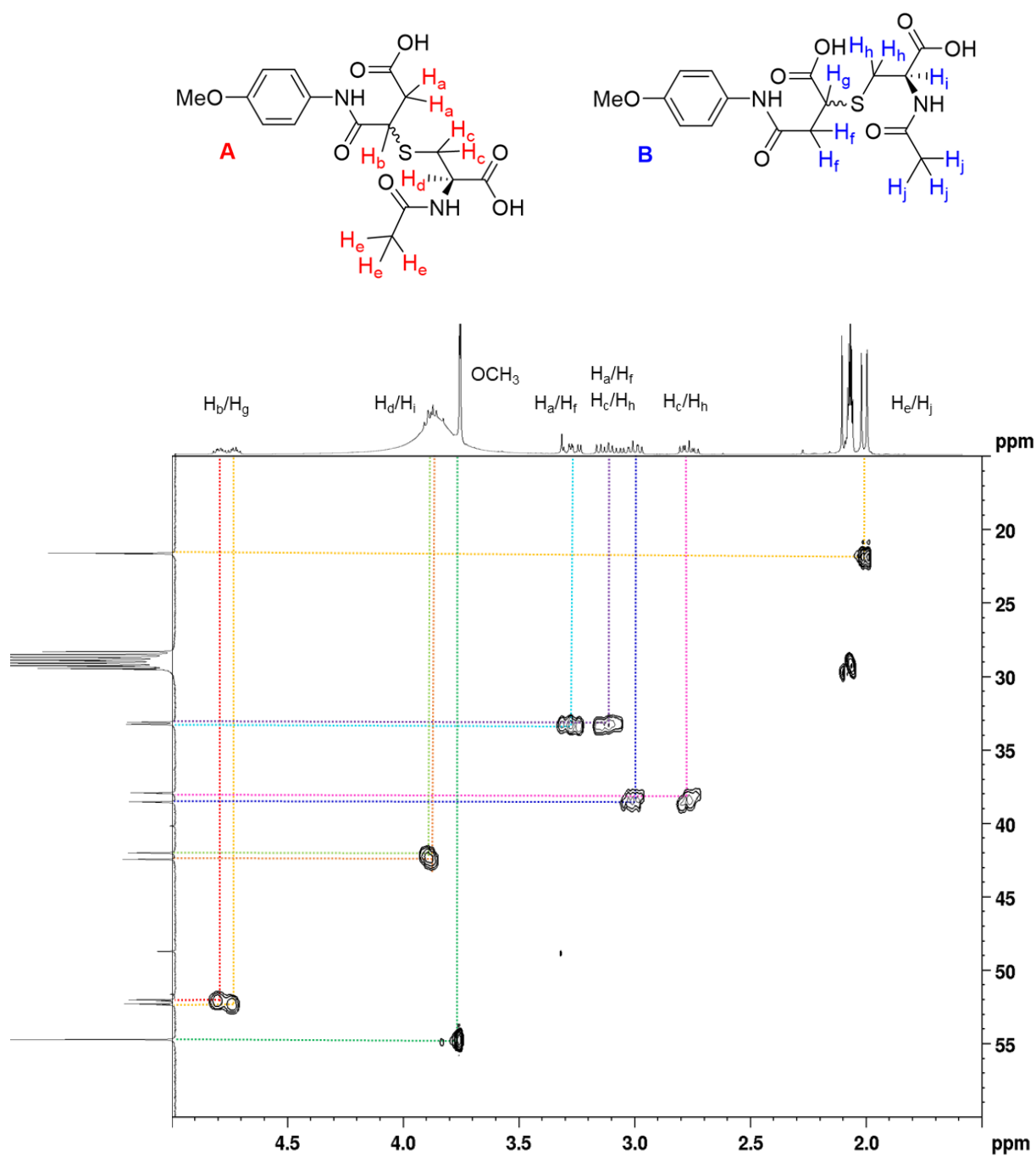
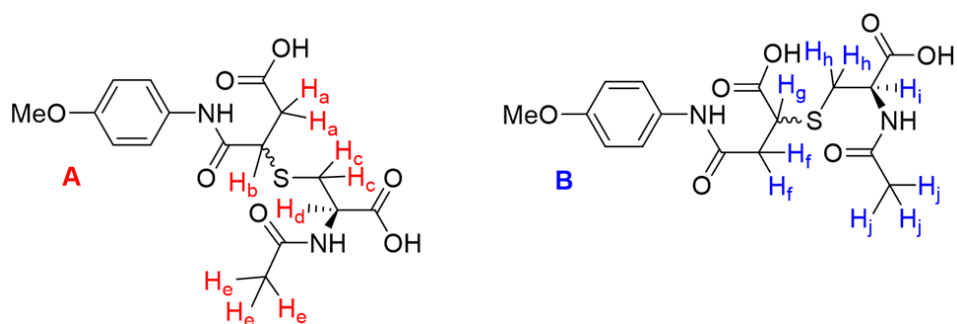


Figure S5: 2D HSQC of the -OMe regioisomeric mixture (**4d**).

Table S3: ^1H and ^{13}C chemical shift allocations of -OMe thio-succinamic acid regio-isomers (4d).

Chemical environment	^1H Chemical Shift	^{13}C Chemical Shift
Hb or Hg	4.80	52.1
Hg or Hb	4.74	52.4
Hd & Hi	3.89	42.4
OCH ₃	3.76	54.8
Ha or Hf	3.27	33.3
Hf or Ha	3.12	33.3
Hc or Hh	3.01	38.6
Hh or Hc	2.76	38.6
He or Hj	2.01	22.2
Hj or He	1.99	22.2



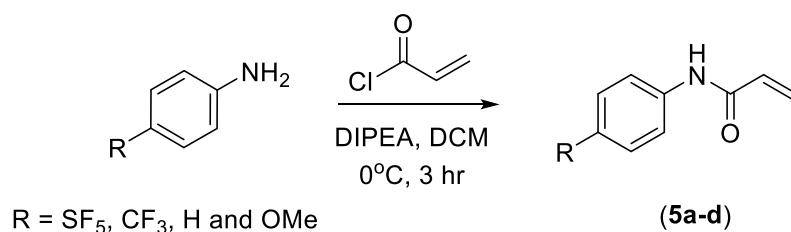


Table S4: Yields obtained of the *N*-phenyl acrylamide derivatives (5a-d).

Compound	R	Yield (%)
5a	SF ₅	69
5b	CF ₃	73
5c	H	86
5d	OMe	81

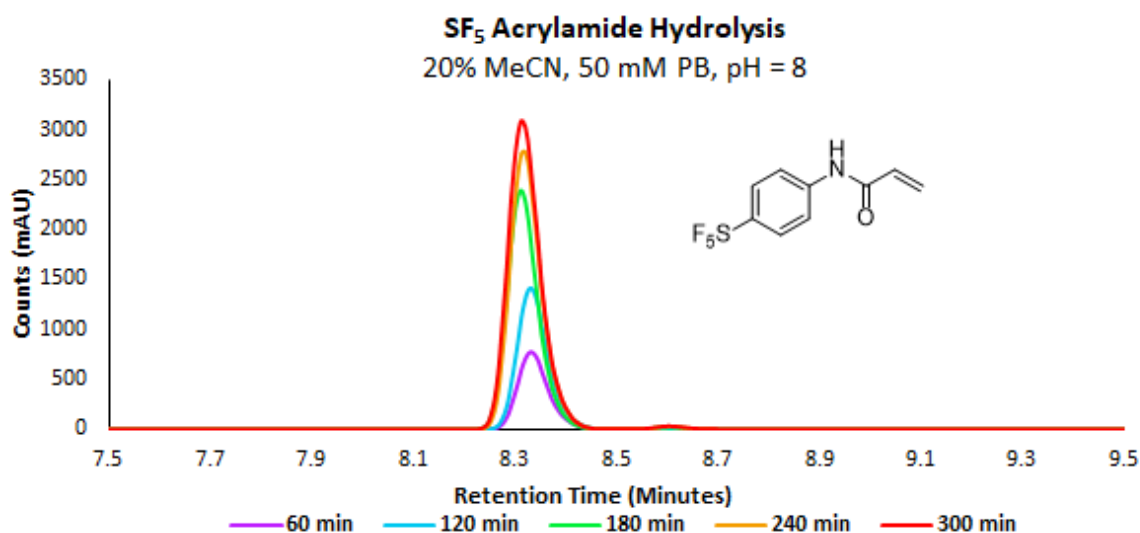


Figure S6: Stacked UV chromatogram showing the unprecedented increase of -SF₅ acrylamide concentration during the decomposition study over the course of 300 minutes.

Table S5: Solvent systems prepared in an attempt to solubilise the -SF₅ acrylamide prosthetic group.

Total volume (mL)	-SF ₅ Acrylamide (mmol)	Co-solvent (% tot. vol.)	Completely Soluble? (Yes/No)
1	0.1	MeCN (20%)	No
1	0.025	MeCN (20%)	No
1	0.025	MeOH (20%)	No
1	0.025	MeOH (40%)	No
1	0.025	DMSO (20%)	No
1	0.025	DMSO (40%)	No
1	0.025	DMF (40%)	No
1	0.025	TFE (40%)	No

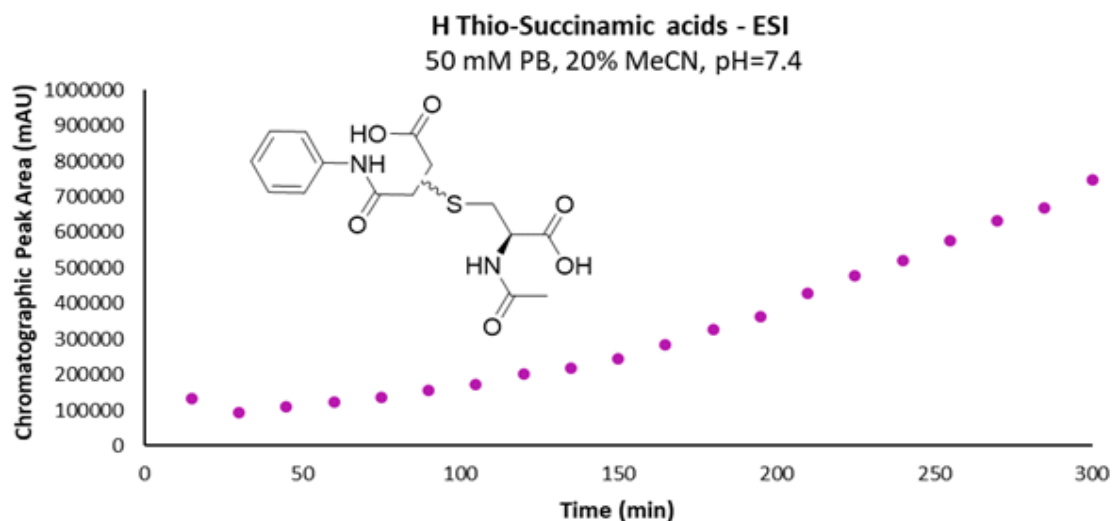


Figure S7: Graph depicting the increase in EIC chromatographic peak area of the H thio-succinamic acid regio-isomers over 300 minutes

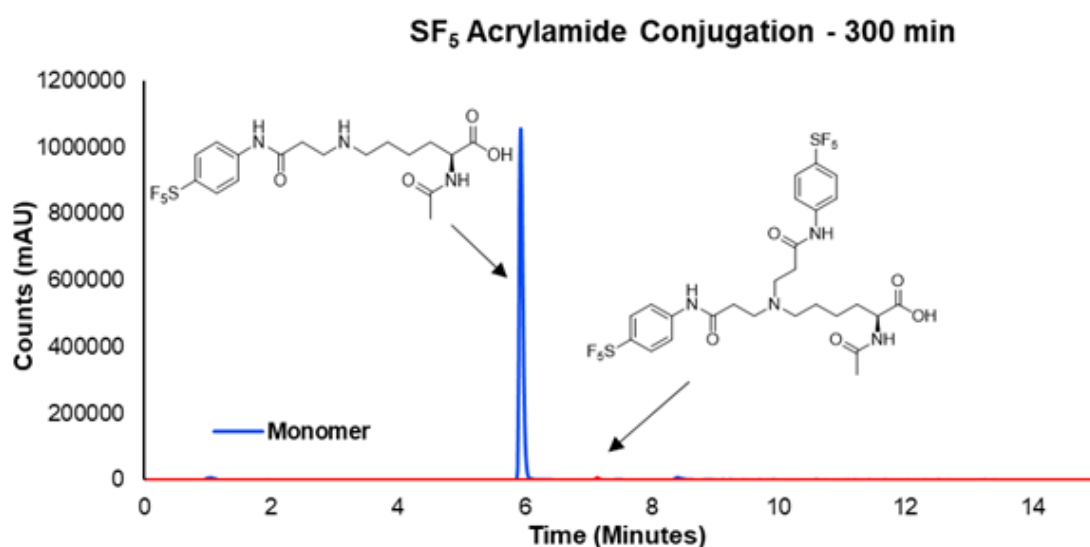


Figure S8: Stacked chromatogram of the crude reaction mixture for the -SF₅ acrylamide-lysine conjugation, comparing the concentration of conjugate monomer and dimer byproduct.

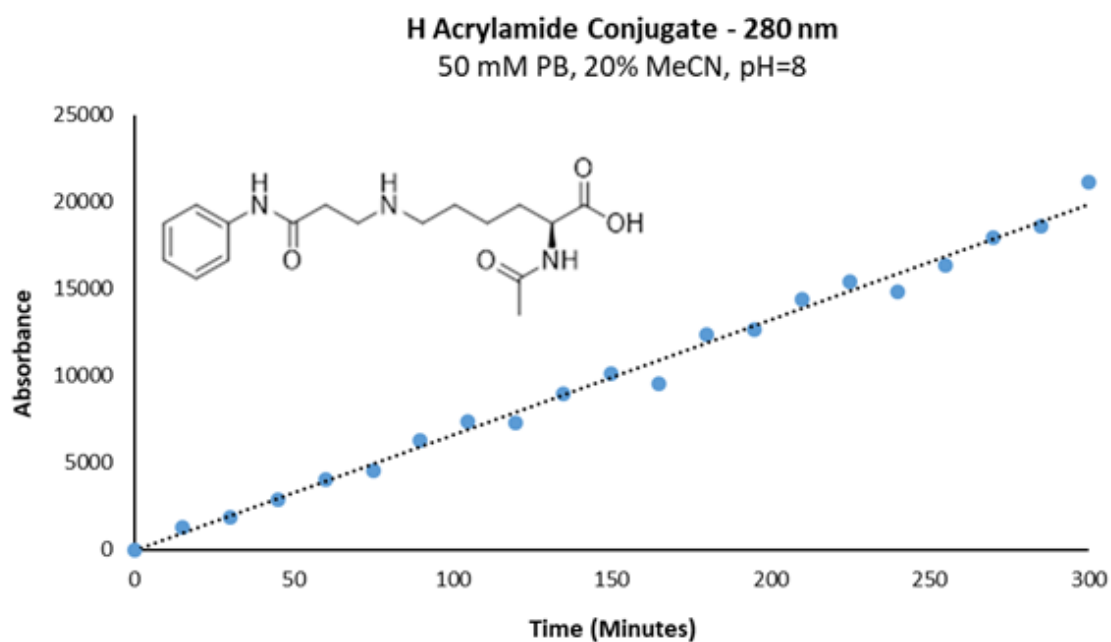


Figure S9: Graph depicting the increase in chromatographic peak area corresponding to the H Acrylamide conjugate over 300 minutes.

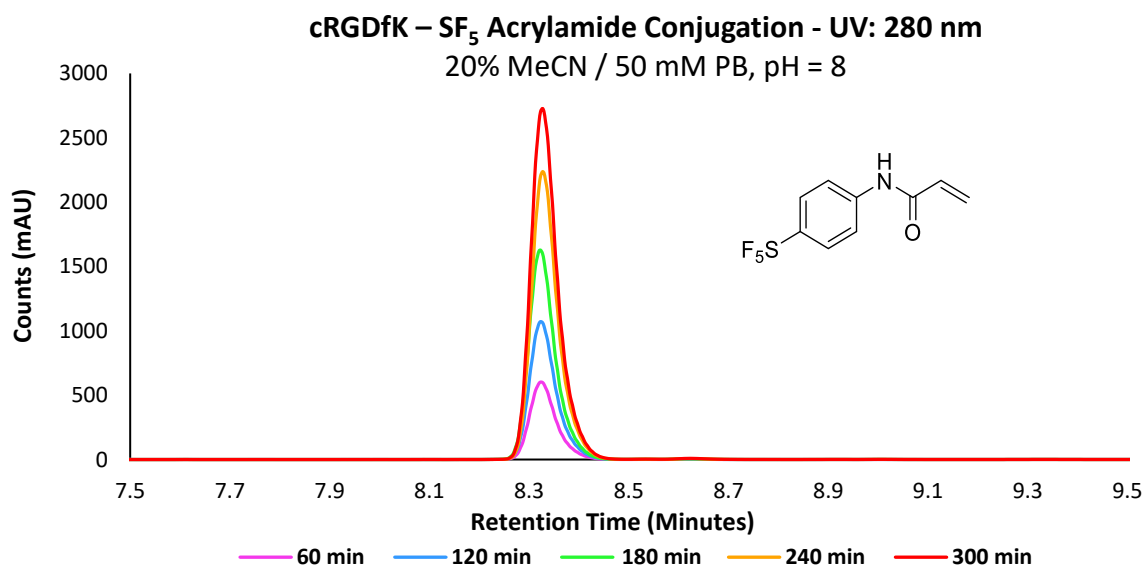


Figure S10: Stacked UV chromatograms showing the apparent increase in acrylamide concentration for the cRGDfK peptide conjugation.

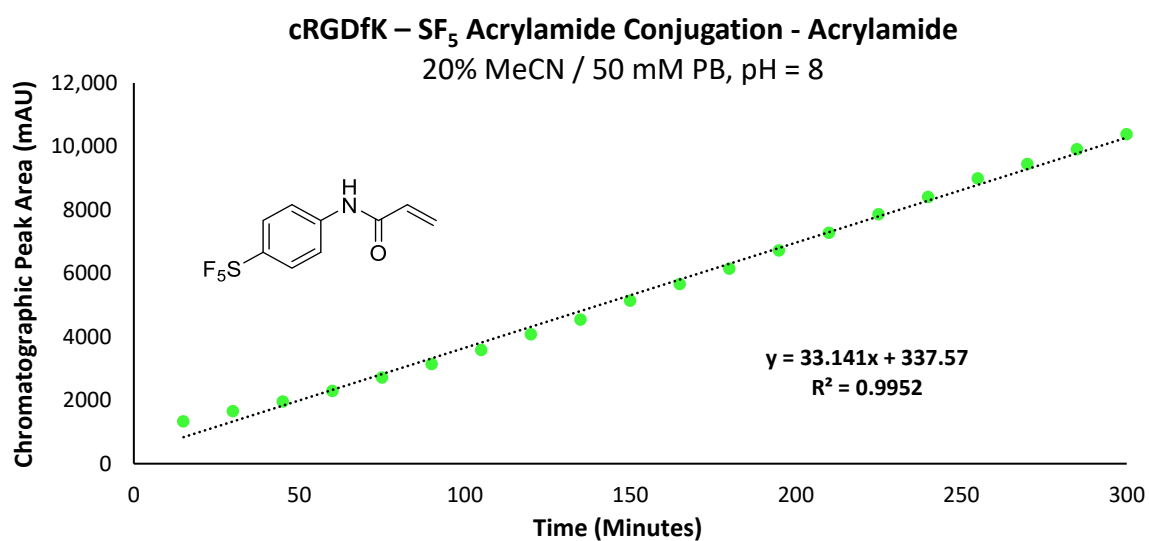
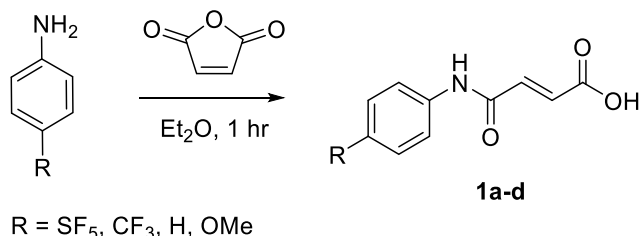
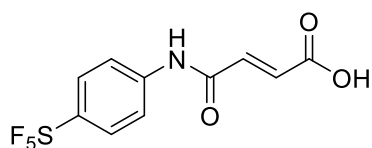


Figure S11: Graph depicting the increase in chromatographic peak area corresponding to the - SF₅ acrylamide reactant over time in the cRGDfK peptide conjugation.



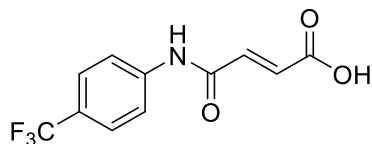
General procedure for the synthesis of (**1a-d**) adapted from the work of De Vivo *et al.* [19]: To a stirred solution of maleic anhydride (196 mg; 2 mmol) in ether (5 mL) was added a solution of 4-(pentafluorosulfonyl) aniline (440 mg; 2 mmol) in ether (3 mL) dropwise. The reaction was allowed to proceed for 1 hr, at which point the evolved precipitate was collected by vacuum filtration and washed with Et₂O (2x5 mL) to afford the pure product.

*4-[4-(pentafluoro- λ^6 -sulfonyl)phenyl]-4-oxo-2-butenoic acid (**1a**)*



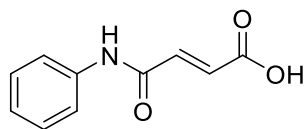
Compound **1a** was obtained as a white solid (1.167 g, 3.72 mmol, 98%). Melting point: 178°C (decomposes). **HRMS (EI)** Calcd for C₁₀H₉F₅NO₃S [M-H]⁻ 316.0066, [M-H]⁻ Found 316.0039; **IR (KBr)**: 3080 (w, br), 1706 (s), 1629 (w), 1589 (m), 1401 (m), 1326 (w), 1266 (w), 1221 (w), 1144 (m), 1117 (m), 975 (w), 813 (s, br) cm⁻¹; **¹H-NMR (d₆-DMSO)**: δ 7.86 (d, J = 9.36 Hz, 2H), 7.81 (d, J = 9.2 Hz, 2H), 6.49 (d, J = 12 Hz, 1H), 6.33 (d, J = 12 Hz, 1H); **¹³C-NMR (d₆-DMSO)**: δ 166.88, 163.90, 147.31 (quin, J = 16 Hz), 142.00, 137.21, 131.68, 130.15, 126.85 (quin, J = 4 Hz), 119.03; **¹⁹F-NMR (d₆-DMSO)**: δ 88.54 (m, 1F), 64.80 (d, J = 160 Hz, 4F).

*4-[4-(trifluoromethyl)phenyl]-4-oxo-2-butenoic acid (**1b**)*



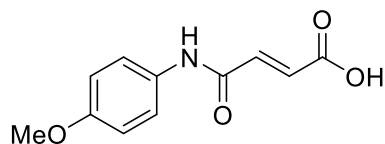
Compound **1b** was obtained as a white solid (953 mg, 3.68 mmol, 92%). Melting point: 183°C (decomposes). **HRMS (EI)** Calcd for C₁₁H₉F₃NO₃ [M+H]⁺ 260.0534, [M+H]⁺ Found 260.0534; **IR (KBr)**: 3070 (w, br), 2268 (w), 2127 (w), 1890 (w), 1715 (s), 1632 (m), 1583 (s), 1536 (s), 1486 (m), 1486 (m), 1407 (m), 1315 (s), 1269 (m), 1165 (m), 1115 (s), 1069 (m), 1016 (m), 973 (m), 850 (s), 837 (s), 668 (m), 610 (m), 586 (m) cm⁻¹; **¹H-NMR (d₆-DMSO)**: δ 7.82 (d, J = 8.4 Hz, 2H), 7.79 (d, J = 8.4 Hz, 2H), 6.49 (d, J = 12 Hz, 1H), 6.32 (d, J = 12 Hz, 1H); **¹³C-NMR (d₆-DMSO)**: δ 166.97, 163.88, 142.34, 131.78, 130.18, 126.16 (q, J = 5 Hz), 123.57, 119.37; **¹⁹F-NMR (d₆-DMSO)**: δ -60.41 (s, 3F).

4-phenyl-4-oxo-2-butenic acid (1c)



Compound **1c** was obtained as a tan-white solid (687 mg, 3.59 mmol, 87%). Melting point: 191°C (Lit. 193-194°C [27]). **HRMS (EI)** Calcd for C₁₀H₁₀NO₃ [M+H]⁺ 192.0660, [M+H]⁺ Found 192.0659; **IR (KBr)**: 3070 (m, br), 2239 (w, br), 2072 (w), 1877 (w), 1694 (m), 1618 (m), 1532 (s), 1489 (s), 1449 (s), 1417 (m), 1329 (m), 1265 (m), 1226 (w), 1189 (w), 995 (m), 969 (s), 908 (w), 843 (s), 769 (s), 653 (m), 606 (s), 535 (s) cm⁻¹; **¹H-NMR (d₆-DMSO)**: δ 7.61 (d, 7.5 Hz, 2H), 7.32 (t, J = 7.36, 14.76, 2H), 7.088 (t, J = 7.36, 14.88, 1H), 6.47 (d, J = 12 Hz, 1H), 6.30 (d, J = 12 Hz, 1H); **¹³C-NMR (d₆-DMSO)**: δ 166.91, 163.28, 138.58, 131.75, 130.47, 128.86, 123.92, 119.58.

4-[4-(methoxy)phenyl]-4-oxo-2-butenic acid (1d)

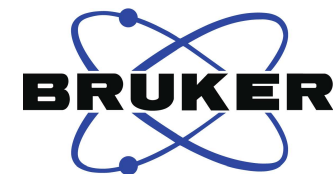


Compound **1d** was obtained as a green-yellow solid (836 mg, 3.78 mmol, 95%). Melting point: 177°C (Lit. 175-178°C [29]). **HRMS (EI)** Calcd for C₁₁H₁₁NO₄ [M+H]⁺ 222.1766, [M+H]⁺ Found 222.1763; **IR (KBr)**: 3067 (w, br), 1695 (m), 1618 (w), 1534 (m), 1504 (s), 1462 (m), 1404 (m), 1307 (w), 1324 (m), 1278 (m), 1176 (m), 1030 (s), 975 (m), 854 (s), 826 (s), 801 (s), 758 (m), 645 (m), 621 (m), 520 (s) cm⁻¹; **¹H-NMR (d₆-DMSO)**: δ 7.54 (d, J = 9 Hz, 2H), 6.91 (d, J = 9 Hz, 2H), 6.46 (d, J = 12 Hz, 1H), 6.30 (J = 12 Hz, 1H), 3.73 (s, 3H); **¹³C-NMR (d₆-DMSO)**: δ 166.66, 162.85, 155.84, 131.65, 131.43, 130.93, 121.21, 113.99, 55.21.

References

19. De Vivo M, Masetti M, Bottegoni G, Cavalli A (2016) Role of Molecular Dynamics and Related Methods in Drug Discovery. *J Med Chem* 59:4035–4061. <https://doi.org/10.1021/acs.jmedchem.5b01684>
27. Sánchez A, Pedroso E, Grandas A (2010) Esterification of maleamic acids without double bond isomerization. *European J Org Chem* 2010:2600–2606. <https://doi.org/10.1002/efoc.200901365>
29. Kumar PP, Rama Devi B, Dubey PK, Mohiuddin SMG (2011) PEG-600 mediated simple, efficient and eco-friendly synthesis of N-substituted imides and chemo selective C = C reduction. *Green Chem Lett Rev* 4:341–348. <https://doi.org/10.1080/17513758.2011.601111>

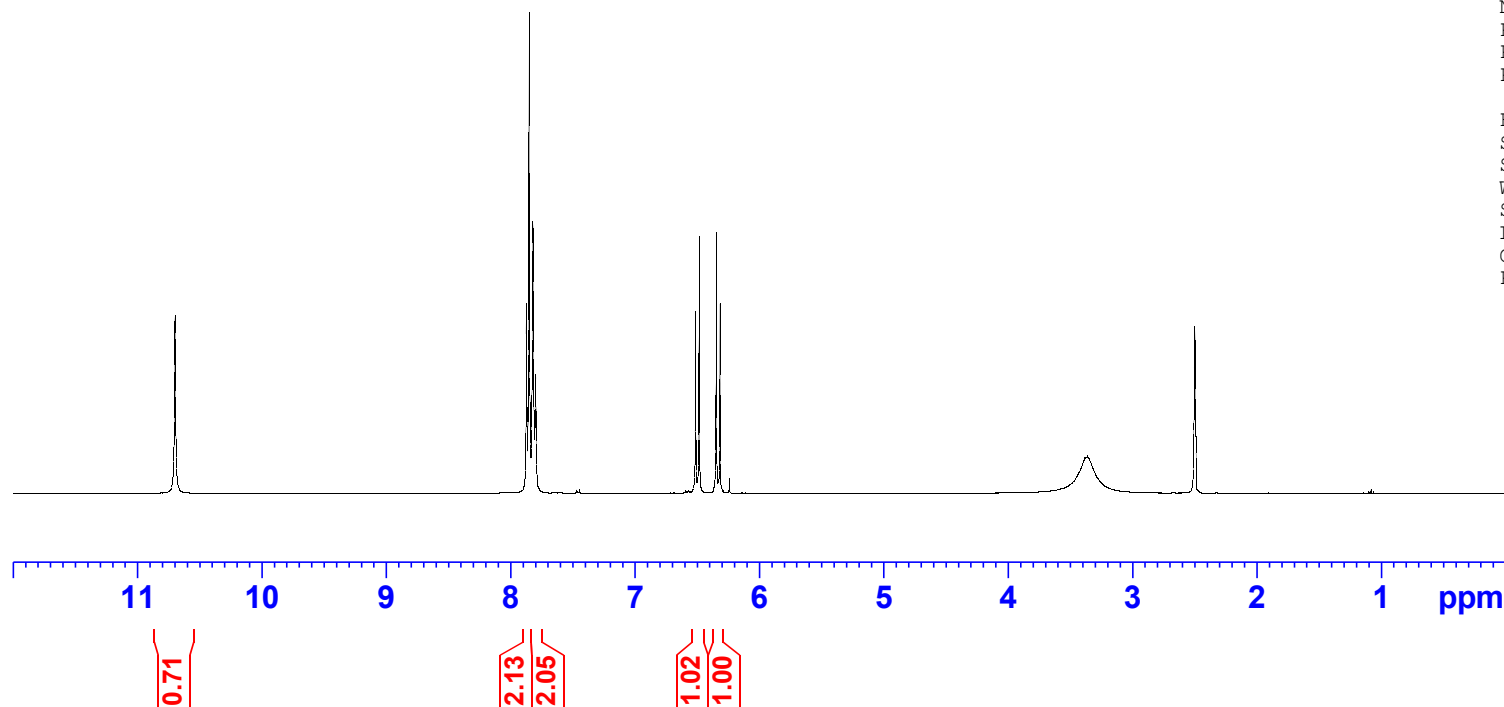
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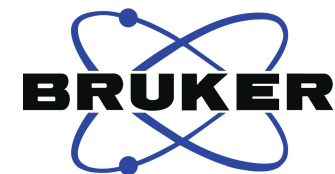
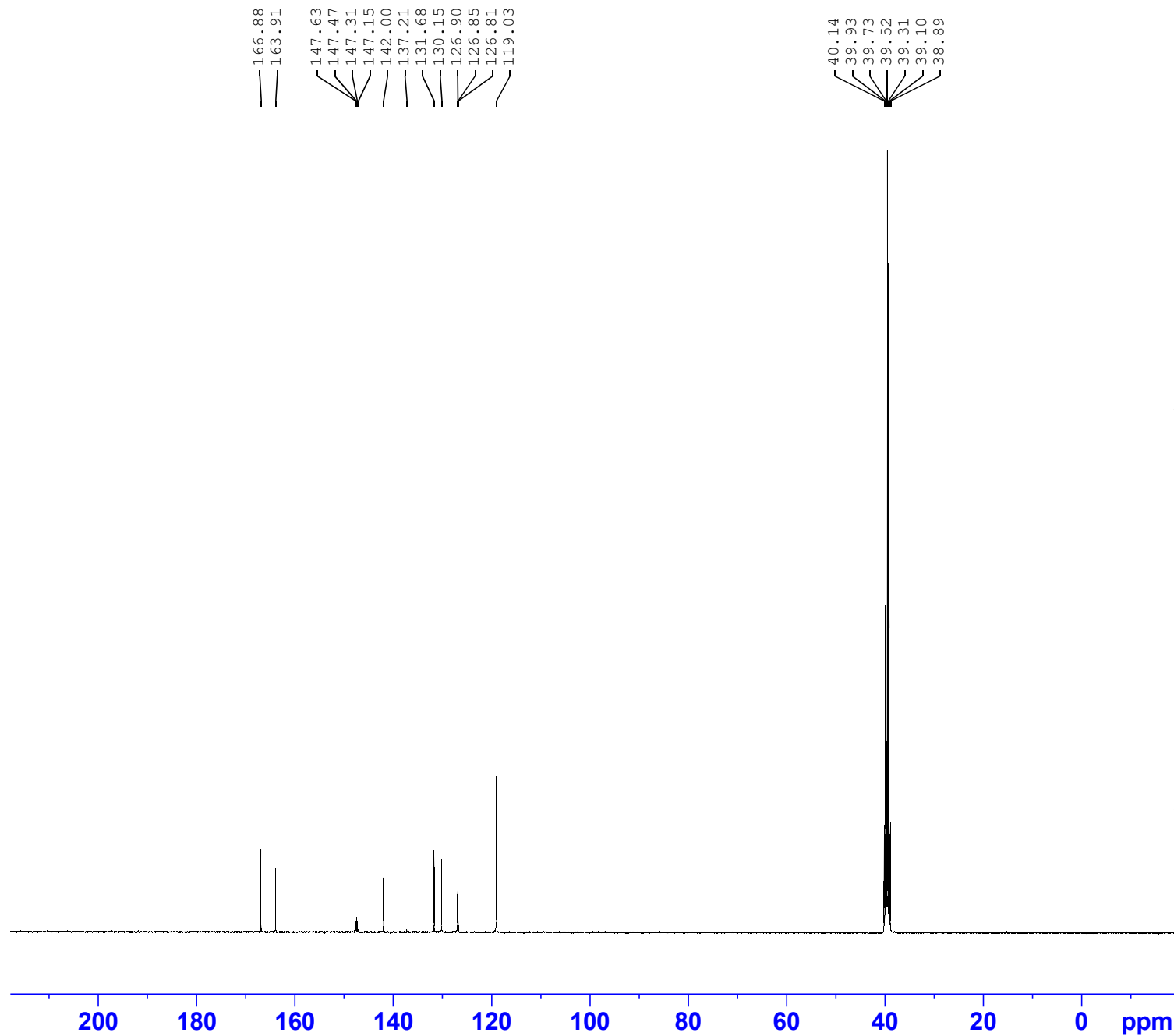
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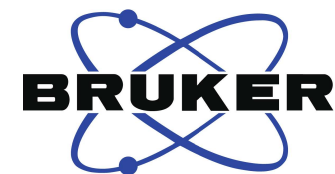
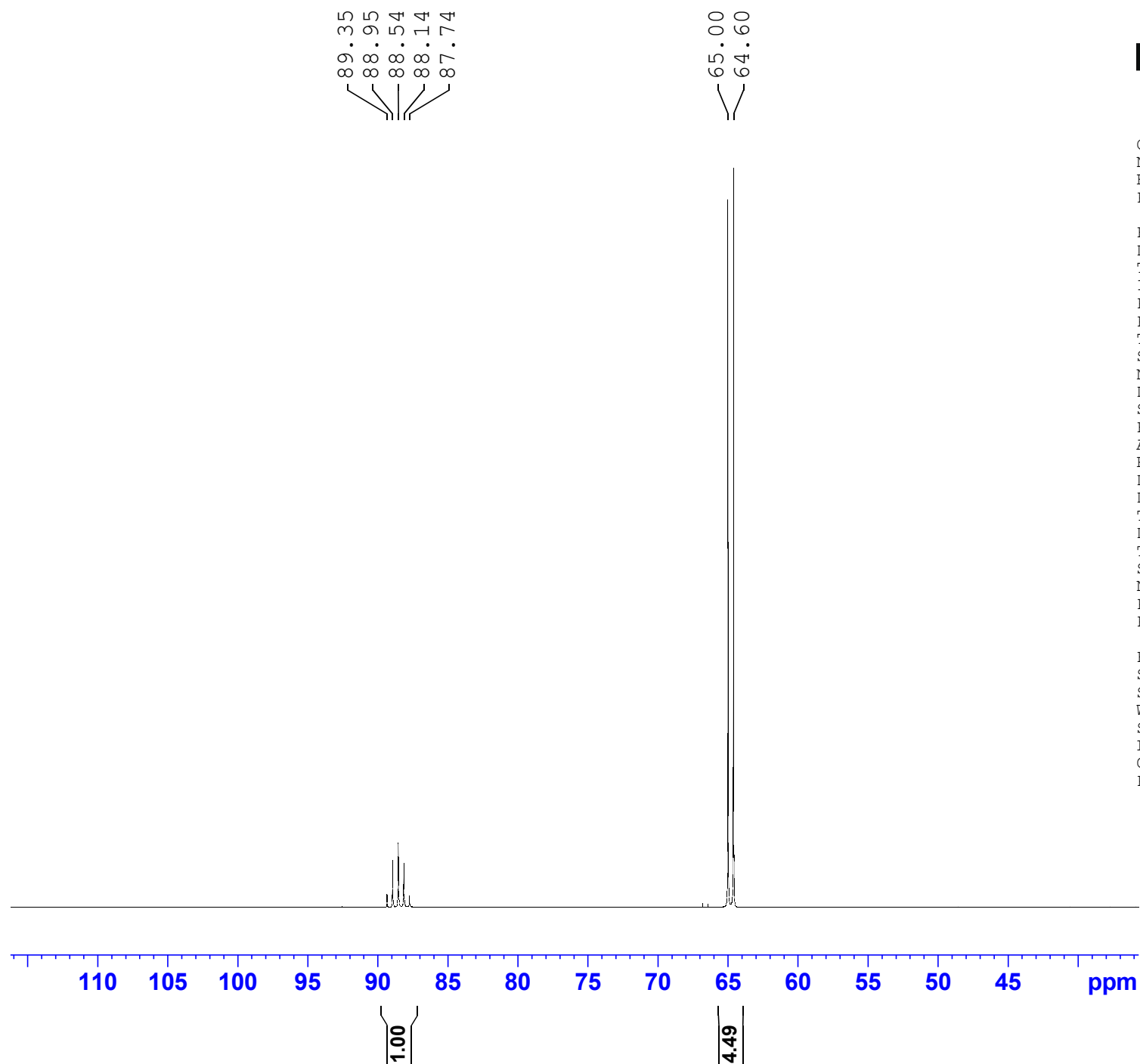


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SF5 Maleamic acid (**1a**)



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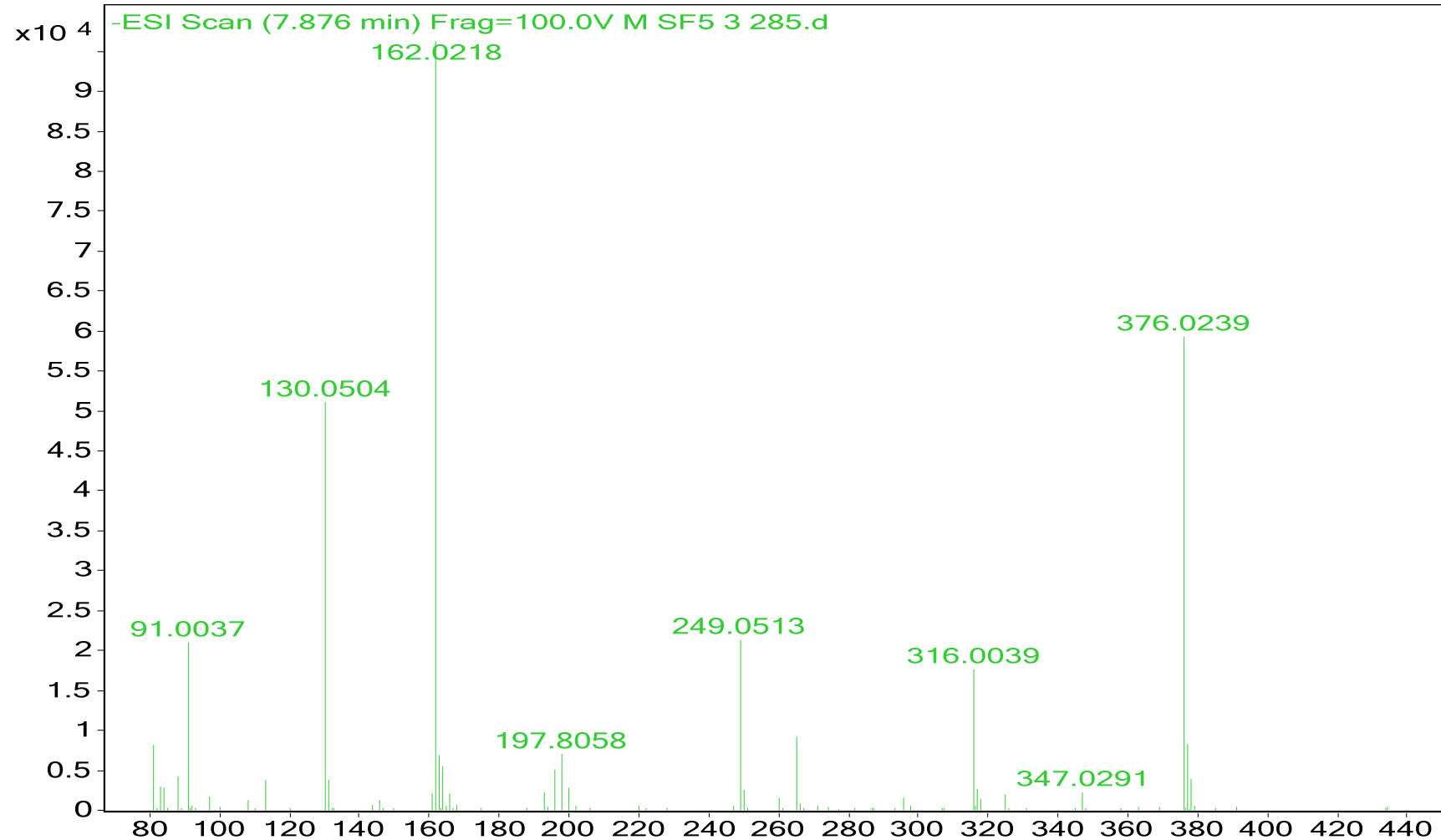
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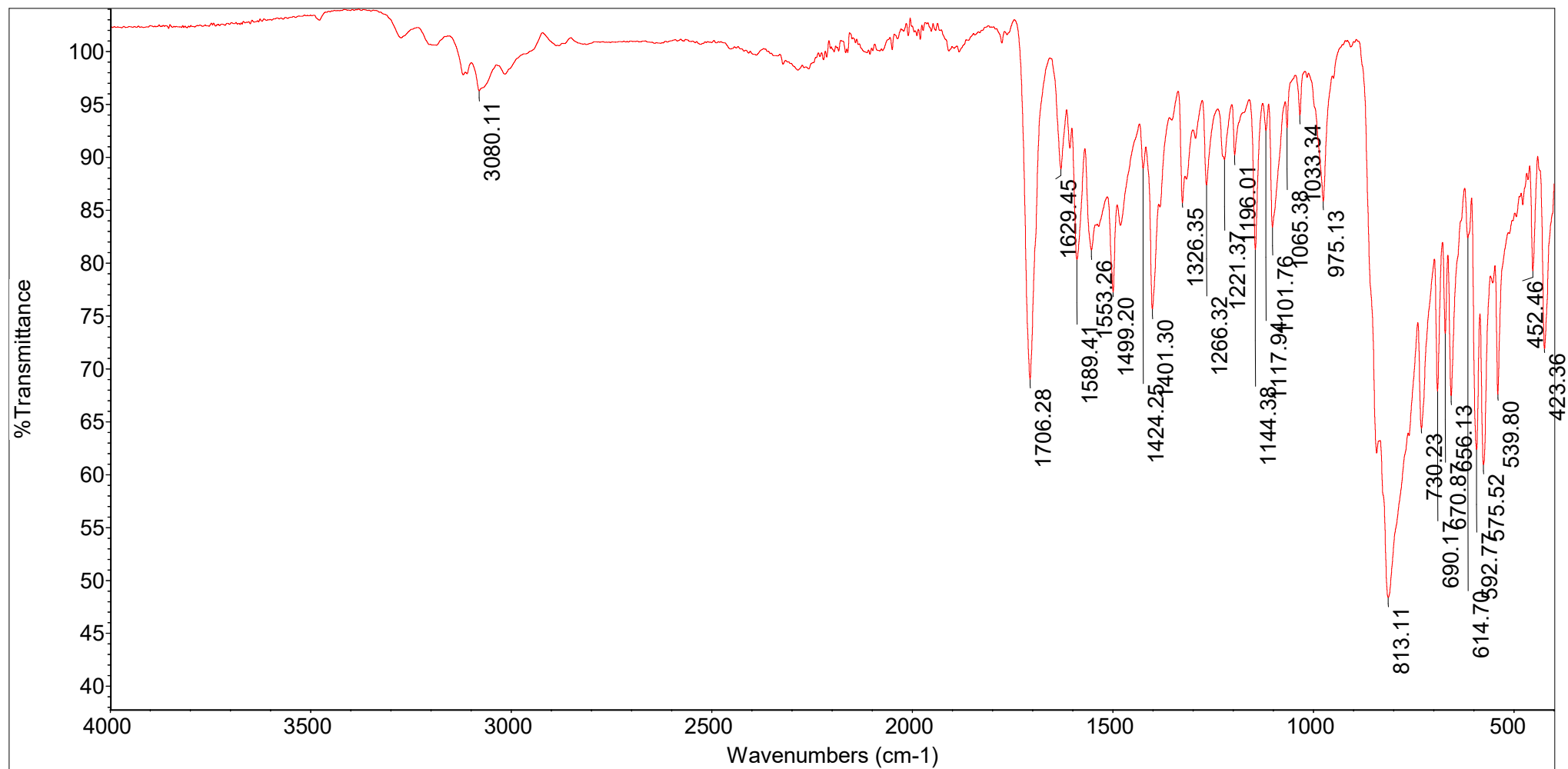
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Instrument Name
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Comment

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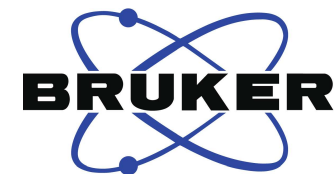


SF5 Maleamic acid (**1a**)

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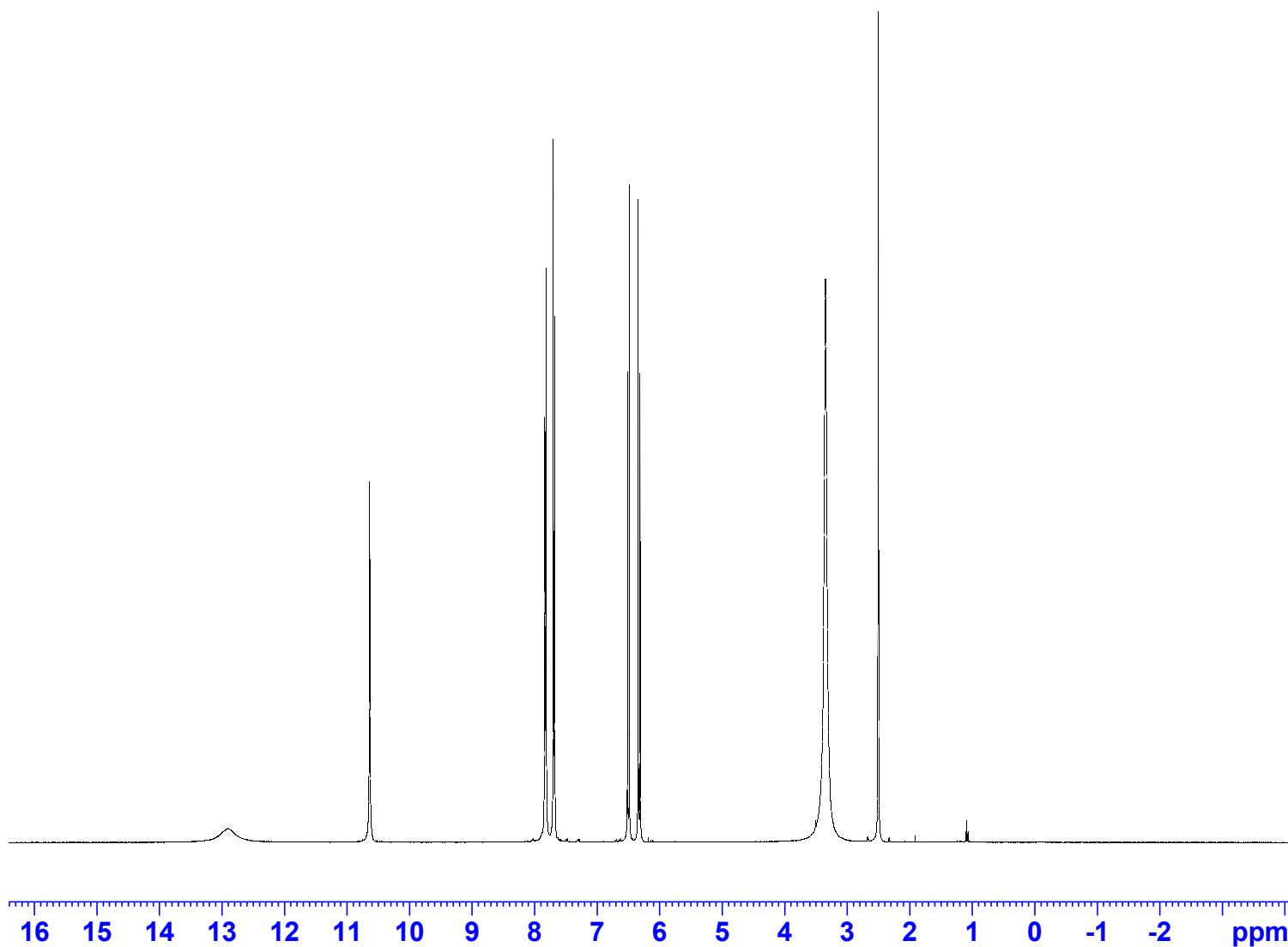
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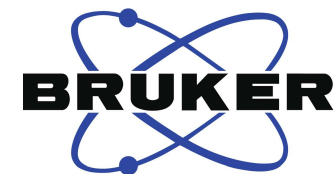
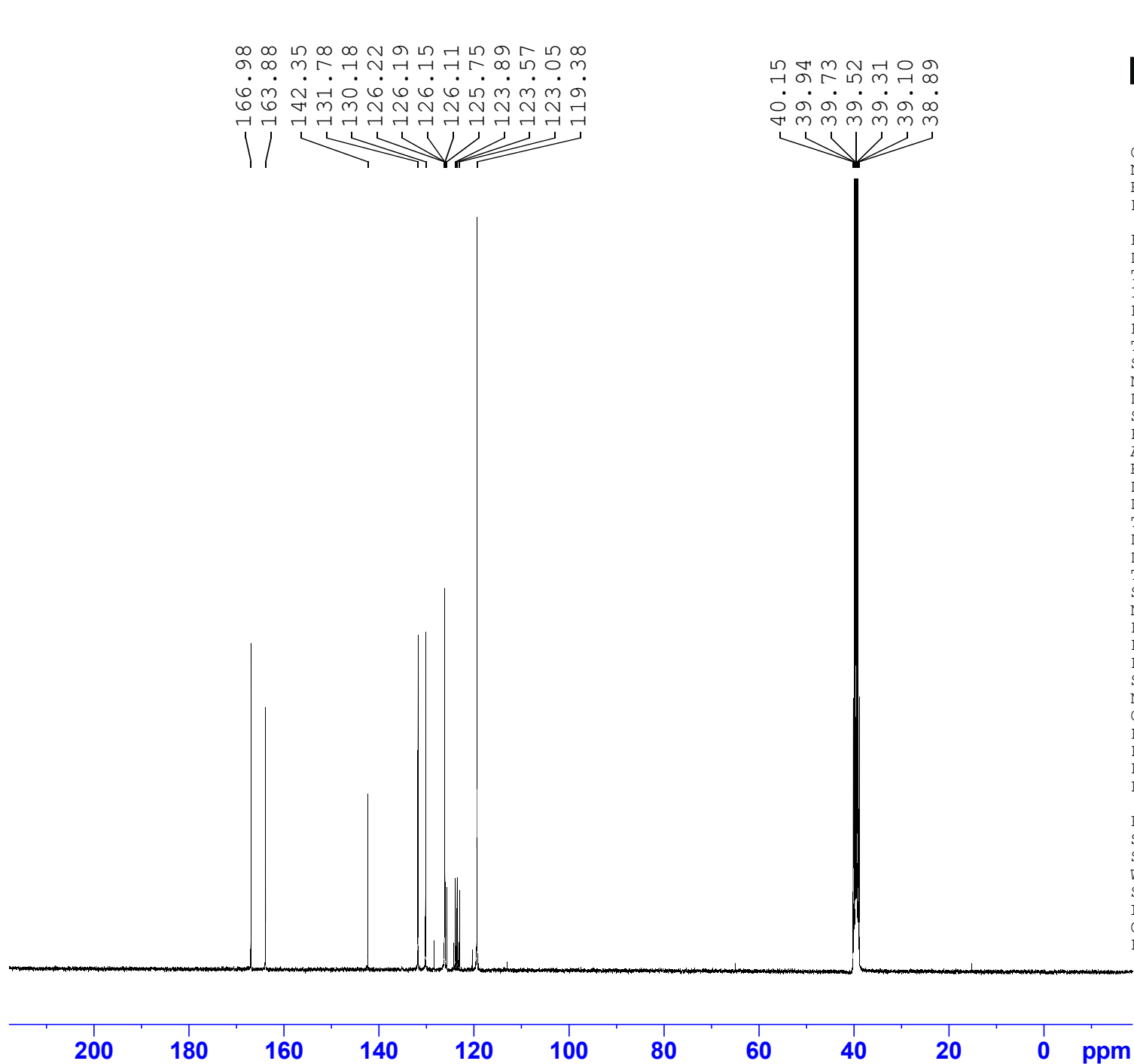
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0.99

1.00

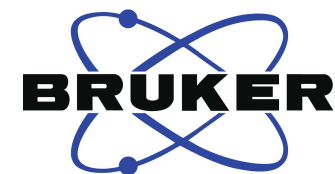
CF3 Maleamic acid (**1b**)



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SFO2 400.1516006 MHz
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TE 298.0 K
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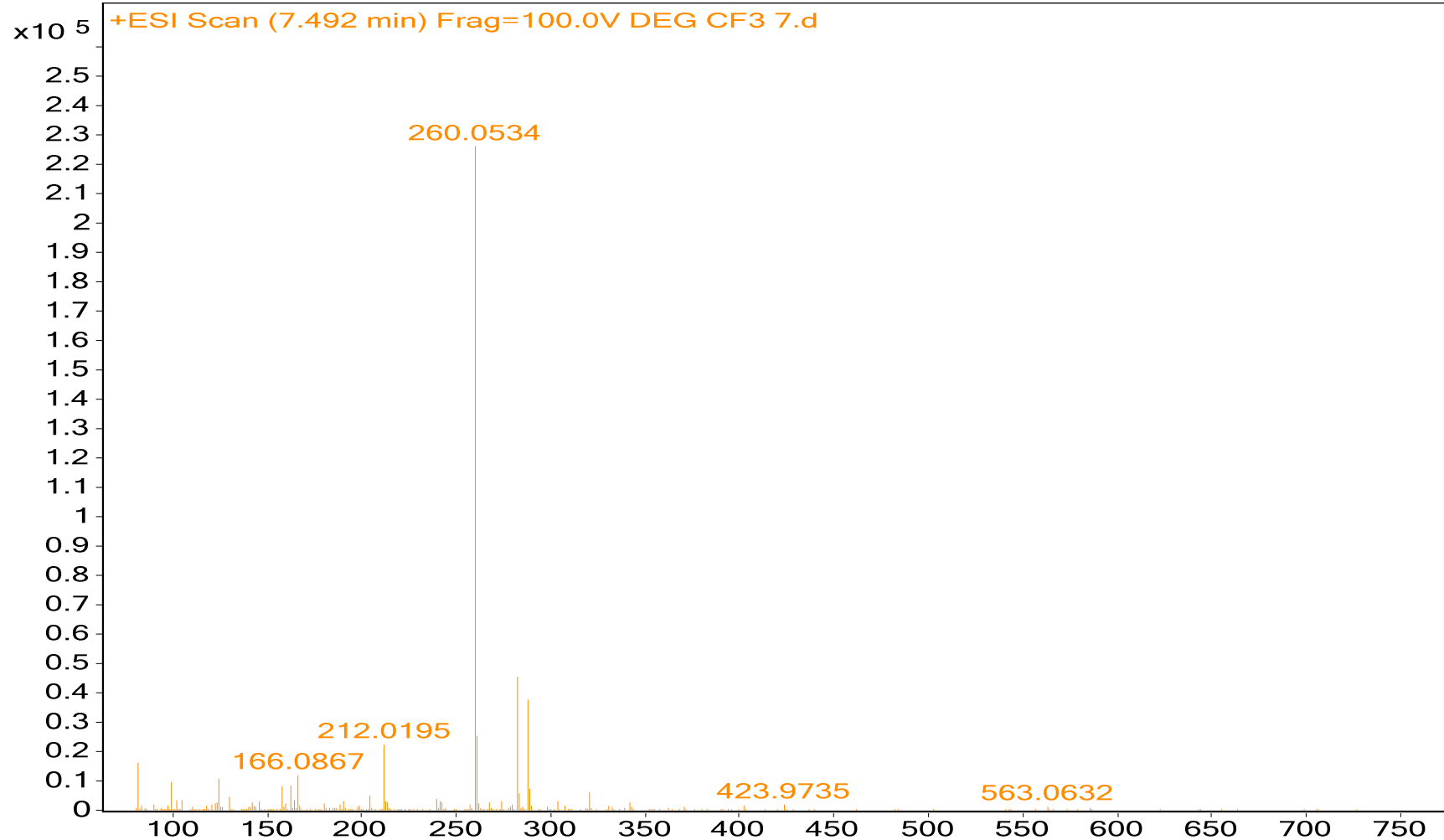
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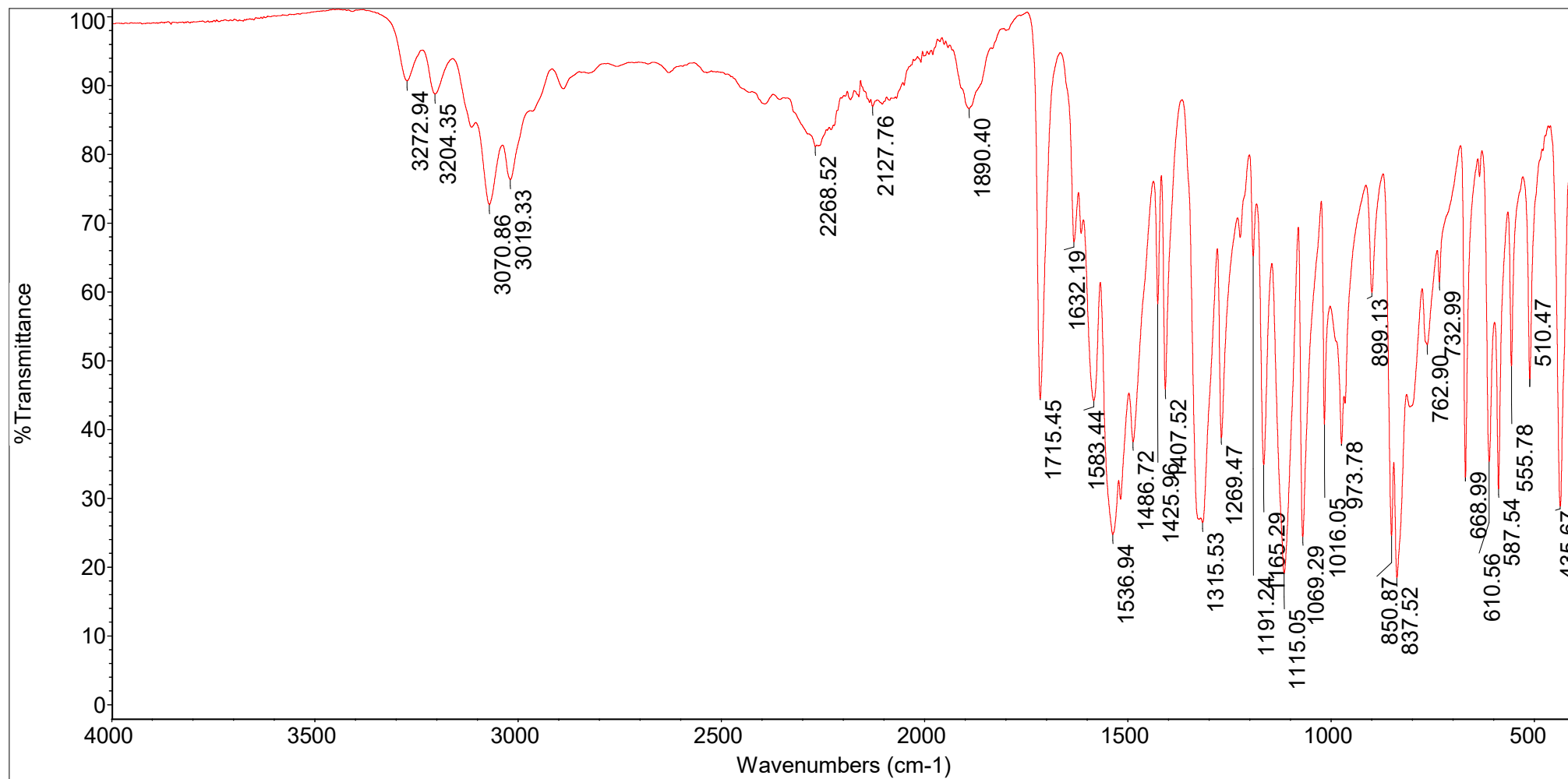
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InjPosition
ACQ Method

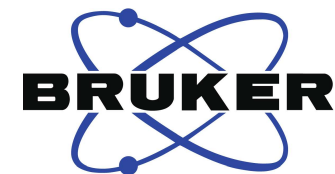
Instrument Name
SampleType
Comment

User Name
IRM Calibration Status
Acquired Time



CF3 Maleamic acid (**1b**)

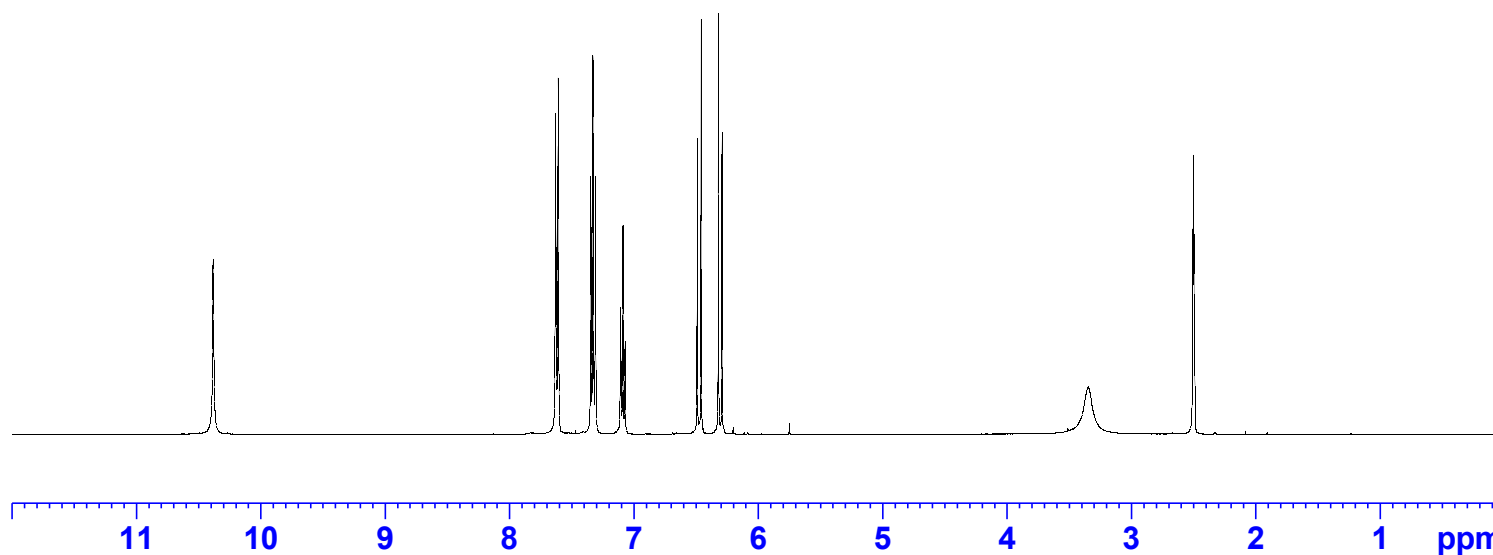
7.629
7.610
7.347
7.328
7.307
7.107
7.089
7.070
6.490
6.460
6.321
6.291



Current Data Parameters
NAME 4H Maleic acid 1H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210329
Time_ 12.42 h
INSTRUM AVNEO
PROBHD Z163739_0206 (
PULPROG zg30
TD 131072
SOLVENT DMSO
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.125072 Hz
AQ 7.9953918 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1524709 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 25.00000000 W

F2 - Processing parameters
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SF 400.1500035 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.00

2.03

2.03

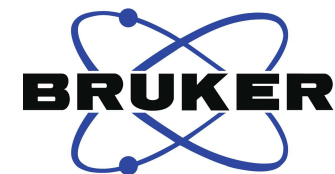
1.04

1.01

1.00

H Maleamic acid (1c)

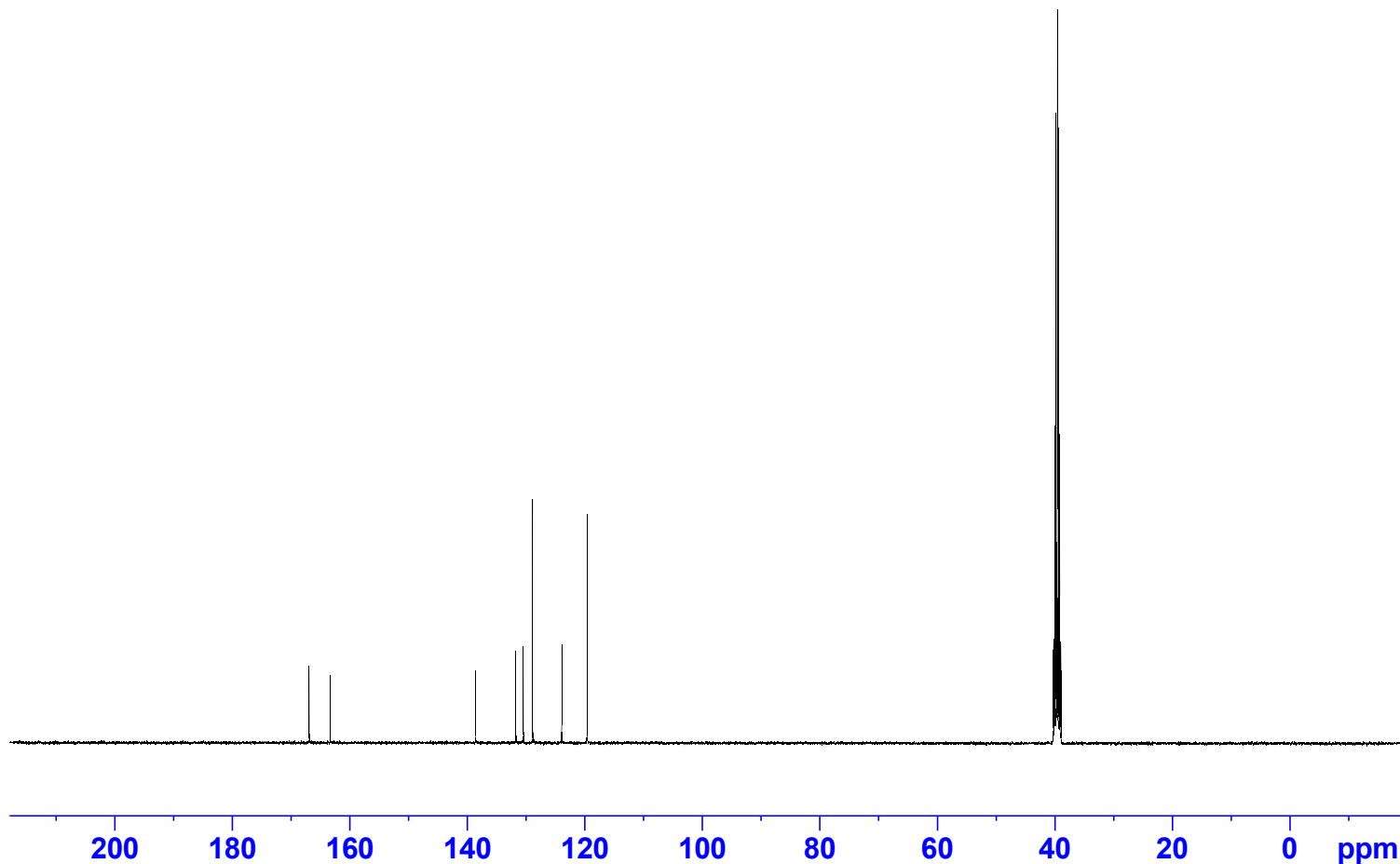
166.91
163.29
138.60
131.75
130.47
128.87
123.93
119.58



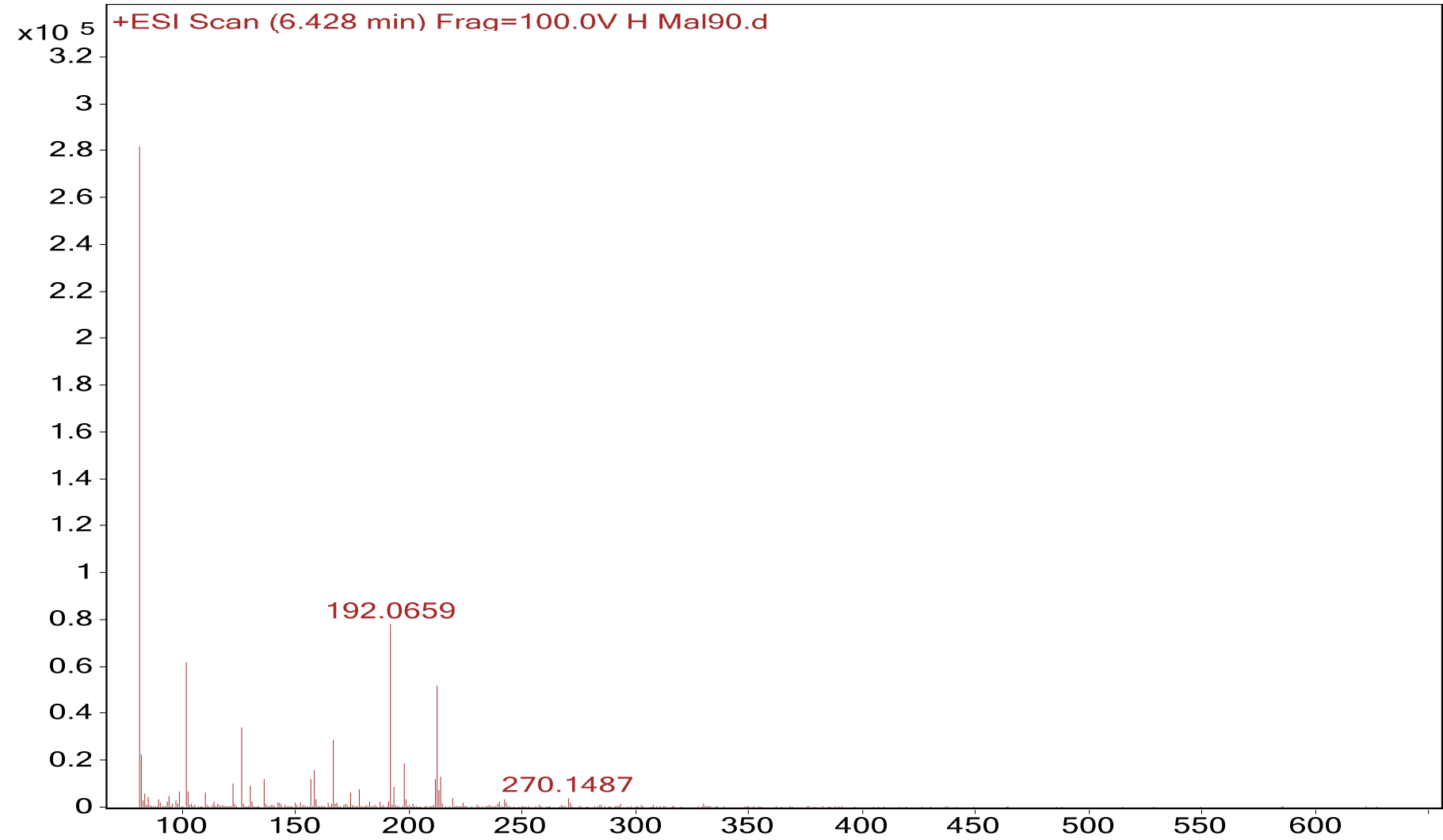
Current Data Parameters
NAME 4H Maleic acid 13C
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210329
Time_ 21.32 h
INSTRUM AVNEO
PROBHD Z163739_0206 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6278593 MHz
NUC1 13C
P0 2.67 usec
P1 8.00 usec
PLW1 93.00000000 W
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 25.00000000 W
PLW12 0.19753000 W
PLW13 0.09935700 W

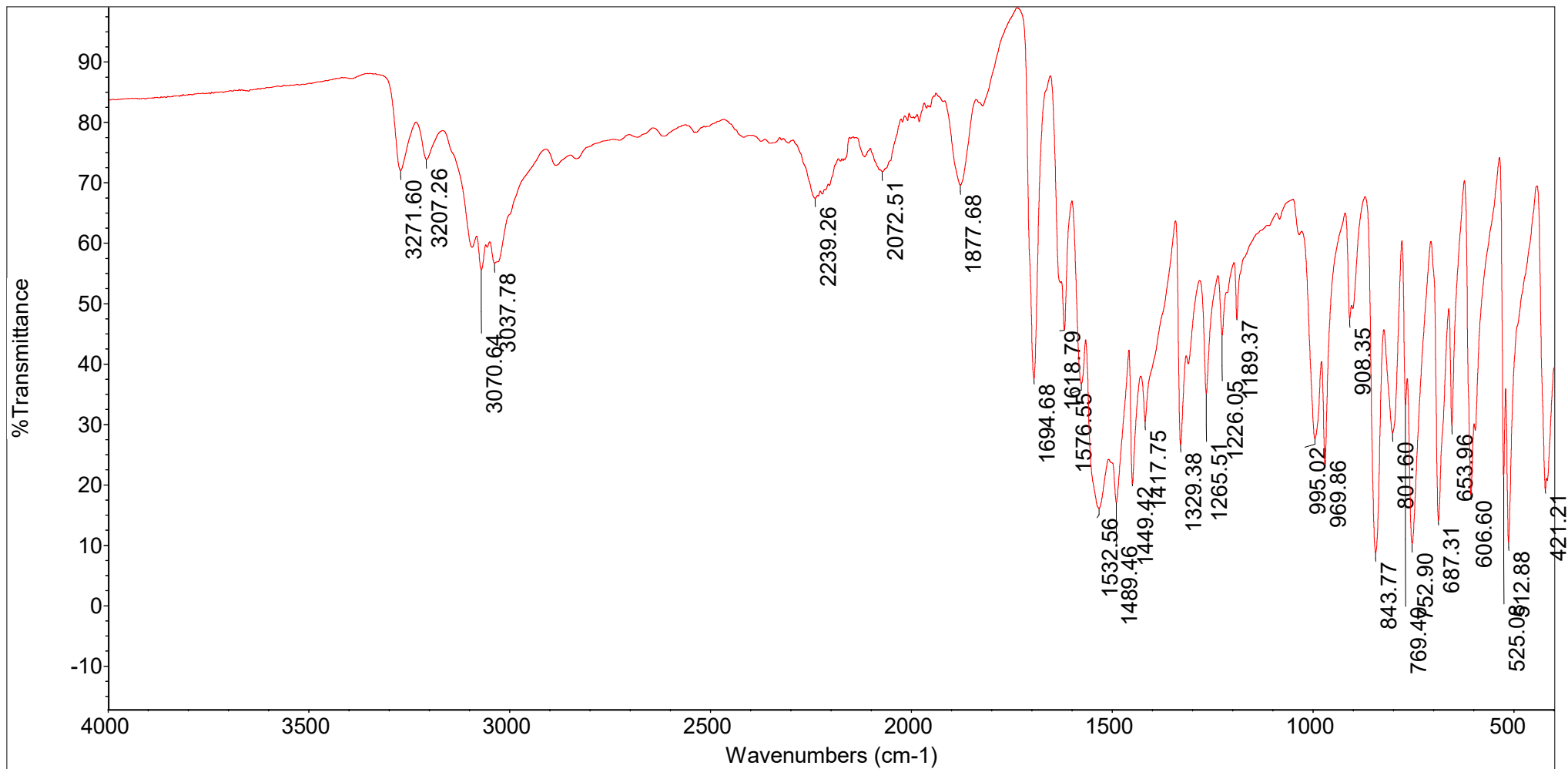
F2 - Processing parameters
SI 32768
SF 100.6178389 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Sample Name H maleamic acid (1c)	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



H Maleamic acid (**1c**)

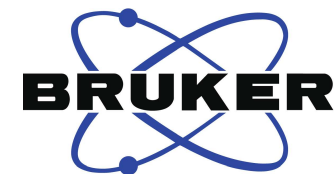


OMe Maleamic acid (1d)

7.559
7.536
6.930
6.907
6.482
6.451
6.320
6.289

3.737

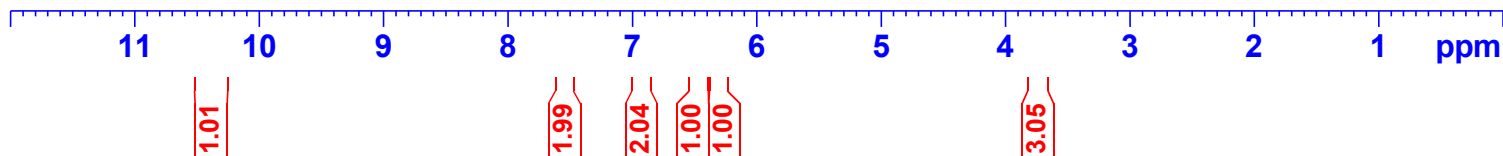
2.507



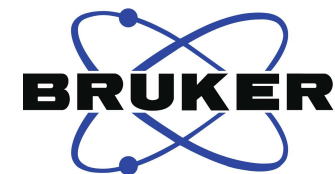
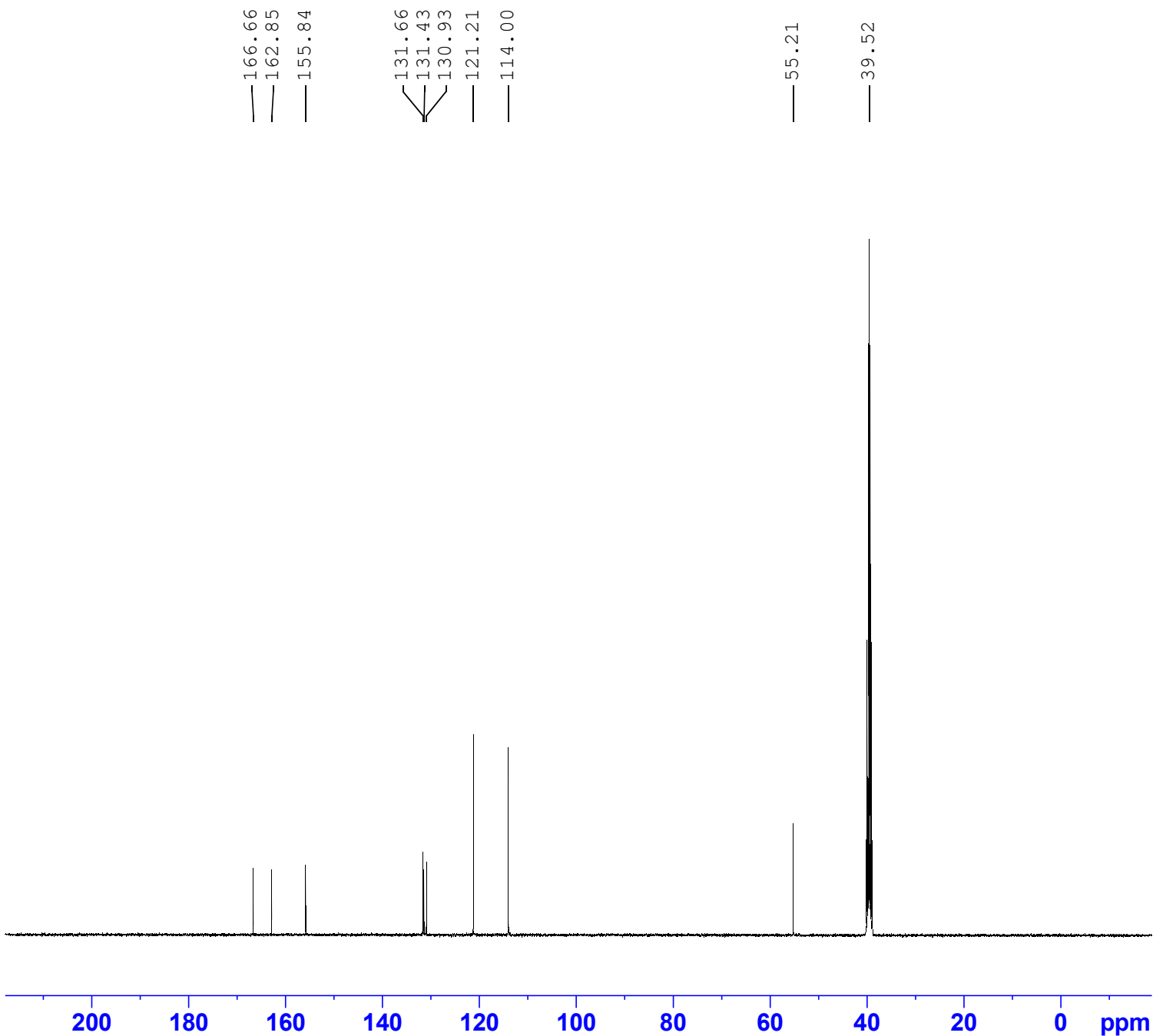
Current Data Parameters
NAME OMe Maleic Acid 1H
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210326
Time_ 11.29 h
INSTRUM AVNEO
PROBHD Z163739_0206 (
PULPROG zg30
TD 131072
SOLVENT DMSO
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.125072 Hz
AQ 7.9953918 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1524709 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 25.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



OMe Maleamic acid (**1d**)



Current Data Parameters
 NAME OMe Maleic acid 13C
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210329
 Time_ 20.27 h
 INSTRUM AVNEO
 PROBHD Z163739_0206 (
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.726609 Hz
 AQ 1.3762560 sec
 RG 101
 DW 21.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6278593 MHz
 NUC1 13C
 P0 2.67 usec
 P1 8.00 usec
 PLW1 93.00000000 W
 SFO2 400.1516006 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 25.00000000 W
 PLW12 0.19753000 W
 PLW13 0.09935700 W

F2 - Processing parameters
 SI 32768
 SF 100.6178432 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Name OMe Maleic acid (1d) OMe Rack Pos. 10
 Inj. Vol. (ul) Plate Pos. OMe 105 Mal Deg 7.4.d
 Data File Method (Acq)

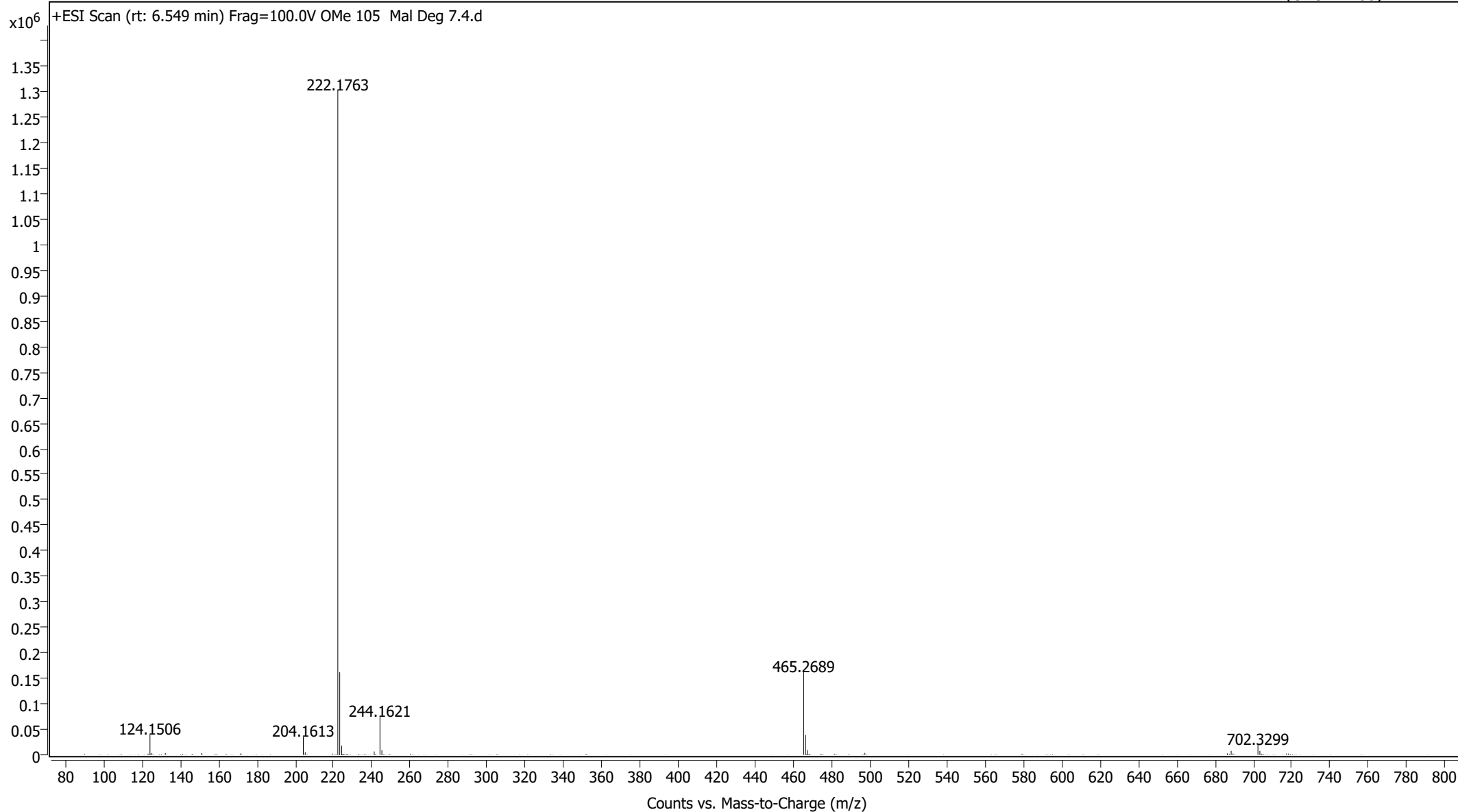
Pos Method (rev).m Instrument
 Comment

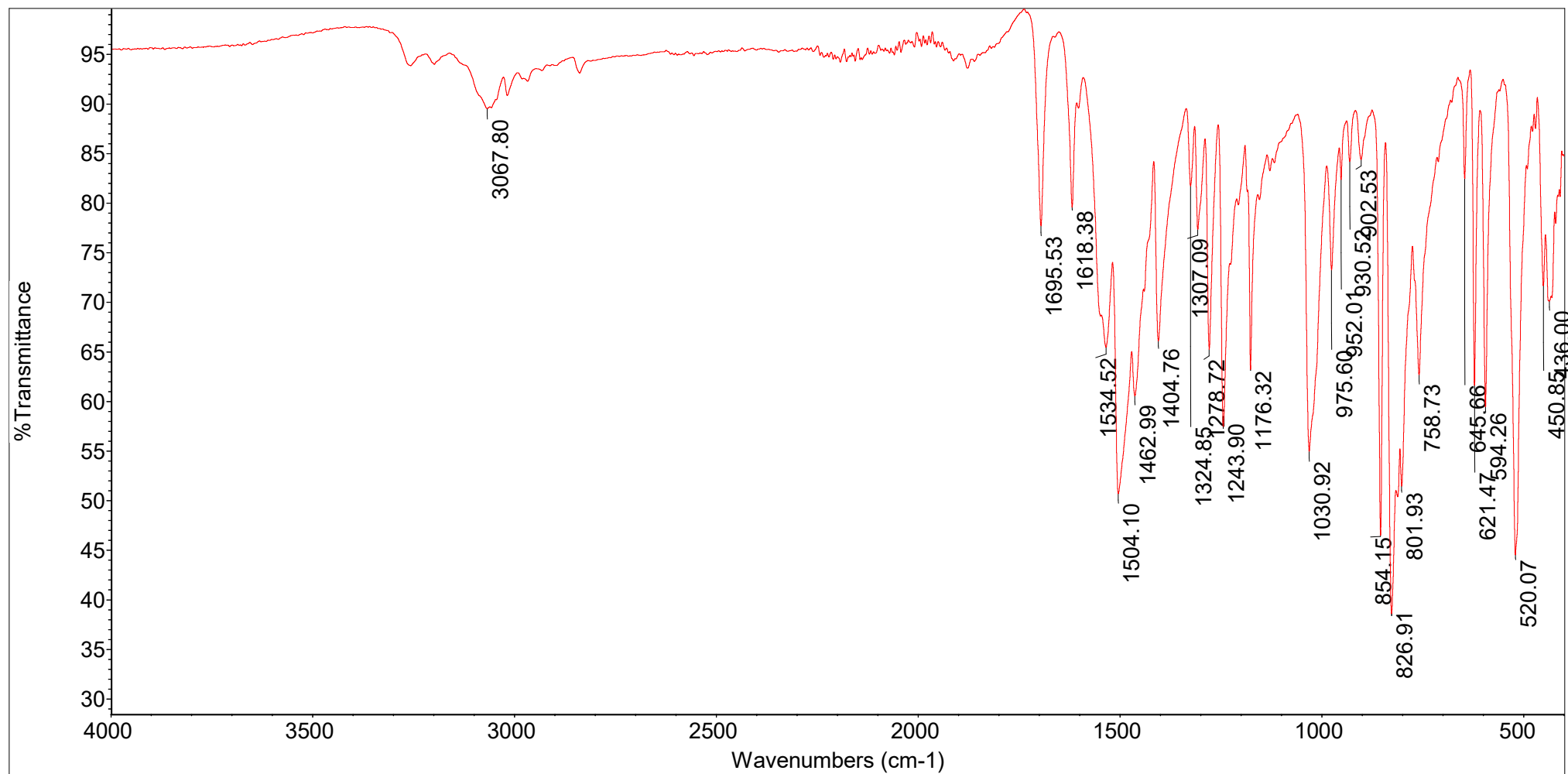
Instrument 1
 Success

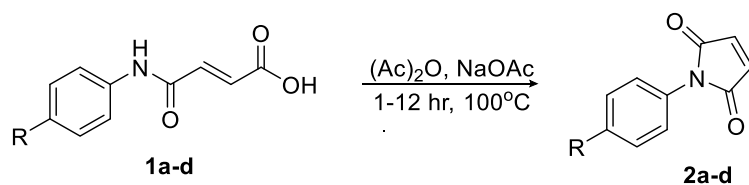
Operator

Acq. Time (Local)

2022-10-15 2:19:31 PM
 (UTC+11:00)

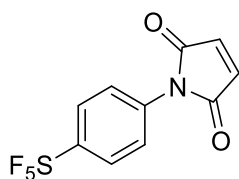






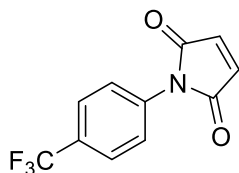
General procedure for the synthesis of (**2a-d**) adapted from the work of Sauers *et al.* [20]: 4-[4-(pentafluoro- λ^6 -sulfanyl)phenyl]-4-oxo-2-butenoic acid (634 mg, 2 mmol) was dissolved in acetic anhydride (5 mL), and sodium acetate (100 mg) was added to the reaction mixture. The reaction mixture was heated to 100°C for 1-12 hr, at which point it was concentrated *in-vacuo*, and the resulting residue was dissolved in Et₂O, dried over sodium carbonate and eluted from a plug of silica gel with Et₂O to afford the pure product.

4-[4-(pentafluoro- λ^6 -sulfanyl)phenyl]pyrrole-2,5-dione (**2a**)



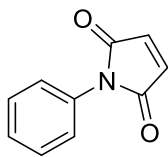
Compound **2a** was obtained as a white solid (502 mg, 1.68 mmol, 84%). Melting point: 126°C. **HRMS (EI)** Calcd for C₁₀H₇F₅NO₂S [M+H]⁺ 300.0117, [M+H]⁺ Found 300.0115; **IR (KBr)**: 1705 (s), 1592 (w), 1498 (m), 1397 (m), 1380 (m), 1219 (w), 1144 (s), 1091 (w), 825 (s, br) cm⁻¹; **¹H-NMR (CDCl₃)**: δ 7.86 (d, J = 9 Hz, 2H), 7.55 (d, J = 9 Hz, 2H), 6.90 (s, 2H); **¹³C-NMR (CDCl₃)**: δ 168.85, 152.42 (quin, J = 18 Hz), 134.49, 134.26, 127.14 (quin, J = 5 Hz), 126.53, 125.46; **¹⁹F-NMR (CDCl₃)**: δ 83.62 (m, 1F), 63.00 (d, J = 160 Hz, 4F).

4-[4-(trifluoromethyl)phenyl]pyrrole-2,5-dione (**2b**)



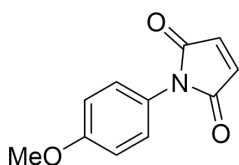
Compound **2b** was obtained as a white solid (424 mg, 1.76 mmol, 88%). Melting point: 130°C. **HRMS (EI)** Calcd for C₁₁H₇F₃NO₂ [M+H]⁺ 242.0428, [M+H]⁺ Found 242.0428; **IR (KBr)**: 1719 (s), 1702 (s), 1614 (w), 1525 (w), 1411 (m), 1330 (m), 1314 (m), 1155 (s), 1125 (m), 1069 (s), 1057 (m), 1037 (w), 1020 (m) cm⁻¹; **¹H-NMR (CDCl₃)**: δ 7.73 (d, J = 8.4 Hz, 2H), 7.54 (d, J = 8.3 Hz, 2H), 6.88 (s, 2H); **¹³C-NMR (CDCl₃)**: δ 169.01, 134.54, 129.95, 126.34 (q, J = 5 Hz), 125.86, 125.22, 122.52; **¹⁹F-NMR (CDCl₃)**: δ -62.64 (s, 3F).

4-(phenyl)pyrrole-2,5-dione (2c)



Compound **2c** was obtained as a light-yellow solid (273 mg, 1.58 mmol, 79%). Melting point 88°C (Lit. 89-90°C [28]). **HRMS (EI)** Calcd for C₁₀H₈NO₂ [M+H]⁺ 174.0555, [M+H]⁺ Found 174.0552; **IR (KBr)**: 1704 (s), 1595 (w), 1507 (m), 1487 (w), 1371 (m), 1310 (w), 1206 (w), 1143 (m), 1070 (m), 1029 (w), 948 (w), 830 (s), 754 (m), 639 (s) cm⁻¹; **¹H-NMR (CDCl₃)**: δ 7.47 (t, J = 7.4, 15.24 Hz, 2H), 7.38-7.33 (m, 3H), 6.84 (s, 2H); **¹³C-NMR (CDCl₃)**: δ 169.64, 134.32, 131.33, 129.27, 128.09, 126.20.

4-[4-(methoxy)phenyl]pyrrole-2,5-dione (2d)

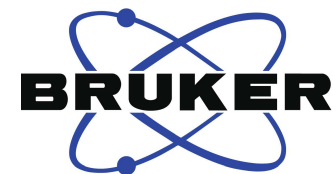


Compound **2d** was obtained as a fluorescent yellow solid (381 mg, 1.86 mmol, 93%). Melting point 154°C (Lit. 154-156°C [29]). **HRMS (EI)** Calcd for C₁₁H₁₀NO₃ [M+H]⁺ 204.0660, [M+H]⁺ Found 204.0660; **IR (KBr)**: 1703 (s), 1607 (w), 1586 (w), 1509 (s), 1467 (w), 1397 (m), 1300 (w), 1246 (m), 1106 (w), 1026 (s), 952 (w), 819 (s), 798 (m), 719 (w), 685 (s) cm⁻¹; **¹H-NMR (CDCl₃)**: δ 7.22 (d, J = 8.8 Hz, 2H), 6.97 (d, J = 8.8 Hz, 2H), 6.82 (s, 2H); **¹³C-NMR (CDCl₃)**: δ 169.96, 159.30, 134.27, 127.72, 123.89, 114.63, 55.63.

References

20. Sauers CK (1969) The Dehydration of N-Arylmaleamic Acids with Acetic Anhydride. J Org Chem 34:2275–2279. <https://doi.org/10.1021/jo01260a008>
28. Fletcher TL, Pan HL (1961) Derivatives of Fluorene. XIV. N-(Ring)-Fluorenylmaleimides. J Org Chem 26:2037–2043. https://doi.org/10.1021/JO01065A087/ASSET/JO01065A087.FP.PNG_V03
29. Kumar PP, Rama Devi B, Dubey PK, Mohiuddin SMG (2011) PEG-600 mediated simple, efficient and eco-friendly synthesis of N-substituted imides and chemo selective C = C reduction. Green Chem Lett Rev 4:341–348. <https://doi.org/10.1080/17518253.2011.571720>

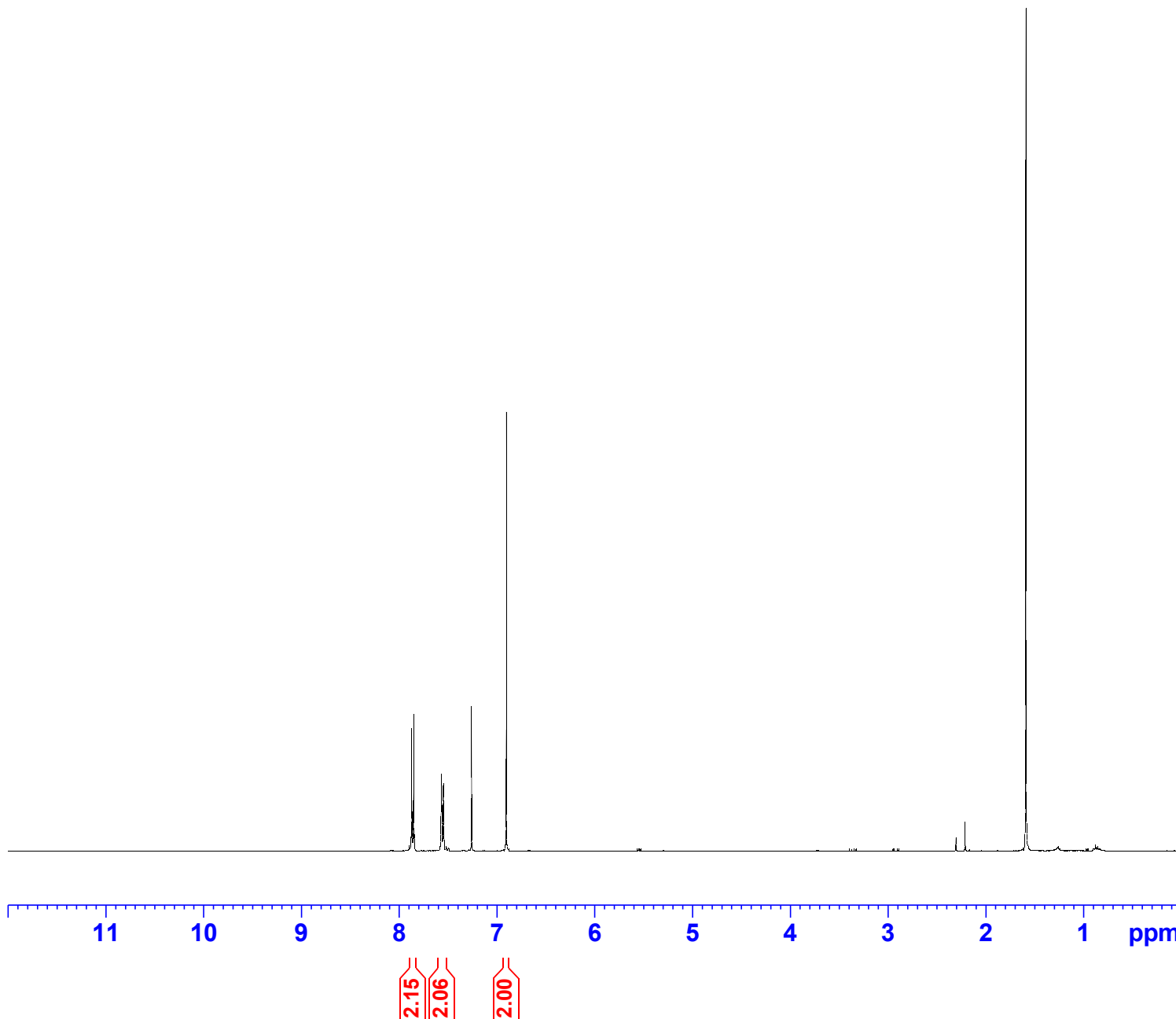
7.874
7.856
7.851
7.569
7.547
7.260
6.904



Current Data Parameters
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EXPNO 4
PROCNO 1

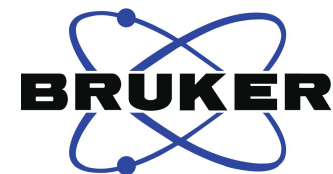
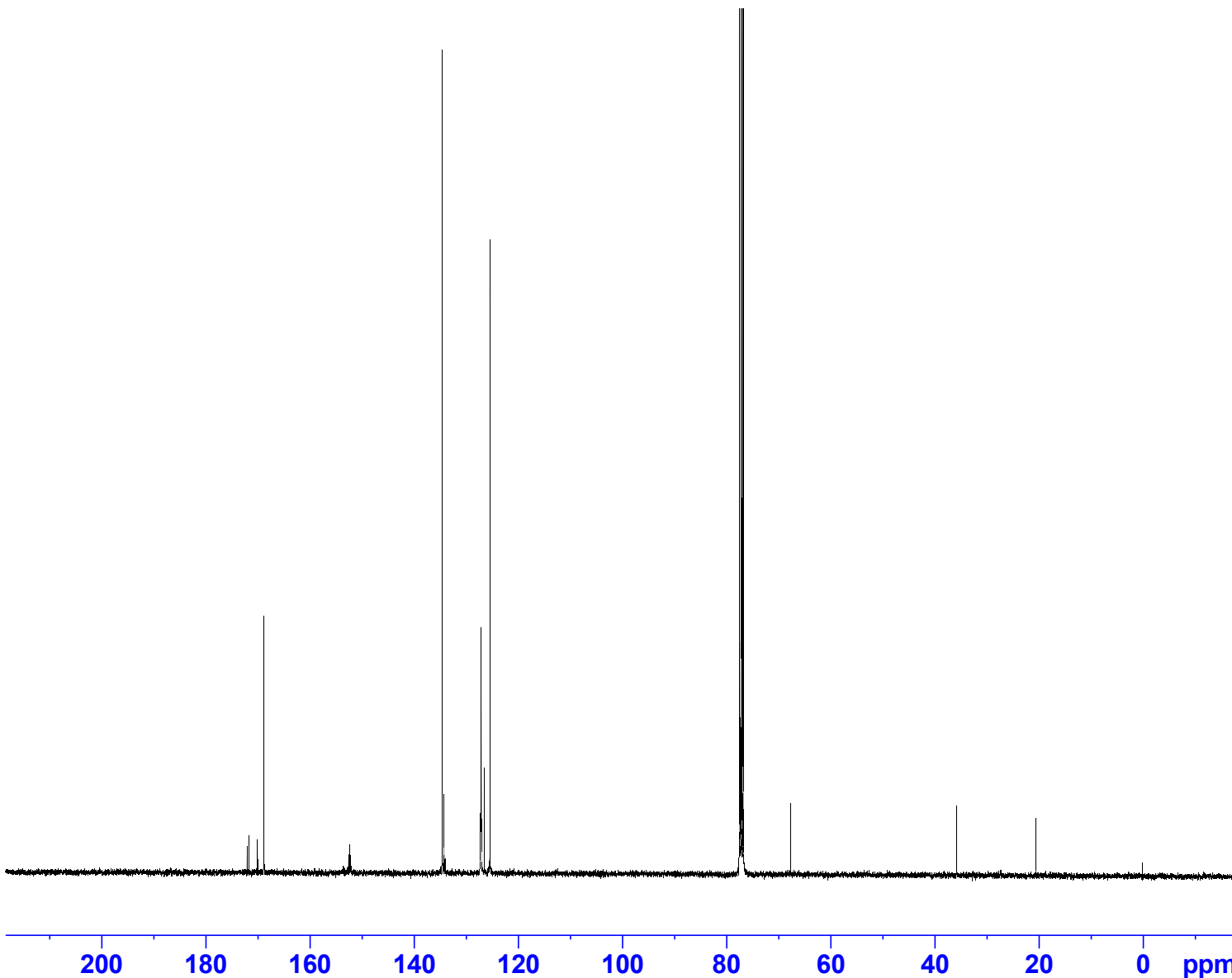
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TD 131072
SOLVENT CDCl3
NS 32
DS 2
SWH 8196.722 Hz
FIDRES 0.125072 Hz
AQ 7.9953918 sec
RG 101
DW 61.000 usec
DE 13.54 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1524709 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 19.63299942 W

F2 - Processing parameters
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SF 400.1500091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



SF5 Maleimide (2a)

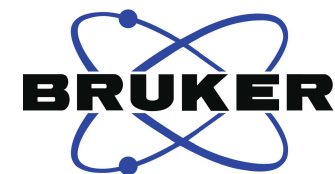
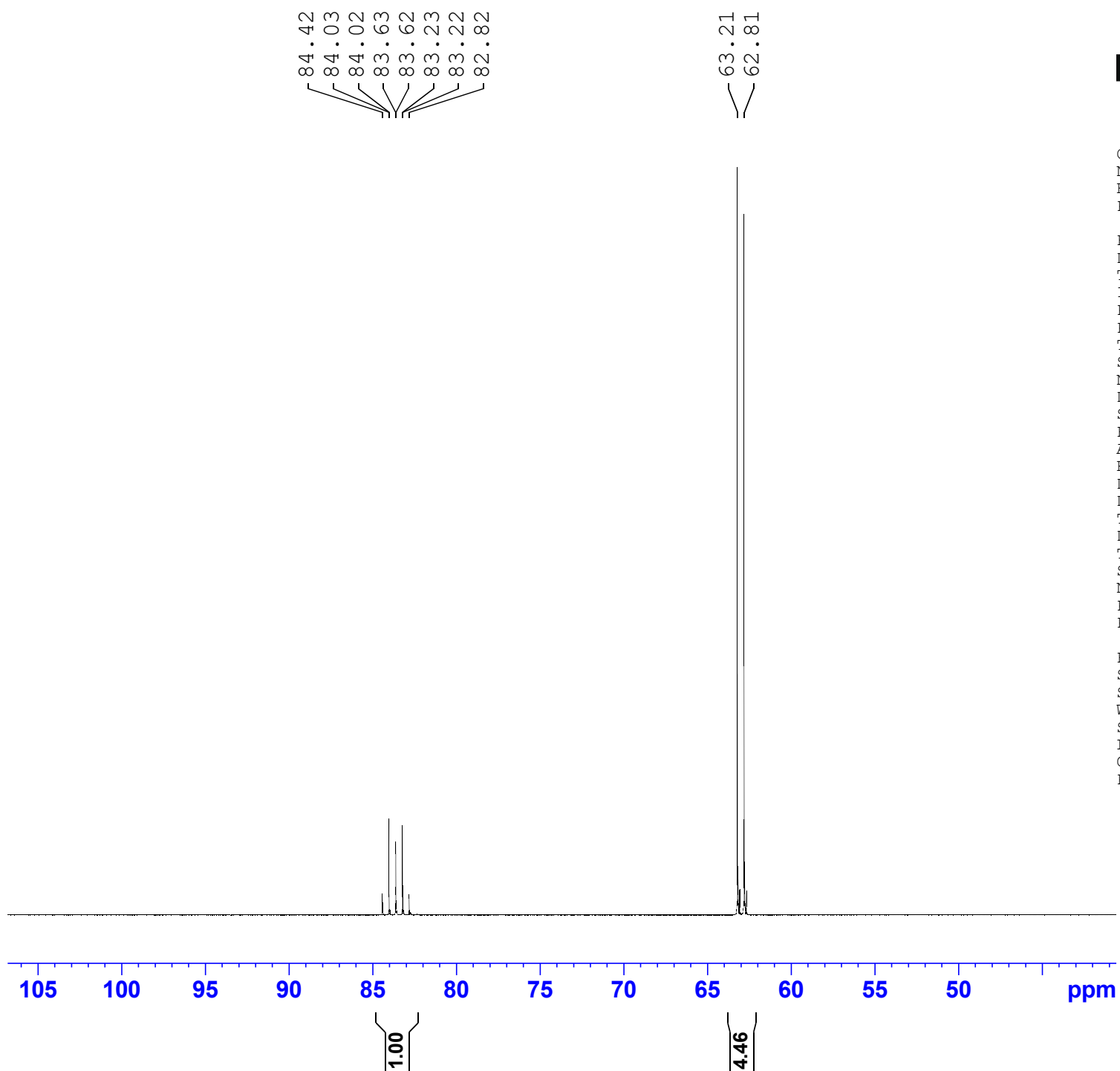
168.85
152.60
152.42
152.24
152.06
134.62
134.27
127.23
127.19
127.14
127.10
127.05
126.53
125.46



Current Data Parameters
NAME SF5 Maleimide 13C
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221208
Time_ 3.24 h
INSTRUM AVNEO
PROBHD Z175272_0008 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3200
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6278593 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 58.38199997 W
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 19.63299942 W
PLW12 0.24237999 W
PLW13 0.12192000 W

F2 - Processing parameters
SI 32768
SF 100.6177842 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME Sep13-2022
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220913
Time_ 20.29 h
INSTRUM AVNEO
PROBHD Z175272_0008 (
PULPROG zg
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 147058.828 Hz
FIDRES 2.243940 Hz
AQ 0.4456448 sec
RG 101
DW 3.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 376.5171850 MHz
NUC1 19F
P1 12.00 usec
PLW1 45.00000000 W

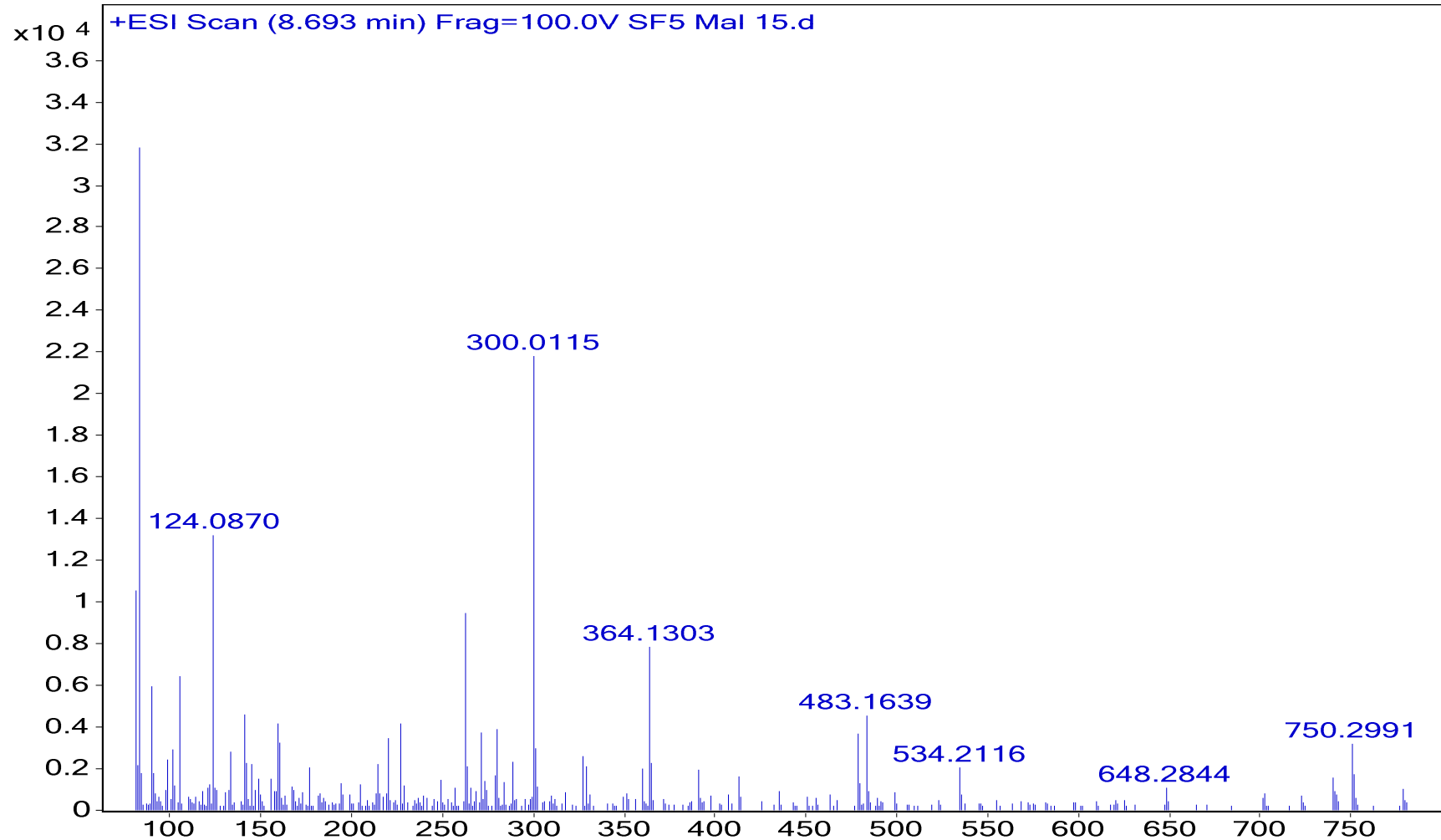
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LB 0.30 Hz
GB 0
PC 1.00

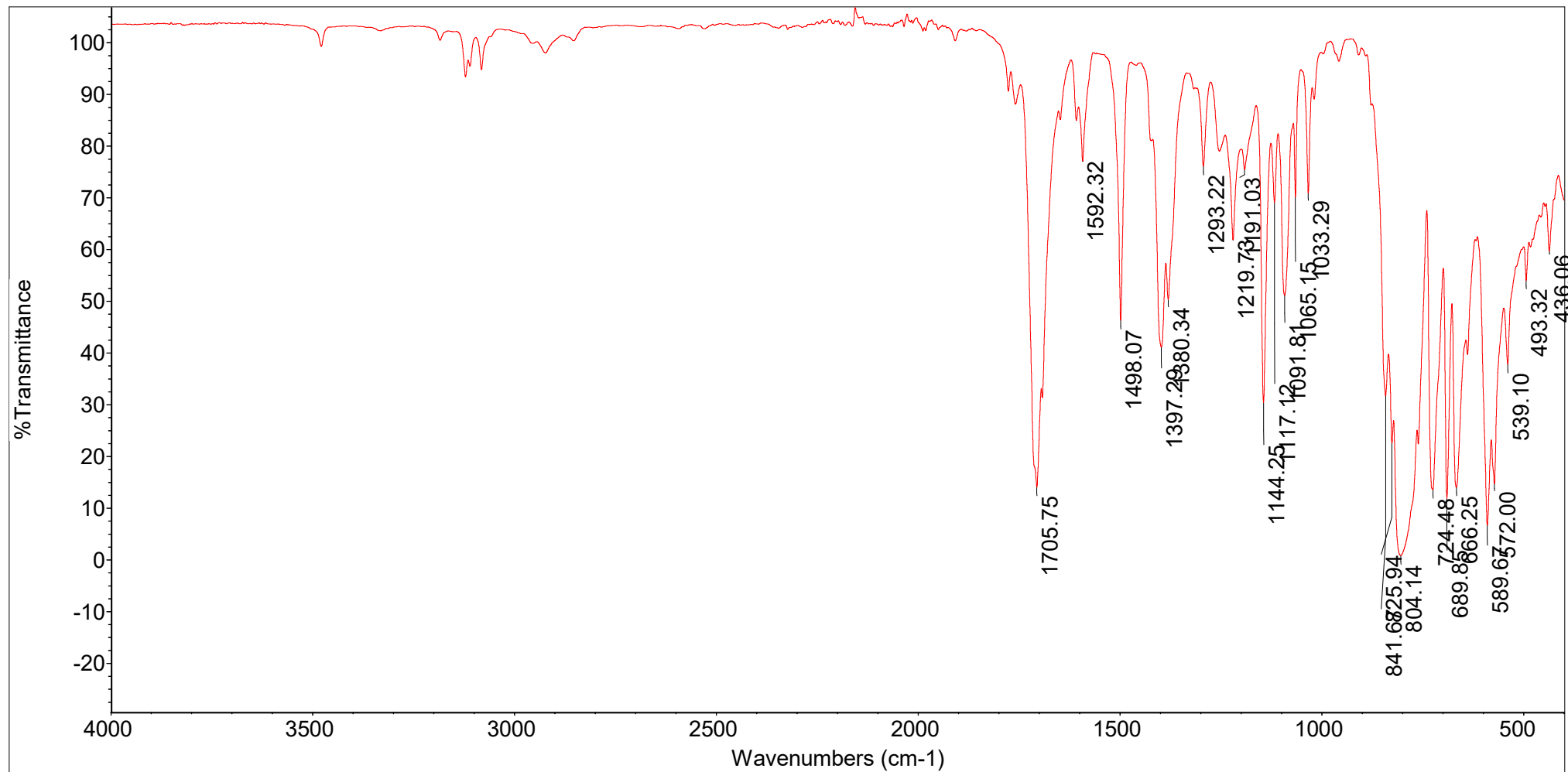
Sample Name SF5 Maleamic acid (2a)
Inj Vol
Data Filename

Position
InjPosition
ACQ Method

Instrument Name
SampleType
Comment

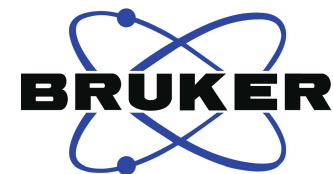
User Name
IRM Calibration Status
Acquired Time





CF3 Maleimide (2b)

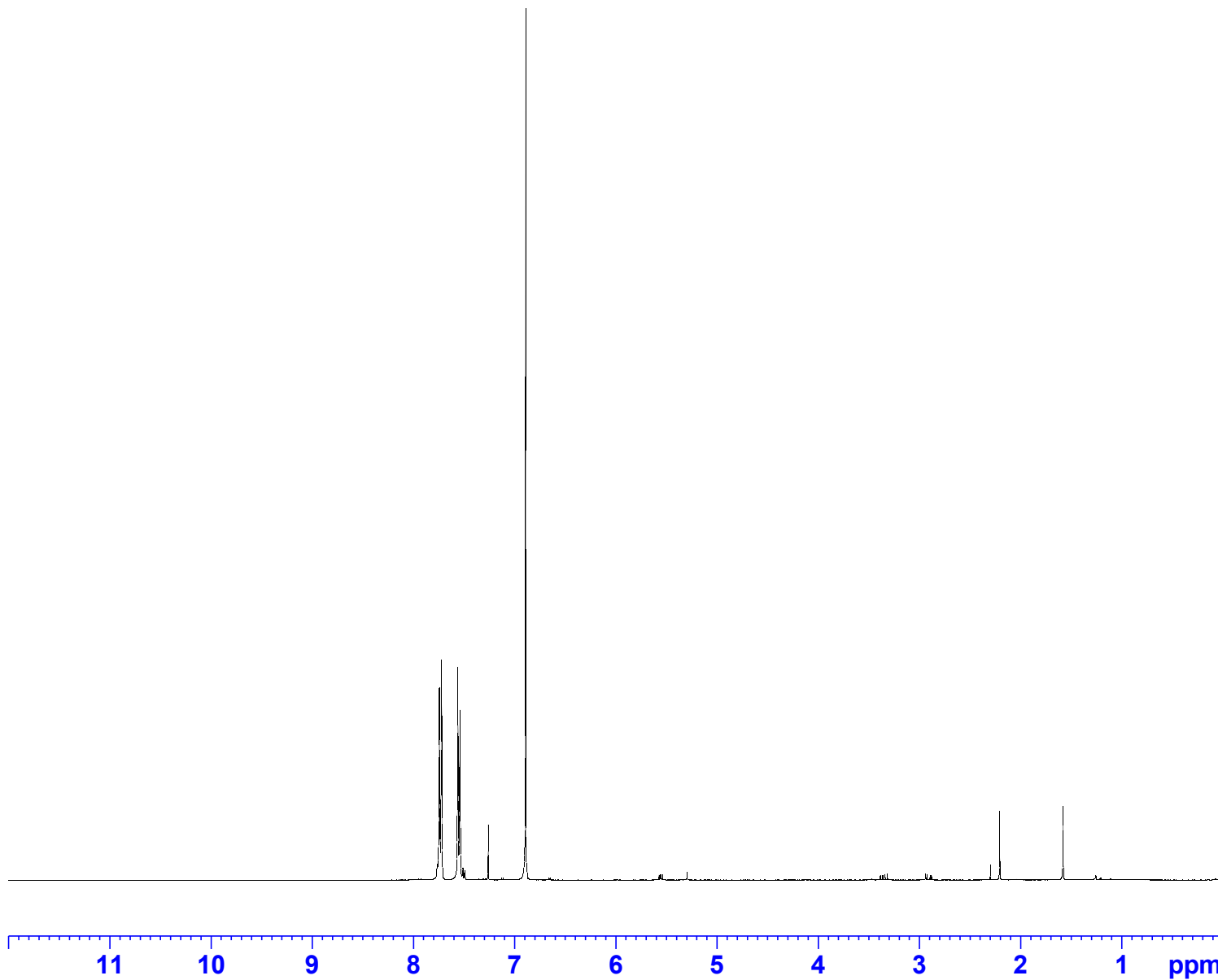
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7.721
7.560
7.539
— 6.890



Current Data Parameters
NAME CF3 Maleimide 1H
EXPNO 15
PROCNO 1

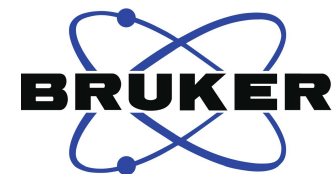
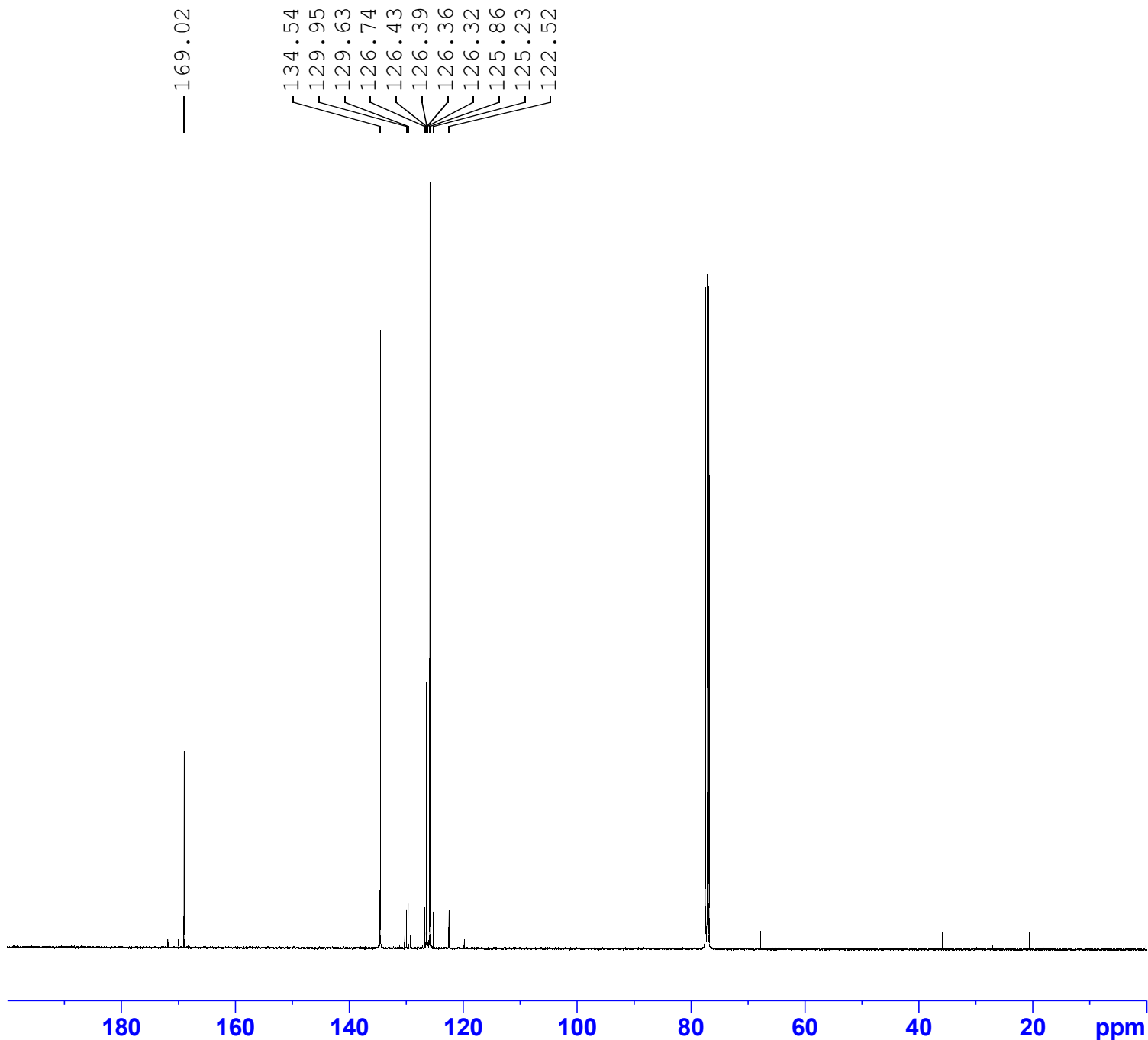
F2 - Acquisition Parameters
Date_ 20220913
Time_ 21.08 h
INSTRUM AVNEO
PROBHD Z175272_0008 (
PULPROG zg30
TD 131072
SOLVENT CDCl3
NS 32
DS 2
SWH 8196.722 Hz
FIDRES 0.125072 Hz
AQ 7.9953918 sec
RG 101
DW 61.000 usec
DE 13.54 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1524709 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 19.63299942 W

F2 - Processing parameters
SI 65536
SF 400.1500088 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2.13
2.09
2.00

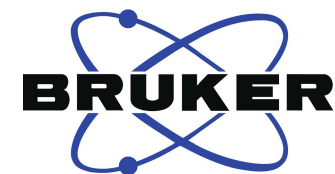
CF3 Maleimide (2b)



Current Data Parameters
 NAME CF3 Maleimide 13C
 EXPNO 16
 PROCNO 1

F2 - Acquisition Parameters
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 Time_ 0.44 h
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 PROBHD Z175272_0008 (
 PULPROG zgpg30
 TD 92160
 SOLVENT CDCl3
 NS 3200
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.516700 Hz
 AQ 1.9353600 sec
 RG 101
 DW 21.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6278593 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 58.38199997 W
 SFO2 400.1516006 MHz
 NUC2 1H
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 PCPD2 90.00 usec
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 PLW12 0.24237999 W
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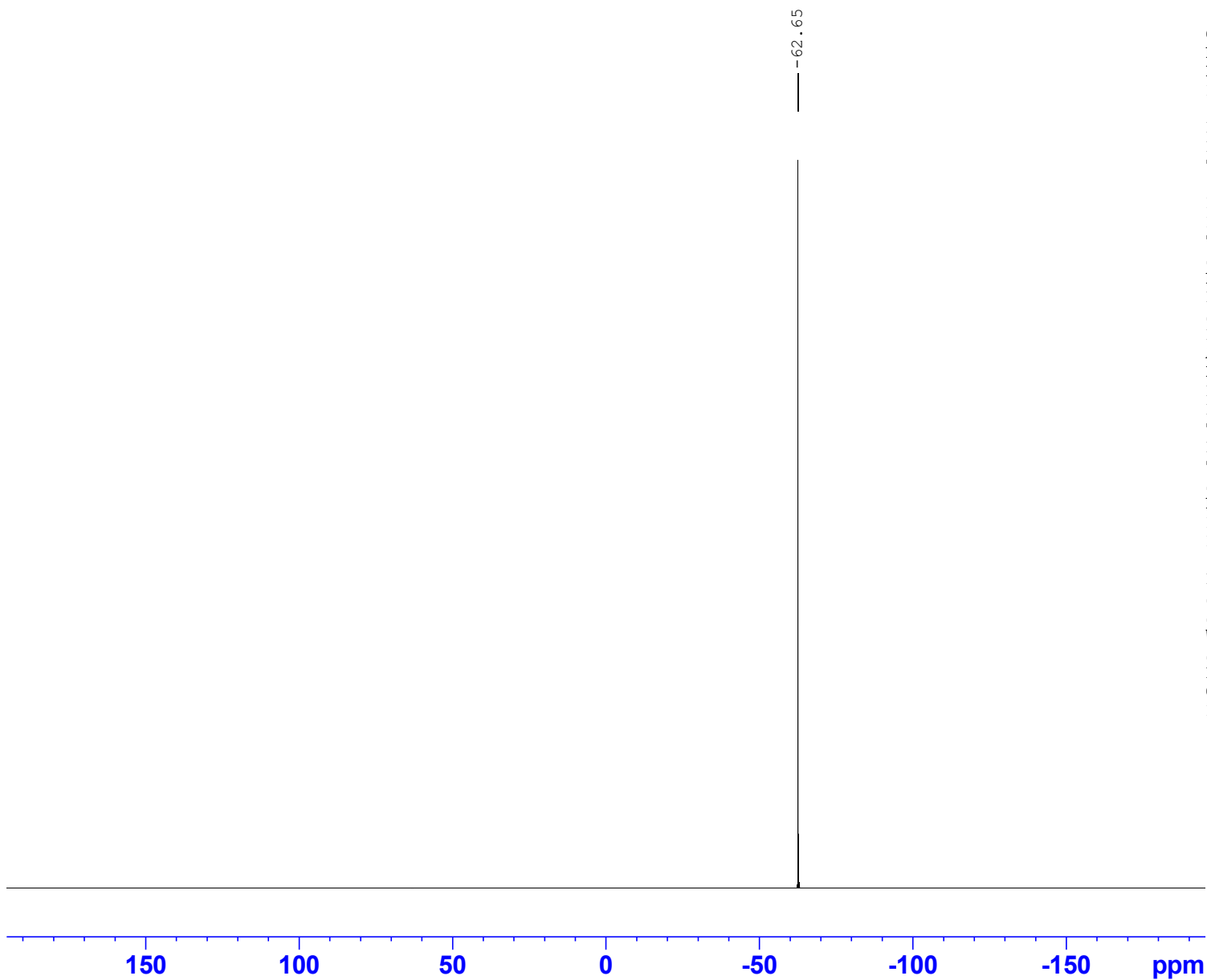
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 PC 1.40



Current Data Parameters
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EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220913
Time_ 20.45 h
INSTRUM AVNEO
PROBHD Z175272_0008 (
PULPROG zg
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 147058.828 Hz
FIDRES 2.243940 Hz
AQ 0.4456448 sec
RG 101
DW 3.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 376.5171850 MHz
NUC1 19F
P1 12.00 usec
PLW1 45.00000000 W

F2 - Processing parameters
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SF 376.5171850 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

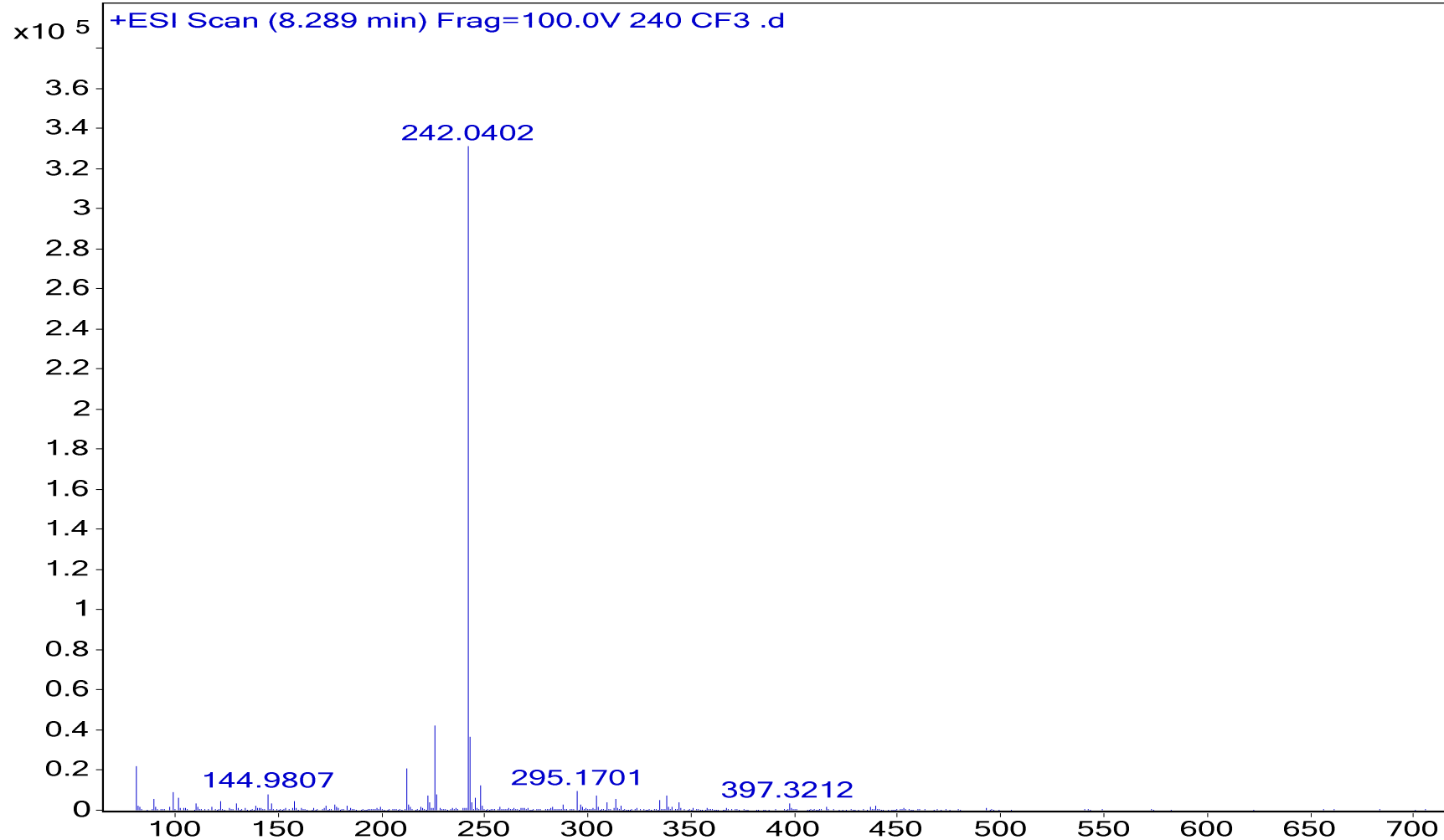


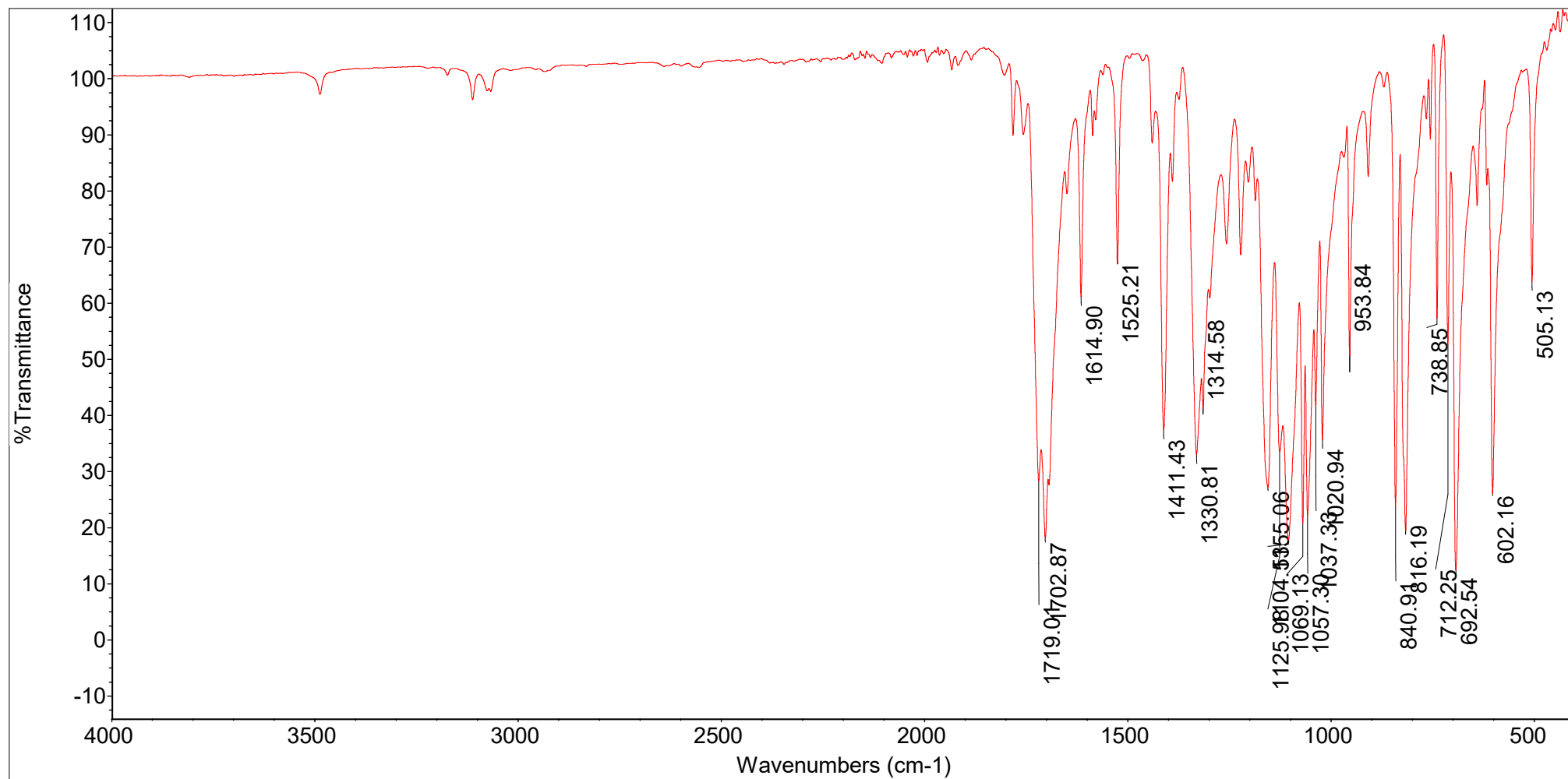
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Inj Vol
Data Filename

Position
InjPosition
ACQ Method

Instrument Name
SampleType
Comment

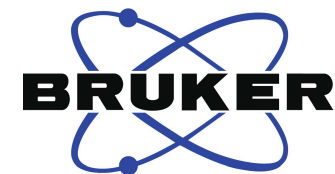
User Name
IRM Calibration Status
Acquired Time





H Maleimide (2c)

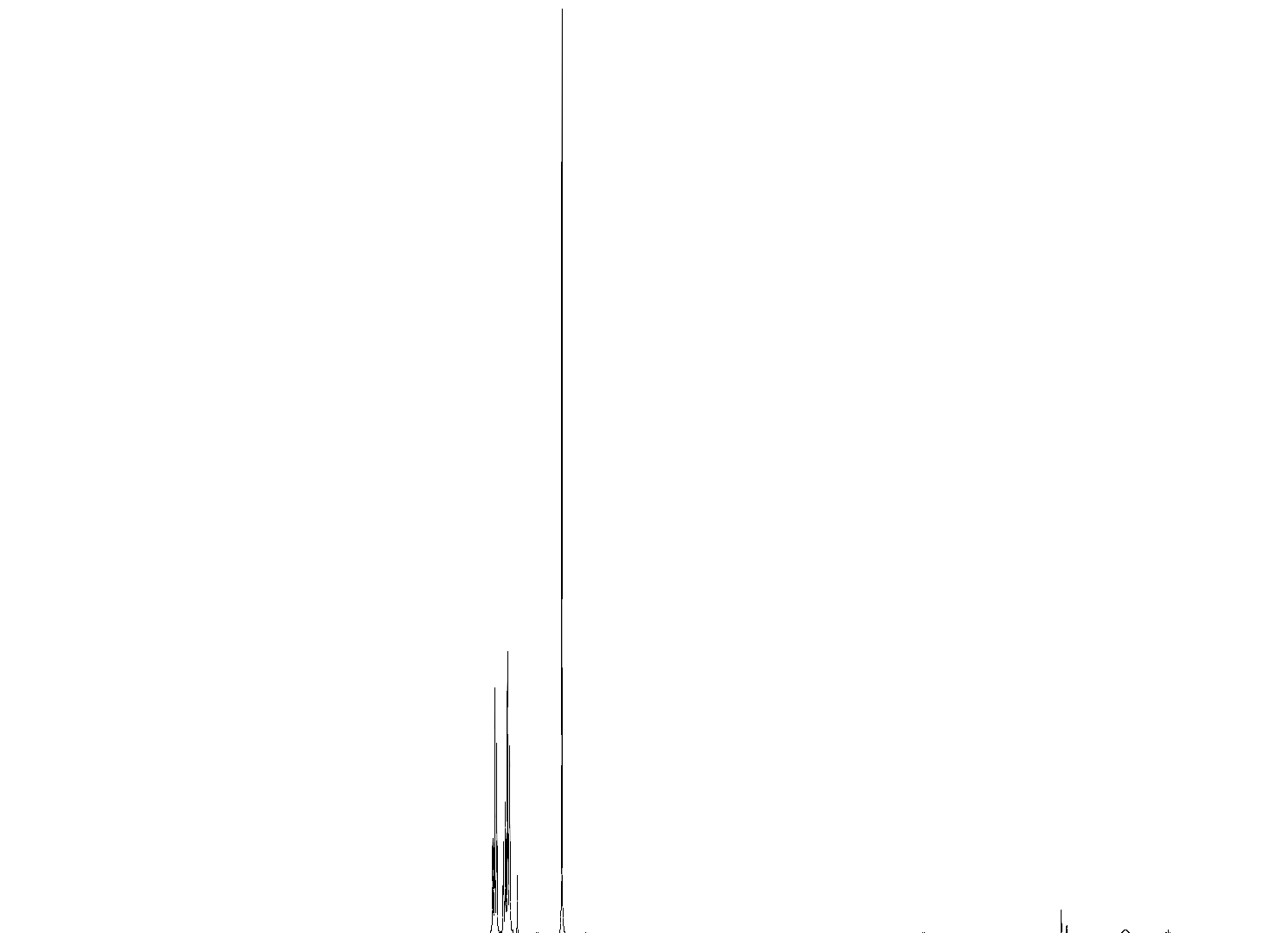
7.490
7.471
7.452
7.389
7.371
7.354
7.350
7.332
7.260
6.846



Current Data Parameters
NAME H Maleimide 1H perf
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220920
Time_ 2.00 h
INSTRUM AVNEO
PROBHD Z175272_0008 (
PULPROG zg30
TD 131072
SOLVENT CDCl3
NS 32
DS 2
SWH 8196.722 Hz
FIDRES 0.125072 Hz
AQ 7.9953918 sec
RG 101
DW 61.000 usec
DE 13.54 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1524709 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 19.63299942 W

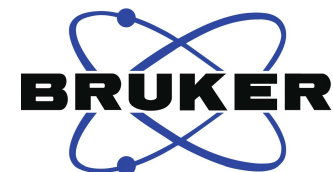
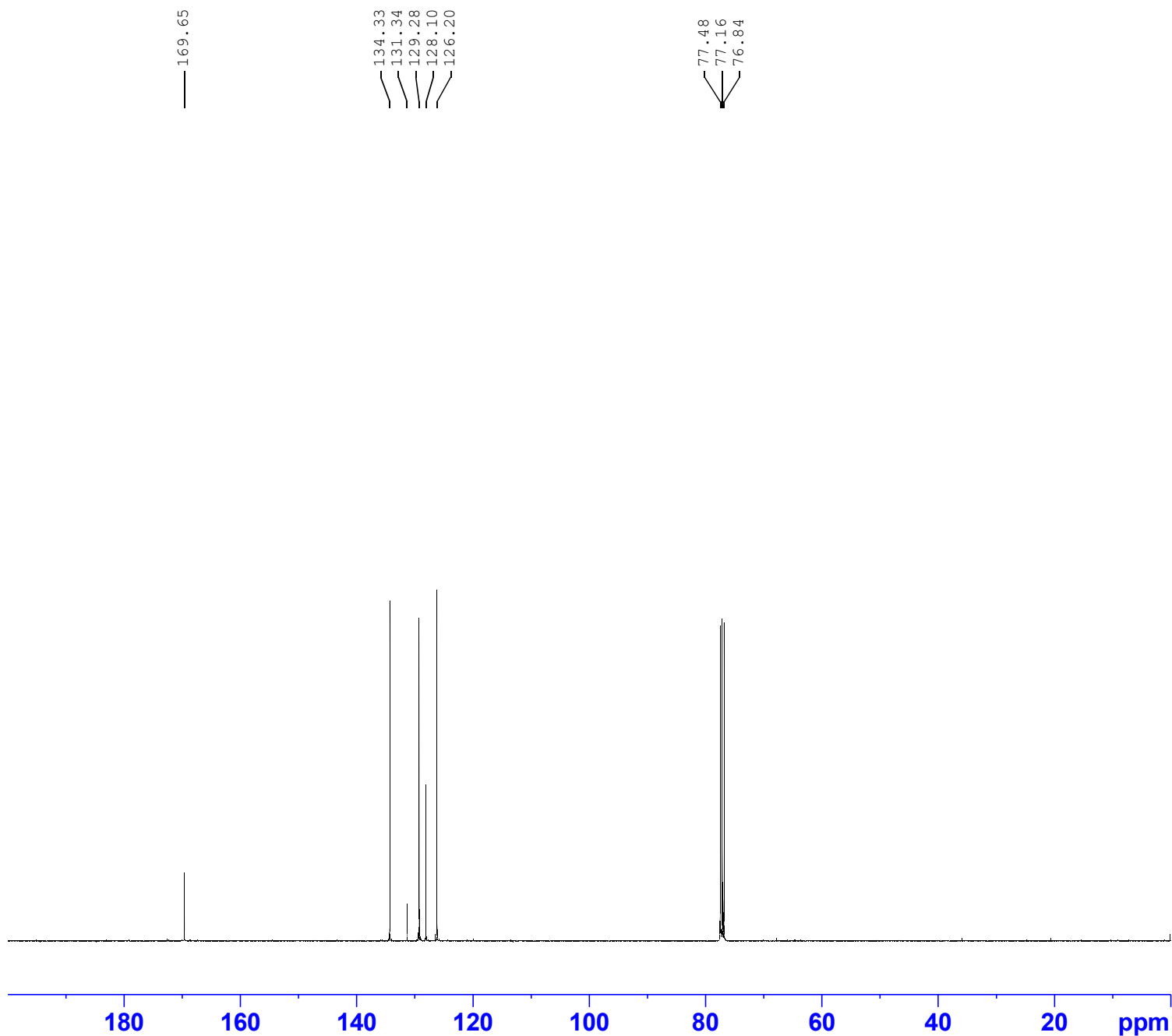
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SF 400.1500094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



11 10 9 8 7 6 5 4 3 2 1 ppm

2.05
2.99
2.00

H Maleimide (**2c**)



Current Data Parameters
NAME H Maleimide 13 C - perf
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220920
Time_ 5.37 h
INSTRUM AVNEO
PROBHD Z175272_0008 (
PULPROG zgpg30
TD 92160
SOLVENT CDCl3
NS 3200
DS 4
SWH 23809.523 Hz
FIDRES 0.516700 Hz
AQ 1.9353600 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6278593 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 58.38199997 W
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 19.63299942 W
PLW12 0.24237999 W
PLW13 0.12192000 W

F2 - Processing parameters
SI 32768
SF 100.6177866 MHz
WDW EM
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LB 1.00 Hz
GB 0
PC 1.40

Sample Name H Maleimide (2c)

Position

Instrument Name

User Name

Inj Vol

InjPosition

SampleType

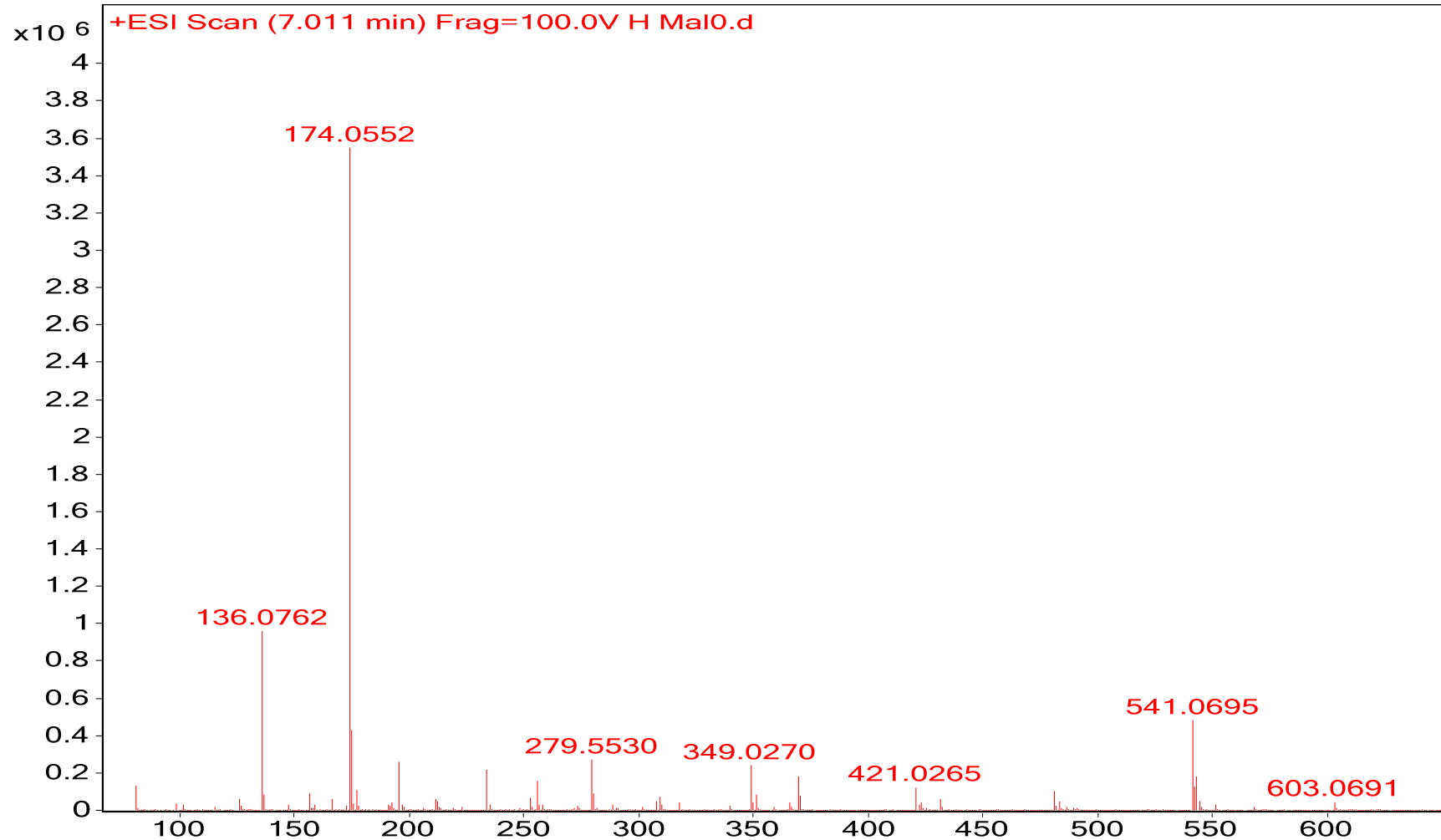
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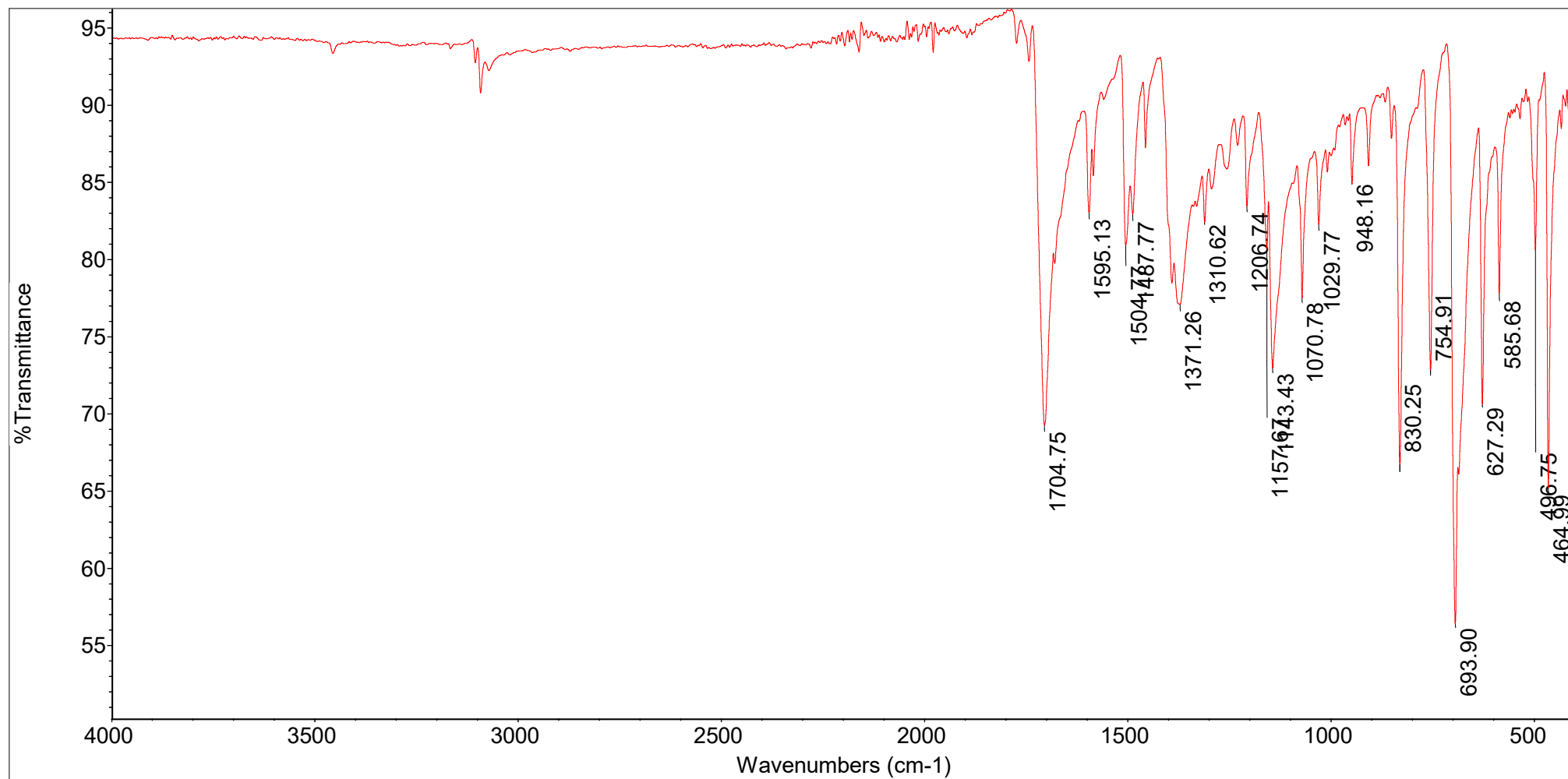
Data Filename

ACQ Method

Comment

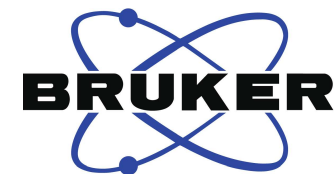
Acquired Time





7.260
7.238
7.216
6.989
6.967
6.827

3.825



Current Data Parameters
NAME 1H OMe Maleimide
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220920
Time_ 5.48 h
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PROBHD Z175272_0008 (
PULPROG zg30
TD 131072
SOLVENT CDCl3
NS 32
DS 2
SWH 8196.722 Hz
FIDRES 0.125072 Hz
AQ 7.9953918 sec
RG 101
DW 61.000 usec
DE 13.54 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1524709 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 19.63299942 W

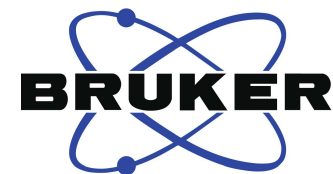
F2 - Processing parameters
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SF 400.1500095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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2.08
2.00

3.32

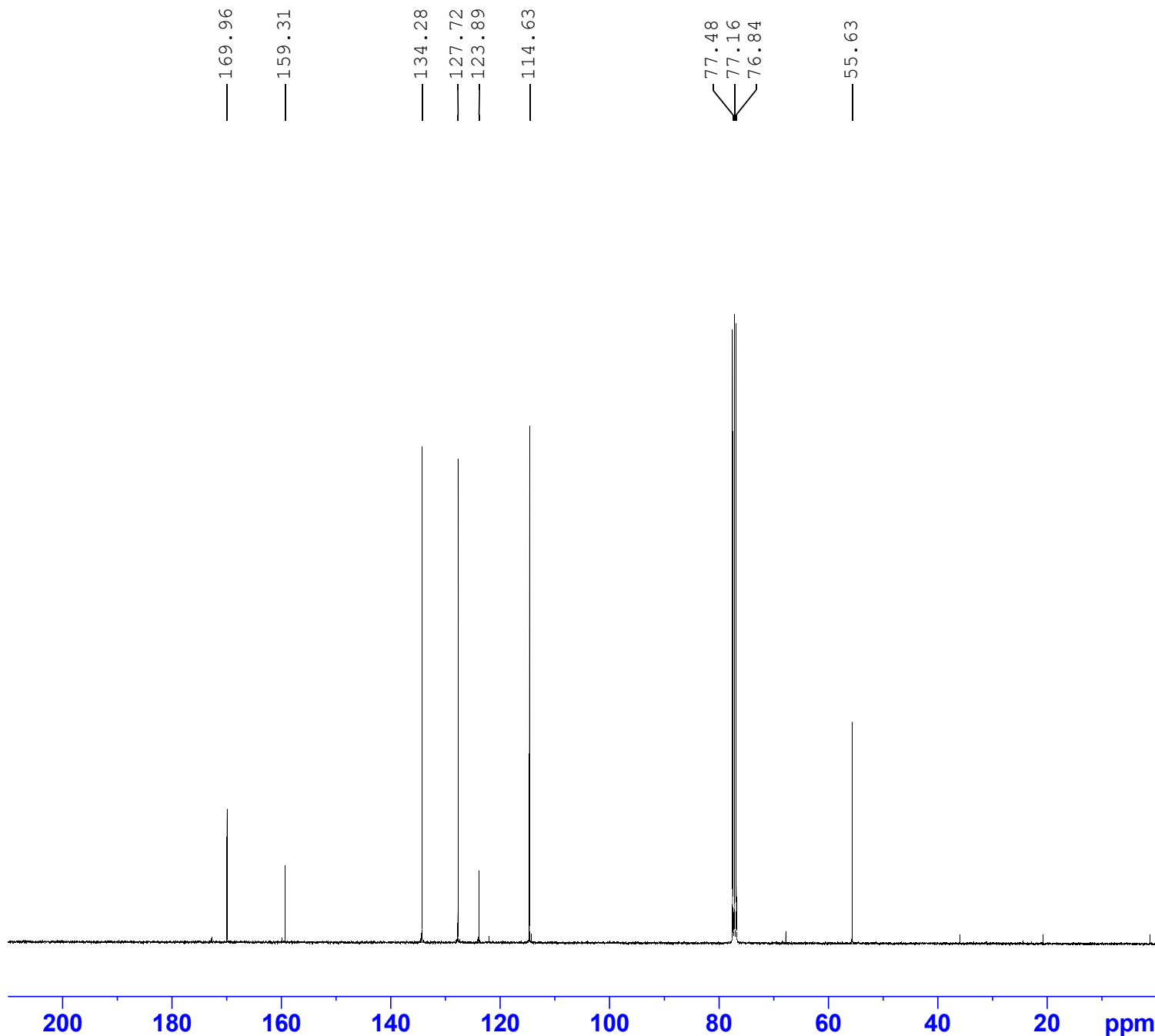
OMe Maleimide (2d)



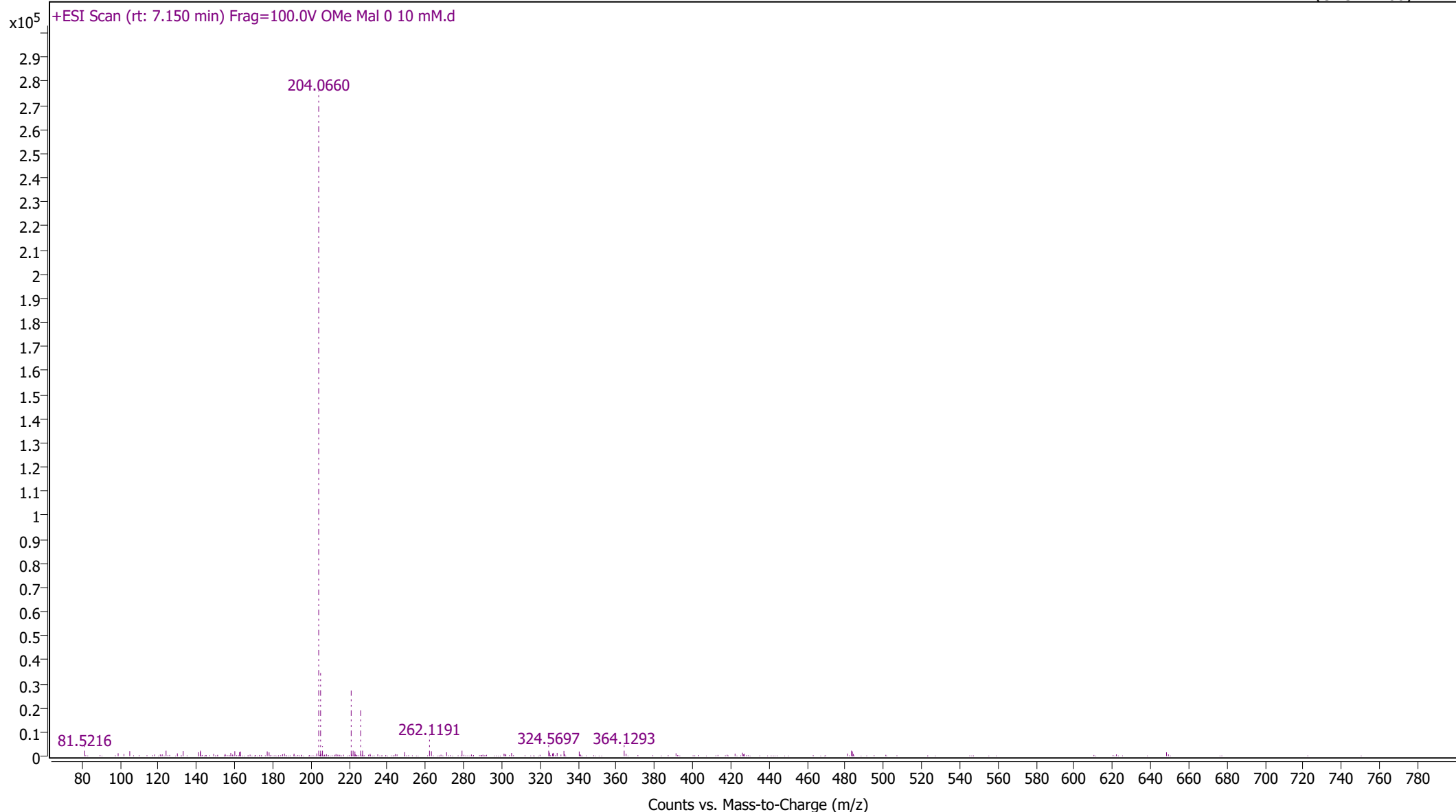
Current Data Parameters
 NAME 13C OMe Maleimide
 EXPNO 4
 PROCNO 1

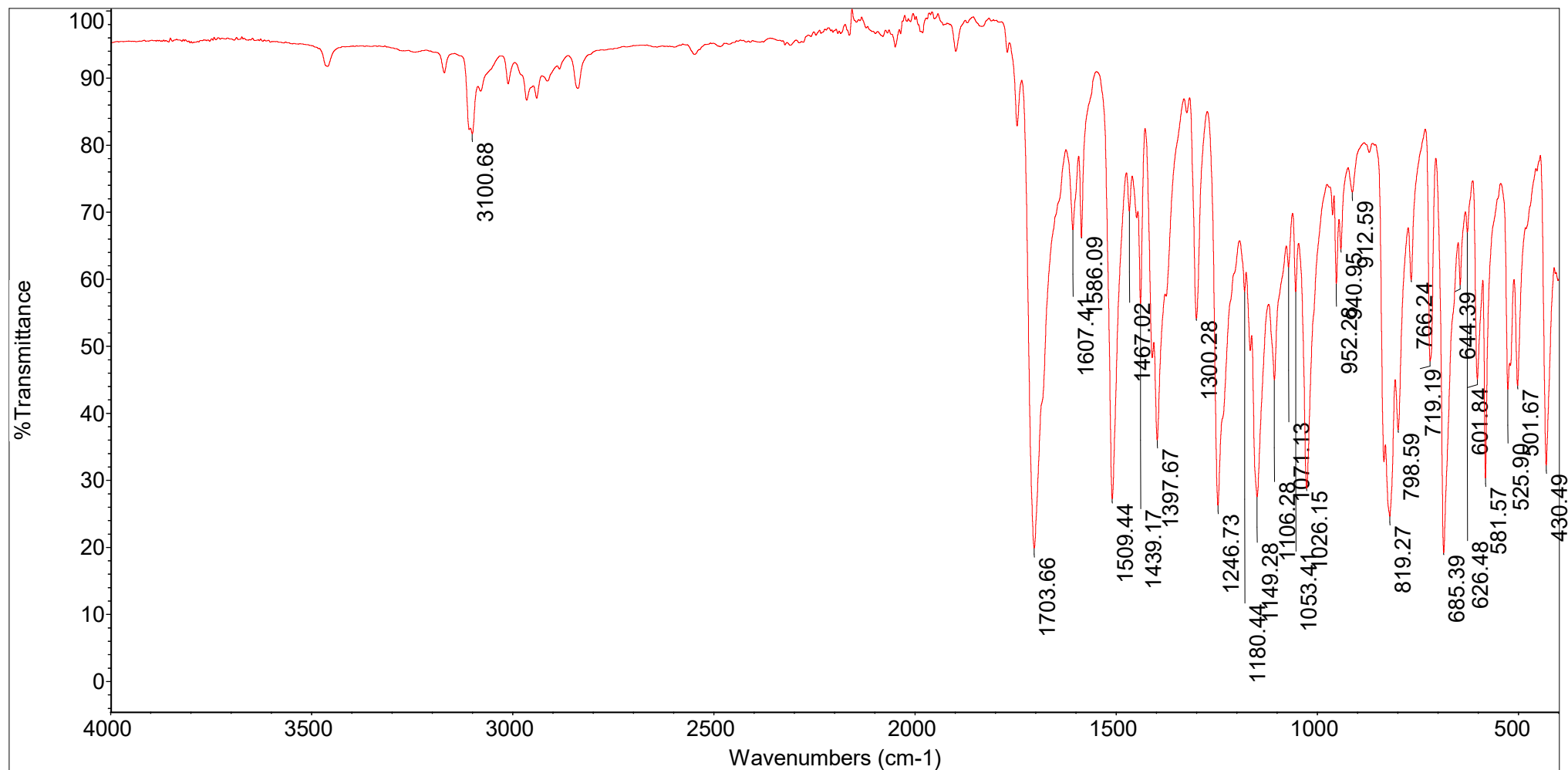
F2 - Acquisition Parameters
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 Time_ 22.40 h
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 PROBHD Z175272_0008 (
 PULPROG zgpg30
 TD 92160
 SOLVENT CDC13
 NS 3200
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.516700 Hz
 AQ 1.9353600 sec
 RG 101
 DW 21.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6278593 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 58.38199997 W
 SFO2 400.1516006 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 19.63299942 W
 PLW12 0.24237999 W
 PLW13 0.12192000 W

F2 - Processing parameters
 SI 32768
 SF 100.6177859 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Name OMe Maleimide (2d)	Transfer	Rack Pos.	Instrument	Instrument 1	Operator
Inj. Vol. (ul)	10	Plate Pos.	IRM Status	Success	
Data File	OMe Mal 0 10 mM.d	Method (Acq)	Degredation Method.m	Comment	Acq. Time (Local)
					2022-08-08 12:38:29 PM (UTC+11:00)

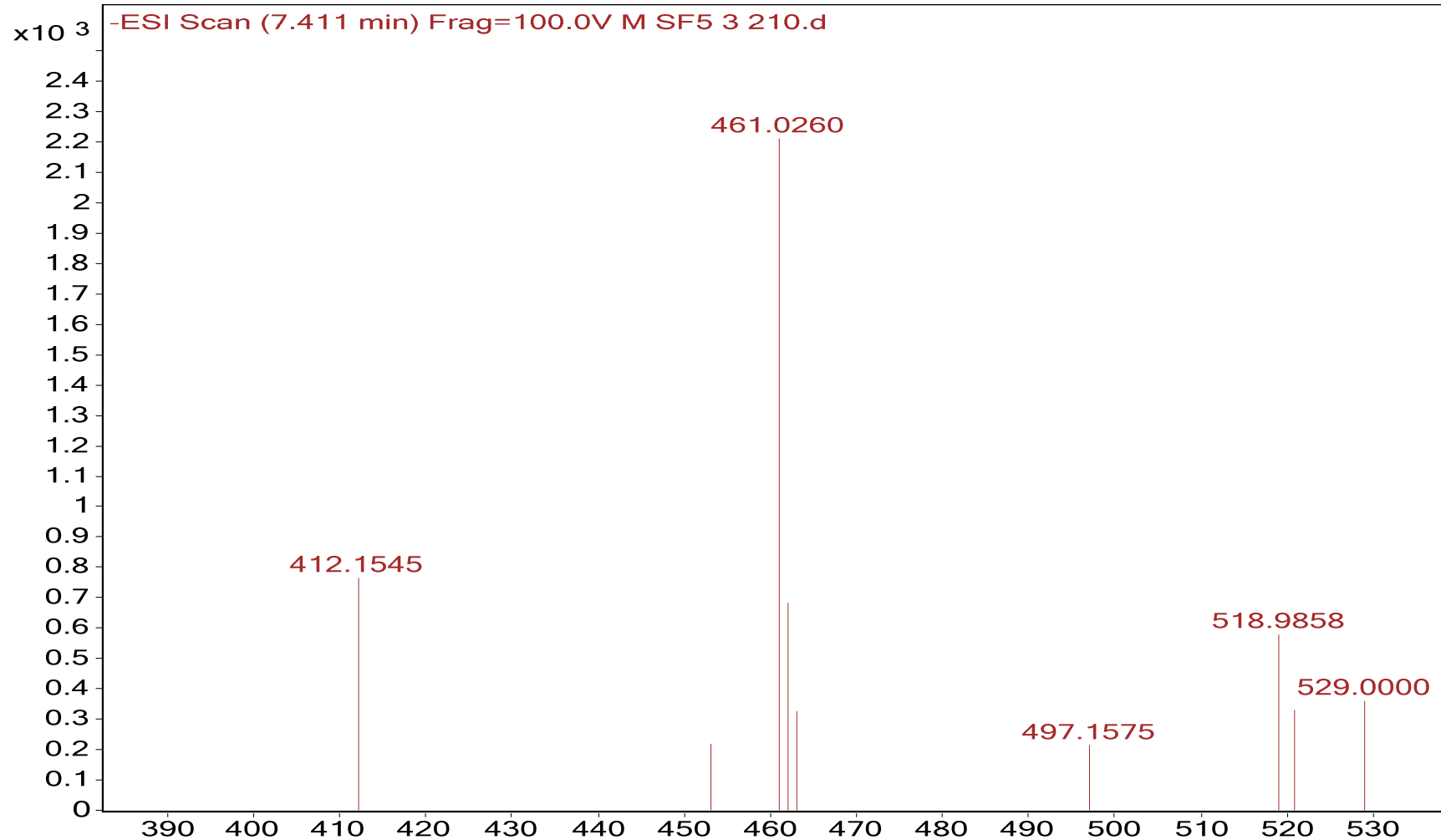




Sample Name SF5 Thio-succinimide (3a) Position
Inj Vol InjPosition
Data Filename ACQ Method

Instrument Name
SampleType
Comment

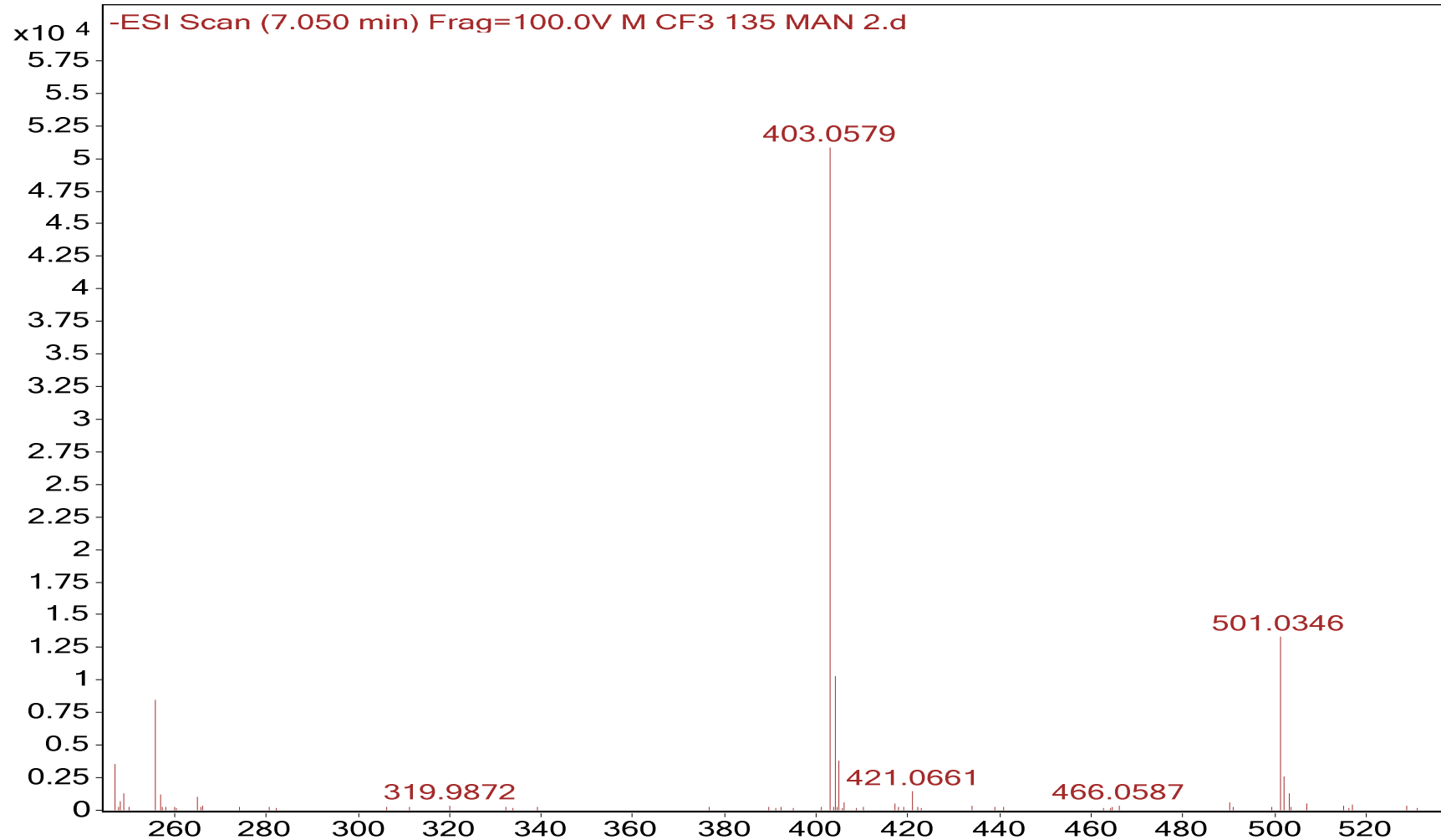
User Name
IRM Calibration Status
Acquired Time



Sample Name: CF3 Thio-succinimide (3b) Position
Inj Vol InjPosition
Data Filename ACQ Method

Instrument Name
SampleType
Comment

User Name
IRM Calibration Status
Acquired Time



Sample Name: H Thio-succinimide (3c)

Position

Instrument Name

User Name

Inj Vol

InjPosition

SampleType

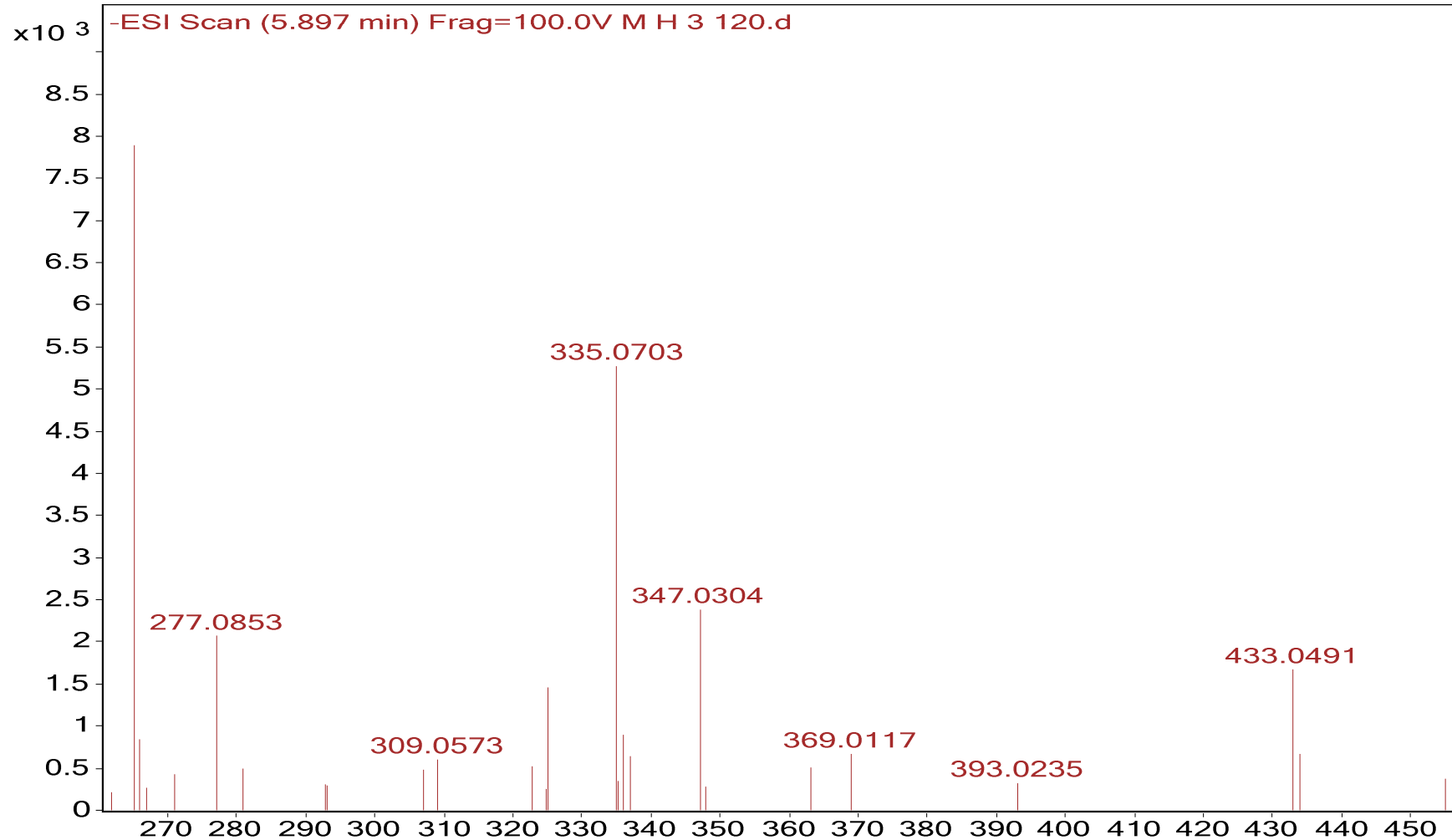
IRM Calibration Status

Data Filename

ACQ Method

Comment

Acquired Time



Sample Name: OMe Thio-succinimide (3d)

Instrument Name

User Name

Inj Vol

InjPosition

SampleType

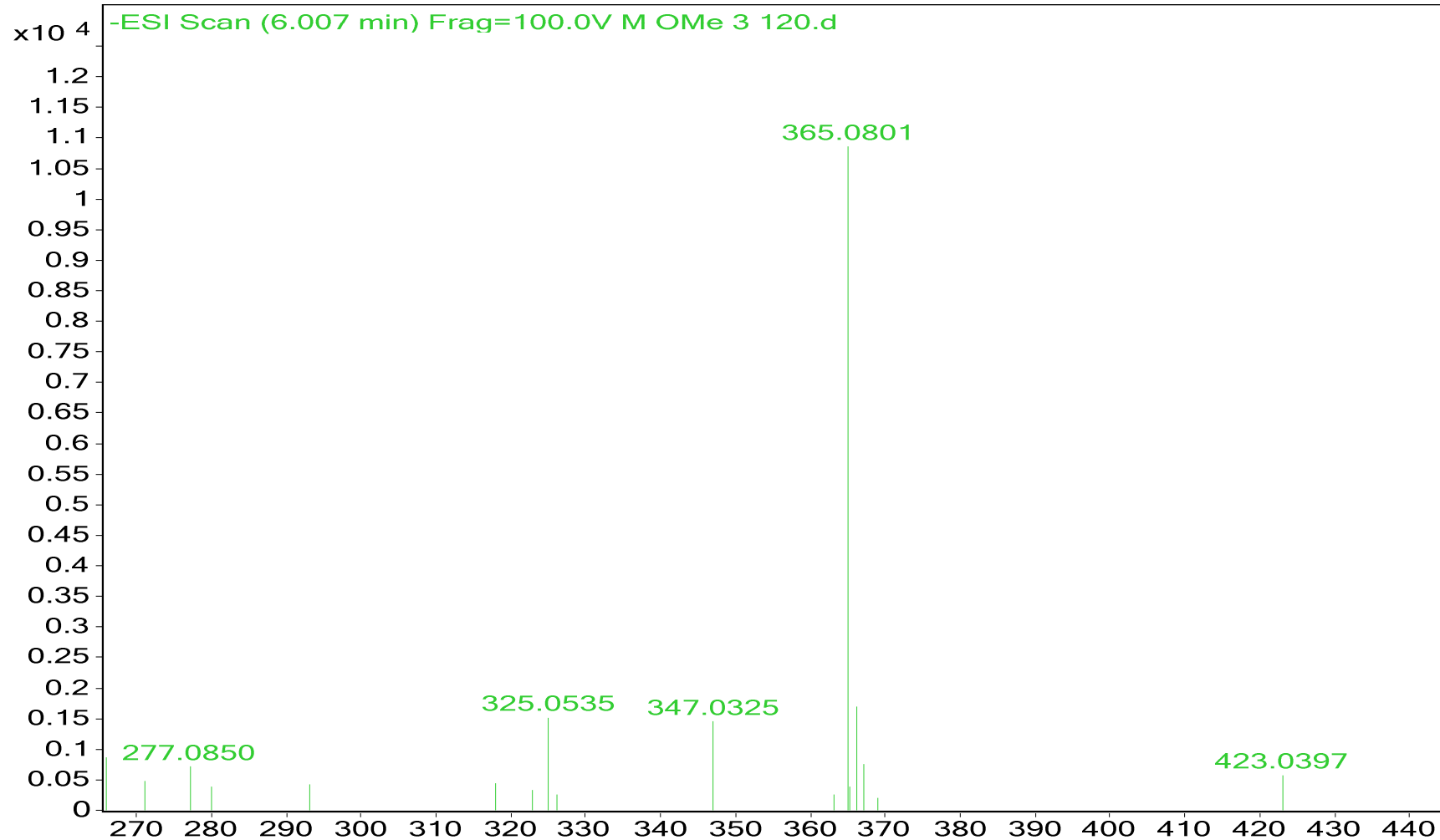
IRM Calibration Status

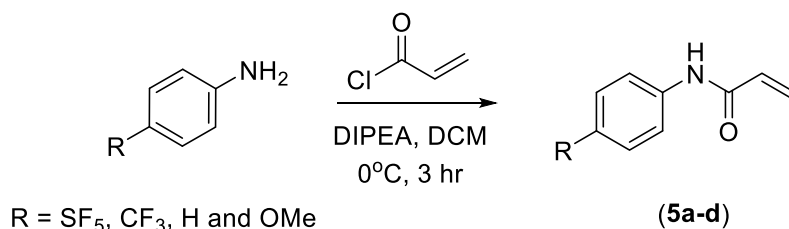
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ACQ Method

Comment

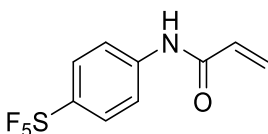
Acquired Time





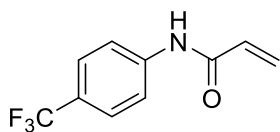
General procedure for the synthesis of **(5a-d)** adapted from the work of Watt *et al.* [25]: A solution of prop-2-enoyl chloride (523 μ L, 3 mmol, 1.5 equiv) and DIPEA (523 μ L, 3 mmol) in DCM (10 mL) was cooled over an ice bath to 0°C. A solution of aniline (2 mmol) in DCM (10 mL) was then added dropwise. The reaction was allowed to proceed for 3 hr. After confirmation by TLC the reaction mixture was then quenched with water (20 mL). The aqueous layer was extracted with DCM (2 \times 20 mL), the combined organics washed with 1 M HCl (20 mL), saturated NaHCO₃ (20 mL), brine (20 mL), dried over MgSO₄ and evaporated to dryness to afford the final product.

N-[4-(pentafluorosulfanyl)phenyl]-2-propenamide (**5a**)



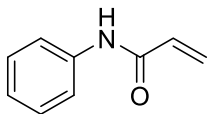
Compound **5a** was obtained as a white solid (377 mg, 1.38 mmol, 69%). Melting point: 111°C. **HRMS (EI)** Calcd for C₉H₇F₅NOS [M-H]⁻ 272.0168, [M-H]⁻ Found 272.0166; **IR (KBr)**: 2922 (w), 1670 (m), 1637 (w), 1513 (m), 1406 (m), 1320 (w), 1193 (m), 1102 (w), 970 (w), 810 (s, br) cm⁻¹; **¹H-NMR (CDCl₃)**: δ 7.73-7.70 (m, 4H), 6.47 (dd, J = 1, 16.8 Hz, 1H), 6.27 (dd, J = 10.2, 16.8 Hz, 1H), 5.83 (dd, J = 1, 8 Hz, 1H); **¹³C-NMR (CDCl₃)**: δ 163.91, 149.53 (quin, J = 18 Hz), 140.53, 130.65, 129.28, 127.20 (quin, J = 4 Hz), 119.35; **¹⁹F-NMR (CDCl₃)**: δ 84.96 (m, 1F), 63.41 (d, J = 150 Hz, 4F).

N-[4-(trifluoromethyl)phenyl]-2-propenamide (**5b**)



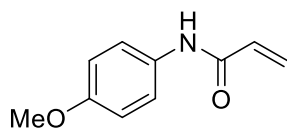
Compound **5b** was obtained as a white solid (314 mg, 1.46 mmol, 73%). Melting point: 126°C. **HRMS (EI)** Calcd for C₁₀H₇F₃NO [M-H]⁻ 214.0479, [M-H]⁻ Found 214.0478; **IR (KBr)**: 2980 (w, br), 1668 (m), 1606 (s), 1544 (m), 1415 (m), 1320 (s), 1255 (m), 1202 (m), 1066 (m), 838 (s) cm⁻¹; **¹H-NMR (CDCl₃)**: δ 7.71 (d, J = 8.4, 2H), 7.59 (d, J = 8.6, 2H), 6.47 (d, J = 16.8 Hz, 1H), 6.26 (dd, J = 10.2, 16.8 Hz, 1H), 5.83 (d, J = 10.2, 1H); **¹³C-NMR (CDCl₃)**: δ 163.83, 140.91, 130.81, 128.97, 126.16 (q, J = 5 Hz), 125.51, 122.81, 119.58; **¹⁹F-NMR (CDCl₃)**: δ -62.13 (s, 3F).

N-phenyl-2-propenamide (**5c**)



Compound **5c** was obtained as a bright yellow solid (253 mg, 1.72 mmol, 86%). Melting point: 102°C (Lit. 104-106°C [30]). **HRMS (EI)** Calcd for C₉H₈NO [M-H]⁻ 146.0605, [M-H]⁻ Found 146.0606; **IR (KBr)**: 3142 (w), 3094 (w), 1664 (s), 1635 (s), 1603 (s), 1548 (s), 1494 (s), 1441 (s), 1406 (s), 1330 (m), 1251 (m), 1200 (w), 939 (w), 750 (s), 686 (s) cm⁻¹; **¹H-NMR (CDCl₃)**: δ 7.58 (d, J = 7.8 Hz, 2H), 7.32 (t, J = 7.8 Hz, 2H), 7.12 (t, J = 7.4 Hz, 1H), 6.42 (d, J = 16.8, 1H), 6.27 (dd, J = 10.2, 16.8 Hz, 1H), 5.74 (d, J = 10.2 Hz, 1H); **¹³C-NMR (CDCl₃)**: δ 163.76, 137.88, 131.34, 129.15, 127.88, 124.65, 120.15.

N-[4-(methoxy)phenyl]-2-propenamide (**5d**)



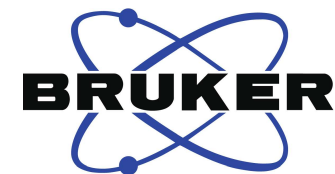
Compound **5d** was obtained as a bright yellow solid (286 mg, 1.62 mmol, 81%). Melting point 95°C (Lit. 97-98°C [30]), **HRMS (EI)** Calcd for C₁₀H₁₀NO₂ [M-H]⁻ 176.0711, [M-H]⁻ Found 176.0709; **IR (KBr)**: 3296 (w), 3007 (w), 1659 (s), 1612 (m), 1538 (m), 1508 (s), 1455 (w), 1412 (m), 1302 (w), 1239 (s), 1171 (m), 1149 (w), 1030 (m), 938 (m), 705 (m, br) cm⁻¹; **¹H-NMR (CDCl₃)**: δ 7.48 (d, J = 8.8 Hz, 2H), 7.86 (d, J = 9 Hz, 2H), 6.41 (dd, J = 0.88, 16.8 Hz, 1H), 6.22 (dd, J = 10.2, 16.8 Hz, 1H), 5.73 (dd, J = 0.8, 10.2 Hz, 1H), 3.79 (s, 3H); **¹³C-NMR (CDCl₃)**: δ 163.63, 156.70, 131.33, 130.98, 127.50, 121.97, 114.30, 55.60.

References

25. Watt SKI, Charlebois JG, Rowley CN, Keillor JW (2022) A mechanistic study of thiol addition to *N*-phenylacrylamide. *Org Biomol Chem* 20:8898–8906. <https://doi.org/10.1039/d2ob01369j>
30. Eriksson J, Åberg O, Långström B (2007) Synthesis of [¹¹C]/[¹³C]acrylamides by palladium-mediated carbonylation. *European J Org Chem* 2007:455–461. <https://doi.org/10.1002/ejoc.200600700>

SF5 Acrylamide (5a)

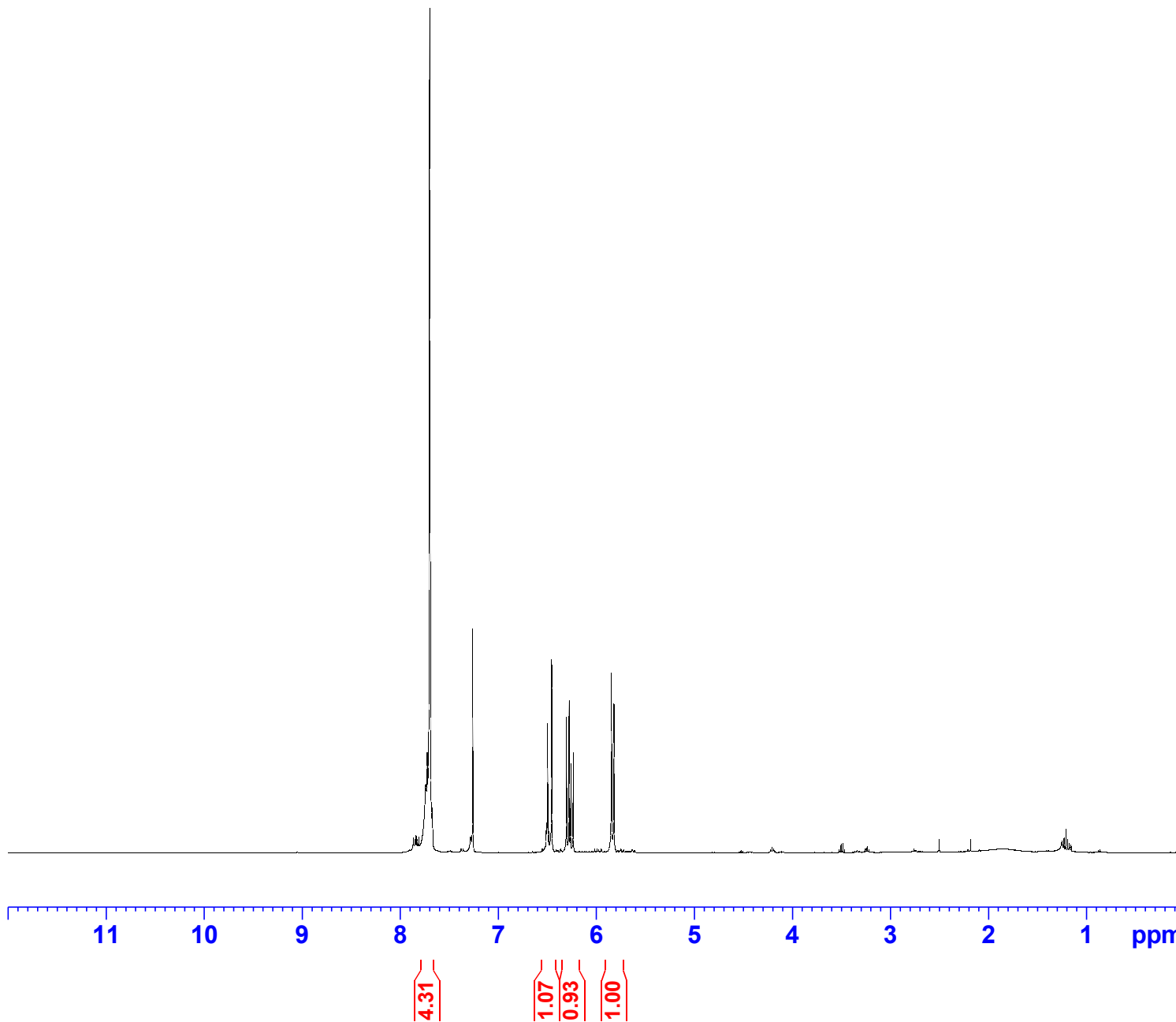
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6.235
5.847
5.844
5.821
5.819



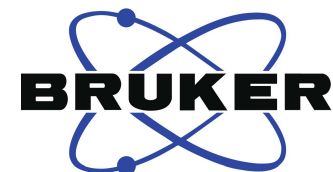
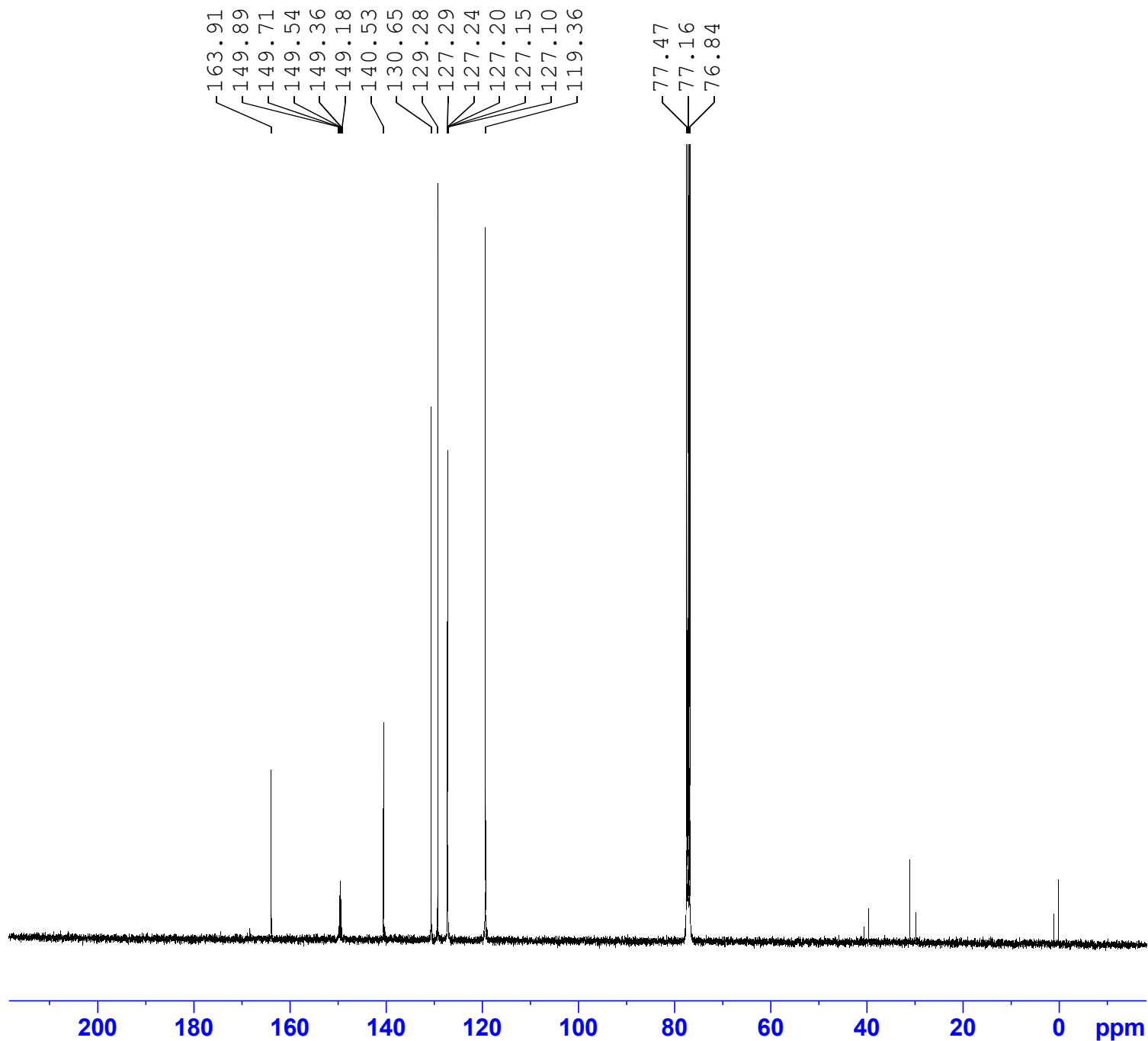
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EXPNO 12
PROCNO 1

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TD 131072
SOLVENT CDC13
NS 32
DS 2
SWH 8196.722 Hz
FIDRES 0.125072 Hz
AQ 7.9953918 sec
RG 101
DW 61.000 usec
DE 13.54 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1524709 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 19.63299942 W

F2 - Processing parameters
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SF5 acrylamide (5a)

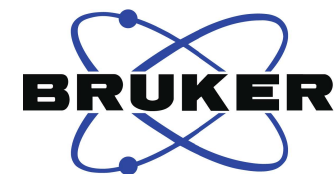
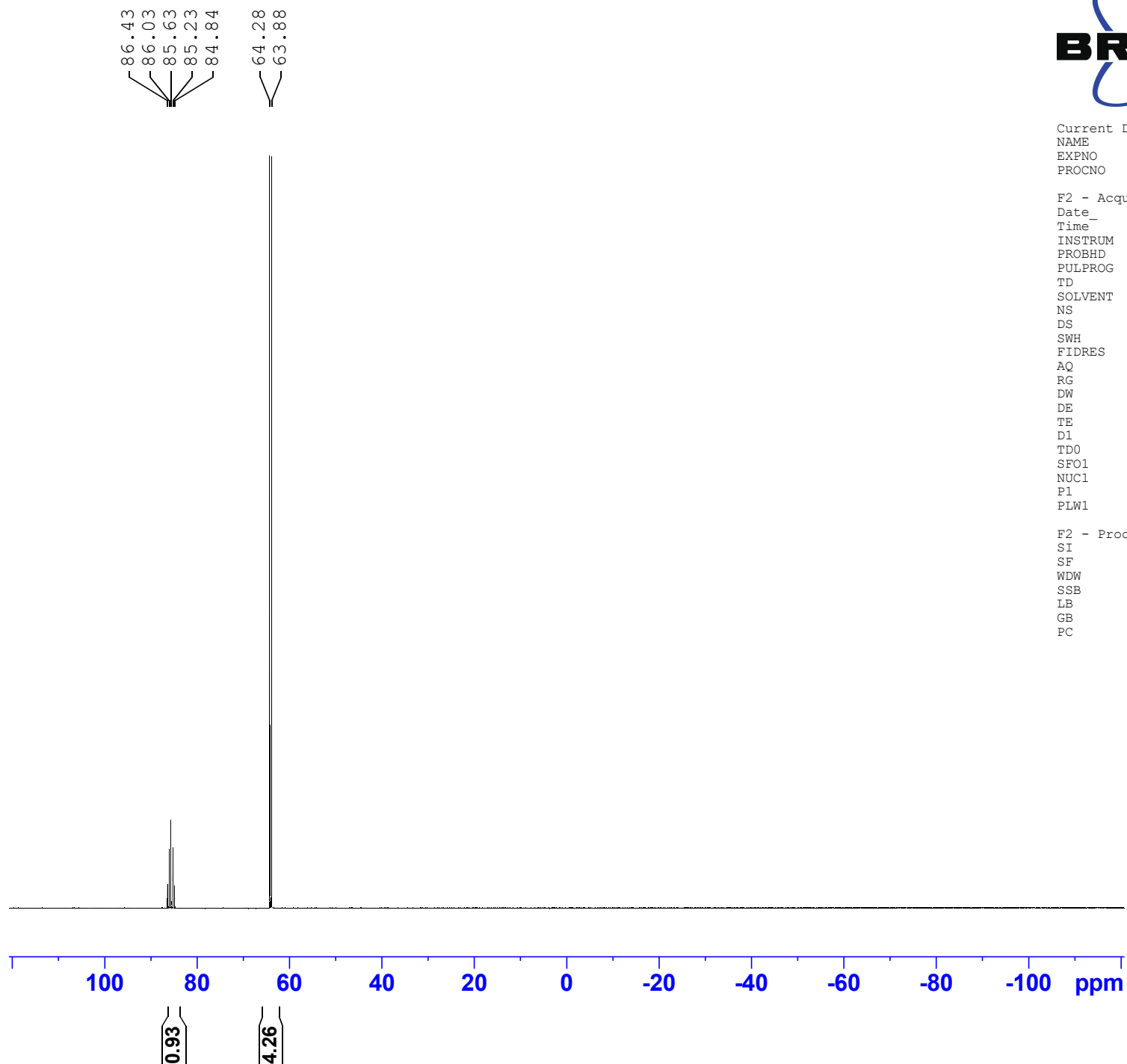


Current Data Parameters
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 EXPNO 11
 PROCNO 1

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 Date_ 20220322
 Time_ 1.14 h
 INSTRUM AVNEO
 PROBHD Z175272_0008 (
 PULPROG zgpg30
 TD 131072
 SOLVENT CDCl3
 NS 4600
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.363304 Hz
 AQ 2.7525120 sec
 RG 101
 DW 21.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SF01 100.6278593 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 58.38199997 W
 SF02 400.1516006 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 19.63299942 W
 PLW12 0.24237999 W
 PLW13 0.12192000 W

F2 - Processing parameters
 SI 32768
 SF 100.6177843 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

SF5 acrylamide (**5a**)



Current Data Parameters
 NAME SF5 Acrylamide 19F - Clean
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220321
 Time_ 17.26 h
 INSTRUM AVNEO
 PROBHD Z175272_0008 (
 PULPROG zg
 TD 131072
 SOLVENT CDCl3
 NS 64
 DS 4
 SWH 147058.828 Hz
 FIDRES 2.243940 Hz
 AQ 0.4456448 sec
 RG 101
 DW 3.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 376.5171850 MHz
 NUC1 19F
 P1 12.00 usec
 PLW1 45.00000000 W

F2 - Processing parameters
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 SF 376.5169352 MHz
 WDW EM
 SSB 0
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 PC 1.00

Name SF5 Acrylamide (5a)
Inj. Vol. (ul)
Data File

Rack Pos.
Plate Pos.

Neg Method (rev).m

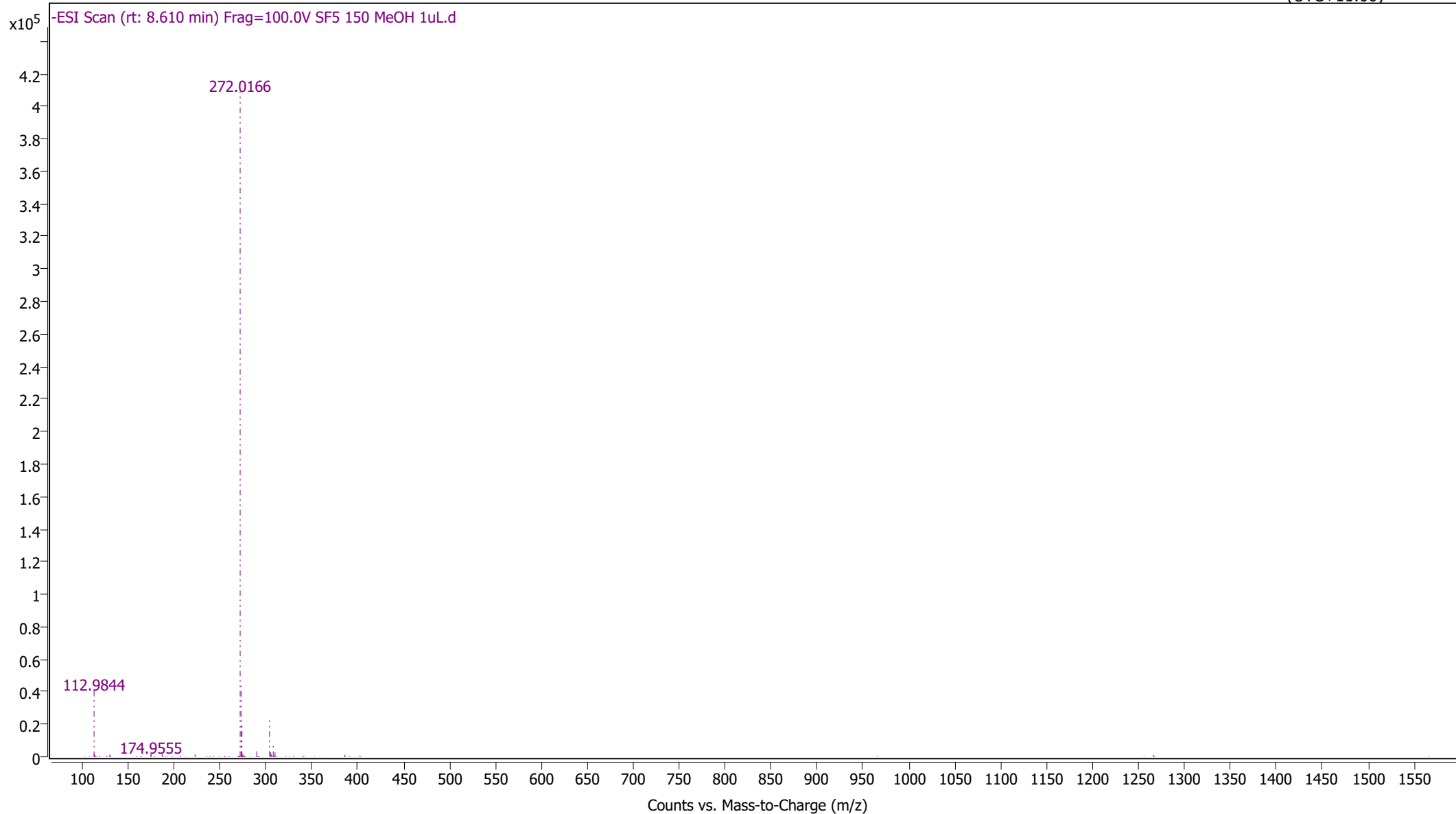
Instrument
IRM Status
Comment

Instrument 1
Success

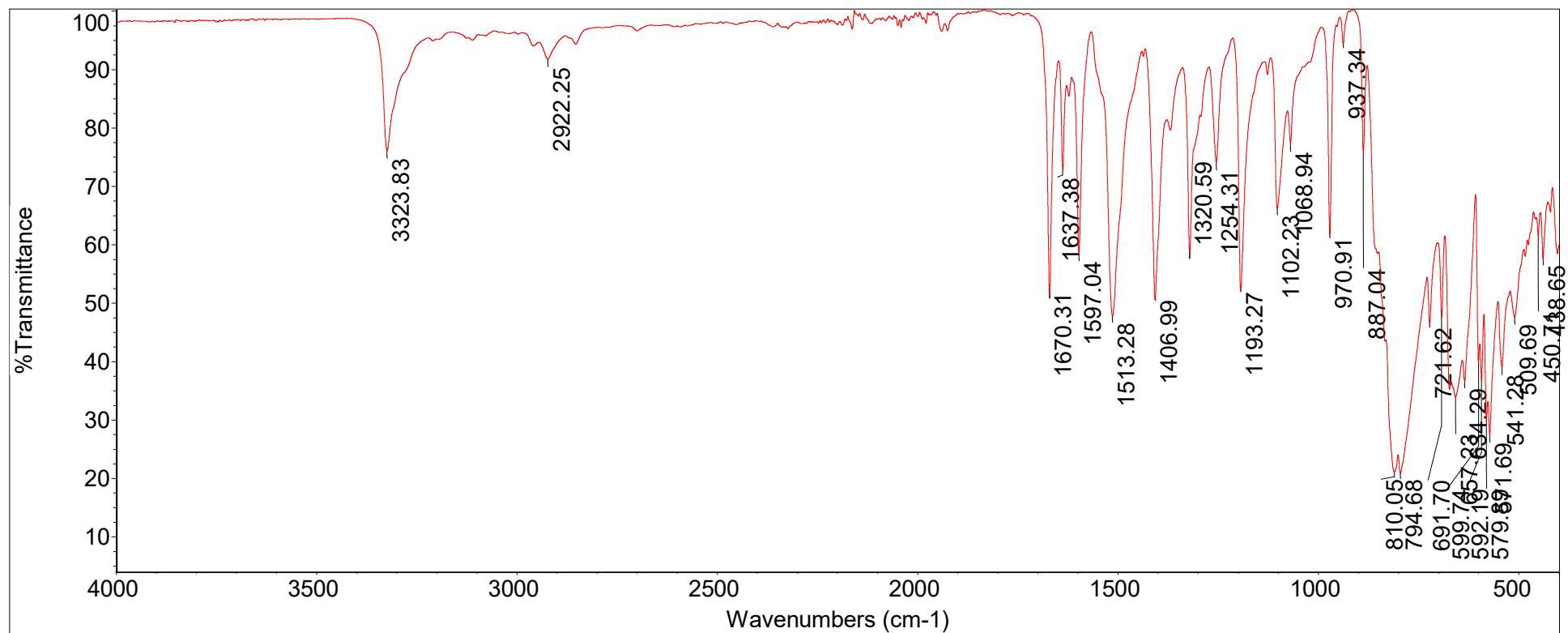
Operator

Acq. Time (Local)

2022-11-30 3:20:55 PM
(UTC+11:00)

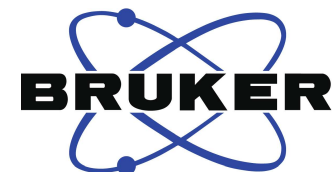


SF5 Acrylamide (5a)



Collection time: Mon Jul 25 11:46:09 2022 (GMT+10)

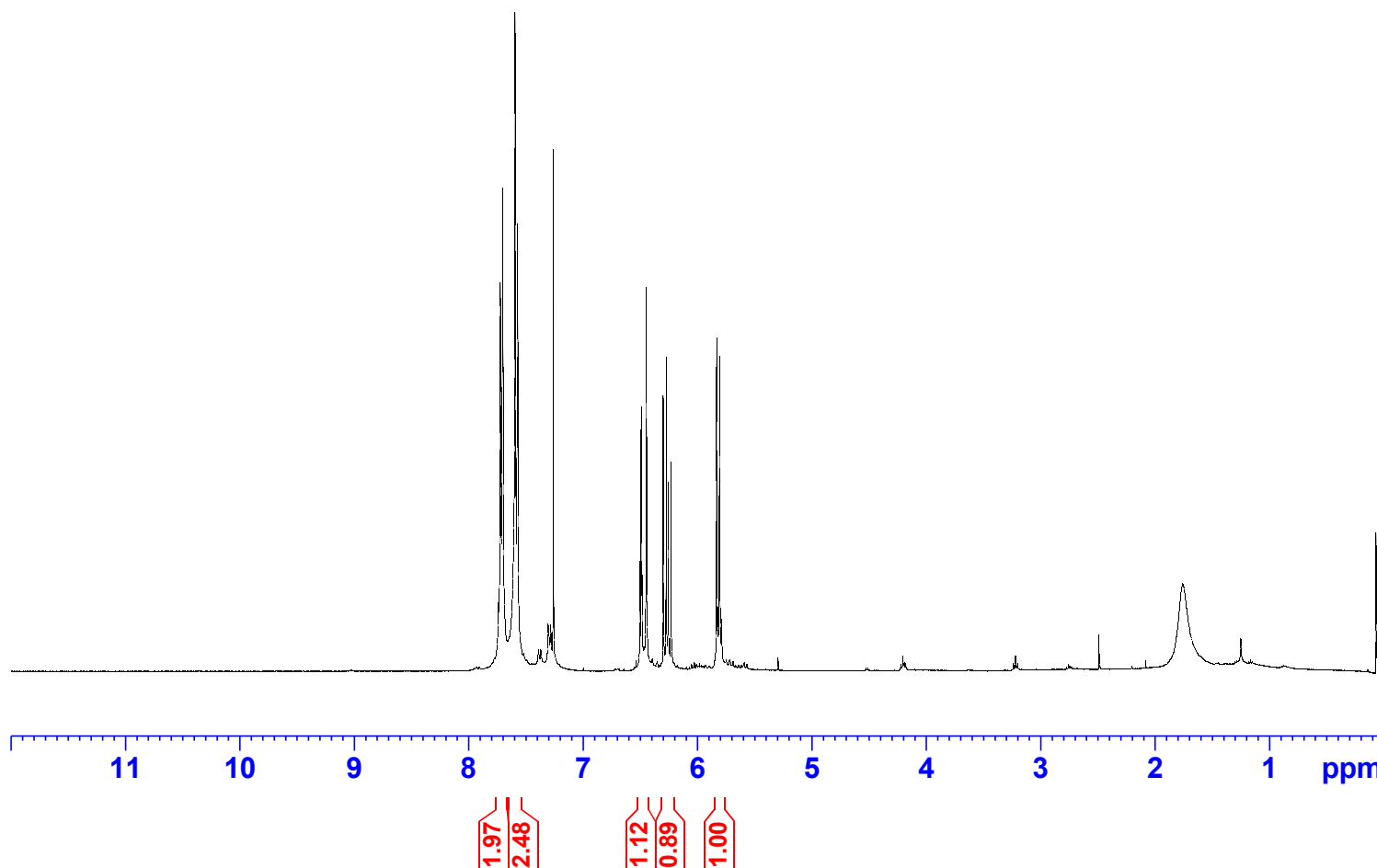
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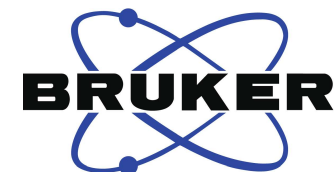
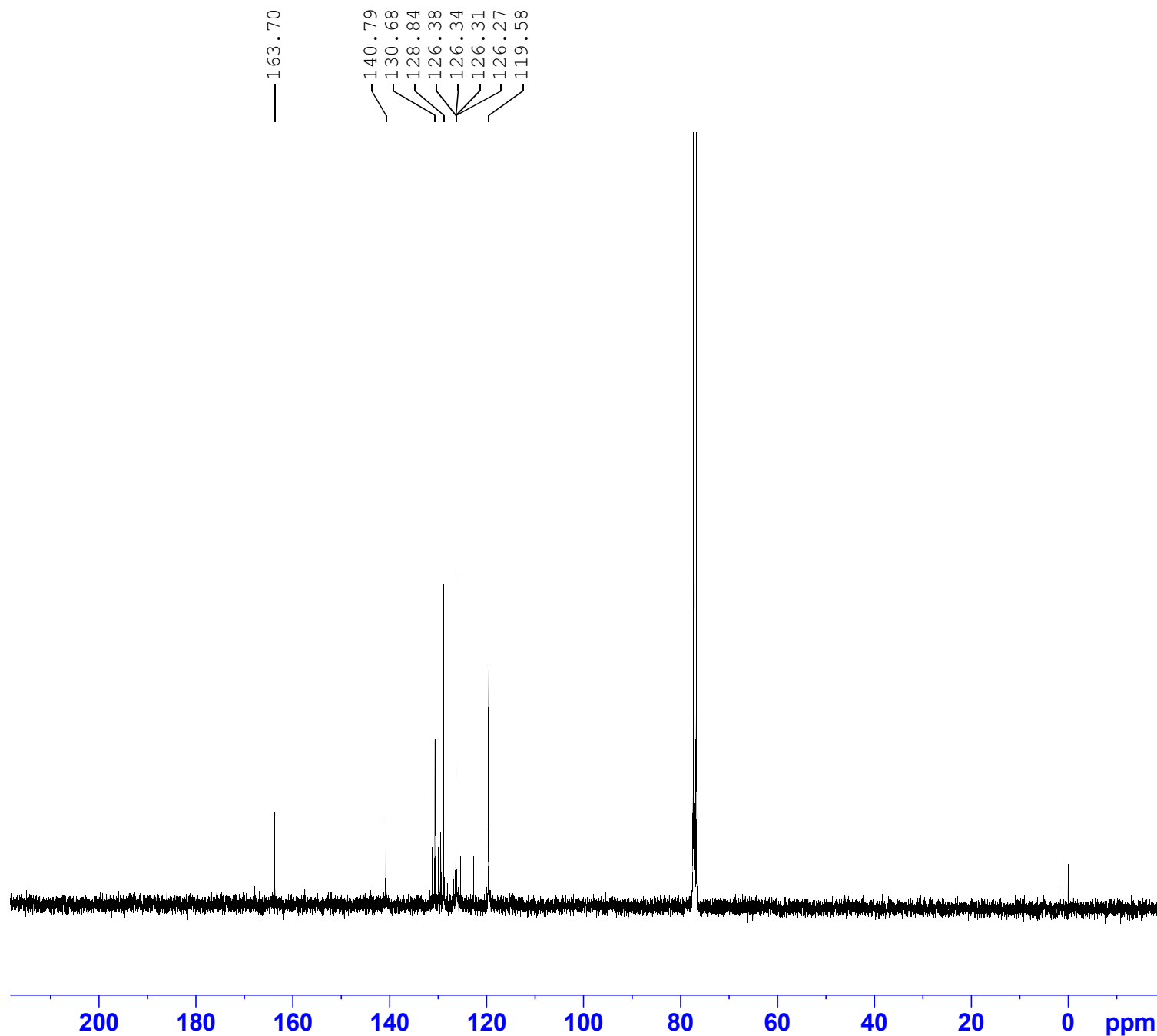
Current Data Parameters
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EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210323
Time_ 16.35 h
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PROBHD Z163739_0206 (
PULPROG zg30
TD 131072
SOLVENT CDC13
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.125072 Hz
AQ 7.9953918 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SF01 400.1524709 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 25.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1500096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



CF3 acrylamide (5b)



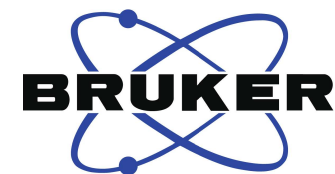
Current Data Parameters
 NAME CF3 Acrylamide 13C - good
 EXPNO 8
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210323
 Time_ 20.54 h
 INSTRUM AVNEO
 PROBHD Z163739_0206 (
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.726609 Hz
 AQ 1.3762560 sec
 RG 101
 DW 21.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SF01 100.6278593 MHz
 NUC1 13C
 P0 2.67 usec
 P1 8.00 usec
 PLW1 93.00000000 W
 SF02 400.1516006 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 25.00000000 W
 PLW12 0.19753000 W
 PLW13 0.09935700 W

F2 - Processing parameters
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 SF 100.6177975 MHz
 WDW EM
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 GB 0
 PC 1.40

CF3 Acrylamide (**5b**)

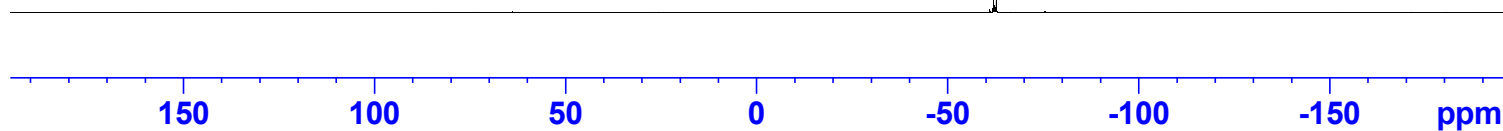
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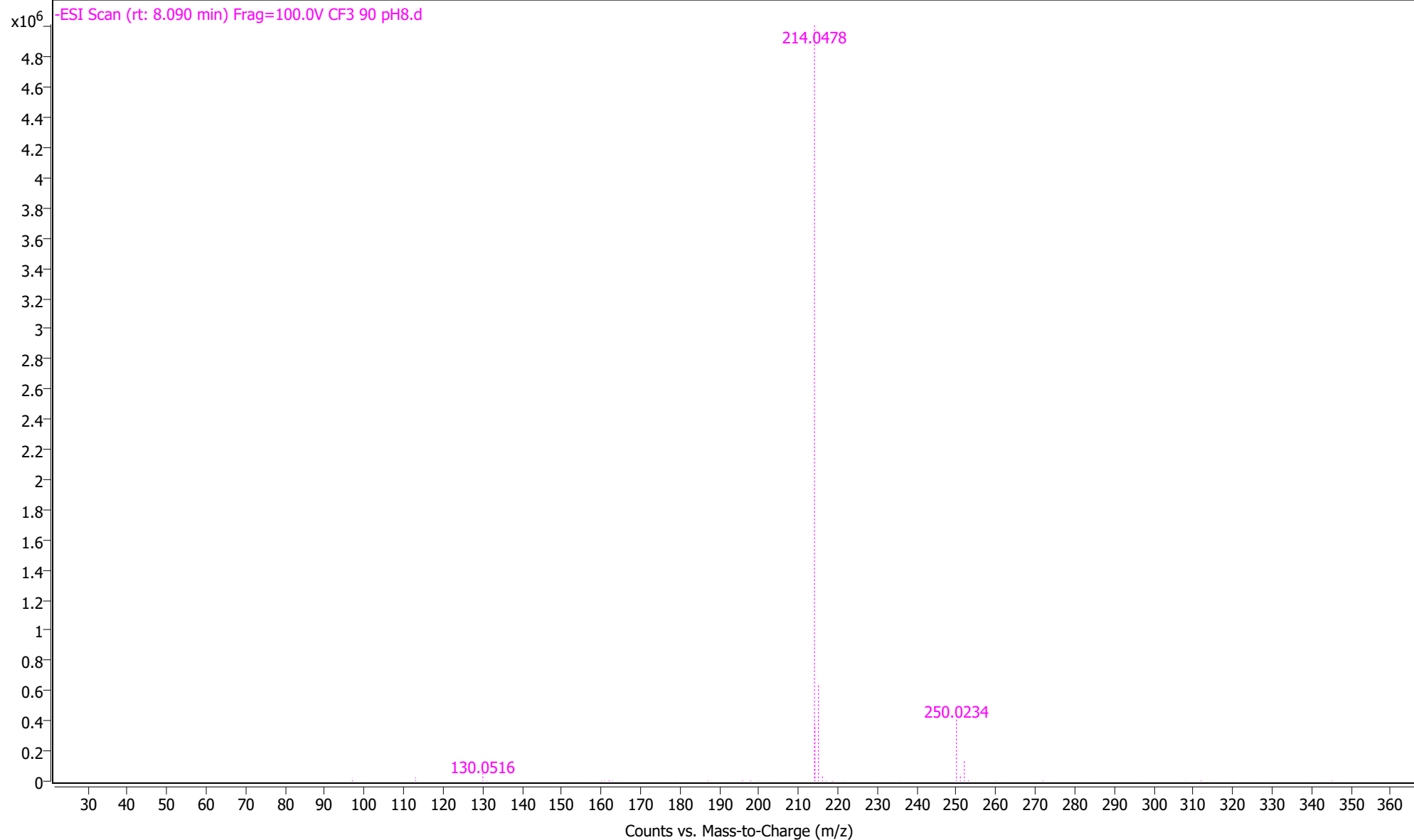
Current Data Parameters
NAME CF3 Acrylamide 19F
EXPNO 9
PROCNO 1

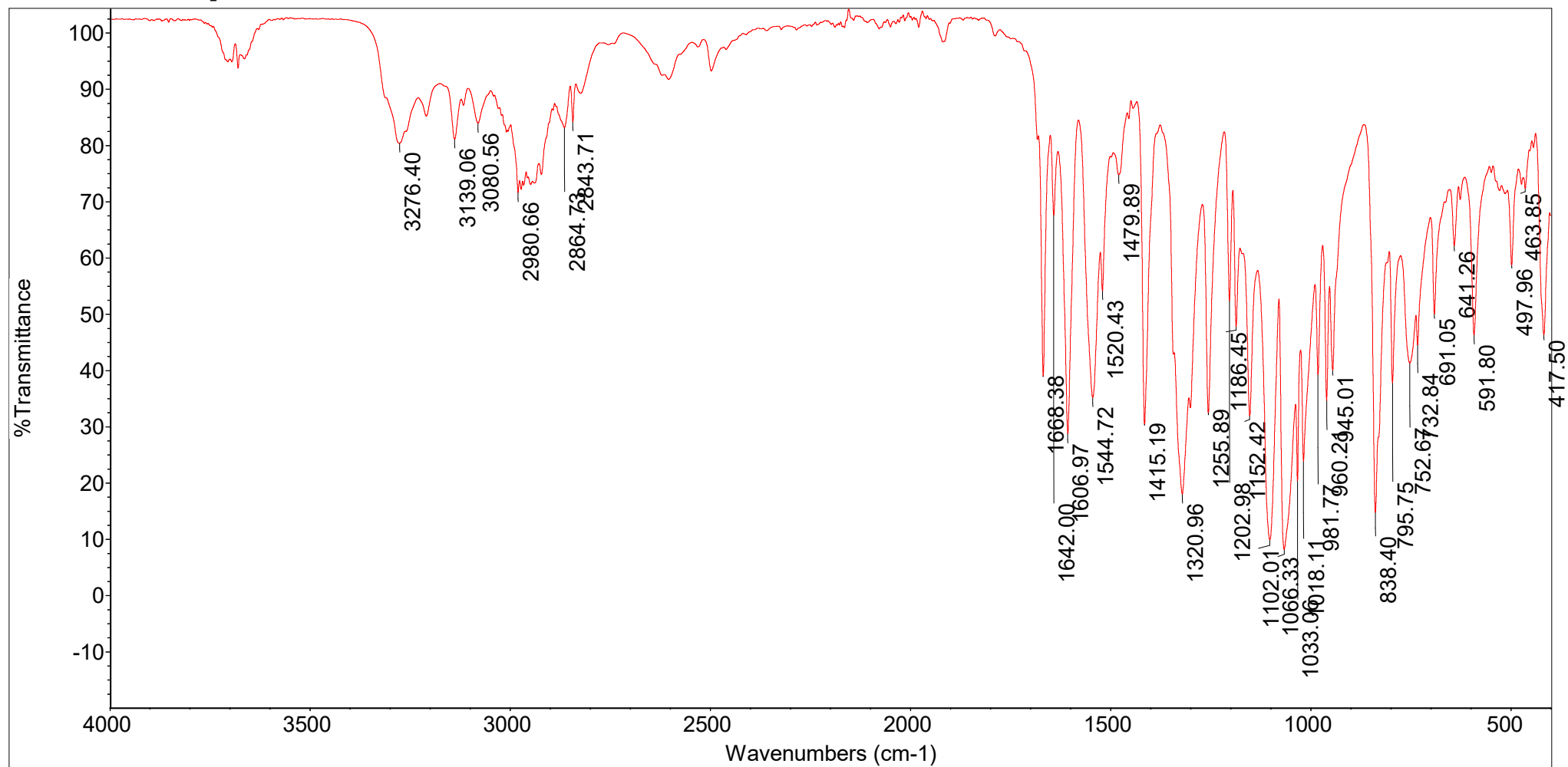
F2 - Acquisition Parameters
Date_ 20220726
Time_ 10.54 h
INSTRUM AVNEO
PROBHD Z175272_0008 (
PULPROG zg
TD 131072
SOLVENT CDC13
NS 128
DS 4
SWH 147058.828 Hz
FIDRES 2.243940 Hz
AQ 0.4456448 sec
RG 101
DW 3.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 376.5171850 MHz
NUC1 19F
P1 12.00 usec
PLW1 45.00000000 W

F2 - Processing parameters
SI 65536
SF 376.5171850 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



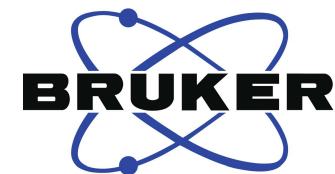
Name CF3 Acrylamide (5b)	Rack Pos.	Instrument	Instrument 1	Operator
Inj. Vol. (ul) 10	Plate Pos.	IRM Status	Success	
Data File CF3 90 pH8.d	Method (Acq)	Neg Method (rev).m	Comment	Acq. Time (Local) 2022-10-11 1:50:20 AM (UTC+11:00)





H acrylamide (5c)

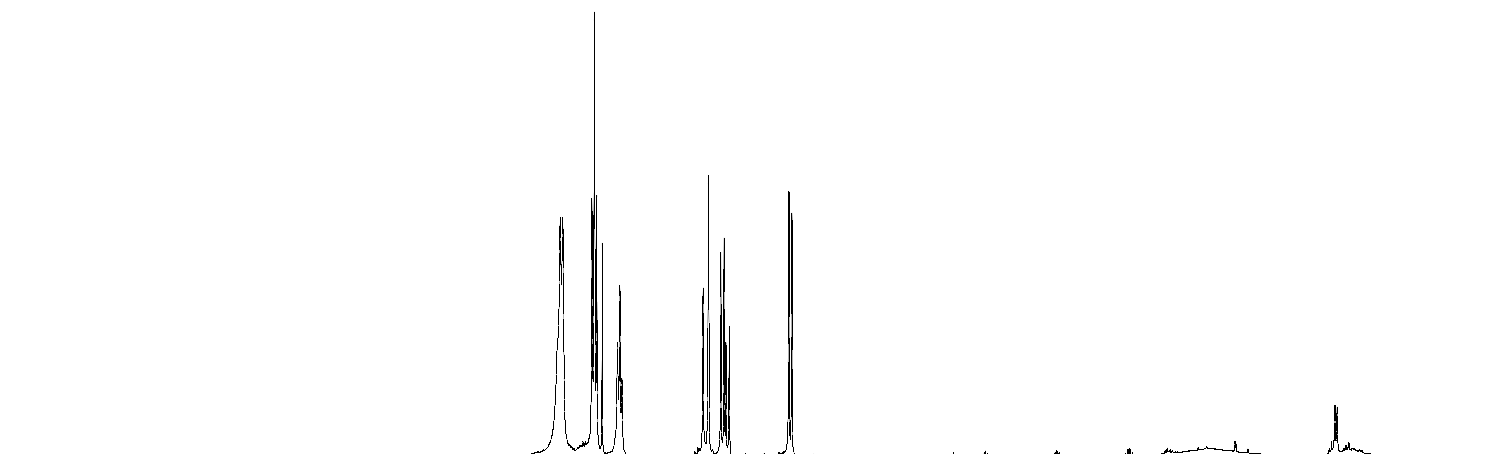
7.597
7.577
7.342
7.322
7.302
7.260
7.137
7.118
7.100
6.446
6.404
6.305
6.280
6.263
6.238
5.761
5.758
5.736
5.733



Current Data Parameters
NAME H Acrylamide 1H- Clean
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210323
Time_ 16.44 h
INSTRUM AVNEO
PROBHD Z163739_0206 (
PULPROG zg30
TD 131072
SOLVENT CDCl3
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.125072 Hz
AQ 7.9953918 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1524709 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 25.00000000 W

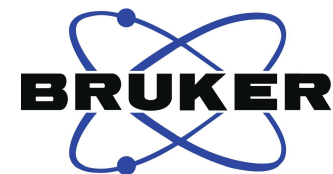
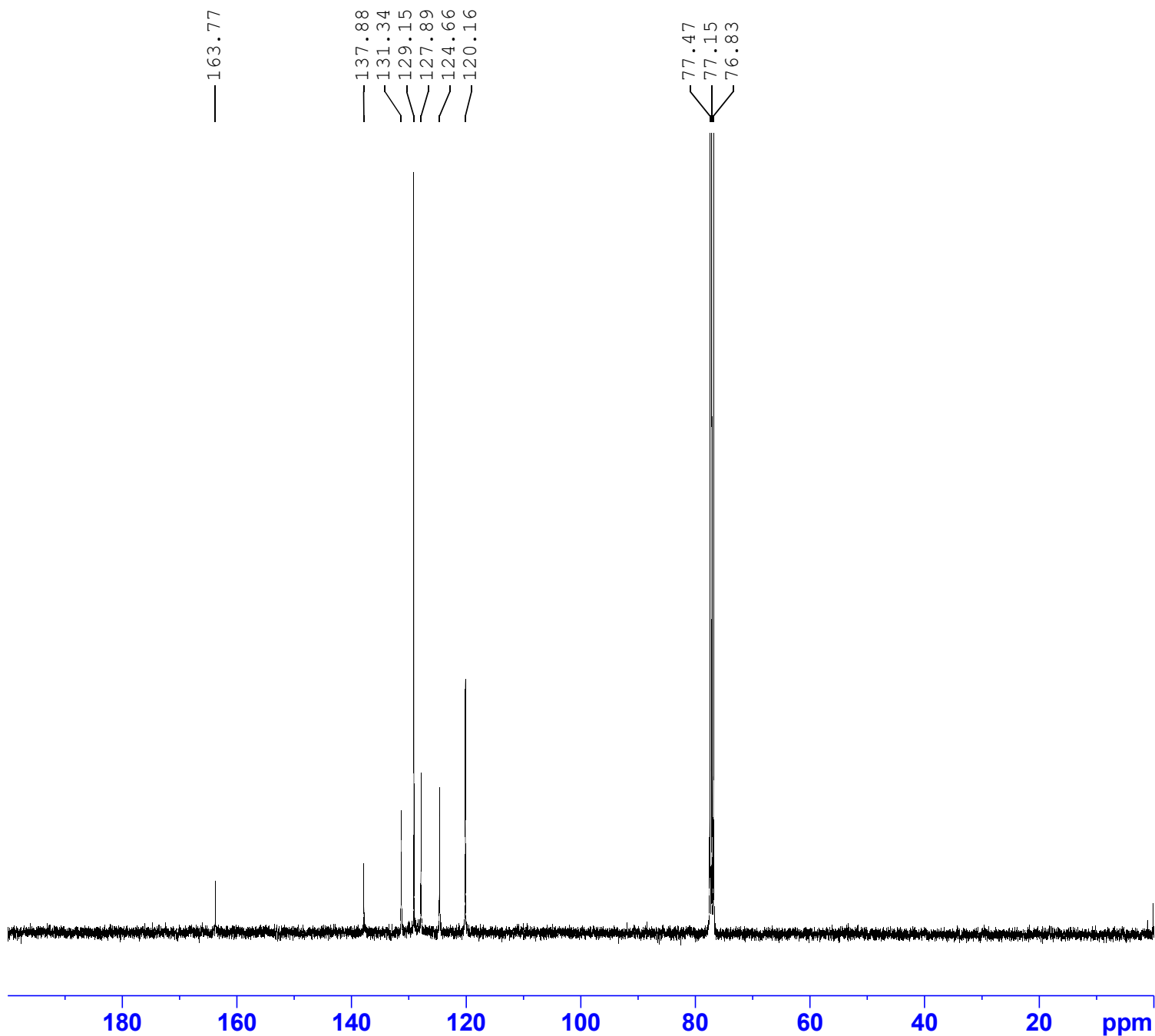
F2 - Processing parameters
SI 65536
SF 400.1500096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



11 10 9 8 7 6 5 4 3 2 1 ppm

2.64
1.60
0.99
0.98
0.91
0.98

H acrylamide (5c)

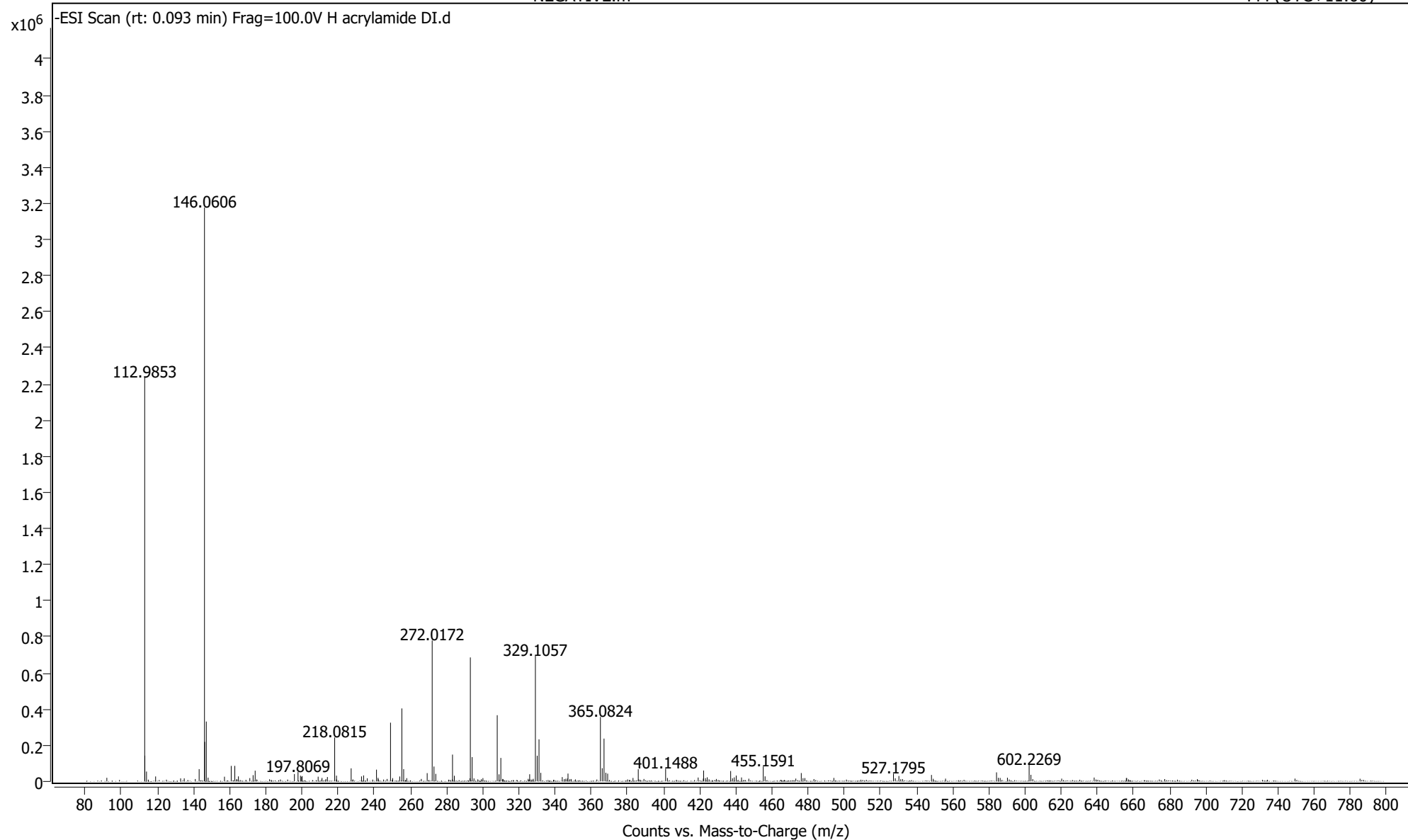


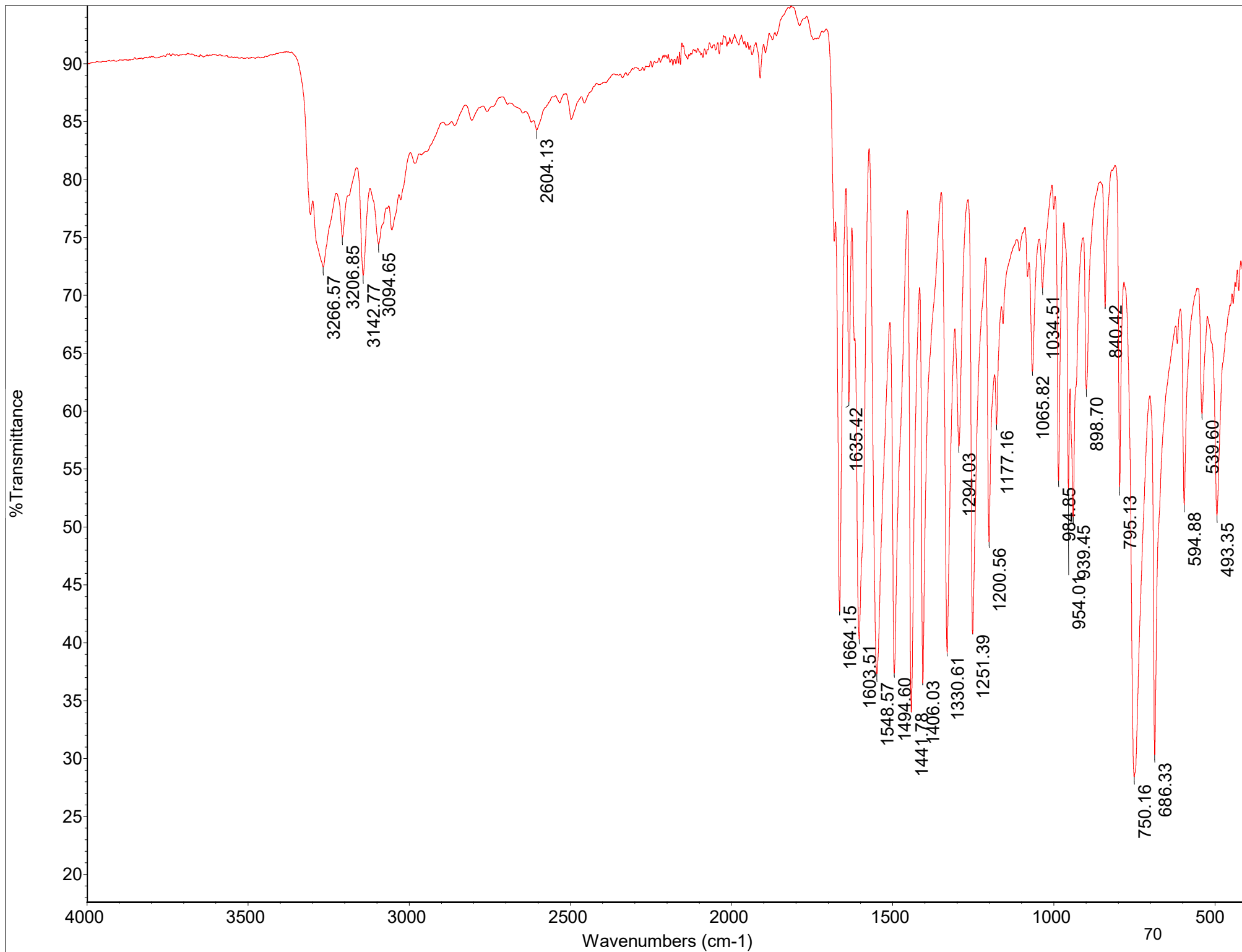
Current Data Parameters
 NAME H Acrylamide 13C - good
 EXPNO 7
 PROCNO 1

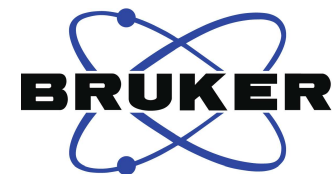
F2 - Acquisition Parameters
 Date 20210323
 Time 19.47 h
 INSTRUM AVNEO
 PROBHD Z163739_0206 (
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.726609 Hz
 AQ 1.3762560 sec
 RG 101
 DW 21.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6278593 MHz
 NUC1 13C
 P0 2.67 usec
 P1 8.00 usec
 PLW1 93.00000000 W
 SFO2 400.1516006 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 25.00000000 W
 PLW12 0.19753000 W
 PLW13 0.09935700 W

F2 - Processing parameters
 SI 32768
 SF 100.6177867 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Name	H Acrylamide (5c)	Rack Pos.	Instrument	Instrument 1	Operator
Inj. Vol. (ul)	5	Plate Pos.	IRM Status	Some ions missed	
Data File	H acrylamide DI.d	Method (Acq)	Hugh Method direct inj	Comment	Acq. Time (Local)
			NEGATIVE.m		2023-01-04 12:42:14 PM (UTC+11:00)



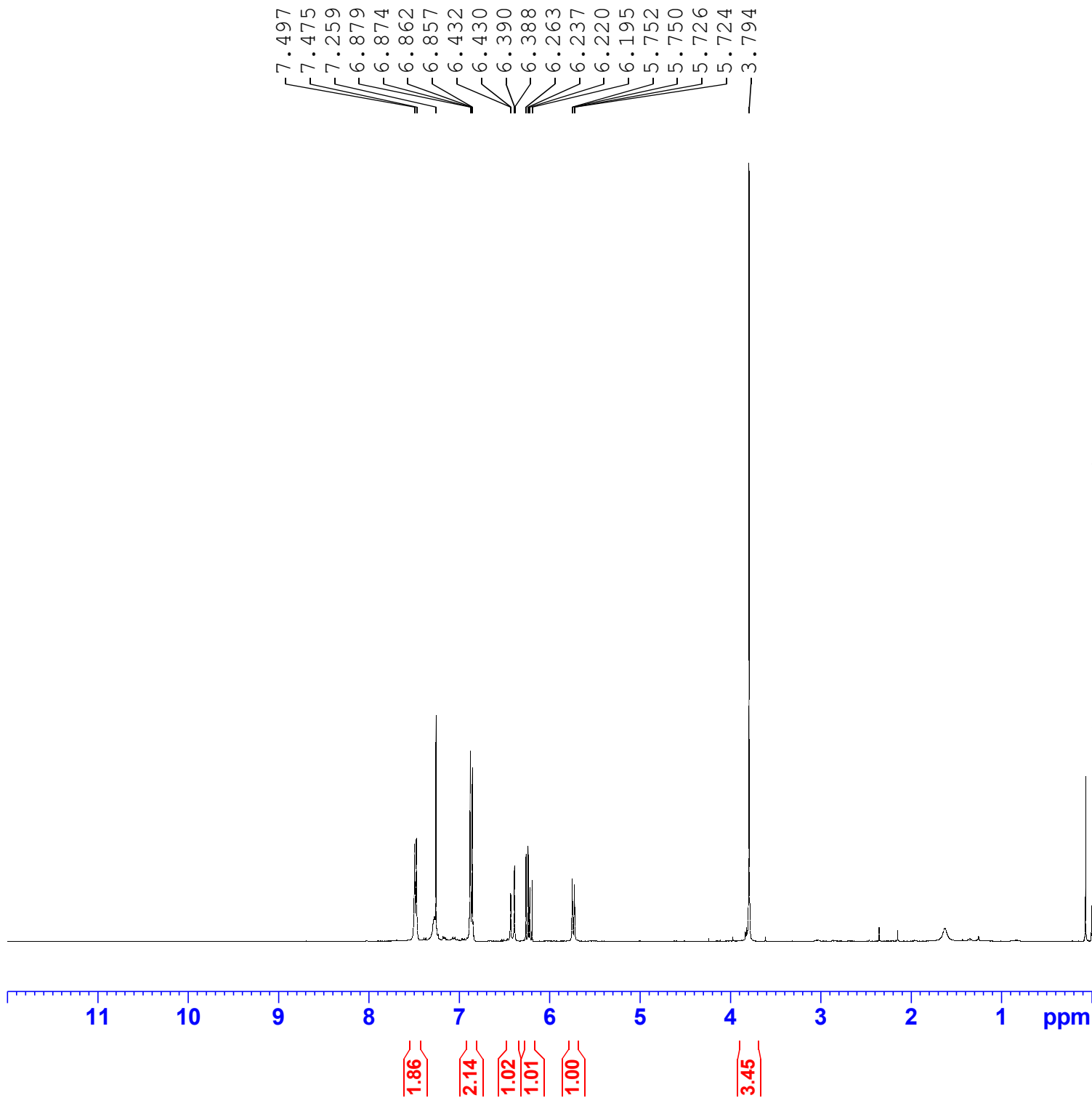




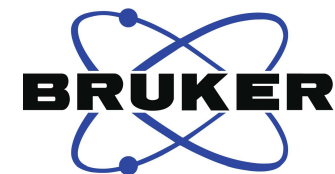
Current Data Parameters
NAME ome acrylamide 1H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220728
Time_ 18.13 h
INSTRUM AVNEO
PROBHD Z175272_0008 (
PULPROG zg30
TD 131072
SOLVENT CDC13
NS 32
DS 2
SWH 8196.722 Hz
FIDRES 0.125072 Hz
AQ 7.9953918 sec
RG 101
DW 61.000 usec
DE 13.54 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1524709 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 19.63299942 W

F2 - Processing parameters
SI 65536
SF 400.1500105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



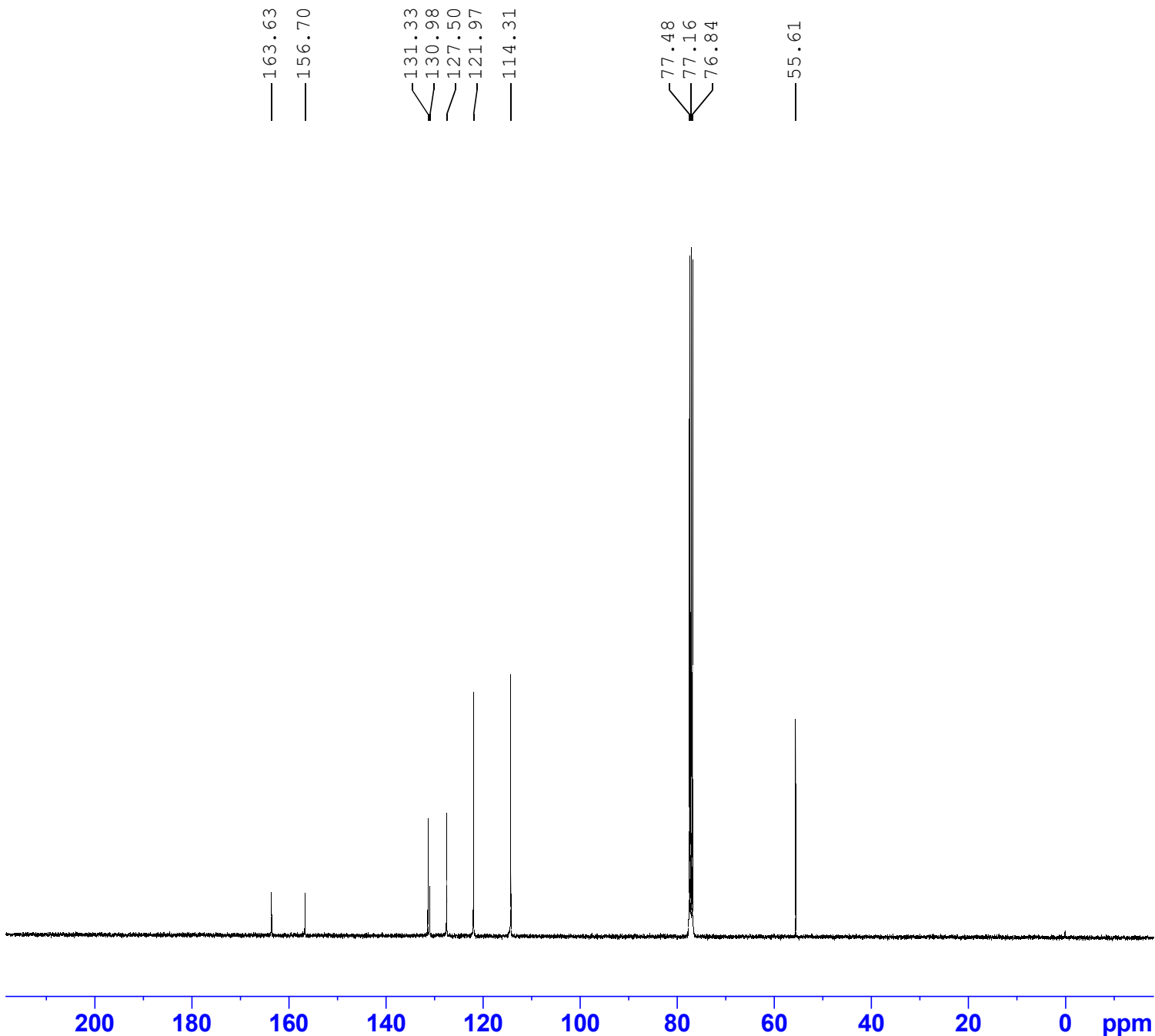
OMe Acrylamide (5d)



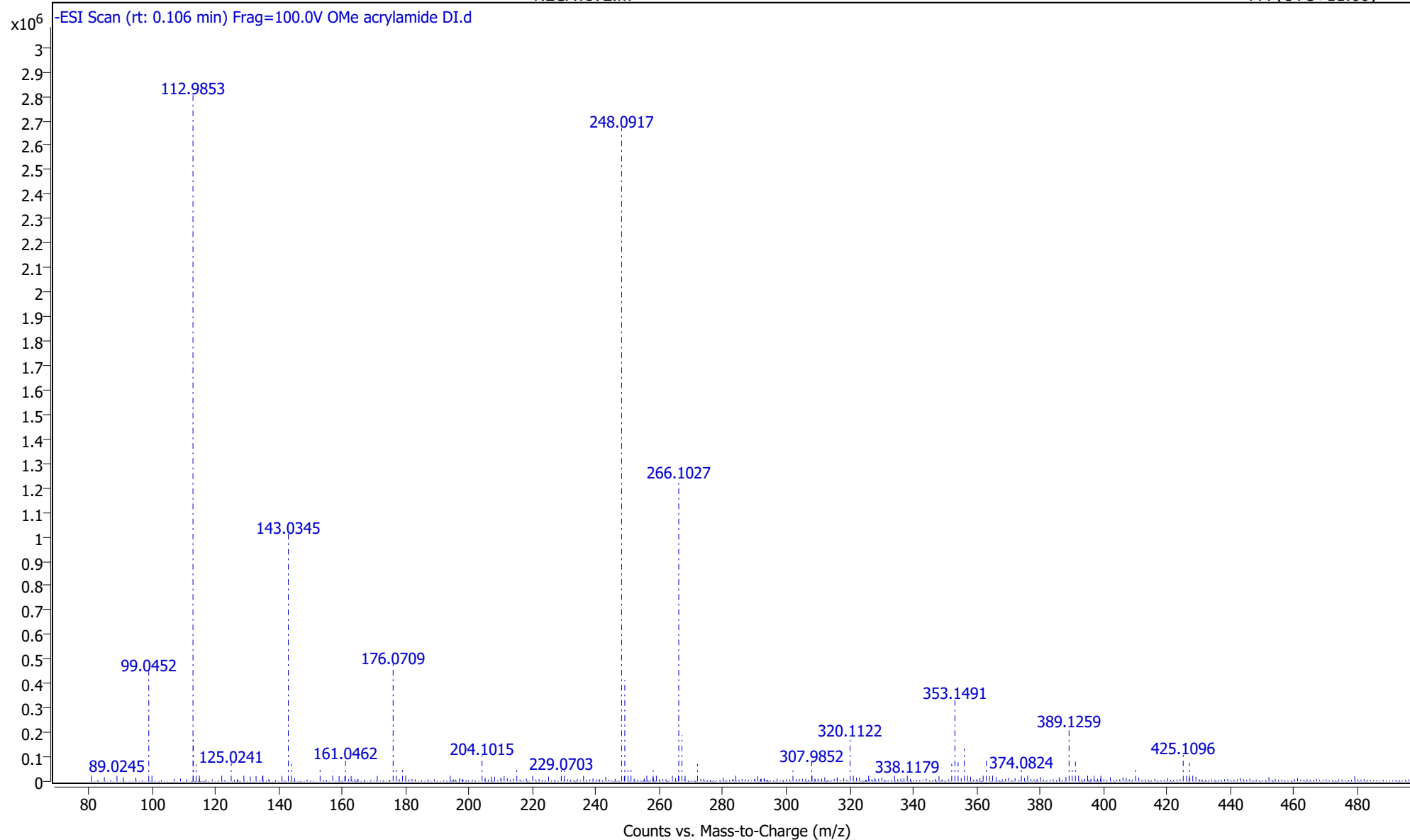
Current Data Parameters
 NAME OMe Acrylamide 13C
 EXPNO 4
 PROCNO 1

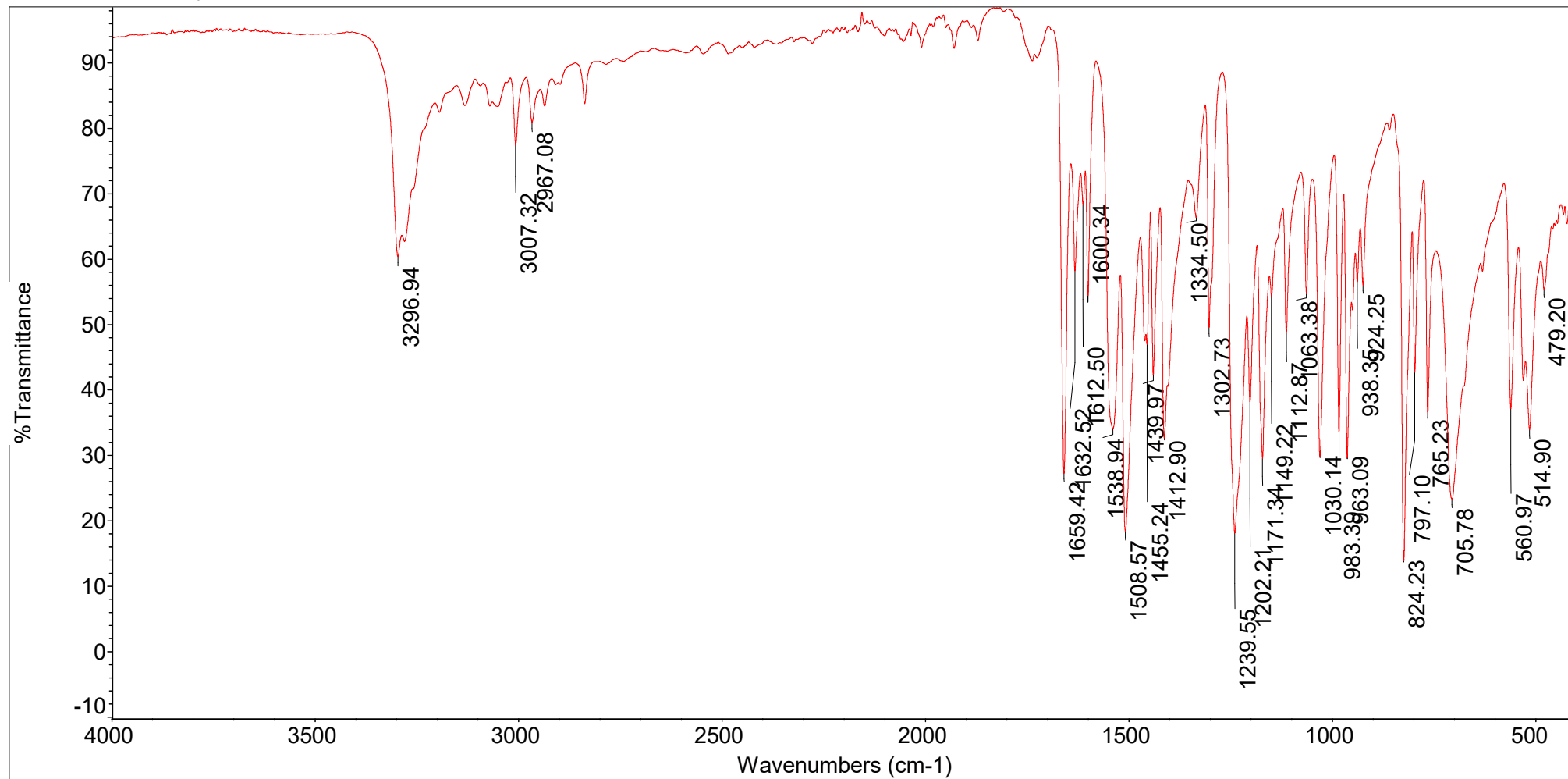
F2 - Acquisition Parameters
 Date_ 20230105
 Time_ 2.21 h
 INSTRUM AVNEO
 PROBHD Z175272_0008 (
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 3800
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.726609 Hz
 AQ 1.3762560 sec
 RG 101
 DW 21.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6278593 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 58.38199997 W
 SFO2 400.1516006 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 19.63299942 W
 PLW12 0.24237999 W
 PLW13 0.12192000 W

F2 - Processing parameters
 SI 32768
 SF 100.6177849 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

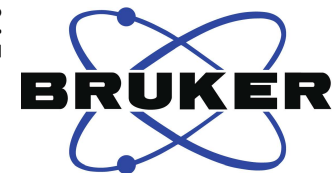
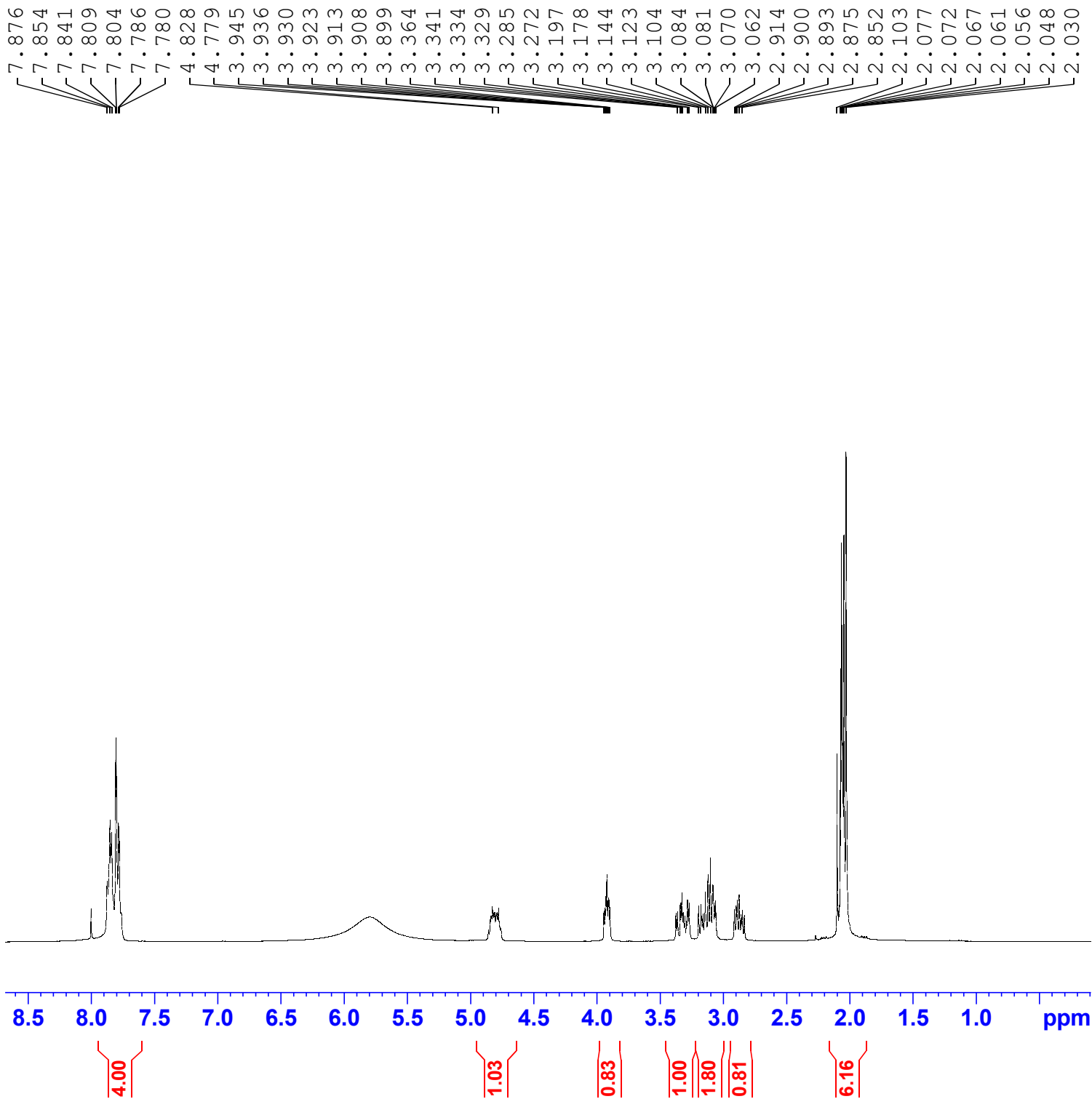


Name	OMe Acrylamide (5d)	Rack Pos.	Instrument	Instrument 1	Operator
Inj. Vol. (ul)	5	Plate Pos.	IRM Status	Some ions missed	
Data File	OMe acrylamide DI.d	Method (Acq)	Hugh Method direct inj	Comment	Acq. Time (Local)
			NEGATIVE.m		2023-01-04 2:13:09 PM (UTC+11:00)





SF5 Cys Conjugate (4a)

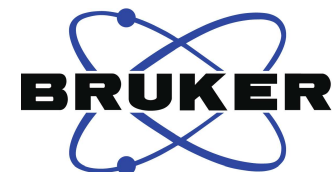
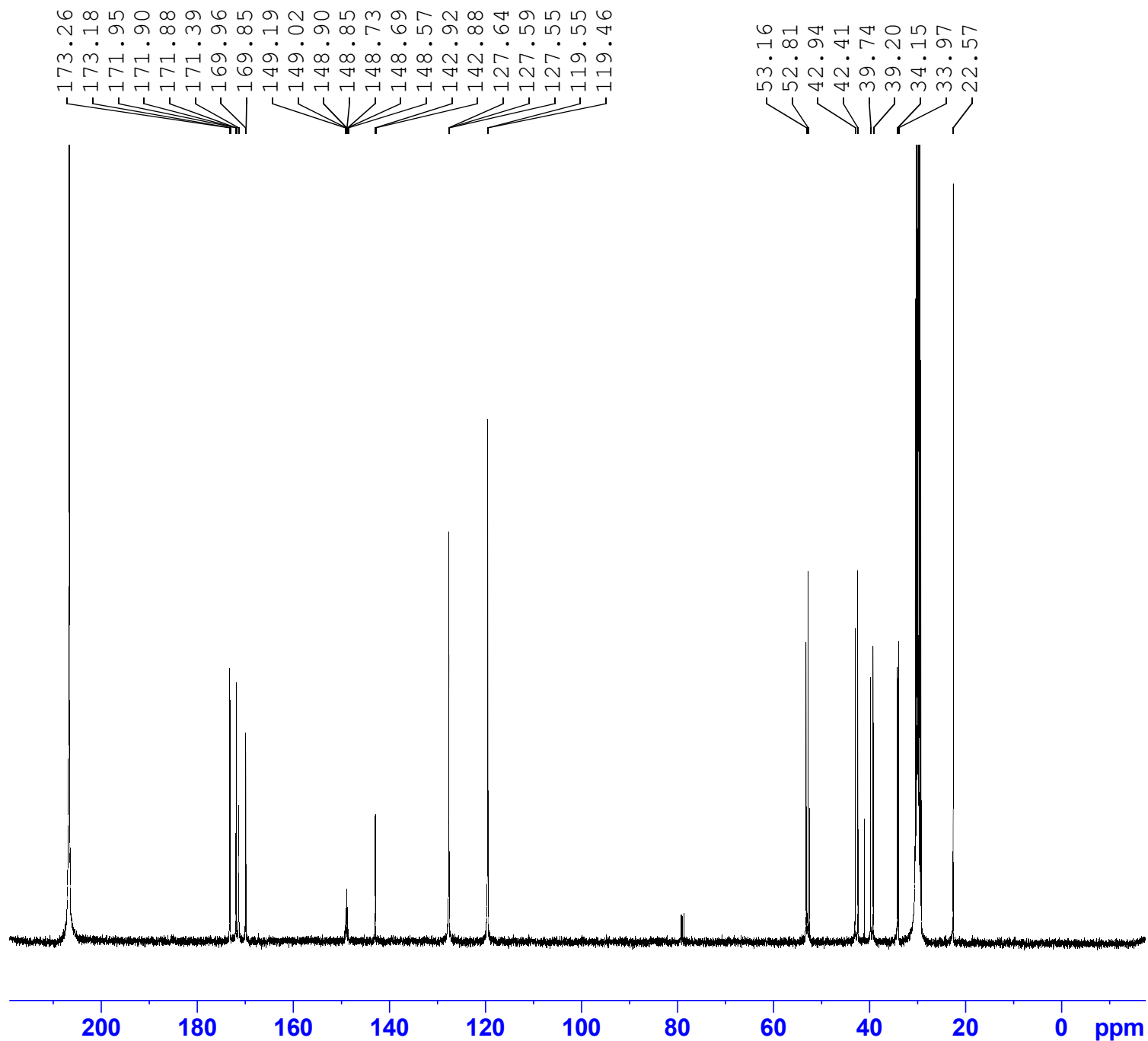


Current Data Parameters
 NAME SF5 Cys Conj Pure - 1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230213
 Time_ 12.02 h
 INSTRUM AVNEO
 PROBHD Z175272_0008 (
 PULPROG zg30
 TD 131072
 SOLVENT Acetone
 NS 32
 DS 2
 SWH 8196.722 Hz
 FIDRES 0.125072 Hz
 AQ 7.9953918 sec
 RG 101
 DW 61.000 usec
 DE 13.54 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1624710 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 19.63299942 W

F2 - Processing parameters
 SI 65536
 SF 400.1600000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

SF5 Cys Conjugate (4a)

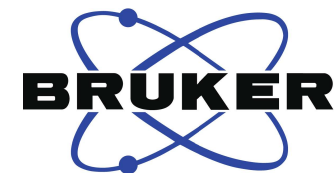
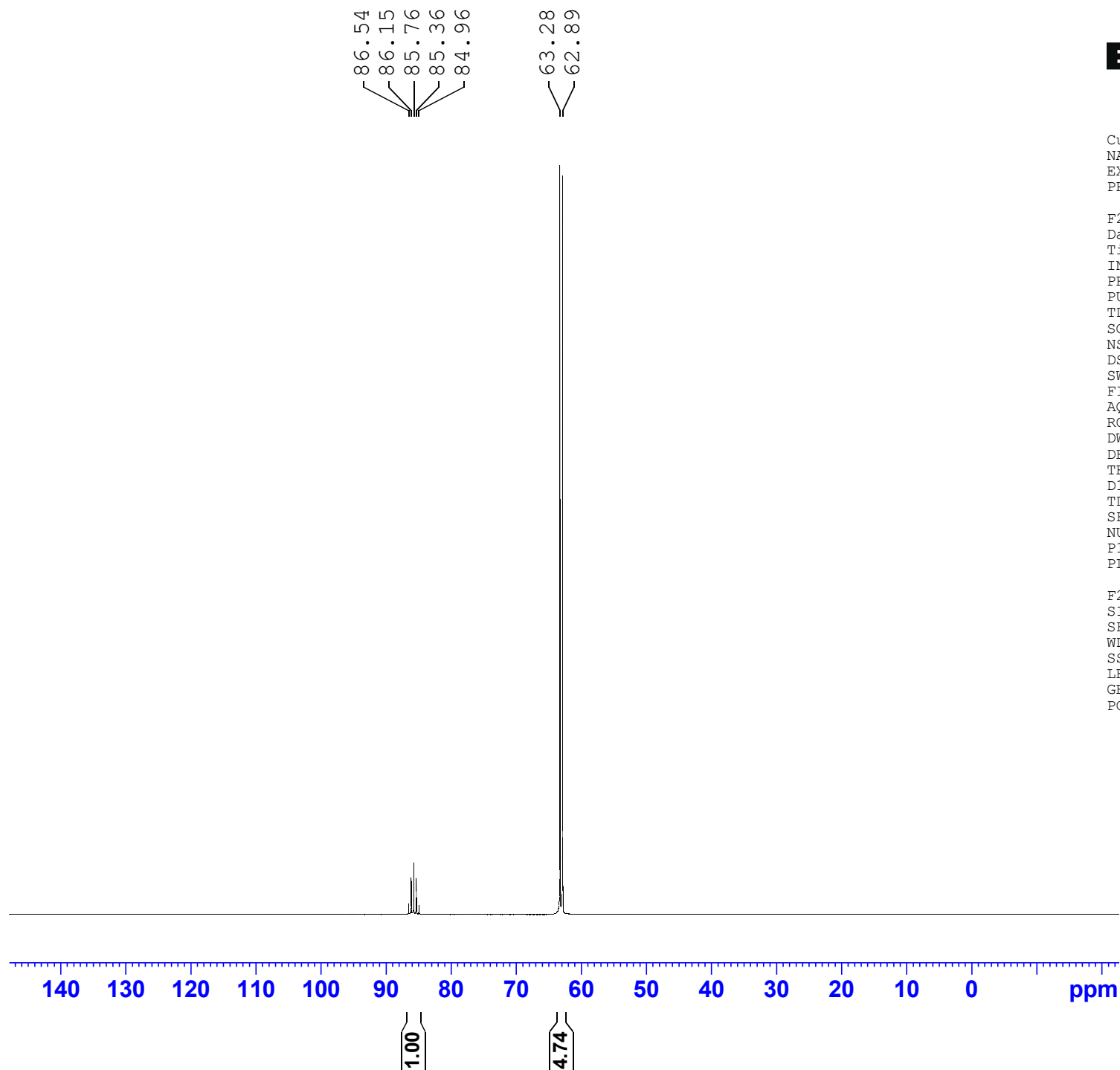


Current Data Parameters
NAME SF5 cys conj. pure - 13C
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230214
Time_ 10.21 h
INSTRUM AVNEO
PROBHD Z175272_0008 (
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 3600
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6303741 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 58.38199997 W
SFO2 400.1616006 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 19.63299942 W
PLW12 0.24237999 W
PLW13 0.12192000 W

F2 - Processing parameters
SI 32768
SF 100.6202299 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

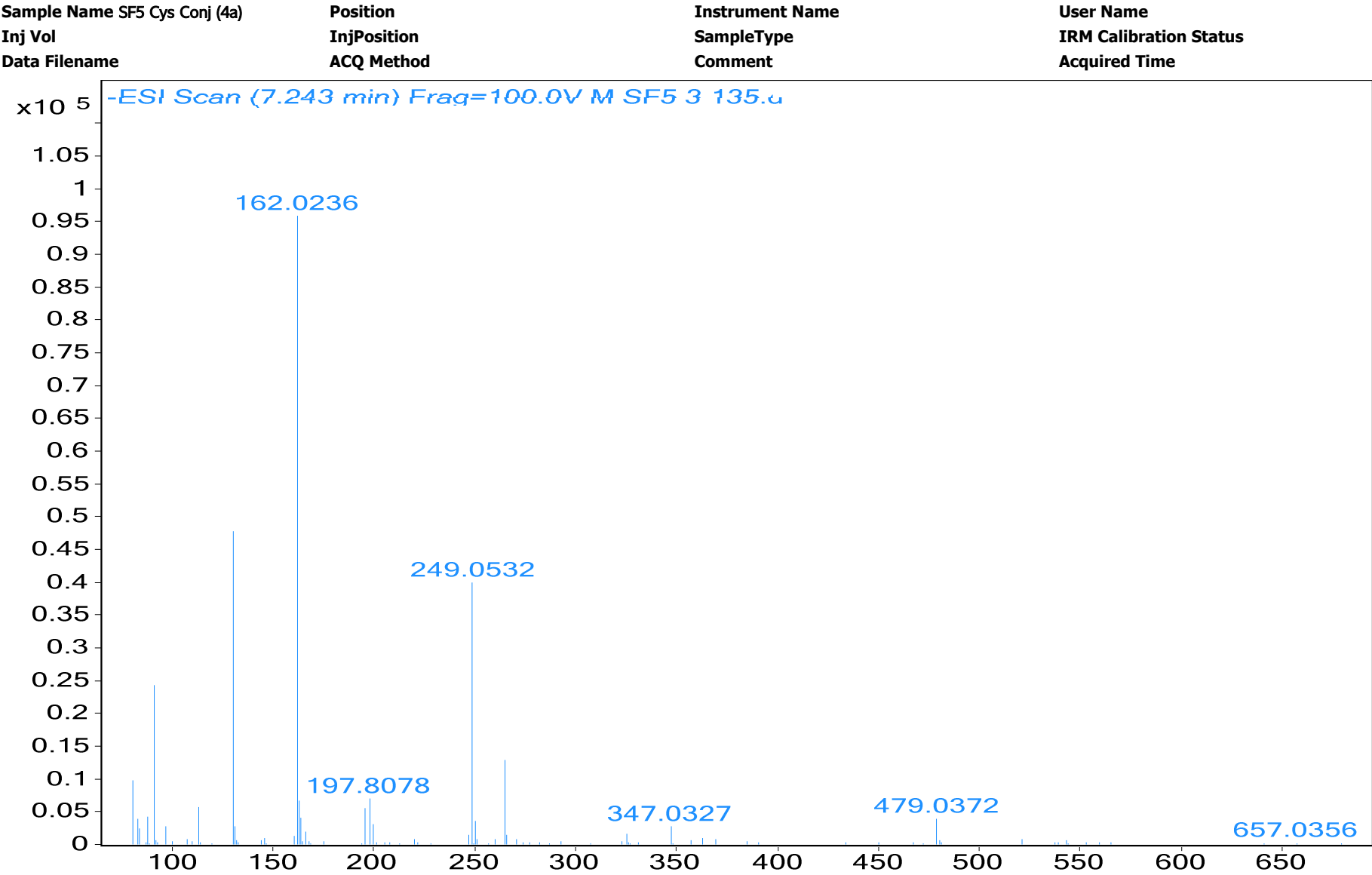
SF5 Cys Conj (4a)



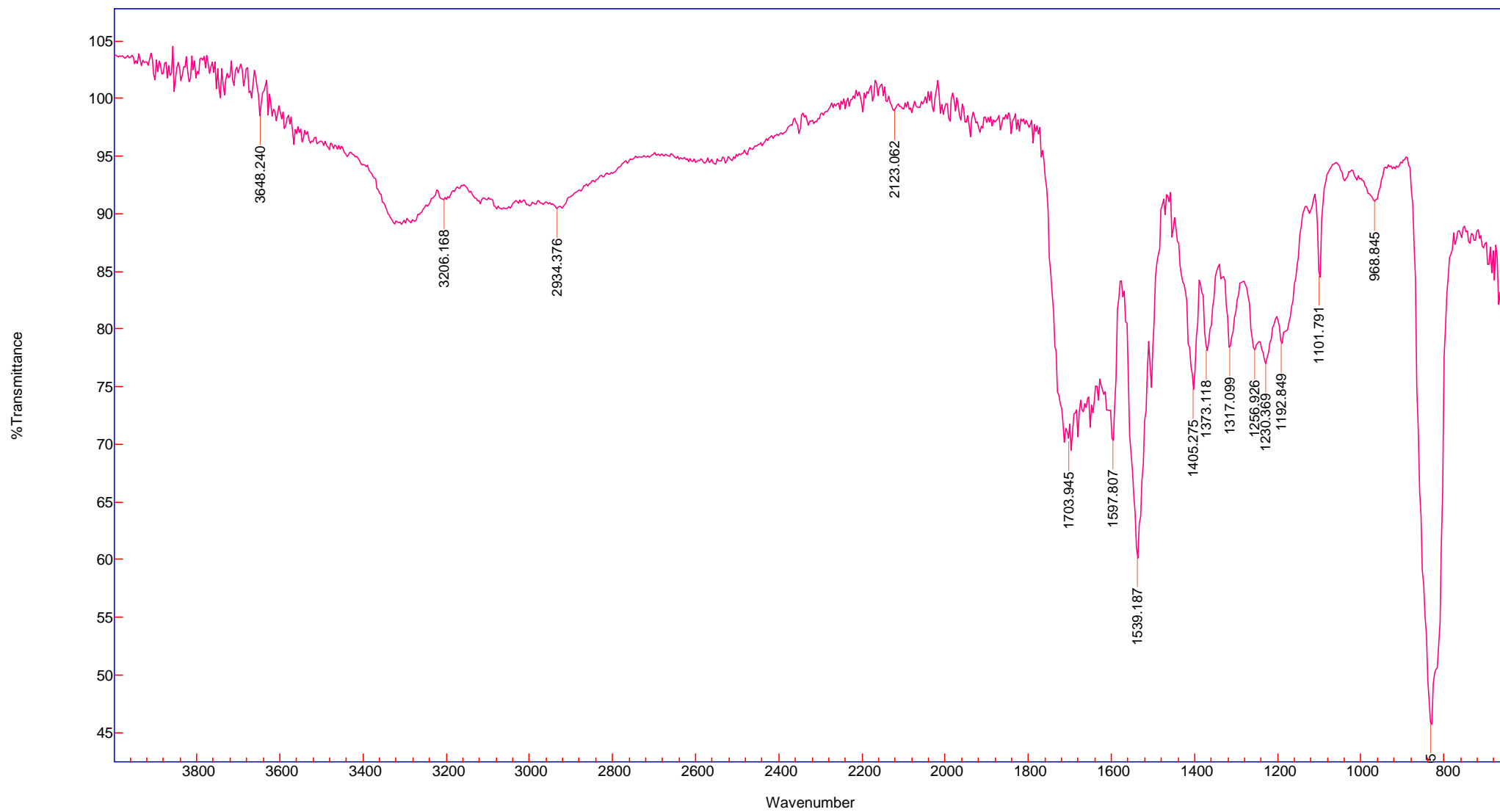
Current Data Parameters
 NAME SF5 Cys Conj. pure 19F
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230213
 Time_ 12.31 h
 INSTRUM AVNEO
 PROBHD Z175272_0008 (zg)
 PULPROG zg
 TD 131072
 SOLVENT Acetone
 NS 128
 DS 4
 SWH 147058.828 Hz
 FIDRES 2.243940 Hz
 AQ 0.4456448 sec
 RG 101
 DW 3.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 376.5265944 MHz
 NUC1 19F
 P1 12.00 usec
 PLW1 45.00000000 W

F2 - Processing parameters
 SI 65536
 SF 376.5265944 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

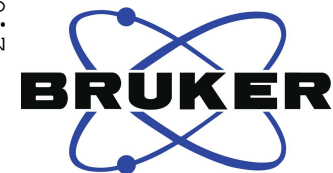
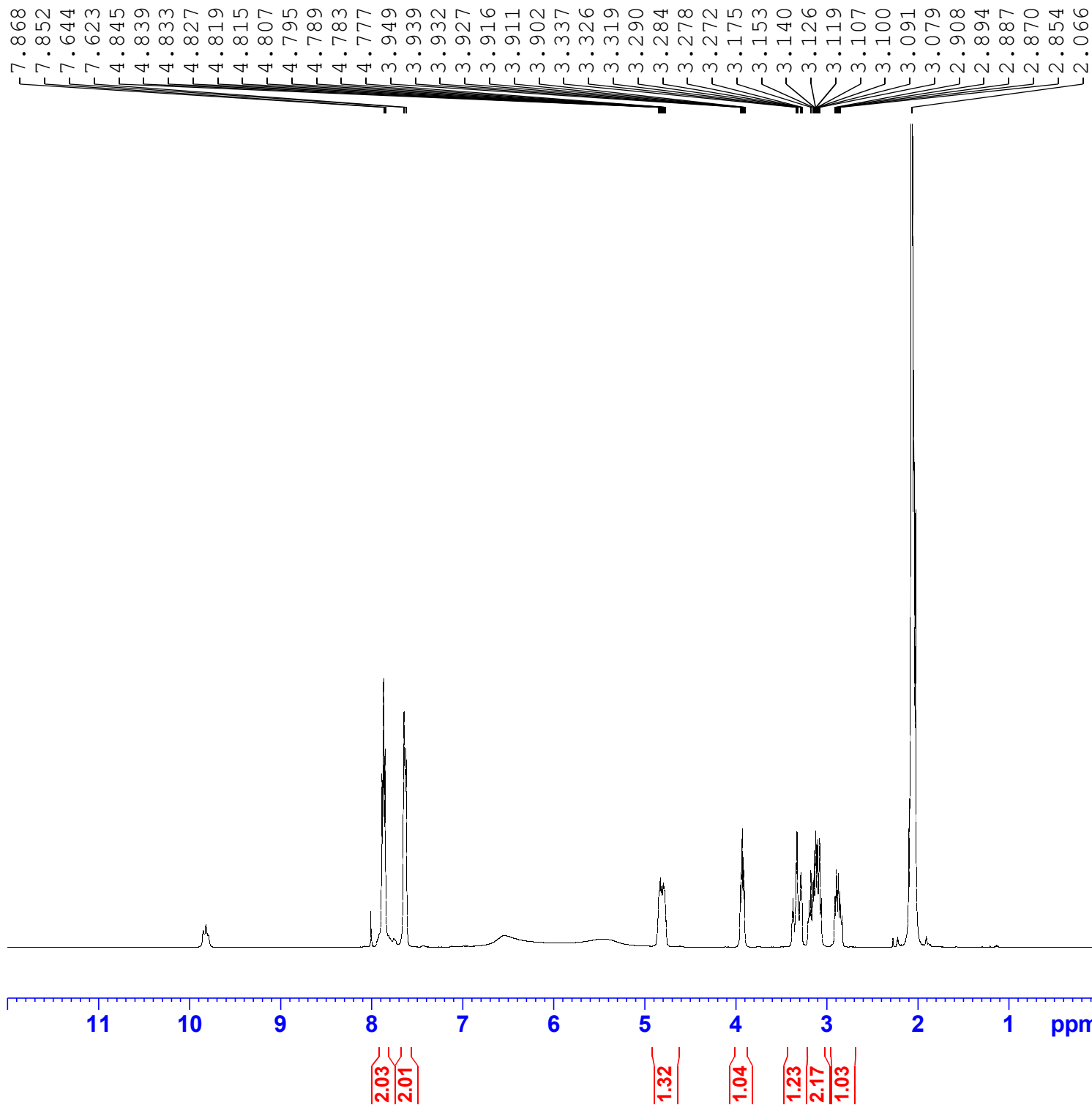


SF5 Cys Conj (**4a**)



Name
SF5 Cys Conj —

CF3 Cys Conjugate (4b)

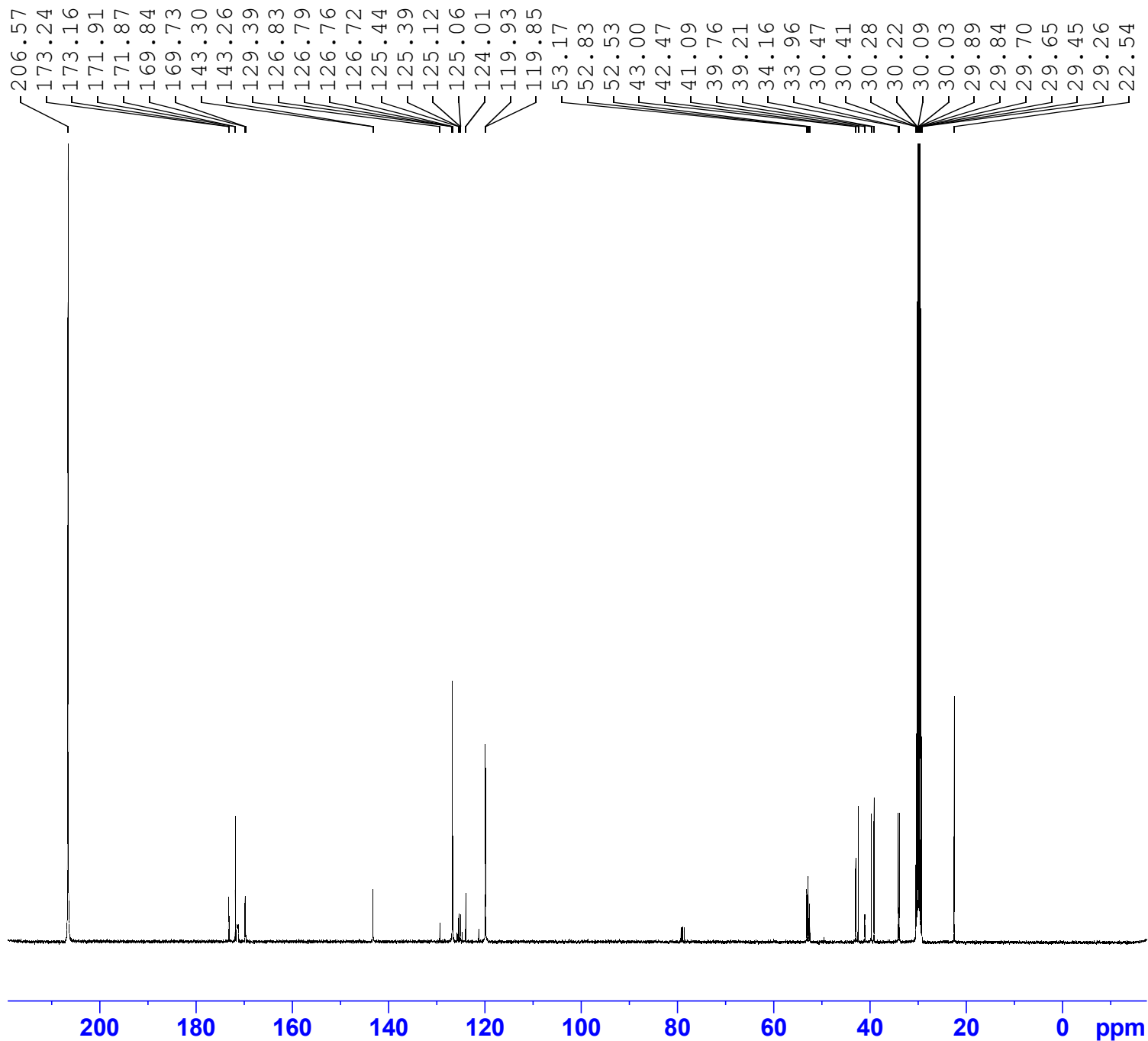
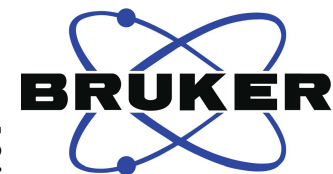


Current Data Parameters
 NAME CF3 Cys Conj. Pure - 1H
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230213
 Time_ 12.41 h
 INSTRUM AVNEO
 PROBHD Z175272_0008 (zg30)
 PULPROG 131072
 TD 131072
 SOLVENT Acetone
 NS 32
 DS 2
 SWH 8196.722 Hz
 FIDRES 0.125072 Hz
 AQ 7.9953918 sec
 RG 101
 DW 61.000 usec
 DE 13.54 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1624710 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 19.63299942 W

F2 - Processing parameters
 SI 65536
 SF 400.1600000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

CF3 Cys Conjugate (4b)



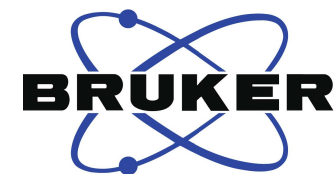
Current Data Parameters
 NAME CF3 Maleimide Conj Pure 13C
 EXPNO 9
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230214
 Time 3.15 h
 INSTRUM AVNEO
 PROBHD Z175272_0008 (
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 3600
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.726609 Hz
 AQ 1.3762560 sec
 RG 101
 DW 21.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6303741 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 58.38199997 W
 SFO2 400.1616006 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 19.63299942 W
 PLW12 0.24237999 W
 PLW13 0.12192000 W

F2 - Processing parameters
 SI 32768
 SF 100.6202287 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

CF3 Cys Conj (4b)

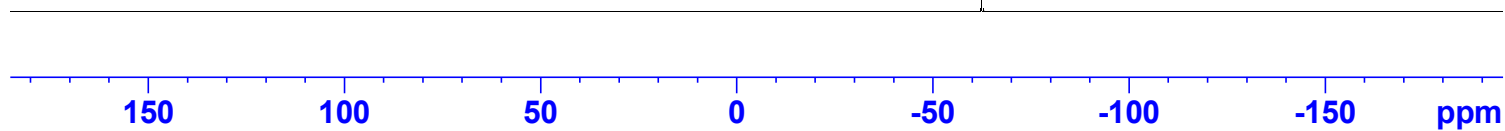
— -62.39



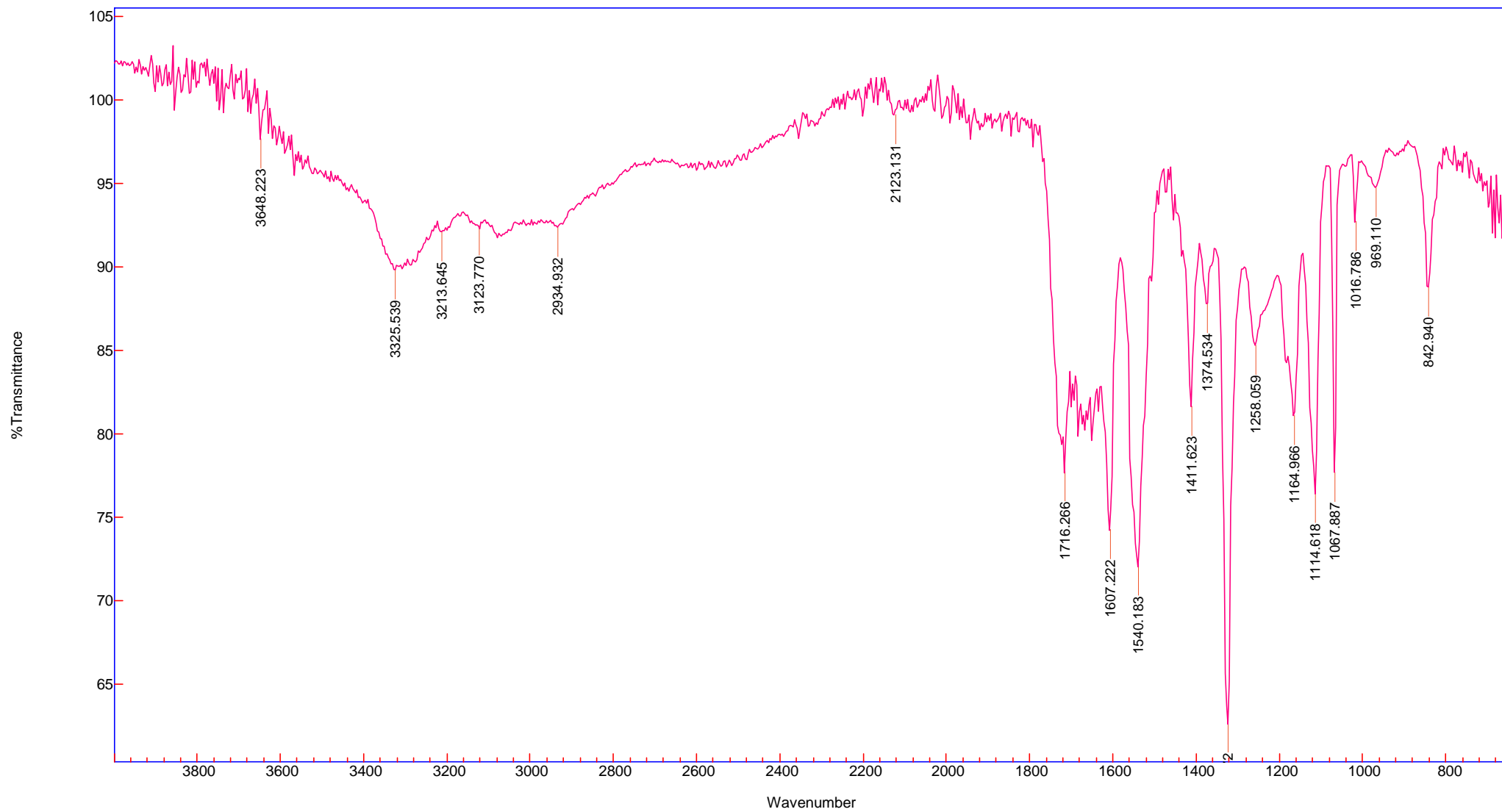
Current Data Parameters
NAME CF3 Mal Conj. pure - 19F
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230213
Time_ 12.47 h
INSTRUM AVNEO
PROBHD Z175272_0008 (
PULPROG zg
TD 131072
SOLVENT Acetone
NS 128
DS 4
SWH 147058.828 Hz
FIDRES 2.243940 Hz
AQ 0.4456448 sec
RG 101
DW 3.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SF01 376.5265944 MHz
NUC1 19F
P1 12.00 usec
PLW1 45.00000000 W

F2 - Processing parameters
SI 65536
SF 376.5265944 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



CF3 Cys Conj (4b)



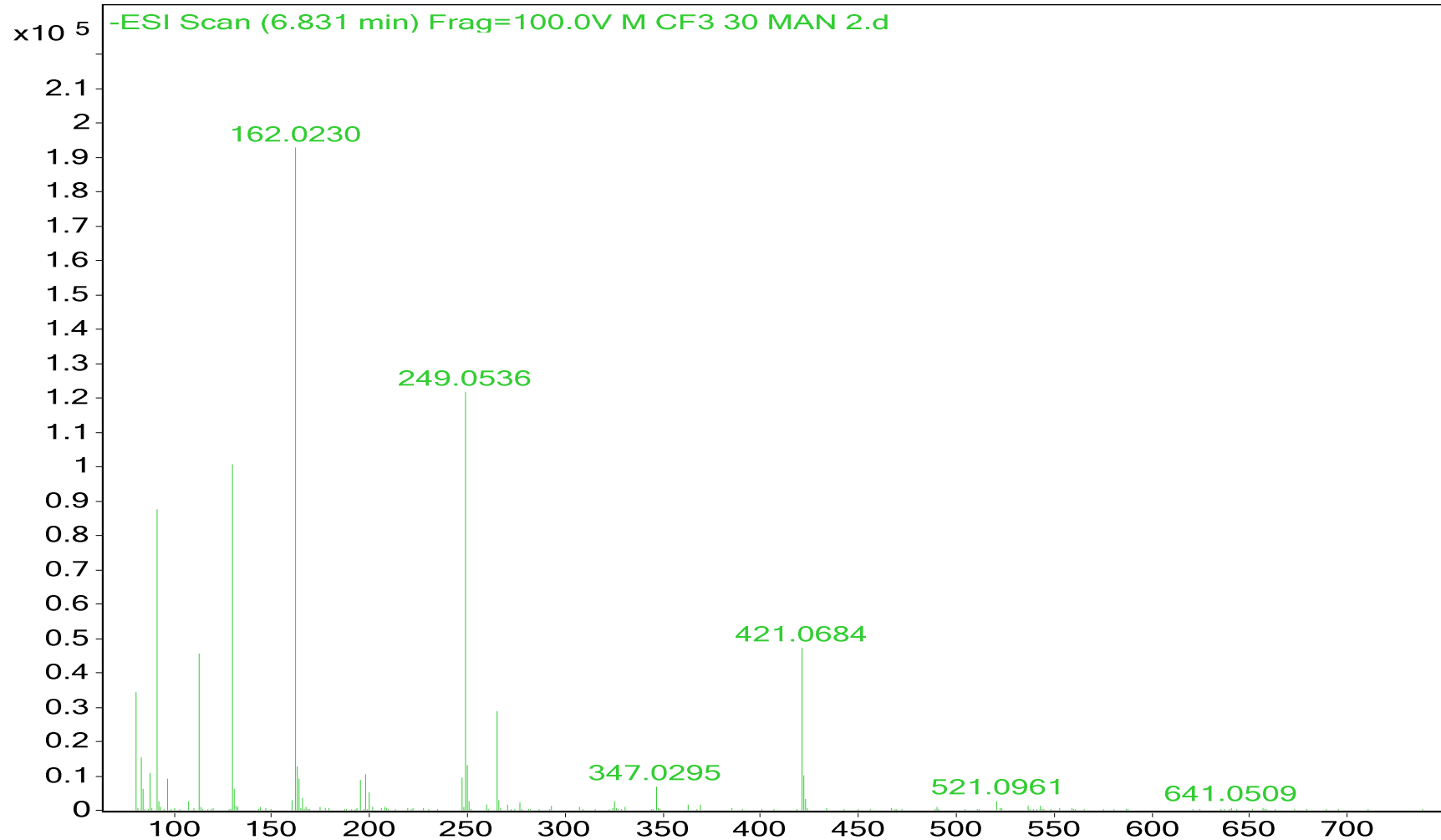
Name
CF3 Cys Conj —

Sample Name CF3 Cys Conj (4b)
Inj Vol
Data Filename

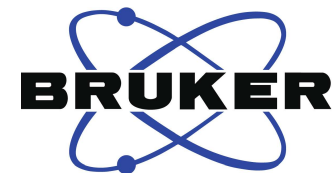
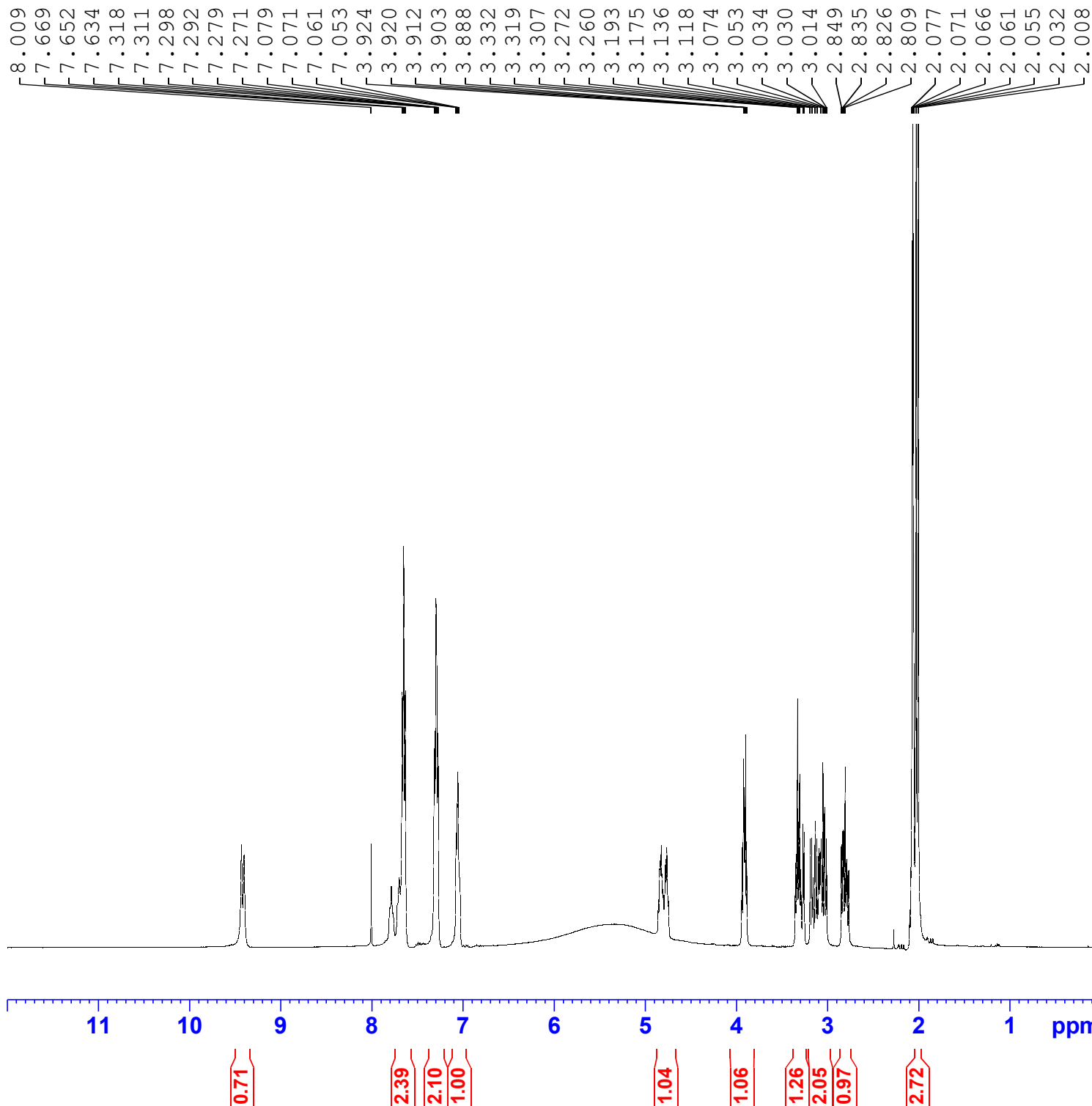
Position
InjPosition
ACQ Method

Instrument Name
SampleType
Comment

User Name
IRM Calibration Status
Acquired Time



H Cys Conjugate (4c)



Current Data Parameters

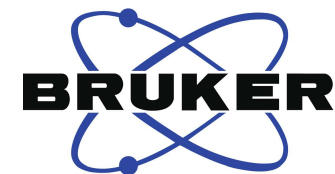
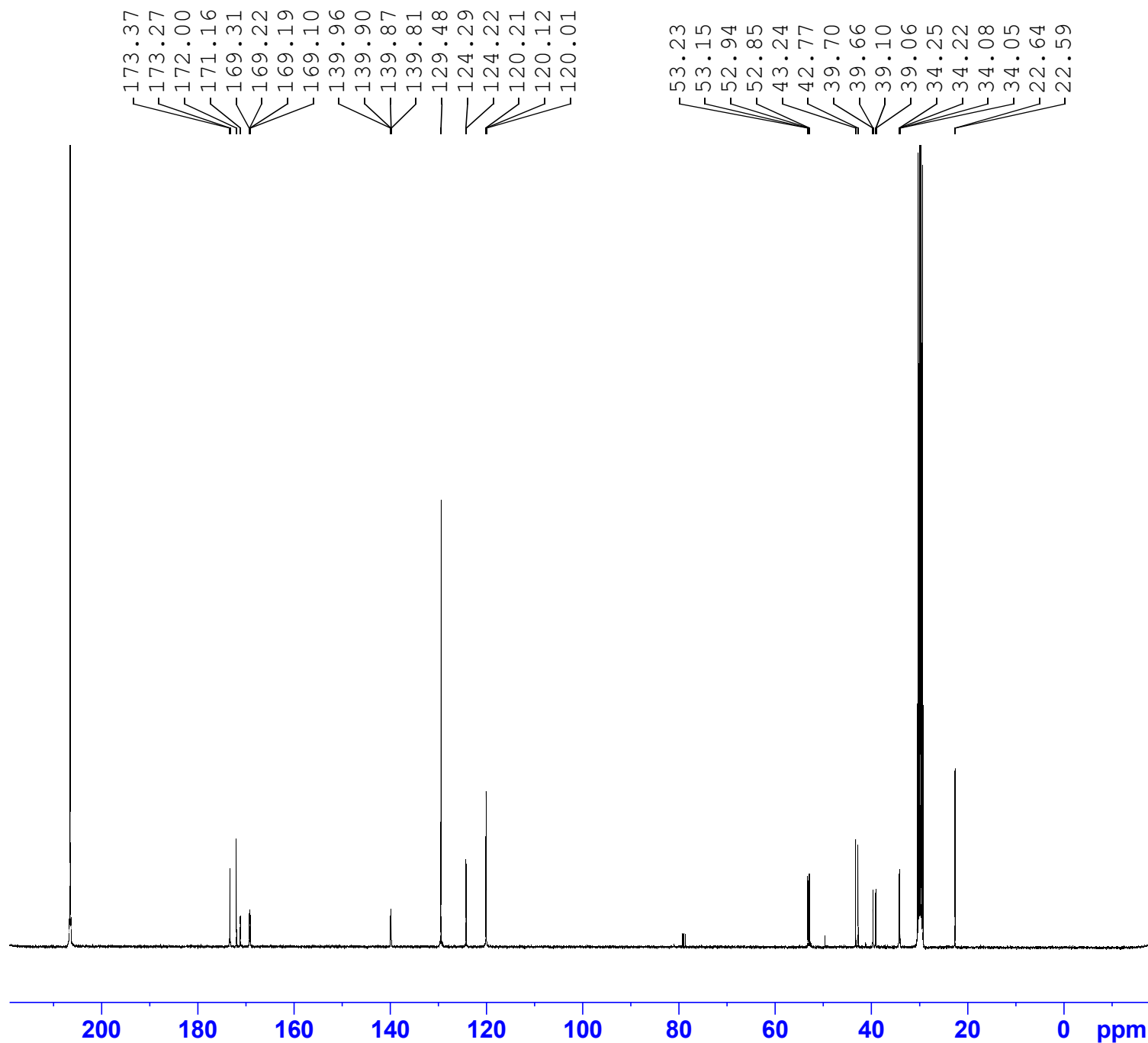
NAME H Cys Conj. Pure - 1H
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters

Date_ 20230213
Time_ 13.47 h
INSTRUM AVNEO
PROBHD Z175272_0008 (
PULPROG zg30
TD 131072
SOLVENT Acetone
NS 32
DS 2
SWH 8196.722 Hz
FIDRES 0.125072 Hz
AQ 7.9953918 sec
RG 101
DW 61.000 usec
DE 13.54 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1624710 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 19.63299942 W

F2 - Processing parameters

SI 65536
SF 400.1600000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

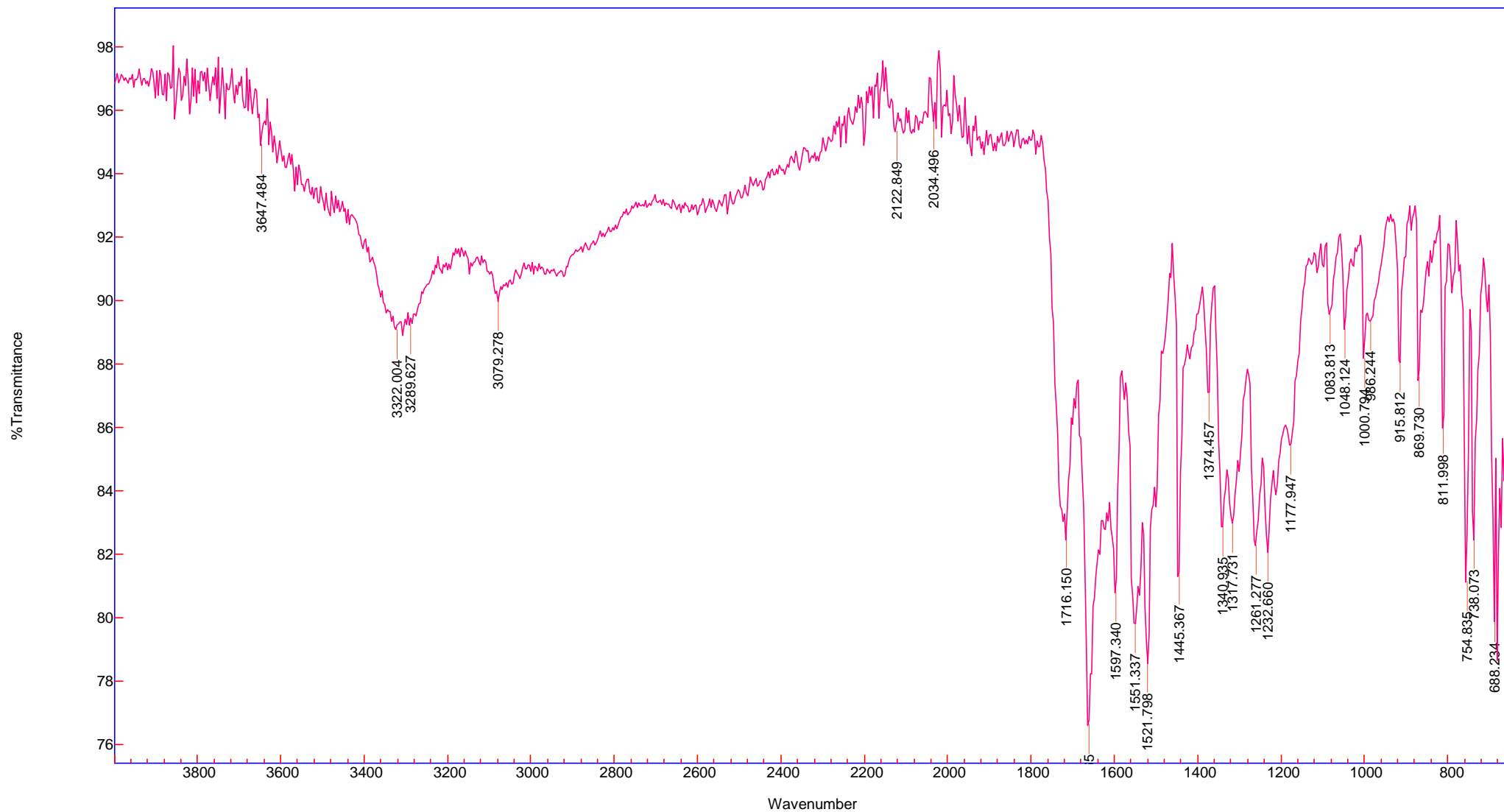


Current Data Parameters
NAME H Cys Conj. Pure 13C
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230214
Time_ 6.47 h
INSTRUM AVNEO
PROBHD Z175272_0008 (
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 3600
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6303741 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 58.38199997 W
SFO2 400.1616006 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 19.63299942 W
PLW12 0.24237999 W
PLW13 0.12192000 W

F2 - Processing parameters
SI 32768
SF 100.6202303 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

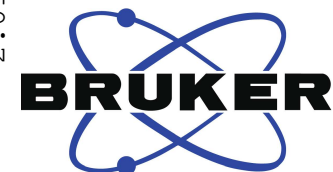
H Cys Conj (4c)



Name
H Cys Conj

OMe Cys Conjugate (4d)

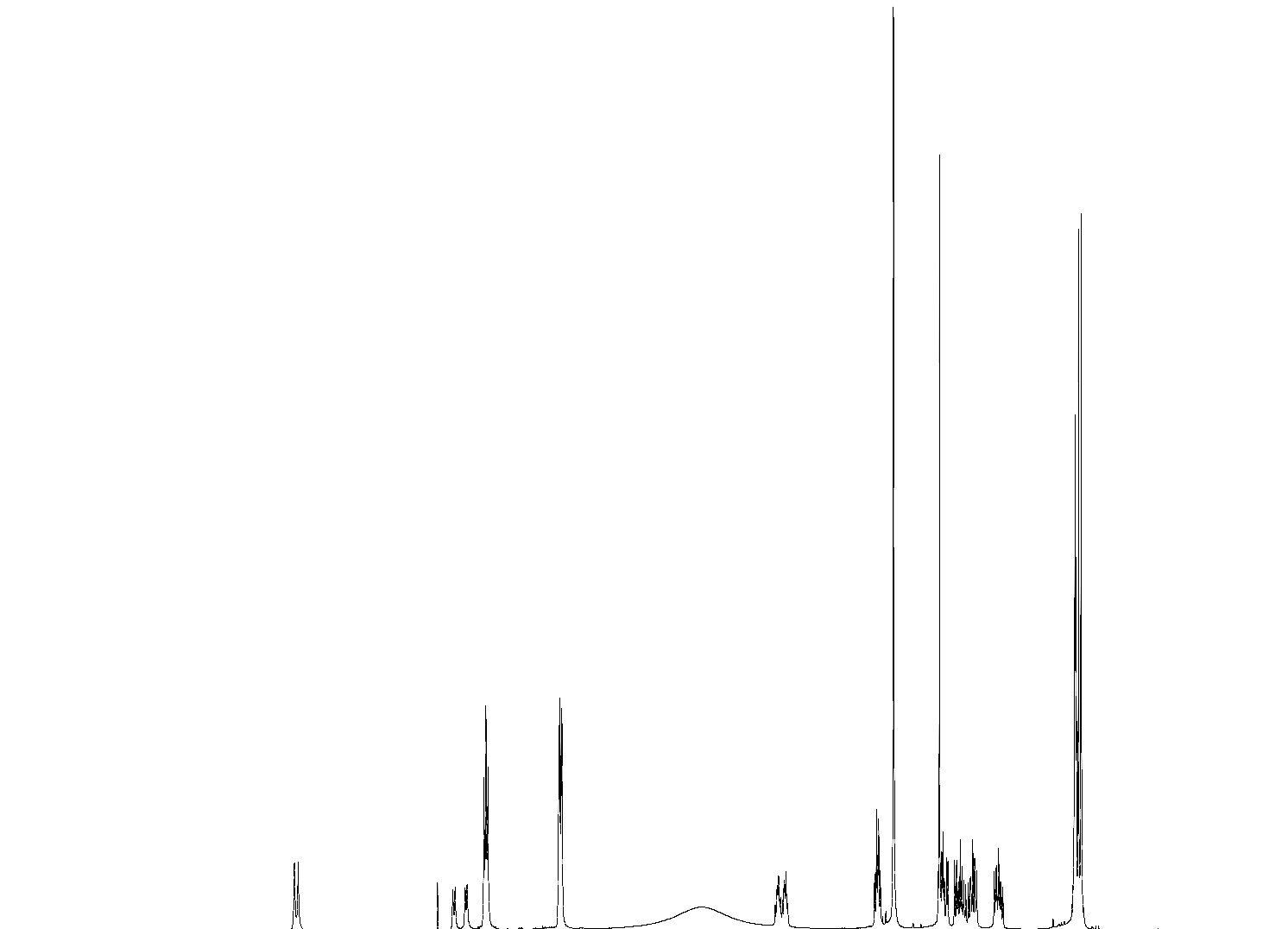
7.558 7.553 7.536 6.878 6.871 6.855 6.848 4.831 4.776 4.763 3.937 3.919 3.906 3.898 3.883 3.762 3.758 3.310 3.299 3.288 3.266 3.253 3.191 3.173 3.157 3.140 3.123 3.106 3.088 3.062 3.045 3.039 3.023 3.005 3.000 2.985 2.823 2.808 2.798 2.782 2.769 2.758 2.037 2.012



Current Data Parameters
NAME OMe Mal Conj. pure - 1H
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230213
Time_ 12.12 h
INSTRUM AVNEO
PROBHD Z175272_0008 (zg30)
PULPROG 131072
TD 32
SOLVENT Acetone
NS 2
DS 8196.722 Hz
FIDRES 0.125072 Hz
AQ 7.9953918 sec
RG 90.5
DW 61.000 usec
DE 13.54 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1624710 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 19.63299942 W

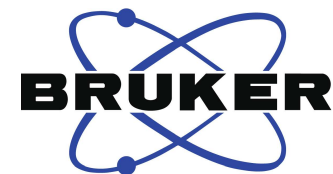
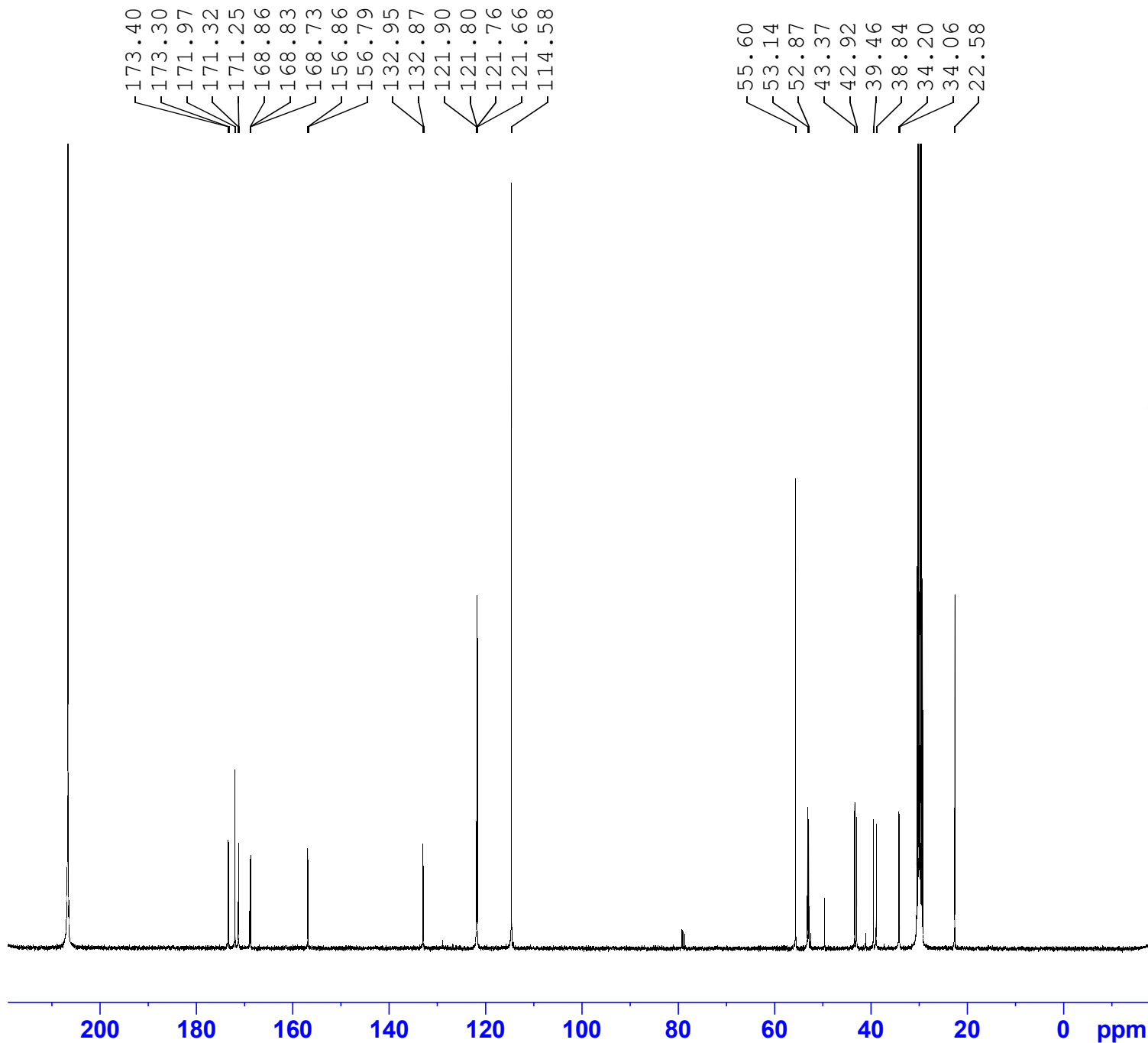
F2 - Processing parameters
SI 65536
SF 400.1600000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



11 10 9 8 7 6 5 4 3 2 1 ppm

2.05 2.00 1.09 1.00 2.99 2.34 2.02 1.02 2.53

OMe Cys Conjugate (4d)



Current Data Parameters
 NAME OMe Cys Conj pure 13C
 EXPNO 8
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230213
 Time_ 22.34 h
 INSTRUM AVNEO
 PROBD Z175272_0008 (
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 3600
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.726609 Hz
 AQ 1.3762560 sec
 RG 101
 DW 21.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6303741 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 58.38199997 W
 SFO2 400.1616006 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 19.63299942 W
 PLW12 0.24237999 W
 PLW13 0.12192000 W

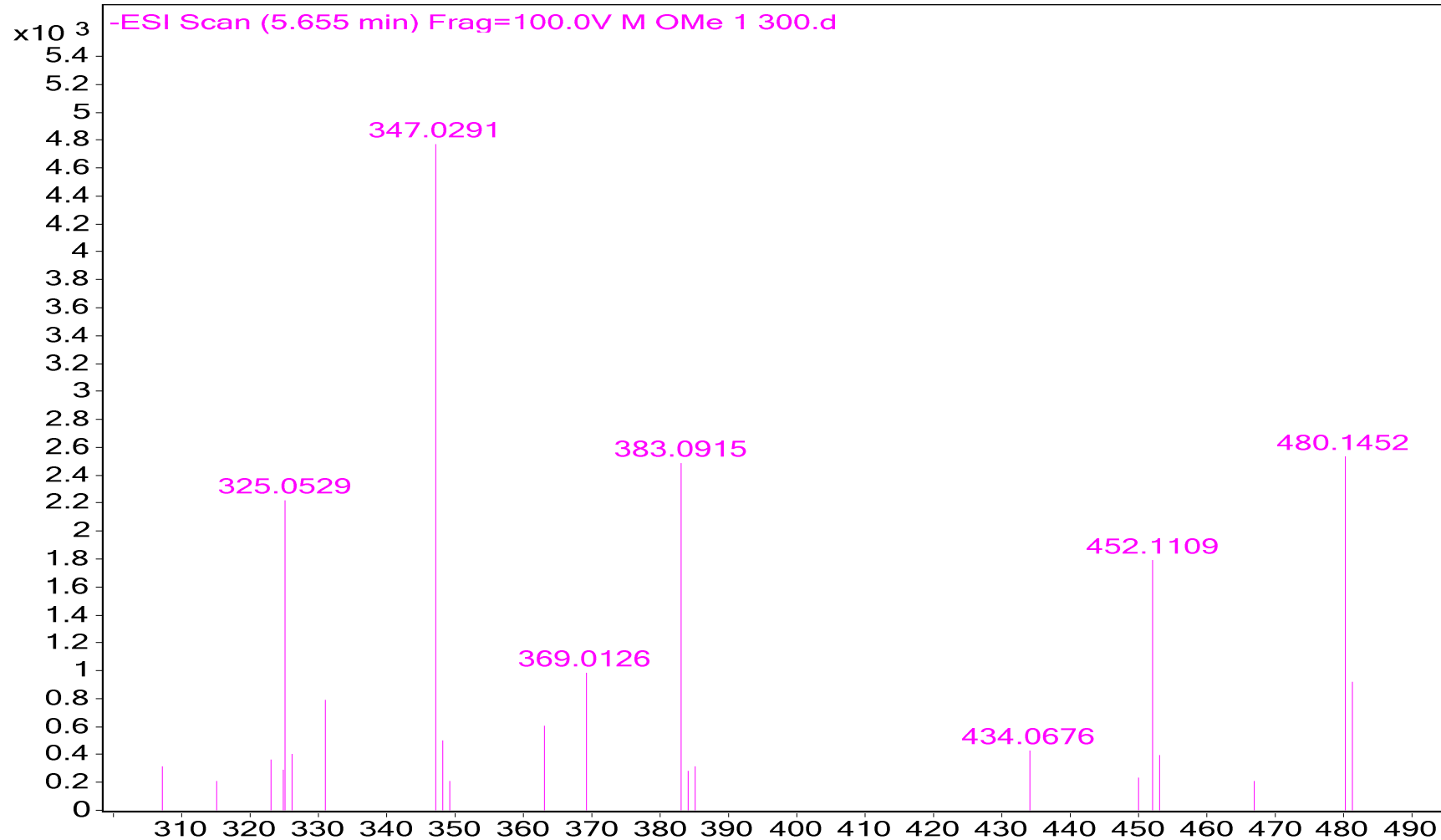
F2 - Processing parameters
 SI 32768
 SF 100.6202307 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Sample Name OMe Cys Conj (4d)
Inj Vol
Data Filename

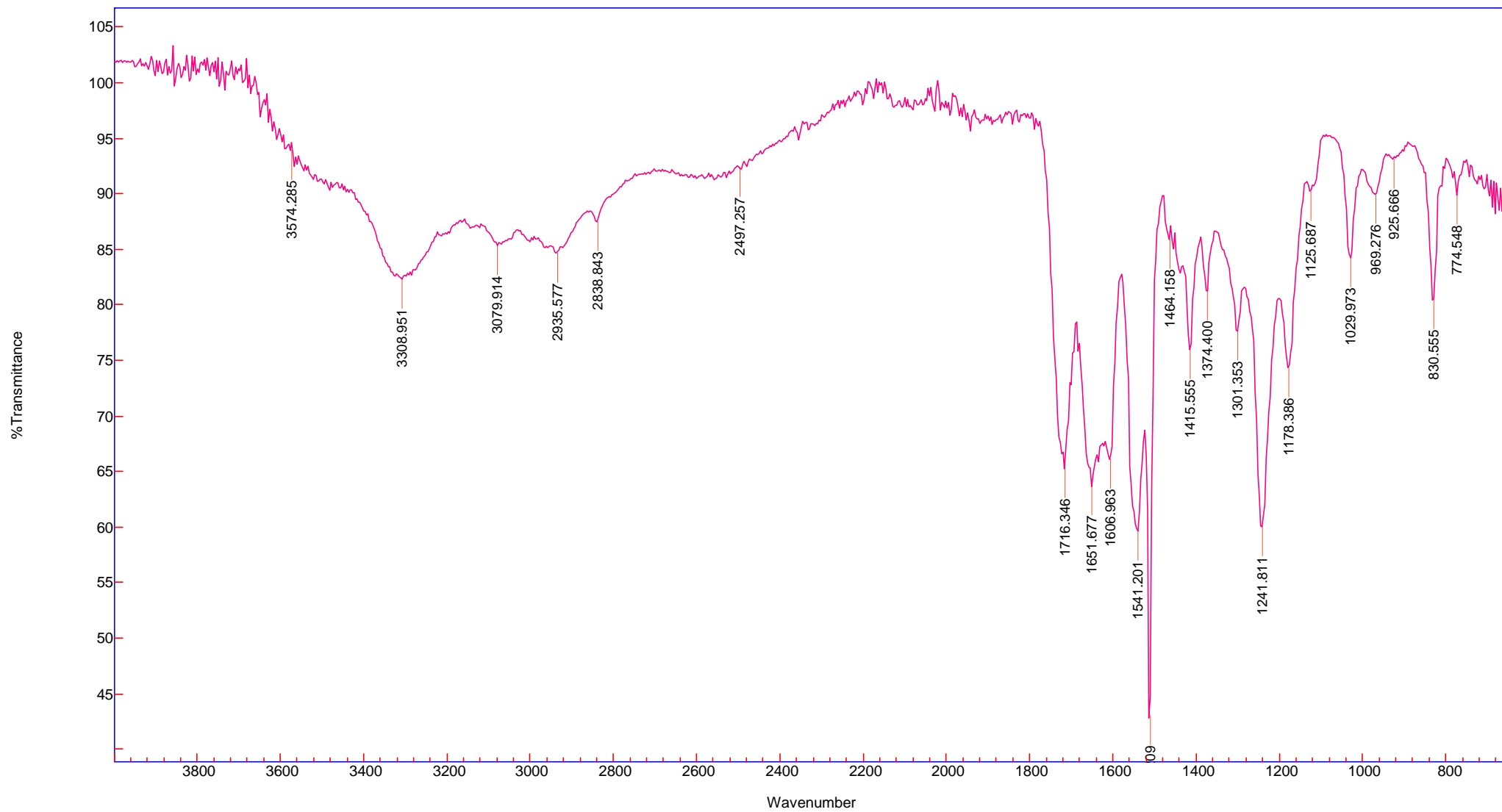
Position
InjPosition
ACQ Method

Instrument Name
SampleType
Comment

User Name
IRM Calibration Status
Acquired Time

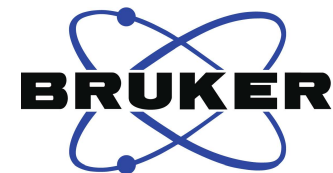
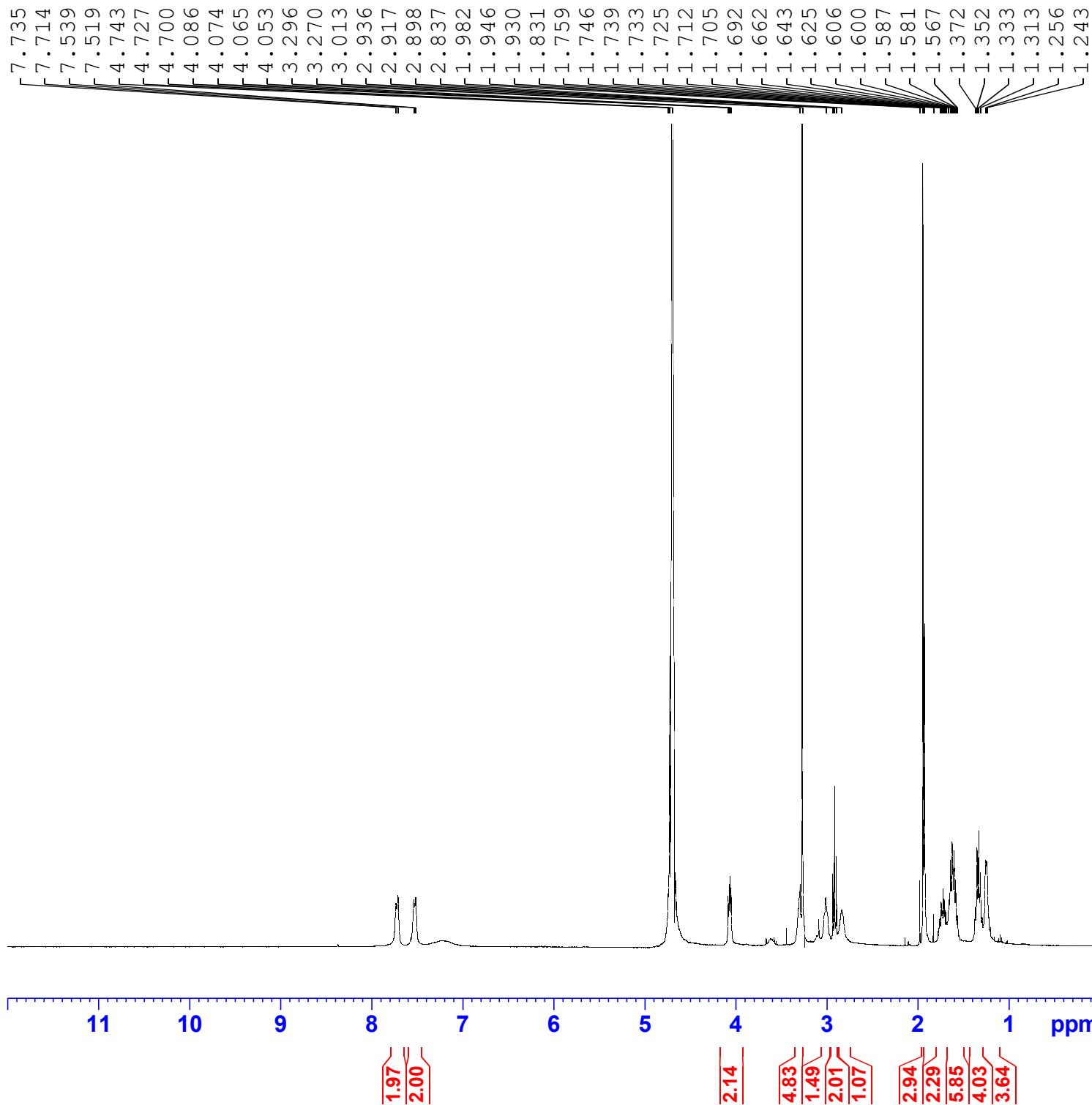


OMe Cys Conj (4d)



Name
OMe Cys Conj

SF5 Acrylamide Conjugate (6a)

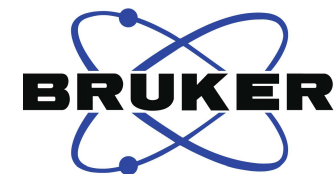


Current Data Parameters
 NAME SF5 Acrylamide Conj - 1H final
 EXPNO 8
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230120
 Time 13.12 h
 INSTRUM AVNEO
 PROBHD Z175272_0008 (
 PULPROG zg30
 TD 131072
 SOLVENT D2O
 NS 32
 DS 2
 SWH 8196.722 Hz
 FIDRES 0.125072 Hz
 AQ 7.9953918 sec
 RG 101
 DW 61.000 usec
 DE 13.54 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1524709 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 19.63299942 W

F2 - Processing parameters
 SI 65536
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

SF5 Acrylamide Conjugate (6a)



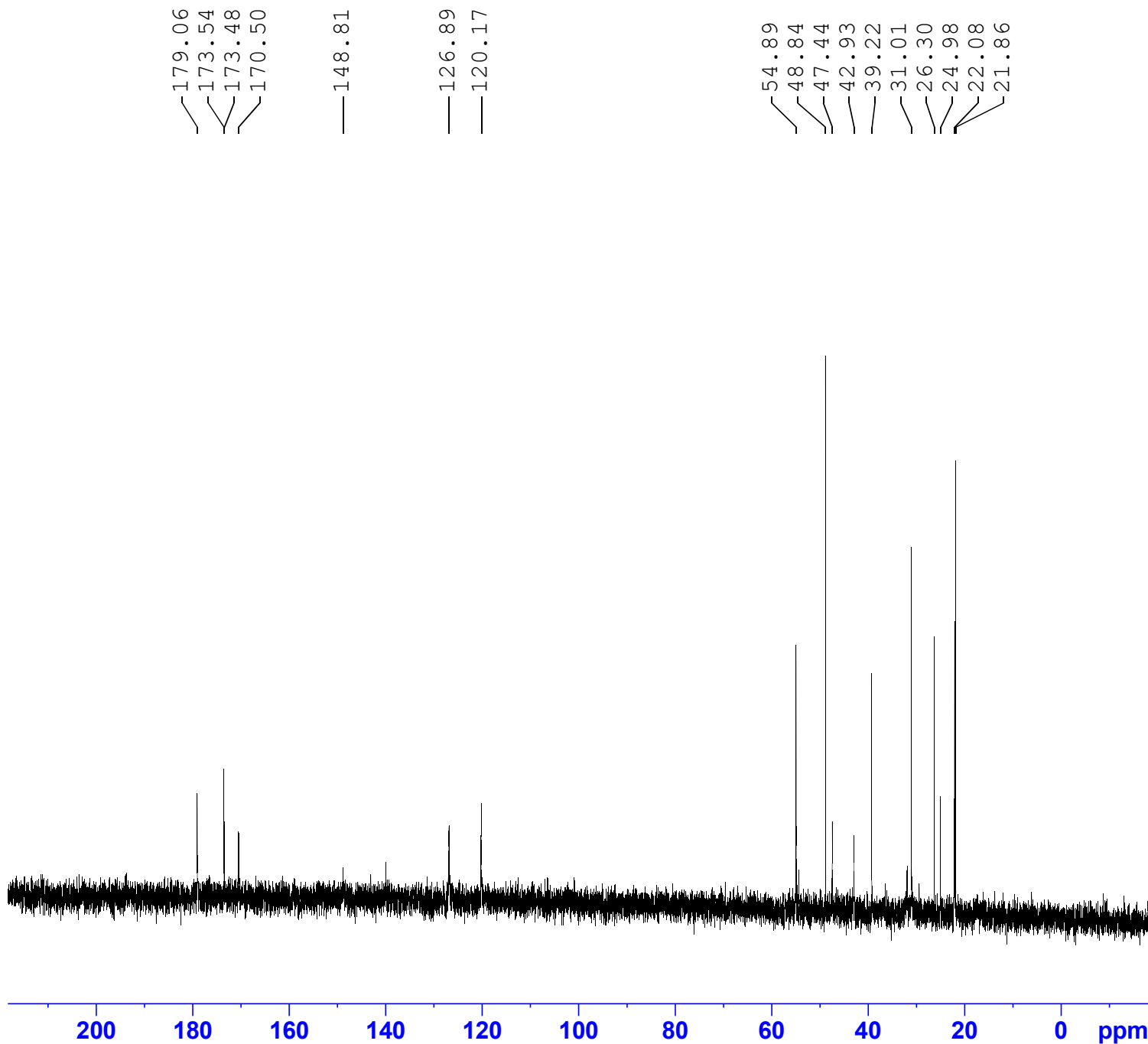
Current Data Parameters
 NAME SF5 Acryl Conj - 13C
 EXPNO 3
 PROCNO 1

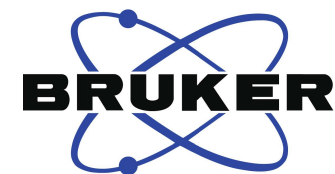
F2 - Acquisition Parameters

Date_ 20230121
 Time 2.04 h
 INSTRUM AVNEO
 PROBHD Z175272_0008 (
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 3600
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.726609 Hz
 AQ 1.3762560 sec
 RG 101
 DW 21.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6278593 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 58.38199997 W
 SFO2 400.1516006 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 90.00 usec
 PLW2 19.63299942 W
 PLW12 0.24237999 W
 PLW13 0.12192000 W

F2 - Processing parameters

SI 32768
 SF 100.6177975 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

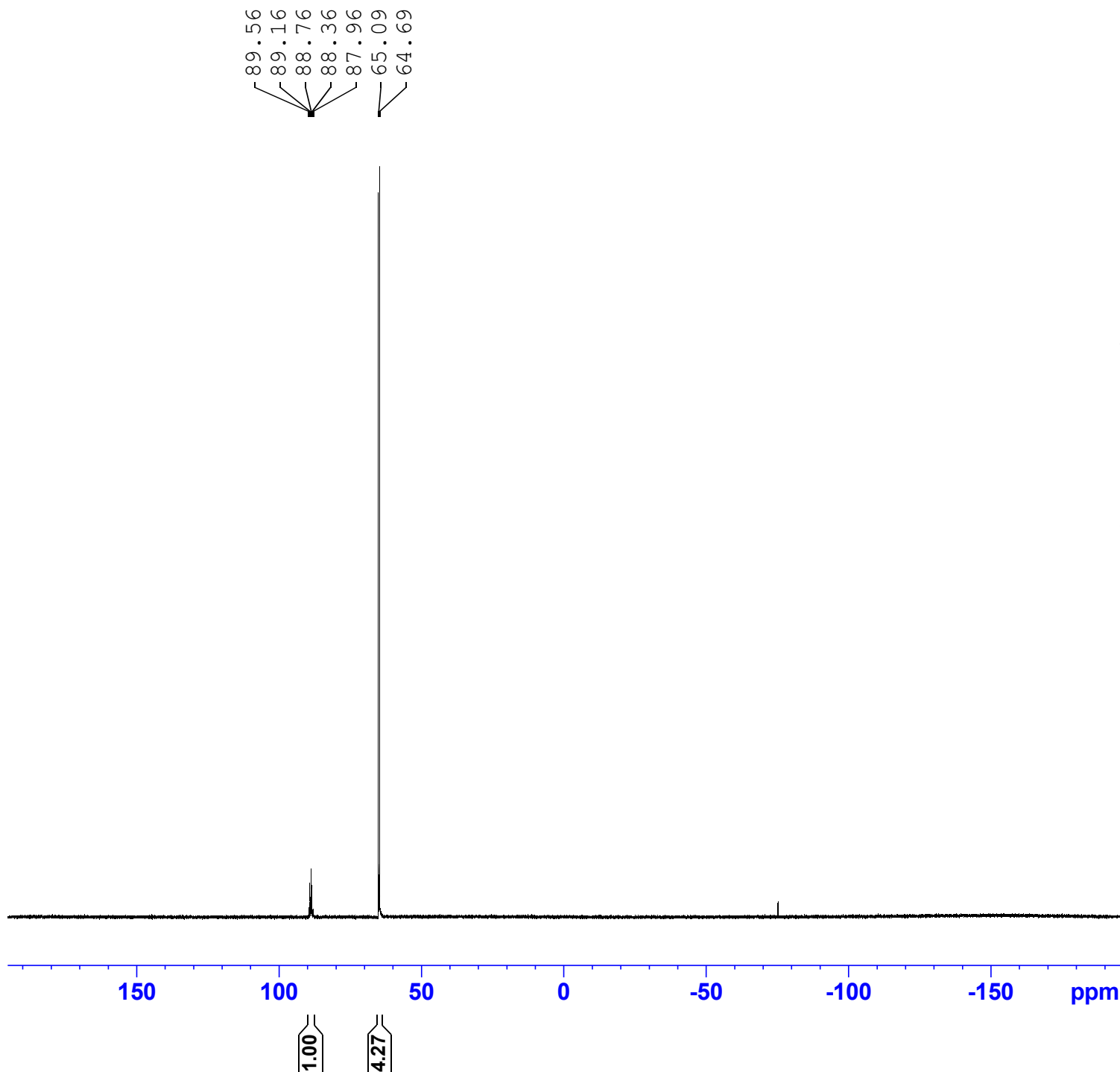




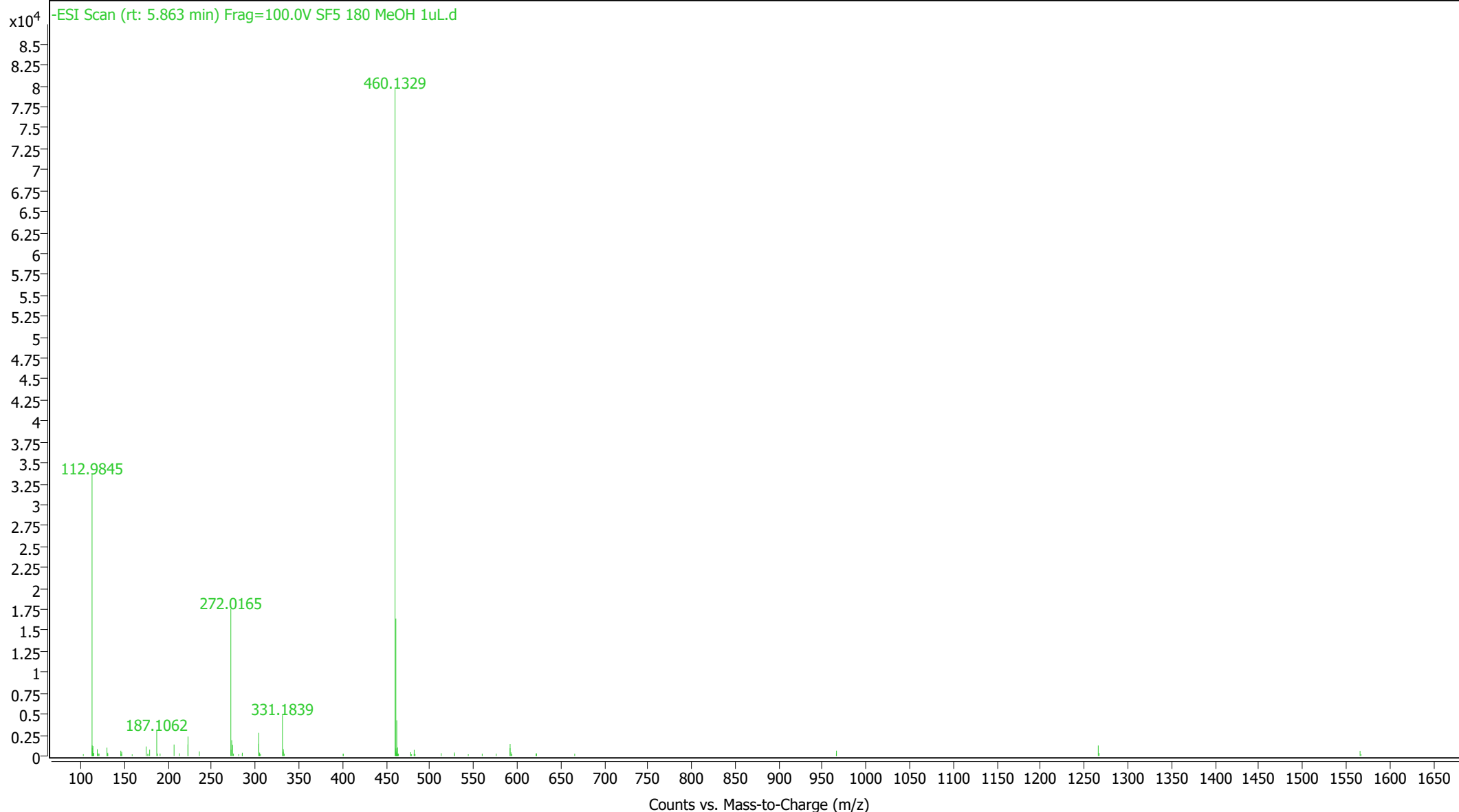
Current Data Parameters
 NAME SF5 Acrylamide Conj - 19F Good
 EXPNO 14
 PROCNO 1

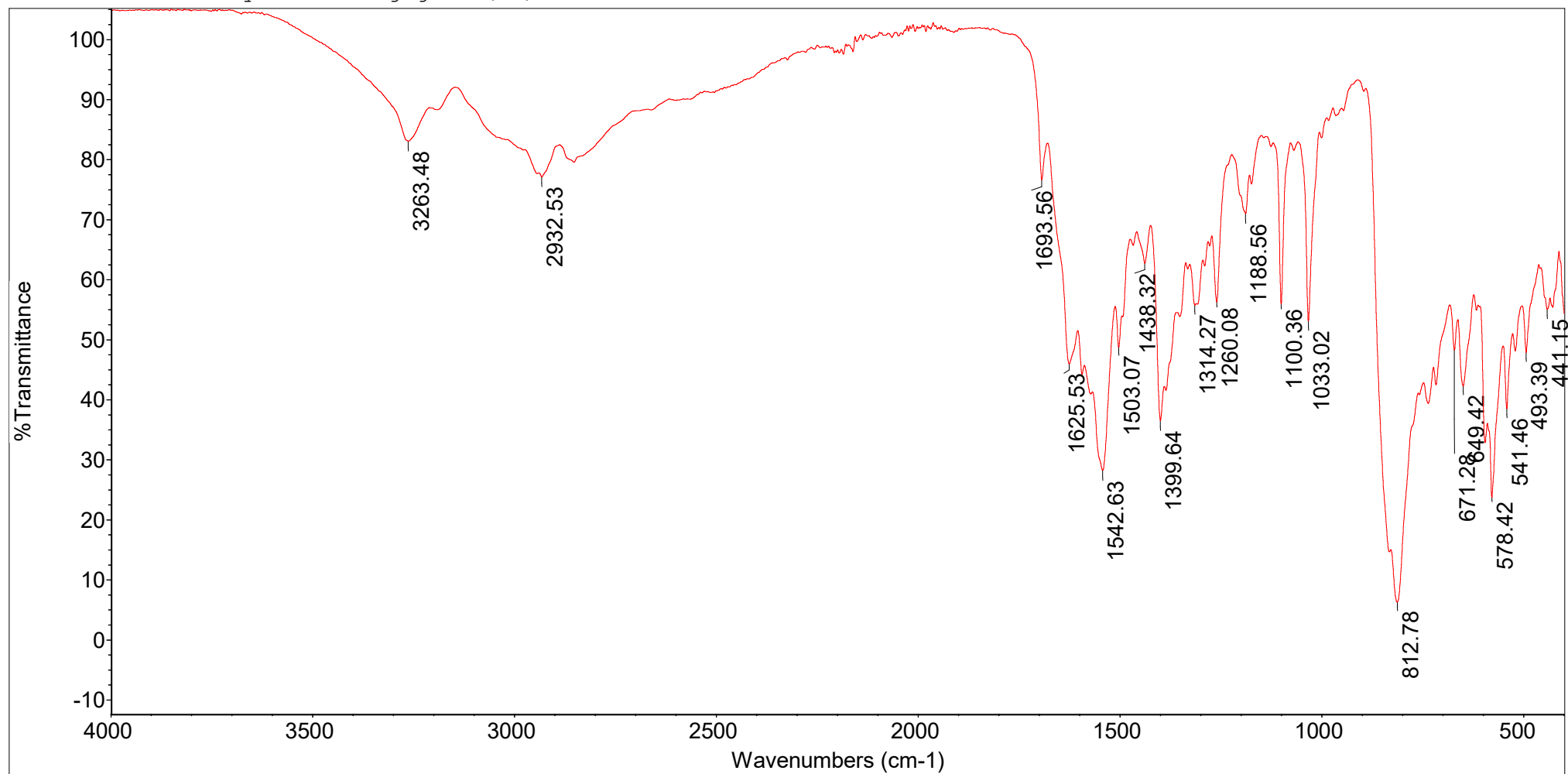
F2 - Acquisition Parameters
 Date_ 20230124
 Time 10.44 h
 INSTRUM AVNEO
 PROBHD Z175272_0008 (
 PULPROG zg
 TD 131072
 SOLVENT DMSO
 NS 128
 DS 4
 SWH 147058.828 Hz
 FIDRES 2.243940 Hz
 AQ 0.4456448 sec
 RG 101
 DW 3.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 376.5171850 MHz
 NUC1 19F
 P1 12.00 usec
 PLW1 45.00000000 W

F2 - Processing parameters
 SI 65536
 SF 376.5171850 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



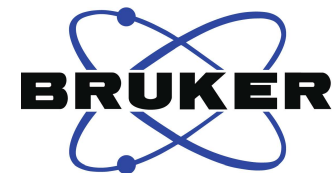
Name	SF5 Acrylamide Conj (6a)	Rack Pos.		Instrument	Instrument 1	Operator	
Inj. Vol. (ul)	10	Plate Pos.		IRM Status	Success		
Data File	SF5 180 MeOH 1uL.d	Method (Acq)	Neg Method (rev).m	Comment		Acq. Time (Local)	2022-11-30 3:53:18 PM (UTC+11:00)





CF3 acryl conj. (6b)

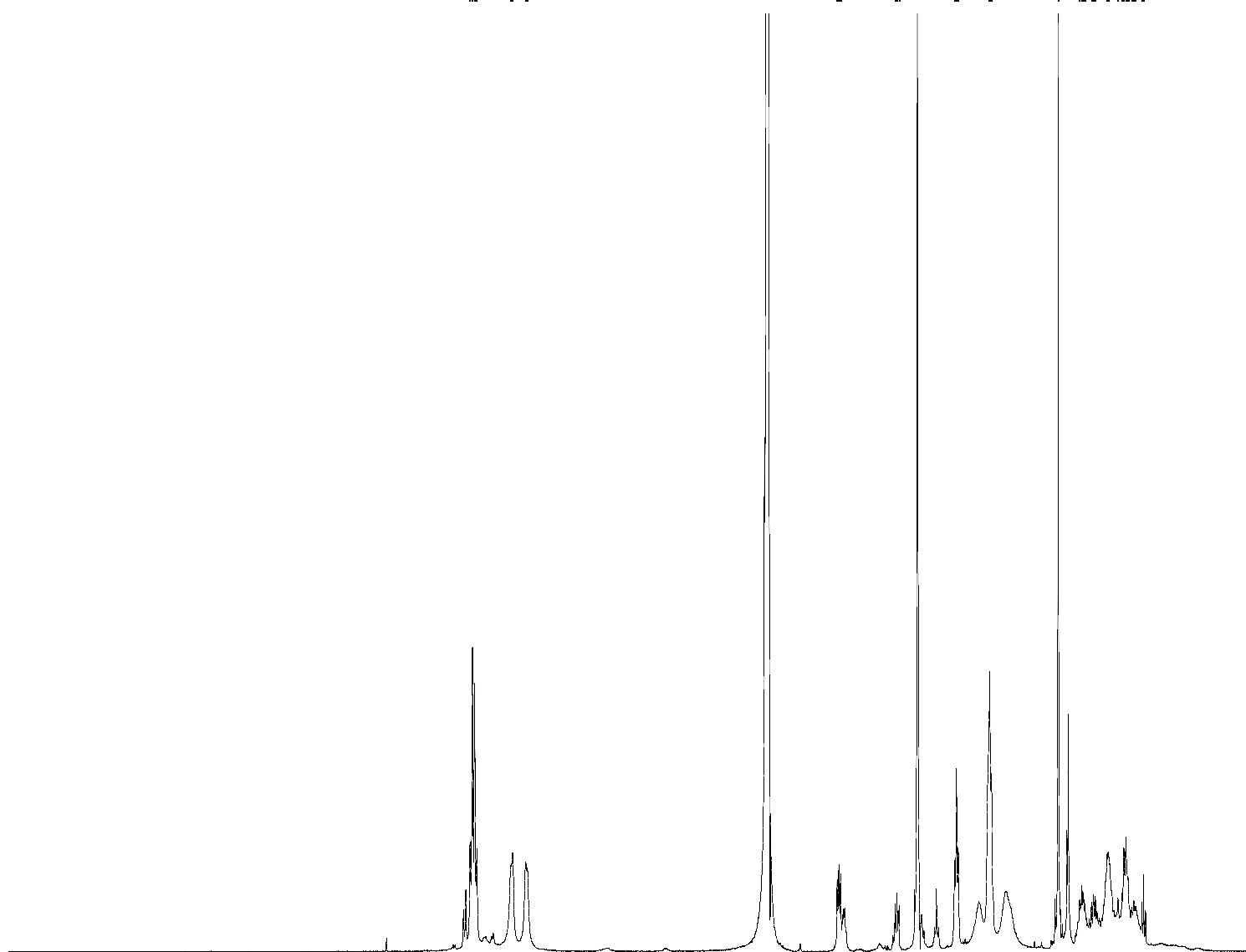
7.562
7.539
7.517
7.496
7.170
7.153
7.028
7.009
4.032
4.020
4.010
3.999
3.474
3.456
3.435
2.902
2.885
2.868
2.572
2.565
2.548
1.906
1.701
1.681
1.669
1.660
1.648
1.585
1.569
1.548
1.435
1.424
1.332
1.294
1.274
1.255
1.244
1.237
1.227
1.199
1.179
1.160
1.101
1.084



Current Data Parameters
NAME CF3 Acrylamide Conj 1H
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230201
Time_ 10.58 h
INSTRUM AVNEO
PROBHD Z175272_0008 (
PULPROG zg30
TD 131072
SOLVENT D2O
NS 32
DS 2
SWH 8196.722 Hz
FIDRES 0.125072 Hz
AQ 7.9953918 sec
RG 101
DW 61.000 usec
DE 13.54 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1524709 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 19.63299942 W

F2 - Processing parameters
SI 65536
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



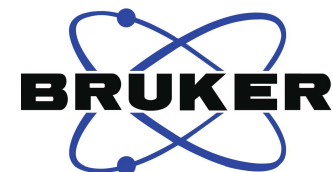
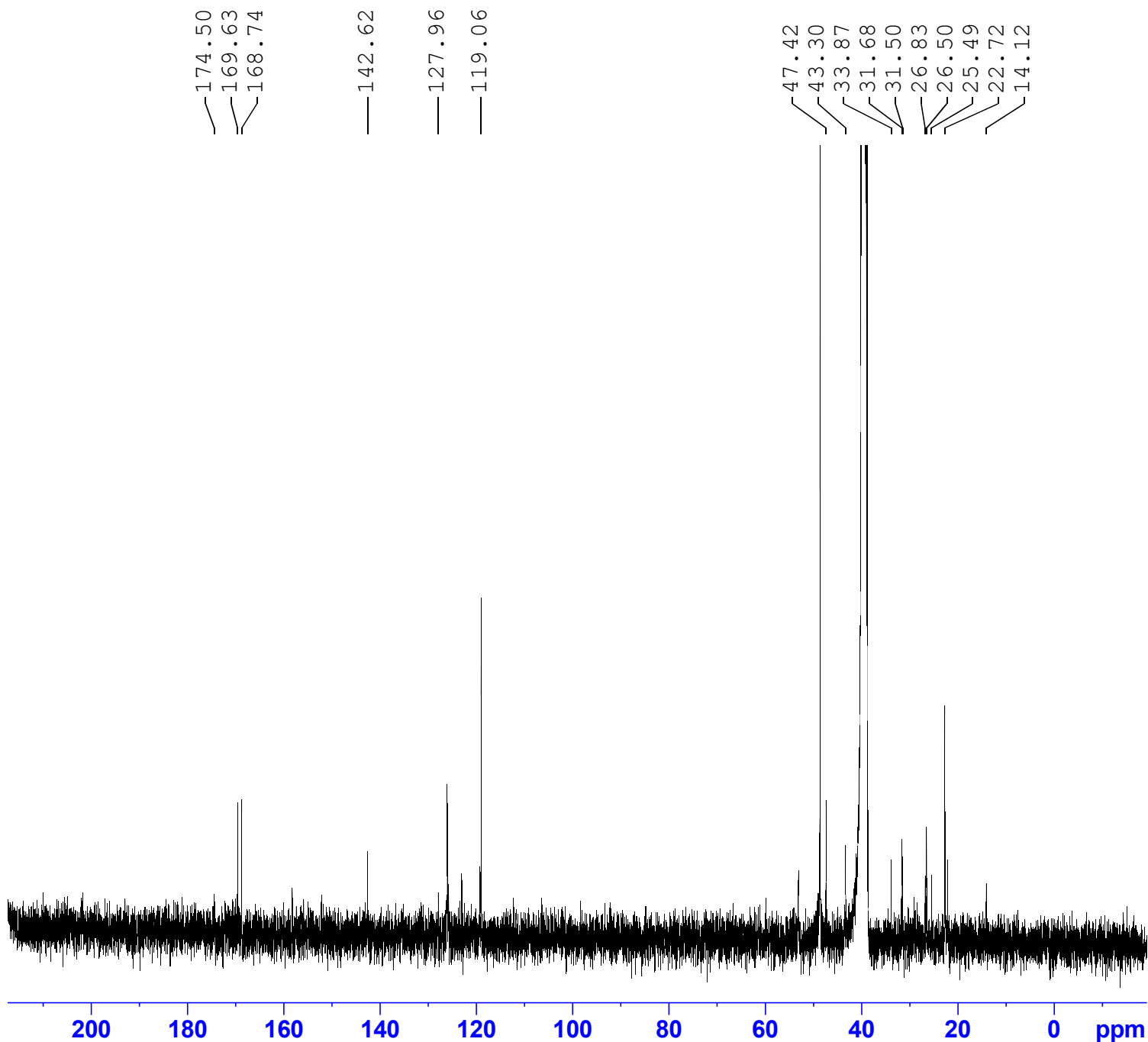
11 10 9 8 7 6 5 4 3 2 1 ppm

4.00
1.69
1.71

1.88
0.79
1.94
3.97

3.03
10.06

CF3 Acrylamide Conj (6b)



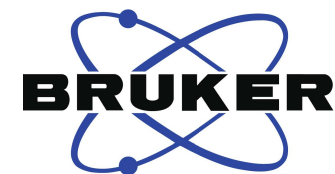
Current Data Parameters
NAME CF3 Acrylamide Conj 13C
EXPNO 17
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230131
Time_ 2.31 h
INSTRUM AVNEO
PROBHD Z175272_0008 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO-Ed
NS 4200
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6278593 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 58.38199997 W
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 19.63299942 W
PLW12 0.24237999 W
PLW13 0.12192000 W

F2 - Processing parameters
SI 32768
SF 100.6178914 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CF3 Acrylamide Conj (6b)

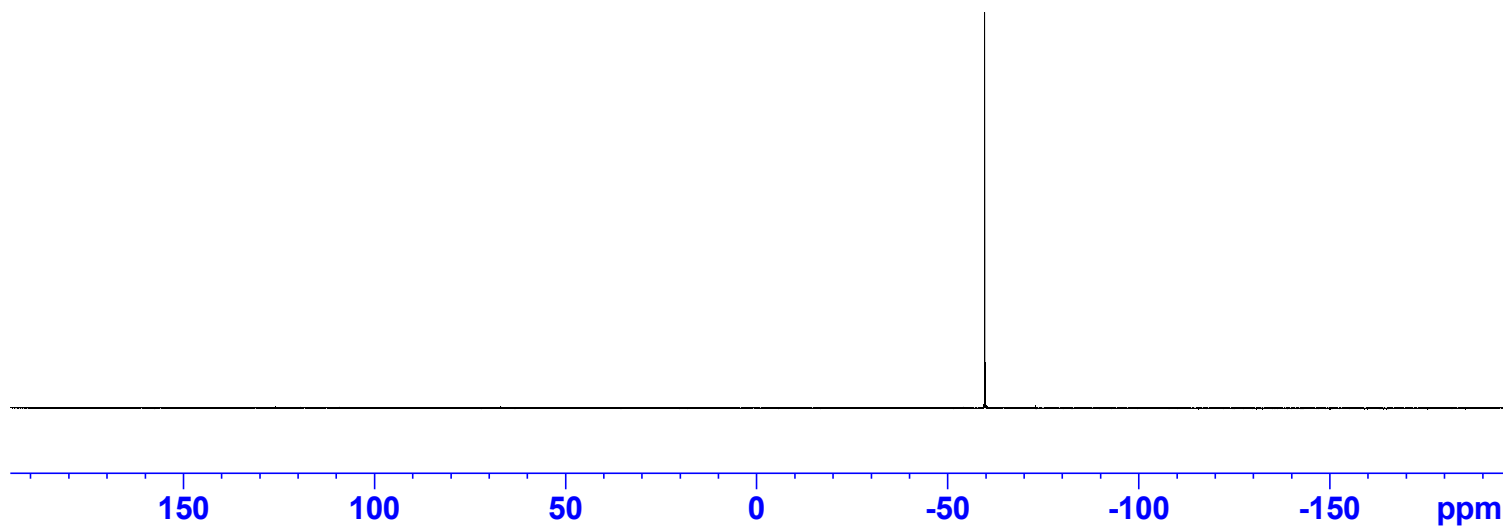
— -59.78



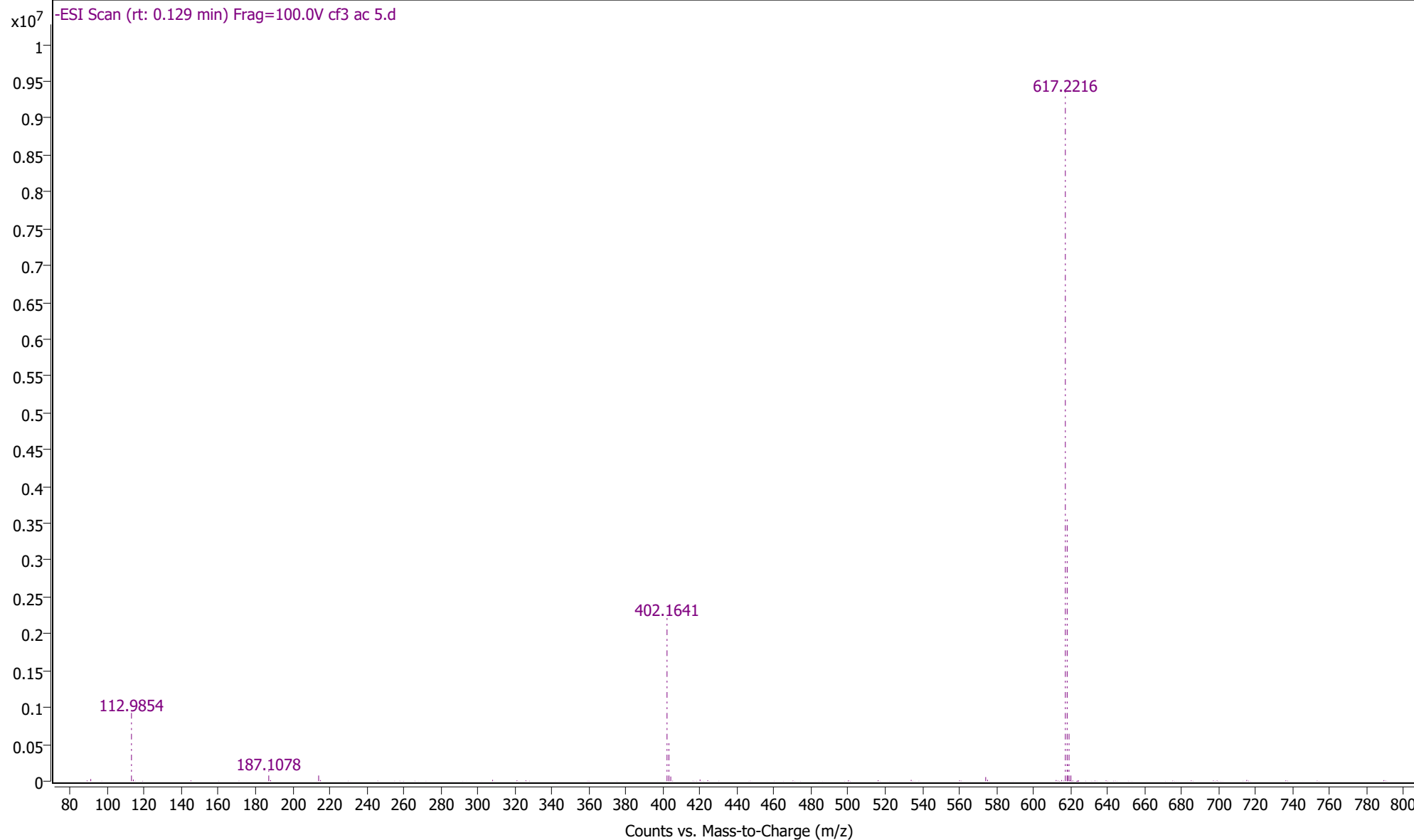
Current Data Parameters
NAME CF3 Acrylamide Conj 19f
EXPNO 16
PROCNO 1

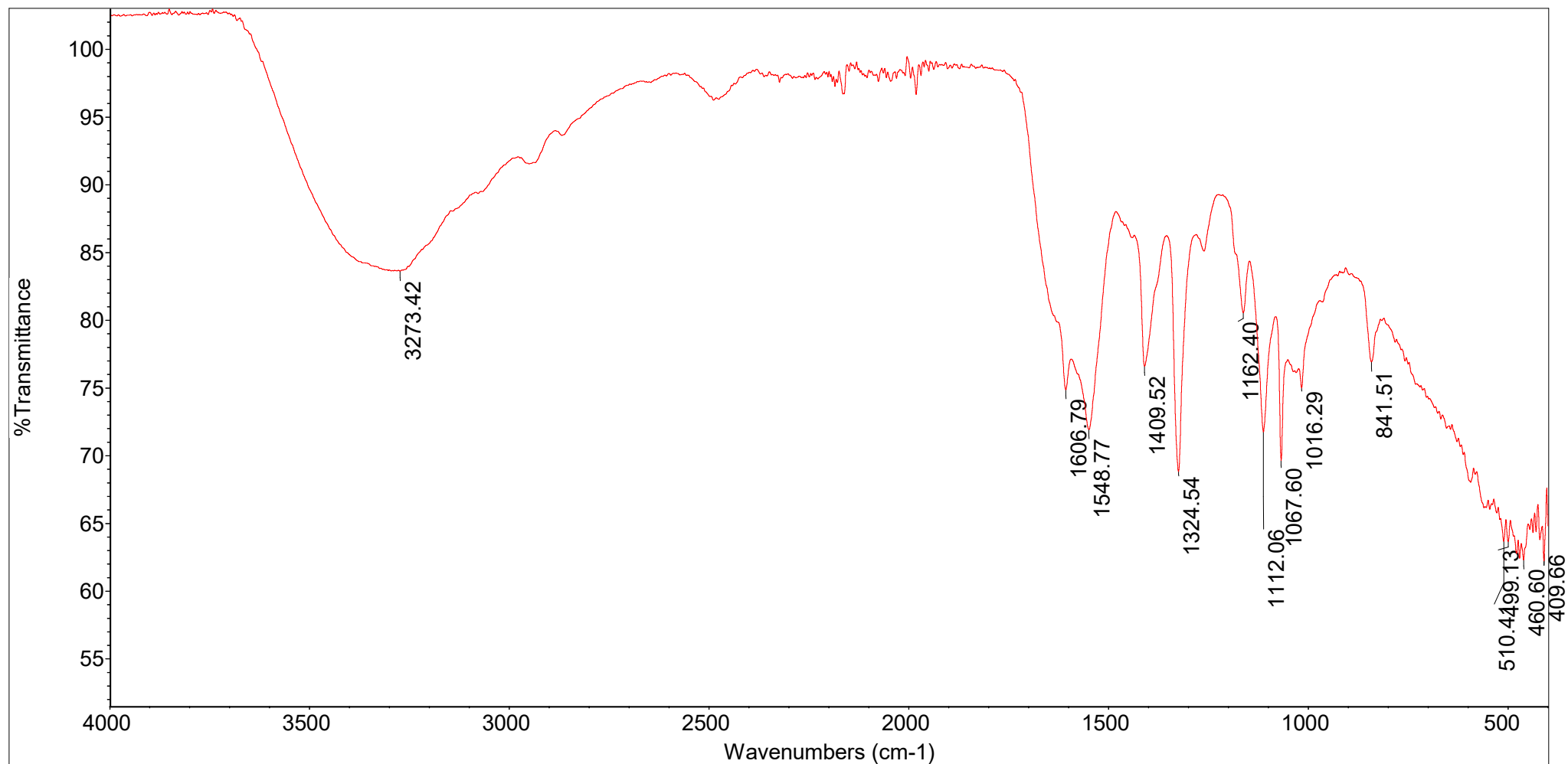
F2 - Acquisition Parameters
Date_ 20230130
Time_ 22.27 h
INSTRUM AVNEO
PROBHD Z175272_0008 (
PULPROG zg
TD 131072
SOLVENT DMSO-Ed
NS 128
DS 4
SWH 147058.828 Hz
FIDRES 2.243940 Hz
AQ 0.4456448 sec
RG 101
DW 3.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 376.5171850 MHz
NUC1 19F
P1 12.00 usec
PLW1 45.00000000 W

F2 - Processing parameters
SI 65536
SF 376.5171850 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

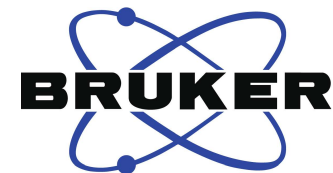
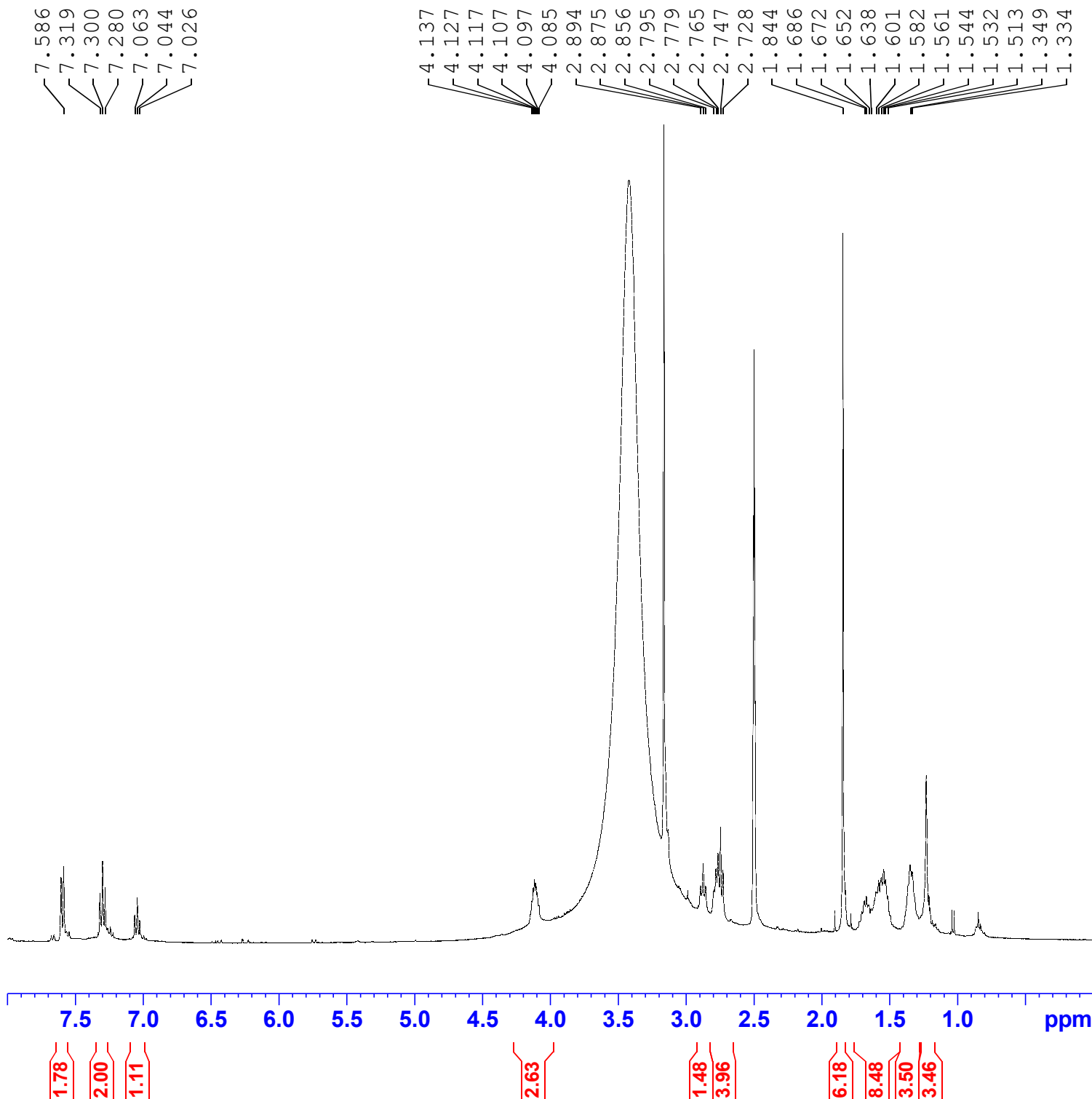


Name	CF3 Acrylamide conjugate (6b)	Rack Pos.		Instrument		Instrument 1	Operator
Inj. Vol. (ul)	5	Plate Pos.		IRM Status		Some ions missed	
Data File	cf3 ac 5.d	Method (Acq)	Hugh Method direct inj	Comment			Acq. Time (Local)
			NEGATIVE.m				2023-01-23 11:23:36 AM (UTC+11:00)





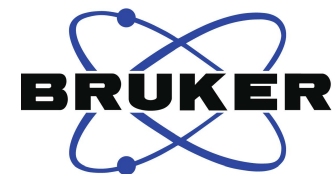
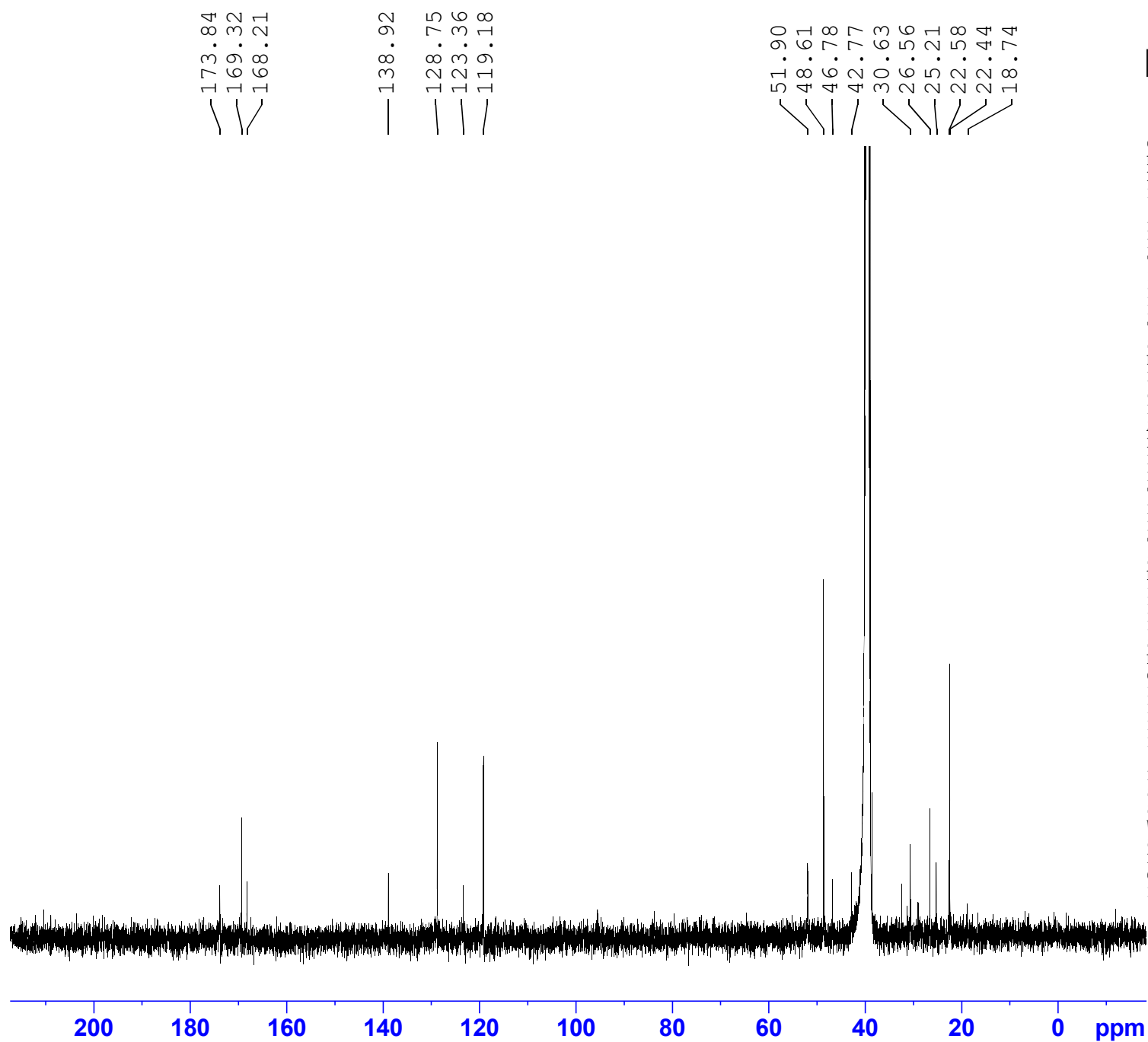
H Acrylamide Conj (6c)



Current Data Parameters
 NAME H Acrylamide Conj 1H
 EXPNO 26
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230131
 Time_ 11.22 h
 INSTRUM AVNEO
 PROBHD Z175272_0008 (
 PULPROG zg30
 TD 131072
 SOLVENT DMSO-Ed
 NS 64
 DS 2
 SWH 8196.722 Hz
 FIDRES 0.125072 Hz
 AQ 7.9953918 sec
 RG 101
 DW 61.000 usec
 DE 13.54 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1524709 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 19.63299942 W

F2 - Processing parameters
 SI 65536
 SF 400.1502111 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

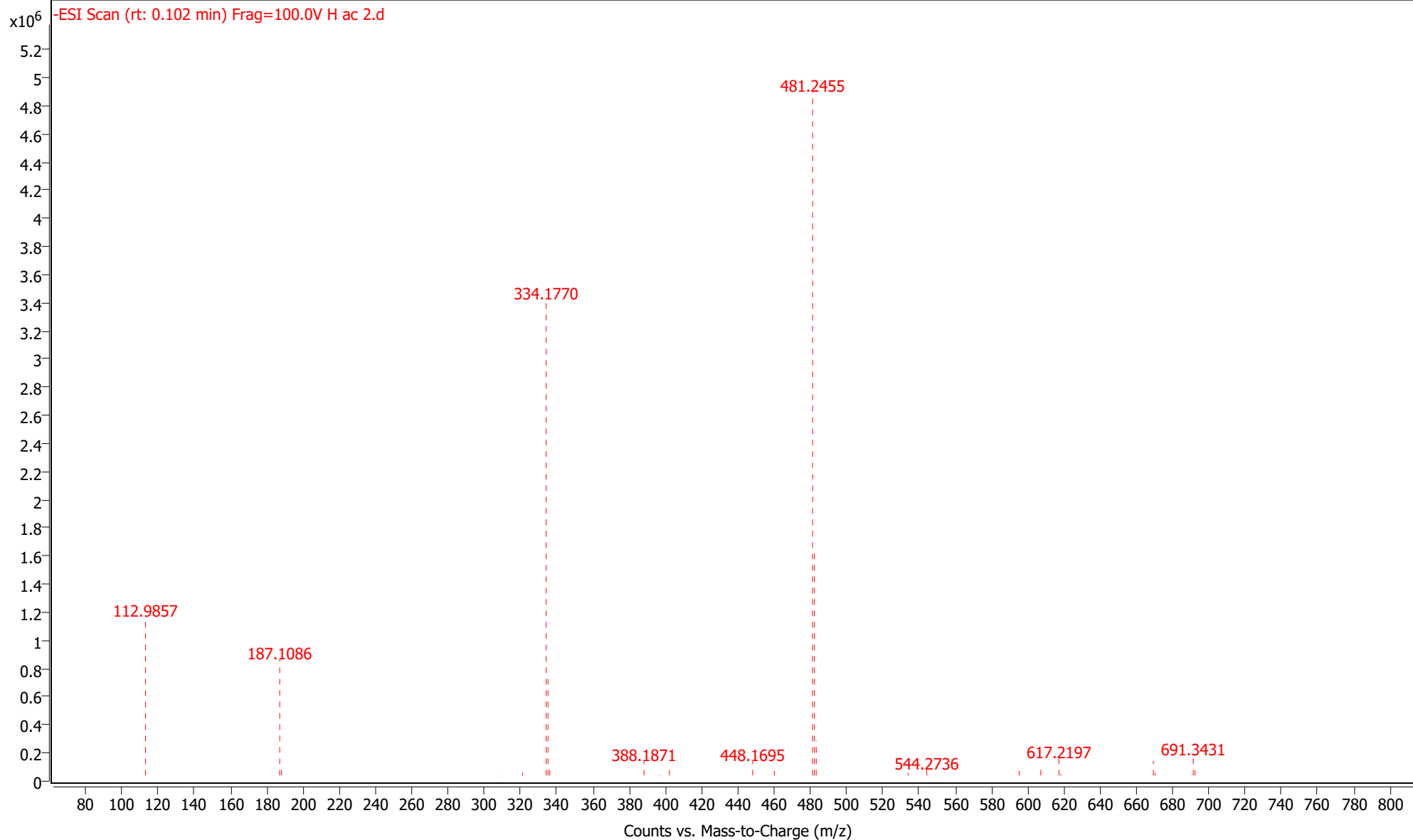


Current Data Parameters
NAME H Acrylamide Conj 13C
EXPNO 27
PROCNO 1

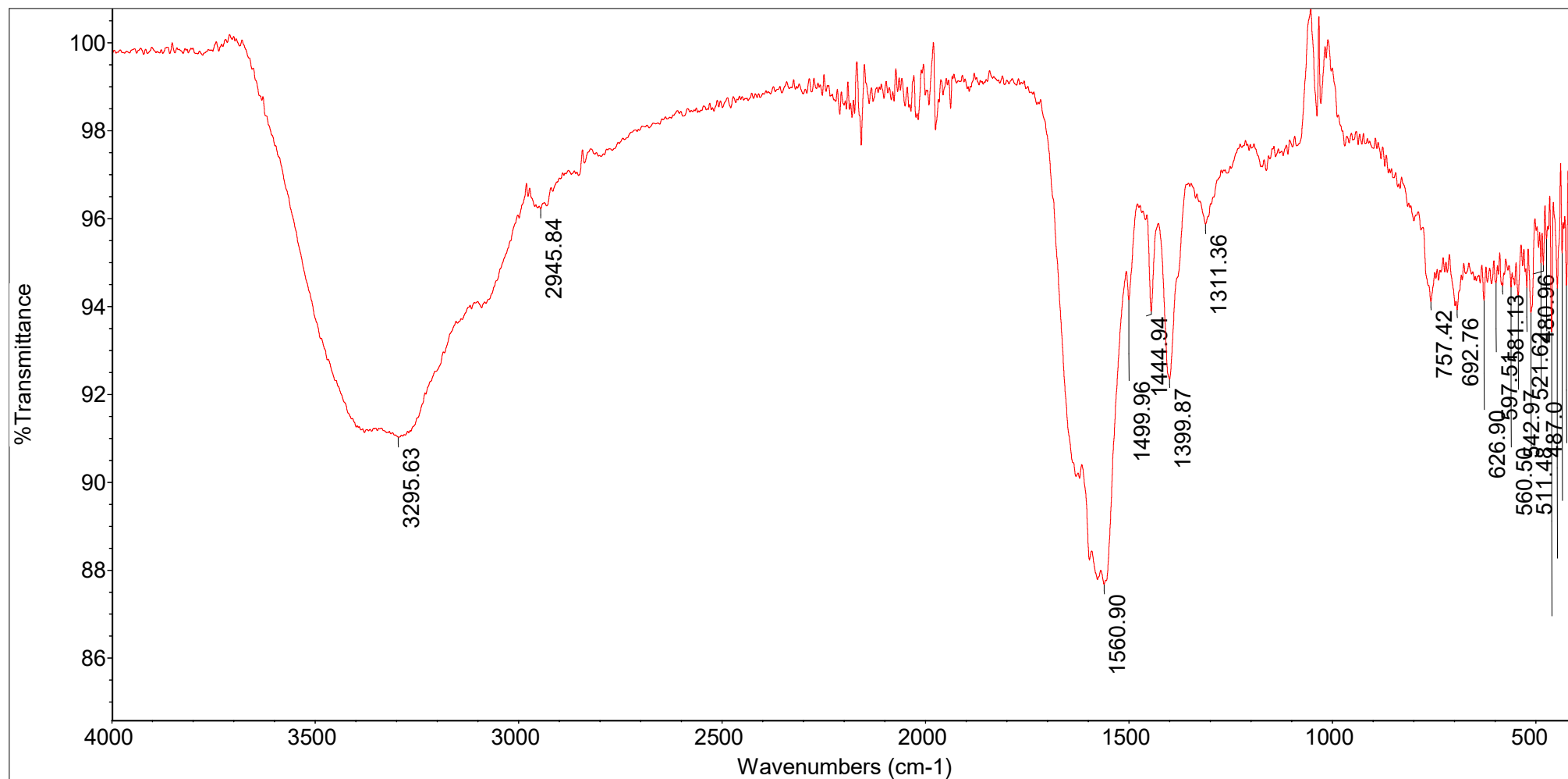
F2 - Acquisition Parameters
Date_ 20230131
Time_ 23.07 h
INSTRUM AVNEO
PROBHD Z175272_0008 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO-Ed
NS 4200
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6278593 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 58.38199997 W
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 19.63299942 W
PLW12 0.24237999 W
PLW13 0.12192000 W

F2 - Processing parameters
SI 32768
SF 100.6178948 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

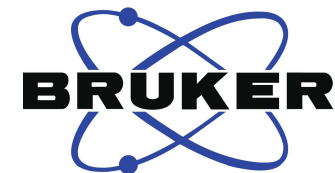
Name	H acrylamide Conjugate (6c)	Rack Pos.		Instrument		Instrument 1	Operator
Inj. Vol. (ul)	5	Plate Pos.		IRM Status		Some ions missed	
Data File	H ac 2.d	Method (Acq)	Hugh Method direct inj	Comment			Acq. Time (Local)
			NEGATIVE.m				2023-01-23 1:42:02 PM (UTC+11:00)



H acrylamide Conjugate (**6c**)



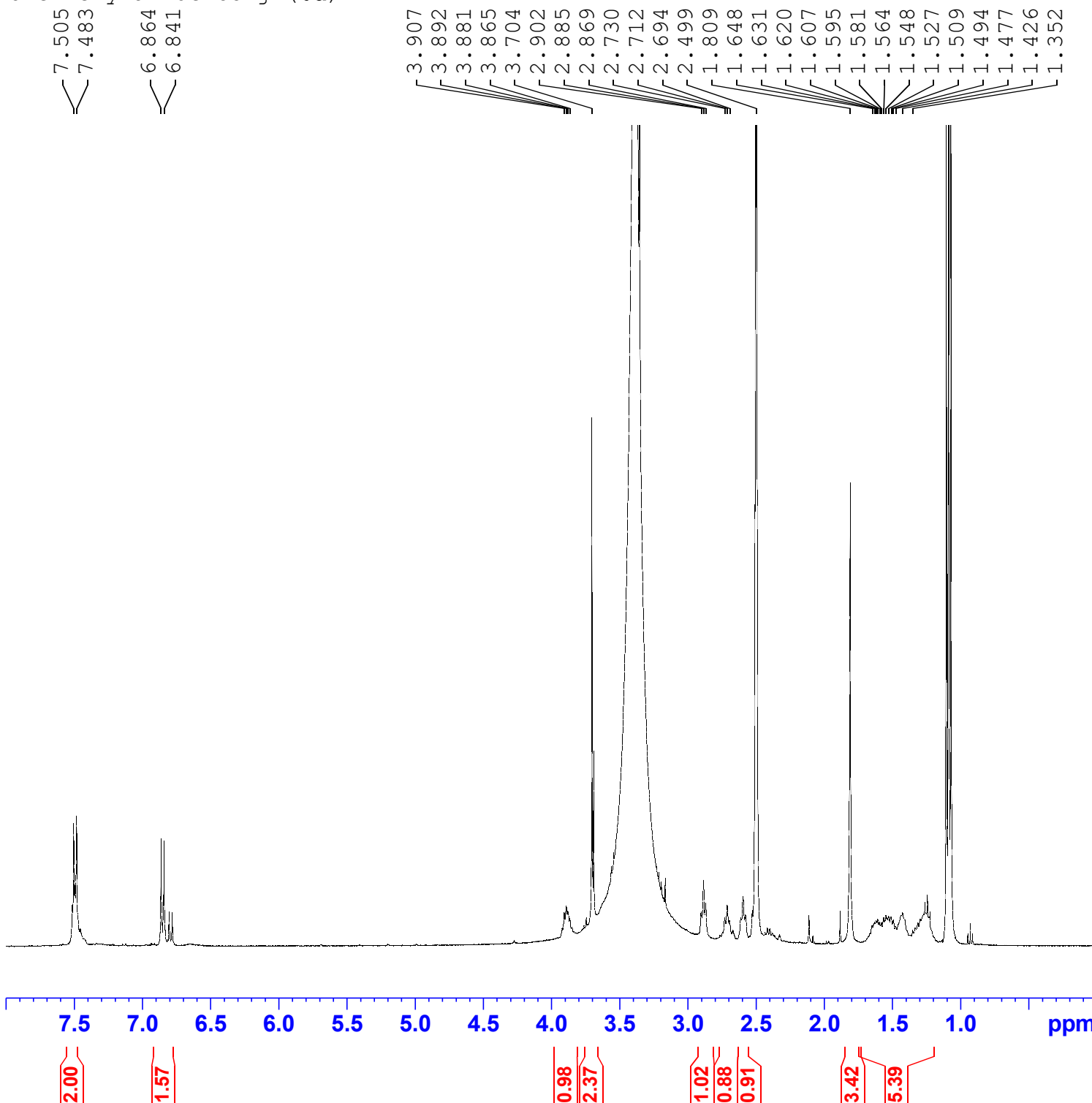
OMe Acrylamide Conj (6d)



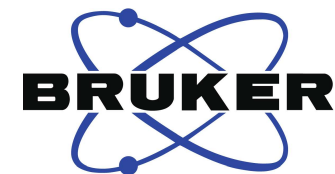
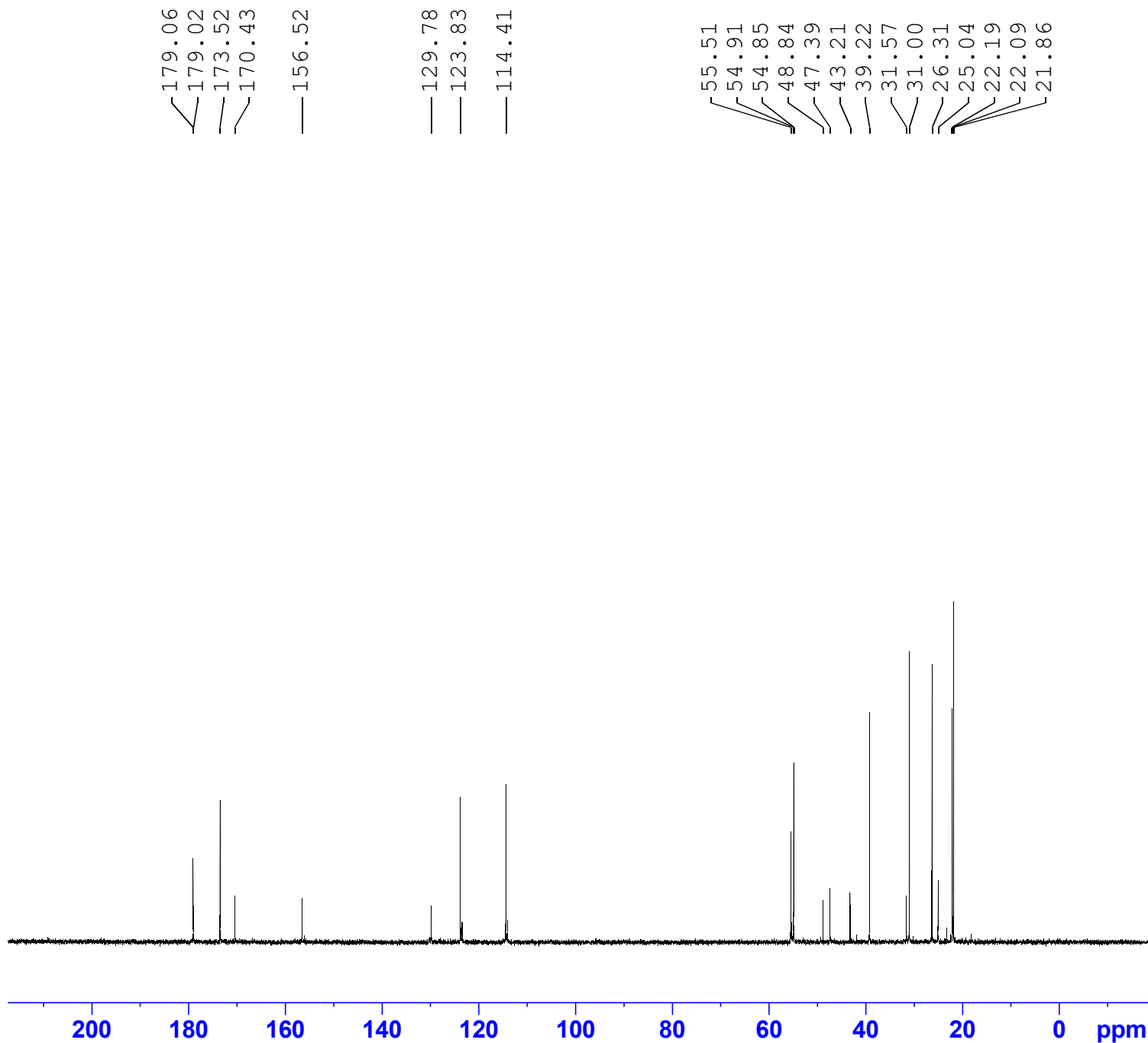
Current Data Parameters
 NAME OMe Acrylamide Conj
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230130
 Time_ 17.02 h
 INSTRUM AVNEO
 PROBHD Z175272_0008 (
 PULPROG zg30
 TD 131072
 SOLVENT DMSO-Ed
 NS 64
 DS 2
 SWH 8196.722 Hz
 FIDRES 0.125072 Hz
 AQ 7.9953918 sec
 RG 101
 DW 61.000 usec
 DE 13.54 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1524709 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 19.63299942 W

F2 - Processing parameters
 SI 65536
 SF 400.1502105 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



OMe Acrylamide Conj. (6d)



Current Data Parameters
NAME OMe Acrylamide conj 13c
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230119
Time_ 3.56 h
INSTRUM AVNEO
PROBHD Z175272_0008 (
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 3600
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6278593 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 58.38199997 W
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 19.63299942 W
PLW12 0.24237999 W
PLW13 0.12192000 W

F2 - Processing parameters
SI 32768
SF 100.6177975 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Name OMe Acrylamide conj (6d)		Rack Pos.	Instrument	Instrument 1	Operator
Inj. Vol. (ul)	5	Plate Pos.	IRM Status	Some ions missed	
Data File	OME ac 3.d	Method (Acq)	Hugh Method direct inj	Comment	Acq. Time (Local)
			NEGATIVE.m		2023-01-23 11:43:06 AM (UTC+11:00)

