Supporting Information

Studies on the [4+2] Cycloaddition and Allylic Substitution of Indole-fused Zwitterionic π-Allylpalladium

Zhengyu Han,[1,2] Yu Xue,[1] Xiang Li,[1] Xinzhe Hu,[1] Xiu-Qin Dong,[4] Jianwei Sun,[3] Hai Huang[1,*]

[1] *Jiangsu Key Laboratory of Advanced Catalytic Materials & Technology, School of Petrochemical Engineering, Changzhou University, Changzhou 213164, China*

[2] *Jiangsu Province Key Laboratory of Fine Petrochemical Engineering, Changzhou University, Changzhou 213164, China*

[3] *Department of Chemistry, The Hong Kong University of Science and Technology, Clethyl acetater Water Bay, Kowloon, Hong Kong SAR (China)*

[4] *College of Chemistry and Molecular Sciences, Engineering Resethyl acetaterch Center of Organosilicon Compounds & Materials, Ministry of Education, Wuhan University, Wuhan, Hubei, 430072, China*

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HPLC and NMR Spectra

I. General Information

Flash column chromatography was performed over silica gel (200-300 mesh) purchased from Qindao Puke Co. Lit., China. All air or moisture sensitive rethyl acetatections were conducted in oven-dried glassware under nitrogen atmosphere using anhydrous solvents. Anhydrous toluene, dichloromethane and tetrahydrofuran were purified by the Innovative® solvent purification system. Other anhydrous solvents were purchased from J&K Scientific. ^{1}H, ^{13}C, and ^{19}F NMR spectra were collected on a Bruker AV 400 or AV 300 MHz NMR spectrometer using residue solvent pethyl acetateks as an internal standard (^{1}H NMR: CDCl$_3$ at 7.26 ppm; ^{13}C NMR: CDCl$_3$ at 77.15 ppm). HRMS spectra were collected on an Agilent GC/MS 5975C system, a MALDI Micro MX mass spectrometer, or an API QSTAR XL System with TOF as mass analyzer.

II. Preparation of Substrates

General Procedure A for the Preparation of Indoloxazinones 1.
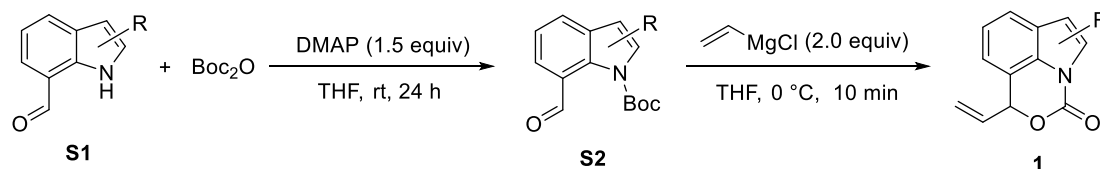
To a solution of indole-7-carboxaldehyde **S1** (0.73 g, 5.0 mmol, 1.0 equiv), *N,N*-dimethylpyridin-4-amine (DMAP) (0.92 g, 7.5 mmol, 1.5 equiv) in THF (15 mL) was added Boc$_2$O (2.18 g, 10.0 mmol, 2.0 equiv). Then the reaction mixture was stirred under room temperature for 24 h. The reaction mixture was quenched by saturated Na$_2$CO$_3$ solution (20 mL), extracted by ethyl acetate (20 mL x 3). Combined organic phase were washed by water, brine and dried over anhydrous Na$_2$SO$_4$, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate = 3:1) to afford the desired product **S2** in 90% Yield (1.10 g).

Under N$_2$ atmosphere at 0 °C, to a solution of **S2** (1.10 g, 4.5 mmol, 1.0 equiv) in anhydrous THF (13.5 mL) was added dropwise vinyl magnesium chloride (4.5 mL, 2.0 M in THF, 2.0 equiv). Then the reaction mixture was stirred at 0 °C for 10 min. The reaction mixture was quenched with saturated NH$_4$Cl solution and extracted with ethyl acetate (20 mL x 3). The combined organic layers were dried with Na$_2$SO$_4$ and evaporated under reduced pressure. The residue was purified by chromatography on silica gel (petroleum ether/ethyl acetate) to afford the desired indoloxazinones **1**.
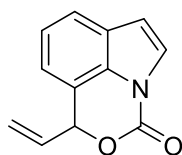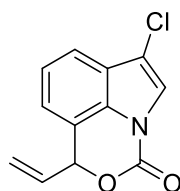

1a

1-Vinyl-1*H*,3*H*-[1,3]oxazino[5,4,3-*hi*]indol-3-one (1a) was prepared according to the General Procedure A as a pink solid (chromatography eluent: petroleum ether/ethyl acetate = 9:1) in 36% yield (322.4 mg).

¹H NMR (400MHz, CDCl$_3$) δ 7.62 (d, *J* = 3.6 Hz, 1H), 7.53 (d, *J* = 7.9 Hz, 1H), 7.27 (t, *J* = 7.5 Hz, 1H), 7.02 (d, *J* = 7.4 Hz, 1H), 6.70 (d, *J* = 3.6 Hz, 1H), 6.31 (d, *J* = 6.9 Hz, 1H), 6.17-6.09 (m, 1H), 5.52-5.43 (m, 2H) ppm.

¹³C NMR (100MHz, CDCl$_3$) δ 145.9, 134.3, 132.0, 127.5, 124.2 (2 C), 120.9, 119.9, 118.7, 117.2, 109.7, 84.3 ppm.

HRMS (CI⁺) Calcd for C$_{12}$H$_9$NNaO$_2$ [M + Na]⁺: 222.0531, Found: 222.0523.

1b

6-Chloro-1-vinyl-1*H*,3*H*-[1,3]oxazino[5,4,3-*hi*]indol-3-one (1b) was prepared according to the General Procedure A as a yellow solid (chromatography eluent: petroleum ether/ethyl acetate = 9:1) in 30% yield (182.2mg).

¹H NMR (400MHz, CDCl$_3$) δ 7.58 (s, 1H), 7.53 (d, *J* = 7.9 Hz, 1H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.08 (d, *J* = 7.3 Hz, 1H), 6.31 (d, *J* = 6.8 Hz, 1H), 6.16-6.07 (m, 1H), 5.51-5.45 (m, 2H) ppm.

¹³C NMR (100MHz, CDCl$_3$) δ 144.8, 133.9, 131.3, 125.4, 124.8, 120.5, 120.3, 119.9, 118.8, 117.3, 115.2, 84.3 ppm.

HRMS (CI⁺) Calcd for C$_{12}$H$_8$ClNNaO$_2$ [M + Na]⁺: 256.0142, Found: 256.0149.

III. Asymmetric Synthesis of Chiral 3a
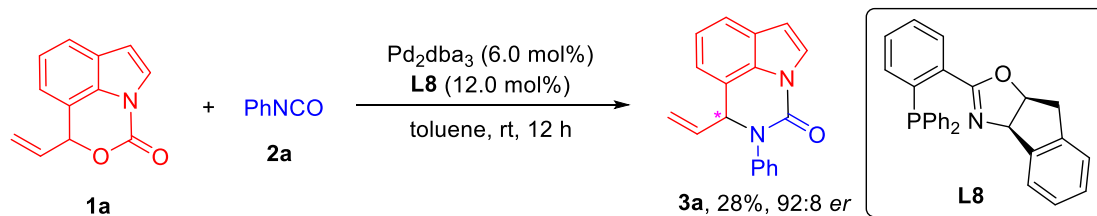
Under N$_2$ at room temperature, to a solution of indoloxazinones **1a** (119.4 mg, 0.6 mmol, 2.0 equiv) and isocyanatobenzene **2a** (35.7 mg, 0.3 mmol, 1.0 equiv) in toluene (5.0 mL) was added Pd$_2$dba$_3$ (16.5 mg, 0.018 mmol, 6.0 mol%) and **L8** (15.1 mg, 0.036 mmol, 12.0 mol%). Then the reaction mixture was stirred at room temperature for 12 h. The reaction mixture was directly concentrated and purified by silica gel column chromatography (petroleum ether/ethyl acetate) to afford the desired products **3a** (23.0 mg, 28%).

[α]$_D^{25}$: +12.3 (c = 0.12, CHCl$_3$). HPLC (AD, i-PrOH/n-hexane = 10/90, flow rate = 1.0 mL/min, l = 210 nm) t$_R$ = 14.17 min (major), 15.92 min (minor).

HPLC and NMR spectra

Agilent Technologies

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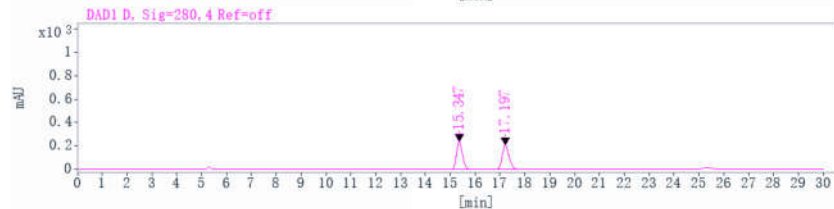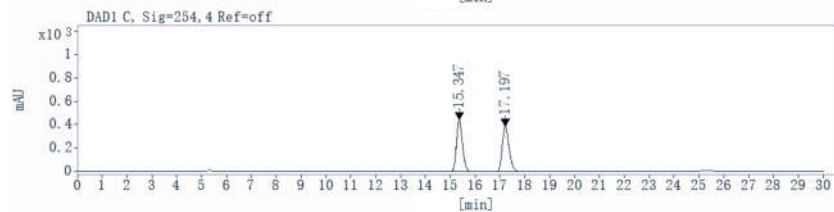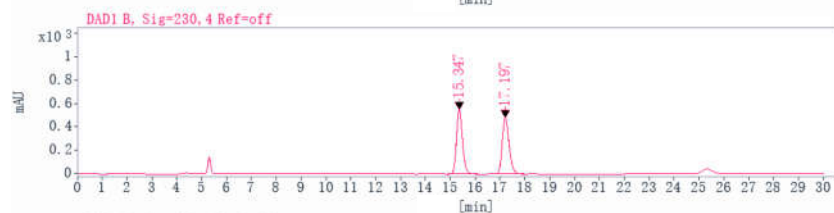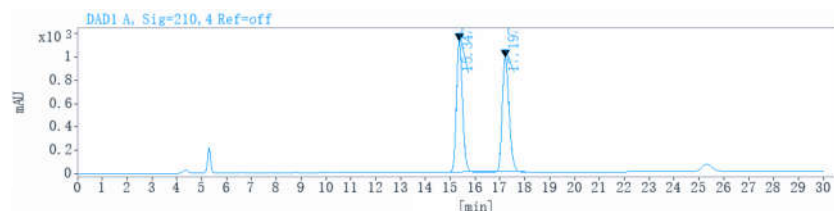
Agilent Technologies

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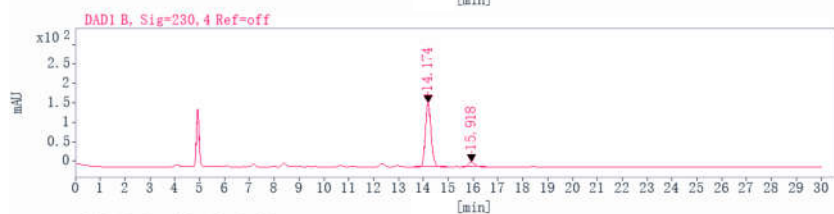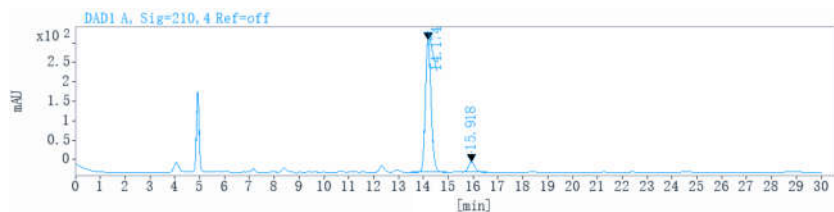| RetTime [min]	Type	Width[min]	Area[mAu*s]	Height [mAu\U]	Area% Name
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rac-**3a**

Agilent Technologies
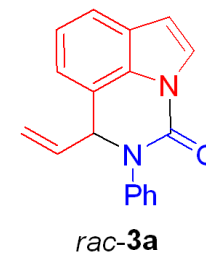
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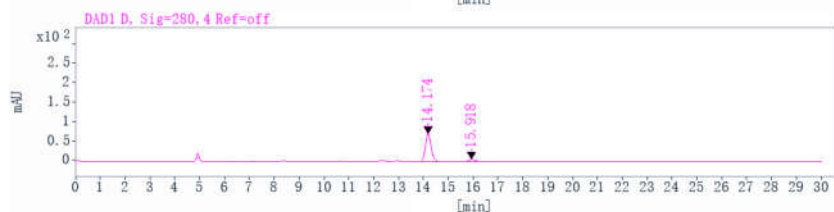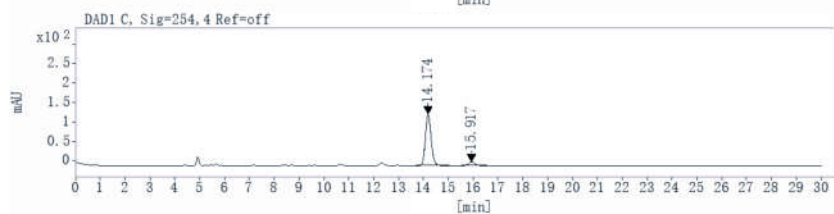
Agilent Technologies

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3a

XY-3-99-H

1a

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7.030
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6.154
6.146
6.129
6.111
6.103
6.086
5.518
5.516
5.514
5.476
5.471
5.456
5.454
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0.93
0.97
2.09

BRUKER
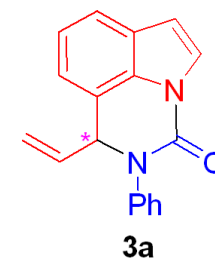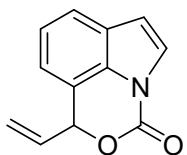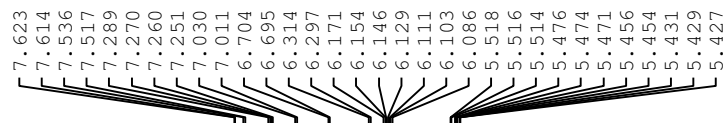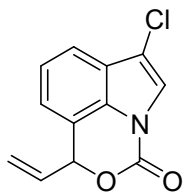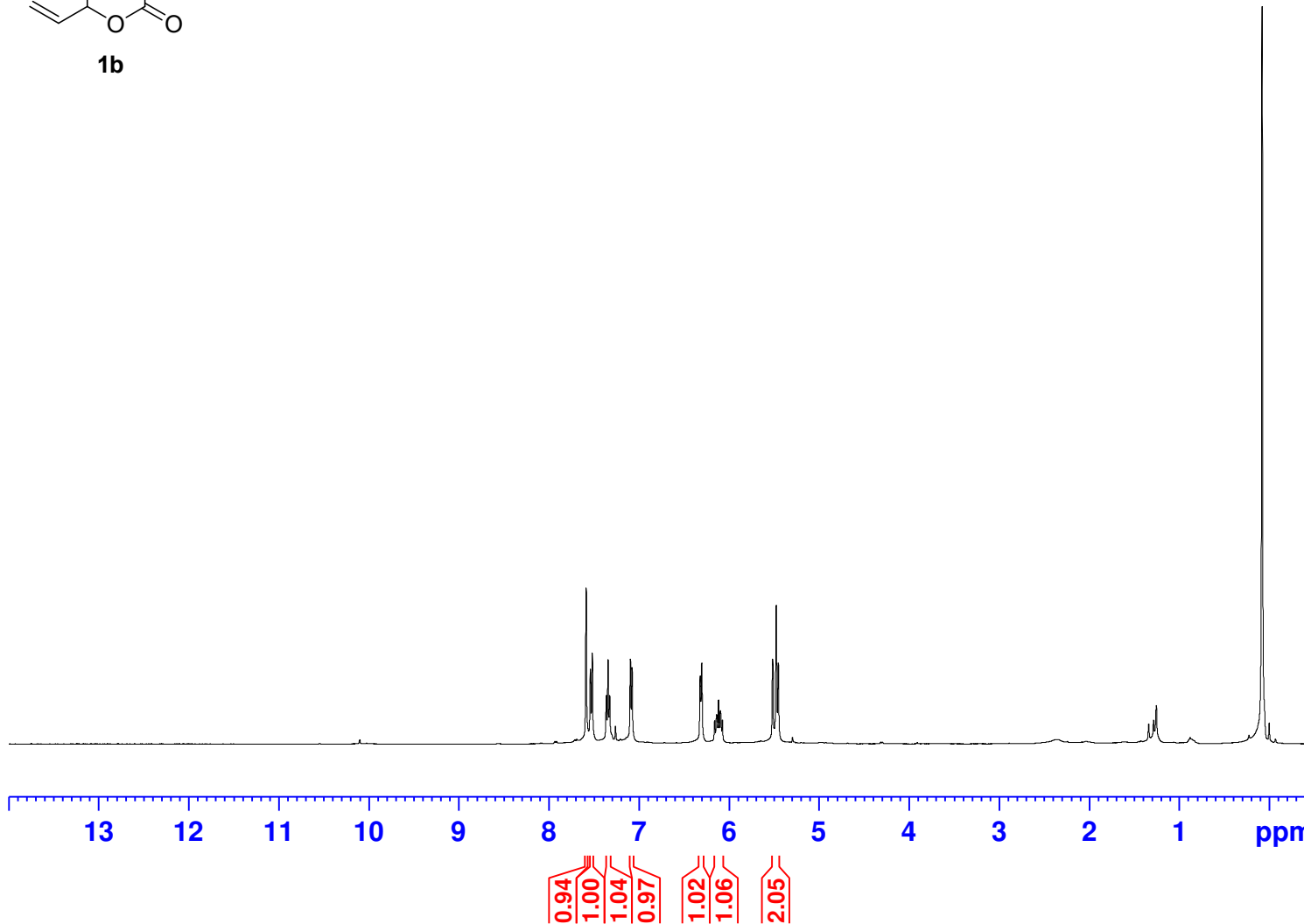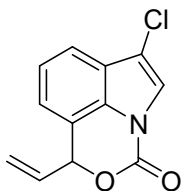
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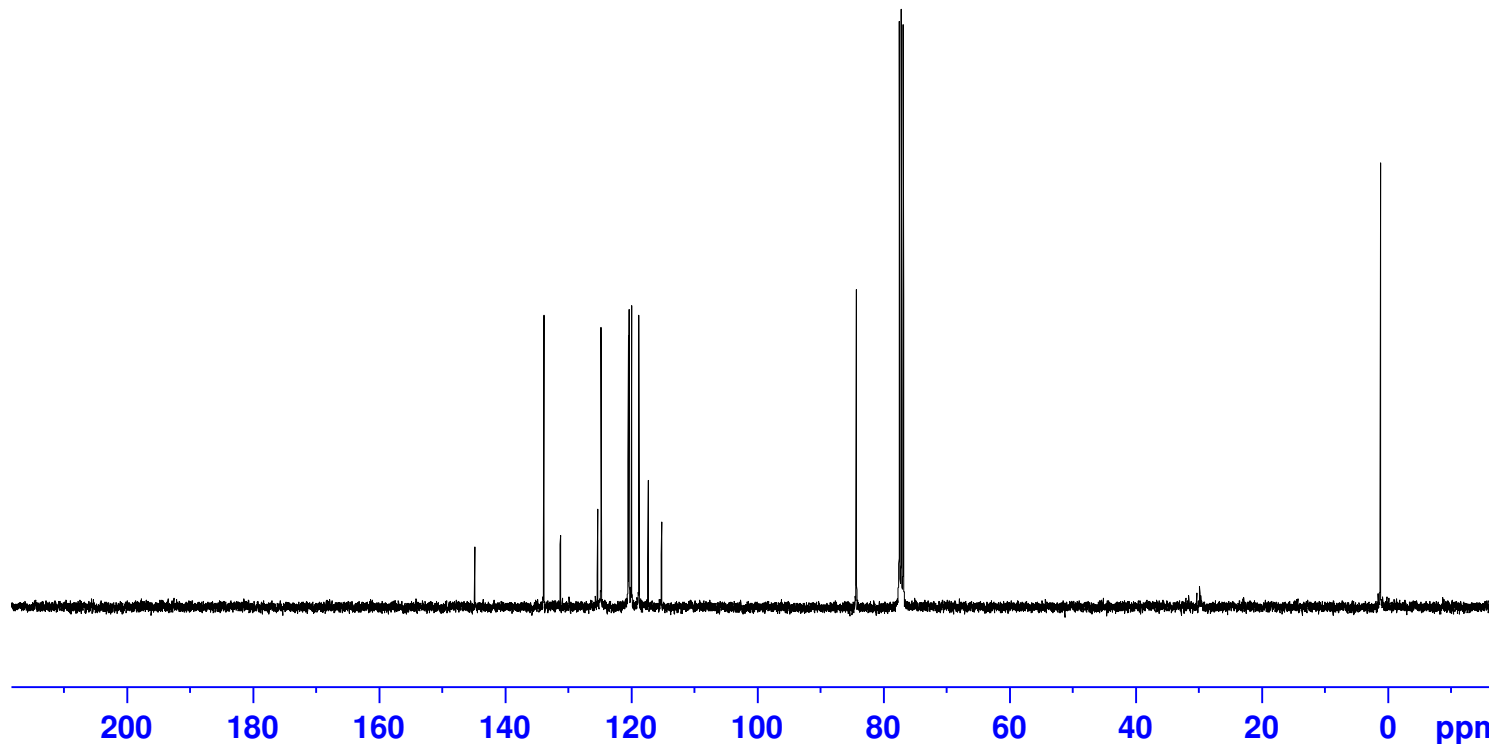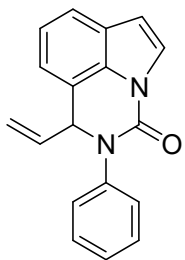SSB   0
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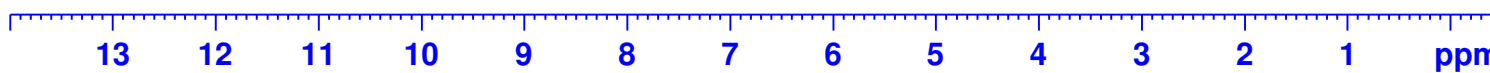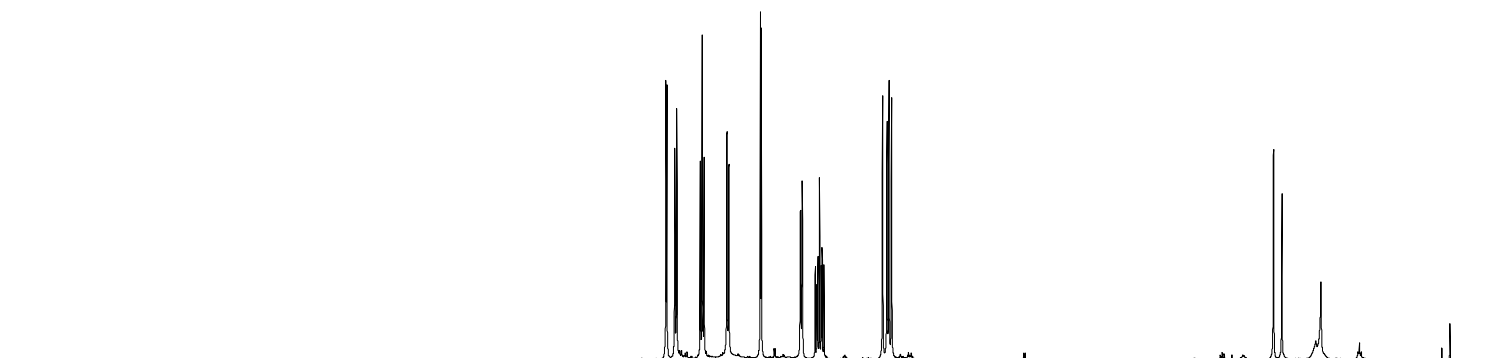
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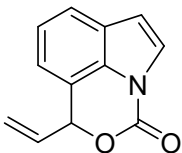
1a

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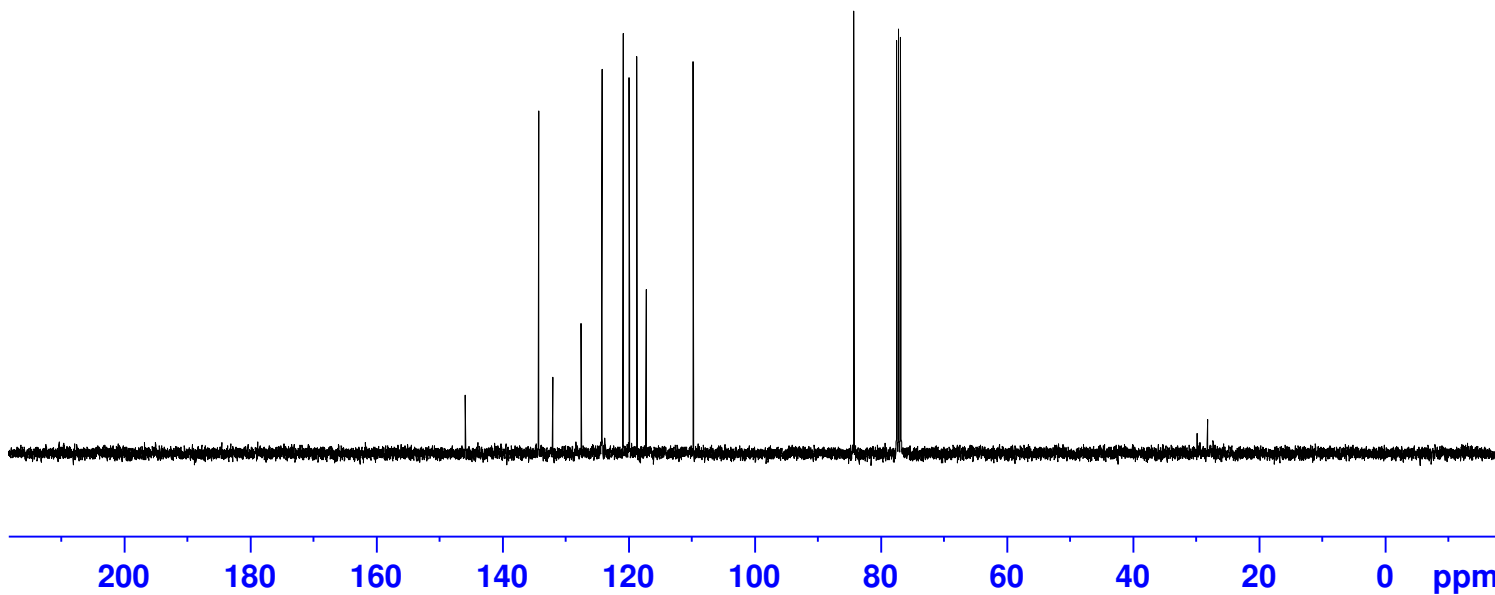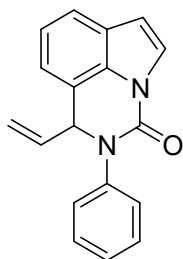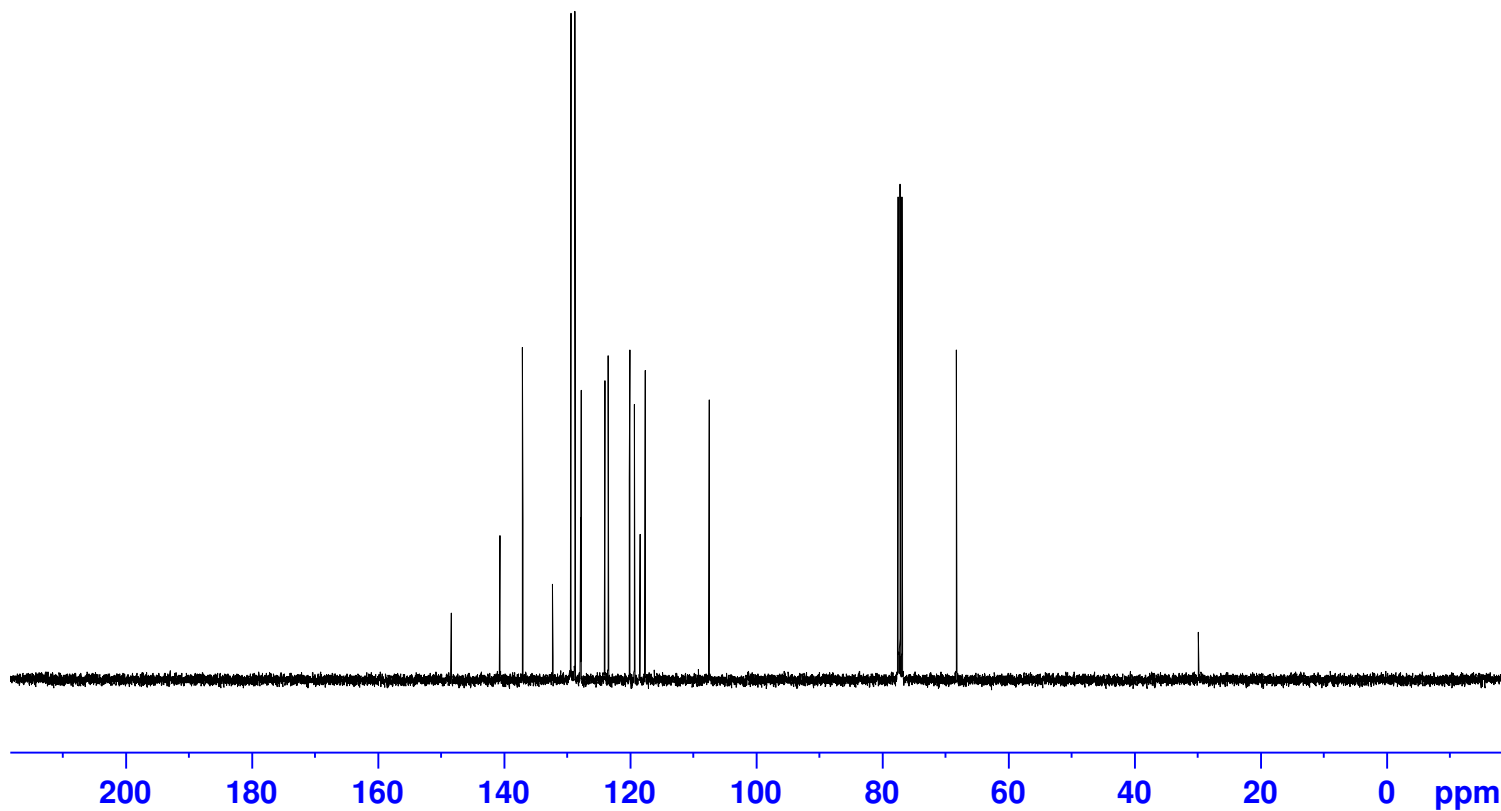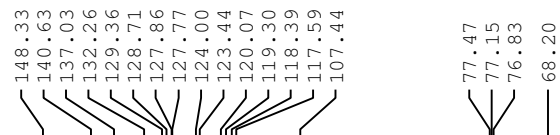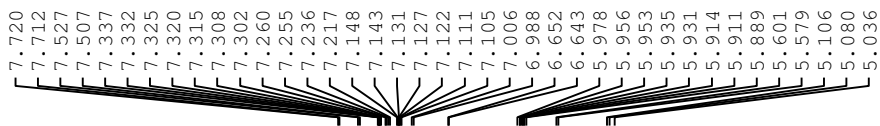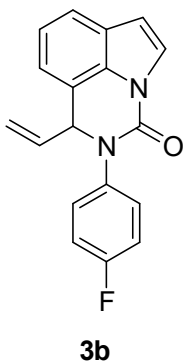
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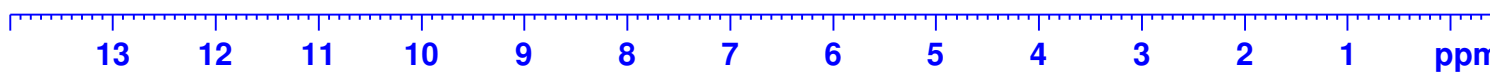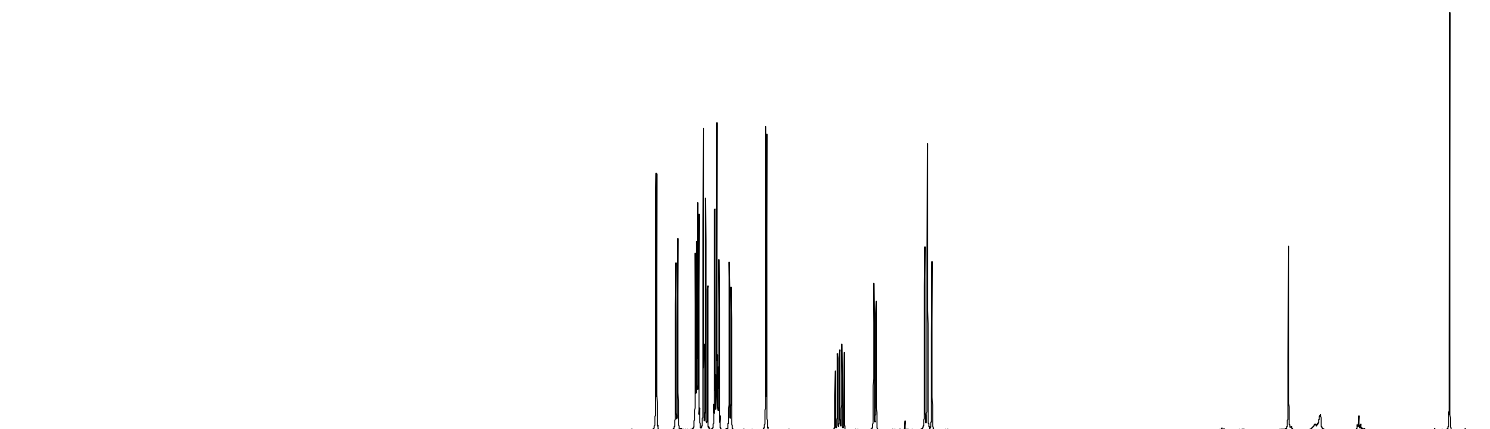SF   100.6127605 MHz
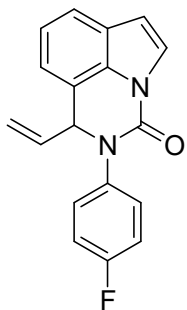WDW   EM
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XY-3-40-N-H

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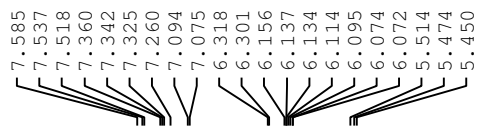
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ppm scale: 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

XY-3-40-N-C

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131.26
125.36
124.78
120.49
120.34
119.94
118.80
117.34
115.20

84.28
77.46
77.15
76.83

1b

200 180 160 140 120 100 80 60 40 20 0 ppm

XY-4-26

3a

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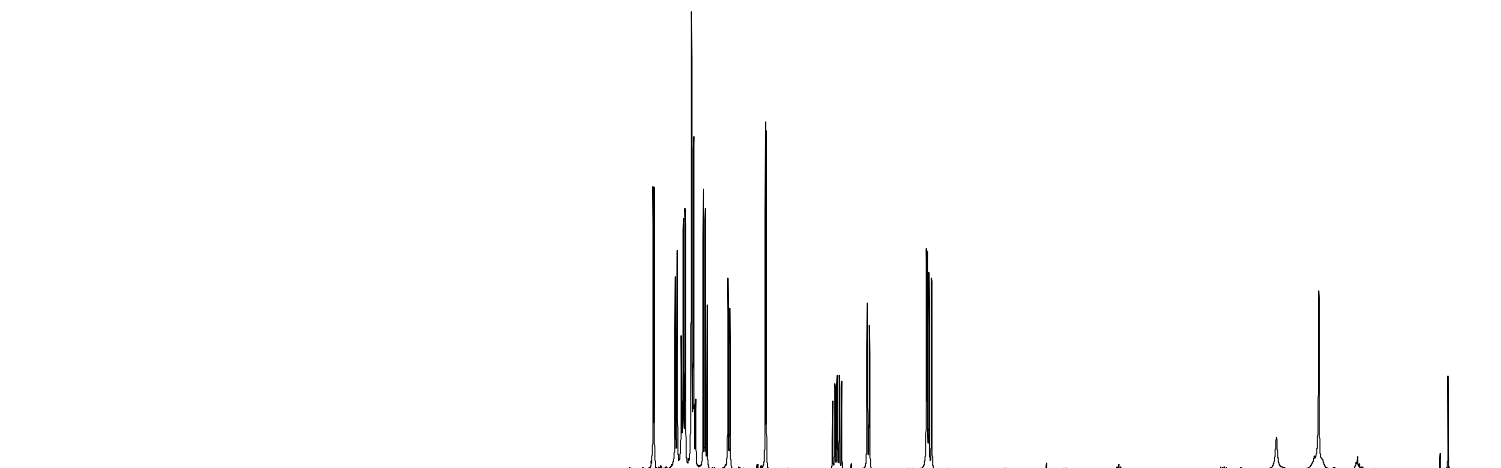
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XY-4-26

3a

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68.20

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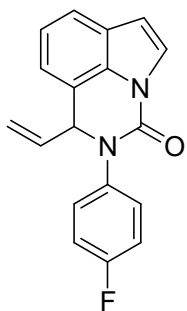NAME   2023-7-25
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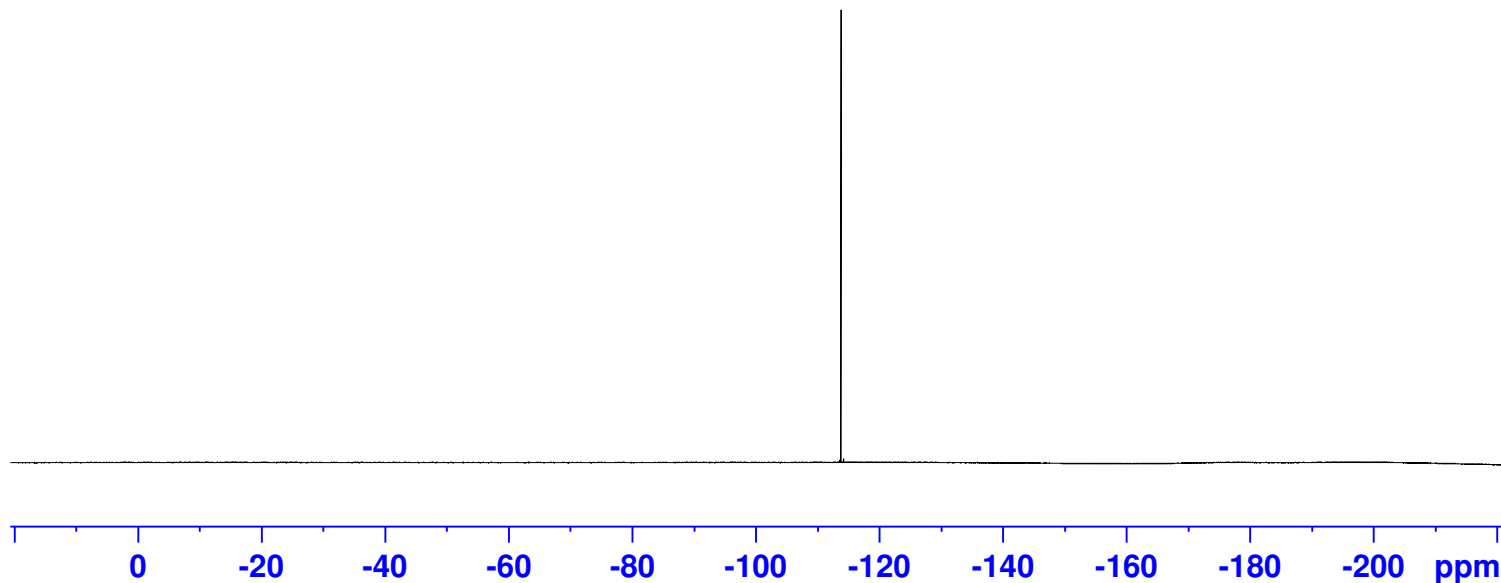PLW2   20.73200035 W
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SF   100.6127628 MHz
WDW   EM
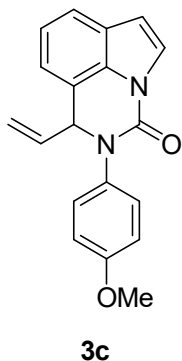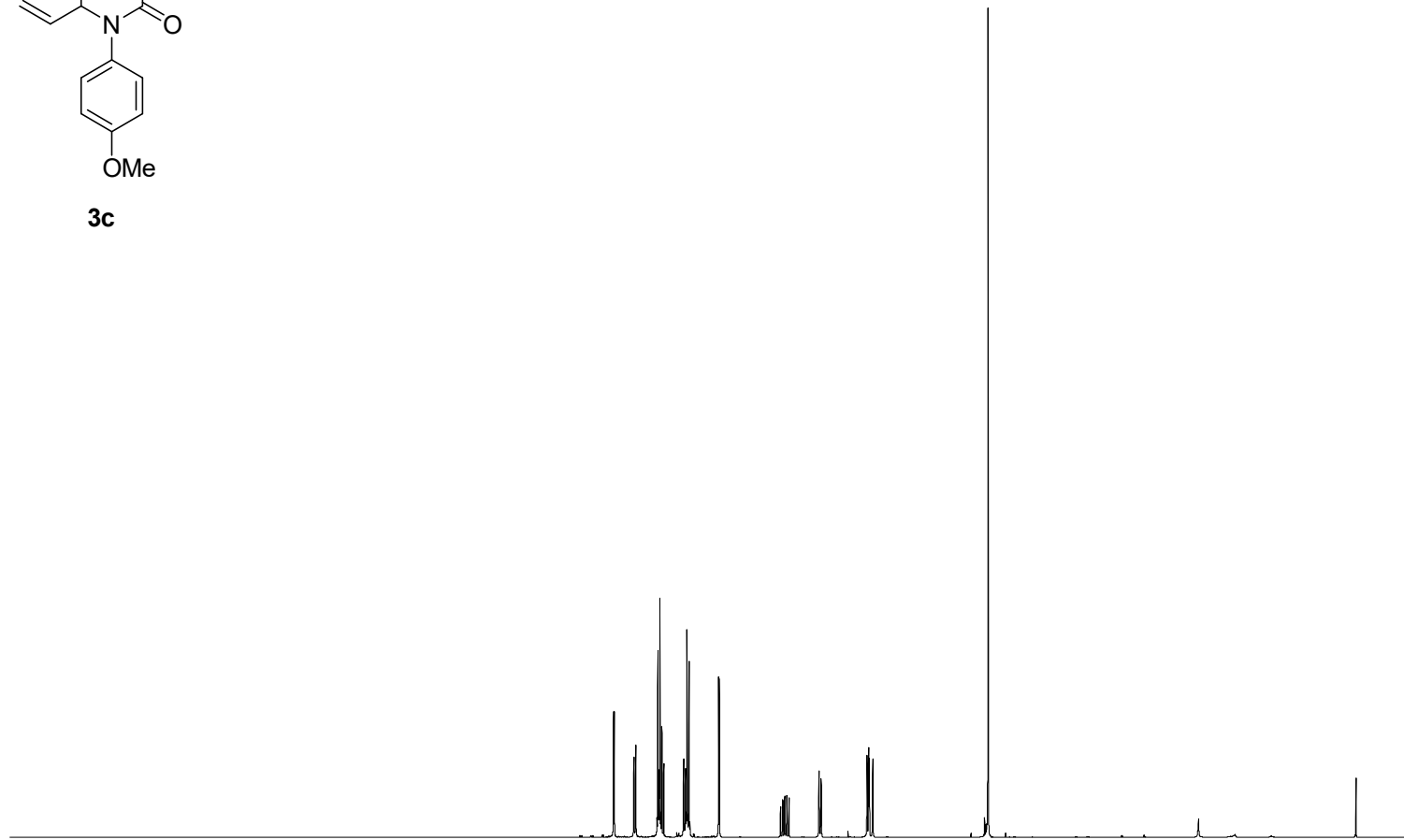SSB   0
LB   1.00 Hz
GB   0
PC   1.40

XY-2-Z1-A

3b

7.720 7.712 7.527 7.507 7.337 7.332 7.325 7.320 7.315 7.308 7.302 7.260 7.255 7.236 7.217 7.148 7.143 7.131 7.127 7.122 7.111 7.105 7.006 6.988 6.652 6.643 5.978 5.956 5.953 5.931 5.914 5.911 5.889 5.601 5.579 5.106 5.080 5.036

Current Data Parameters
NAME   xy-2-81-A
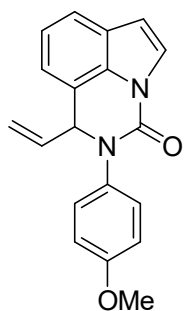EXPNO   5
PROCNO   1

F2 - Acquisition Parameters
Date_   20230303
Time   23.27 h
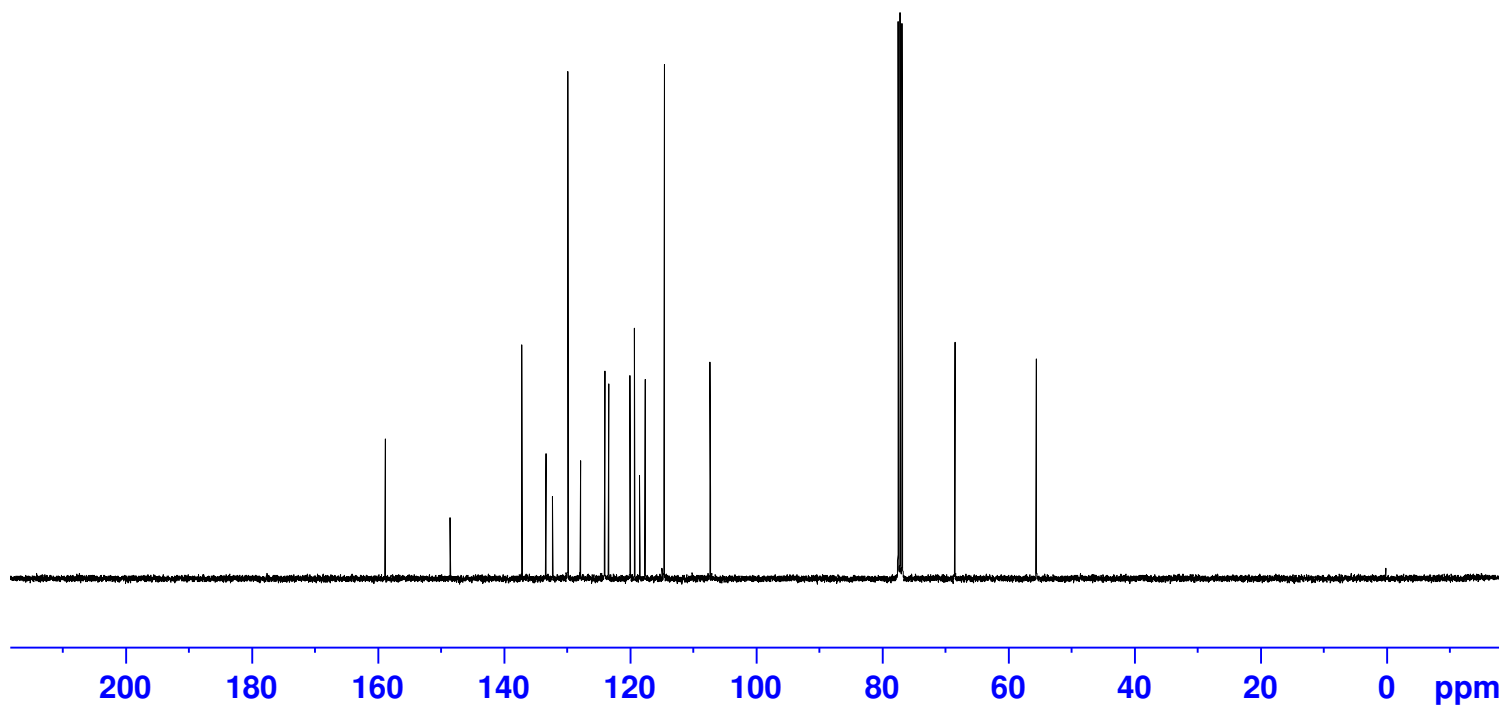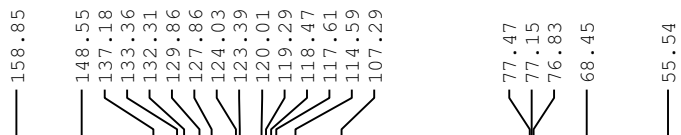INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zg30
TD   65536
SOLVENT   CDCl3
NS   16
DS   2
SWH   8196.722 Hz
FIDRES   0.250144 Hz
AQ   3.9976959 sec
RG   101
DW   61.000 usec
DE   13.54 usec
TE   295.2 K
D1   1.00000000 sec
TD0   1
SFO1   400.1324708 MHz
NUC1   1H
P0   3.33 usec
P1   10.00 usec
PLW1   20.73200035 W

F2 - Processing parameters
SI   65536
SF   400.1300097 MHz
WDW   EM
SSB   0
LB   0.30 Hz
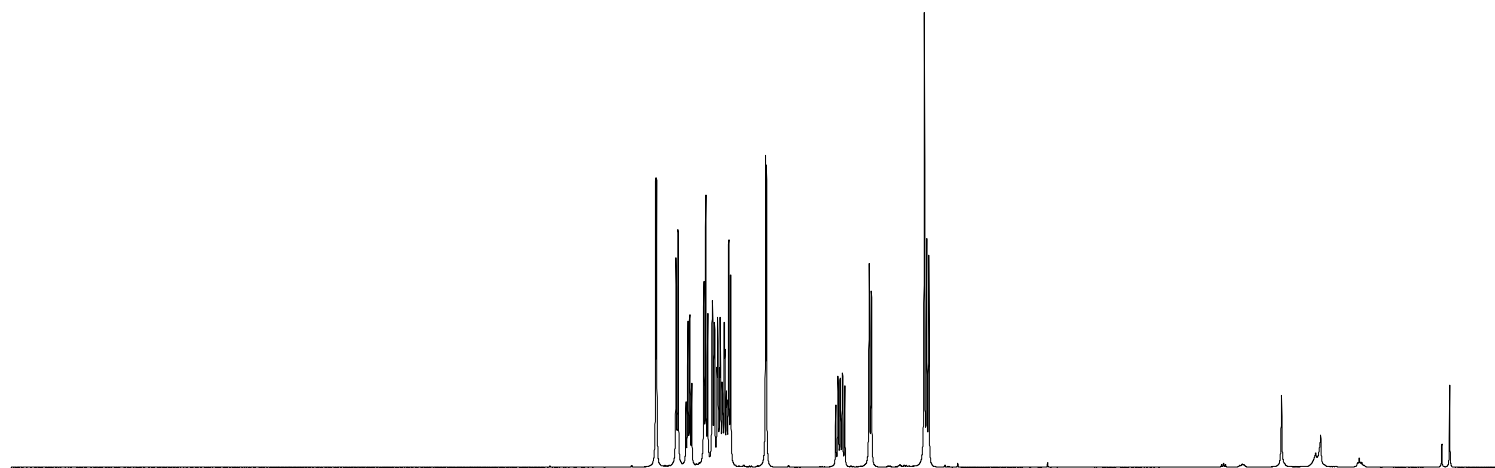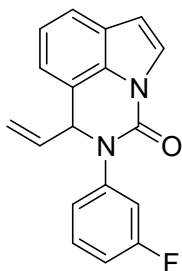GB   0
PC   1.00

13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

1.00 1.04 2.15 1.08 2.15 1.03 1.01 1.06 1.07 2.17

XY-2-81-A-C

163.00
160.54
148.38
136.88
136.56
136.53
132.22
130.62
130.54
127.93
123.96
123.54
120.18
119.38
118.23
117.93
116.41
116.19
107.58

77.47
77.15
76.83

68.48

3b

200   180   160   140   120   100   80   60   40   20   0   ppm

XY-2-81-A-F

3b

-113.83

XY-2-81-B-H

3c

7.720 7.711 7.508 7.489 7.260 7.254 7.249 7.243 7.237 7.229 7.217 7.198 6.991 6.972 6.965 6.957 6.951 6.940 6.934 6.628 6.620 5.984 5.963 5.959 5.942 5.938 5.921 5.917 5.896 5.583 5.562 5.085 5.070 5.068 5.066 5.060 5.028 5.026 5.024 3.827

0.94 0.98 3.16 3.00 0.93 0.97 0.98 1.99 3.00

13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

XY-2-81-B-C

3c

158.85

148.55
137.18
133.36
132.31
129.86
127.86
124.03
123.39
120.01
119.29
118.47
117.61
114.59
107.29

77.47
77.15
76.83

68.45

55.54

Current Data Parameters
NAME   Scope
EXPNO   4
PROCNO   1

F2 - Acquisition Parameters
Date_   20230308
Time   23.41 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   500
DS   4
SWH   23809.523 Hz
FIDRES   0.726609 Hz
AQ   1.3762560 sec
RG   48.6724
DW   21.000 usec
DE   6.50 usec
TE   298.1 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1
SFO1   100.6228298 MHz
NUC1   13C
P0   3.33 usec
P1   10.00 usec
PLW1   87.89900208 W
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz65
PCPD2   90.00 usec
PLW2   20.73200035 W
PLW12   0.25595000 W
PLW13   0.12874000 W

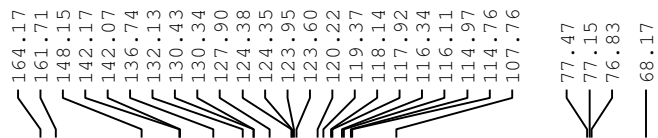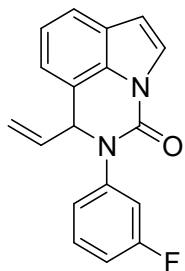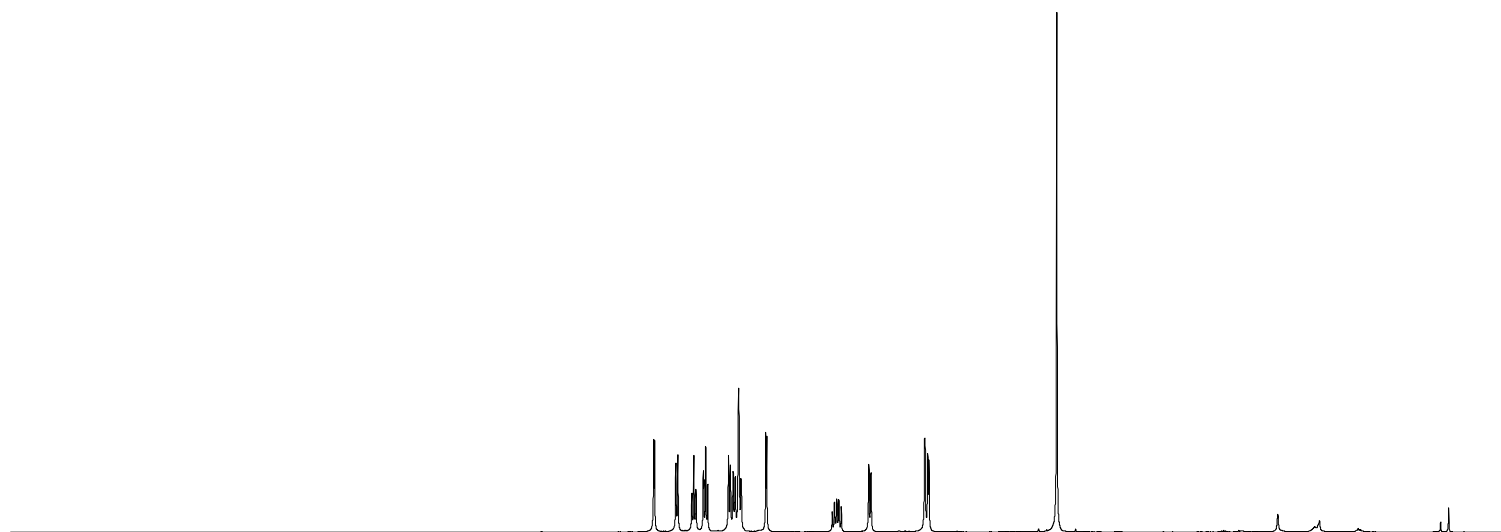F2 - Processing parameters
SI   32768
SF   100.6127605 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

XY-3-9-A-H
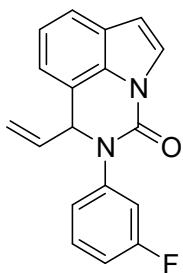
3d
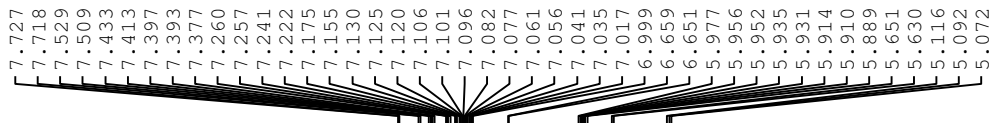
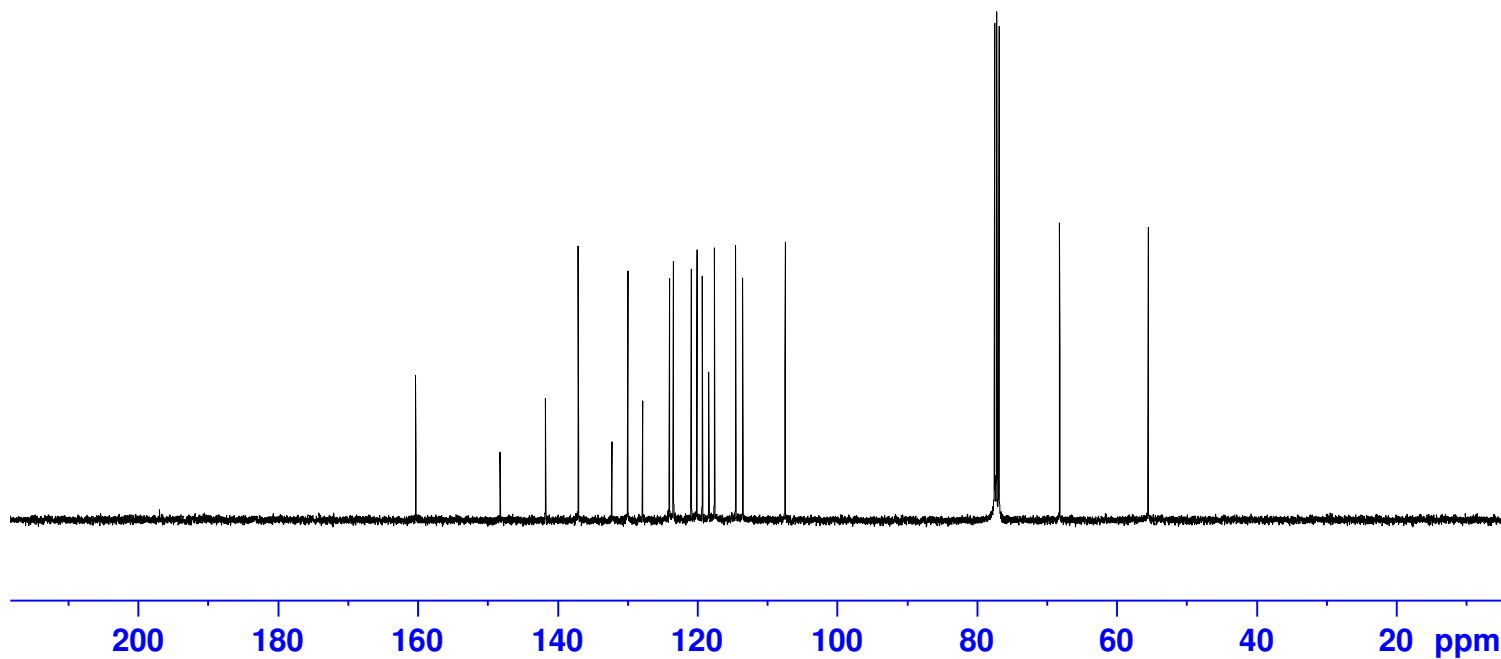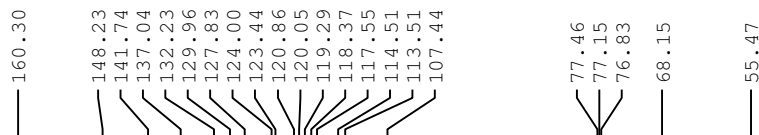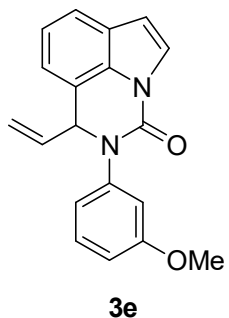Current Data Parameters
NAME   Scope1
EXPNO   4
PROCNO   1

F2 - Acquisition Parameters
Date_   20230311
Time   1.13 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zg30
TD   65536
SOLVENT   CDCl3
NS   16
DS   2
SWH   8196.722 Hz
FIDRES   0.250144 Hz
AQ   3.9976959 sec
RG   101
DW   61.000 usec
DE   13.54 usec
TE   292.7 K
D1   1.00000000 sec
TD0   1
SFO1   400.1324708 MHz
NUC1   1H
P0   3.33 usec
P1   10.00 usec
PLW1   20.73200035 W

F2 - Processing parameters
SI   65536
SF   400.1300112 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00

XY-3-9-A-C

3d

164.17
161.71
148.15
142.17
142.07
136.74
132.13
130.43
130.34
127.90
124.38
124.35
123.95
123.60
120.22
119.37
118.14
117.92
116.34
116.11
114.97
114.76
107.76

77.47
77.15
76.83

68.17
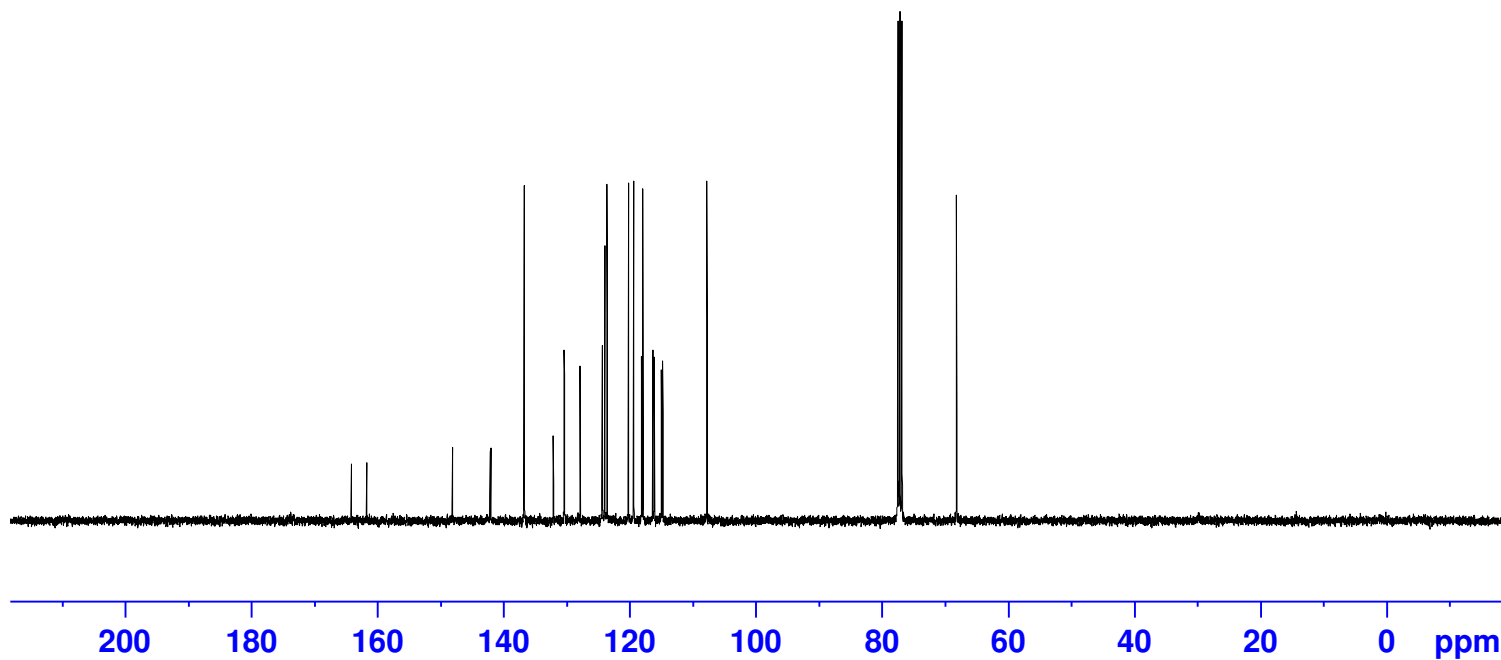
Current Data Parameters
NAME   2023-3-16
EXPNO   2
PROCNO   1

F2 - Acquisition Parameters
Date_   20230315
Time   0.41 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   500
DS   4
SWH   23809.523 Hz
FIDRES   0.726609 Hz
AQ   1.3762560 sec
RG   51.55
DW   21.000 usec
DE   6.50 usec
TE   294.5 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1
SFO1   100.6228298 MHz
NUC1   13C
P0   3.33 usec
P1   10.00 usec
PLW1   87.89900208 W
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz65
PCPD2   90.00 usec
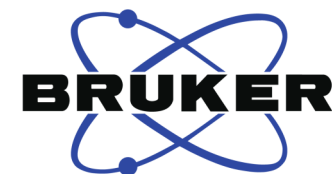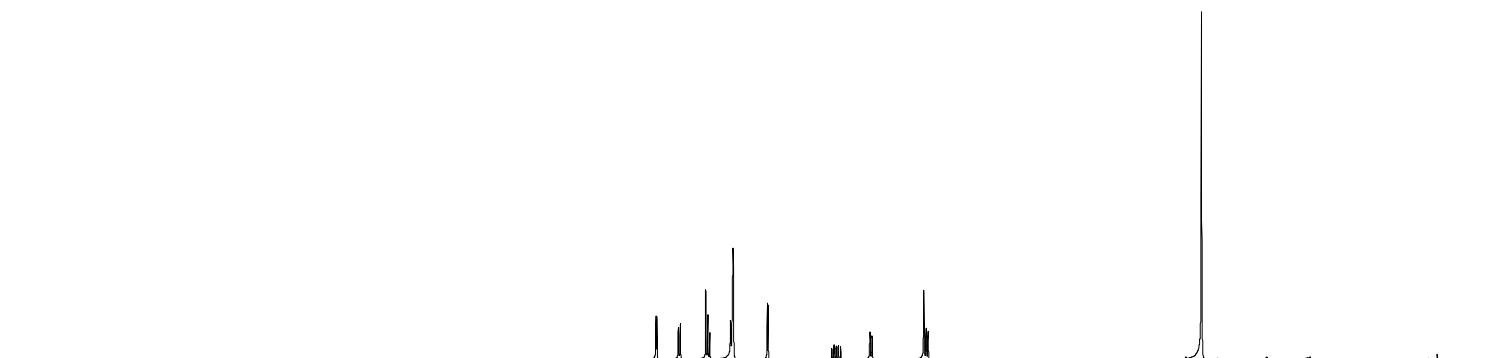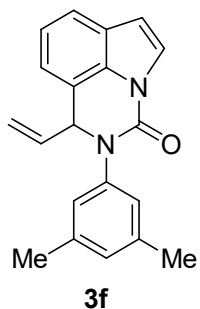PLW2   20.73200035 W
PLW12   0.25595000 W
PLW13   0.12874000 W

F2 - Processing parameters
SI   32768
SF   100.6127613 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

200   180   160   140   120   100   80   60   40   20   0   ppm

xy-3-9a

3d

—111.54

0   -20   -40   -60   -80   -100   -120   -140   -160   -180   ppm

XY-3-9-B-H

7.742
7.733
7.526
7.506
7.370
7.350
7.331
7.260
7.255
7.236
7.216
7.014
6.996
6.969
6.948
6.914
6.894
6.888
6.651
6.642
6.005
5.984
5.982
5.962
5.942
5.939
5.918
5.650
5.629
5.107
5.103
5.077
5.066
3.822

3e

0.91 0.94 0.98 0.99 4.00 0.91 0.98 1.00 2.05 3.03

XY-3-9-B-C

3e

160.30
148.23
141.74
137.04
132.23
129.96
127.83
124.00
123.44
120.86
120.05
119.29
118.37
117.55
114.51
113.51
107.44

77.46
77.15
76.83
68.15

55.47

Current Data Parameters
NAME   2023-3-16
EXPNO   1
PROCNO   1

F2 - Acquisition Parameters
Date_   20230315
Time   0.08 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   500
DS   4
SWH   23809.523 Hz
FIDRES   0.726609 Hz
AQ   1.3762560 sec
RG   50.1934
DW   21.000 usec
DE   6.50 usec
TE   294.5 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1
SFO1   100.6228298 MHz
NUC1   13C
P0   3.33 usec
P1   10.00 usec
PLW1   87.89900208 W
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz65
PCPD2   90.00 usec
PLW2   20.73200035 W
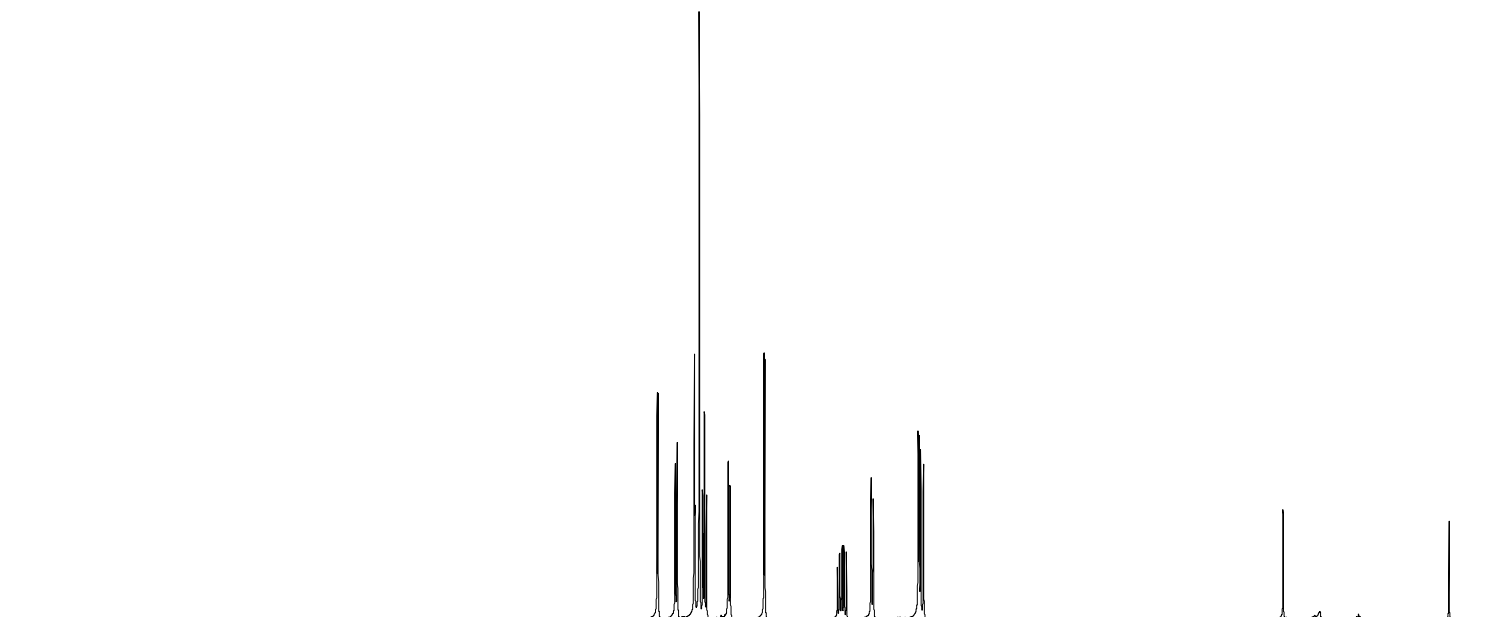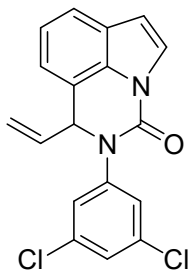PLW12   0.25595000 W
PLW13   0.12874000 W

F2 - Processing parameters
SI   32768
SF   100.6127635 MHz
WDW   EM
SSB   0
LB   1.00 Hz
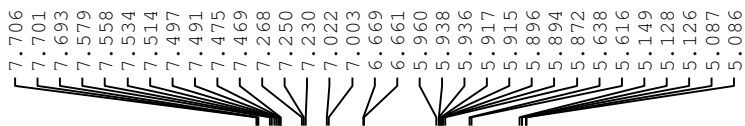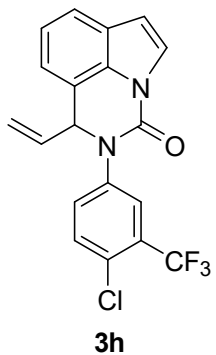GB   0
PC   1.40

200 180 160 140 120 100 80 60 40 20 ppm

3f
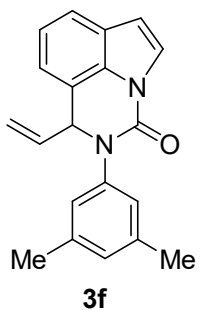
7.752
7.743
7.531
7.511
7.260
7.239
7.220
7.016
6.991
6.651
6.643
6.014
5.993
5.989
5.972
5.968
5.952
5.947
5.926
5.637
5.616
5.106
5.081
5.062

2.361

Integration values: 1.00, 1.04, 1.09, 4.13, 0.94, 1.11, 1.01, 0.94, 0.91, 5.99

ppm scale: 13 12 11 10 9 8 7 6 5 4 3 2 1

XY-3-25-A-C

3f

148.36, 140.37, 138.96, 137.18, 132.26, 129.59, 127.79, 126.25, 123.99, 123.35, 119.95, 119.23, 118.45, 117.33, 107.27

77.47, 77.15, 76.83

68.06

21.38

XY-3-21-A-H

7.708, 7.699, 7.533, 7.513, 7.351, 7.346, 7.342, 7.300, 7.296, 7.267, 7.260, 7.248, 7.228, 7.017, 6.999, 6.669, 6.660, 5.955, 5.934, 5.931, 5.913, 5.910, 5.892, 5.889, 5.868, 5.628, 5.607, 5.170, 5.160, 5.145, 5.118

3g

1.00 1.03 1.00 1.99 1.03 0.98 1.00 1.06 1.07 2.14

13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

XY-3-21-A-C

3g

147.97
142.51
136.36
135.33
131.99
128.11
127.96
127.52
123.90
123.77
120.39
119.47
118.42
117.84
108.12

77.47
77.15
76.83

68.16
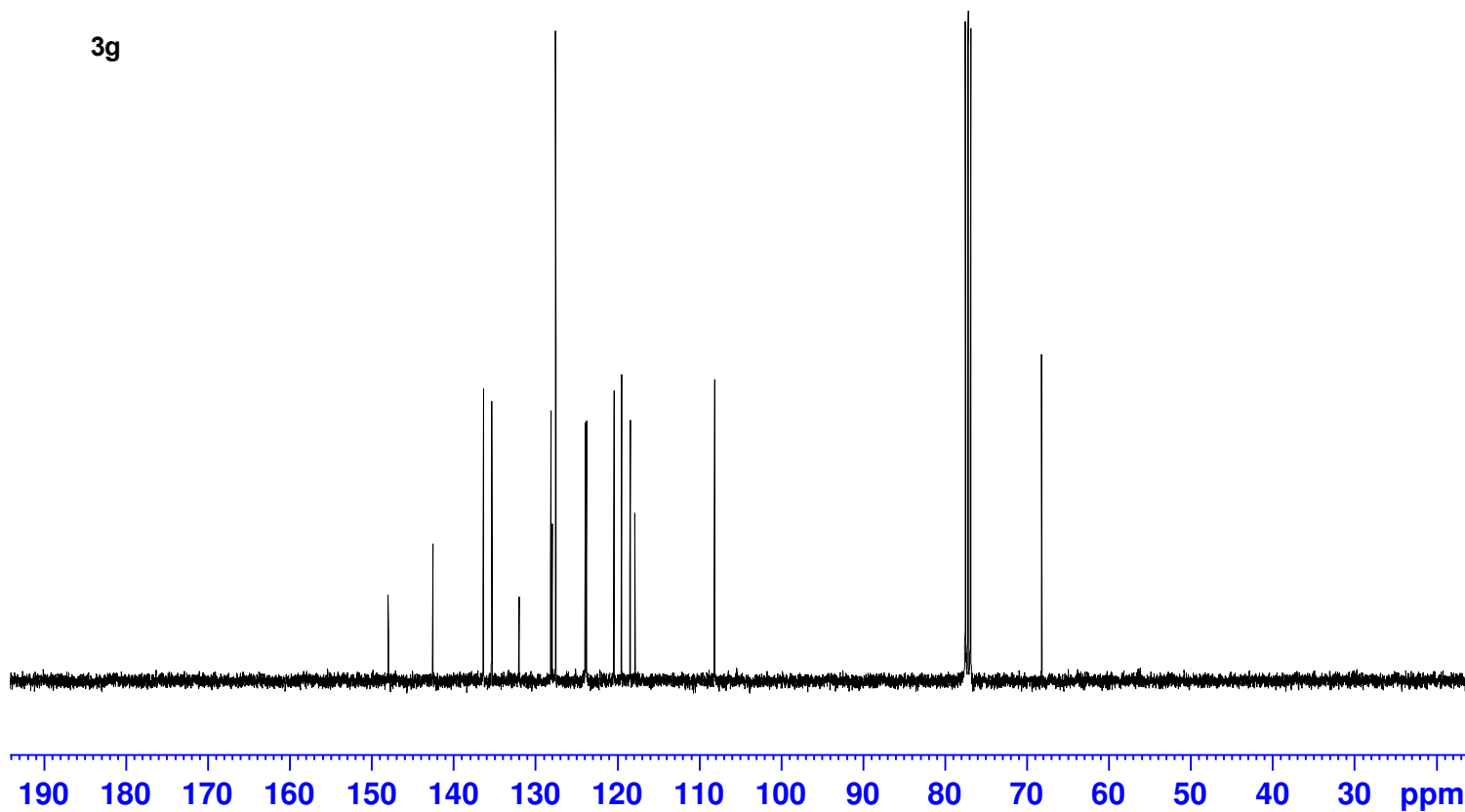
Current Data Parameters
NAME   2023-3-20
EXPNO   2
PROCNO   1

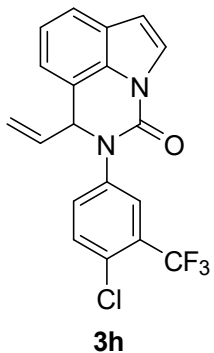F2 - Acquisition Parameters
Date_   20230321
Time   2.25 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   200
DS   4
SWH   23809.523 Hz
FIDRES   0.726609 Hz
AQ   1.3762560 sec
RG   50.1934
DW   21.000 usec
DE   6.50 usec
TE   294.2 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1
SFO1   100.6228298 MHz
NUC1   13C
P0   3.33 usec
P1   10.00 usec
PLW1   87.89900208 W
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz65
PCPD2   90.00 usec
PLW2   20.73200035 W
PLW12   0.25595000 W
PLW13   0.12874000 W

F2 - Processing parameters
SI   32768
SF   100.6127605 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

XY-3-37-H

3h

7.706
7.701
7.693
7.579
7.558
7.534
7.514
7.497
7.491
7.475
7.469
7.268
7.250
7.230
7.022
7.003
6.669
6.661
5.960
5.938
5.936
5.917
5.915
5.896
5.894
5.872
5.638
5.616
5.149
5.128
5.126
5.087
5.086
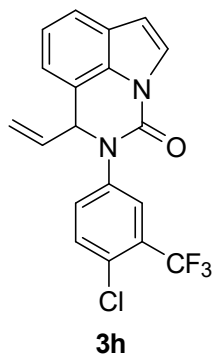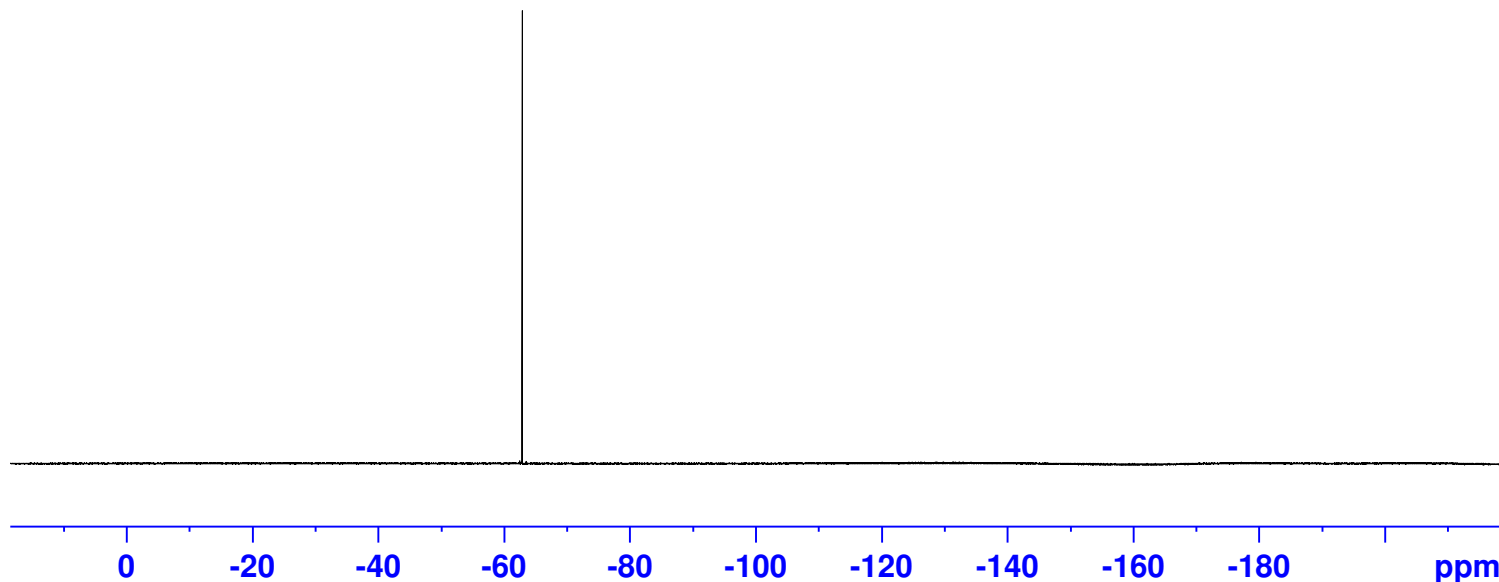
Current Data Parameters
NAME   2023-4-3
EXPNO   2
PROCNO   1

F2 - Acquisition Parameters
Date_   20230404
Time   1.59 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zg30
TD   65536
SOLVENT   CDCl3
NS   16
DS   2
SWH   8196.722 Hz
FIDRES   0.250144 Hz
AQ   3.9976959 sec
RG   101
DW   61.000 usec
DE   13.54 usec
TE   293.7 K
D1   1.00000000 sec
TD0   1
SFO1   400.1324708 MHz
NUC1   1H
P0   3.33 usec
P1   10.00 usec
PLW1   20.73200035 W
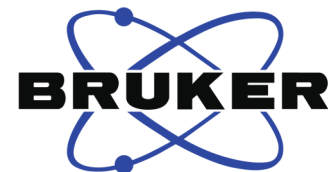
F2 - Processing parameters
SI   65536
SF   400.1300136 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00

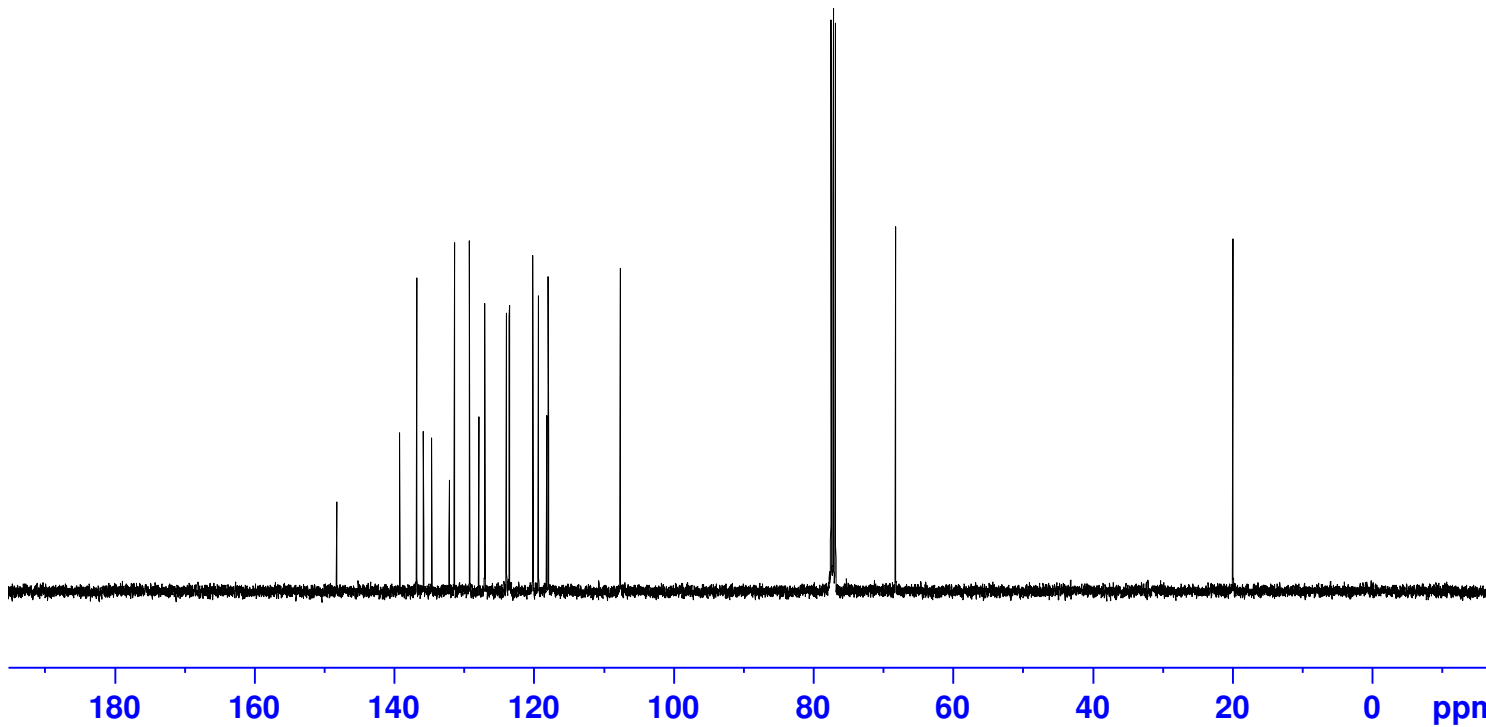13   12   11   10   9   8   7   6   5   4   3   2   1   ppm

1.95 3.00 1.07 0.96 0.94   1.01 0.97   1.95
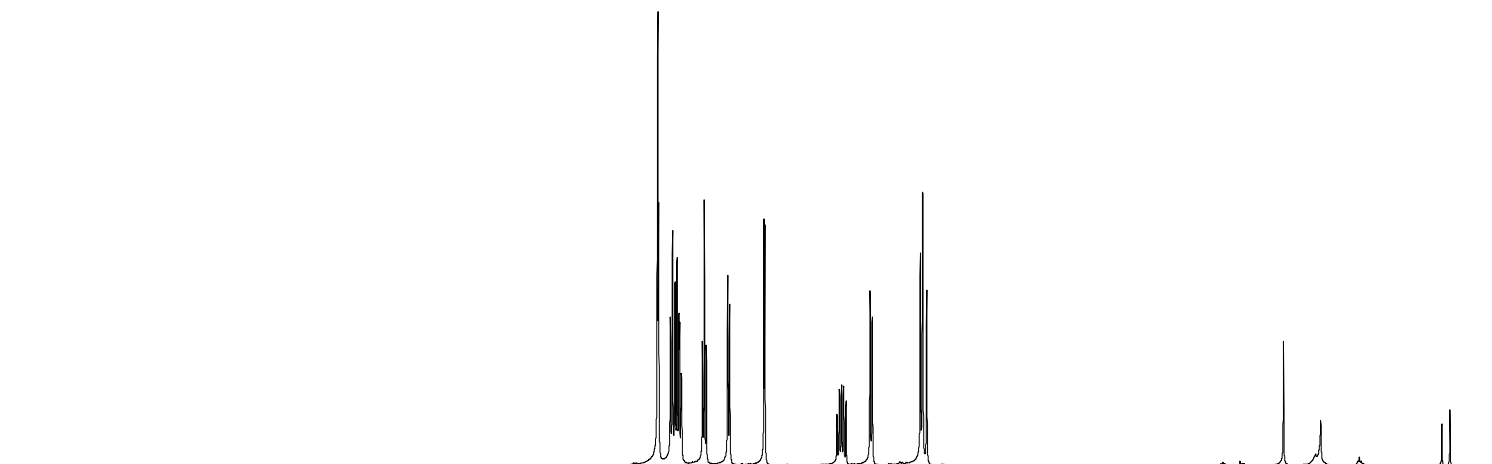
XY-3-37-C

148.14
139.46
136.41
133.37
132.41
132.03
131.40
129.57
129.25
128.00
127.98
127.93
126.56
123.88
123.85
123.80
121.13
120.44
119.51
118.51
118.41
117.80
108.16

77.46
77.15
76.83

68.23

3h
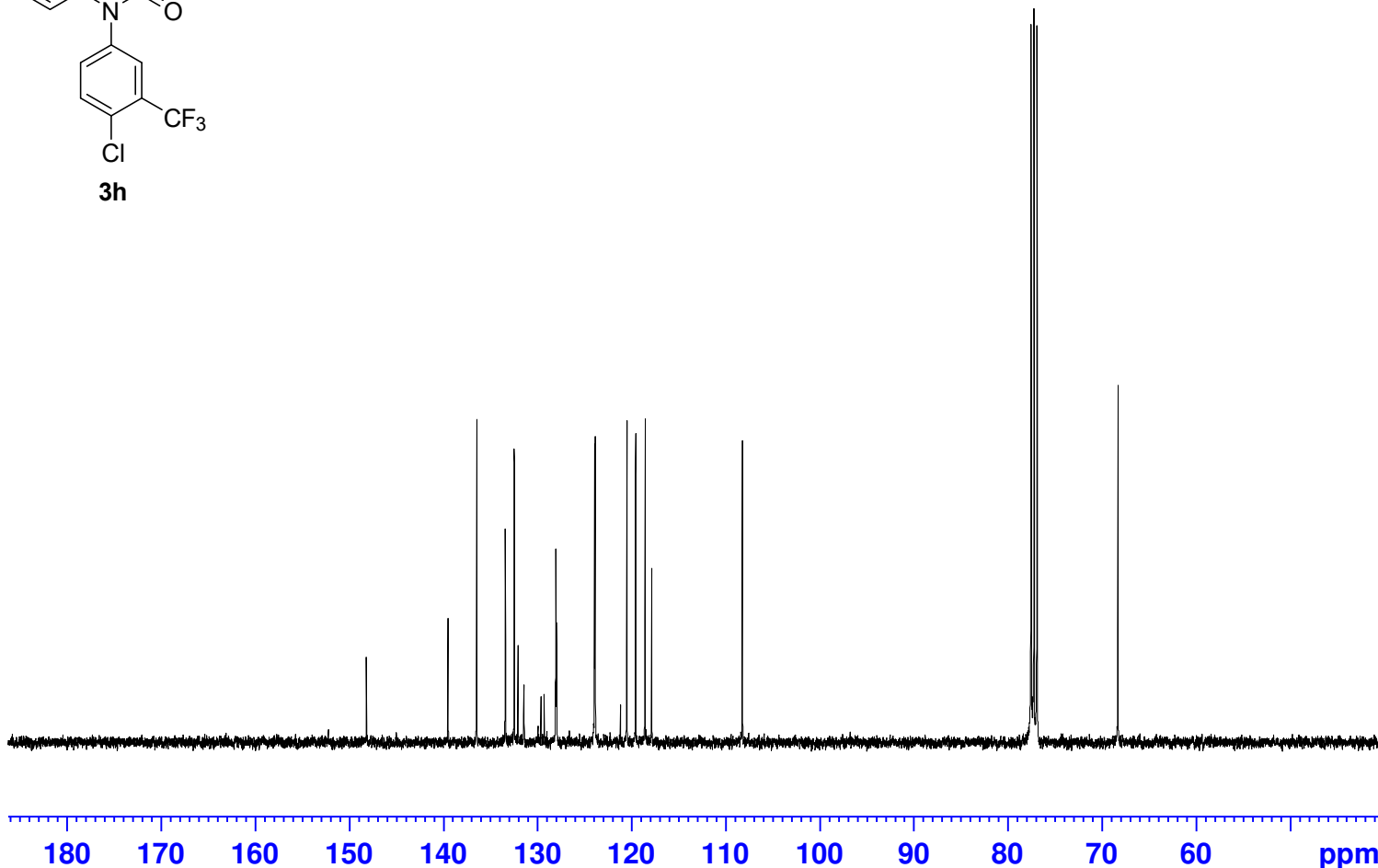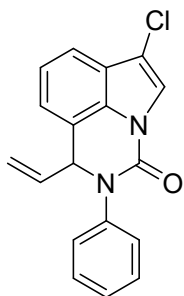
Current Data Parameters
NAME   2023-4-3
EXPNO   3
PROCNO   1

F2 - Acquisition Parameters
Date_   20230404
Time   2.29 h
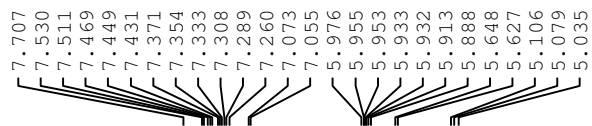INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   500
DS   4
SWH   23809.523 Hz
FIDRES   0.726609 Hz
AQ   1.3762560 sec
RG   47.4244
DW   21.000 usec
DE   6.50 usec
TE   294.2 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1
SFO1   100.6228298 MHz
NUC1   13C
P0   3.33 usec
P1   10.00 usec
PLW1   87.89900208 W
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz65
PCPD2   90.00 usec
PLW2   20.73200035 W
PLW12   0.25595000 W
PLW13   0.12874000 W

F2 - Processing parameters
SI   32768
SF   100.6127604 MHz
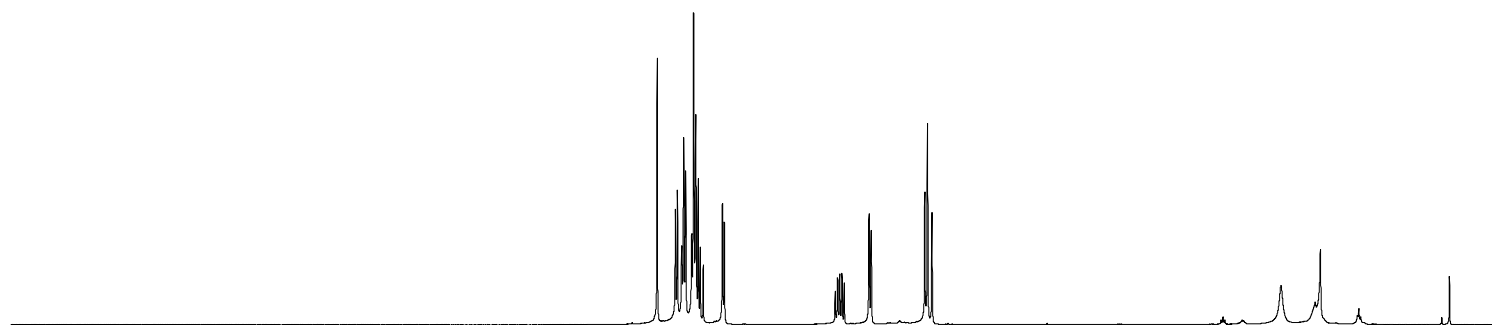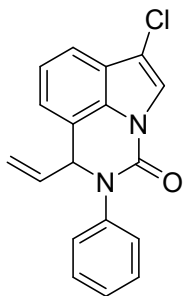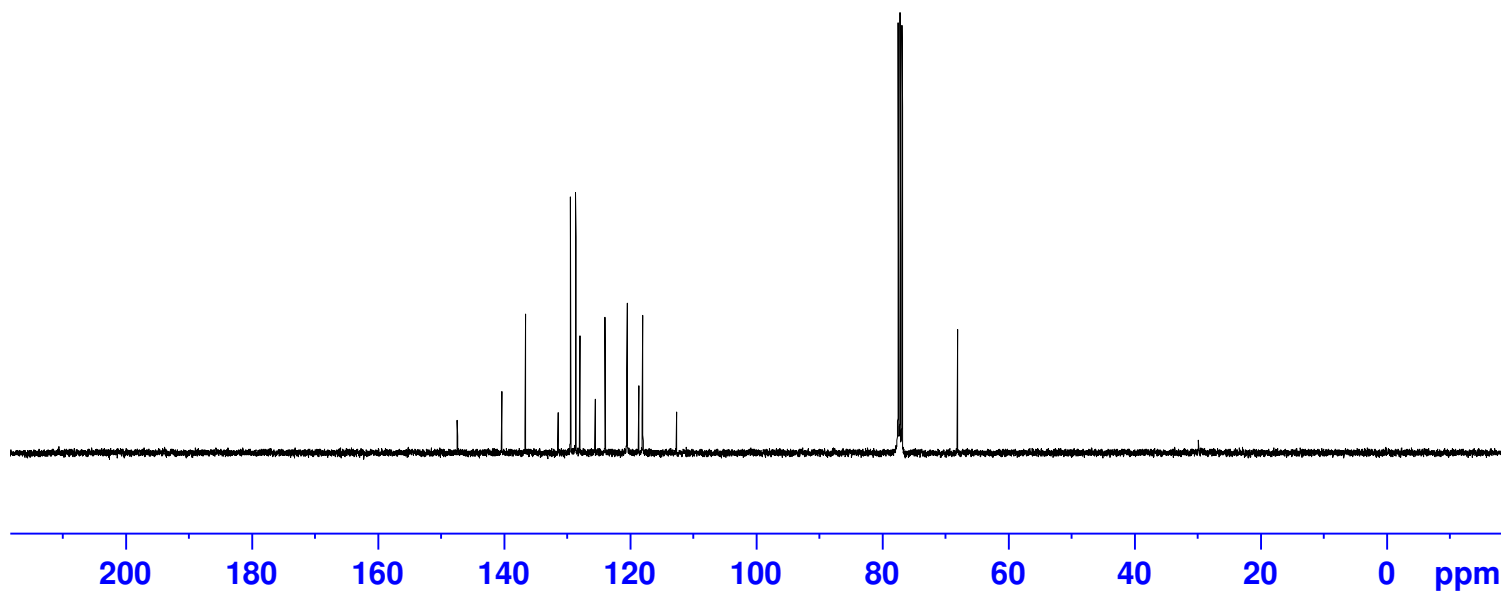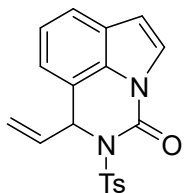WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

xy-3-37

−62.86

3h

0   -20   -40   -60   -80   -100   -120   -140   -160   -180   ppm

XY-3-38-H

7.726
7.717
7.526
7.507
7.376
7.371
7.305
7.285
7.260
7.257
7.237
7.218
7.177
7.172
7.157
7.152
7.010
6.991
6.654
6.645
5.976
5.955
5.951
5.934
5.930
5.913
5.909
5.888
5.619
5.598
5.125
5.116
5.100
5.074

2.405

3i

Current Data Parameters
NAME   2023-3-31
EXPNO   1
PROCNO   1
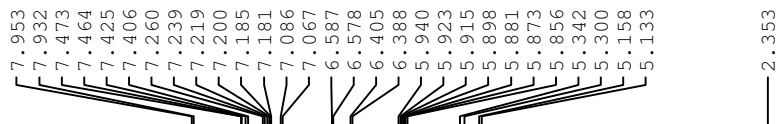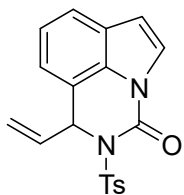
F2 – Acquisition Parameters
Date_   20230401
Time   7.37 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zg30
TD   65536
SOLVENT   CDCl3
NS   16
DS   2
SWH   8196.722 Hz
FIDRES   0.250144 Hz
AQ   3.9976959 sec
RG   93.7735
DW   61.000 usec
DE   13.54 usec
TE   293.4 K
D1   1.00000000 sec
TD0   1
SFO1   400.1324708 MHz
NUC1   1H
P0   3.33 usec
P1   10.00 usec
PLW1   20.73200035 W

F2 – Processing parameters
SI   65536
SF   400.1300101 MHz
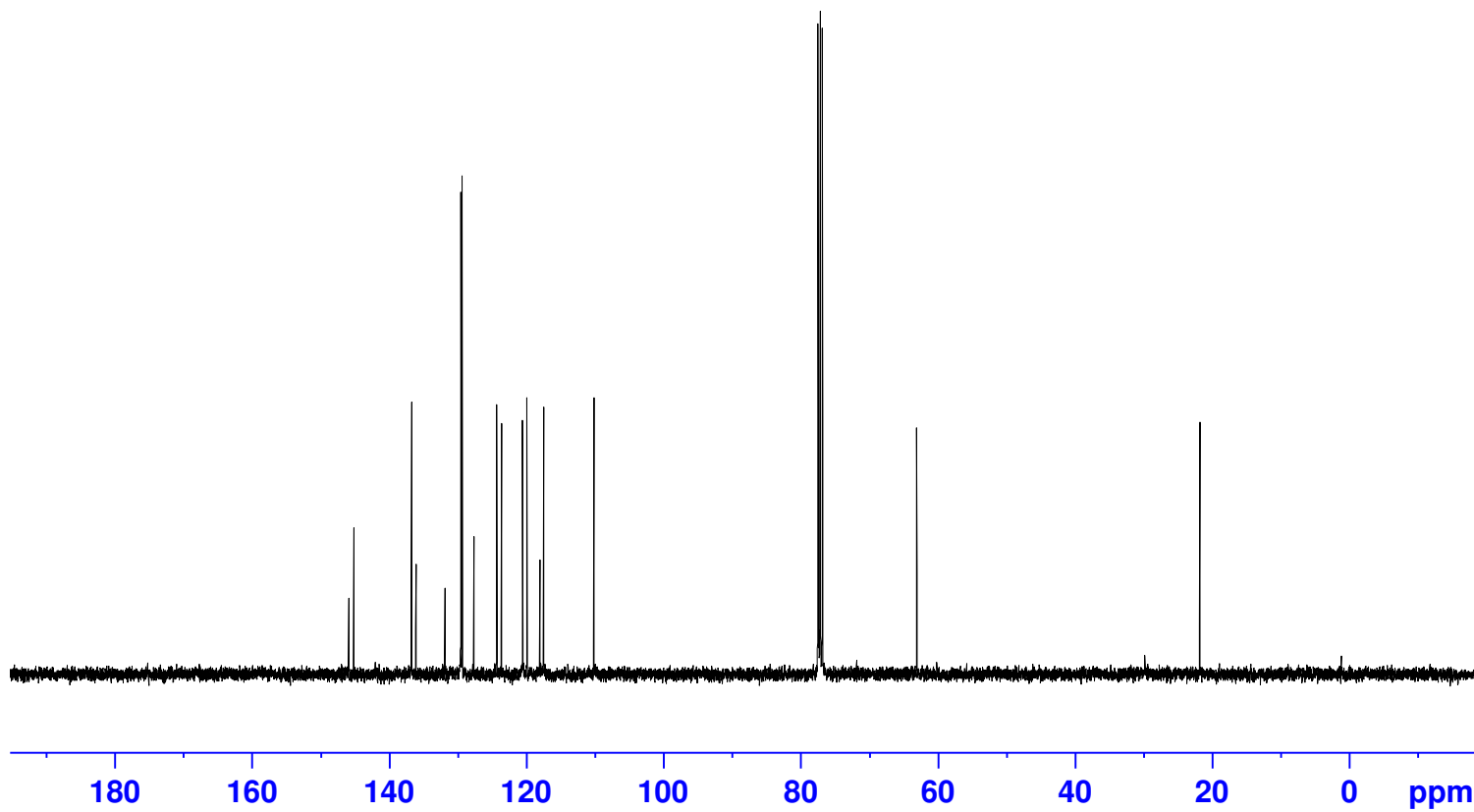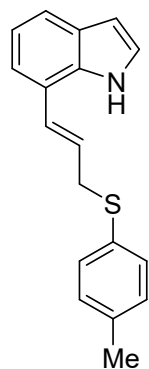WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00
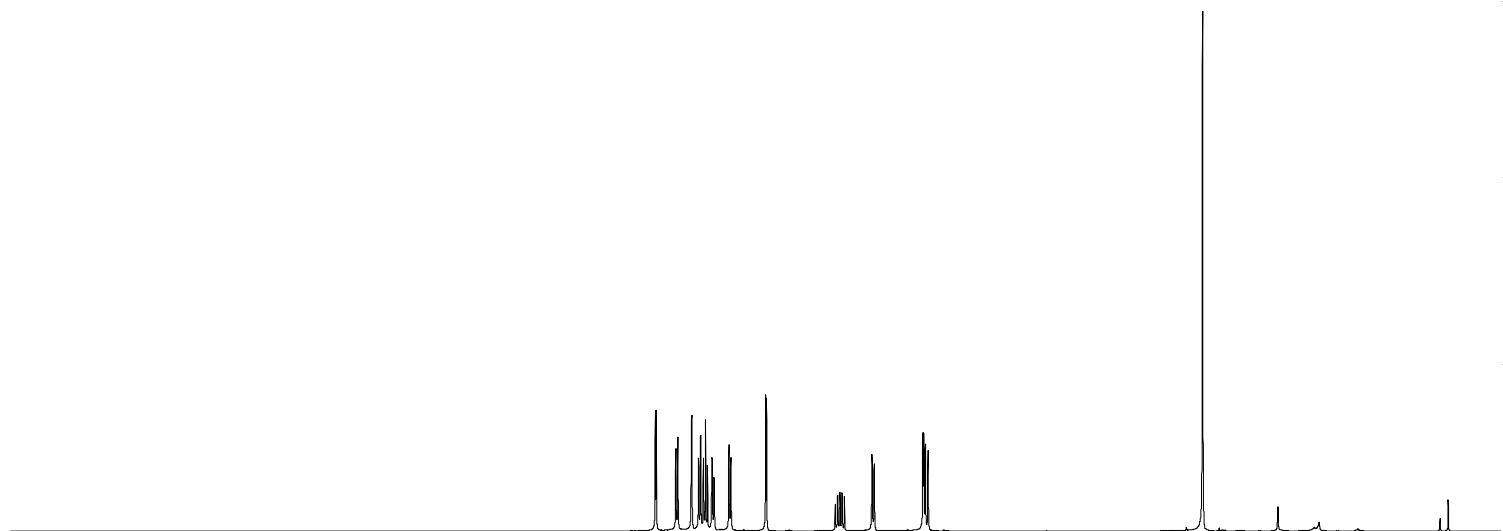
0.96 0.96 0.94 0.98 1.00 0.96 0.98 0.94 1.00 0.98 1.00 0.95   2.99

XY-3-38-C
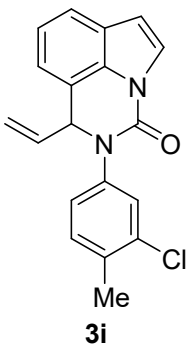
148.23
139.24
136.79
135.82
134.66
132.14
131.40
129.24
127.88
127.05
123.94
123.53
120.15
119.36
118.17
117.95
107.62

77.46
77.15
76.83
68.22

19.90

3i

180 160 140 120 100 80 60 40 20 0 ppm

XY-3-89-H

3j

7.707, 7.530, 7.511, 7.469, 7.449, 7.431, 7.371, 7.354, 7.333, 7.308, 7.289, 7.260, 7.073, 7.055, 5.976, 5.955, 5.953, 5.933, 5.932, 5.913, 5.888, 5.648, 5.627, 5.106, 5.079, 5.035

13   12   11   10   9   8   7   6   5   4   3   2   1   ppm

0.92 1.01 2.01 3.96 0.94   1.00 0.98   2.00

XY-3-89-H

3j

147.42
140.38
136.63
131.42
129.46
128.63
127.97
125.56
123.99
120.50
120.46
118.61
118.05
117.99
112.63

77.46
77.15
76.83

68.04

XY-3-25-B-H

3k

7.953
7.932
7.473
7.464
7.425
7.406
7.260
7.239
7.219
7.200
7.185
7.181
7.086
7.067
6.587
6.578
6.405
6.388
5.940
5.923
5.915
5.898
5.881
5.873
5.856
5.342
5.300
5.158
5.133

2.353

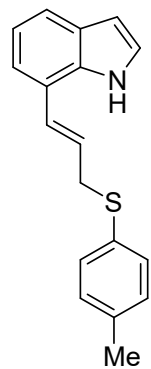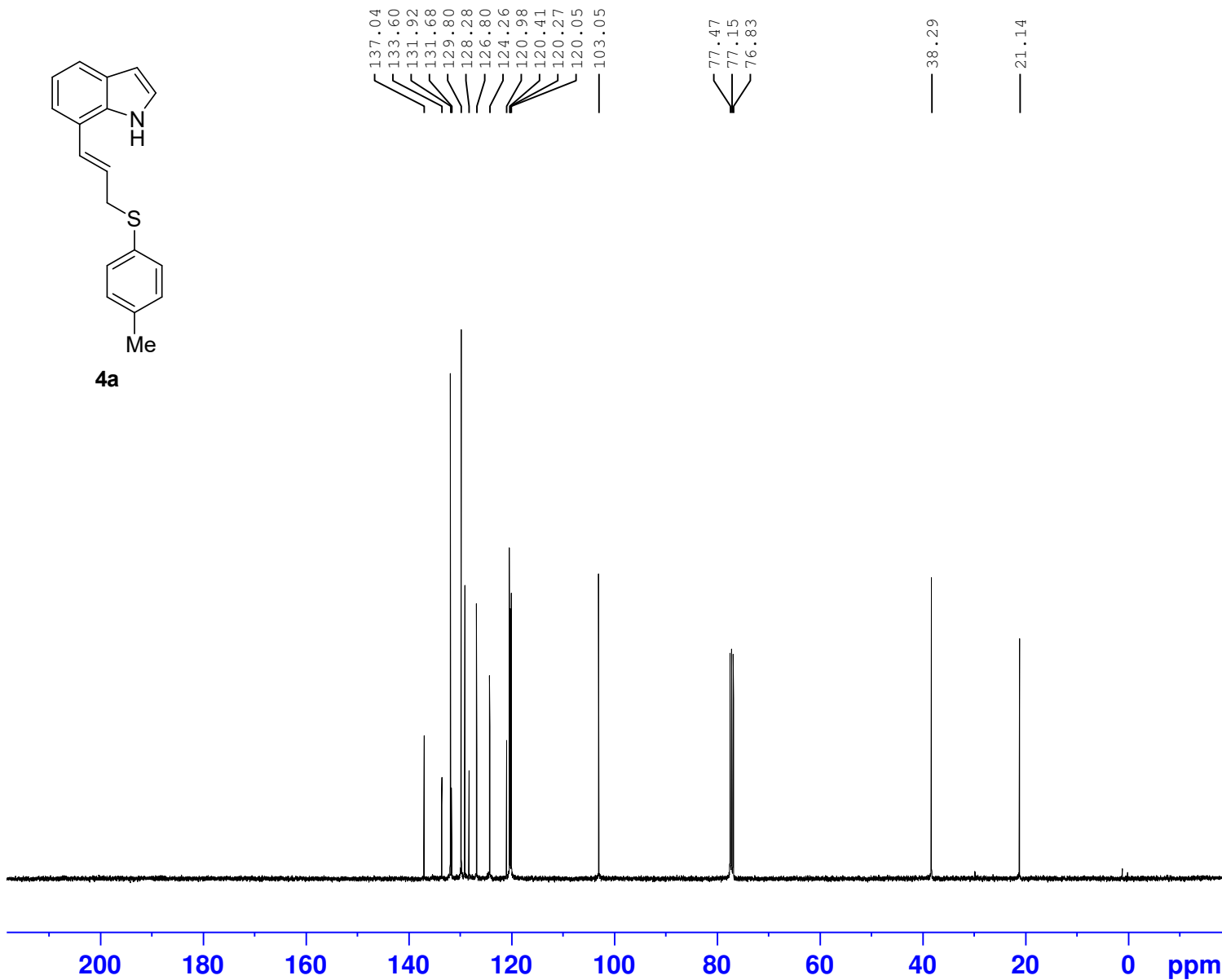Current Data Parameters
NAME   2023-3-22
EXPNO   1
PROCNO   1

F2 - Acquisition Parameters
Date_   20230322
Time   21.11 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zg30
TD   65536
SOLVENT   CDCl3
NS   16
DS   2
SWH   8196.722 Hz
FIDRES   0.250144 Hz
AQ   3.9976959 sec
RG   101
DW   61.000 usec
DE   13.54 usec
TE   293.2 K
D1   1.00000000 sec
TD0   1
SFO1   400.1324708 MHz
NUC1   1H
P0   3.33 usec
P1   10.00 usec
PLW1   20.73200035 W

F2 - Processing parameters
SI   65536
SF   400.1300397 MHz
WDW   EM
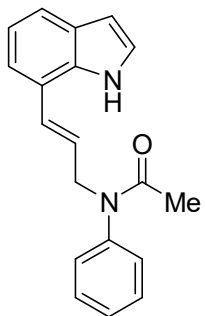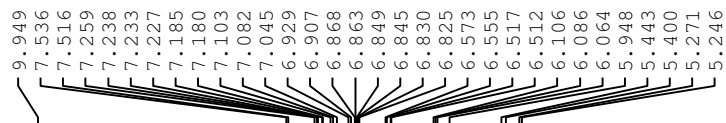SSB   0
LB   0.30 Hz
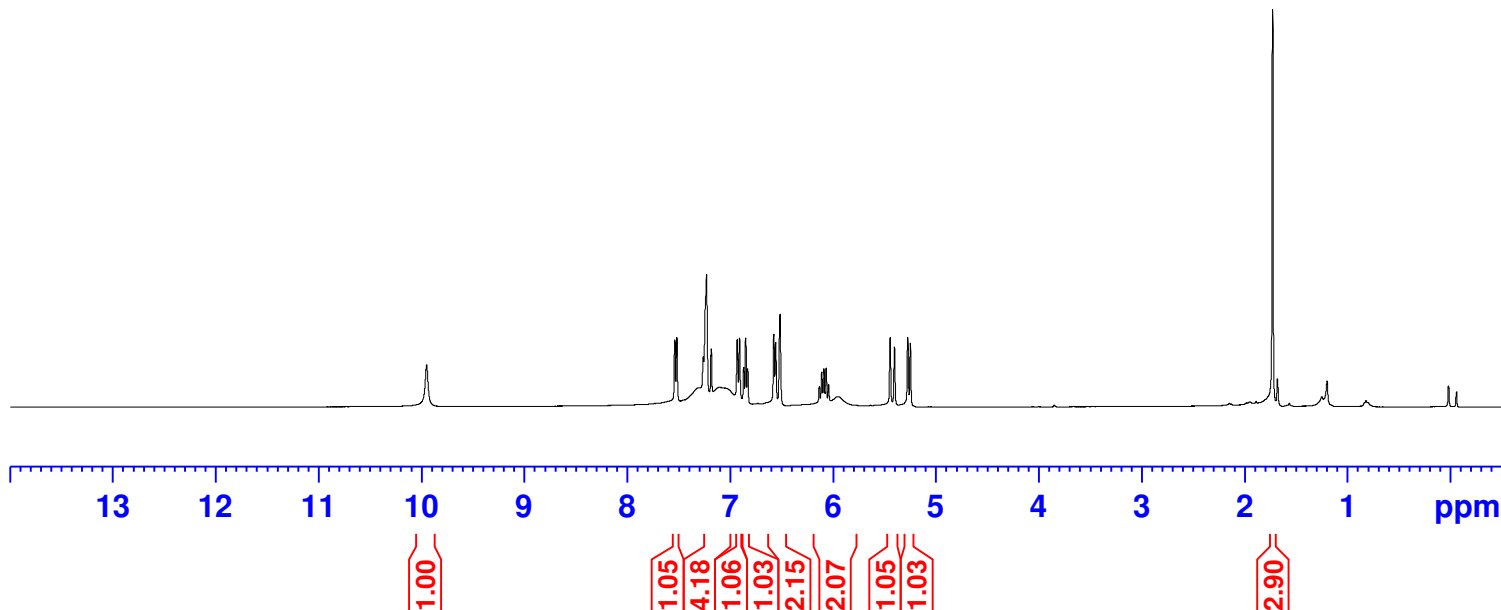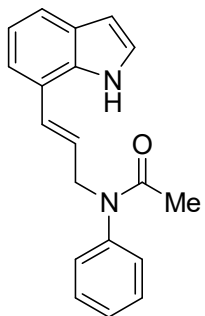GB   0
PC   1.00

2.02 0.99 0.99 3.24 0.97 0.95 0.99 1.00 1.04 1.02   3.11

XY-3-25-B-C

3k

145.90
145.17
136.77
136.12
131.85
129.56
129.37
127.67
124.34
123.65
120.56
119.92
119.04
117.48
110.15

77.47
77.15
76.83

63.07

21.80

BRUKER

180   160   140   120   100   80   60   40   20   0   ppm

8.071, 7.597, 7.577, 7.402, 7.382, 7.260, 7.179, 7.165, 7.155, 7.147, 7.141, 7.137, 7.118, 7.099, 6.618, 6.593, 6.588, 6.585, 6.580, 6.304, 6.286, 6.268, 6.265, 6.247, 6.229, 3.763, 3.760, 3.745, 3.742, 2.365

4a

0.95 0.95 1.84 5.00 1.91 0.99 1.99 3.10

4a

137.04
133.60
131.92
131.68
129.80
128.28
126.80
124.26
120.98
120.41
120.27
120.05
103.05

77.47
77.15
76.83

38.29

21.14

Current Data Parameters
NAME   2023-5-4
EXPNO   2
PROCNO   1

F2 - Acquisition Parameters
Date_   20230429
Time   2.32 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   500
DS   4
SWH   23809.523 Hz
FIDRES   0.726609 Hz
AQ   1.3762560 sec
RG   47.2408
DW   21.000 usec
DE   6.50 usec
TE   295.2 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1
SFO1   100.6228298 MHz
NUC1   13C
P0   3.33 usec
P1   10.00 usec
PLW1   87.89900208 W
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz65
PCPD2   90.00 usec
PLW2   20.73200035 W
PLW12   0.25595000 W
PLW13   0.12874000 W
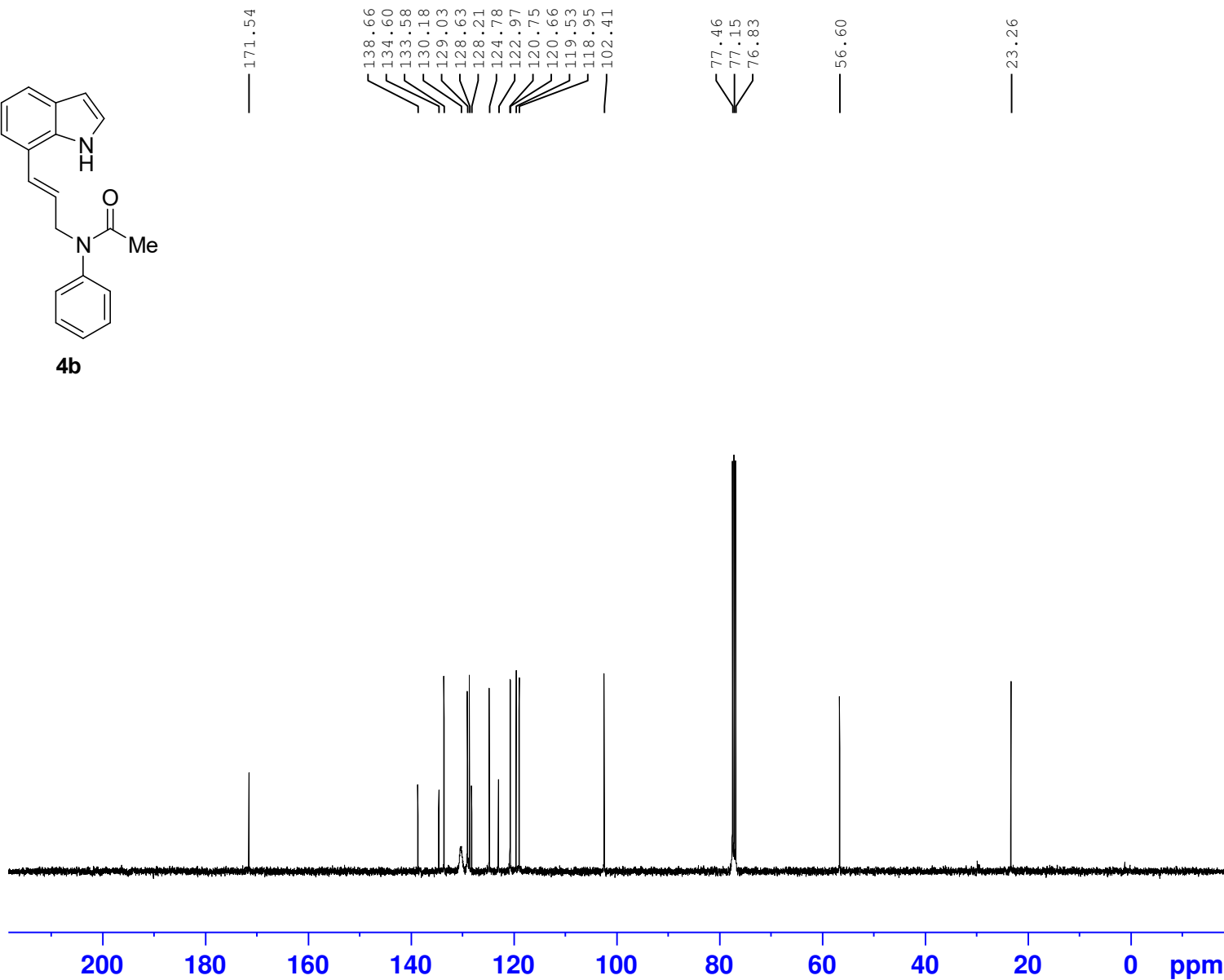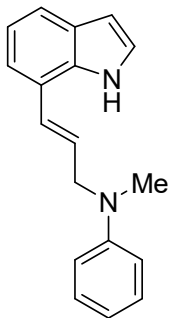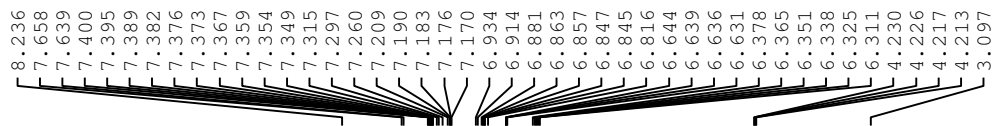
F2 - Processing parameters
SI   32768
SF   100.6127704 MHz
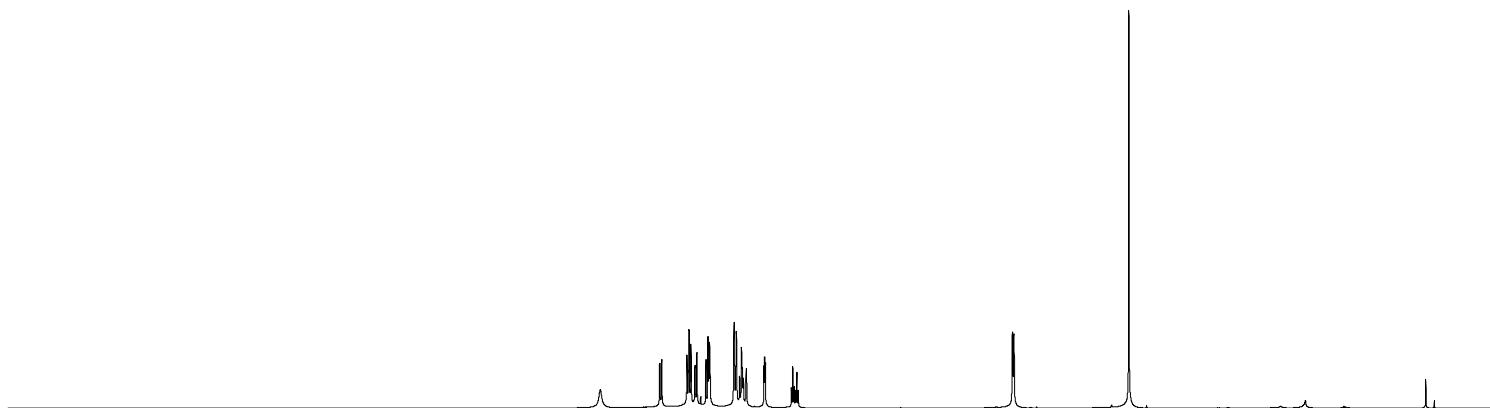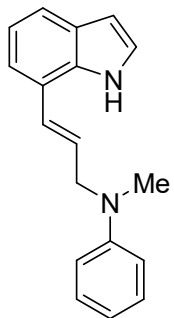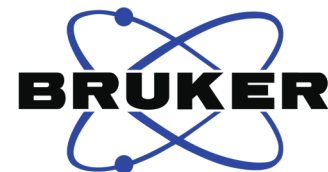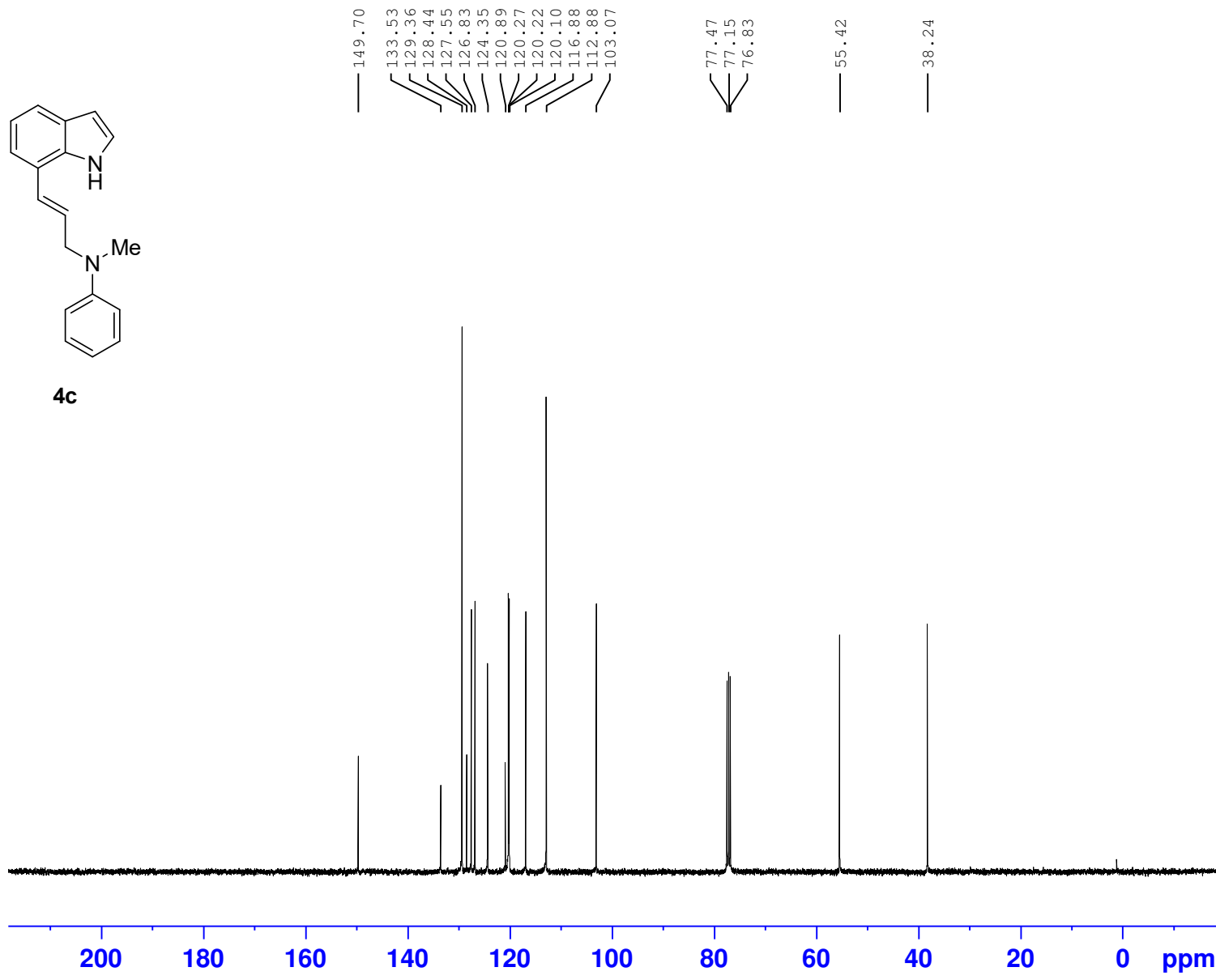WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

XY-3-71-H

9.949
7.536
7.516
7.259
7.238
7.233
7.227
7.185
7.180
7.103
7.082
7.045
6.929
6.907
6.868
6.863
6.849
6.845
6.830
6.825
6.573
6.555
6.517
6.512
6.106
6.086
6.064
5.948
5.443
5.400
5.271
5.246

1.727
1.722

4b

1.00   1.05 4.18 1.06 1.03 2.15 2.07 1.05 1.03   2.90

13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

XY-3-71-C

171.54

138.66
134.60
133.58
130.18
129.03
128.63
128.21
124.78
122.97
120.75
120.66
119.53
118.95
102.41

77.46
77.15
76.83

56.60

23.26

4b

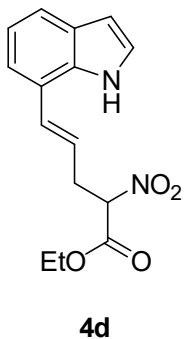Current Data Parameters
NAME   2023-4-27
EXPNO   7
PROCNO   1

F2 - Acquisition Parameters
Date_   20230428
Time   2.30 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   500
DS   4
SWH   23809.523 Hz
FIDRES   0.726609 Hz
AQ   1.3762560 sec
RG   47.4244
DW   21.000 usec
DE   6.50 usec
TE   295.0 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1
SFO1   100.6228298 MHz
NUC1   13C
P0   3.33 usec
P1   10.00 usec
PLW1   87.89900208 W
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz65
PCPD2   90.00 usec
PLW2   20.73200035 W
PLW12   0.25595000 W
PLW13   0.12874000 W

F2 - Processing parameters
SI   32768
SF   100.6127620 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

XY-3-79-H

Peak list (ppm): 8.236, 7.658, 7.639, 7.400, 7.395, 7.389, 7.382, 7.376, 7.373, 7.367, 7.359, 7.354, 7.349, 7.315, 7.297, 7.260, 7.209, 7.190, 7.183, 7.176, 7.170, 6.934, 6.914, 6.881, 6.863, 6.857, 6.847, 6.845, 6.816, 6.639, 6.636, 6.644, 6.631, 6.378, 6.365, 6.351, 6.338, 6.325, 6.311, 4.230, 4.226, 4.217, 4.213, 3.097

4c

Integrations: 1.00, 0.98, 1.98, 1.00, 2.01, 4.00, 1.03, 0.99, 1.94, 3.06

XY-3-79-C

149.70
133.53
129.36
128.44
127.55
126.83
124.35
120.89
120.27
120.22
120.10
116.88
112.88
103.07

77.47
77.15
76.83

55.42

38.24

4c

200 180 160 140 120 100 80 60 40 20 0 ppm

XY-3-69-H

8.430 7.597 7.577 7.260 7.242 7.235 7.228 7.173 7.155 7.117 7.098 7.079 6.850 6.810 6.589 6.584 6.581 6.576 6.198 6.180 6.161 6.140 6.122 5.305 5.291 5.284 5.269 4.349 4.347 4.331 4.330 4.313 4.295 3.232 3.214 3.195 3.189 3.185 3.173 3.156 3.153 3.134 1.332 1.315 1.297

4d

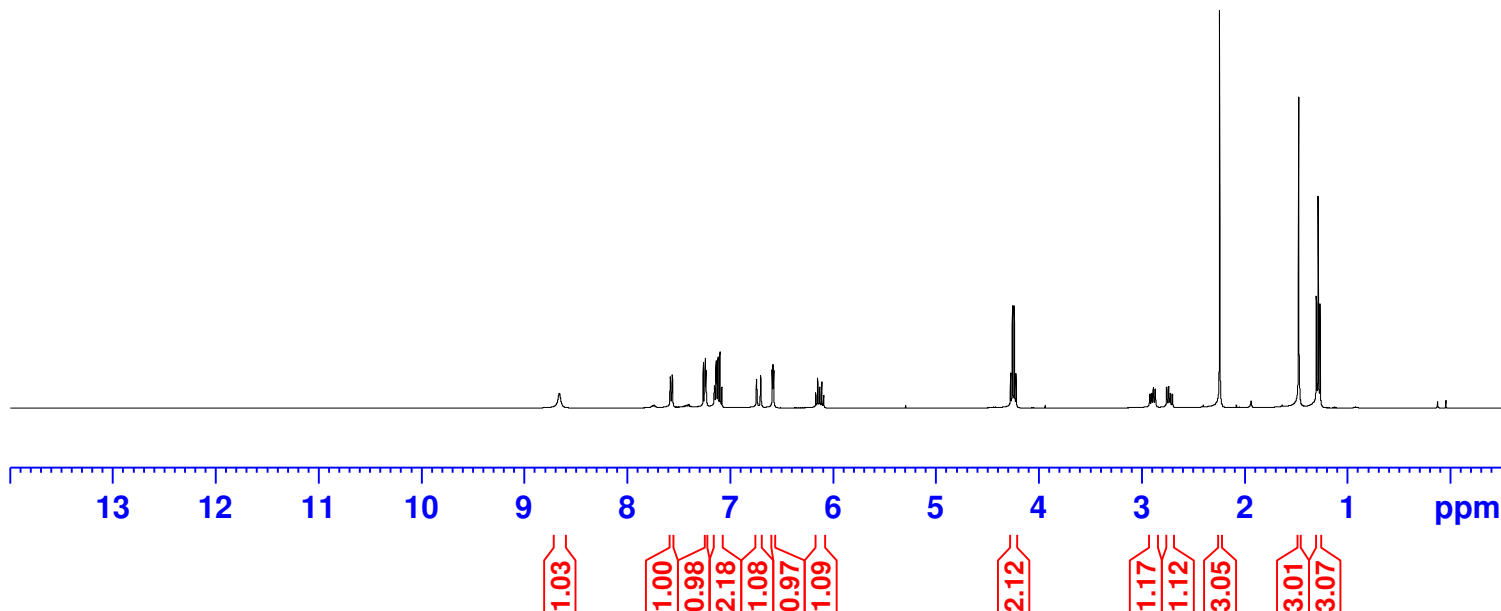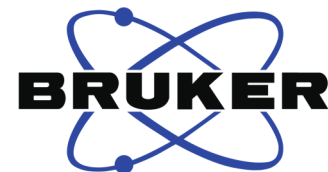Current Data Parameters
NAME   2023-4-27
EXPNO   4
PROCNO   1

F2 - Acquisition Parameters
Date_   20230428
Time   0.53 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zg30
TD   65536
SOLVENT   CDCl3
NS   16
DS   2
SWH   8196.722 Hz
FIDRES   0.250144 Hz
AQ   3.9976959 sec
RG   98.3478
DW   61.000 usec
DE   13.54 usec
TE   294.5 K
D1   1.00000000 sec
TD0   1
SFO1   400.1324708 MHz
NUC1   1H
P0   3.33 usec
P1   10.00 usec
PLW1   20.73200035 W

F2 - Processing parameters
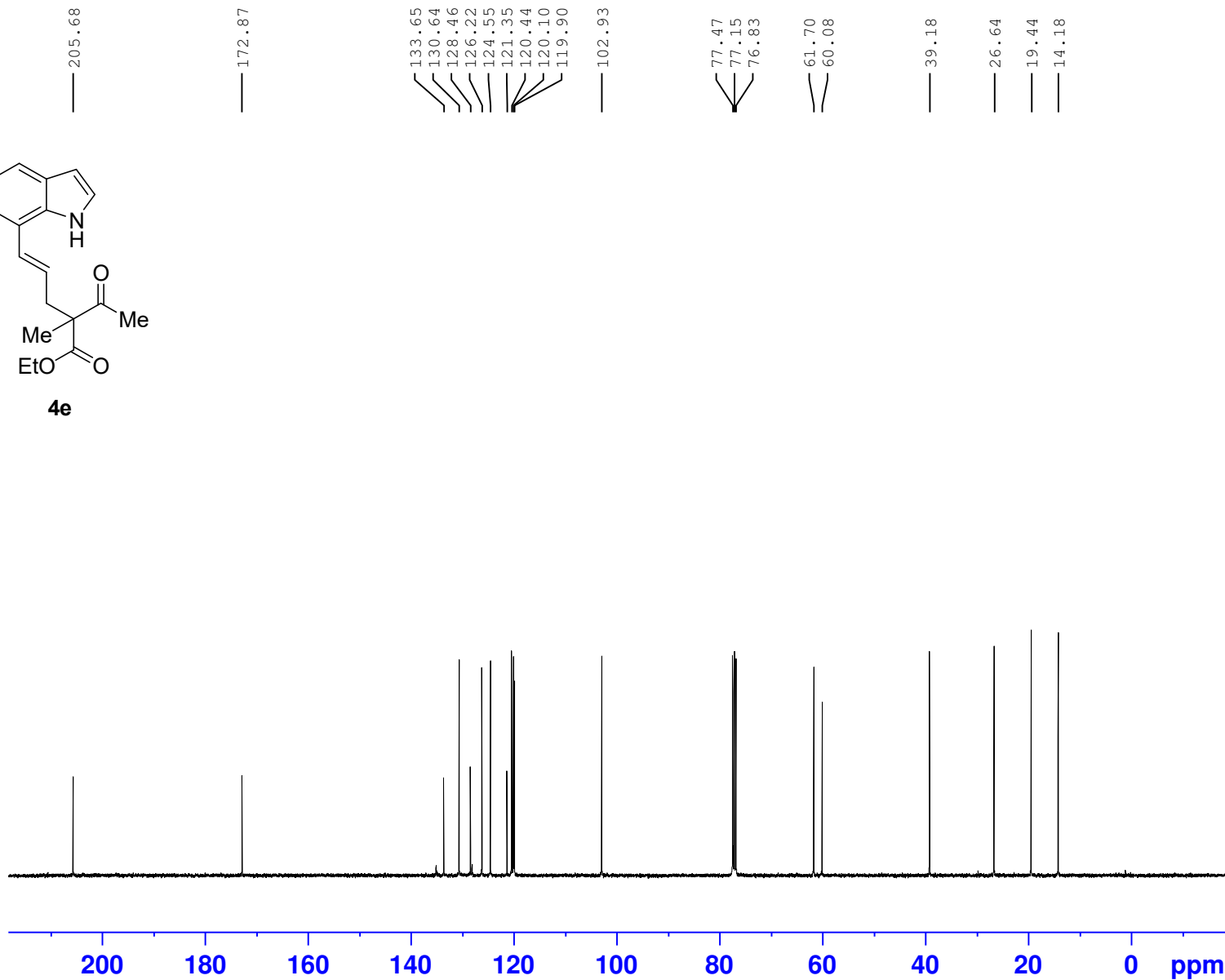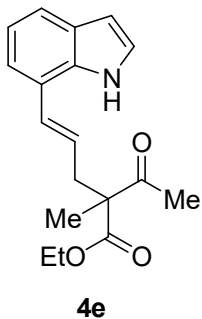SI   65536
SF   400.1300098 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00

Integrals: 0.95 0.95 0.96 1.00 1.01 1.00 0.91 1.04 1.00 2.03 2.13 3.11
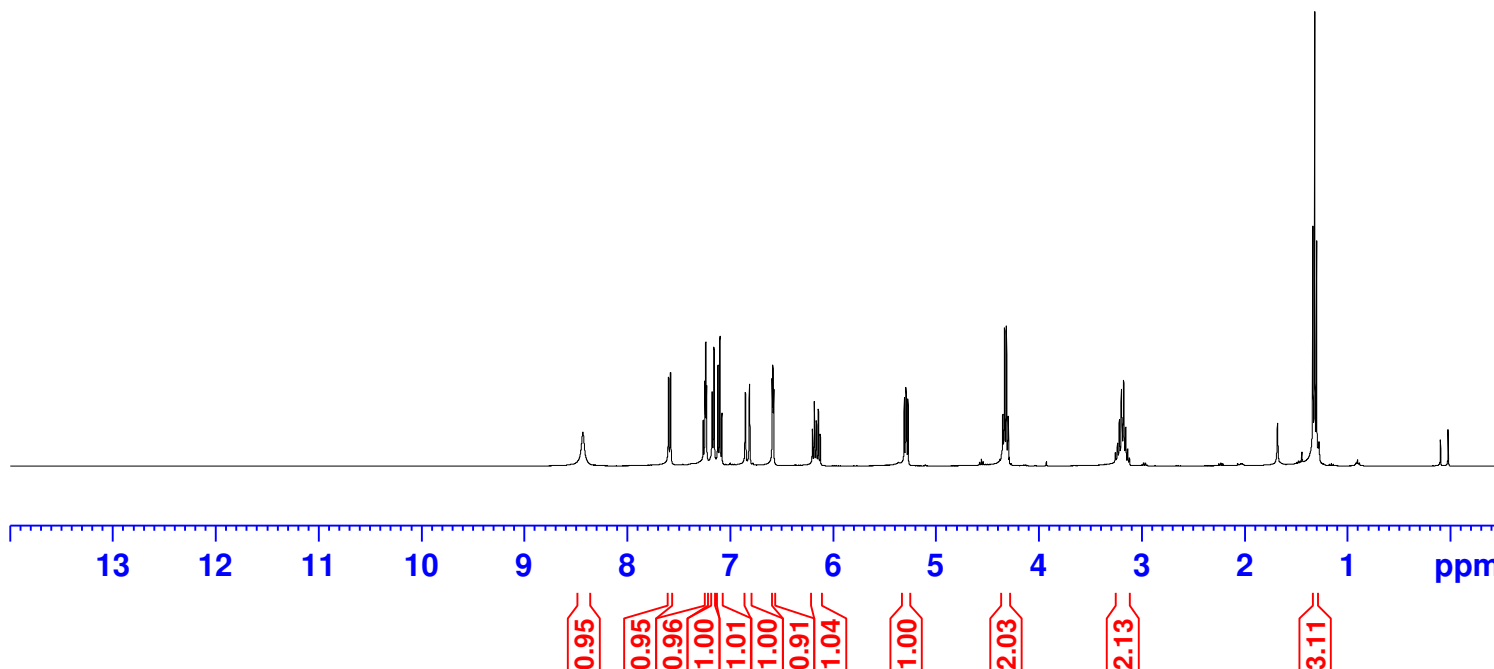
XY-3-69-C
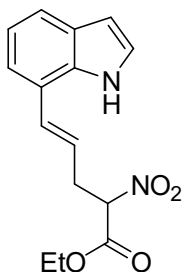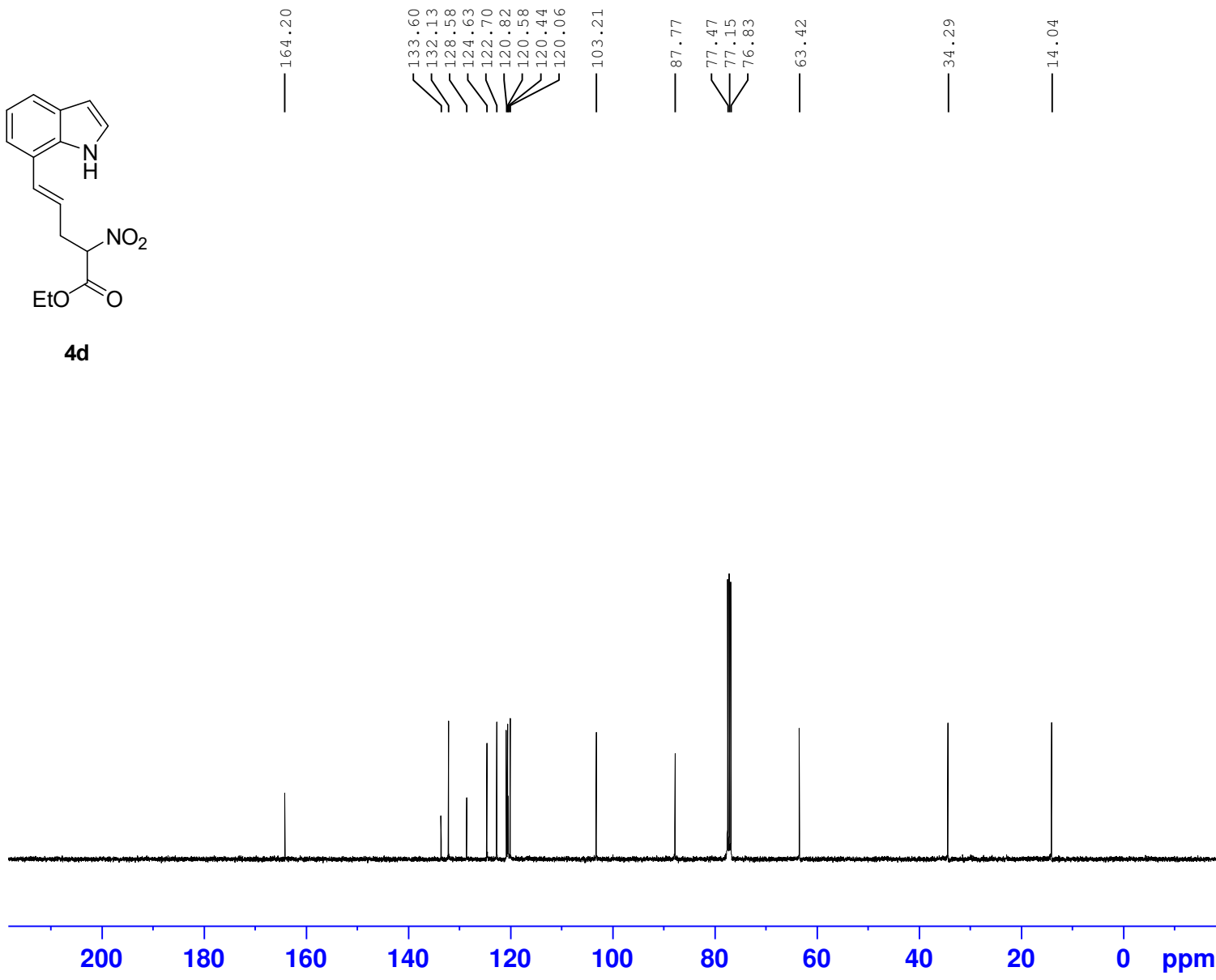
164.20
133.60
132.13
128.58
124.63
122.70
120.82
120.58
120.44
120.06
103.21
87.77
77.47
77.15
76.83
63.42
34.29
14.04

4d

200 180 160 140 120 100 80 60 40 20 0 ppm

XY-3-70-H

8.659
7.580
7.561
7.260
7.246
7.238
7.231
7.150
7.135
7.117
7.098
7.080
6.741
6.701
6.588
6.583
6.581
6.575
6.166
6.147
6.127
6.107
6.089
4.272
4.254
4.236
4.218
2.920
2.917
2.901
2.898
2.885
2.882
2.866
2.863
2.755
2.752
2.735
2.732
2.720
2.717
2.700
2.697
2.239
1.471
1.299
1.281
1.263

BRUKER

Current Data Parameters
NAME   2023-4-27
EXPNO   8
PROCNO   1

F2 - Acquisition Parameters
Date_   20230428
Time   15.59 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zg30
TD   65536
SOLVENT   CDCl3
NS   16
DS   2
SWH   8196.722 Hz
FIDRES   0.250144 Hz
AQ   3.9976959 sec
RG   41.6667
DW   61.000 usec
DE   13.54 usec
TE   293.7 K
D1   1.00000000 sec
TD0   1
SFO1   400.1324708 MHz
NUC1   1H
P0   3.33 usec
P1   10.00 usec
PLW1   20.73200035 W

F2 - Processing parameters
SI   65536
SF   400.1300097 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00

4e

1.03
1.00
0.98
2.18
1.08
0.97
1.09
2.12
1.17
1.12
3.05
3.01
3.07

XY-3-70-C

205.68

172.87

133.65
130.64
128.46
126.22
124.55
121.35
120.44
120.10
119.90

102.93

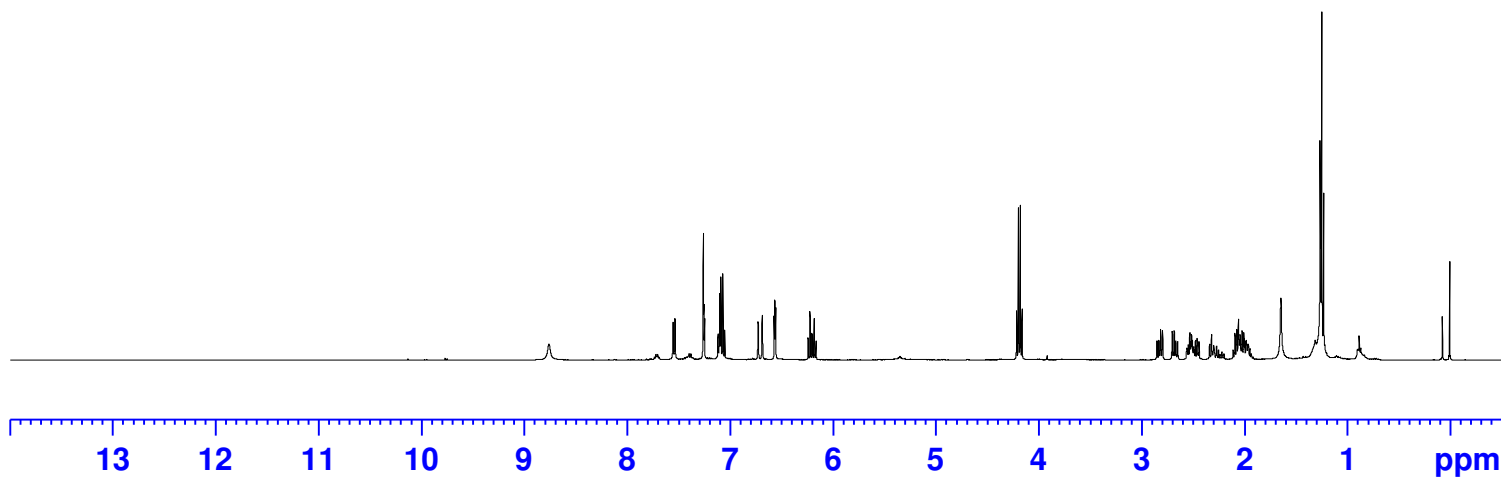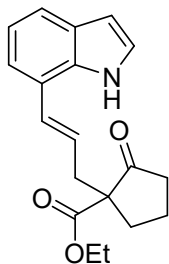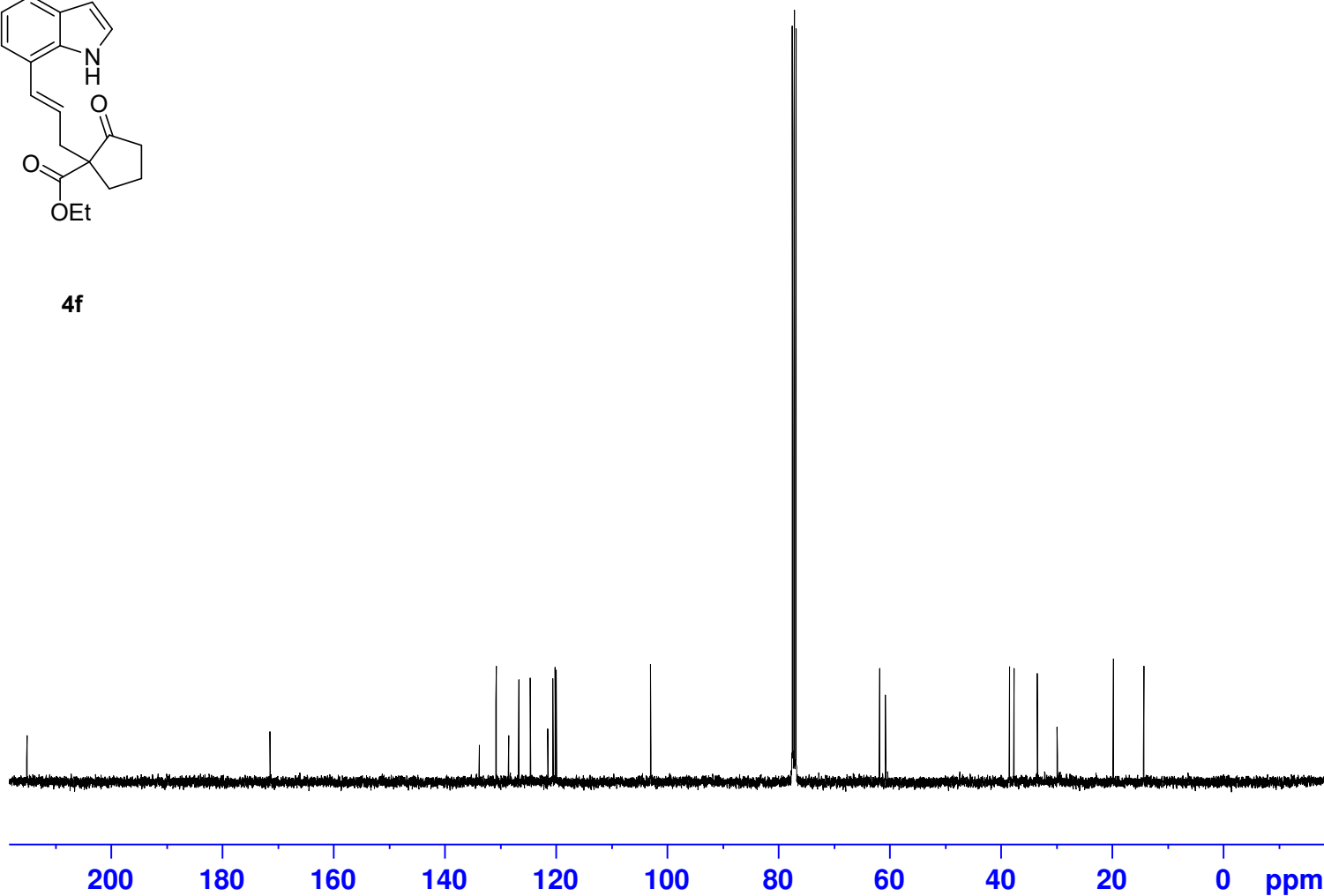77.47
77.15
76.83

61.70
60.08

39.18

26.64

19.44
14.18
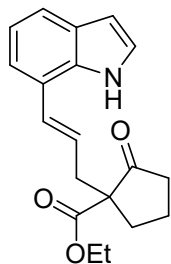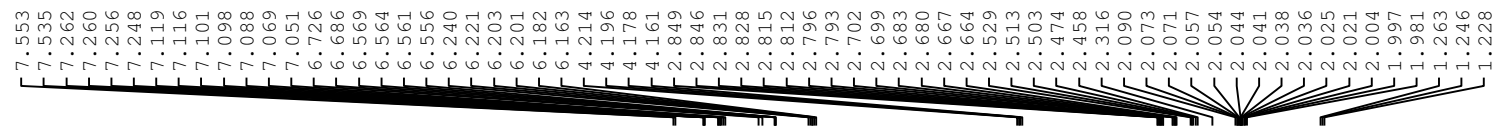
BRUKER

Current Data Parameters
NAME   2023-4-27
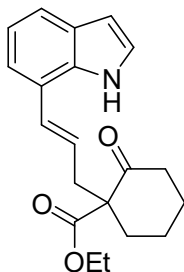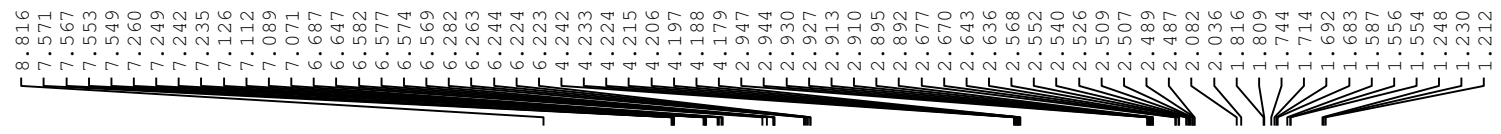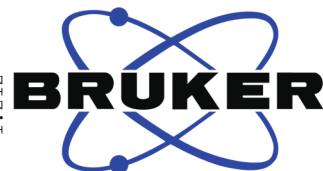EXPNO   6
PROCNO   1

F2 - Acquisition Parameters
Date_   20230428
Time   1.57 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   500
DS   4
SWH   23809.523 Hz
FIDRES   0.726609 Hz
AQ   1.3762560 sec
RG   46.0295
DW   21.000 usec
DE   6.50 usec
TE   294.8 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1
SFO1   100.6228298 MHz
NUC1   13C
P0   3.33 usec
P1   10.00 usec
PLW1   87.89900208 W
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz65
PCPD2   90.00 usec
PLW2   20.73200035 W
PLW12   0.25595000 W
PLW13   0.12874000 W

F2 - Processing parameters
SI   32768
SF   100.6127675 MHz
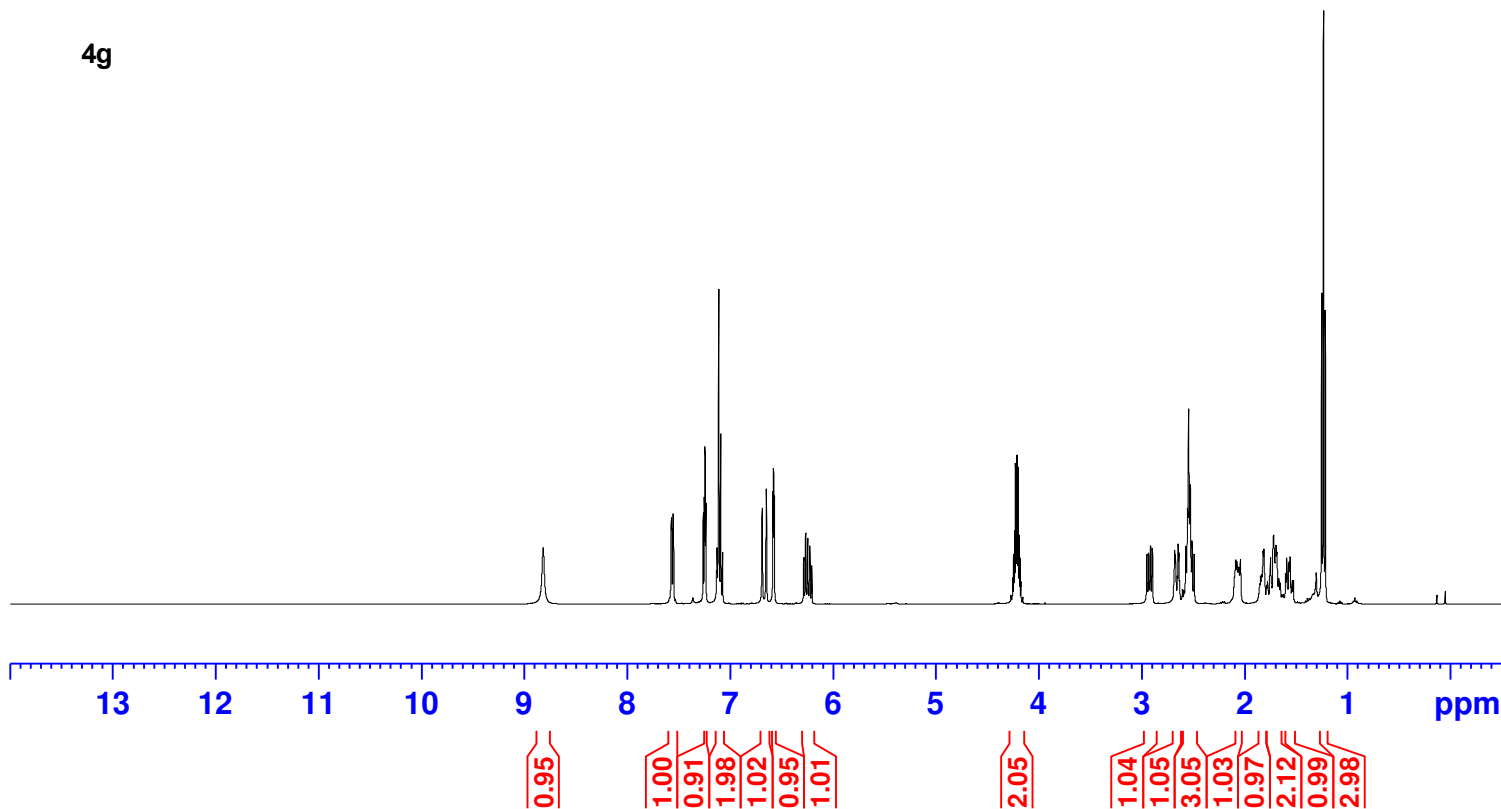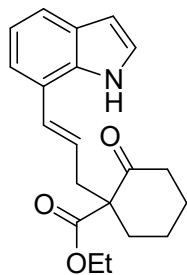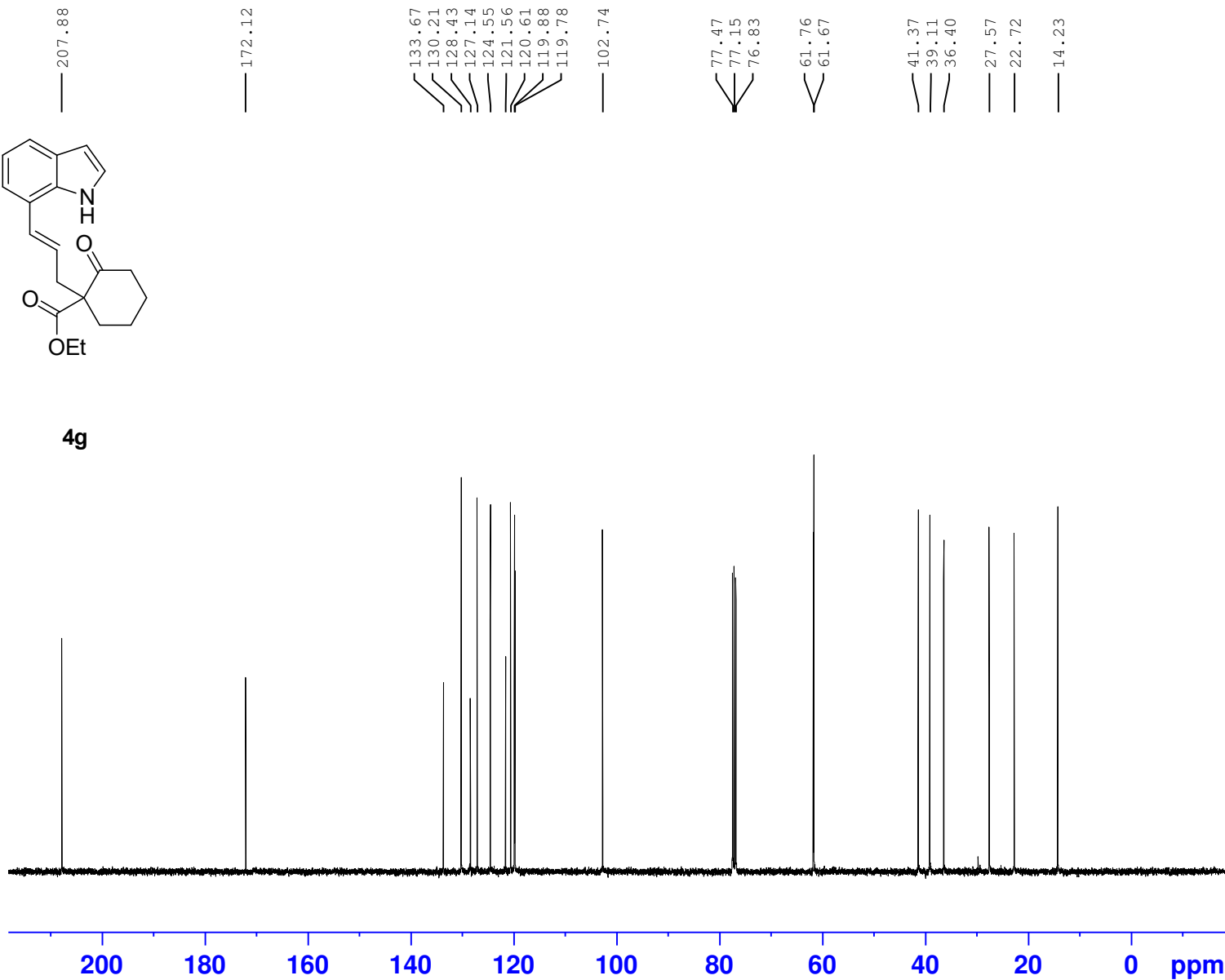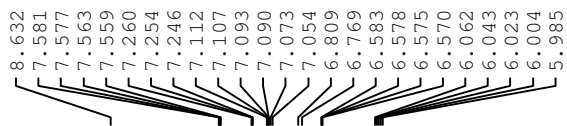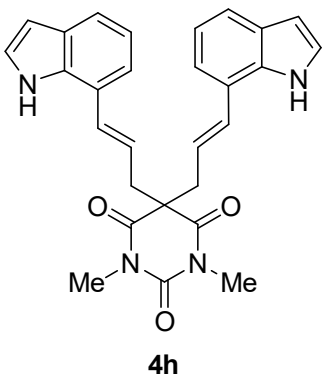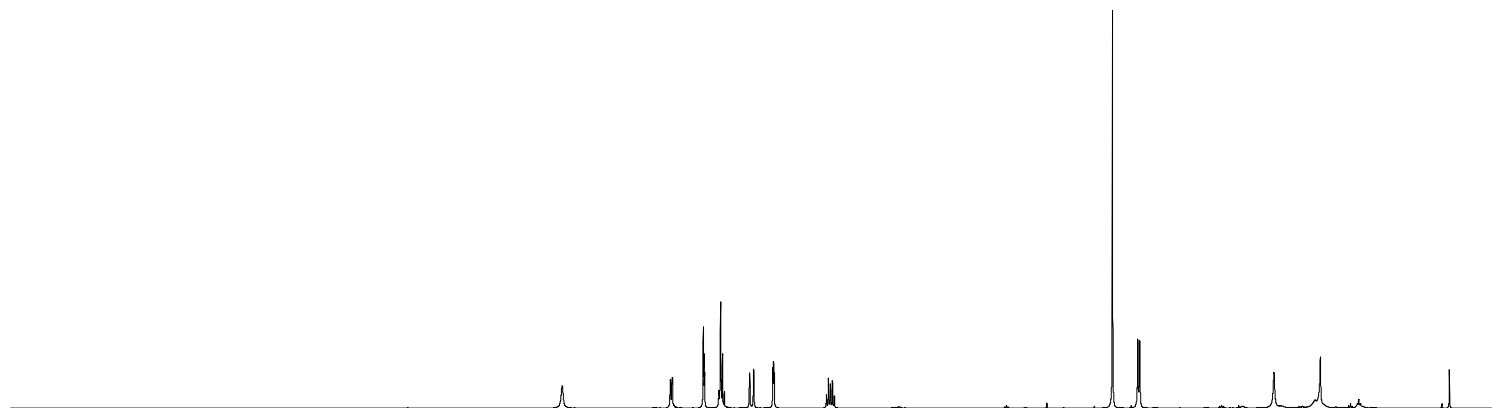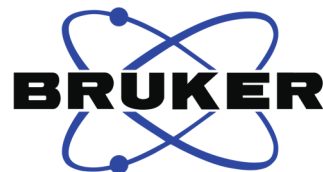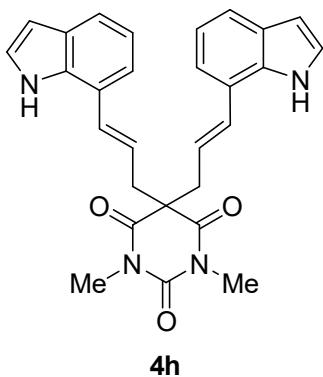WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

4e

200   180   160   140   120   100   80   60   40   20   0   ppm

XY-4-8-H

7.553 7.535 7.262 7.260 7.256 7.248 7.119 7.116 7.101 7.098 7.088 7.069 7.051 6.726 6.686 6.569 6.564 6.561 6.556 6.240 6.221 6.203 6.201 6.182 6.163 4.214 4.196 4.178 4.161 2.846 2.831 2.828 2.815 2.812 2.796 2.793 2.702 2.699 2.683 2.680 2.667 2.664 2.529 2.513 2.503 2.474 2.458 2.316 2.090 2.073 2.071 2.057 2.054 2.044 2.041 2.038 2.036 2.025 2.021 2.004 1.997 1.981 1.263 1.246 1.228

4f

0.88 0.93 1.14 1.96 0.89 0.88 0.93 1.93 0.97 0.97 2.00 1.18 3.17 1.01 2.05

XY-4-8-C

215.17

171.43

133.77
130.77
128.51
126.69
124.59
121.46
120.55
120.15
119.92

102.96

77.46
77.15
76.83

61.79
60.70

38.41
37.58
33.39

19.75
14.26

4f

200   180   160   140   120   100   80   60   40   20   0   ppm

XY-4-22-H

8.816
7.571
7.567
7.553
7.549
7.260
7.249
7.242
7.235
7.126
7.112
7.089
7.071
6.687
6.647
6.582
6.577
6.574
6.569
6.263
6.244
6.224
6.223
4.242
4.233
4.224
4.215
4.206
4.197
4.188
4.179
2.947
2.944
2.930
2.927
2.913
2.910
2.895
2.892
2.677
2.670
2.643
2.636
2.568
2.552
2.540
2.526
2.509
2.507
2.489
2.487
2.082
2.036
1.816
1.809
1.744
1.714
1.692
1.683
1.587
1.556
1.554
1.248
1.230
1.212

4g

0.95 1.00 0.91 1.98 1.02 0.95 1.01 2.05 1.04 1.05 3.05 1.03 0.97 2.12 0.99 2.98

13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

XY-4-22-C

207.88

172.12

133.67
130.21
128.43
127.14
124.55
121.56
120.61
119.88
119.78

102.74

77.47
77.15
76.83

61.76
61.67

41.37
39.11
36.40

27.57
22.72

14.23

4g

Current Data Parameters
NAME   2023-6-16-1
EXPNO   4
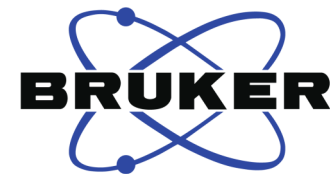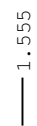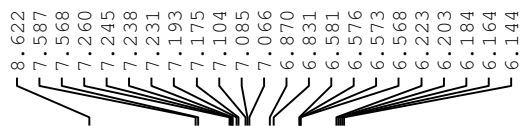PROCNO   1
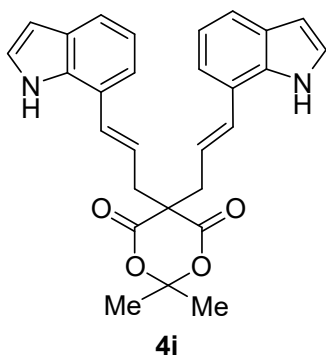
F2 - Acquisition Parameters
Date_   20230617
Time   4.33 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   200
DS   4
SWH   23809.523 Hz
FIDRES   0.726609 Hz
AQ   1.3762560 sec
RG   47.4244
DW   21.000 usec
DE   6.50 usec
TE   294.8 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1
SFO1   100.6228298 MHz
NUC1   13C
P0   3.33 usec
P1   10.00 usec
PLW1   87.89900208 W
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz65
PCPD2   90.00 usec
PLW2   20.73200035 W
PLW12   0.25595000 W
PLW13   0.12874000 W

F2 - Processing parameters
SI   32768
SF   100.6127705 MHz
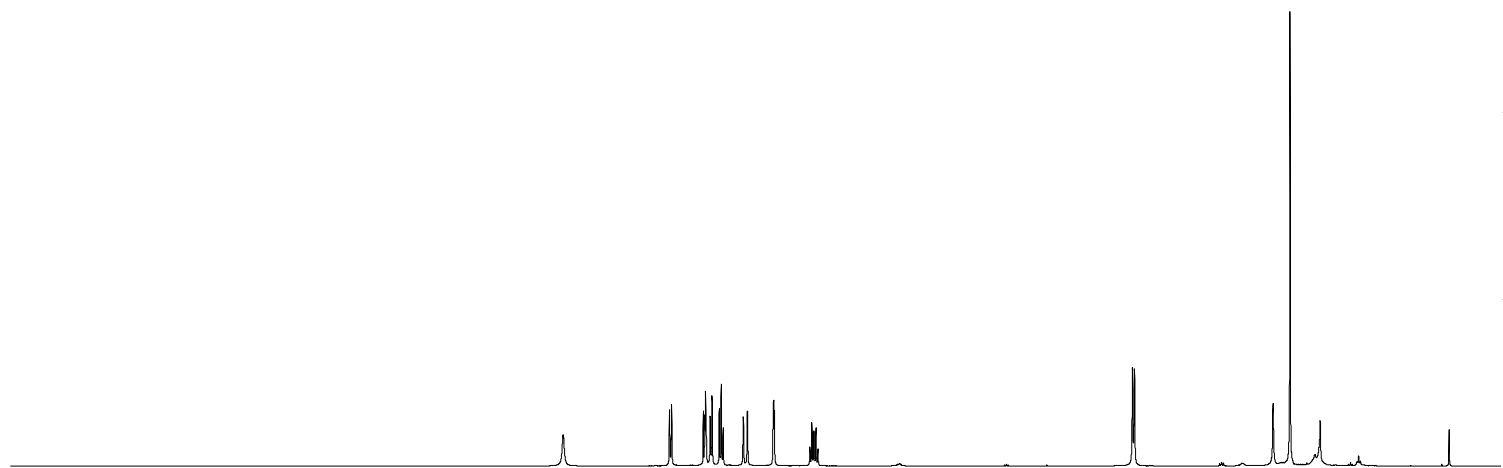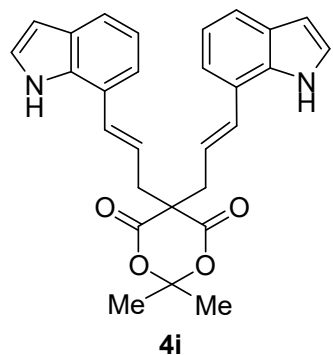WDW   EM
SSB   0
LB   1.00 Hz
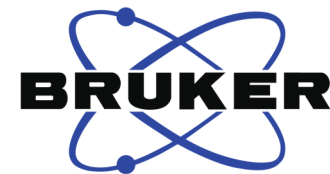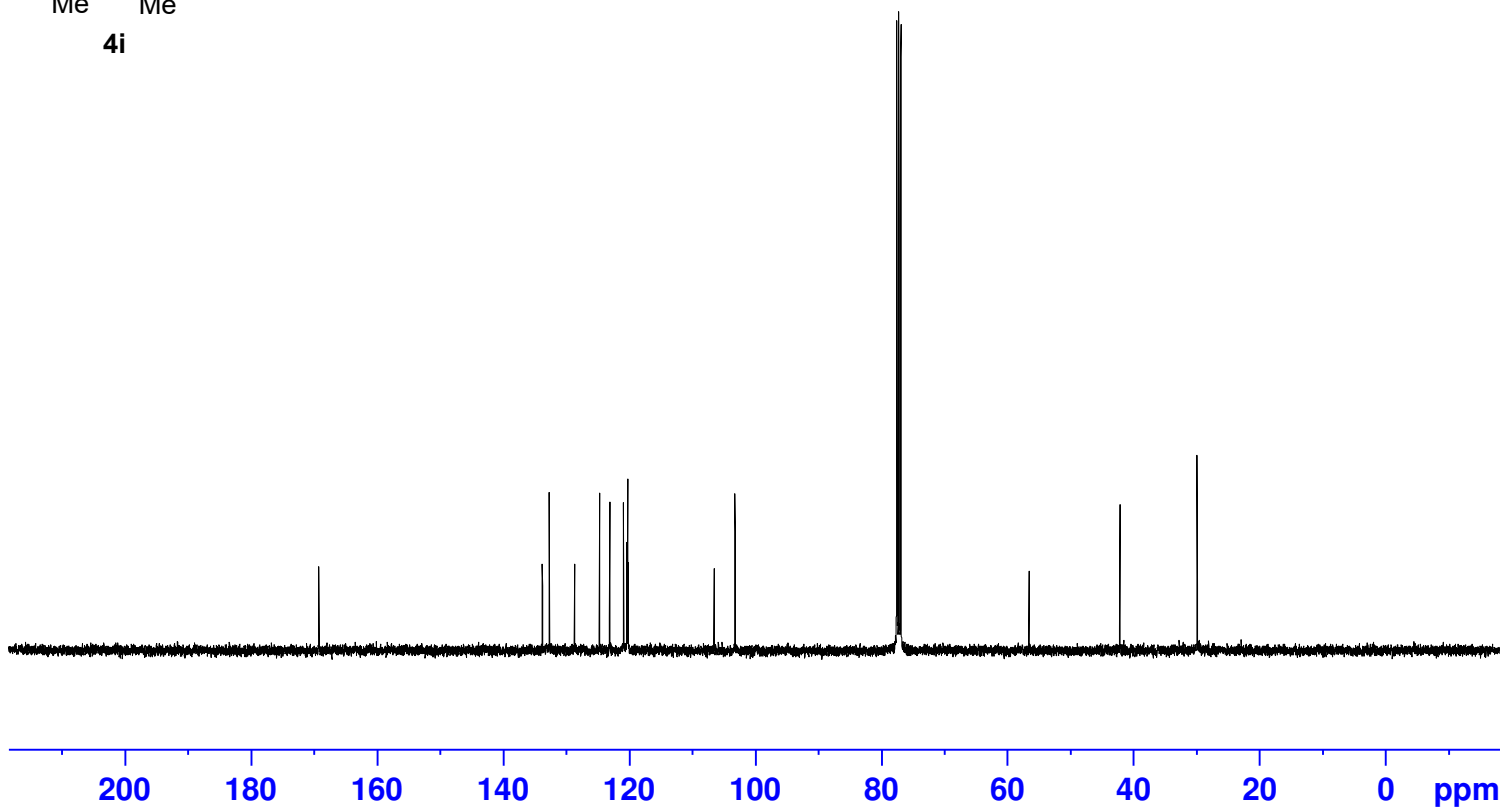GB   0
PC   1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

XY-4-15-H

4h

8.632
7.581
7.577
7.563
7.559
7.260
7.254
7.246
7.112
7.107
7.093
7.090
7.073
7.054
6.809
6.769
6.583
6.578
6.575
6.570
6.062
6.043
6.023
6.004
5.985

3.280
3.036
3.016

BRUKER

Current Data Parameters
NAME   2023-6-12
EXPNO   2
PROCNO   1

F2 – Acquisition Parameters
Date_   20230613
Time   2.49 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zg30
TD   65536
SOLVENT   CDCl3
NS   16
DS   2
SWH   8196.722 Hz
FIDRES   0.250144 Hz
AQ   3.9976959 sec
RG   101
DW   61.000 usec
DE   13.54 usec
TE   294.3 K
D1   1.00000000 sec
TD0   1
SFO1   400.1324708 MHz
NUC1   1H
P0   3.33 usec
P1   10.00 usec
PLW1   20.73200035 W

F2 – Processing parameters
SI   65536
SF   400.1300098 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00

1.83   2.00 2.08 4.12 2.03 1.89 2.06   5.83 3.97

13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

XY-4-15-C

XY-4-20-H

4i

8.622
7.587
7.568
7.260
7.245
7.238
7.231
7.193
7.175
7.104
7.085
7.066
6.870
6.831
6.581
6.576
6.573
6.568
6.223
6.203
6.184
6.164
6.144

3.086
3.067

1.555

2.01 | 2.00 | 1.93 | 2.03 | 2.05 | 2.07 | 1.98 | 2.09 | 4.00 | 6.01

XY-4-20-C

169.17

133.71
132.64
128.61
124.64
123.03
120.85
120.35
120.20
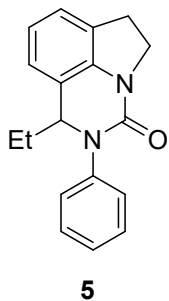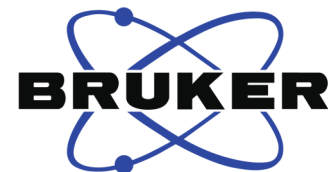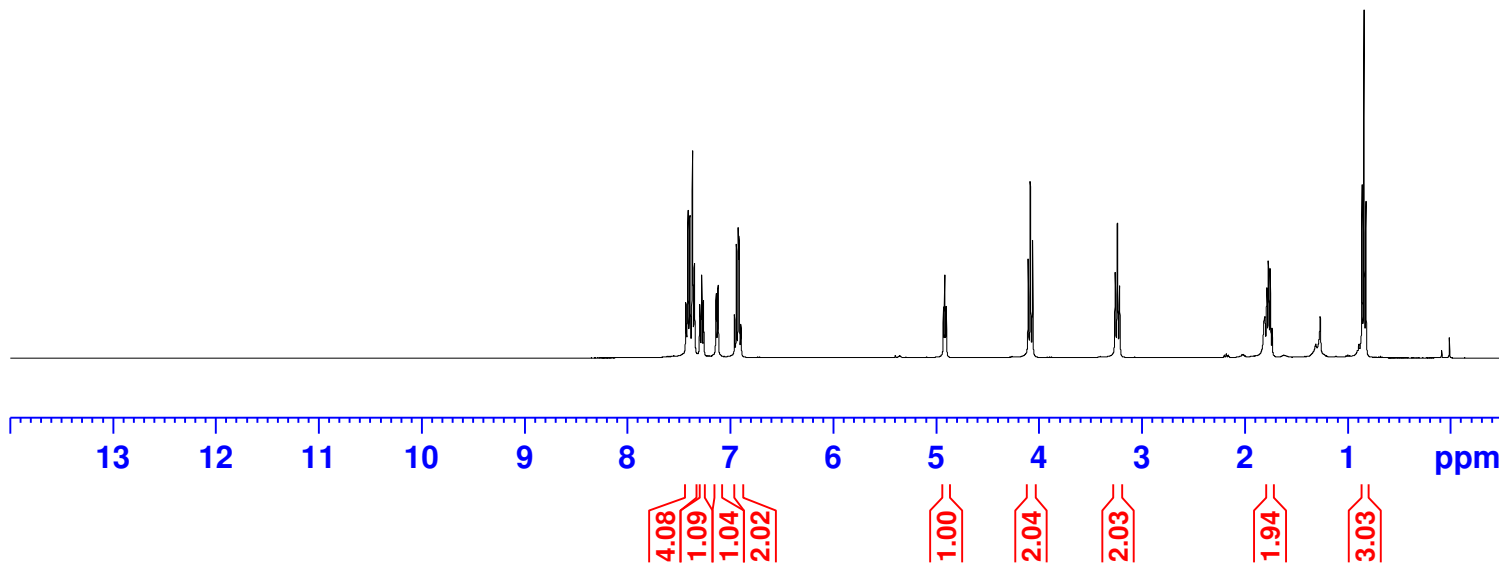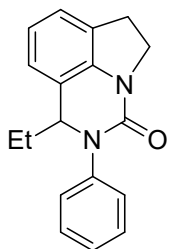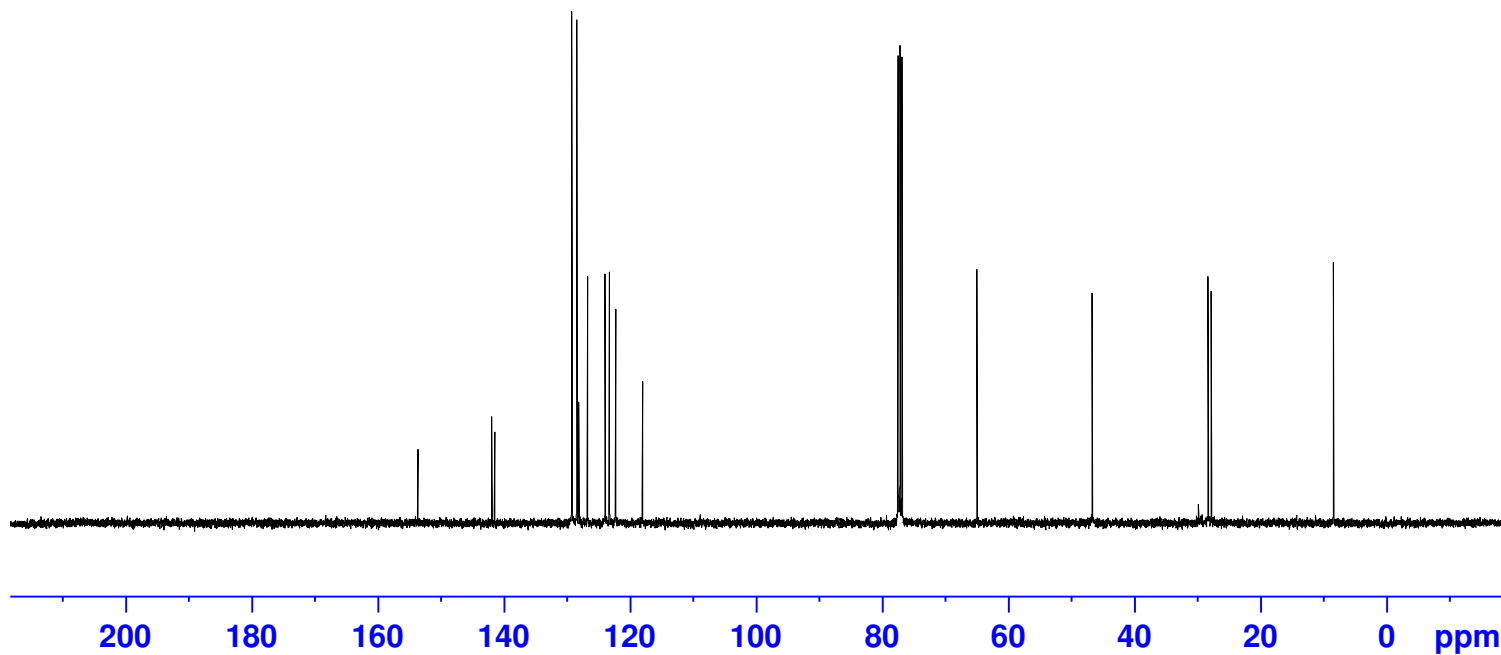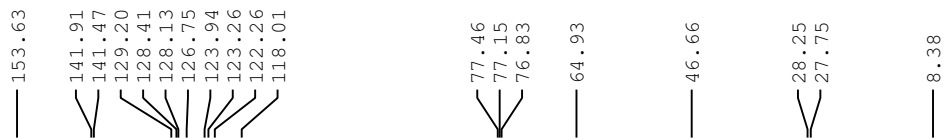120.11
106.46
103.14

77.47
77.15
76.83

56.48

42.08

29.82

4i

200 180 160 140 120 100 80 60 40 20 0 ppm

XY-4-32-H

5

4.08 1.09 1.04 2.02   1.00   2.04   2.03   1.94   3.03

XY-4-32-H

5

153.63
141.91
141.47
129.20
128.41
128.13
126.75
123.94
123.26
122.26
118.01
77.46
77.15
76.83
64.93
46.66
28.25
27.75
8.38

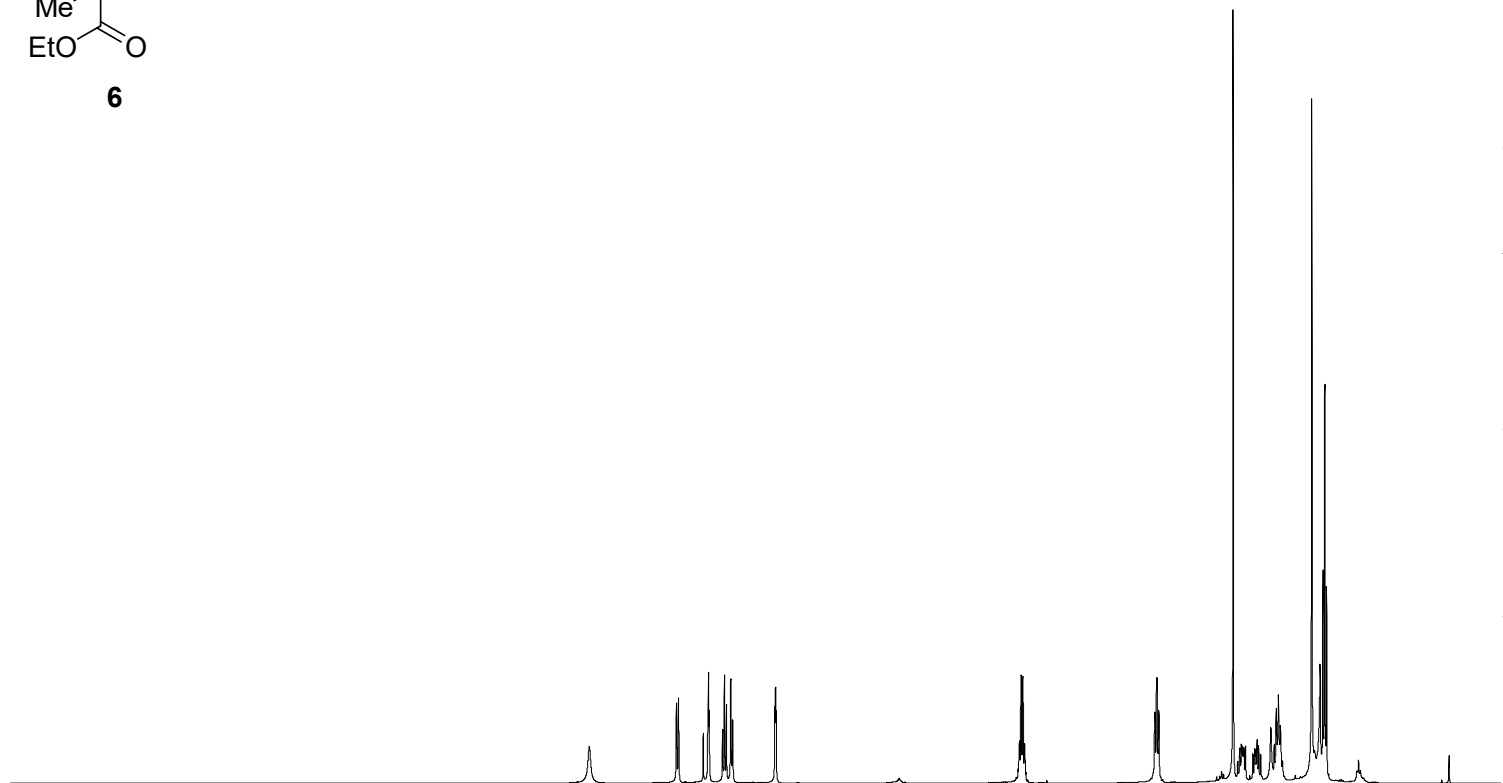200 180 160 140 120 100 80 60 40 20 0 ppm

XY-4-27-H

8.368
7.520
7.500
7.260
7.215
7.208
7.201
7.072
7.054
7.035
6.992
6.974
6.564
6.559
6.556
6.551
4.190
4.185
4.172
4.168
4.154
4.150
4.137
4.132
2.869
2.852
2.848
2.831
2.109
2.042
2.029
2.022
2.014
2.008
2.003
1.988
1.915
1.898
1.890
1.881
1.874
1.861
1.840
1.708
1.688

0.97 1.00 1.04 1.07 1.02 0.98   2.13   2.04 2.94 1.12 1.14 2.19 3.05 3.16

XY-4-27-C

206.10

173.22

134.88
127.88
124.28
124.06
121.46
120.01
118.85

103.06

77.46
77.15
76.83

61.50
59.74

34.83
31.83
26.32
24.62
19.18
14.11

6

XY-4-48-H

9.120
7.557
7.538
7.260
7.242
7.235
7.228
7.138
7.121
7.088
7.069
7.050
6.810
6.771
6.557
6.552
6.549
6.544
6.210
6.191
6.172
6.152
6.133
4.224
4.206
4.203
4.188
4.185
4.171
4.167
3.710
3.696
3.682
2.707
2.686
2.673
2.667
2.649
2.631
1.288
1.270
1.253

Current Data Parameters
NAME   2023-7-6
EXPNO   1
PROCNO   1

F2 - Acquisition Parameters
Date_   20230707
Time   6.11 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zg30
TD   65536
SOLVENT   CDCl3
NS   16
DS   2
SWH   8196.722 Hz
FIDRES   0.250144 Hz
AQ   3.9976959 sec
RG   101
DW   61.000 usec
DE   13.54 usec
TE   294.5 K
D1   1.00000000 sec
TD0   1
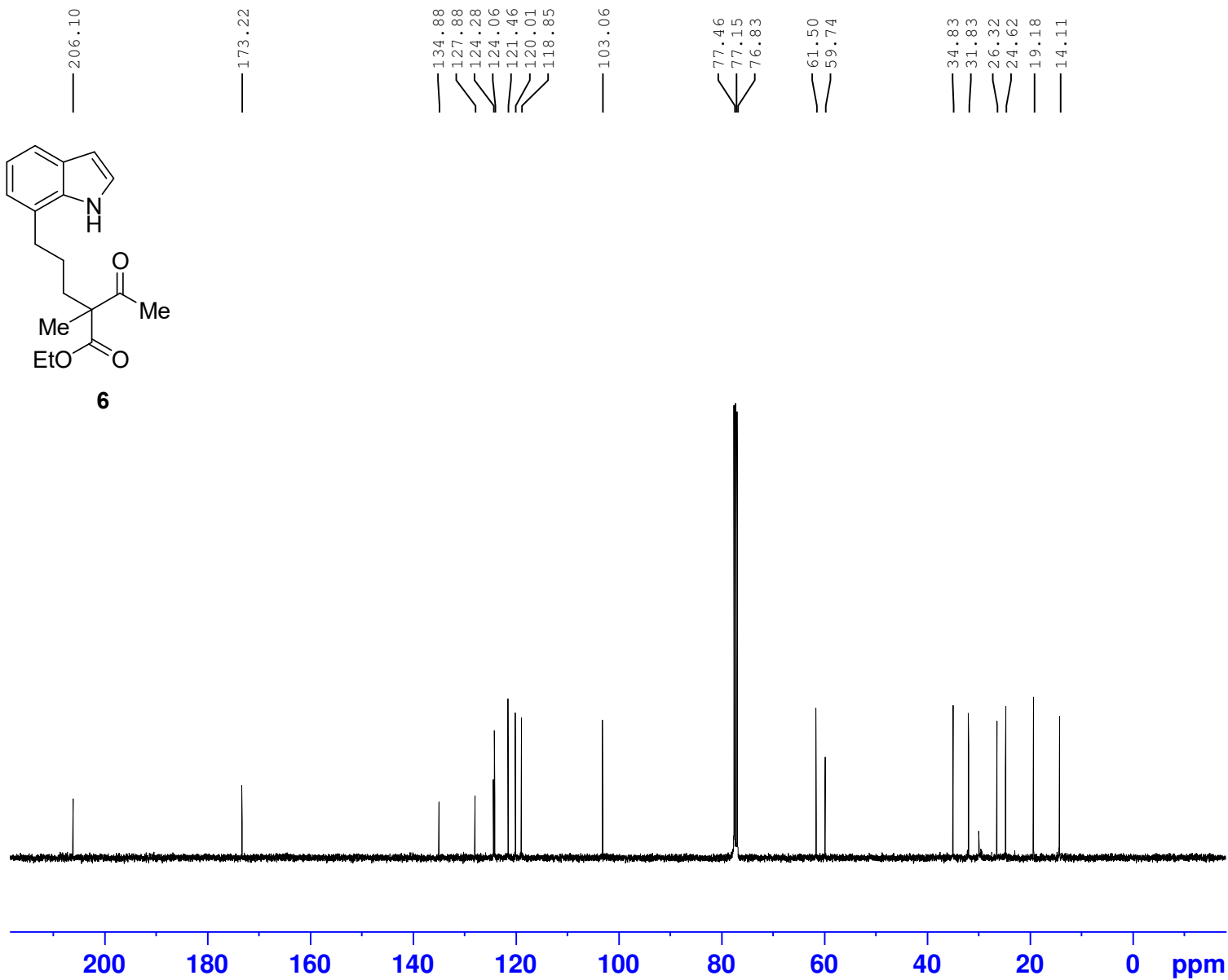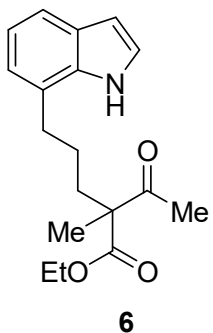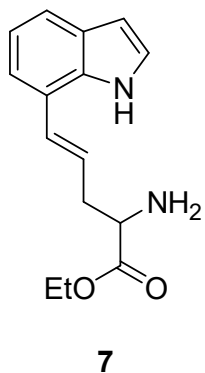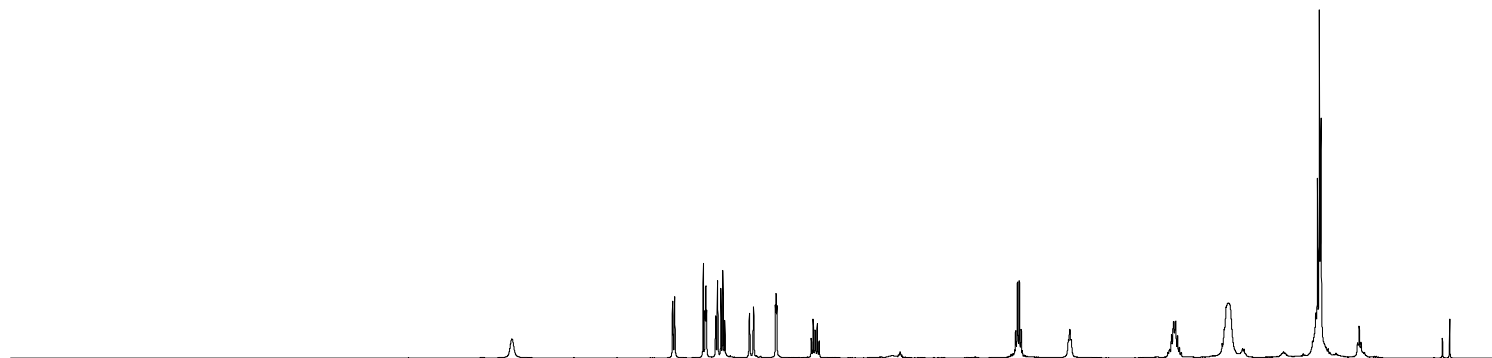SFO1   400.1324708 MHz
NUC1   1H
P0   3.33 usec
P1   10.00 usec
PLW1   20.73200035 W

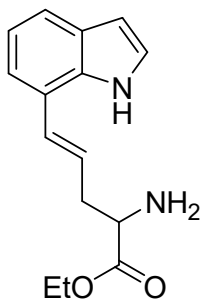F2 - Processing parameters
SI   65536
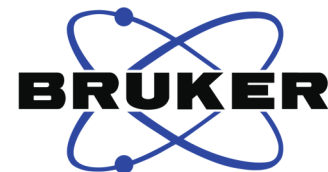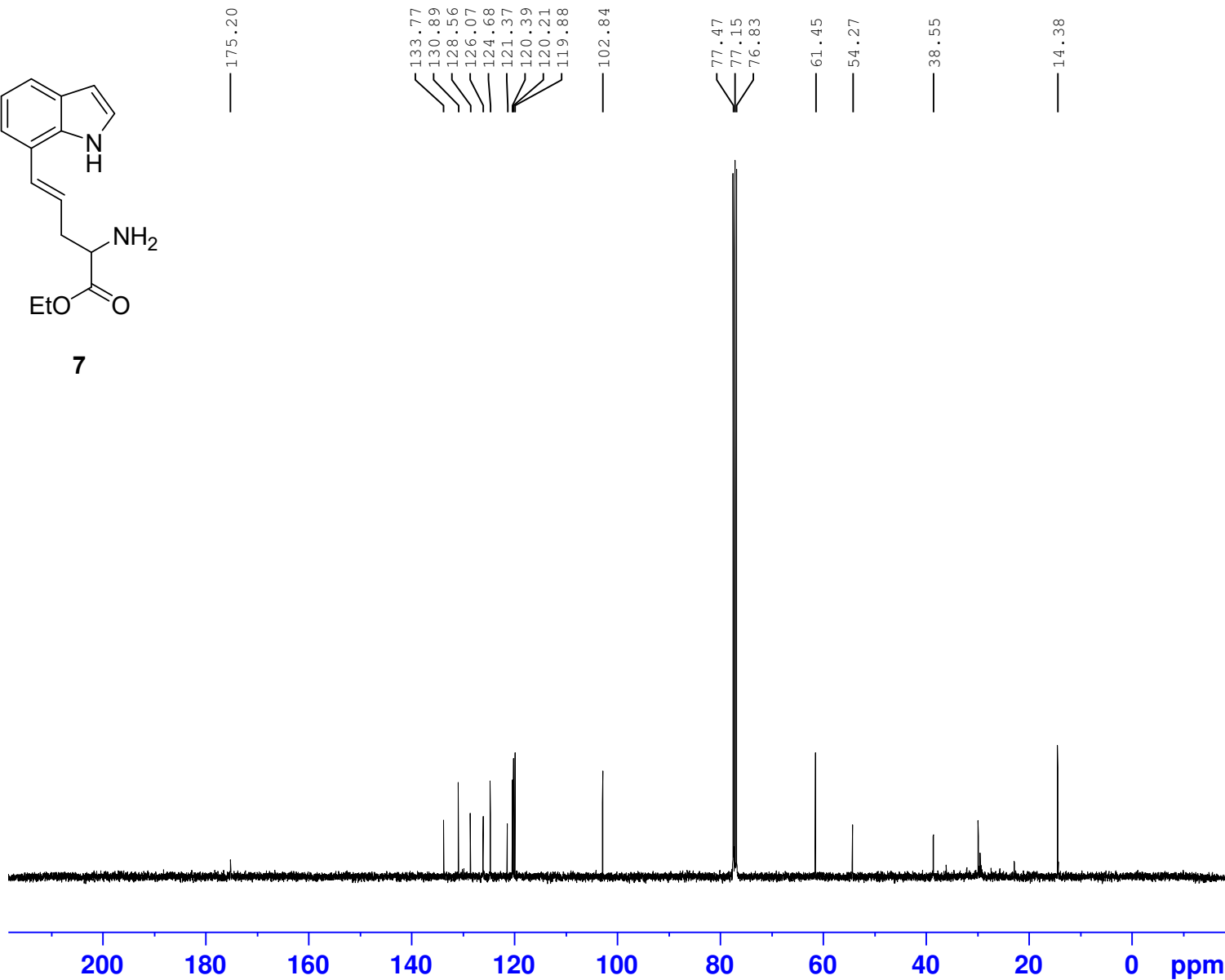SF   400.1300098 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00

Integrations: 0.93 1.00 0.96 1.00 1.08 1.04 1.00 1.05 2.00 0.94 2.14 3.04

XY-4-48-C

175.20
133.77
130.89
128.56
126.07
124.68
121.37
120.39
120.21
119.88
102.84
77.47
77.15
76.83
61.45
54.27
38.55
14.38

7
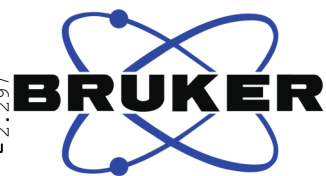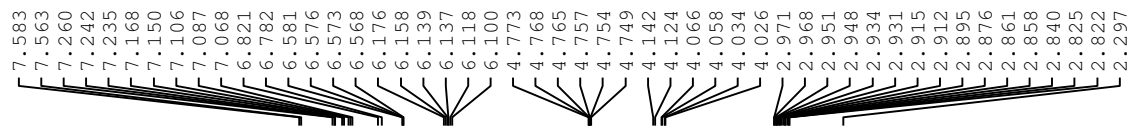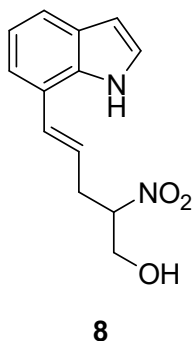
Current Data Parameters
NAME   2023-7-6
EXPNO   2
PROCNO   1

F2 - Acquisition Parameters
Date_   20230707
Time   6.58 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   800
DS   4
SWH   23809.523 Hz
FIDRES   0.726609 Hz
AQ   1.3762560 sec
RG   46.5207
DW   21.000 usec
DE   6.50 usec
TE   294.6 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1
SFO1   100.6228298 MHz
NUC1   13C
P0   3.33 usec
P1   10.00 usec
PLW1   87.89900208 W
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz65
PCPD2   90.00 usec
PLW2   20.73200035 W
PLW12   0.25595000 W
PLW13   0.12874000 W

F2 - Processing parameters
SI   32768
SF   100.6127685 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

XY-4-53-H

Current Data Parameters
NAME   2023-7-7
EXPNO   1
PROCNO   1

F2 – Acquisition Parameters
Date_   20230707
Time   21.10 h
INSTRUM   Avance
PROBHD   Z116098_0833 (
PULPROG   zg30
TD   65536
SOLVENT   CDCl3
NS   24
DS   2
SWH   8196.722 Hz
FIDRES   0.250144 Hz
AQ   3.9976959 sec
RG   101
DW   61.000 usec
DE   13.54 usec
TE   294.5 K
D1   1.00000000 sec
TD0   1
SFO1   400.1324708 MHz
NUC1   1H
P0   3.33 usec
P1   10.00 usec
PLW1   20.73200035 W

F2 – Processing parameters
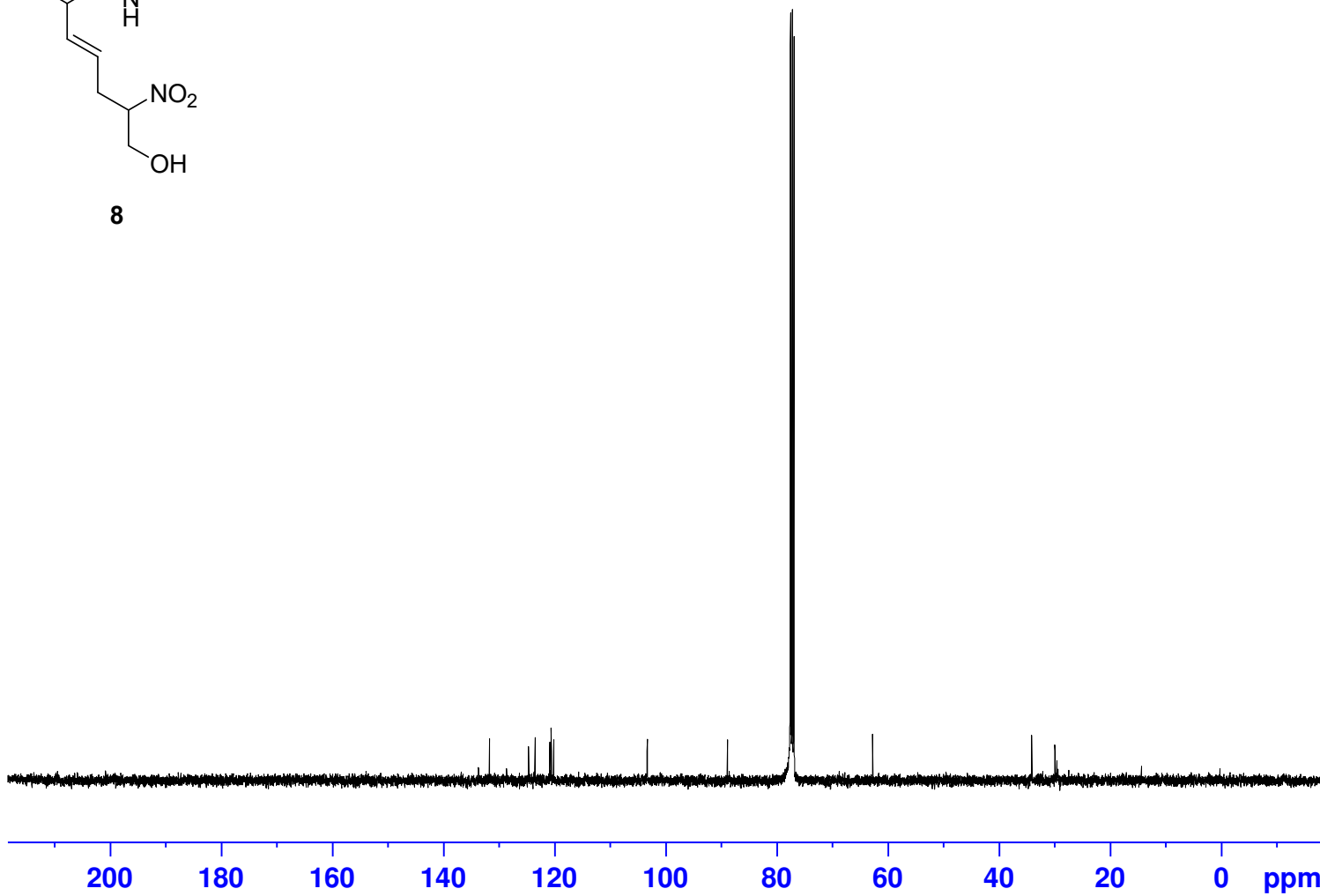SI   65536
SF   400.1300100 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00
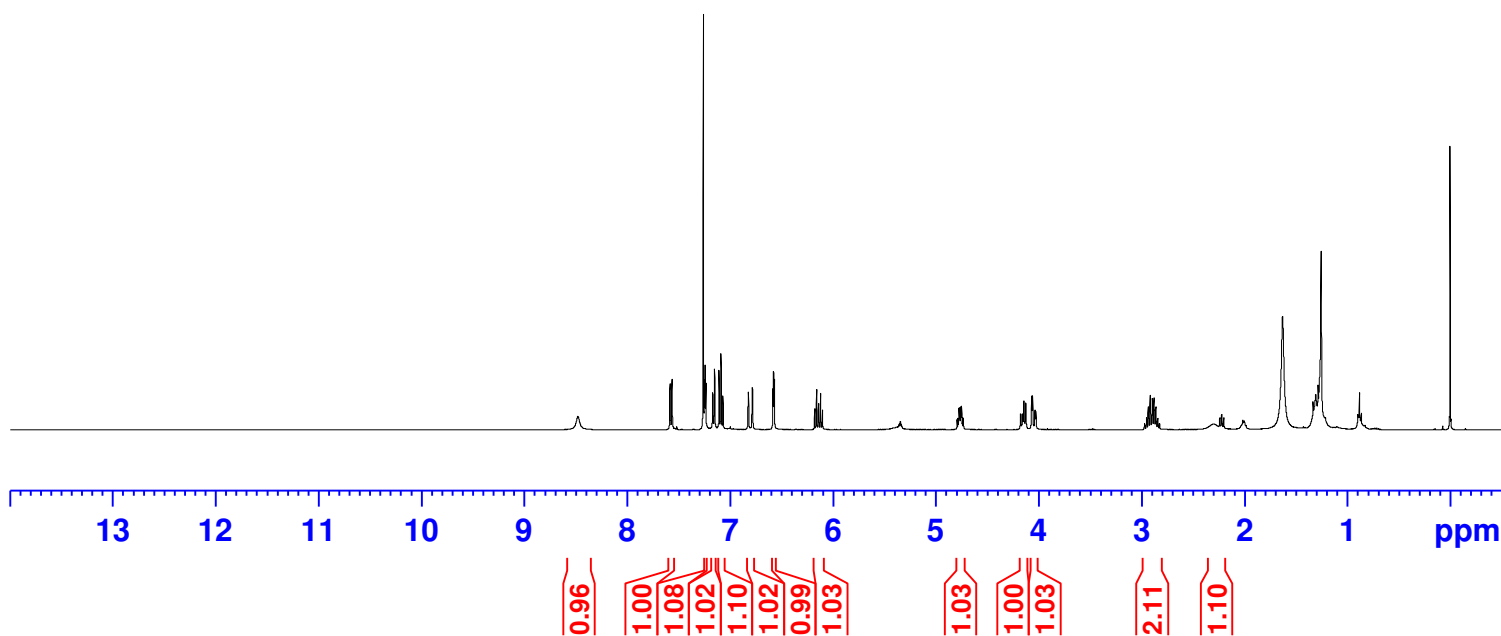
XY-4-56-C
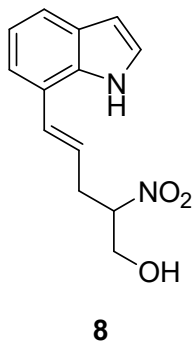
133.632
131.654
128.623
124.602
123.467
120.775
120.534
120.093
103.260
88.766
77.465
77.148
76.830
62.685
34.030
14.263

8