

Stereoselective Sulfenylation of Oxindole-derived Propargyl Alcohols to access Sulfenylated-3-Alkenyloxindoles

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General Information:

All solvents used were of analytical grade and used as purchased without further purification. Reactions were monitored by thin-layer chromatography (TLC). Visualization of the spots on TLC plates was done under UV light. Commercial silica gel (60-120 and 100-200 mesh size) was used for column chromatography. ^1H s were recorded in CDCl_3 and ^{13}C NMR samples were recorded in CDCl_3 , and 1-2 drops of $\text{DMSO}-d_6$, chemical shifts are expressed in parts per million (δ) scale using tetramethylsilane as an internal standard. The standard abbreviations s, d, dd, t, and m refer to singlet, doublet, and doublet of doublet, triplet, and multiplet respectively. Coupling constants (J) have been reported in Hz. Oxindole derived propargyl alcohols synthesized using a reported procedure. Isatins, alkynes, KO^tBu , thiophenols, 2-naphthalenethiol, 1-naphthalenethiols, $\text{Ca}(\text{OTf})_2$, Bu_4NPF_6 and other reagents required were purchased from Sigma-Aldrich, Alfa Aesar, Spectrochem, TCI Chemicals and Avra Synthesis. Solvents and silica gel (60–120 mesh) and other common reagents were procured from local suppliers. Thin-layer chromatography (TLC) was carried out on Merck silica gel plates (60 F254). ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR were recorded on a Bruker Ultrashield 500 and 400 MHz or Bruker Ascend 500 MHz instrument. Melting points were measured with a MEPA LABINDIA melting point apparatus. Single-crystal X-ray diffraction data were collected in Bruker D8-Quest diffractometers.

Data for Single X-Ray Crystal Structure 3a:

Vapour diffusion crystallization method was used for crystal growth for **3a**, where compound was dissolved in chloroform by heating to make saturated solution in small vial which was placed in closed bottle with other solvent as *n*-hexane.

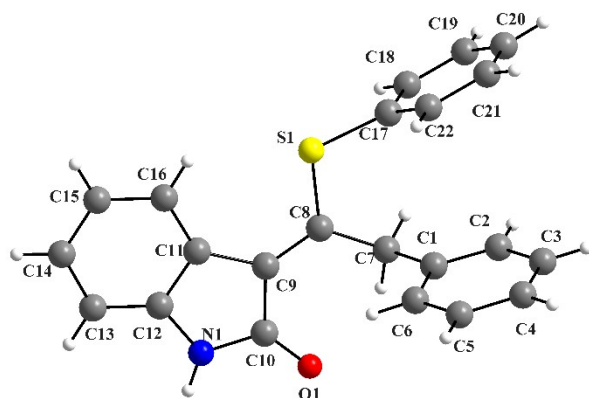


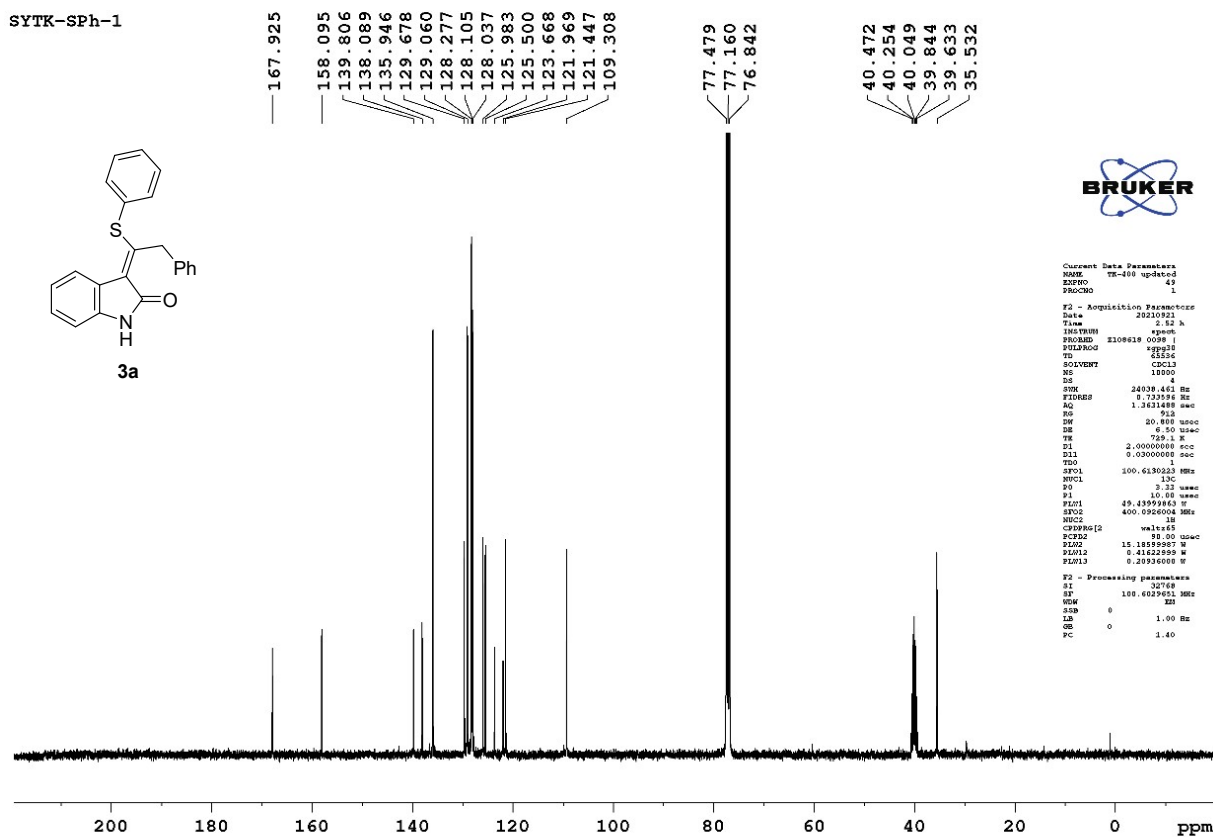
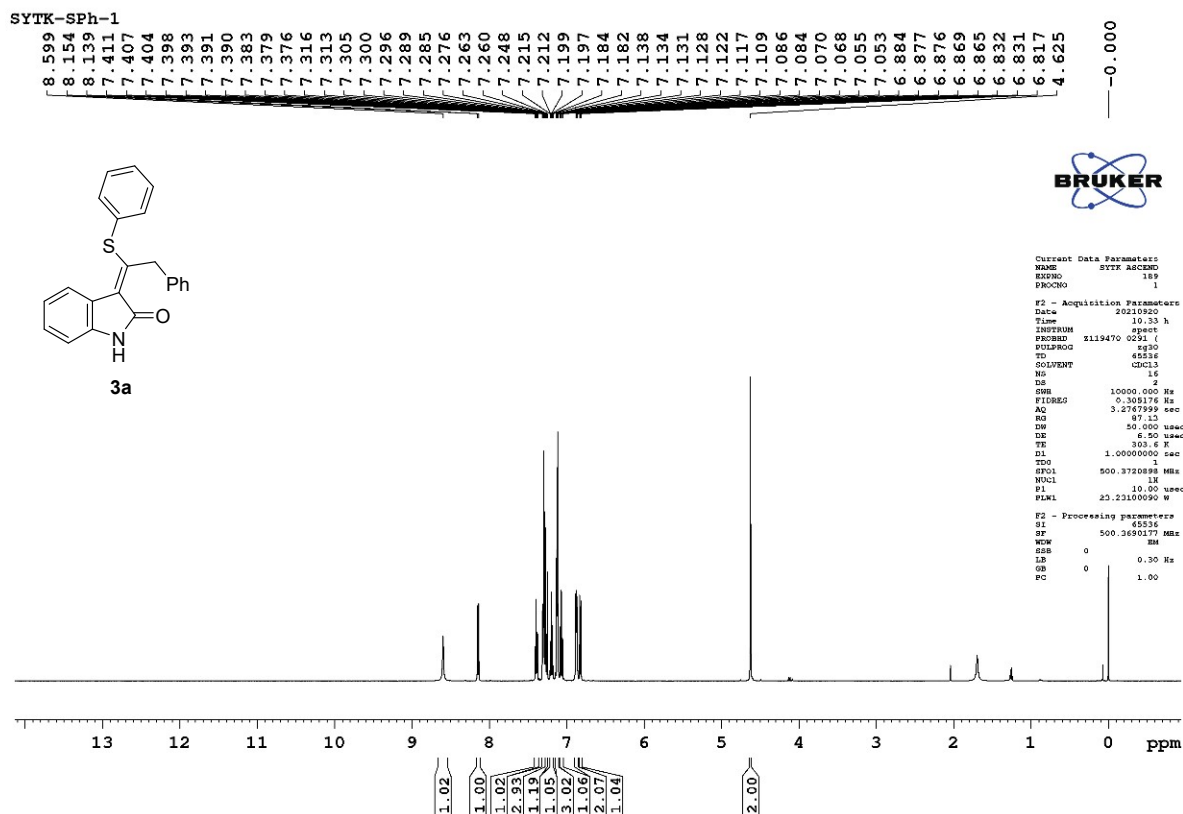
Figure S1. ORTEP representation of compound **3a** and thermal ellipsoids are drawn with 50% probability.

Crystal data and structure refinement for **3a**:

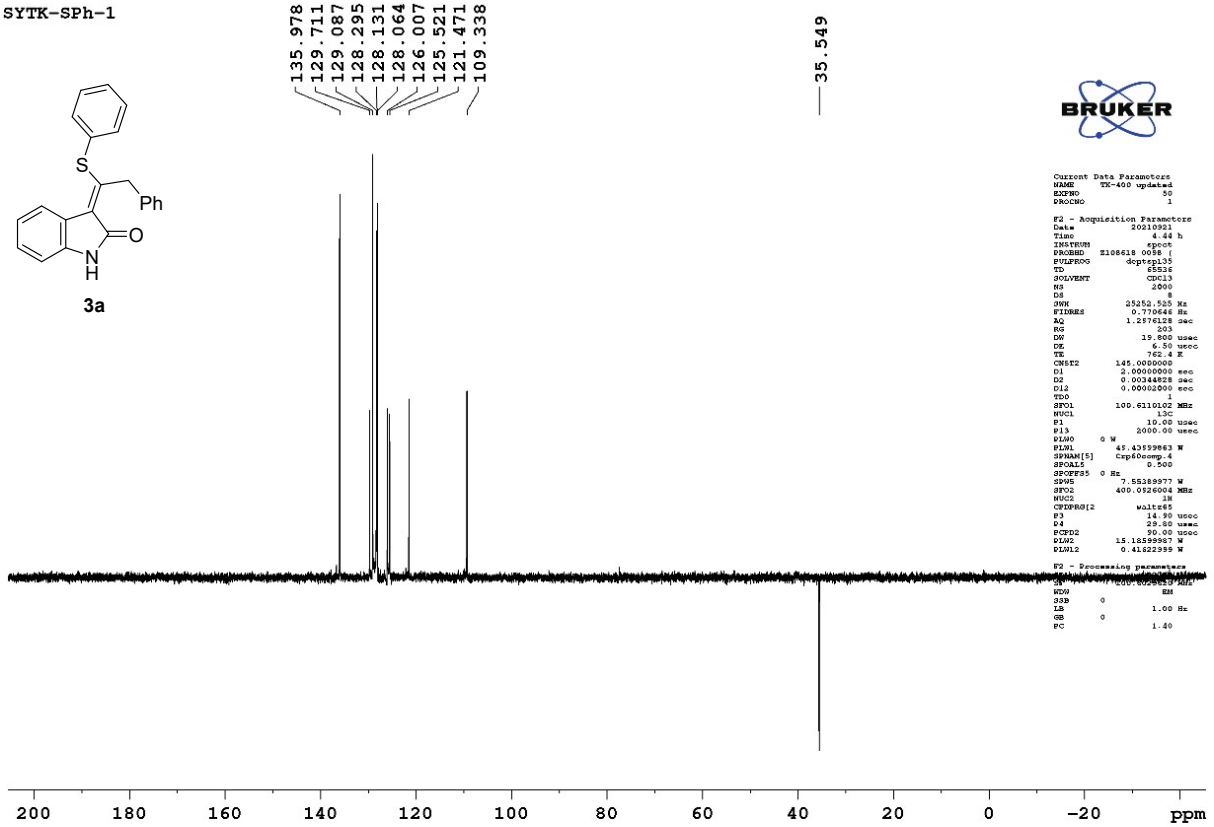
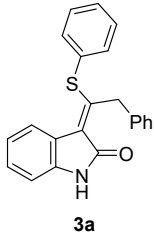
Identification code	ysr32a
Empirical formula	C ₂₂ H ₁₇ NOS
Formula weight	343.42
Temperature	293 K
Wavelength	0.71073 Å
Crystal system	'Triclinic'
Space group	P 1 21/c 1
Unit cell dimensions	a = 7.472 (2) Å α = 115.159(12). b = 10.980 (3) Å β = 102.060 (13). c = 12.170 (4) Å γ = 95.668 (13).
Volume	863.7 (5)
Z	2
Density	1.320 Mg/m ³
Absorption coefficient	0.196 mm ⁻¹

F(000)	36.0
Crystal size	0.16 x 0.14 x 0.12 mm ³
Theta range for data collection	2.852 to 27.750.
Index ranges	-9<=h<=9,-14<=k<=14,-15<=l<=15
Reflections collected	27526
Independent reflections	1946 [R(int) = 0.0779]
restraints / parameters	0/226
Goodness-of-fit on F ²	1.076
Final R indices [I>2sigma(I)]	R1 = 0.0779, wR2 = 0.1640
CCDC number	2109891

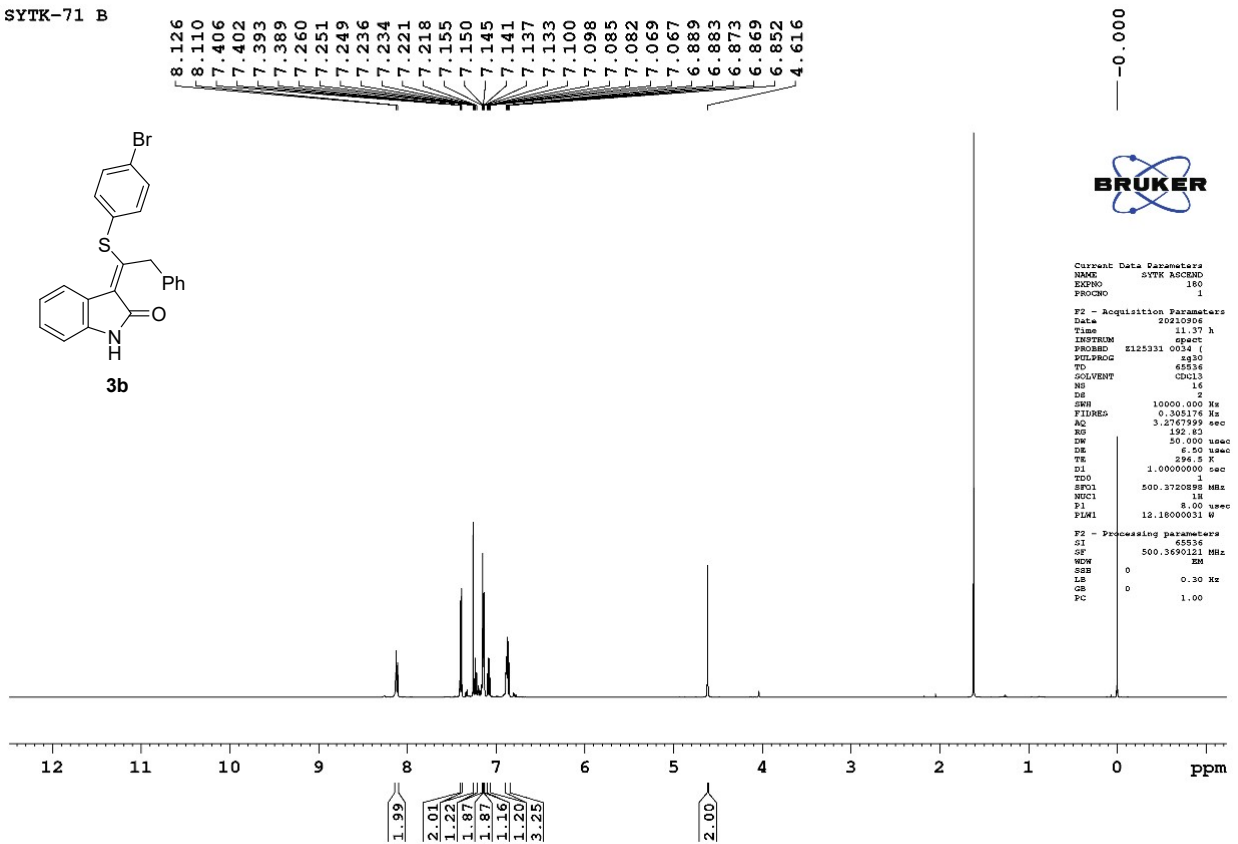
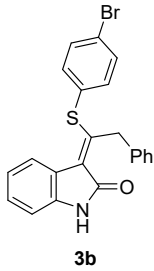
Spectral copies:



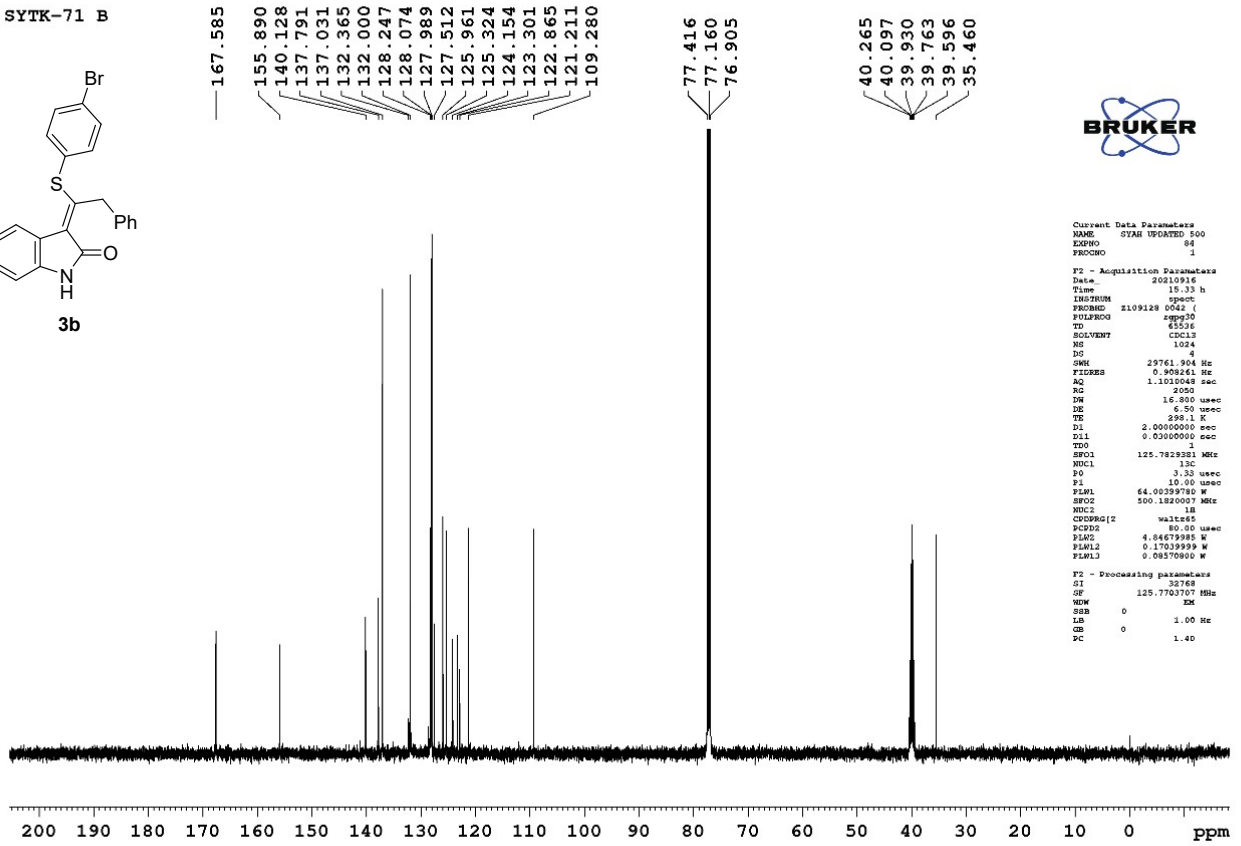
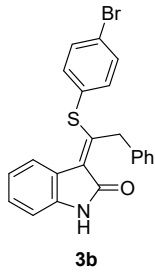
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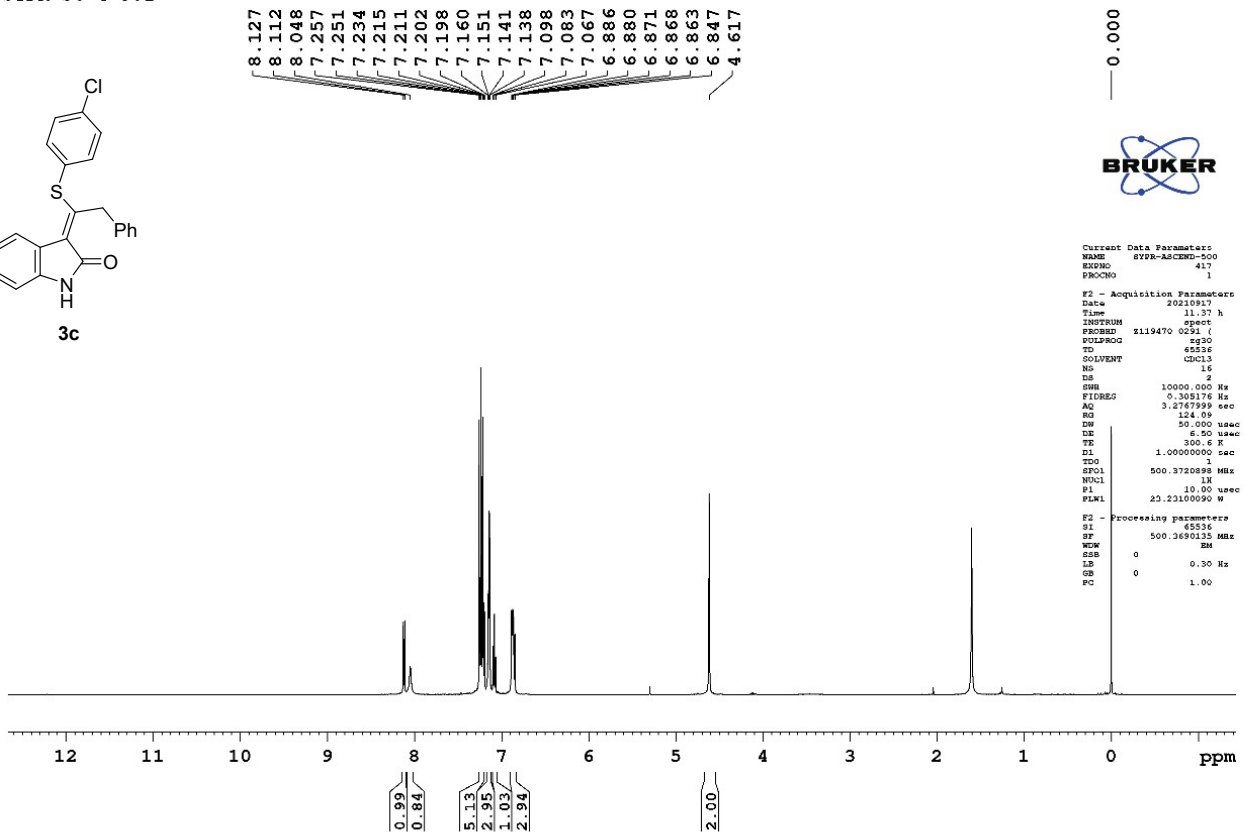
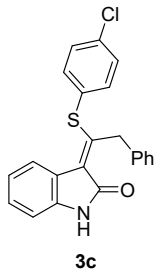
SYTK-71 B



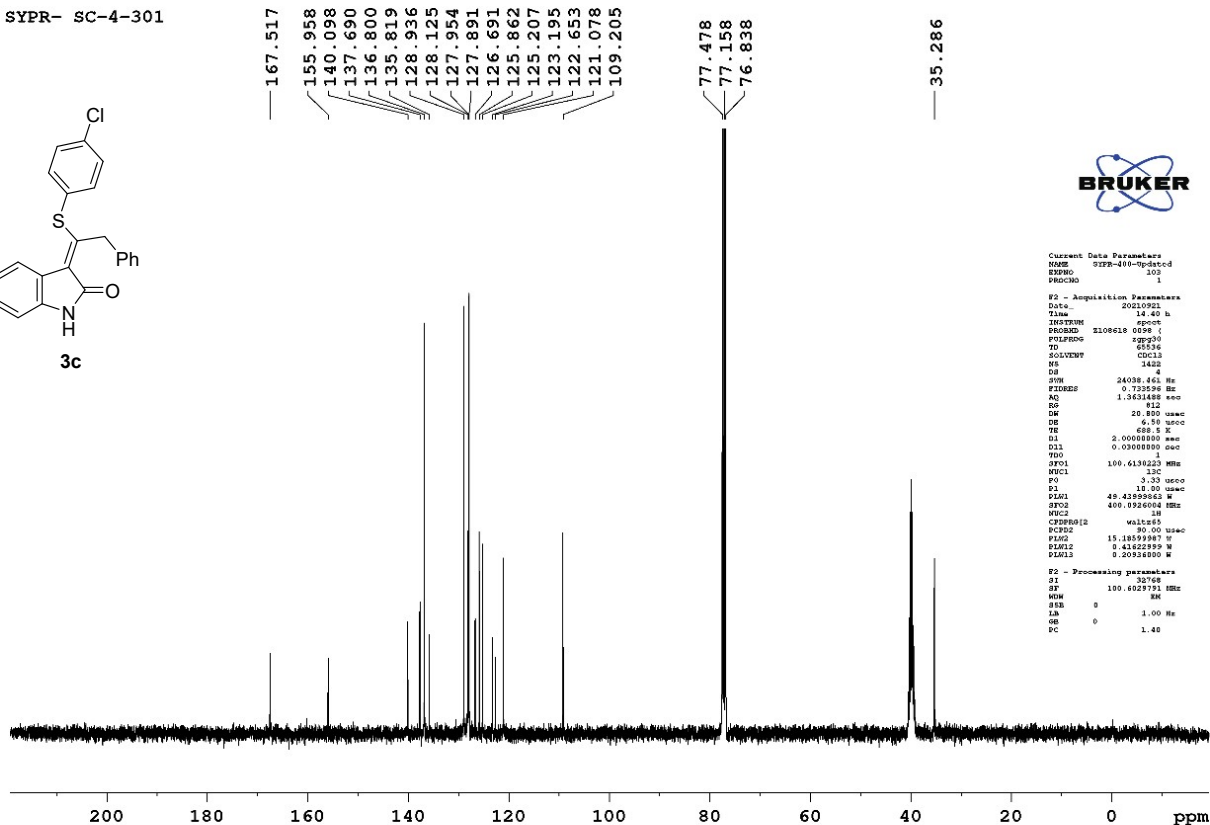
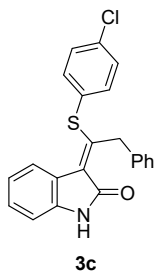
SYTK-71 B



SYPR-SC-4-301



SYPR- SC-4-301



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PROCNO 1

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Date_ 20210921
Time 14.40 h
INSTRUM spect
PROBHD 110618 059 (1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1422
DS 4
SW 24038.461 Hz
FIDRES 0.732296 Hz
AQ 1.3631488 sec
RG 812
DM 20.800 usac
DE 6.50 usac
TE 68.5 K
D1 2.0000000 sec
D11 0.0300000 sec
TPO 1
SFO1 100.6136223 MHz
NUC1 13C
P1 3.33 usac
D1 15.00 usac
SFO2 49.416006163 MHz
SFO3 400.0926004 MHz
NUC2 1H
CPRPR012 waltz165
DPR2 90.00 usac
PLN2 15.18599987 W
PLM2 0.41622959 W
PLM13 0.20934000 W

F2 - Processing parameters
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SSB 0
LB 1.00 Hz
GB 0
PC 1.40

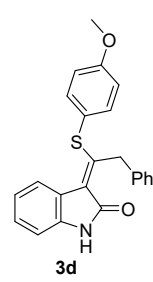
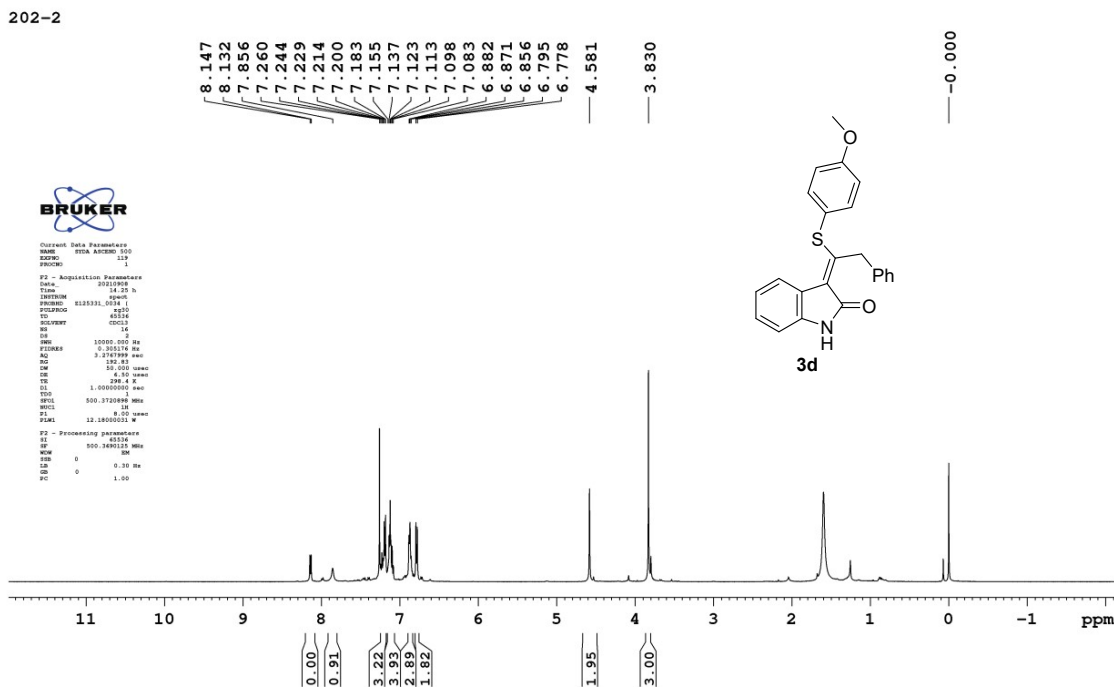
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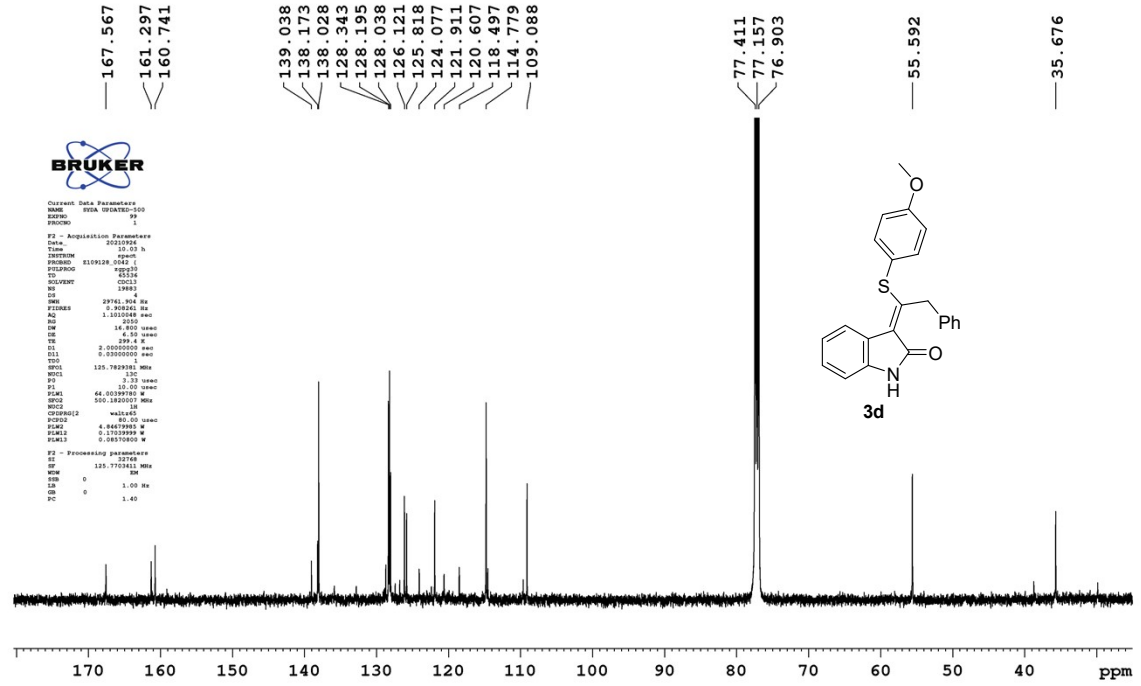
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EXPNO 1
PROCNO 1

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PROBHD 110618 059 (1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1422
DS 4
SW 24038.461 Hz
FIDRES 0.732296 Hz
AQ 1.3631488 sec
RG 812
DM 20.800 usac
DE 6.50 usac
TE 68.5 K
D1 2.0000000 sec
D11 0.0300000 sec
TPO 1
SFO1 100.6136223 MHz
NUC1 13C
P1 3.33 usac
D1 15.00 usac
SFO2 49.416006163 MHz
SFO3 400.0926004 MHz
NUC2 1H
CPRPR012 waltz165
DPR2 90.00 usac
PLN2 15.18599987 W
PLM2 0.41622959 W
PLM13 0.20934000 W

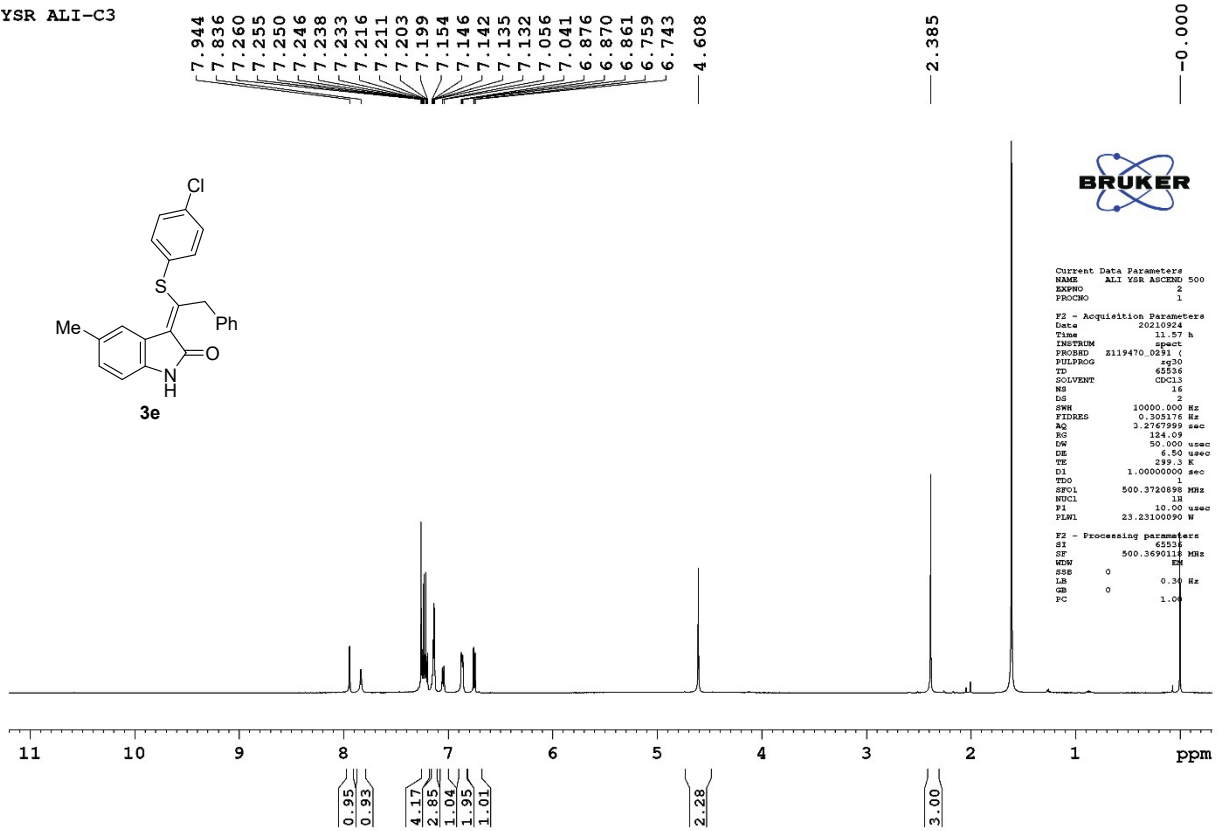
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



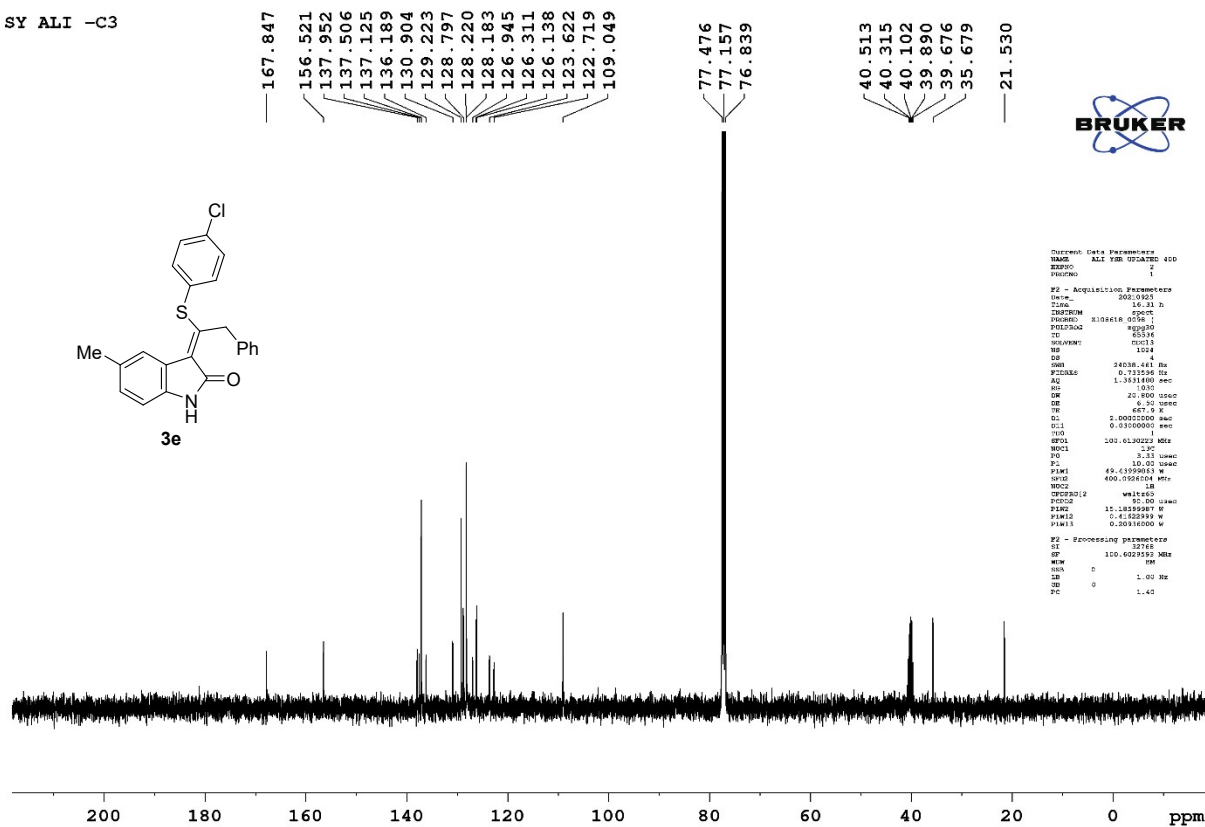
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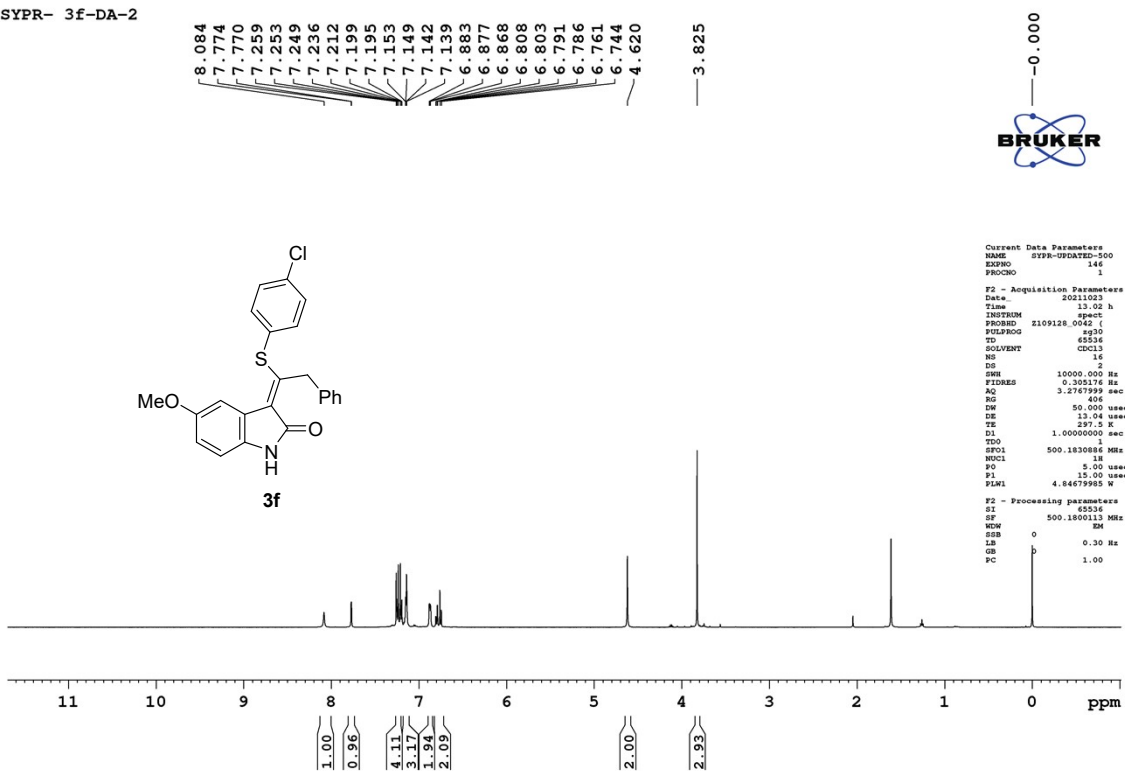
YSR ALI-C3



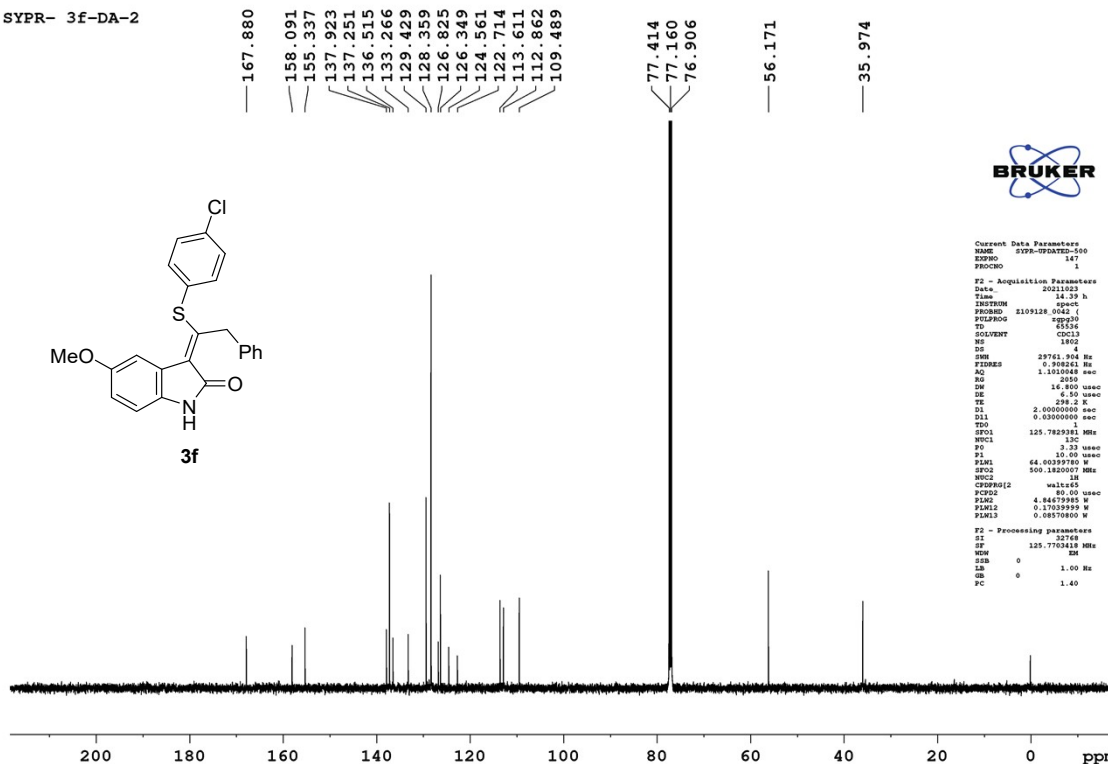
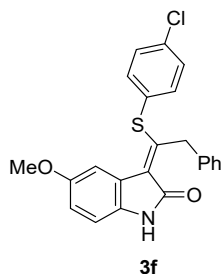
SY ALI -C3



SYPR- 3f-DA-2



SYPR- 3f-DA-2

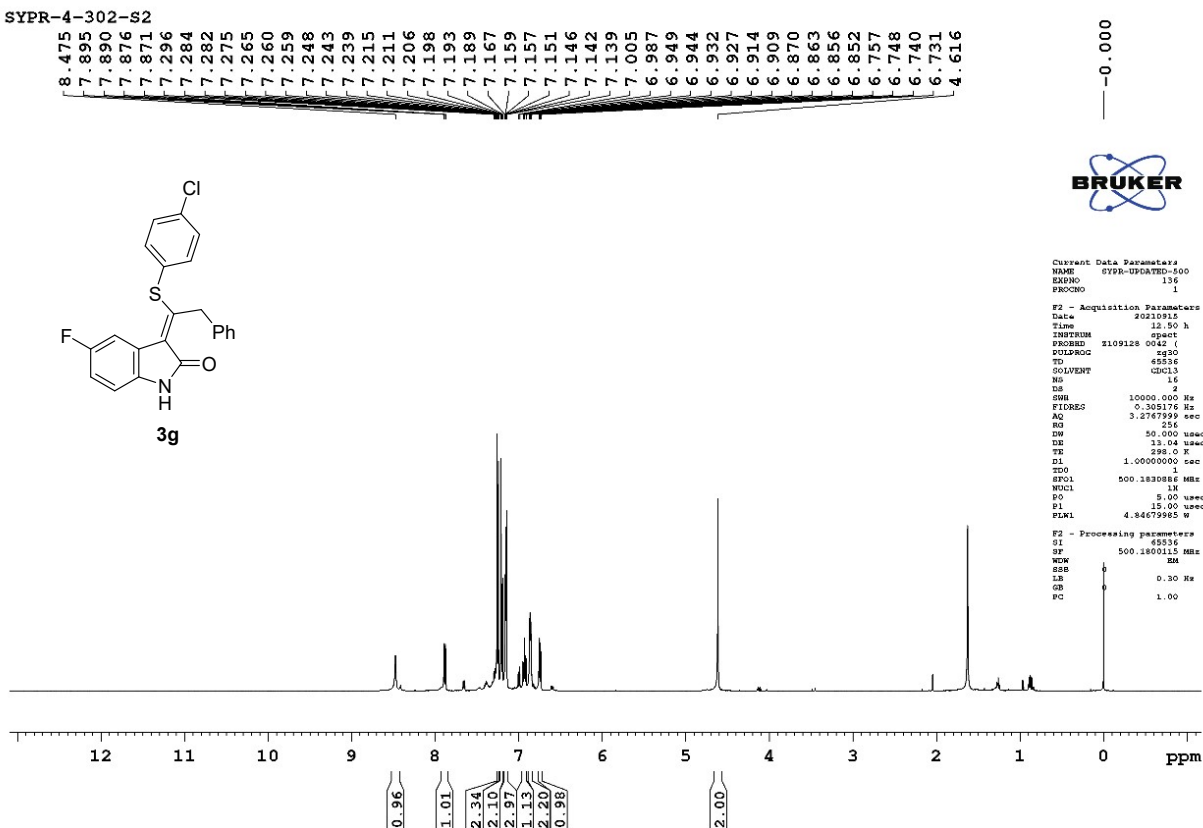
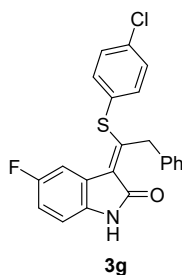


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EXPNO 147
PROCNO 1

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INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1802
DS 2
SWH 29761.904 Hz
FIDRES 0.298281 Hz
AQ 1.1010248 sec
RG 3200
DE 16.800 usac
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 125.7629381 MHz
NUC1 13C
P1 130
PC 150.000 usac
FREQ1 84.8697888 MHz
SFO2 500.1820007 MHz
NUC2 1H
CPRP02(1) waltz165
PCPD2 85.00 usac
PLM2 4.84679985 W
PLM12 0.17039999 W
PLM13 0.08570800 W

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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

SYPR-4-302-S2

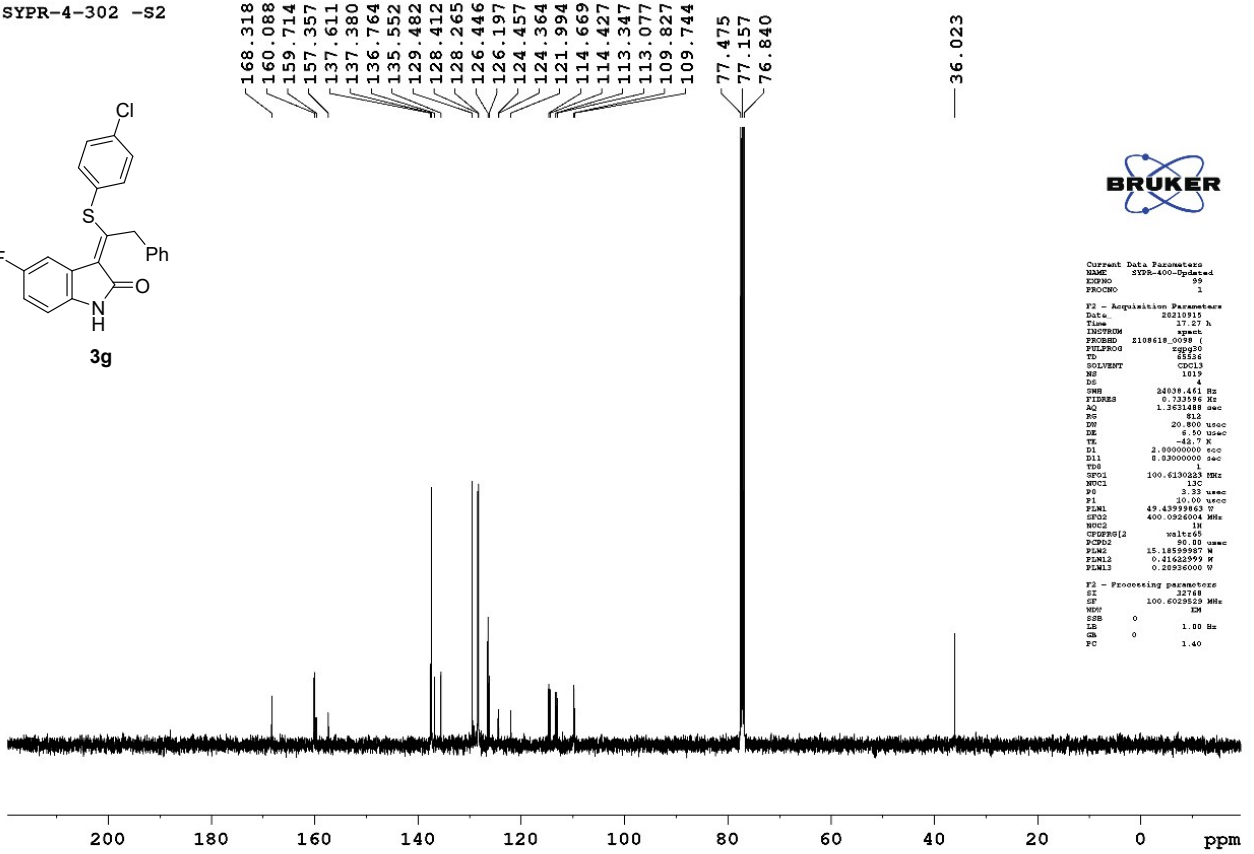
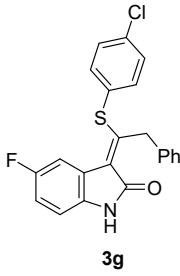


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EXPNO 136
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210915
Time 12:50 h
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 18
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 320
DE 16.800 usac
TE 298.2 K
D1 1.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 500.1820007 MHz
NUC1 1H
P1 150.000 usac
FREQ1 500.1800115 MHz
PLM1 4.84679985 W

F2 - Processing parameters
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SF 500.1800115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

SYPR-4-302 -S2



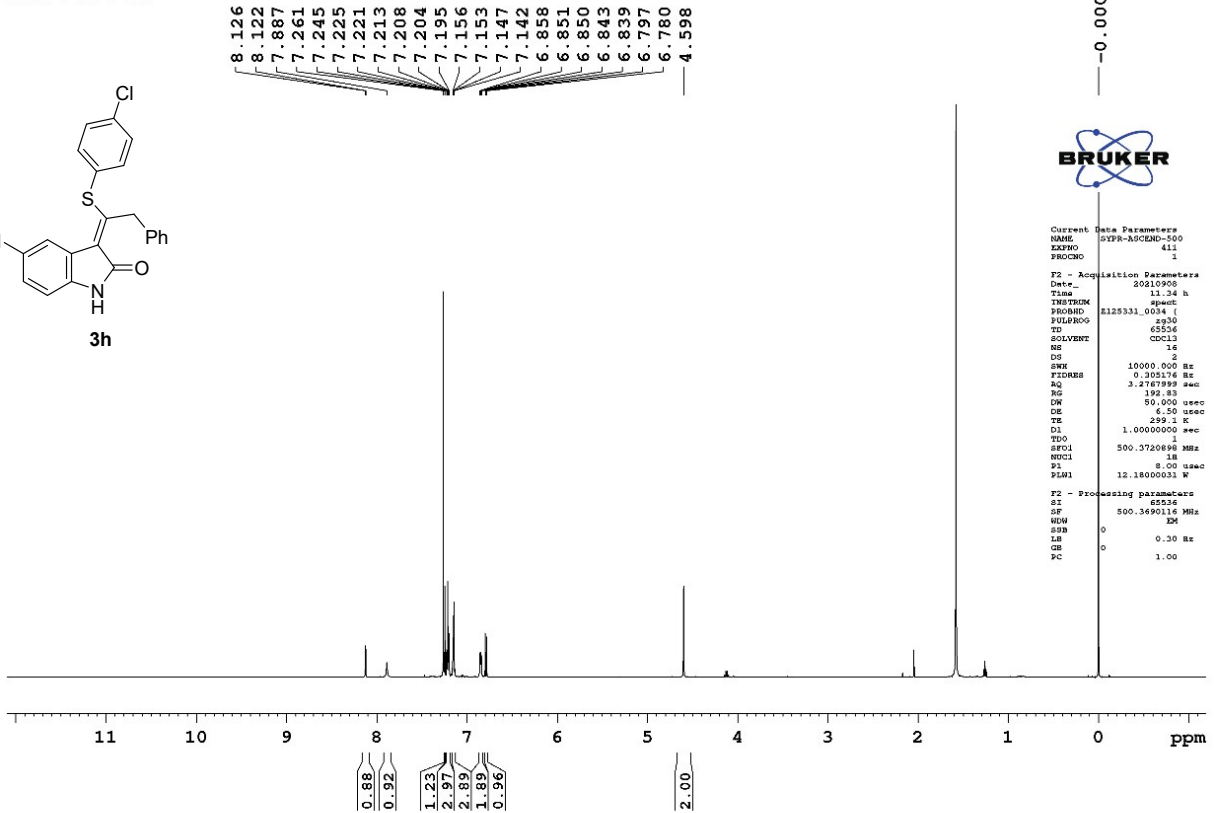
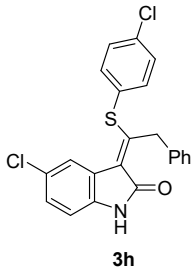
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EXPNO    1
PROCNO   1

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Date_    20210915
Time     17:57 A
INSTRUM  spect
PROBHD   1H601
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        411
DS        4
SWH       24938.461 Hz
FIDRES   0.733596 Hz
AQ        1.303489 sec
RG        818
DW        20.000 usec
DE        6.50 usec
TE        300.2 K
D1        2.00000000 sec
D11       0.03000000 sec
TDO       1
SFO1      100.6130253 MHz
NUC1      13C
P1         3.33 usec
PI         30.00 usec
FDM1      49.43999863 Hz
SFO2      400.0000000 MHz
NUC2      1H
CFPRG2    waltz16
PCPD2     30.00 usec
P1M2      15.18558987 Hz
P1M13     0.21625999 Hz
P1M13     0.20250000 Hz

F2 - Processing parameters
SI         32768
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SSB        0
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PC         1.40
    
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SYPR-4-294-S2



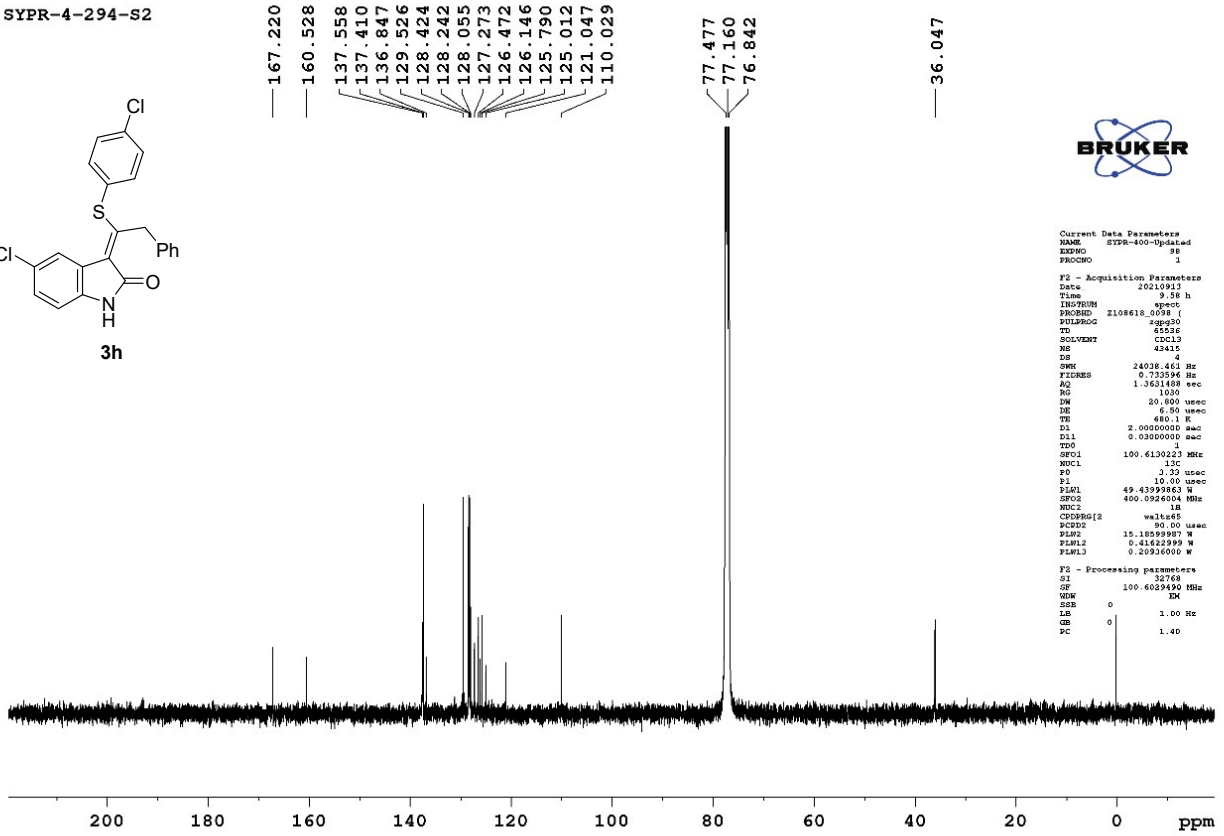
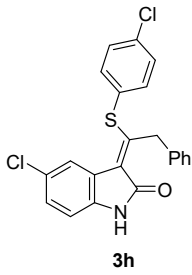
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EXPNO    1
PROCNO   1

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Time     11:34 h
INSTRUM  spect
PROBHD   1H601
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        411
DS        2
SWH       10000.000 Hz
FIDRES   0.393176 Hz
AQ        3.2767999 sec
RG        350.43
DW        50.000 usec
DE        6.50 usec
TE        299.1 K
D1        1.00000000 sec
TDO       1
SFO1      500.3720898 MHz
NUC1      13C
P1         8.00 usec
PI         12.18000031 Hz

F2 - Processing parameters
SI         65536
SF         500.3690116 MHz
WDW        DM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
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SYPR-4-294-S2



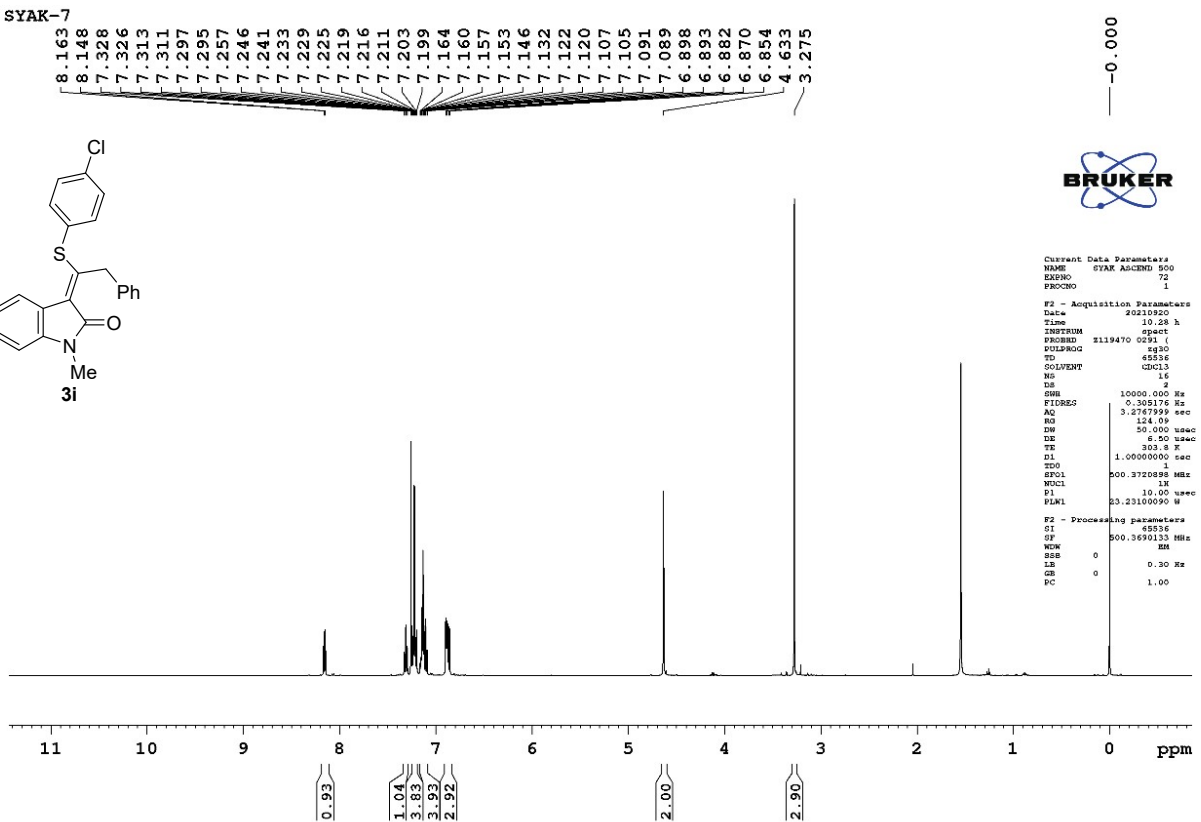
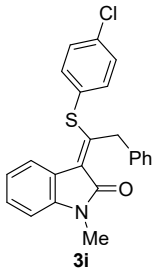
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EXPNO    2
PROCNO   1

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Date_    20210912
Time     9.58 h
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PROBHD   110618.0058 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        43412
DS        4
SWH       24038.461 Hz
FIDRES   0.71594 Hz
AQ        1.3631488 sec
RG        1020
DM        20.800 usec
DE        8.50 usec
TE        480.1 K
D1        2.0000000 sec
d11       0.0200000 sec
TD0       1
SFO1      100.6130133 MHz
NUC1      13C
P2        3.32 usec
P3        10.00 usec
PL1L1     49.4399863 W
SFO2      400.0924804 MHz
MDC2      1B
CROSSPO2  waltz16
PCPDFT    90.00 usec
PL1R2     15.1839987 W
PL1L2     0.41622999 W
PL1L3     0.20310000 W

F2 - Processing parameters
SI        32768
SF        100.6029490 MHz
RG        0
WDW       0
SSB       0
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GB        0
PC        1.40
    
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SYAK-7



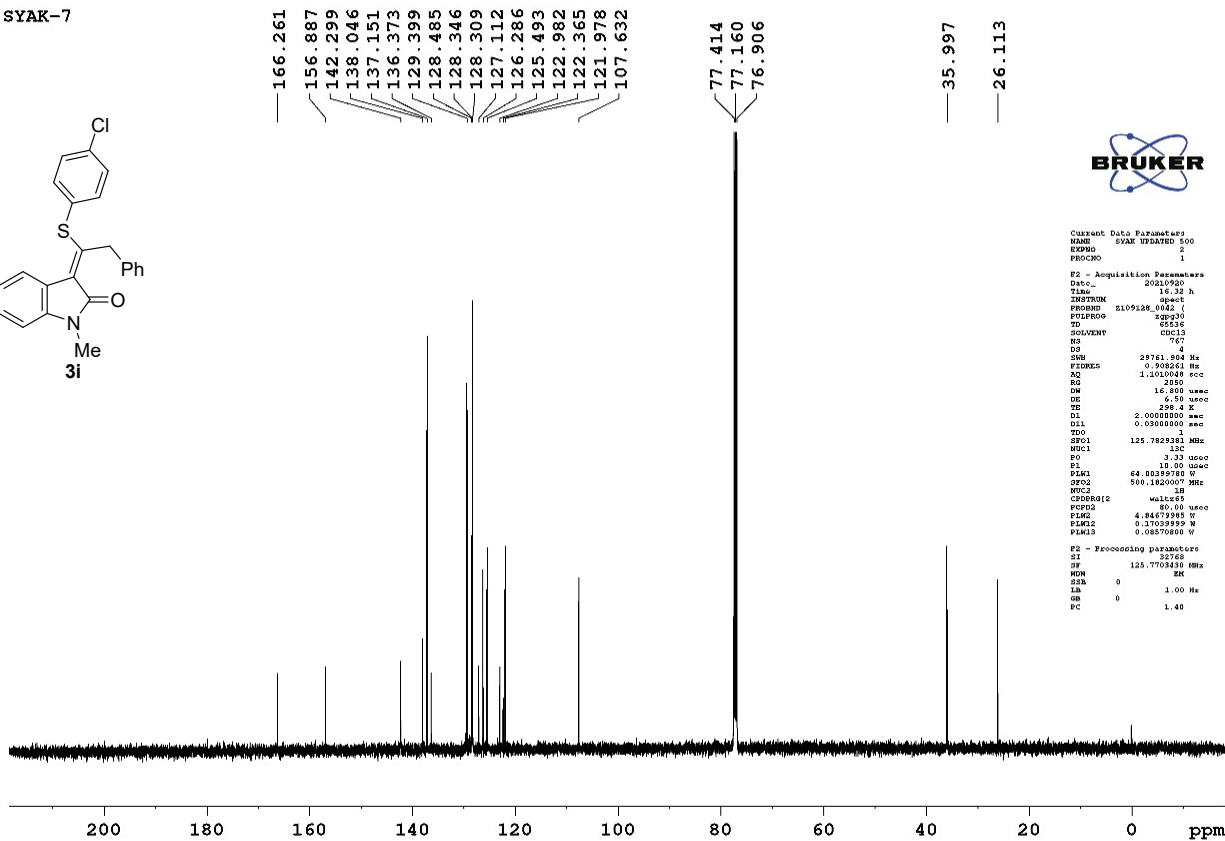
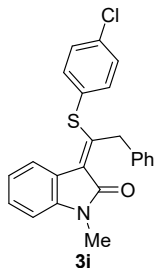
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NAME      SYAK-AS000
EXPNO    72
PROCNO   1

F2 - Acquisition Parameters
Date_    20210920
Time     10.28 h
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PROBHD   1119470.0291 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       10000.000 Hz
FIDRES   0.305176 Hz
AQ        3.2747929 sec
RG        124.00
DM        50.000 usec
DE        8.50 usec
TE        303.2 K
D1        1.0000000 sec
d11       0.0200000 sec
TD0       1
SFO1      500.3720988 MHz
NUC1      13C
P2        10.00 usec
PL1L1     23.23100090 W

F2 - Processing parameters
SI        65536
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SSB       0
LB        0.30 Hz
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PC        1.00
    
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SYAK-7



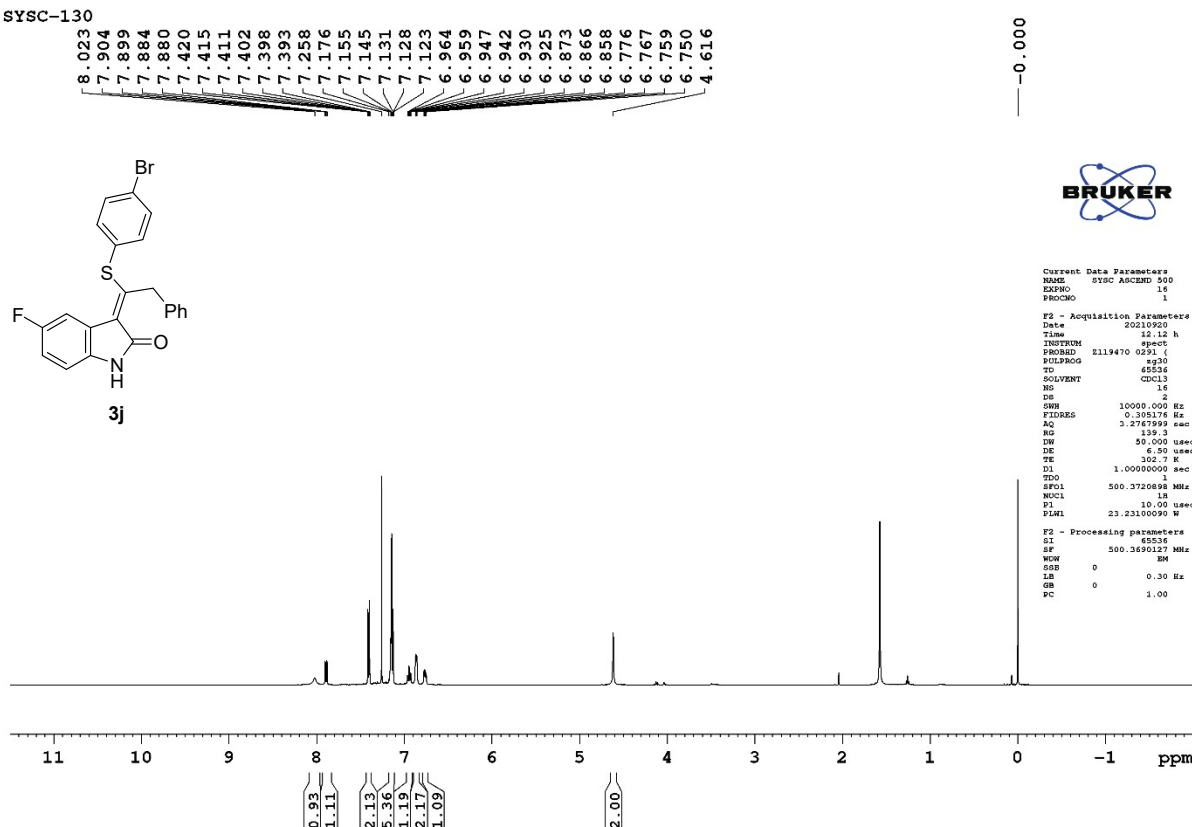
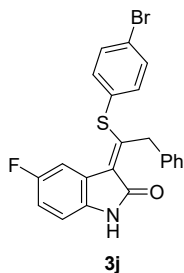
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Current Data Parameters
NAME SYAK_UPDATED_500
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210920
Time 16.32 h
INSTRUM spect
PROBHD z109128_0042 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 2
SWH 28761.904 Hz
FIDRES 0.900000 Hz
AQ 1.1010048 sec
RG 2500
OR 16.888 usec
DE 1.50 usec
TE 298.2 K
D1 2.0000000 sec
d11 0.0300000 sec
SFO1 125.7629151 MHz
NUC1 13C
P1 3.33 usec
PL1 0.00 usec
PL12 64.80395780 W
PL13 500.1820000 MHz
SFO2 500.1313131 MHz
NUC2 1H
CROSSP2 80.00 usec
SFO3 4.84673985 W
PLM2 0.1310000 W
PLM3 0.08570888 W

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GB 0
PC 1.40
    
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SYSC-130



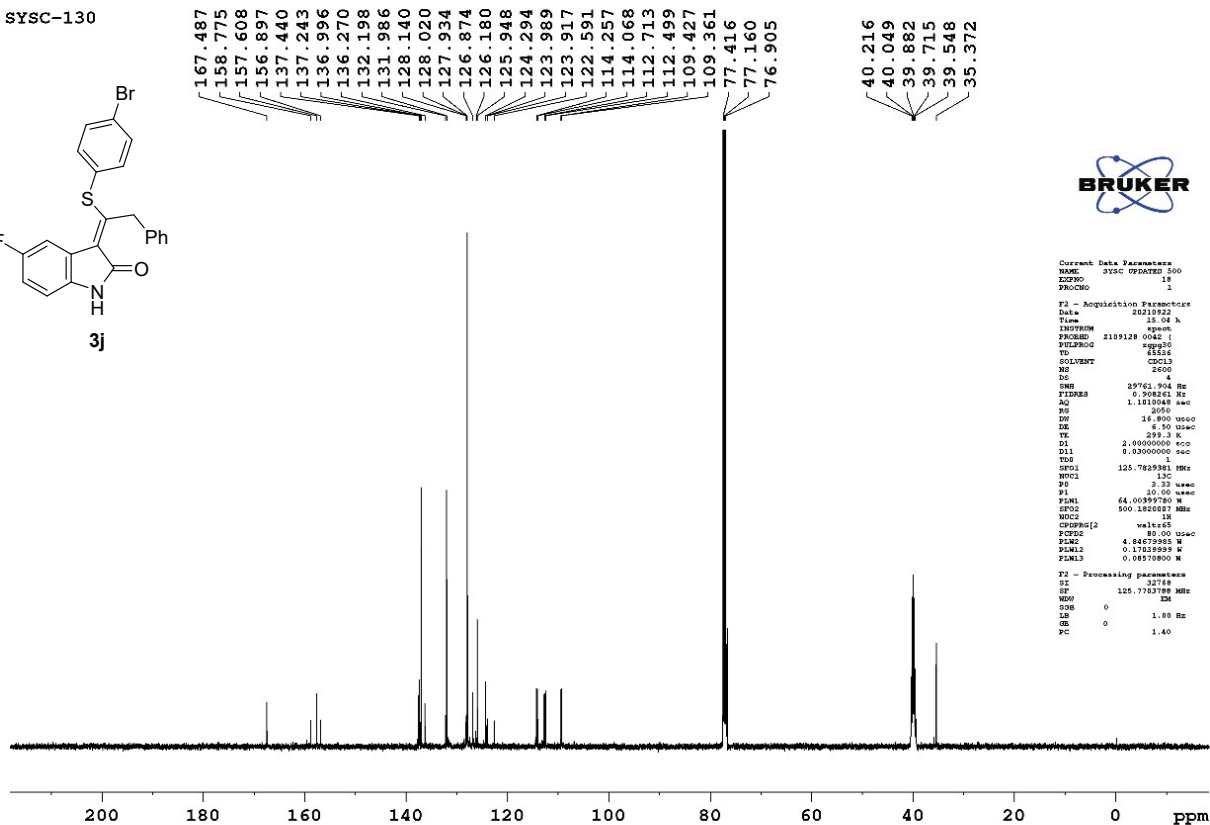
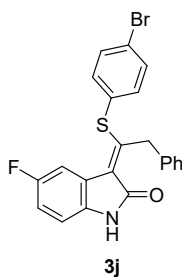
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EXPNO 18
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210920
Time 12.12 h
INSTRUM spect
PROBHD z119470_0291 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.205176 Hz
AQ 5.2167090 sec
RG 132.3
OR 50.000 usec
DE 6.50 usec
TE 302.2 K
D1 1.0000000 sec
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PL1 23.23100090 W

F2 - Processing parameters
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LB 0.30 Hz
GB 0
PC 1.00
    
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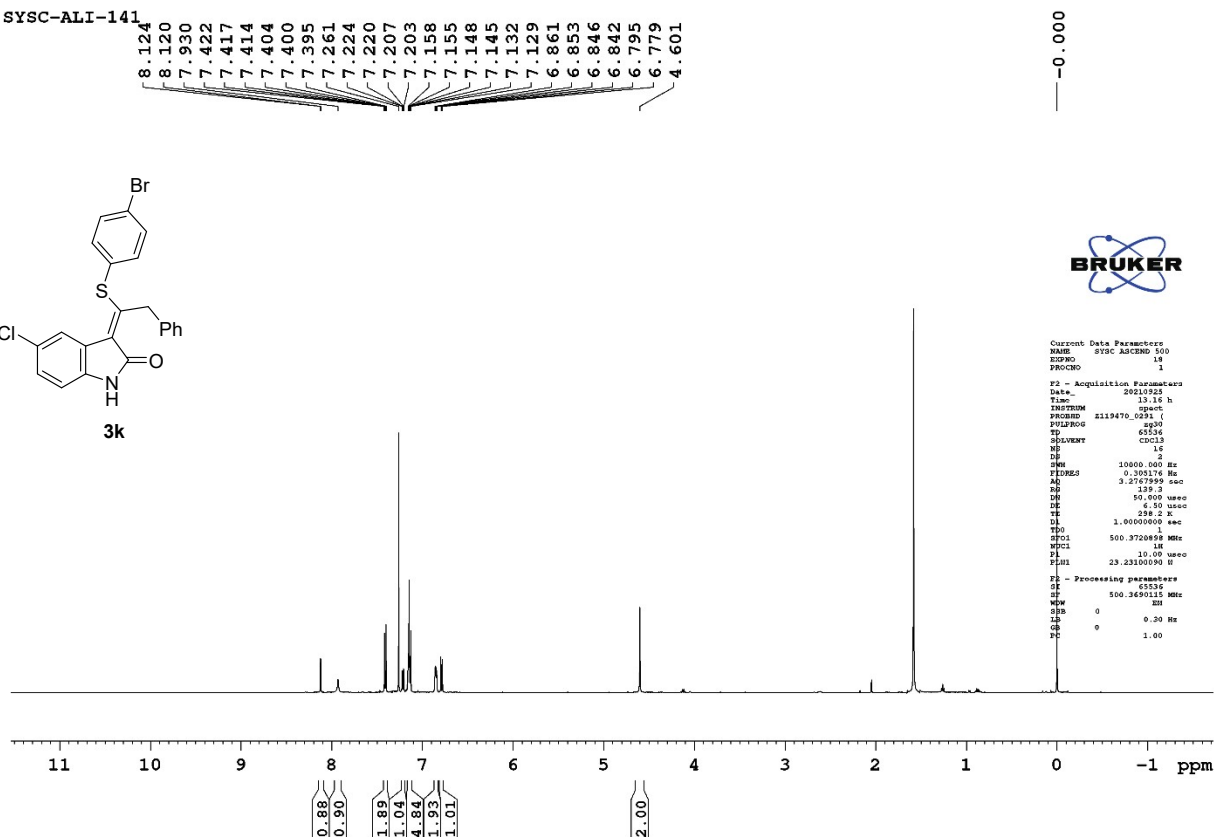
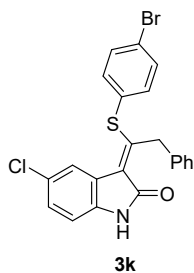
SYSC-130



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Current Data Parameters
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EXPNO: 18
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20210922
Time: 15:34 h
INSTRUM: spect
PROBHD: 1H9120 0042 1
PULPROG: zgpg30
TE: 300.2
SOLVENT: CDCl3
NS: 2000
DS: 4
SWH: 29761.904 Hz
FIDRES: 0.508261 Hz
AQ: 1.1810048 sec
RG: 2050
DQ: 18.890 usec
DE: 8.50 usec
TE: 299.2 K
D1: 2.00000000 sec
d11: 0.03000000 sec
TDS: 1
SFO1: 125.762951 MHz
NUC1: 13C
P1: 1.33 usec
PL1: 10.00 usec
P1M1: 64.0099780 MHz
SFO2: 500.135067 MHz
NUC2: 1H
CPDPRG2: waltz16
PCPD2: 89.00 usec
PLAC: 4.8467288 MHz
PLM12: 0.1783988 MHz
PLM13: 0.0870800 MHz
F2 - Processing parameters
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WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
    
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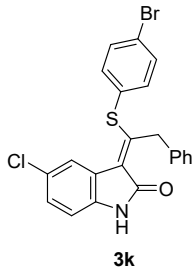
SYSC-ALI-141



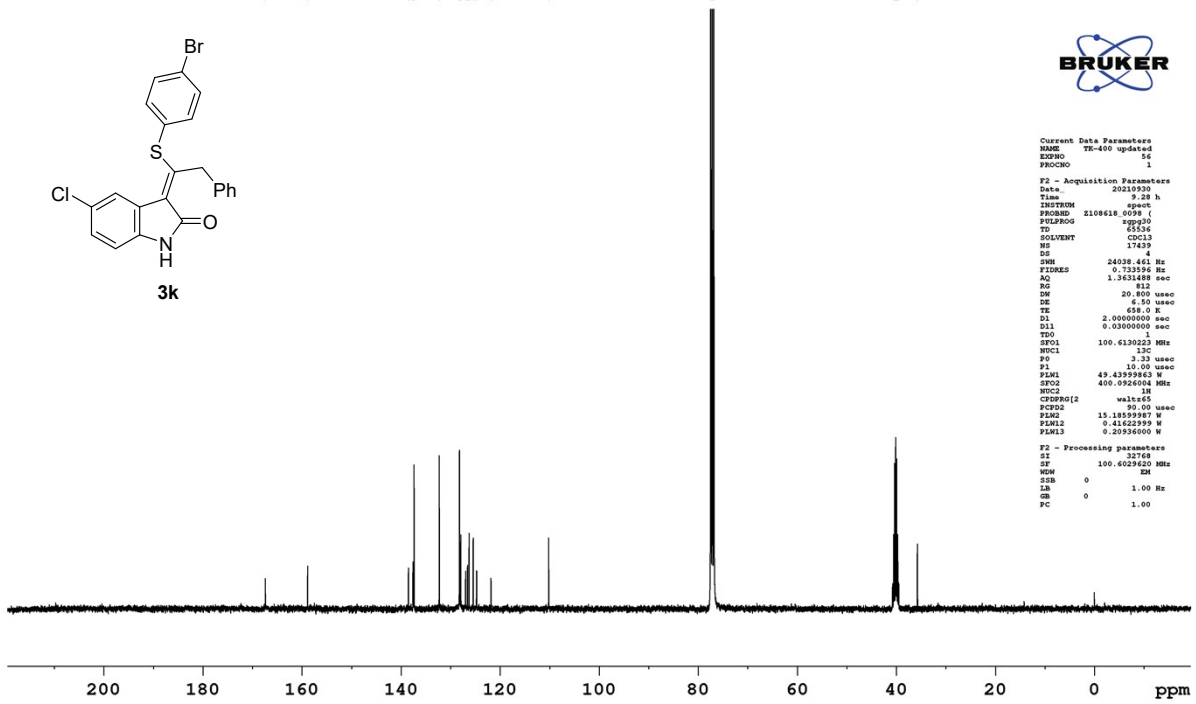
```

Current Data Parameters
NAME: SYSC ASCEND 500
EXPNO: 18
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20210925
Time: 13:16 h
INSTRUM: spect
PROBHD: z119470_0291 1
PULPROG: zgpg30
TE: 300.2
SOLVENT: CDCl3
NS: 16
DS: 2
SWH: 10800.000 Hz
FIDRES: 0.200170 Hz
AQ: 3.2567899 sec
RG: 358
DQ: 50.000 usec
DE: 8.50 usec
TE: 298.2 K
TDS: 1.00000000 sec
SFO1: 500.3720678 MHz
NUC1: 1H
P1: 10.00 usec
PL1: 23.23300390 dB
F2 - Processing parameters
SI: 65536
SF: 500.3690115 MHz
WDW: EM
SSB: 0
LB: 0.00 Hz
GB: 0
PC: 1.00
    
```

SYTK-ALI-141

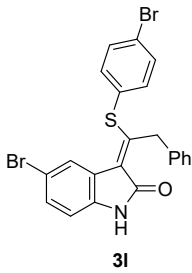


167.406
158.851
138.507
137.583
137.369
132.284
128.234
128.166
127.924
126.957
126.589
126.252
125.435
124.765
124.723
121.839
110.185

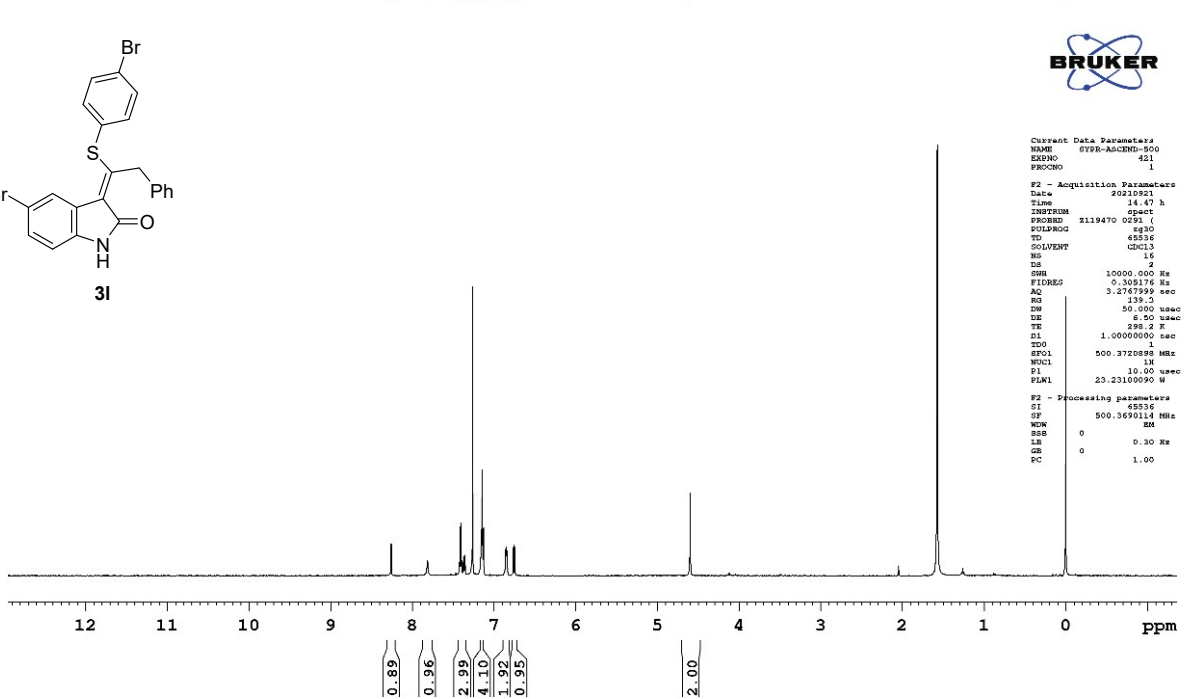


Current Data Parameters
NAME: SYTK-ALI-141
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20210930
Time: 9.28 h
INSTRUM: spect
PROBHD: Z108618.0098 (C
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 1749
DS: 4
SWH: 24039.464 Hz
FIDRES: 0.733594 Hz
AQ: 1.2631488 sec
RG: 812
DM: 20.800 usec
DE: 6.50 usec
TE: 300.2 K
D1: 2.0000000 sec
D11: 0.0300000 sec
TDO: 0
SFO1: 100.6130223 MHz
NUC1: 13C
P1: 3.13 usec
PL1: 10.00 usec
PLM1: 49.4399989 W
SFO2: 400.0924004 MHz
NUC2: 1H
CPDPRG2: waltz165
PCPD2: 998.00 usec
PLM2: 15.1859989 W
PLM3: 0.4302099 W
PLM13: 0.20936000 W
F2 - Processing parameters
SI: 32768
SF: 100.6029620 MHz
WDW: EM
SSB: 0 1.00 Hz
LB: 0
GB: 0 1.00
PC: 1.00

SYPR-4-309 N

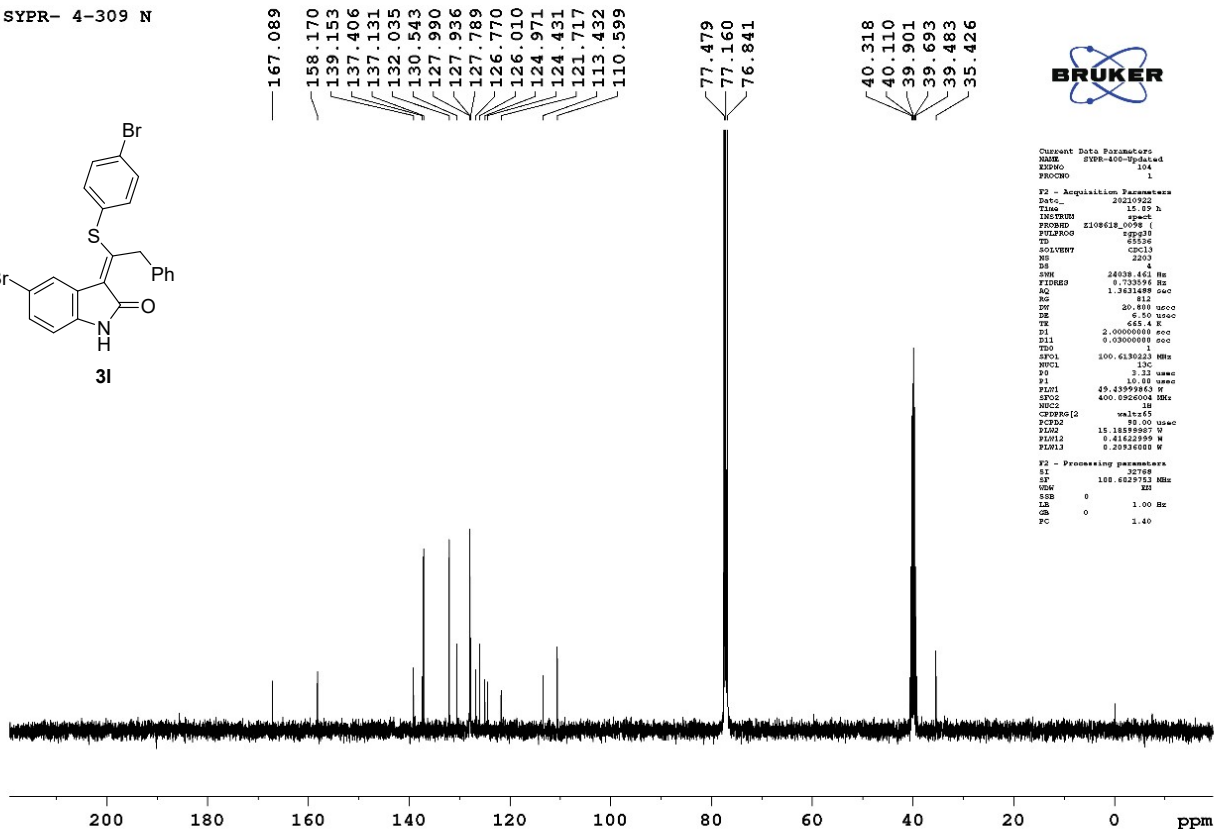
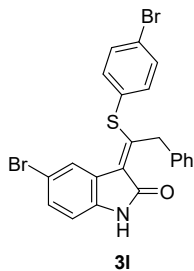


8.259
7.814
7.417
7.401
7.374
7.370
7.357
7.354
7.261
7.156
7.154
7.144
7.128
6.856
6.850
6.842
6.760
6.743



Current Data Parameters
NAME: SYPR-4-309 N
EXPNO: 421
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20210921
Time: 14.47 h
INSTRUM: spect
PROBHD: Z119470.0299 (C
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 15
DS: 2
SWH: 10000.000 Hz
FIDRES: 0.308176 Hz
AQ: 3.2707594 sec
RG: 399.5
DM: 50.000 usec
DE: 6.50 usec
TE: 300.2 K
D1: 1.0000000 sec
TDO: 0
SFO1: 500.3720898 MHz
NUC1: 13C
P1: 10.00 usec
PLM1: 23.23100090 W
F2 - Processing parameters
SI: 65536
SF: 500.3690114 MHz
WDW: EM
SSB: 0 0.30 Hz
LB: 0
GB: 0 1.00
PC: 1.00

SYPR- 4-309 N



SYPR-4-316

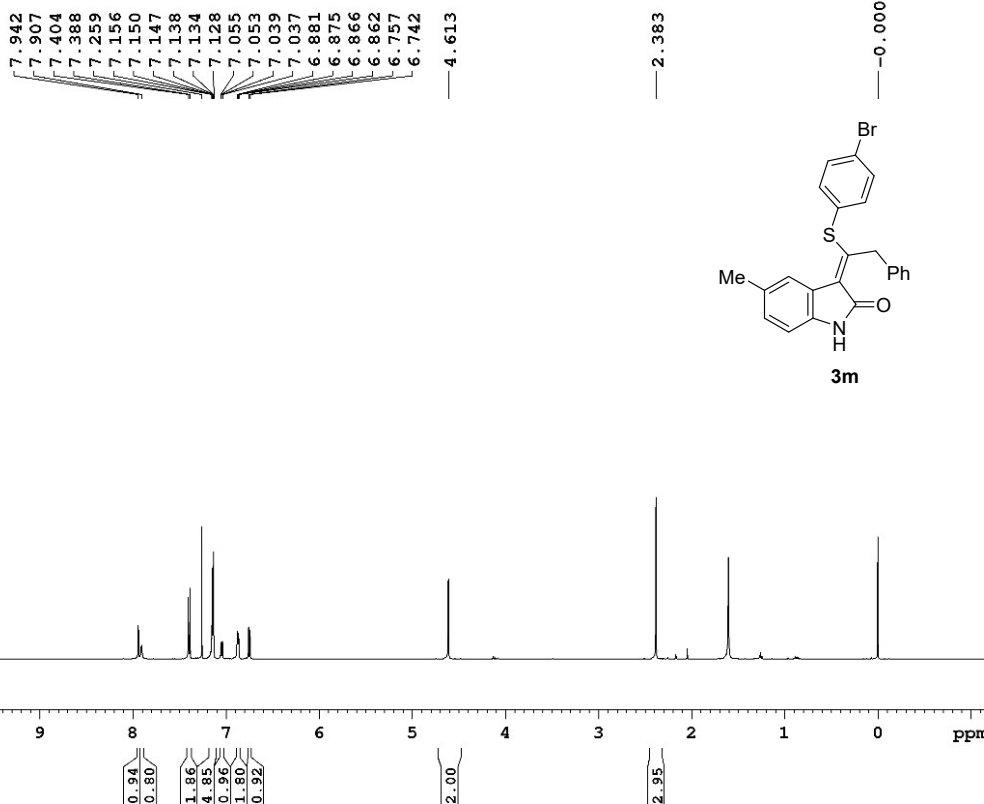


```

Current Data Parameters
NAME  SYPR-400-Updated
EXPNO  1
PROCNO  1

F2 - Acquisition Parameters
Date_  20210922
Time  16:19:14
INSTRUM  spect
PROBHD  zgpg30 (
PULPROG  zgpg30
TD  65536
SOLVENT  cdcl3
NS  2033
DS  4
SWH  10000.000 Hz
FIDRES  0.305176 Hz
AQ  3.2767999 sec
RG  134.09
DE  50.090 usec
TE  6.50 usec
T1  298.2 K
D1  1.00000000 sec
T20  1
SFO1  500.3720998 MHz
NUC1  13C
P1  10.00 usec
PL1  23.23100000 W

F2 - Processing parameters
SI  65536
SF  500.3690124 MHz
WDW  0
SSB  0
LB  0.30 Hz
GB  0
PC  1.00
    
```

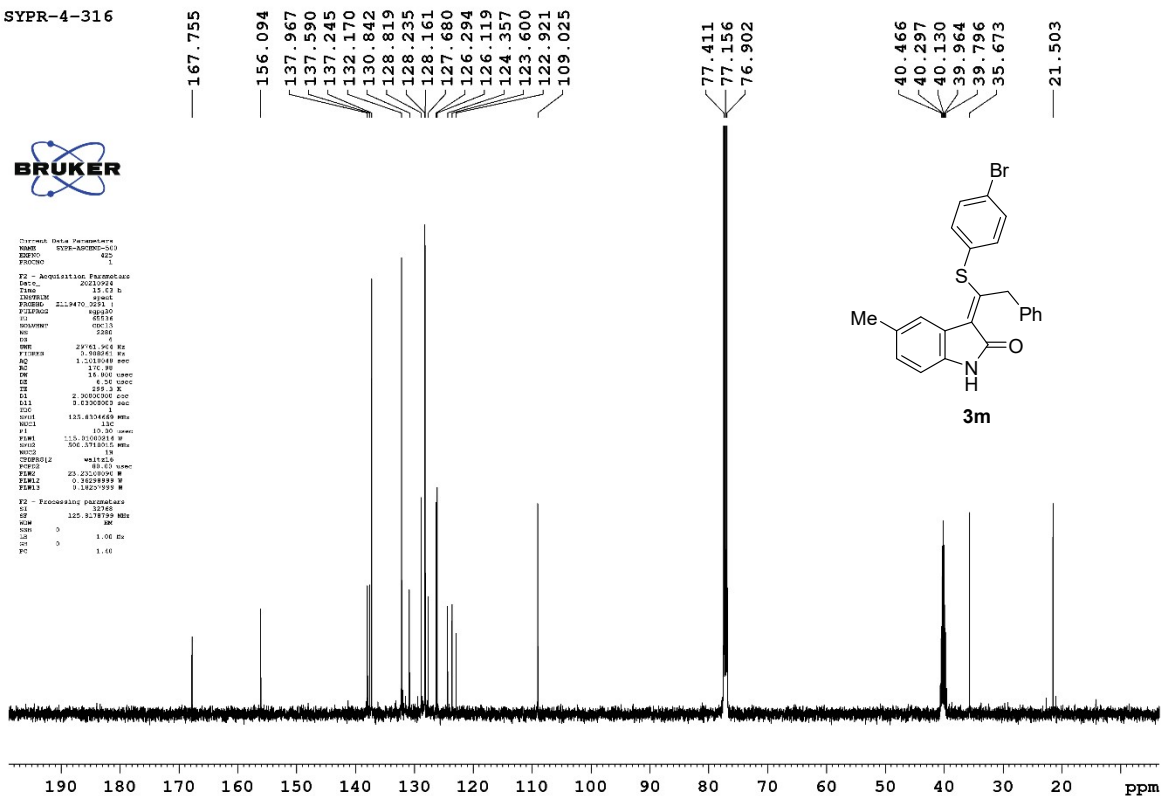


SYPR-4-316



```

Current Data Parameters
NAME: SYPR-ASCPD-316
EXPNO: 422
PROCNO: 1
F2 - Acquisition Parameters
Date_ 20121212
Time: 12:12:48
INSTRUM: spect
PROBHD: 513470-QNP-1
PULPROG: zgpg30
PC: zgpg30
SOLVENT: CDCl3
NS: 2048
DS: 4
SWH: 24961.916 Hz
FIDRES: 0.00048 Hz
AQ: 1.1218048 sec
RG: 312.88
AQ: 16.800 usec
DE: 6.00 usec
TE: 299.2 K
NUC1: 13C
NUC2: 13C
NUC3: 13C
NUC4: 13C
P1: 12.00 usec
P2: 110.0000016 M
P3: 500.1300010 MHz
NUC1P2: 13C
NUC2P2: 13C
NUC3P2: 13C
NUC4P2: 13C
PCPDSP12: white16
PCPDSP13: white16
P2M2: 23.2500000 M
P2M3: 0.1620000 M
P2M12: 0.1620000 M
F2 - Processing parameters
SI: 32768
SF: 125.017950 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00
  
```

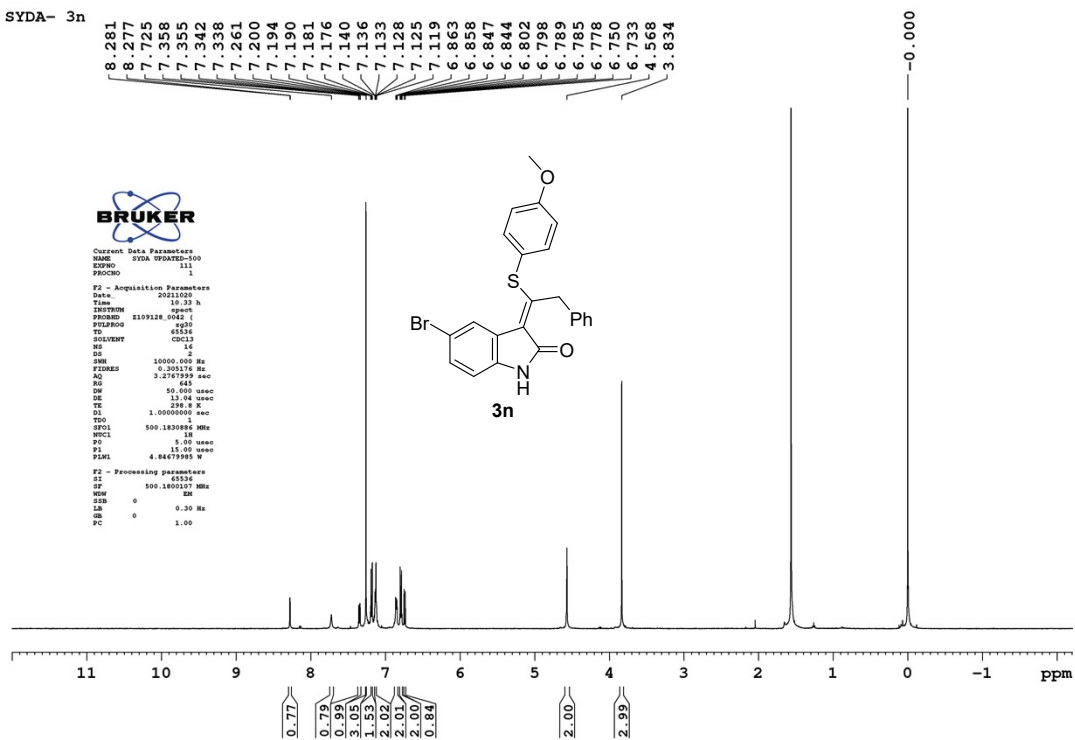


SYDA- 3n

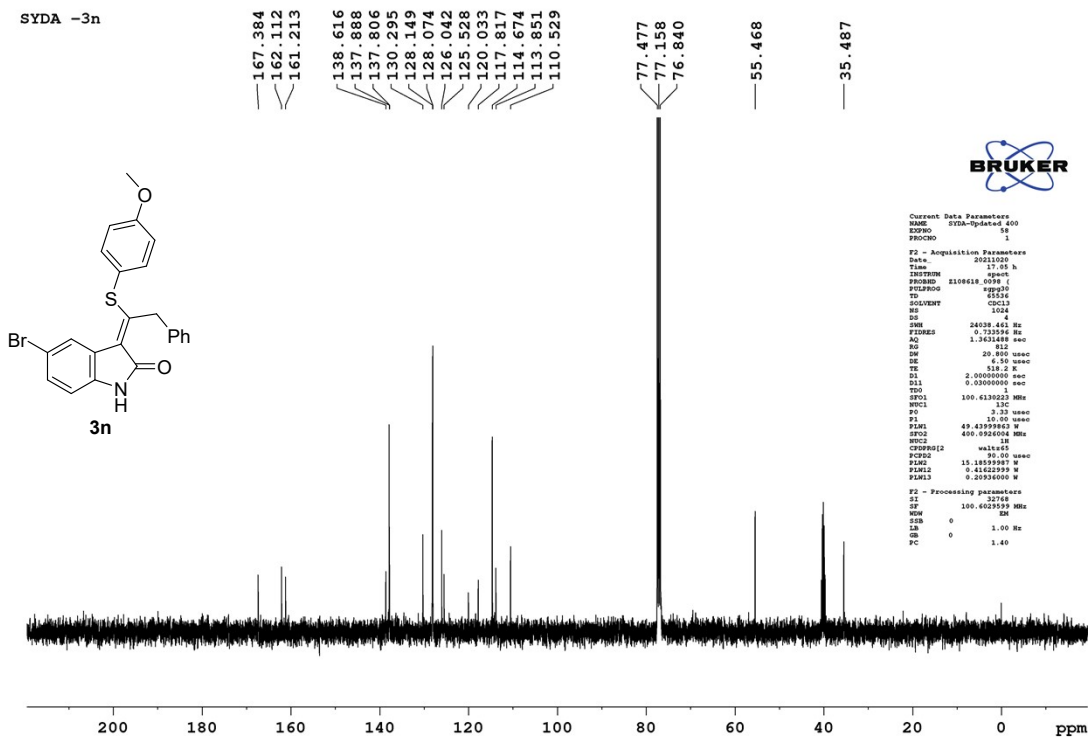


```

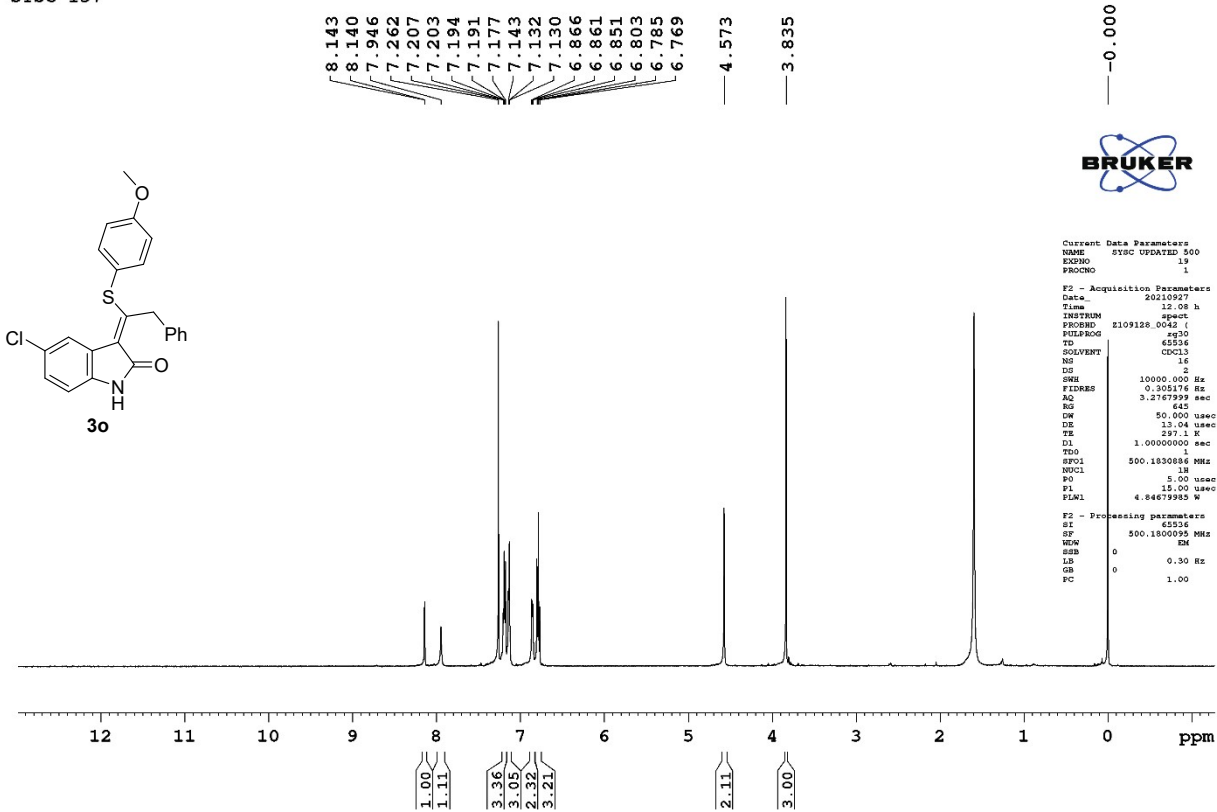
Current Data Parameters
NAME: SYDA-3n-111
EXPNO: 111
PROCNO: 1
F2 - Acquisition Parameters
Date_ 20121020
Time: 10:23:14
INSTRUM: spect
PROBHD: 513470-QNP-1
PULPROG: zgpg30
PC: zgpg30
SOLVENT: CDCl3
NS: 2048
DS: 4
SWH: 10000.000 MHz
FIDRES: 0.0001516 MHz
AQ: 3.2707959 sec
RG: 640
AQ: 50.000 usec
DE: 13.04 usec
TE: 299.2 K
NUC1: 13C
NUC2: 13C
NUC3: 13C
NUC4: 13C
P1: 12.00 usec
P2: 500.1300010 MHz
P3: 500.1300010 MHz
P2M2: 23.2500000 M
P2M3: 0.1620000 M
P2M12: 0.1620000 M
F2 - Processing parameters
SI: 32768
SF: 500.1300010 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
  
```



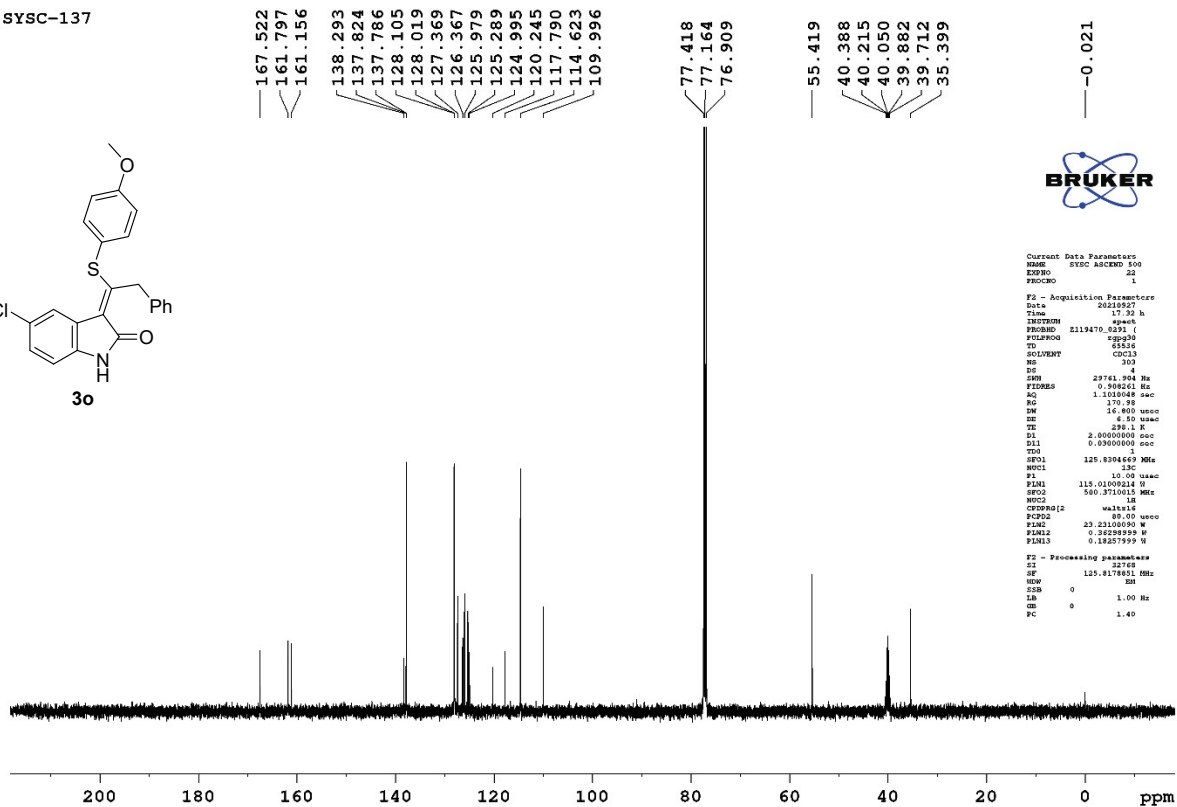
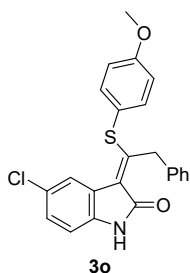
SYDA -3n



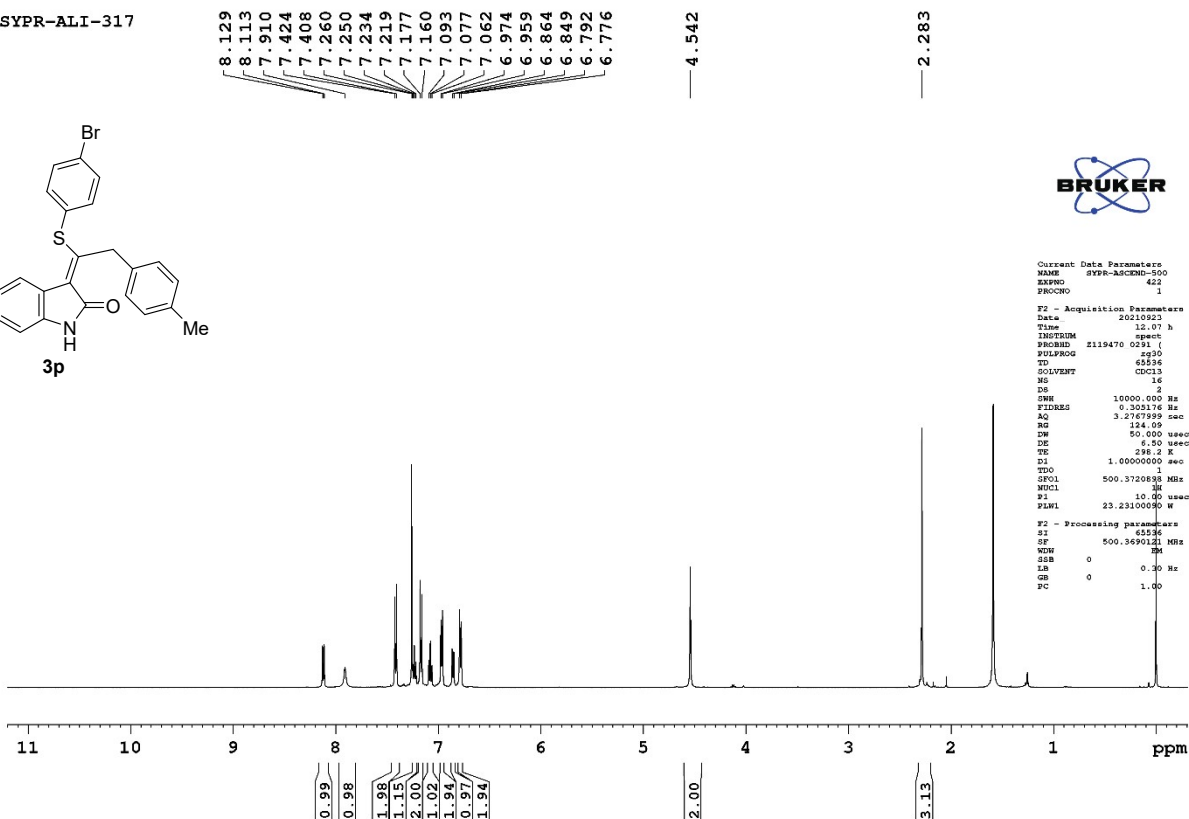
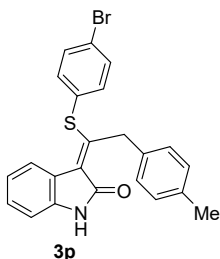
SYSC-137



SYSC-137



SYPR-ALI-317



SYPR-ALI-317



```

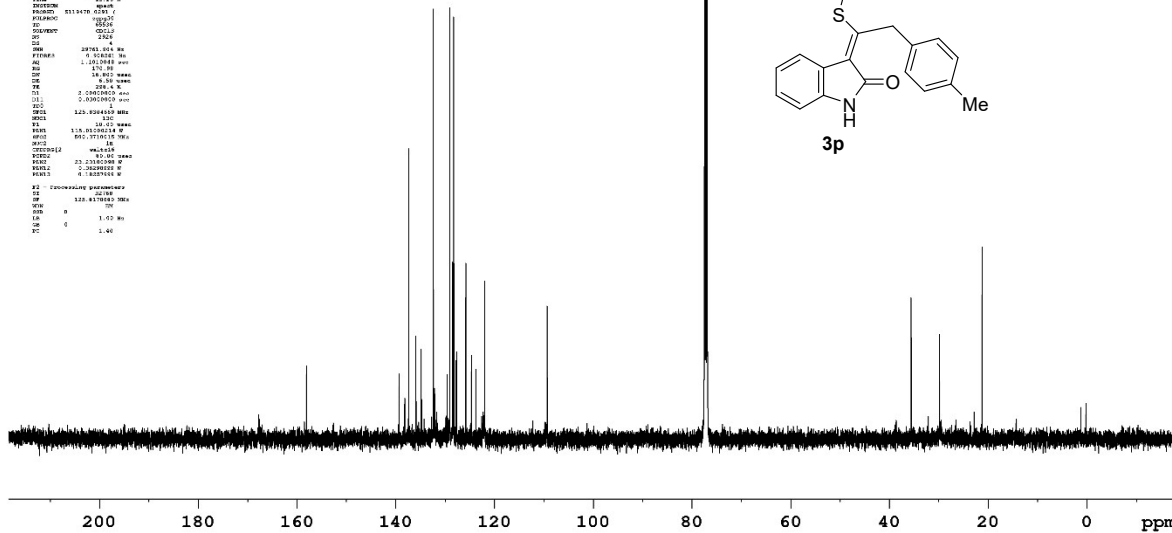
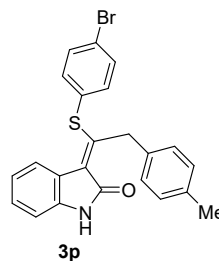
Current Data Parameters
NAME: SYPR-ACBND-317
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_   : 20120202
Time    : 10:21 h
INSTRUM : spect
PROBHD  : 5mm QNP 1H/1
PULPROG : zgpg30
TD      : 65536
SOLVENT : CDCl3
NS      : 128
DS      : 4
SWH     : 20414.614 Hz
FIDRES  : 0.000000 Hz
AQ      : 1.012088 sec
RG      : 327.50
DE      : 18.00 umax
TE      : 300.2 K
D1      : 1.0000000 sec
d11     : 0.0000000 sec
DELTA   : 2.0000000 sec
SFO1    : 500.1370993 MHz
NUC1    : 1H
SFO2    : 125.7611550 MHz
NUC2    : 13C
AQ2     : 1.012088 sec
RG2     : 327.50
DE2     : 18.00 umax
TE2     : 300.2 K
D12     : 1.0000000 sec
d121    : 0.0000000 sec
DELTA2  : 2.0000000 sec
SFO3    : 75.2611550 MHz
NUC3    : 13C
AQ3     : 1.012088 sec
RG3     : 327.50
DE3     : 18.00 umax
TE3     : 300.2 K
D13     : 1.0000000 sec
d131    : 0.0000000 sec
DELTA3  : 2.0000000 sec
SFO4    : 150.5223100 MHz
NUC4    : 13C
AQ4     : 1.012088 sec
RG4     : 327.50
DE4     : 18.00 umax
TE4     : 300.2 K
D14     : 1.0000000 sec
d141    : 0.0000000 sec
DELTA4  : 2.0000000 sec
F2 - Processing parameters
SI      : 65536
SF      : 500.1370993 MHz
WDW     : EM
SSB     : 0
LB      : 0.30 Hz
GB      : 0
PC      : 1.00
  
```

- 167.708
- 158.071
- 137.369
- 135.896
- 134.814
- 132.400
- 129.052
- 128.477
- 128.242
- 127.709
- 125.795
- 124.640
- 121.975
- 109.303

- 77.410
- 77.156
- 76.902

- 35.569

- 21.186

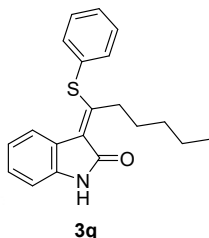


SYTK-SPh-2



```

Current Data Parameters
NAME: SYTK-ACBND-184
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_   : 20120314
Time    : 10:30 h
INSTRUM : spect
PROBHD  : 5mm QNP 1H/1
PULPROG : zgpg30
TD      : 65536
SOLVENT : CDCl3
NS      : 128
DS      : 4
SWH     : 10000.000 Hz
FIDRES  : 0.005176 Hz
AQ      : 3.2767999 sec
RG      : 192.83
DE      : 50.000 umax
TE      : 300.2 K
D1      : 1.0000000 sec
d11     : 0.0000000 sec
DELTA   : 2.0000000 sec
SFO1    : 500.1370993 MHz
NUC1    : 1H
SFO2    : 125.7611550 MHz
NUC2    : 13C
AQ2     : 1.012088 sec
RG2     : 327.50
DE2     : 18.00 umax
TE2     : 300.2 K
D12     : 1.0000000 sec
d121    : 0.0000000 sec
DELTA2  : 2.0000000 sec
SFO3    : 75.2611550 MHz
NUC3    : 13C
AQ3     : 1.012088 sec
RG3     : 327.50
DE3     : 18.00 umax
TE3     : 300.2 K
D13     : 1.0000000 sec
d131    : 0.0000000 sec
DELTA3  : 2.0000000 sec
SFO4    : 150.5223100 MHz
NUC4    : 13C
AQ4     : 1.012088 sec
RG4     : 327.50
DE4     : 18.00 umax
TE4     : 300.2 K
D14     : 1.0000000 sec
d141    : 0.0000000 sec
DELTA4  : 2.0000000 sec
F2 - Processing parameters
SI      : 65536
SF      : 500.1370993 MHz
WDW     : EM
SSB     : 0
LB      : 0.30 Hz
GB      : 0
PC      : 1.00
  
```

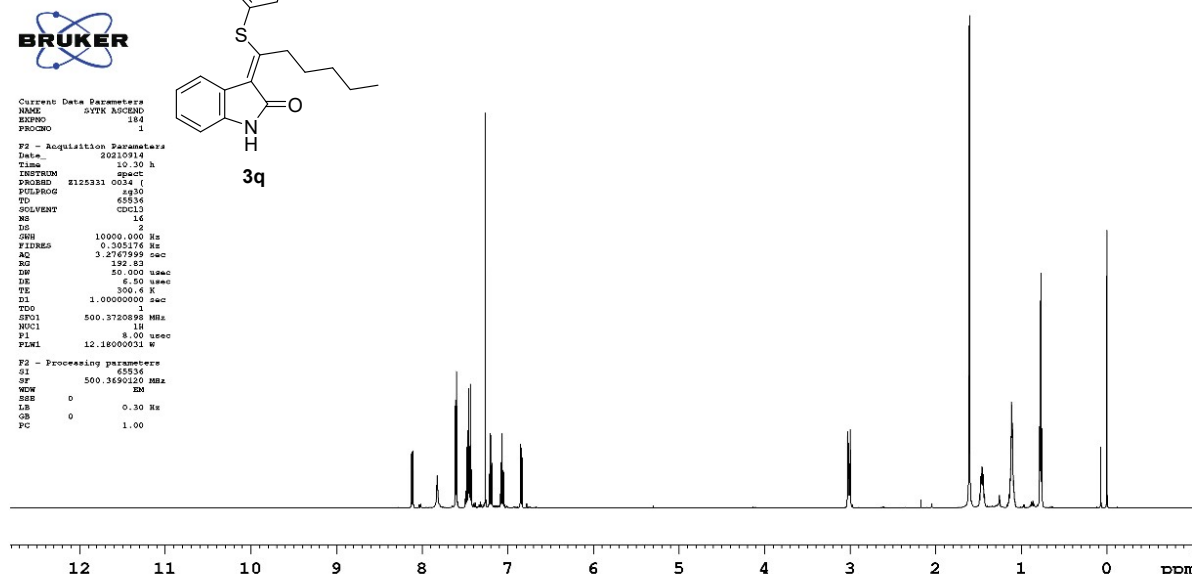


- 8.121
- 8.106
- 7.823
- 7.612
- 7.610
- 7.606
- 7.601
- 7.596
- 7.593
- 7.477
- 7.466
- 7.463
- 7.460
- 7.452
- 7.449
- 7.441
- 7.437
- 7.424
- 7.260
- 7.215
- 7.213
- 7.200
- 7.197
- 7.184
- 7.182
- 7.082
- 7.080
- 7.067
- 7.065
- 7.052
- 7.049
- 6.851
- 6.850
- 6.835
- 6.835
- 3.030
- 3.019
- 3.014
- 3.008
- 2.998
- 1.607
- 1.475
- 1.465
- 1.458
- 1.453
- 1.444
- 1.131
- 1.126
- 1.122
- 1.118
- 1.115
- 1.108
- 1.104
- 1.101
- 0.787
- 0.773
- 0.759
- 0.000

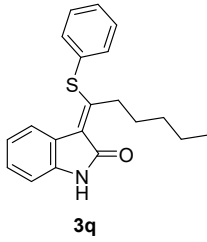
- 0.94
- 0.91
- 1.94
- 3.08
- 1.02
- 1.06
- 0.95

- 2.00

- 2.11
- 4.11
- 3.06



SYTK-SPh-2



167.868
167.781
163.116

139.298
139.242
136.060
129.990
129.504
129.382
129.086
127.711
125.343
124.189
121.676
119.808
109.094
109.069

77.414
77.161
76.907

31.723
31.119
29.879
22.226
14.033



```

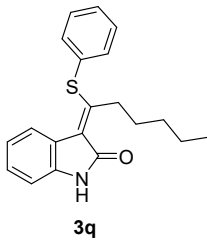
Current Data Parameters
NAME      SYTK-SPh-2
EXPNO    186
PROCNO   1

F2 - Acquisition Parameters
Date_    20210915
Time     17:31 A
INSTRUM  spect
PROBHD   1H1470-QNP1 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        377
DS        4
SWH       20761.904 Hz
FIDRES   0.998261 Hz
AQ        1.1810048 sec
RG         270.98
DF         14.800 usec
DE         6.50 usec
TE        301.2 K
D1        2.0000000 sec
D11       1.0300000 sec
SFO1      125.8304669 MHz
NUC1       13C
P1         130.00 usec
PL1        115.0190214 W
PCPD2     20.00 usec
NUC2       1H
SFO2      500.1360514 MHz
PCPD2     18.00 usec
PCPD2     mult16
PLM1      23.2310099 W
PLM2      0.3629899 W
PLM3      0.1825799 W

F2 - Processing parameters
SI        32768
SF        125.8178664 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

SYTK-SPh-2



136.062
129.992
129.492
127.686
125.309
121.656

109.082

31.704
31.082
29.863
22.212
14.033



```

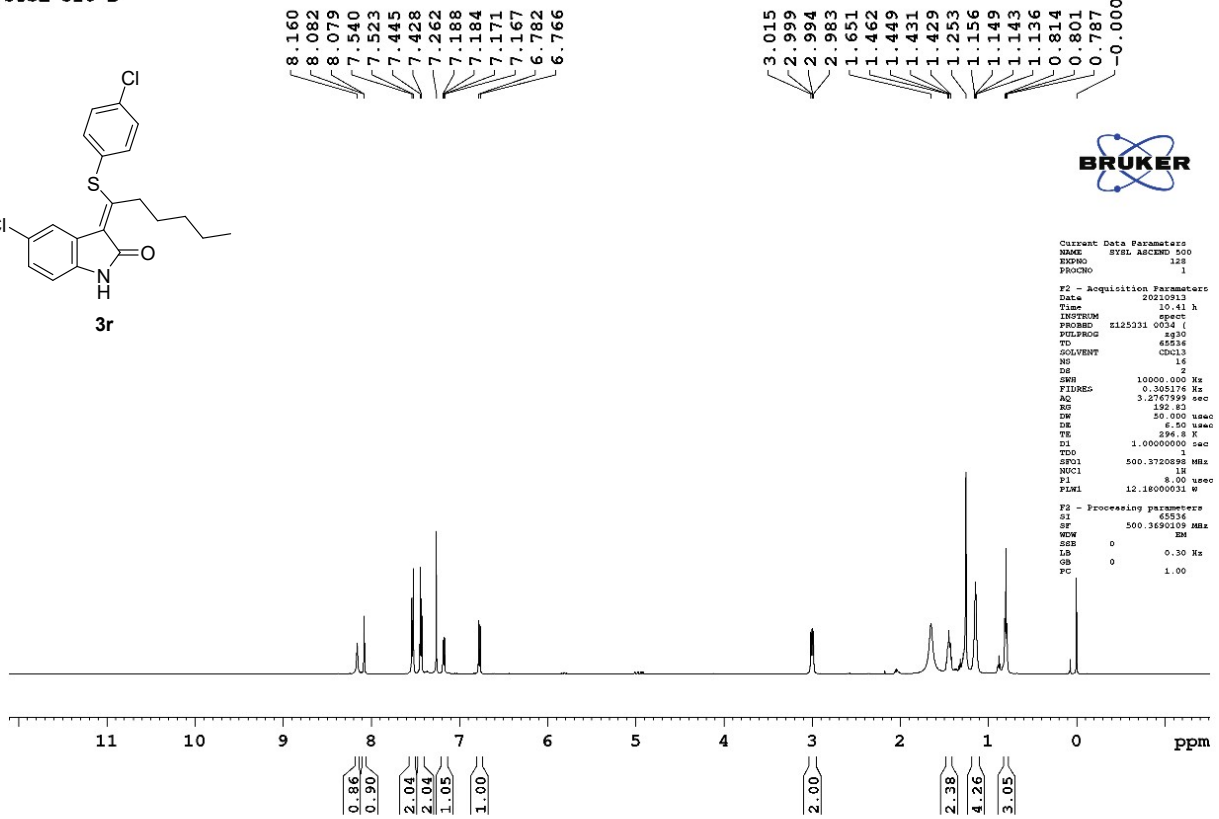
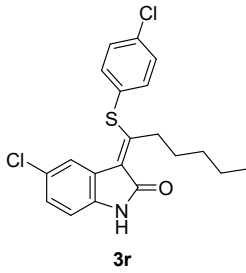
Current Data Parameters
NAME      SYTK-SPh-2
EXPNO    185
PROCNO   1

F2 - Acquisition Parameters
Date_    20210915
Time     17:10 h
INSTRUM  spect
PROBHD   1H1470-QNP1 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        125
DS        4
SWH       31250.000 Hz
FIDRES   0.933076 Hz
AQ        1.0485760 sec
RG         250.83
DF         14.000 usec
DE         6.50 usec
TE        300.5 K
CHFTZ    145.0000000
D1        2.0000000 sec
D11       0.00348828 sec
D12       0.00002000 sec
SFO1      125.8279504 MHz
NUC1       13C
P1         19.00 usec
PL1        115.01000214 W
PCPD2     20.00 usec
SFO2      500.1360514 MHz
PCPD2     18.00 usec
PCPD2     mult16
PLM1      23.2310099 W
PLM2      0.3629899 W
PLM3      0.1825799 W

F2 - Processing parameters
SI        32768
SF        125.8178664 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 -20 ppm

SYSL-328-B



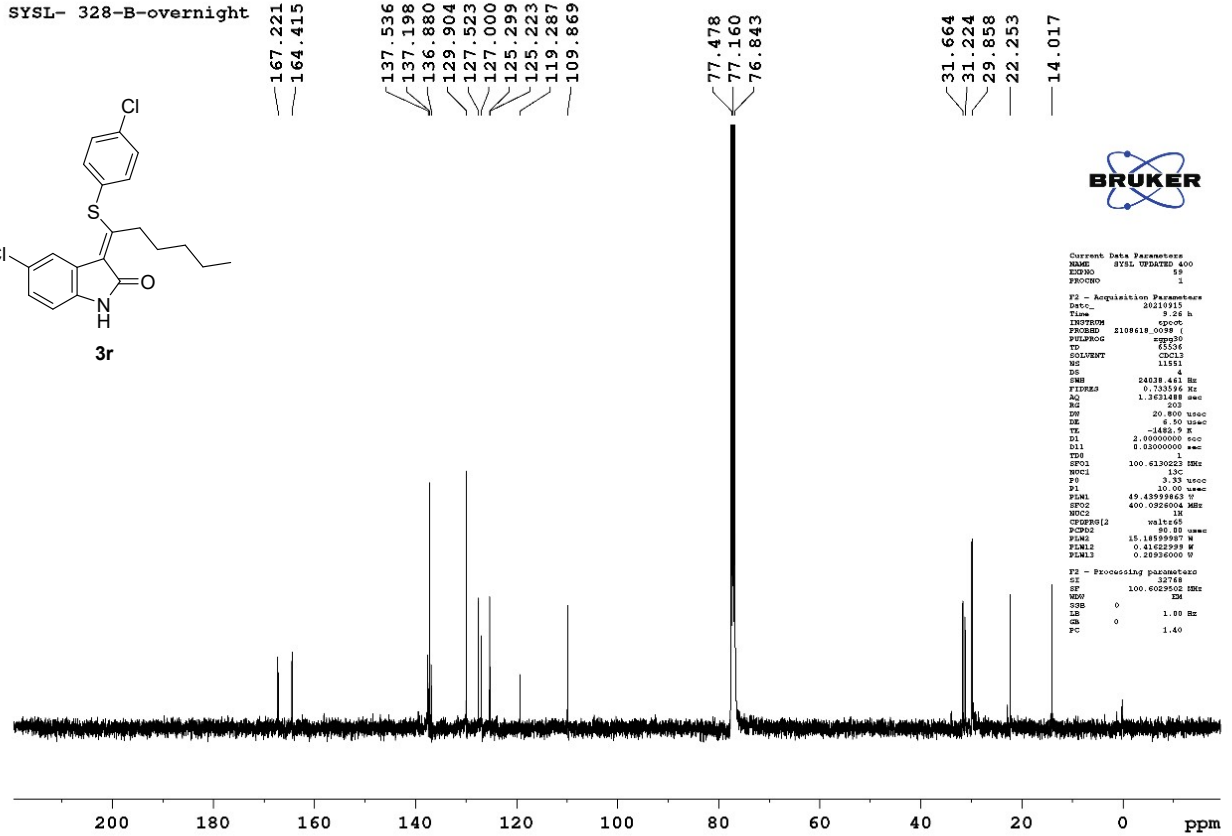
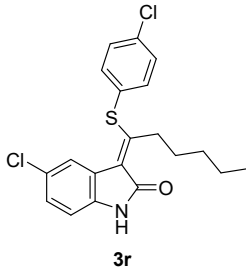
Current Data Parameters
 NAME SYSL-328-B-500
 EXPNO 128
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210913
 Time 10:41 h
 INSTRUM spect
 PROBRD z12531 0034 (420
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SSB 10000.000 Ks
 FIDRES 0.305176 Hz
 AQ 3.2767599 sec
 RG 192.83
 DW 20.000 usec
 DE 6.50 usec
 TE 296.2 K
 D1 1.00000000 sec
 TDO 1
 SFO1 500.3720688 MHz
 NUC1 1H
 P1 8.00 usec
 PLM1 12.18000031 W

F2 - Processing parameters
 SI 65536
 SF 500.3690109 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



SYSL- 328-B-overnight



Current Data Parameters
 NAME SYSL-328-B-400
 EXPNO 19
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210915
 Time 9:26 h
 INSTRUM spect
 PROBRD z12531 0034 (420
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SSB 24838.441 Hz
 FIDRES 0.233556 Hz
 AQ 1.361448 sec
 RG 203
 DW 20.000 usec
 DE 6.50 usec
 TE -182.9 K
 D1 2.00000000 sec
 D11 8.00000000 sec
 TDO 1
 SFO1 100.6130263 MHz
 NUC1 13C
 P1 3.15 usec
 P1 10.00 usec
 PLM1 49.4259980 W
 SFO2 400.0926004 MHz
 NUC2 1H
 CPOFFS(2) wait63
 PPRG 90.00 usec
 PLM2 15.1859987 W
 PLM3 0.4162299 W
 PLM4 0.2592600 W

F2 - Processing parameters
 SI 23748
 SF 100.6095002 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

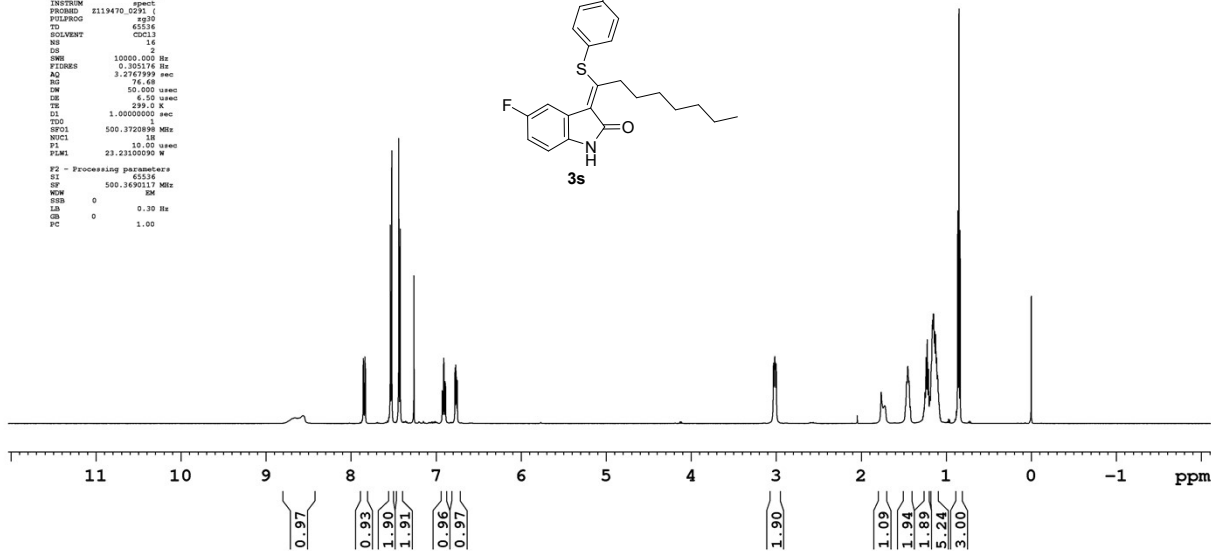
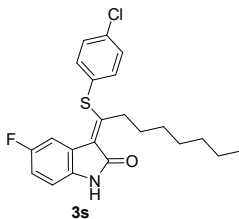


SYDA-209-1

8.565
7.856
7.851
7.836
7.832
7.543
7.538
7.534
7.525
7.521
7.516
7.444
7.439
7.435
7.426
7.422
7.260
6.928
6.923
6.910
6.905
6.893
6.888
6.777
6.768
6.760
6.751
3.031
3.015
2.999
1.765
1.466
1.451
1.451
1.437
1.249
1.237
1.223
1.209
1.209
1.161
1.153
1.147
1.136
1.124
1.113
1.103
1.092
0.864
0.850
0.836
-0.000



Current Data Parameters
NAME SYDA ASCND 500
EXPNO 128
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210924
Time 12.11 h
INSTRUM spect
PROBHD 519470_0291_0
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2
DS 2
SWH 10000.000 Hz
FIDRES 0.355176 Hz
AQ 3.278799 sec
RG 36.69
DM 50.000 usec
DE 6.50 usec
TE 299.2 K
D1 1.00000000 sec
TSD
SFO1 500.3720898 MHz
NUC1 1H
P1 10.00 usec
PL1 23.23100000 W
F2 - Processing parameters
SI 65536
SF 500.3695117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

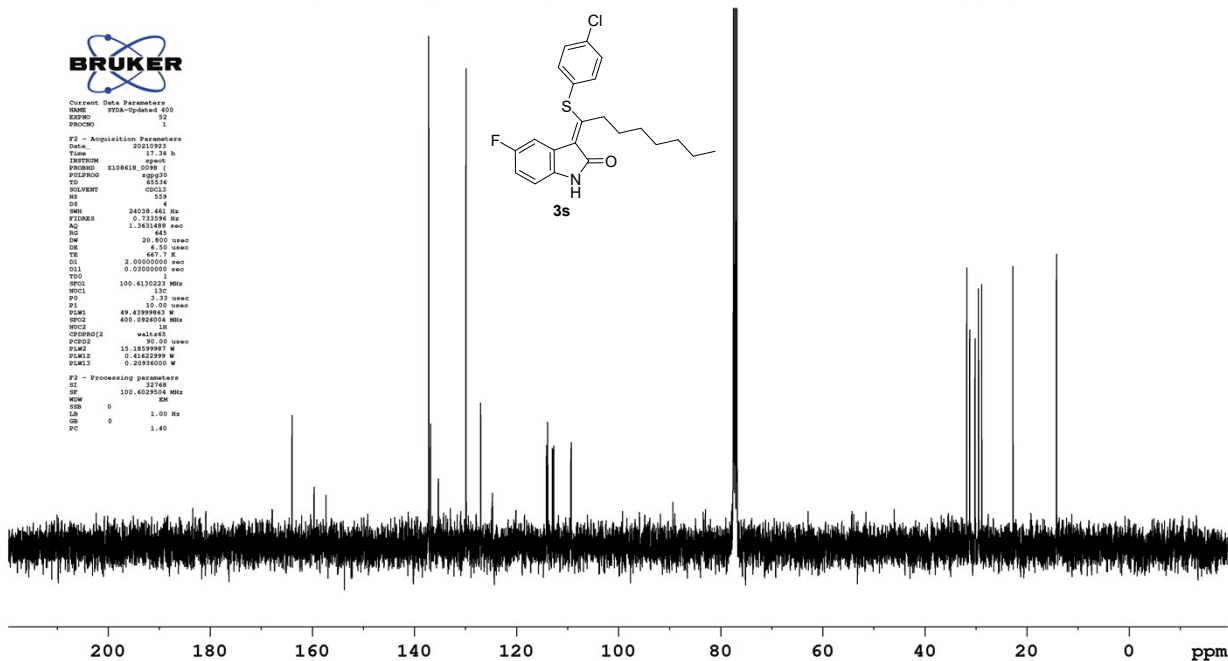
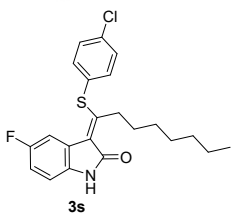


SYDA - 209-1

163.970
159.658
157.305
137.195
136.837
129.882
127.011
124.708
114.120
113.879
112.973
112.699
109.289
31.777
31.207
30.164
29.489
28.851
22.732
14.199

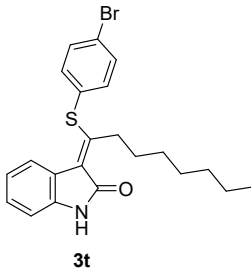


Current Data Parameters
NAME SYDA-Detected 400
EXPNO 32
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210923
Time 17.14 h
INSTRUM spect
PROBHD 519470_0291_0
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2
DS 2
SWH 24038.461 Hz
FIDRES 0.733204 Hz
AQ 1.363488 sec
RG 645
DM 20.800 usec
DE 6.50 usec
TE 667.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TSD
SFO1 100.6300203 MHz
NUC1 13C
P1 2.13 usec
PL1 10.00 usec
PL2 69.4399860 W
SFO2 400.3926004 MHz
NUC2 1H
CPDPRG2 waltz165
F2 - Processing parameters
SI 65536
SF 100.6299977 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

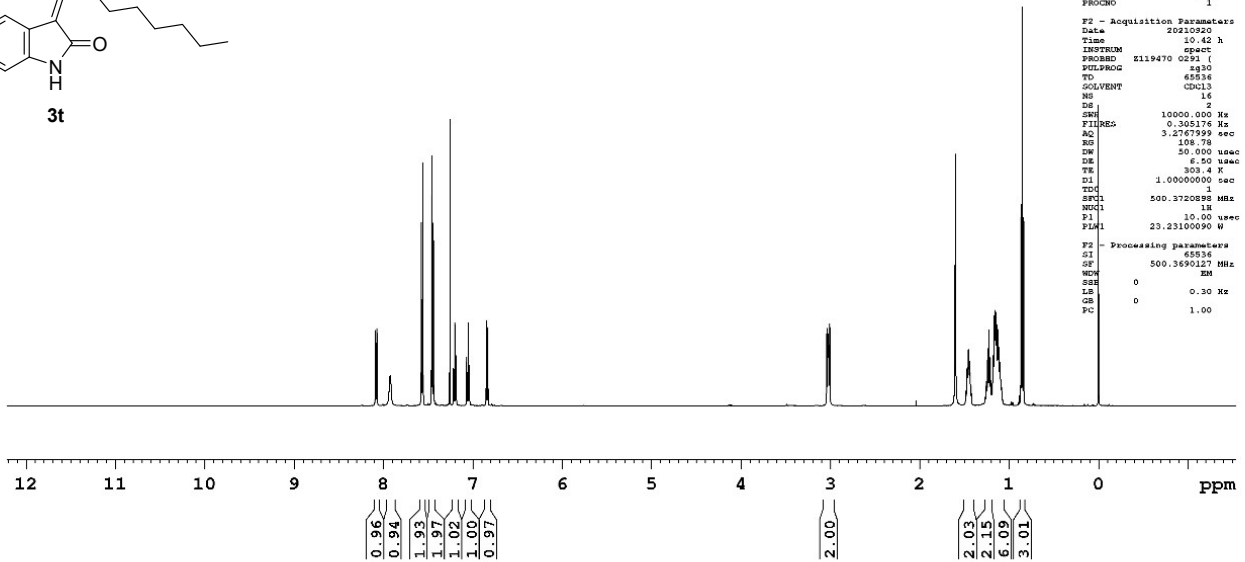


SYPR-4-304-S3

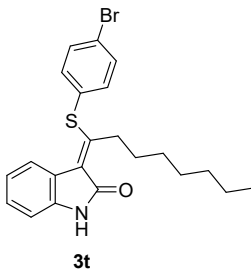
8.089
8.073
7.926
7.577
7.573
7.564
7.560
7.555
7.464
7.459
7.455
7.446
7.442
7.258
7.218
7.216
7.203
7.201
7.187
7.185
7.070
7.068
7.055
7.053
7.039
7.037
6.849
6.834
3.038
3.028
3.023
3.018
3.007
3.001
1.601
1.470
1.460
1.455
1.448
1.440
1.251
1.239
1.225
1.211
1.180
1.166
1.154
1.150
1.143
1.137
1.126
1.114
1.105
1.101
0.866
0.851
0.837
-0.000



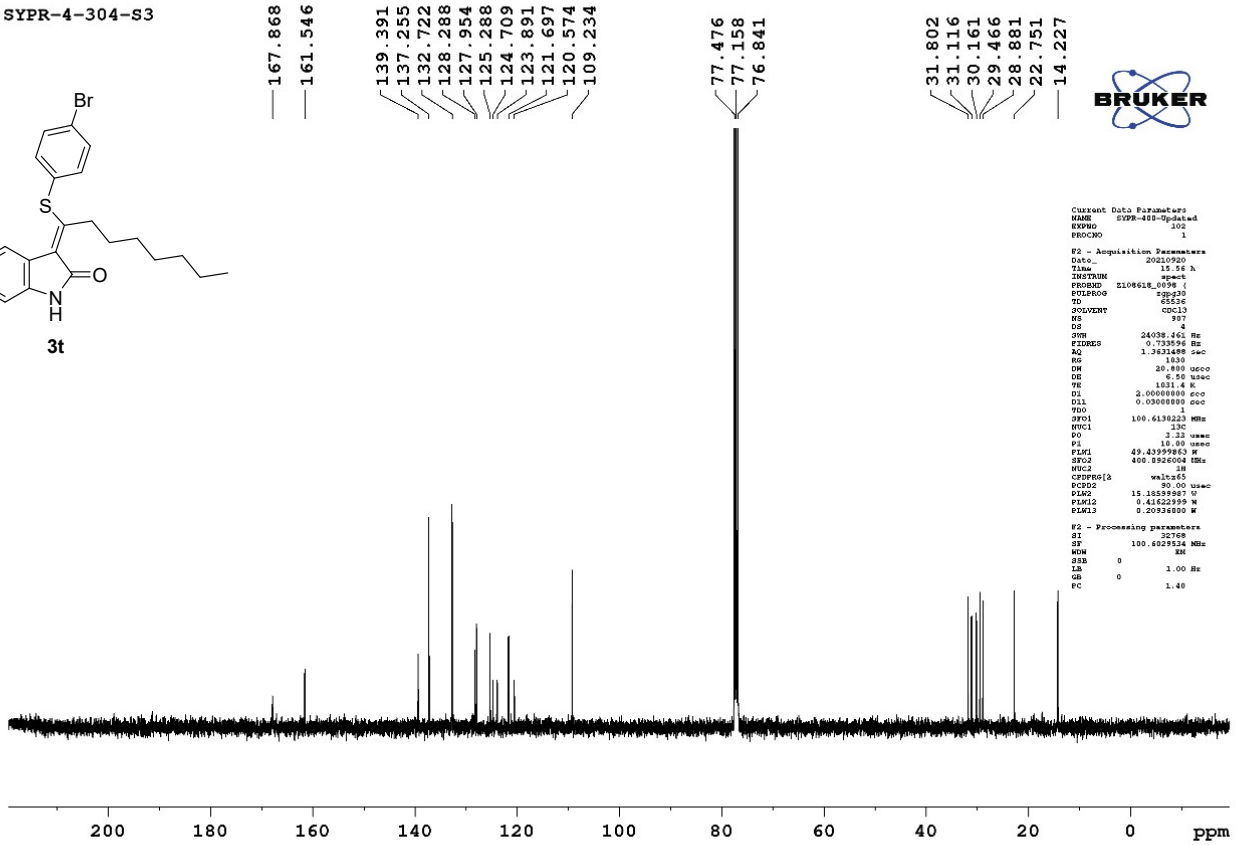
Current Data Parameters
NAME SYPR-ASCEND-500
EXPNO 419
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210920
Time 10.42 h
INSTRUM spect
PROBHD 519470 0294 (i
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 KHz
FIDRES 0.305176 KHz
AQ 3.2787399 sec
RG 108.78
DM 50.000 usec
DE 6.50 usec
TE 303.4 K
D1 1.00000000 sec
TEC 2
SFO1 500.372088 MHz
NUC1 1H
P1 10.00 usec
PL1 23.23100090 W
F2 - Processing Parameters
SI 65536
SF 500.3690127 MHz
WDW EM
SS 0
LB 0.30 KHz
GB 0
PC 1.00



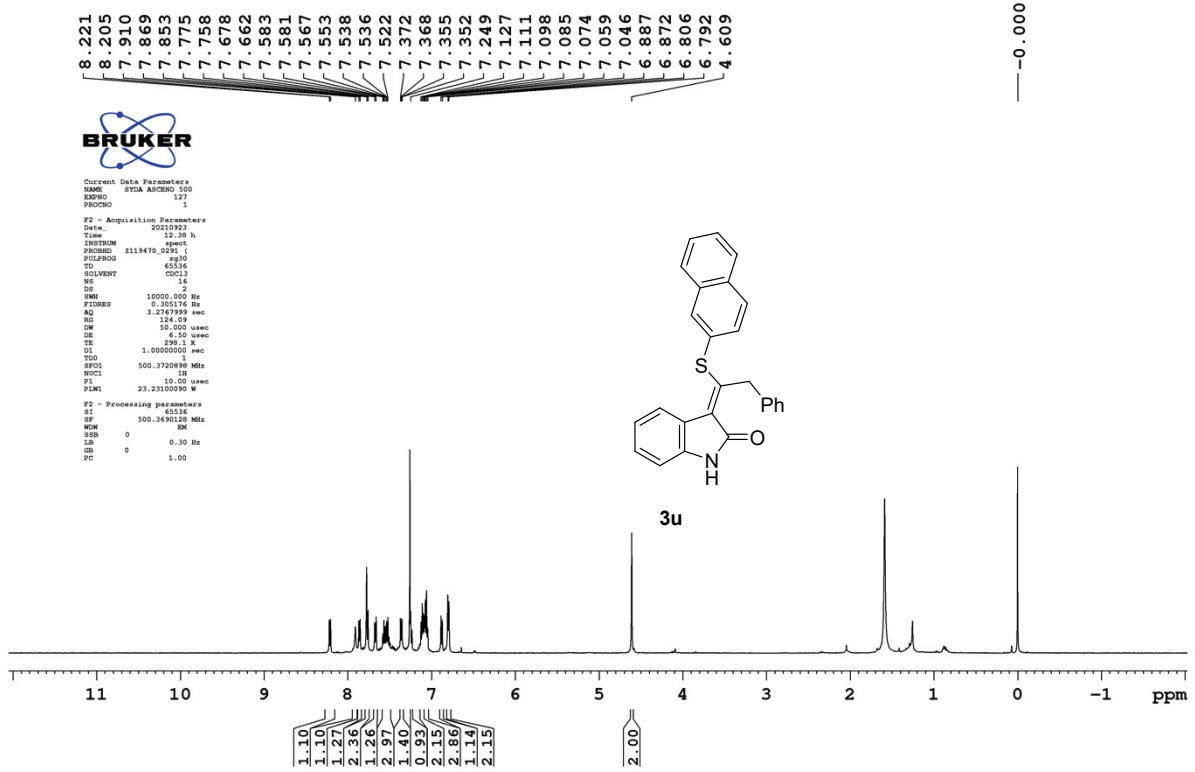
SYPR-4-304-S3



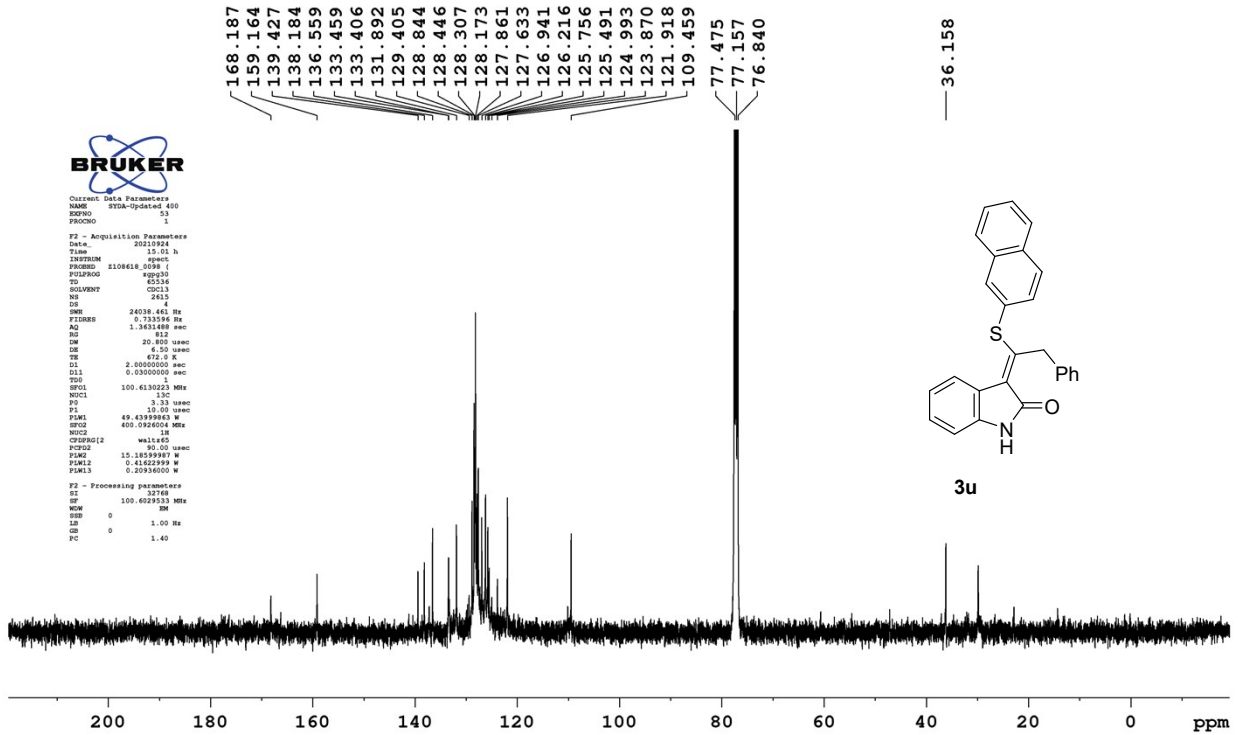
Current Data Parameters
NAME SYPR-400-000-001
EXPNO 200
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210920
Time 15.56 h
INSTRUM spect
PROBHD 5106618_0098 (i
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 997
DS 4
SWH 24038.461 KHz
FIDRES 0.733056 KHz
AQ 1.3631488 sec
RG 1030
DM 20.800 usec
DE 6.50 usec
TE 303.4 K
D1 2.00000000 sec
D11 0.03000000 sec
FID 1
SFO1 100.6138223 MHz
NUC1 13C
P1 2.33 usec
PL1 15.80 usec
PL12 49.43997803 W
SFO2 400.8926004 MHz
NUC2 13C
CPDPRG2 waltz160
PCPD2 90.00 usec
PLM2 15.18599887 W
PLM12 0.41622998 W
PLM13 0.20936000 W
F2 - Processing Parameters
SI 20708
SF 100.6029324 MHz
WDW EM
SS 0
LB 1.00 KHz
GB 0
PC 1.40



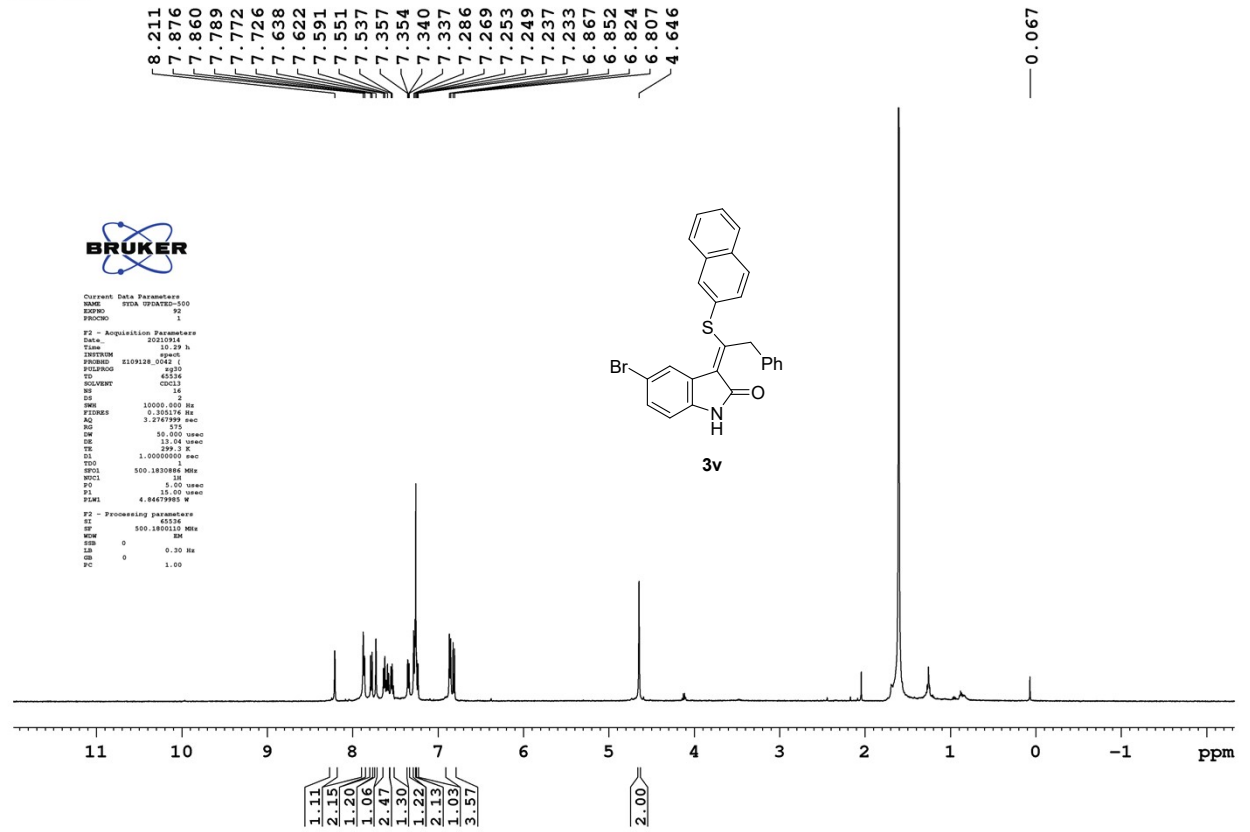
204-1



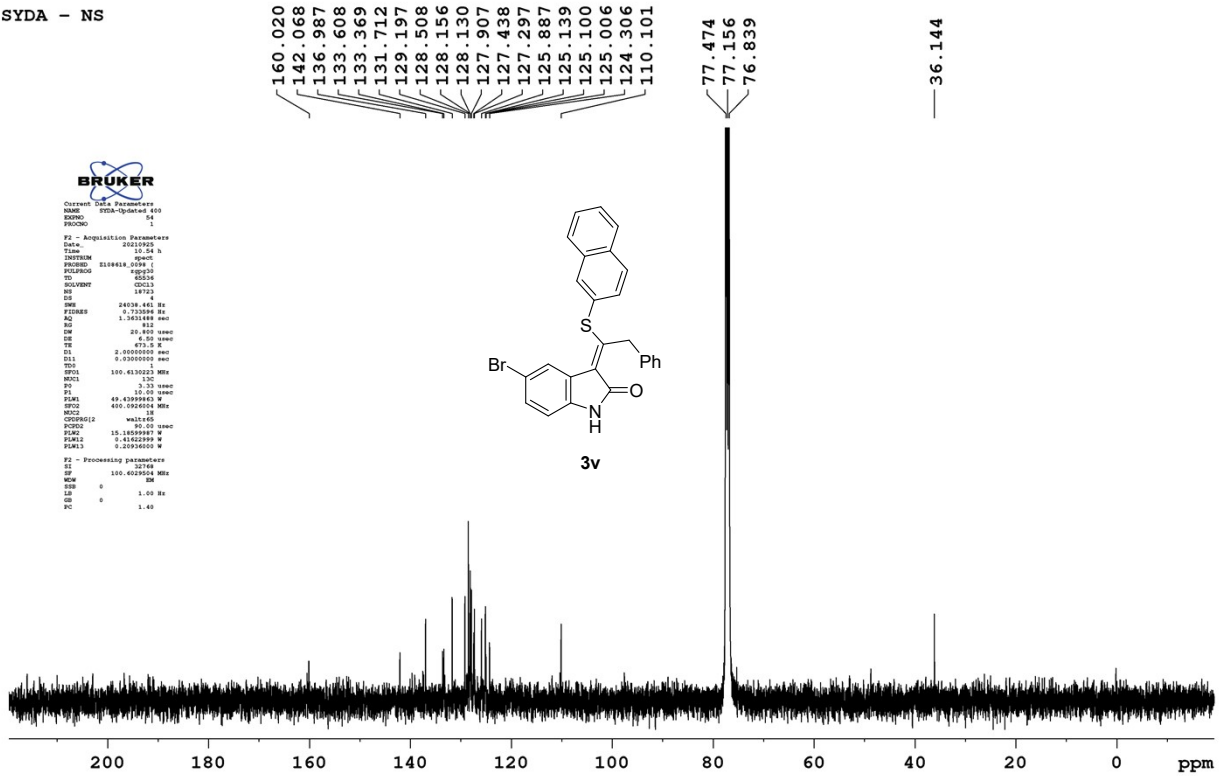
SYDA - 204-1



SYDA-NS

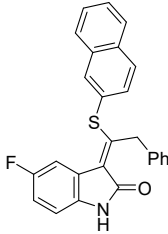


SYDA - NS

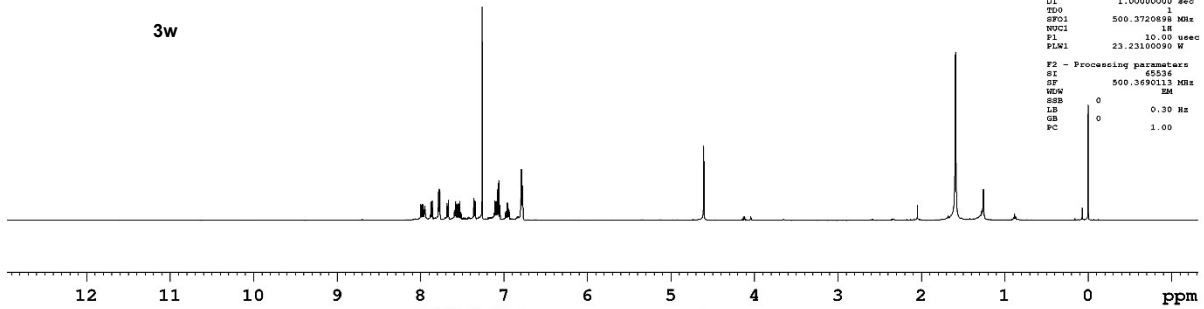


SY ALI-C4

7.937
7.932
7.977
7.972
7.949
7.875
7.859
7.785
7.775
7.772
7.770
7.682
7.666
7.594
7.592
7.580
7.578
7.564
7.562
7.547
7.544
7.531
7.517
7.382
7.359
7.345
7.342
7.260
7.106
7.092
7.078
7.066
7.063
7.049
6.977
6.960
6.955
6.942
6.937
6.800
6.791
6.782
6.776
6.774
4.606



3w



1.20
0.92
1.30
2.40
1.32
1.26
1.16
1.19
3.31
1.20
3.17
2.00



Current Data Parameters
NAME: ALI YOR ASCEND 500
EXPNO: 3
PROCNO: 1

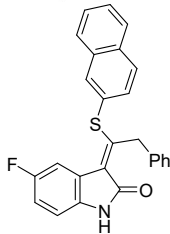
F2 - Acquisition Parameters
Date_: 20210921
Time: 16.09 h
INSTRUM: spect
PROBHD: Z113470 0291 (4
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 16
DS: 4
SWH: 10000.000 Hz
FIDRES: 0.300176 Hz
AQ: 3.276789 sec
RG: 139.3
DM: 50.000 usec
DE: 6.50 usec
TE: 298.2 K
D1: 1.0000000 sec
TDO: 0
SFO1: 500.3720898 MHz
NUC1: 1H
P1: 10.00 usec
PLW1: 23.23100090 W

F2 - Processing parameters
SI: 65536
SF: 500.3690113 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

-0.000

YSR ALI C4

167.723
161.398
137.910
136.771
135.160
133.587
133.435
131.833
129.004
128.419
128.253
128.217
127.910
127.806
127.056
126.352
124.895
114.502
114.308
113.511
113.256
109.424
109.354
100.140
77.415
77.160
76.907
36.227

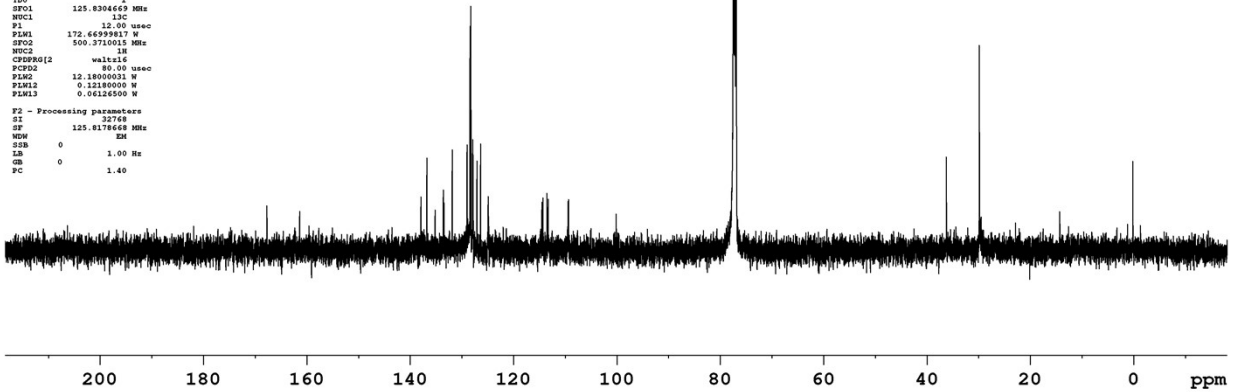


3w

Current Data Parameters
NAME: ALI YOR ASCEND 500
EXPNO: 7
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20211023
Time: 10.44 h
INSTRUM: spect
PROBHD: Z113331 0056 (4
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 1571
DS: 4
SWH: 29761.908 Hz
FIDRES: 0.98261 Hz
AQ: 1.1010048 sec
RG: 15.92
DM: 16.800 usec
DE: 6.50 usec
TE: 298.2 K
D1: 2.0000000 sec
D11: 0.03000000 sec
TDO: 0
SFO1: 125.8304669 MHz
NUC1: 13C
P1: 12.00 usec
PLW1: 173.6699817 W
SFO2: 500.3710015 MHz
NUC2: 1H
CPDPRG2: waltz16
PCPD2: 88.00 usec
PLM2: 12.18000001 W
PLM3: 0.12180000 W
PLM4: 0.00121800 W

F2 - Processing parameters
SI: 32768
SF: 125.8174668 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40



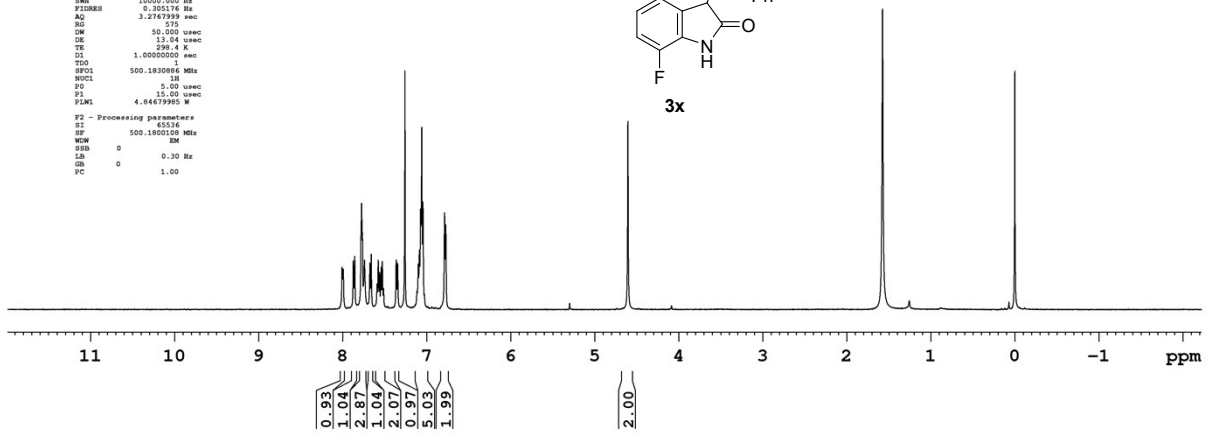
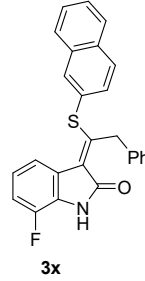
SYDA-208-2

8.007
 7.992
 7.873
 7.857
 7.774
 7.765
 7.741
 7.676
 7.660
 7.577
 7.562
 7.543
 7.528
 7.363
 7.346
 7.259
 7.101
 7.087
 7.073
 7.058
 7.044
 6.787
 6.773
 4.605

-0.000



Current Data Parameters
 NAME SYDA-UPDATE-500
 EXPNO 4
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20210921
 Time 15:17 h
 INSTRUM spect
 FREQID 5109128.0042 f
 PULPROG zgpg30
 TD 65536
 SOLVENT CMC13
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2747079 sec
 RG 575
 DW 50.0000 usec
 DE 13.04 usec
 TE 298.4 K
 D1 1.00000000 sec
 TDO
 SFO1 500.1830886 MHz
 NUC1 1H
 PD 5.00 usec
 P1 151.00 usec
 PL1 4.84679985 W
 F2 - Processing parameters
 SI 65536
 SF 500.1800100 MHz
 WDW RM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



SYDA - 208-2

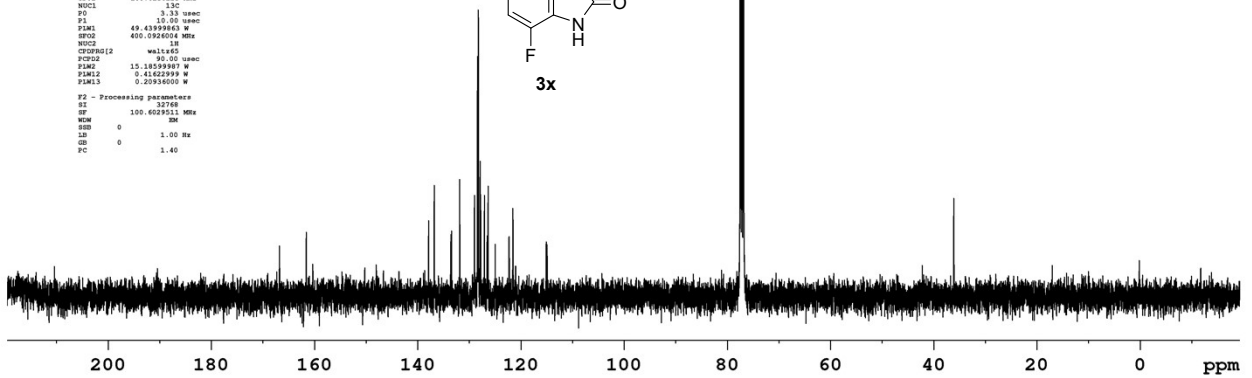
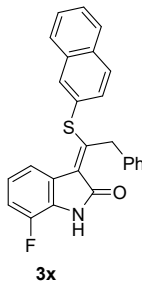
166.782
 161.585
 137.865
 136.767
 133.561
 133.408
 131.850
 128.974
 128.400
 128.228
 127.893
 127.789
 127.039
 126.519
 126.323
 124.979
 122.298
 121.537
 115.078
 114.904

77.474
77.157
76.839

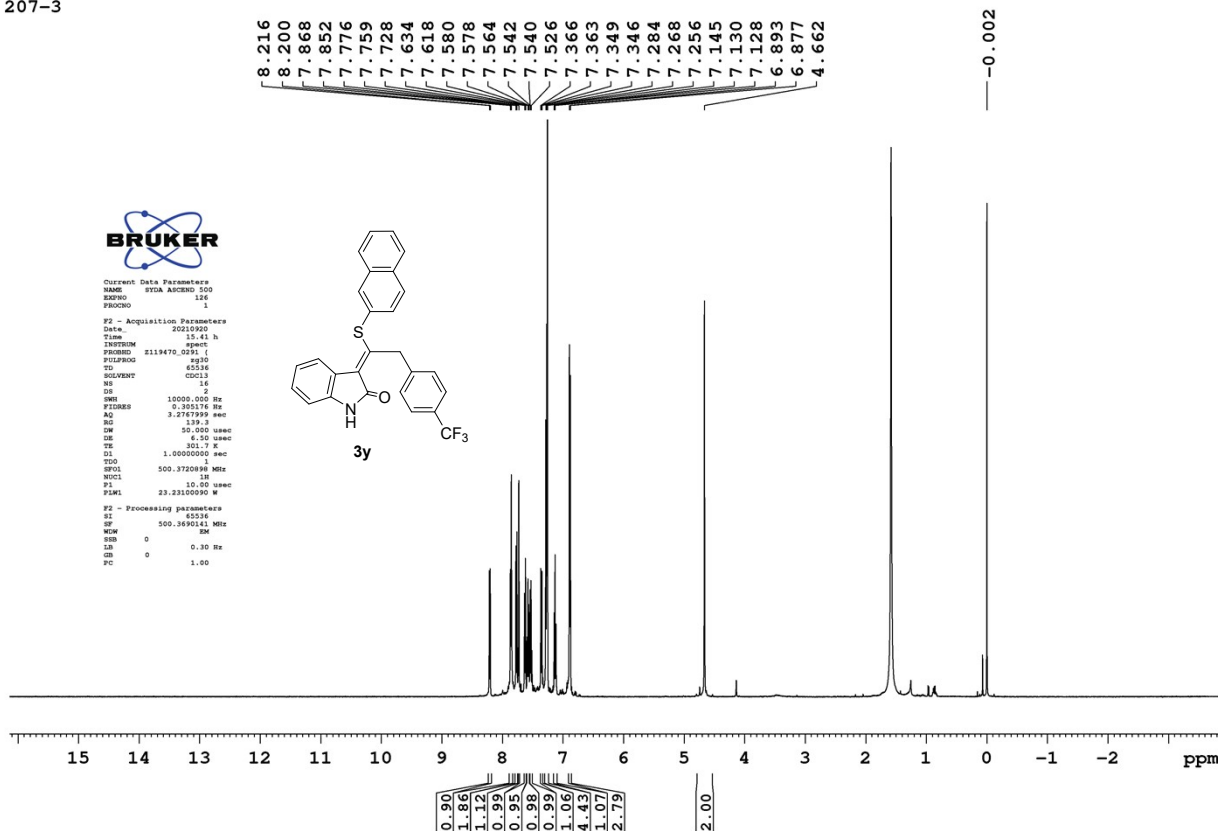
36.072



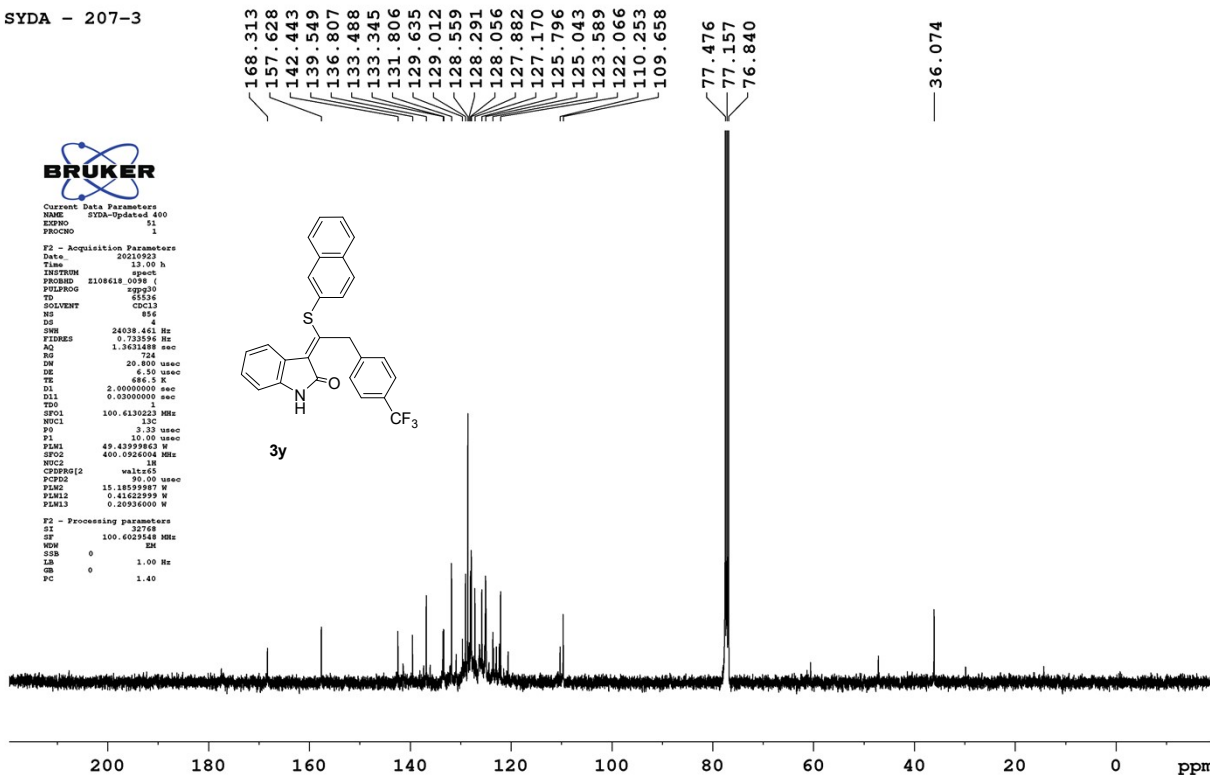
Current Data Parameters
 NAME SYDA-UPDATE-600
 EXPNO 50
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20210922
 Time 12:56 h
 INSTRUM spect
 FREQID 5108619.0098 f
 PULPROG zgpg30
 TD 65536
 SOLVENT CMC13
 NS 16
 DS 2
 SWH 24038.461 Hz
 FIDRES 0.733396 Hz
 AQ 1.3631488 sec
 RG 512
 DW 20.800 usec
 DE 6.50 usec
 TE 871.7 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO
 SFO1 100.6130223 MHz
 NUC1 13C
 PD 3.33 usec
 P1 10.00 usec
 PL1 49.43999603 W
 PL2 400.00000004 MHz
 NUC2 1H
 CPOPRG2 waltz165
 PFG2 90.00 usec
 PLM2 10.18599987 W
 PLM3 0.41622999 W
 PLM13 0.20936000 W
 F2 - Processing parameters
 SI 32768
 SF 100.6029511 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



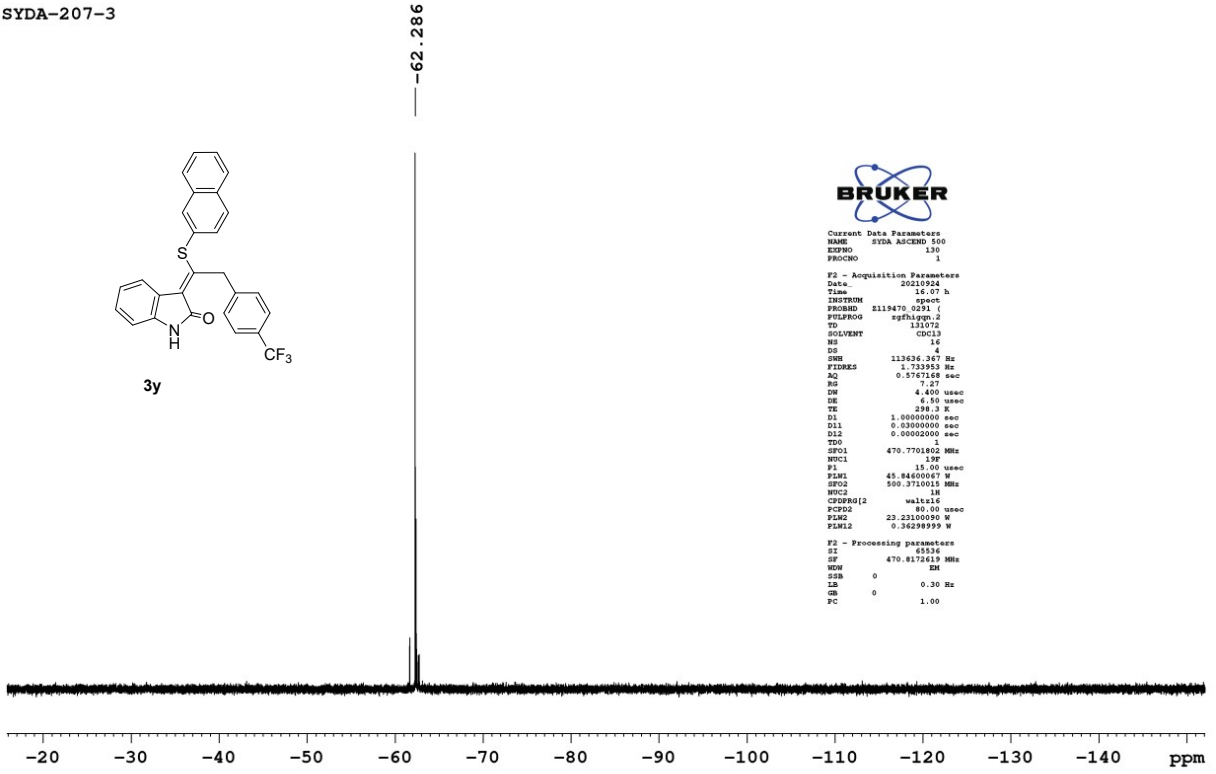
207-3



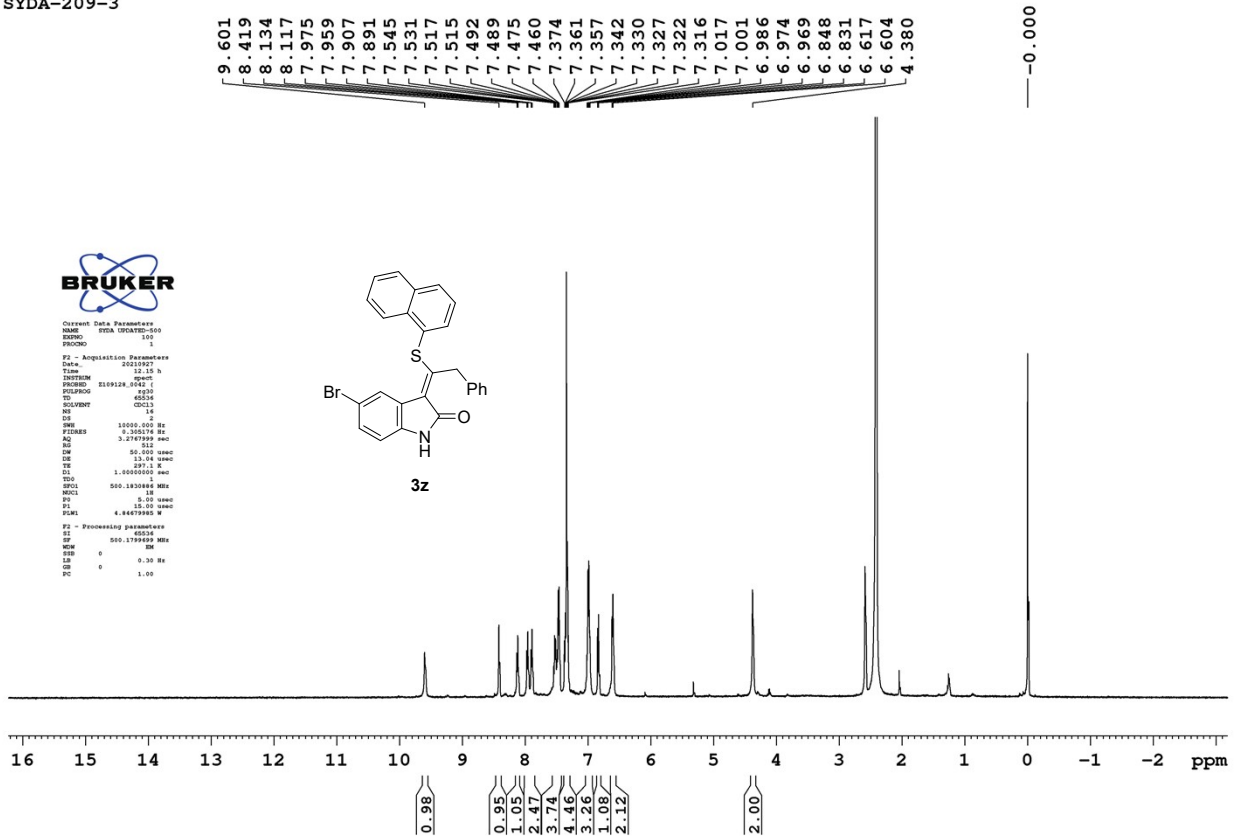
SYDA - 207-3



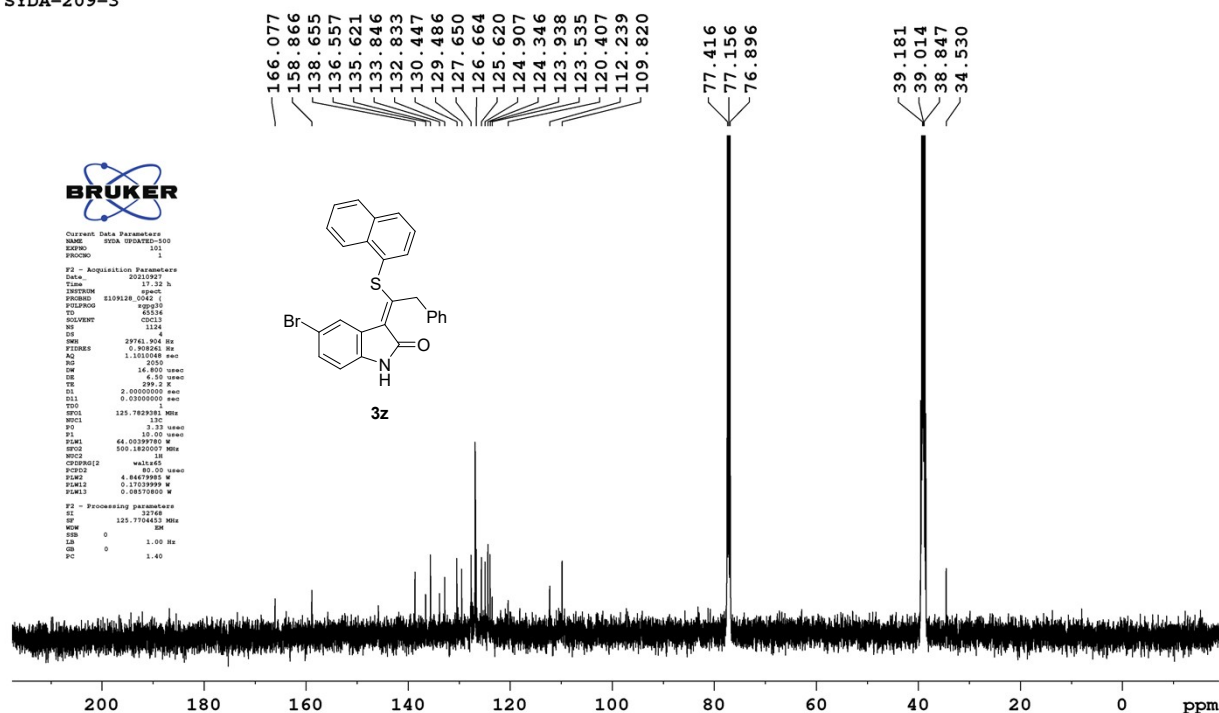
SYDA-207-3



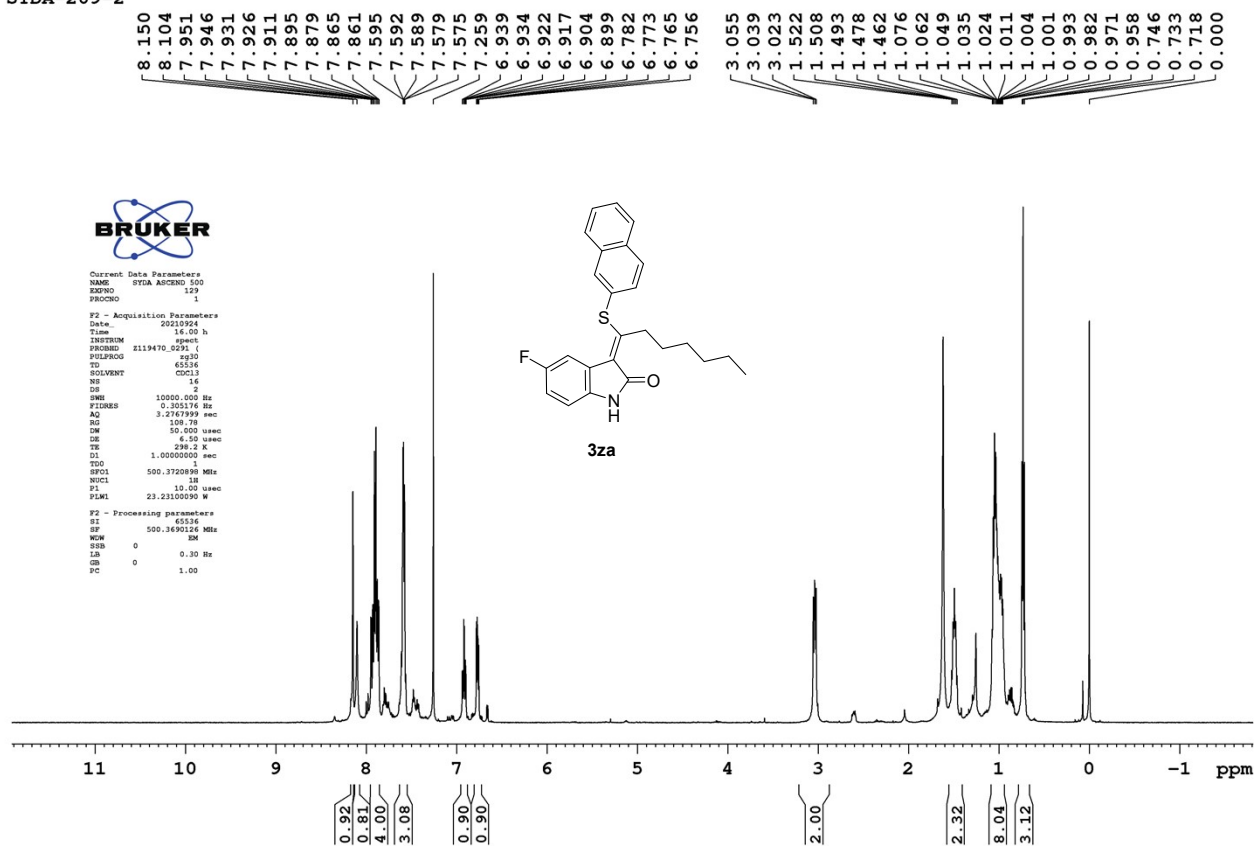
SYDA-209-3

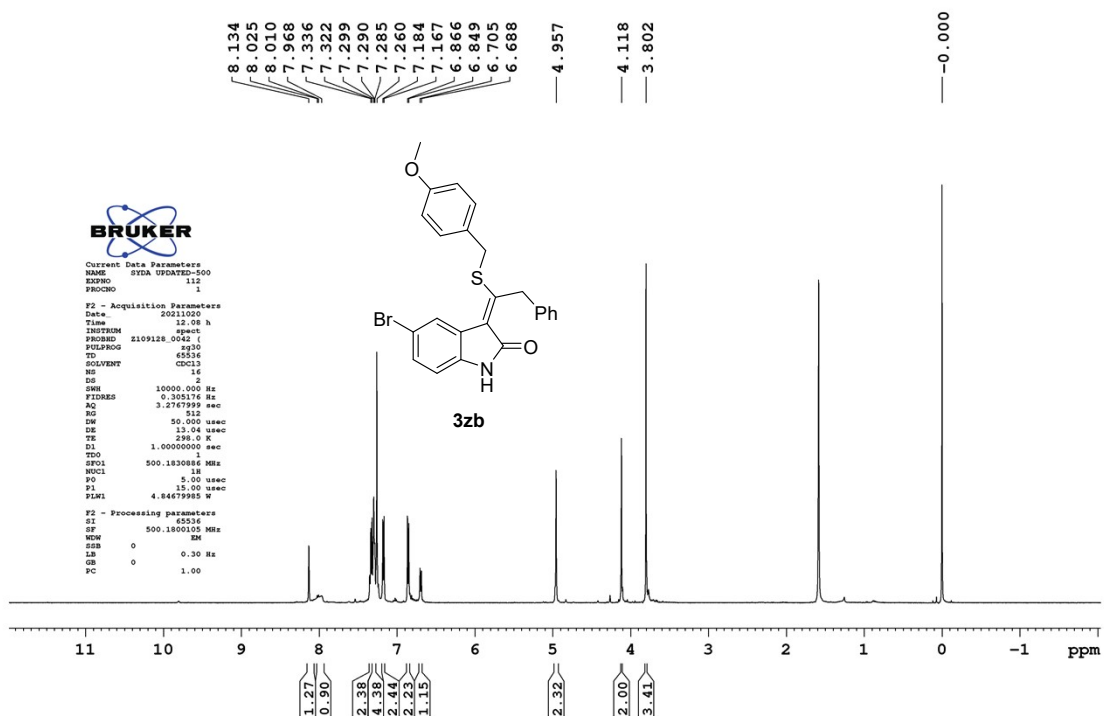
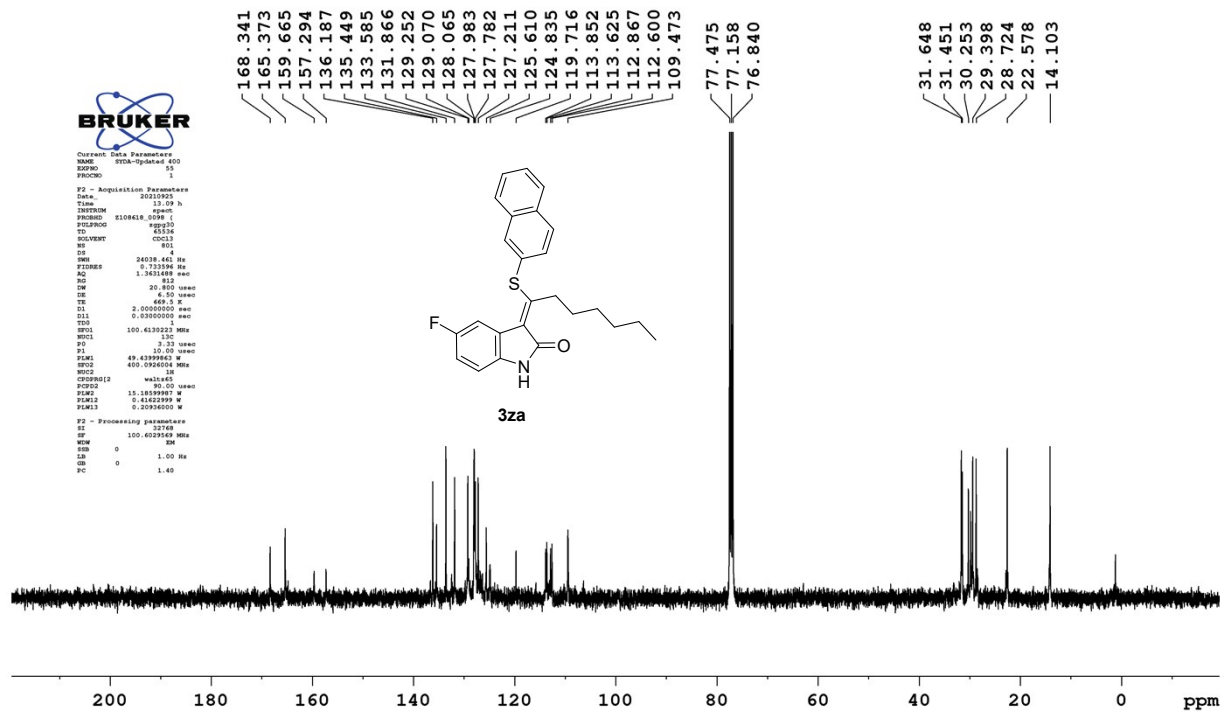


SYDA-209-3

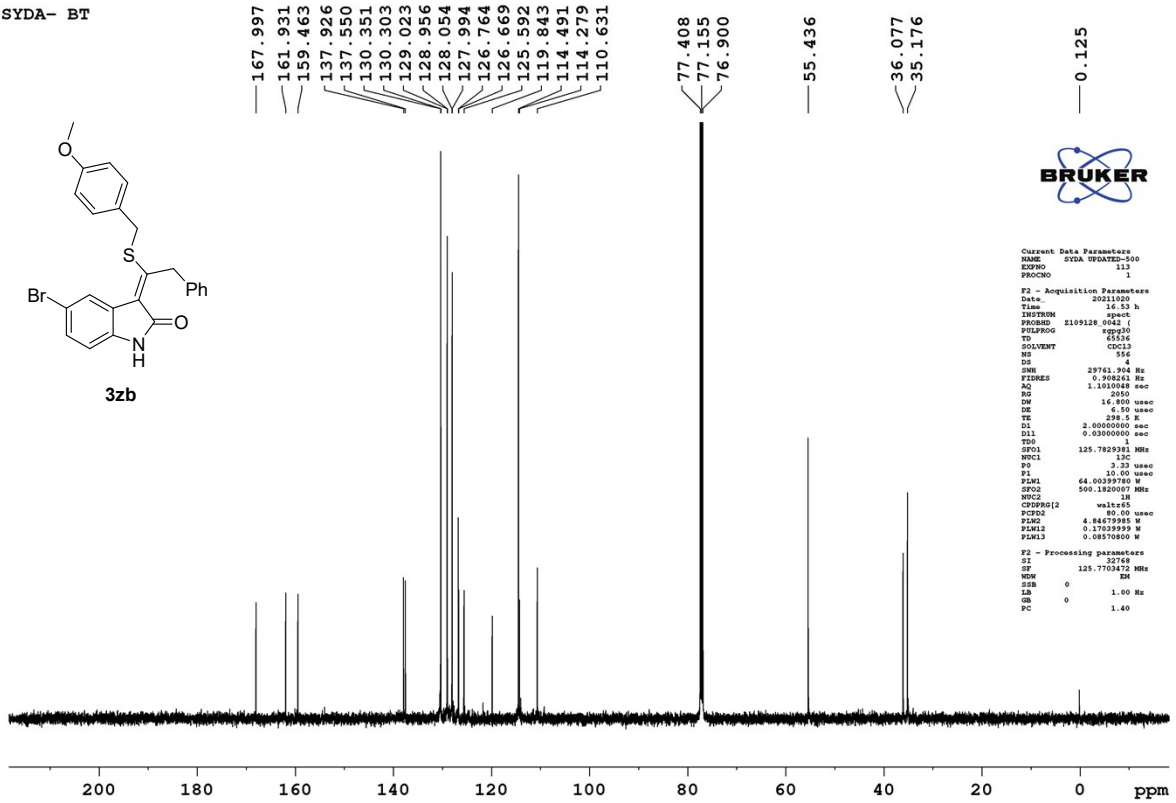


SYDA-209-2

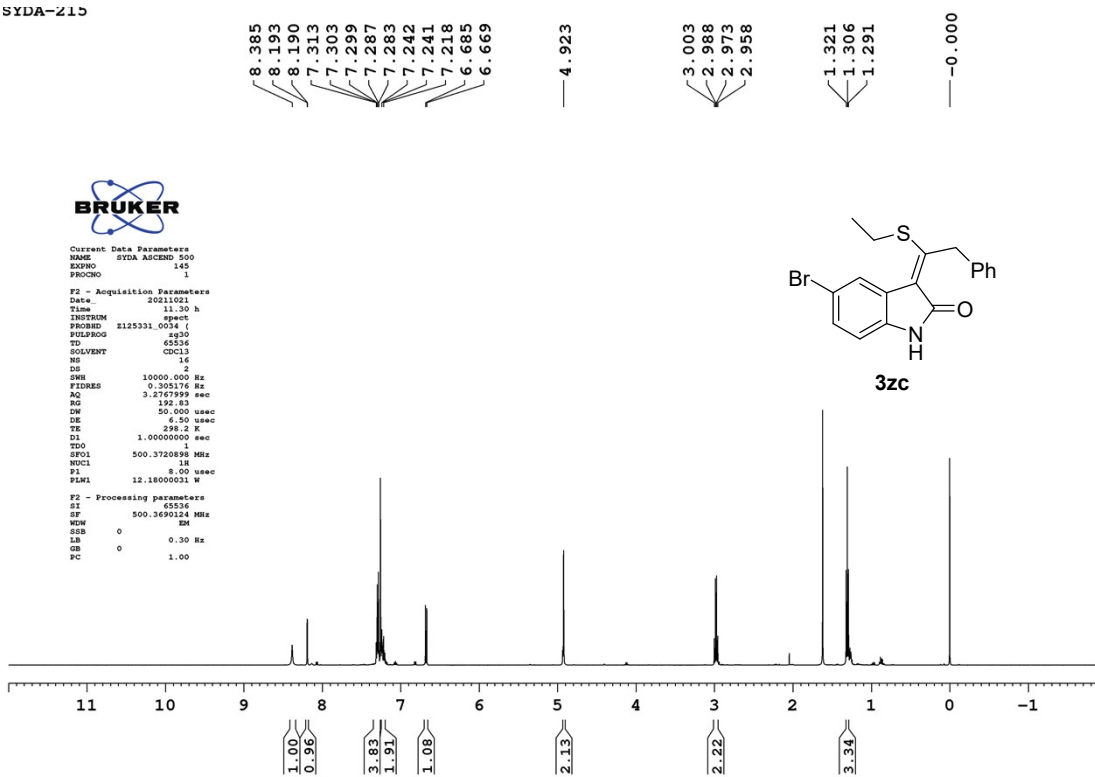


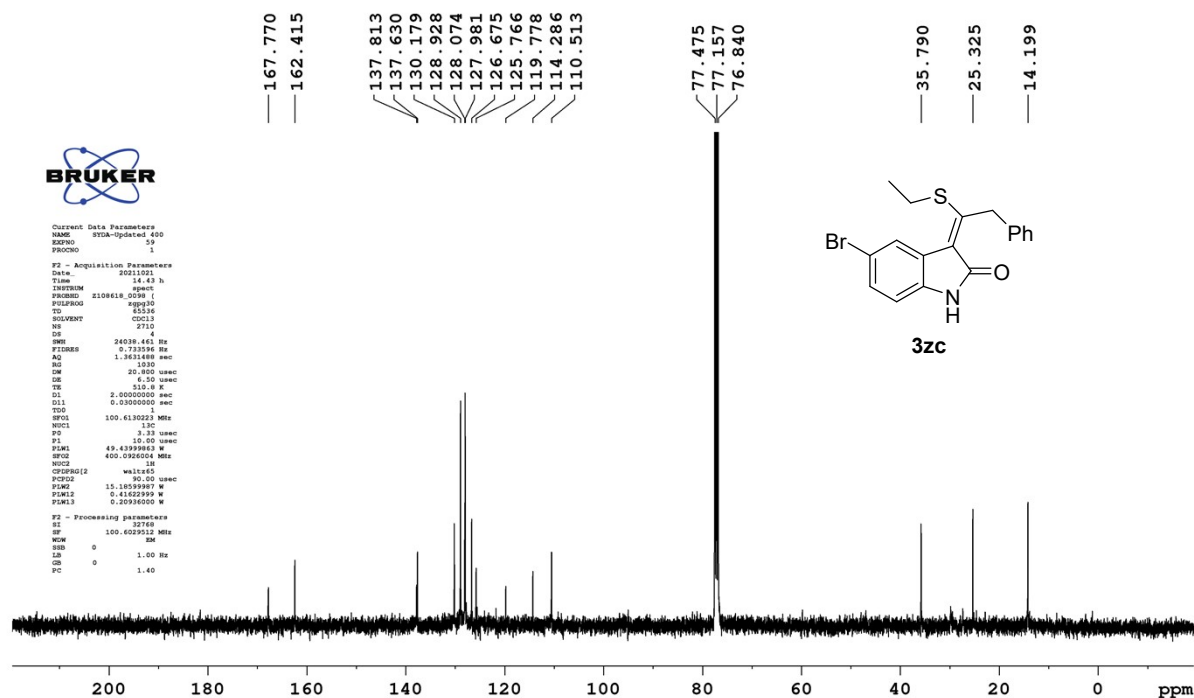


SYDA-BT

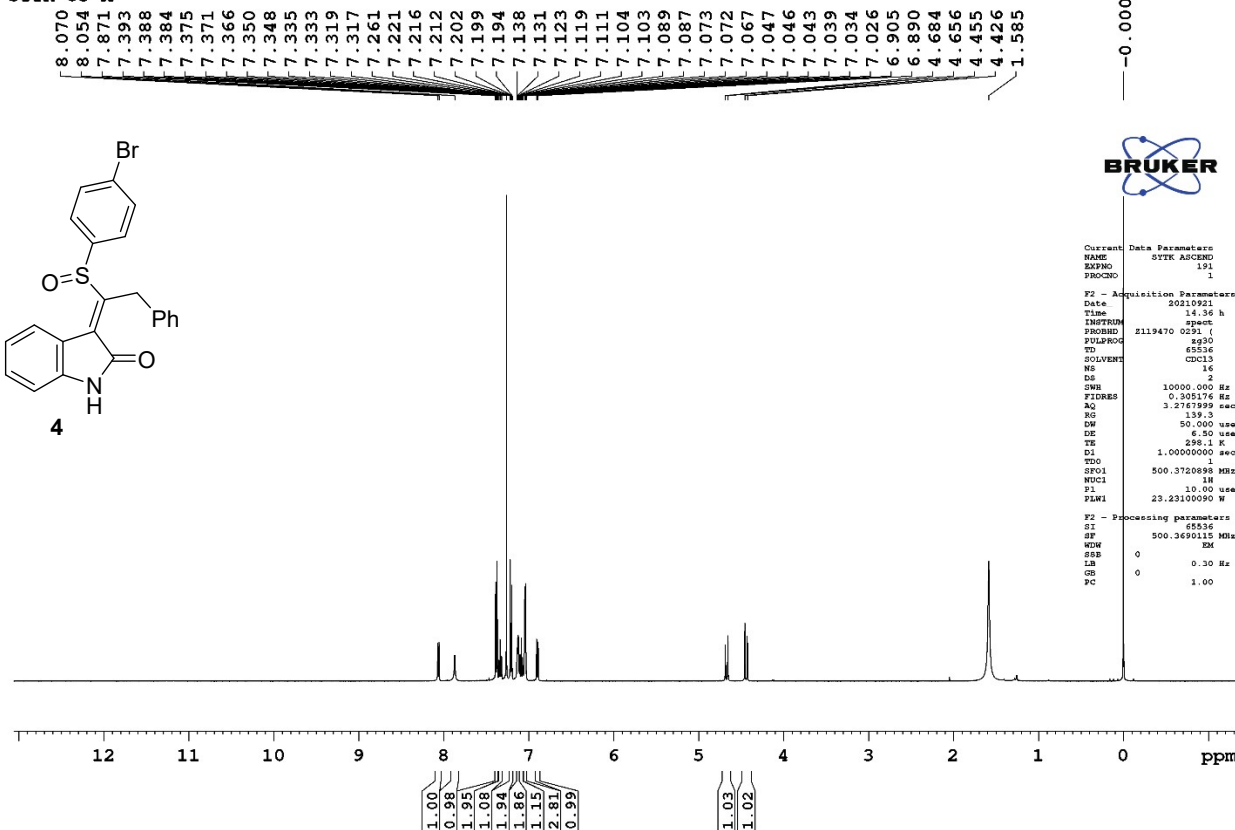


SYDA-Z15

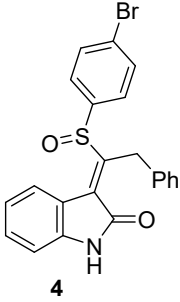




SYTK-83 A



SYTK-83 A



167.115
158.567
142.706
140.183
137.458
136.743
131.011
130.168
129.069
129.023
127.783
127.038
125.742
125.091
122.041
121.464
110.694

77.479
77.160
76.841

40.612
40.391
40.181
39.972
39.764
39.559
39.345
27.395

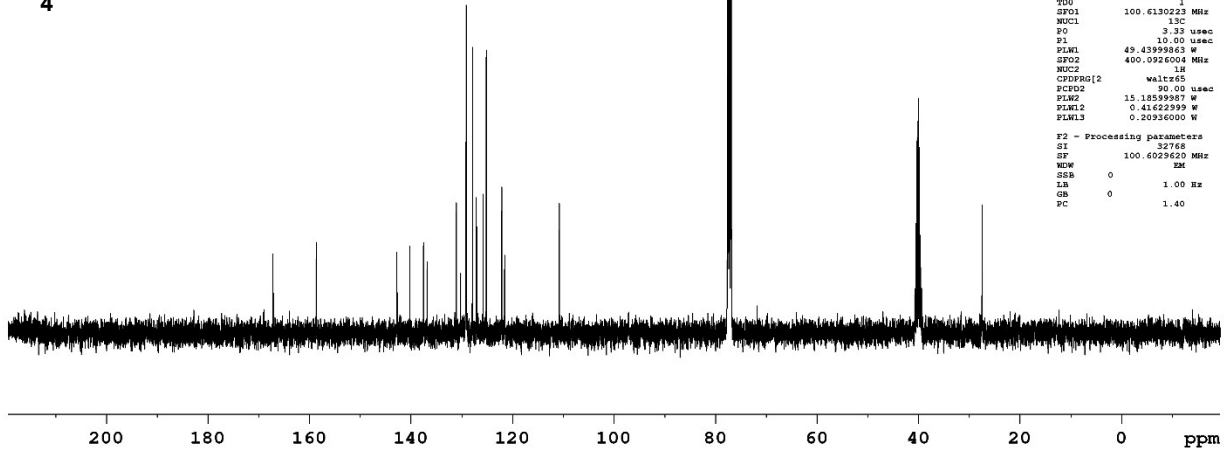


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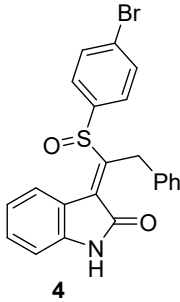
Current Data Parameters
NAME      TK-400 updated
EXPNO    52
PROCNO   1

F2 - Acquisition Parameters
Date_    20210923
Time     15:43 h
INSTRUM  spect
PROBHD   Z108618_0098 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        1024
DS        4
SWH       24038.461 Hz
FIDRES   0.73396 Hz
AQ        1.3631489 sec
RG        203
DM        20.800 usec
DE        6.50 usec
TE        666.3 K
D1        2.0000000 sec
d11       0.0300000 sec
TDO       1
SFO1     100.6130223 MHz
NUC1      13C
P1        3.33 usec
P2        10.00 usec
PLH1     45.45999863 W
SFO2     400.0926004 MHz
NUC2      1H
CPDPRG2  waltz65
PCPD2    90.00 usec
PLH2     15.18599987 W
PLH3     0.41622999 W
PLH4     0.20936000 W

F2 - Processing parameters
SI        32768
SF        100.6026620 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```



SYTK-83 A



131.008
129.065
129.018
127.781
127.035
125.739
125.085
122.036
110.696

27.395

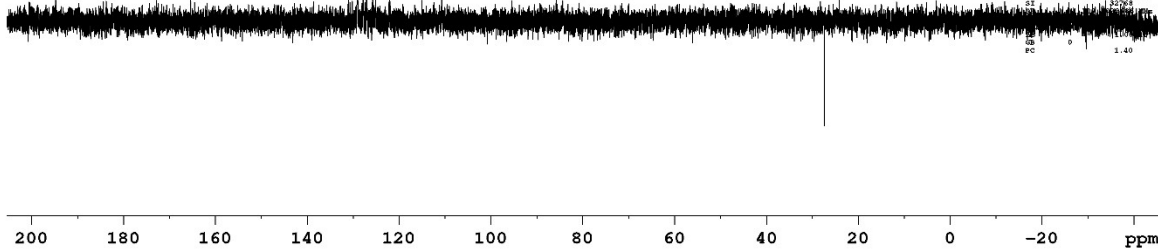


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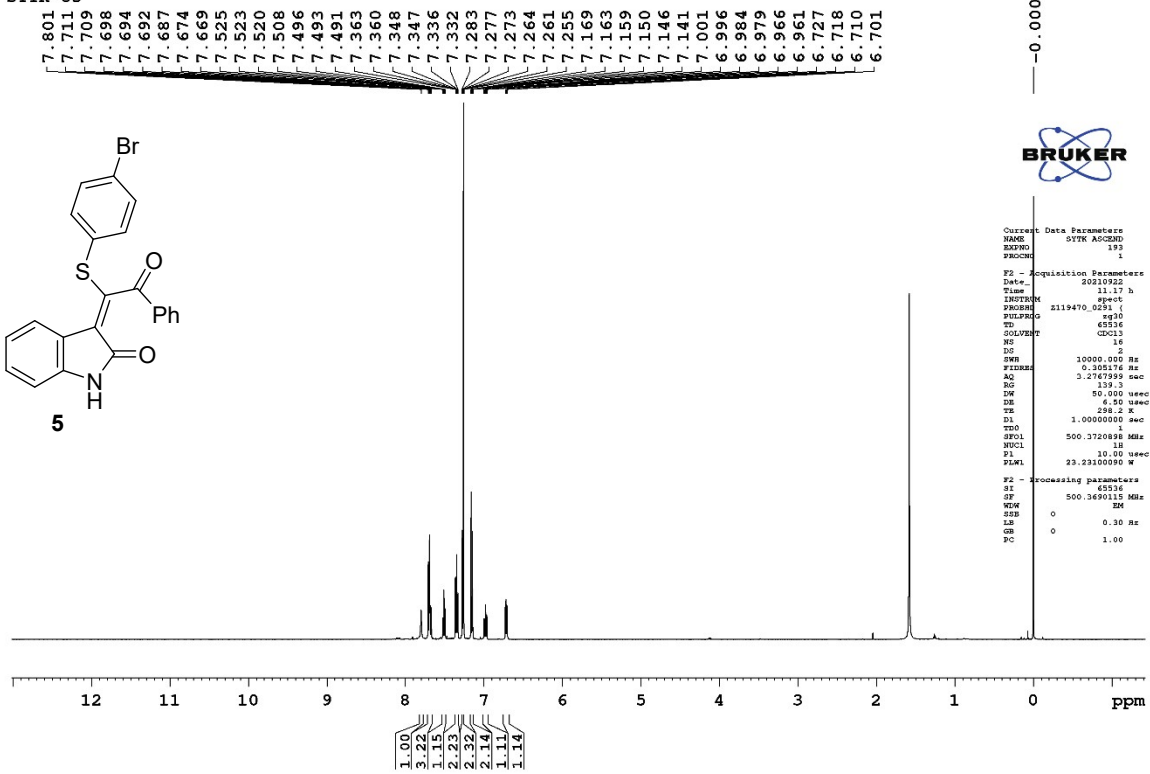
Current Data Parameters
NAME      TK-400 updated
EXPNO    51
PROCNO   1

F2 - Acquisition Parameters
Date_    20210923
Time     14:45 h
INSTRUM  spect
PROBHD   Z108618_0098 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        1024
DS        4
SWH       24038.461 Hz
FIDRES   0.73396 Hz
AQ        1.3631489 sec
RG        203
DM        20.800 usec
DE        6.50 usec
TE        666.3 K
D1        2.0000000 sec
d11       0.0300000 sec
TDO       1
SFO1     100.6130223 MHz
NUC1      13C
P1        3.33 usec
P2        10.00 usec
PLH1     45.45999863 W
SFO2     400.0926004 MHz
NUC2      1H
CPDPRG2  waltz65
PCPD2    90.00 usec
PLH2     15.18599987 W
PLH3     0.41622999 W
PLH4     0.20936000 W

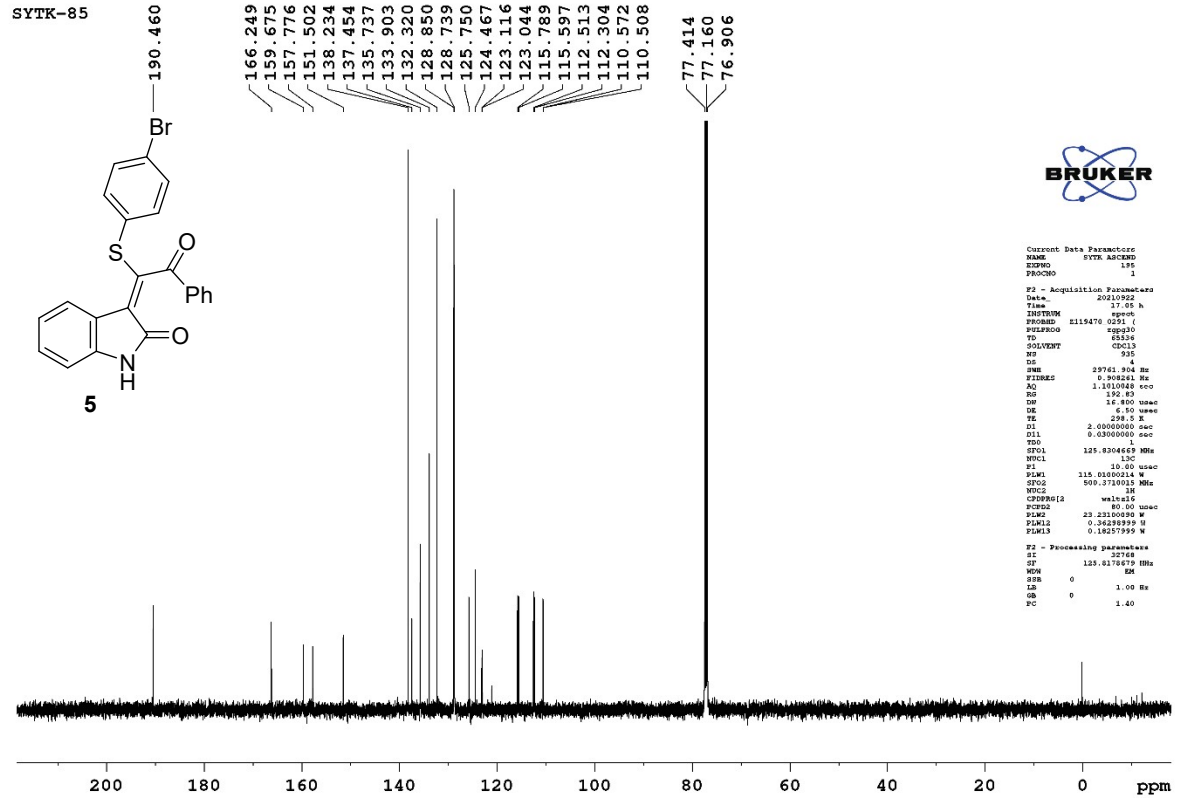
F2 - Processing parameters
SI        32768
SF        100.6026620 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```



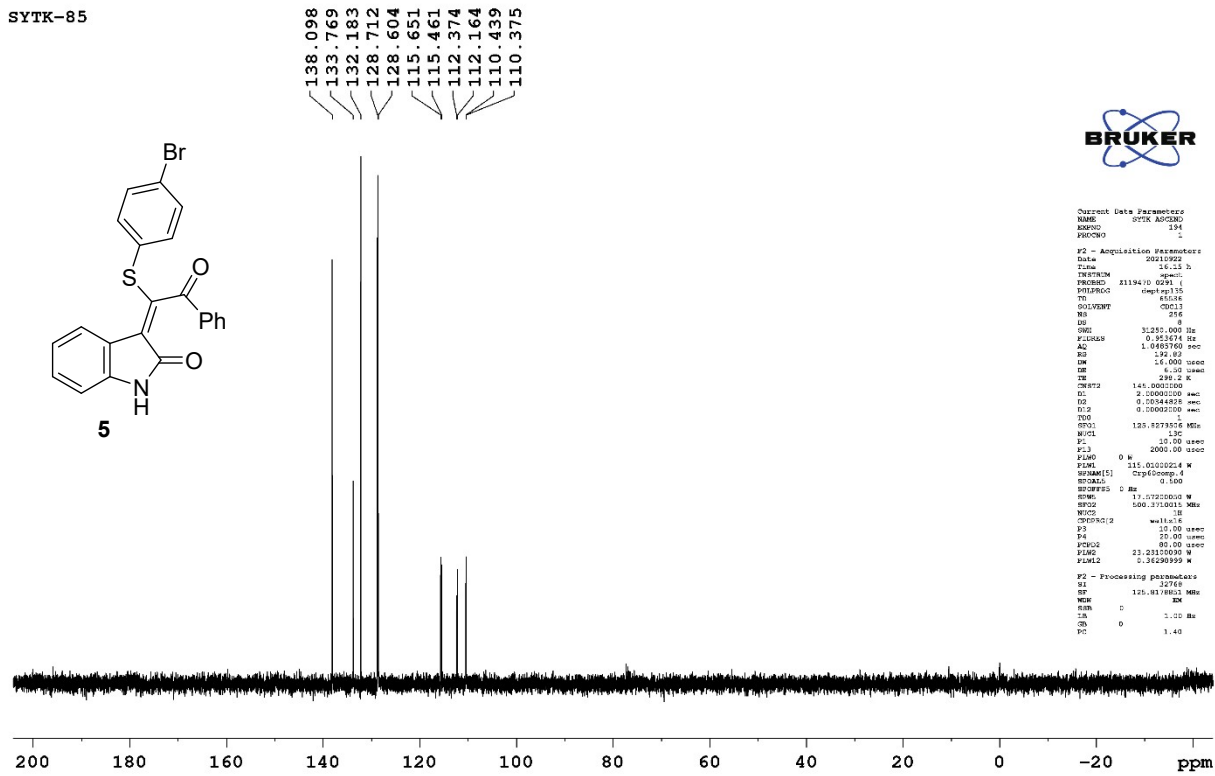
SYTK-85



SYTK-85



SYTK-85



```

Current Date Parameters
NAME: sytk_85
PROCNO: 1
PROC9: 1

F2 - Acquisition Parameters
Date_ 20210922
Time 16:11 h
INSTRUM spect
PROBHD: EBB-5mm
PULPROG zgpg30
TD 65536
SOLVENT cdm3
NS 256
DS 4
SFO1 125.7612500 MHz
F2ACQ99 0.92476 Hz
AQ 1.0493760 sec
RG 328.00
DM 1.6000 usec
DE 6.00 usec
TE 296.2 K
CMT2 145.0000000
IC 2.000000000
IG 0.000000000
D12 0.000000000
TD0 1
SFO1 125.7612500 MHz
NUC1 13
PC 10.00 usec
PC9 2000.00 usec
P1M0 0 W
P1M1 115.0000021 W
SFO1M1 125.7612500 MHz
PC1M1 0.100
SFO1M2 500.1300010 MHz
SFO2 500.1300010 MHz
SFO2M2 500.1300010 MHz
PC2M2 0.100 usec
P4 20.00 usec
SFO4 80.00 usec
P1M2 23.23150000 W
SFO1M2 0.10280000 W

F2 - Processing parameters
SI 32768
SF 125.7612500 MHz
MR 13
AQ 1.0493760
RG 328
DM 1.6000
DE 6.00
TE 296.2
PC 10.00
PC9 2000.00
PC1M1 0.100
PC1M2 23.23150000
PC2M2 0.10280000

```