

AlFe₂O₄@Ph-SO₃H Innovative Nanocatalyst: A Sustainable Approach for the A3 Coupling Reaction in DES for 2-Thioarylbenzoazoles

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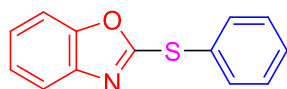
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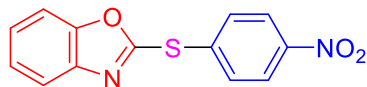
^a Department of Allied Science, Graphic Era Hill University, Dehradun, India.

^b Adjunct Professor, Graphic Era Deemed to be University, Dehradun, Uttarakhand, India.

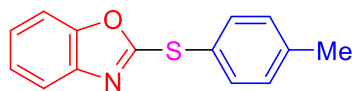
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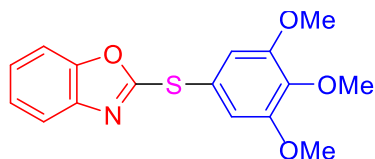
2-(phenylthio)benzo[d]oxazole: Colorless oil, ¹H NMR (400 MHz, CDCl₃) δ 7.76 (d, J = 7.8 Hz, 2H), 7.66 (d, J = 8.0 Hz, 2H), 7.52 (d, J = 8.6 Hz, 2H), 7.47 – 7.42 (m, 3H).; ¹³C NMR (101 MHz, CDCl₃) δ 154.9, 152.0, 141.3, 134.8, 126.8, 126.5, 125.7, 124.3, 123.6, 122.7, 121.0, 109.3.



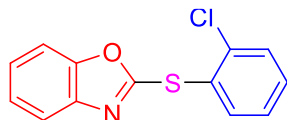
2-(4-nitrophenylthio)benzo[d]oxazole: mp: 93-95 °C, ¹H NMR (400 MHz, CDCl₃) δ 7.91 (d, J = 7.7 Hz, 2H), 7.64 (dd, J = 9.1, 3.5 Hz, 4H), 7.38 (d, J = 8.6 Hz, 2H).; ¹³C NMR (101 MHz, CDCl₃) δ 154.0, 147.6, 143.2, 136.9, 131.1, 124.7, 123.2, 122.0, 121.3, 120.8, 119.8, 119.1, 101.5.



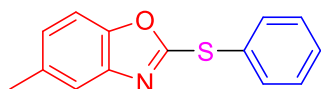
2-(4-methylphenylthio)benzo[d]oxazole: Colorless oil, ¹H NMR (400 MHz, CDCl₃) δ 7.83 (d, J = 7.7 Hz, 2H), 7.65-7.63 (m, 2H), 7.46 (d, J = 8.6 Hz, 2H), 7.34 (d, J = 9.0 Hz, 2H), 2.39 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 155.0, 153.1, 142.8, 137.6, 127.5, 126.0, 124.3, 123.7, 122.6, 121.0, 119.8, 108.5, 20.1.



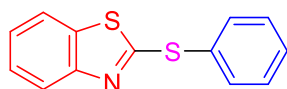
2-((3,4,5-trimethoxyphenyl)thio)benzo[d]oxazole: mp: 129-131 °C, ^1H NMR (400 MHz, CDCl_3) δ 7.71 (d, J = 8.0 Hz, 2H), 7.43 (d, J = 8.6 Hz, 2H), 7.12 (s, 2H), 3.85 (s, 6H), 3.71 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 154.3, 151.9, 142.7, 134.1, 130.7, 129.8, 128.4, 127.4, 119.7, 112.6, 61.9, 55.4.



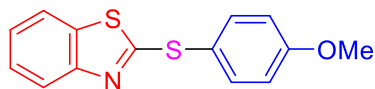
2-((2-chlorophenyl)thio)benzo[d]oxazole: mp: 46-48 °C, ^1H NMR (400 MHz, CDCl_3) δ 7.81 (d, J = 7.8 Hz, 1H), 7.75 (d, J = 7.7 Hz, 2H), 7.68 (d, J = 8.0 Hz, 2H), 7.61 (d, J = 7.6 Hz, 1H), 7.33 – 7.30 (m, 1H), 7.11 (t, J = 7.7 Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 145.1, 152.6, 143.2, 134.7, 132.8, 131.5, 129.0, 128.6, 126.4, 119.8, 112.5.



5-methyl-2-(phenylthio)benzo[d]oxazole: mp: 48-50 °C, ^1H NMR (400 MHz, CDCl_3) δ 7.88 (d, J = 7.4 Hz, 1H), 7.71 (s, 1H), 7.69 (d, J = 7.6 Hz, 1H), 7.54 (d, J = 8.6 Hz, 2H), 7.30 (d, J = 7.7 Hz, 2H), 7.16 – 7.09 (m, 1H), 2.61 (s, 3H).; ^{13}C NMR (101 MHz, CDCl_3) δ 153.2, 138.9, 131.5, 126.7, 125.1, 123.6, 120.1, 100.7, 21.0.

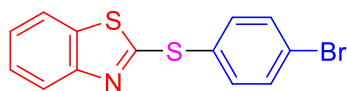


2-(phenylthio)benzo[d]thiazole: mp: 33-35 °C, ^1H NMR (400 MHz, CDCl_3) δ 8.03 (d, J = 8.0 Hz, 2H), 7.91 (d, J = 7.7 Hz, 2H), 7.37 (t, J = 8.6 Hz, 2H), 7.20 (d, J = 7.8 Hz, 2H), 7.08-7.04 (m, 1H); ^{13}C NMR (126 MHz, CDCl_3) δ 163.2, 156.7, 138.0, 133.9, 127.6, 126.5, 124.3, 123.7, 122.1, 121.0, 120.5.

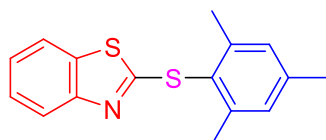


2-((4-methoxyphenyl)thio)benzo[d]thiazole: mp: 55-57 °C, ^1H NMR (400 MHz, CDCl_3) δ 7.34 (d, J = 7.4 Hz, 1H), 8.09 (d, J = 7.5 Hz, 1H), 7.54-7.48 (m, 2H), 7.37–7.33 (m, 2H), 7.04 (d, J = 7.0 Hz, 2H), , 3.83

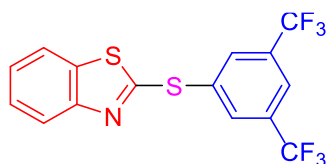
(s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 163.8, 156.0, 152.1, 138.7, 128.9, 127.4, 126.1, 125.7, 124.3, 113.1, 54.9.



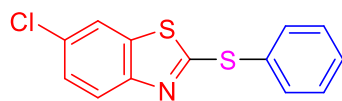
2-((4-bromophenyl)thio)benzo[d]thiazole: mp: 50-52 °C, ^1H NMR (400 MHz, CDCl_3) δ 8.06 (d, J = 7.7 Hz, 1H), 7.81 (d, J = 7.6 Hz, 1H), 7.53 (d, J = 8.0 Hz, 2H), 7.38-7.30 (m, 4H); ^{13}C NMR (101 MHz, CDCl_3) δ 167.3, 156.1, 134.7, 129.8, 128.4, 127.1, 124.9, 121.5, 120.3..



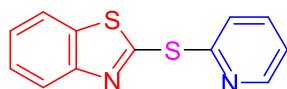
2-(mesitylthio)benzo[d]thiazole: Colorless oil, ^1H NMR (400 MHz, CDCl_3) δ 8.11 (d, J = 8.0 Hz, 1H), 8.01 (d, J = 8.4 Hz, 1H), 7.63-7.55 (m, 2H), 7.01 (s, 2H), 2.42 (s, 6H), 2.18 (s 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 163.1, 152.8, 138.7, 135.9, 131.0, 124.7, 123.1, 122.6, 121.0, 120.3, 22.1 19.8..



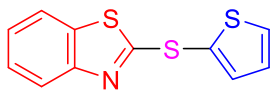
2-((3,5-bis(trifluoromethyl)phenyl)thio)benzo[d]thiazole: Colorless oil, ^1H NMR (400 MHz, CDCl_3) δ 8.21 (d, J = 7.4 Hz, 1H), 8.07 (dd, J = 8.9, 2.3 Hz, 1H), 7.73 (s, 1H), 7.46-7.58 (m, 2H), 7.43 (s, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.5, 154.8, 137.4, 129.8, 128.1, 127.3, 126.0, 125.3, 124.7, 123.1, 120.7.



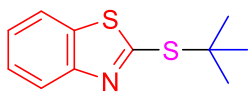
6-chloro-2-(phenylthio)benzo[d]thiazole: mp: 69-71 °C, ^1H NMR (400 MHz, CDCl_3) δ 8.10 (s, 1H), 7.83 (d, J = 7.8 Hz, 1H), 7.64 (d, J = 8.6 Hz, 1H), 7.33 (d, J = 8.0 Hz, 2H), 7.25-7.19 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 163.2, 153.1, 138.6, 126.5, 125.3, 124.6, 123.0, 121.8.



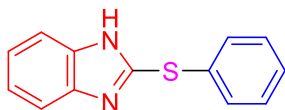
2-(pyridin-2-ylthio)benzo[d]thiazole: mp: 66-68 °C, ^1H NMR (400 MHz, CDCl_3) δ 8.41 (d, J = 8.0 Hz, 1H), 8.23 (d, J = 7.5 Hz, 1H), 8.03 (d, J = 8.1 Hz, 1H), 7.46 (t, J = 8.1 Hz, 1H), 7.21–7.18 (m, 2H), 7.04–7.00 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 161.0, 154.3, 153.9, 149.8, 134.9, 133.6, 125.4, 123.6, 121.4.



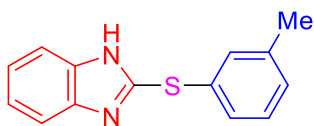
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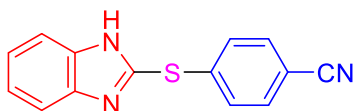
2-(tert-butylthio)benzo[d]thiazole: Colorless oil, ^1H NMR (400 MHz, CDCl_3) δ 7.89 (d, J = 8.4 Hz, 1H), 7.76 (d, J = 7.9 Hz, 1H), 7.43–7.37 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 164.1, 155.8, 132.9, 126.3, 125.1, 124.7, 122.0, 45.6, 30.7.



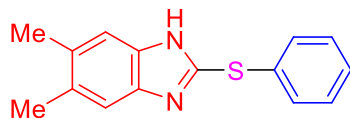
2-(phenylthio)-1H-benzo[d]imidazole : mp: 202-204 °C, ^1H NMR (400 MHz, CDCl_3) δ 9.76 (s, 1H), 7.98 (d, J = 8.4 Hz, 2H), 7.43 (d, J = 8.0 Hz, 2H), 7.36 (t, J = 7.6 Hz, 2H), 7.27–7.20 (m, 1H), 7.04–6.97 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 141.9, 139.5, 136.7, 129.8, 128.1, 126.7, 116.5.



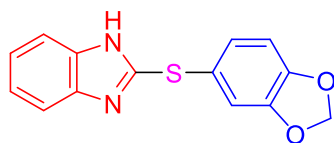
2-(m-tolylthio)-1H-benzo[d]imidazole: Colorless oil, ^1H NMR (400 MHz, CDCl_3) δ 9.80 (s, 1H), 7.83 (d, J = 8.6 Hz, 2H), 7.66 (dd, J = 8.8, 3.1 Hz, 1H), 7.48–7.43 (m, 3H), 7.32 (s, 1H), 7.11 (dd, J = 9.2, 1.4 Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 139.0, 131.6, 123.1, 122.6, 121.9, 120.5, 120.3, 119.8, 114.3, 114.0, 21.5.



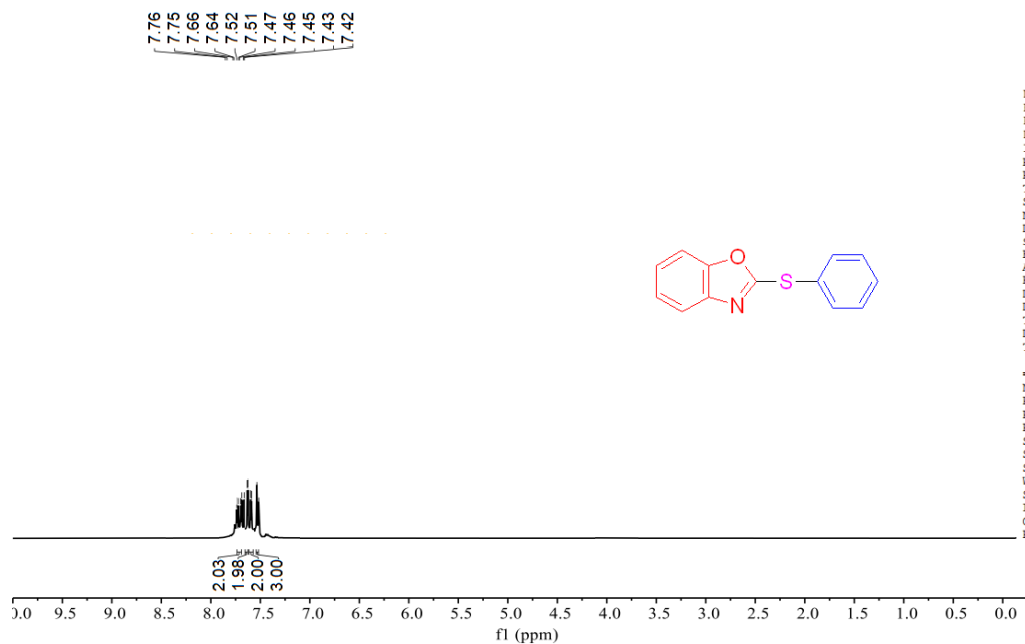
4-((1*H*-benzo[*d*]imidazol-2-yl)thio)benzonitrile: mp: 178-180 °C, ¹H NMR (400 MHz, CDCl₃) δ 9.82 (s, 1H), 7.75 (d, *J* = 7.4 Hz, 2H), 7.62 (d, *J* = 7.7 Hz, 2H), 7.41 (d, *J* = 8.6 Hz, 2H), 7.35-7.29 (m, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 140.7, 138.5, 137.2, 133.0, 131.4, 121.3, 119.5, 117.0.



5,6-dimethyl-2-(phenylthio)-1*H*-benzo[*d*]imidazole: mp: 167-169 °C, ¹H NMR (400 MHz, CDCl₃) δ 9.79 (s, 1H), 7.85-7.81 (m, 3H), 7.63 (dd, *J* = 8.7, 3.6 Hz, 2H), 7.50 (s, 2H), 2.34 (s, 6H); ¹³C NMR (101 MHz, CDCl₃) δ 138.7, 130.6, 130.3, 129.8, 129.2, 128.0, 127.4, 120.4, 120.0, 116.9.

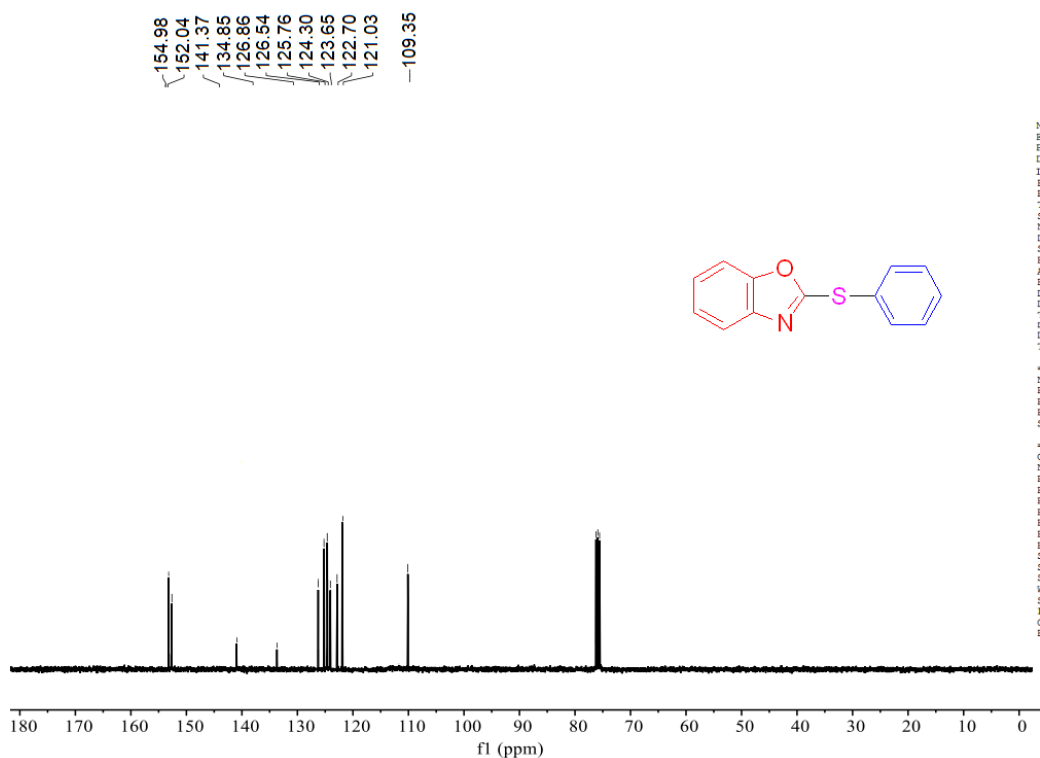


2-(benzo[*d*][1,3]dioxol-5-ylthio)-1*H*-benzo[*d*]imidazole: mp: 183-185 °C, ¹H NMR (400 MHz, CDCl₃) δ 9.74 (s, 1H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.66-7.61 (m, 2H), 7.37-7.32 (m, 1H), 7.16 (s, 1H), 7.09 (d, *J* = 8.0 Hz, 1H), 6.07 (s, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 150.1, 138.7, 131.7, 129.8, 124.8, 123.1, 122.0, 121.5, 120.7, 116.7, 101.3.



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D1 6.0000000 sec
TD0 1

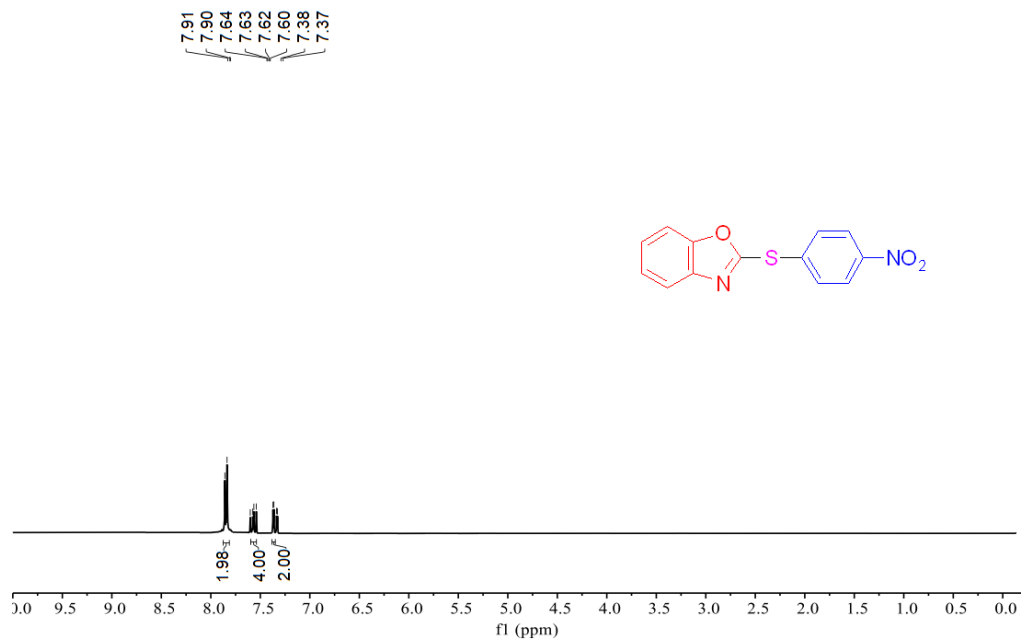
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SF 400.2200000 MHz
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SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME UN
EXPNO 435
PROCNO 2
Date_ 20240908
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TD0 1

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PL13 17.90 dB
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PL12W 0.28722104 W
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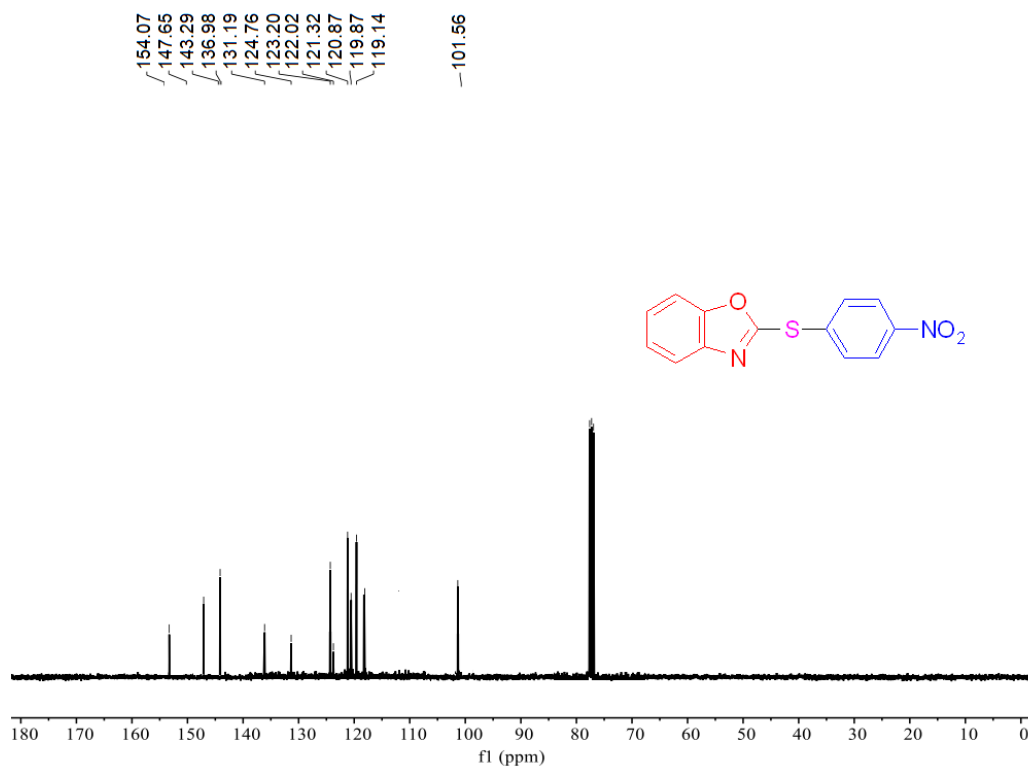


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AQ         4.089496 sec
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TE         293.2 K
D1         6.0000000 sec
D11        1
TD0        1
  
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===== CHANNEL f1 =====
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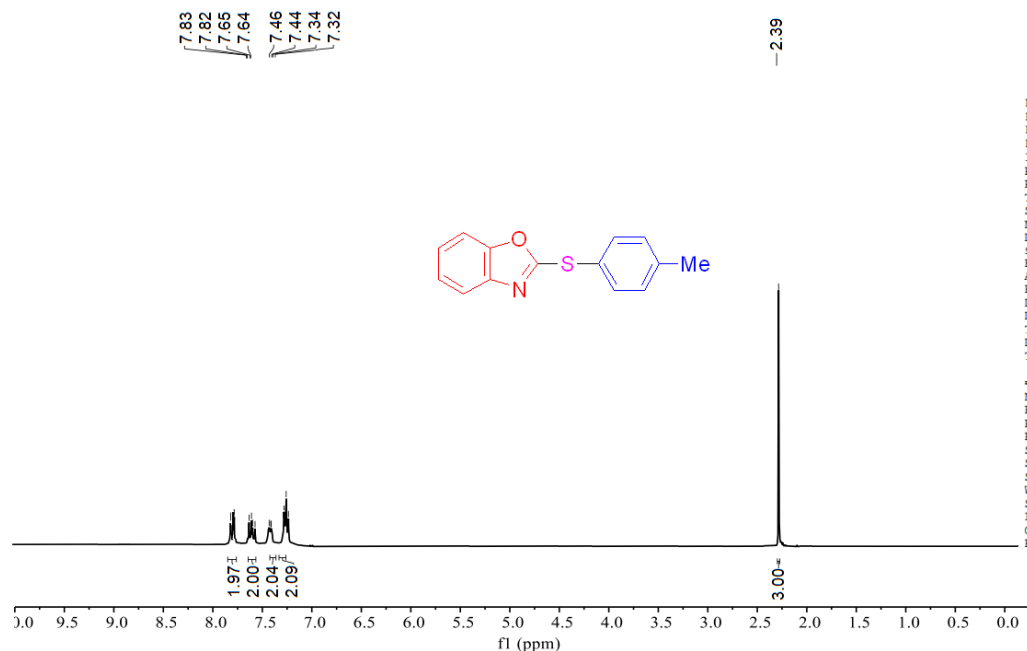
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RG         2050
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TE         293.4 K
D1         3.0000000 sec
D11        1
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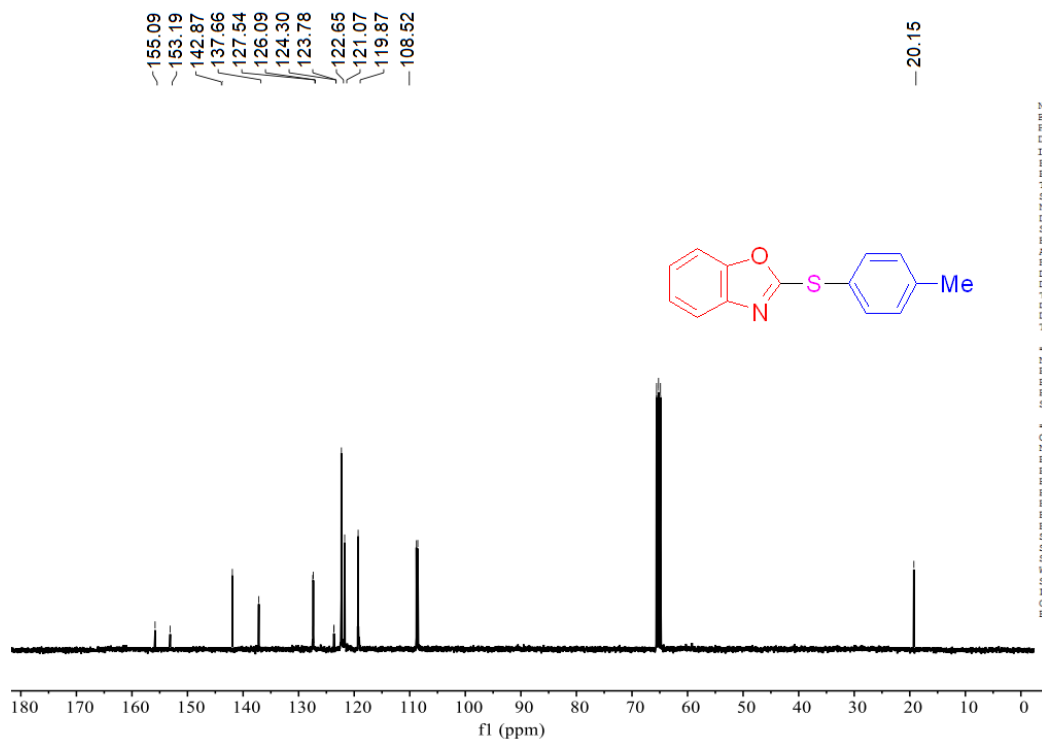
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PL12W     6.28722104 W
PL13W     0.12139934 W
SFO2      400.2216009 MHz
SI        32768
SF        100.6353990 MHz
WDW       EM
SSB       0
LB        1.00 Hz
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PC         1.40
  
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NAME UN
EXPNO 426
PROCNO 1
Date_ 20240908
INSTRUM spect
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PULPROG zg30
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SOLVENT CDCl₃
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
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RG 406
DW 62.400 usec
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TE 293.2 K
D1 6.0000000 sec
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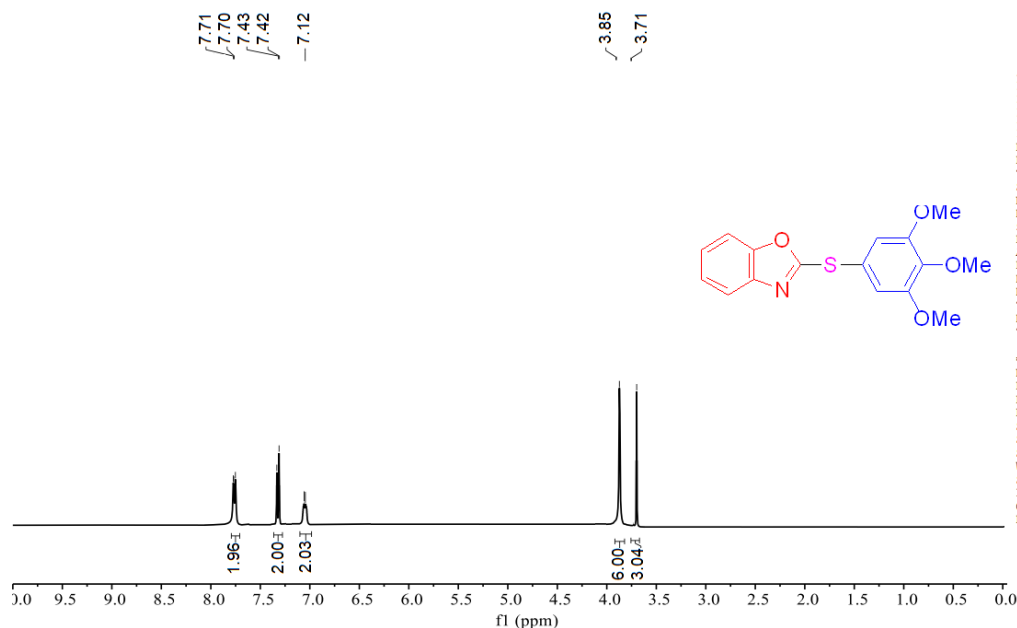
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PL1 -2.00 dB
PL1W 11.86359406 W
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SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME UN
EXPNO 435
PROCNO 2
Date_ 20240908
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT CDCl₃
NS 31
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FIDRES 0.385323 Hz
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RG 2050
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TE 293.4 K
D1 3.0000000 sec
D11 0.0300000 sec
TD0 1

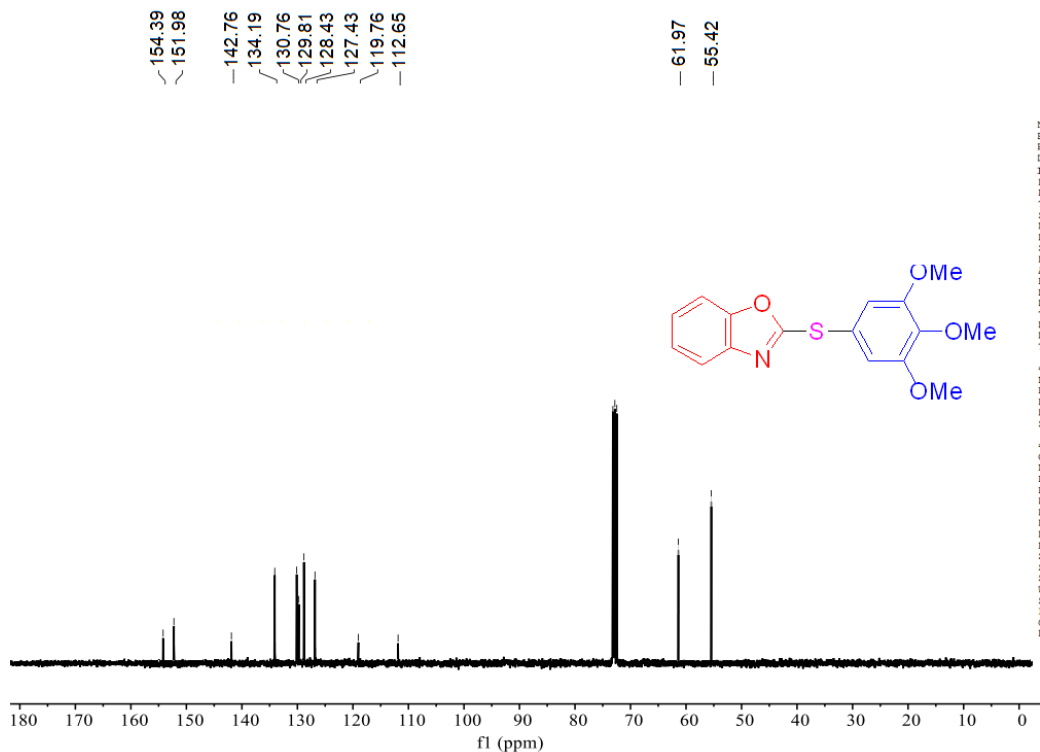
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PL1W 42.02801895 W
SFO1 100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



NAME UN
EXPNO 426
PROCNO 1
Date 20240912
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 6.0000000 sec
D10 1

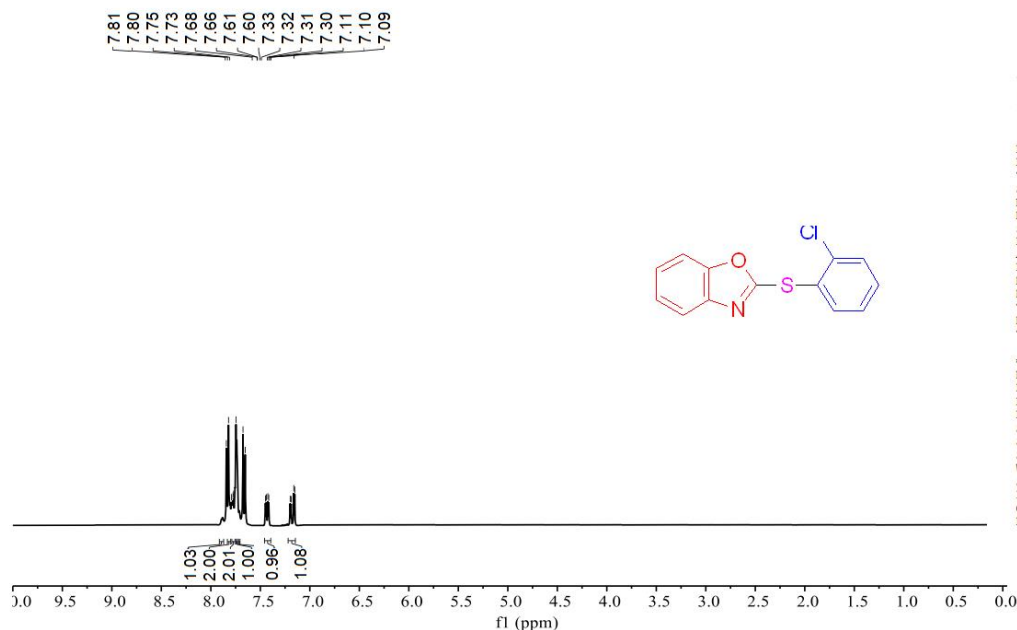
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME UN
EXPNO 435
PROCNO 2
Date 20240912
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT CDCl₃
NS 31
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2376629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 293.4 K
D1 3.0000000 sec
D11 6.0300000 sec
D10 1

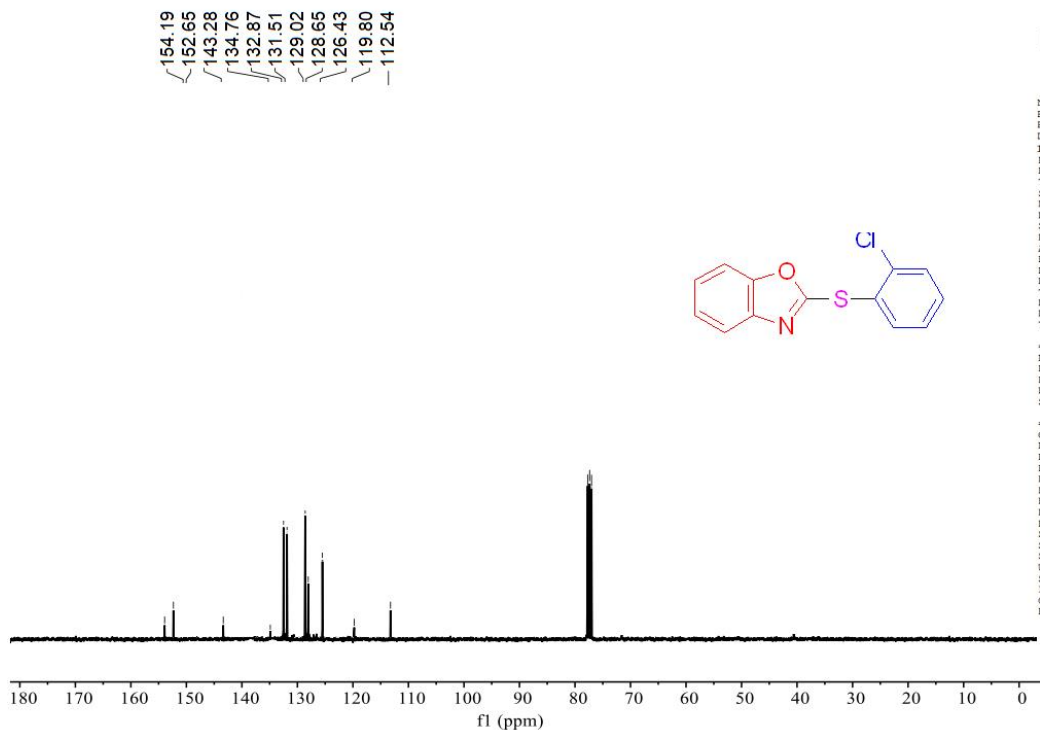
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



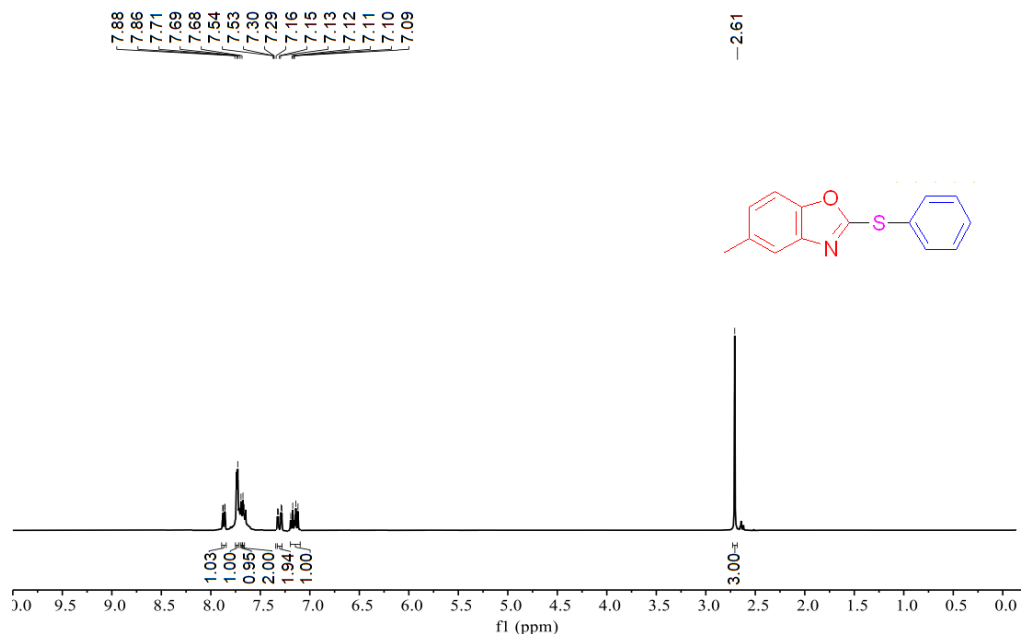
NAME UN
EXPNO 426
PROCNO 1
Date_ 20240912
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 6.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME UN
EXPNO 435
PROCNO 2
Date_ 20240912
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT CDCl₃
NS 31
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 293.2 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL12W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

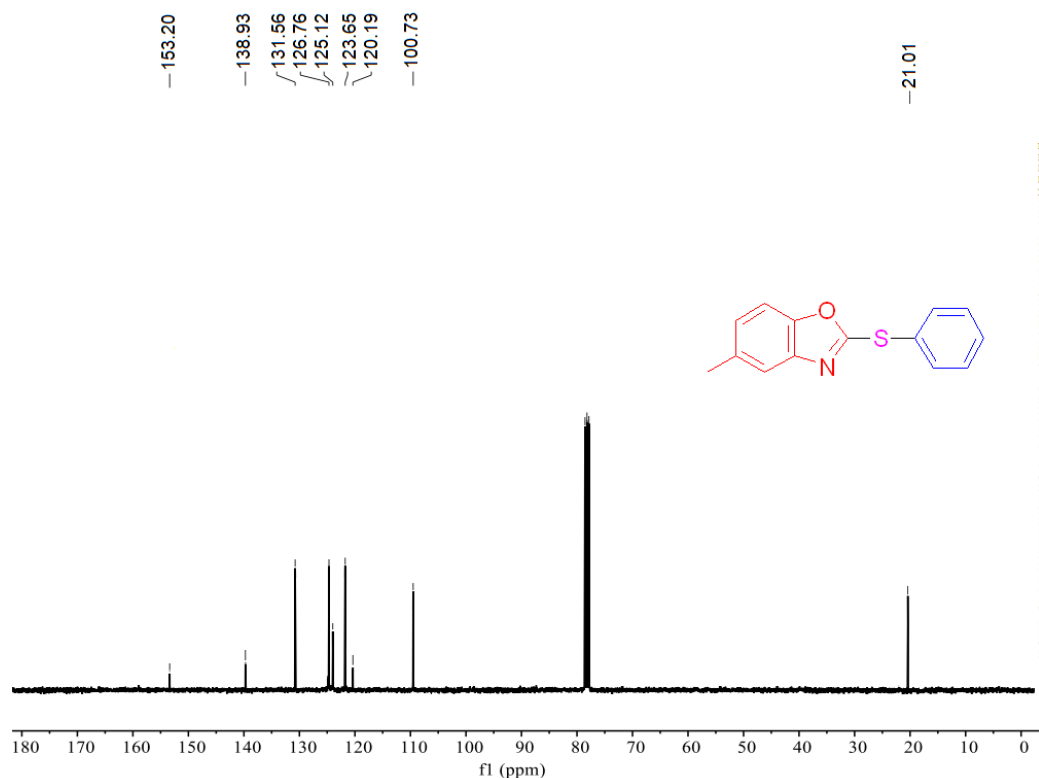


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NAME      UN
EXPNO     425
PROCNO    1
Date_     20240908
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zg30
TD         65536
SOLVENT    CDCl3
NS         24
DS         0
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0894968 sec
RG         406
DW         62.400 usec
DE         6.50 usec
TE         293.2 K
D1         6.00000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1       1H
P1         14.00 usec
PL1        -2.00 dB
PL1W       11.86359406 W
SFO1       400.2236020 MHz
SI         32768
SF         400.2200000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



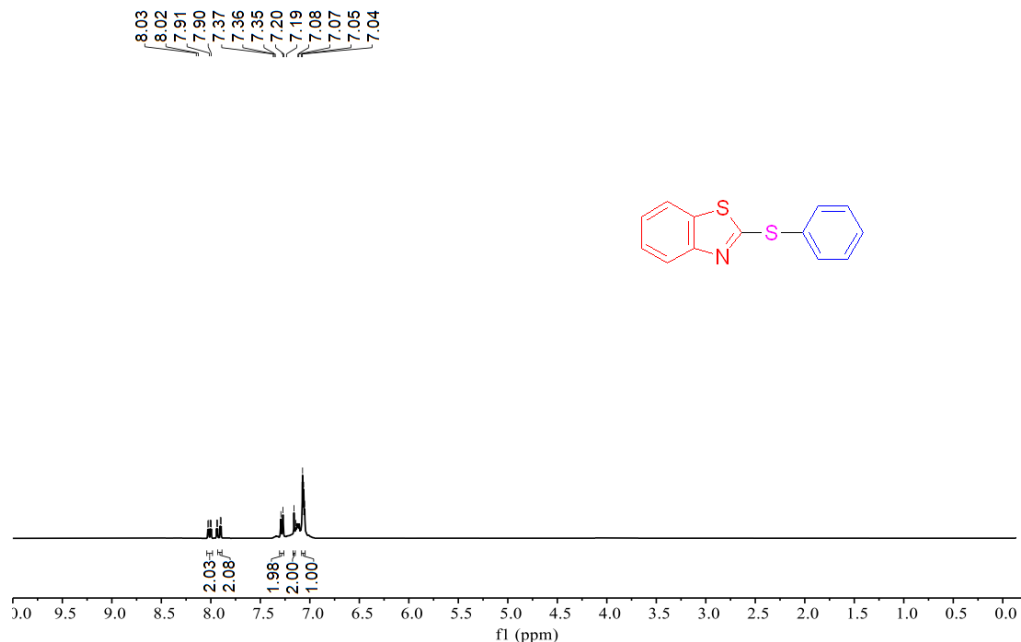
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NAME      UN
EXPNO     435
PROCNO    2
Date_     20240908
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zgpg
TD         65536
SOLVENT    CDCl3
NS         31
DS         0
SWH        25252.525 Hz
FIDRES     0.385323 Hz
AQ         1.2976629 sec
RG         2050
DW         19.800 usec
DE         6.50 usec
TE         293.2 K
D1         3.00000000 sec
D11        0.03000000 sec
TD0        1
  
```

```

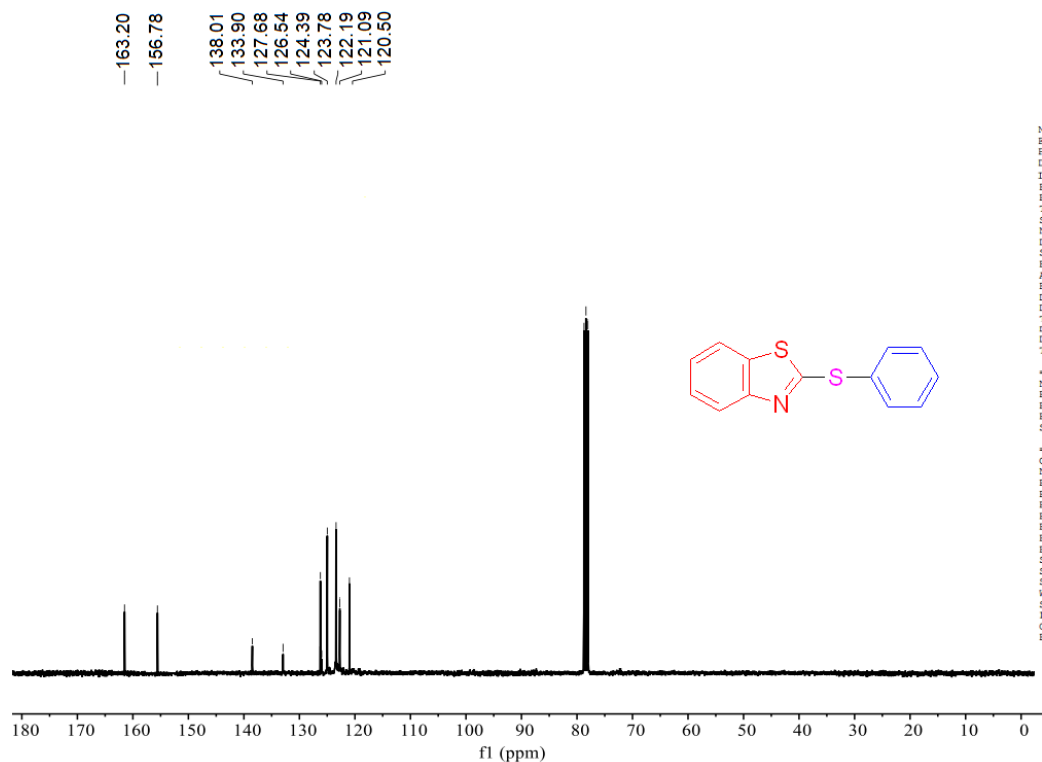
===== CHANNEL f1 =====
NUC1       13C
P1         9.00 usec
PL1        -0.90 dB
PL1W       42.02801895 W
SFO1       100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -2.00 dB
PL12       14.16 dB
PL13       17.90 dB
PL1W       11.86359406 W
PL12W      6.28722104 W
PL13W      6.12139934 W
SFO2       400.2216009 MHz
SI         32768
SF         100.6353990 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



NAME UN
EXPNO 425
PROCNO 1
Date_ 20240908
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894968 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 6.00000000 sec
TD0 1

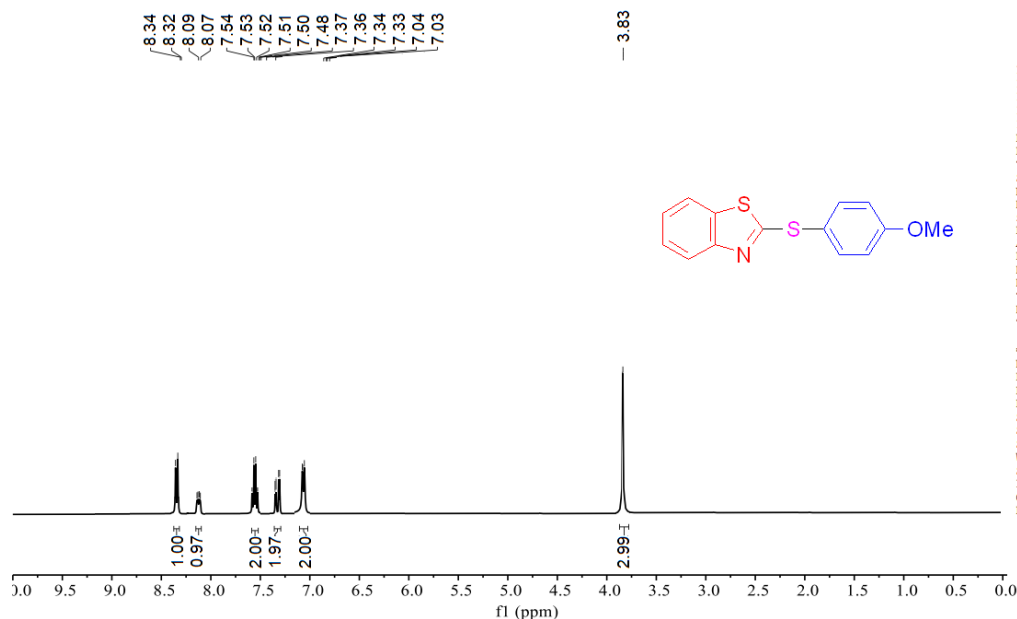
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359405 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME UN
EXPNO 435
PROCNO 2
Date_ 20240908
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT CDCl₃
NS 31
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 293.4 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1

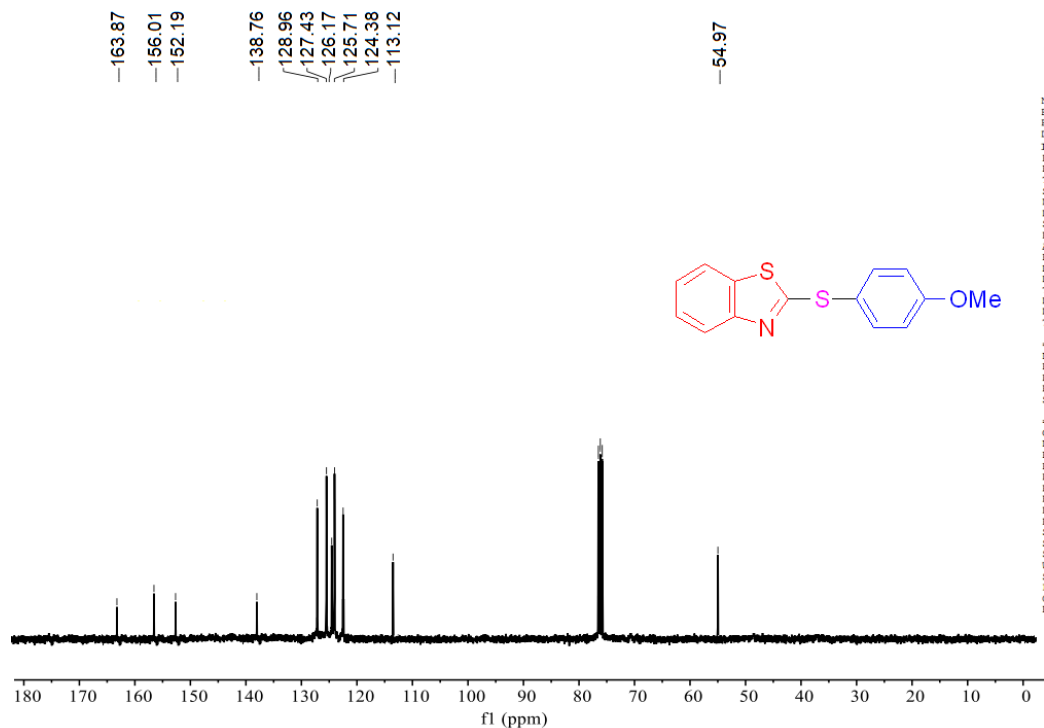
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL1W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



NAME UN
EXPNO 426
PROCNO 1
Date_ 20240912
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 6.00000000 sec
TD0 1

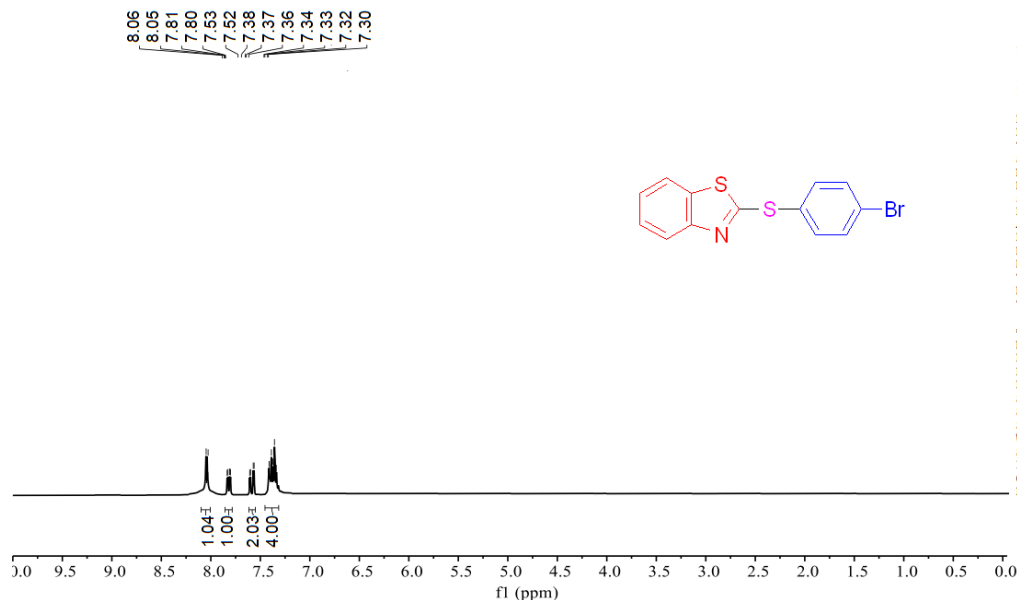
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME UN
EXPNO 435
PROCNO 2
Date_ 20240912
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT CDCl₃
NS 31
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 293.4 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1

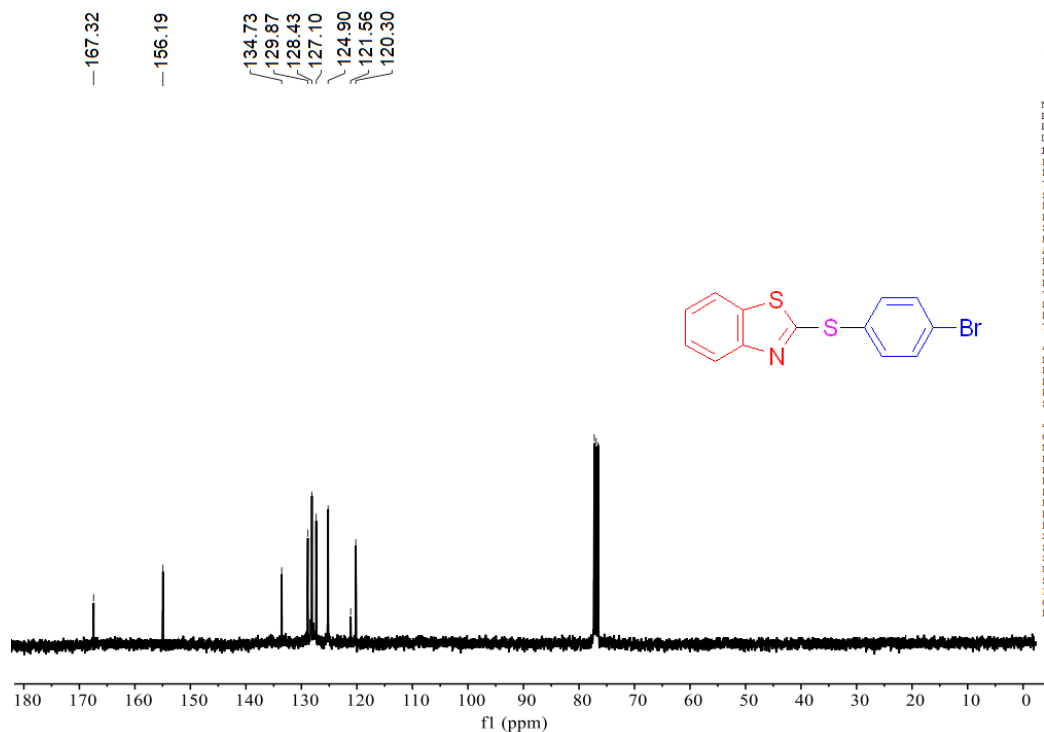
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



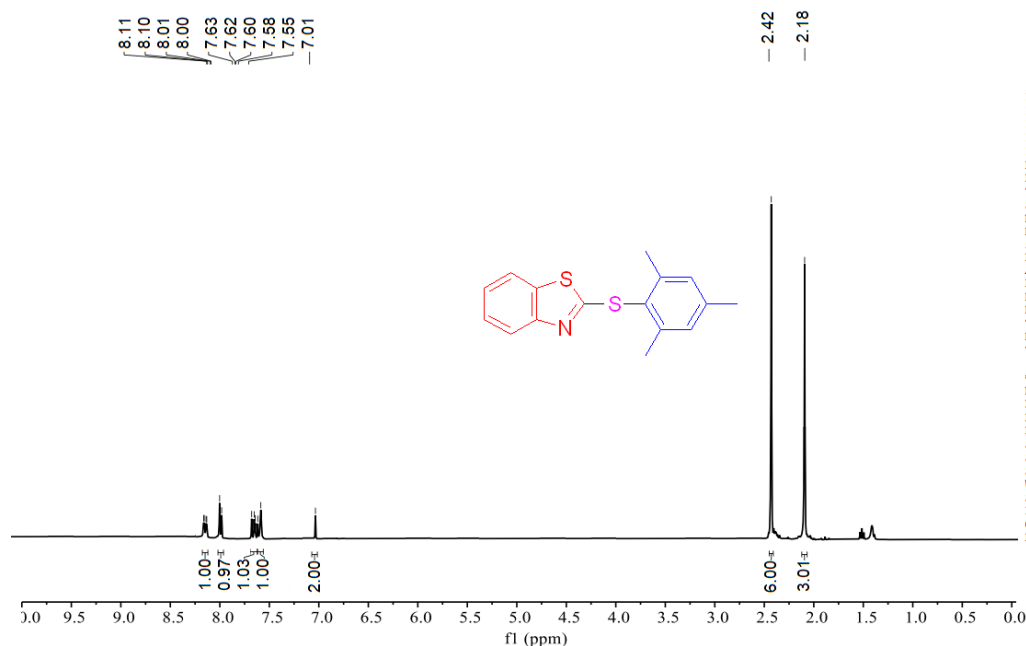
NAME UN
EXPNO 426
PROCNO 1
Date_ 20240912
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 6.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



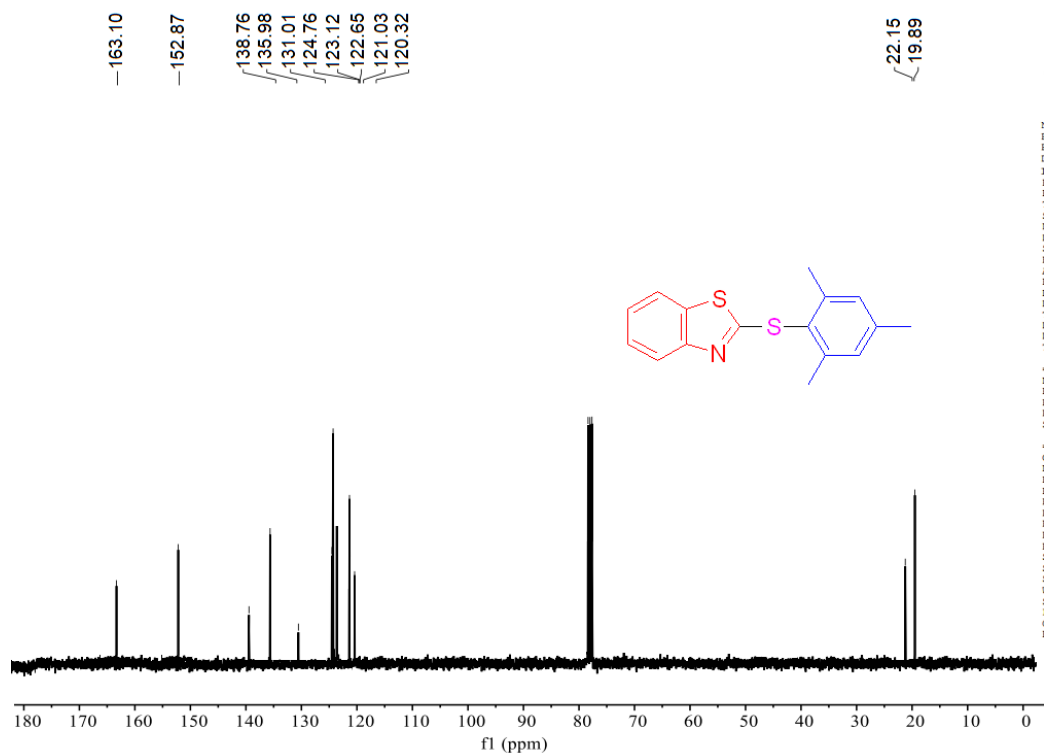
NAME UN
EXPNO 435
PROCNO 2
Date_ 20240912
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT CDCl₃
NS 31
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 293.4 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL1W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



NAME UN
EXPNO 426
PROCNO 1
Date_ 20240912
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 6.0000000 sec
TD0 1

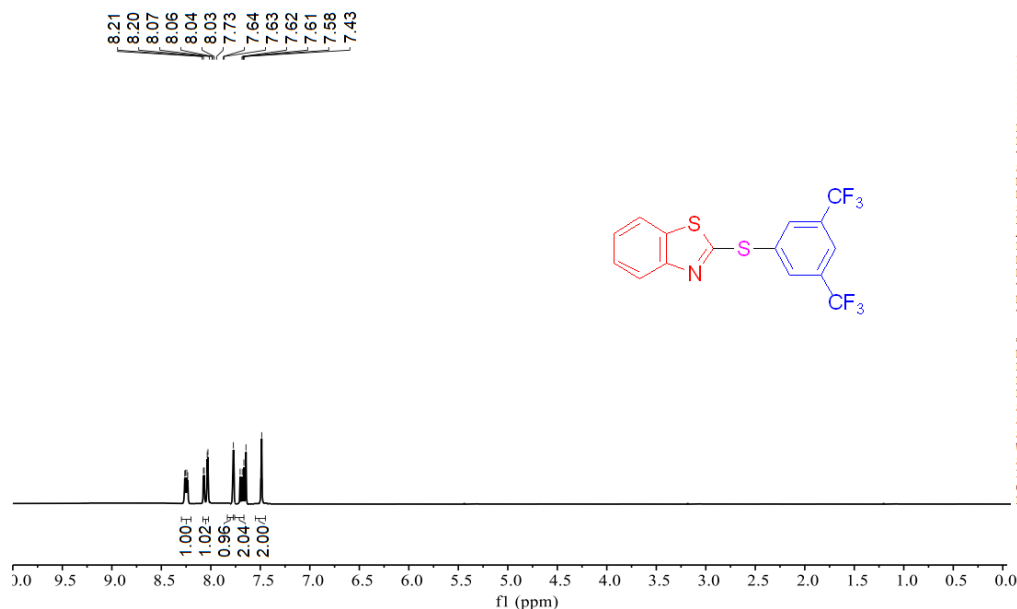
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME UN
EXPNO 435
PROCNO 2
Date_ 20240912
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT CDCl₃
NS 31
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 293.4 K
D1 3.0000000 sec
D11 0.0300000 sec
TD0 1

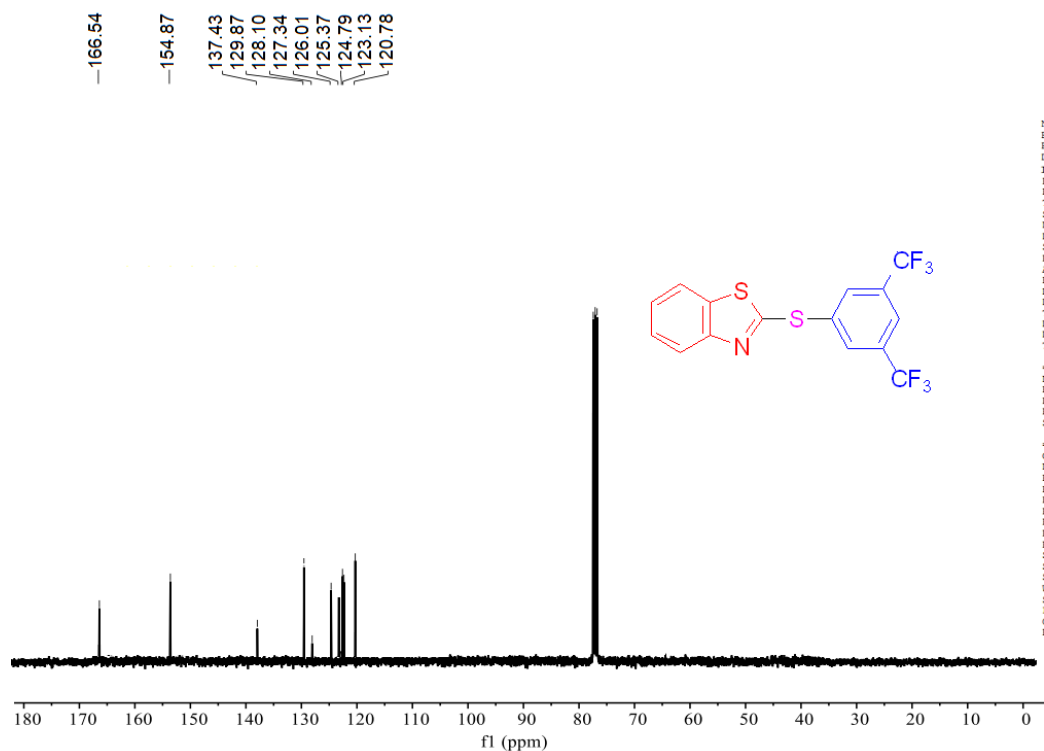
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 6.28722104 W
PL13W 6.12139834 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



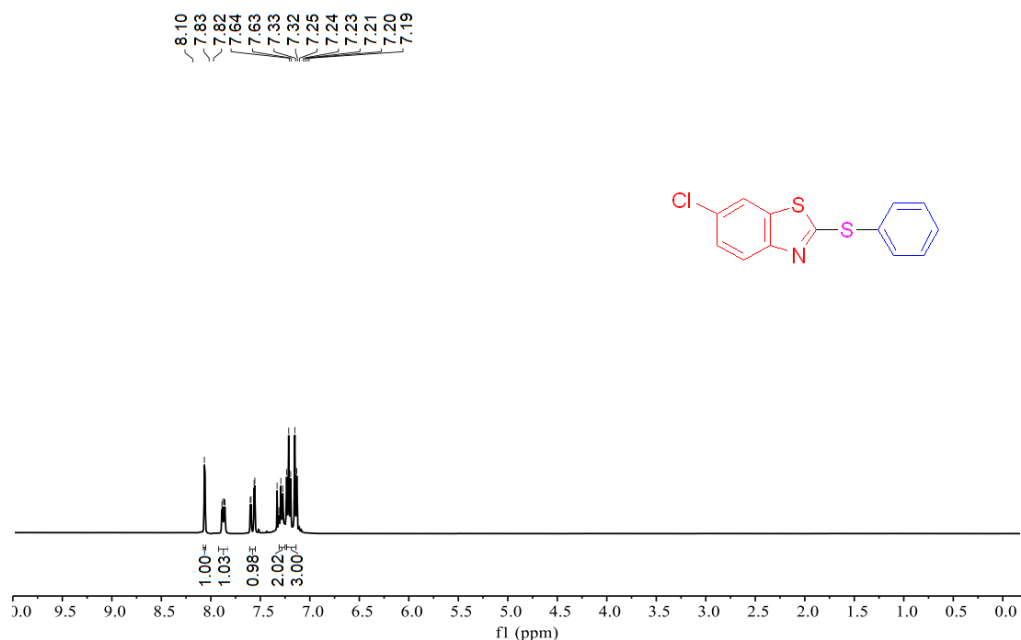
NAME UN
EXPNO 426
PROCNO 1
Date_ 20240912
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 6.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



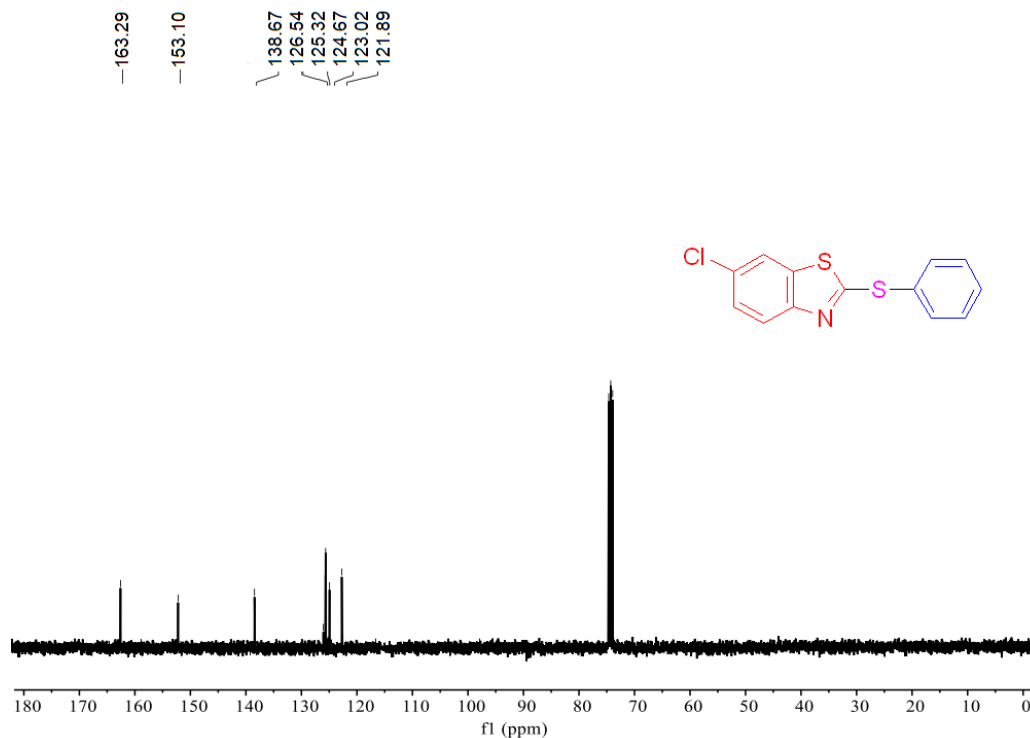
NAME UN
EXPNO 435
PROCNO 2
Date_ 20240912
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT CDCl₃
NS 31
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 293.4 K
D1 3.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL1W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



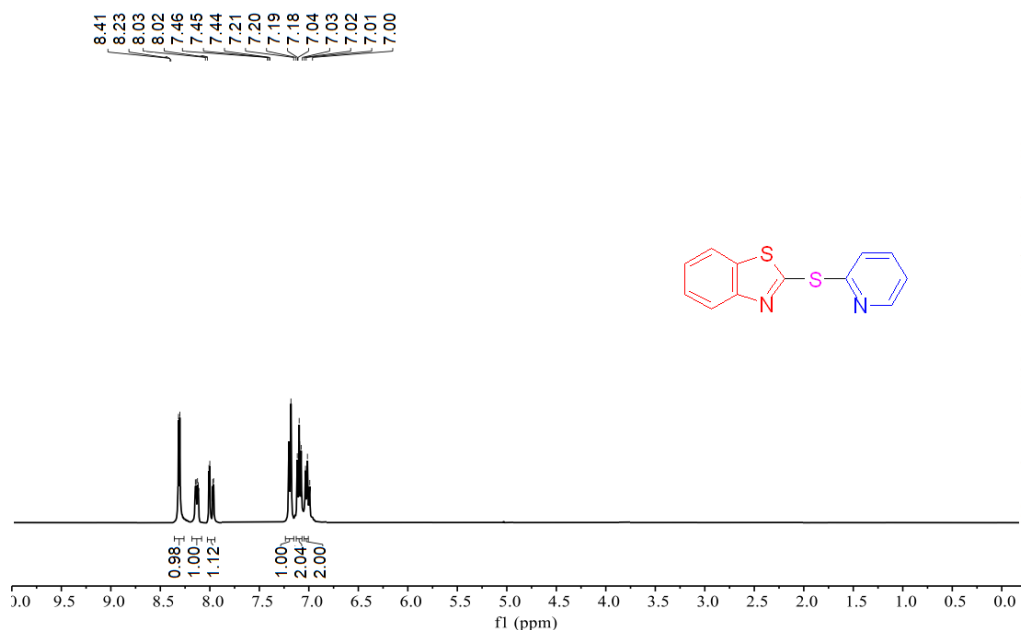
NAME UN
EXPNO 426
PROCNO 1
Date_ 20240915
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.089496 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 6.0000000 sec
D10 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



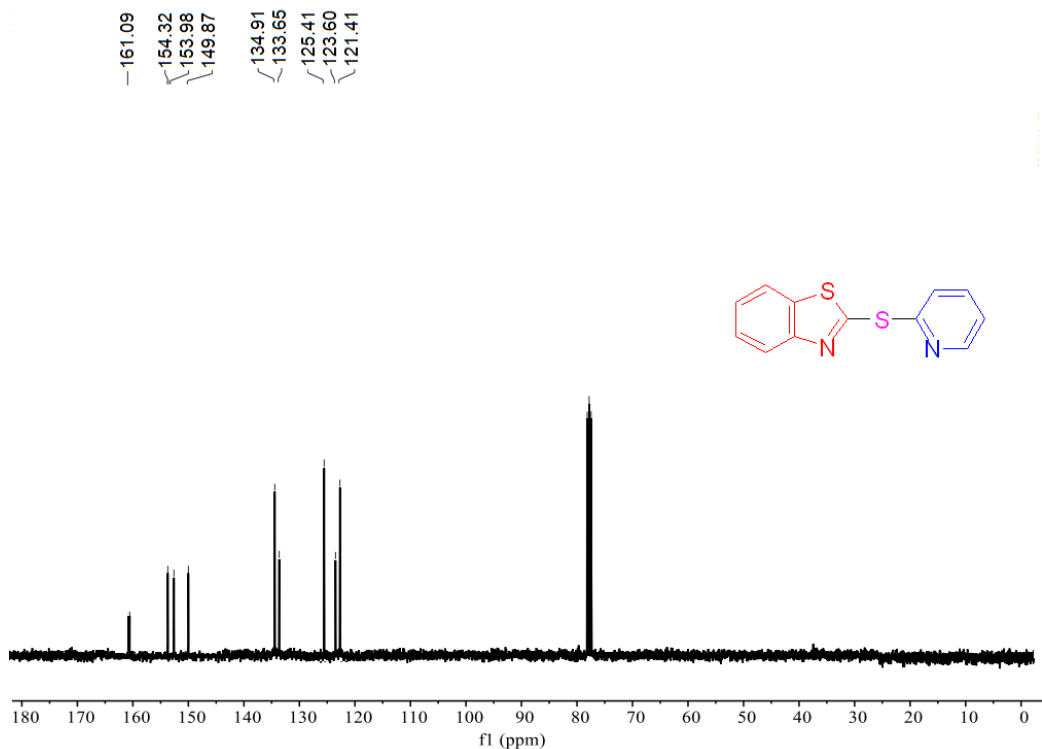
NAME UN
EXPNO 426
PROCNO 2
Date_ 20240915
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT CDCl₃
NS 31
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 293.4 K
D1 3.0000000 sec
D11 0.0300000 sec
D10 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



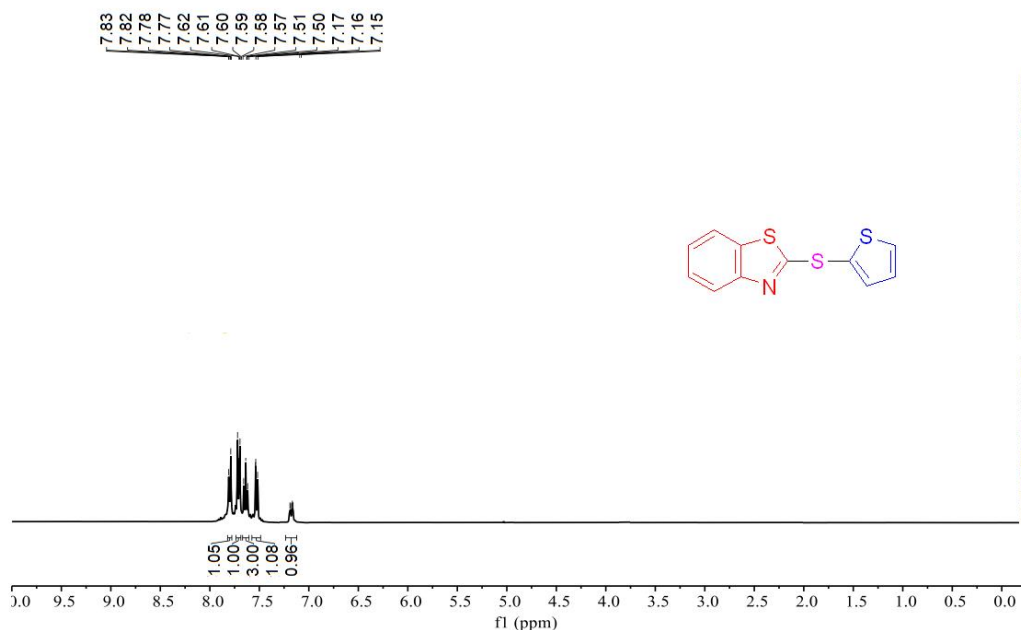
NAME UN
EXPNO 426
PROCNO 1
Date_ 20240915
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 6.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



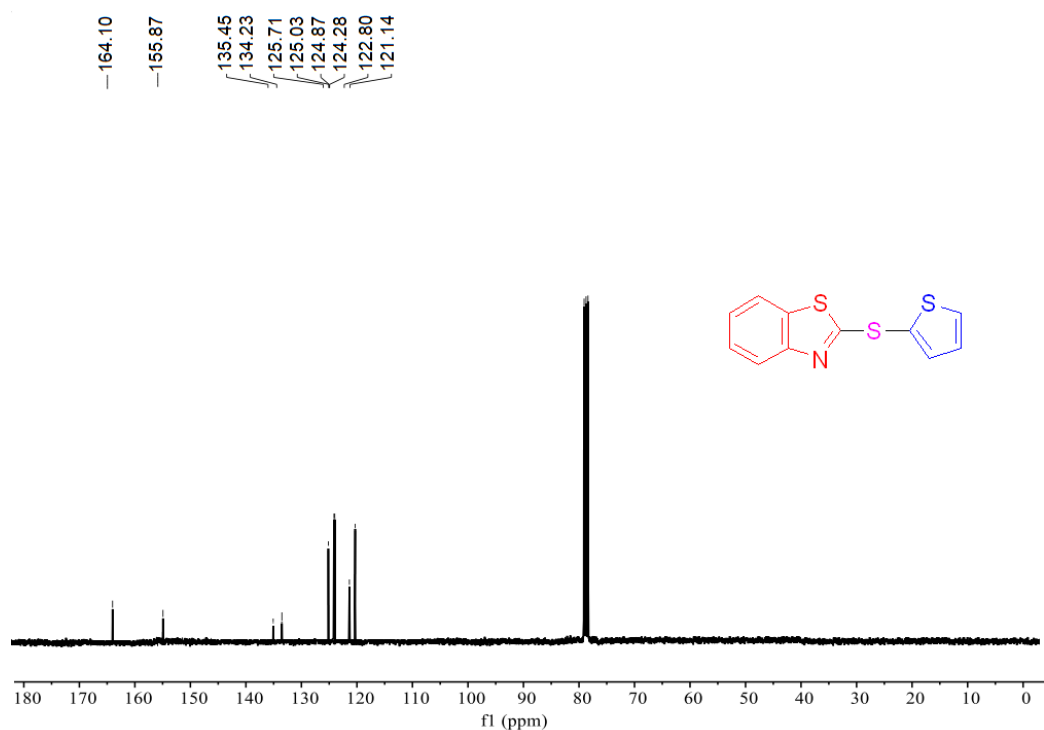
NAME UN
EXPNO 436
PROCNO 2
Date_ 20240915
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT CDCl₃
NS 31
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 293.4 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6478784 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



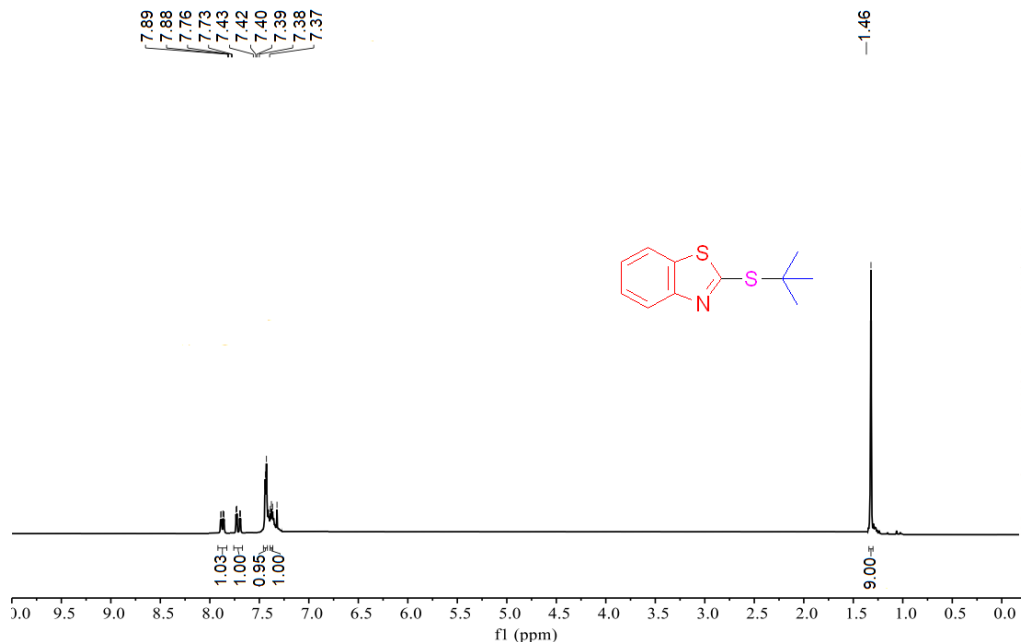
NAME UN
EXPNO 426
PROCNO 1
Date_ 20240915
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.089496 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 6.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



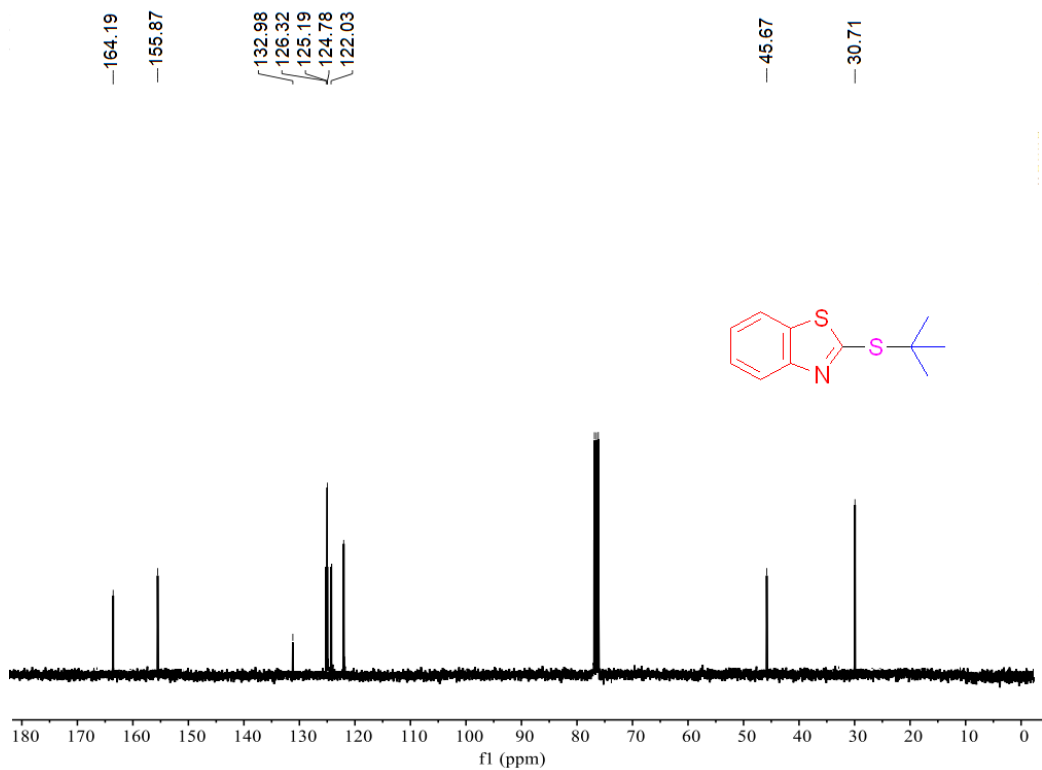
NAME UN
EXPNO 436
PROCNO 2
Date_ 20240915
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT CDCl₃
NS 31
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 293.2 K
D1 3.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6478784 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



NAME UN
EXPNO 426
PROCNO 1
Date_ 20240915
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.089496 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 6.0000000 sec
TD0 1

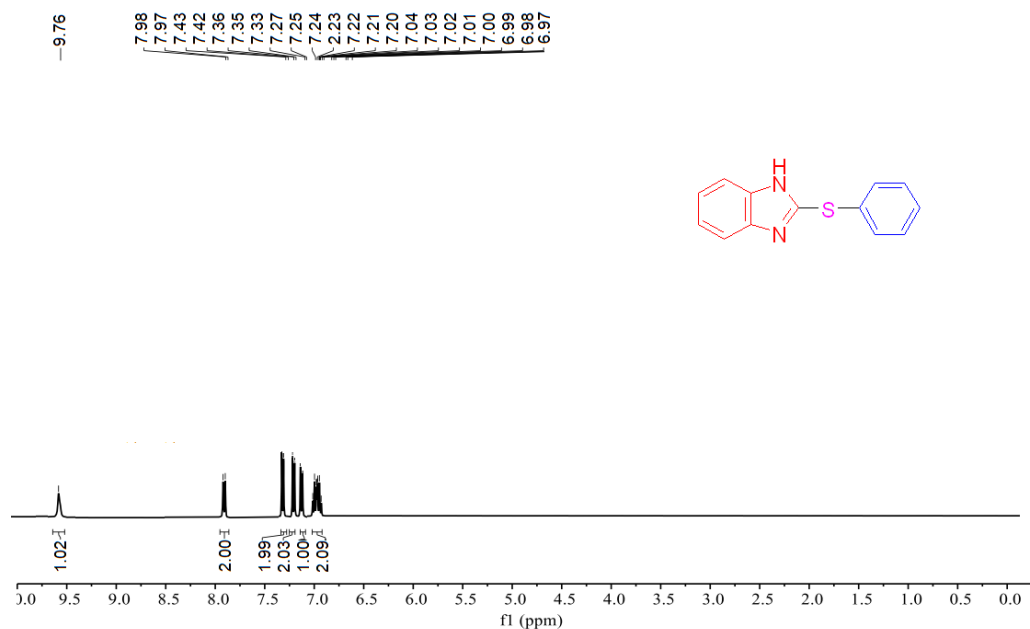
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME UN
EXPNO 436
PROCNO 2
Date_ 20240915
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT CDCl₃
NS 31
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 293.2 K
D1 3.0000000 sec
D11 0.0300000 sec
TD0 1

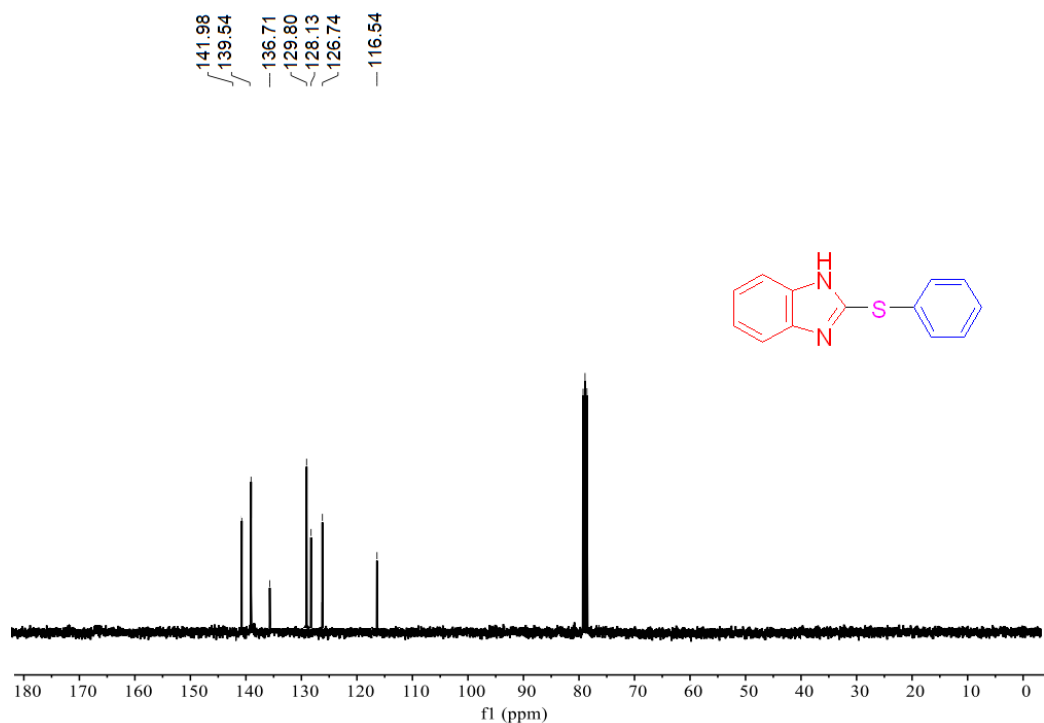
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



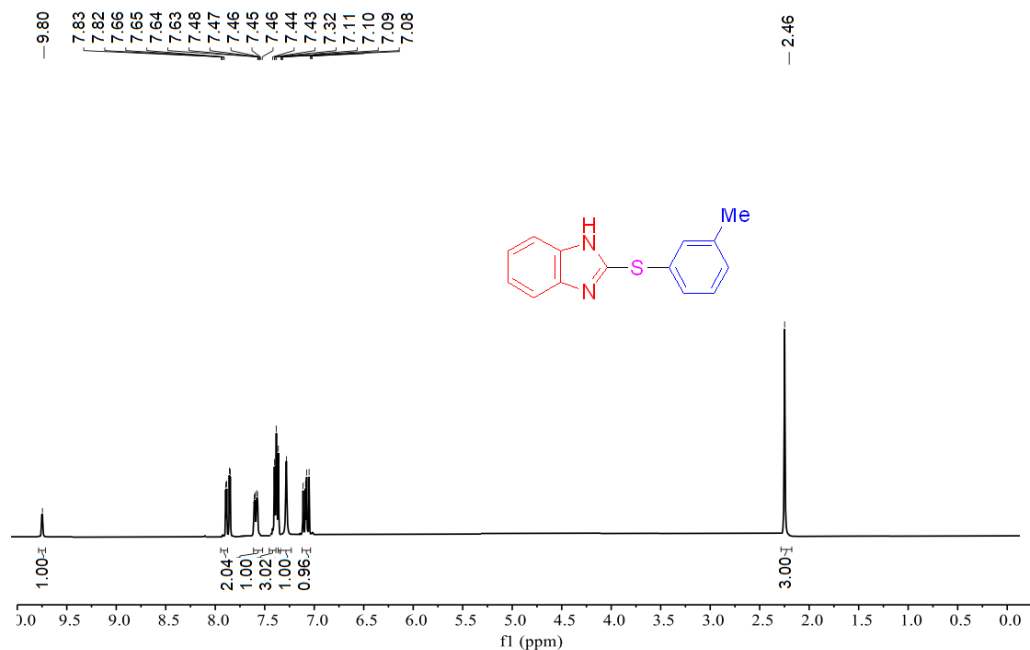
NAME UN
EXPNO 425
PROCNO 1
Date_ 20240922
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894968 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 6.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



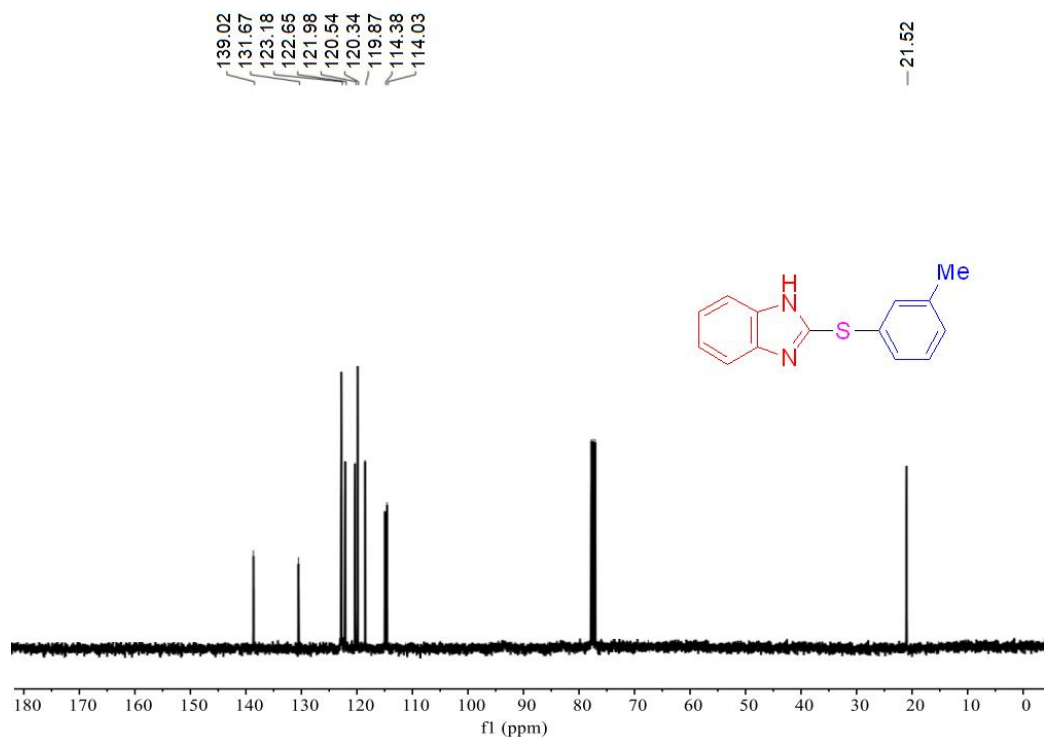
NAME UN
EXPNO 435
PROCNO 2
Date_ 20240922
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 31
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 293.4 K
D1 3.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL12W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



NAME UN
EXPNO 425
PROCNO 1
Date_ 20240922
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 6.0000000 sec
TD0 1

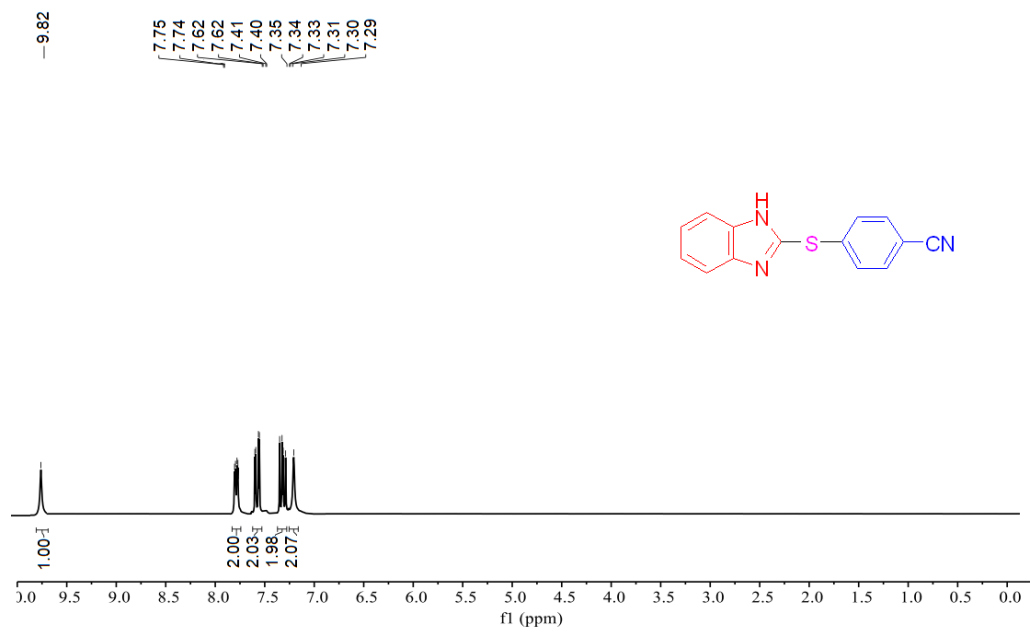
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME UN
EXPNO 435
PROCNO 2
Date_ 20240922
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT CDCl₃
NS 31
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 293.2 K
D1 3.0000000 sec
D11 0.0300000 sec
TD0 1

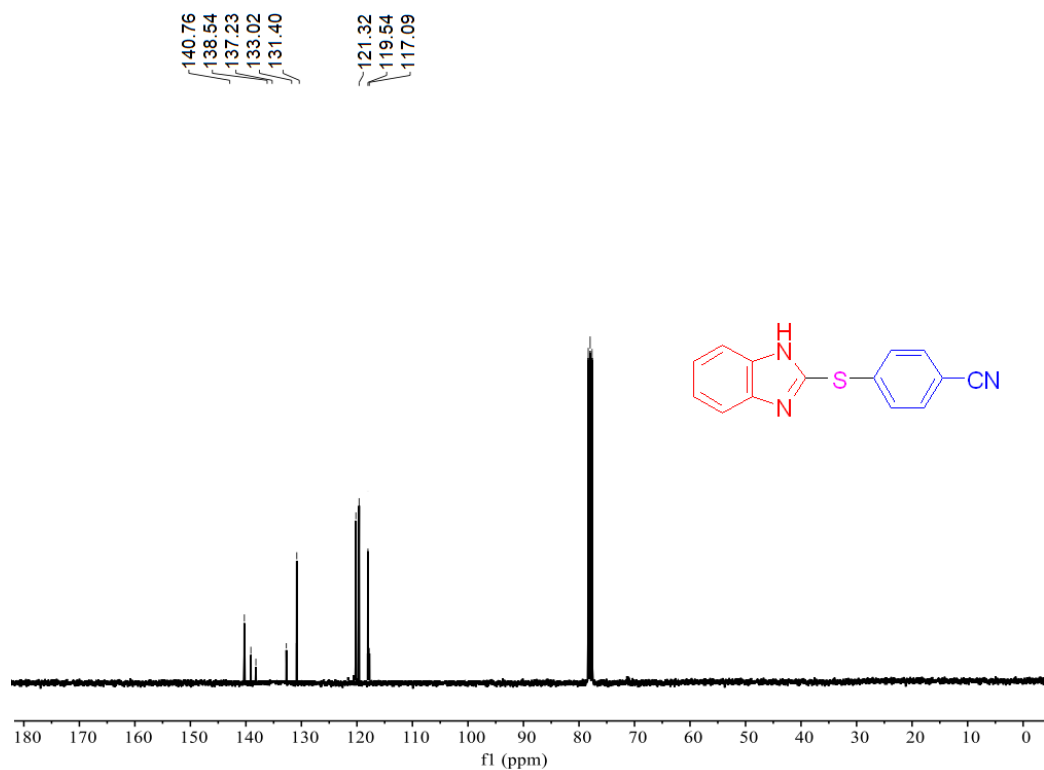
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL1W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



NAME UN
EXPNO 426
PROCNO 1
Date_ 20240922
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 6.0000000 sec
TD0 1

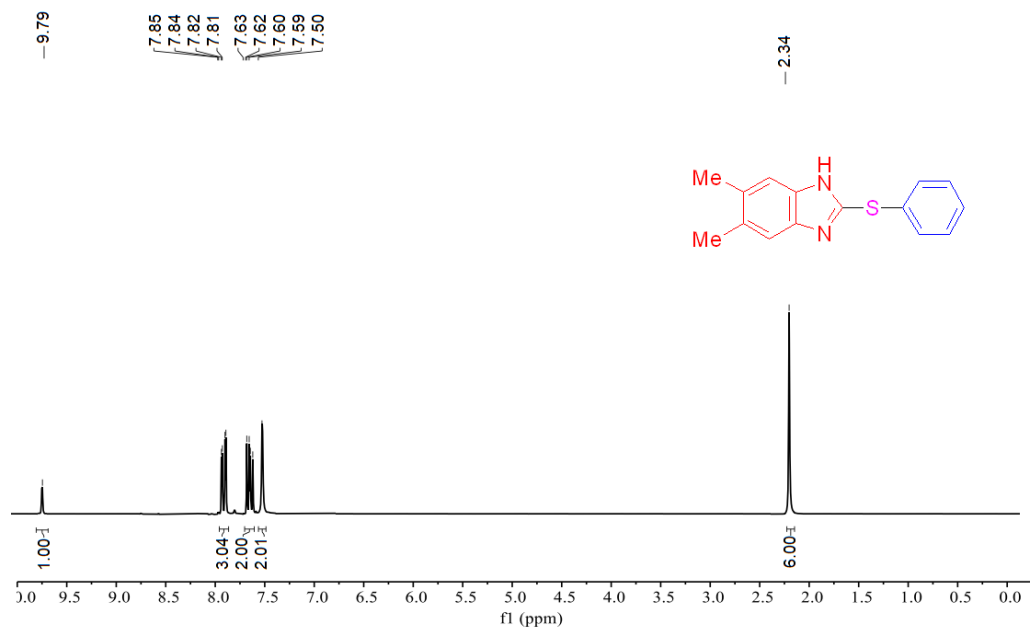
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME UN
EXPNO 435
PROCNO 2
Date_ 20240922
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT CDCl₃
NS 31
DS 0
SWH 25252.523 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 293.4 K
D1 3.0000000 sec
D11 0.0300000 sec
TD0 1

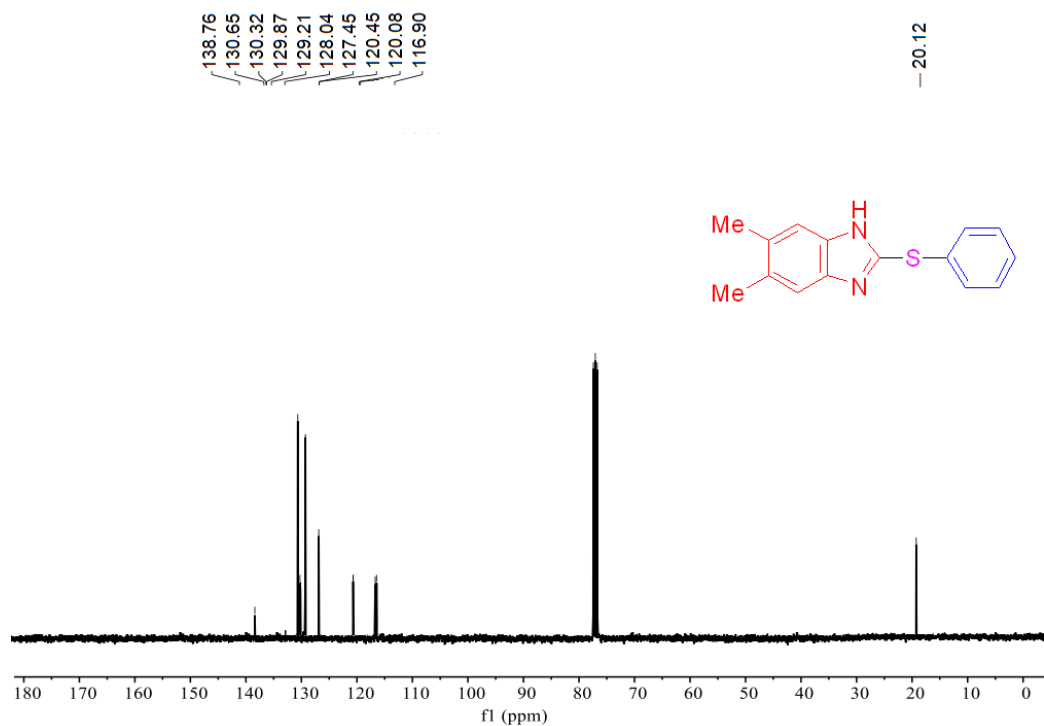
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



NAME UN
EXPNO 425
PROCNO 1
Date_ 20240922
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 6.0000000 sec
TD0 1

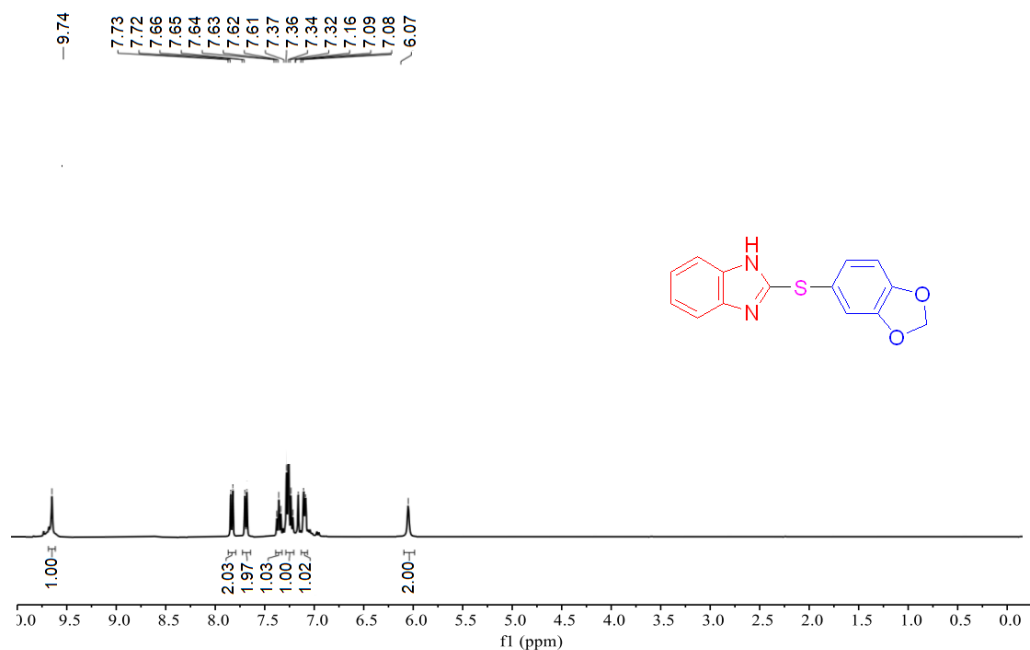
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME UN
EXPNO 435
PROCNO 2
Date_ 20240922
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT CDCl₃
NS 31
DS 0
SWH 25252.523 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 293.4 K
D1 3.0000000 sec
D11 0.0300000 sec
TD0 1

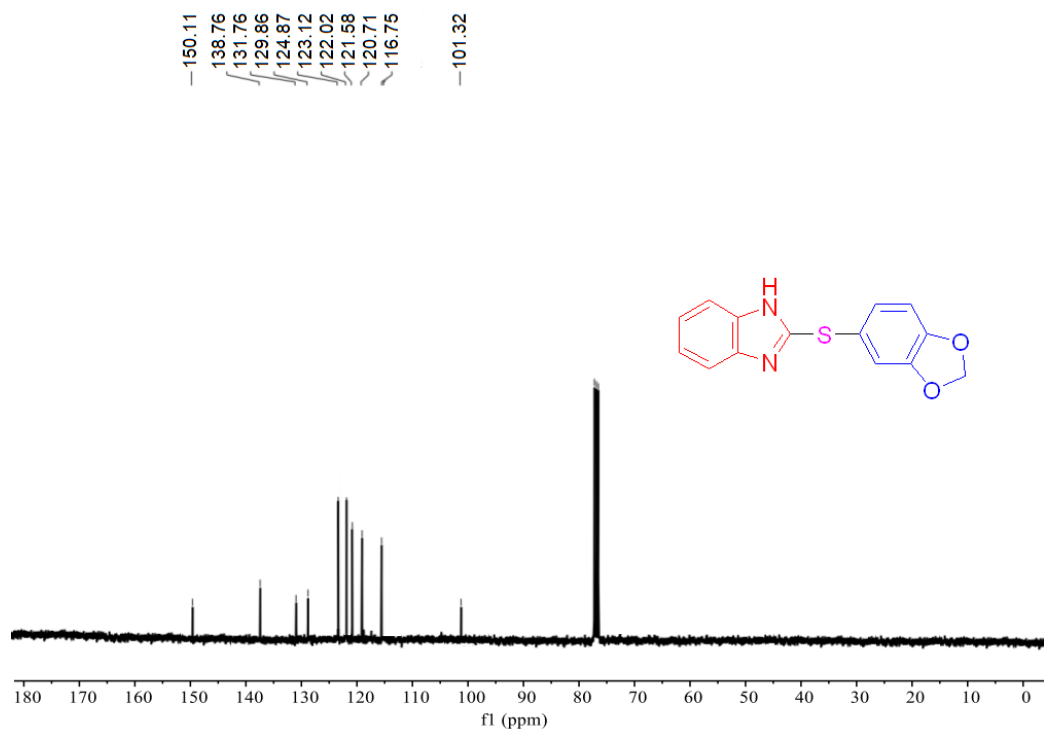
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL1W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



NAME UN
EXPNO 425
PROCNO 1
Date_ 20240922
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 24
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 406
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 6.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
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PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME UN
EXPNO 435
PROCNO 2
Date_ 20240922
INSTRUM spect
PROBHD 5 mm PABBO BB-
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TD 65536
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NS 31
DS 0
SWH 25252.523 Hz
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TD0 1

===== CHANNEL f1 =====
NUC1 13C
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PL1W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40