

## Supporting Information

# **Palladium(II) Complexes bearing Mesoionic Carbene Ligands: Catalytic Application in Domino Sonogashira Coupling/Cyclization Reactions for One-pot Synthesis of Benzofuran and Indole Derivatives**

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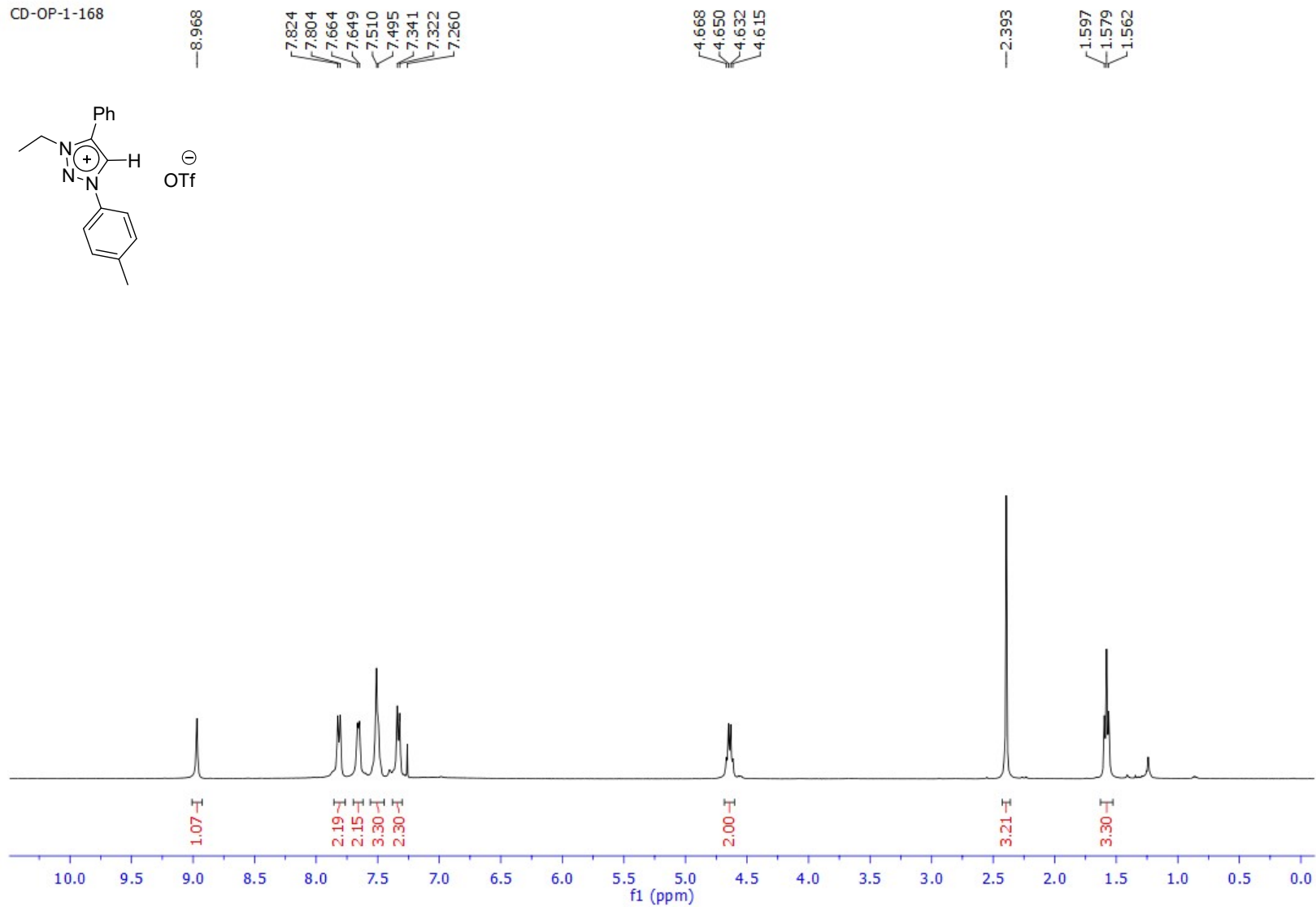
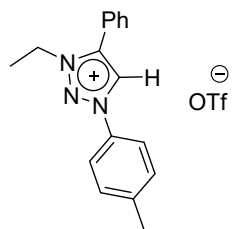
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<sup>b</sup>Catalytic Applications Laboratory, Department of Chemistry, School of Basic Sciences, Faculty of Science, Manipal University Jaipur, Dehmi Kalan, Jaipur – 303007, Rajasthan, India.

\*Corresponding author:

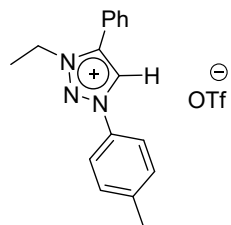
Email: [ckdash@curaj.ac.in](mailto:ckdash@curaj.ac.in); [sriparna.ray@gmail.com](mailto:sriparna.ray@gmail.com)

CD-OP-1-168



**Figure S1.**  $^1\text{H}$  NMR spectrum of **1a** in  $\text{CDCl}_3$

CD-OP-1-168



143.737  
142.579  
132.672  
131.900  
130.879  
129.721  
129.672  
126.559  
121.795  
121.480

77.478  
77.160  
76.841

47.990

21.369

14.139

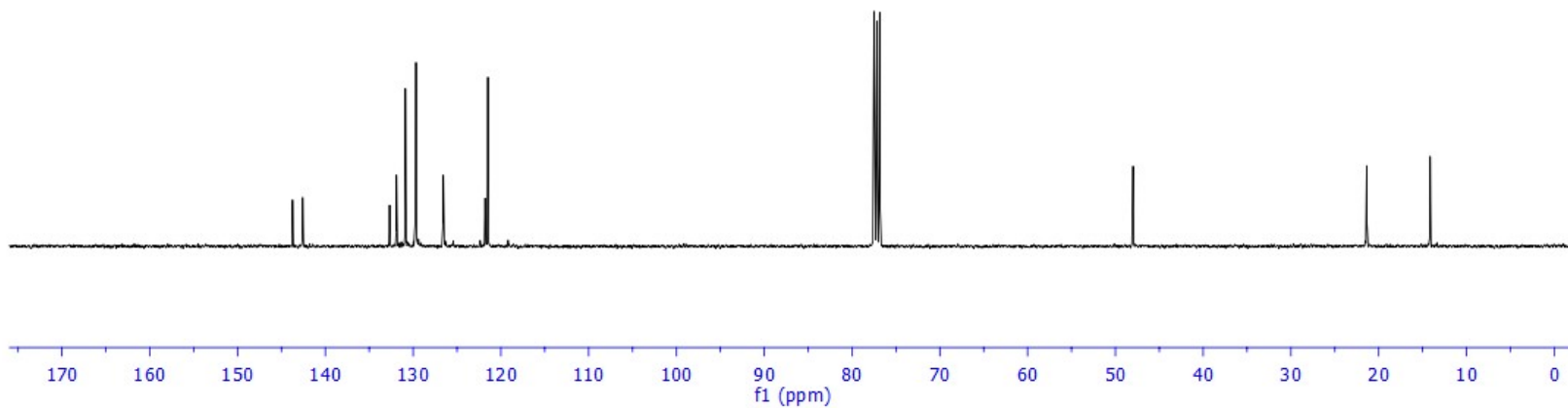
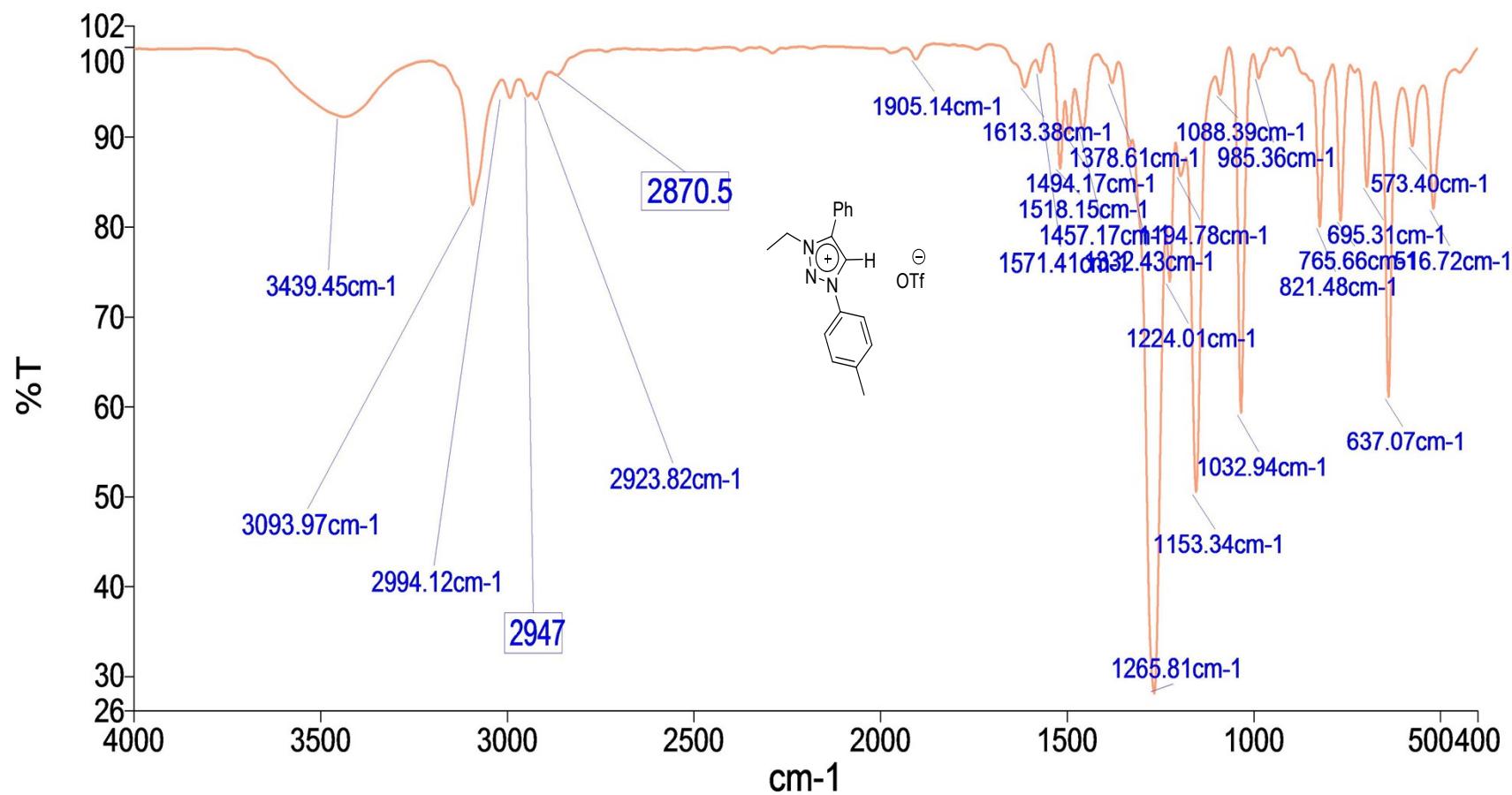


Figure S2.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1a** in  $\text{CDCl}_3$



**Figure S3.** IR spectrum of **1a** in KBr



CD-OP-1-235-13C-14-07-2022

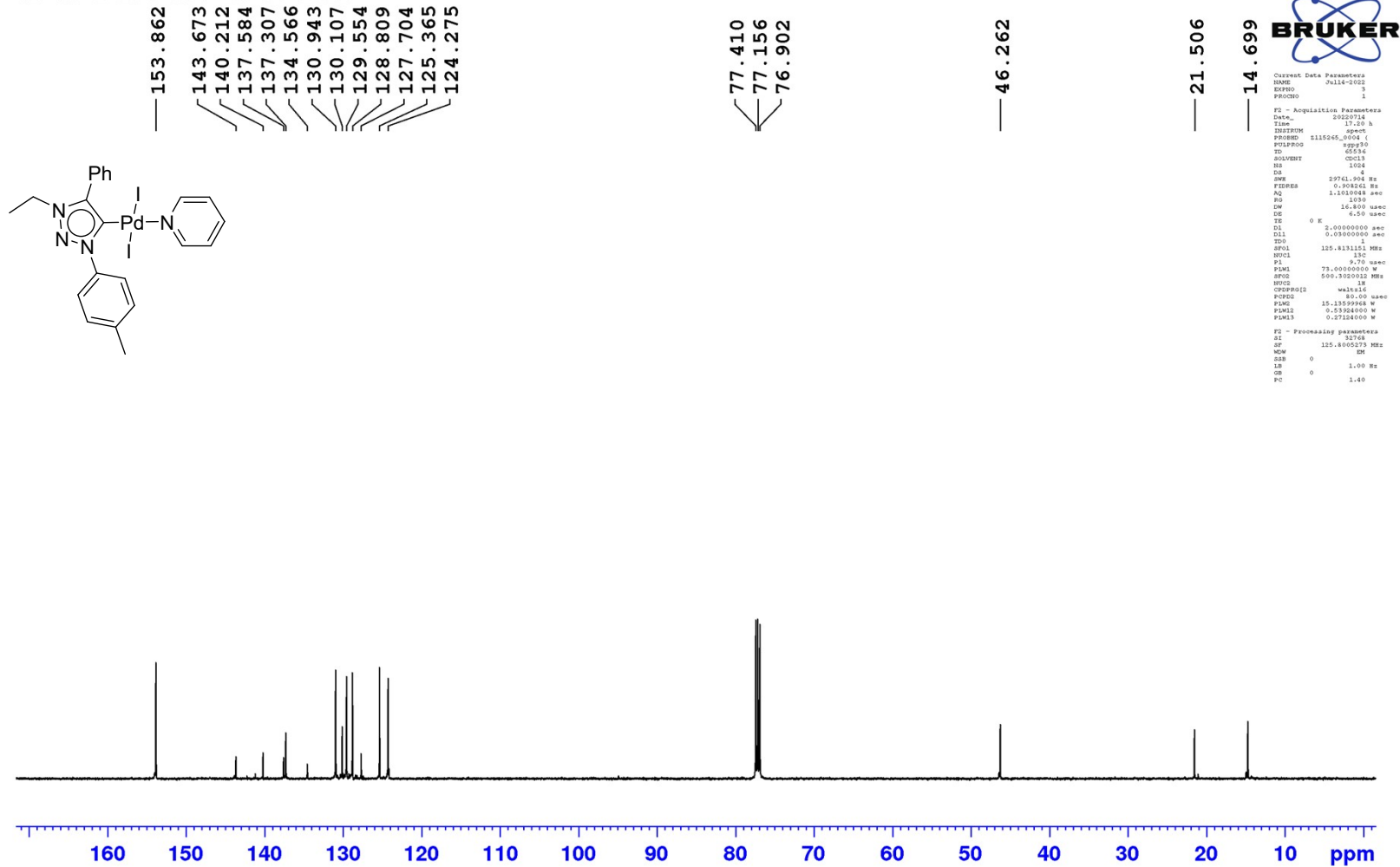


Figure S5.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **2a** in  $\text{CDCl}_3$

CD-OP-1-235-DEPT-135-14.7.22

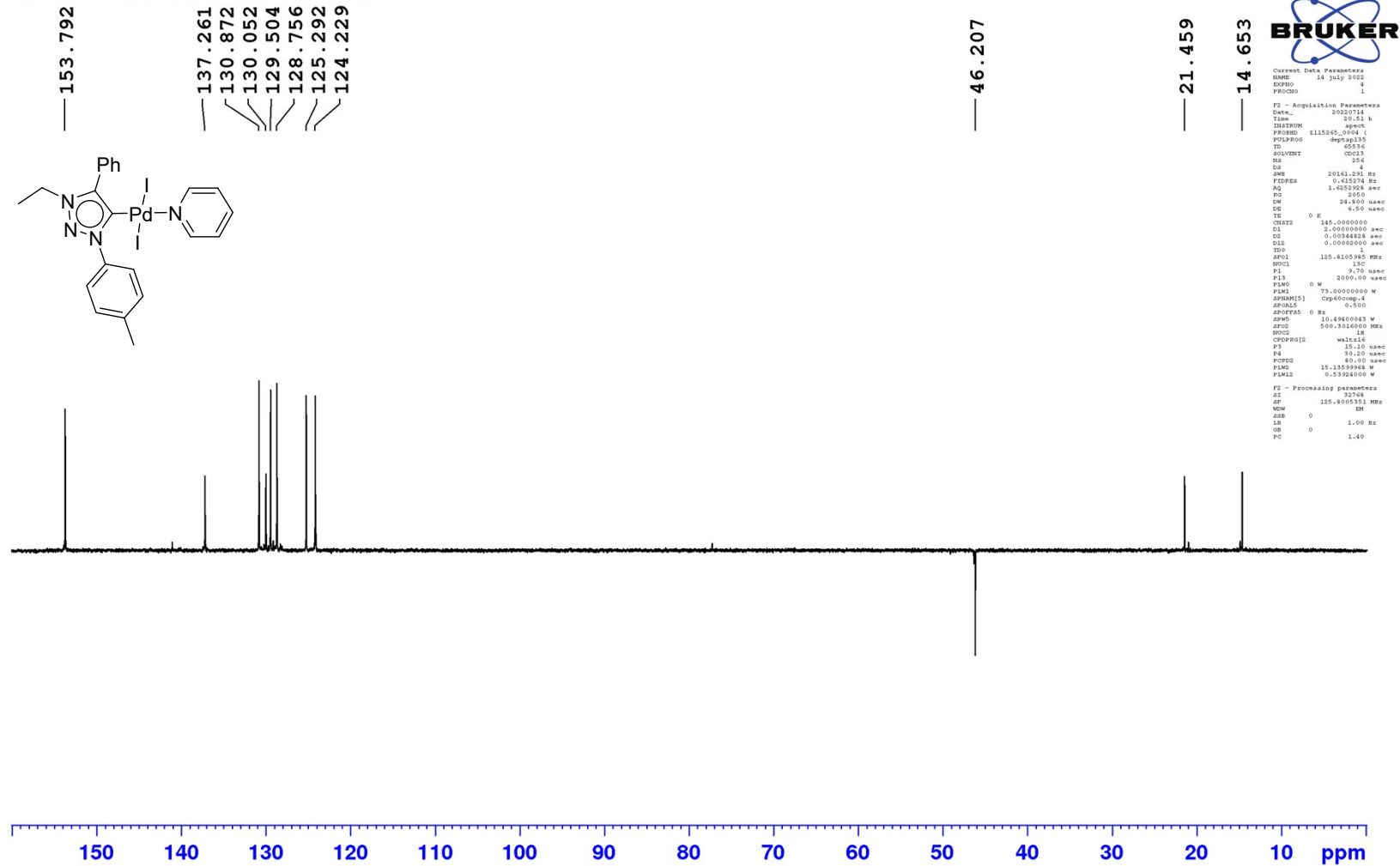


Figure S6. DEPT135 NMR spectrum of 2a in CDCl<sub>3</sub>

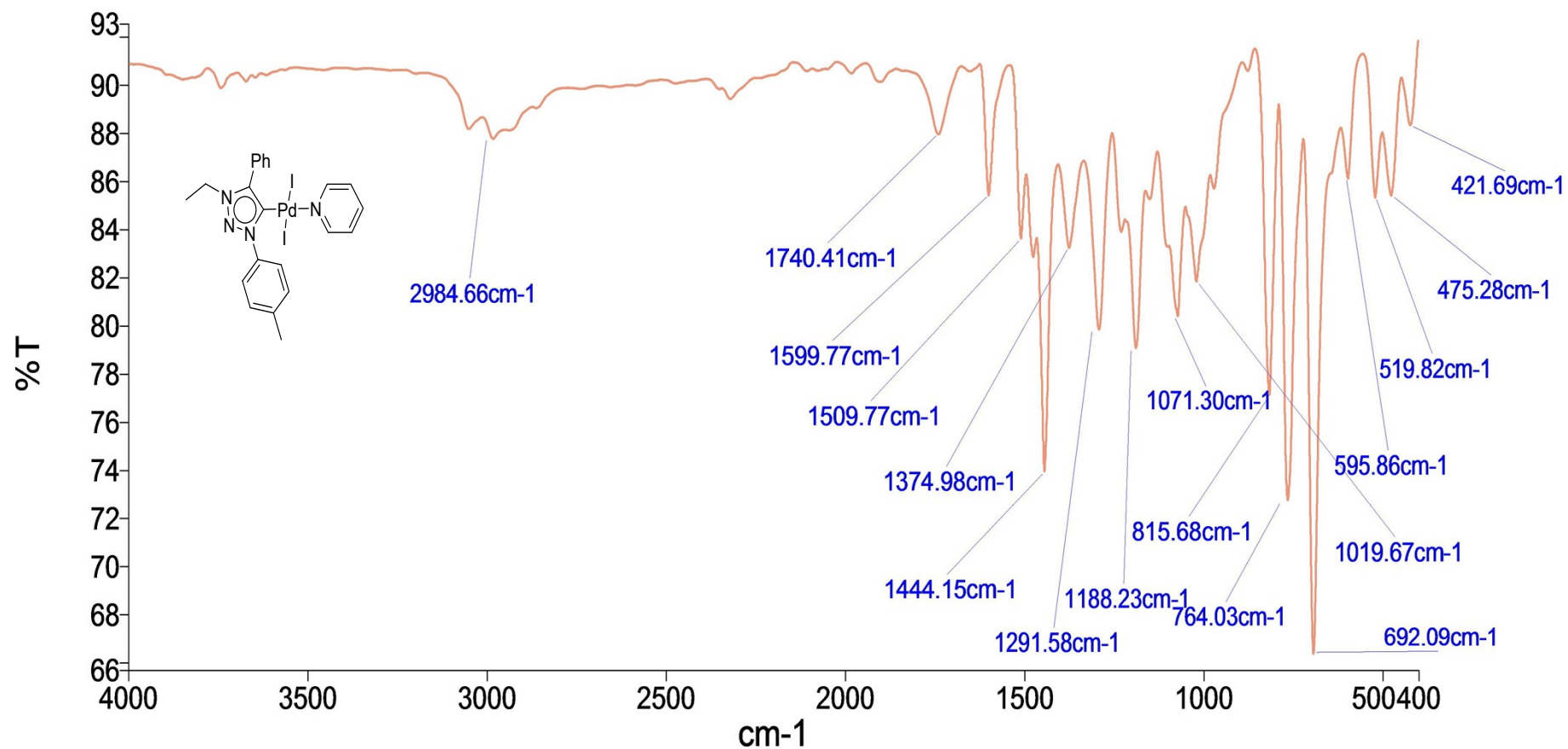
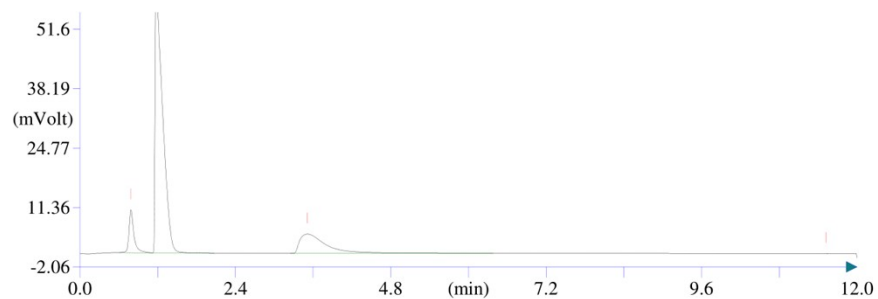


Figure S7. IR spectrum of 2a in KBr



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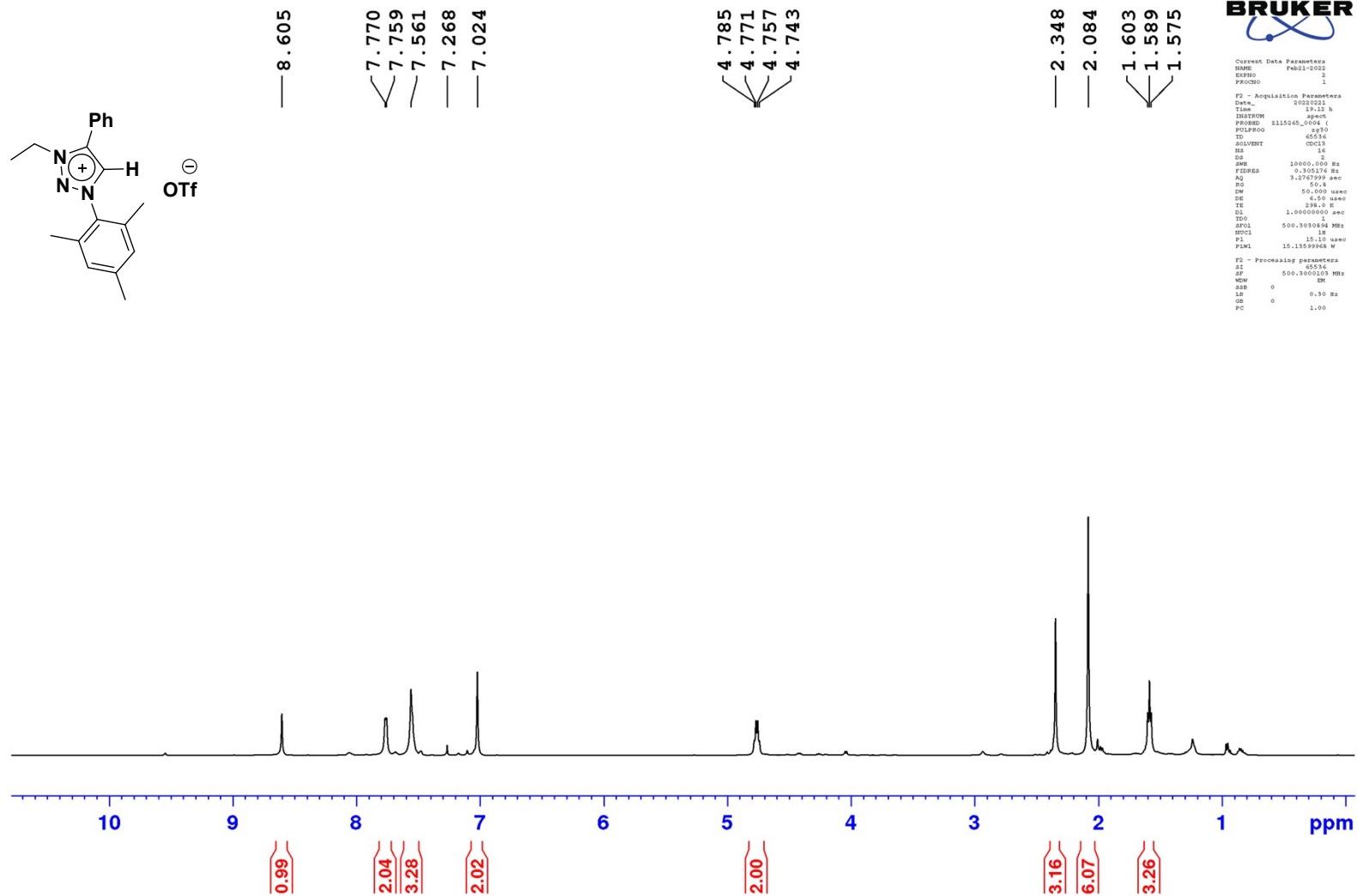
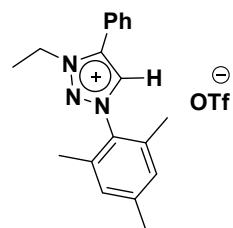
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 Printed: 02-19-2021 18:33  
 Elemental Analyser method:  
 Sampler method:  
 Sample ID: CD-OP-1-226 (# 28)  
 Analysis type: UnkNown  
 Chromatogram filename: CD-OP-1-226-19-2--2021.dat  
 Calibration method: K Factors  
 Sample weight: 2.666  
 Protein factor: 6.25



Retention Time (min)	Area (.1* $\mu$ V*sec)	Component Name	Element %
0.783	505311	Nitrogen	7.428
1.175	4919907	Carbon	37.591
3.508	1256201	Hydrogen	3.123
11.525	9913		0.000
	6691331		48.142

**Figure S8.** Elemental Analysis data of **2a**

CD-OP-1-335-OTf-1H



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PROCNO 1

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PROBHD z115245\_0094 (1  
PULPROG zgpg30  
ID 65516  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.300276 Hz  
AQ 3.2787959 sec  
RG 65.8  
DM 50.000 usec  
DE 4.50 usec  
TE 298.0 K  
DQ 1.00000000 sec  
TD 1  
FID 500.3030494 MHz  
SFO1 18  
NUC1 15.10 usec  
PL 15.13599948 W

F2 - Processing parameters  
SI 65516  
SF 500.3000103 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Figure S9. <sup>1</sup>H NMR spectrum of **1b** in CDCl<sub>3</sub>

CD-OP-1-335-OTf-13C

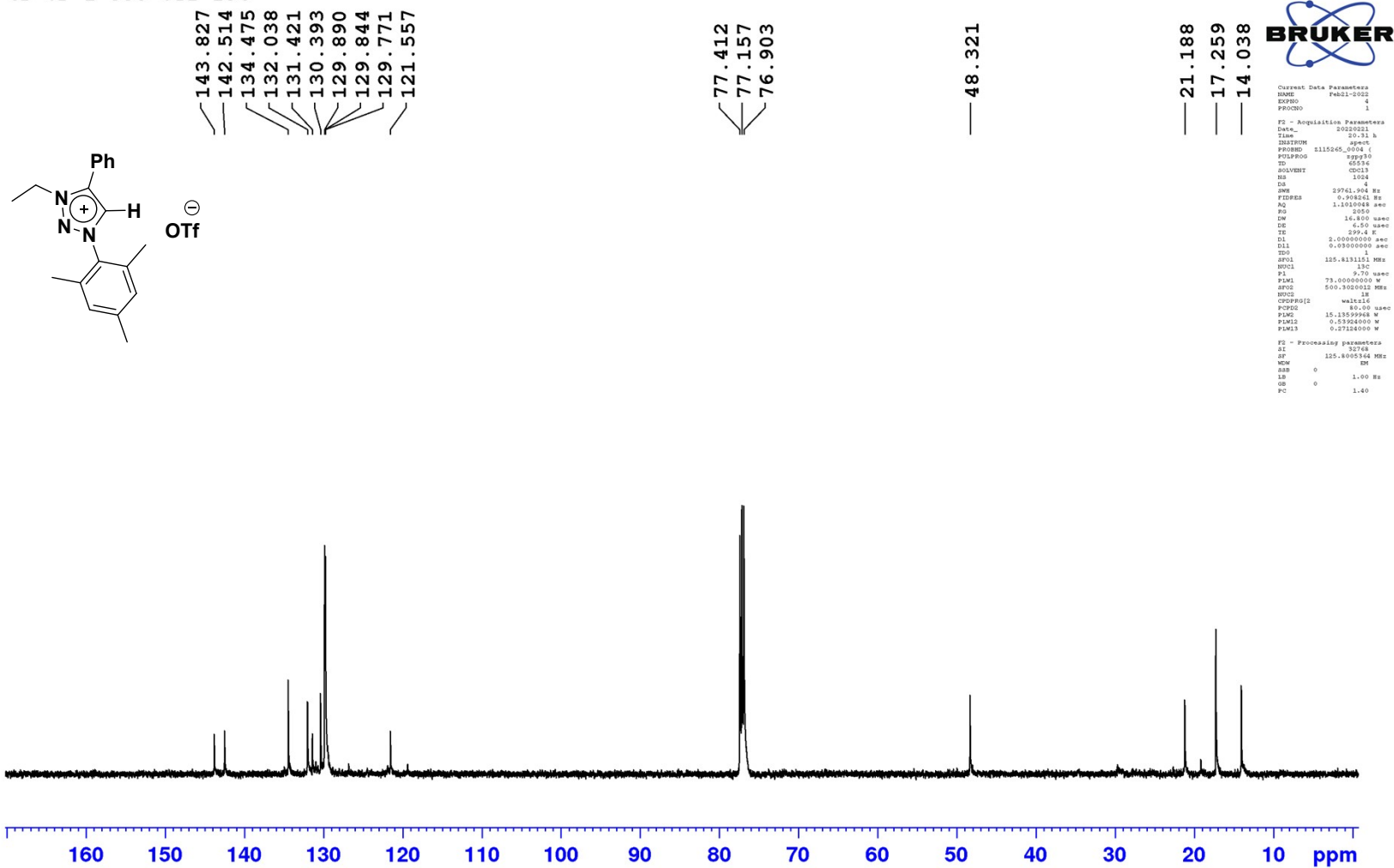


Figure S10.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1b** in  $\text{CDCl}_3$

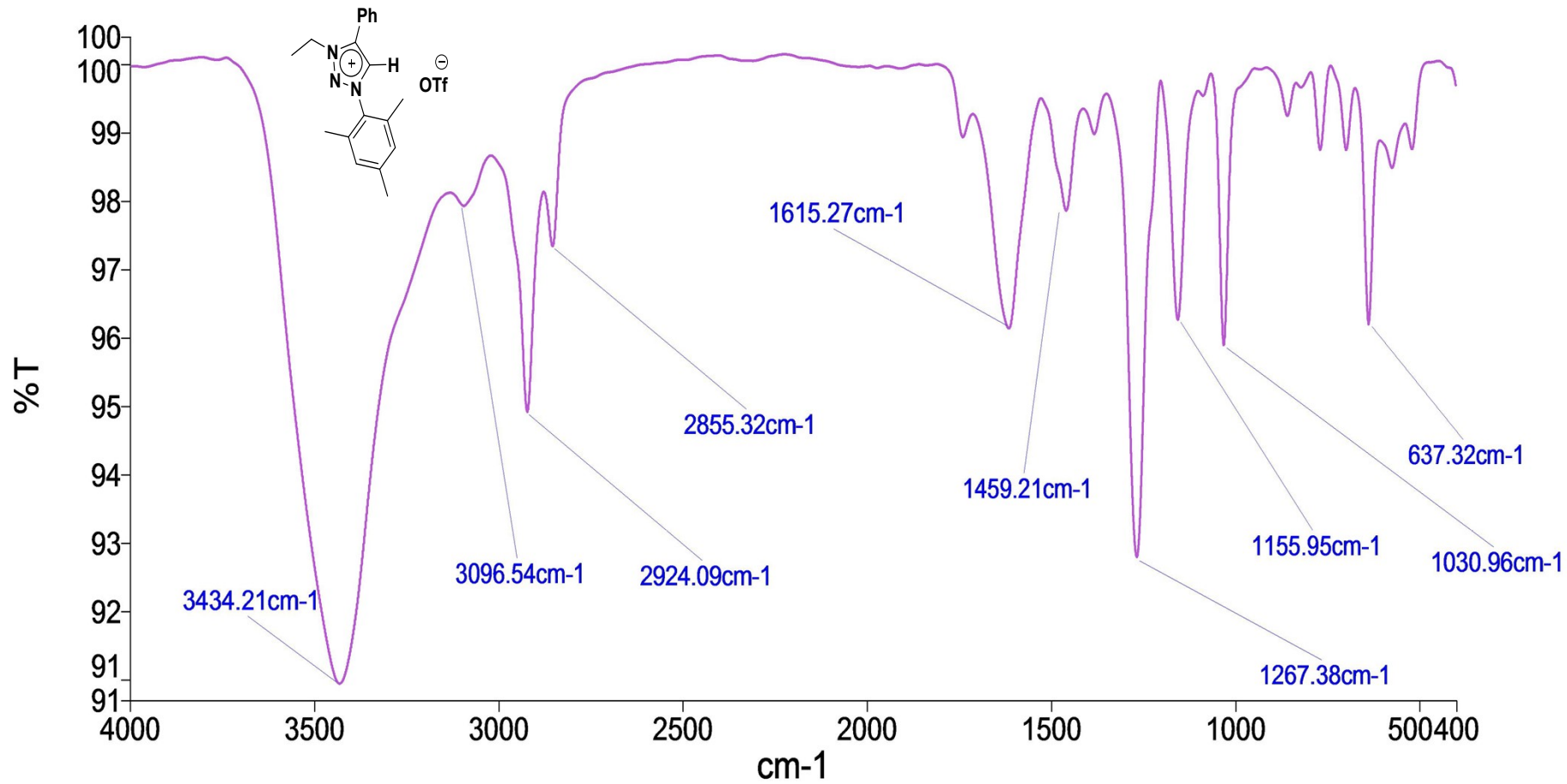


Figure S11. IR spectrum of **1b** in KBr

CD-OP-1-236

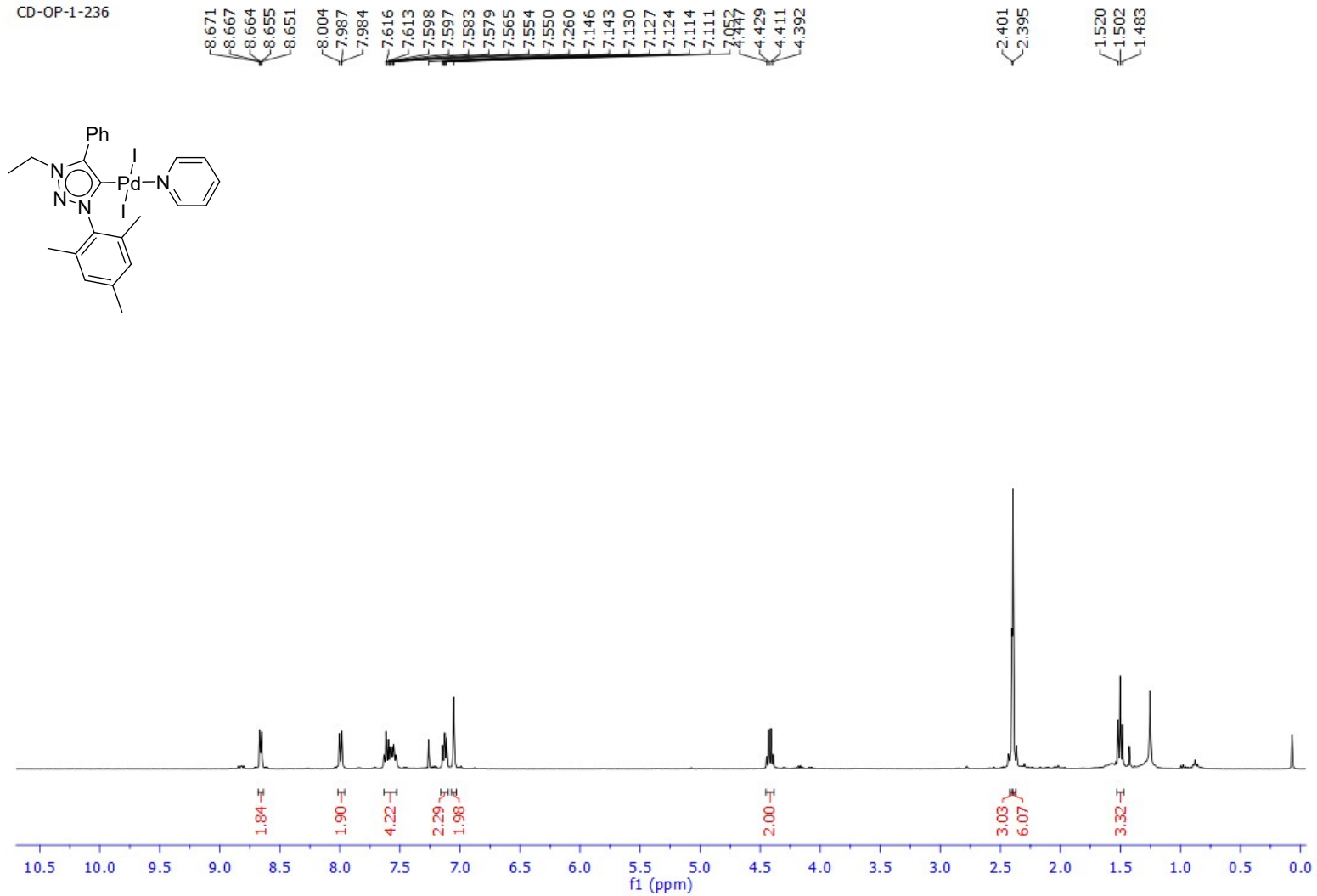
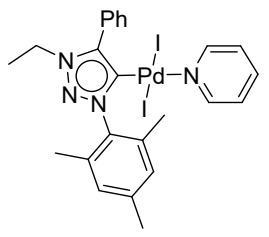


Figure S12. <sup>1</sup>H NMR spectrum of **2b** in CDCl<sub>3</sub>

CD-OP-1-236-13C-30.7.22



153.828  
144.829  
140.412  
137.703  
137.126  
135.896  
135.791  
131.245  
130.099  
129.625  
128.686  
128.312  
124.102

77.411  
77.157  
76.904

46.204

21.485  
21.387  
14.909



```
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EXPNO         4
PROCNO        1

F2 - Acquisition Parameters
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Time          22:24.8
INSTRUM       spect
PROBHD        1H5265_0104 (
PULPROG       zgpg30
SU            GSSG
SOLVENT       CDCl3
DS            2048
DA            4
SHE           29761.904 Hz
FIDRES        0.208261 Hz
AQ            1.1020848 sec
RG            2050
DM            16.850 usec
DE            6.50 usec
TE            0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD           1
SFO1          125.811111 MHz
NUC1           13C
P1            9.70 usec
PL1           75.00000000 W
SFO2          500.1302012 MHz
NUC2           1H
PCPD012       waltz16
PCPD0         80.00 usec
PLM0          15.1359968 W
PLM12         0.53924000 W
PLM13         0.27224000 W

F2 - Processing parameters
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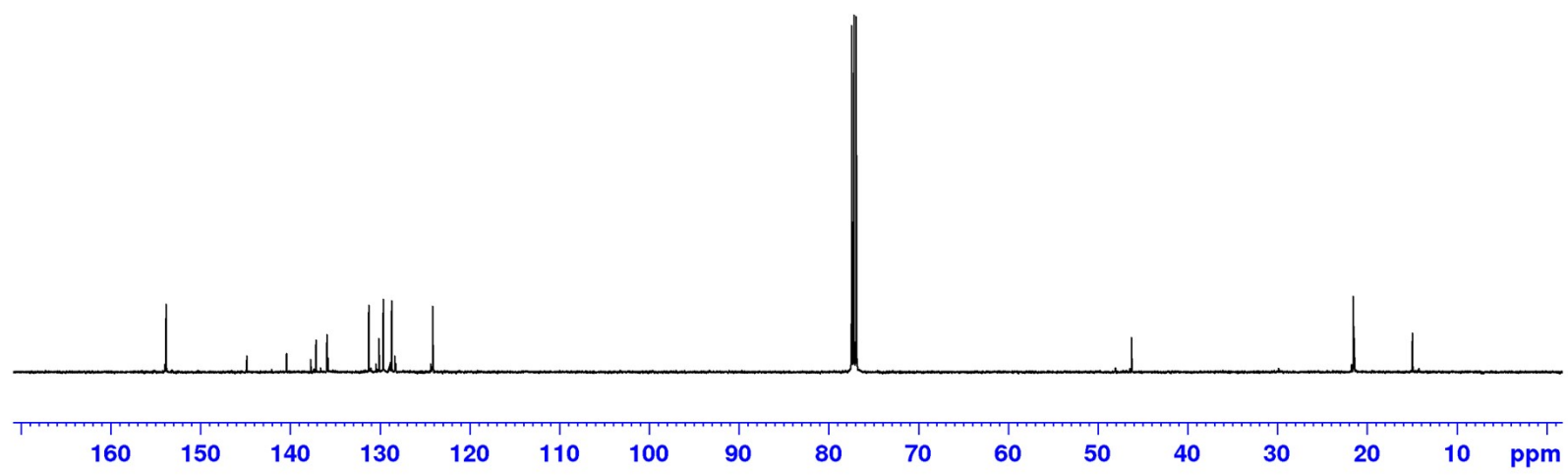


Figure S13.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **2b** in  $\text{CDCl}_3$

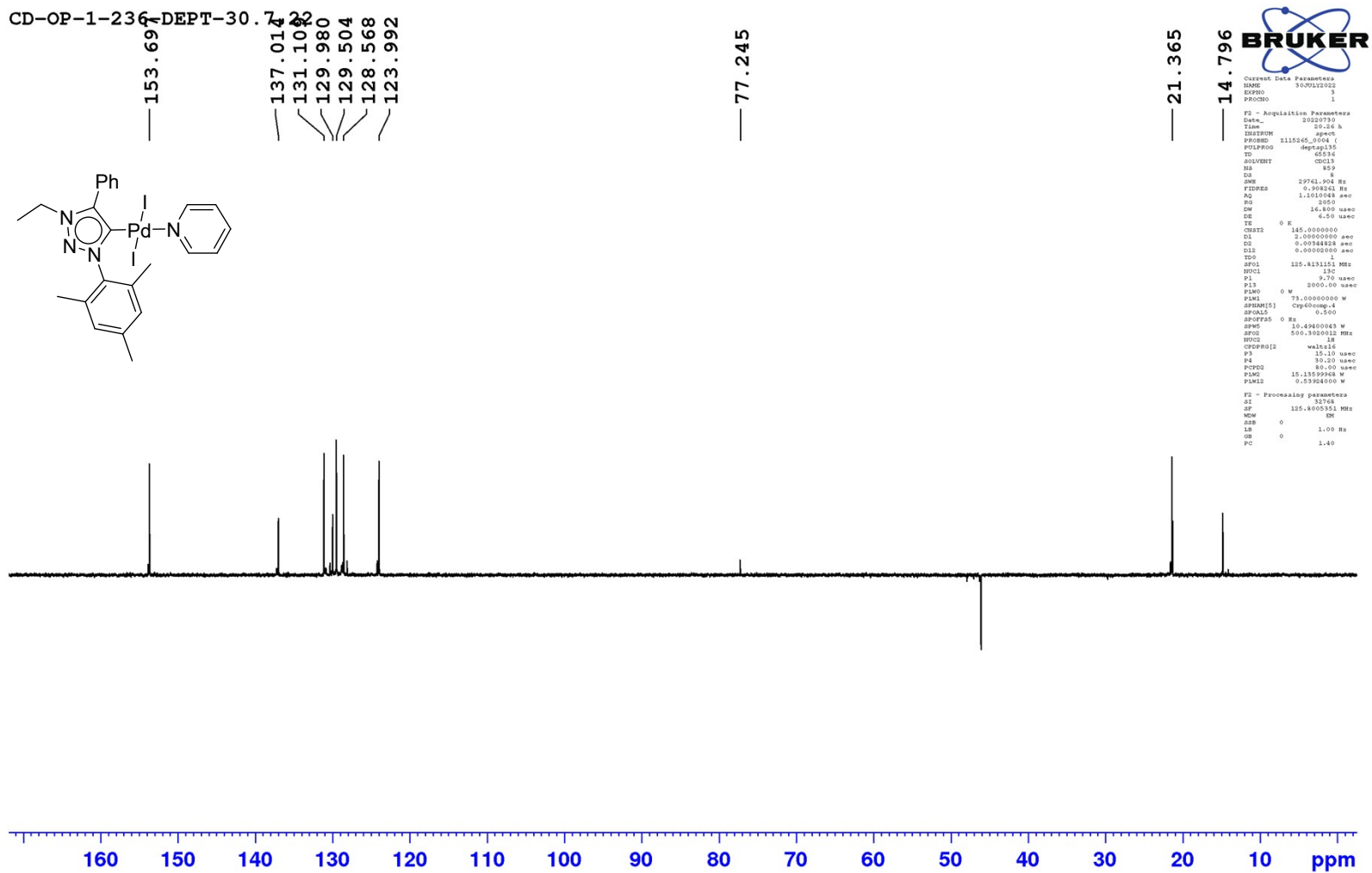


Figure S14. DEPT135 NMR spectrum of **2b** in  $\text{CDCl}_3$

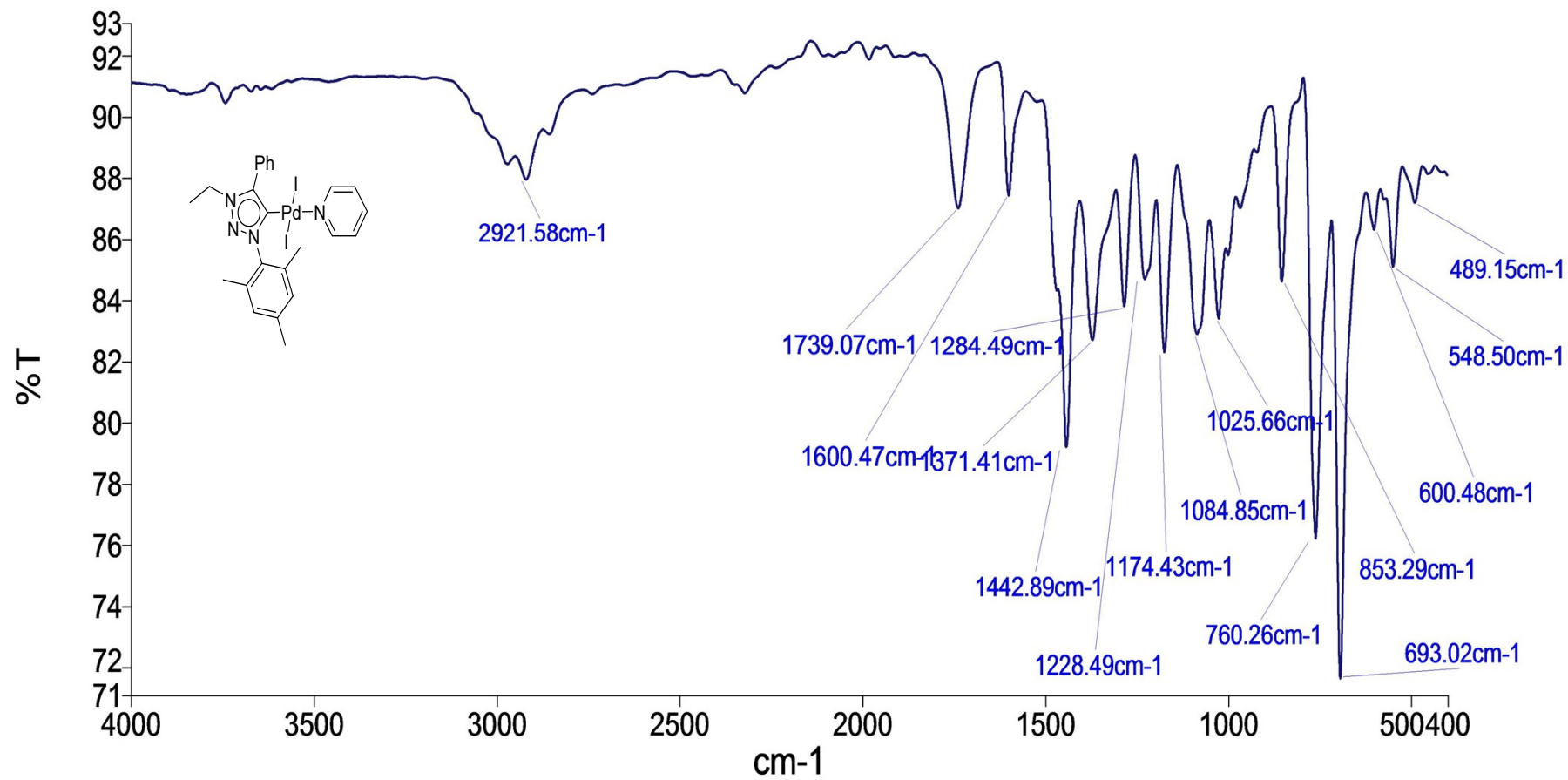
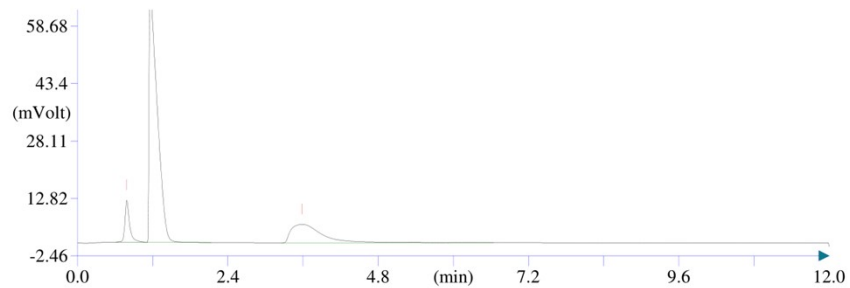


Figure S15. IR spectrum of **2b** in KBr



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Operator ID:  
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 Elemental Analyser method:  
 Sampler method:  
 Sample ID: CD-OP-1-215 (# 26)  
 Analysis type: UnkNown  
 Chromatogram filename: CD-OP-1-215-19-02-2021.dat  
 Calibration method: K Factors  
 Sample weight: 3.175  
 Protein factor: 6.25



Retention Time (min)	Area (.1* $\mu$ V*sec)	Component Name	Element %
0.783	567889	Nitrogen	7.208
1.158	6062293	Carbon	38.901
3.583	1704203	Hydrogen	3.563
	8334385		49.672

**Figure S16.** Elemental Analysis data of **2b**

CD-OP-1-343-1H

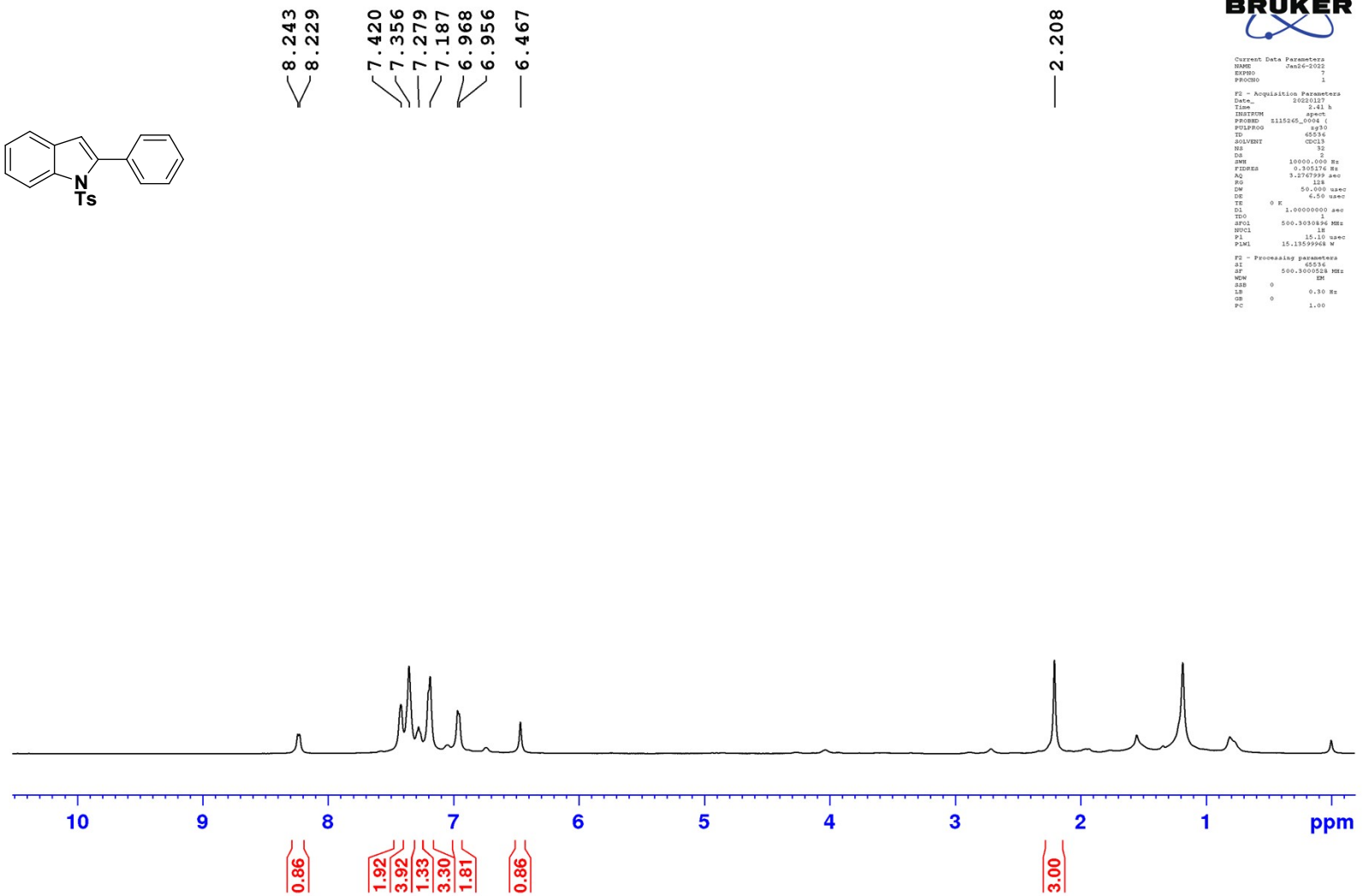
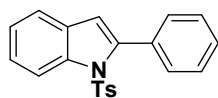


Figure S17. <sup>1</sup>H NMR spectrum of 3ah in CDCl<sub>3</sub>

CD-OP-1-343-13C

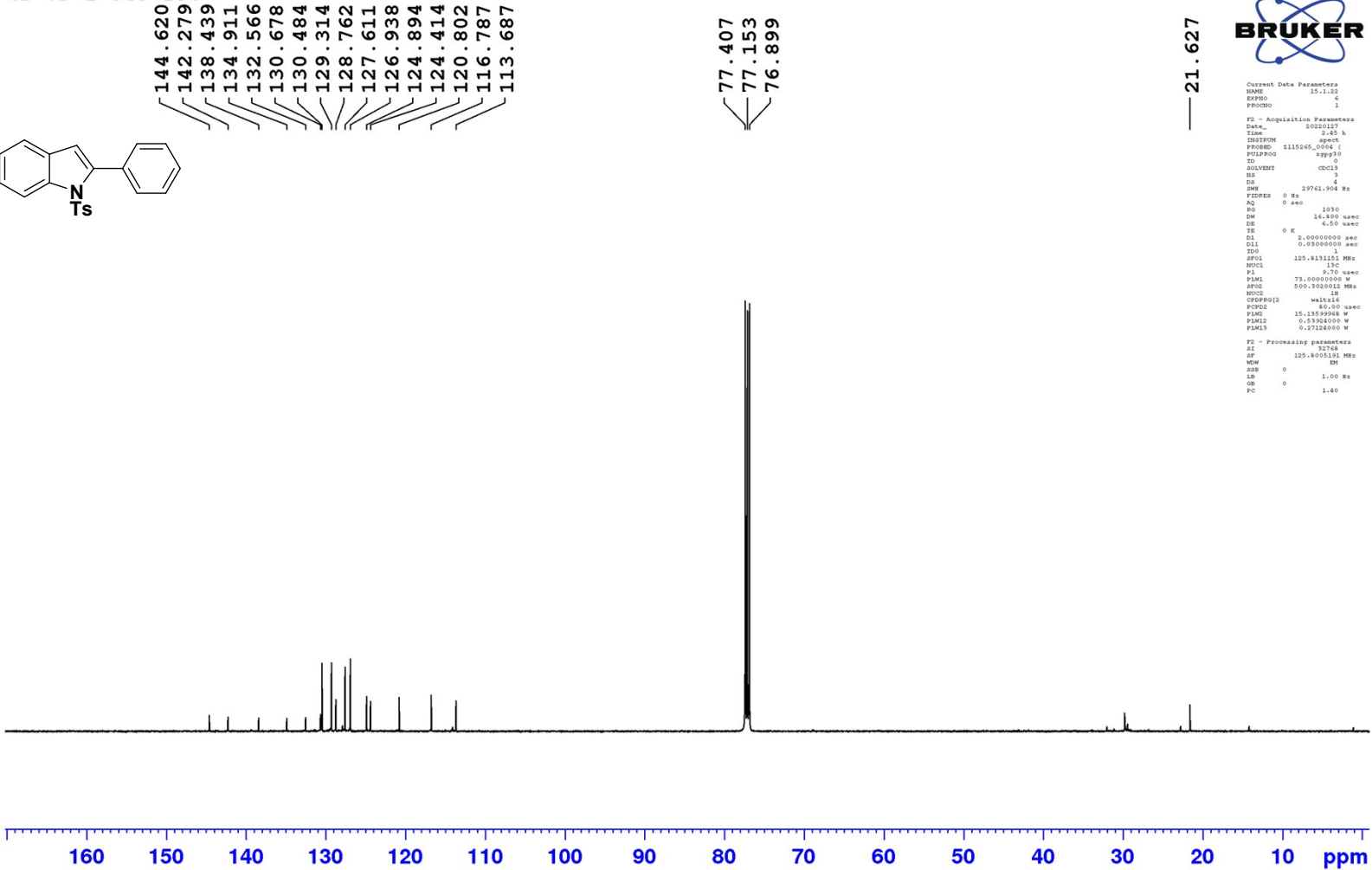
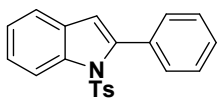
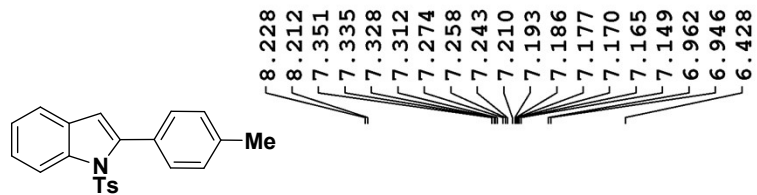


Figure S18.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3ah** in  $\text{CDCl}_3$

CD-OP-1-345



8.228  
8.212  
7.351  
7.335  
7.328  
7.312  
7.274  
7.258  
7.243  
7.210  
7.193  
7.186  
7.177  
7.170  
7.165  
7.149  
6.962  
6.946  
6.428

2.361  
2.198



Current Data Parameters  
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EXPNO 1  
PROCNO 1  
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Date\_ 20220220  
Time 18.41 h  
INSTRUM spect  
PROBHD E115265\_004 (4  
PULPROG zgpg  
TD 65536  
SOLVENT CDCl3  
NS 32  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.246174 Hz  
AQ 3.2747599 sec  
RG 300  
EW 50.000 kHz  
EQ 6.50 kHz  
TE 300 K  
D1 1.00000000 sec  
TDO 0.00000000 sec  
SFO1 500.305054 MHz  
HFQC1 1H  
P1 15.10000000 sec  
PLM1 15.13599968 W  
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SI 65536  
SF 500.305054 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

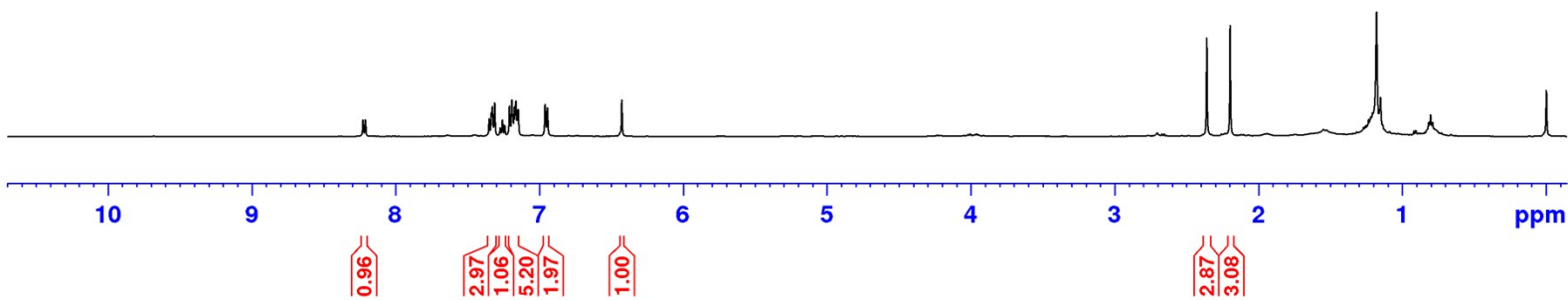
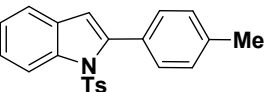


Figure S19. <sup>1</sup>H NMR spectrum of 3ai in CDCl<sub>3</sub>

CD-OP-1-345C13

144.5673  
142.4533  
138.735  
138.370  
134.869  
130.792  
130.343  
129.695  
129.286  
128.382  
126.940  
124.736  
124.389  
120.703  
116.802  
113.386



77.409  
77.156  
76.902

29.829  
21.557



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PROBHD   515245_004 1
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
DE        32.77
DS        4
SWH       23741.904 Hz
FIDRES   0.392641 Hz
AQ        1.1010048 sec
RG         1030
DE         16.800 usec
QE         6.50 usec
TE        0 K
D1         2.00000000 sec
d11       0.03000000 sec
SFO1      125.8131151 MHz
NUC1       13C
P1         9.70 usec
PL1        73.00000000 W
SFO2      500.3000152 MHz
NUC2       1H
PCPD02    waltz16
PCPD0     80.00 usec
PAC        15.11359948 W
PLM1      0.53924000 W
PLM3      0.27124000 W
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GB         0
OR         1.00 Hz
PC         1.40
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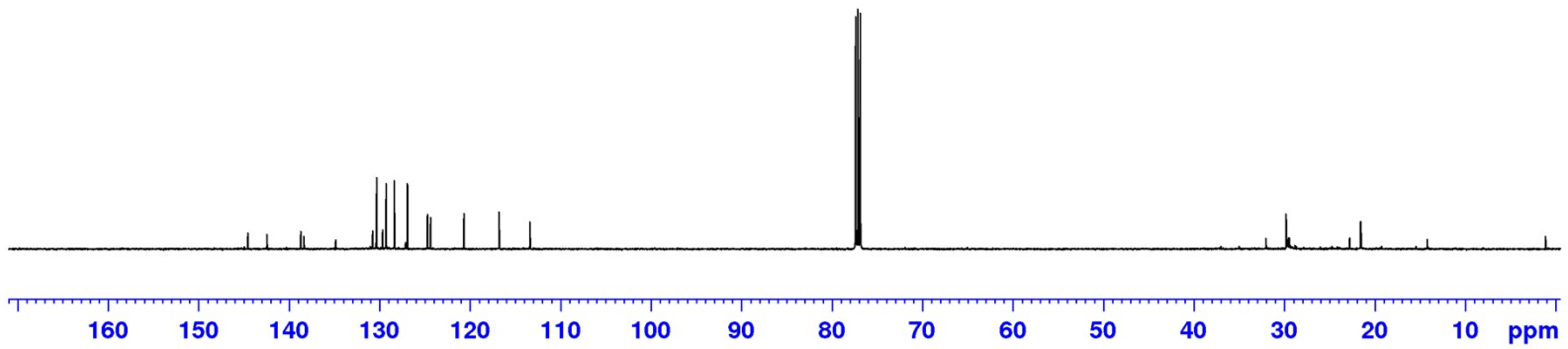
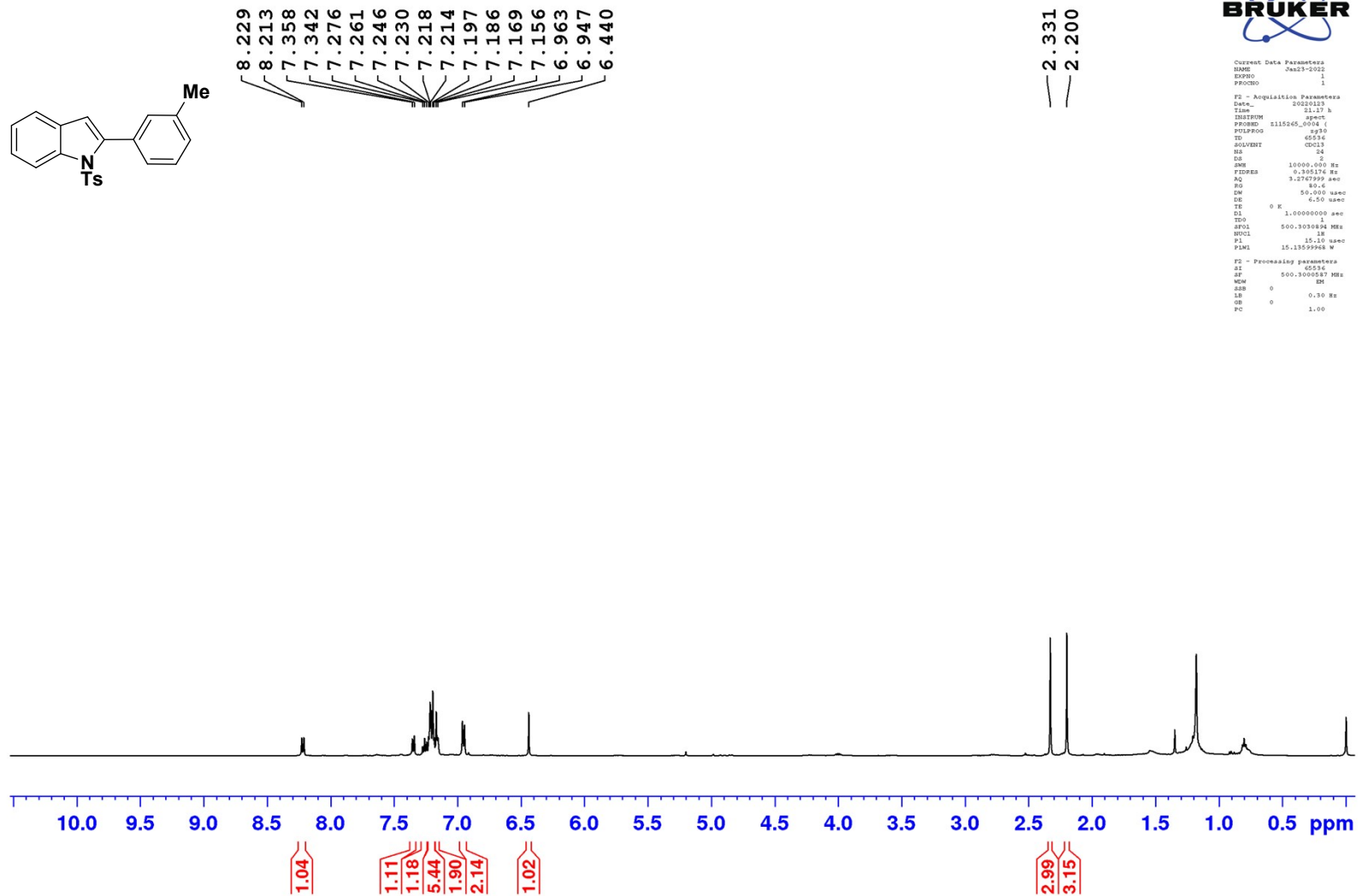
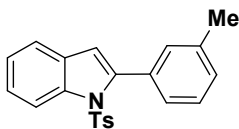


Figure S20.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3ai** in  $\text{CDCl}_3$

CD-OP-351-1H



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PROCNO 1

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PROBHD 1H5245\_0094 f  
PULPROG zgpg30  
TD 65534  
SOLVENT CDCl3  
NS 54  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 1.2747999 sec  
RG 80.4  
EM 50.000 usec  
DE 6.50 usec  
TE 0 K  
DQ 1.0000000 sec  
DI 11  
SFO 500.1308194 MHz  
NUC1 15.10 usec  
PI 15.11559948 W  
PLM1 15.11559948 W

F2 - Processing parameters  
SI 65534  
SF 500.1308194 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Figure S21. <sup>1</sup>H NMR spectrum of 3aj in CDCl<sub>3</sub>

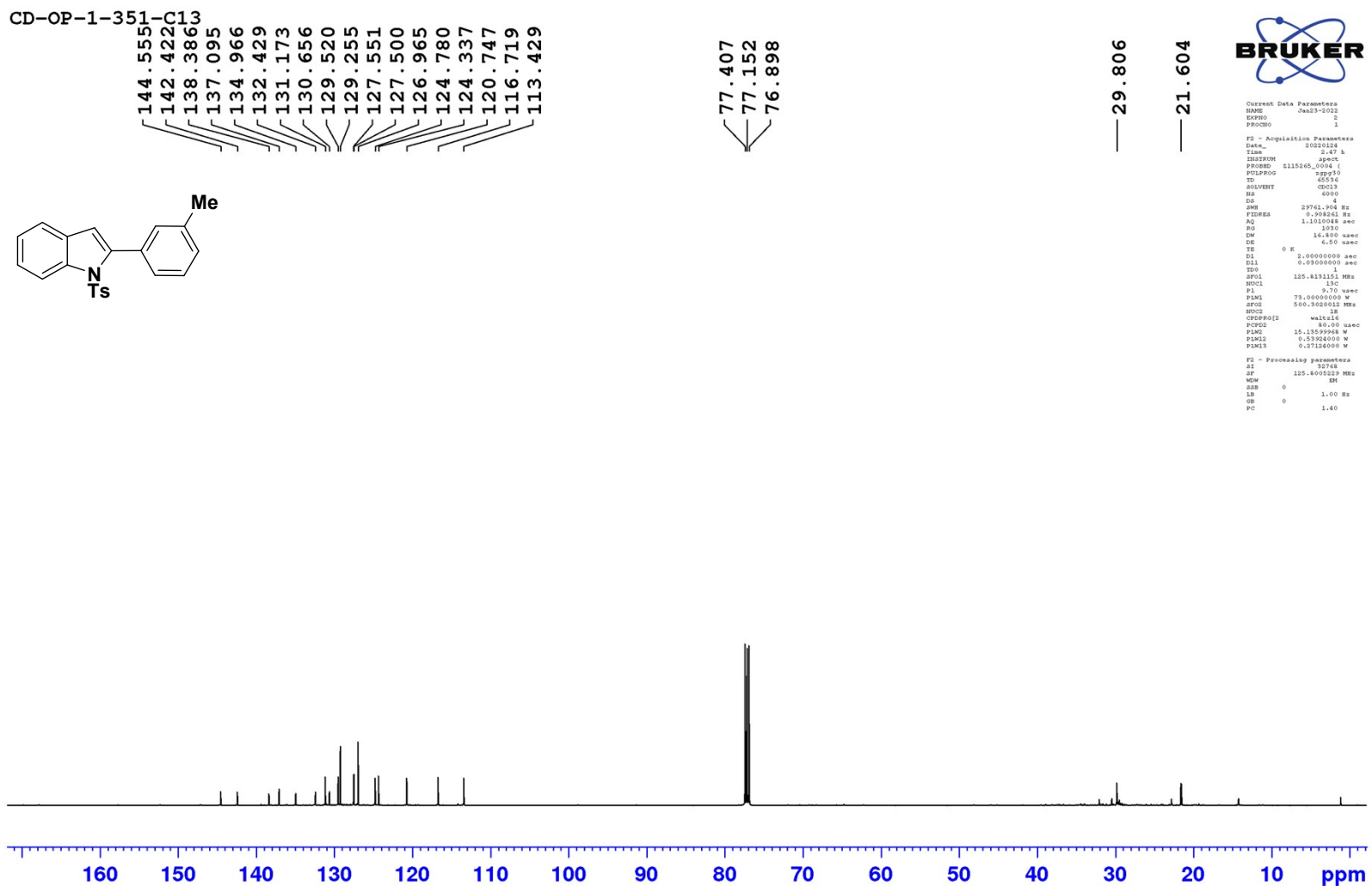
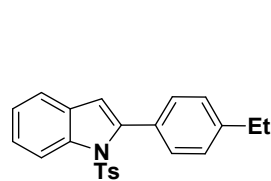


Figure S22.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3aj** in  $\text{CDCl}_3$

CD-OP-1-349



8.219  
8.203  
7.332  
7.317  
7.254  
7.239  
7.223  
7.187  
7.169  
7.150  
7.136  
6.932  
6.916  
6.412

2.667  
2.653  
2.638  
2.624  
2.170

1.231  
1.217  
1.203



Current Data Parameters  
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PROBHD 1H5265\_0004 (1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 24  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.1276799 sec  
RG 64  
DM 50.000 usec  
DE 4.50 usec  
TE 0 K  
D1 1.0000000 sec  
TD0 1  
SFO1 500.130824 MHz  
NUC1 1H  
P1 15.10 usec  
P1M1 15.13559968 M  
F2 - Processing parameters  
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SF 500.130824 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

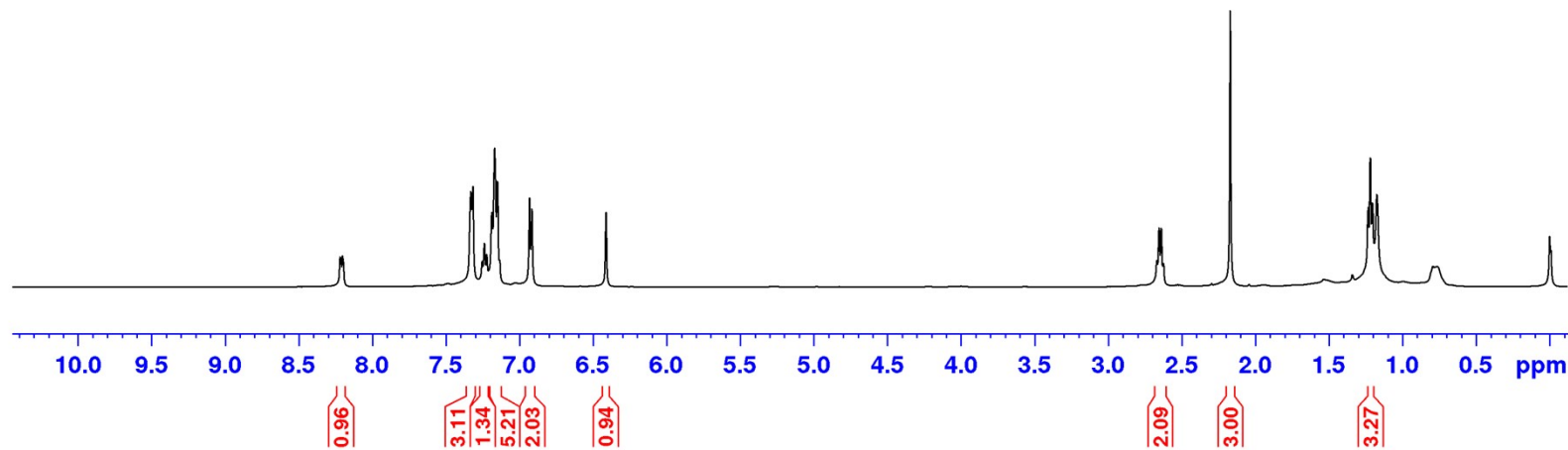


Figure S23. <sup>1</sup>H NMR spectrum of 3ak in CDCl<sub>3</sub>



CD-OP-1-349C13

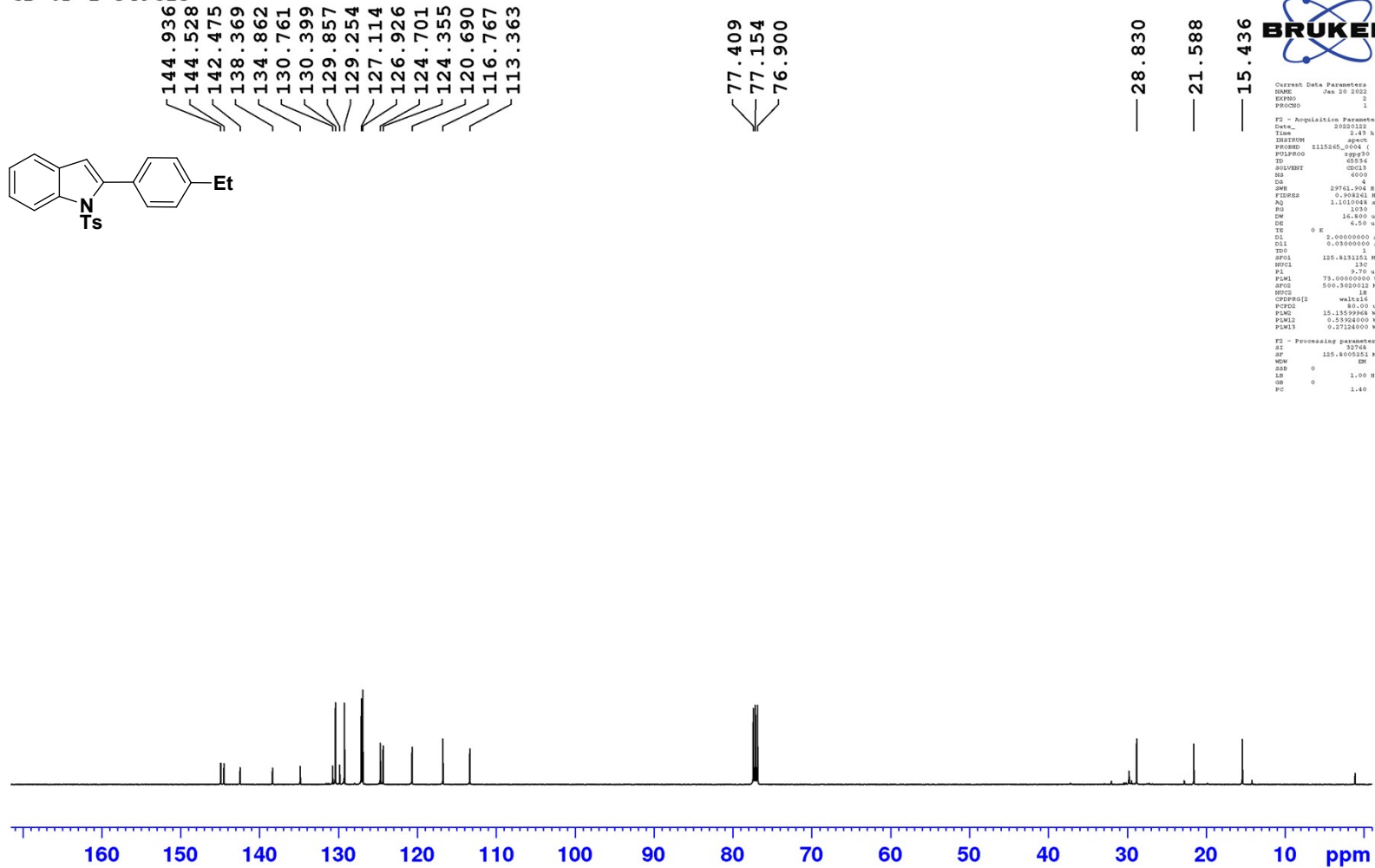
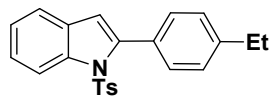


Figure S24.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 3ak in  $\text{CDCl}_3$



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PROCNO   1

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INSTRUM  spect
PROBHD   5mmQNP1
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        600
DS        4
SWH       29761.904 Hz
FIDRES    0.598261 Hz
AQ        1.1010048 sec
RG         1020
CW         16.800 usec
DE         4.50 usec
TE        0 K
D1         2.00000000 sec
d11        0.03000000 sec
TPO       1
AQF1      125.8131151 MHz
NUC1       13C
P1         8.70 usec
PL1L       73.0000000 W
AF1        500.3000012 MHz
NUC2
CPDPRG2   waltz16
P2FC1     81.00 usec
PL2L      15.1359998 W
PL2R      0.3300000 W
PLM1      0.27124000 W

F2 - Processing parameters
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SF         125.8055151 MHz
WDW        EM
SSB        0
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GB         0
PC         1.40
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CD-OP-1-352. 1H CDCl3

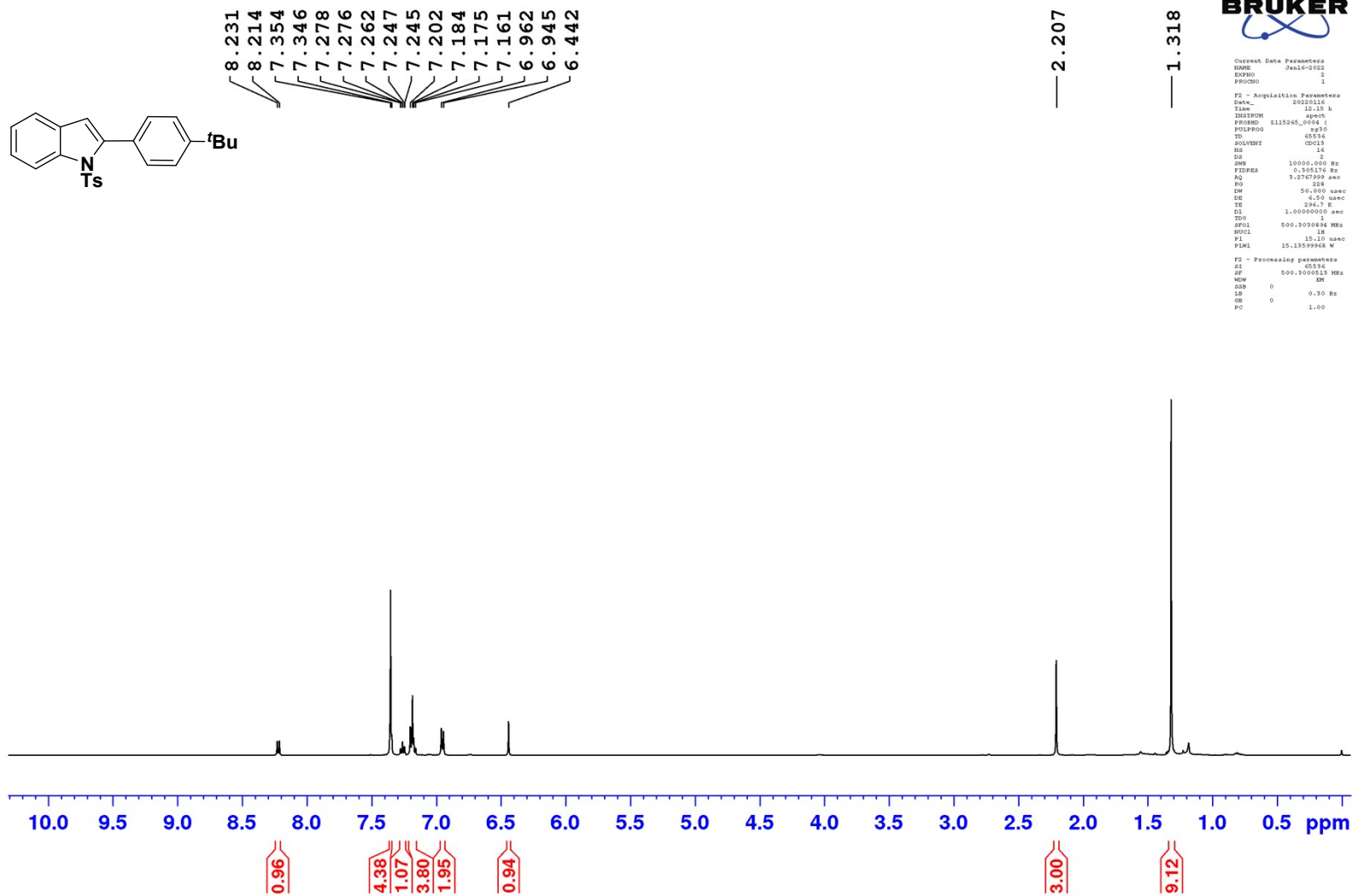


Figure S25. <sup>1</sup>H NMR spectrum of 3al in CDCl<sub>3</sub>

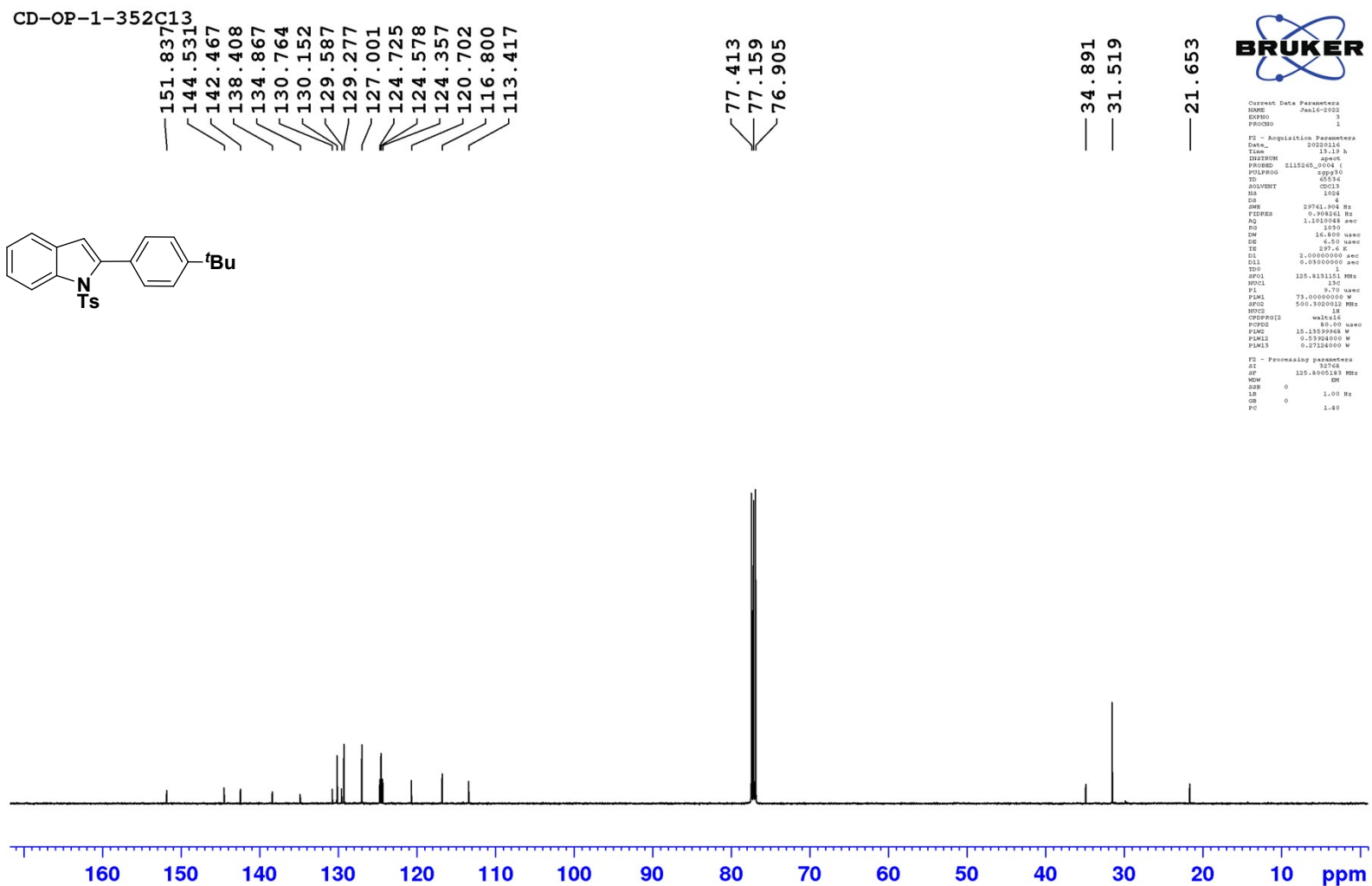


Figure S26.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3al** in  $\text{CDCl}_3$

CD-OP-1-356

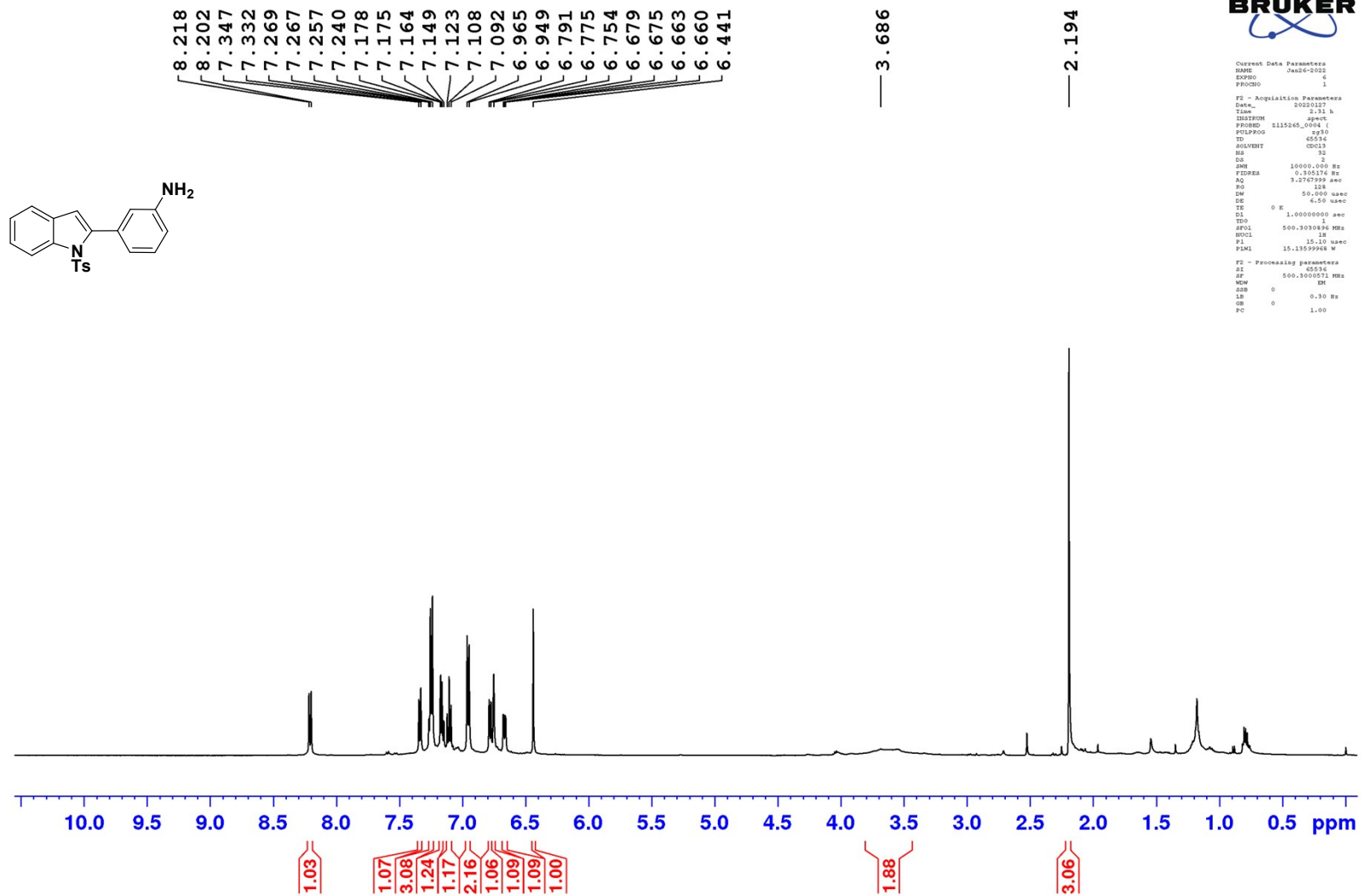
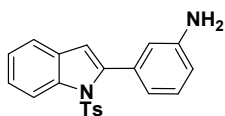


Figure S27. <sup>1</sup>H NMR spectrum of 3am in CDCl<sub>3</sub>

CD-OP-1-356-13c-CDCl<sub>3</sub>



145.687  
144.546  
142.532  
138.407  
134.871  
133.480  
130.690  
129.254  
128.532  
127.015  
124.756  
124.339  
120.777  
120.760  
117.426  
116.763  
115.604  
113.388

77.407  
77.153  
76.899

21.613



Current Data Parameters  
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PROCNO 1  
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PROBHD 1H1266\_0004 (1  
PULPROG zgpg30  
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SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 29761.294 Hz  
FIDRES 0.000461 Hz  
AQ 1.1010048 sec  
RG 2000  
DM 16.800 usec  
DE 0.500 usec  
TE 0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD 1  
SFO1 125.8131151 MHz  
NUC1 13C  
P1 9.70 usec  
PLM1 73.00000000 W  
SFO2 500.3020012 MHz  
NUC2 1H  
PCPDPRG2 waltz16  
PCPD 89.00 usec  
PLM2 15.13599968 W  
PLM3 0.23020000 W  
PLM3 0.27124000 W  
F2 - Processing parameters  
SI 32768  
SF 125.8095211 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

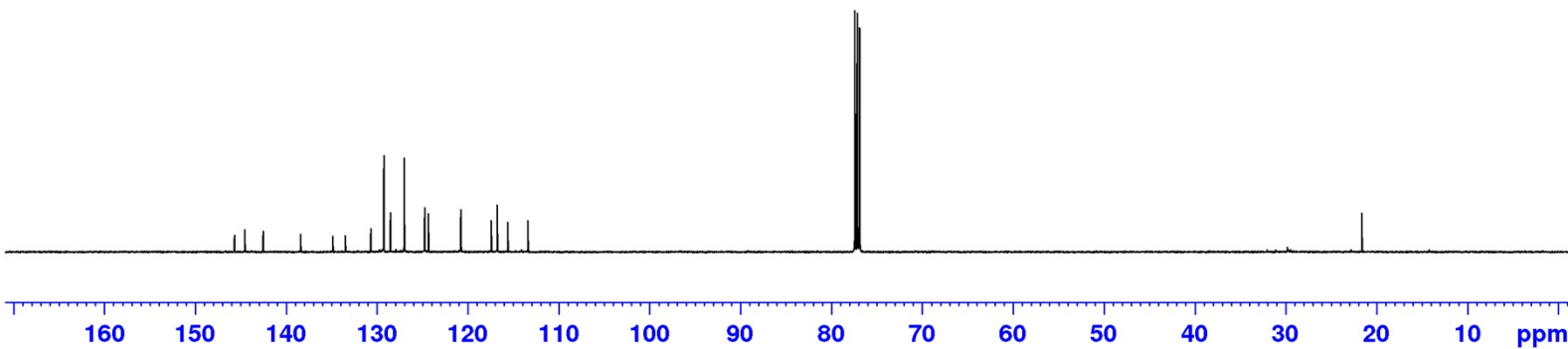


Figure S28. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 3am in CDCl<sub>3</sub>

# Spectrum Plot Report



Name	GM-354	Rack Pos.		Instrument	Instrument 1	Operator
Inj. Vol. (ul)	1	Plate Pos.		IRM Status	Success	
Data File	GM-354.d	Method (Acq)	KAMAL Method.m	Comment		Acq. Time (Local)
						15-12-2022 11:38:52 (UTC+05:30)

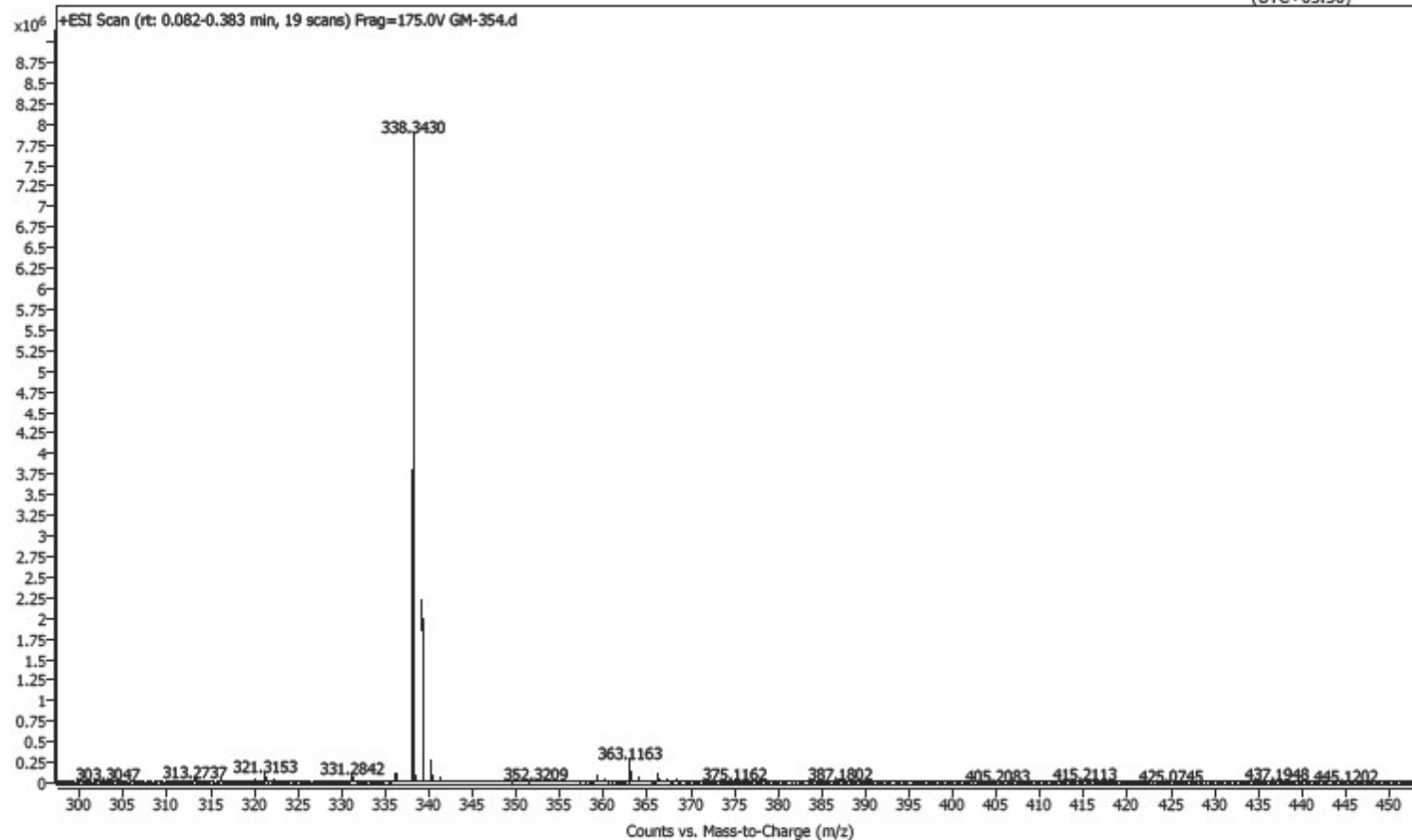


Figure S29. High Resolution Mass Spectrometry (HRMS) data of **3am**

CD-op-1-305

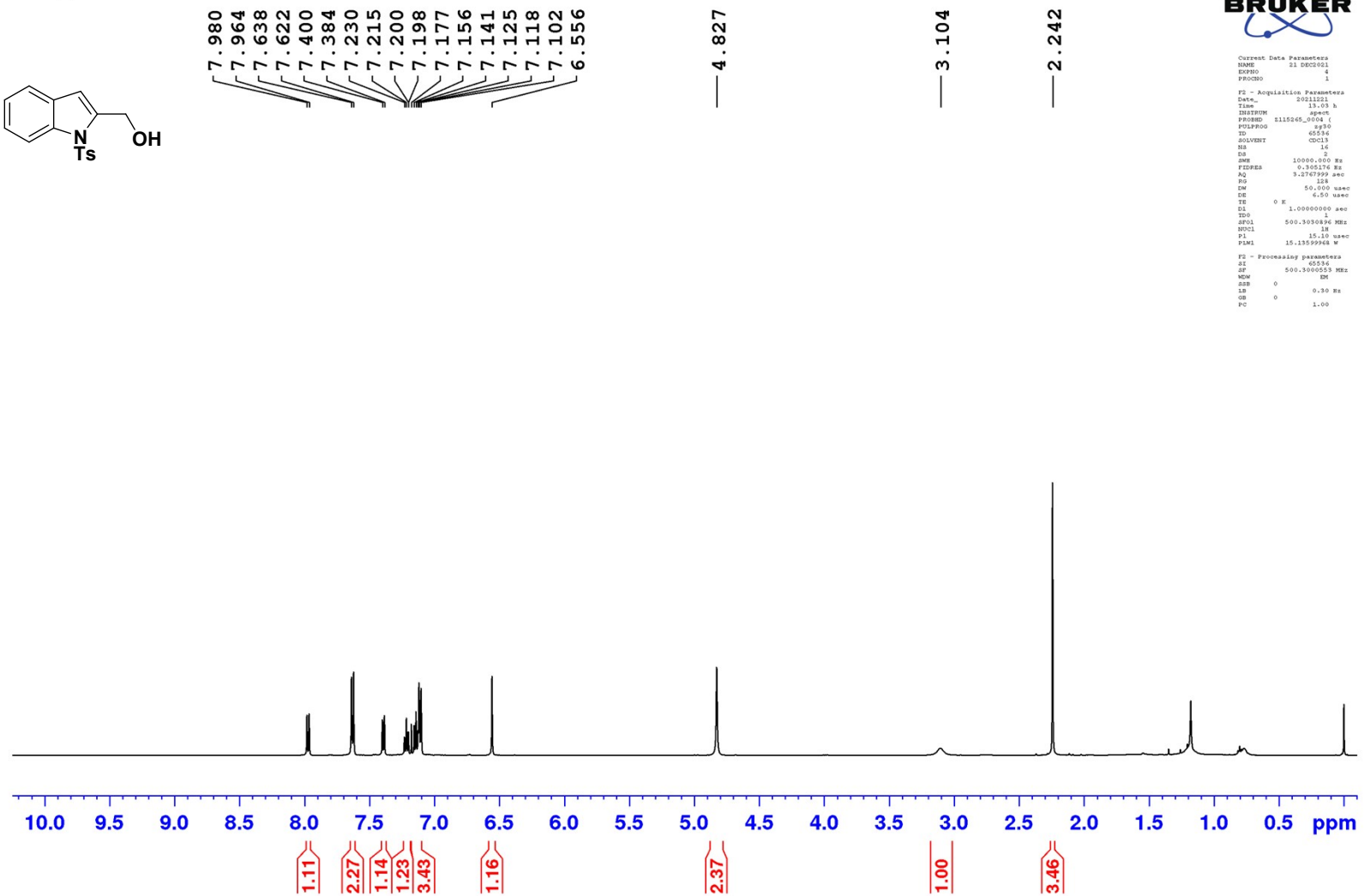
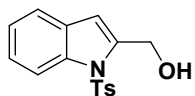
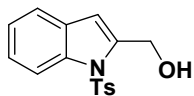


Figure S30.  $^1\text{H}$  NMR spectrum of **3an** in  $\text{CDCl}_3$

CD-OP-1-305C13



145.246  
140.328  
137.130  
135.710  
130.073  
129.219  
126.534  
125.084  
123.848  
121.292  
114.479  
111.330

77.411  
77.157  
76.903

58.689

21.653



```
Current Data Parameters
NAME      D1 DDC001
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    2011021
Time     19.01 h
INSTRUM  spect
PROBHD   E115260_0004 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS       381
DS        4
SFO1     29741.994 Hz
FIDRES   0.298261 Hz
AQ       1.1012048 sec
RG        2000
DW       16.800 usec
DE       5.50 usec
TE       0 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1
SFO1     125.8131151 MHz
NUC1      13C
P1       9.70 usec
PL1      78.00000000 W
SFO2     500.3620012 MHz
NUC2      1H
CPDPRG2  waltz16
PCPD2    80.00 usec
PLM2     15.13559968 W
PLM3     0.23924000 W
PLM13    0.27124000 W

F2 - Processing parameters
SI       32768
SF       125.8005337 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
```

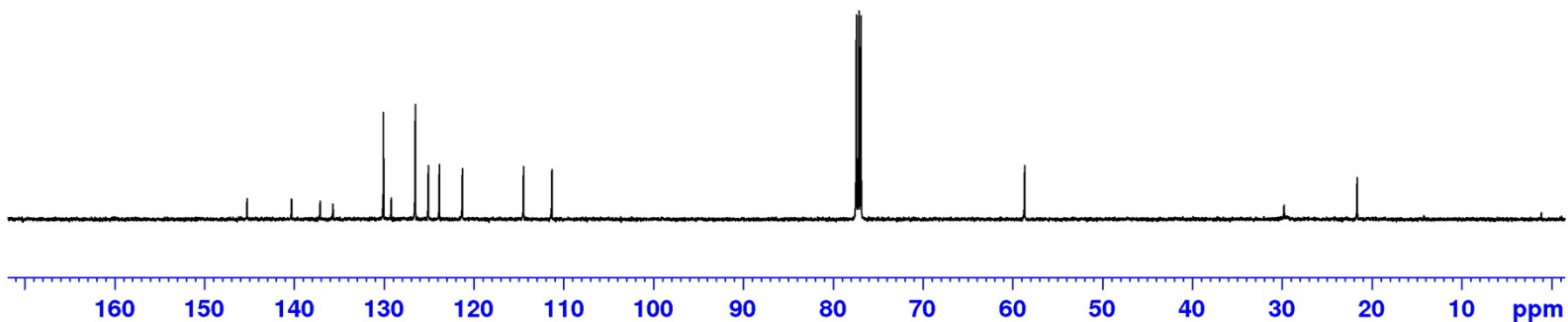
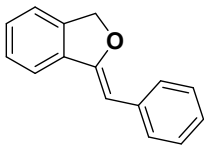


Figure S31.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3an** in  $\text{CDCl}_3$



CD-OP-1-358



7.788  
7.772  
7.606  
7.594  
7.388  
7.373  
7.359  
7.270  
7.196  
7.181  
7.167  
— 5.984  
— 5.543



```
Current Data Parameters
NAME      Jan25-2022
EXPNO    1
PROCNO   1
F2 - Acquisition Parameters
Date_    20220225
Time     11:02 h
INSTRUM  spect
PROBHD   5110245_0004 (
PULPROG  zgpg30
ID       65536
SOLVENT  CDCl3
NS       16
DS       2
SFO      600.115 Hz
FIDRES   0.001680 Hz
AQ       4.9632597 sec
RG       101
DW       75.733 usec
DE       6.50 usec
TE       0 K
D1       1.00000000 sec
TDO      500.302745 MHz
SFO1     500.302745 MHz
NUC1      1H
P1       15.10 usec
PL1      15.1359968 M
F2 - Processing parameters
SI       65536
SF       500.300194 MHz
WDW      EM
SSB      0
LB       0.10 Hz
GB       0
PC       1.00
```

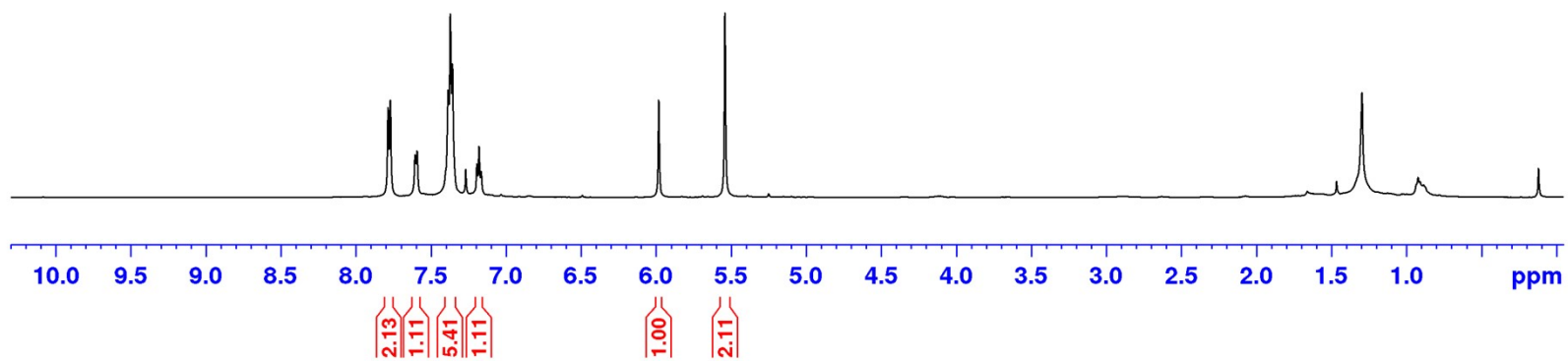


Figure S32. <sup>1</sup>H NMR spectrum of **4aa** in CDCl<sub>3</sub>

CD-OP-1-358-C13

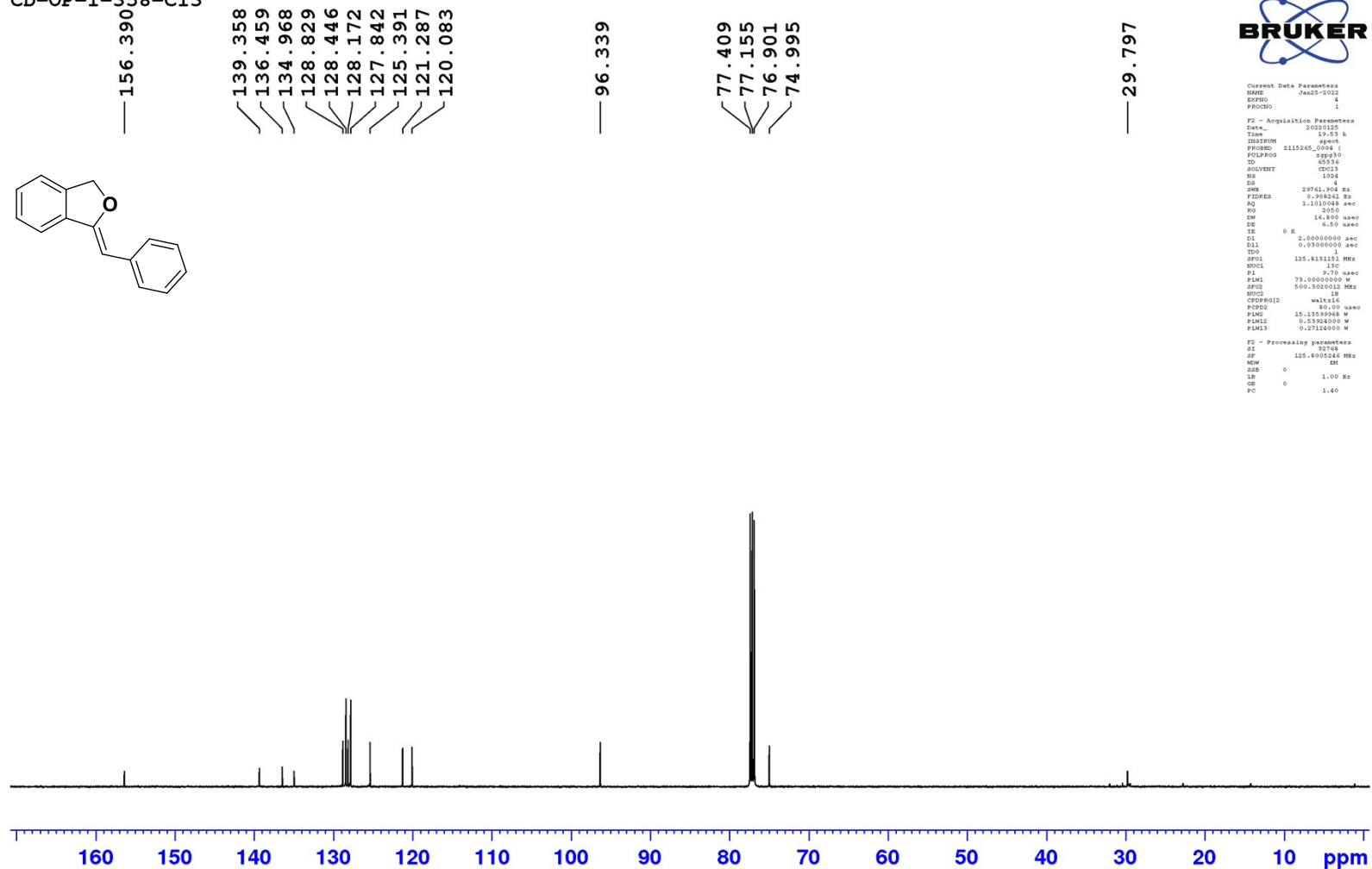
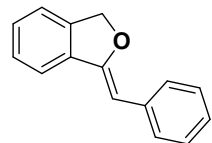


Figure S33.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **4aa** in  $\text{CDCl}_3$

CD-OP-1-375-1H

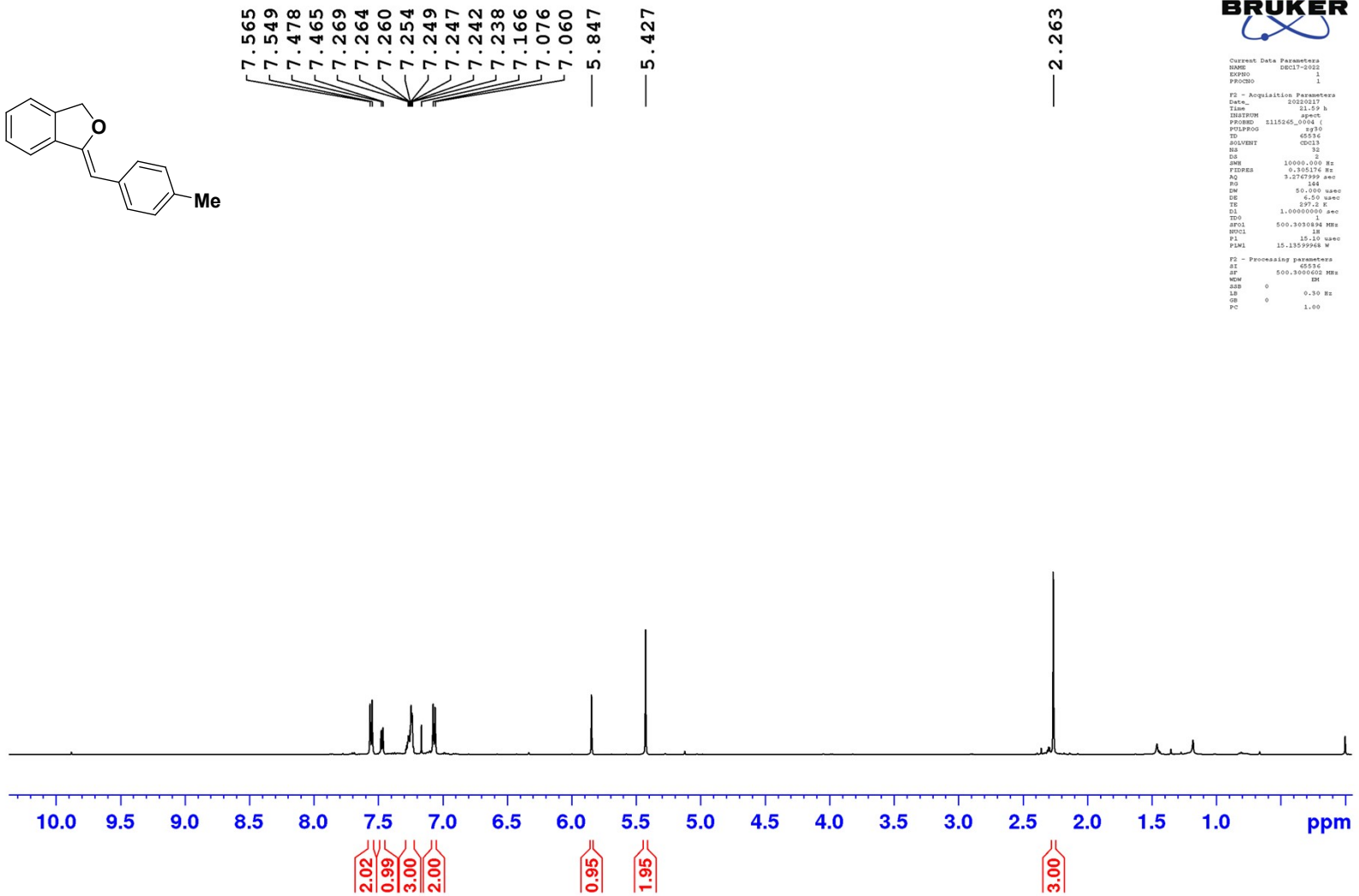
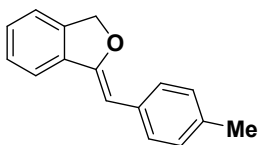


Figure S34. <sup>1</sup>H NMR spectrum of 4ab in CDCl<sub>3</sub>

CD-OP-1-375-13C

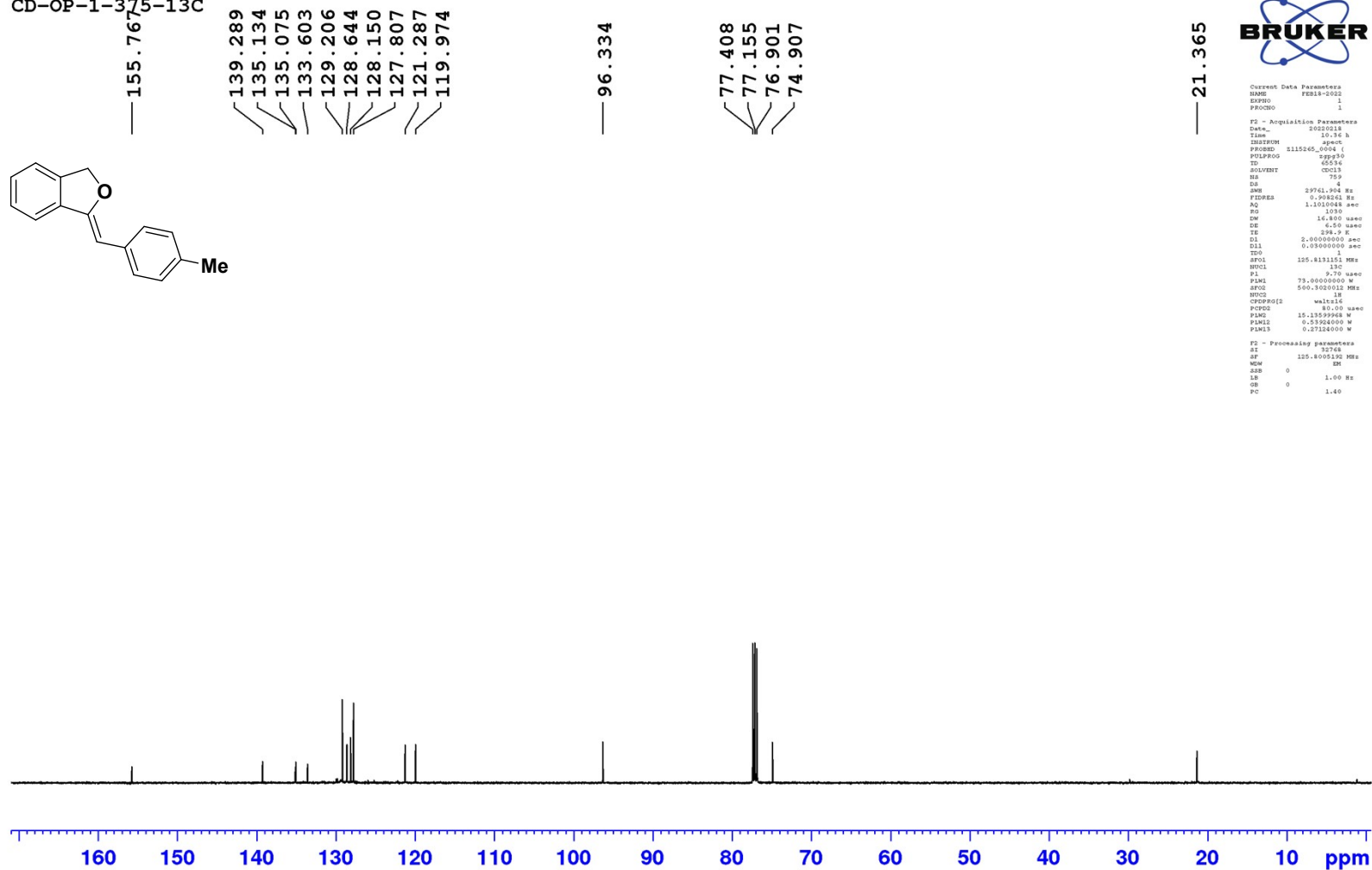
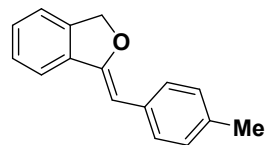
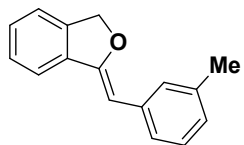


Figure S35.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **4ab** in  $\text{CDCl}_3$

CD-OP-1-376-1H



7.482  
7.463  
7.458  
7.451  
7.447  
7.261  
7.247  
7.240  
7.231  
7.228  
7.223  
7.217  
7.204  
7.154  
7.139  
7.123  
6.887  
6.872  
5.825  
5.403

2.282



```
Current Data Parameters
NAME      FEB14-2022
EXPNO    7
PROCNO   1

F2 - Acquisition Parameters
Date_    20220218
Time     20:11:5
INSTRUM  spect
PROBHD   1H5005_004 1
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS       16
DS       2
SWH       10000.000 Hz
FIDRES   0.305176 Hz
AQ        3.274799 sec
RG        64
RW        50.000 nsec
DE        6.50 nsec
TE        296.2 K
D1        1.00000000 sec
D2        1
SFO1     500.3030894 MHz
SFO2     18
SFO3     15.10000000 MHz
P1        15.10 nsec
PL1      15.10000000 W

F2 - Processing parameters
SI        65536
SF        500.300014 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
```

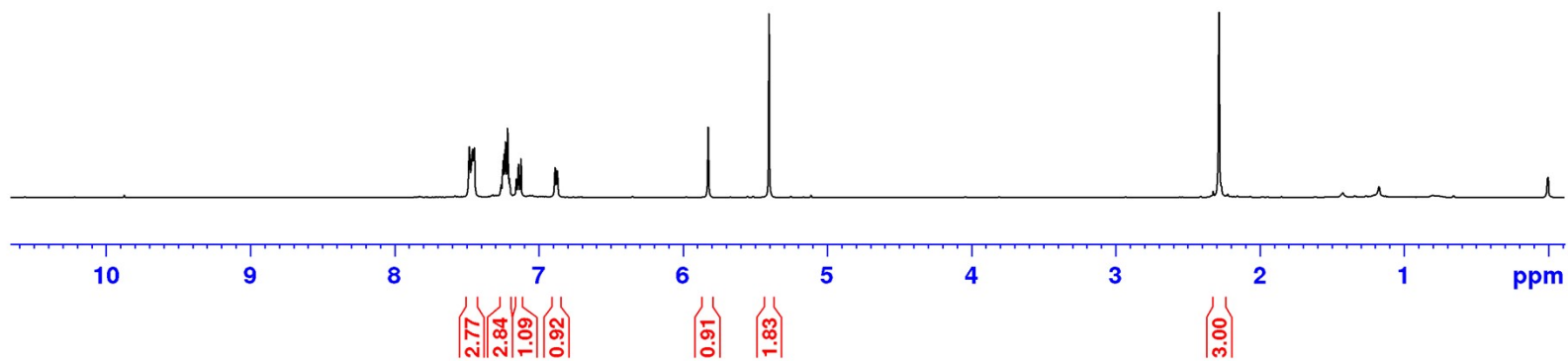
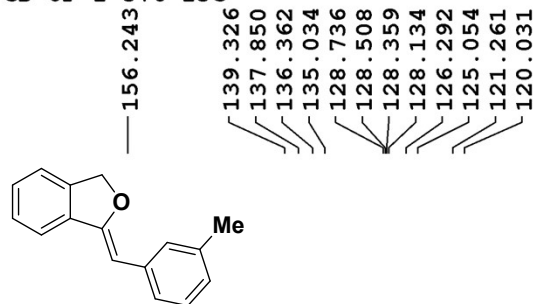


Figure S36. <sup>1</sup>H NMR spectrum of **4ac** in CDCl<sub>3</sub>

CD-OP-1-376-13C



96.420

77.411  
77.157  
76.903  
74.949

21.699



```
Current Data Parameters
NAME      FE18-2022
EXPNO    4
PROCNO   1
F2 - Acquisition Parameters
Date_    20220218
Time     21:03 h
INSTRUM  spect
PROBHD   E115245_0904 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        832
DS        4
SWH       29761.904 Hz
FIDRES    0.903601 Hz
AQ         1.1010048 sec
RG         3200
DE         16.800 usec
TE         300.2 K
DQ         6.00 usec
DE         297.9 Hz
DIL        1.00000000 sec
D11        0.03000000 sec
D12        1
D13        1
AF01      125.813151 MHz
NUC1       13C
P1         9.70 usec
PL1        71.00000000 W
RF12       500.3020151 MHz
NUC2
PCPPROG2  waltz16
PCPD2     80.00 usec
PLPG      15.1359968 W
PLM15     0.5324000 W
PLM13     0.2118000 W
F2 - Processing parameters
SI         32768
SF         125.8100521 MHz
WDW        EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
```

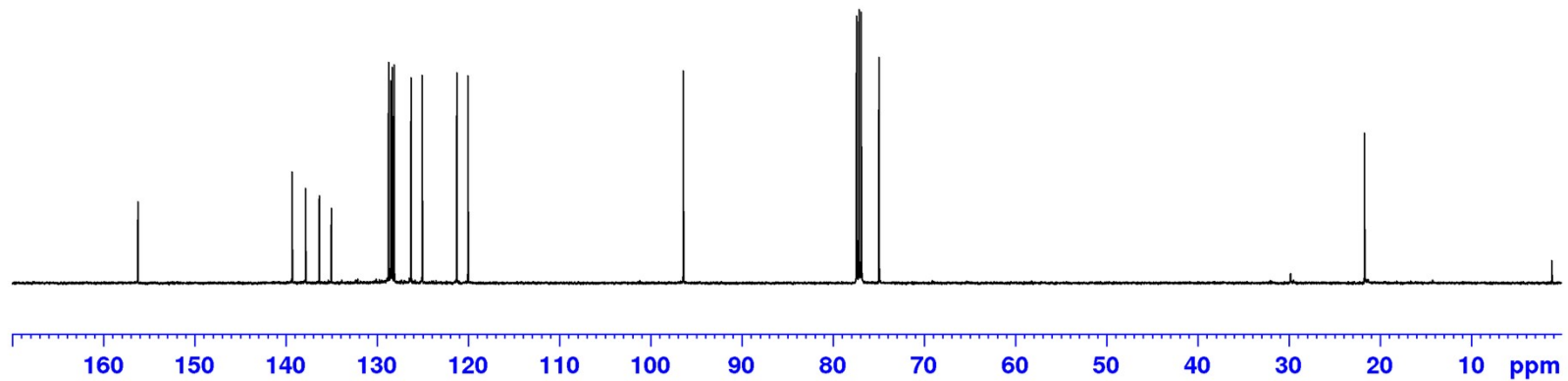


Figure S37.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **4ac** in  $\text{CDCl}_3$

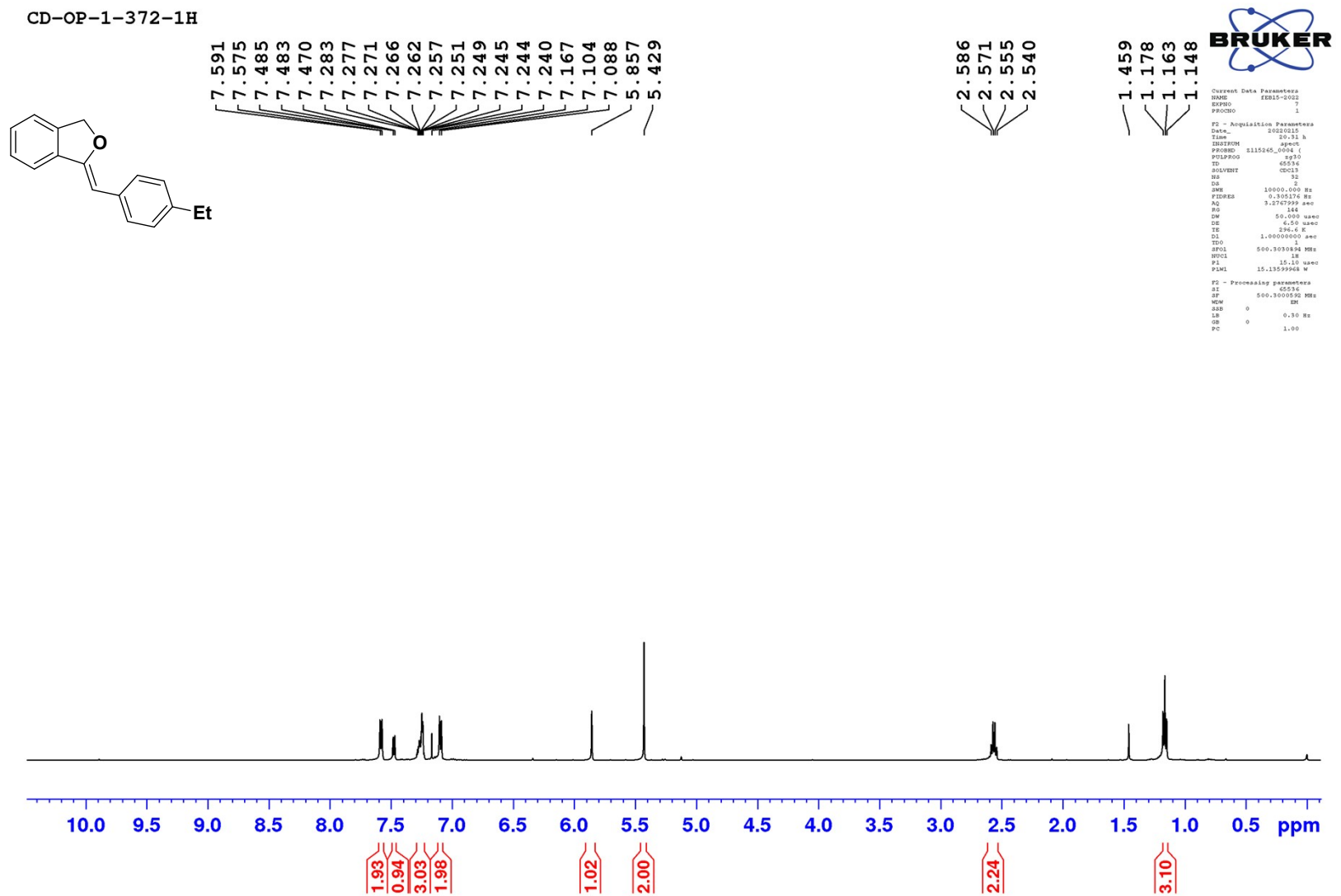
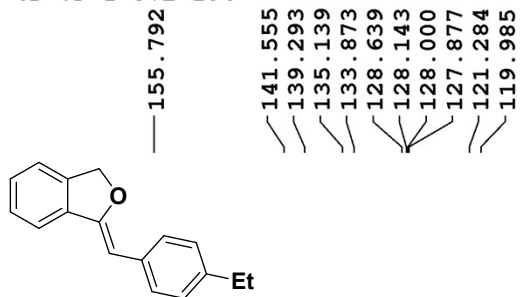


Figure S38. <sup>1</sup>H NMR spectrum of 4ad in CDCl<sub>3</sub>

CD-OP-1-372-13C



96.344

77.409  
77.155  
76.901  
74.897

28.791

15.760



```
Current Data Parameters
NAME      FEB15-2022
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20220215
Time     21:26 h
INSTRUM  spect
PROBHD   E115265_0904 (
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       2048
DS       4
SWH      29761.904 Hz
FIDRES   0.368248 Hz
AQ       1.1012084 sec
RG       3000
DN       16.800 usec
DE       4.00 usec
TE       298.2 K
D1       2.00000000 sec
d11      0.03000000 sec
TD0      1
SFO1     125.813151 MHz
HPC1     130
PI       9.70 usec
P1L1     73.00000000 W
SFO2     500.3020012 MHz
HPC2     18
CPDPRG2  waltz16
PCPD2    81.00 usec
PLM2     15.13599948 W
PLM3     0.53964000 W
PLM13    0.27124000 W

F2 - Processing parameters
SI       32768
SF       125.8005301 MHz
MSB      0
SGB      0
SGB      0
GB       0
PC       1.60
```

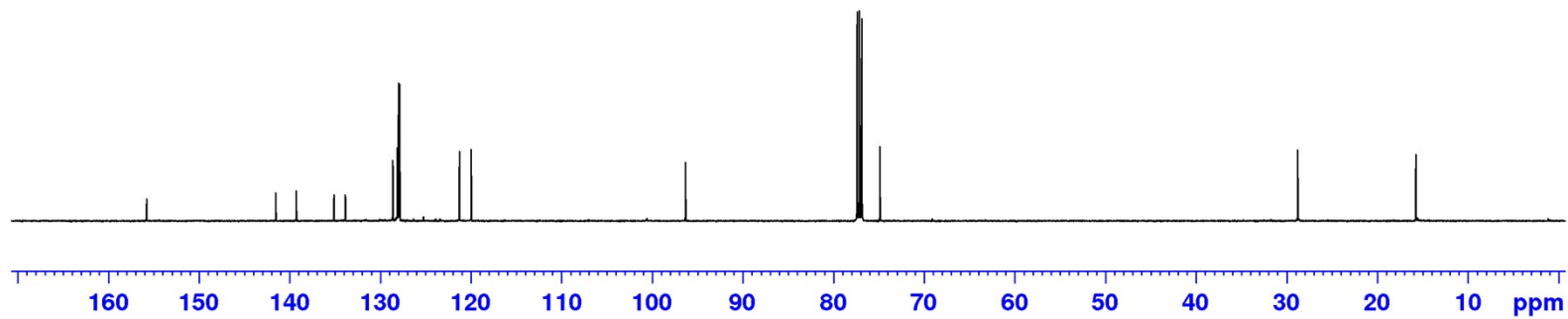


Figure S39.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **4ad** in  $\text{CDCl}_3$



CD-OP-1-370-1H

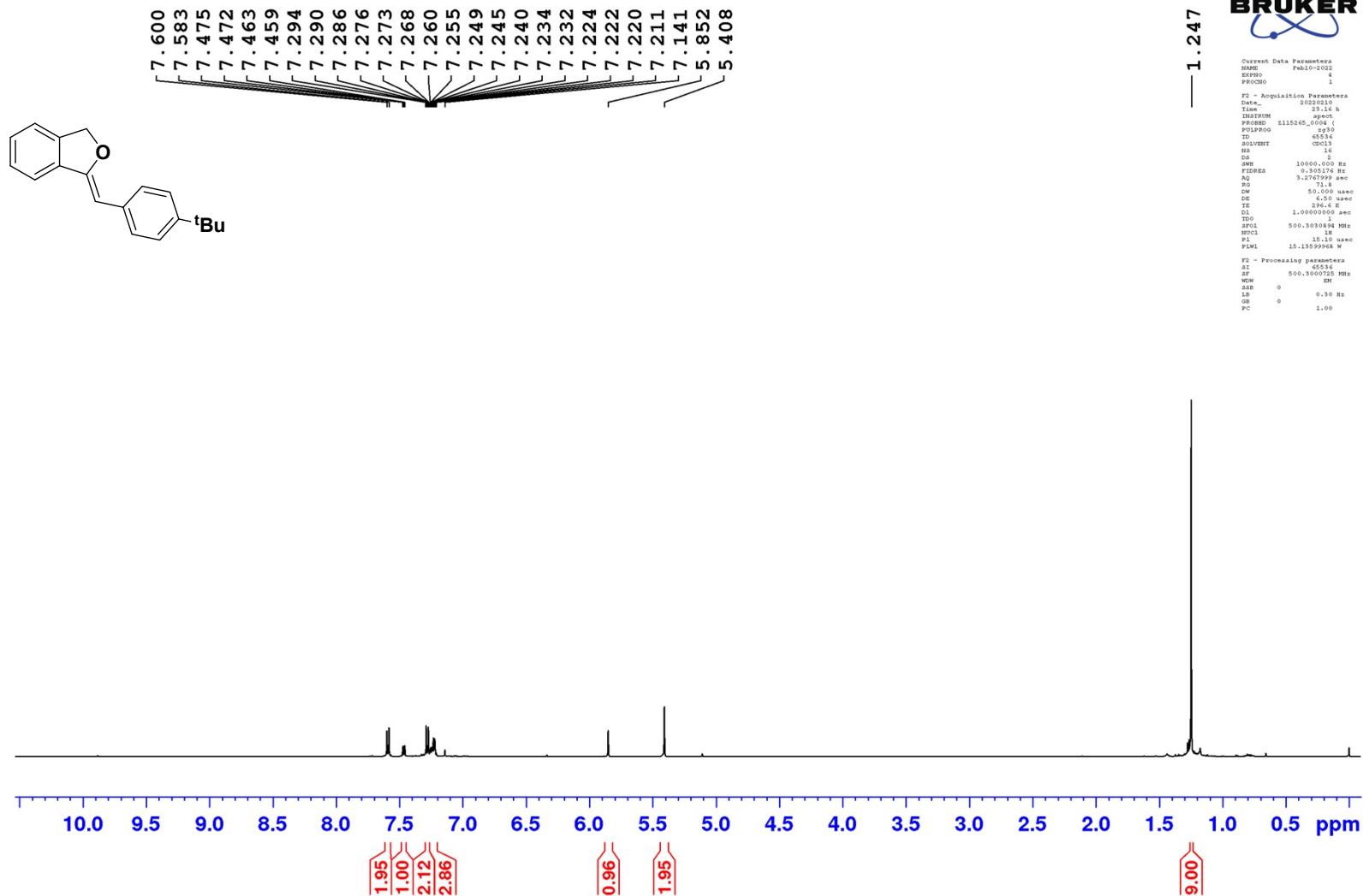
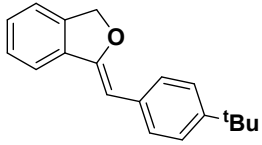


Figure S40. <sup>1</sup>H NMR spectrum of 4ae in CDCl<sub>3</sub>

CD-OP-1-370-13C



155.911

148.352

139.313

135.127

133.645

128.636

128.130

127.607

125.378

121.278

120.004

96.194

77.412

77.158

76.904

74.875

34.609

31.491



```
Current Data Parameters
NAME      Fabio-2022
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20220211
Time     1:13 h
INSTRUM  spect
PROBHD   E115265_6004 (
PULPROG  zgpg30
TD        65556
SOLVENT  CDCl3
NS        2048
DS        4
SWH       20761.994 Hz
FIDRES    0.998241 Hz
AQ         1.1018048 sec
RG         3200
DW         16.800 usec
DE         6.600 usec
TE         298.2 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
SFO1      125.811151 MHz
NUC1       13C
P1         9.70 usec
PLM1       73.00000000 W
SFO2      500.3020913 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2      90.00 usec
PLM2       15.13599968 W
PLM3       0.53984000 W
PLM33      0.27124000 W

F2 - Processing parameters
SI         32768
SF         125.8095228 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

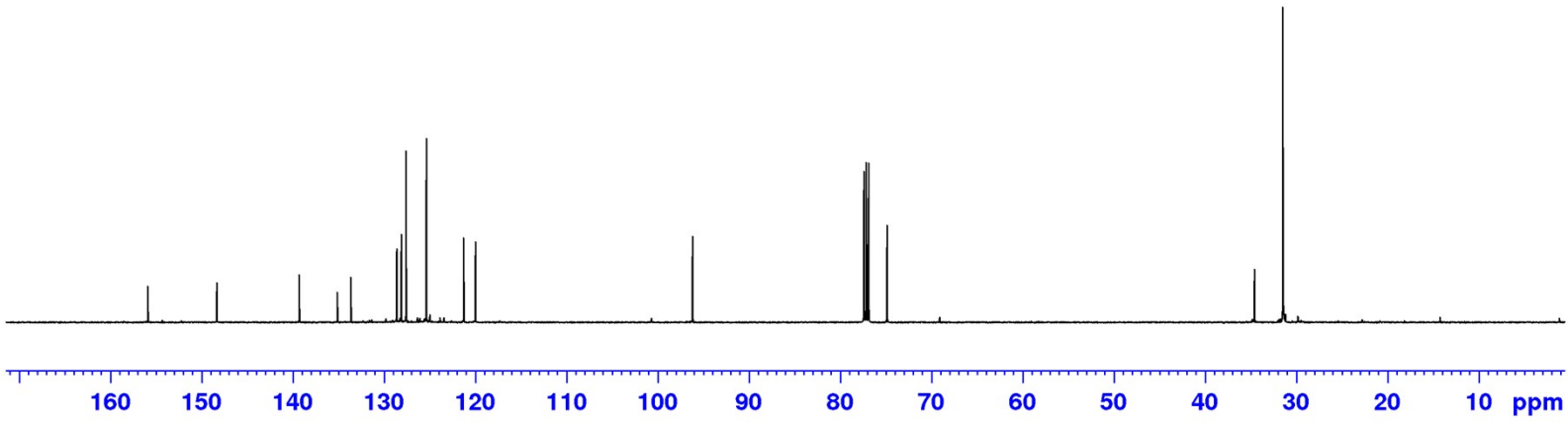


Figure S41.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 4ae in  $\text{CDCl}_3$

# Spectrum Plot Report



Name	GM-370	Rack Pos.		Instrument	Instrument 1	Operator
Inj. Vol. (ul)	1	Plate Pos.		IRM Status	Success	
Data File	GM-370.d	Method (Acq)	KAMAL Method.m	Comment		Acq. Time (Local)
						15-12-2022 11:34:19 (UTC+05:30)

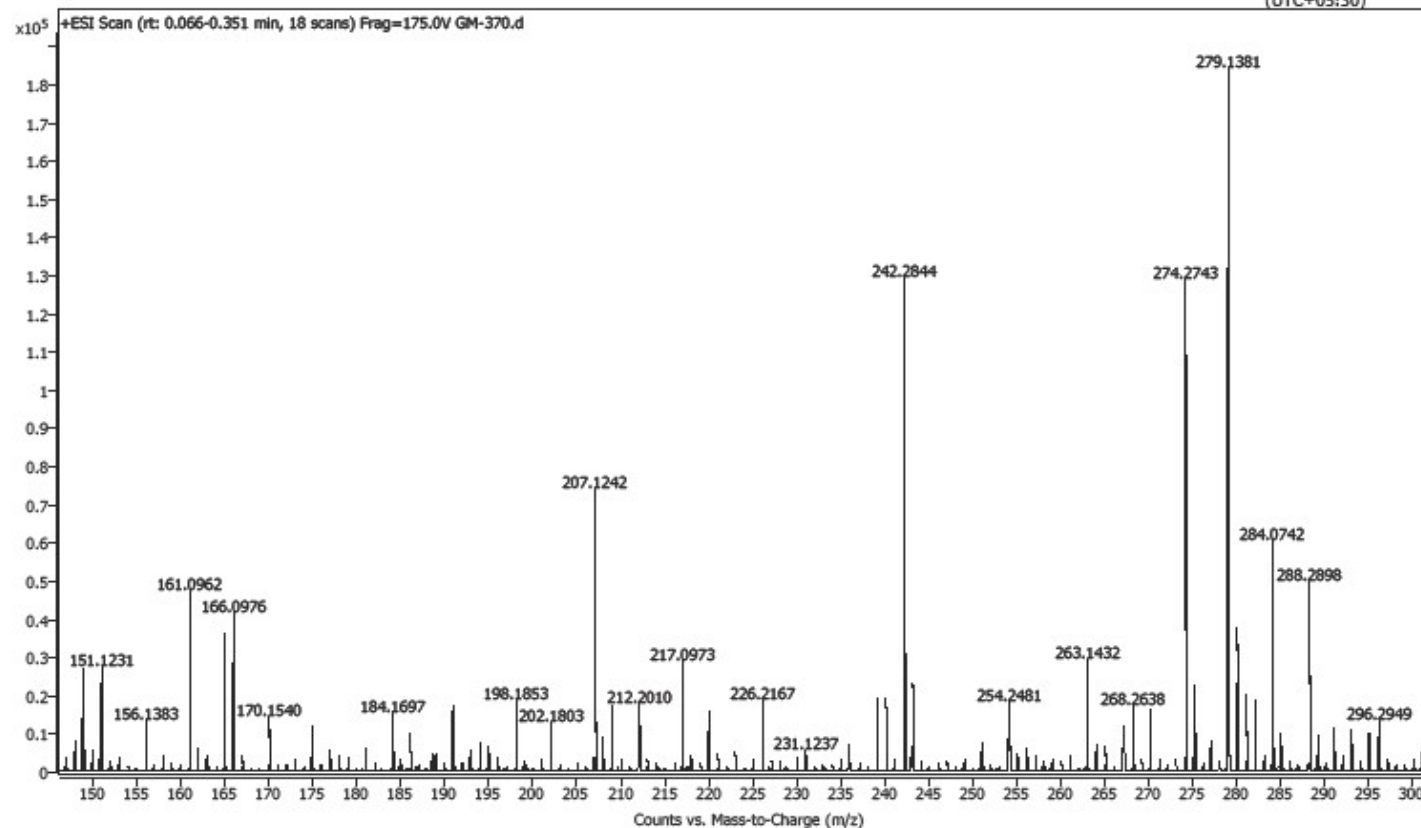


Figure S42. High Resolution Mass Spectrometry (HRMS) data of **4ae**

CD-OP-1-366-1H

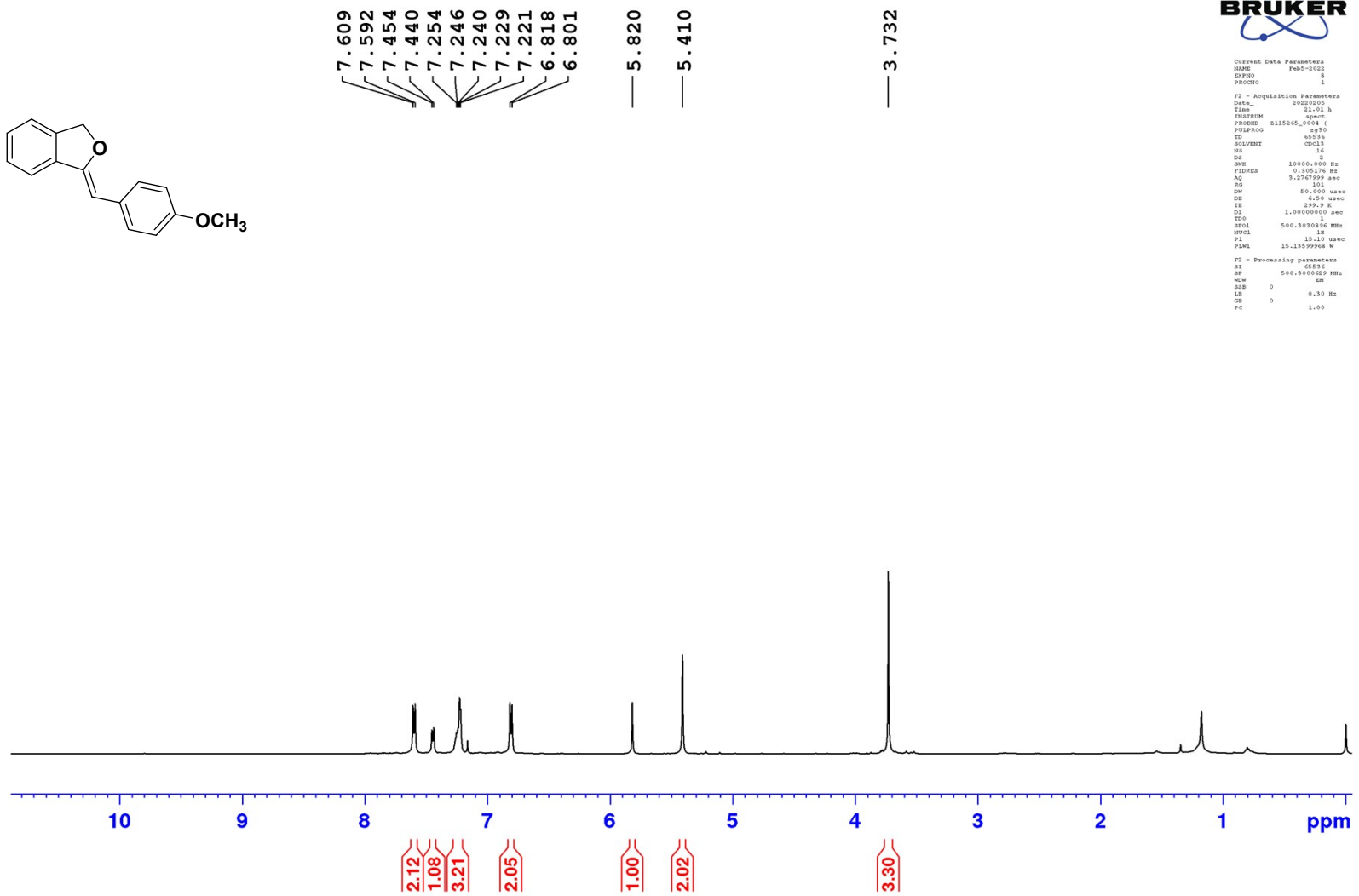
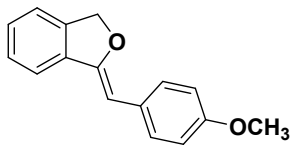
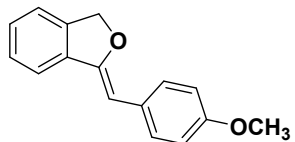


Figure S43.  $^1\text{H}$  NMR spectrum of **4af** in  $\text{CDCl}_3$

CD-OP-1-366-13C



157.566  
154.879

139.082  
135.147  
129.333  
129.059  
128.455  
128.111  
121.259  
119.781  
114.011

95.936

77.413  
77.158  
76.904  
74.790

55.396

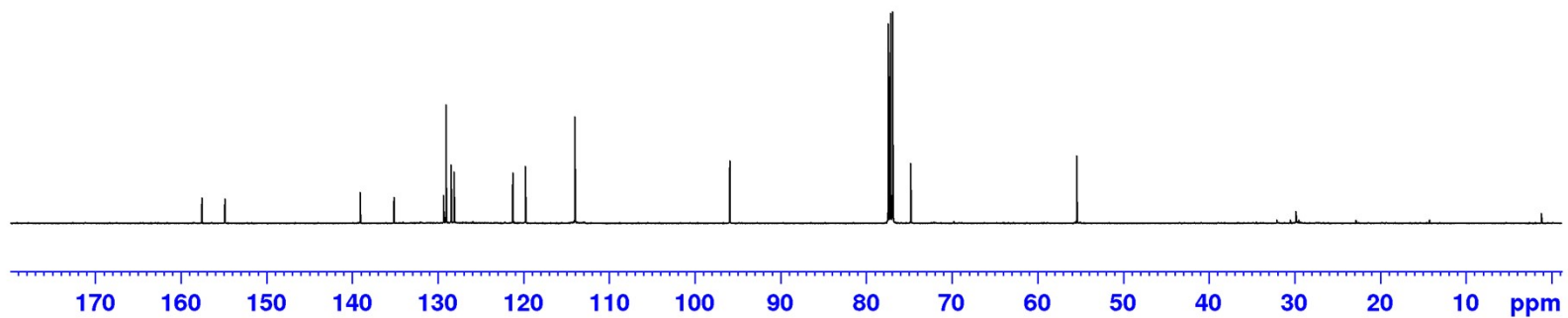


Figure S44.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **4af** in  $\text{CDCl}_3$

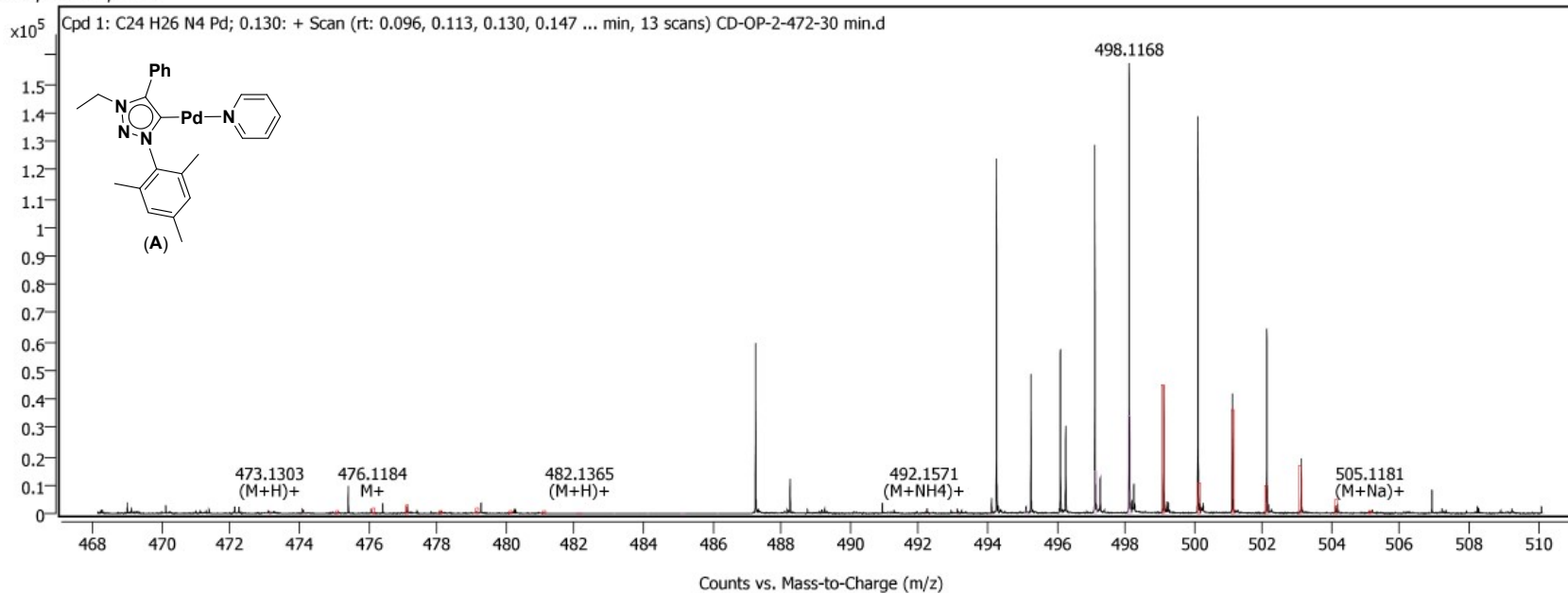


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Userfile Data Parameters
NAME      Feb 5 2022  9
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20220204
Time     01:40 h
INSTRUM  spect
PROBHD   1H5MMQ_0004 (
PULPROG  zgpg30
TE       300.2
SOLVENT  CDCl3
NS       4000
DS       4
SWH      29761.904 Hz
FIDRES   0.904241 Hz
AQ       1.101048 sec
RG       1030
DW       16.800 usec
DE       6.50 usec
TE       303.14 K
D1       2.00000000 sec
D11      0.08000000 sec
TD       65536
SFO1     125.811115 MHz
NUC1     13C
P1       130
PC1      9.70 usec
PL1      78.00000000 W
SFO2     500.1328012 MHz
NUC2     1H
PCPD2    80.00 usec
PL2      15.1859968 W
PL12     0.53924000 W
PL13     0.27124000 W

F2 - Processing parameters
SI       32768
SF       125.800528 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
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Compound Spectra

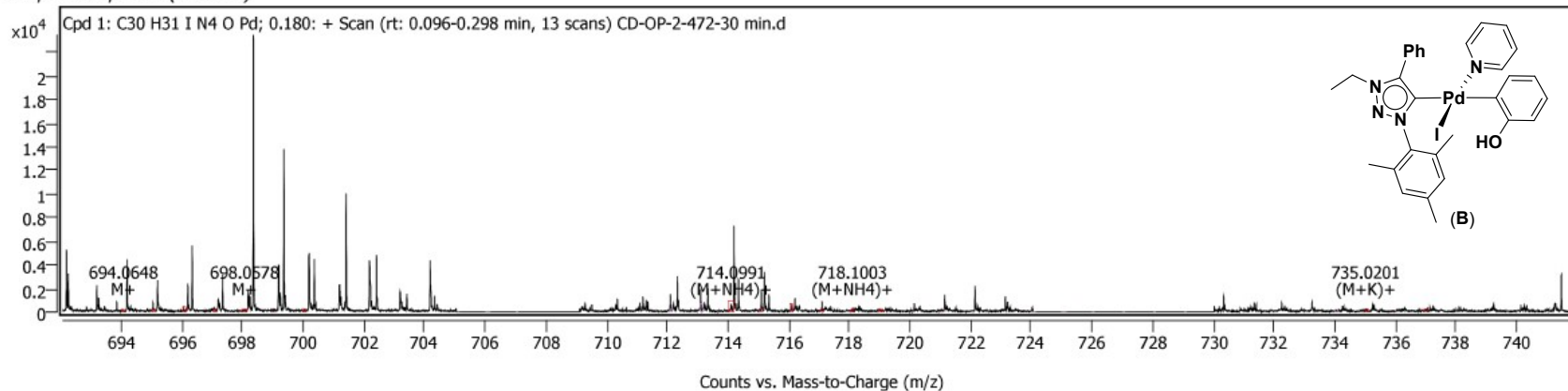


Spectrum Peaks

m/z	Z	Abund	Diff (ppm)	Height %	Height % (Calc)	Ion Species	Formula
473.1303	1	418	3.45	16.11	3.01	(M+H) <sup>+</sup>	C <sub>24</sub> H <sub>26</sub> N <sub>4</sub> Pd
475.1301	1	248	6.41	9.55	32.94	(M+H) <sup>+</sup>	C <sub>24</sub> H <sub>26</sub> N <sub>4</sub> Pd
476.1184	1	249	-2.45	100.00	100.00	M <sup>+</sup>	C <sub>24</sub> H <sub>26</sub> N <sub>4</sub> Pd
477.1257	1	2594	-3.73	100.00	100.00	(M+H) <sup>+</sup>	C <sub>24</sub> H <sub>26</sub> N <sub>4</sub> Pd
482.1365	1	157	10.77	6.06	9.82	(M+H) <sup>+</sup>	C <sub>24</sub> H <sub>26</sub> N <sub>4</sub> Pd
492.1571	1	167	6.94	48.66	32.84	(M+NH <sub>4</sub> ) <sup>+</sup>	C <sub>24</sub> H <sub>26</sub> N <sub>4</sub> Pd
494.1466	1	343	-14.91	100.00	100.00	(M+NH <sub>4</sub> ) <sup>+</sup>	C <sub>24</sub> H <sub>26</sub> N <sub>4</sub> Pd
499.1196	1	44955	20.50	100.00	100.00	(M+Na) <sup>+</sup>	C <sub>24</sub> H <sub>26</sub> N <sub>4</sub> Pd
505.1181	1	763	3.61	1.70	1.29	(M+Na) <sup>+</sup>	C <sub>24</sub> H <sub>26</sub> N <sub>4</sub> Pd
498.1168		158250					

Figure S45. High Resolution Mass Spectrometry (HRMS) data of Intermediate A

Compound Spectra (overlaid)

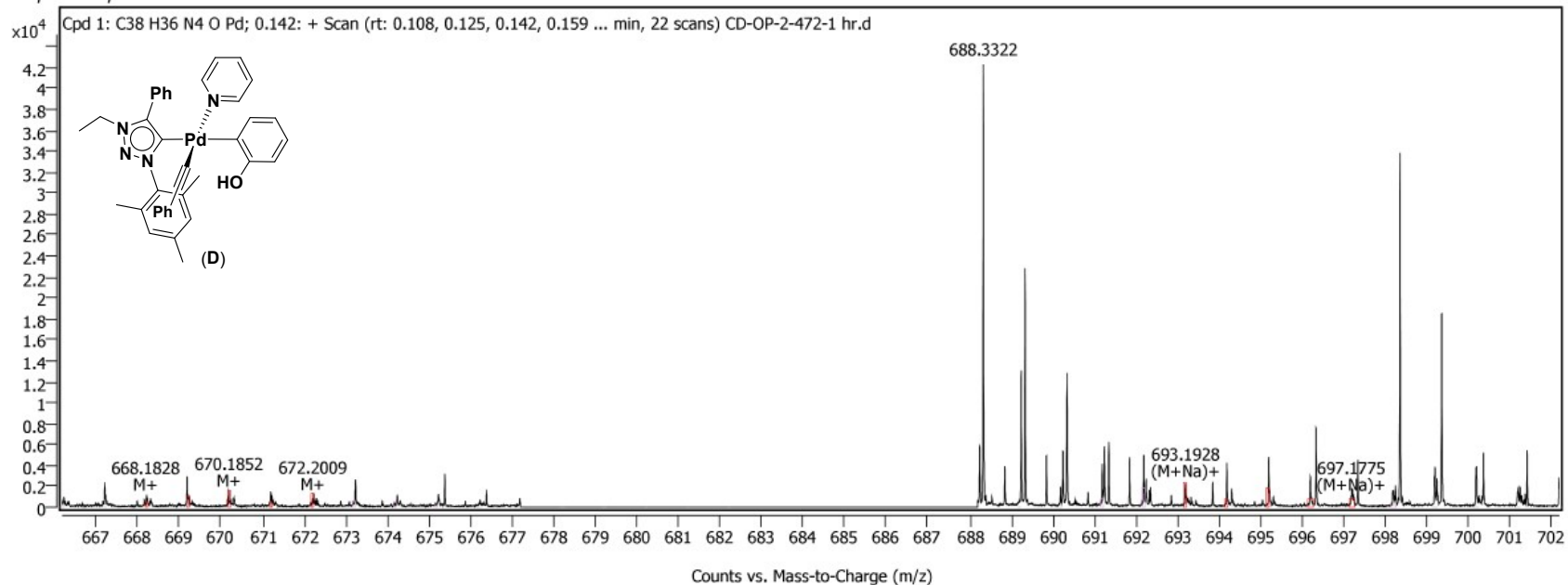


Spectrum Peaks

m/z	Z	Abund	Diff (ppm)	Height %	Height % (Calc)	Ion Species	Formula
694.0648	1	135	10.11	32.44	31.42	M+	C <sub>30</sub> H <sub>31</sub> I N <sub>4</sub> O Pd
695.0669	1	331	11.21	79.74	73.38	M+	C <sub>30</sub> H <sub>31</sub> I N <sub>4</sub> O Pd
696.0511	1	415	-10.38	100.00	100.00	M+	C <sub>30</sub> H <sub>31</sub> I N <sub>4</sub> O Pd
698.0578	1	225	-0.22	54.34	79.20	M+	C <sub>30</sub> H <sub>31</sub> I N <sub>4</sub> O Pd
699.0613	1	134	0.66	32.35	26.02	M+	C <sub>30</sub> H <sub>31</sub> I N <sub>4</sub> O Pd
700.0534	1	157	-8.61	37.95	37.31	M+	C <sub>30</sub> H <sub>31</sub> I N <sub>4</sub> O Pd
714.0991	1	718	9.01	98.60	100.00	(M+NH <sub>4</sub> ) <sup>+</sup>	C <sub>30</sub> H <sub>31</sub> I N <sub>4</sub> O Pd
716.0991	1	728	9.37	100.00	79.09	(M+NH <sub>4</sub> ) <sup>+</sup>	C <sub>30</sub> H <sub>31</sub> I N <sub>4</sub> O Pd
718.1003	1	366	8.99	50.22	37.31	(M+NH <sub>4</sub> ) <sup>+</sup>	C <sub>30</sub> H <sub>31</sub> I N <sub>4</sub> O Pd
719.0553	1	129	9.96	100.00	100.00	(M+Na) <sup>+</sup>	C <sub>30</sub> H <sub>31</sub> I N <sub>4</sub> O Pd
719.1026	1	135	8.53	18.48	11.91	(M+NH <sub>4</sub> ) <sup>+</sup>	C <sub>30</sub> H <sub>31</sub> I N <sub>4</sub> O Pd
735.0201	1	266	-2.49	100.00	100.00	(M+K) <sup>+</sup>	C <sub>30</sub> H <sub>31</sub> I N <sub>4</sub> O Pd
737.0221	1	162	0.71	60.64	84.50	(M+K) <sup>+</sup>	C <sub>30</sub> H <sub>31</sub> I N <sub>4</sub> O Pd

Figure S46. High Resolution Mass Spectrometry (HRMS) data of Intermediate B

Compound Spectra



Spectrum Peaks

m/z	Z	Abund	Diff (ppm)	Height %	Height % (Calc)	Ion Species	Formula
668.1828	1	333	-14.49	21.57	29.59	M+	C <sub>38</sub> H <sub>36</sub> N <sub>4</sub> OPd
670.1852	1	1545	-11.94	100.00	100.00	M+	C <sub>38</sub> H <sub>36</sub> N <sub>4</sub> OPd
672.2009	1	855	11.91	55.31	77.16	M+	C <sub>38</sub> H <sub>36</sub> N <sub>4</sub> OPd
693.1928	1	2269	14.09	100.00	100.00	(M+Na)+	C <sub>38</sub> H <sub>36</sub> N <sub>4</sub> OPd
697.1775	1	1114	-9.54	49.11	37.41	(M+Na)+	C <sub>38</sub> H <sub>36</sub> N <sub>4</sub> OPd
688.3322		42712					

Figure S47. High Resolution Mass Spectrometry (HRMS) data of Intermediate D



**Table S1.** Crystal data and structure refinement for **2b**

Identification code	<b>2b</b>
Empirical formula	C <sub>24</sub> H <sub>26</sub> N <sub>4</sub> PdI <sub>2</sub>
Formula weight	730.69
Temperature/K	145(2)
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /n
a/Å	9.5780(3)
b/Å	16.2412(6)
c/Å	33.3733(12)
α/°	90
β/°	96.3530(10)
γ/°	90
Volume/Å <sup>3</sup>	5159.6(3)
Z	8
ρ <sub>calc</sub> /g/cm <sup>3</sup>	1.881
μ/mm <sup>-1</sup>	3.131
F(000)	2800.0
Crystal size/mm <sup>3</sup>	0.2 × 0.17 × 0.14
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.456 to 51.448
Index ranges	-11 ≤ h ≤ 10, -19 ≤ k ≤ 19, -40 ≤ l ≤ 40
Reflections collected	52632
Independent reflections	9808 [R <sub>int</sub> = 0.0509, R <sub>sigma</sub> = 0.0365]
Data/restraints/parameters	9808/0/567
Goodness-of-fit on F <sup>2</sup>	1.206
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0430, wR <sub>2</sub> = 0.0883
Final R indexes [all data]	R <sub>1</sub> = 0.0498, wR <sub>2</sub> = 0.0906
Largest diff. peak/hole / e Å <sup>-3</sup>	1.57/-0.87

**Table S2.** Bond lengths for **2b**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.383(8)	C27	C28	1.383(8)
C1	N4	1.379(7)	C27	C32	1.397(8)
C1	Pd1	1.970(5)	C28	C29	1.391(9)
C2	C3	1.466(8)	C29	C30	1.374(9)
C2	N2	1.358(7)	C30	C31	1.382(9)
C3	C4	1.401(8)	C31	C32	1.379(9)
C3	C8	1.390(9)	C33	C34	1.497(10)
C4	C5	1.386(9)	C33	N6	1.478(8)
C5	C6	1.382(9)	C35	C36	1.398(9)
C6	C7	1.388(9)	C35	C40	1.384(9)
C7	C8	1.377(9)	C35	N8	1.451(8)

C9	C10	1.506(12)	C36	C37	1.387(10)
C9	N2	1.478(8)	C36	C41	1.516(10)
C11	C12	1.397(8)	C37	C38	1.410(11)
C11	C16	1.389(9)	C38	C39	1.378(10)
C11	N4	1.452(8)	C38	C42	1.523(10)
C12	C13	1.382(9)	C39	C40	1.387(9)
C12	C17	1.495(9)	C40	C43	1.510(9)
C13	C14	1.401(10)	C44	C45	1.390(9)
C14	C15	1.373(10)	C44	N5	1.321(8)
C14	C18	1.505(9)	C45	C46	1.361(10)
C15	C16	1.404(9)	C46	C47	1.382(10)
C16	C19	1.499(9)	C47	C48	1.376(9)
C20	C21	1.375(9)	C48	N5	1.347(8)
C20	N1	1.331(8)	N1	Pd1	2.116(5)
C21	C22	1.397(10)	N2	N3	1.322(7)
C22	C23	1.374(10)	N3	N4	1.328(7)
C23	C24	1.378(9)	N5	Pd2	2.107(5)
C24	N1	1.338(8)	N6	N7	1.319(7)
C25	C26	1.394(8)	N7	N8	1.331(7)
C25	N8	1.382(7)	Pd1	I1	2.6208(6)
C25	Pd2	1.980(6)	Pd1	I2	2.5973(6)
C26	C27	1.477(8)	Pd2	I3	2.5801(6)
C26	N6	1.359(7)	Pd2	I4	2.6281(6)

**Table S3. Bond angles for 2b**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C1	Pd1	126.1(4)	C40	C35	C36	123.1(6)
N4	C1	C2	103.2(5)	C40	C35	N8	120.0(5)
N4	C1	Pd1	130.7(4)	C35	C36	C41	123.0(6)
C1	C2	C3	128.7(5)	C37	C36	C35	117.3(6)
N2	C2	C1	106.1(5)	C37	C36	C41	119.7(6)
N2	C2	C3	125.2(5)	C36	C37	C38	121.5(6)
C4	C3	C2	119.2(5)	C37	C38	C42	120.2(7)
C8	C3	C2	121.7(5)	C39	C38	C37	118.0(6)
C8	C3	C4	119.0(6)	C39	C38	C42	121.7(7)
C5	C4	C3	119.6(6)	C38	C39	C40	122.7(7)
C6	C5	C4	120.9(6)	C35	C40	C39	117.1(6)
C5	C6	C7	119.6(6)	C35	C40	C43	122.7(6)
C8	C7	C6	120.0(6)	C39	C40	C43	120.1(6)
C7	C8	C3	121.0(6)	N5	C44	C45	123.0(6)
N2	C9	C10	112.1(6)	C46	C45	C44	119.1(7)
C12	C11	N4	118.7(5)	C45	C46	C47	118.8(6)
C16	C11	C12	123.2(6)	C48	C47	C46	118.7(6)
C16	C11	N4	118.1(5)	N5	C48	C47	122.9(6)
C11	C12	C17	121.2(6)	C20	N1	C24	118.5(5)
C13	C12	C11	117.1(6)	C20	N1	Pd1	122.1(4)
C13	C12	C17	121.7(6)	C24	N1	Pd1	119.4(4)
C12	C13	C14	122.2(6)	C2	N2	C9	128.6(5)
C13	C14	C18	120.3(7)	N3	N2	C2	113.5(5)
C15	C14	C13	118.2(6)	N3	N2	C9	117.9(5)
C15	C14	C18	121.5(7)	N2	N3	N4	103.1(4)
C14	C15	C16	122.5(6)	C1	N4	C11	128.5(5)
C11	C16	C15	116.6(6)	N3	N4	C1	114.1(5)
C11	C16	C19	122.7(6)	N3	N4	C11	117.4(5)
C15	C16	C19	120.7(6)	C44	N5	C48	117.4(5)
N1	C20	C21	123.2(6)	C44	N5	Pd2	126.2(4)
C20	C21	C22	118.3(6)	C48	N5	Pd2	116.4(4)
C23	C22	C21	118.4(6)	C26	N6	C33	128.9(5)
C22	C23	C24	119.7(7)	N7	N6	C26	113.2(5)
N1	C24	C23	122.0(6)	N7	N6	C33	117.4(5)
C26	C25	Pd2	126.8(4)	N6	N7	N8	103.8(5)
N8	C25	C26	102.9(5)	C25	N8	C35	129.2(5)
N8	C25	Pd2	130.2(4)	N7	N8	C25	113.8(5)
C25	C26	C27	130.5(5)	N7	N8	C35	116.4(5)
N6	C26	C25	106.3(5)	C1	Pd1	N1	176.0(2)
N6	C26	C27	122.9(5)	C1	Pd1	I1	87.90(17)
C28	C27	C26	121.9(5)	C1	Pd1	I2	88.99(17)
C28	C27	C32	118.5(6)	N1	Pd1	I1	92.12(14)
C32	C27	C26	119.5(5)	N1	Pd1	I2	90.49(14)
C27	C28	C29	120.6(6)	I2	Pd1	I1	172.31(2)
C30	C29	C28	120.2(6)	C25	Pd2	N5	172.8(2)
C29	C30	C31	119.6(6)	C25	Pd2	I3	89.24(16)
C32	C31	C30	120.5(6)	C25	Pd2	I4	90.91(16)
C31	C32	C27	120.4(6)	N5	Pd2	I3	90.93(14)
N6	C33	C34	110.7(6)	N5	Pd2	I4	88.96(14)
C36	C35	N8	116.7(6)	I3	Pd2	I4	179.62(3)

