

Supporting Information

Synthesis of 4-Isoxazolines through Gold(I)-Catalyzed Cyclization of Propargylic *N*-Hydroxylamines

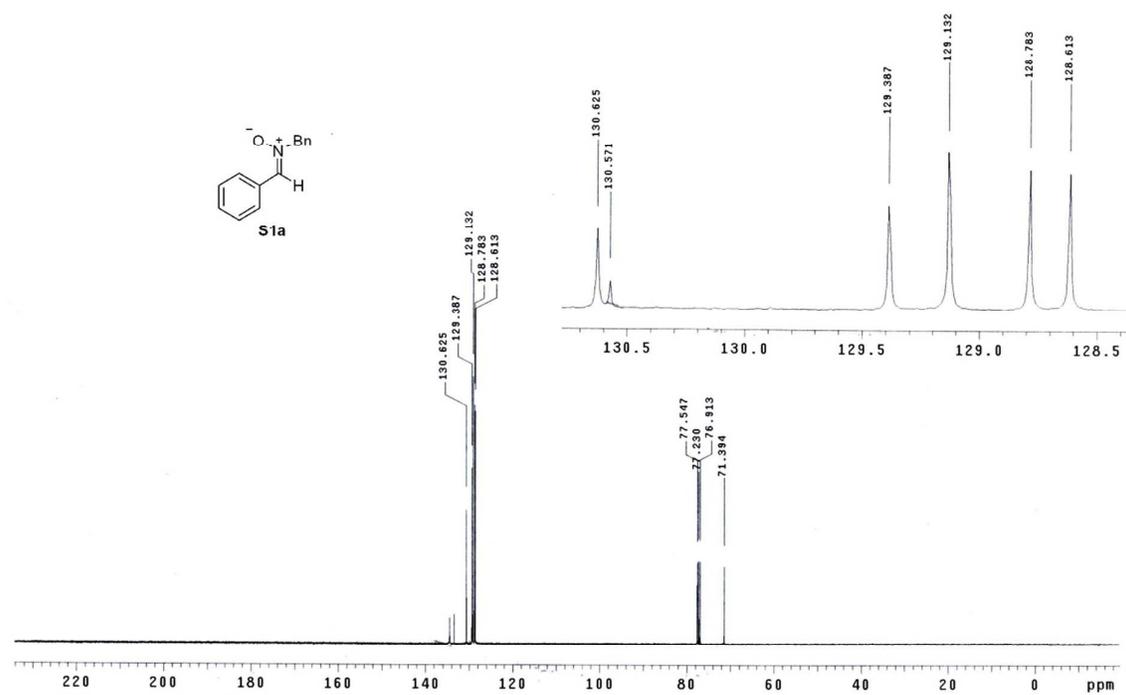
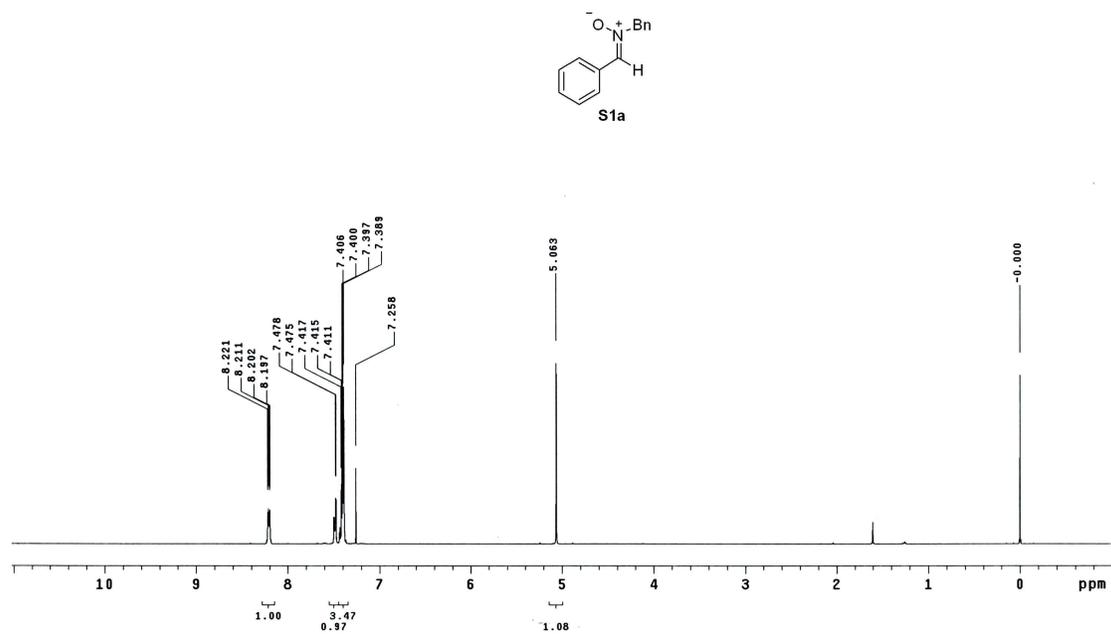
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University, 52 Ewhayeodae-gil, Seodaemun-Gu, Seoul 03760, Republic of Korea.*

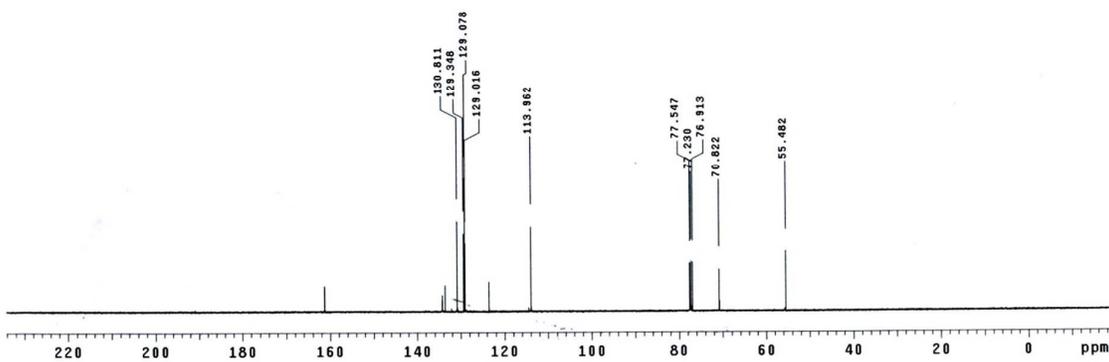
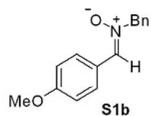
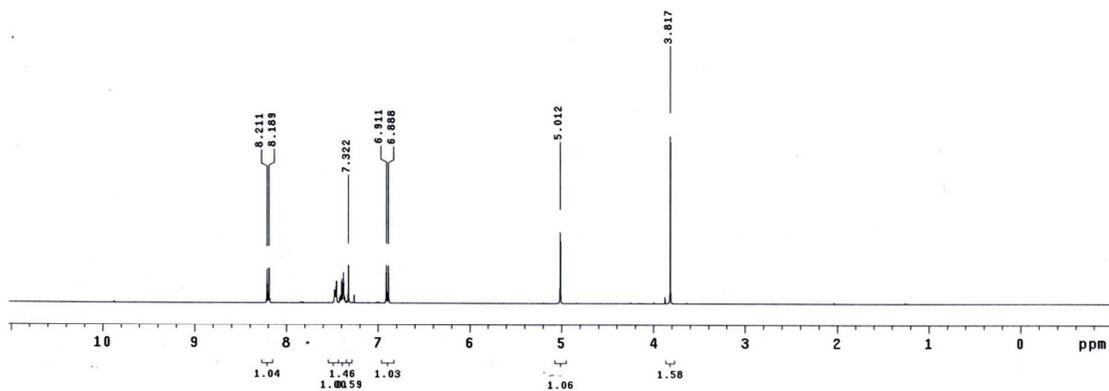
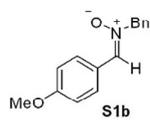
E-mail: ryuj@ewha.ac.kr; Fax+82 2 3277 2851; Tel: +82 2 3277 3008

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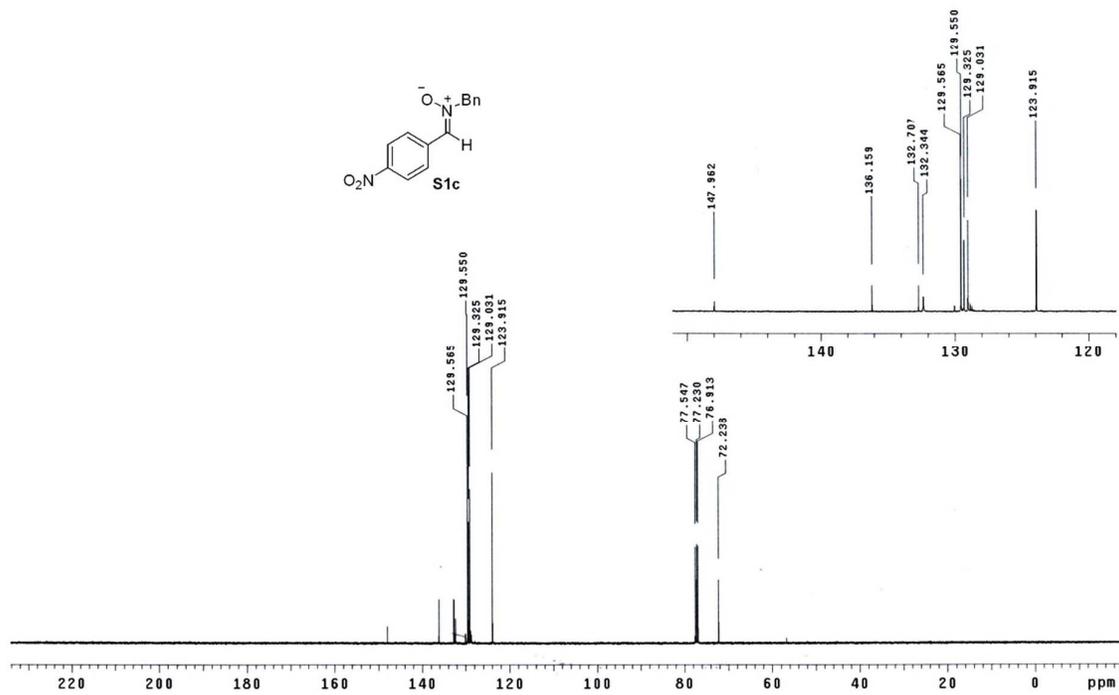
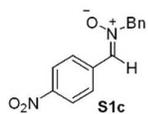
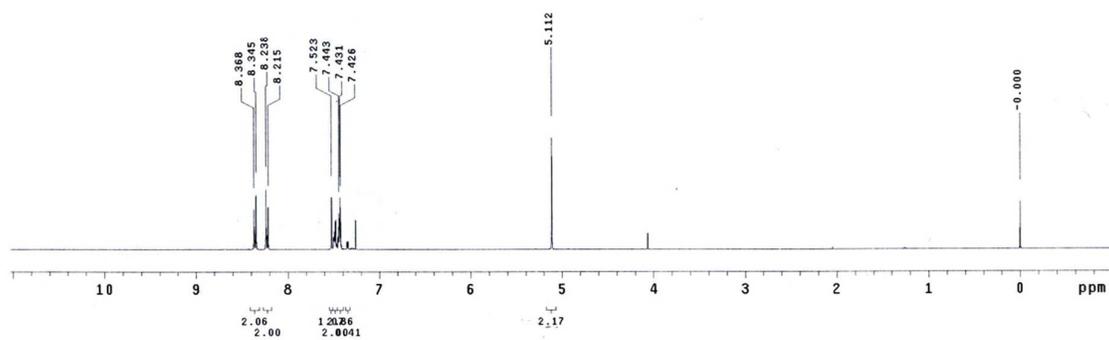
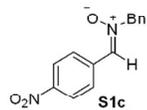
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A. $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ chart for S1a-f, 1a-s, and 2a-s.

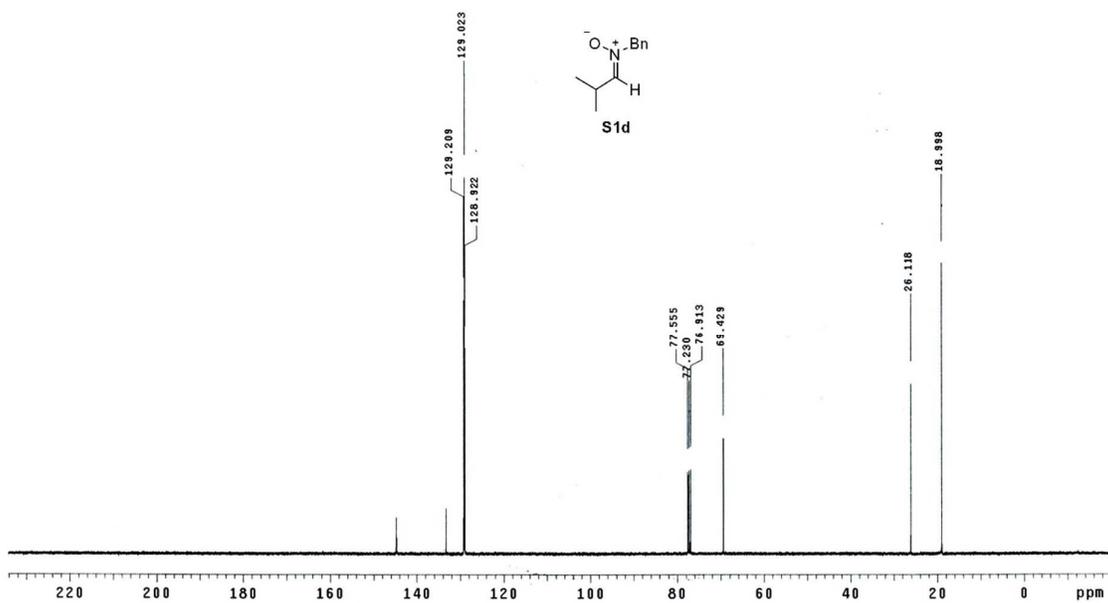
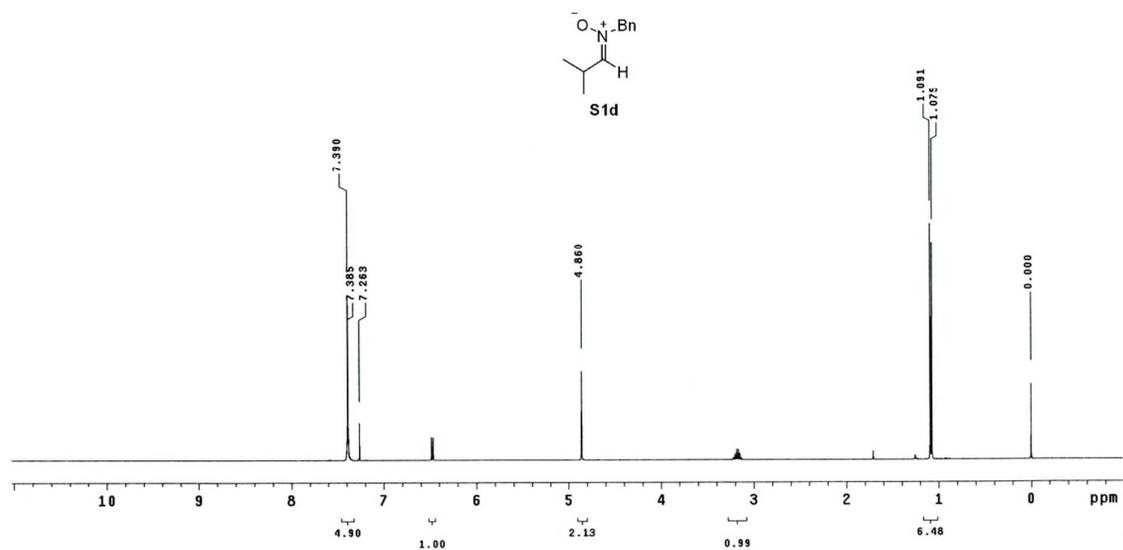
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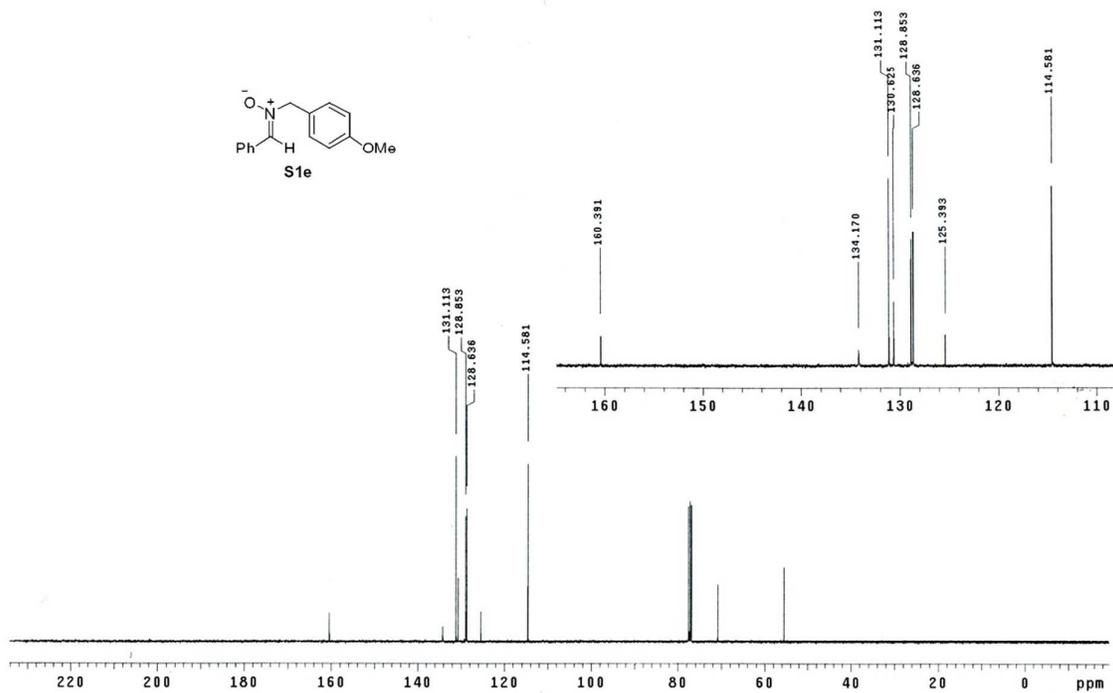
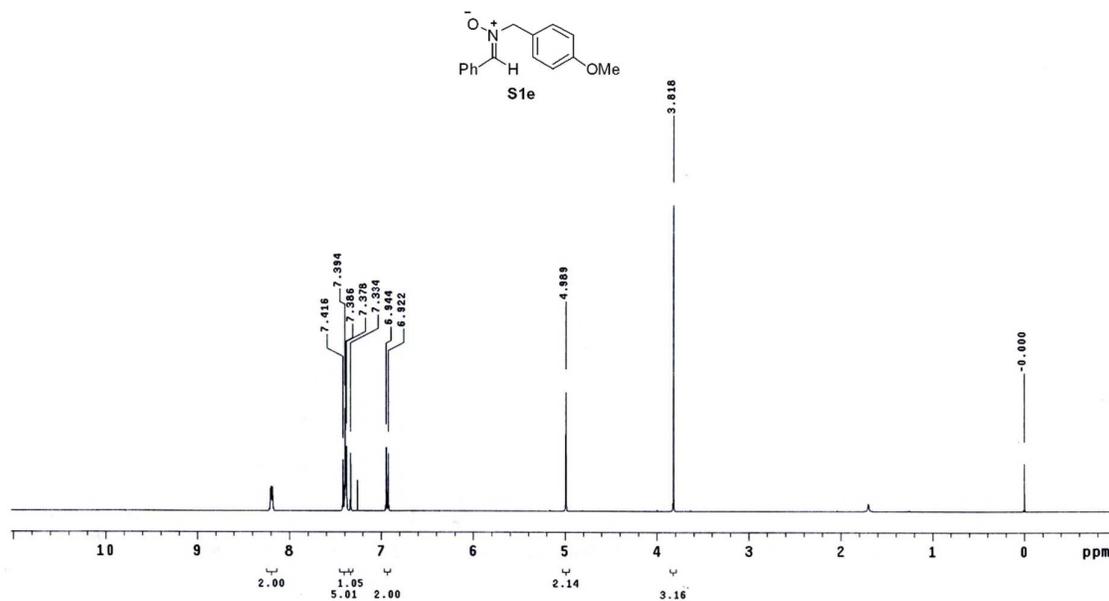
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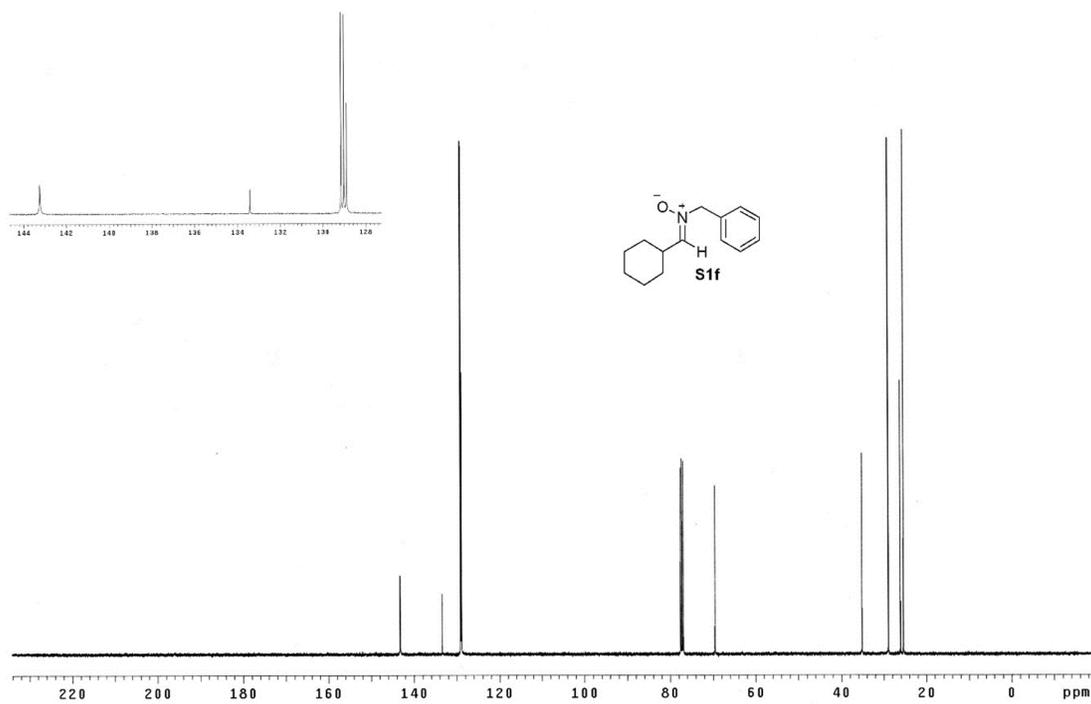
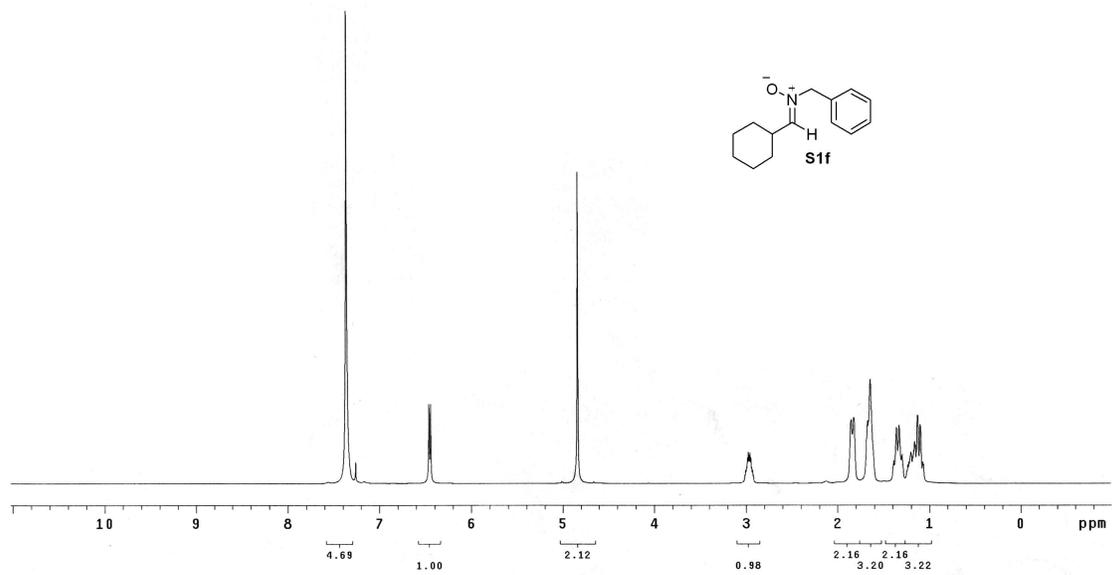
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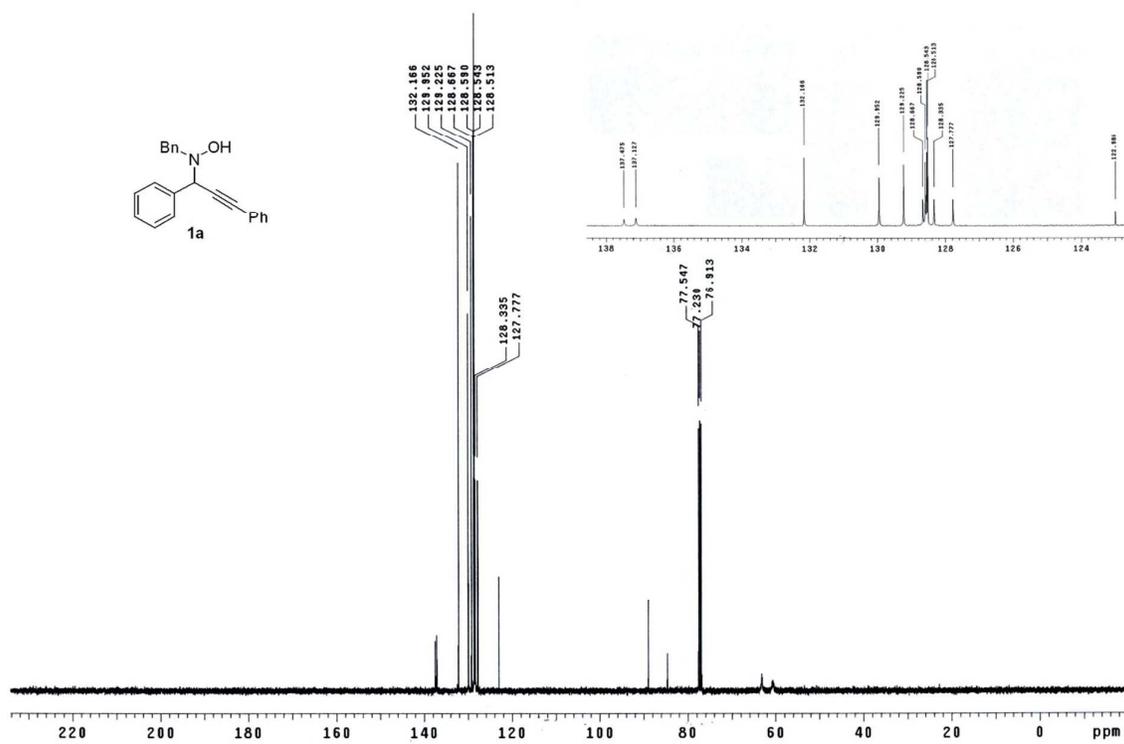
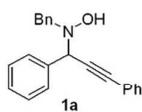
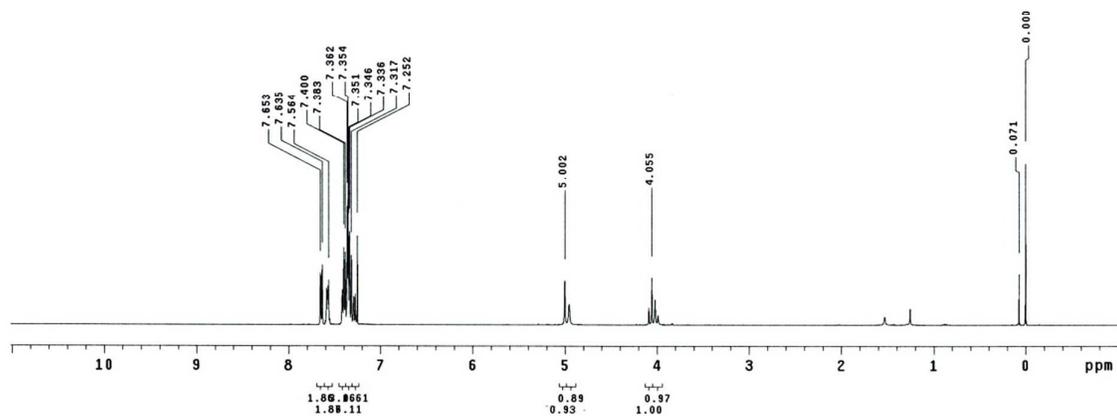
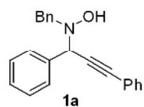
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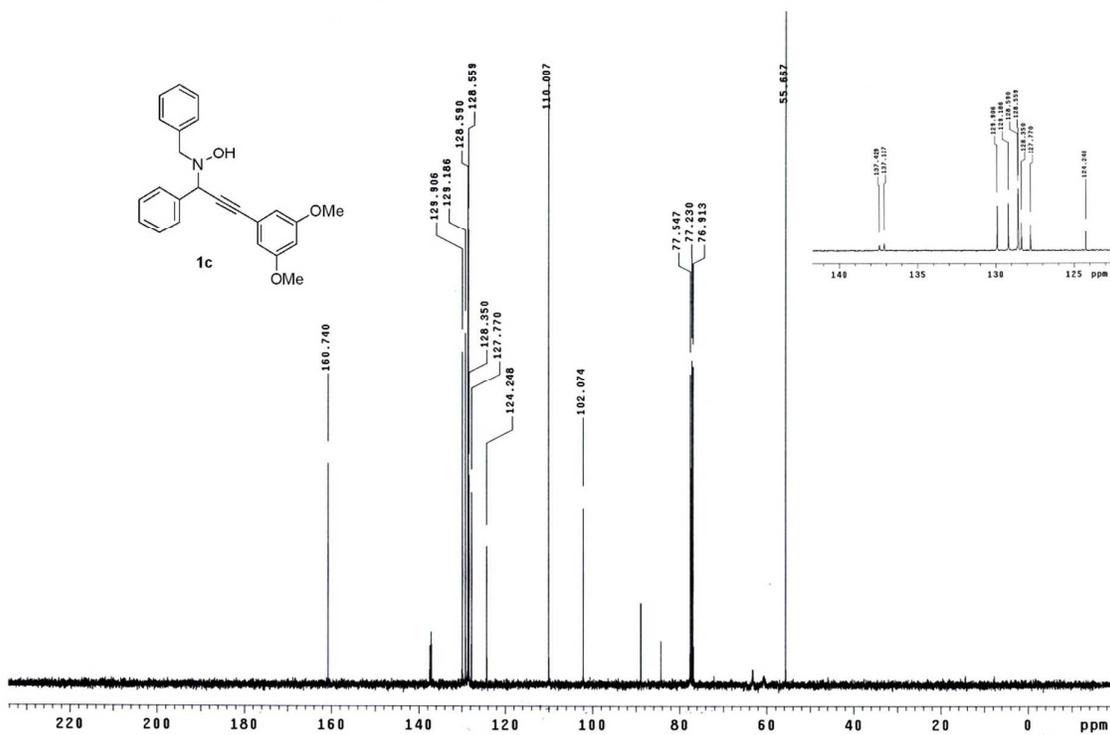
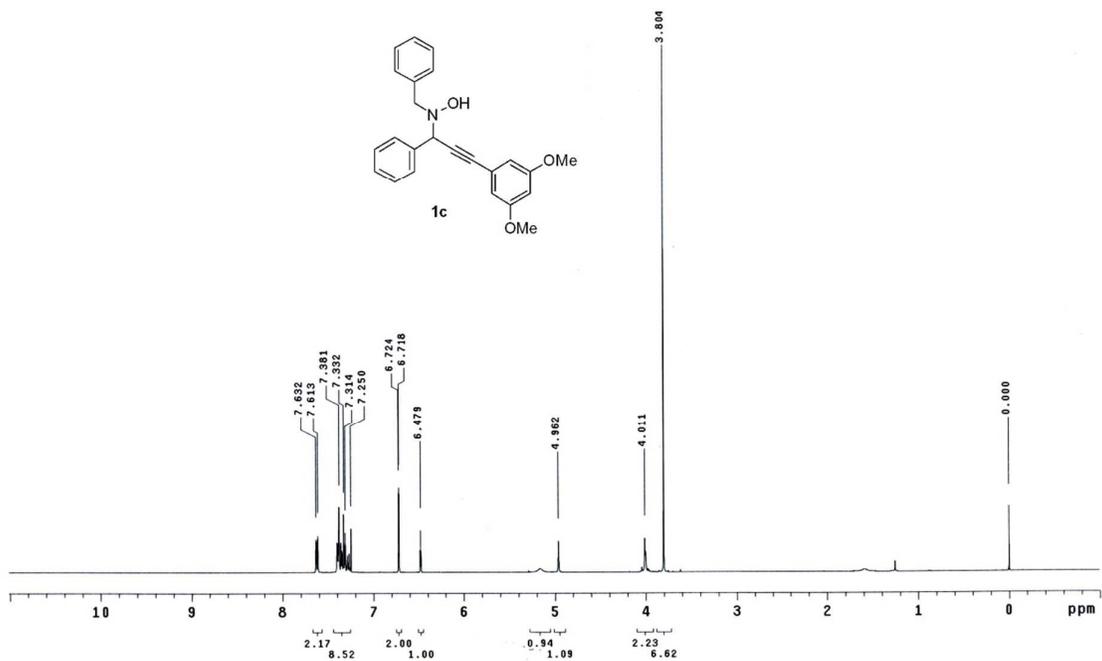
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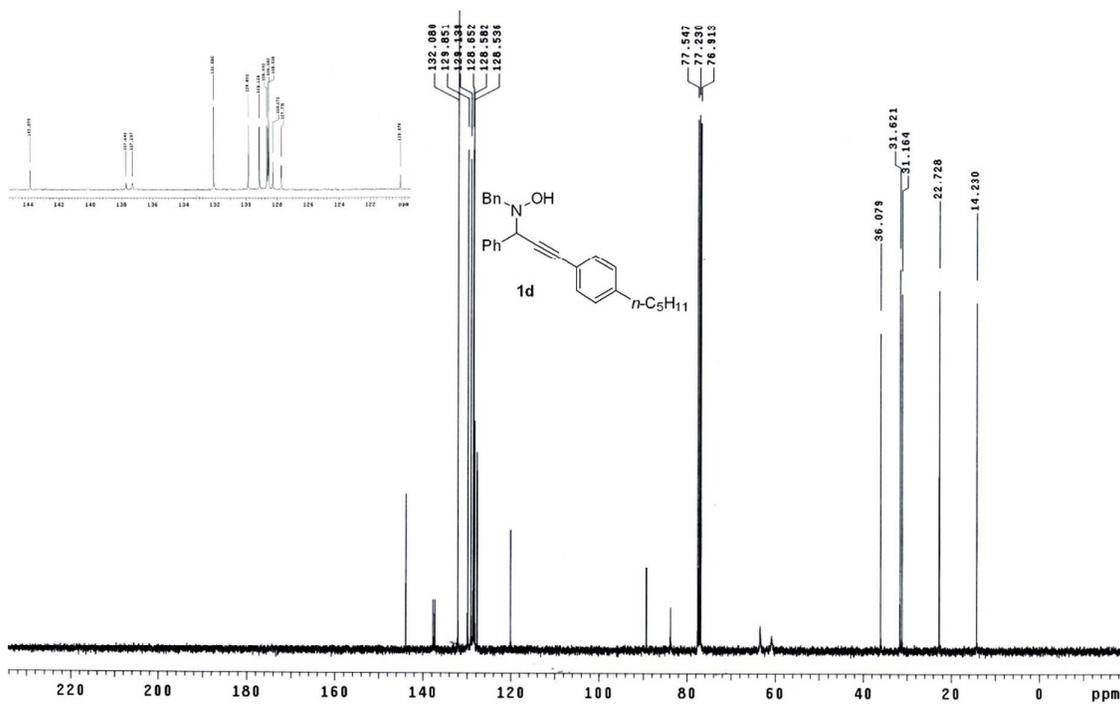
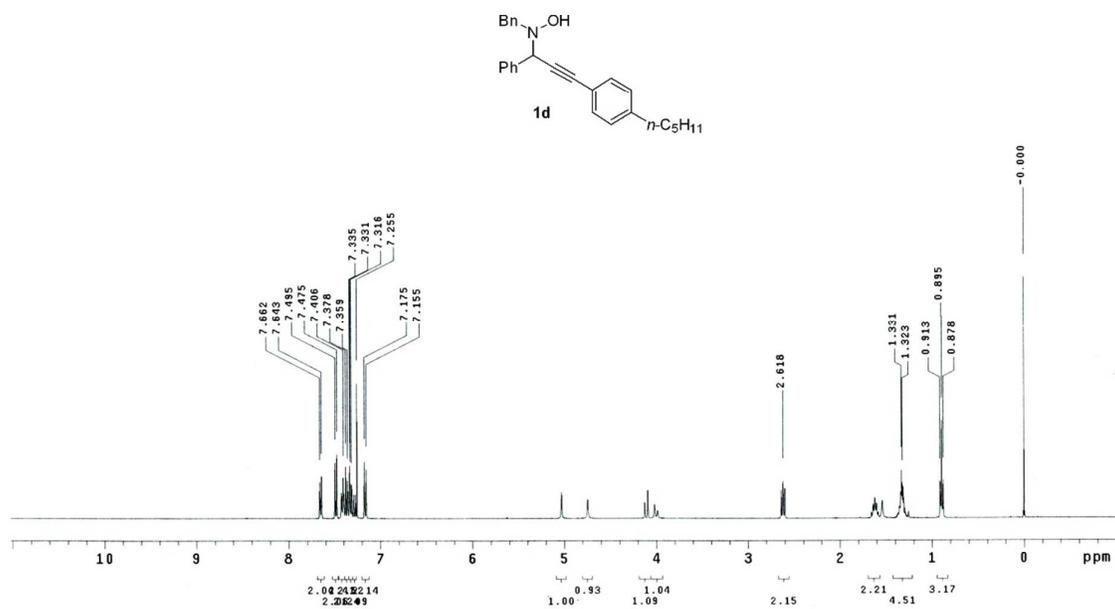
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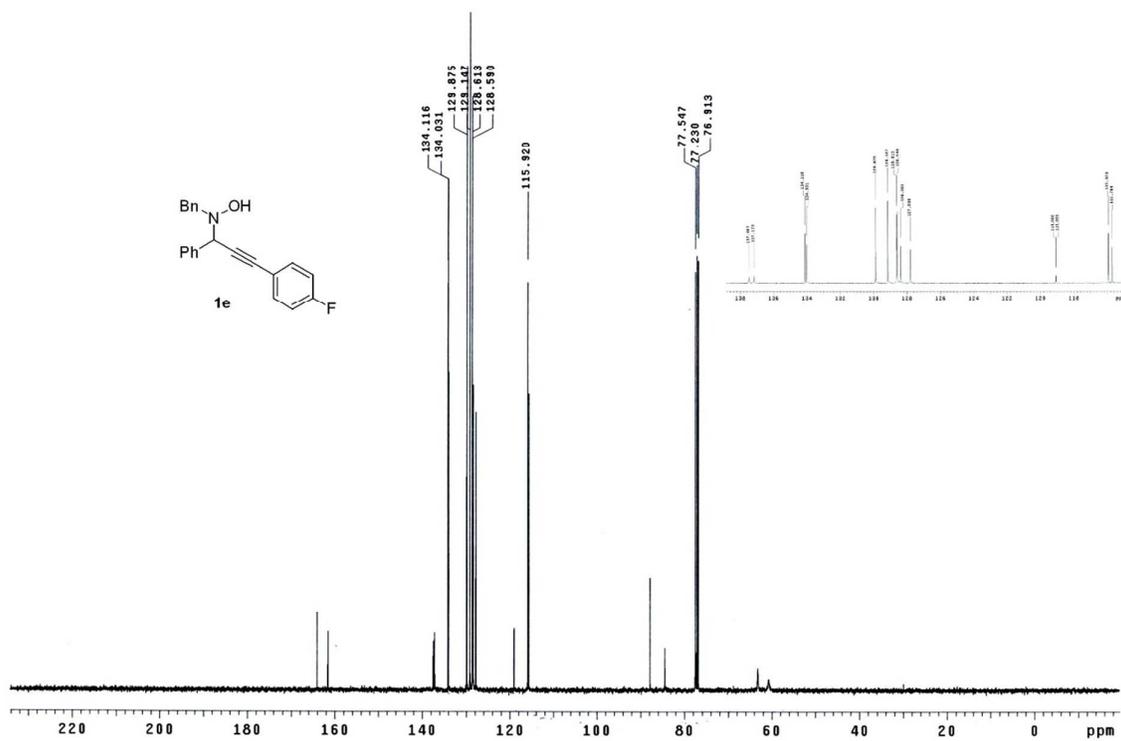
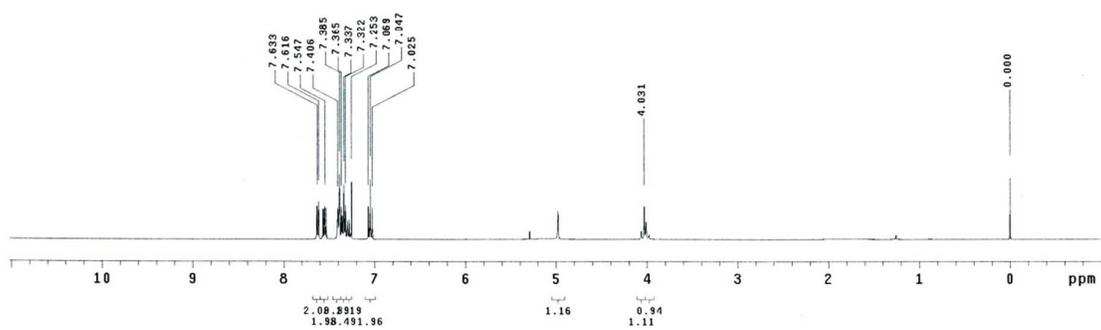
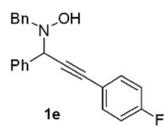
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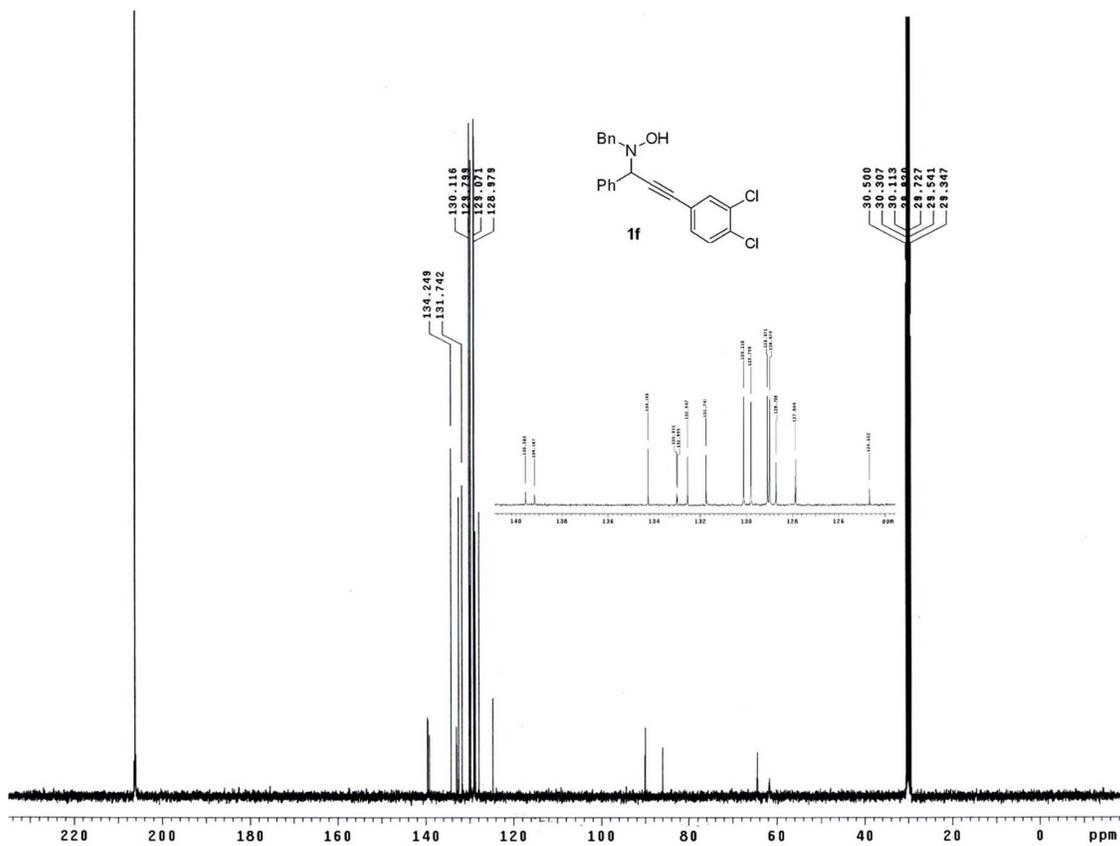
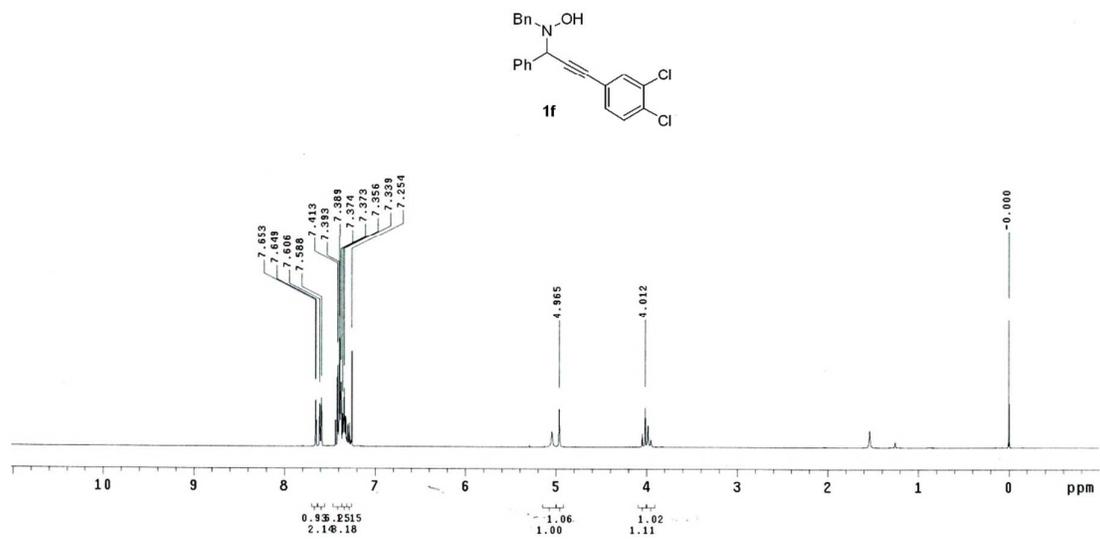
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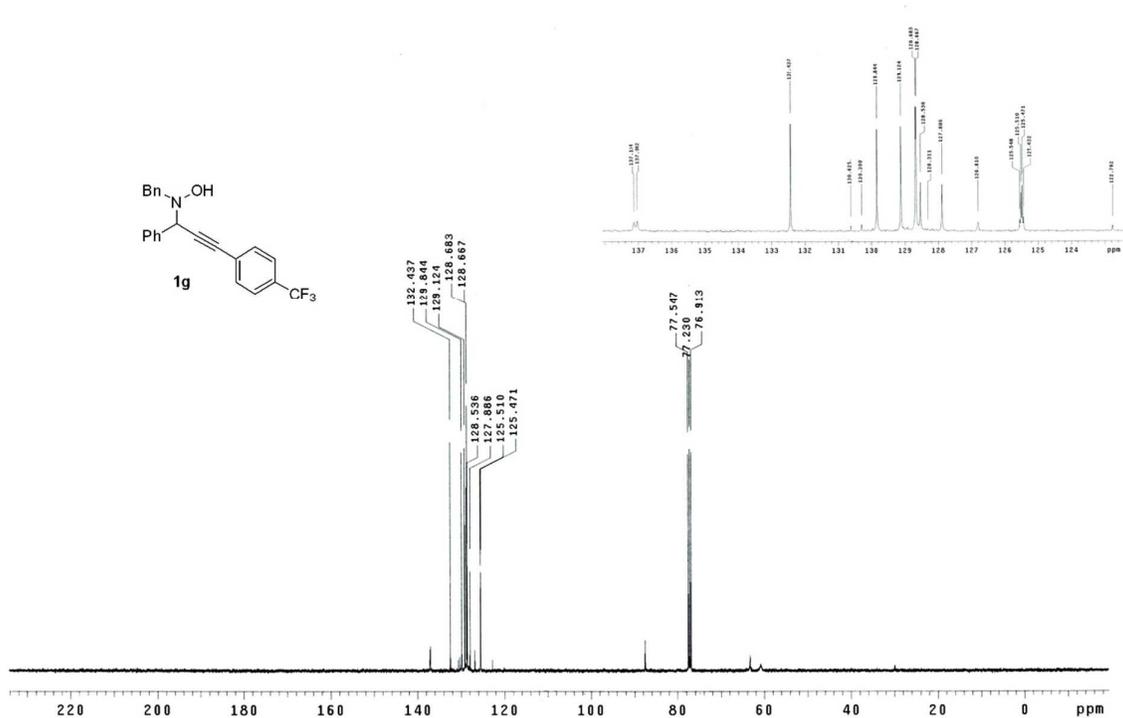
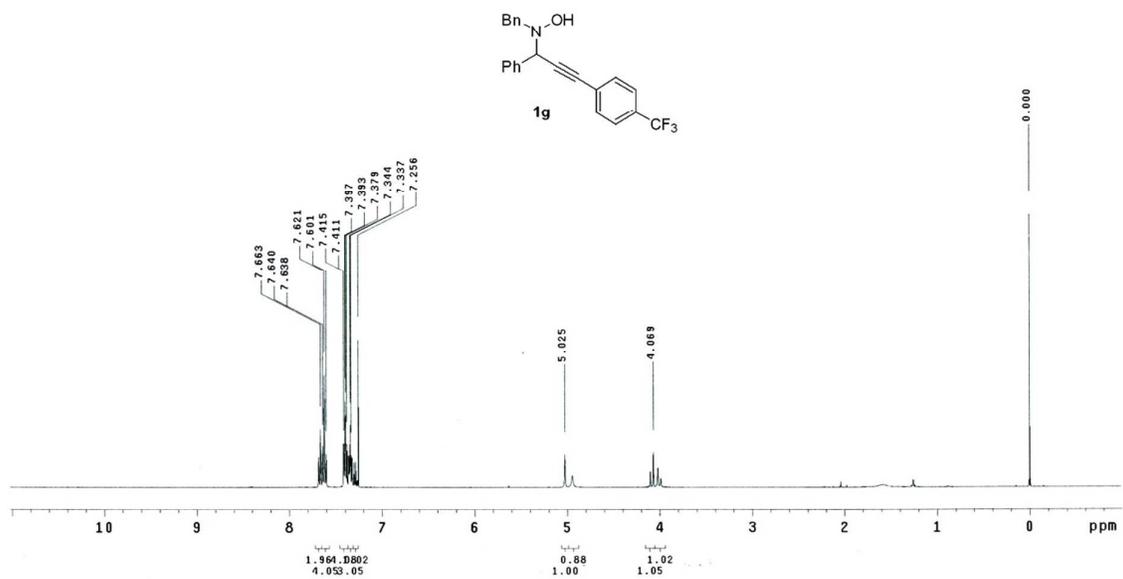
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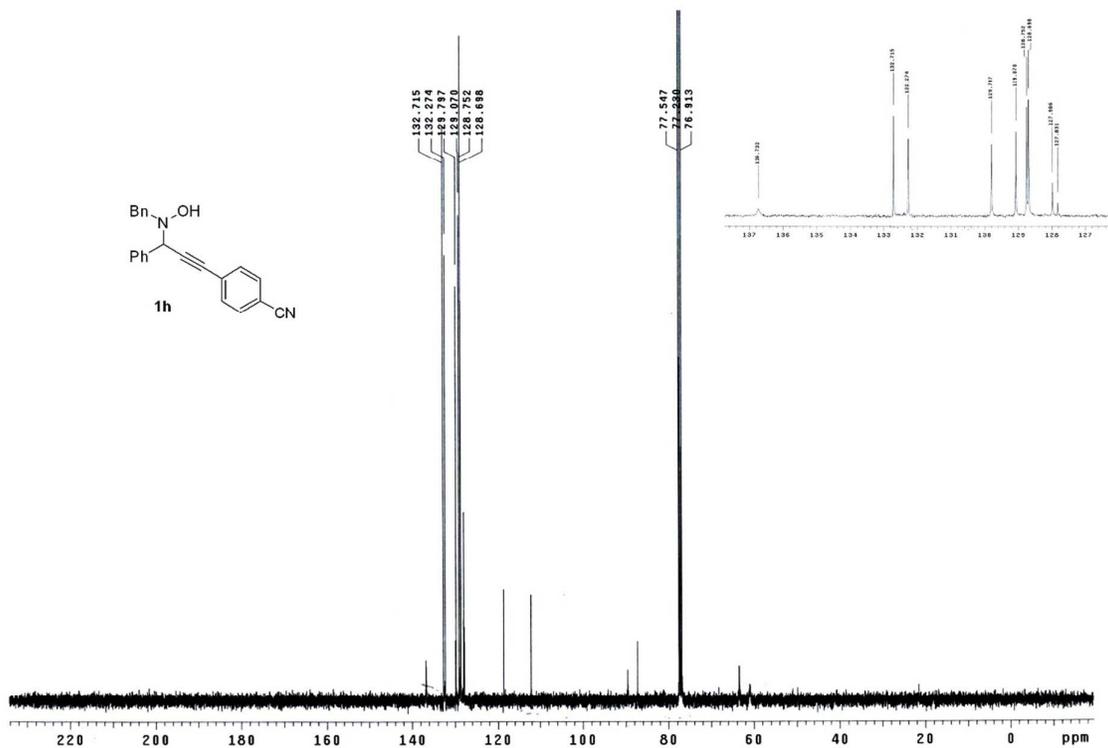
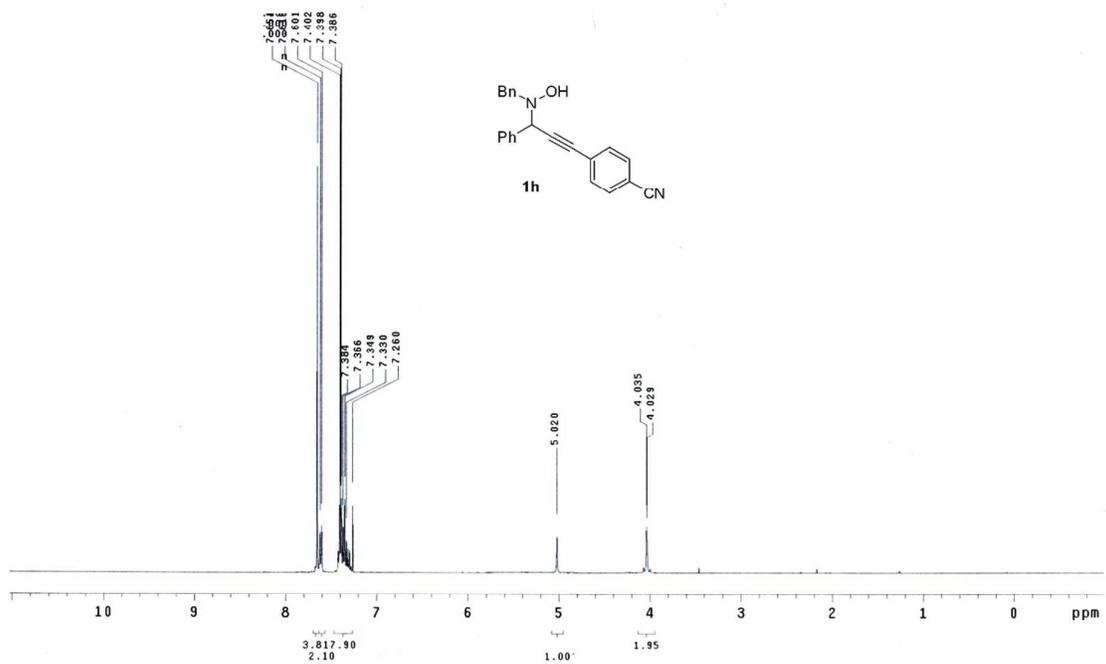
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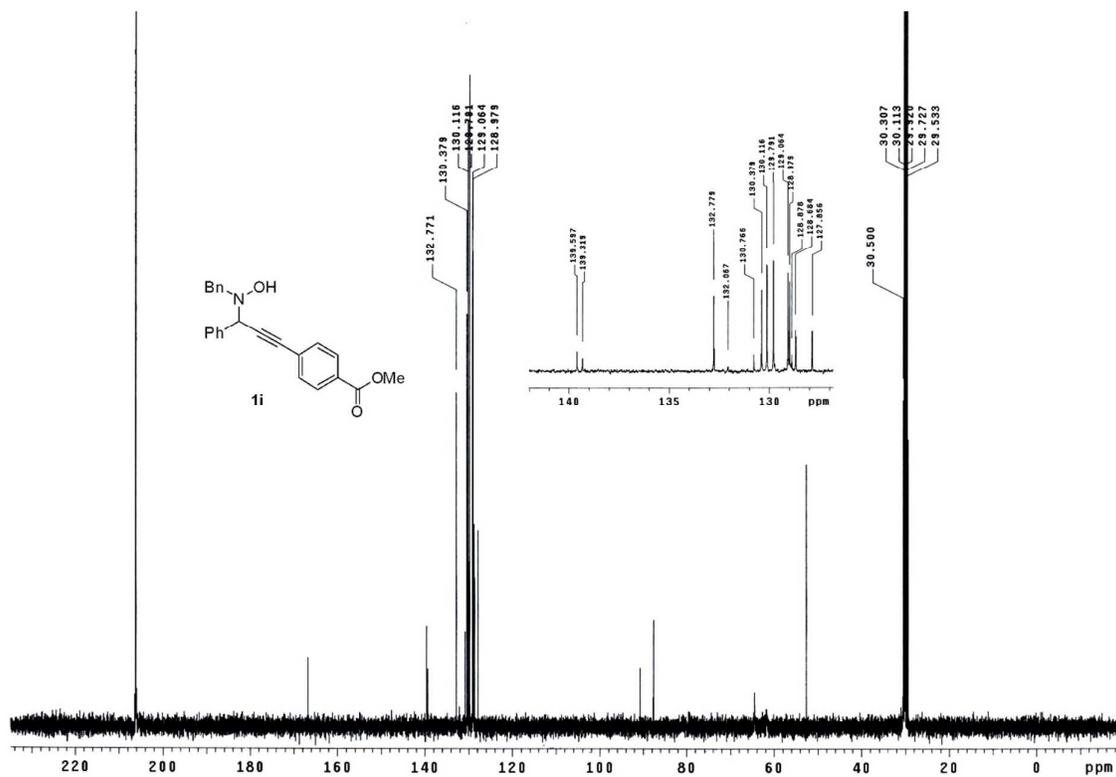
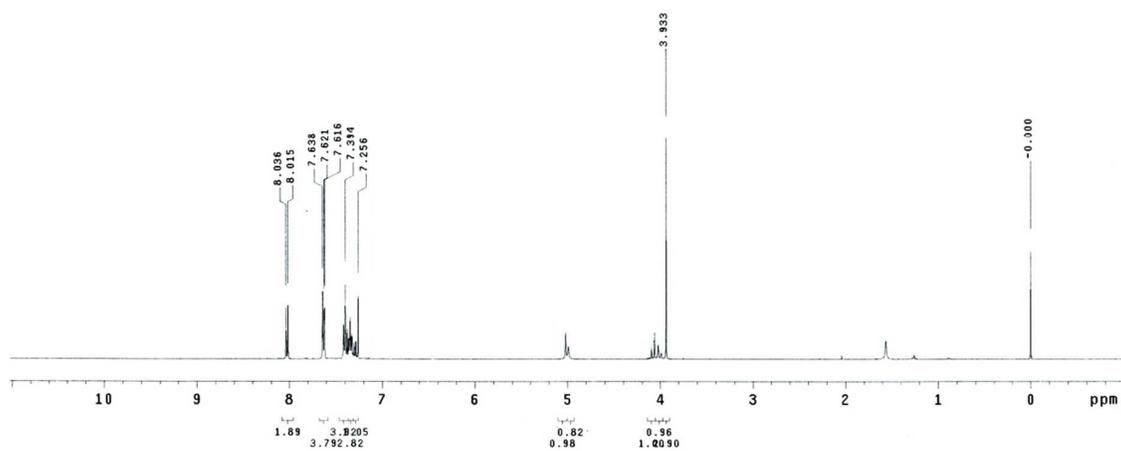
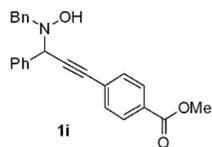
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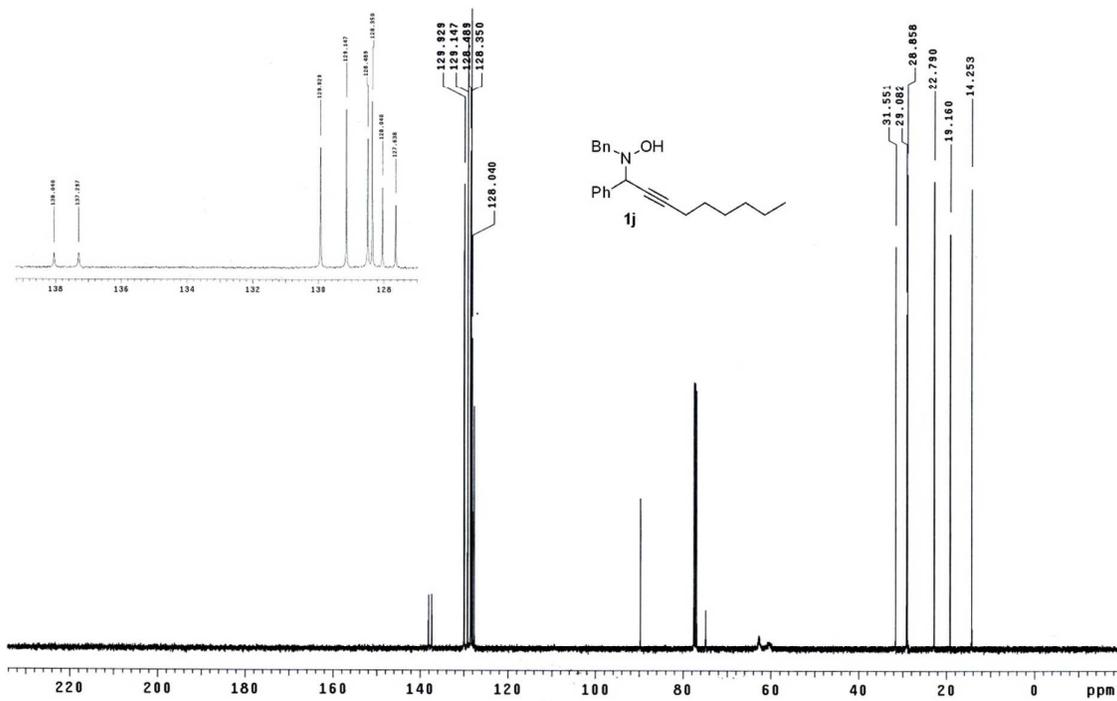
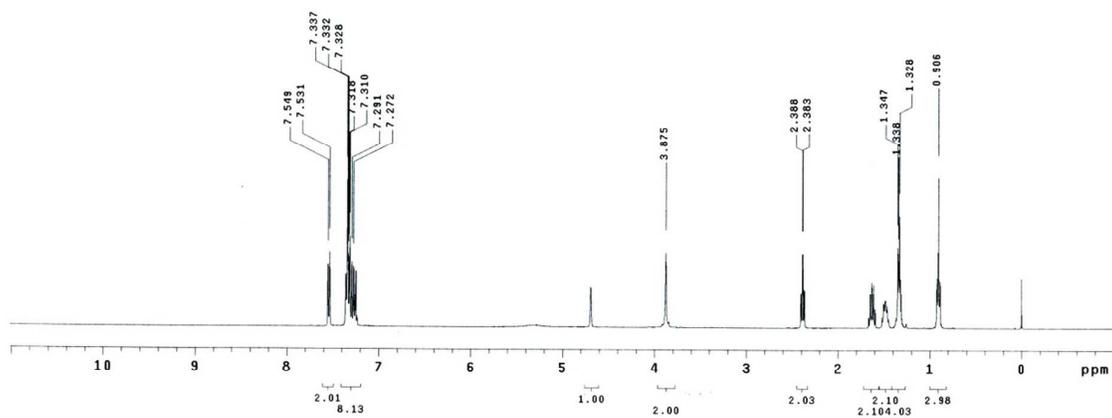
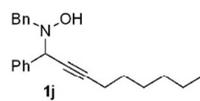
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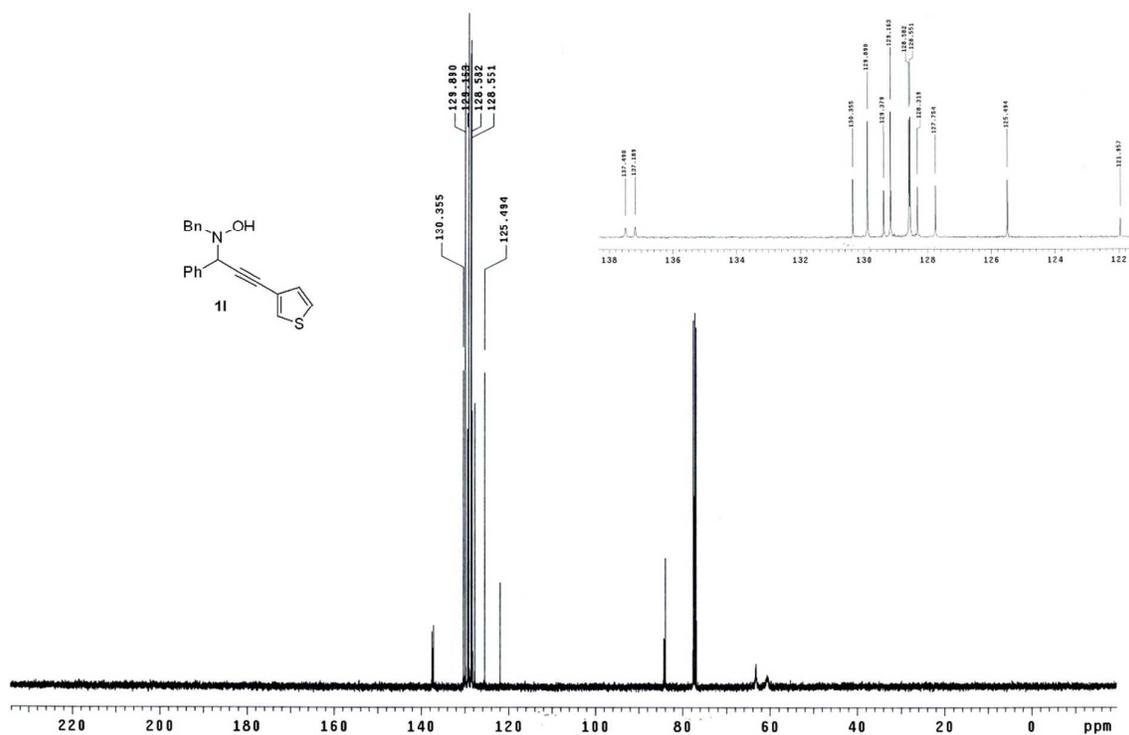
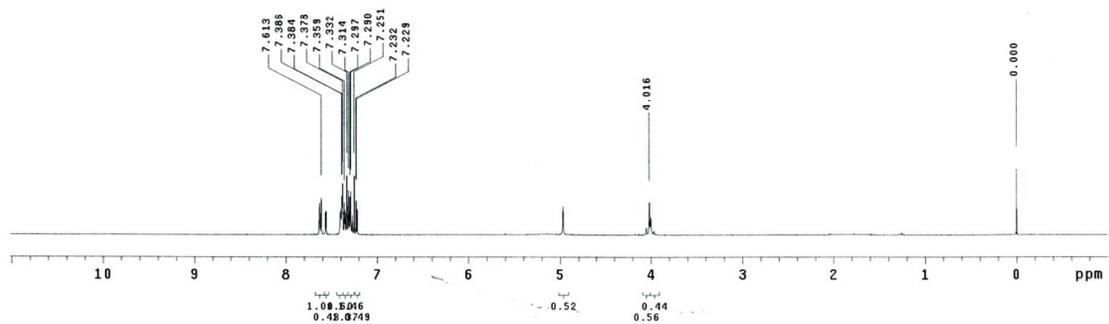
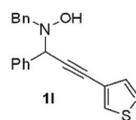
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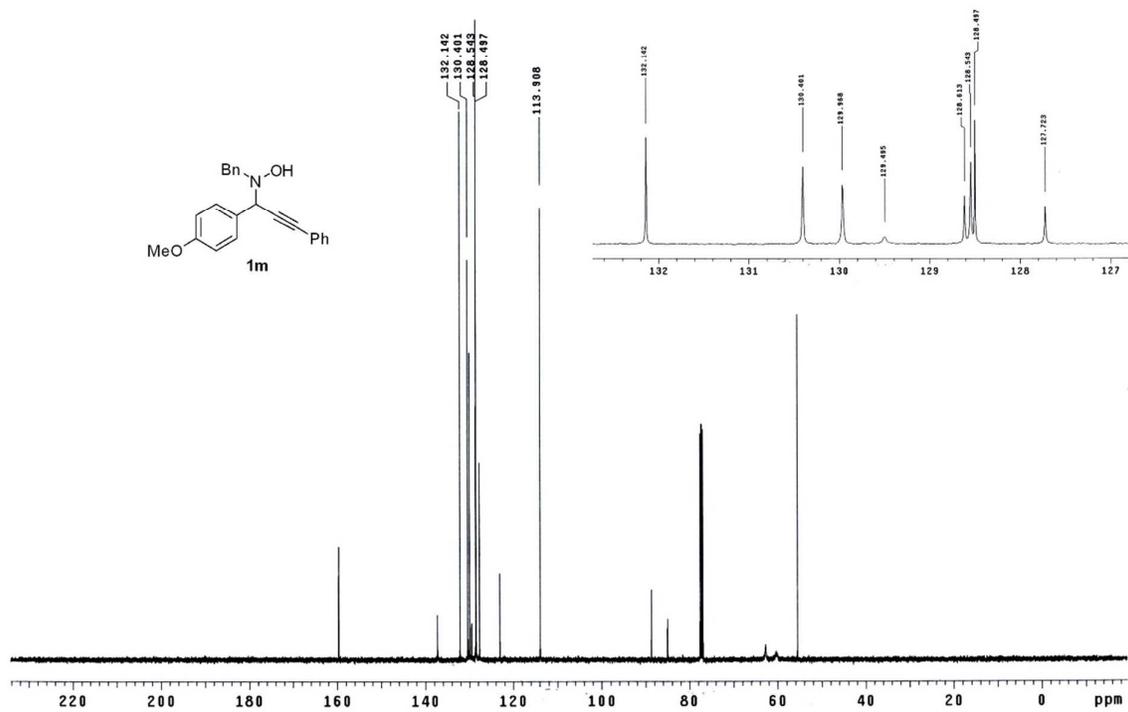
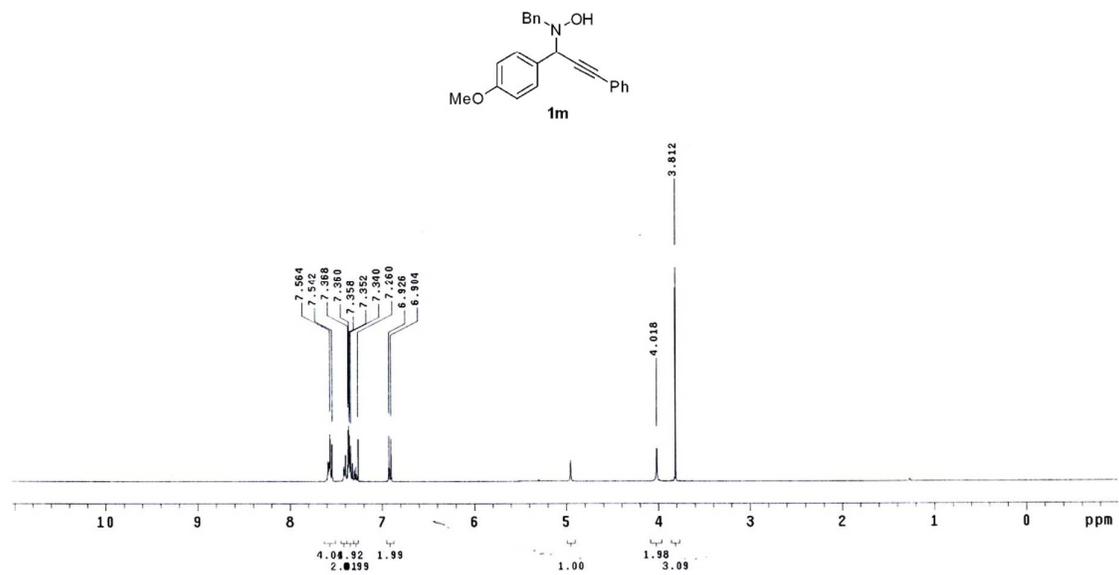
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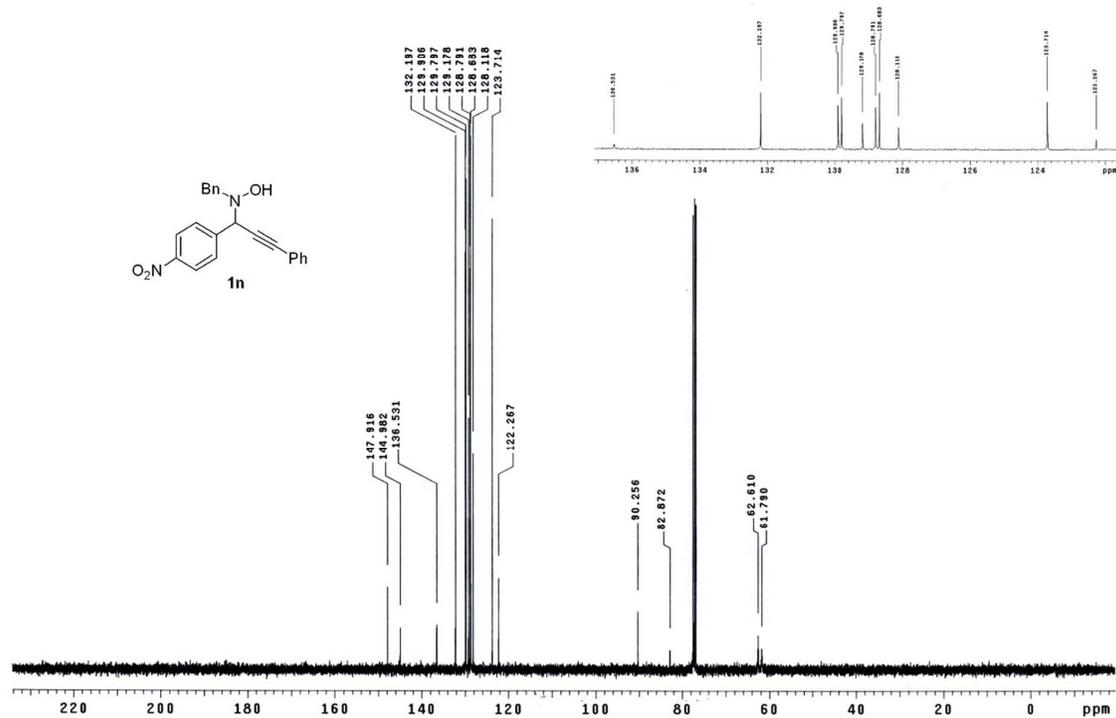
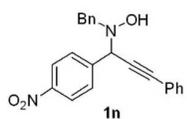
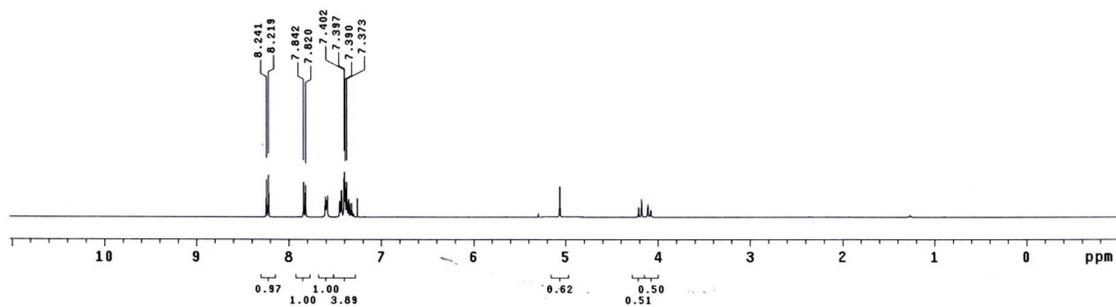
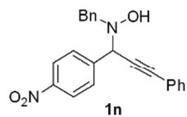
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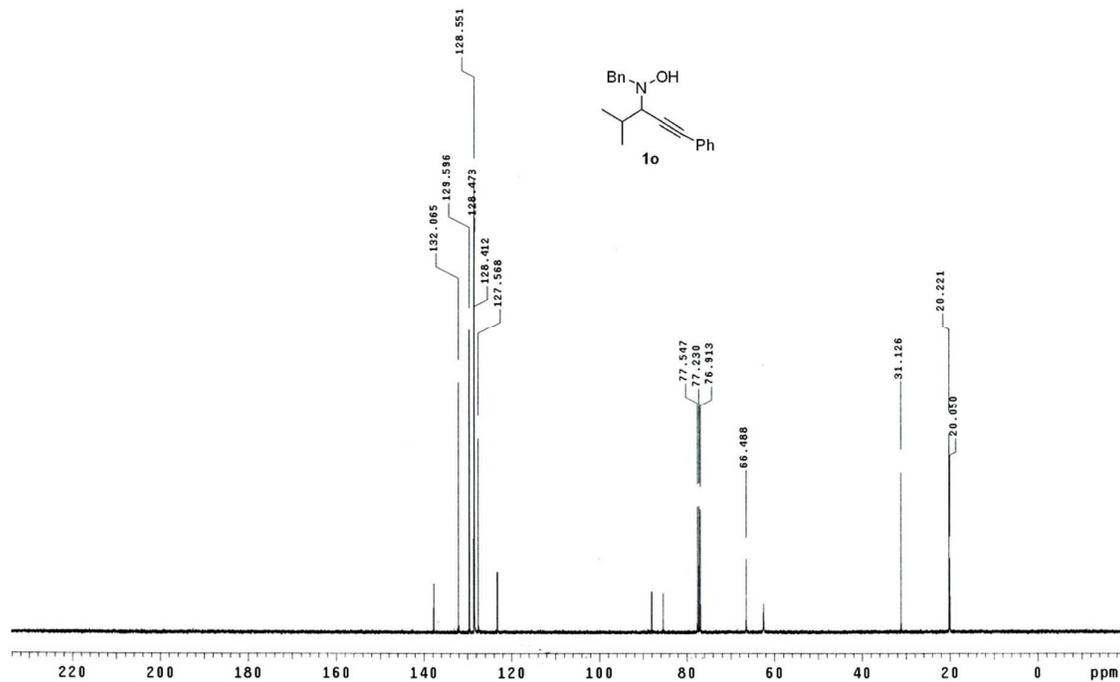
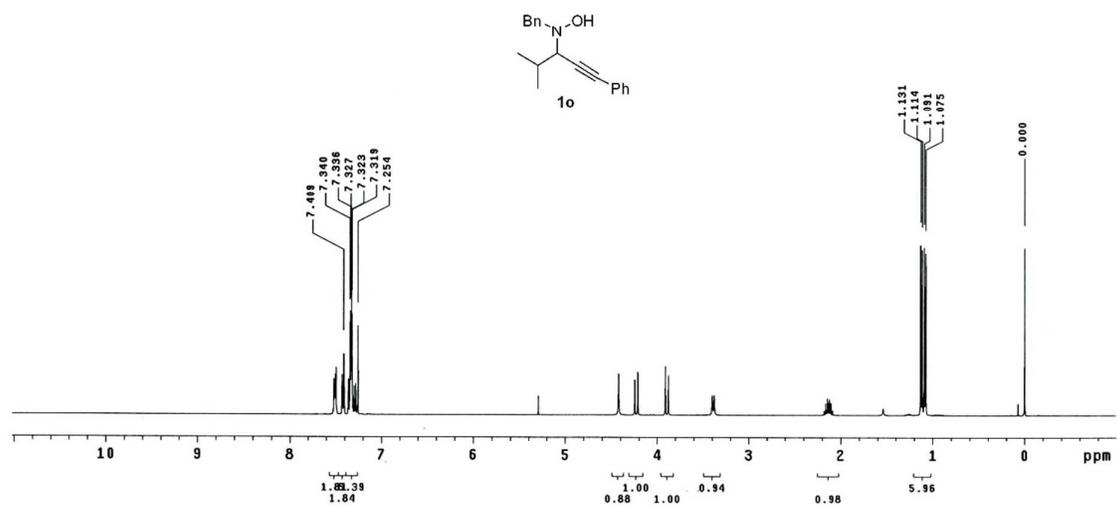
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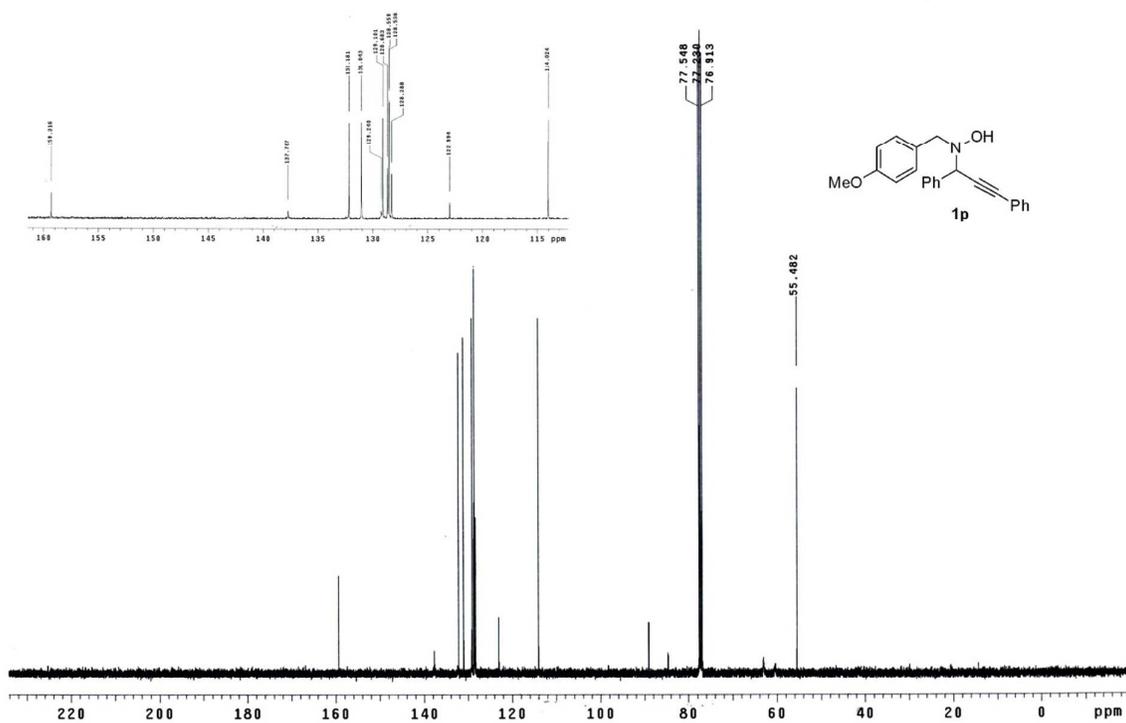
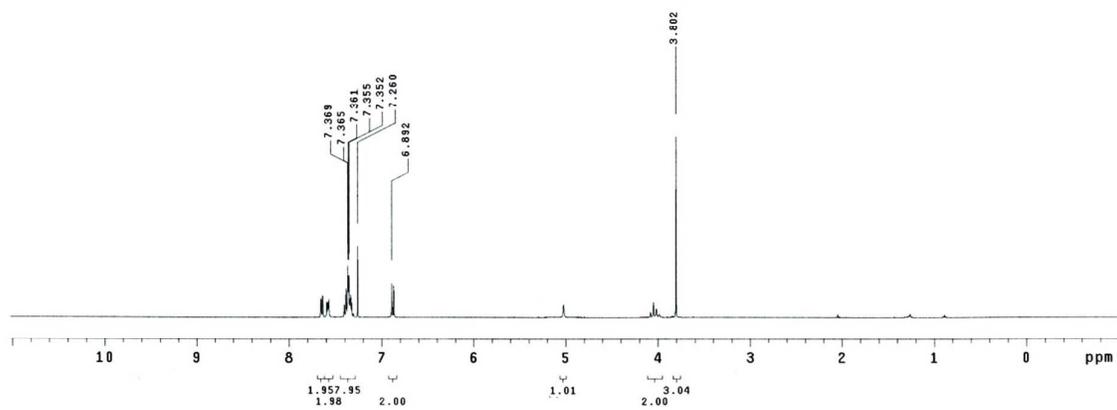
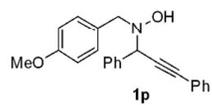
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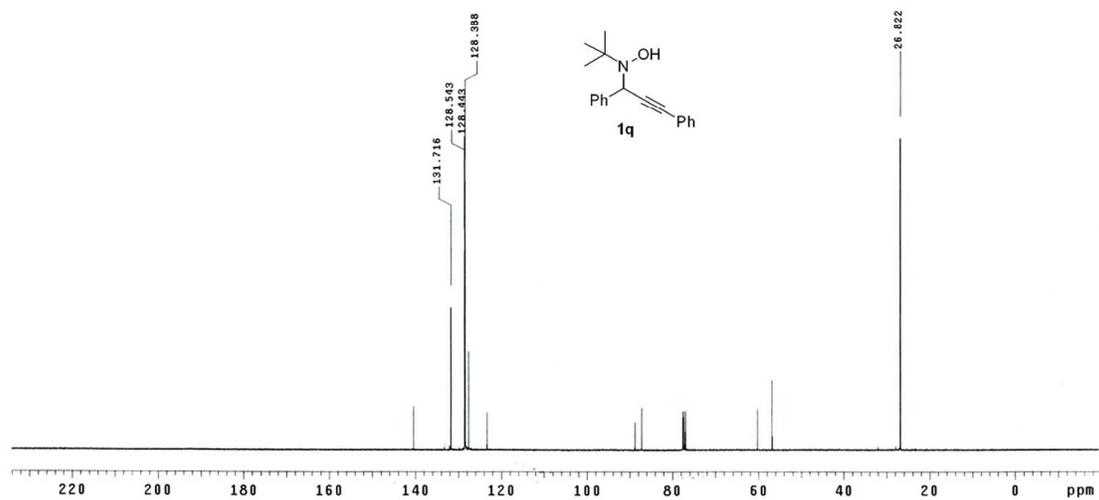
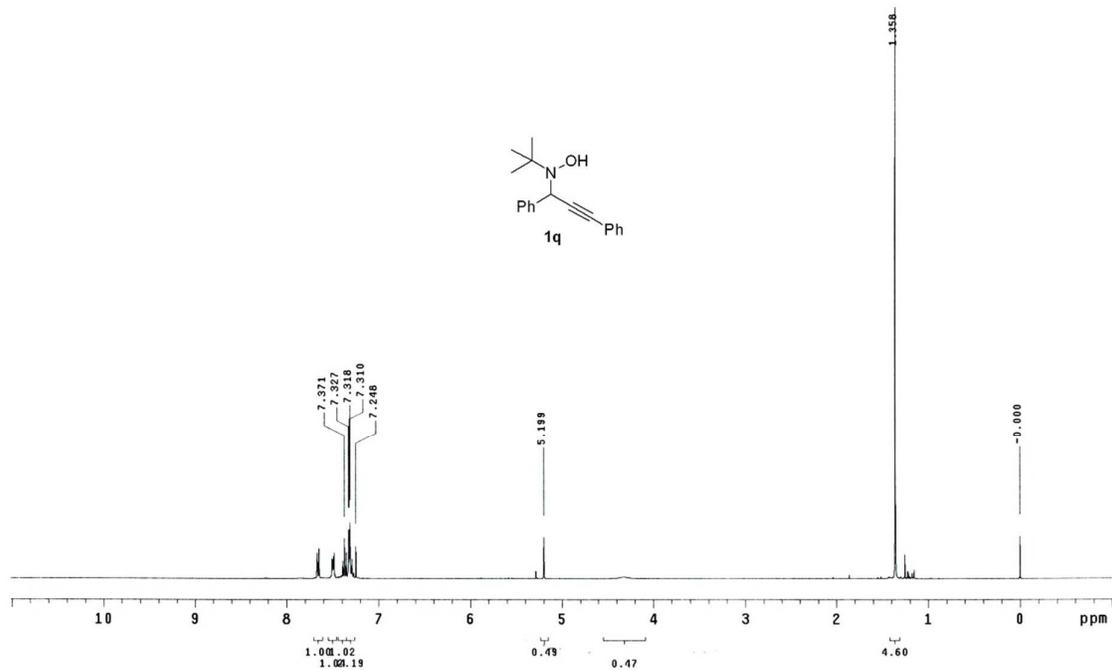
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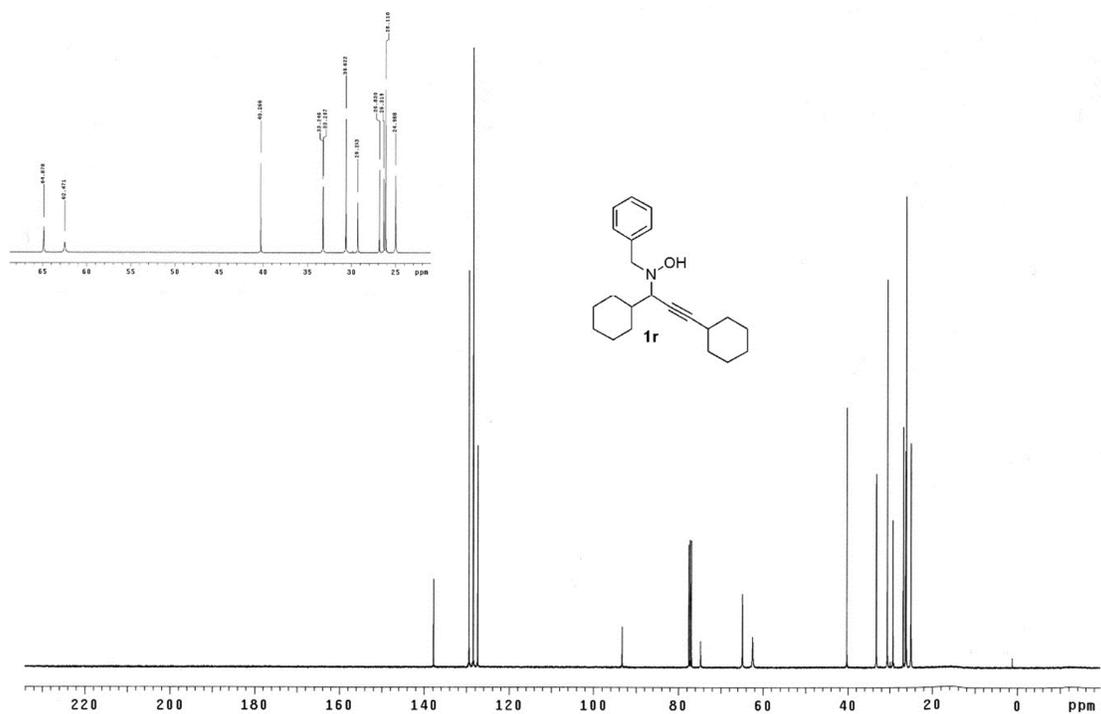
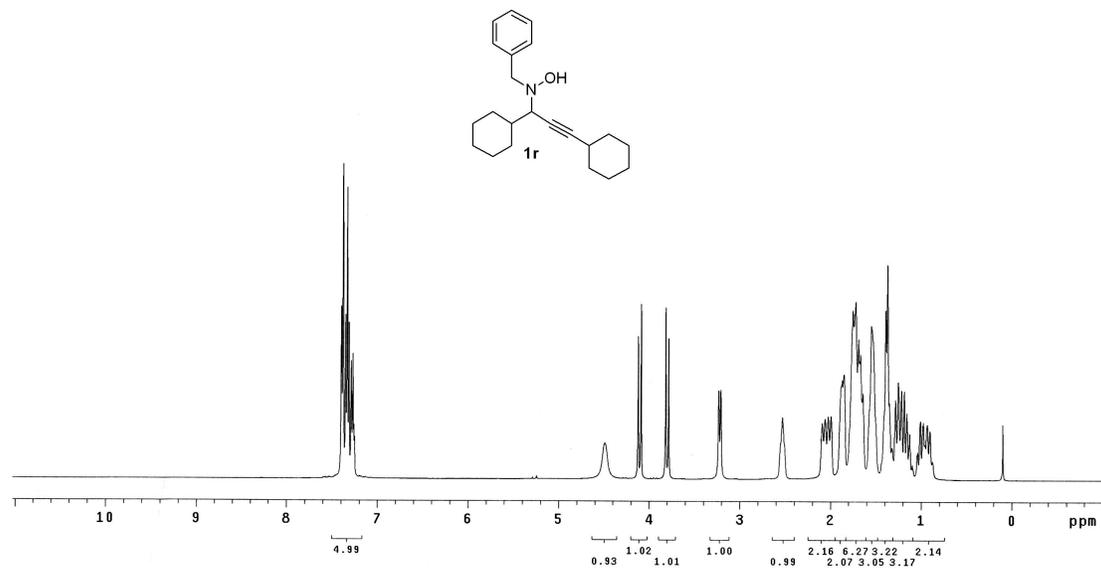


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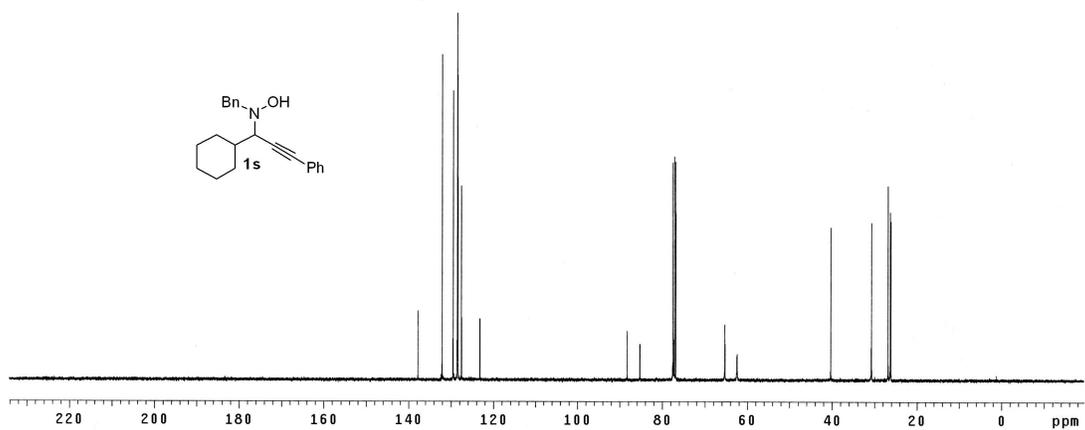
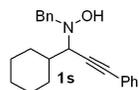
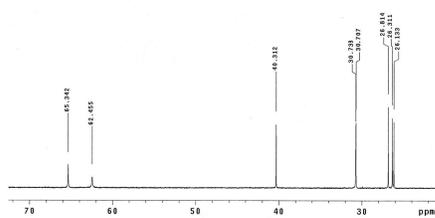
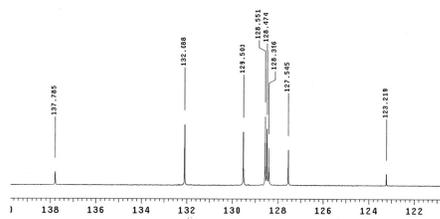
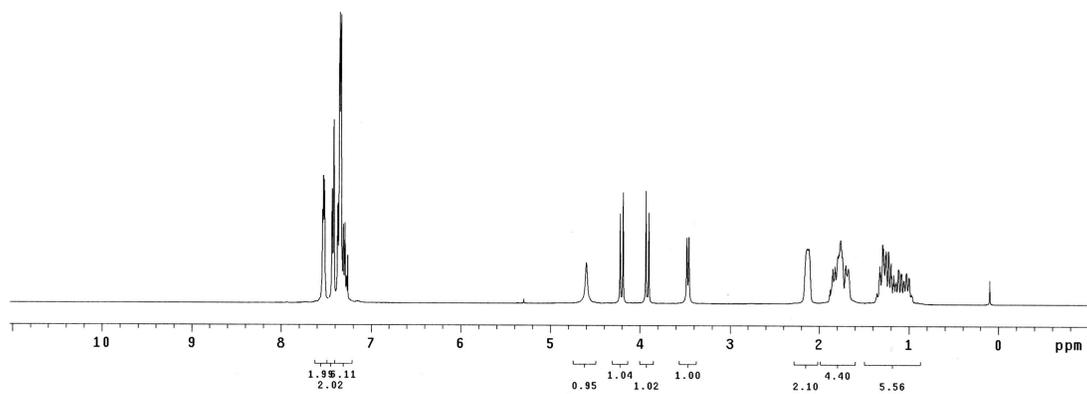
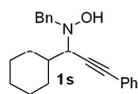


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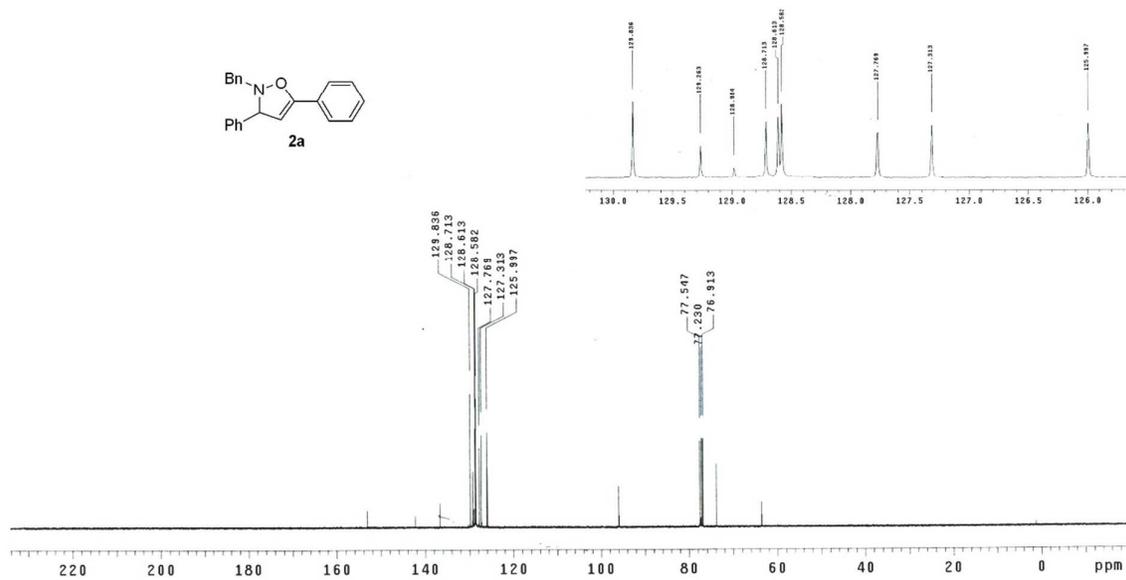
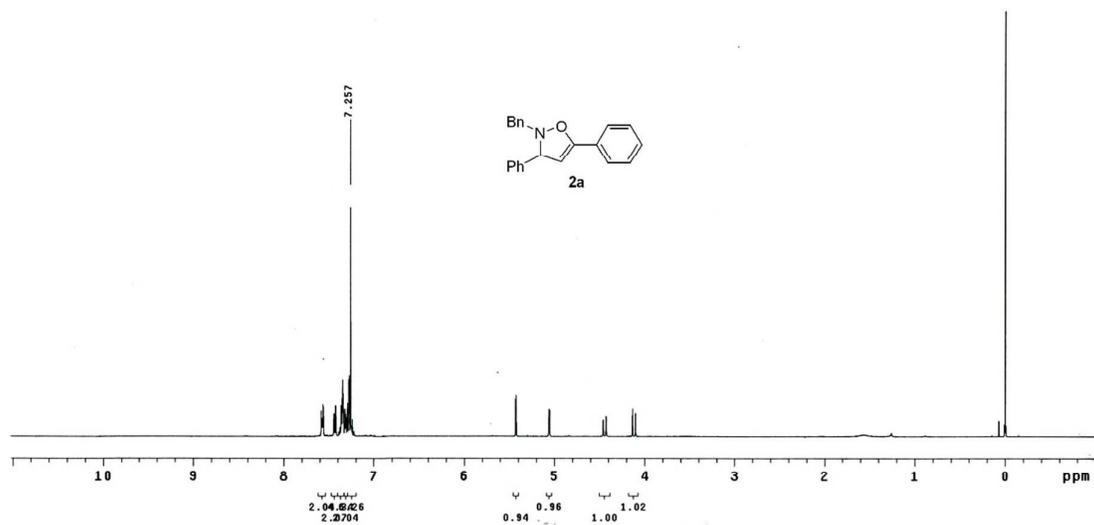


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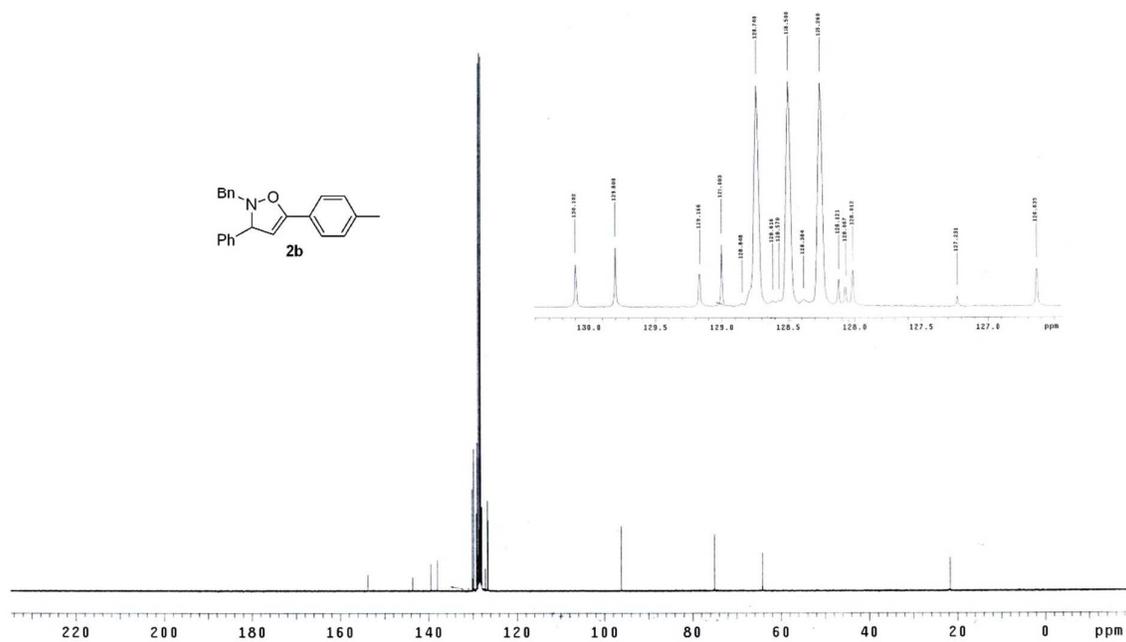
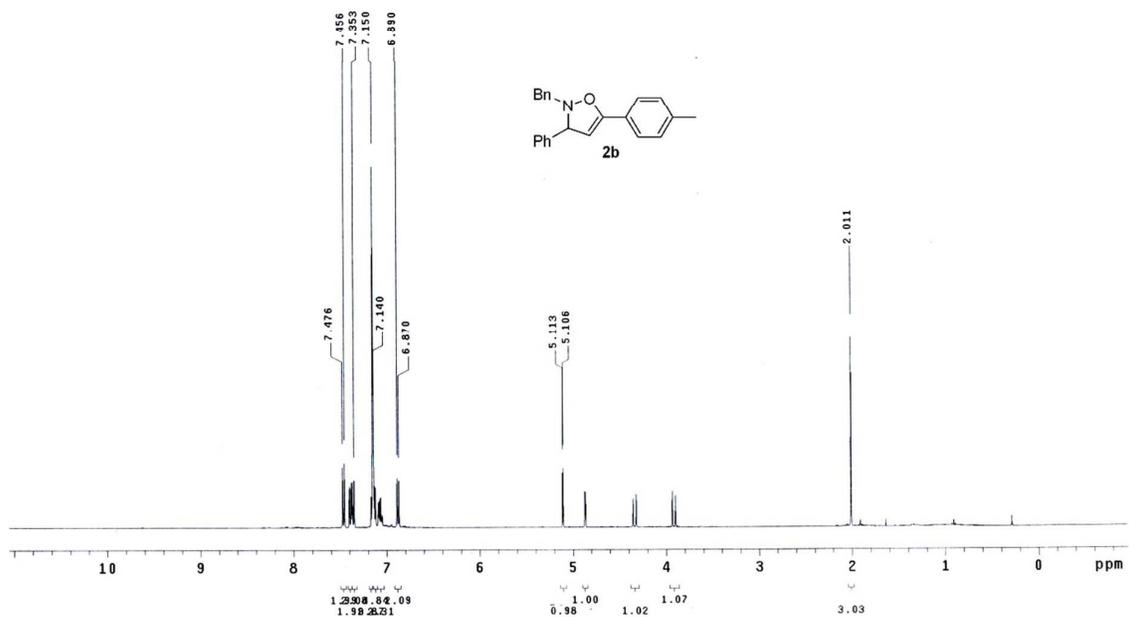


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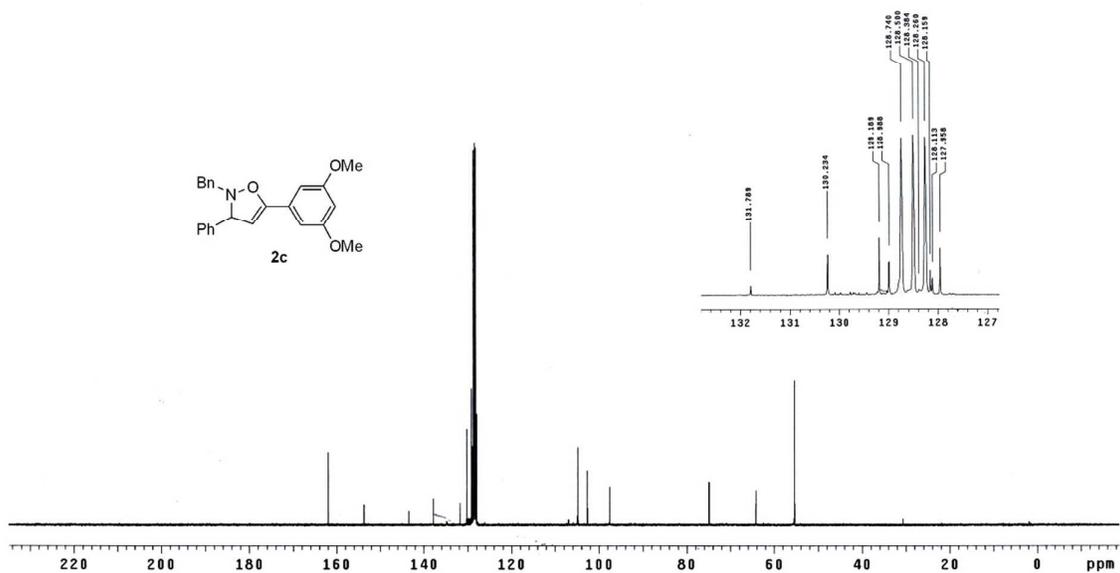
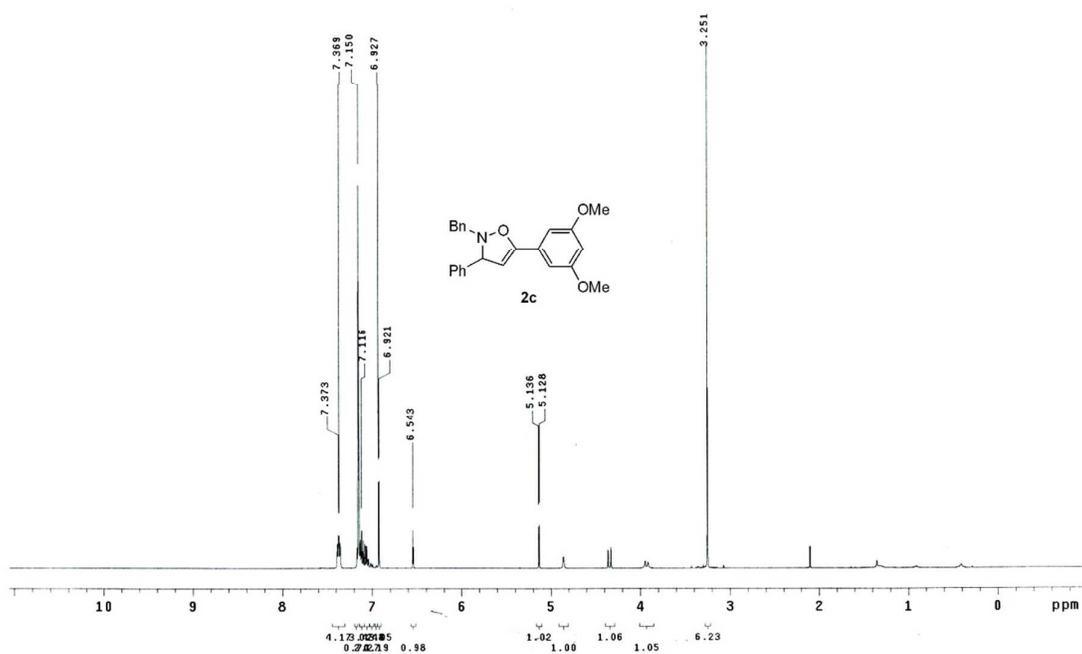
$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ chart for **2a** ([Table 2, entry 14], $(\text{PPh}_3)\text{AuNTf}_2$ used)



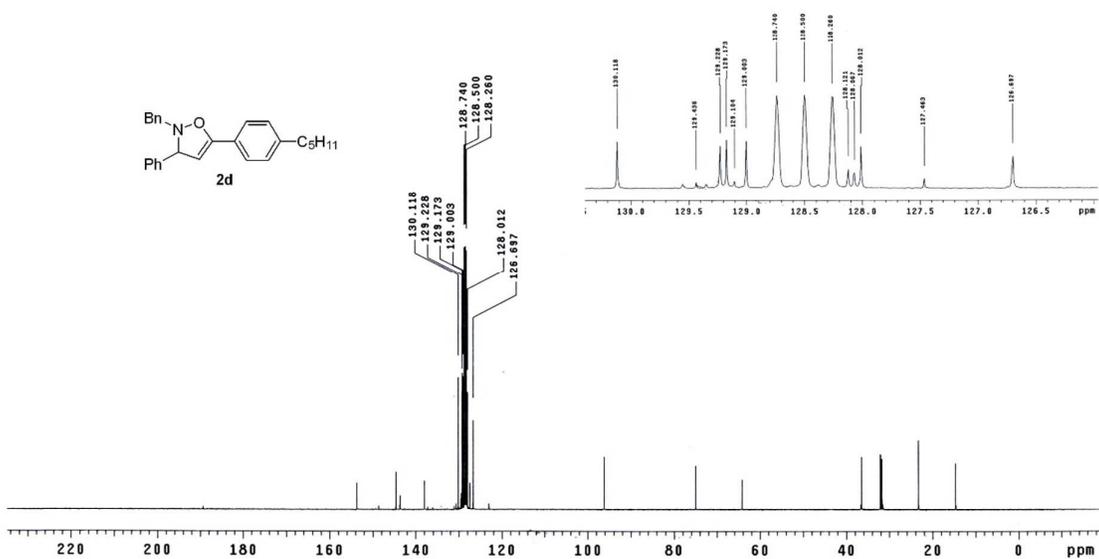
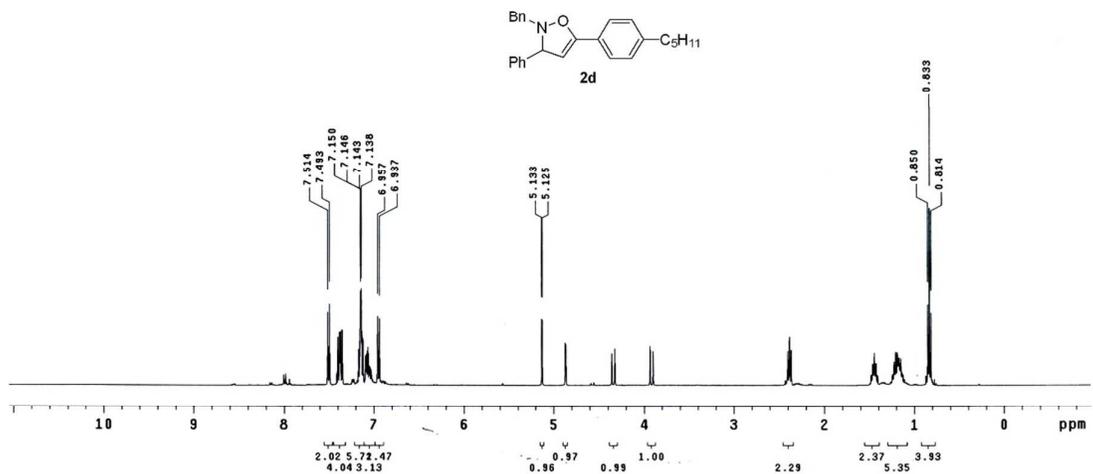
$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ chart for **2b** ([Scheme 2], $(\text{PPh}_3)\text{AuNTf}_2$ used)



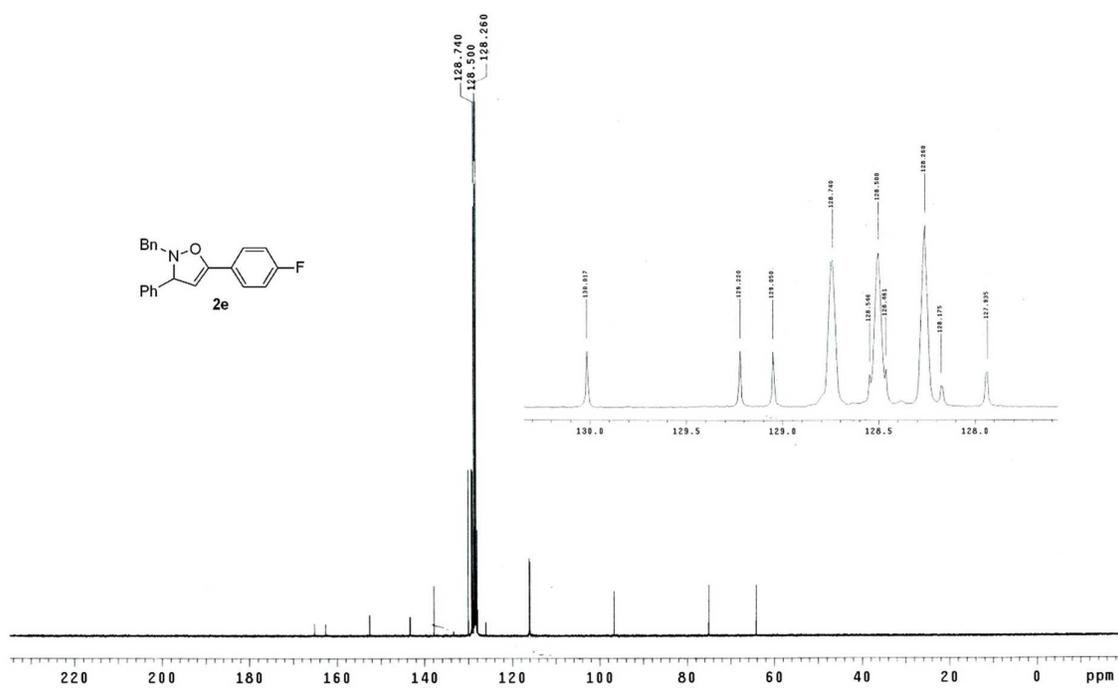
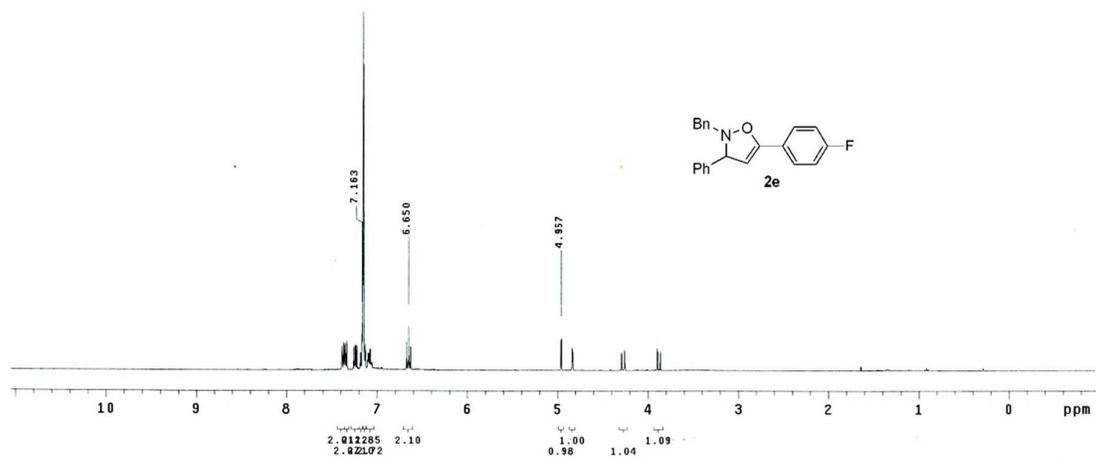
$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ chart for **2c** ([Scheme 2], $(\text{PPh}_3)\text{AuCl}/\text{AgOTf}$ used)



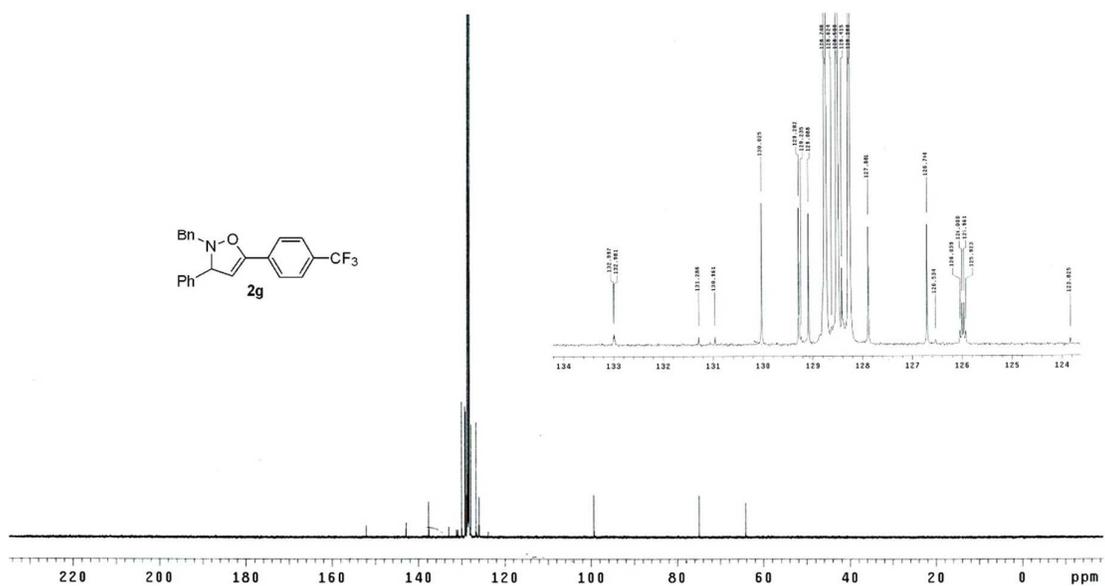
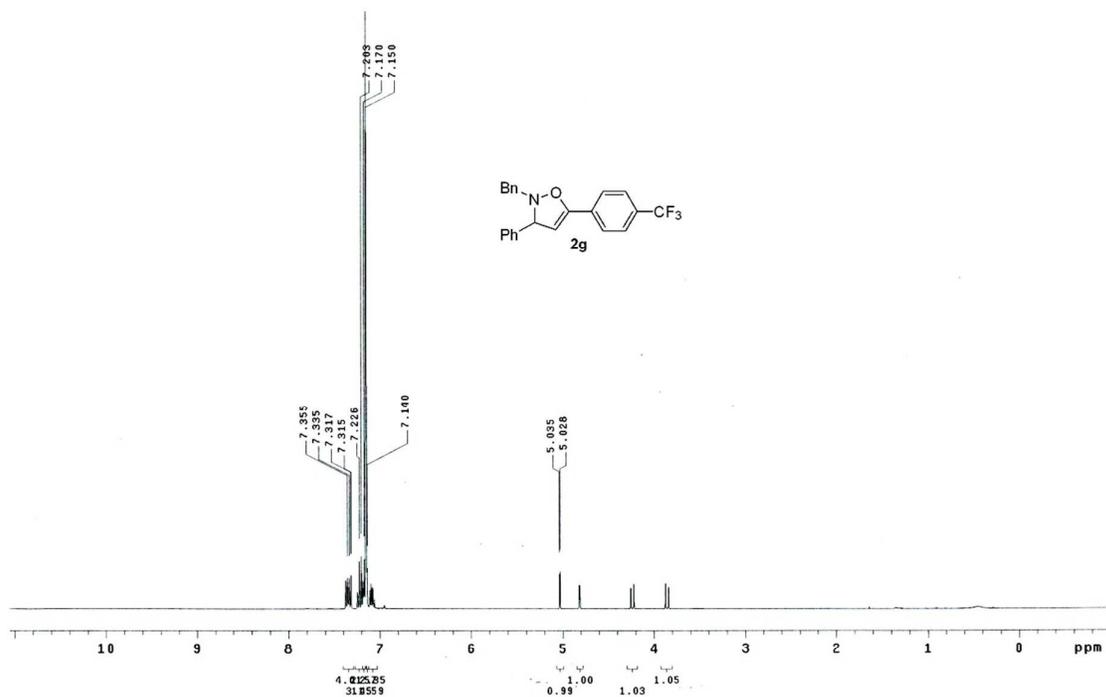
$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ chart for **2d** ([Scheme 2], $(\text{PPh}_3)\text{AuCl}/\text{AgOTf}$ used)

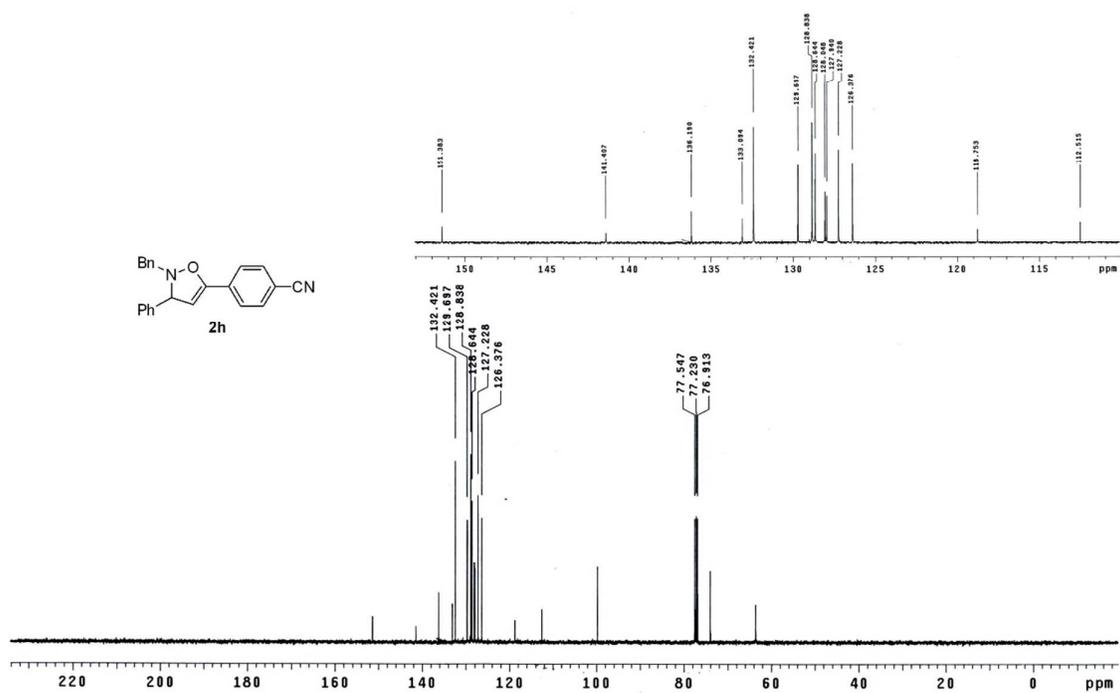
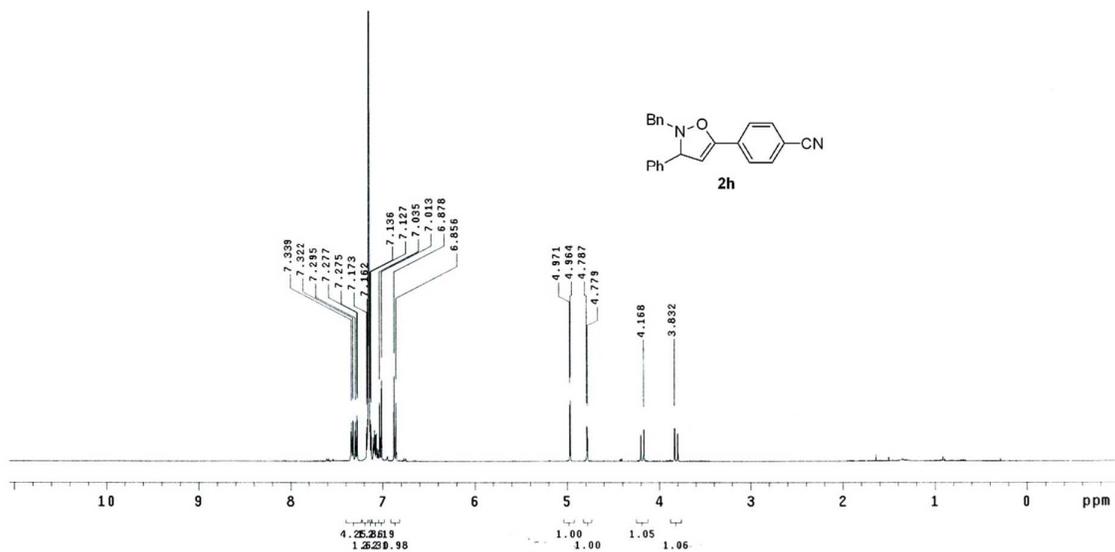


$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ chart for **2e** ([Scheme 2], $(\text{PPh}_3)\text{AuCl/AgOTf}$ used)

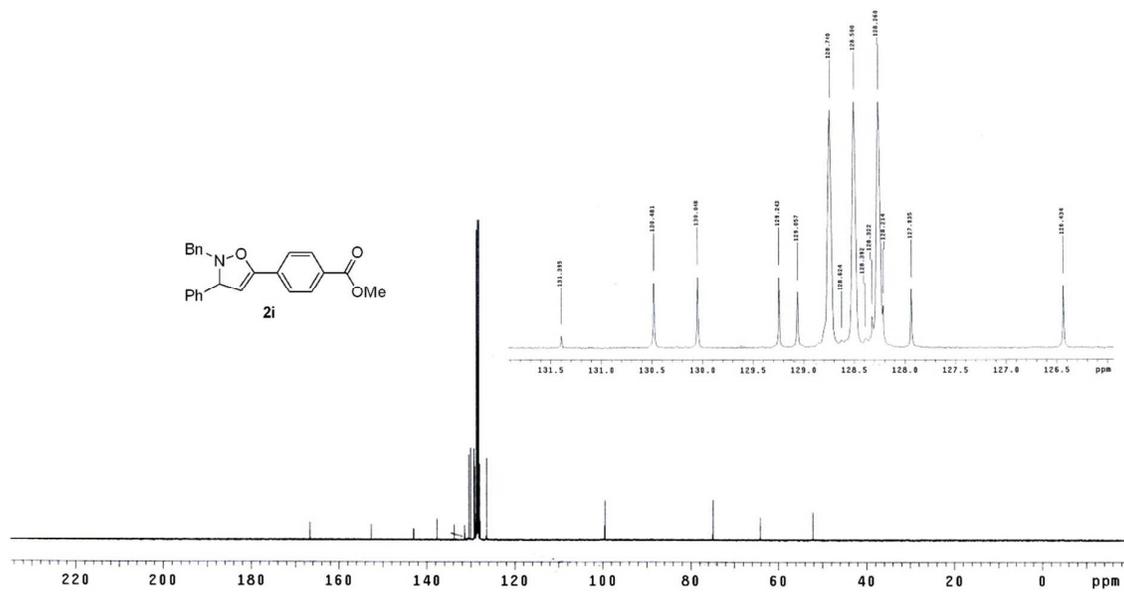
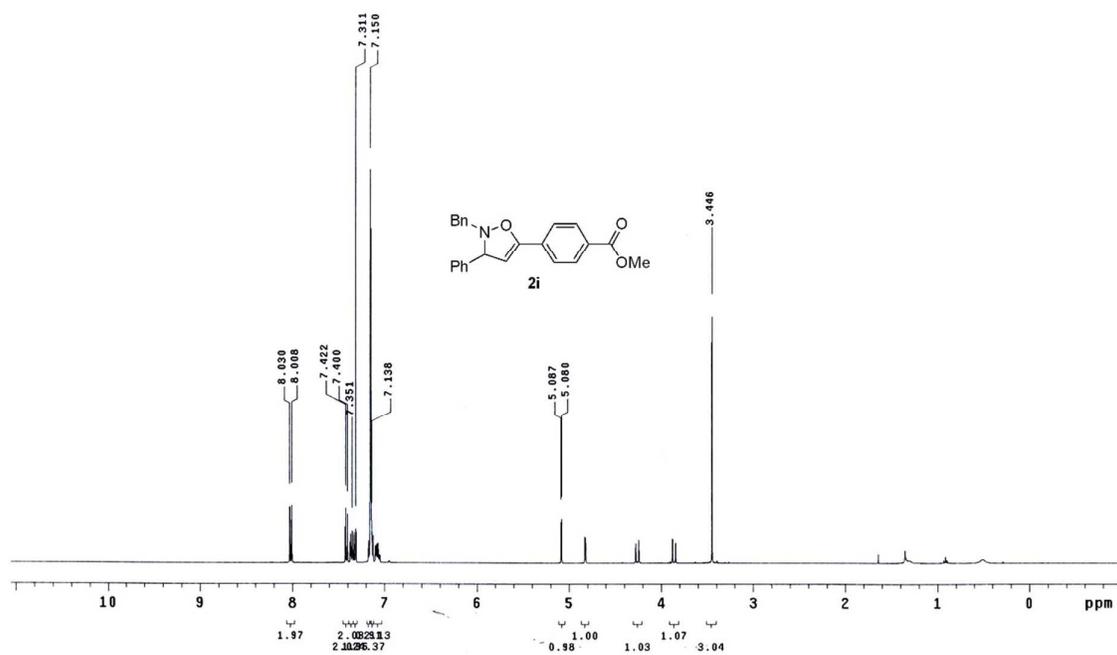


$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ chart for **2g** ([Scheme 2], $(\text{PPh}_3)\text{AuCl}/\text{AgOTf}$ used)

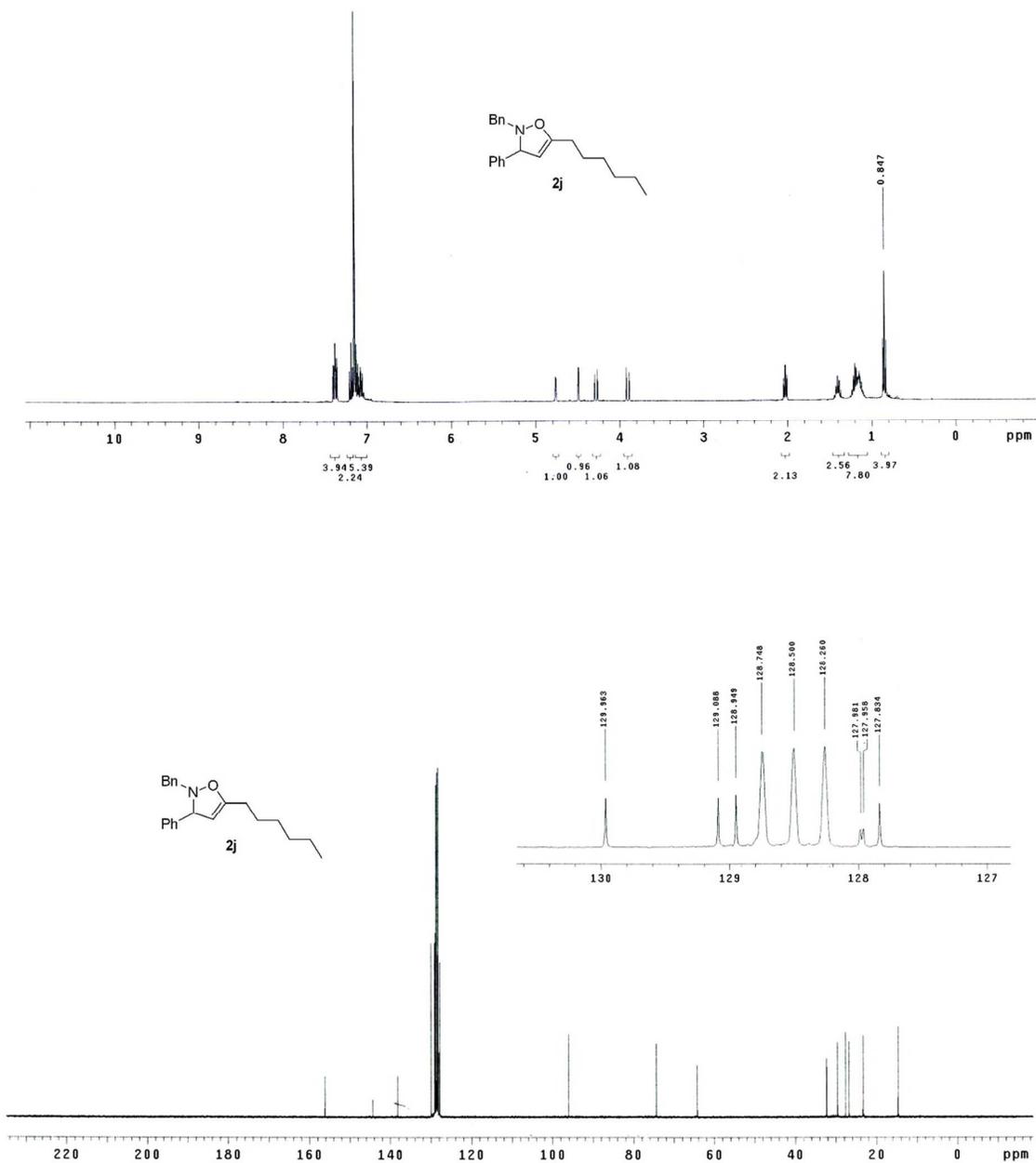


¹H-NMR and ¹³C-NMR chart for **2h** ([Scheme 2], (PPh₃)AuCl/AgOTf used)

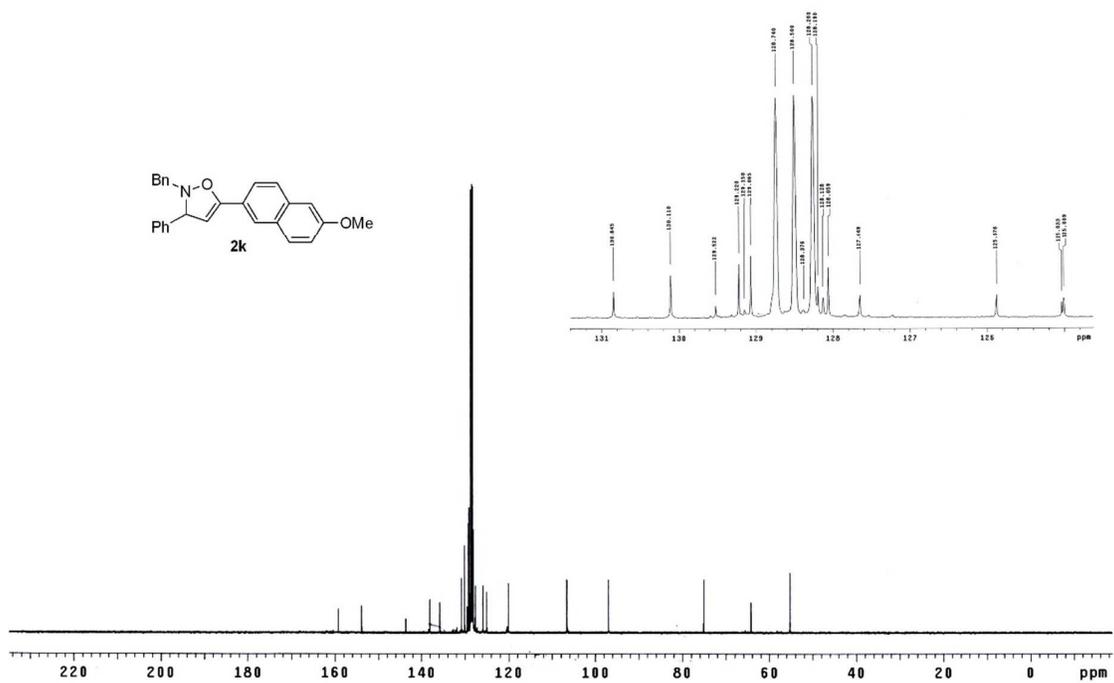
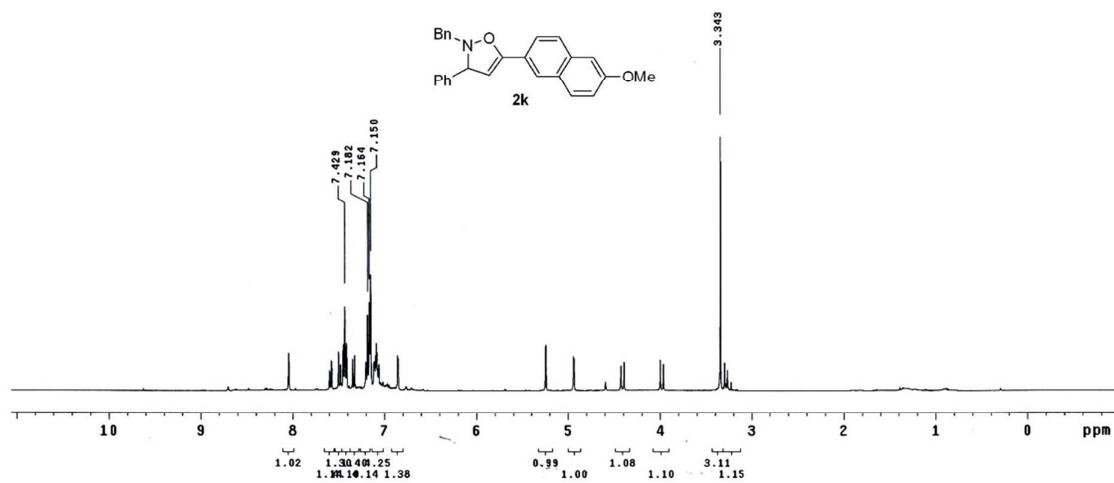
$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ chart for **2i** ([Scheme 2], $(\text{PPh}_3)\text{AuNTf}_2$ used)



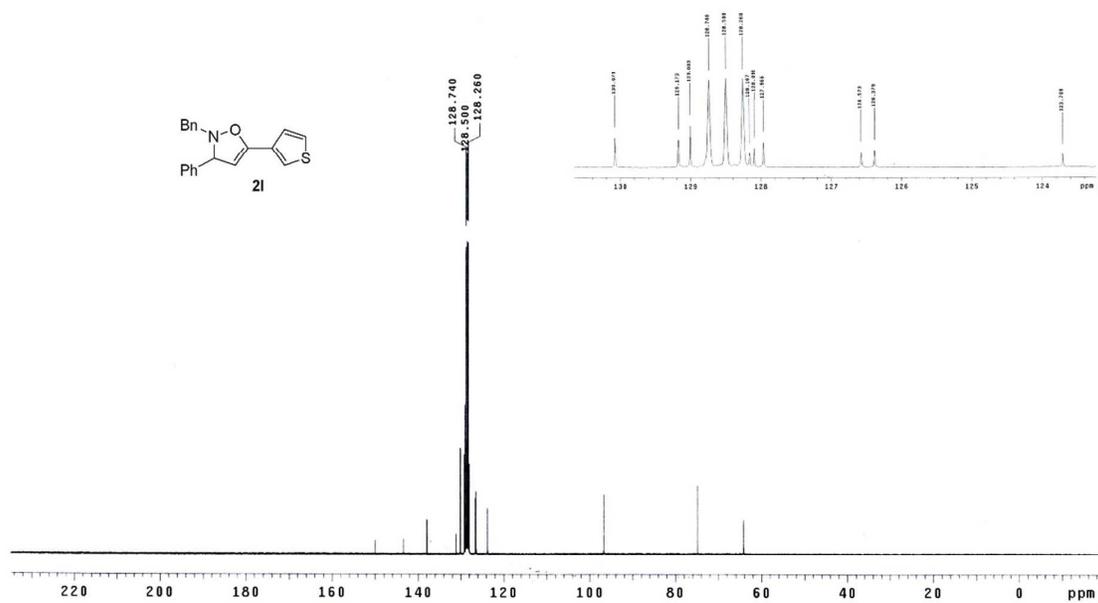
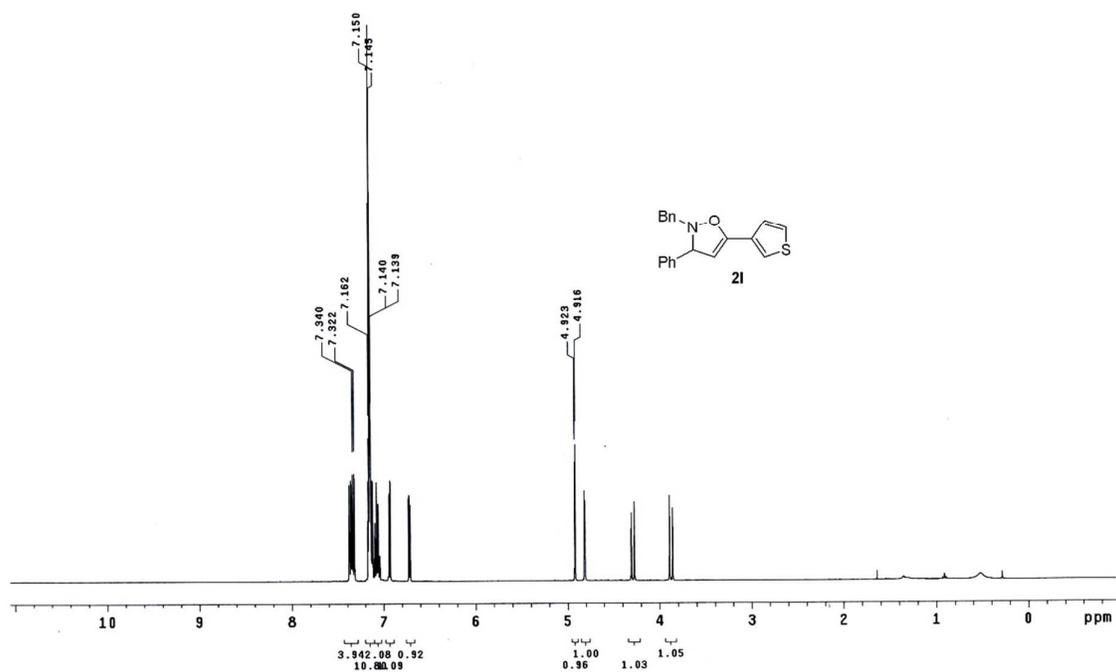
$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ chart for **2j** ([Scheme 2], $(\text{PPh}_3)\text{AuNTf}_2$ used)



$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ chart for **2k** ([Scheme 2], $(\text{PPh}_3)\text{AuNTf}_2$ used)

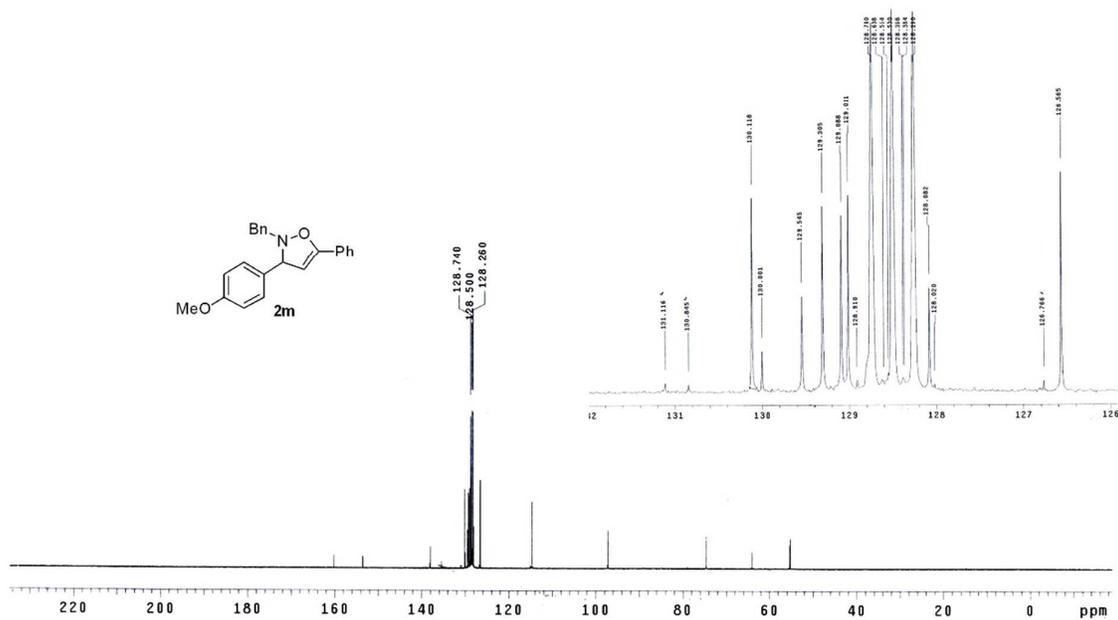
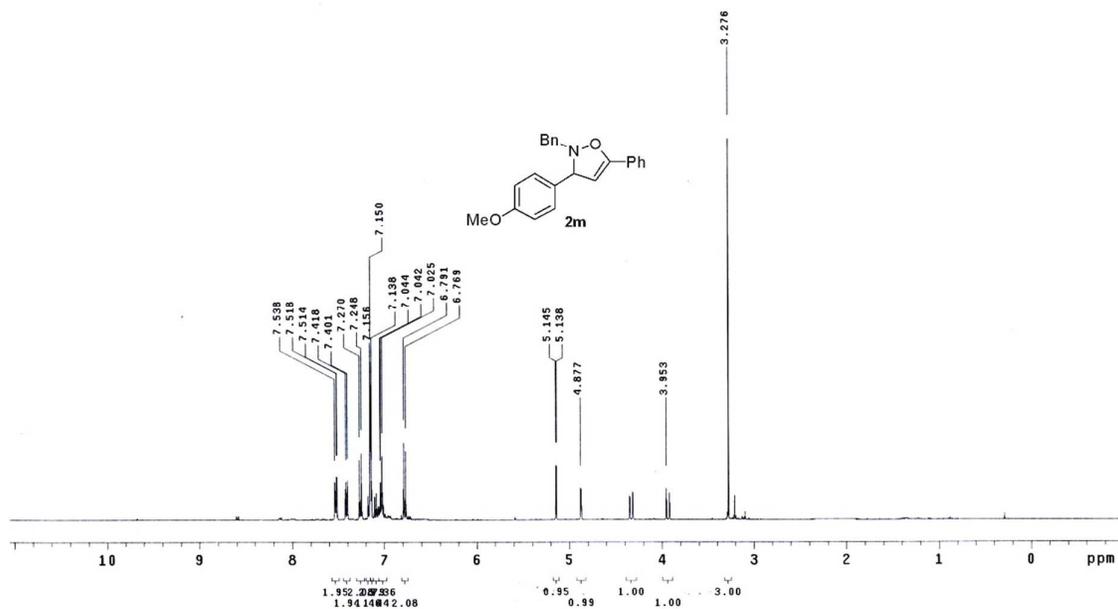


$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ chart for **2I** ([Scheme 2], $(\text{PPh}_3)\text{AuNTf}_2$ used)

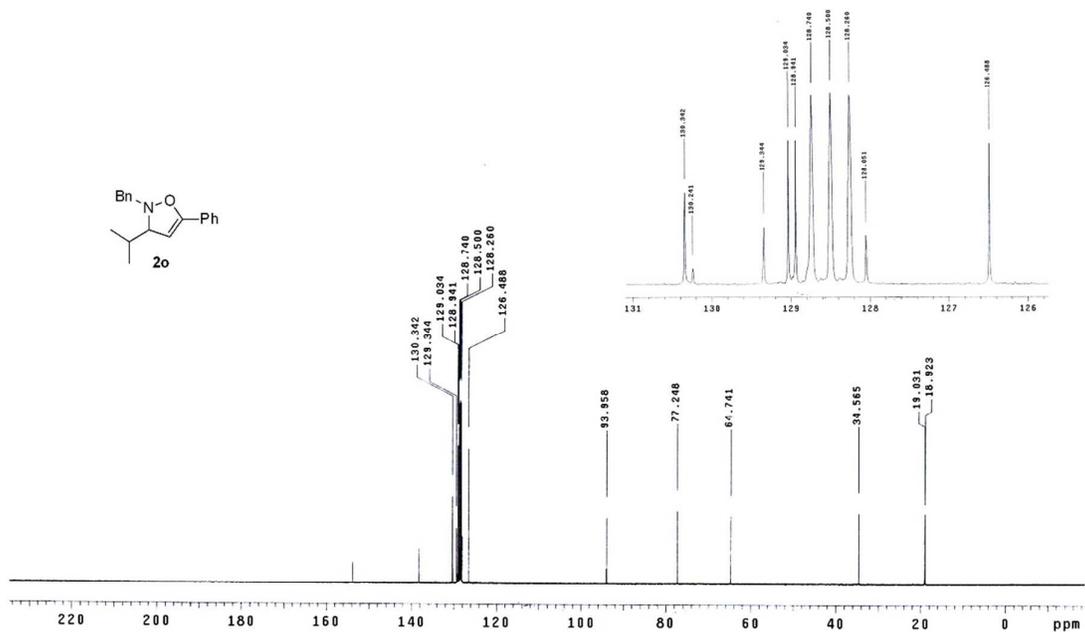
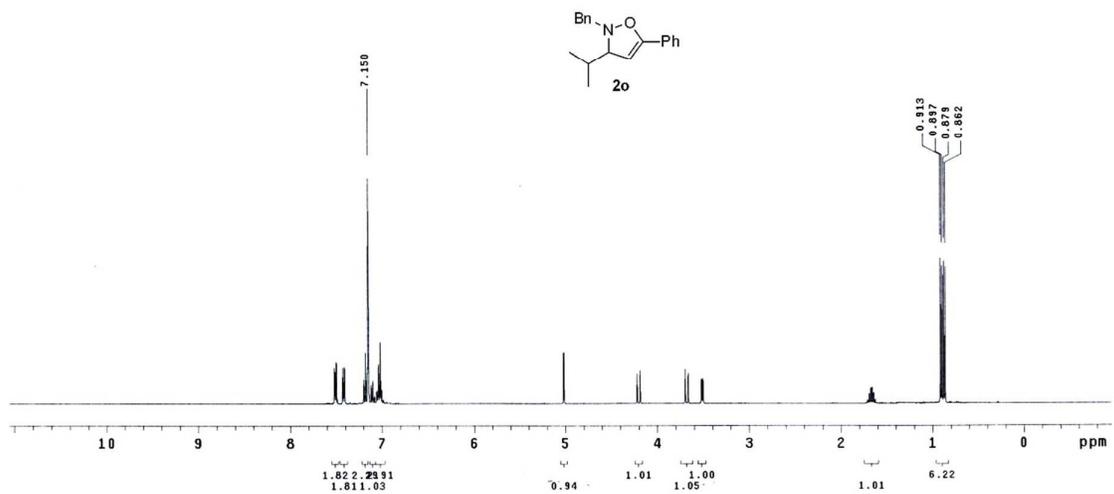


Supporting information

$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ chart for **2m** ([Scheme 2], $(\text{PPh}_3)\text{AuCl/AgOTf}$ used)

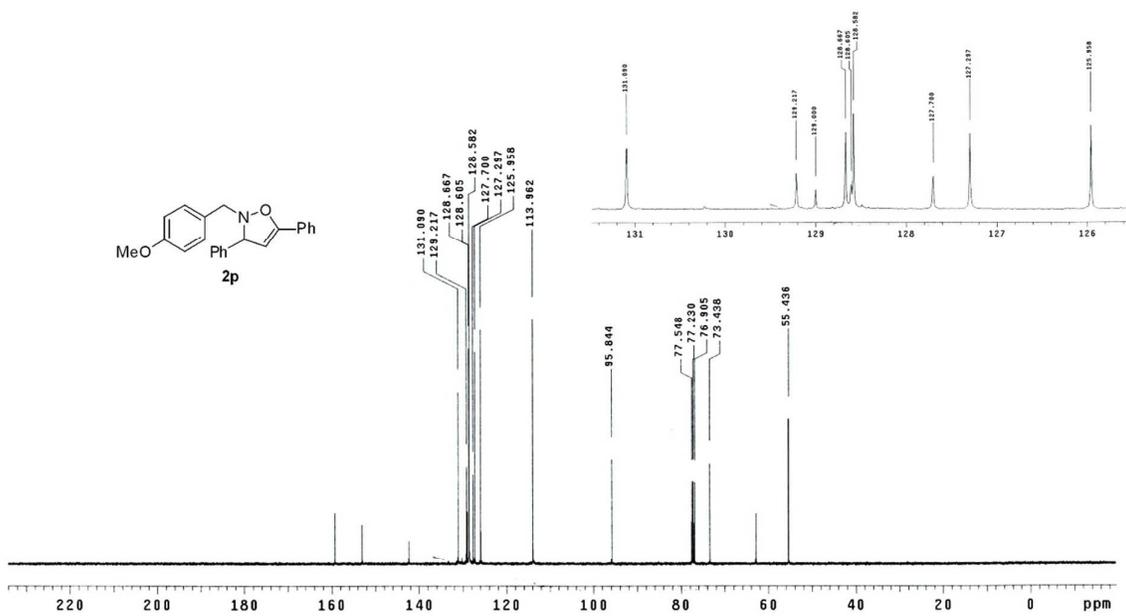
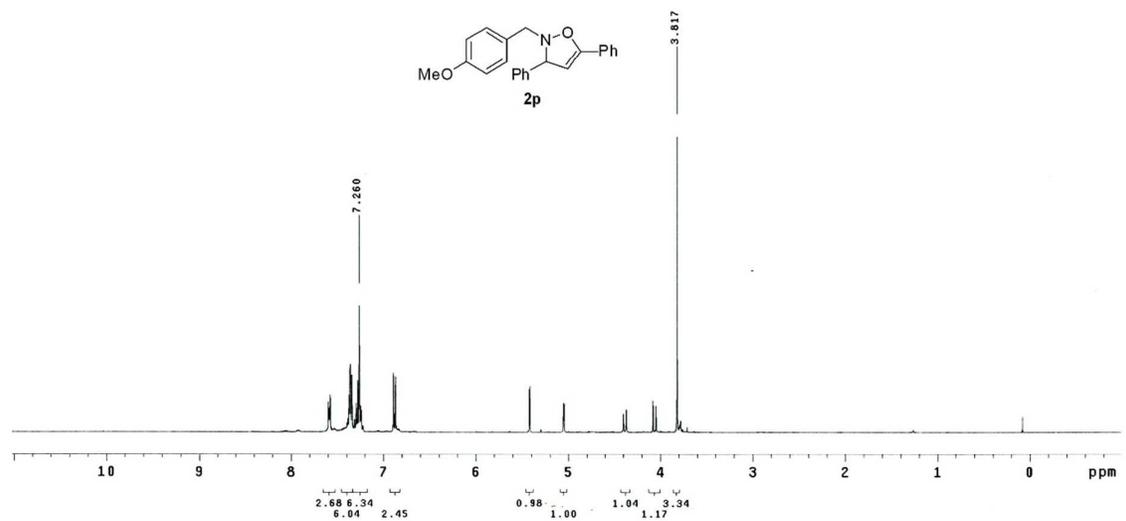


$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ chart for **2o** ([Scheme 2], $(\text{PPh}_3)\text{AuCl}/\text{AgOTf}$ used)

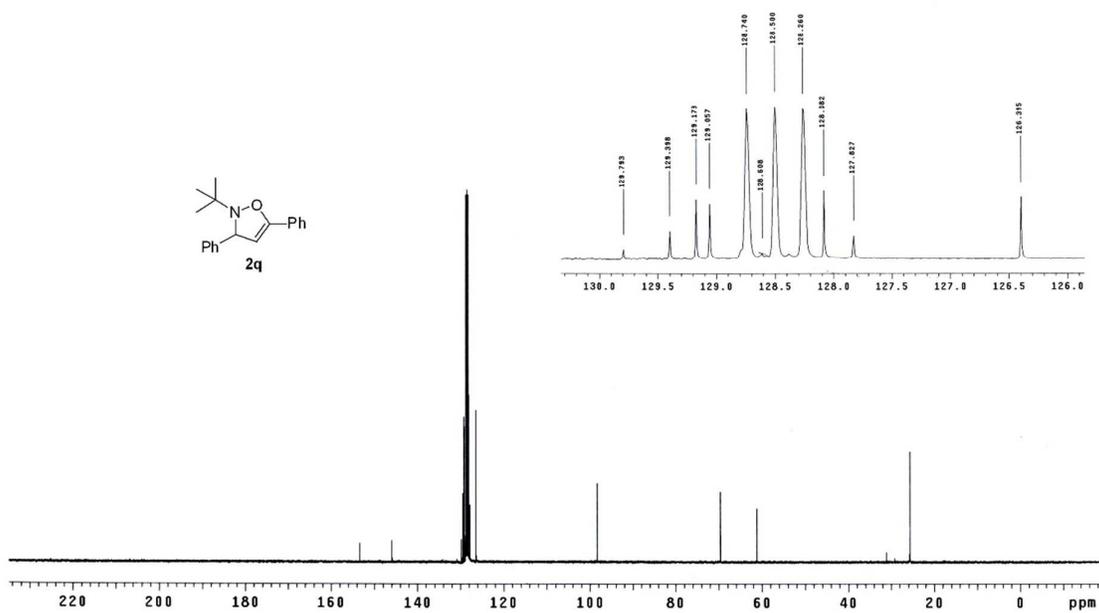
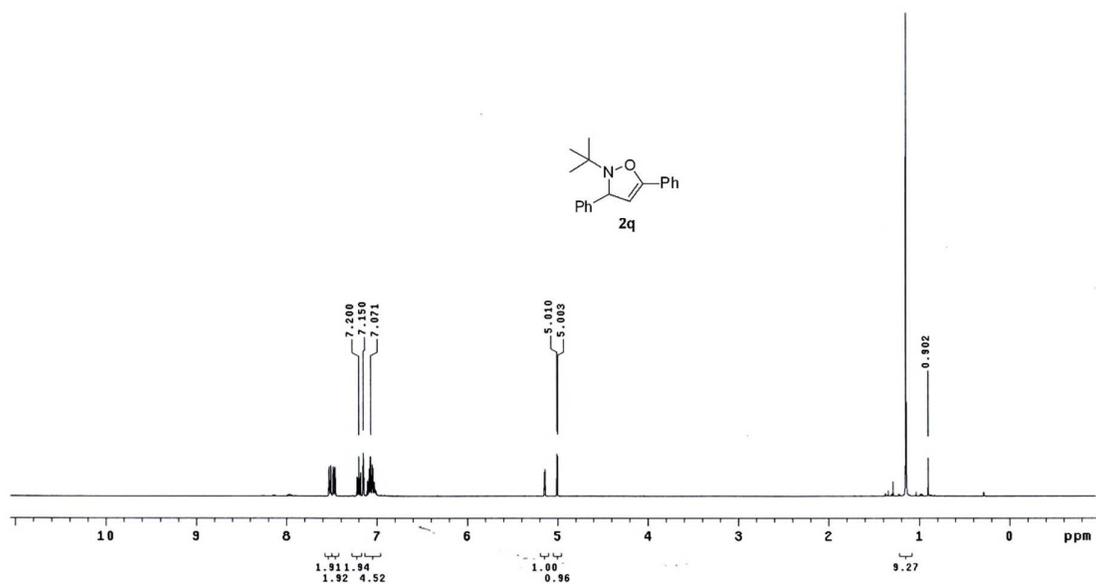


Supporting information

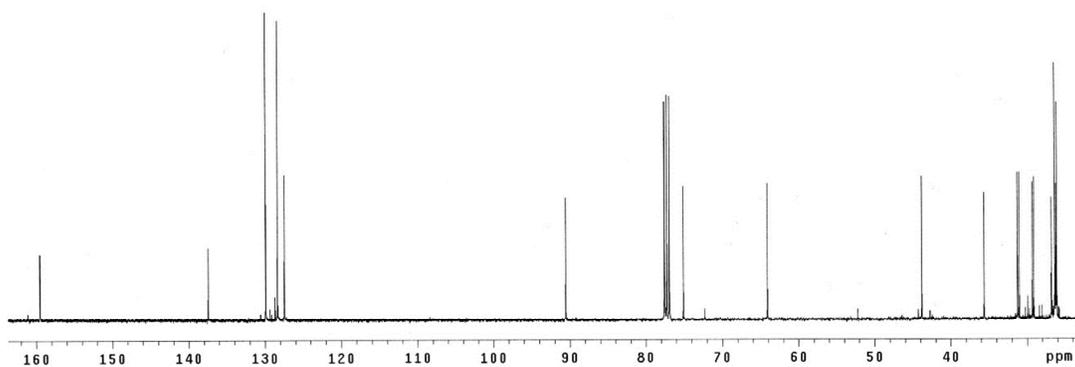
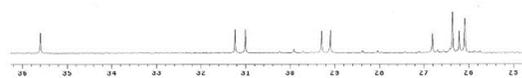
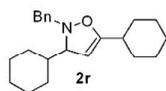
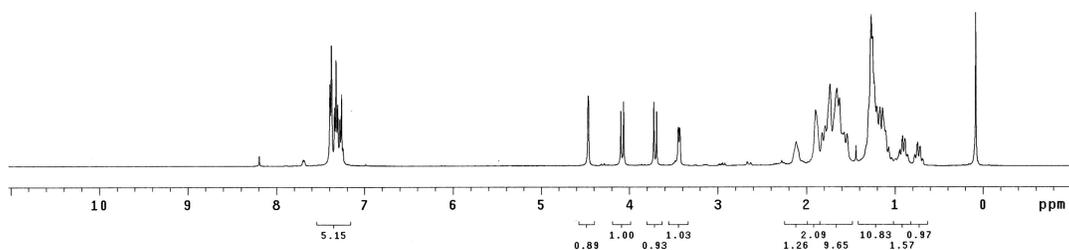
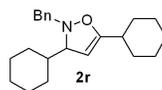
$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ chart for **2p** ([Scheme 2], $(\text{PPh}_3)\text{AuCl}/\text{AgOTf}$ used)



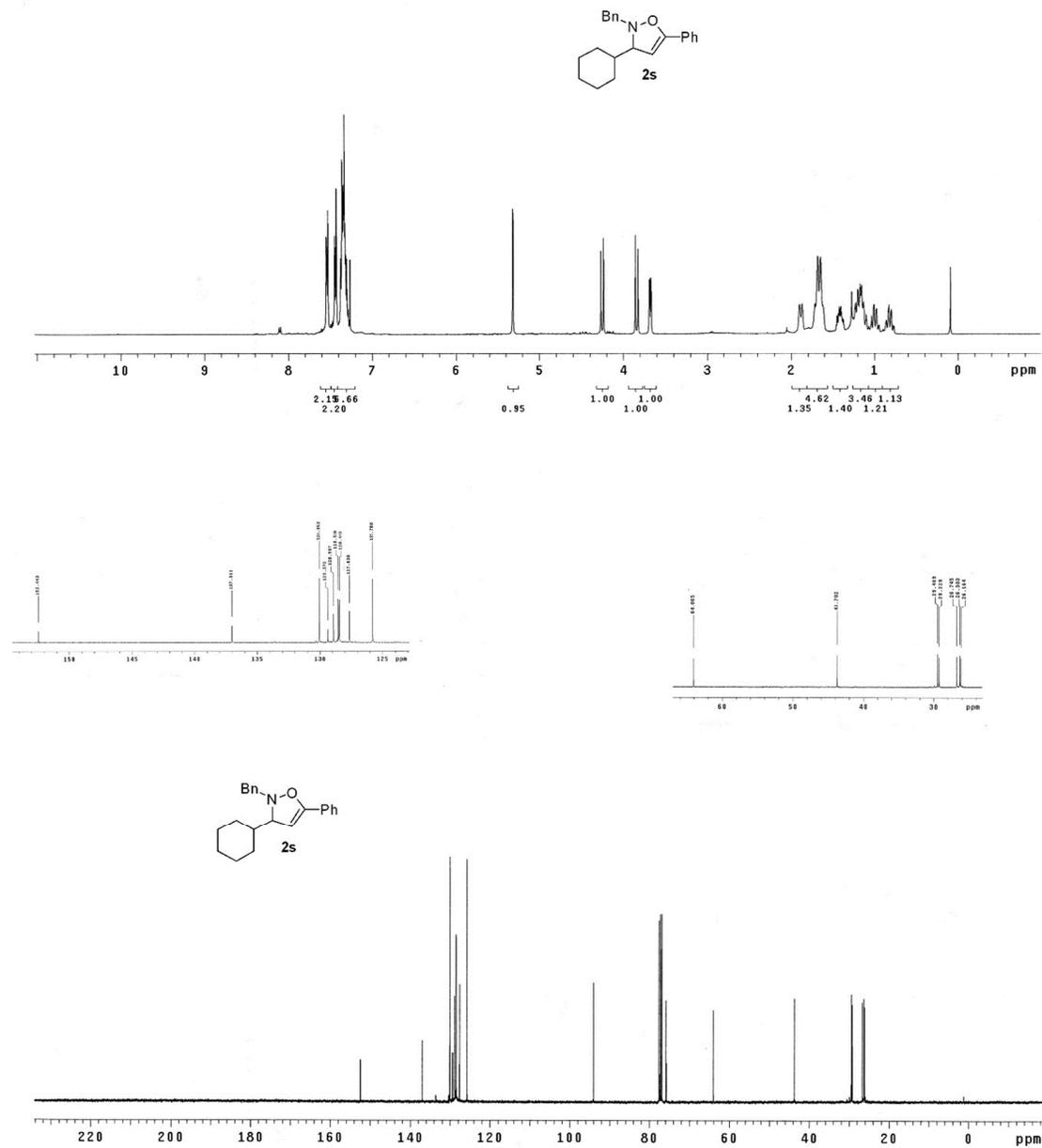
$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ chart for **2q** ([Scheme 2], $(\text{PPh}_3)\text{AuNTf}_2$ used)



$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ chart for **2r** ([Scheme 2], $(\text{PPh}_3)\text{AuNTf}_2$ used)

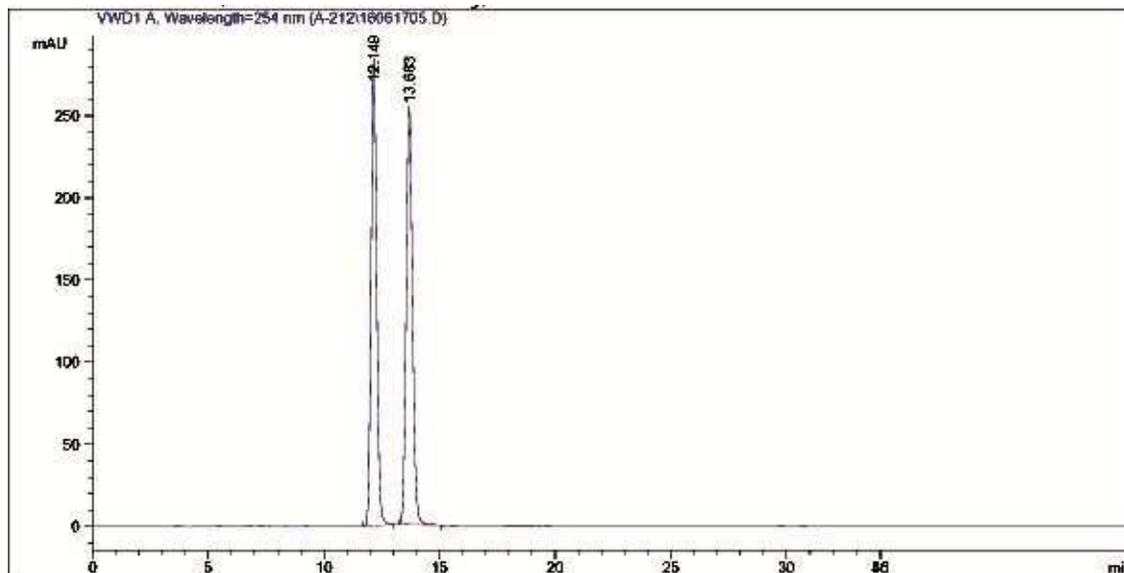


$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ chart for **2s** ([Scheme 2], $(\text{PPh}_3)\text{AuNTf}_2$ used)



B. HPLC chromatogram for (R)-1a and (S)-2a

a) Racemic 1a



=====
 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Sample Amount : 1.00000 [ng/ul] (not used in calc.)
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

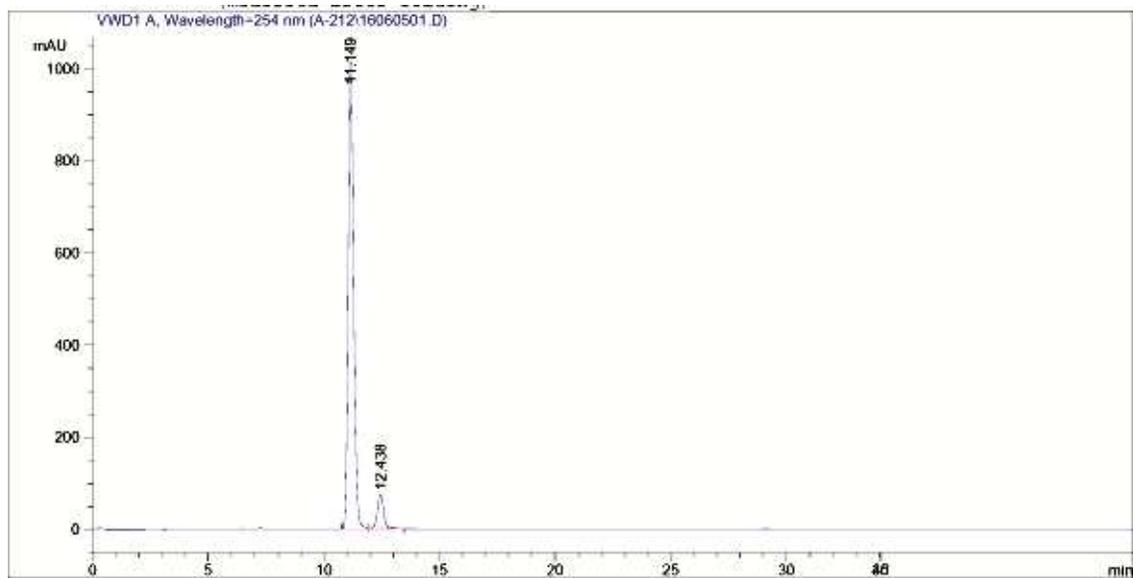
| Peak # | RetTime [min] | Type | Width [min] | Area mAU | Area % | Height [mAU] |
|--------|---------------|------|-------------|------------|---------|--------------|
| 1 | 12.149 | PB | 0.2544 | 4708.60400 | 49.3651 | 284.32306 |
| 2 | 13.683 | BB | 0.2931 | 4829.72510 | 50.6349 | 254.06660 |

Totals : 9538.32910 538.38966

Results obtained with enhanced integrator!

=====
 *** End of Report ***

b) (R)-1a (84% ee)



```

=====
                          Area Percent Report
=====
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Sample Amount  :      1.00000 [ng/ul] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

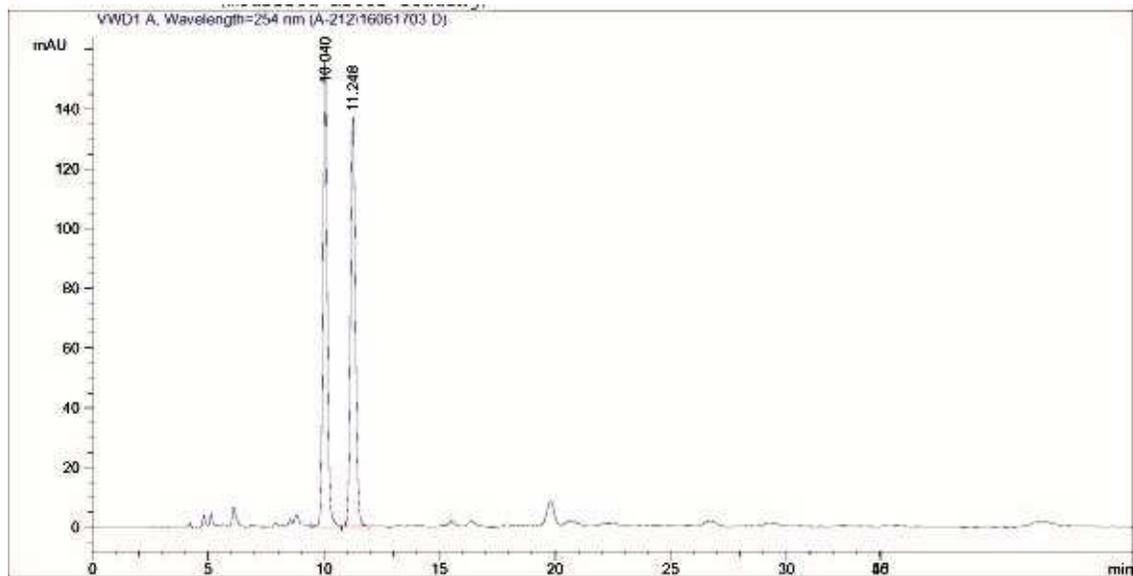
Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type Width Area Height Area
# [min] [min] mAU *s [mAU ] %
----|-----|-----|-----|-----|-----|
  1 11.149 PV 0.2524 1.66693e4 1016.91522 92.0206
  2 12.438 VB 0.2891 1449.44702 75.43888 7.9794

Totals :                1.81148e4 1092.35410

Results obtained with enhanced integrator!
=====
*** End of Report ***
    
```

c) Racemic 2a



=====
 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Sample Amount : 1.00000 [ng/ul] (not used in calc.)
 Use Multiplier & Dilution Factor with ISTDs

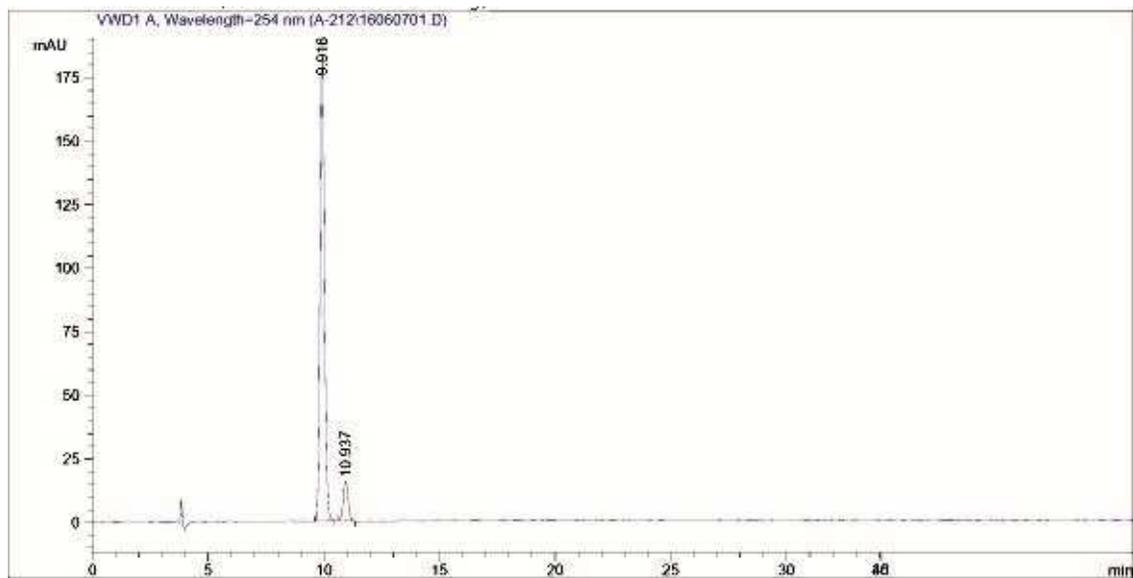
Signal 1: VWD1 A, Wavelength=254 nm

| Peak # | RetTime [min] | Type | Width [min] | Area mAU *s | Height [mAU] | Area % |
|--------|---------------|------|-------------|-------------|--------------|---------|
| 1 | 10.040 | VB | 0.2008 | 2045.85779 | 156.29192 | 50.3936 |
| 2 | 11.248 | BB | 0.2265 | 2013.89893 | 137.25471 | 49.6064 |

Totals : 4059.75671 293.54663

Results obtained with enhanced integrator!

=====
 *** End of Report ***

d) (S)-2a ((PPh₃)AuCl/AgOTf reaction: 83% ee)

```

=====
                          Area Percent Report
=====

```

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution      :      1.0000
Sample Amount  :      1.00000 [ng/ul] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

```

```

Signal 1: VWD1 A, Wavelength=254 nm

```

| Peak # | RetTime [min] | Type | Width [min] | Area MAU *s | Height [mAU] | Area % |
|--------|---------------|------|-------------|-------------|--------------|---------|
| 1 | 9.916 | PB | 0.2039 | 2399.28394 | 181.26244 | 91.5792 |
| 2 | 10.937 | BP | 0.2218 | 220.61707 | 15.45930 | 8.4208 |

```

Totals :                2619.90100  196.72173

```

```

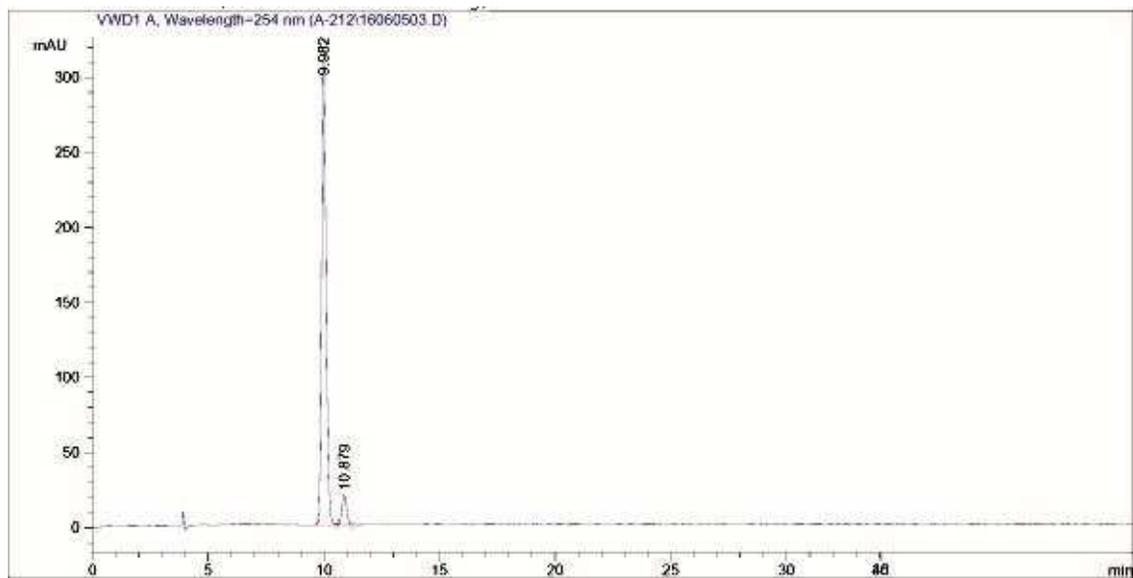
Results obtained with enhanced integrator!

```

```

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*** End of Report ***

```

e) (S)-2a ((PPh₃)AuNTf₂ reaction: 87% ee)

```

=====
                          Area Percent Report
=====
  
```

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution      :      1.0000
Sample Amount  :      1.00000 [ng/ul] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs
  
```

```

Signal 1: VWD1 A, Wavelength=254 nm
  
```

| Peak # | RetTime [min] | Type | Width [min] | Area MAU *s | Height [mAU] | Area % |
|--------|---------------|------|-------------|-------------|--------------|---------|
| 1 | 9.982 | PV | 0.2038 | 4138.13135 | 309.93823 | 93.4969 |
| 2 | 10.873 | VB | 0.2199 | 287.82288 | 20.22880 | 5.5031 |

```

Totals :                4425.95422  330.16704
  
```

```

Results obtained with enhanced integrator!
  
```

```

=====
*** End of Report ***
  
```