

# Synthesis and transformations of a few 9-(pent-4-yn-1-yl)anthracene-type systems

Eason M. Mathew, Tomson Devassia, Sreedharan Prathapan, and  
Perupparampil A. Unnikrishnan\*

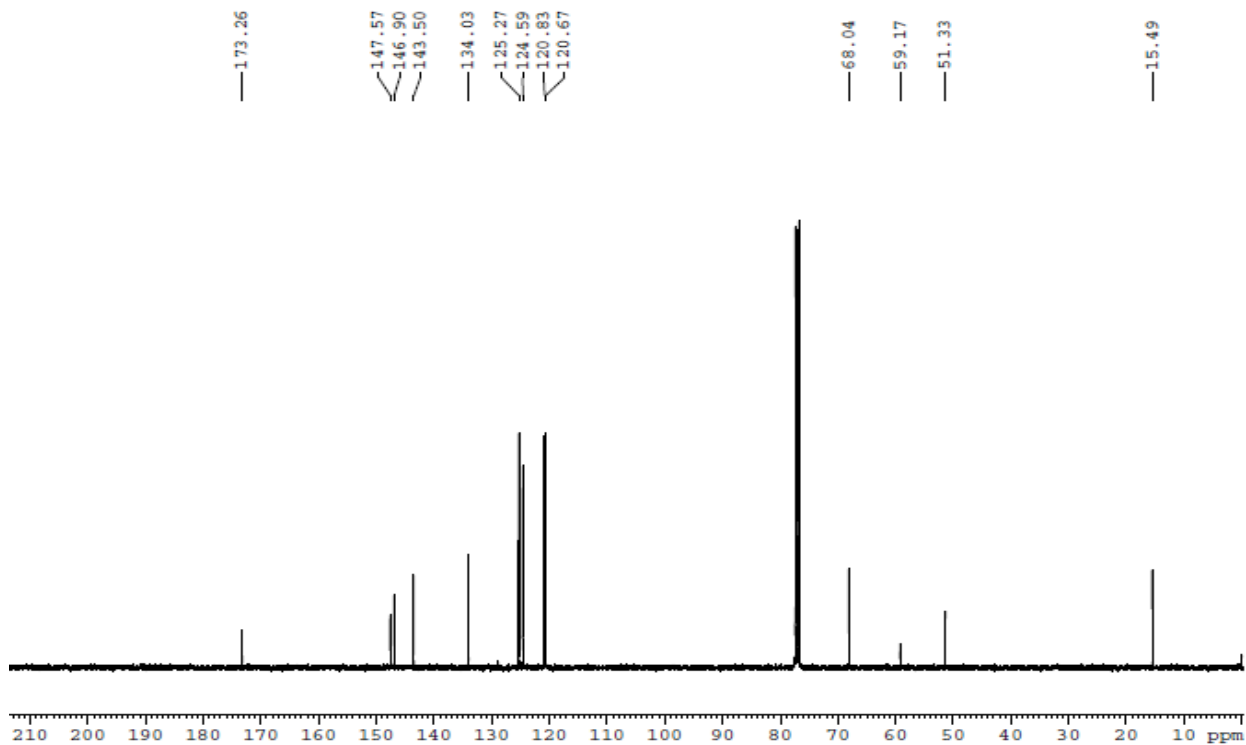
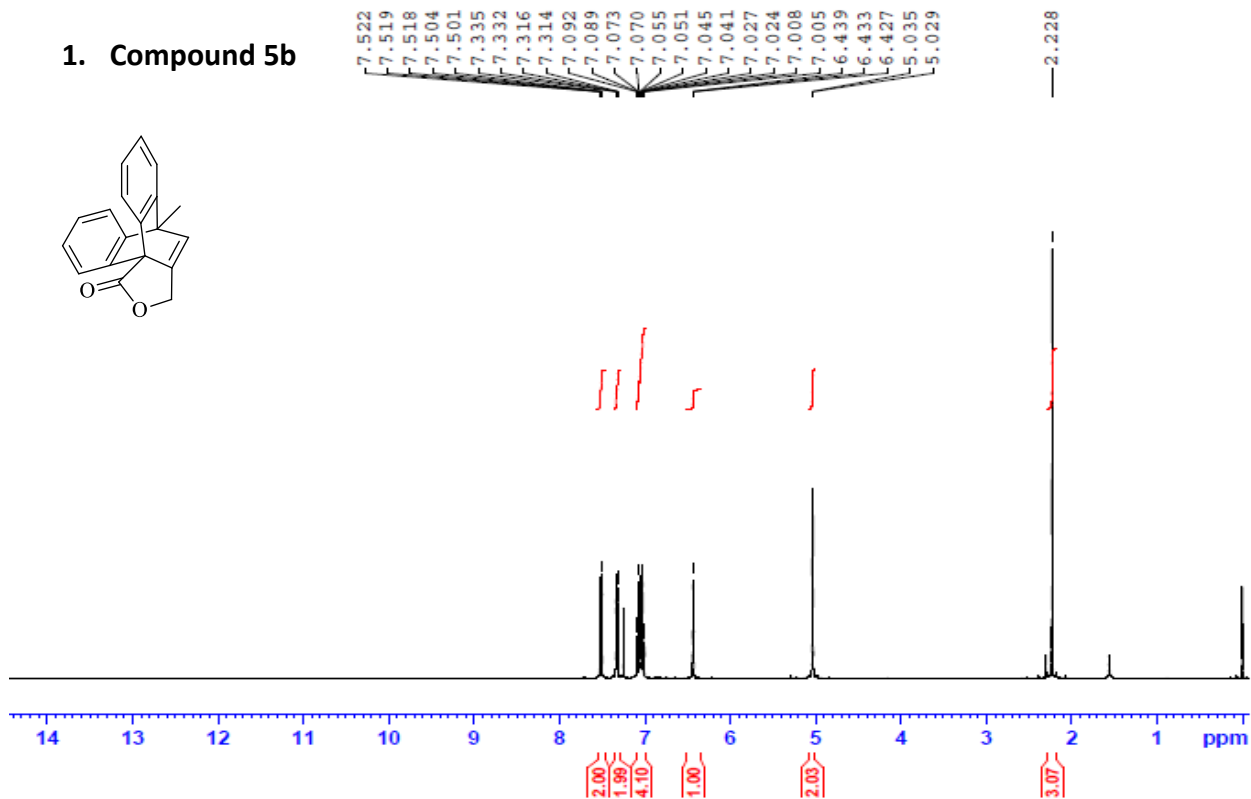
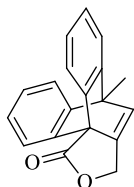
*Department of Applied Chemistry, CUSAT, Kochi-22, India*

*Email: [paunni@gmail.com](mailto:paunni@gmail.com)*

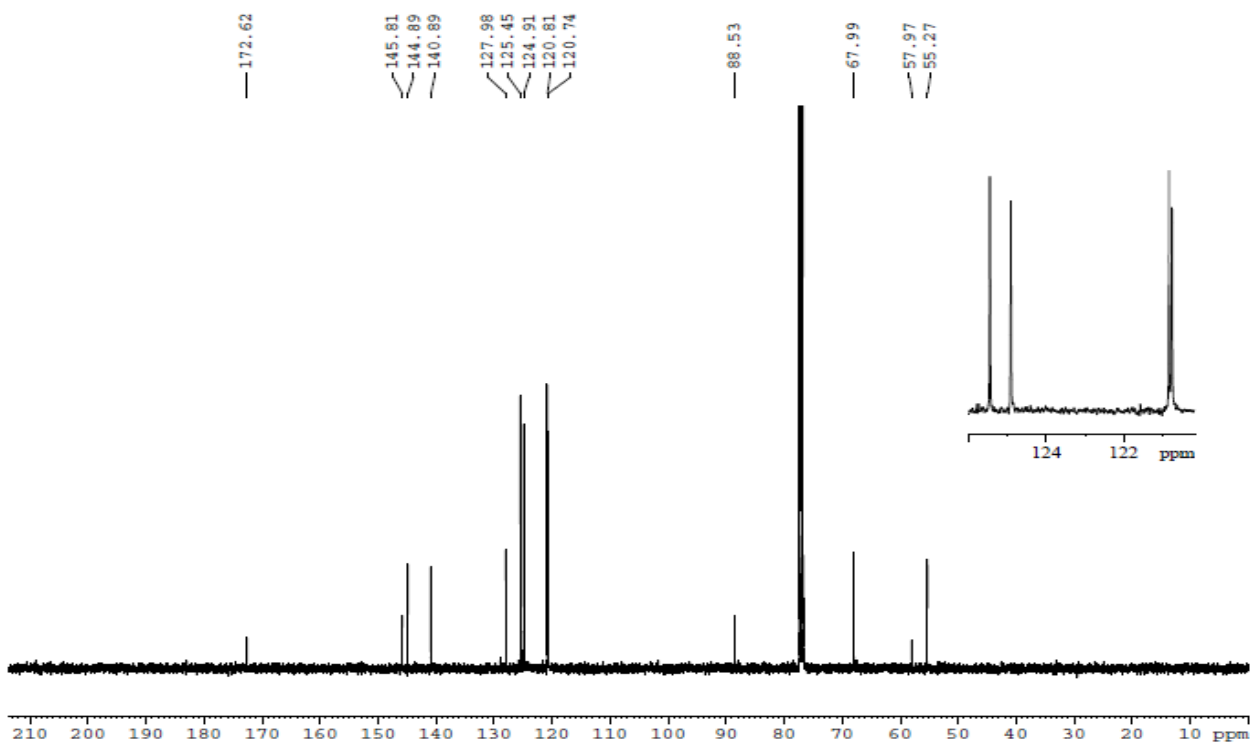
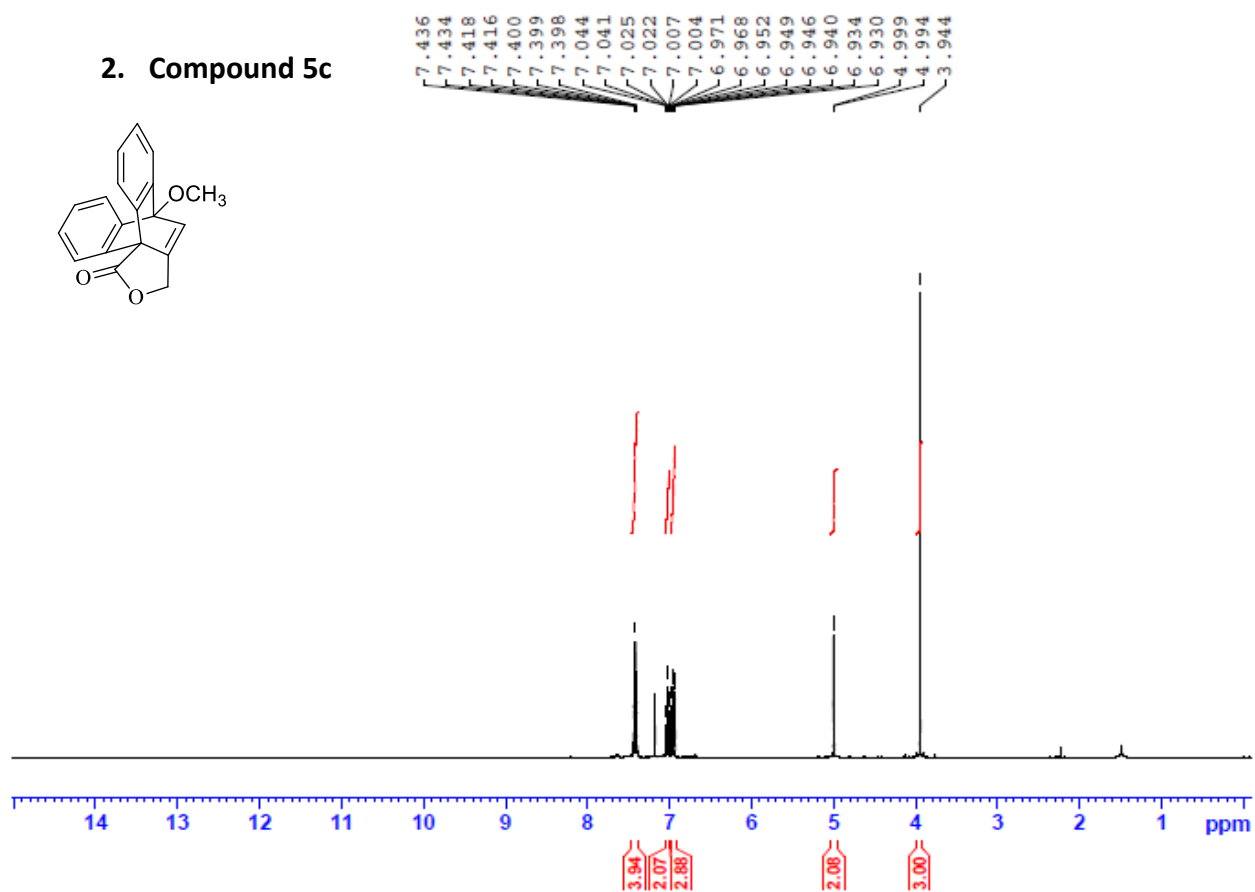
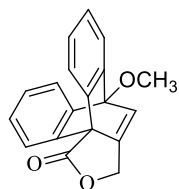
**Content:  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of novel compounds**

Unless otherwise mentioned, all  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on a 400 MHz Bruker Avance III FT-NMR spectrometer with tetramethylsilane (TMS) as internal standard. Chemical shifts ( $\delta$ ) are reported in parts per million (ppm) downfield of TMS.

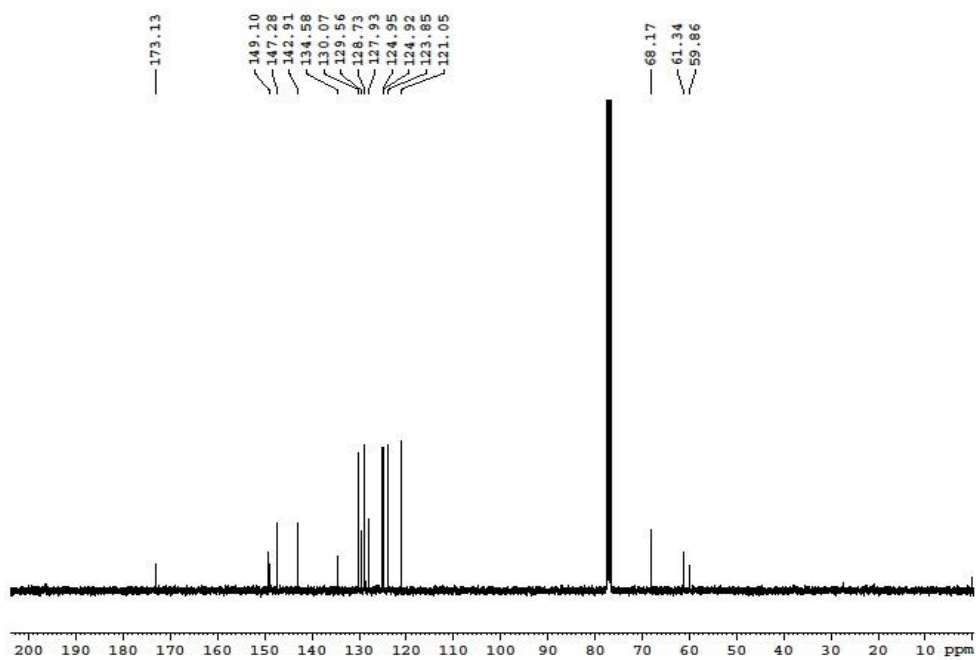
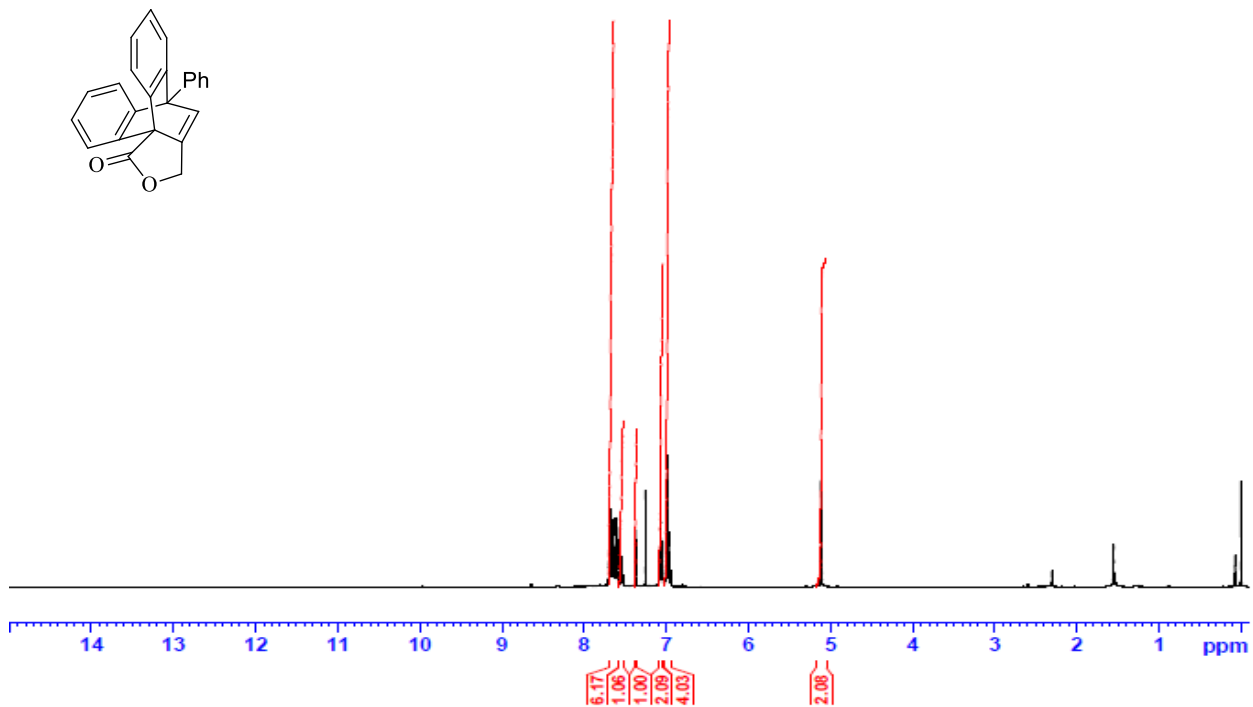
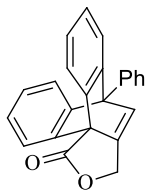
1. Compound 5b



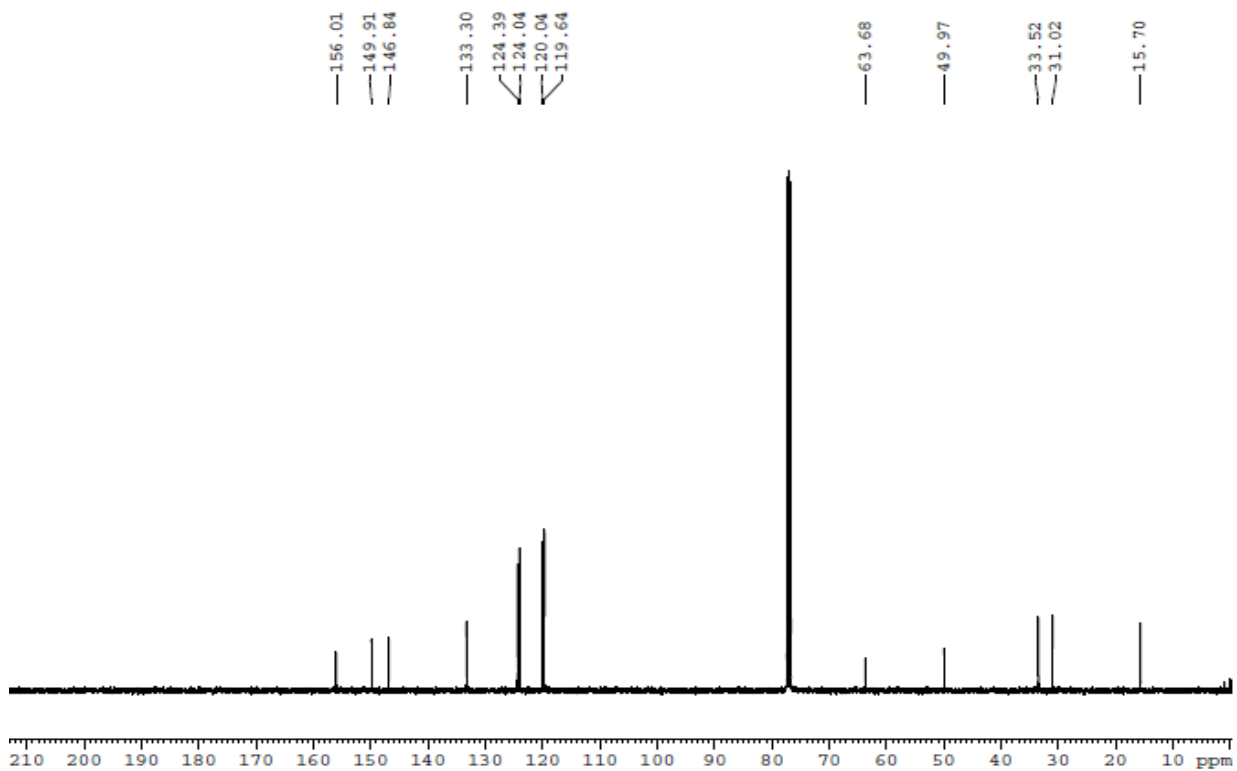
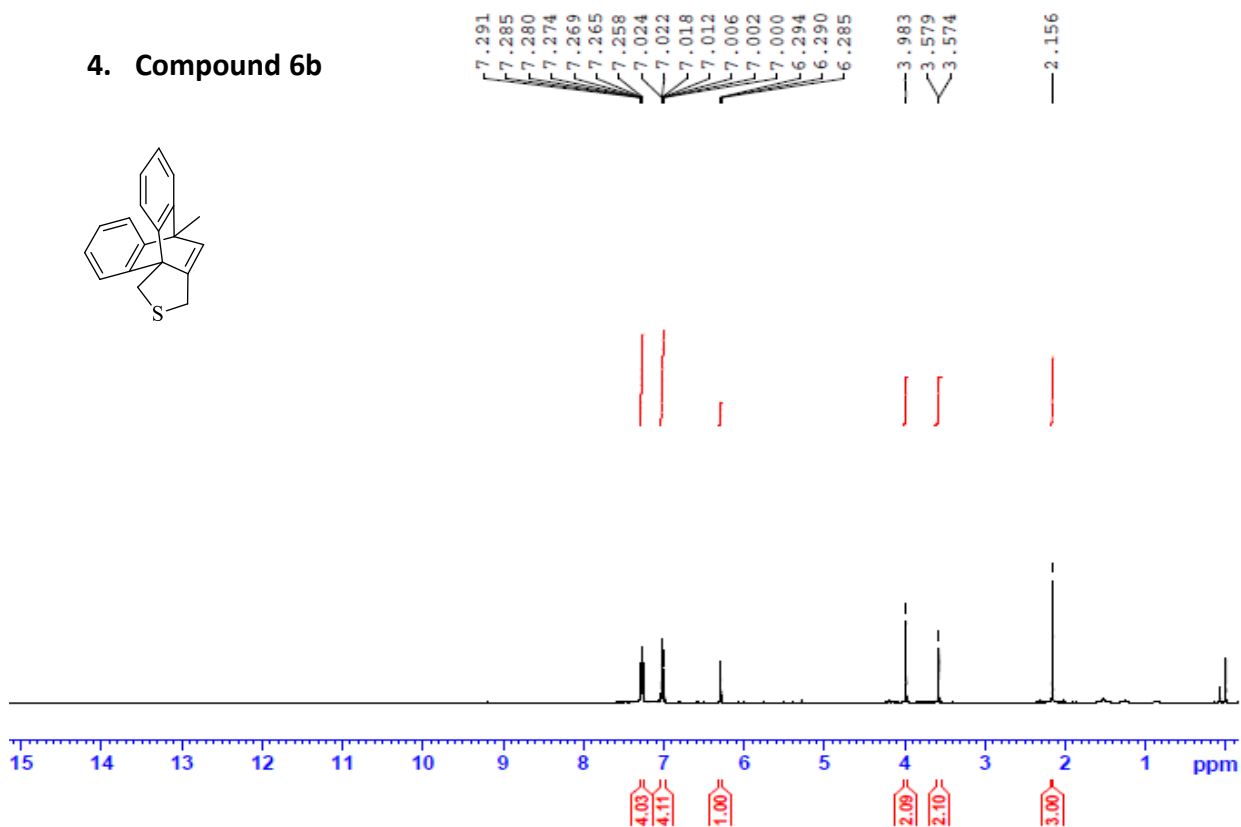
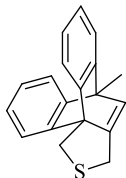
## 2. Compound 5c



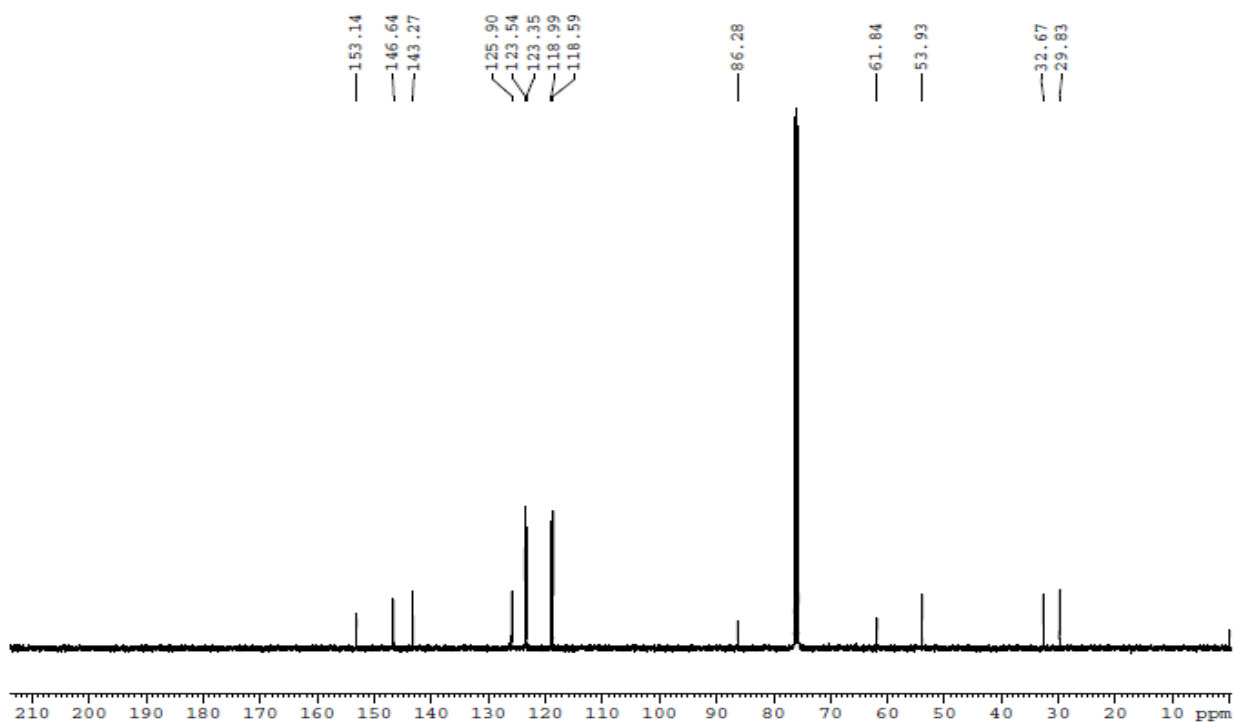
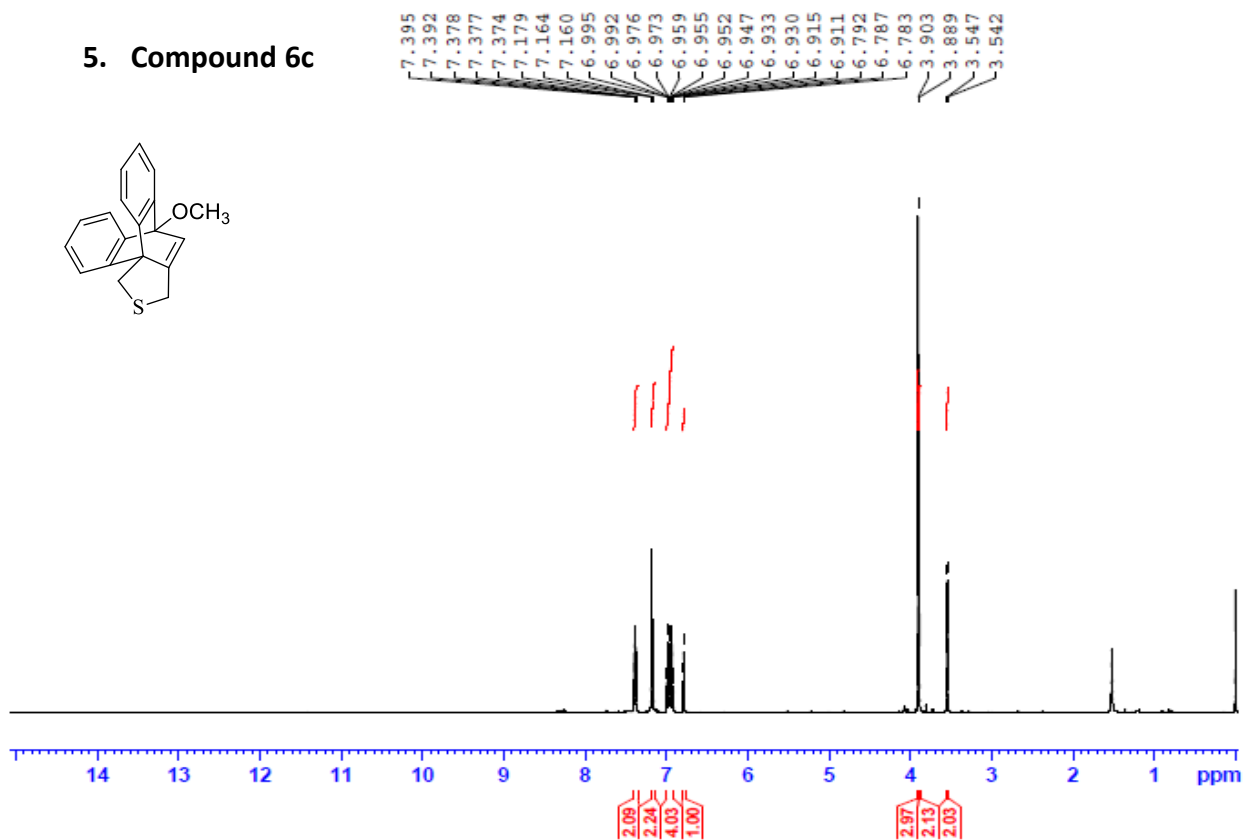
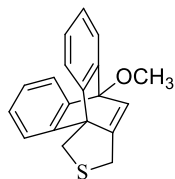
## 3. Compound 5d



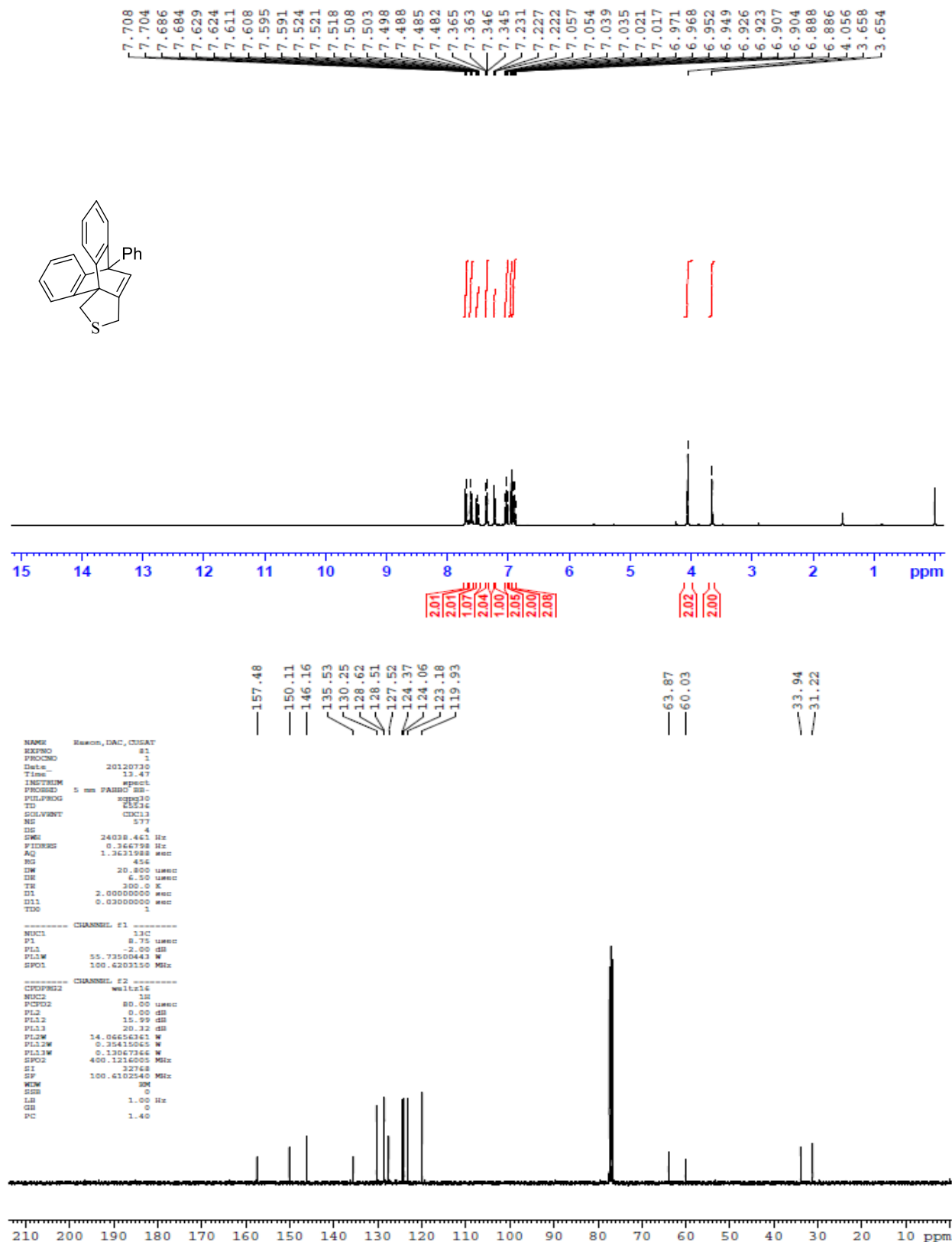
4. Compound 6b



## 5. Compound 6c

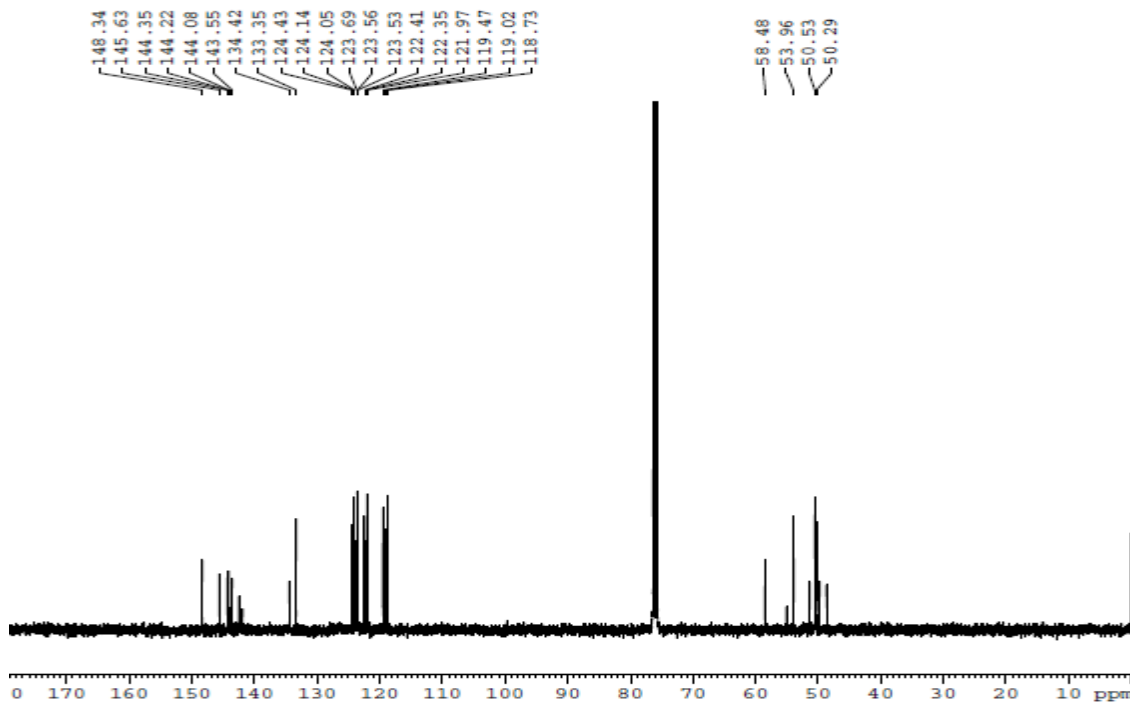
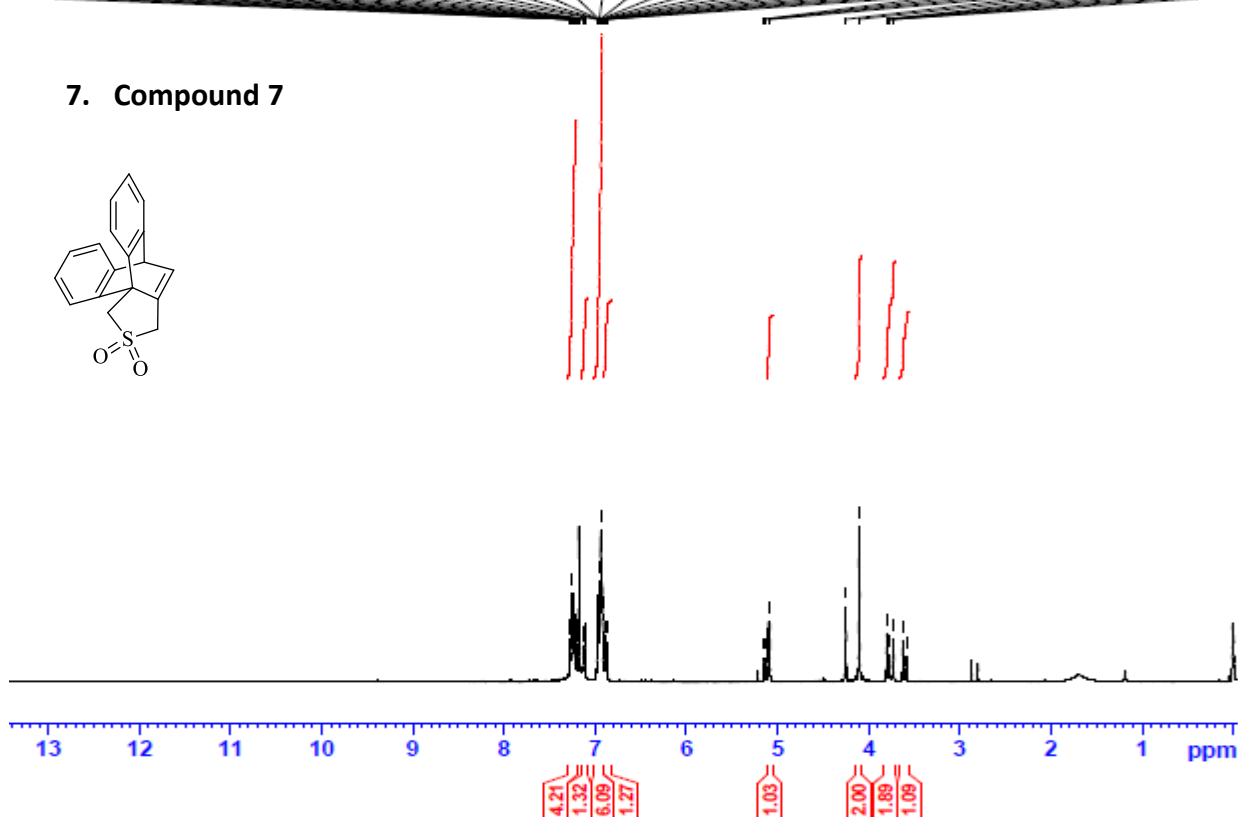
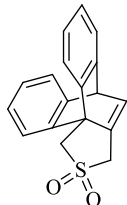


6. Compound 6d



7.279  
7.274  
7.265  
7.257  
7.252  
7.245  
7.235  
7.229  
7.226  
7.216  
7.212  
7.193  
7.172  
7.133  
7.125  
7.115  
7.111  
6.974  
6.969  
6.964  
6.963  
6.958  
6.954  
6.943  
6.938  
6.933  
6.928  
6.922  
6.920  
6.917  
6.891  
6.886  
6.881  
6.877  
6.871  
5.148  
5.133  
5.099  
5.084  
4.250  
4.103  
3.801  
3.796  
3.771  
3.766  
3.732  
3.728

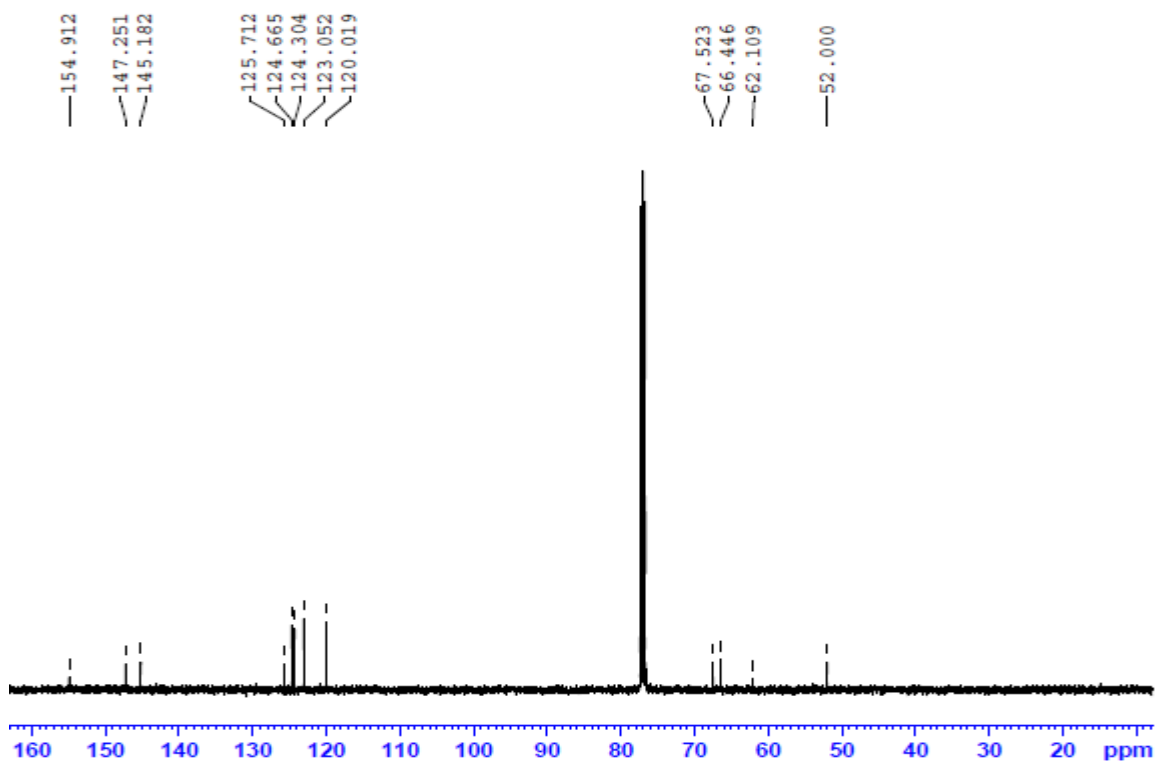
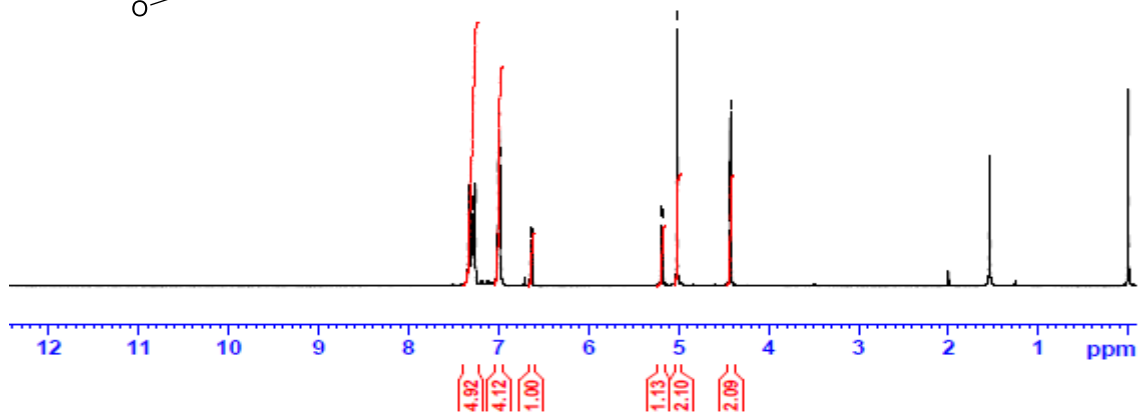
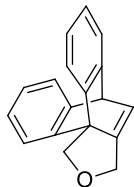
7. Compound 7



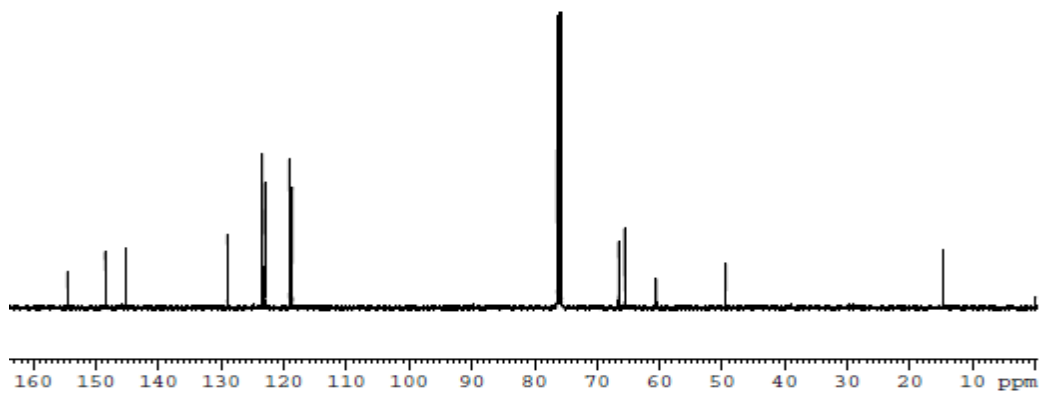
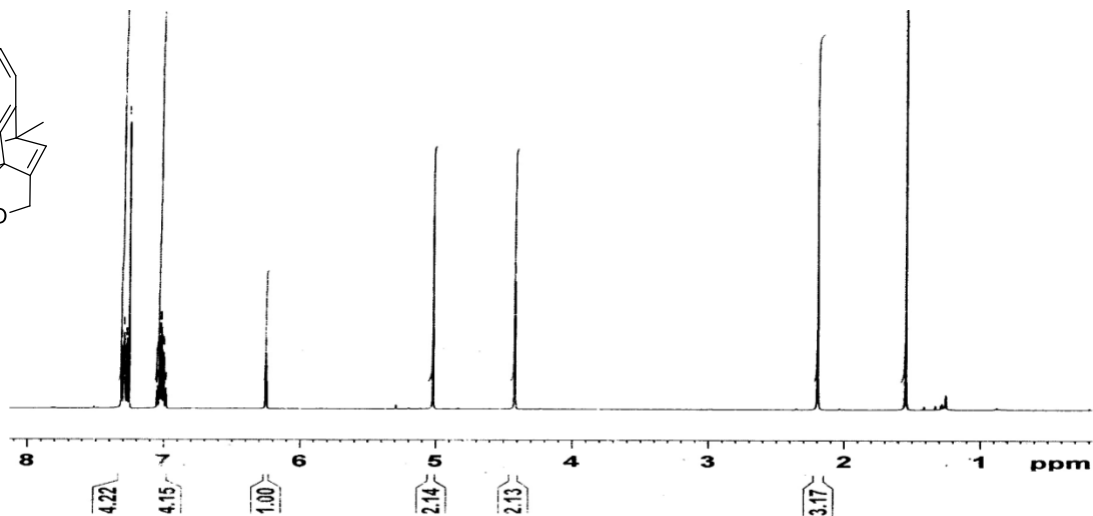
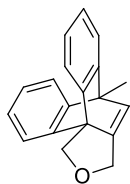


7.333  
7.328  
7.321  
7.312  
7.292  
7.282  
7.275  
7.271  
7.004  
7.002  
6.999  
6.993  
6.987  
6.983  
6.640  
6.634  
6.630  
6.625  
5.189  
5.174  
5.013  
4.422  
4.417

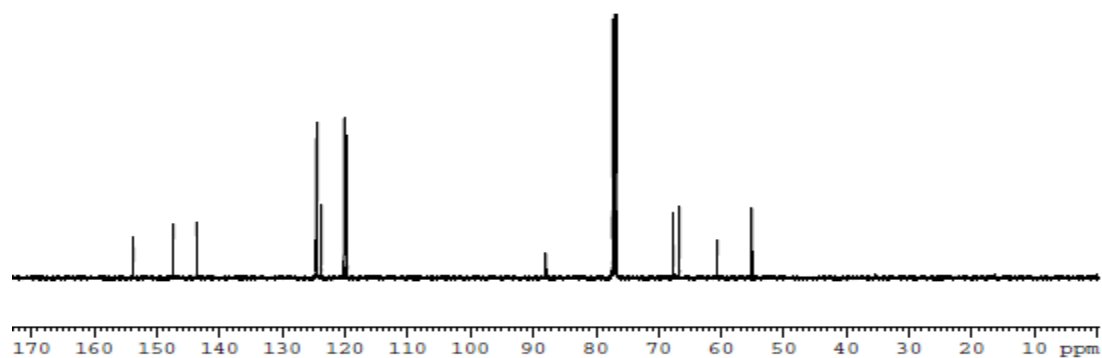
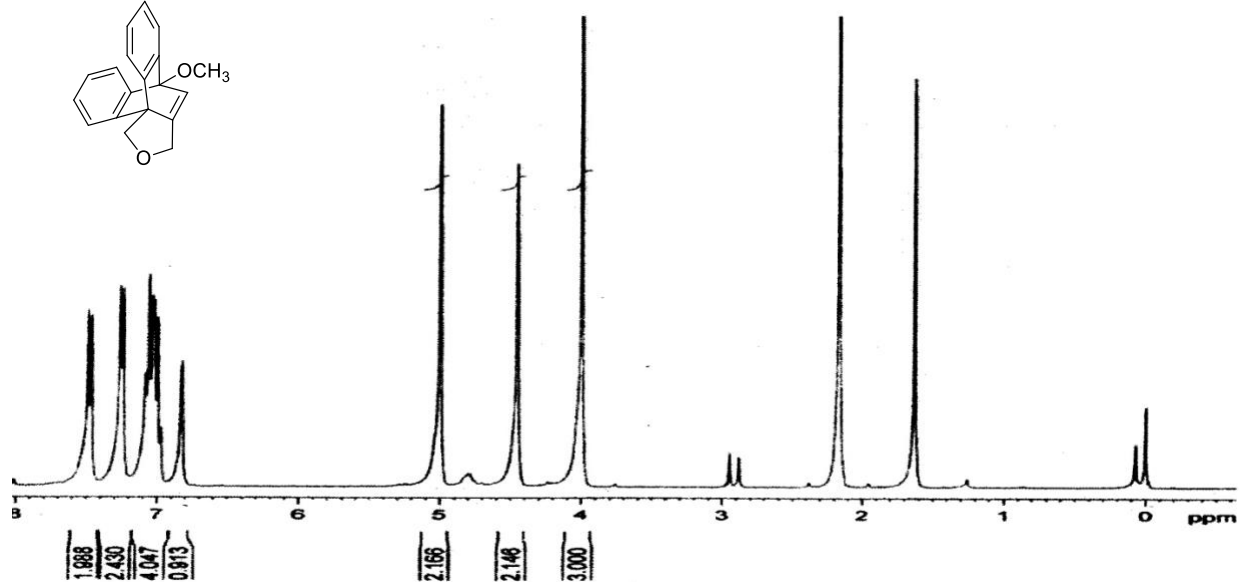
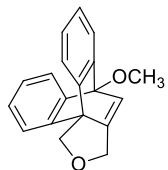
## 8. Compound 8a



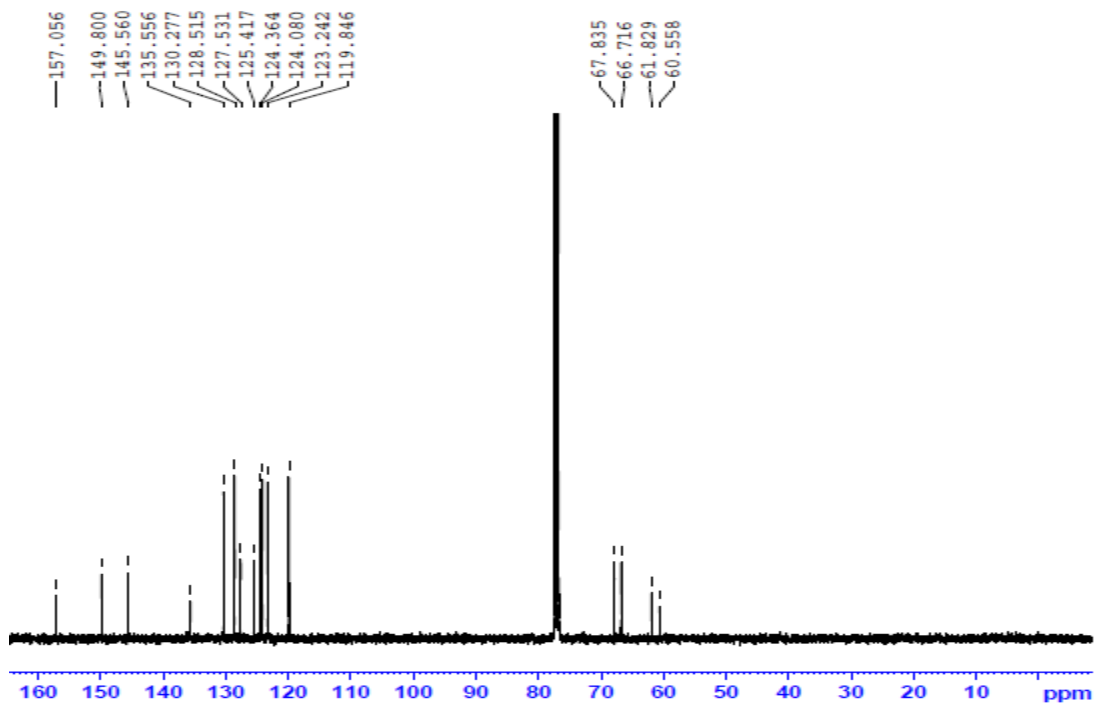
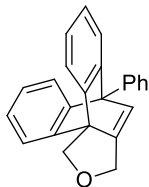
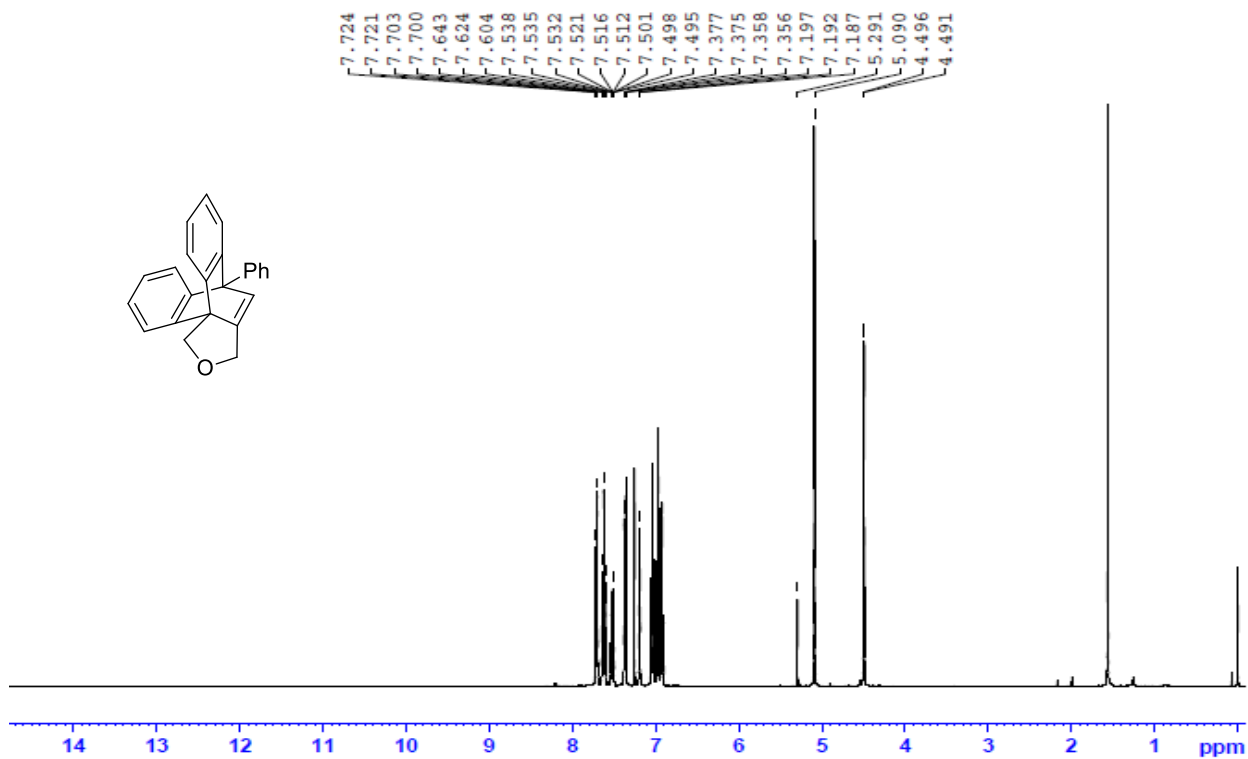
## 9. Compound 8b

 $^1\text{H}$  NMR on a 500 M Hz instrument

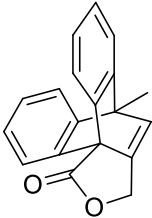
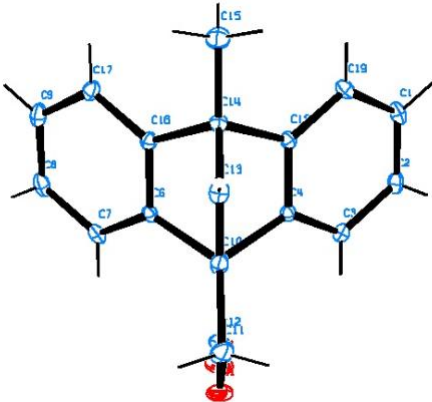
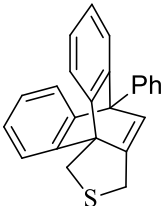
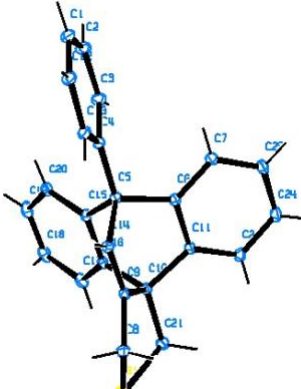
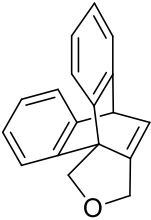
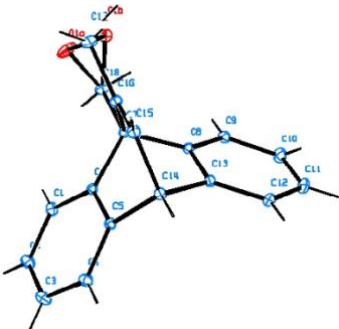
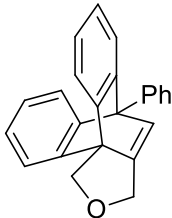
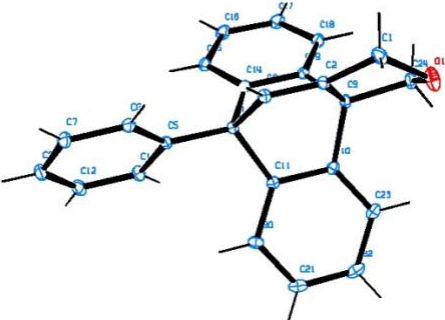
## 10. Compound 8c

 $^1\text{H}$  NMR on a 500 M Hz instrument)

## 11. Compound 8d



## Single Crystal XRD obtained for a few tethered barrelenes

<p><b>1. Compound 5b</b></p>  <p>Chemical structure of Compound 5b, a tethered barrelene derivative with an oxygen atom in the bridgehead position.</p>	 <p>ORTEP diagram of Compound 5b, showing the molecular structure with atoms labeled C1 through C19 and O1. Thermal ellipsoids are drawn at the 50% probability level.</p>
<p><b>2. Compound 6c</b></p>  <p>Chemical structure of Compound 6c, a tethered barrelene derivative with a sulfur atom in the bridgehead position and a phenyl group (Ph).</p>	 <p>ORTEP diagram of Compound 6c, showing the molecular structure with atoms labeled C1 through C28 and S1. Thermal ellipsoids are drawn at the 50% probability level.</p>
<p><b>3. Compound 8a</b></p>  <p>Chemical structure of Compound 8a, a tethered barrelene derivative with an oxygen atom in the bridgehead position.</p>	 <p>ORTEP diagram of Compound 8a, showing the molecular structure with atoms labeled C1 through C16 and O1. Thermal ellipsoids are drawn at the 50% probability level.</p>
<p><b>4. Compound 8d</b></p>  <p>Chemical structure of Compound 8d, a tethered barrelene derivative with an oxygen atom in the bridgehead position and a phenyl group (Ph).</p>	 <p>ORTEP diagram of Compound 8d, showing the molecular structure with atoms labeled C1 through C23 and O1. Thermal ellipsoids are drawn at the 50% probability level.</p>