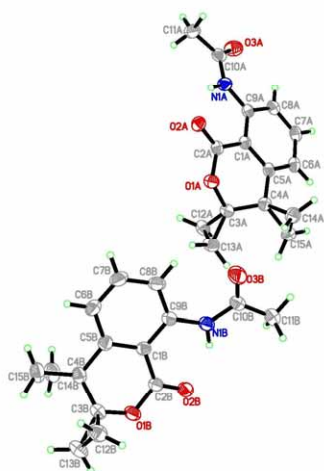


Electronic Supplementary Information

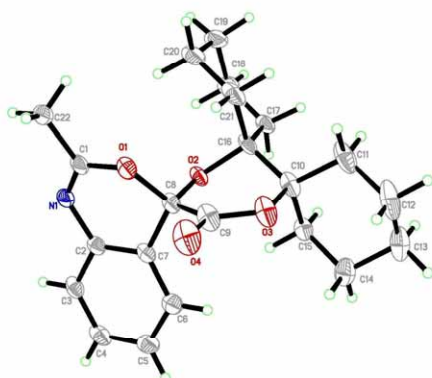
Photo-induced Reactions of Bicycloalkylidenes with Isatin and Isoquinolinetriene

Dong-Dong Wu, Ming-Tao He, Qi-Di Liu, Wei Wang, Jie Zhou, Lei Wang, Hoong-Kun Fun,
Jian-Hua Xu and Yan Zhang*

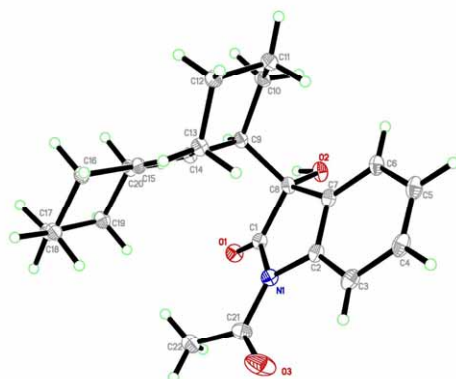
Crystal structure of compound 12



Crystal structure of compound 31

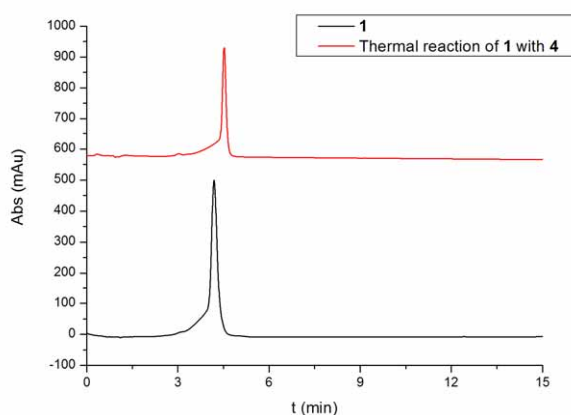


Crystal structure of compound 32



Control experiments

Thermal reaction of 1 with 4. A solution of **1** (0.02M) and **4** (2 equiv) in anhydrous benzene was stirred at room temperature or under reflux. The reaction was monitored by HPLC and no obvious conversion of starting material was observed.



Photolysis of 1 with 4 in the presence of 1,4-Cyclohexadiene. A solution of **1** and **4** (2 equiv) in anhydrous benzene containing 1,4-Cyclohexadiene (2 equiv) was photolyzed and the reaction was monitored by TLC in different time course. No products corresponding to **9-12** were observed during the whole photolysis course for 12 hours.

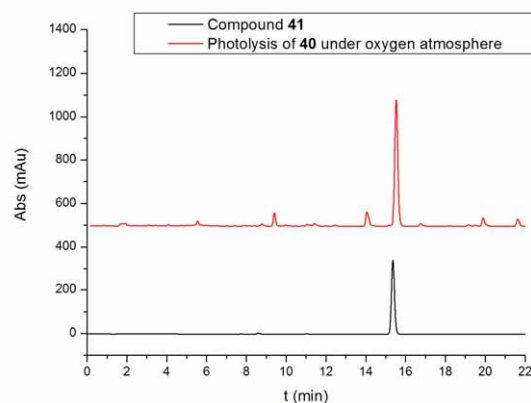
Photolysis of 9-11. A solution of **9** (**10** or **11**, 0.02M) in anhydrous benzene was photolyzed with inert gas bubbling. The reaction was monitored by TLC and no product **12** was observed by extend the reaction time to 24h.

Thermal decomposition of 9-11. A solution of **9** (**10** or **11**, 0.02M) in anhydrous benzene was stirred with silica gel in 25°C. The reaction was monitored by TLC and no product **12** was observed.

Photolysis of 30 under oxygen atmosphere. A solution of **30** (0.02M) in anhydrous benzene was photolyzed with O₂ bubbling. The reaction was monitored by TLC and **30** could be convert completely. The ¹H NMR of the crude product showed that it was **31**.

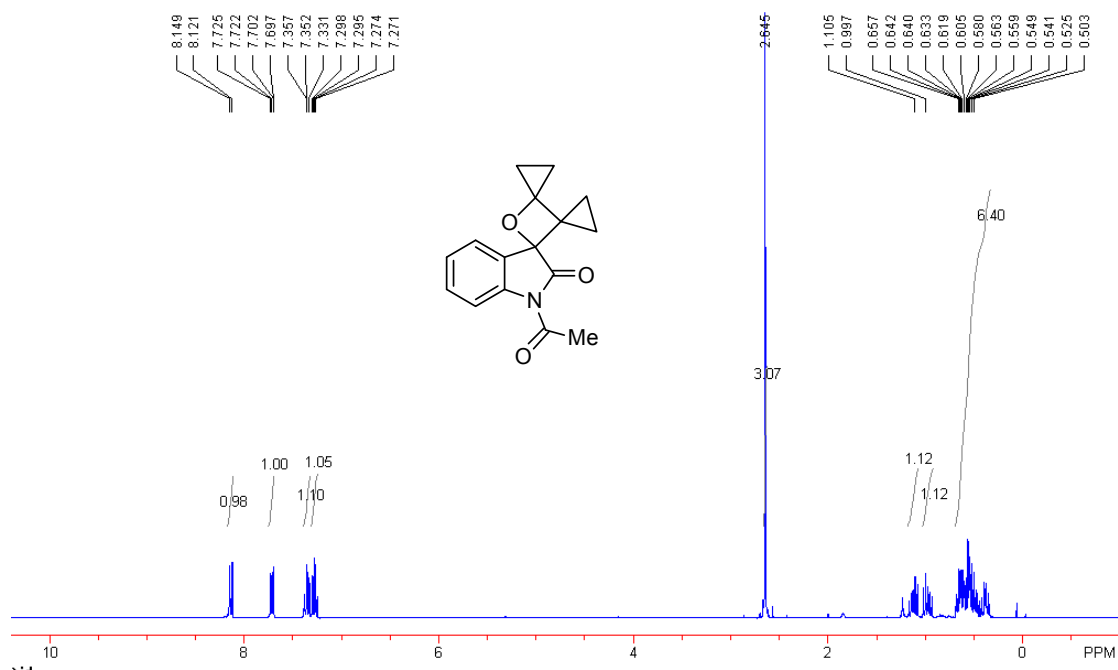
Photolysis of 35. A solution of **35** (0.02M) in anhydrous acetonitrile was photolyzed with inert gas bubbling. The reaction was monitored by TLC and **35** could be convert to **36** smoothly in 12h.

Photolysis of 40 under oxygen atmosphere. A solution of **40** (0.02M) in anhydrous acetonitrile was photolyzed with O₂ bubbling. The reaction was monitored by HPLC and **40** could be convert to **41** smoothly.

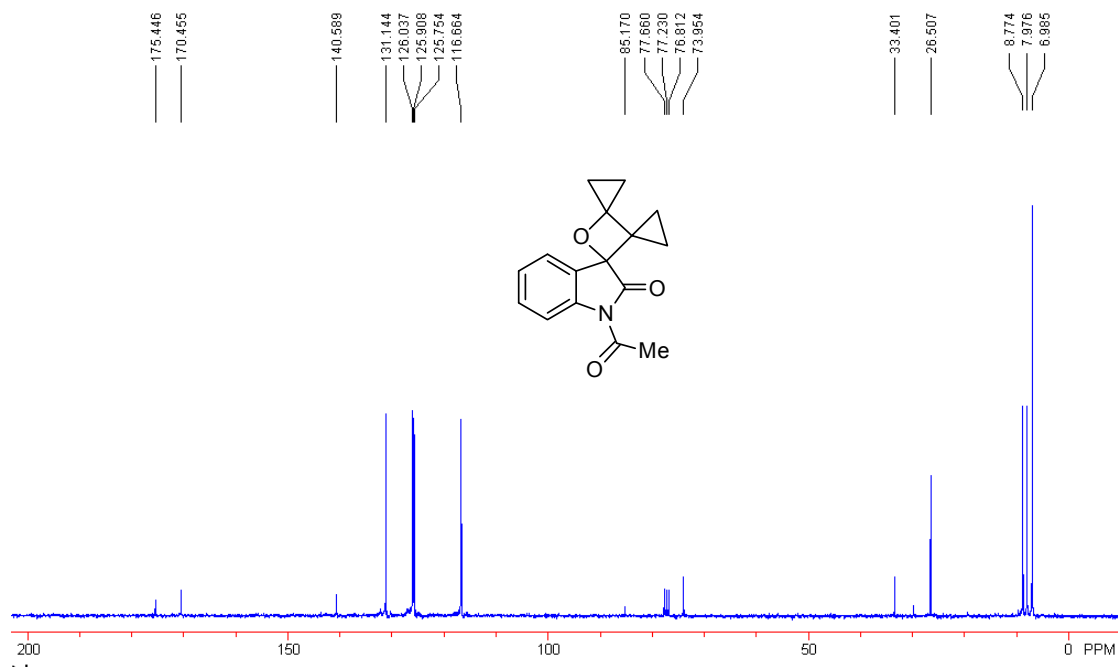


Copies of ^1H NMR and ^{13}C NMR spectra of all new compounds

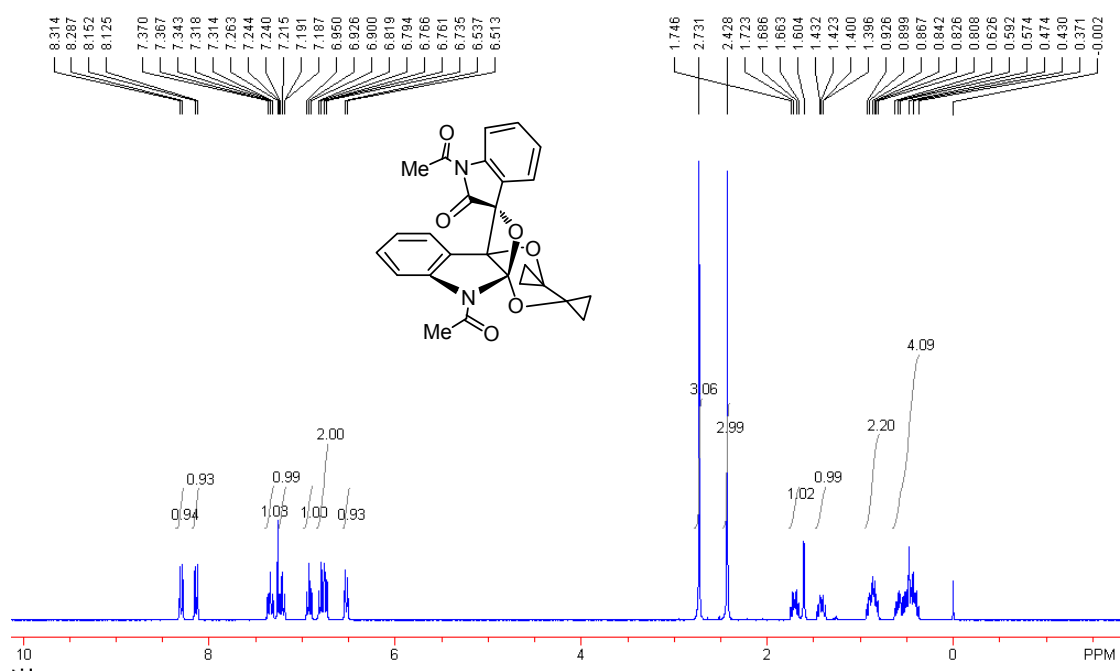
9- ^1H NMR(CDCl_3)



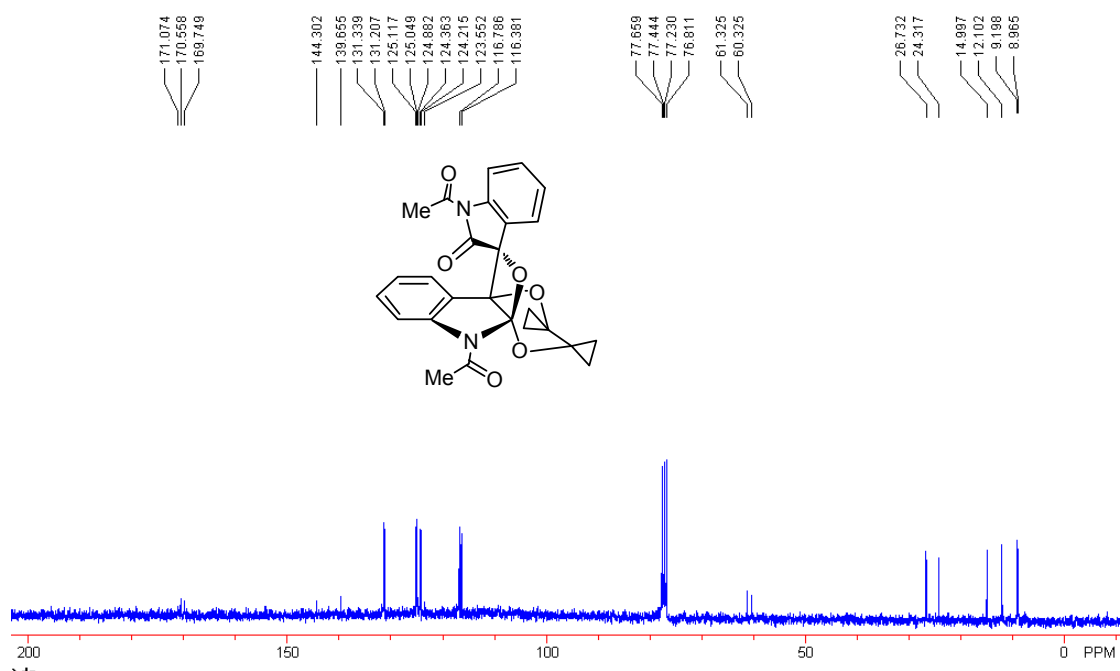
9- ^{13}C NMR(CDCl_3)



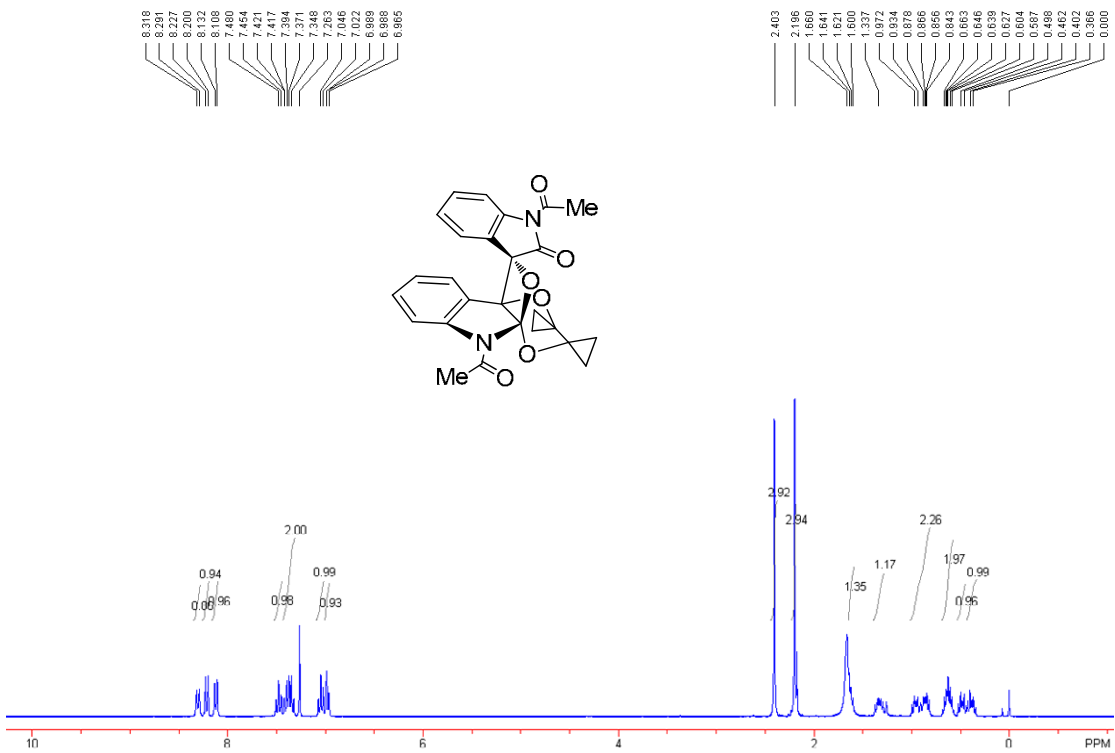
10-¹H NMR(CDCl₃)



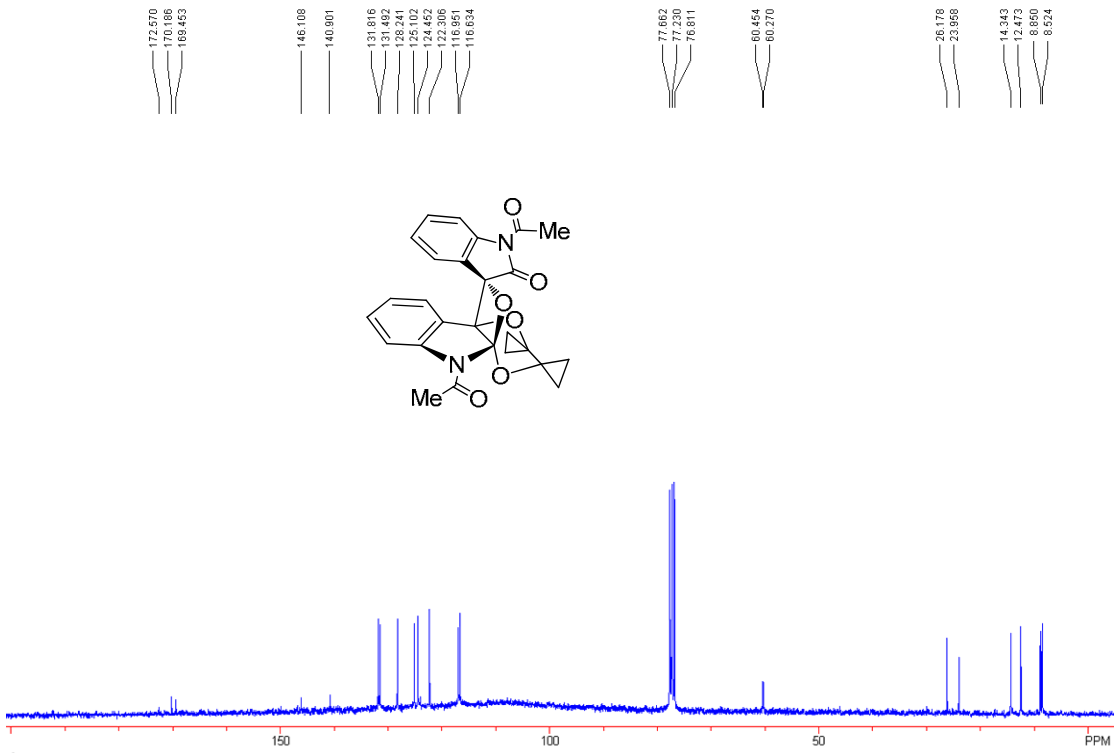
10-¹³C NMR(CDCl₃)



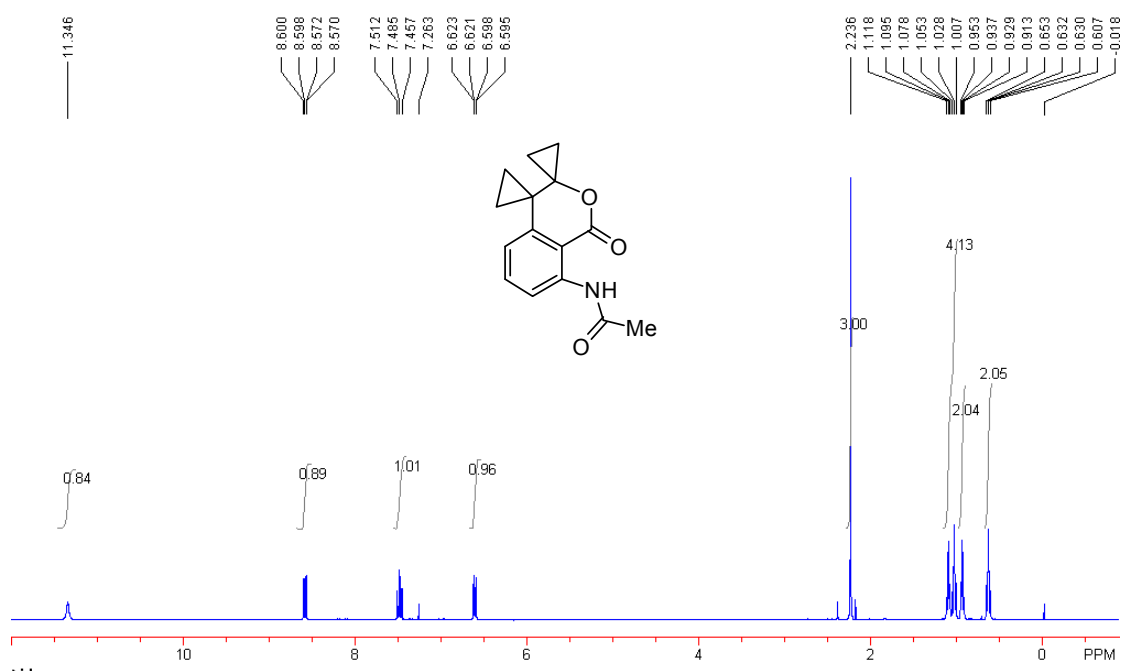
11-¹H NMR(CDCl₃)



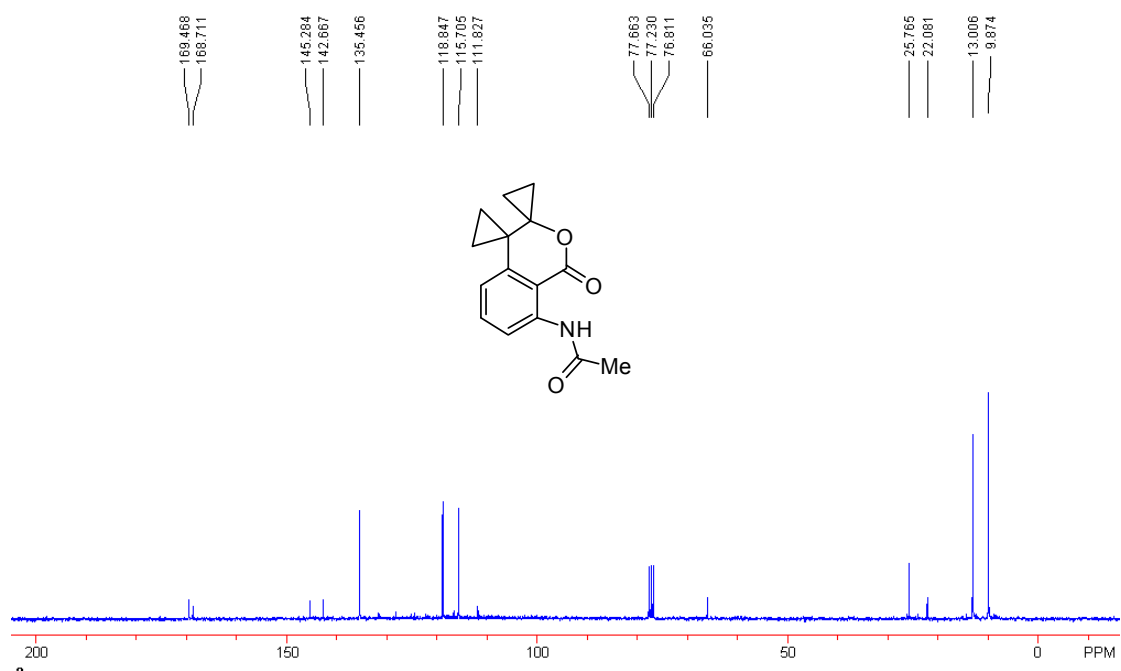
11-¹³C NMR(CDCl₃)



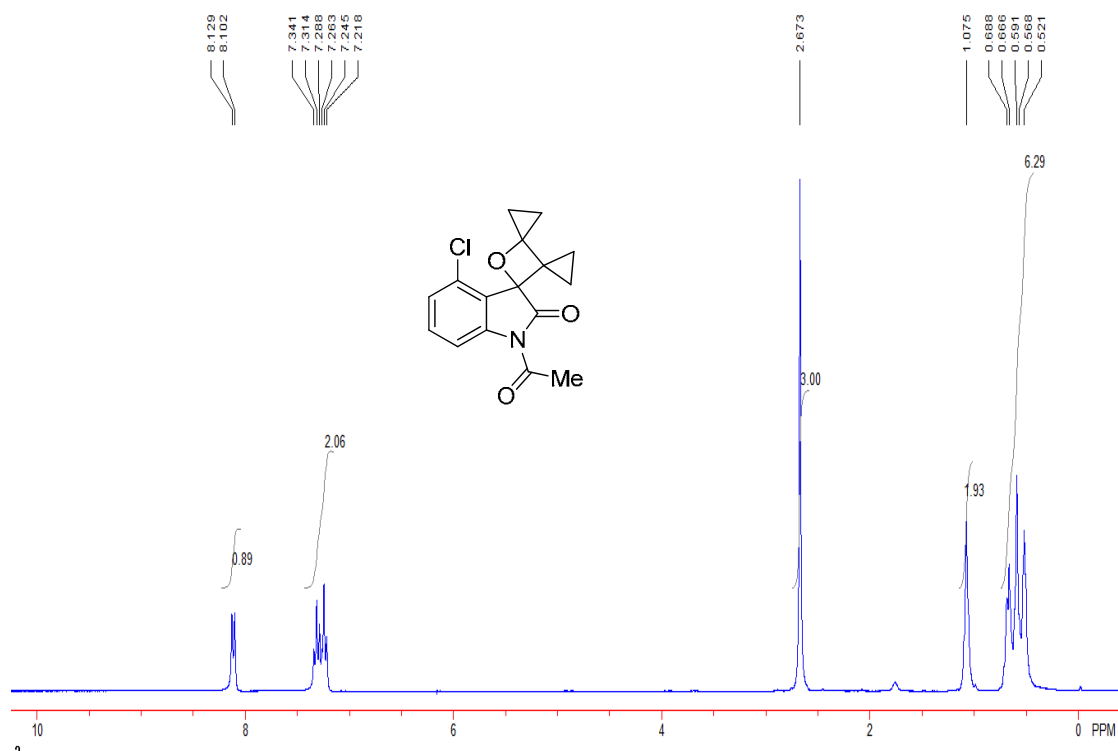
12-¹H NMR(CDCl₃)



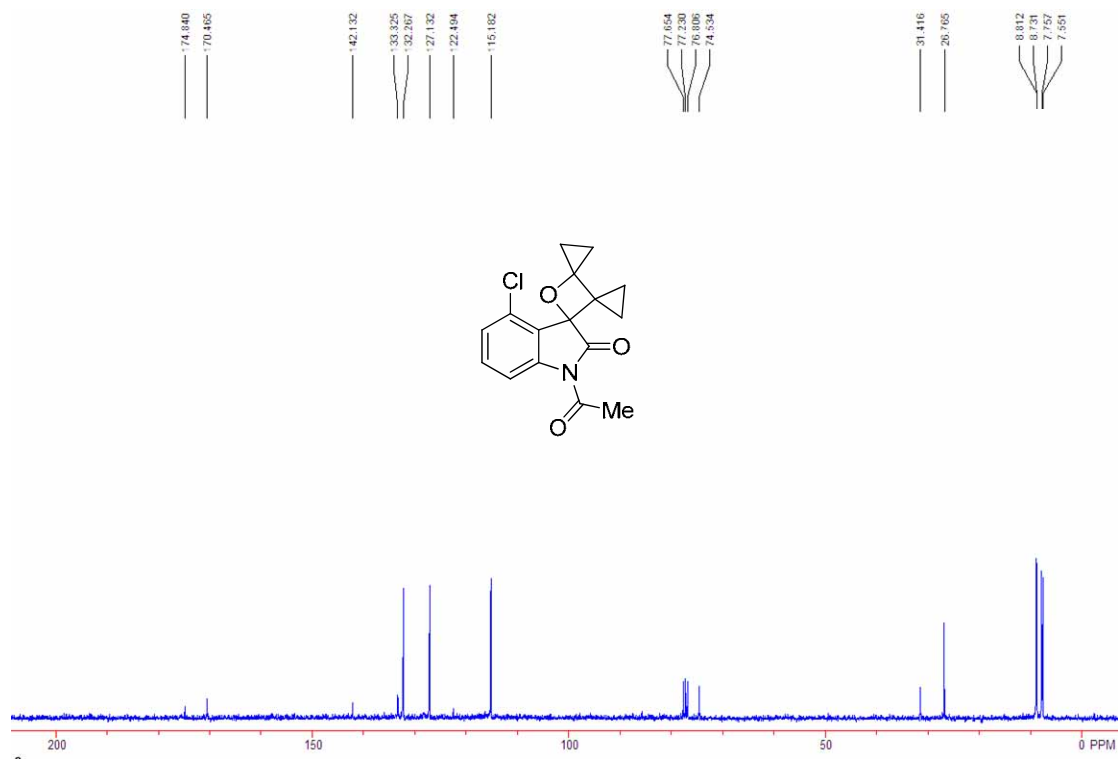
12-¹³C NMR(CDCl₃)



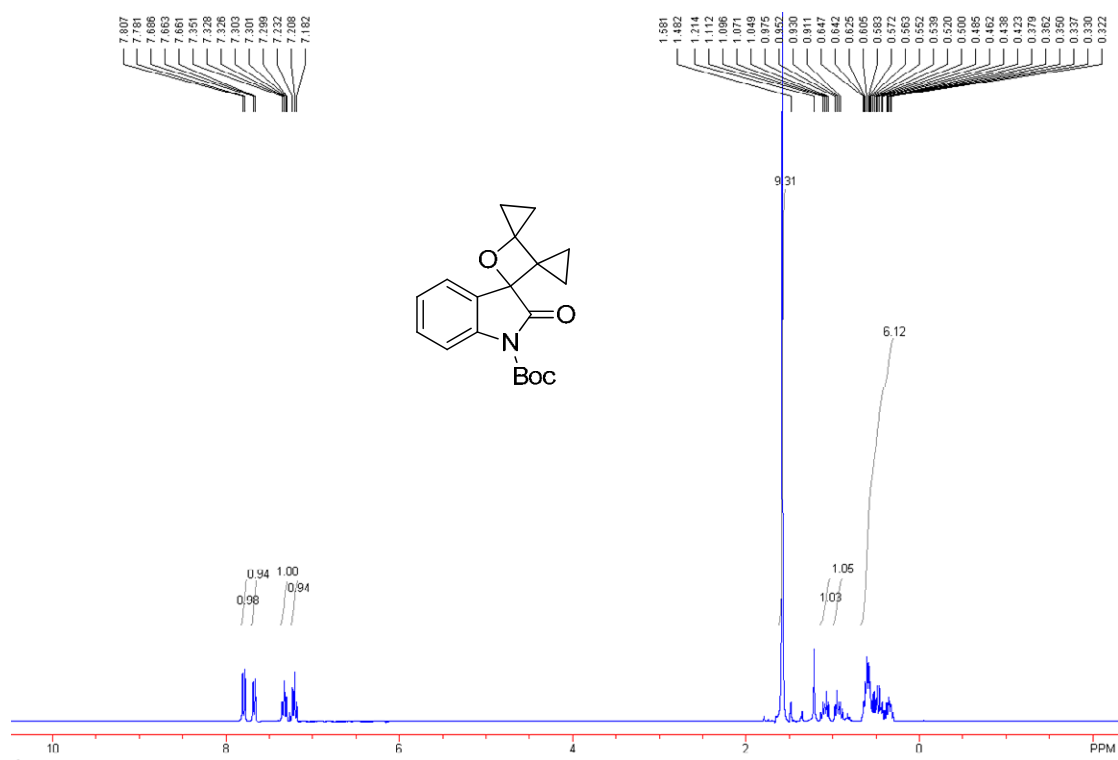
15-¹H NMR(CDCl₃)



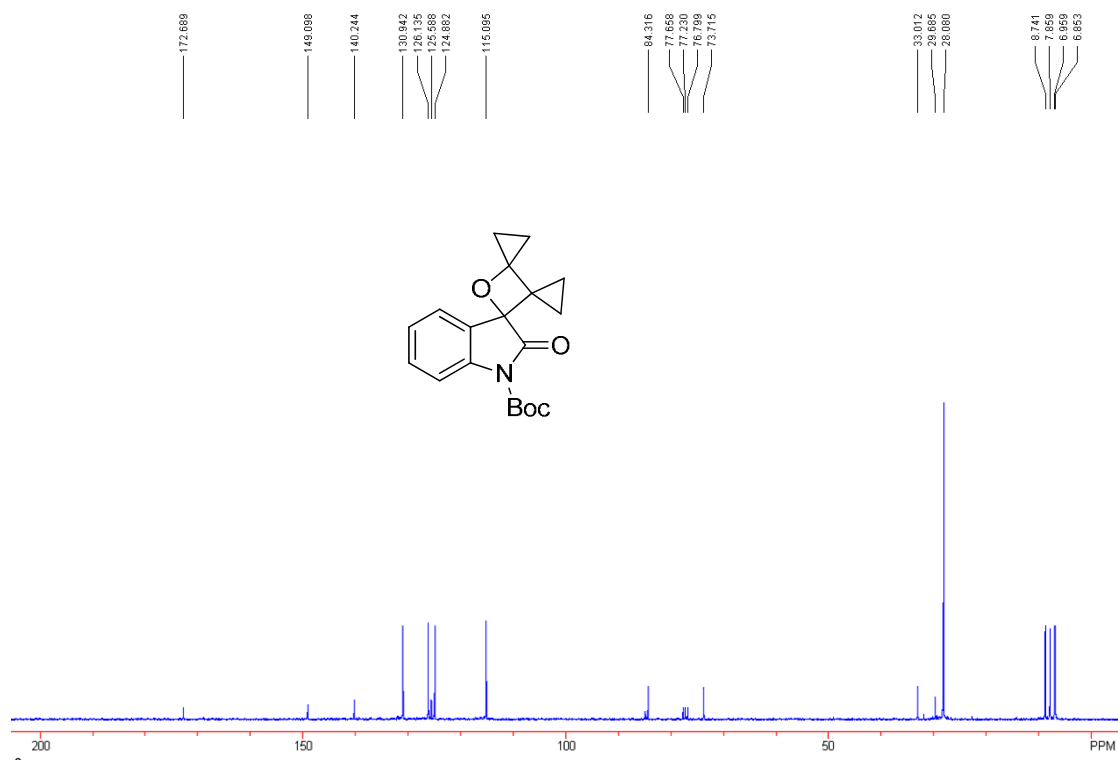
15-¹³C NMR(CDCl₃)



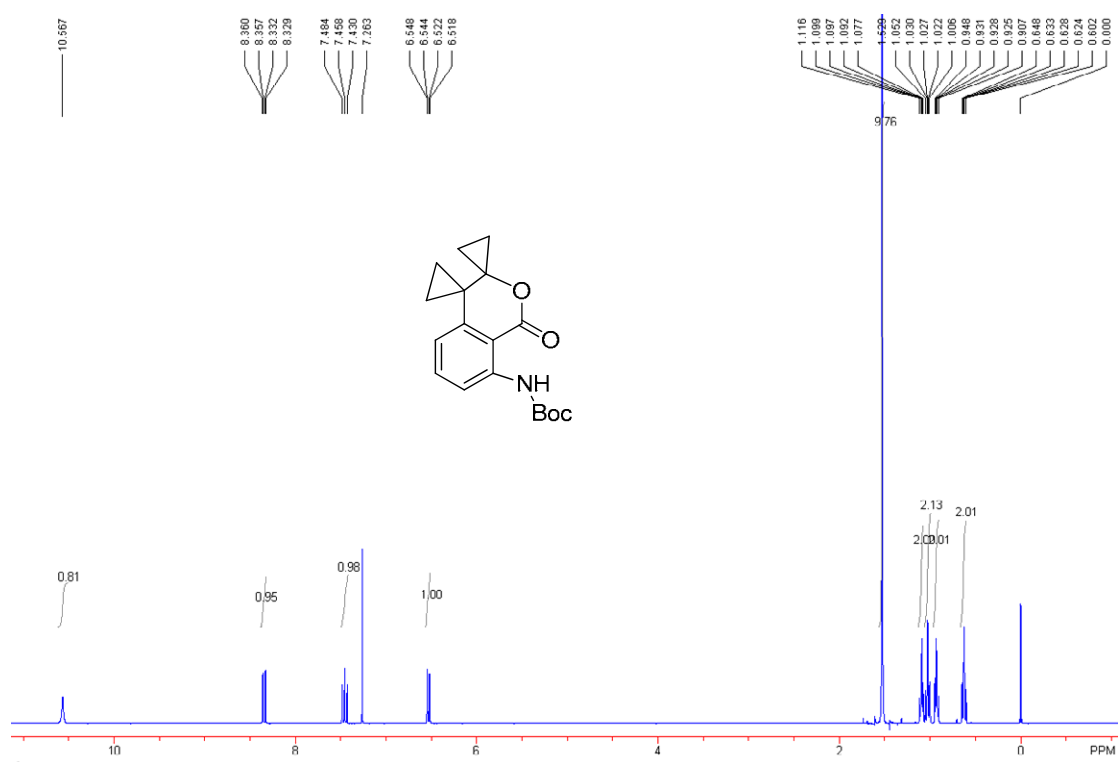
16-¹H NMR(CDCl₃)



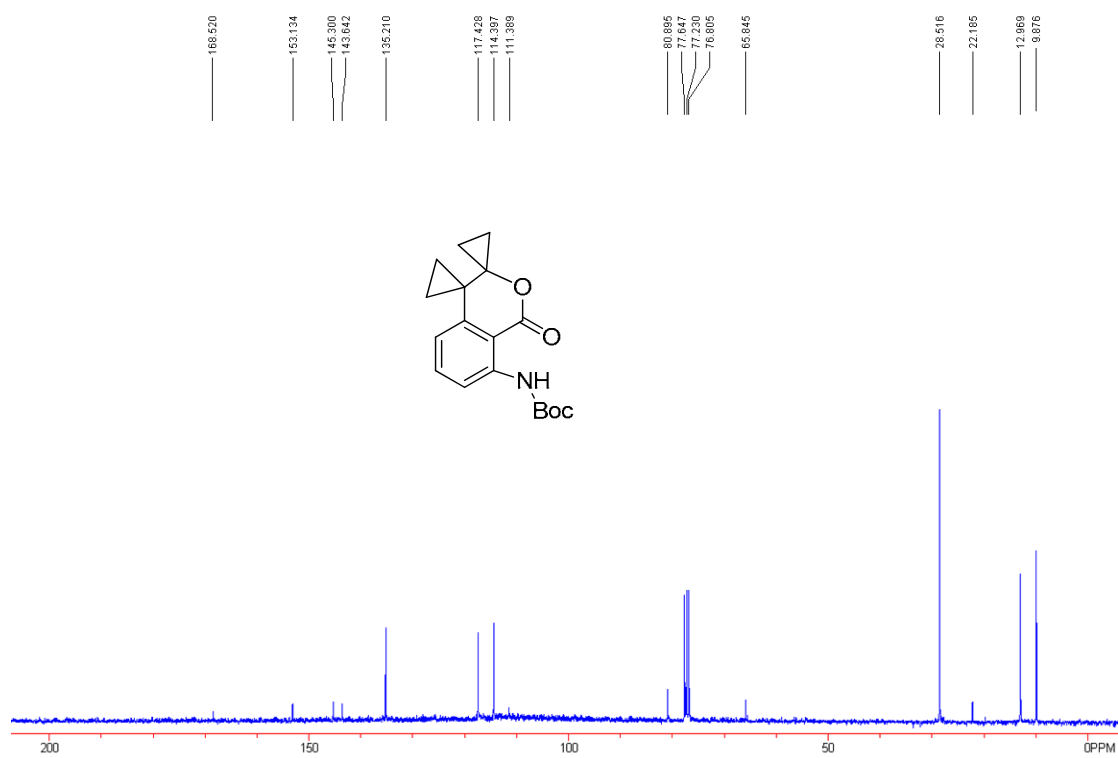
16-¹³C NMR(CDCl₃)



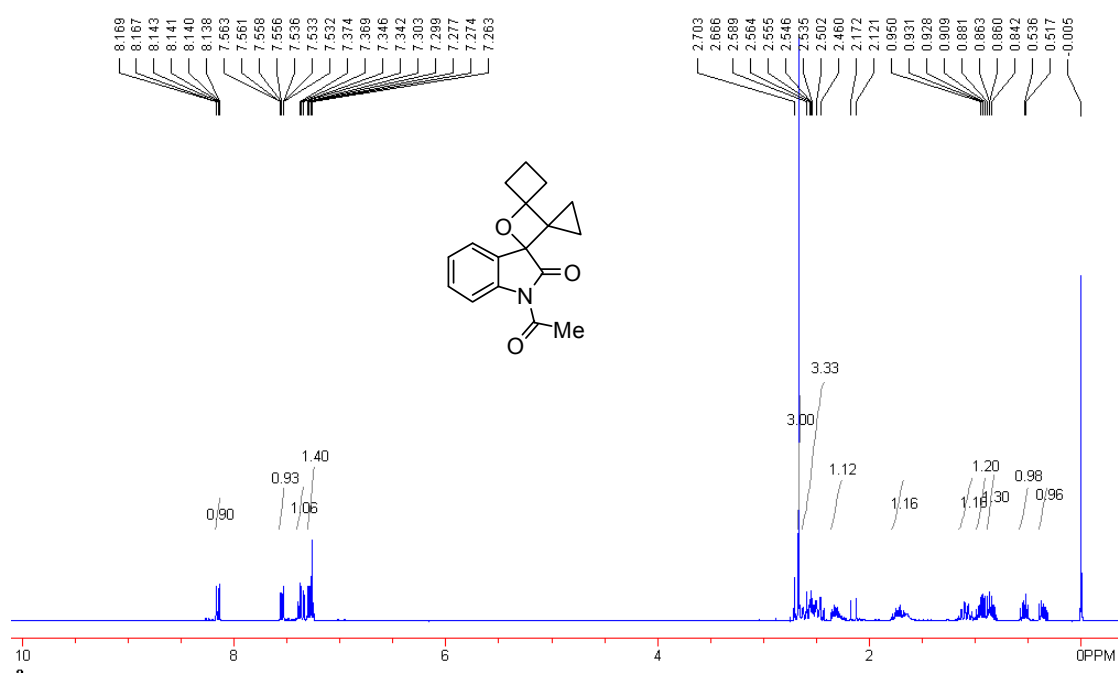
17-¹H NMR(CDCl₃)



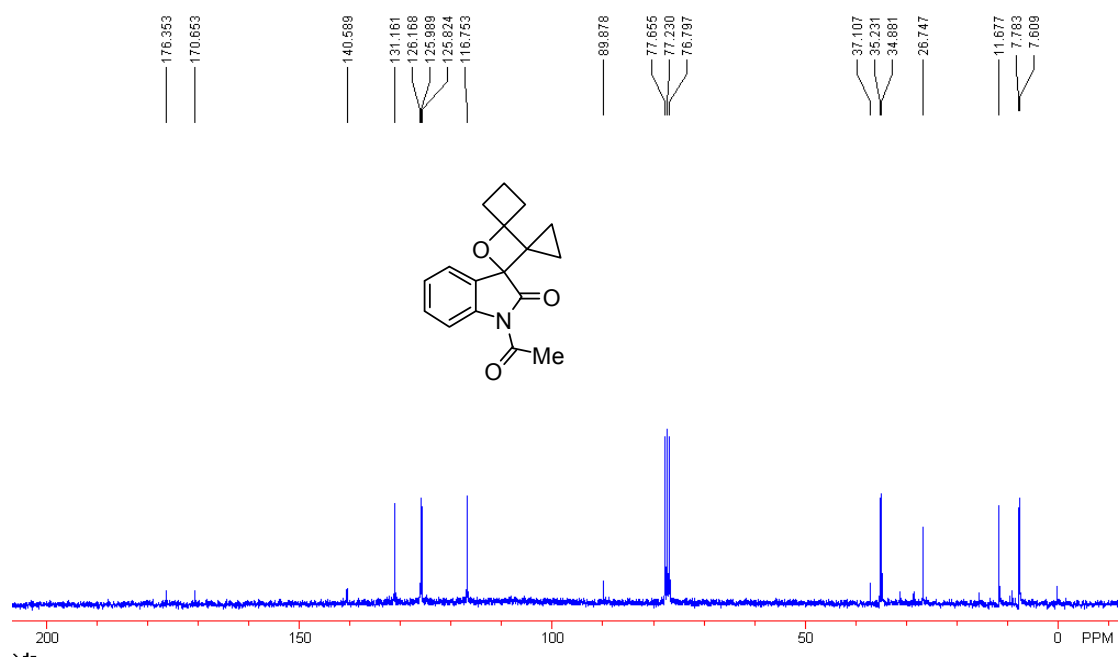
17-¹³C NMR(CDCl₃)



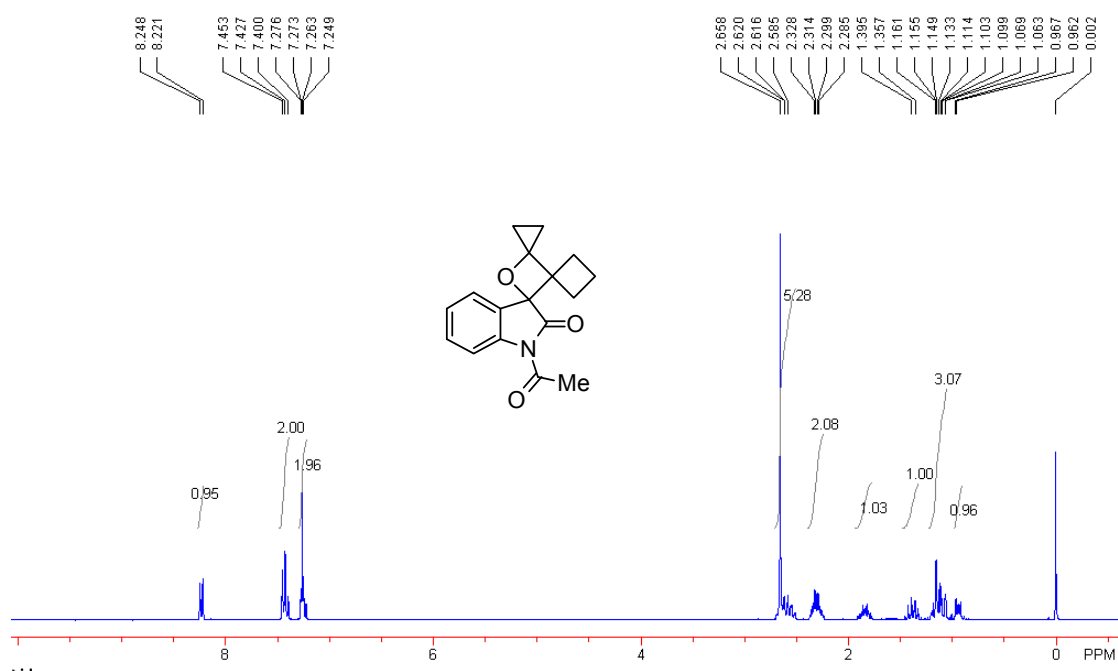
18-¹H NMR(CDCl₃)



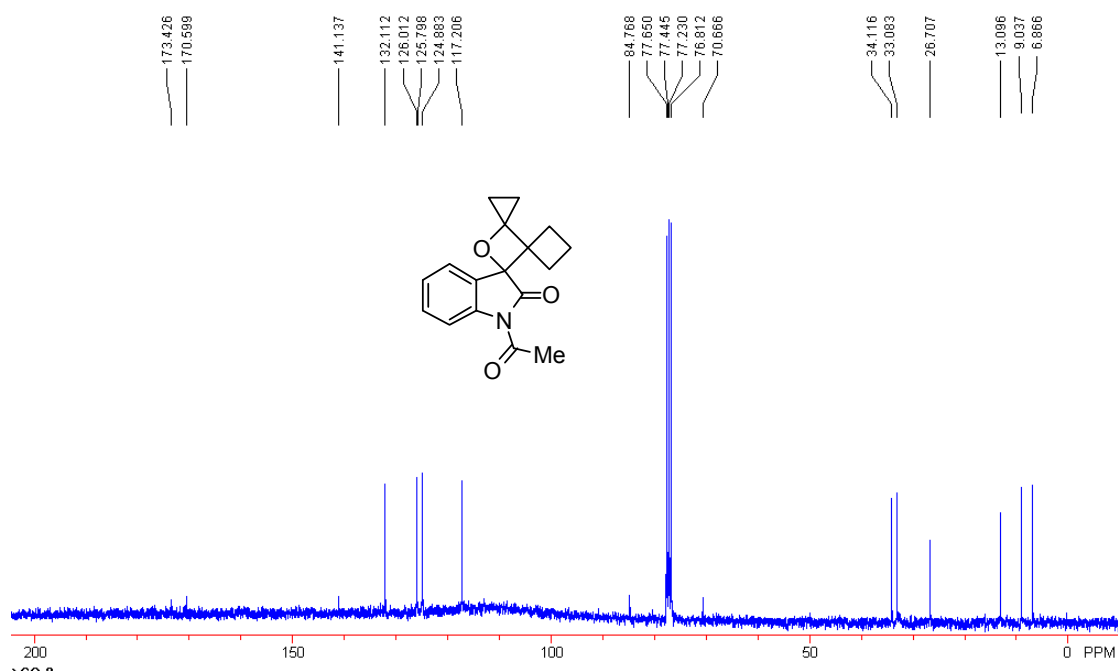
18-¹³C NMR(CDCl₃)



19-¹H NMR(CDCl₃)

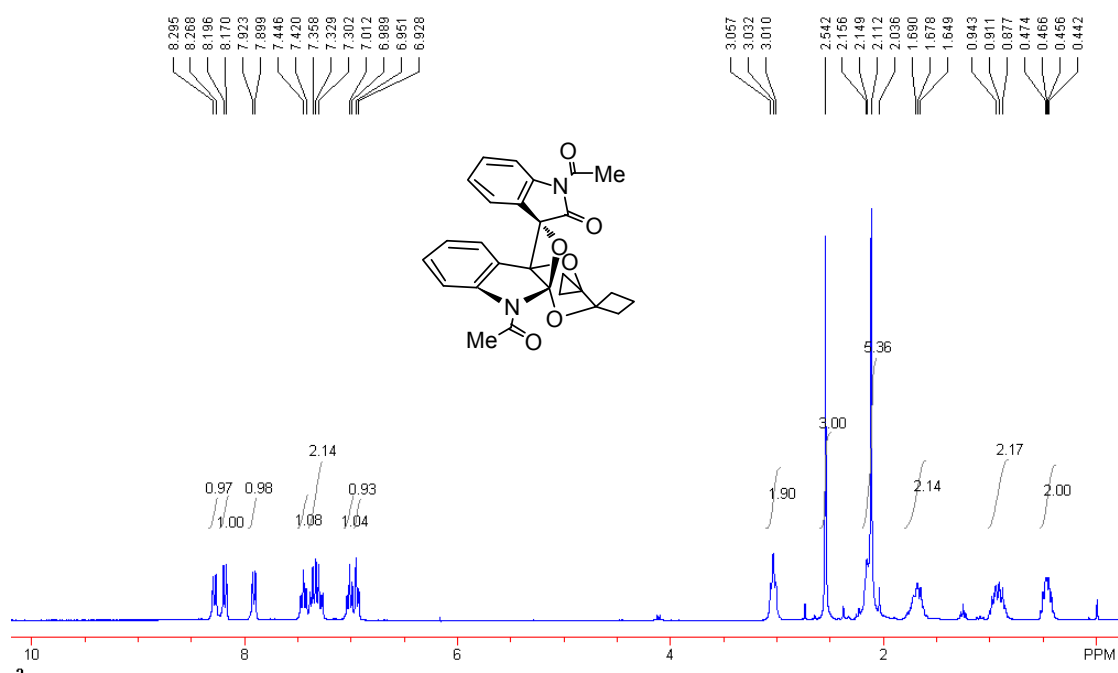


19-¹³C NMR(CDCl₃)

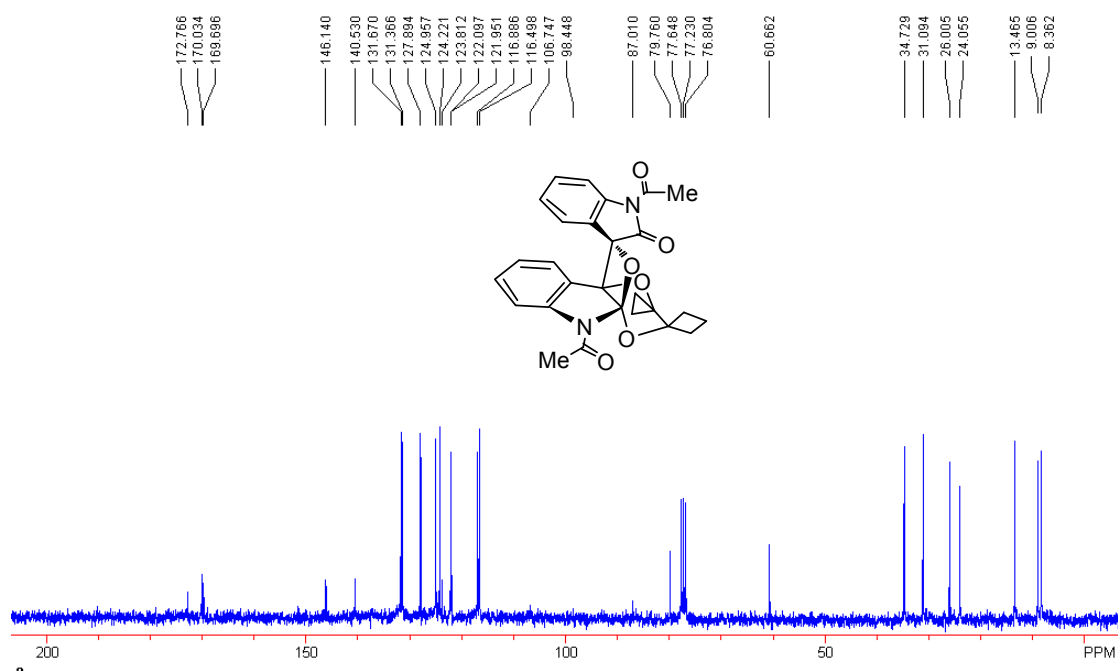




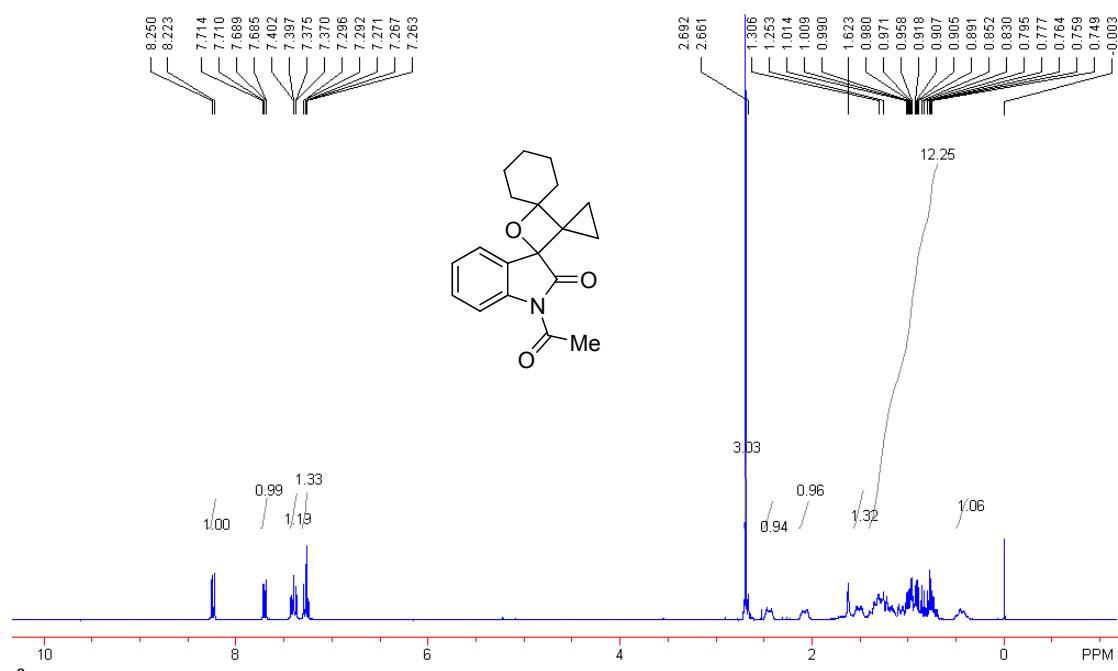
21-¹H NMR(CDCl₃)



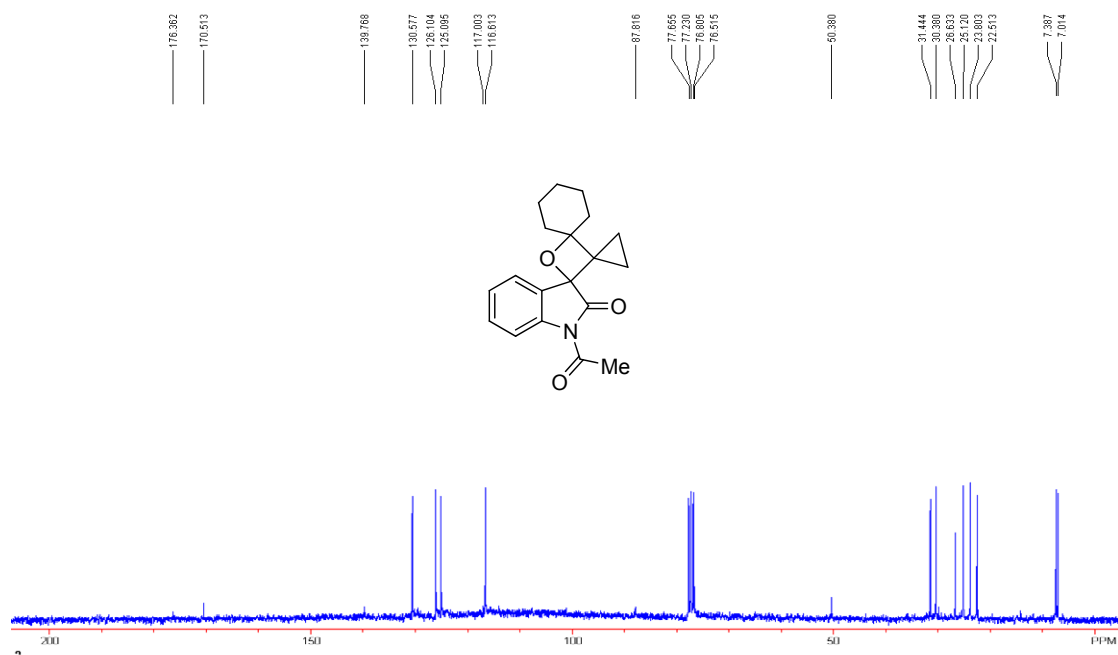
21-¹³C NMR(CDCl₃)



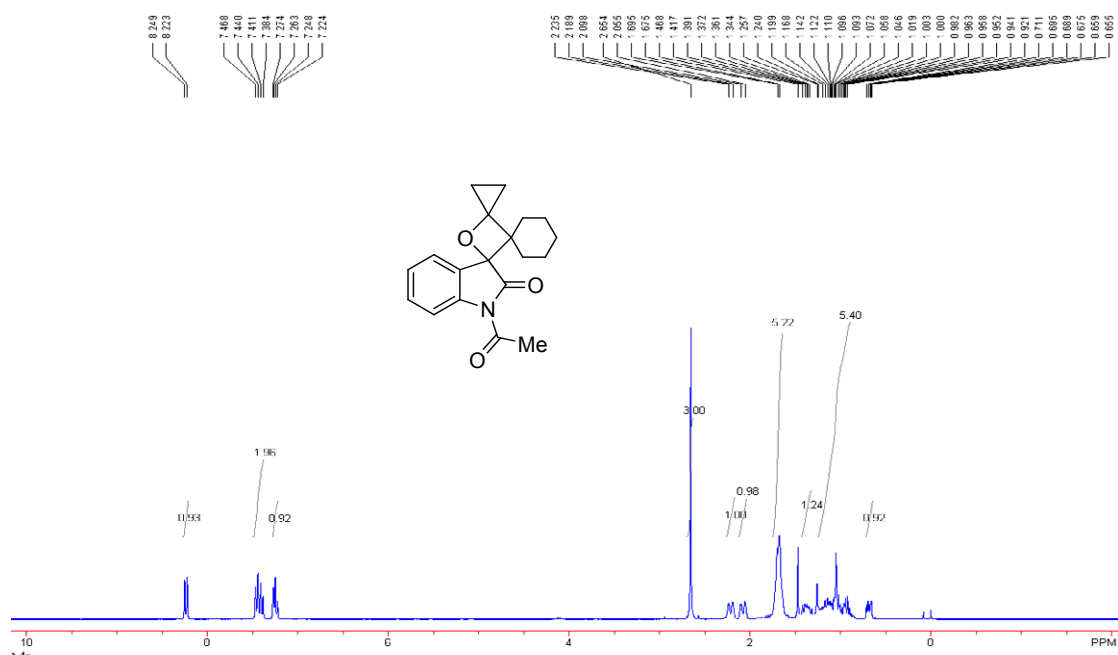
23-¹H NMR(CDCl₃)



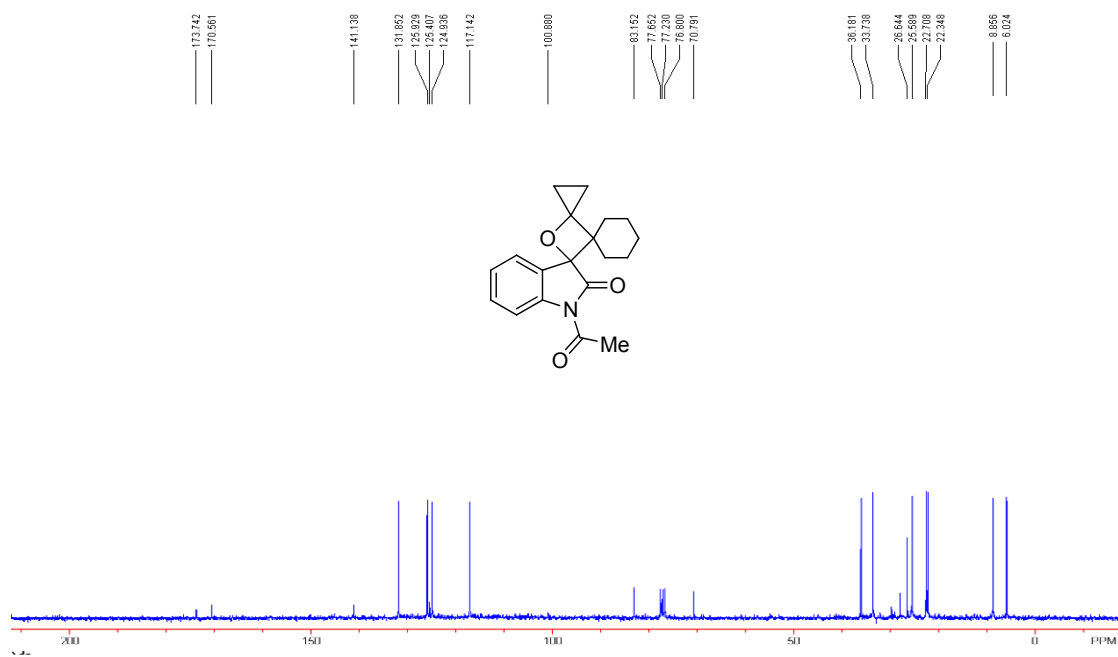
23-¹³C NMR(CDCl₃)



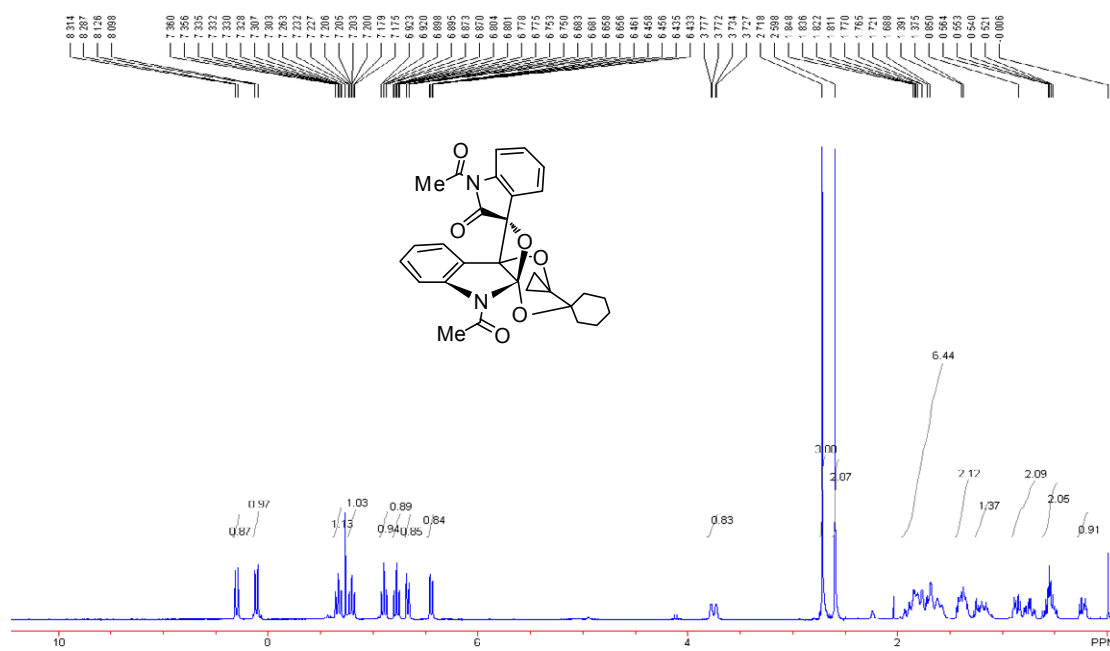
24-¹H NMR(CDCl₃)



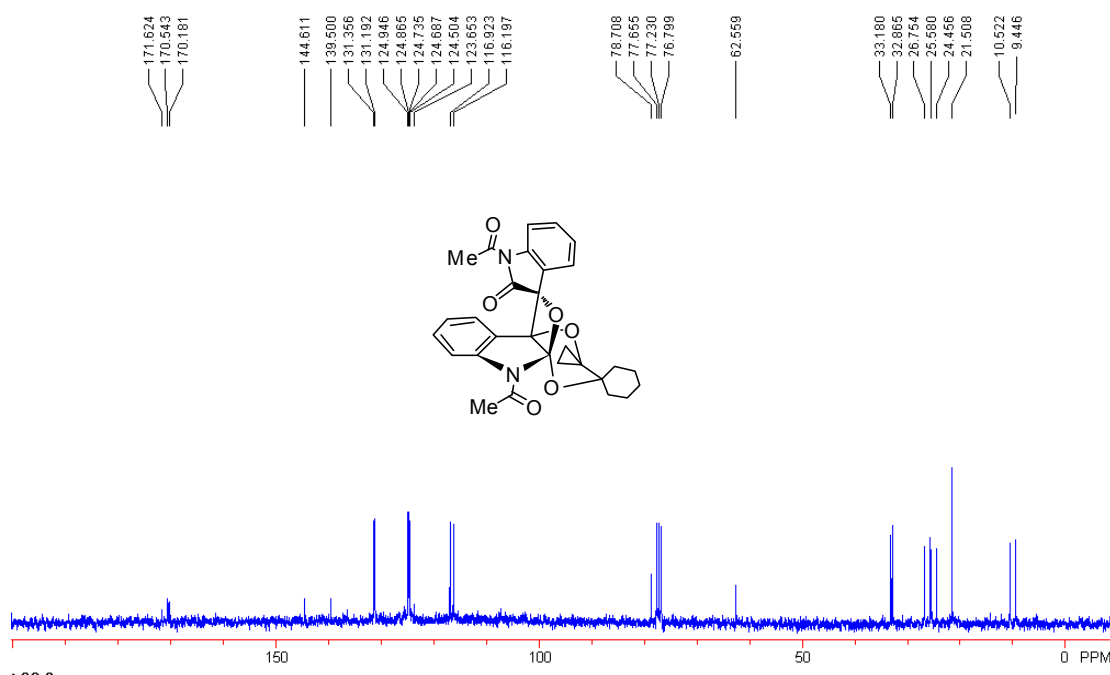
24-¹³C NMR(CDCl₃)



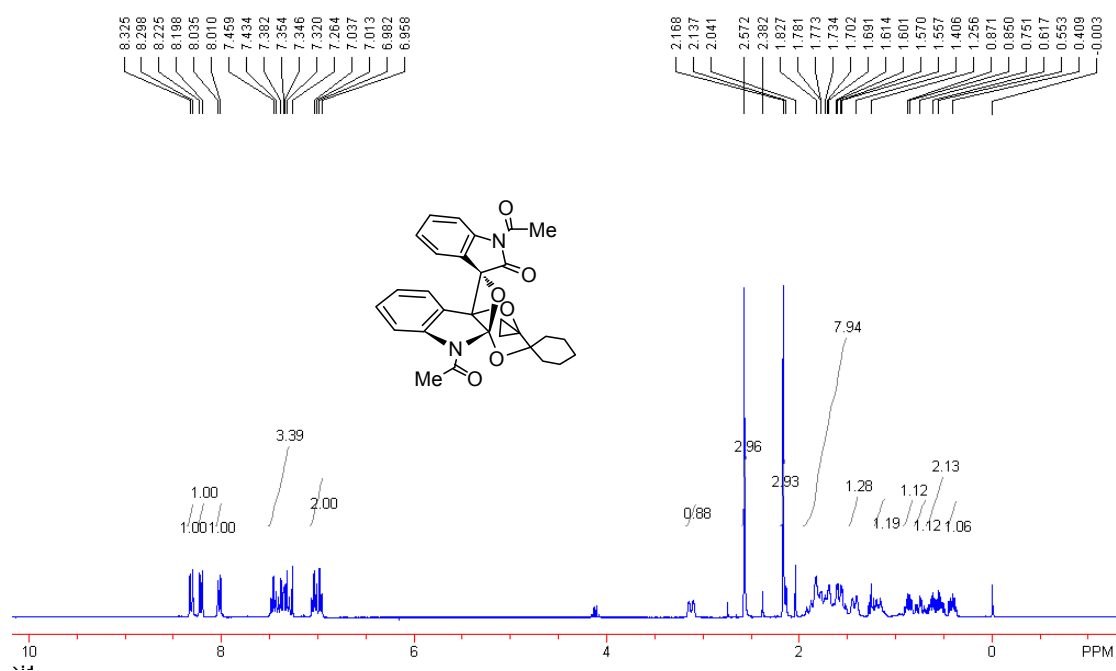
25-¹H NMR(CDCl₃)



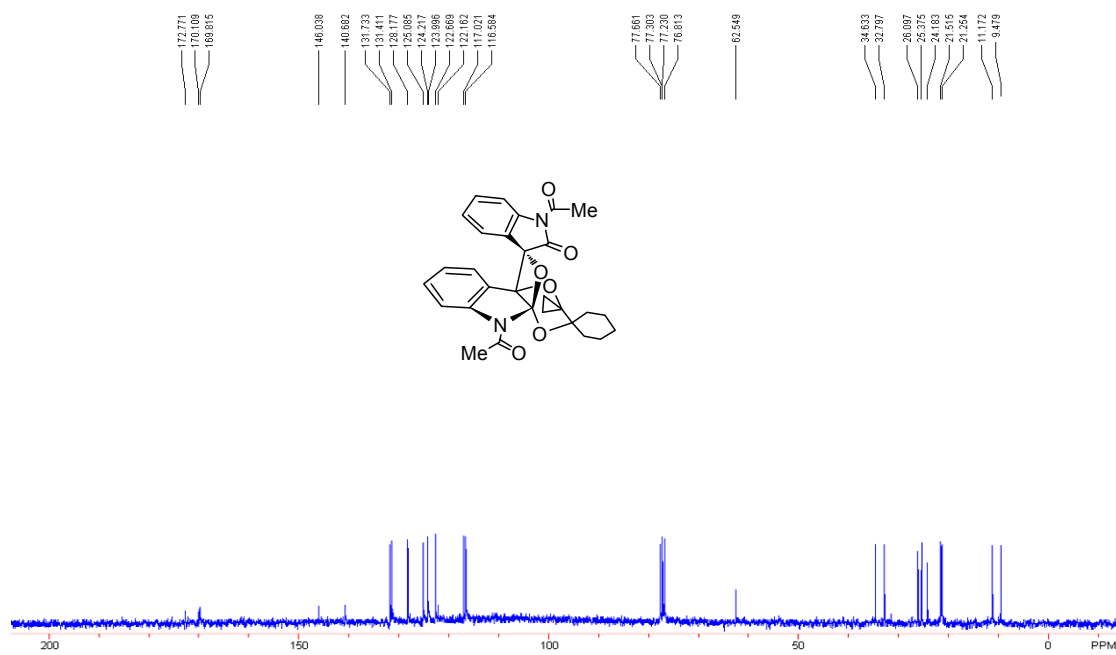
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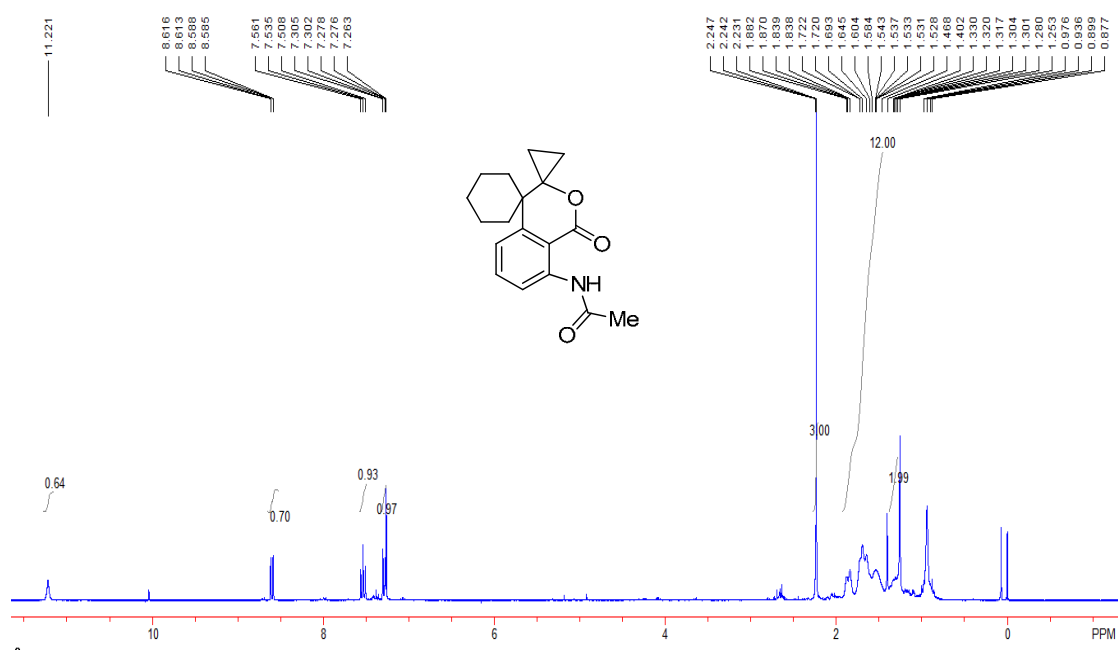
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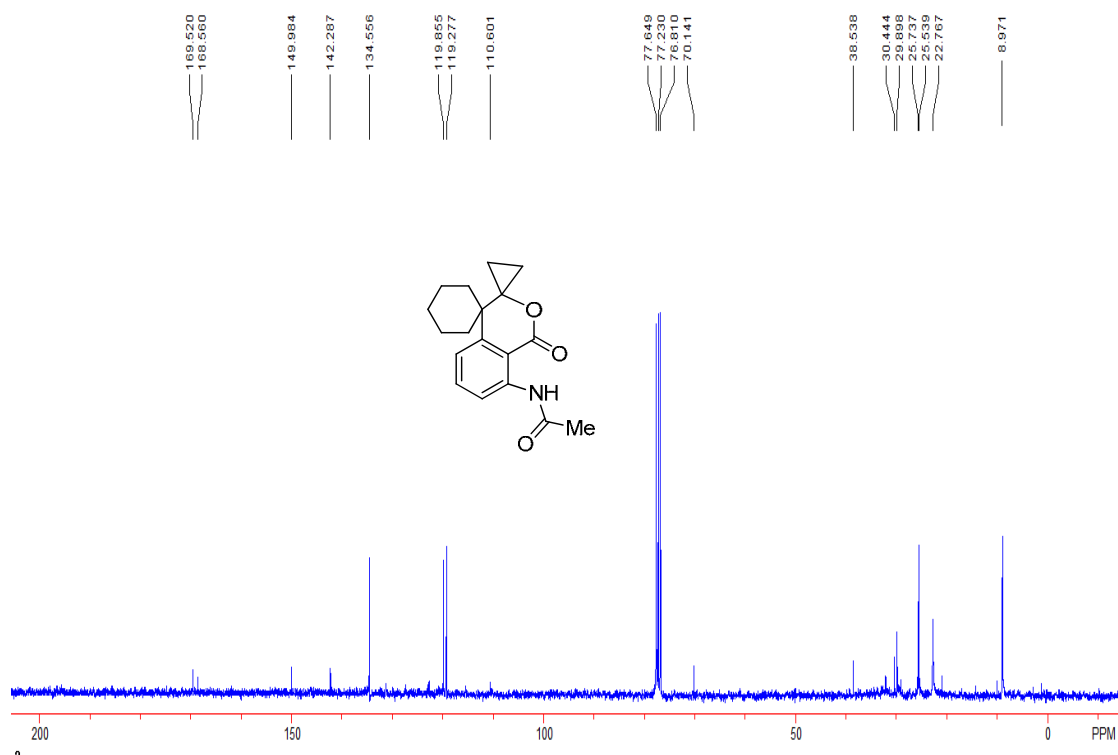
26-¹³C NMR(CDCl₃)



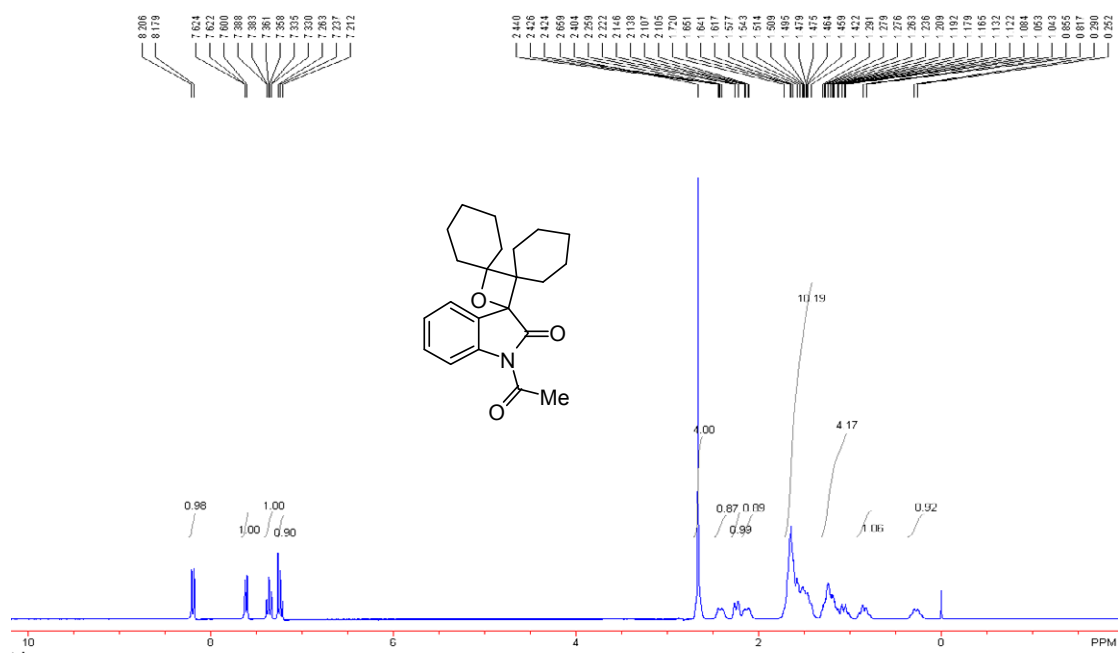
27-¹H NMR(CDCl₃)



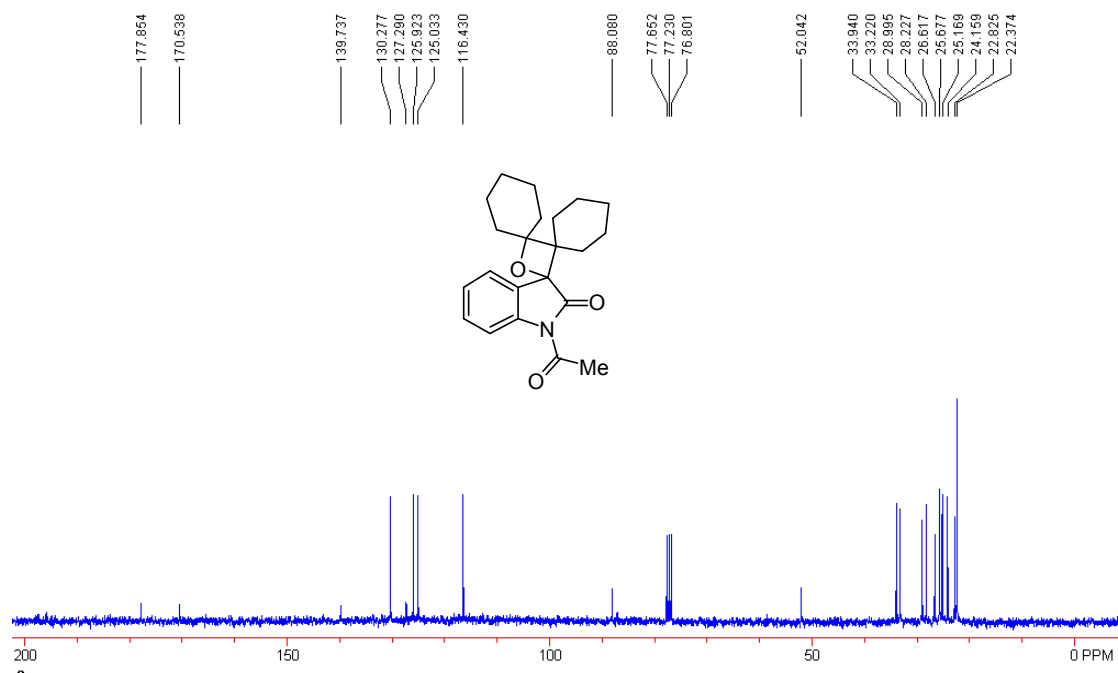
27-¹³C NMR(CDCl₃)



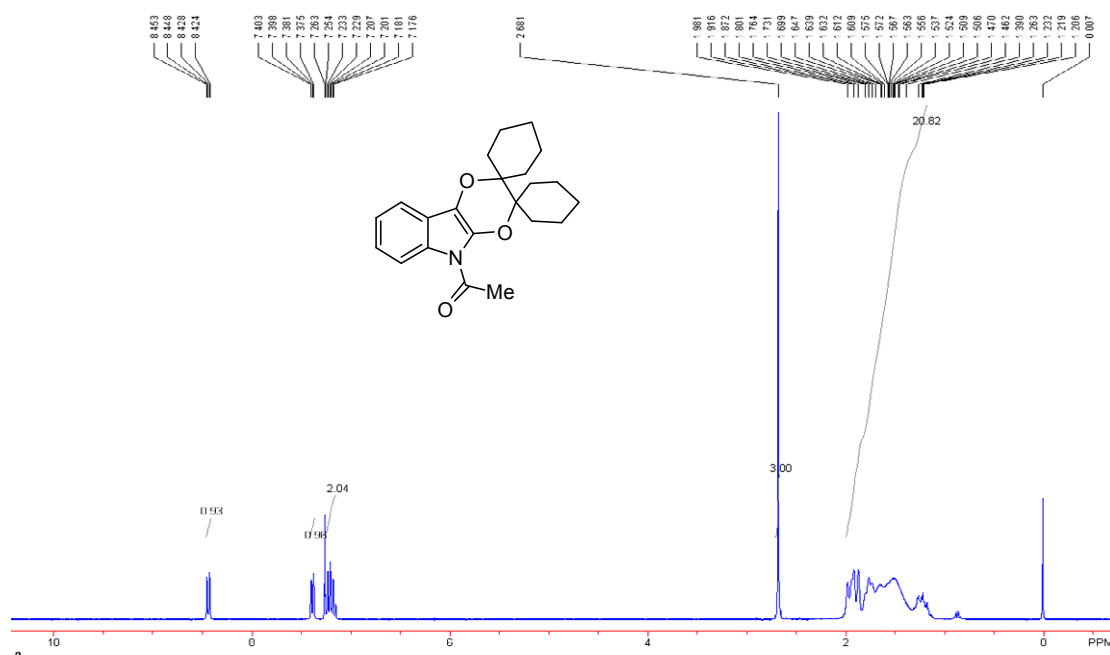
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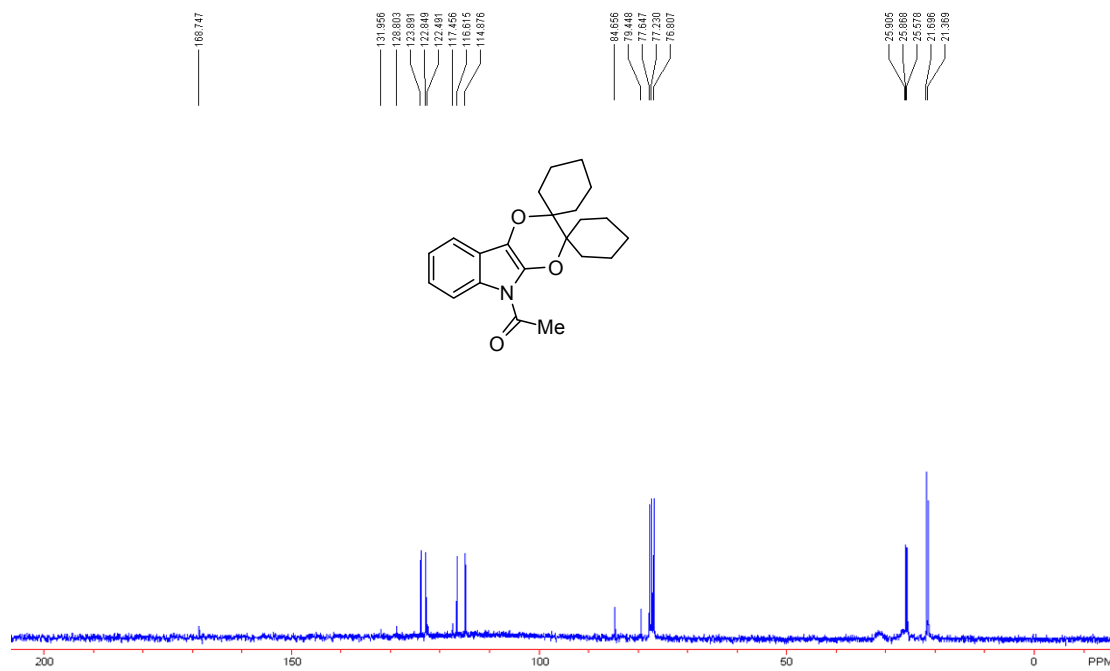
29-¹³C NMR(CDCl₃)



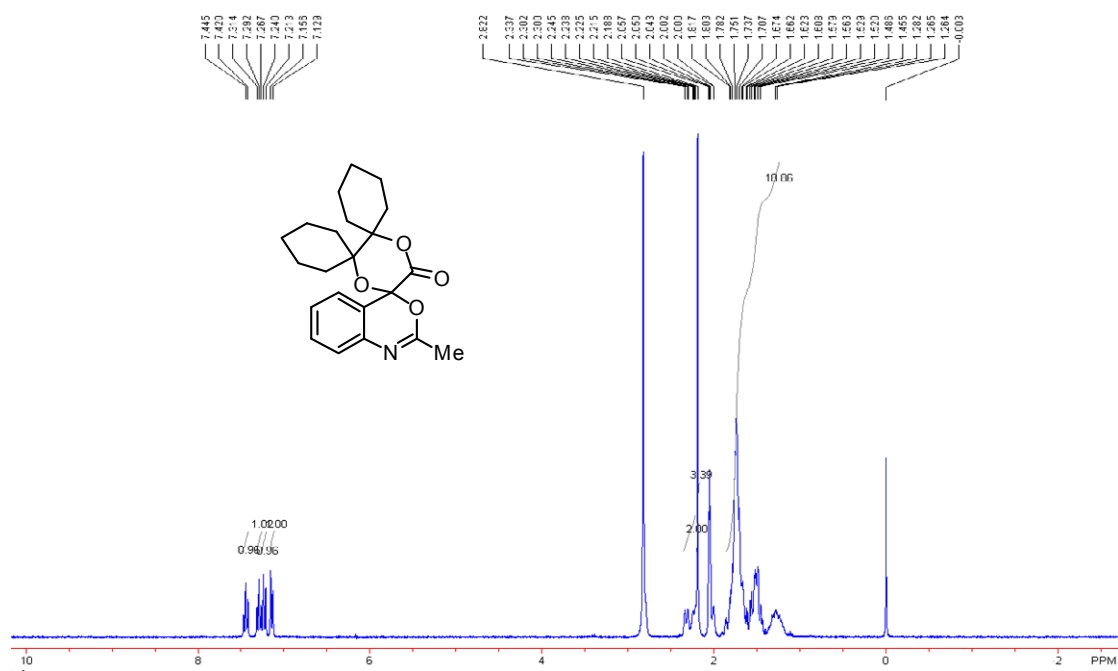
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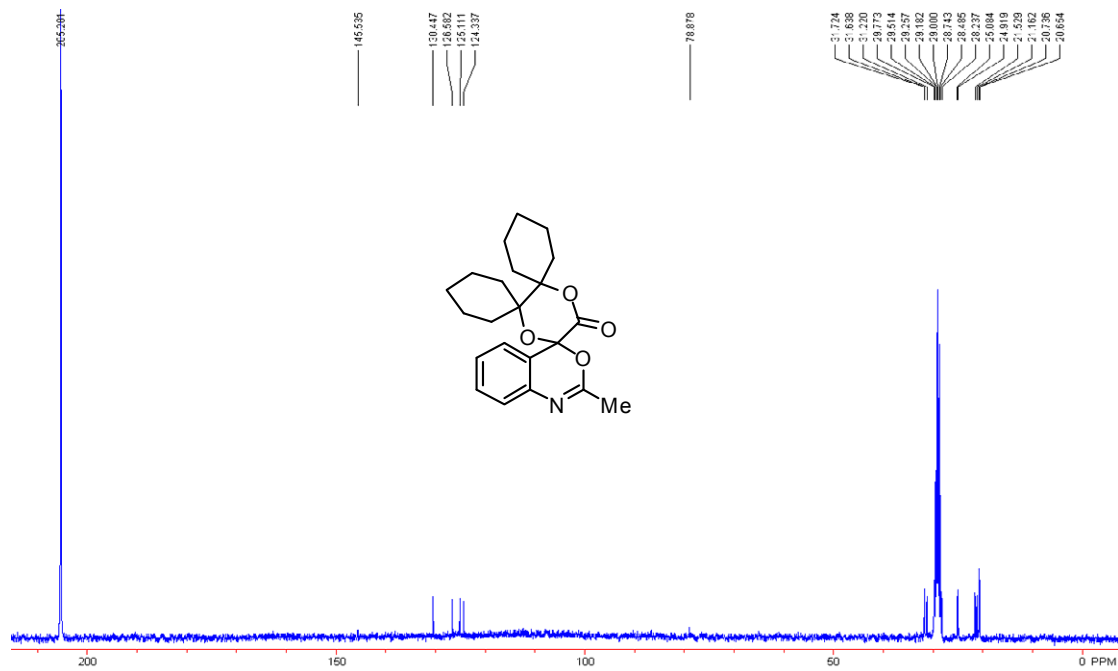
30-¹³C NMR(CDCl₃)



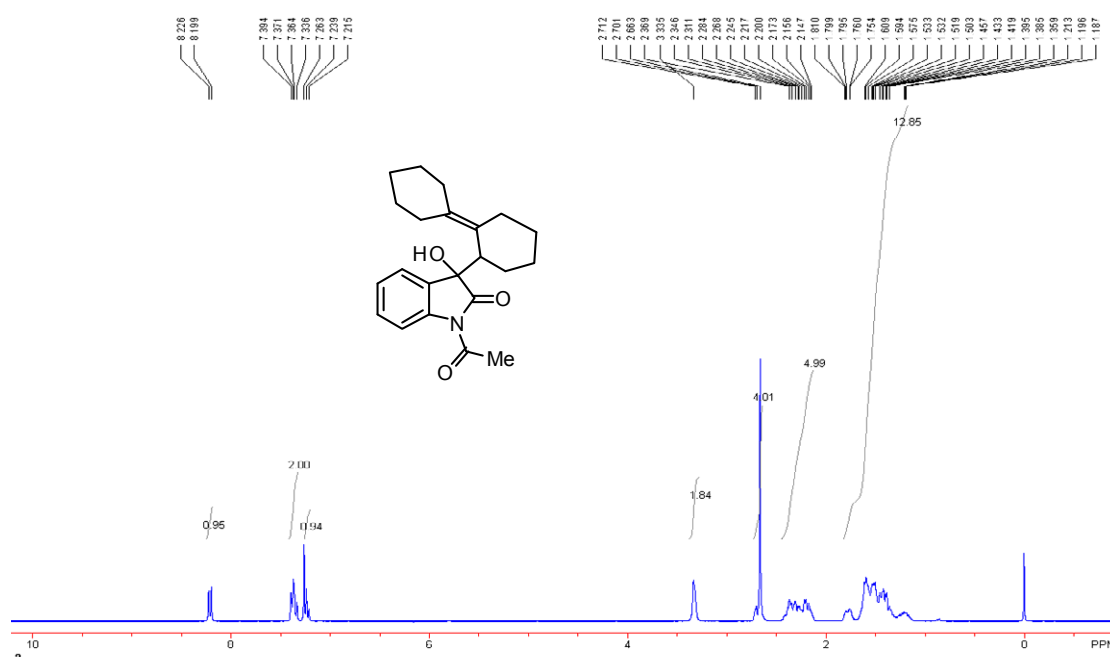
$31\text{-}^1\text{H NMR}(\text{CD}_3\text{COCD}_3)$



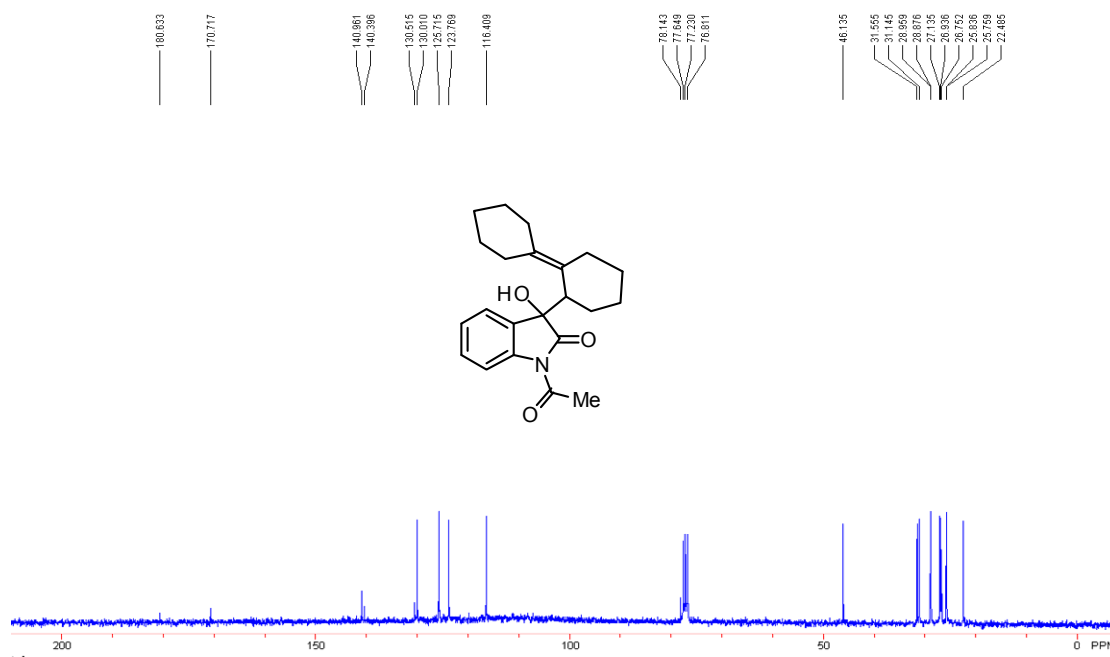
$31\text{-}^{13}\text{C NMR}(\text{CD}_3\text{COCD}_3)$



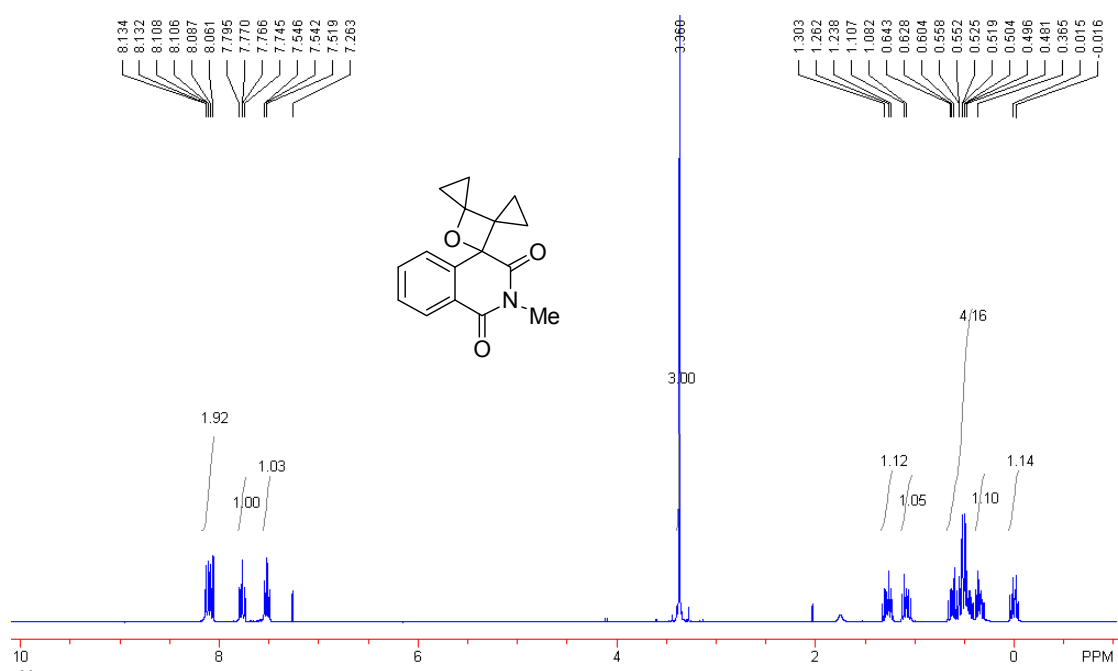
32-¹H NMR(CDCl₃)



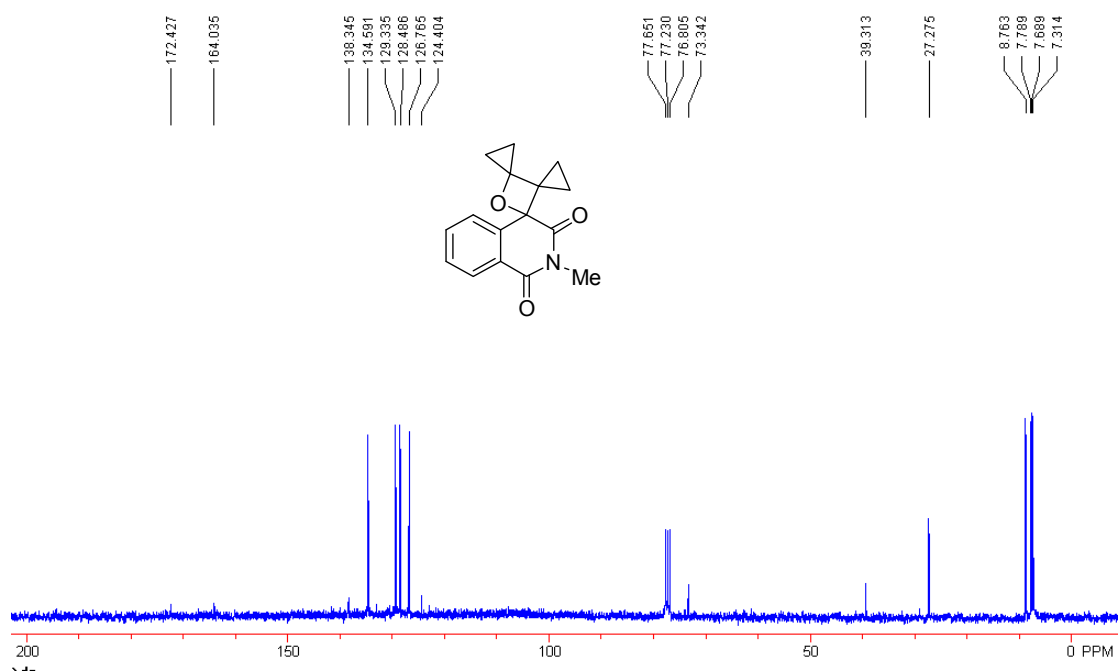
32-¹³C NMR(CDCl₃)



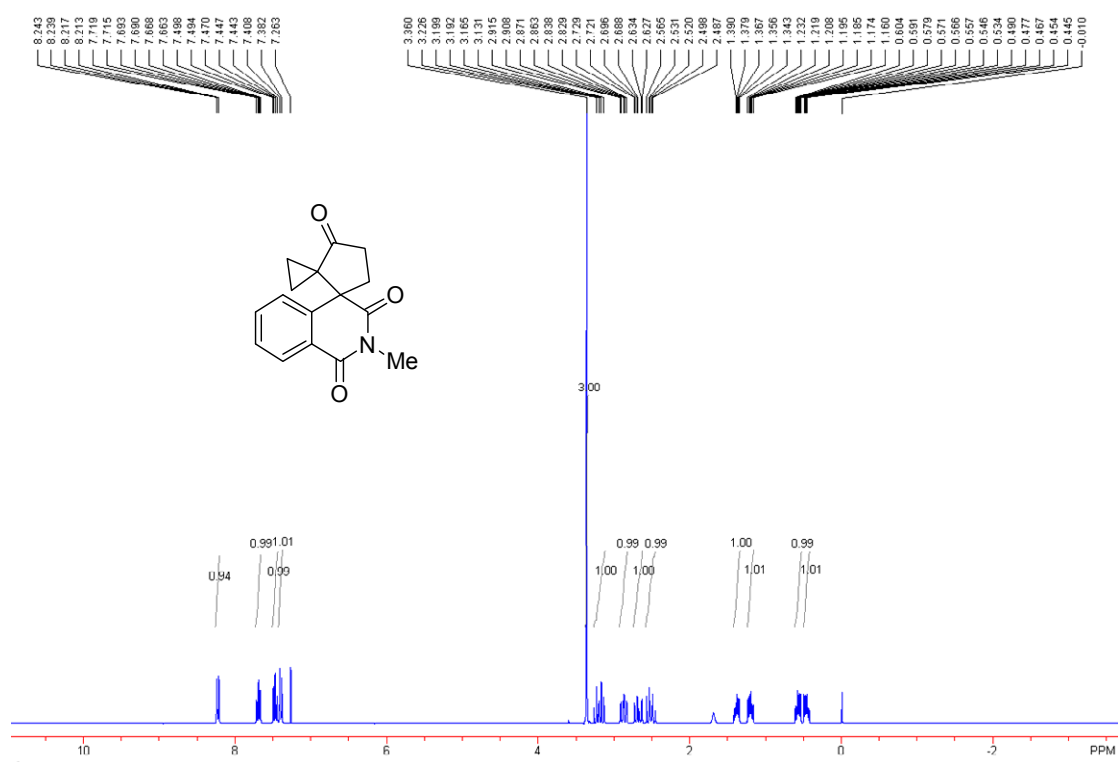
35-¹H NMR(CDCl₃)



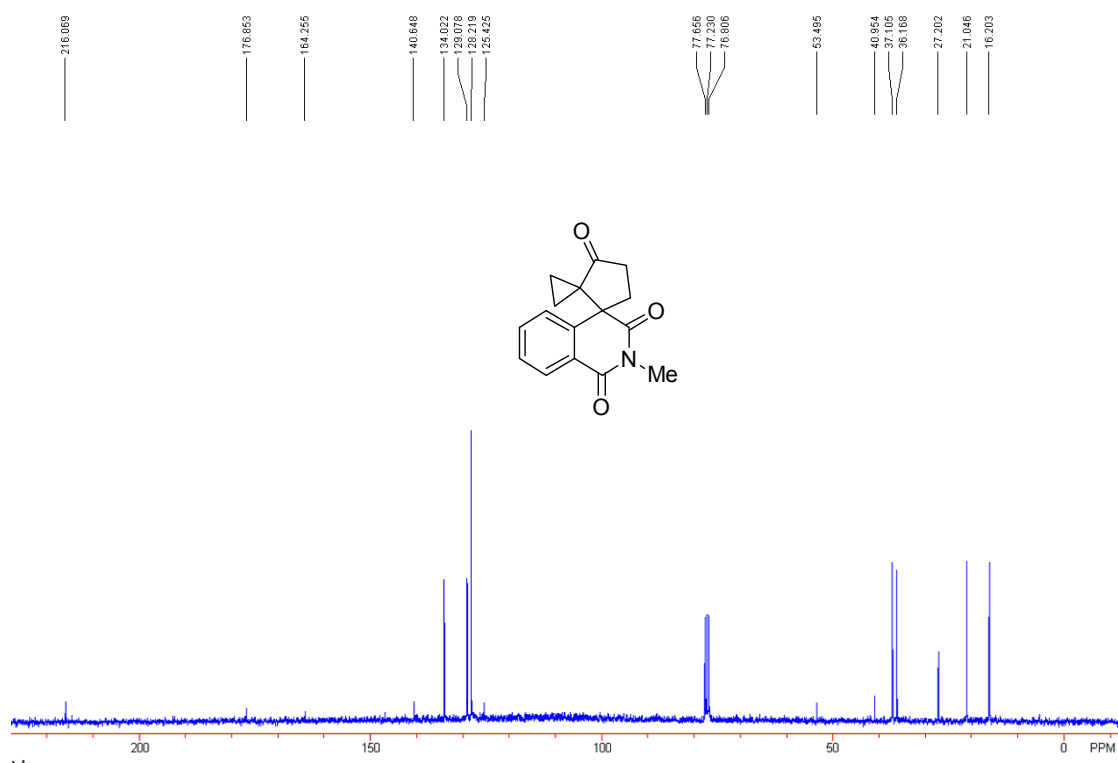
35-¹³C NMR(CDCl₃)



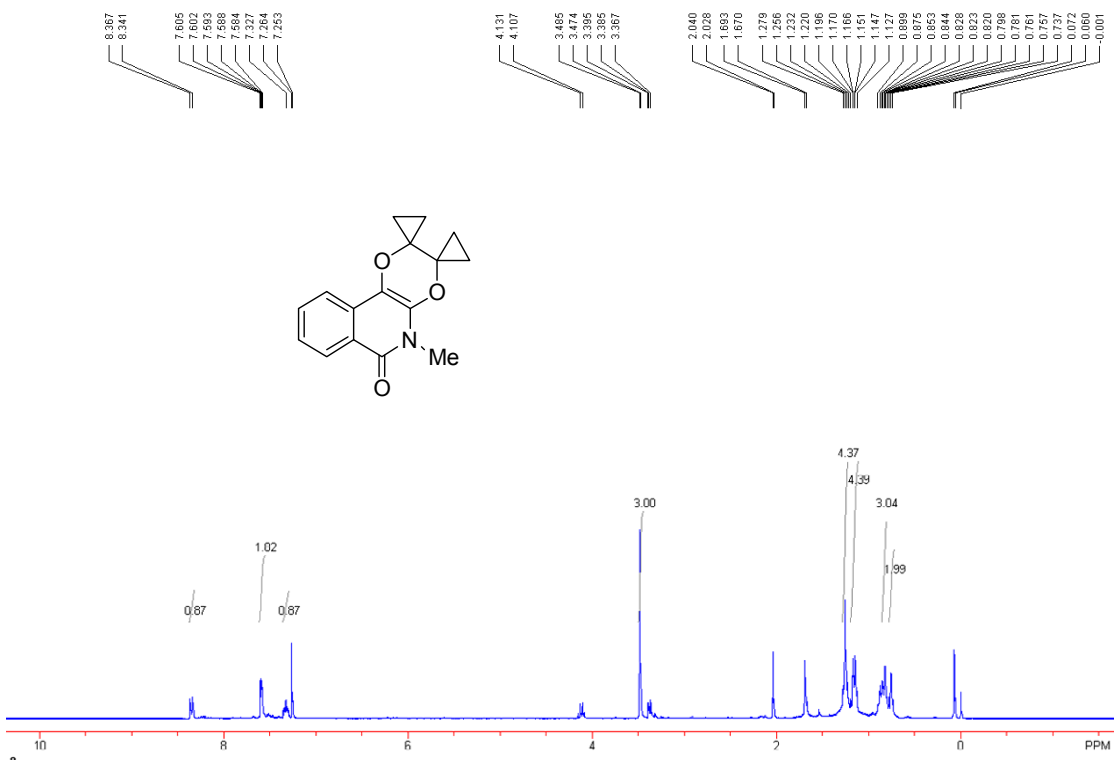
36-¹H NMR(CDCl₃)



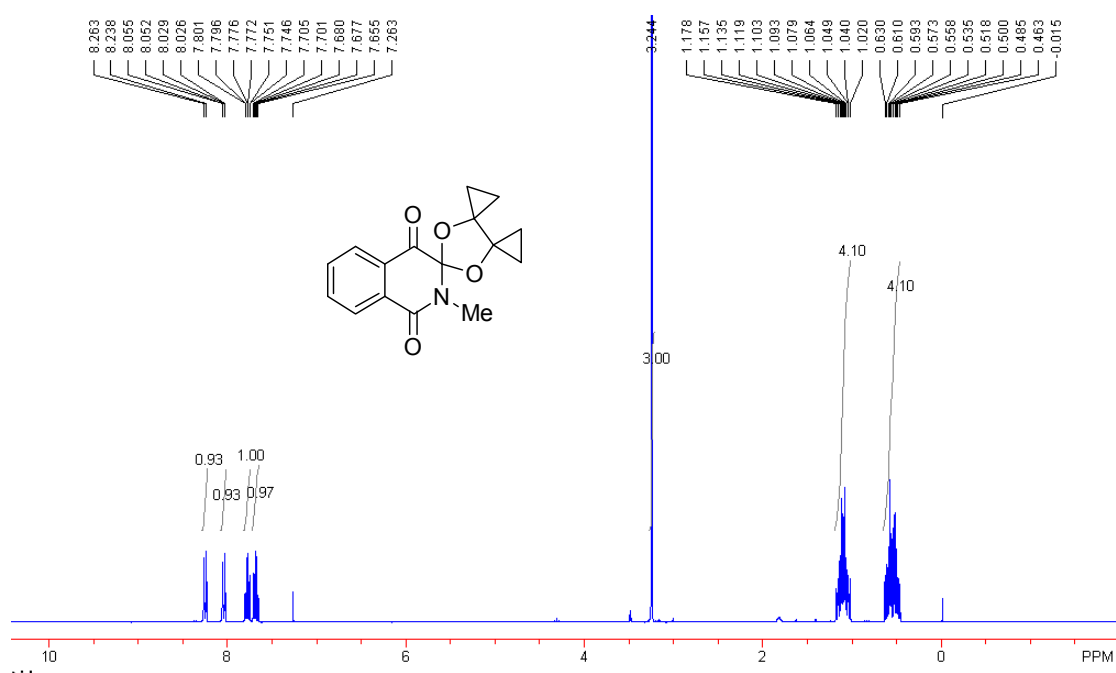
36-¹³C NMR(CDCl₃)



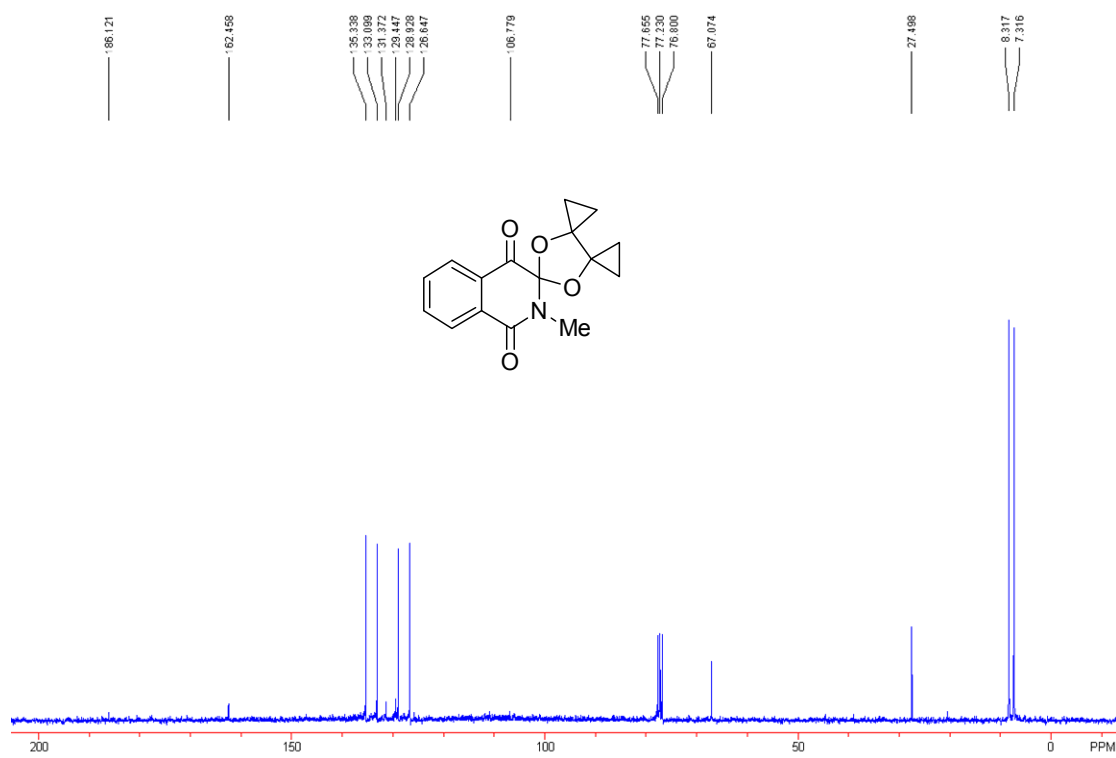
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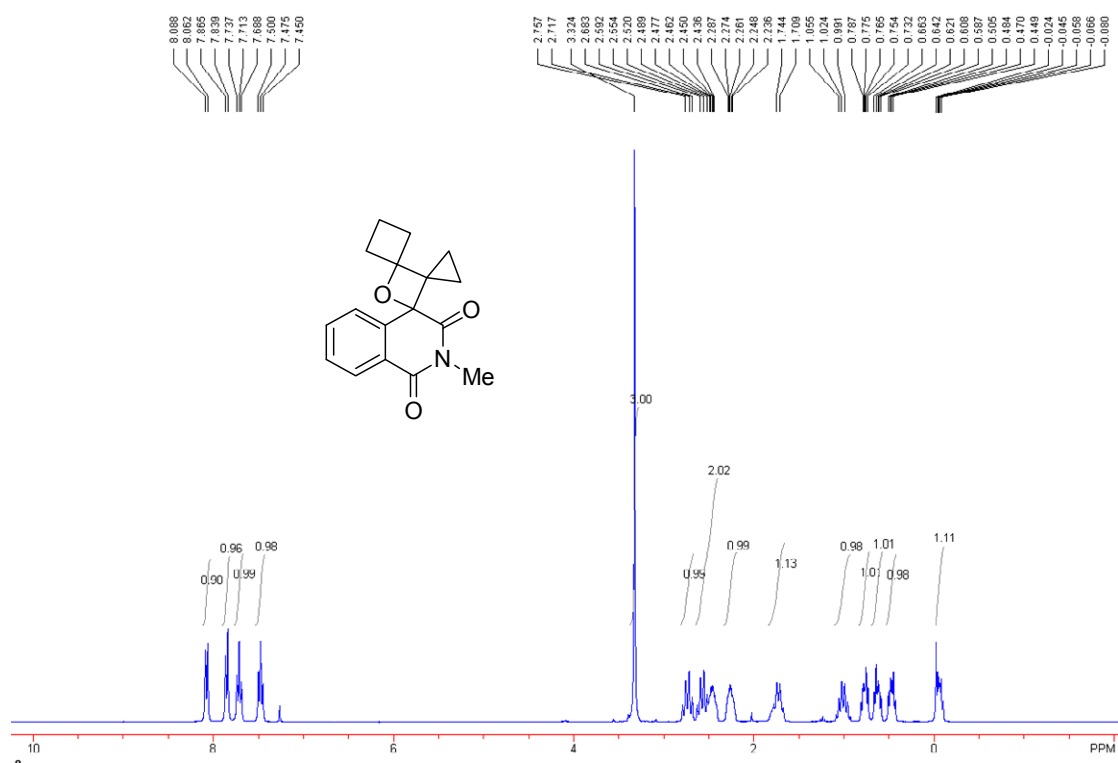
38-¹H NMR(CDCl₃)



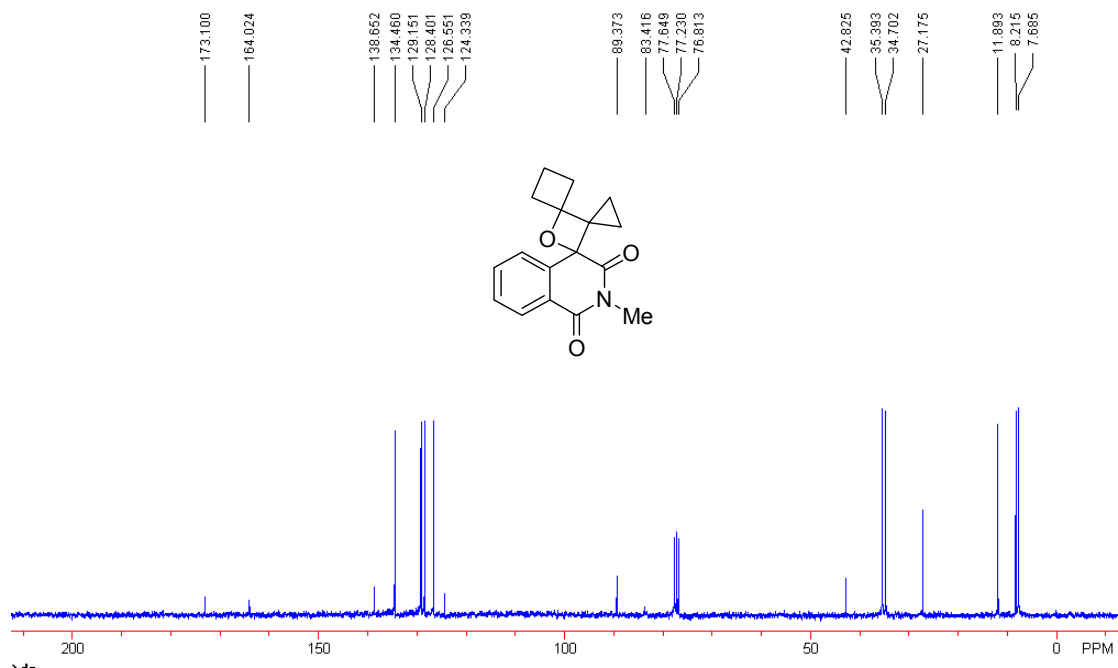
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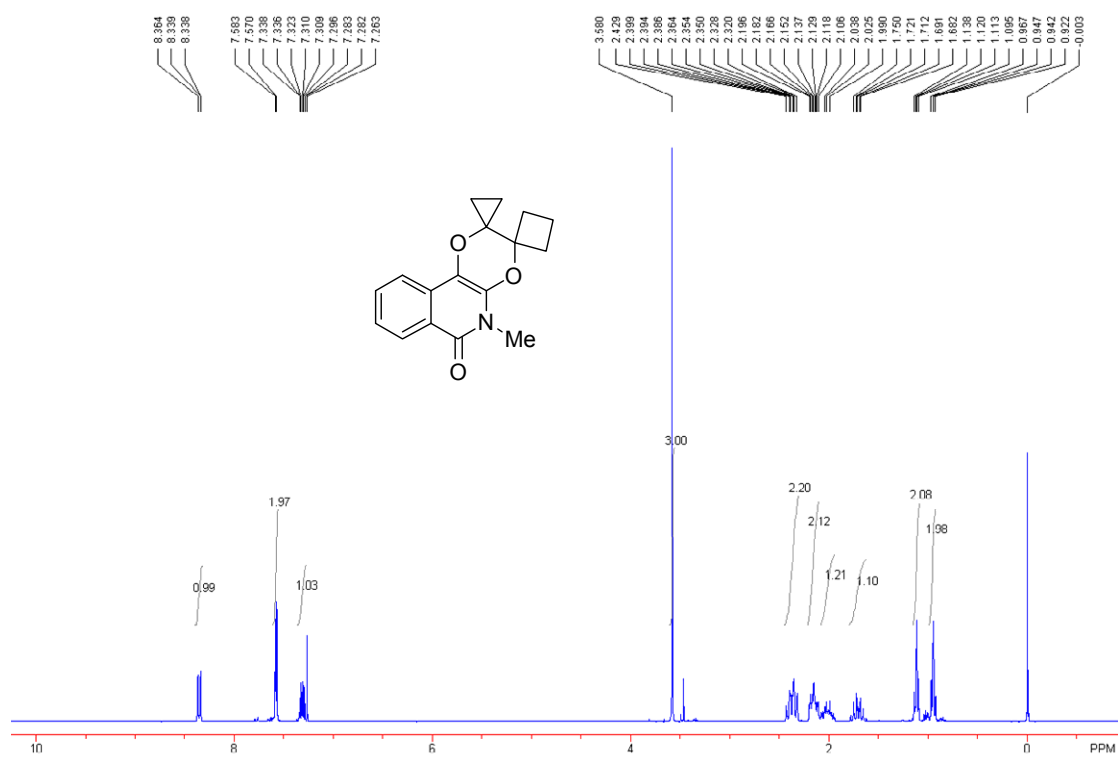
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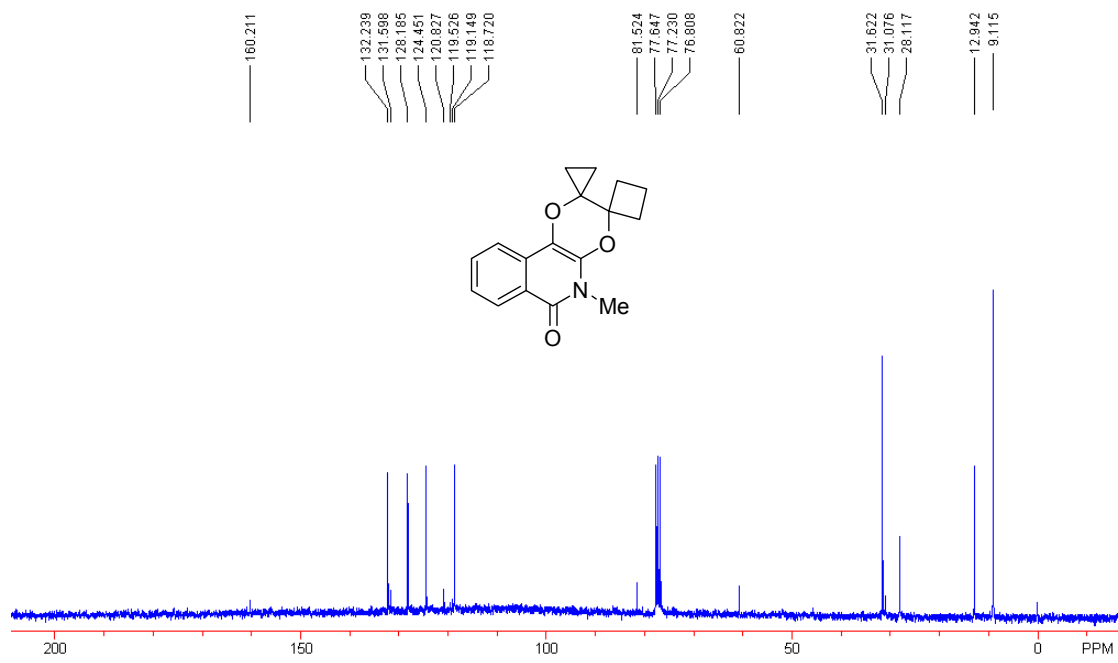
39-¹³C NMR(CDCl₃)



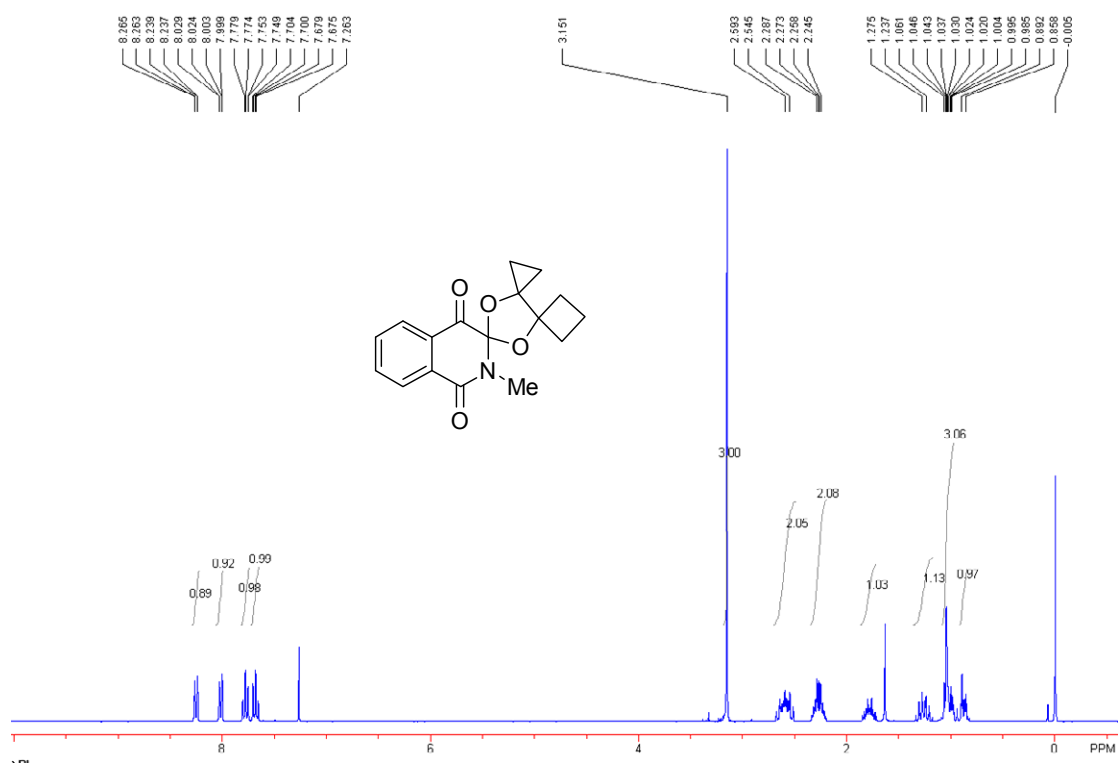
40-¹H NMR(CDCl₃)



40-¹³C NMR(CDCl₃)



41-¹H NMR(CDCl₃)



41-¹³C NMR(CDCl₃)

