

## Supporting Information

for

### **C–C (alkynylation) vs C–O (ether) bond formation under Pd/C–Cu catalysis: synthesis and pharmacological evaluation of 4-alkynylthieno[2,3-*d*]pyrimidines**

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E-mail: Manojit Pal\* - [manojitpal@rediffmail.com](mailto:manojitpal@rediffmail.com)

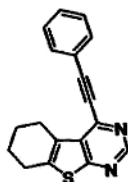
\*Corresponding author

### **NMR spectra of compounds 3a–n**

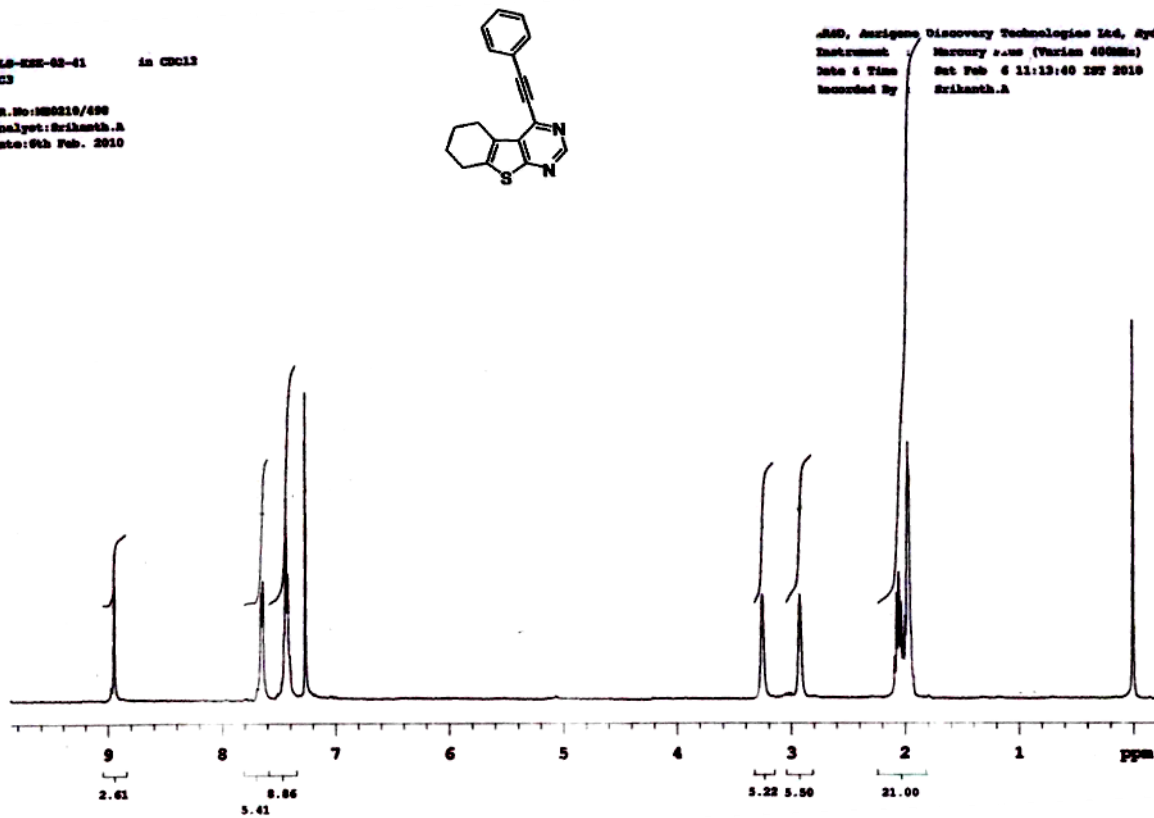
3a <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

118-828-02-01 in CDCl<sub>3</sub>  
NCS

AR.No:MS0210/698  
Analyst:Srikanth.A  
Date:04h Feb. 2010



MSD, Amgen Discovery Technologies Ltd, Hyderabad  
Instrument Mercury 400 (Varian 400MHz)  
Date & Time Sat Feb 6 11:13:40 IST 2010  
Recorded By Srikanth.A



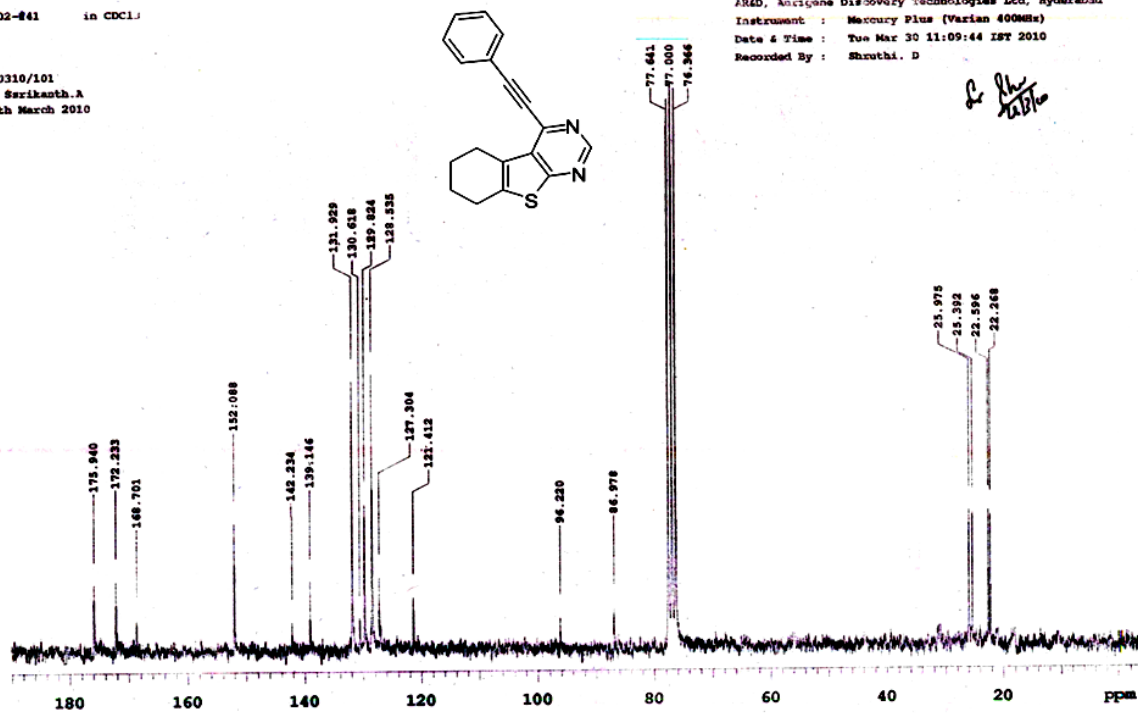
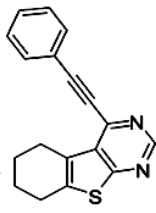
3a <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)

ILS-RSK-02-#41 in CDCl<sub>3</sub>  
ILS-MC3

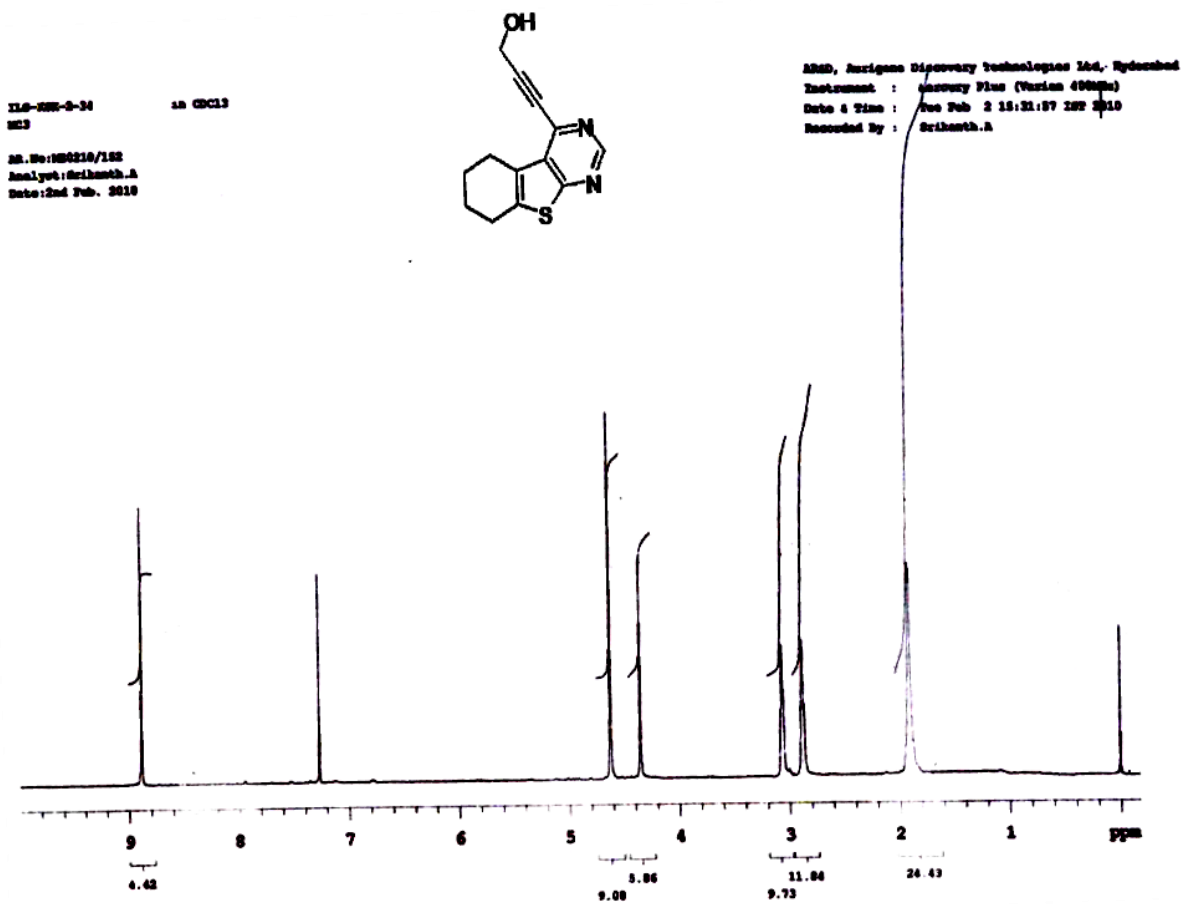
MR. NO: 020310/101  
Analyst: Srikanth.A  
Date: 26th March 2010

ARL0, Arisone Discovery Technologies Ltd, Hyderabad  
Instrument : Mercury Plus (Varian 400MHz)  
Date & Time : Tue Mar 30 11:09:44 IST 2010  
Recorded By : Shruthi. D

*S. Srikanth*



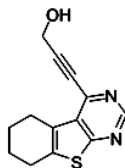
**3b**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



**3b**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

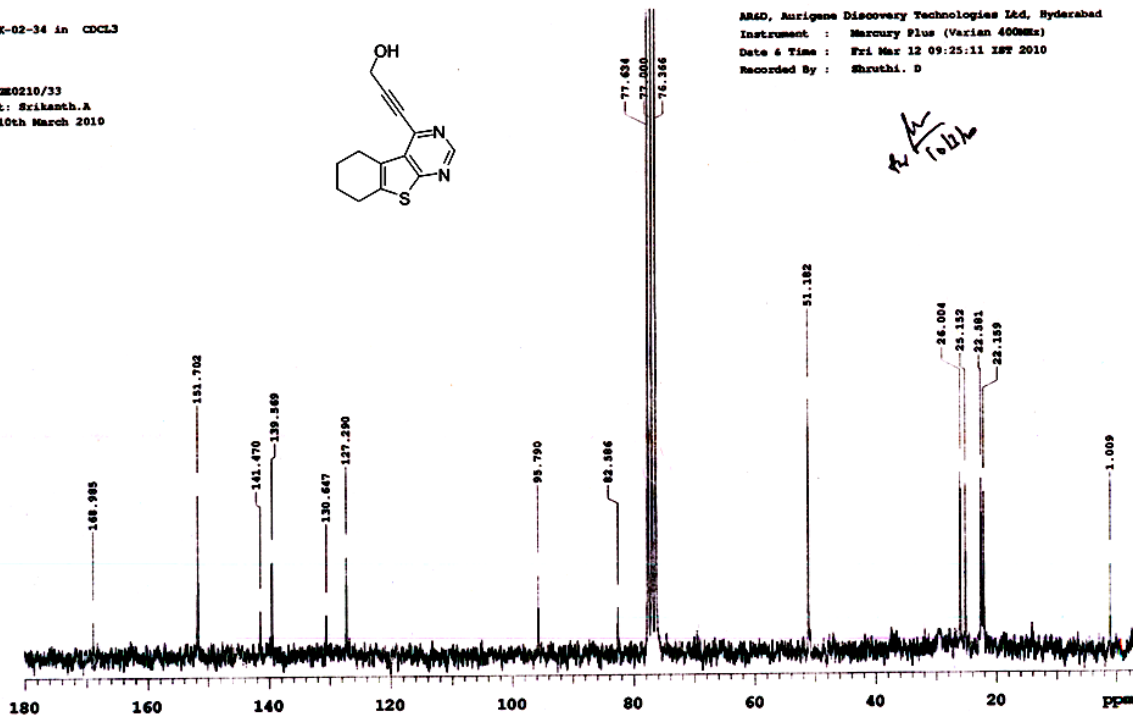
ILS-KSK-02-34 in  $\text{CDCl}_3$   
MCS

AN.WO:G80210/33  
Analyst: Srikanth.A  
Date: 10th March 2010

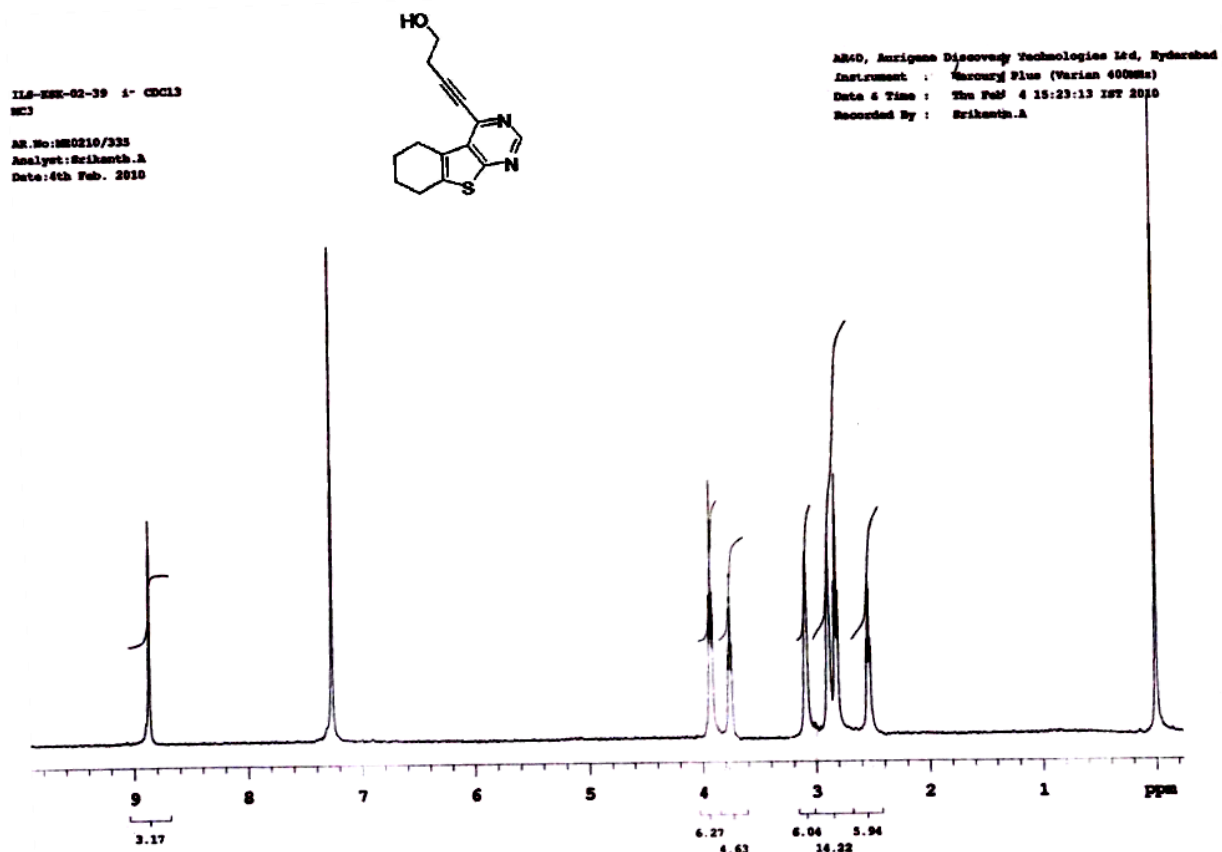


AR&D, Aurigene Discovery Technologies Ltd, Hyderabad  
Instrument : Mercury Plus (Varian 400MHz)  
Date & Time : Fri Mar 12 09:25:11 IST 2010  
Recorded By : Shruthi. D

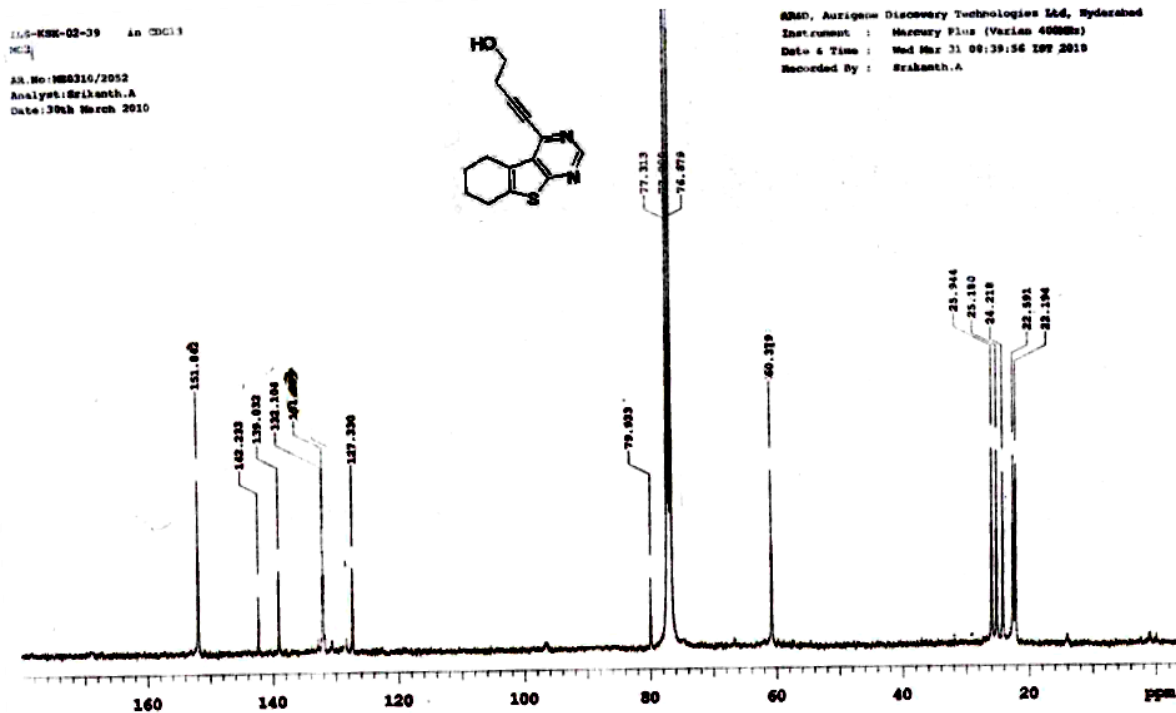
*Handwritten signature*  
10/3/10



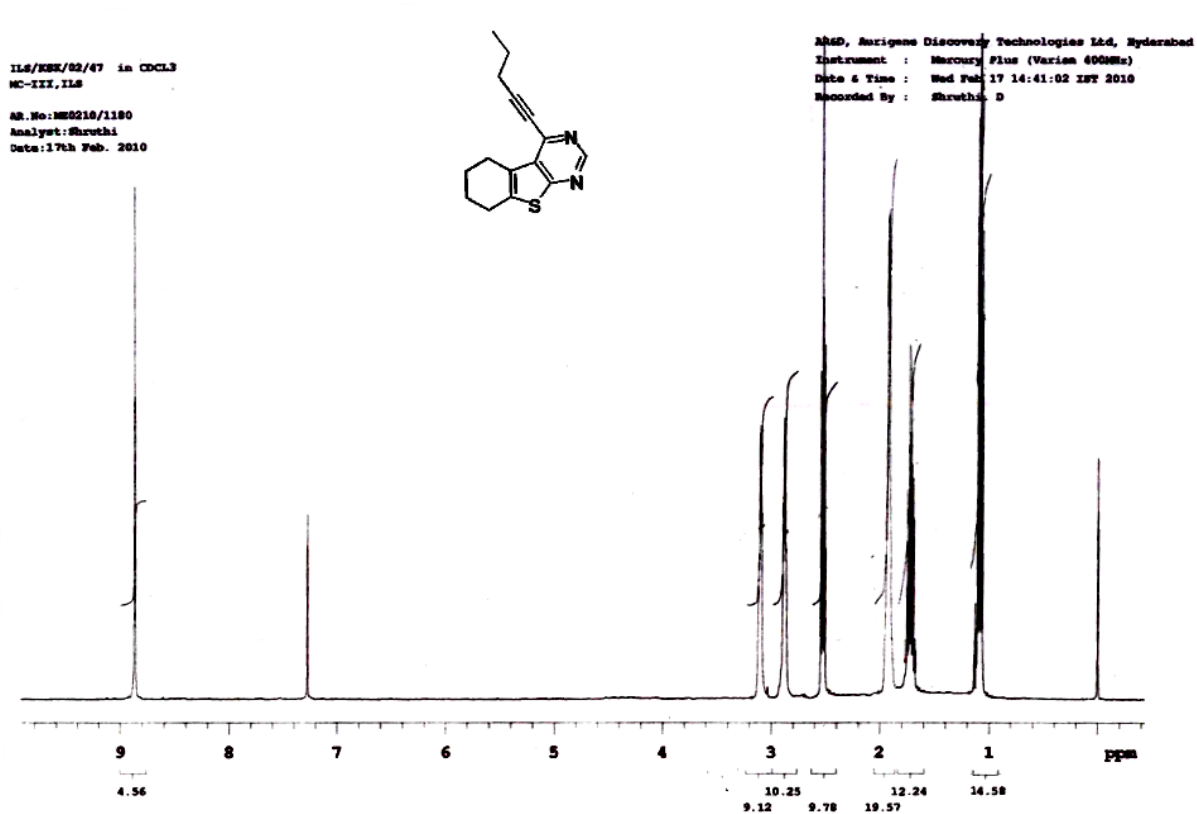
3c <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



3c <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)



3d <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

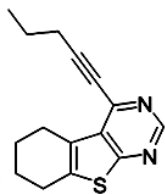




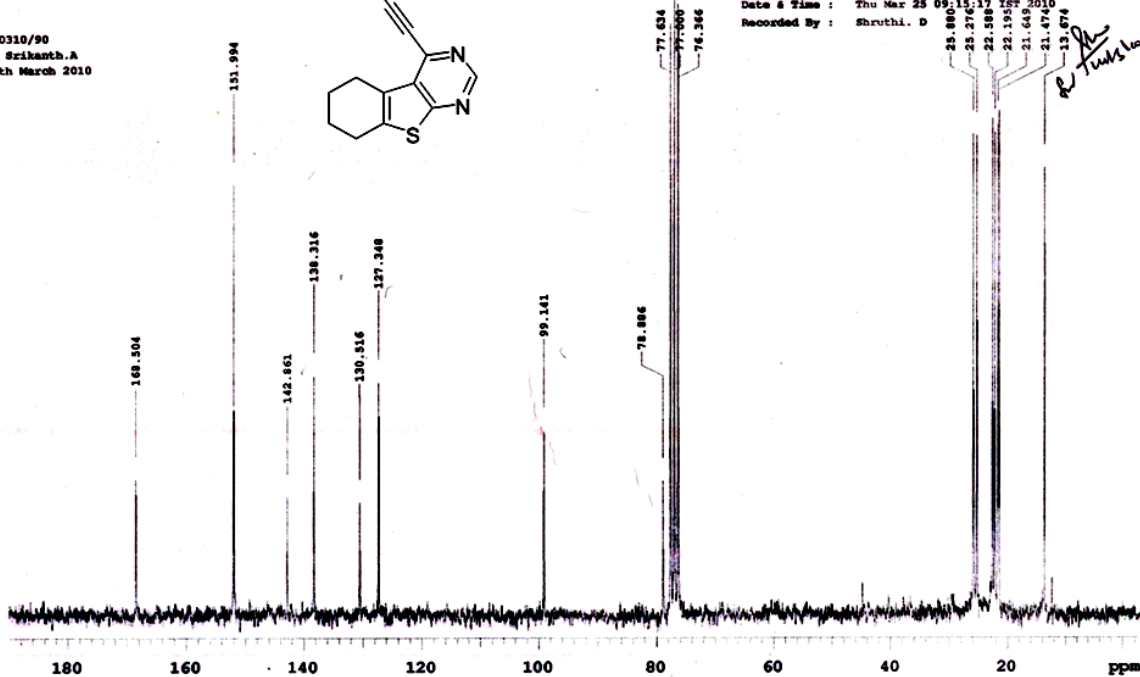
3d <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)

ILS-KSK-02-47 in CDCl<sub>3</sub>  
ILS, MC3

AN.NO: GE0310/90  
Analyst: Srikanth.A  
Date: 24th March 2010

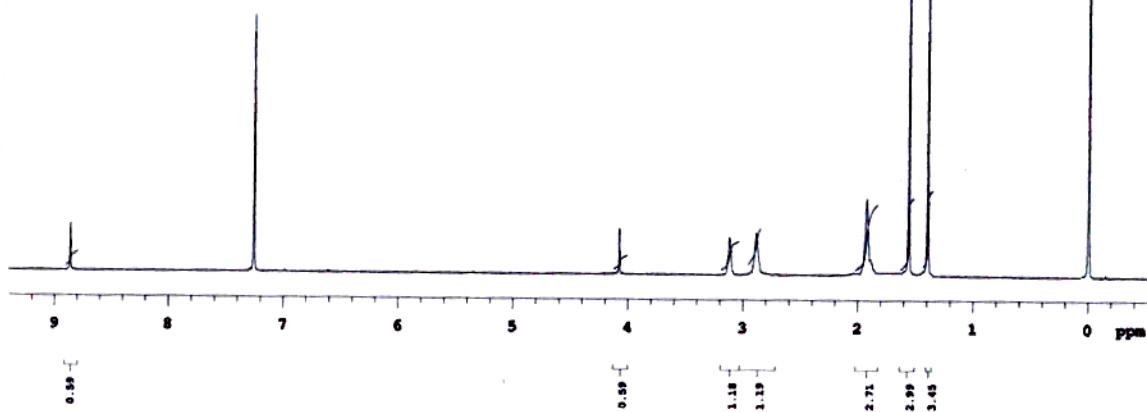
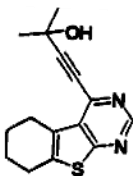


ARSD, Arvigene Discovery Technologies Ltd, Hyderabad  
Instrument : Mercury Plus (Varian 400MHz)  
Date & Time : Thu Mar 25 09:13:17 IST 2010  
Recorded By : Shruthi. D



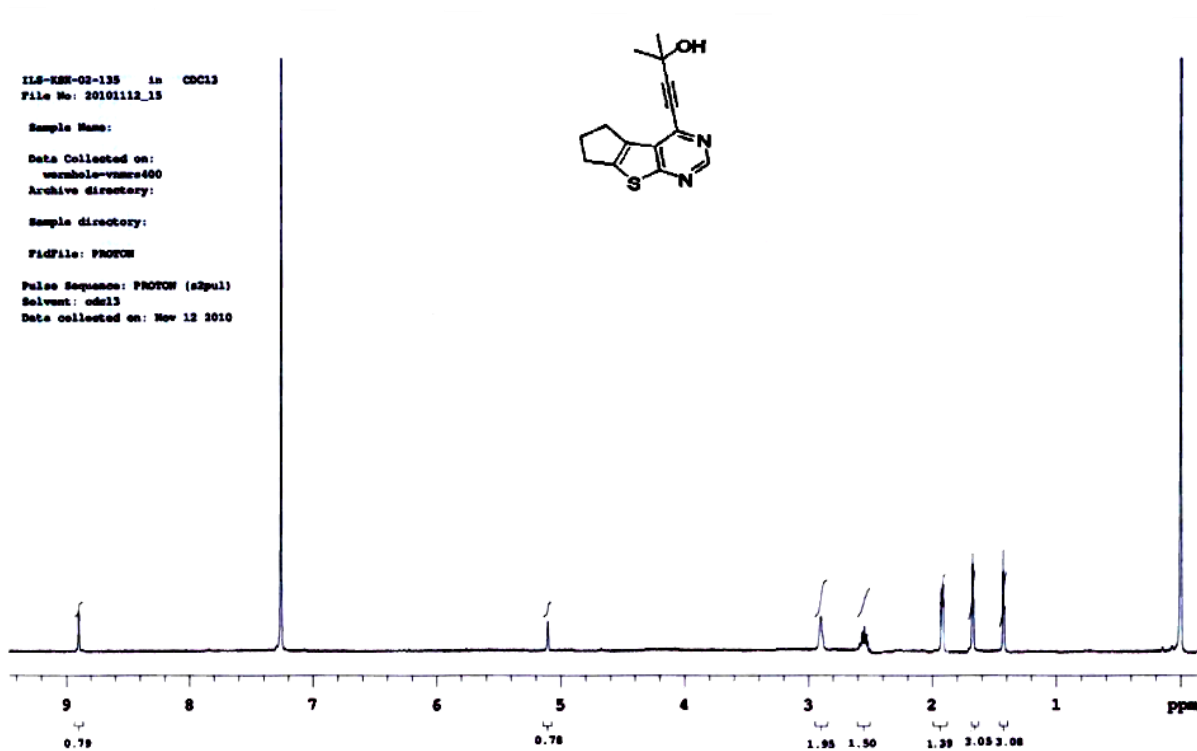
3e <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

ILS-MSK-03-134  
File No: 20101112\_5  
Sample Name:  
Data Collected on:  
vornhole-vmsr48C  
Archive directory:  
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File: PROTON  
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 12 2010



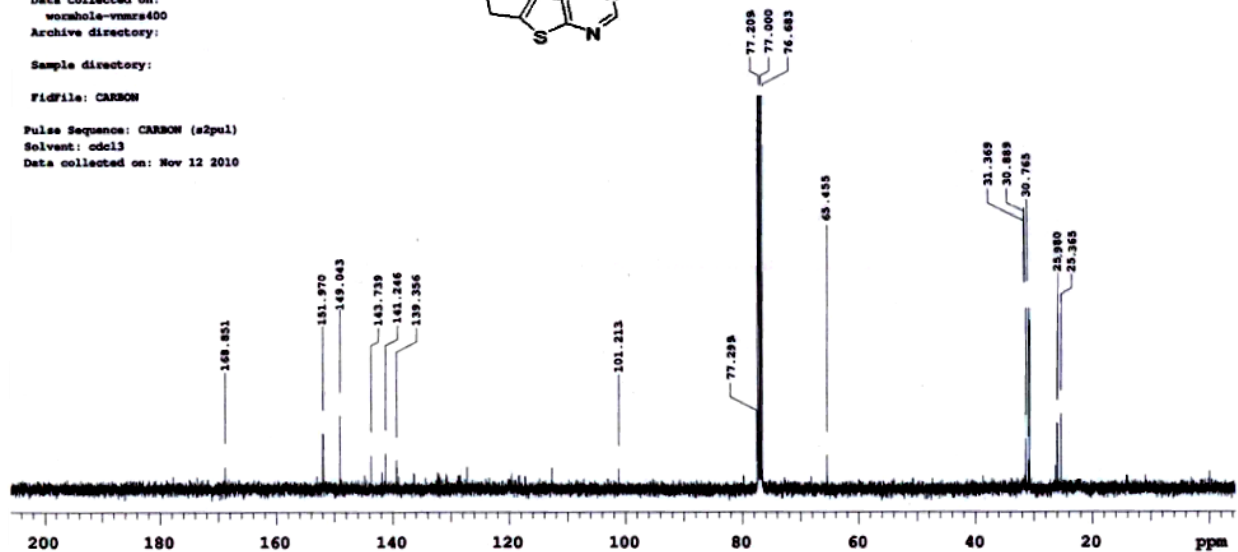
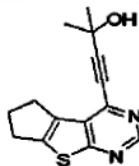


3f  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

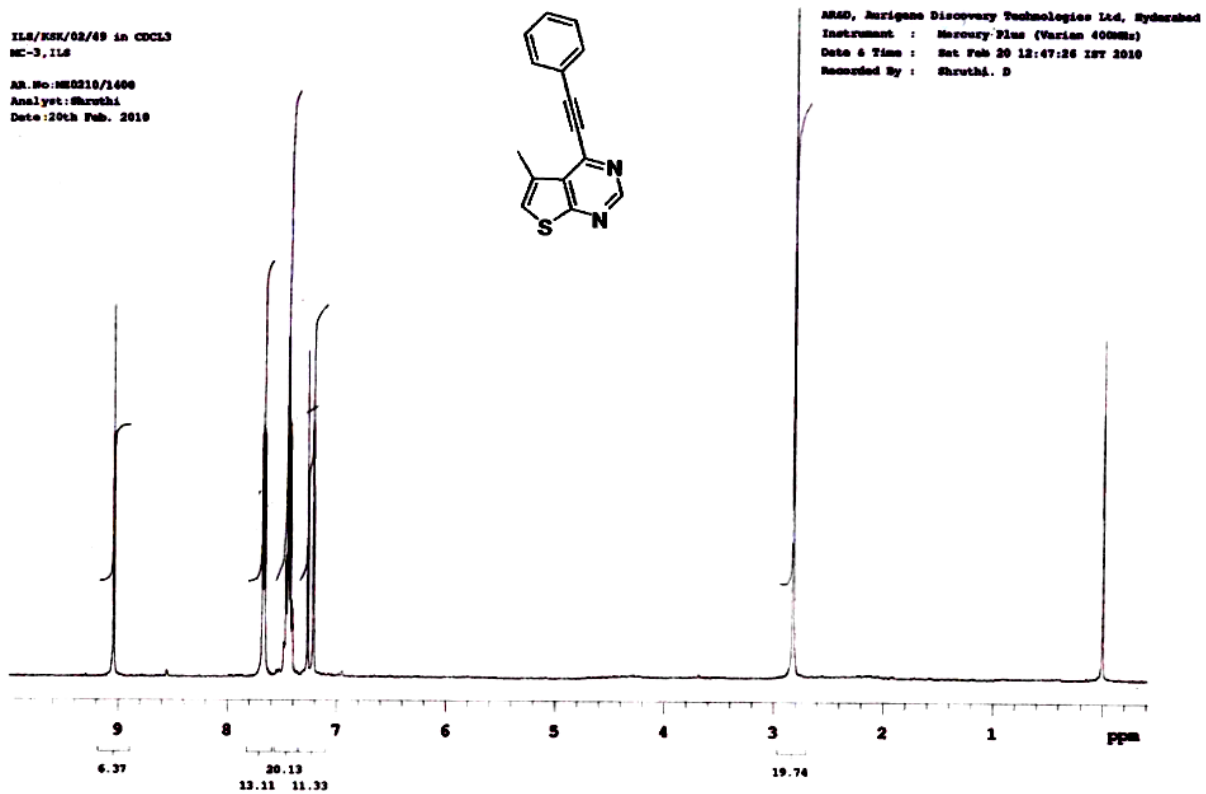


3f <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)

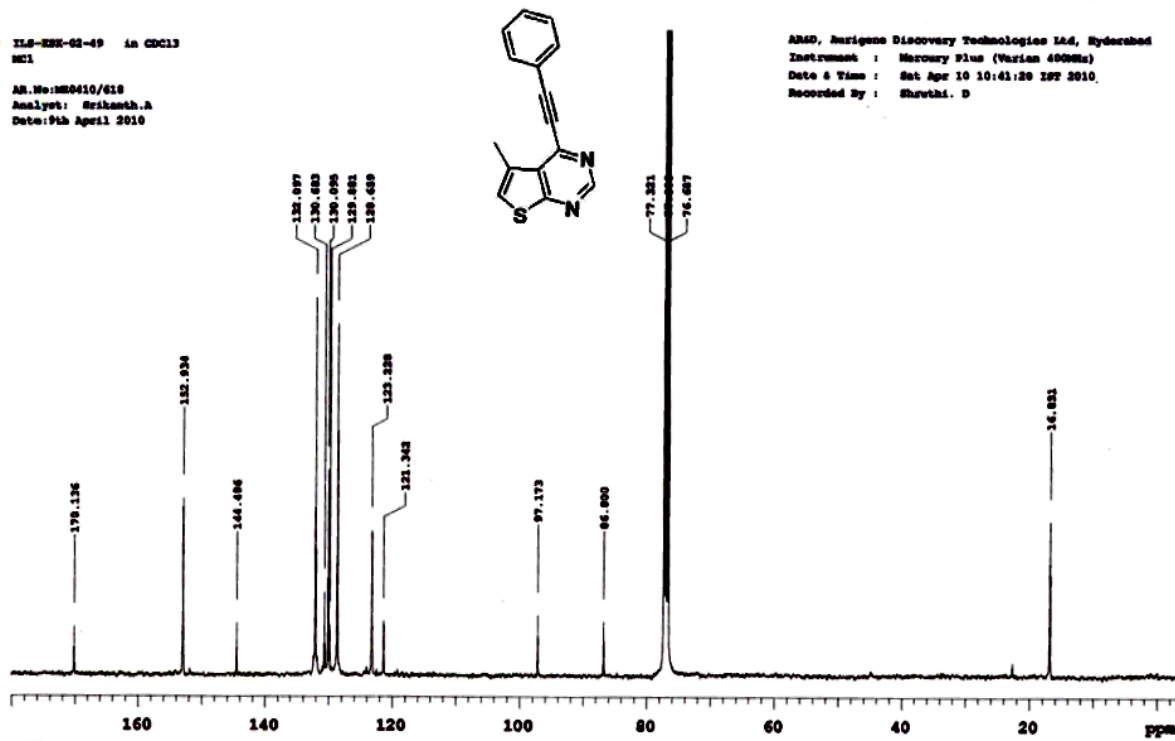
ILS-KSK-02-135 in CDCl<sub>3</sub>  
13C Exp.  
File No:20101112\_18  
Sample Name:  
Data Collected on:  
wornhole-vmrs400  
Archive directory:  
Sample directory:  
Fid#file: CARBON  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 12 2010



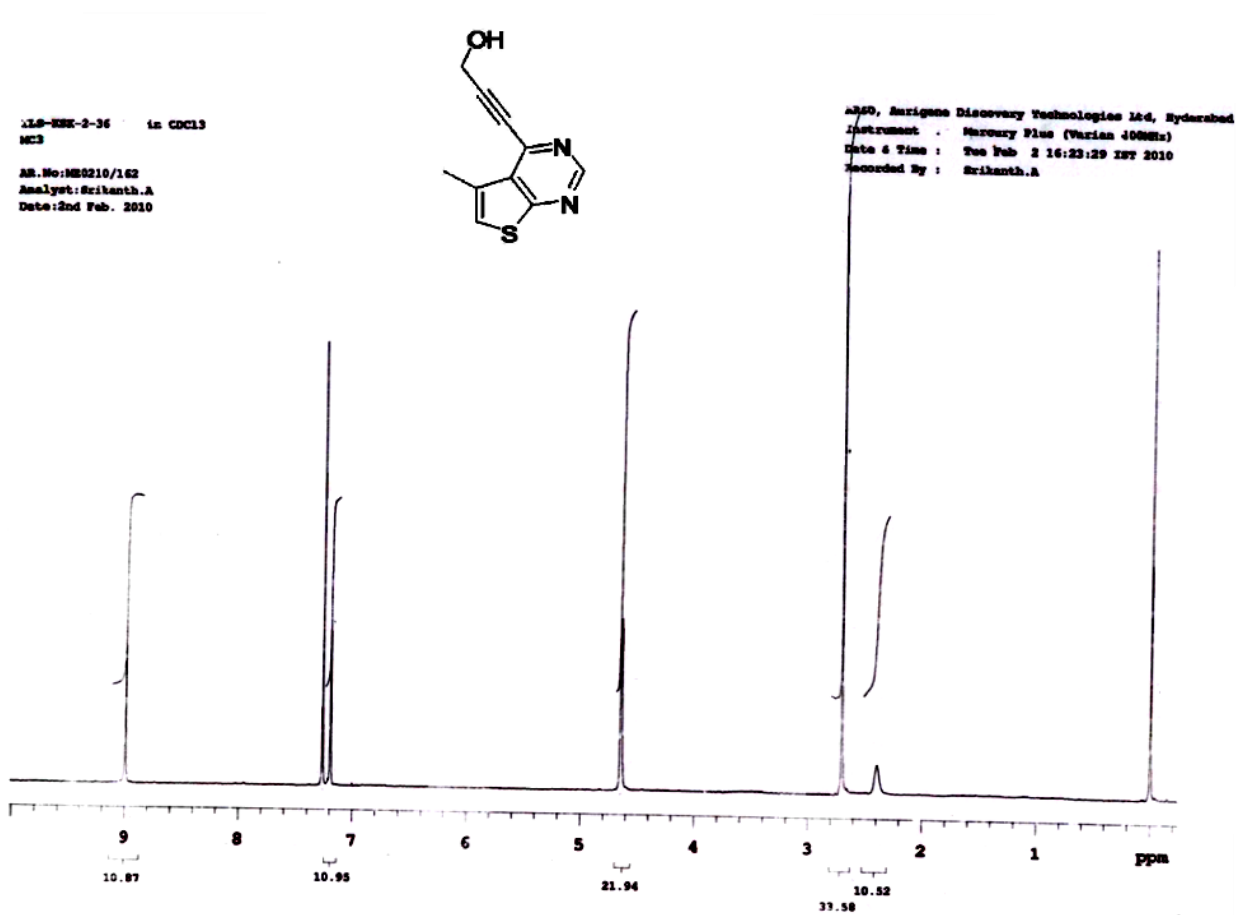
3g <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



3g <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)

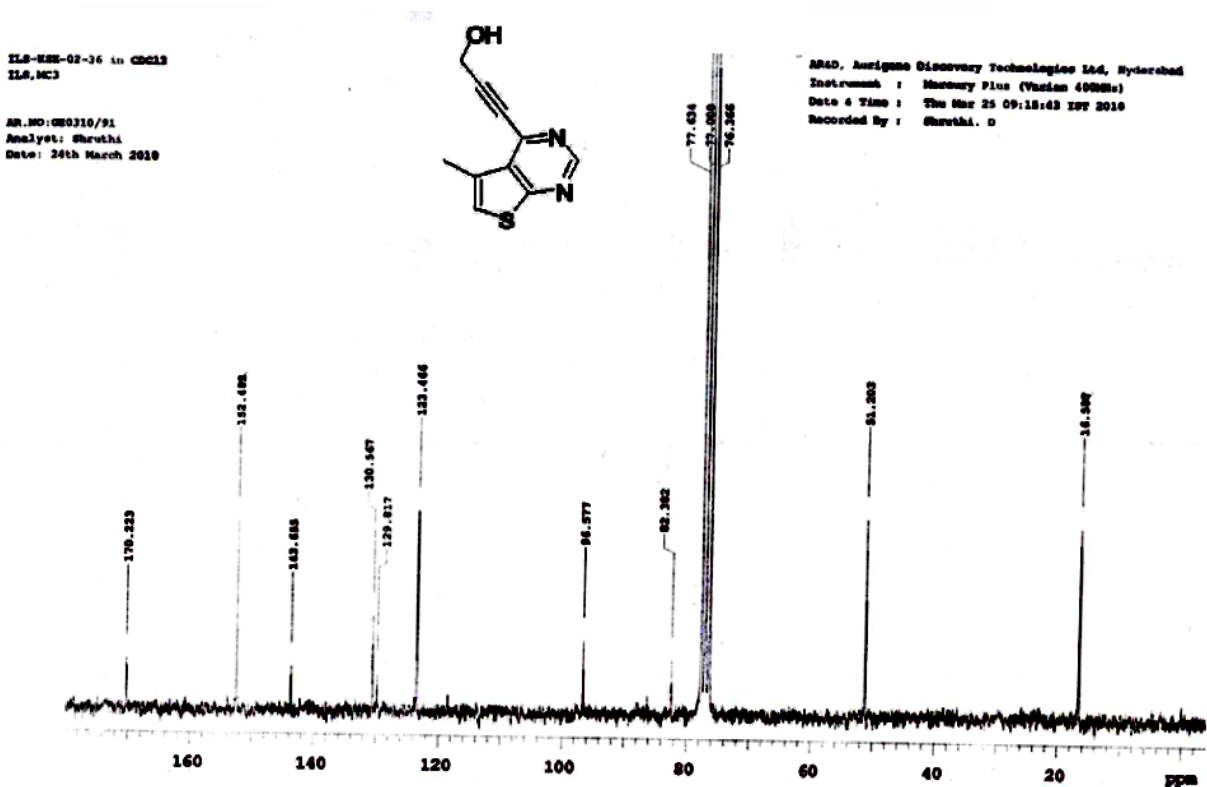


3h <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

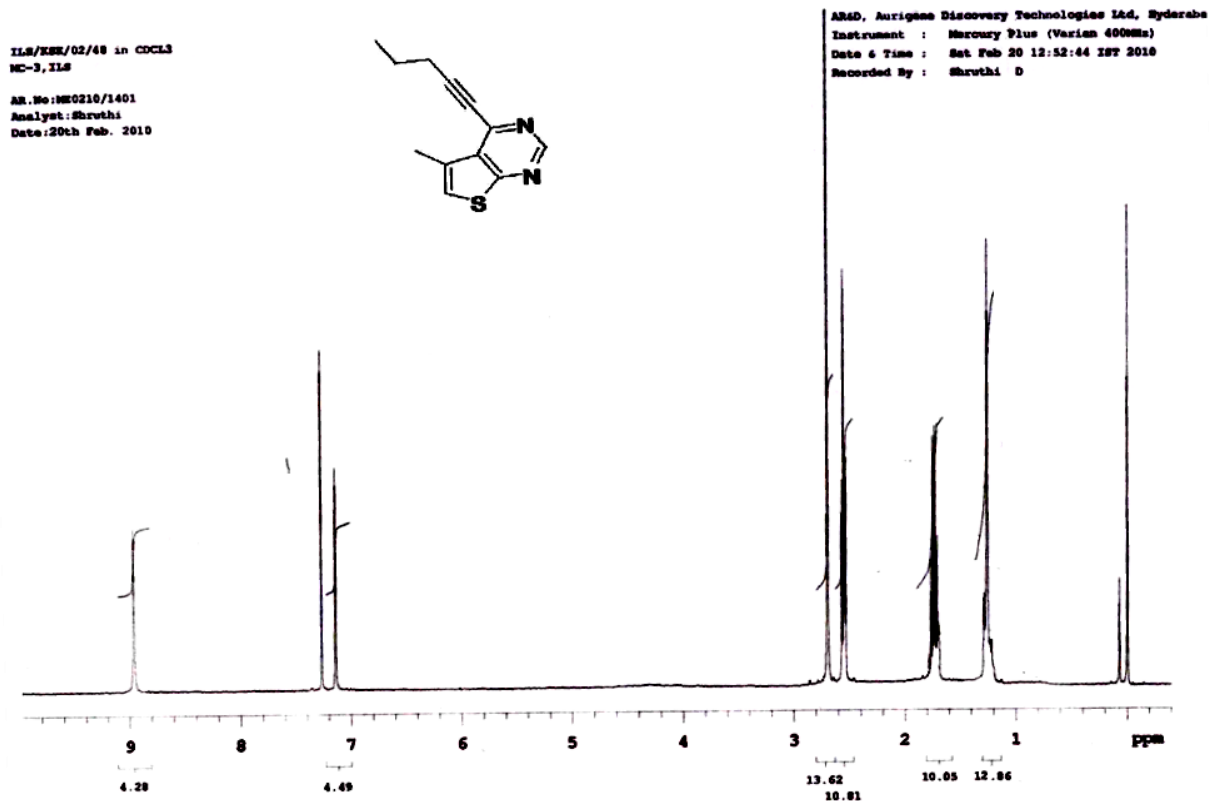




3h  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )



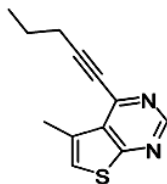
3i <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



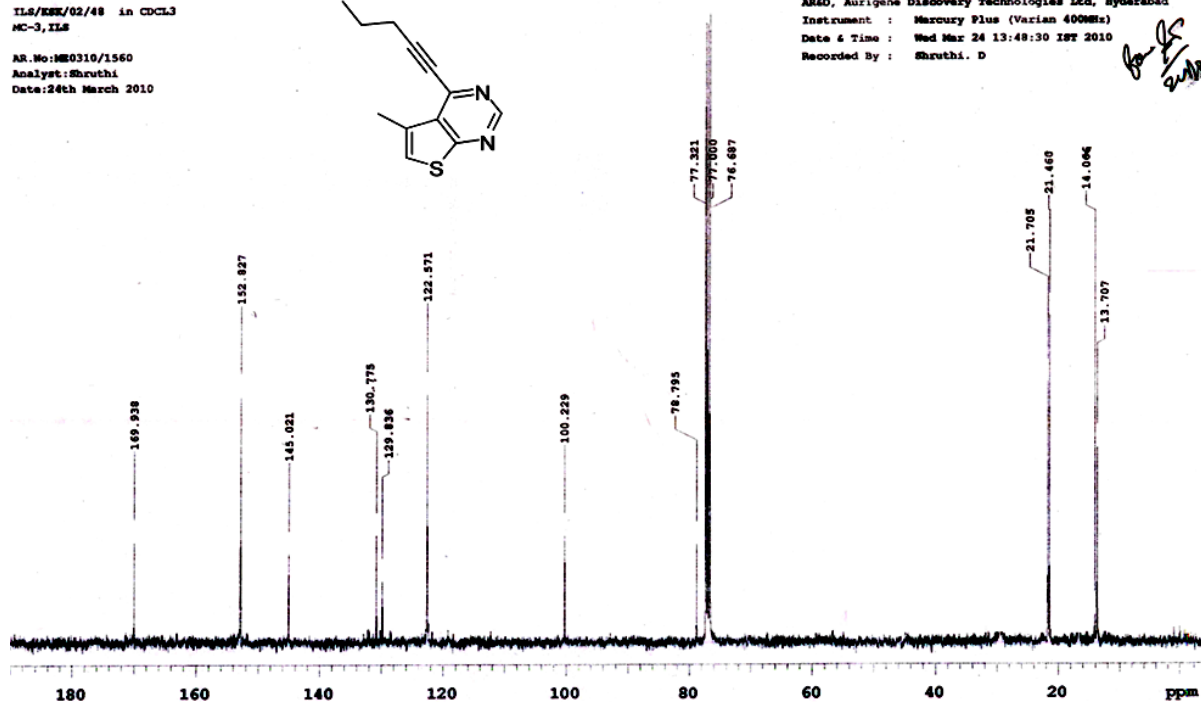
3i <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)

ILS/RRR/02/48 in CDCl<sub>3</sub>  
MC-3, ILS

AR.No:MR0310/1560  
Analyst:Shruthi  
Date:24th March 2010



AR&D, Aurigene Discovery Technologies Ltd, Hyderabad  
Instrument : Mercury Plus (Varian 400MHz)  
Date & Time : Wed Mar 24 13:48:30 IST 2010  
Recorded By : Shruthi. D



3j <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

ILS-KSK-02-130-2 in CDCl<sub>3</sub>  
File No: 20101124\_10

Sample Name:

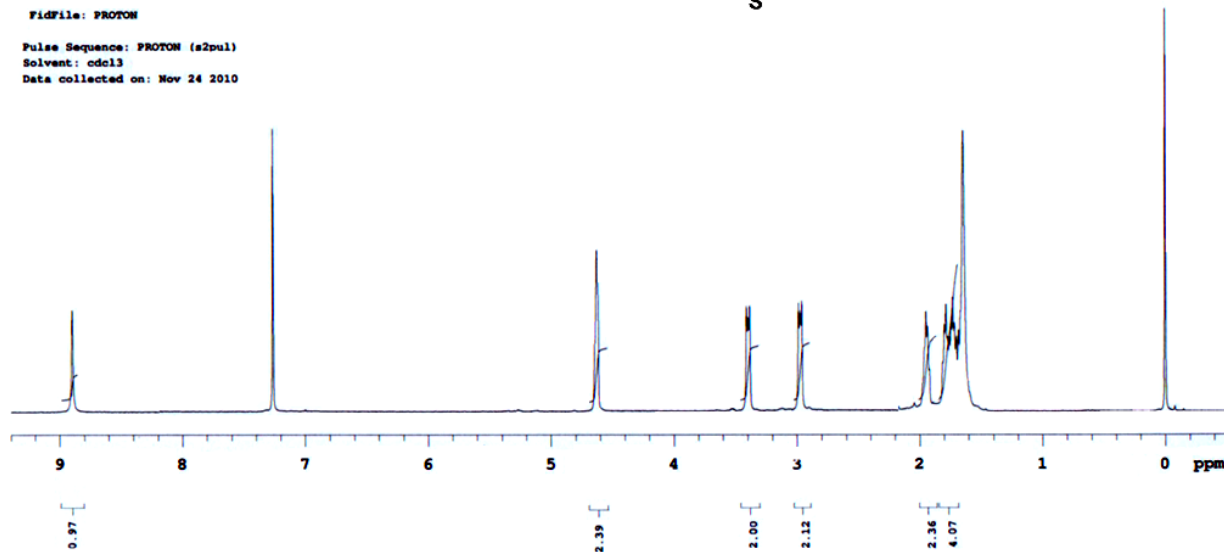
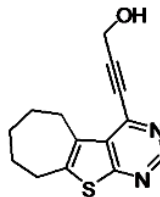
Data Collected on:  
wormhole-vnmrs400

Archive directory:

Sample directory:

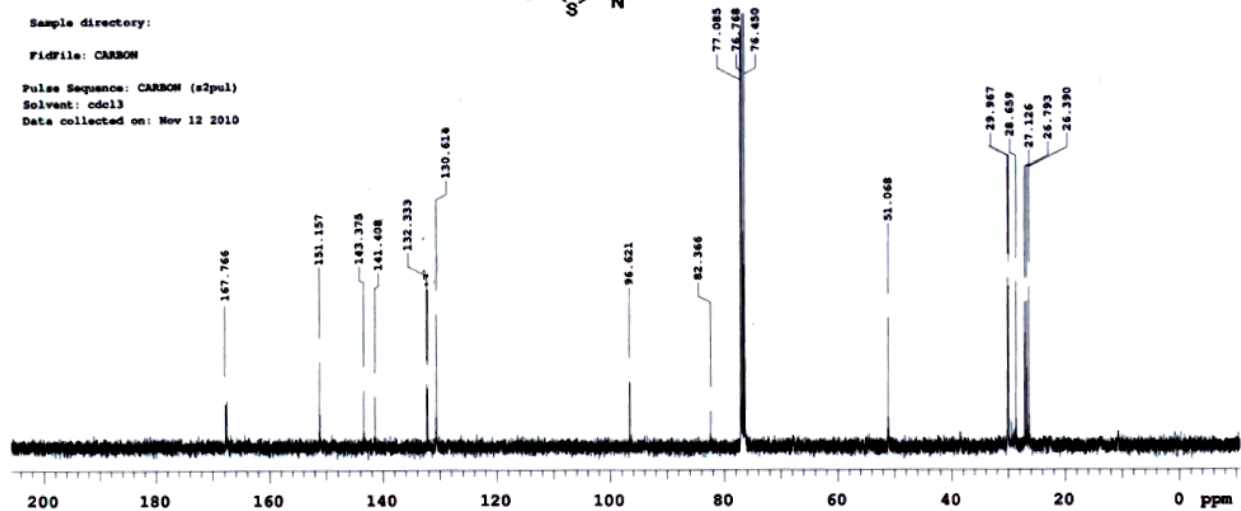
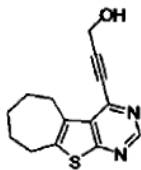
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 24 2010

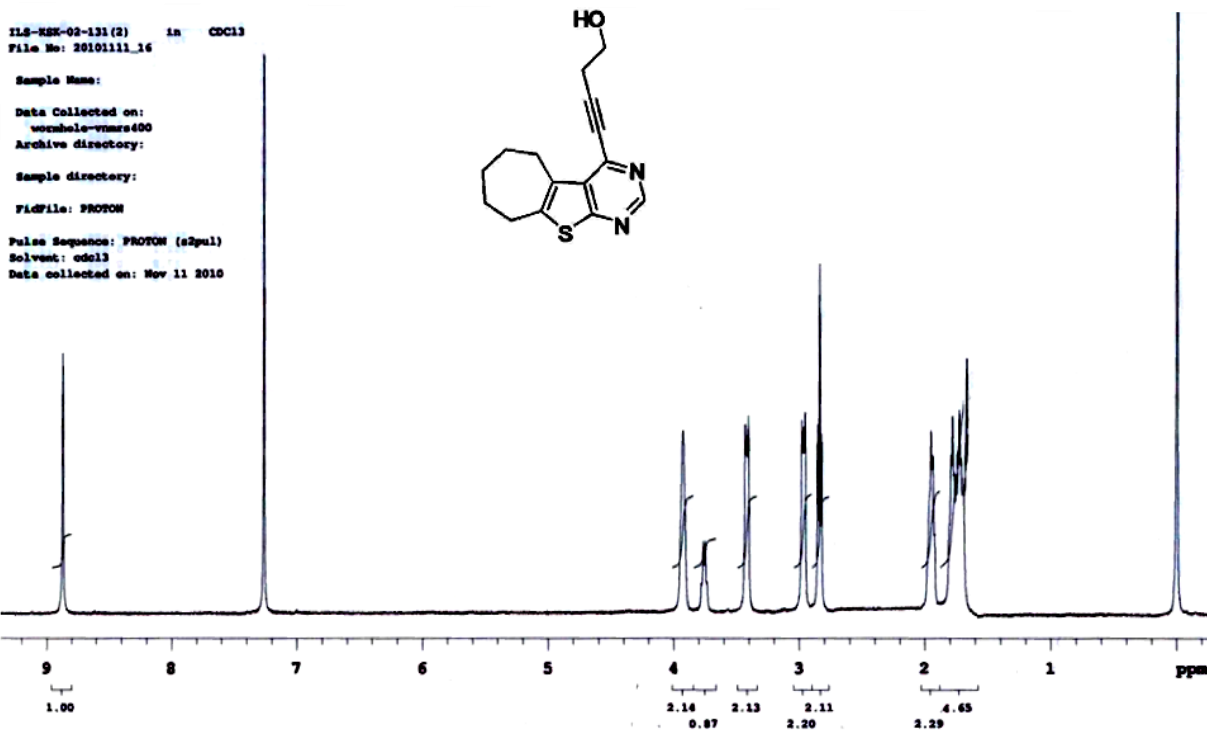


3j <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)

ILS-KSR-02-130 in CDCl<sub>3</sub>  
13C Expt.  
File No: 20101112\_7  
Sample Name:  
Data Collected on:  
wormhole-vvms400  
Archive directory:  
Sample directory:  
Fidfile: CARBON  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 12 2010

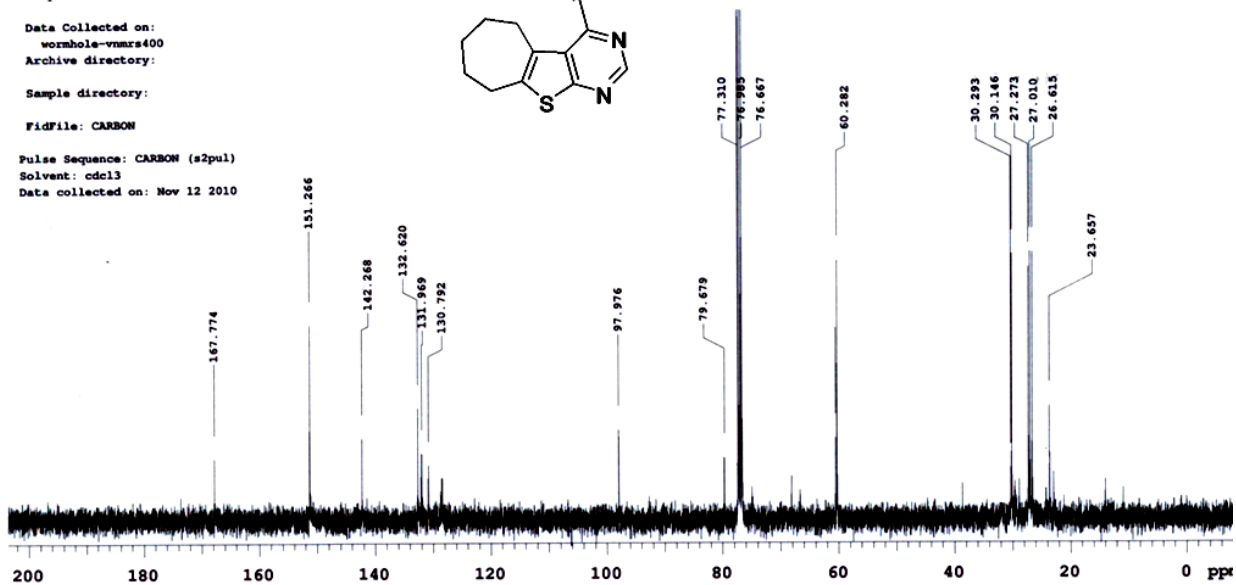
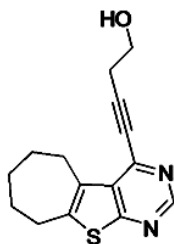


3k  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

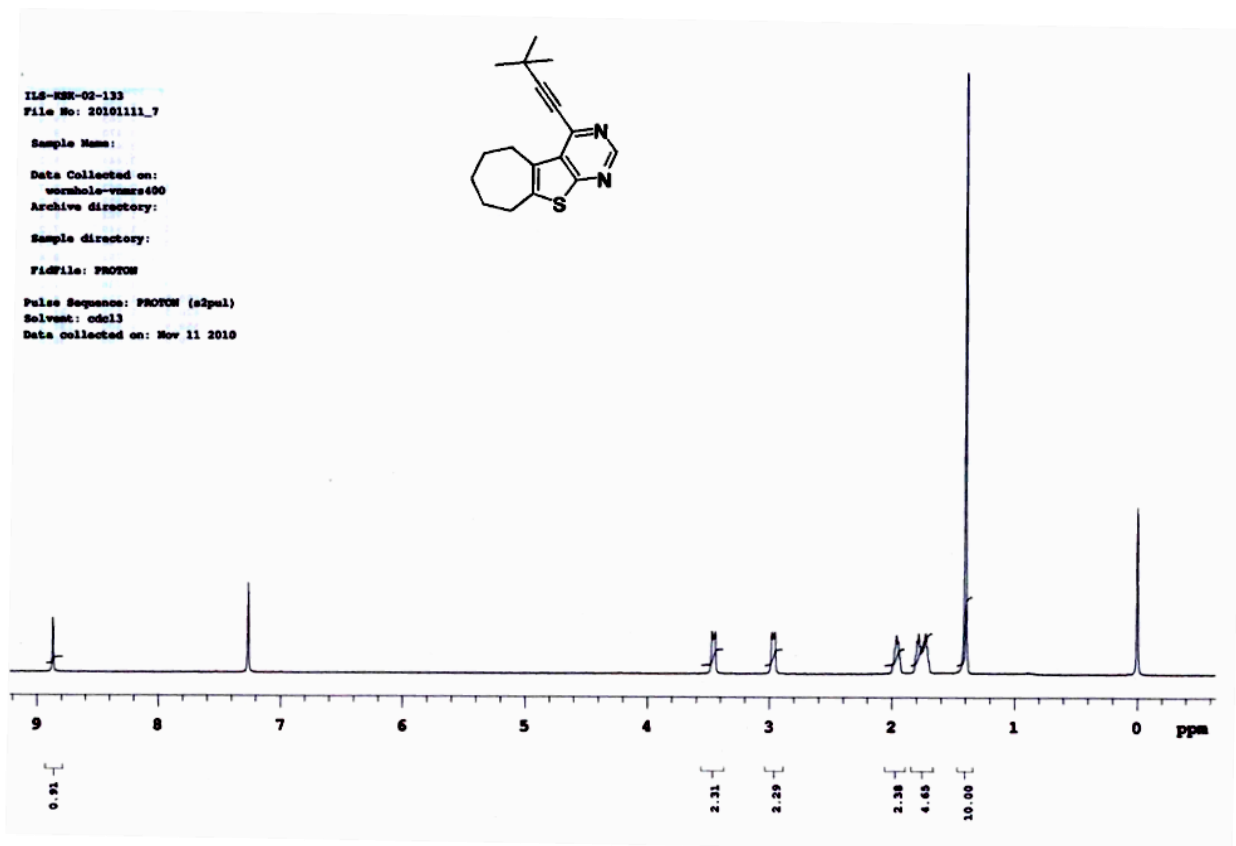


3k  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

ILS-KSK-02-131-2 in  $\text{CDCl}_3$   
13C Expt.  
File No:20101112\_3  
Sample Name:  
Data Collected on:  
wormhole-vnmr400  
Archive directory:  
Sample directory:  
Fidfile: CARBON  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 12 2010



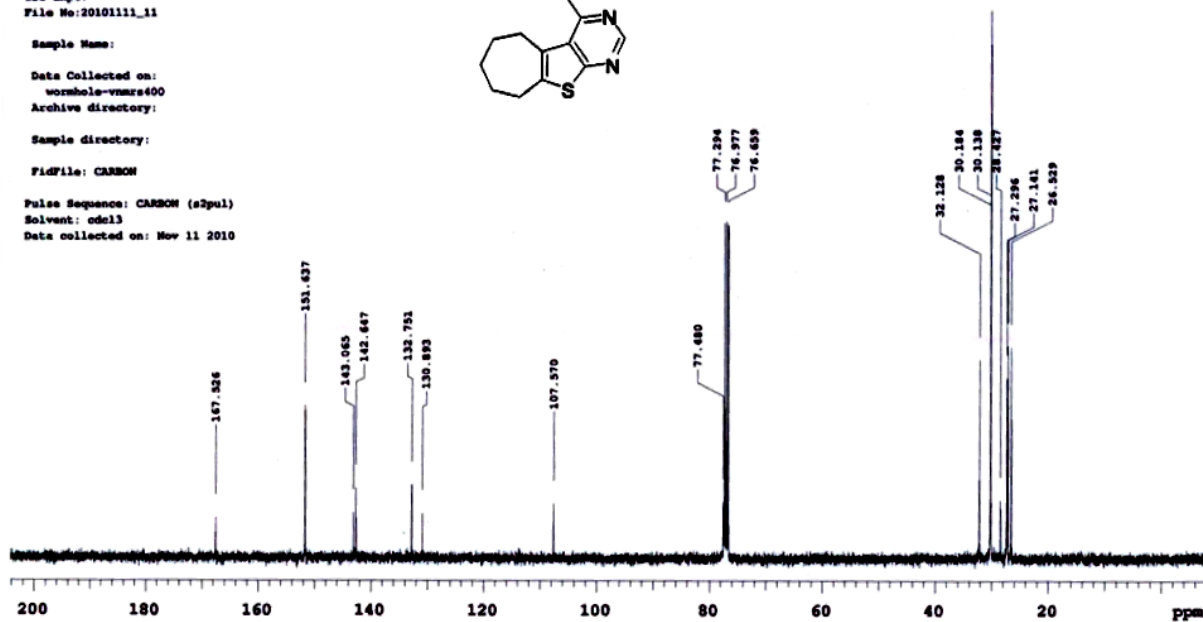
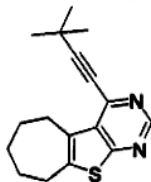
31  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )





31 <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)

ILS-KSK-02-133\_13C  
13C Expt.  
File No:20101111\_11  
Sample Name:  
Data Collected on:  
wormhole-vmsr400  
Archive directory:  
Sample directory:  
FidFile: CARBON  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 11 2010



3m  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

118-NM-08-128-2  
File No: 20101111\_10

Sample Name:

Data Collected on:

Acquire directory:

Archive directory:

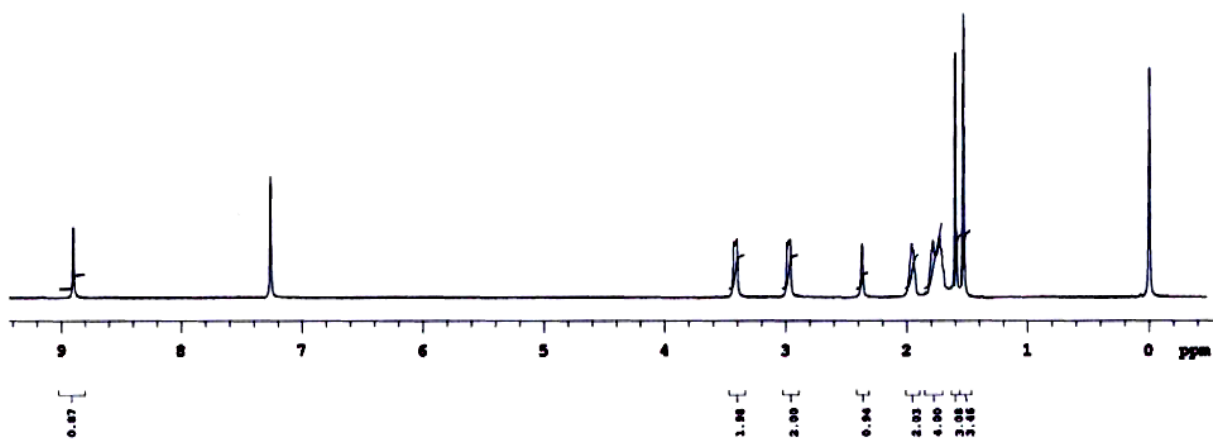
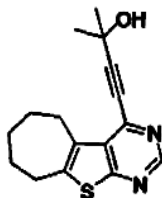
Sample directory:

Fidfile: PROTON

Pulse Sequence: PROTON (zgpg3)

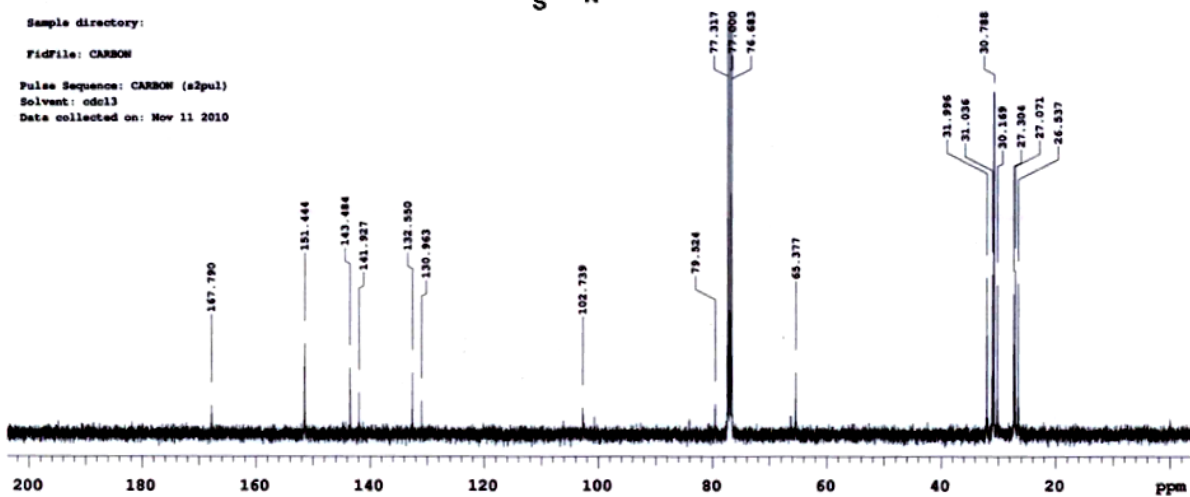
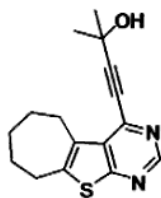
Solvent: cdcl3

Data collected on: Nov 11 2010

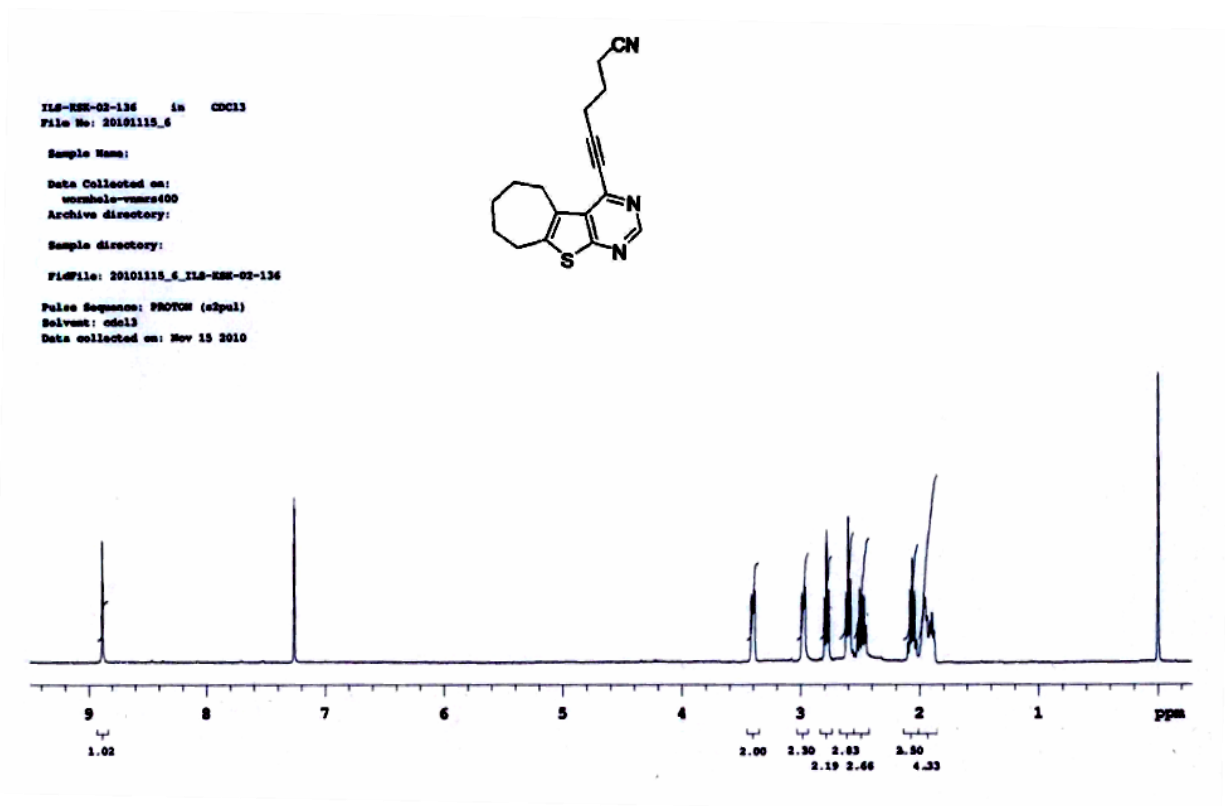


**3m**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

ILS-RSK-02-132(2) in  $\text{CDCl}_3$   
13C Expt.  
File No: 20101111\_17  
Sample Name:  
Data Collected on:  
wormhole-vnmr600  
Archive directory:  
Sample directory:  
FidFile: CARBON  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 11 2010



3n <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



3n <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)

ILS-RSR-02-136 in CDCl<sub>3</sub>  
13C Expt.  
File No: 20101115\_10  
Sample Name:  
Data Collected on:  
wormhole-vmars400  
Archive directory:  
Sample directory:  
FidFile: CARBON  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Nov 15 2010

