

Support information

One-pot Synthesis of 2-Amino-4(3*H*)-Quinazolinones via Ring-opening of Isatoic anhydride with amines and Palladium-catalyzed Oxidative Isocyanide-insertion

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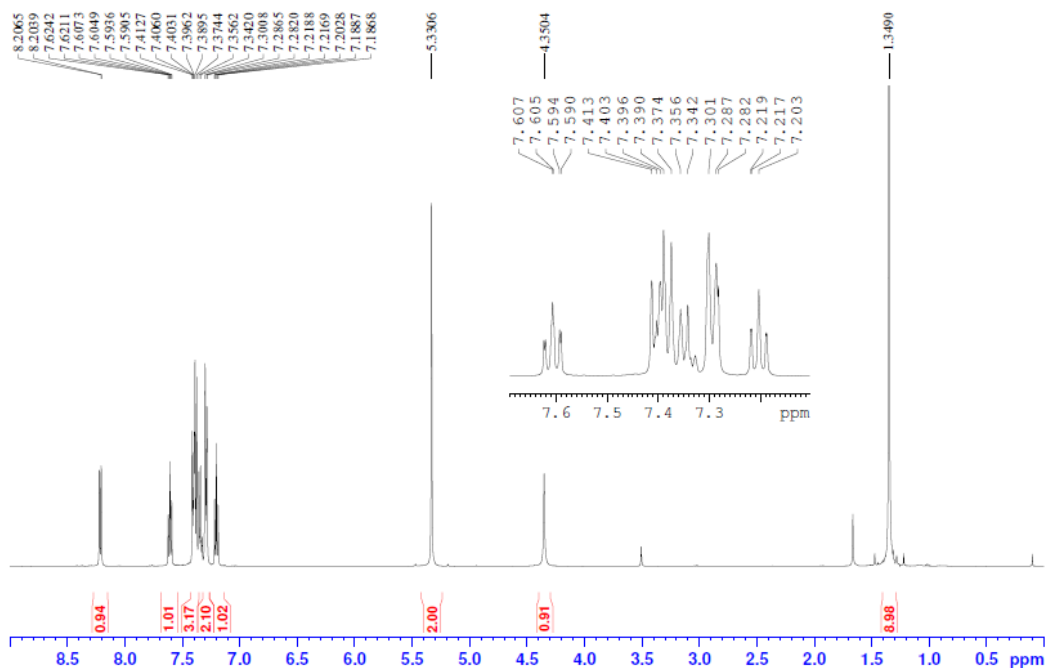
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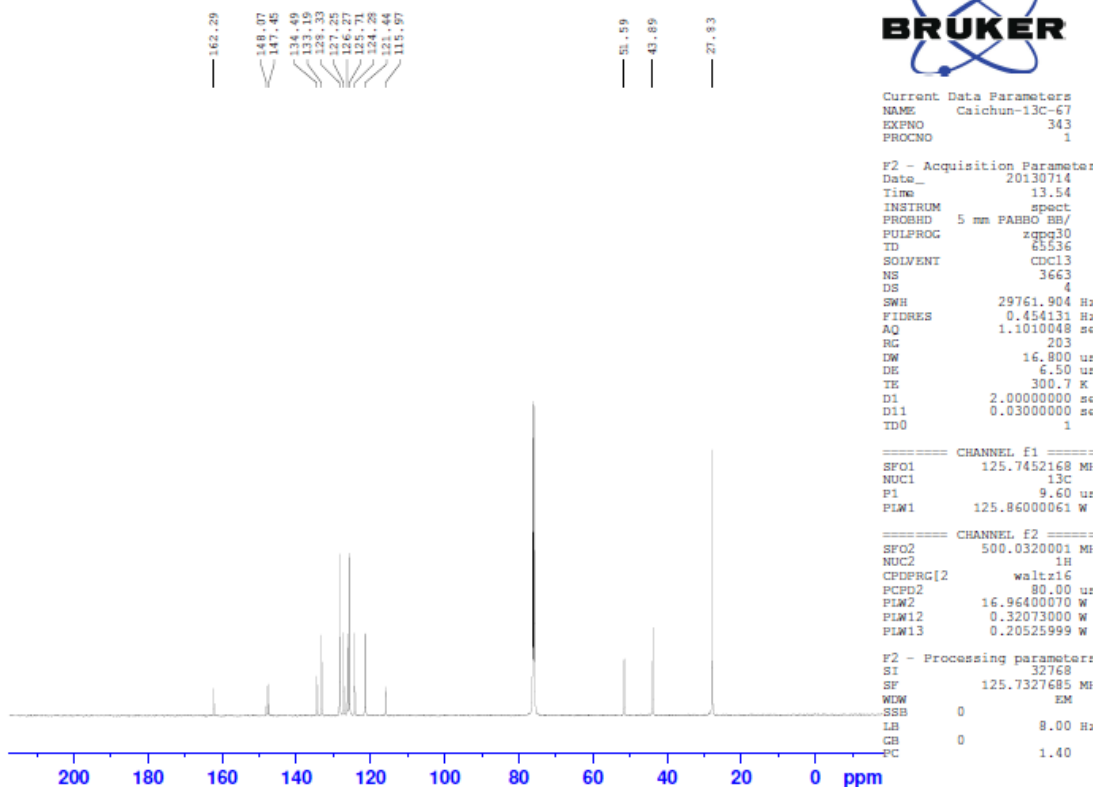
Copies of ¹H, ¹³C NMR

2013-07-13 1H-9 cdcl3 CC-1258 (JF-1 dianhongsuangan shudingjiyijing bianan)



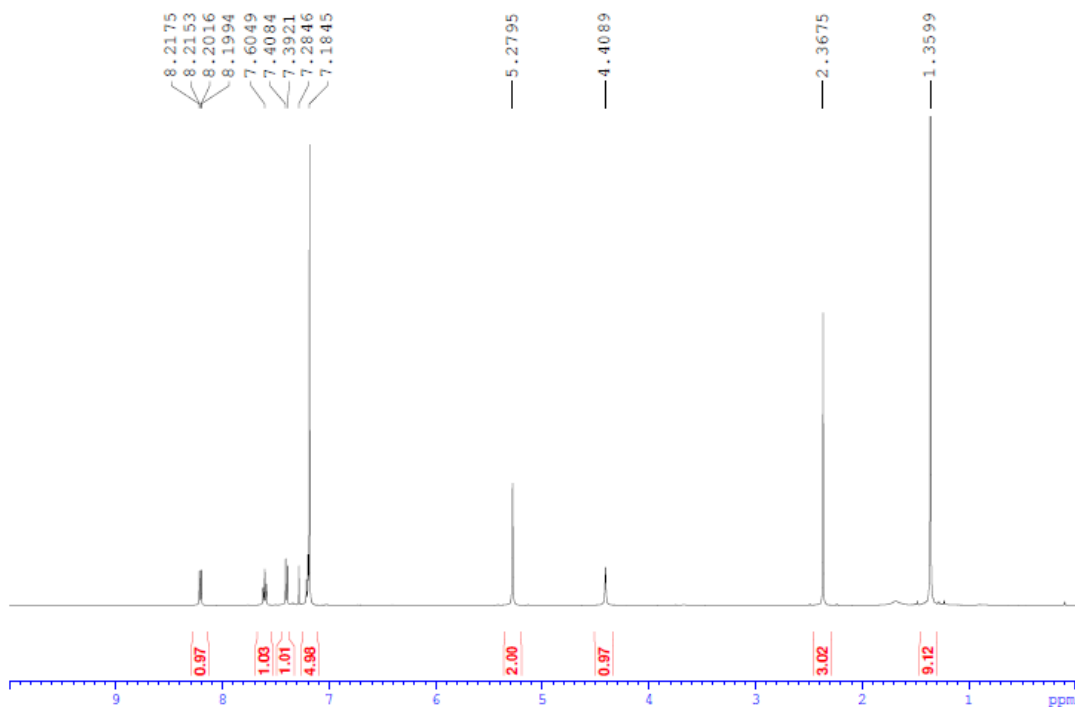
¹H NMR of compound 4a

2013-7-14 13C-1 cdcl3 CC-343 (jF-1 dianhongsuangan bianan shudingjiyijing)



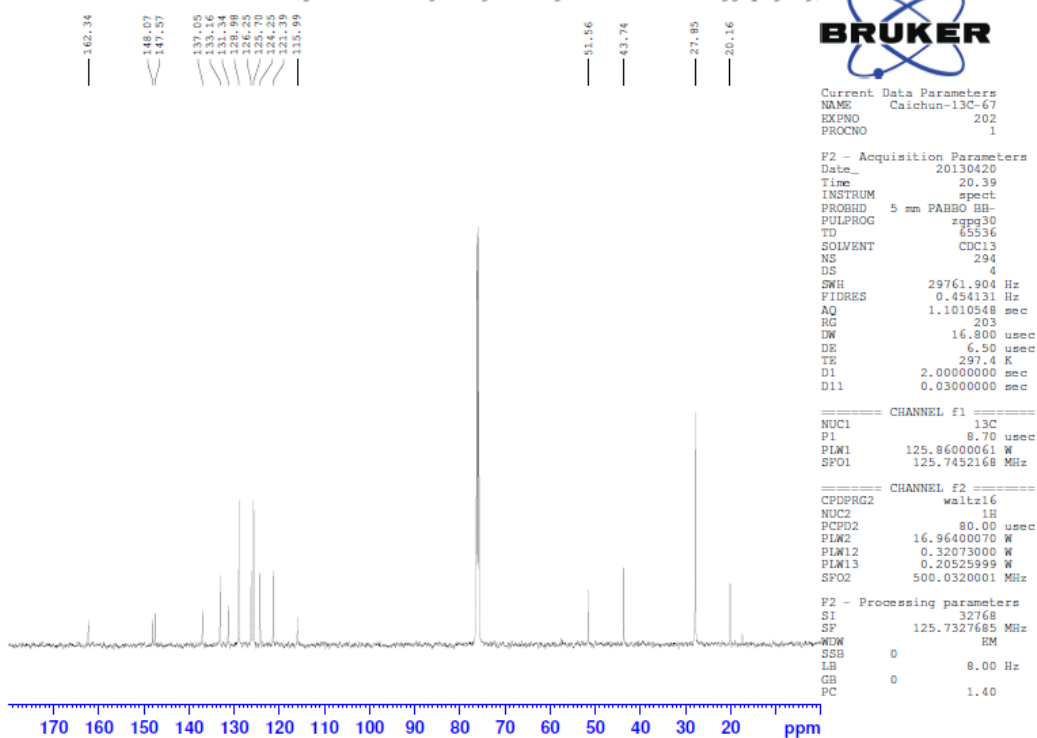
¹³C NMR of compound 4a

2013-3-18 1H-2 CDCL3 CC-33(JF-2)



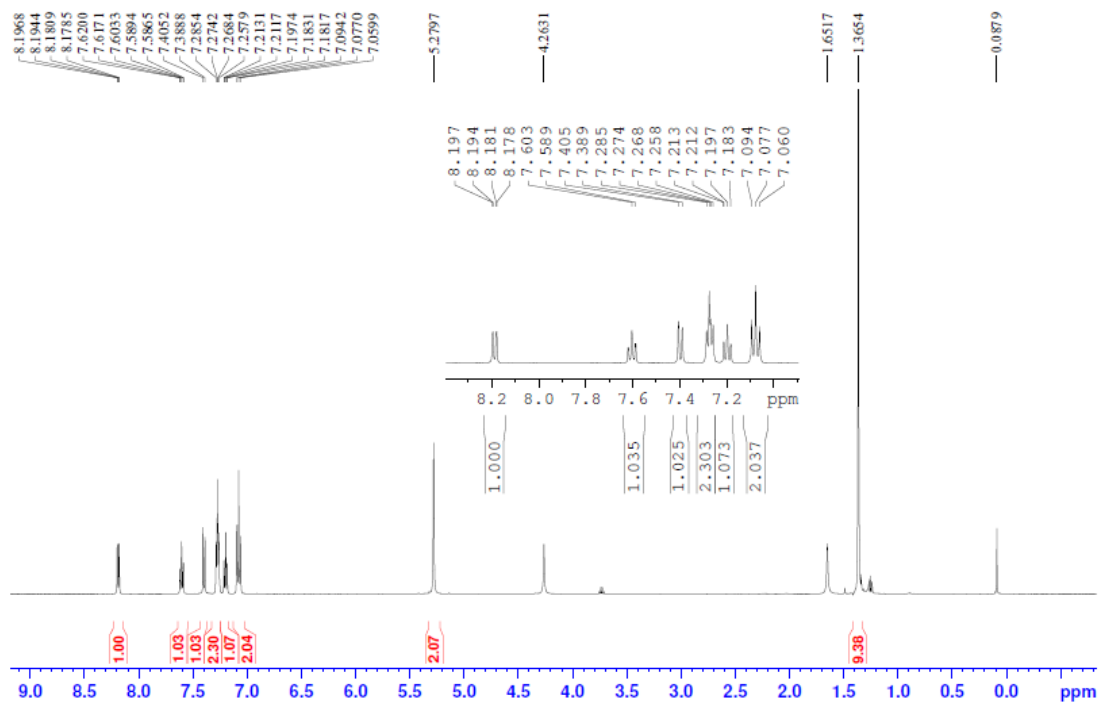
¹H NMR of compound **4b**

2013-4-20 13C-5 dms0 CC-202(jf-2 dianhongsuangan duijiabianan shudingjiyijing)



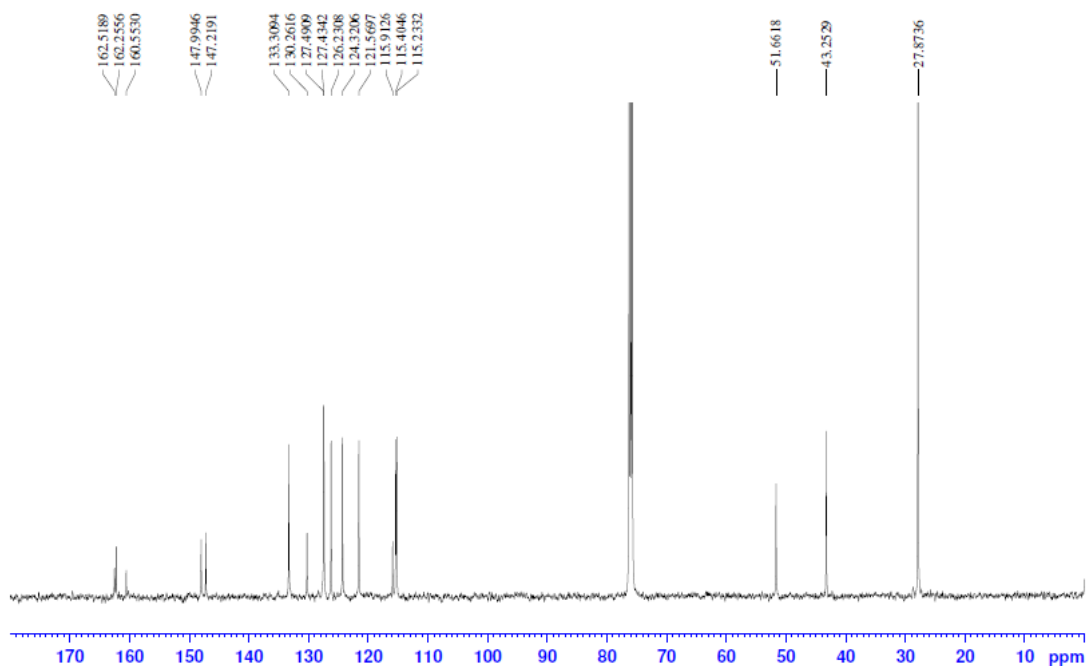
¹³C NMR of compound **4b**

2013-07-23 1H-4 CDCL3 CC-1319 (JF)



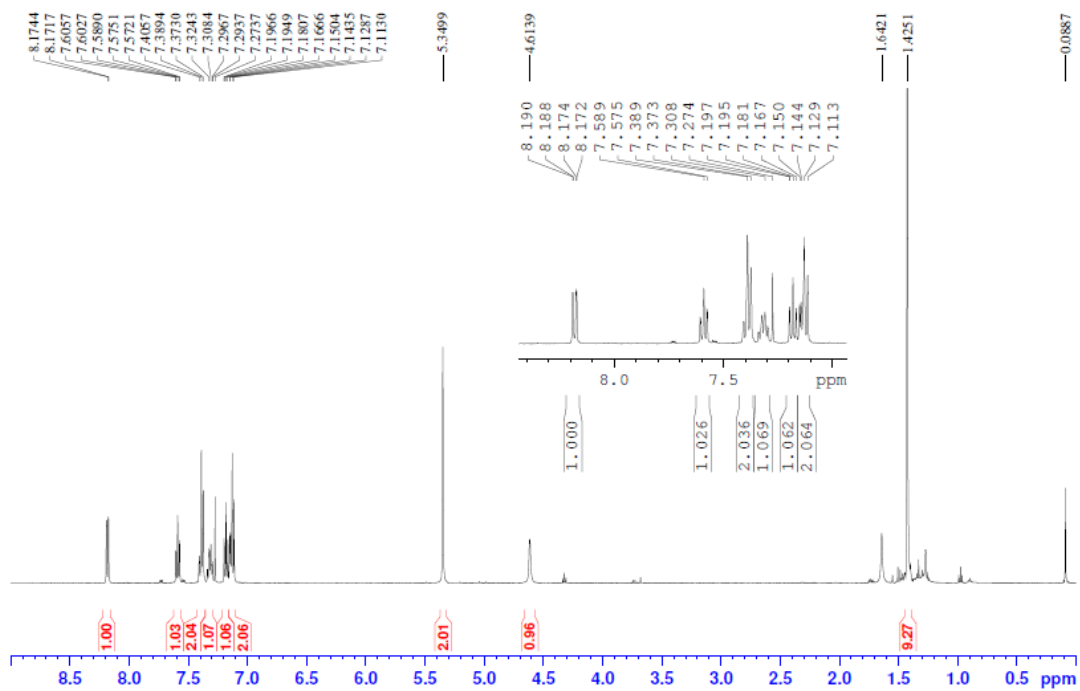
¹H NMR of compound 4c

2013-7-23 13C-2 cdcl3 CC-365 (jf-duifubianan+shudingjiyijing+dianhongsuangan)



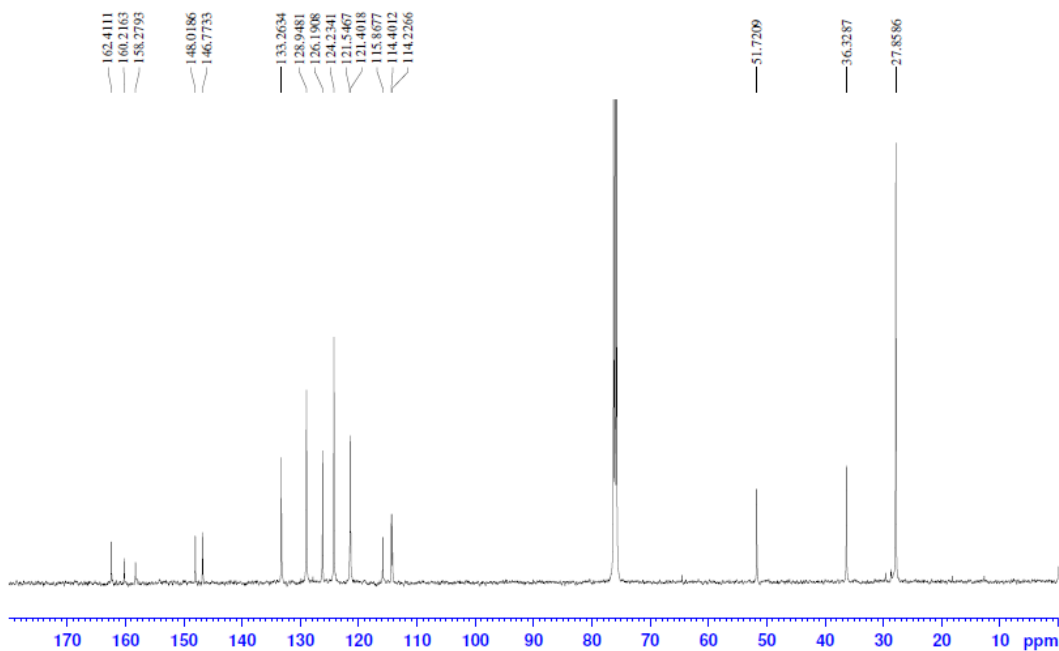
¹³C NMR of compound 4c

2013-07-23 1H-3 CDCL3 CC-1318 (JF-LINFU)



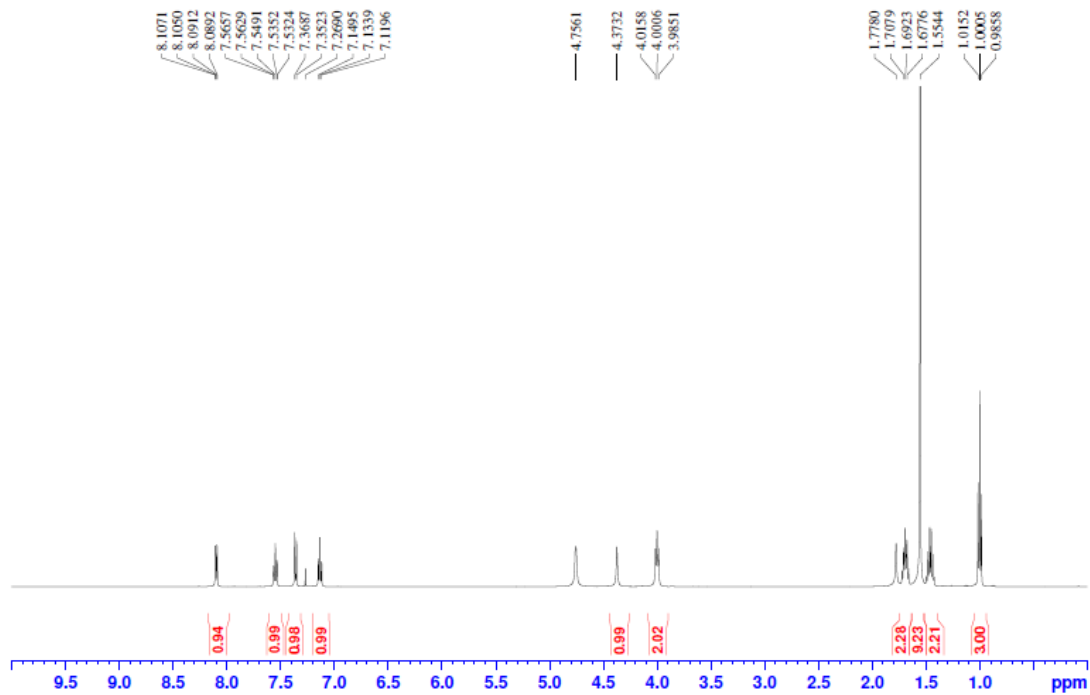
¹H NMR of compound **4d**

2013-7-24 13C-4 cdc13 CC-370 (jf)



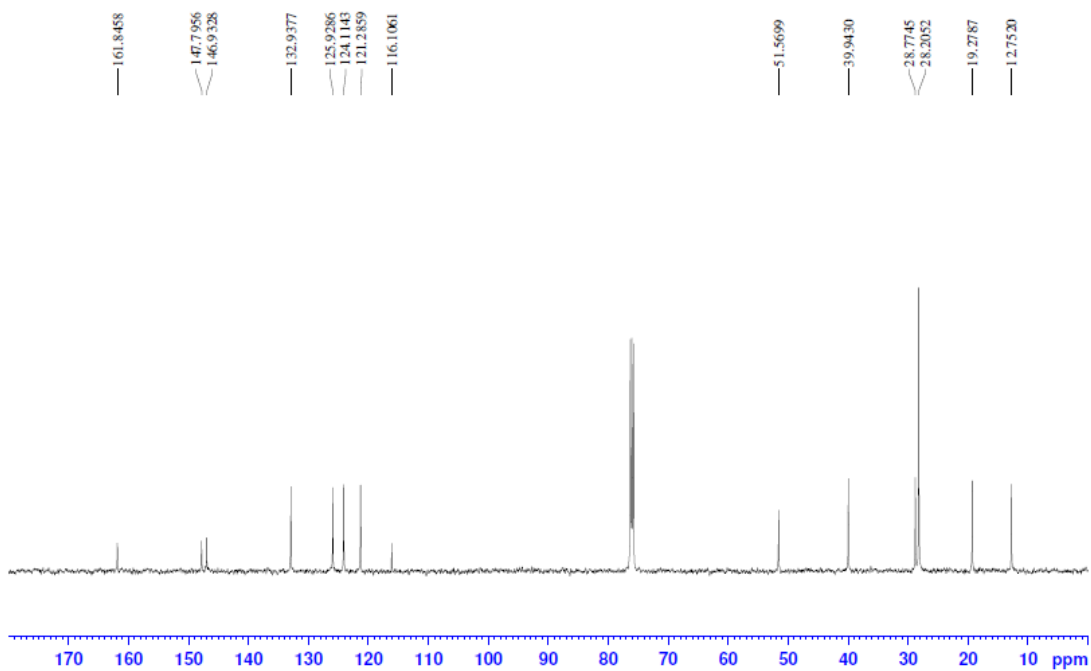
¹³C NMR of compound **4d**

2013-08-22 1H-5 CDCL3 CC-1359 (JF-1)



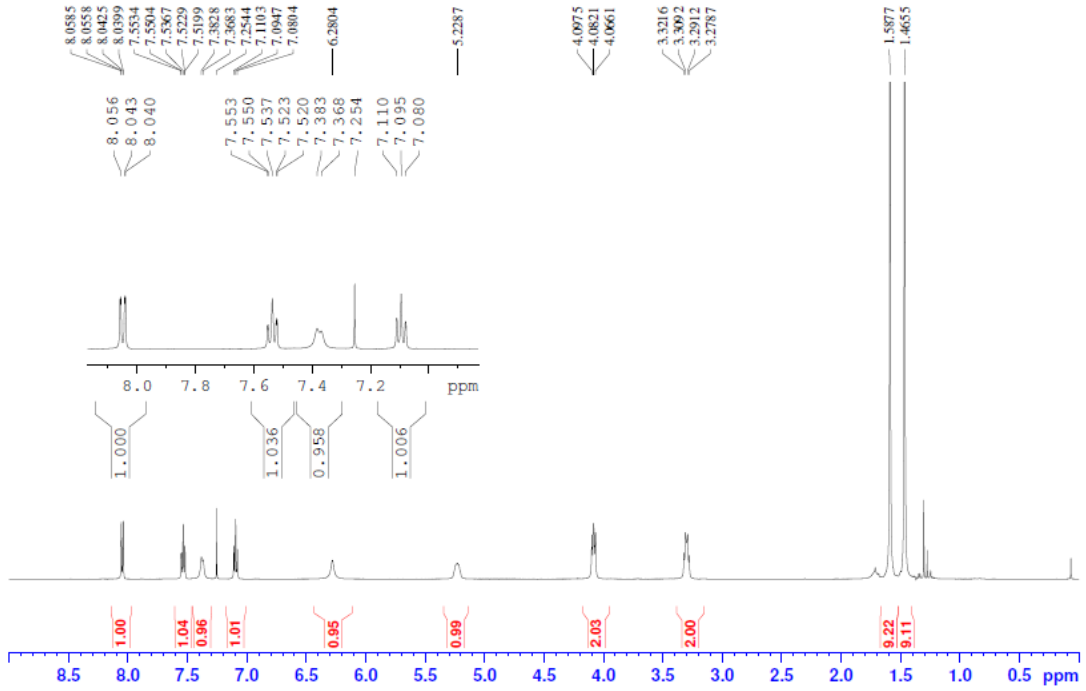
¹H NMR of compound **4e**

2013-8-22 13C-3 CDCL3 CC-389 (JF-1)



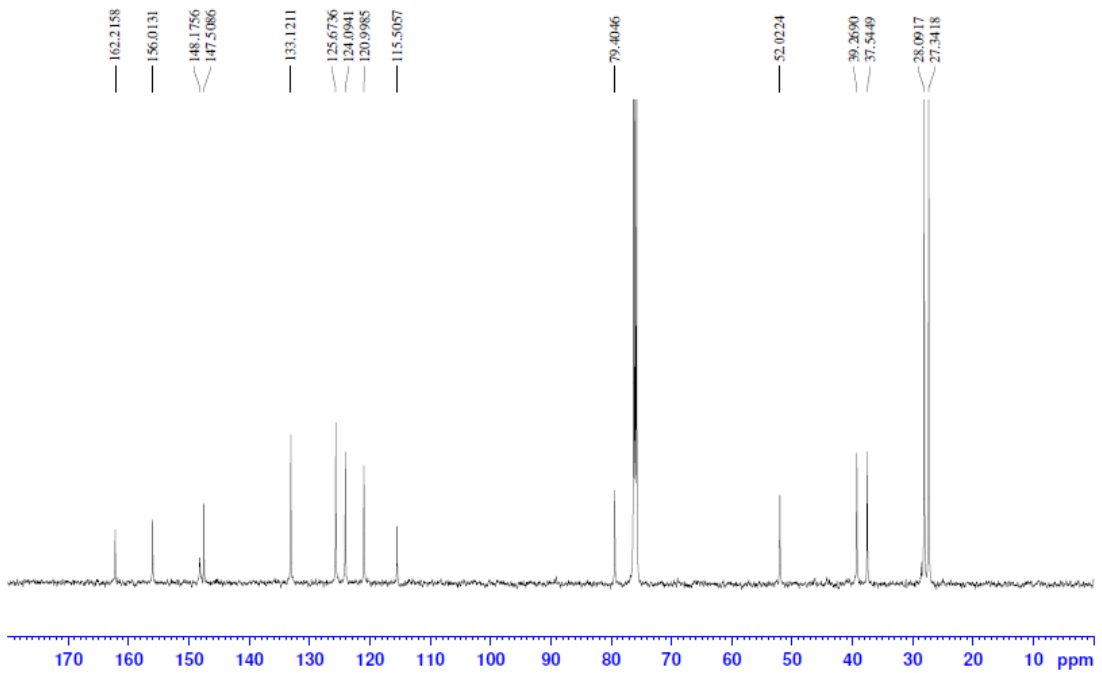
¹³C NMR of compound **4e**

2013-10-20 1H-11 CDCL3 CC-1573 (JF-3 dianhongsuangan Boc-yieran shudingjiyijing)



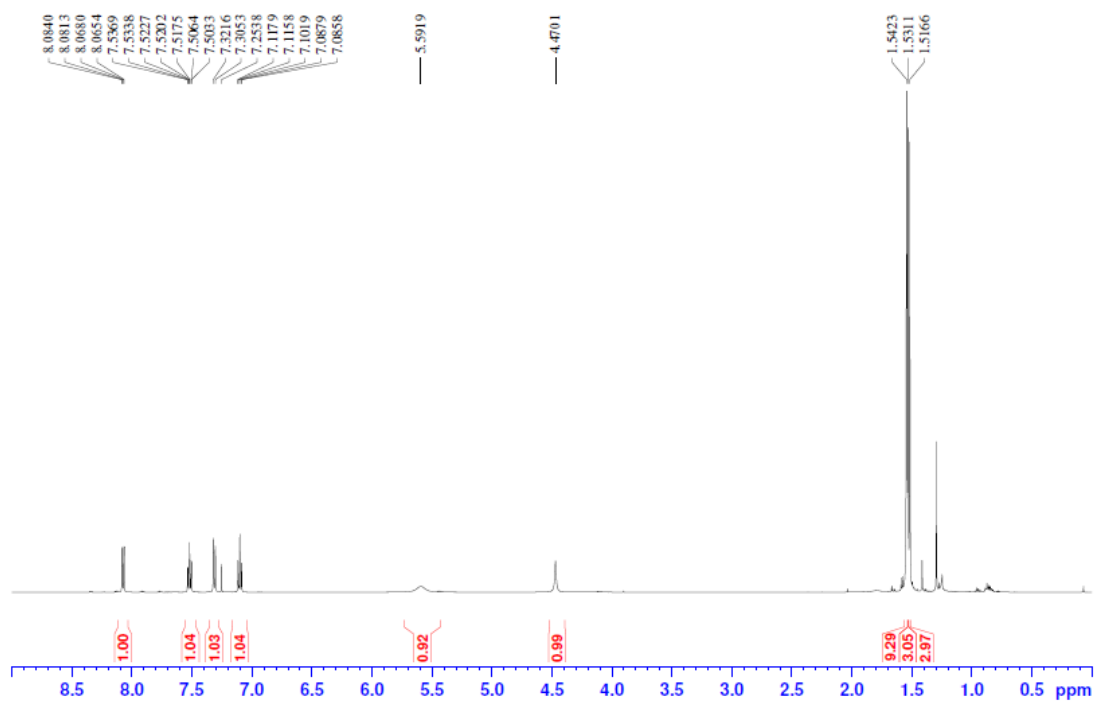
¹H NMR of compound **4f**

2013-10-20 13C-4 cdcl3 CC-467 (jf-2 dianhongsuangan bocyieran shudingjiyijing)



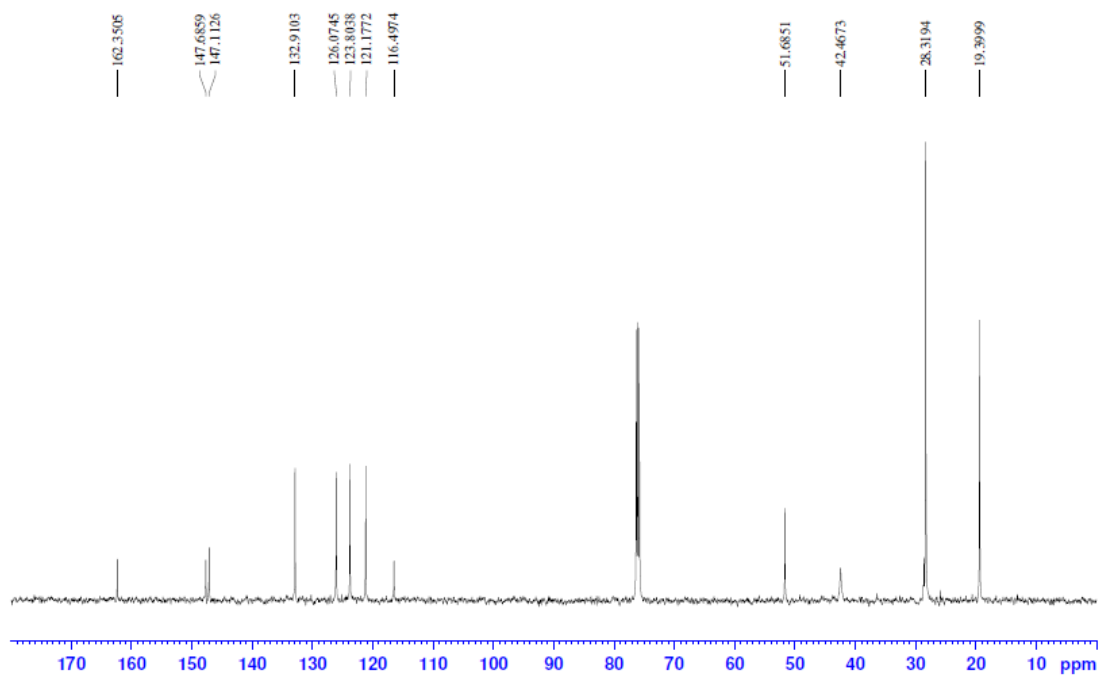
¹³C NMR of compound **4f**

2013-10-20 1H-9 CDCL3 CC-1571 (JF-1 YIBINGAN)



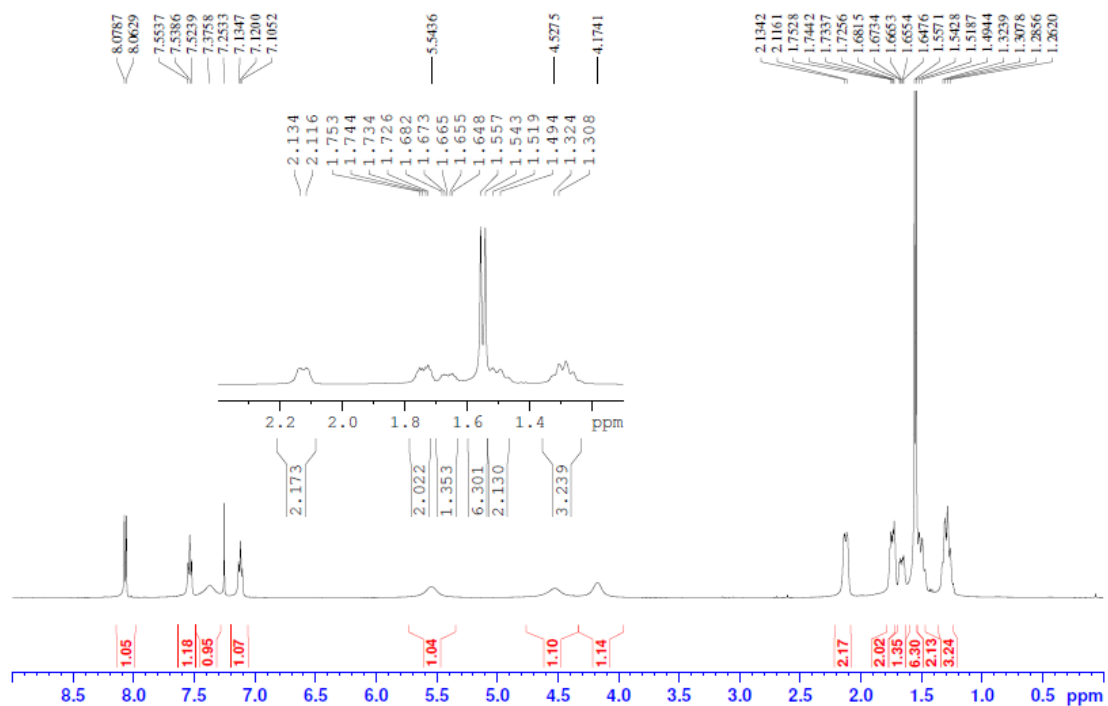
¹H NMR of compound **4g**

2013-10-20 13C-3 cdcl3 CC-466 (jf-1 dianhongsuangan yibingan shudingjiyijing)



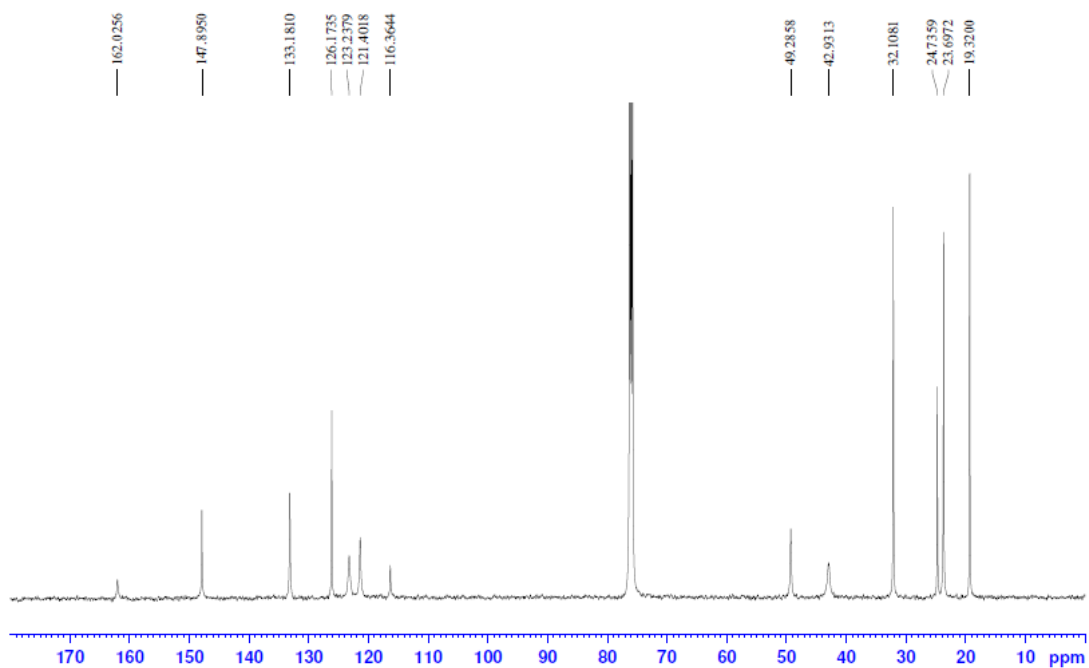
¹³C NMR of compound **4g**

2013-10-26 1H-25 CDCL3 CC-1617(JF yibingan dianhongsuangan huanjijiyijing)



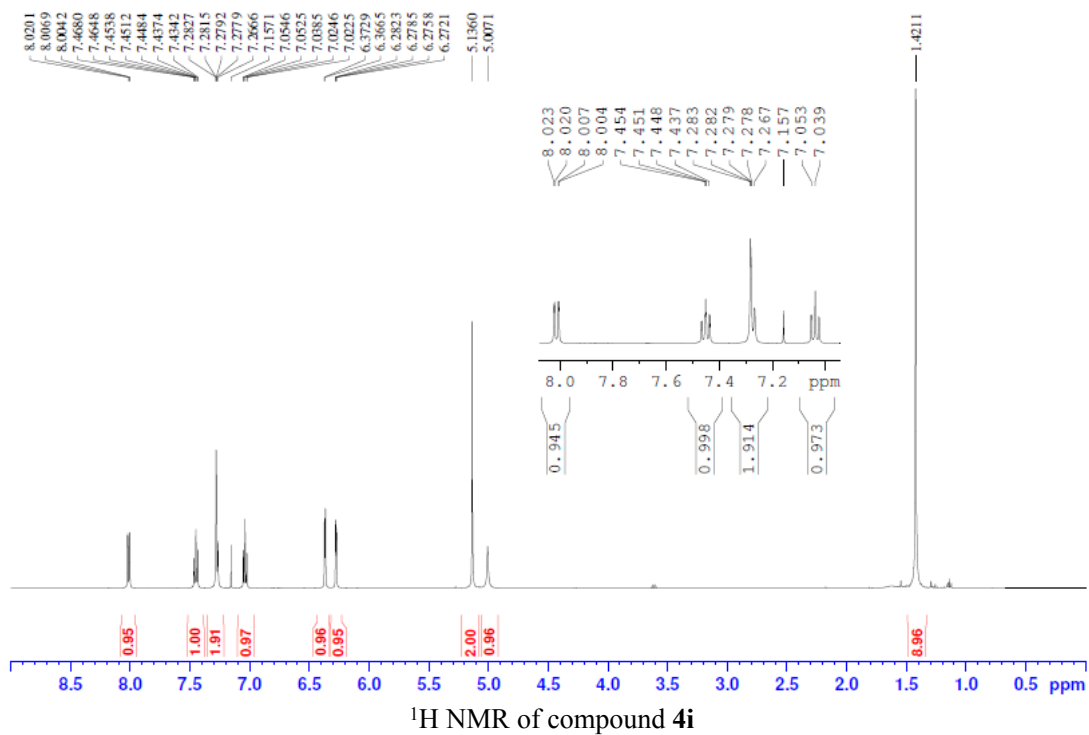
¹H NMR of compound **4h**

2013-10-26 13C-5 cdc13 CC-477 (jf-1 dianhongsuangan yibingan huanjijiyijing)



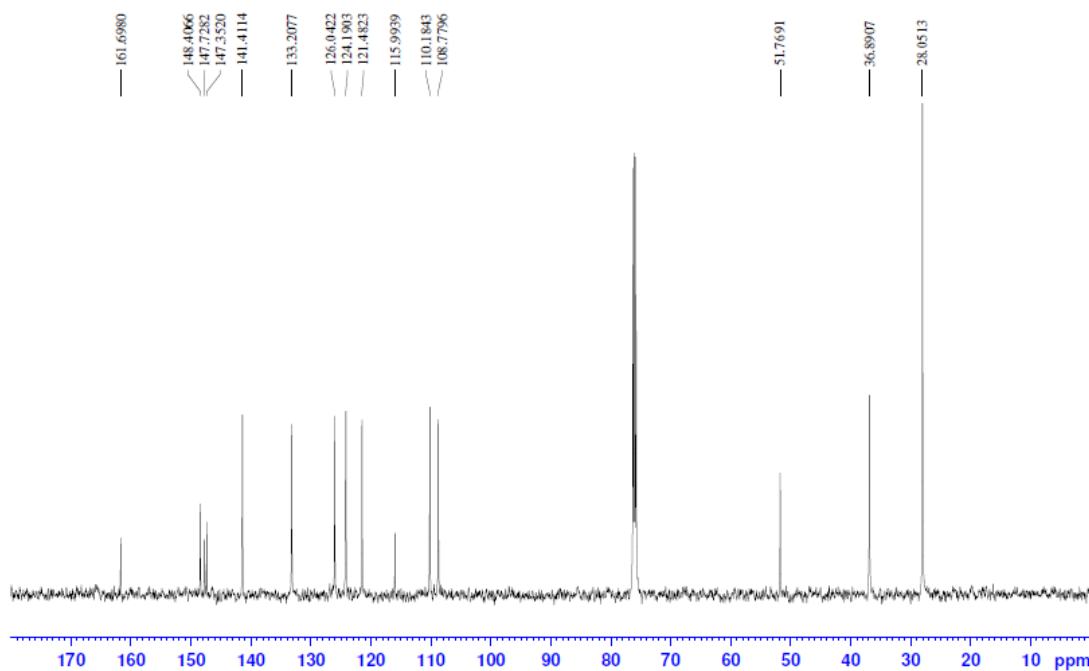
¹³C NMR of compound **4h**

2013-10-19 1H-15 CDCL3 CC-1558 (JF DIANHONGSUANGAN KANGAN SHUDINGJIYIJING)



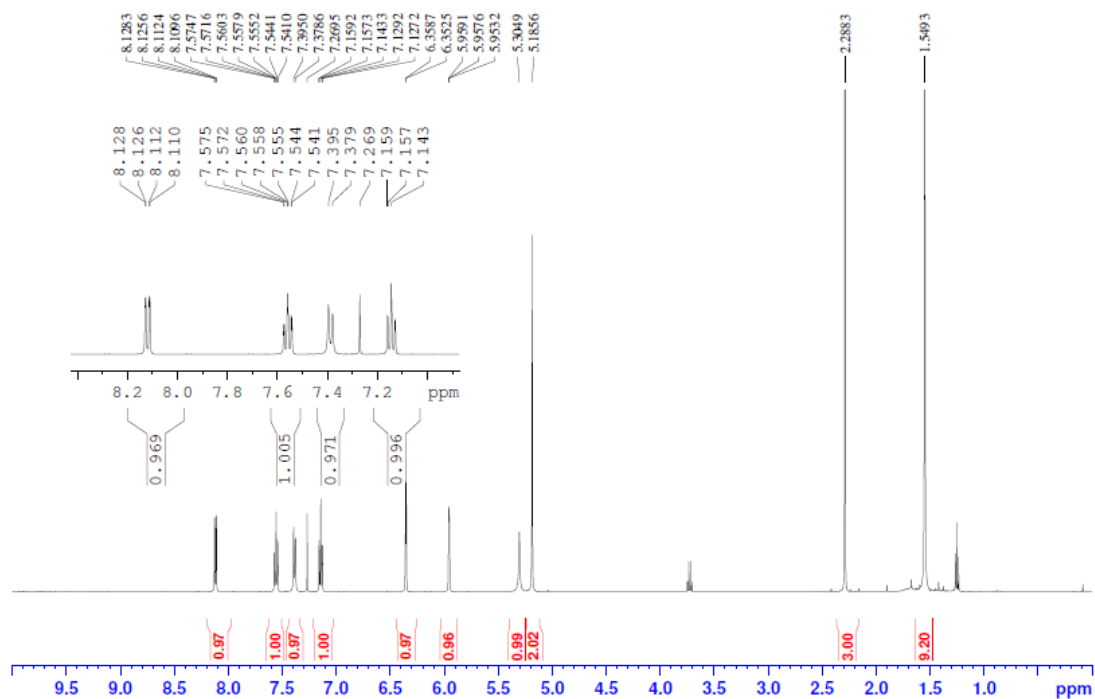
¹H NMR of compound **4i**

2013-10-19 13C-6 CDCL3 CC-454 (jf-2 dianhongsuangan kangan shudingjiyijing)



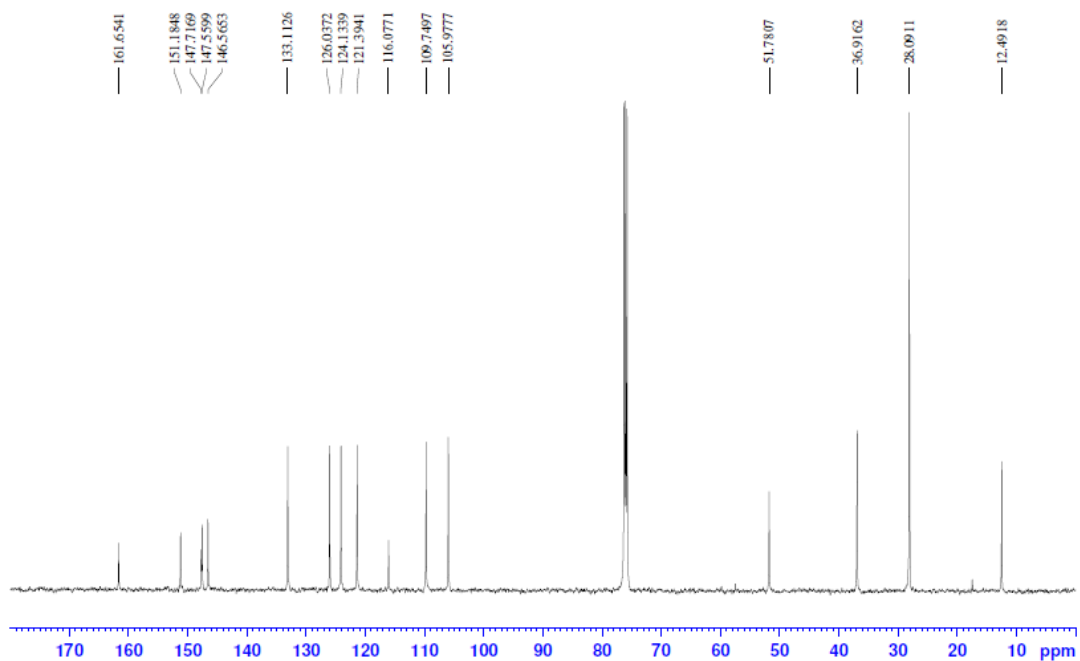
¹³C NMR of compound **4i**

2013-10-12 1H-30 CDCL3 CC-1502 (jf-1 2-jiajikangan dianhongsuangan shudingjiyijing)



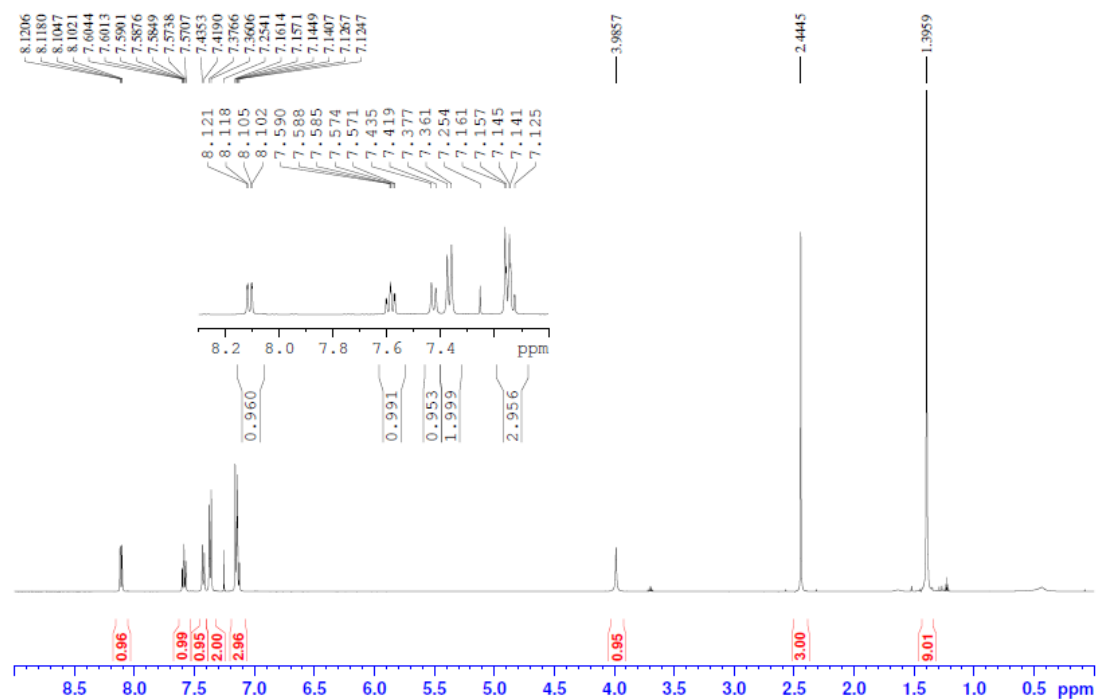
¹H NMR of compound **4j**

2013-10-12 13C-8 CDCL3 CC-436 (jf-1 2jiajikangan dianhongsuangan shudingjiyijing)



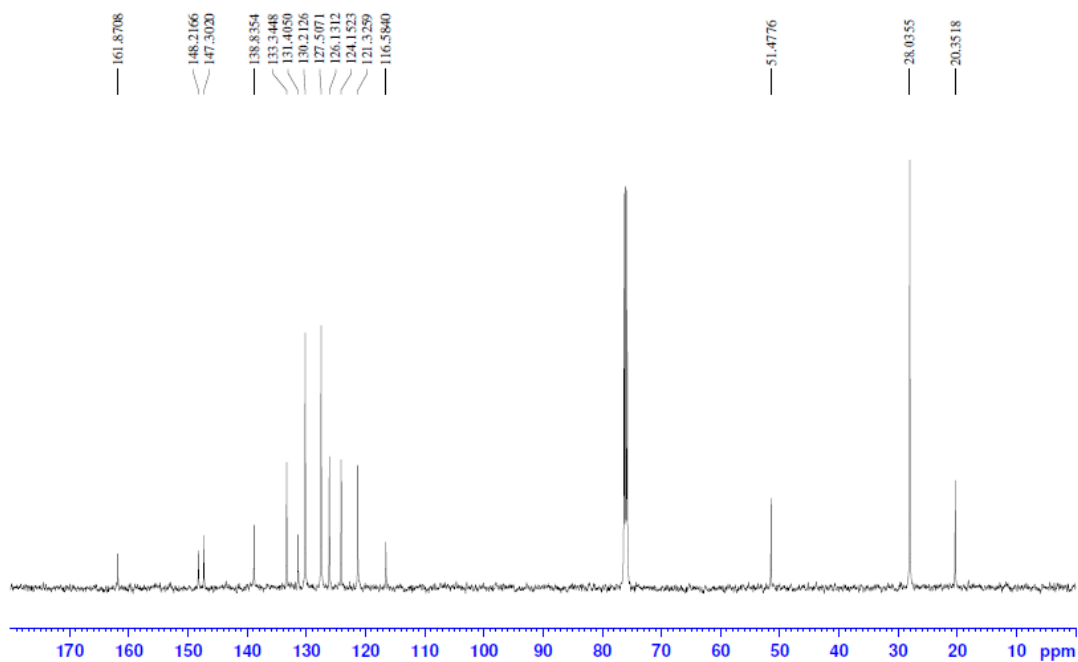
¹³C NMR of compound **4j**

2013-10-26 1H-23 CDCL3 CC-1615 (JF duijiabenan dianhongsuangan shudingjiyijing)



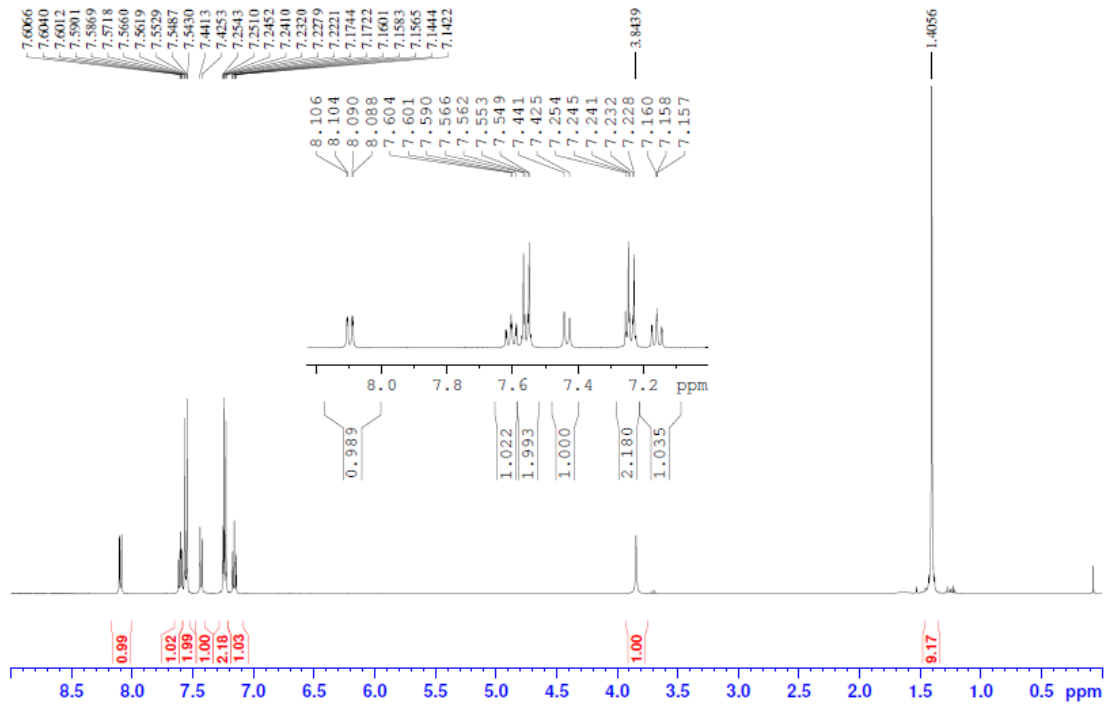
^1H NMR of compound **4k**

2013-10-26 13C-11 cdcl3 CC-484 (jf-3 dianhongsuangan duijiabenan shudingjiyijing)



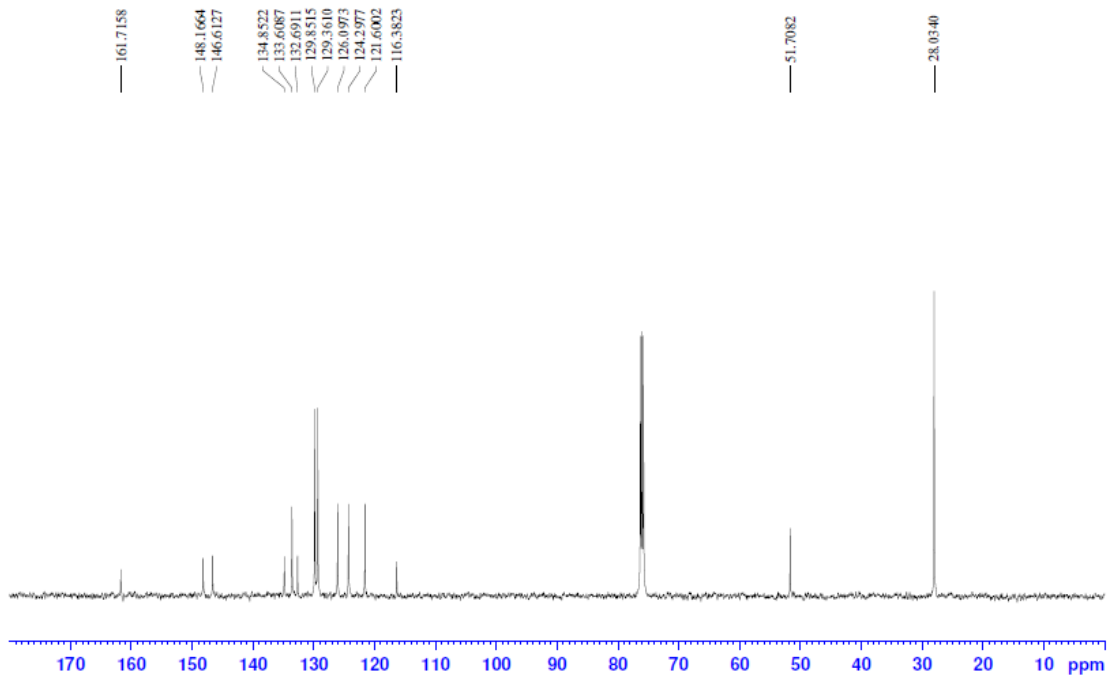
^{13}C NMR of compound **4k**

2013-11-10 1H-1 CDCL3 CC-1755 (JF-DUILVBENAN)



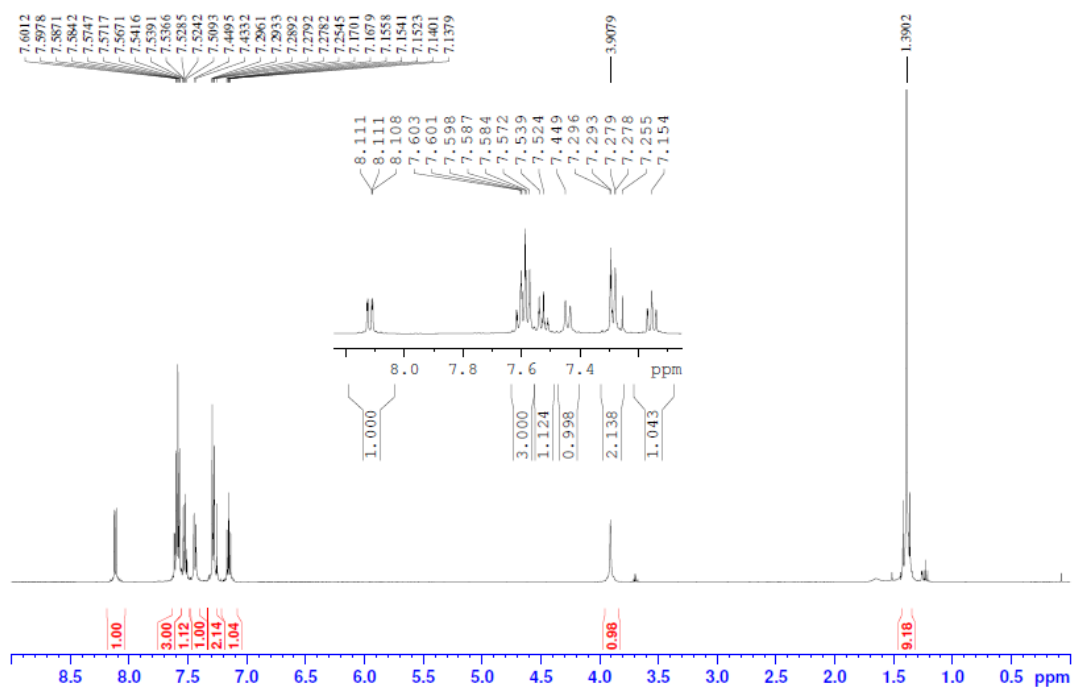
¹H NMR of compound **4I**

2013-11-10 13C-1 CDCL3 CC-511 (jf-duilvbenan)



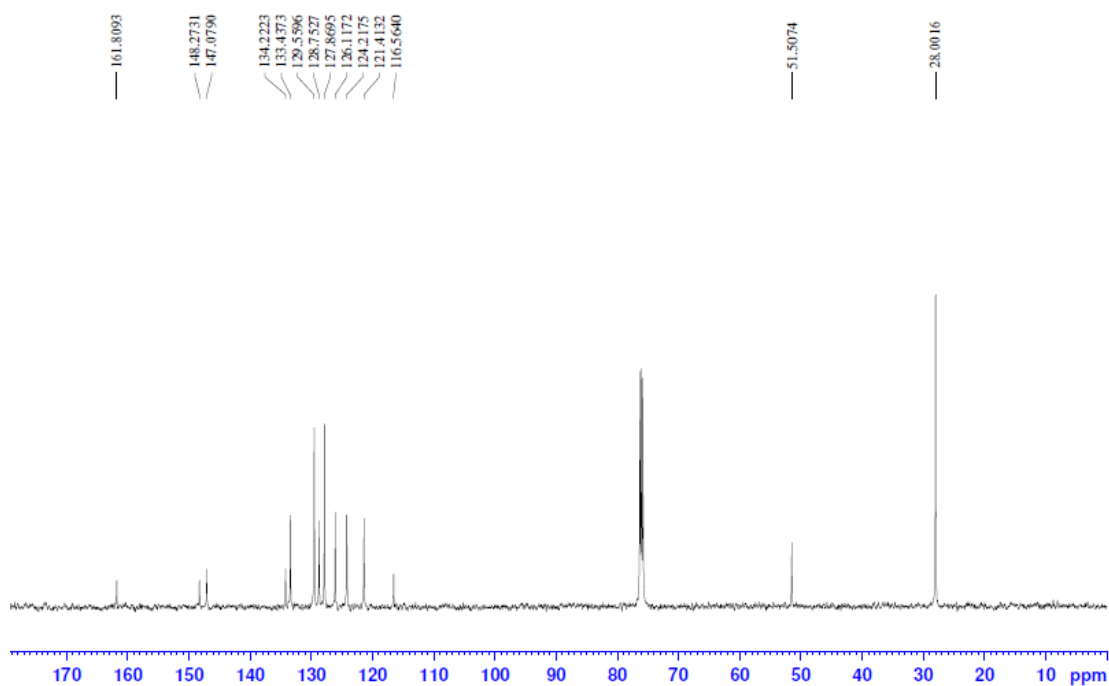
¹³C NMR of compound **4I**

2013-11-24 1H-18 CDCL3 CC-1868 (JF-1)



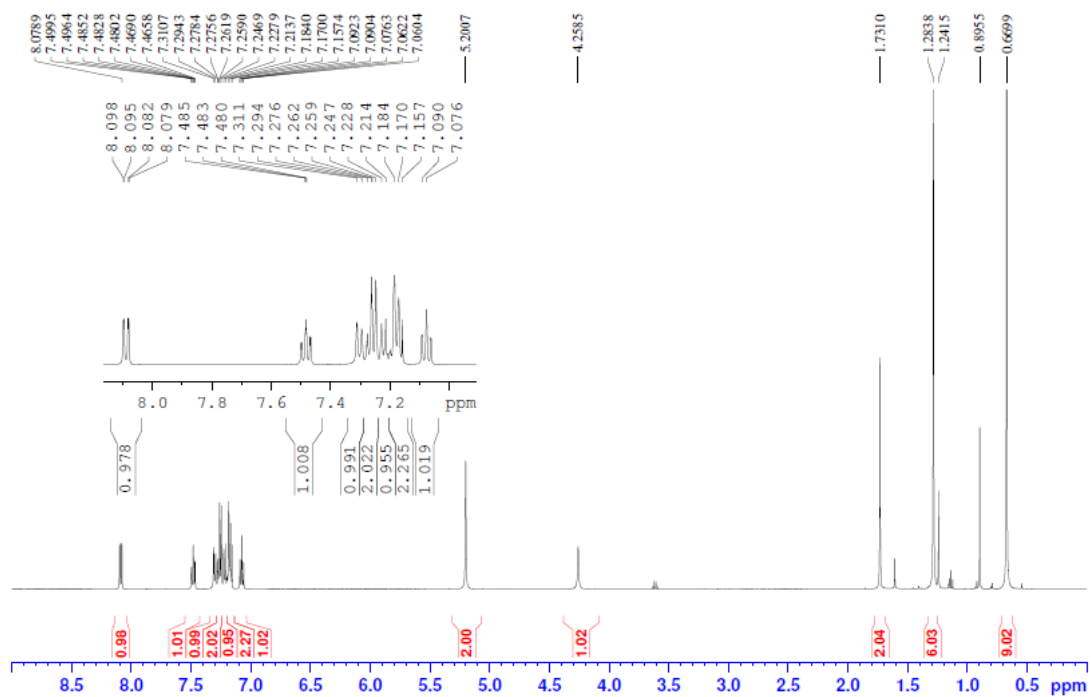
¹H NMR of compound **4m**

2013-11-24 13C-5 CDCL3 CC-551 (jF-2 dianhongsuangan benan shudingjiyijing)



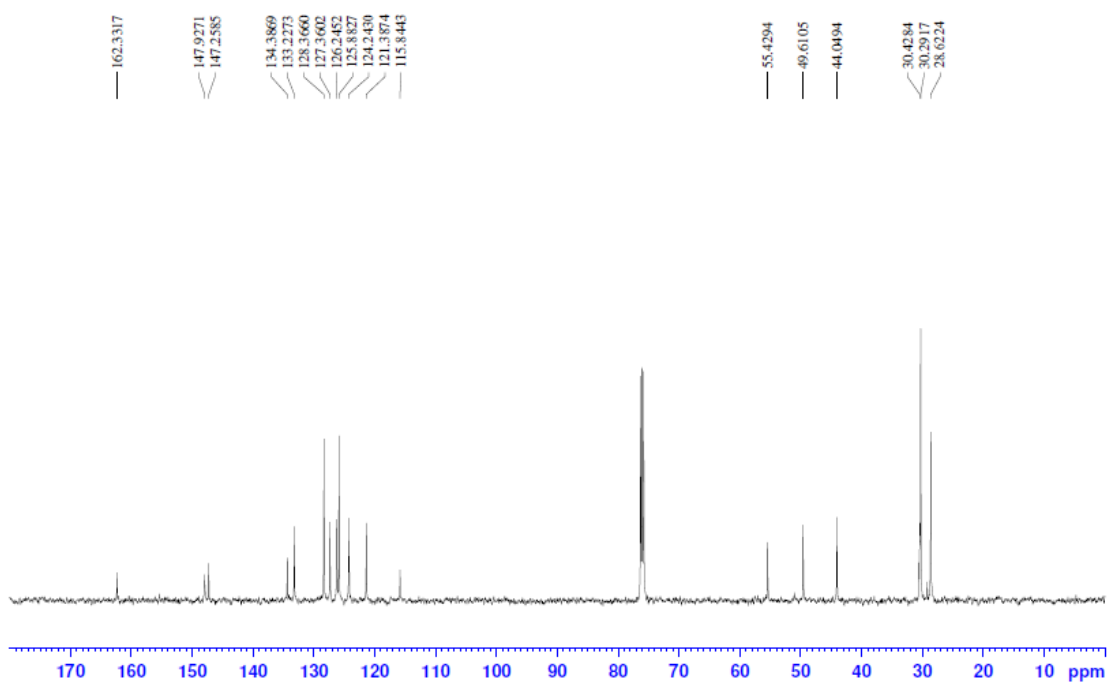
¹³C NMR of compound **4m**

2013-10-19 1H-16 CDCL3 CC-1559 (JF DIANHONGSUANGAN BIANAN 1,1,3,3-SHUDINGJIYIJING)



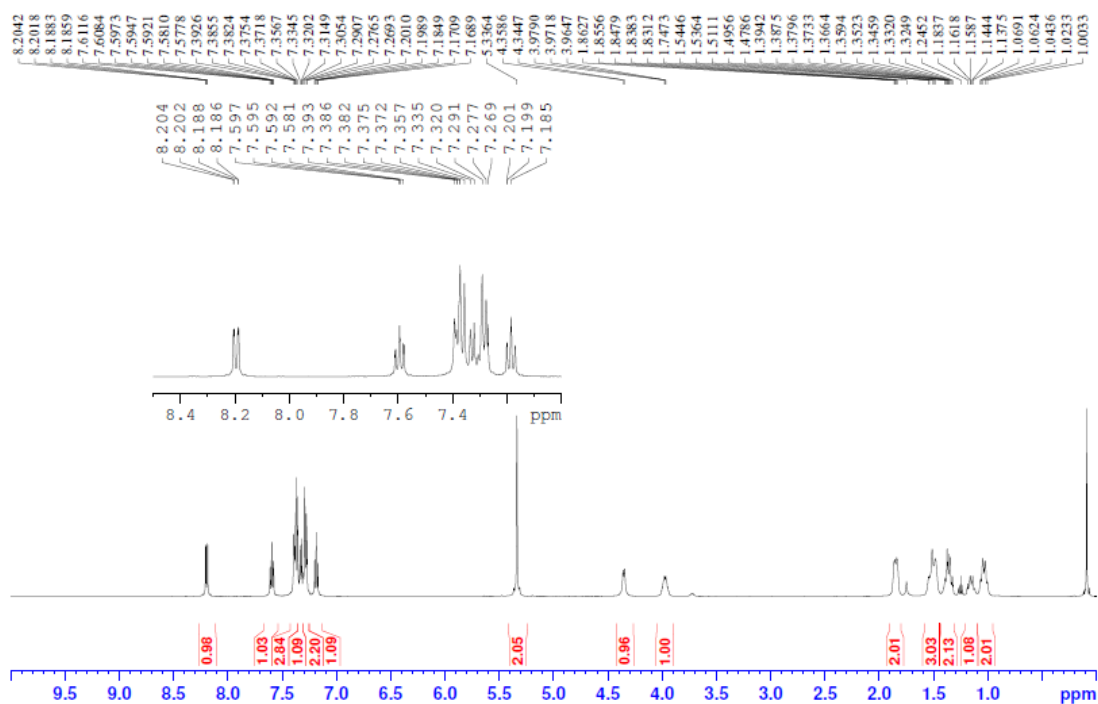
¹H NMR of compound **4n**

2013-10-19 13C-5 CDCL3 CC-453 (jf-1 dianhongsuangan bianan 1,1,3,3-sijiajizhengdingjiyi)



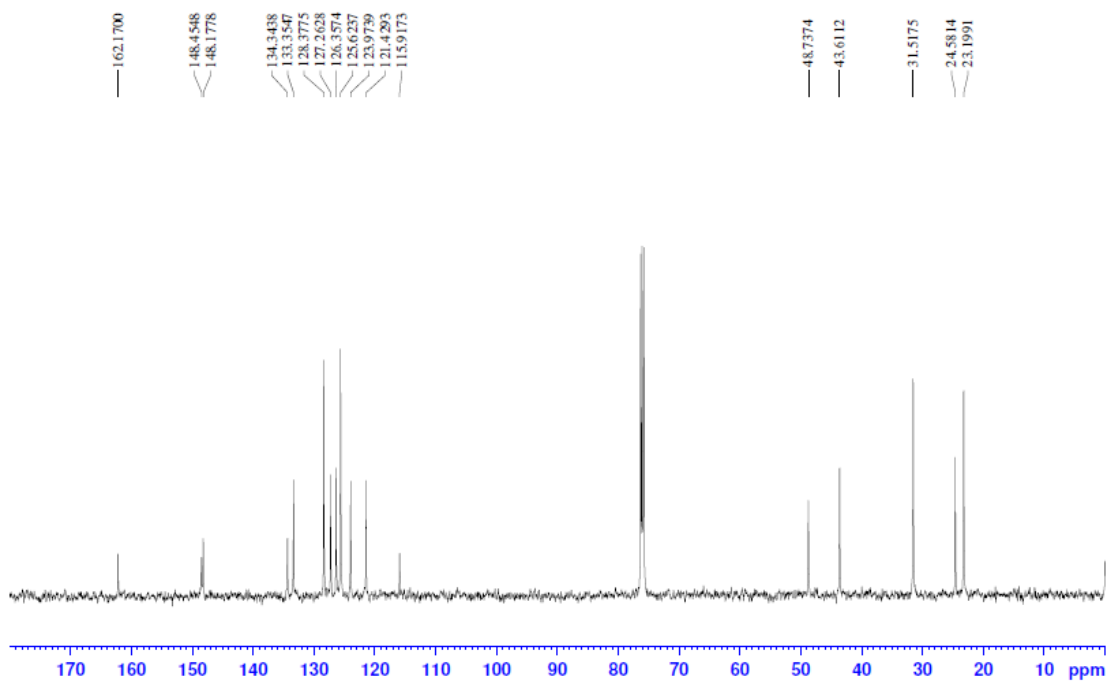
¹³C NMR of compound **4n**

2013-08-31 1H-9 CDCL3 CC-1380 (JF-1 DIANHONGSUANGAN BIANAN SHUDINGJIYIJING)



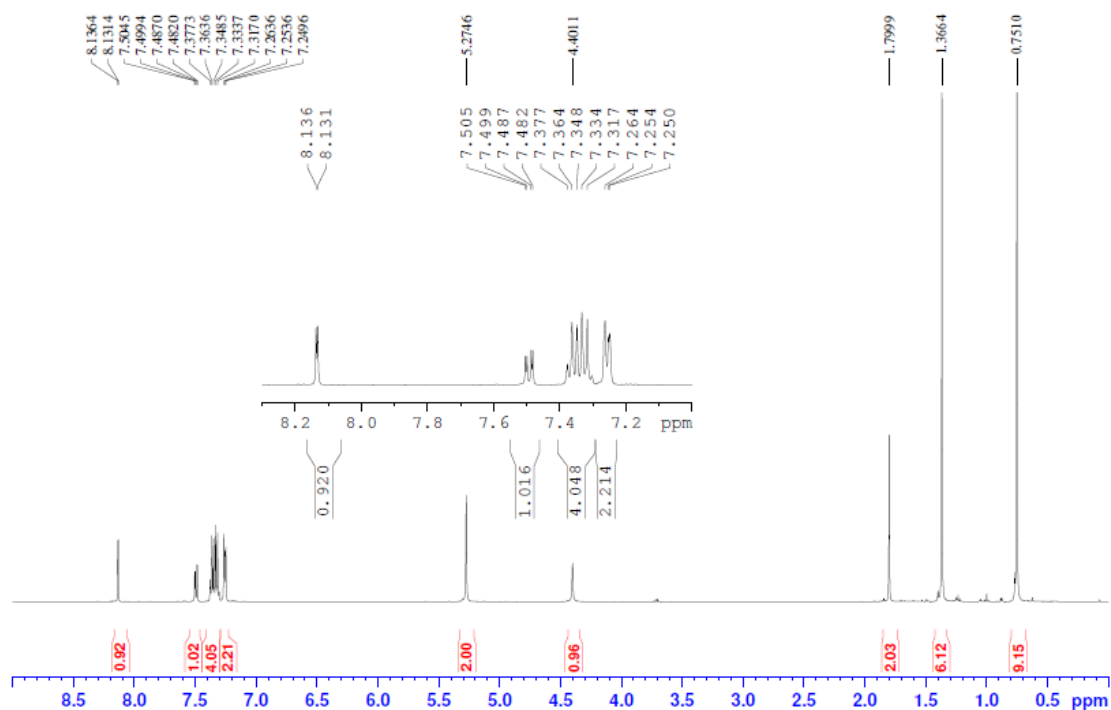
¹H NMR of compound **4o**

2013-8-31 13C-5 CDCL3 CC-397 (JF-1 DIANHONGSUANGAN BIANAN HUANJJIYIJING)



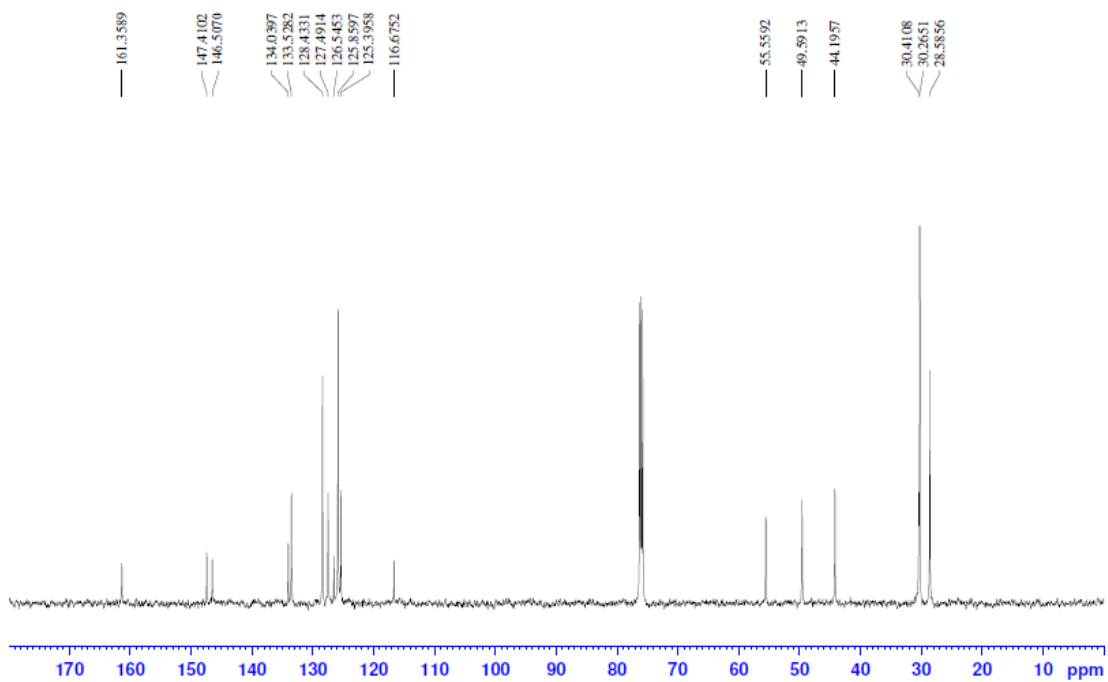
¹³C NMR of compound **4o**

2013-10-26 1H-26 CDCL3 CC-1618(JF bianan dianhongsuangan xinxingyijing)



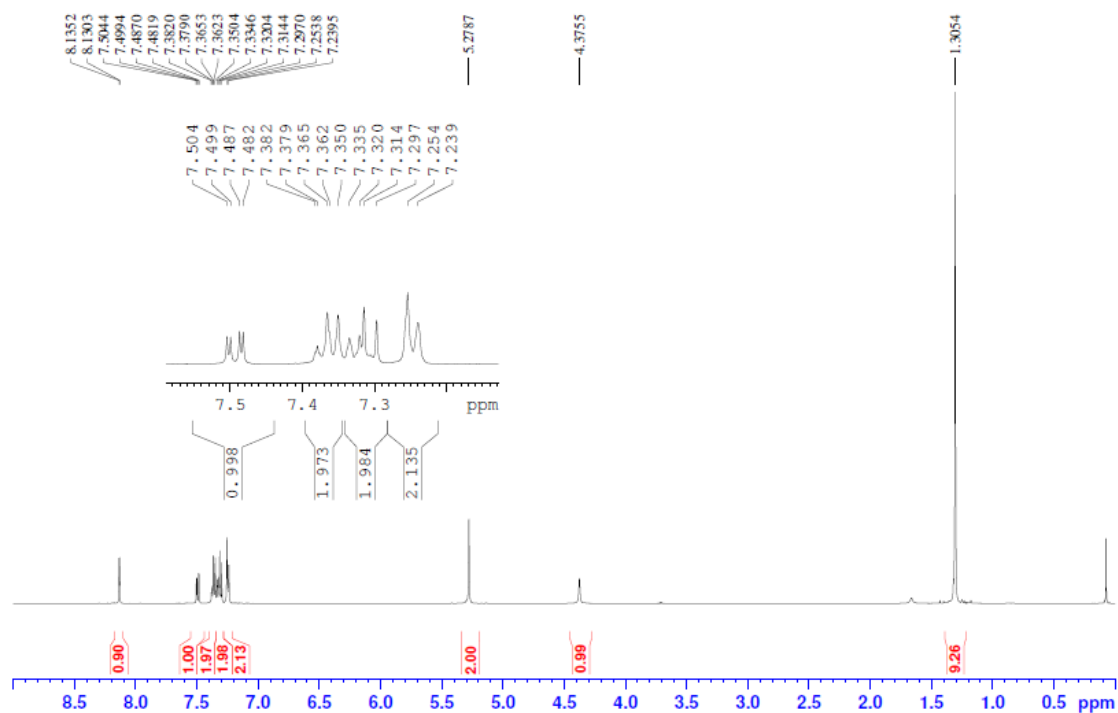
^1H NMR of compound **4p**

2013-10-26 13C-4 cdcl3 CC-476 (jf-1 5-1vdianhongsuangan bianan xinxingyijing)



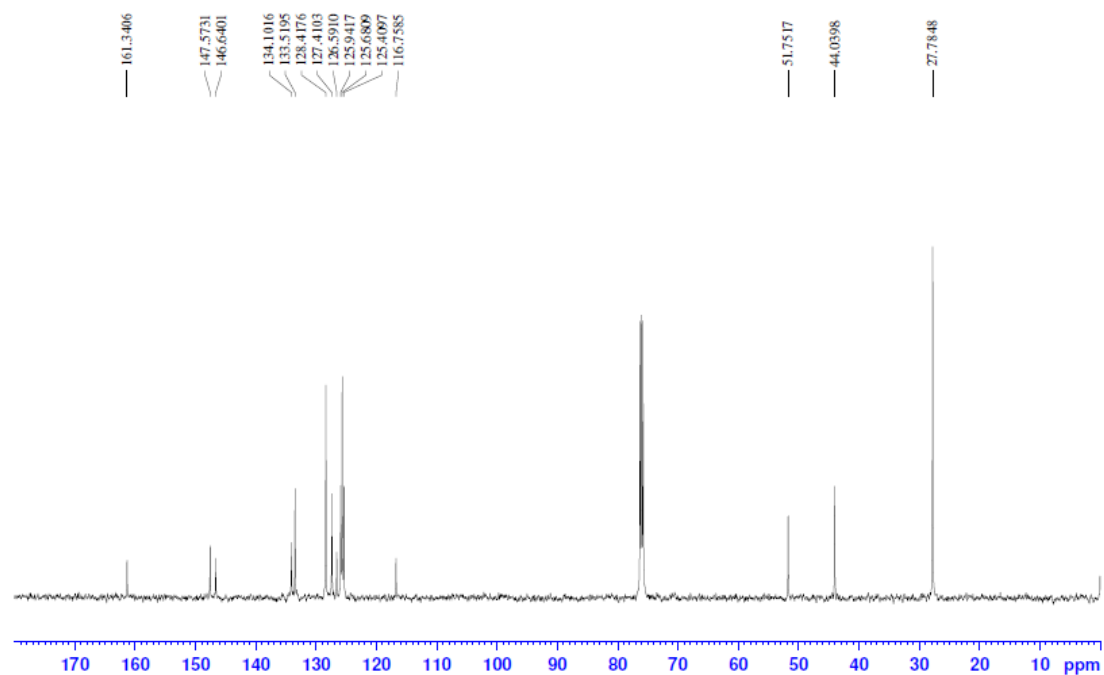
^{13}C NMR of compound **4p**

2013-10-20 1H-10 CDCL3 CC-1572 (JF-2 5-lvdianhongsuangan bianan shudingjiyijing)



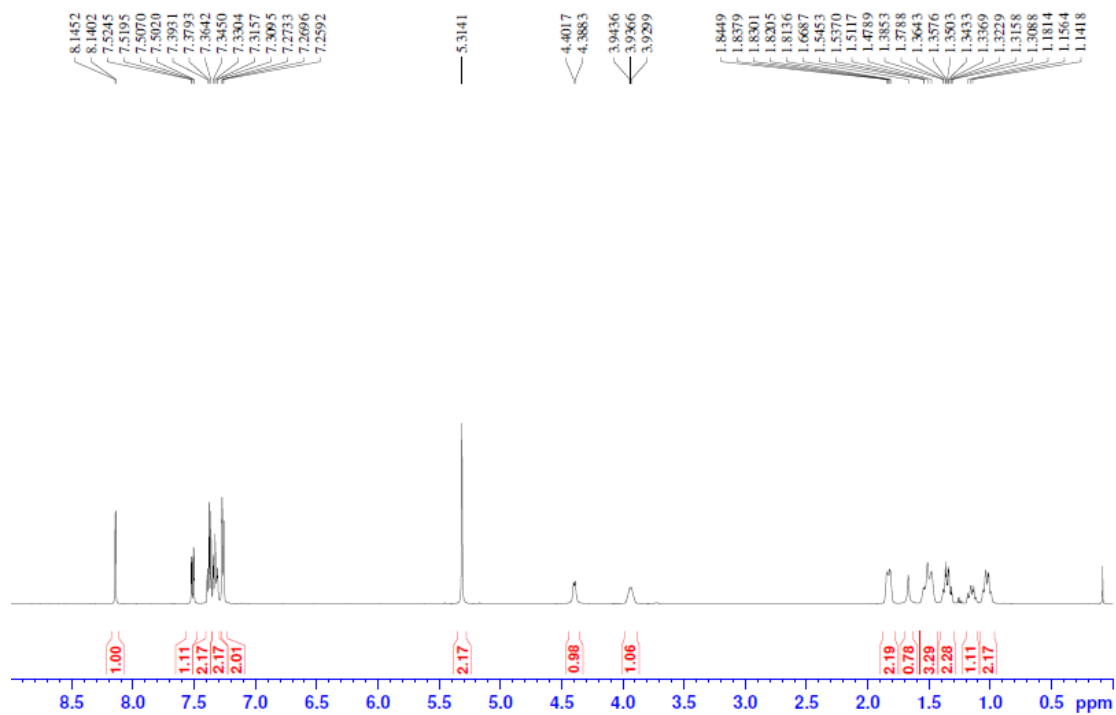
¹H NMR of compound **4q**

2013-10-20 13C-5 cdcl3 CC-468 (jf-3 5-lvdianhongsuangan bianan shudingjiyijing)



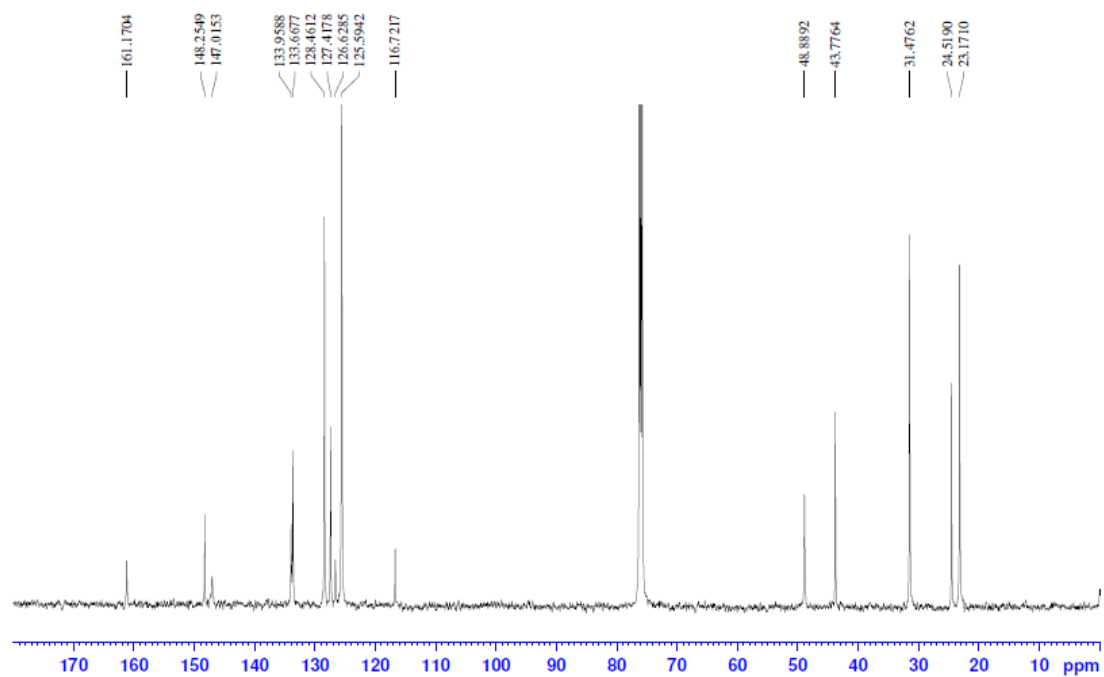
¹³C NMR of compound **4q**

2013-09-08 1H-8 CDCL3 CC-1422 (JF-1)

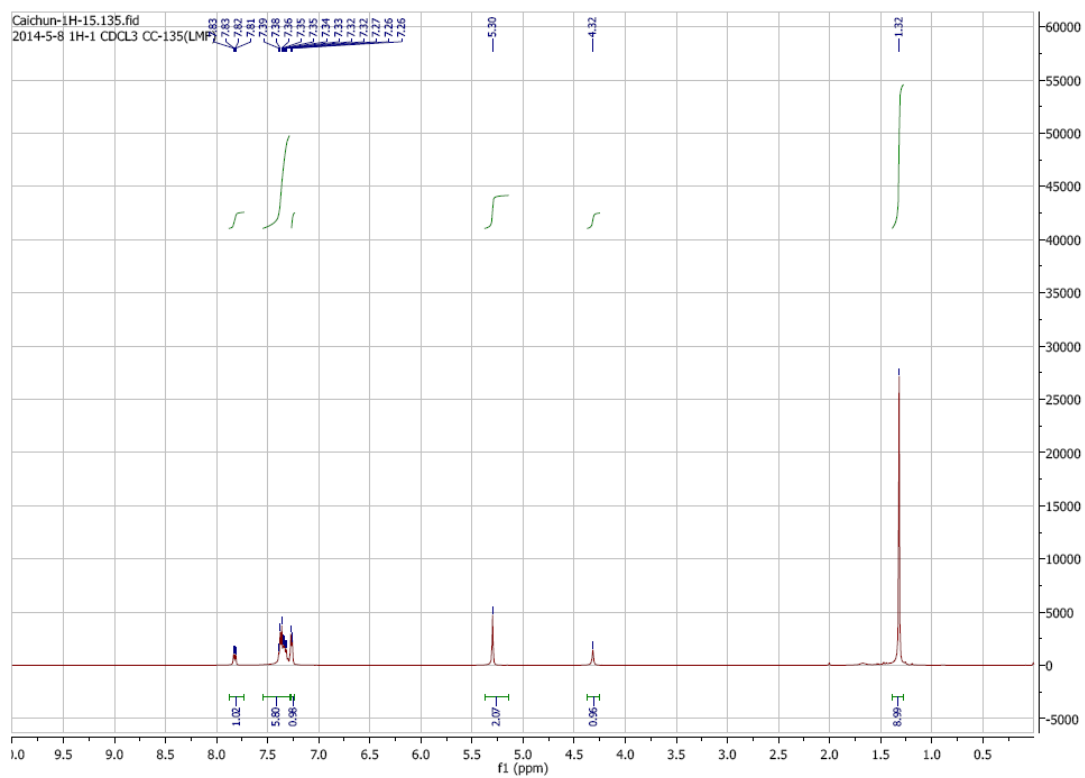


¹H NMR of compound **4r**

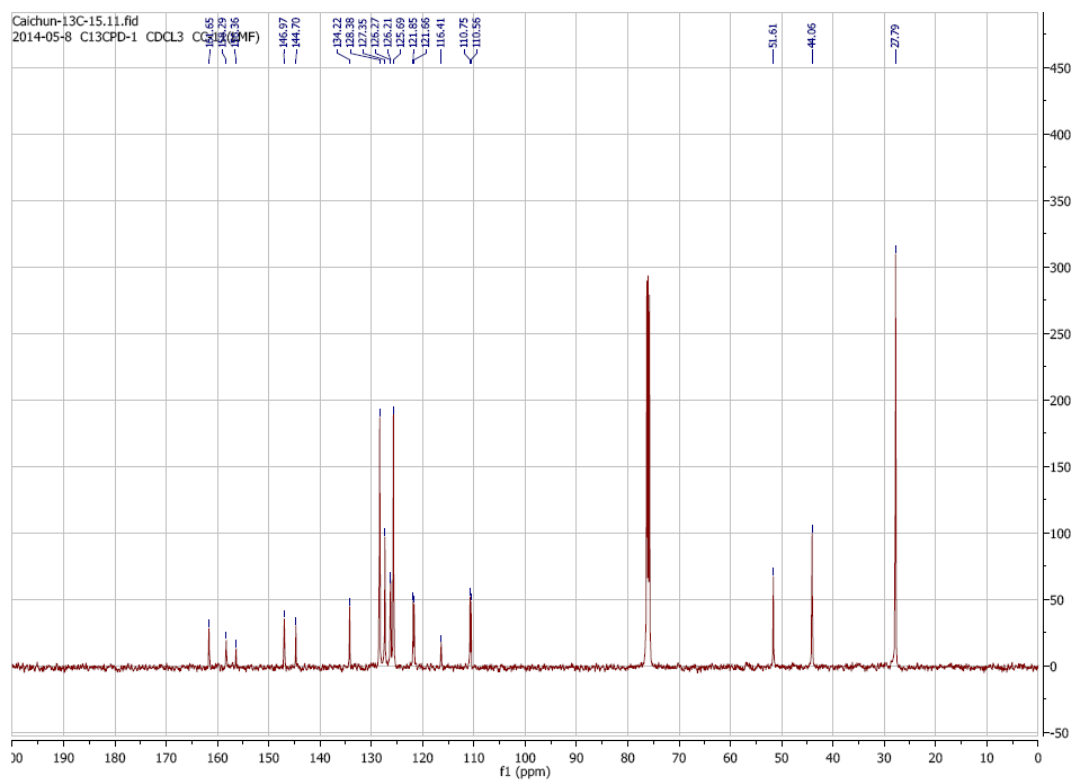
2013-10-12 13C-9 CDCL3 CC-437 (jf-2 2jiajikangan dianhongsuangan shudingyijing)



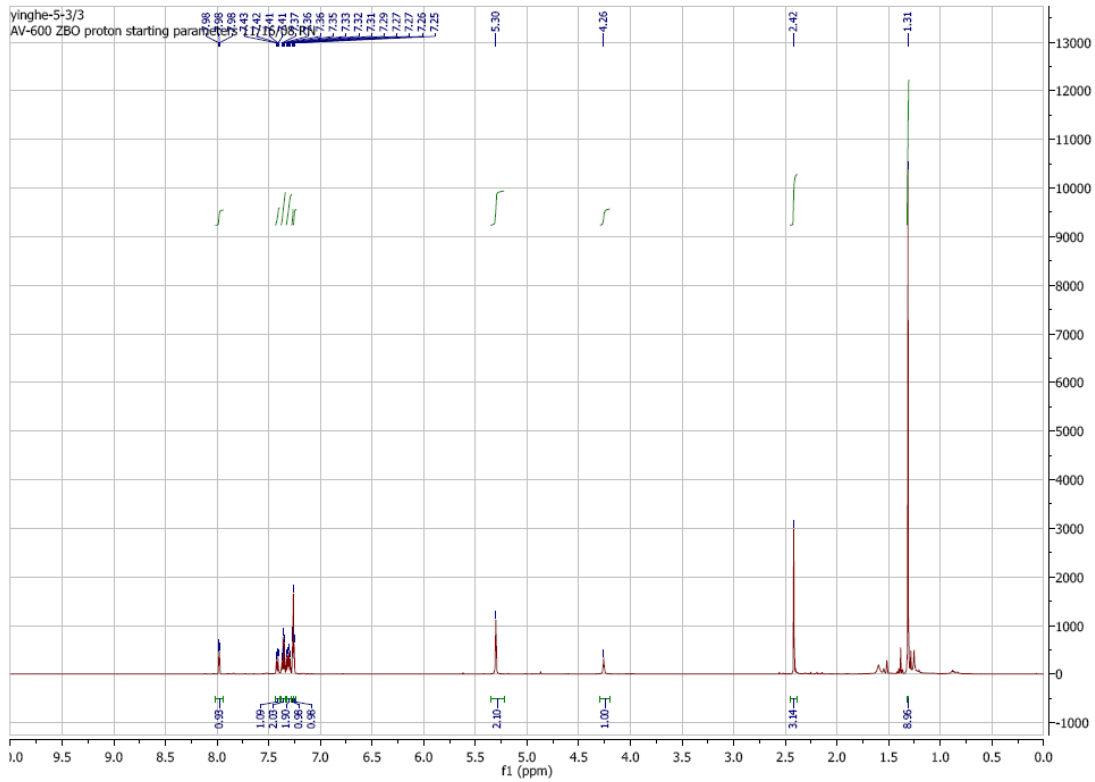
¹³C NMR of compound **4r**



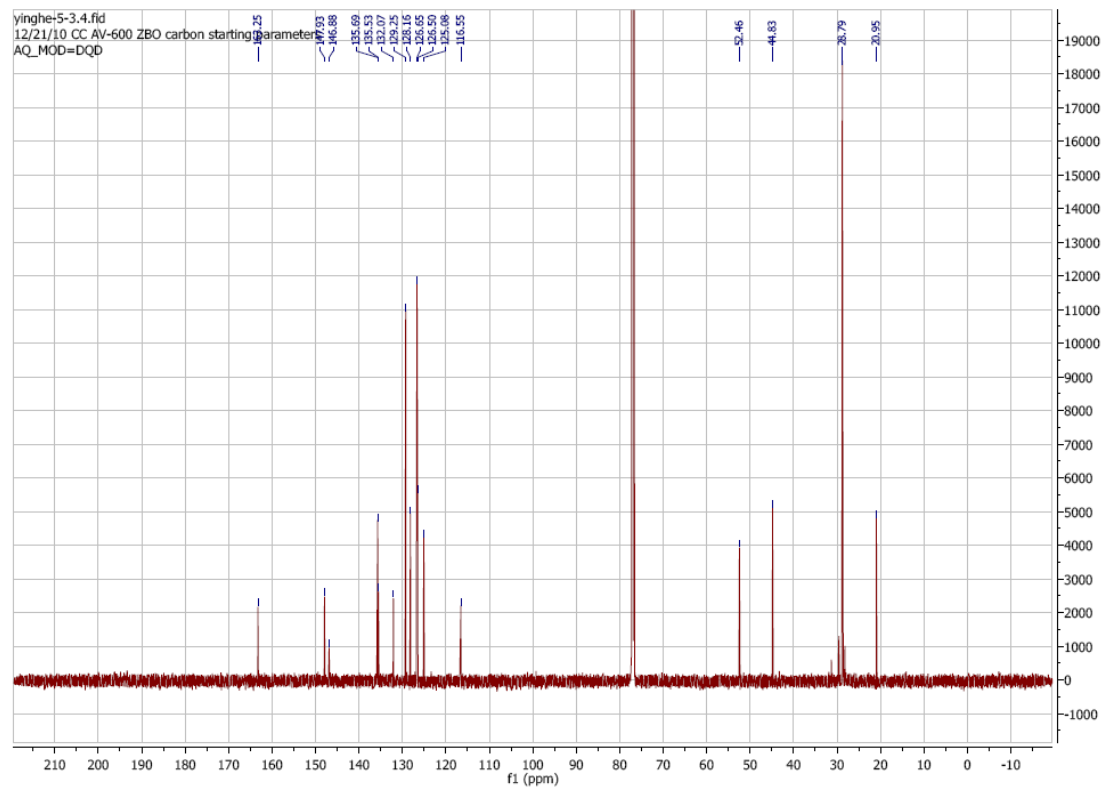
¹H NMR of compound **4s**



¹³C NMR of compound **4s**

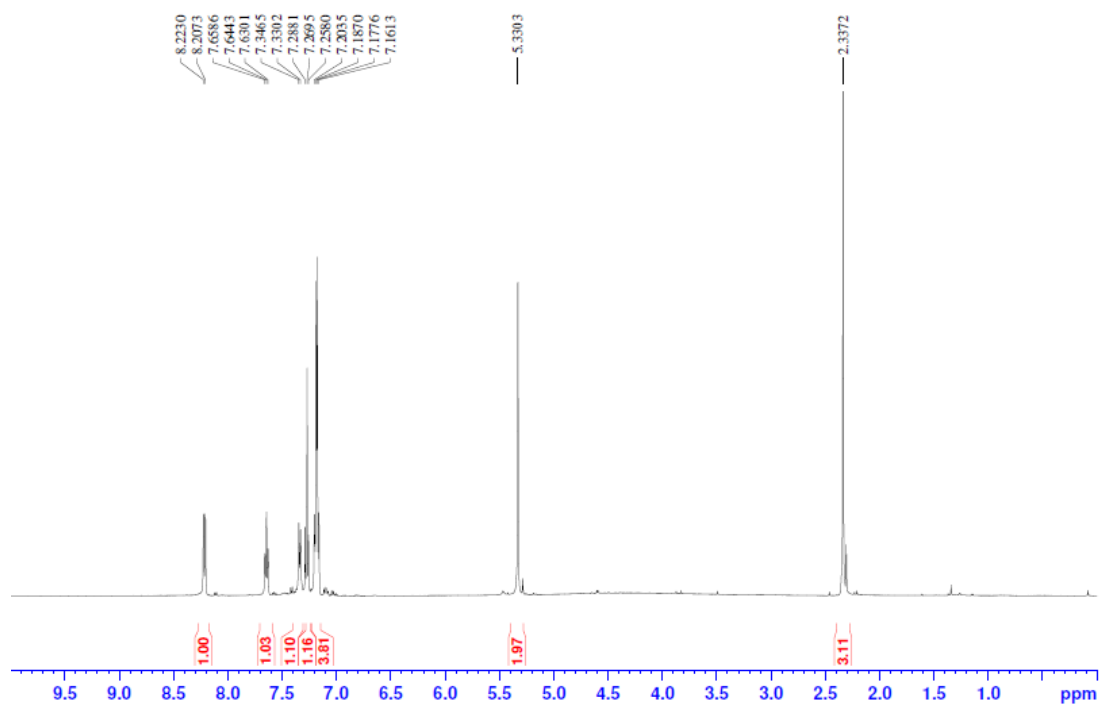


¹H NMR of compound **4t**



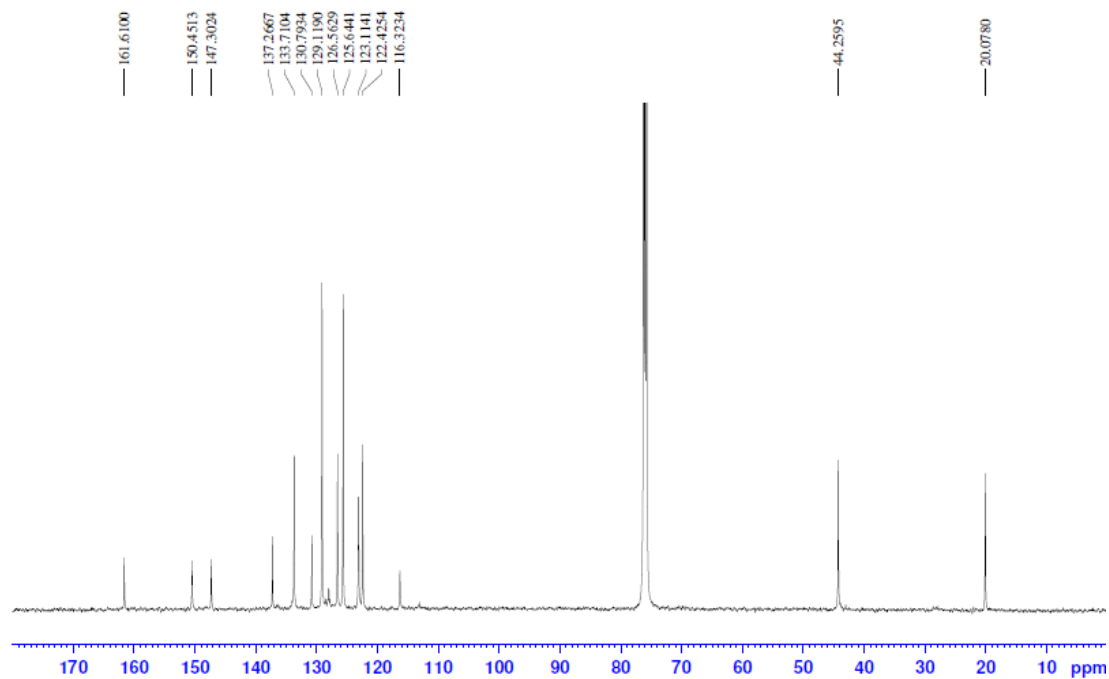
¹³C NMR of compound **4t**

2013-09-21 1H-1 CDCL3 CC-1445 (JF-1)



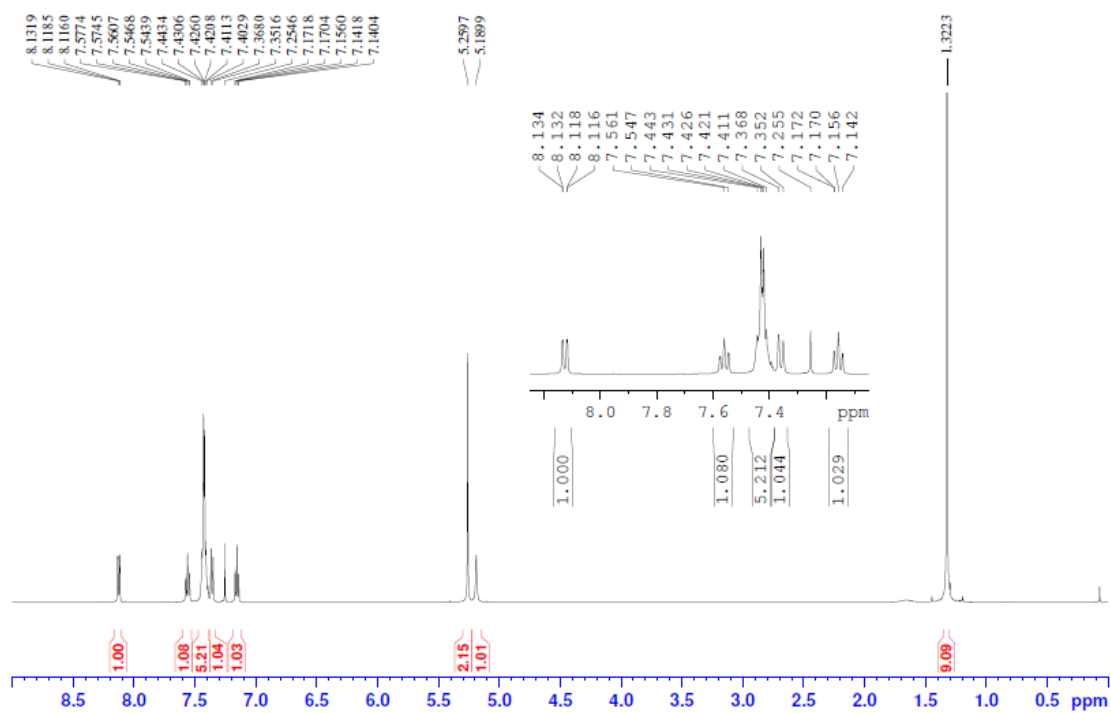
¹H NMR of compound **4u**

2013-9-21 13C-3 CDCL3 CC-418 (JF-2)



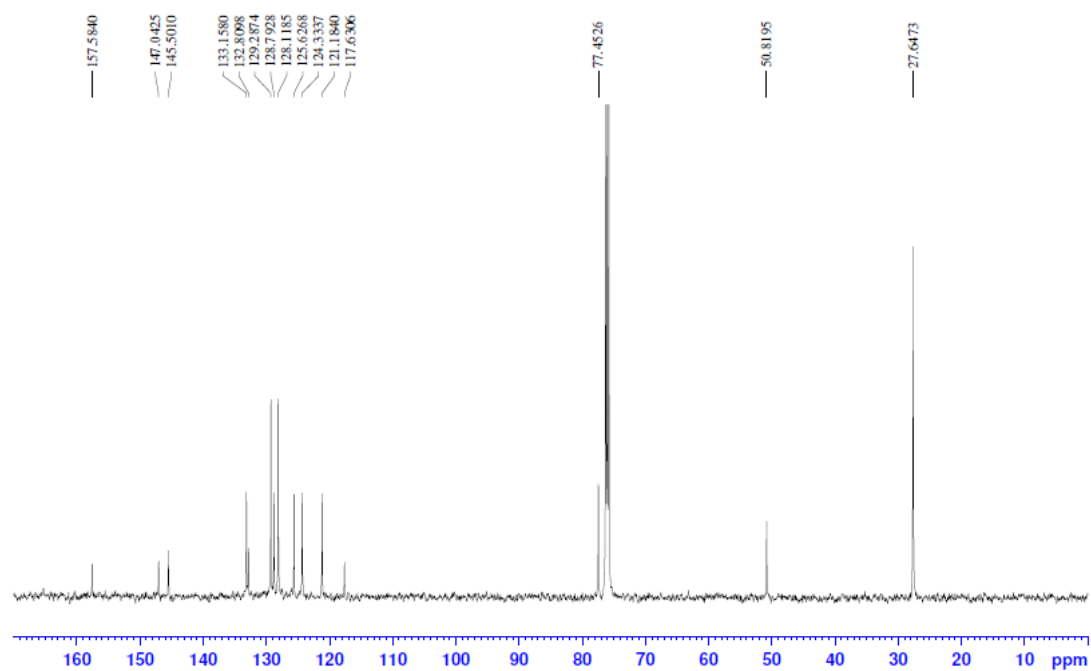
¹³C NMR of compound **4u**

2013-11-16 1H-22 CDCL3 CC-1799(JF-1 BIANJIQIANGAN)



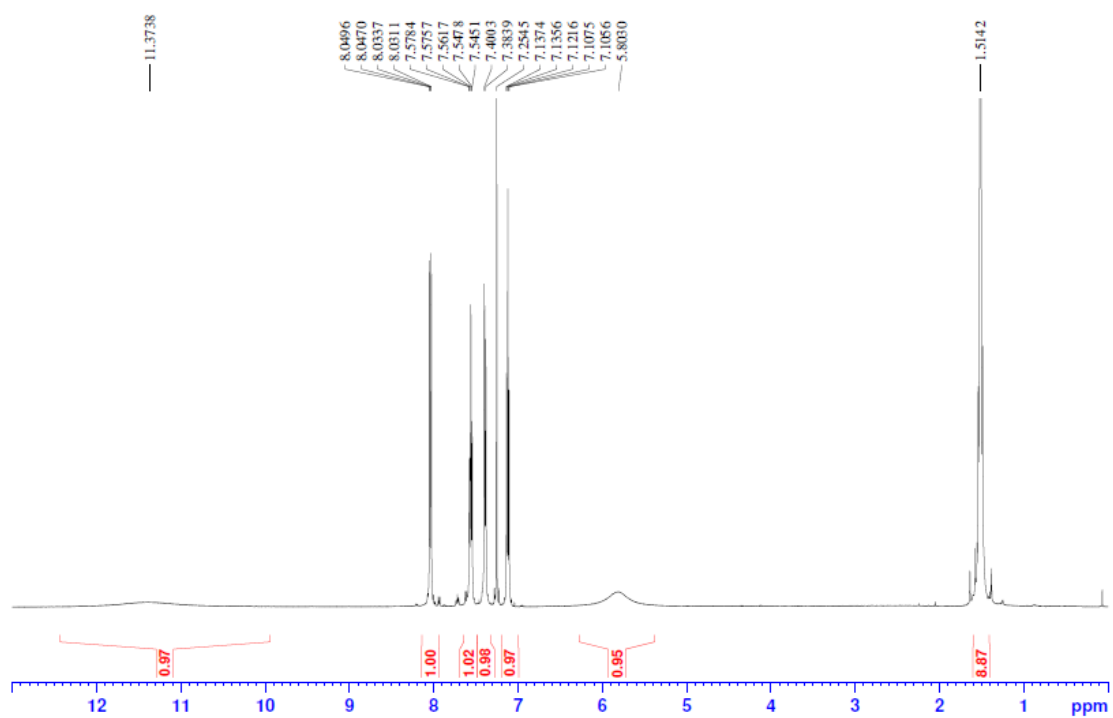
¹H NMR of compound 4v

2013-11-16 13C-8 CDCL3 CC-528(jf-1 dianhongsuangan bianjiqiangan shudingjiyijing)



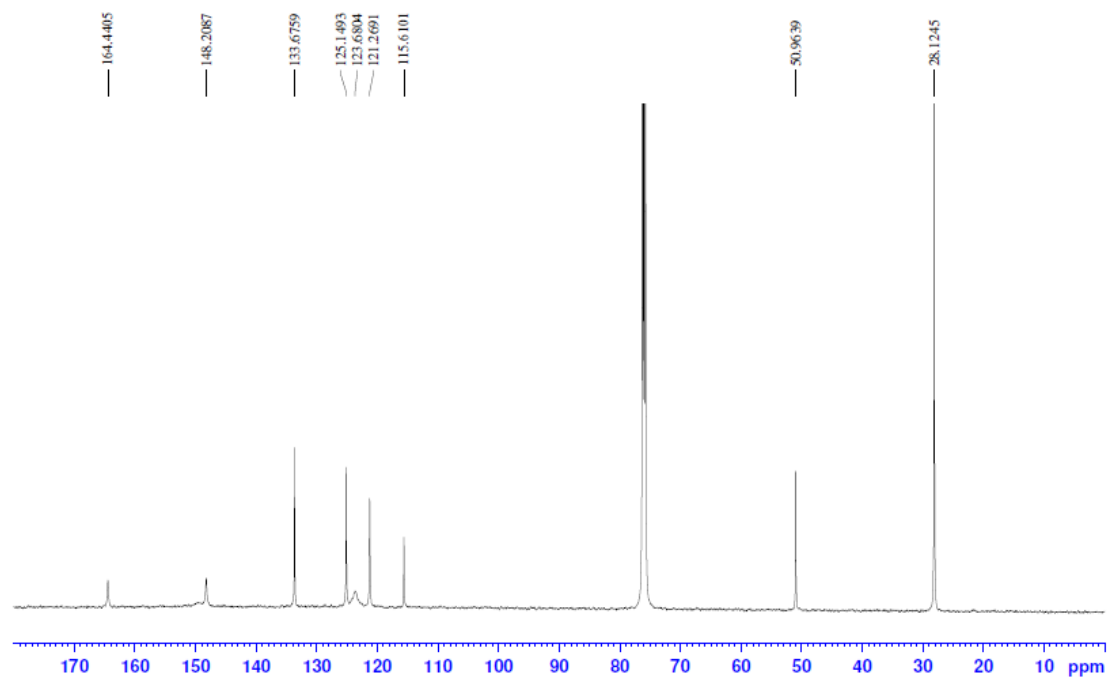
¹³C NMR of compound 4v

2013-11-23 1H-7 CDCL3 CC-1840 (JF-1)



¹H NMR of compound **4w**

2013-11-23 13C-5 CDCL3 CC-546 (jf-2 dianhongsuangan bianjiqianan shudingjiyijing qinghua)

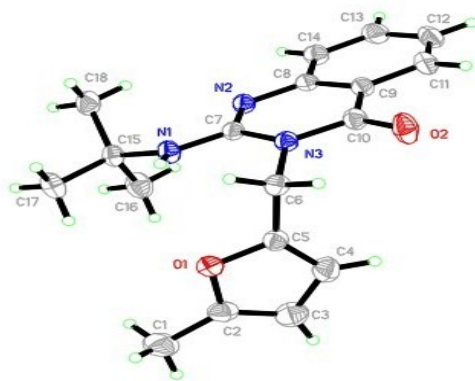


¹³C NMR of compound **4w**

Single-crystal X-ray analysis of product 4j

Crystallographic data (excluding structure factors) for compound **4j** (CCDC 966928) have been deposited with the Cambridge Crystallographic Data Centre. Crystallographic data of complexes was collected at 296 K on a Bruker SMART CCD system equipped with graphite-monochromated Mo-K α radiation ($\lambda = 0.071073$ nm) using ω - ϕ scan technique. Diffraction data were integrated by the SAINT program, which was also used for intensity corrections for Lorentz and polarization effects. Semi-empirical absorption correction was applied using SADABS. The structures were solved by direct methods and all non-hydrogen atoms were refined anisotropically on F² by full-matrix least-squares using the SHELXL-97 crystallographic software package.

complex	4j
Formula	C ₁₈ H ₂₁ N ₃ O ₂
Formula weight	311.38
Crystal system	Monoclinic
space group	P2(1)/n
a (Å)	12.3807(10)
b (Å)	10.2922(8)
c (Å)	13.3591(10)
α (°)	90.00
β (°)	102.8390(10)
γ (°)	90.00
Volume(Å ³)	1659.7(2)
Z	4
T, (K)	296(2)
D _{calcd} (g/m ³)	1.246
F(000)	664
Reflections collected	3094
Unique reflections	2409
Goof	1.028
R ₁ [I > 2 σ (I)]	0.0412
wR ₂ [I > 2 σ (I)]	0.1086
CCDC number	CCDC 966928



Single-crystal X-ray analysis of **4j**