

CHEMBIOCHEM

Supporting Information

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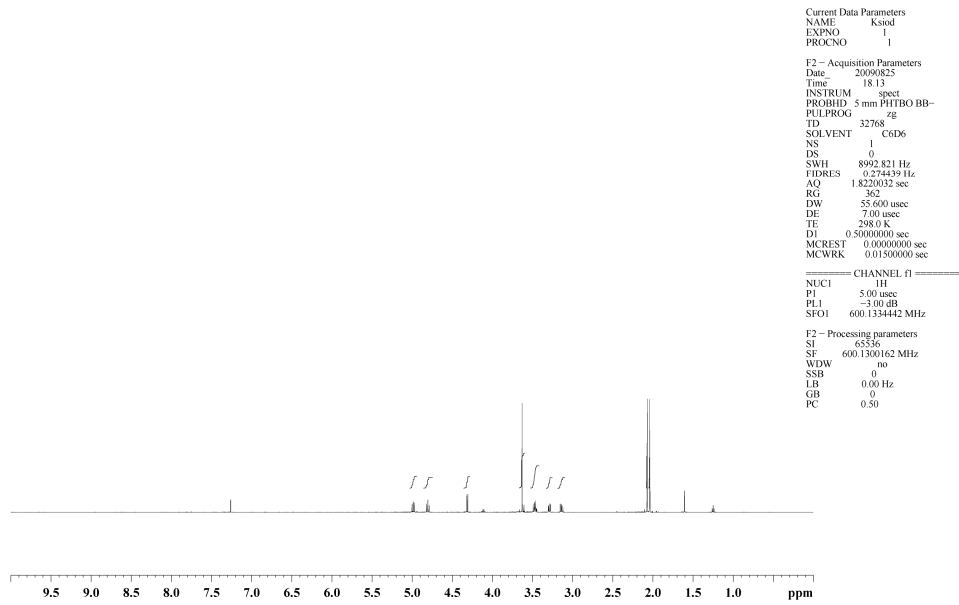
The Development of Selective Inhibitors of NagZ: Increased Susceptibility of Gram-Negative Bacteria to β - Lactams

Keith A. Stubbs,^{*[a]} John-Paul Bacik,^[b, d] G. Evan Perley-Robertson,^[c] Garrett E. Whitworth,^[c, e]
Tracey M. Gloster,^[c, f] David J. Vocadlo,^[c] and Brian L. Mark^{*[b]}

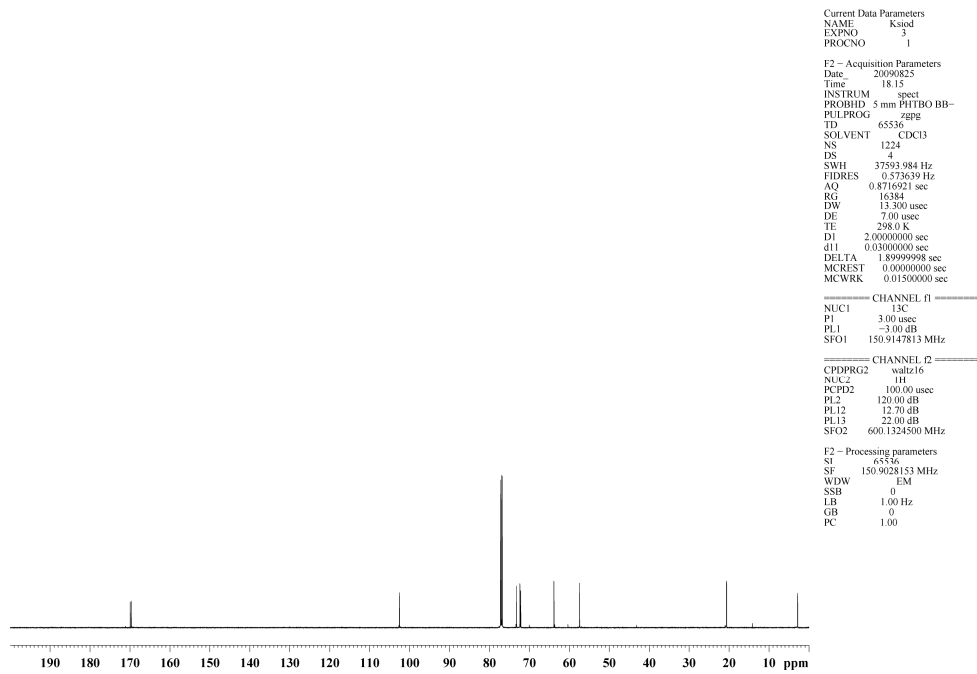
cbic_201300395_sm_miscellaneous_information.pdf

Table S1: Crystallographic data and model refinement

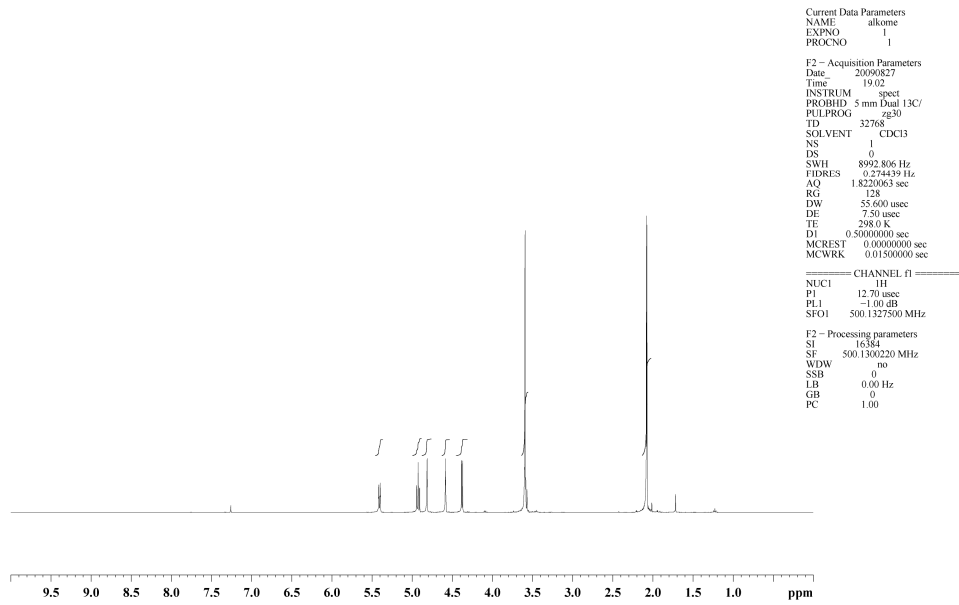
StNagZ-21 (PDB:4HZM)	
Data Collection^a	
Space group	P1 2 ₁ 1
Unit cell (Å)	a=49.77, b=66.19, c=95.07 $\alpha = 90, \beta = 99.21, \gamma = 90^\circ$
Wavelength (Å)	0.9795
Resolution range (Å)	49.12 – 1.45 (1.53 – 1.45)
Total observations	378412
Total unique observations	105765
I/ σ ₁	13.0 (3.1)
Completeness (%)	98.0 (87.5)
R _{merge}	0.065 (0.365)
Redundancy	3.6 (2.5)
Refinement Statistics	
Resolution (Å)	49.12 – 1.45
Reflections (total)	105697
Reflections (test)	3160
Total atoms refined	6089
Solvent	920
R _{work} (R _{free})	0.169 (0.193)
Mean B values (Å ²)	14.5
Overall	
Bound ligand (A/B subunit)	7.9/7.9
RMSDs	0.008/1.172
Bond lengths (Å) / angles (°)	
Ramachandran plot	97.1/2.9
Favored/allowed (%)	



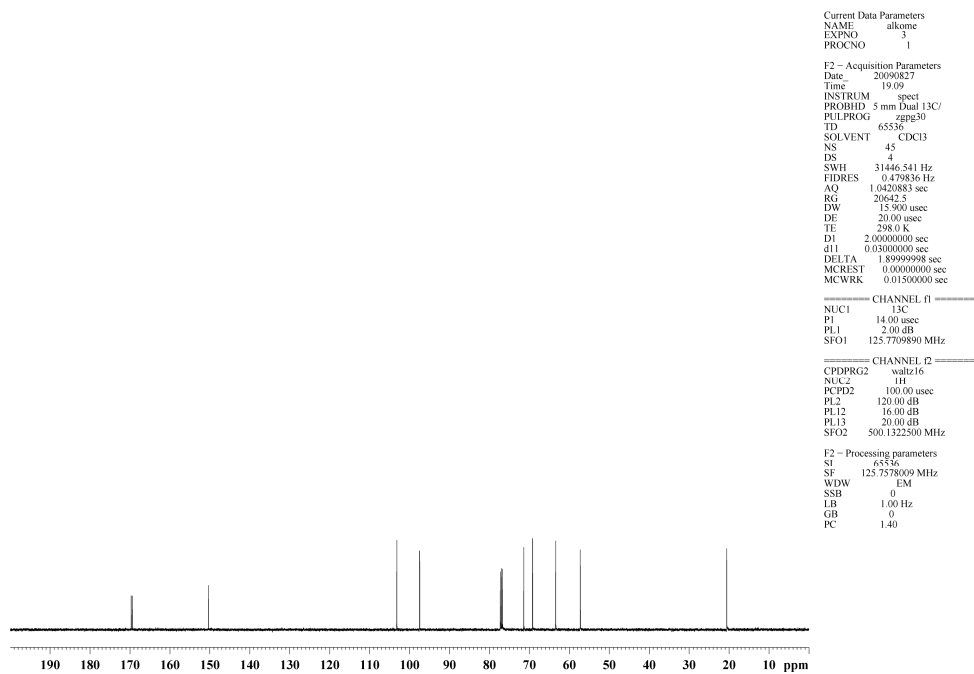
^1H NMR of **5**.



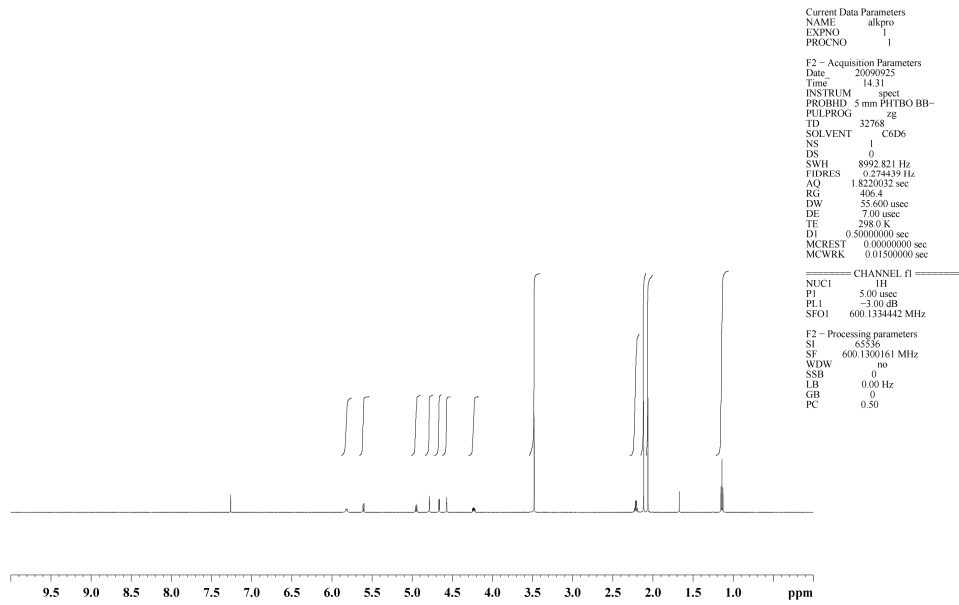
^{13}C NMR of **5**.



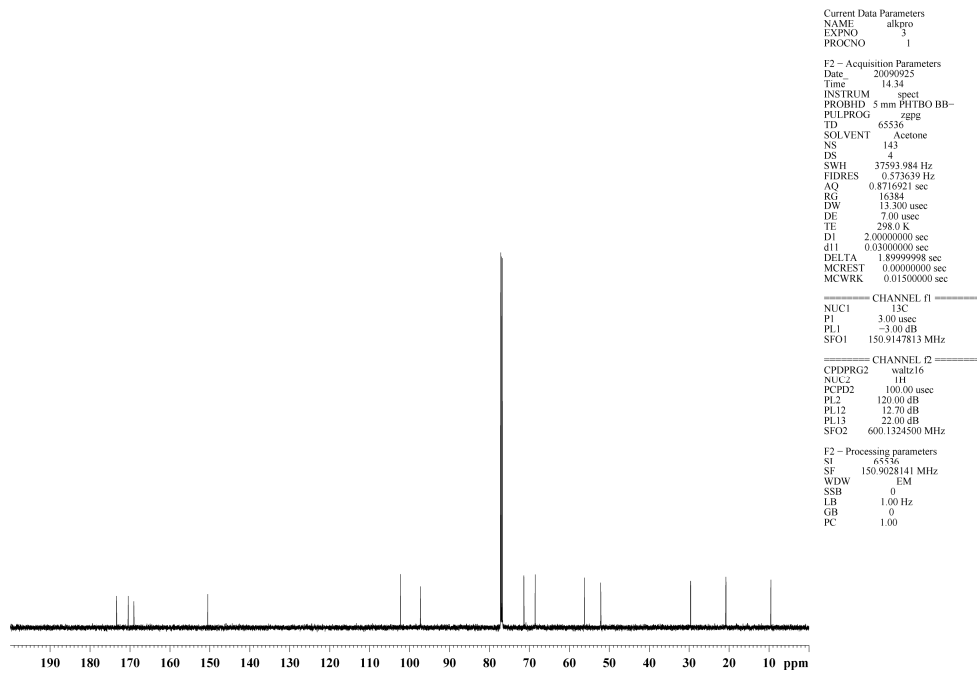
¹H NMR of 2.



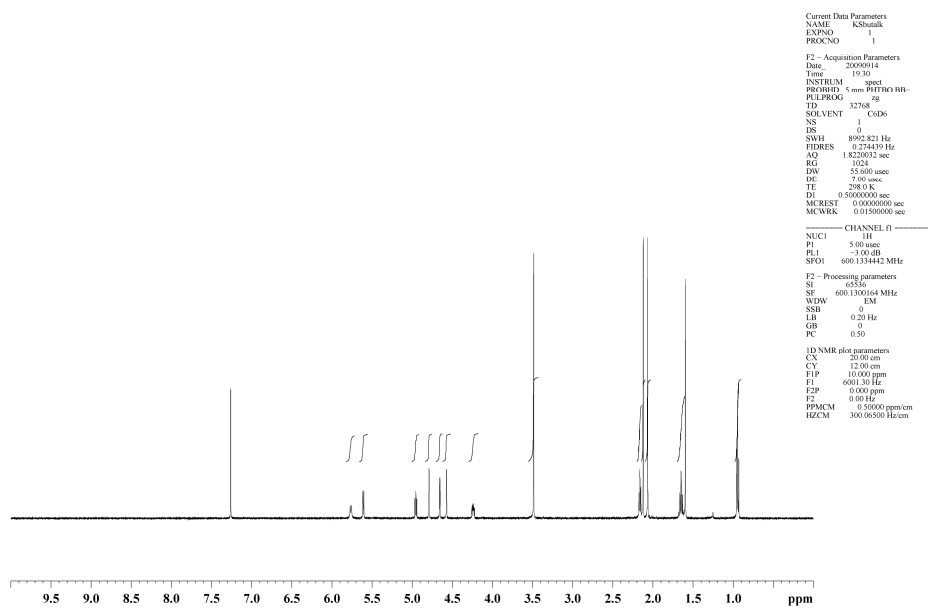
¹³C NMR of 2.



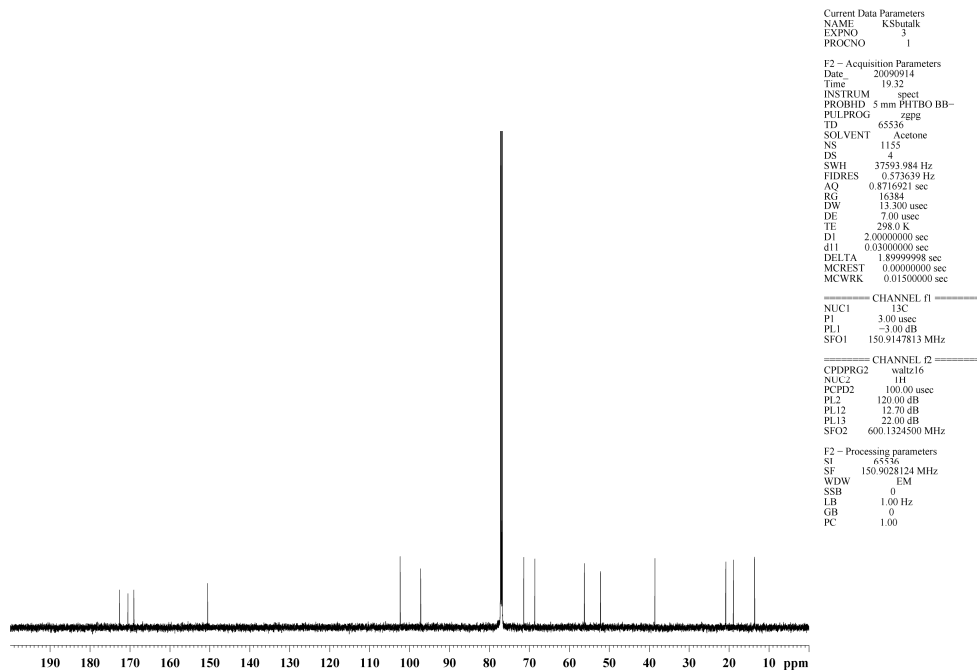
^1H NMR of **7**.



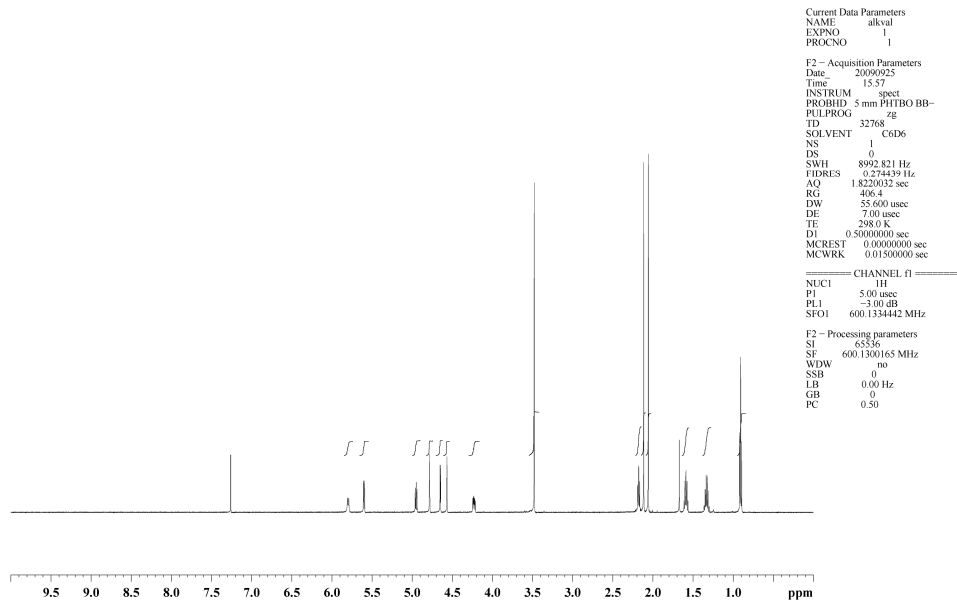
^{13}C NMR of **7**.



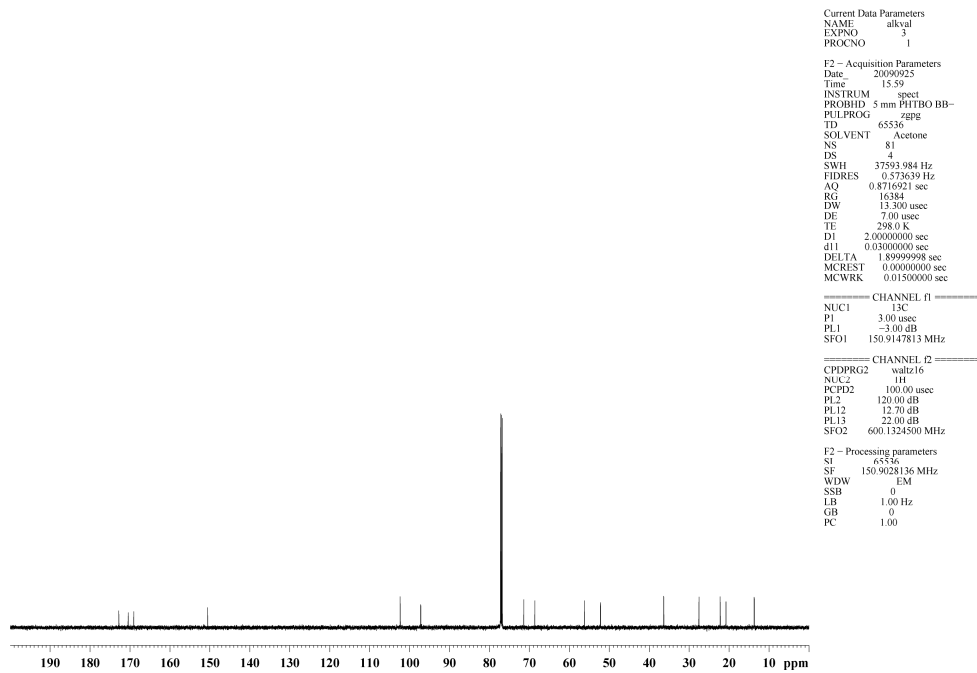
^1H NMR of **8**.



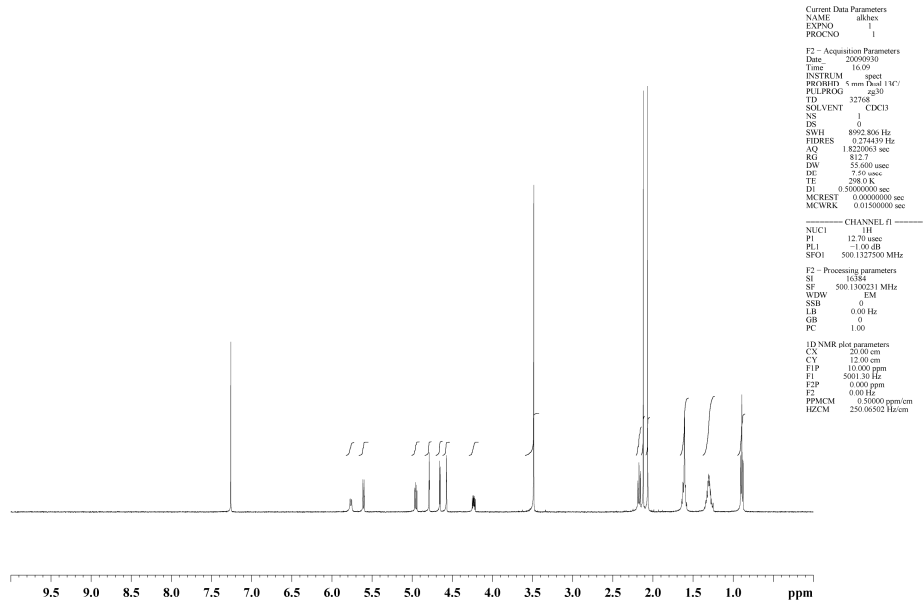
^{13}C NMR of **8**.



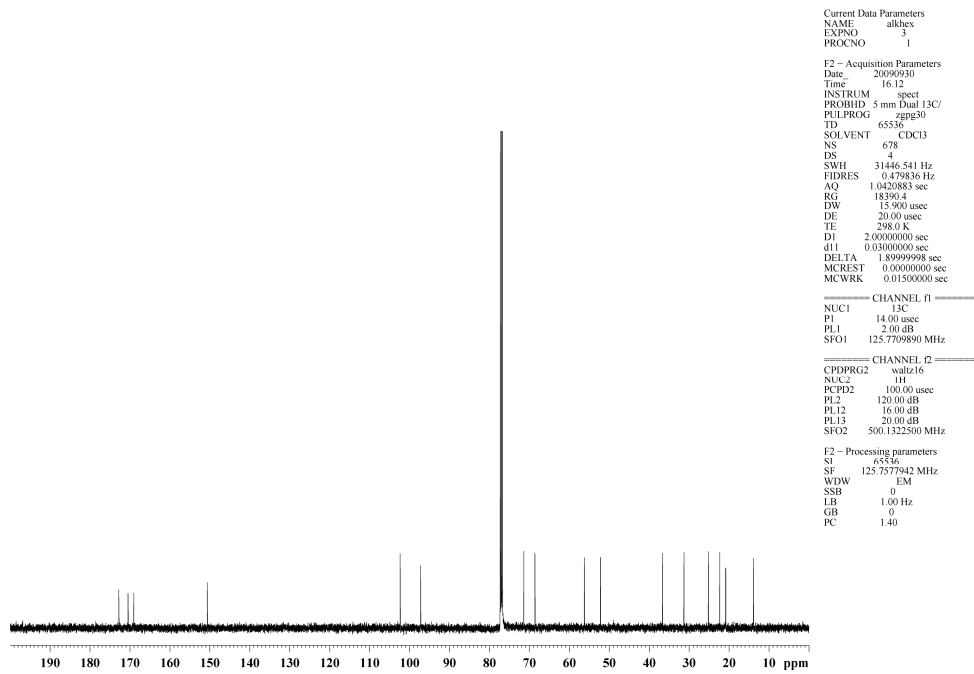
¹H NMR of **9**.



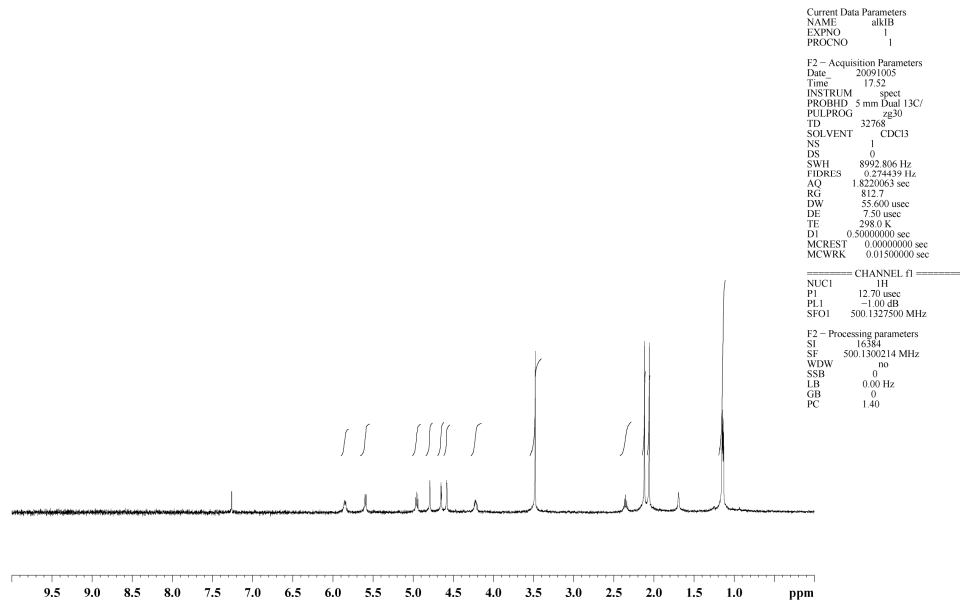
¹³C NMR of **9**.



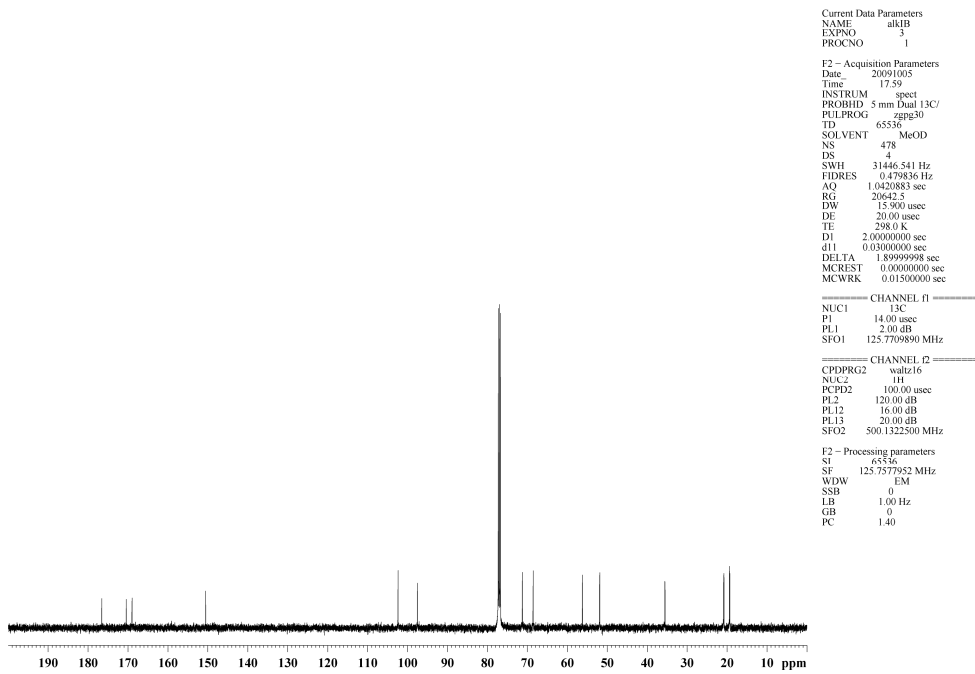
¹H NMR of 10.



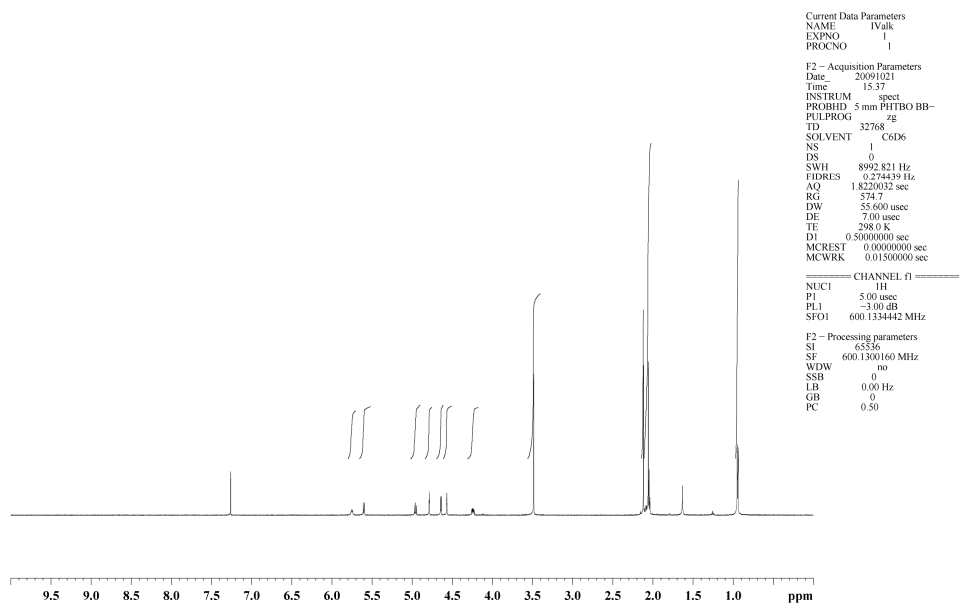
¹³C NMR of 10.



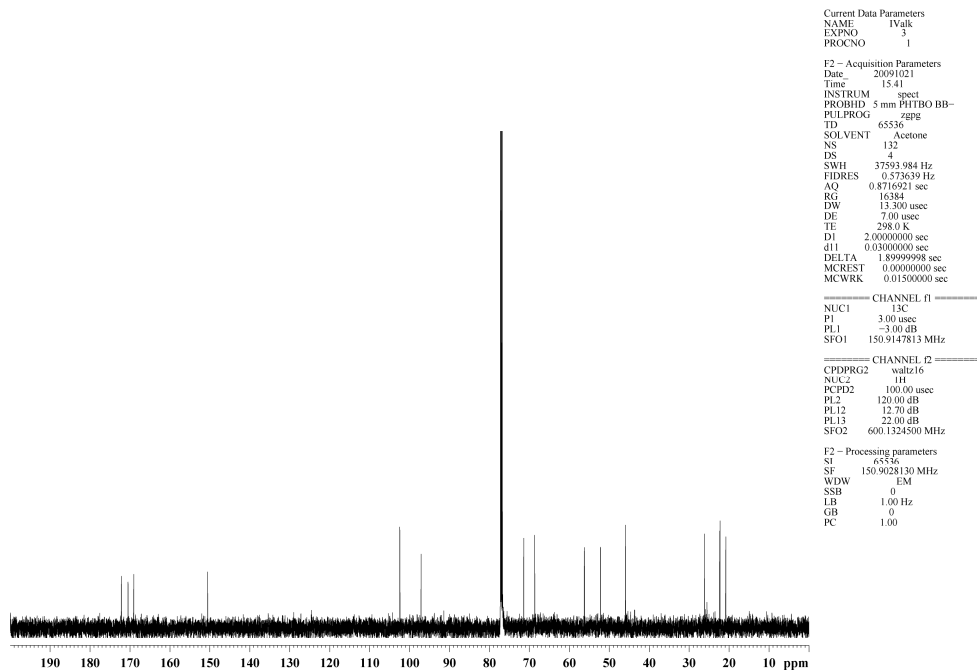
¹H NMR of **11**.



¹³C NMR of **11**.



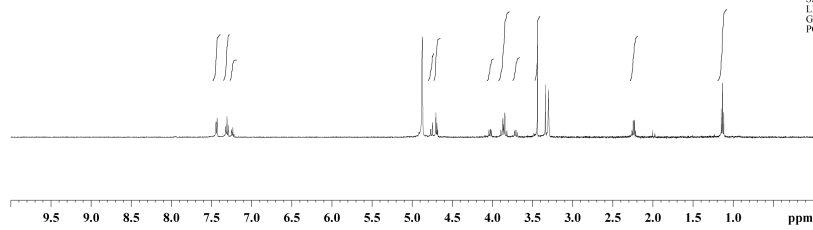
^1H NMR of **12**.



^{13}C NMR of **12**.

Current Data Parameters
 NAME pro0bn
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
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 Time 18.31
 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 1
 DS 0
 SWH 892.806 Hz
 FIDRES 0.274439 Hz
 AQ 1.822063 sec
 RG 812.7
 DW 55.600 usec
 DE 7.20 usec
 TE 297.5 K
 D1 0.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.01500000 sec

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 P1 12.70 usec
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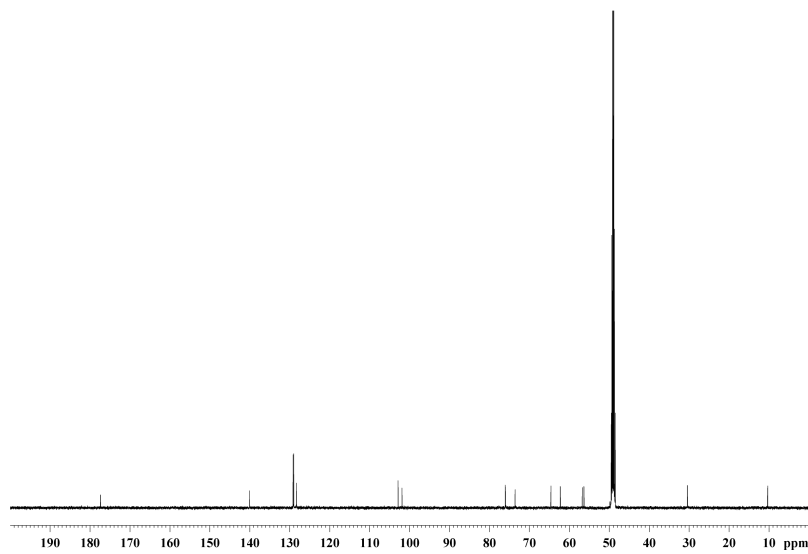


¹H NMR of 14.

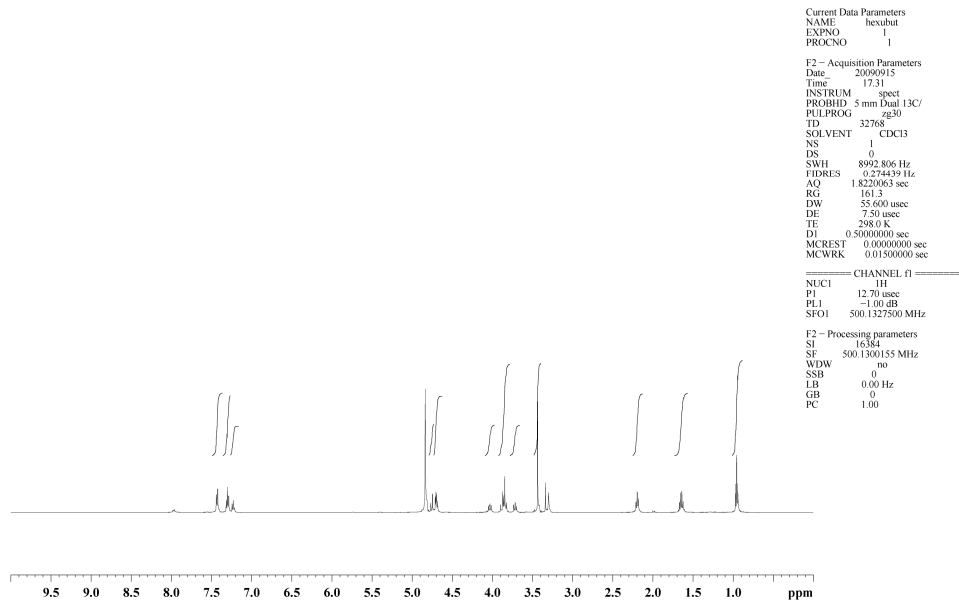
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 PROCNO 1
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 TD 65536
 SOLVENT MeOD
 NS 1022
 DS 4
 SWH 31446.541 Hz
 FIDRES 0.479836 Hz
 AQ 1.0420883 sec
 RG 20642.5
 DW 15.900 usec
 DE 20.00 usec
 TE 298.0 K
 D1 2.0000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 MCREST 0.0000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 14.00 usec
 PL1 2.00 dB
 SFO1 125.7709890 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
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 PL2 120.00 dB
 PL12 16.00 dB
 PL13 20.00 dB
 SFO2 500.1322500 MHz

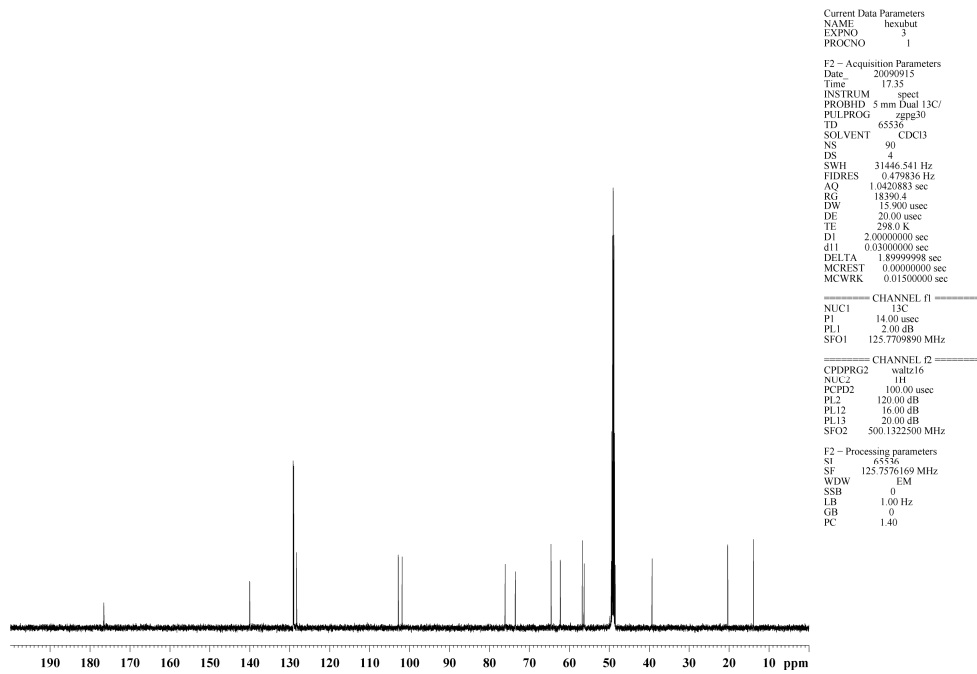
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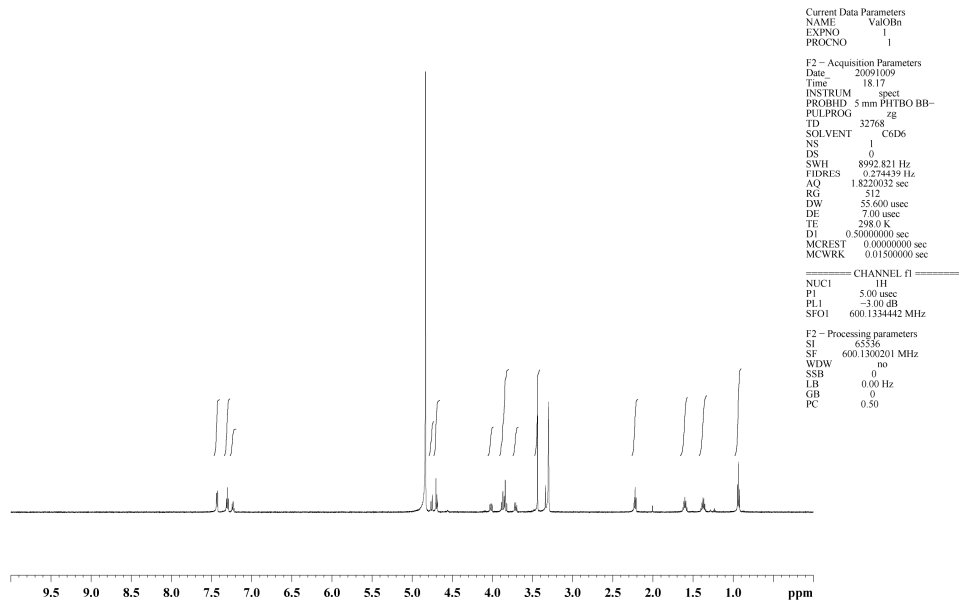
¹³C NMR of 14.



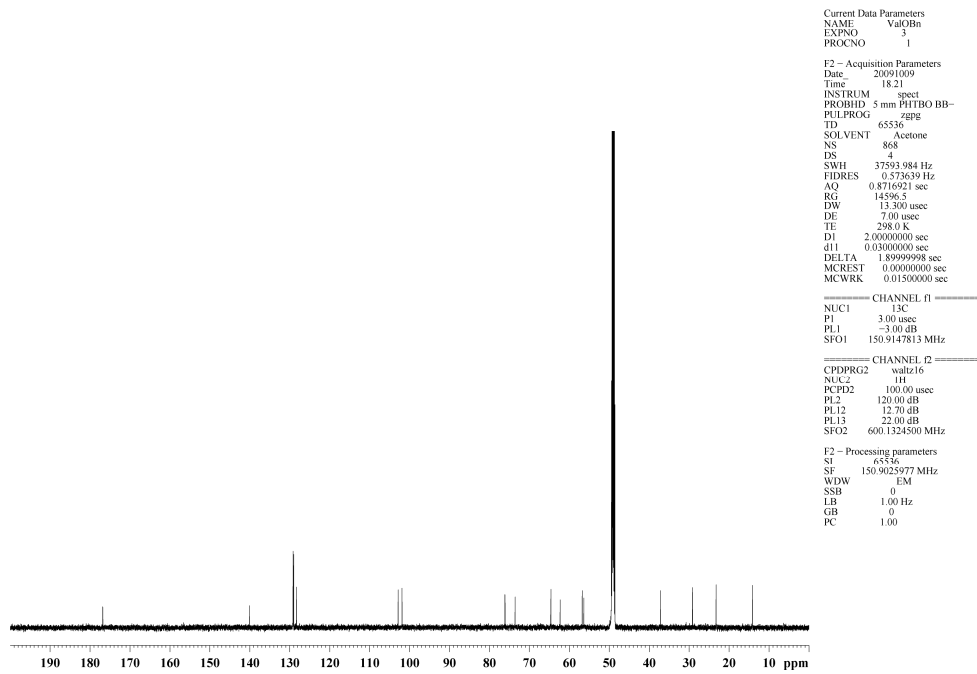
^1H NMR of **15**.



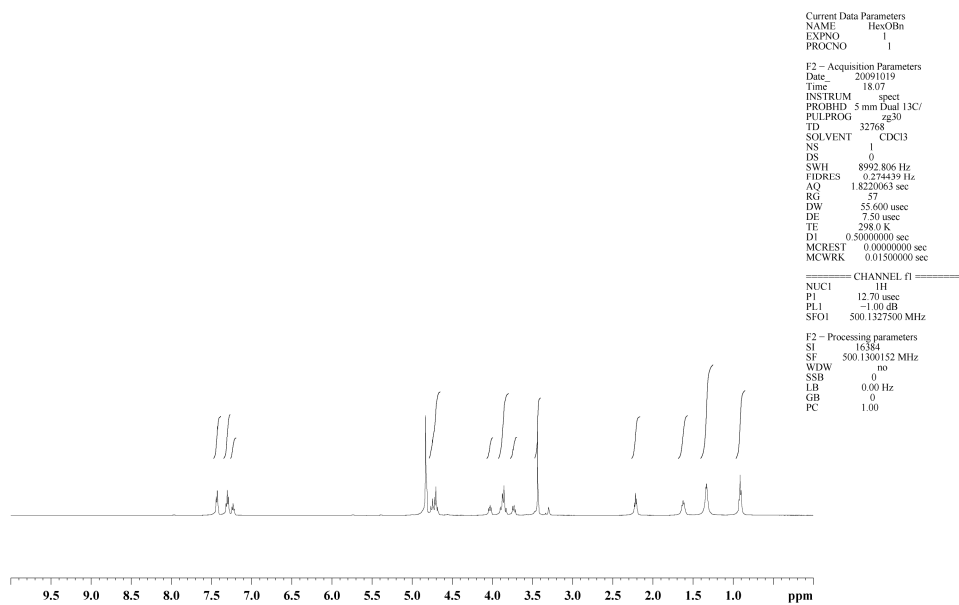
^{13}C NMR of **15**.



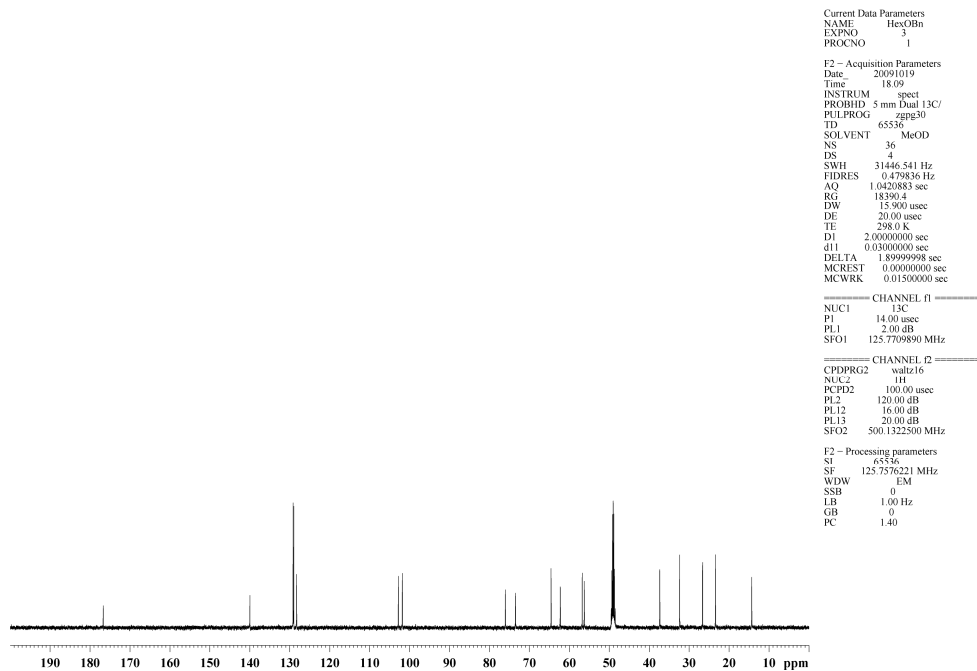
^1H NMR of 16.



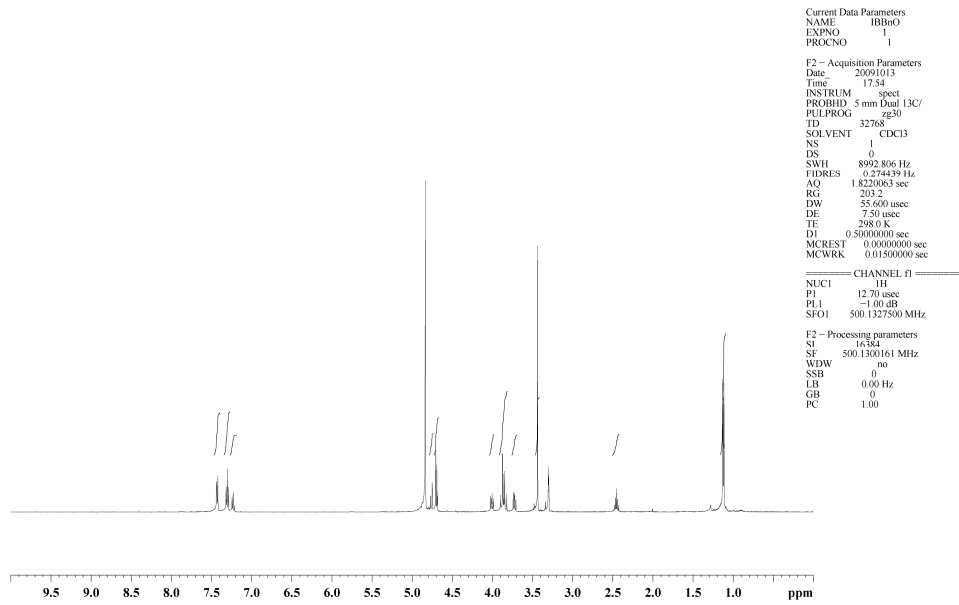
^{13}C NMR of 16.



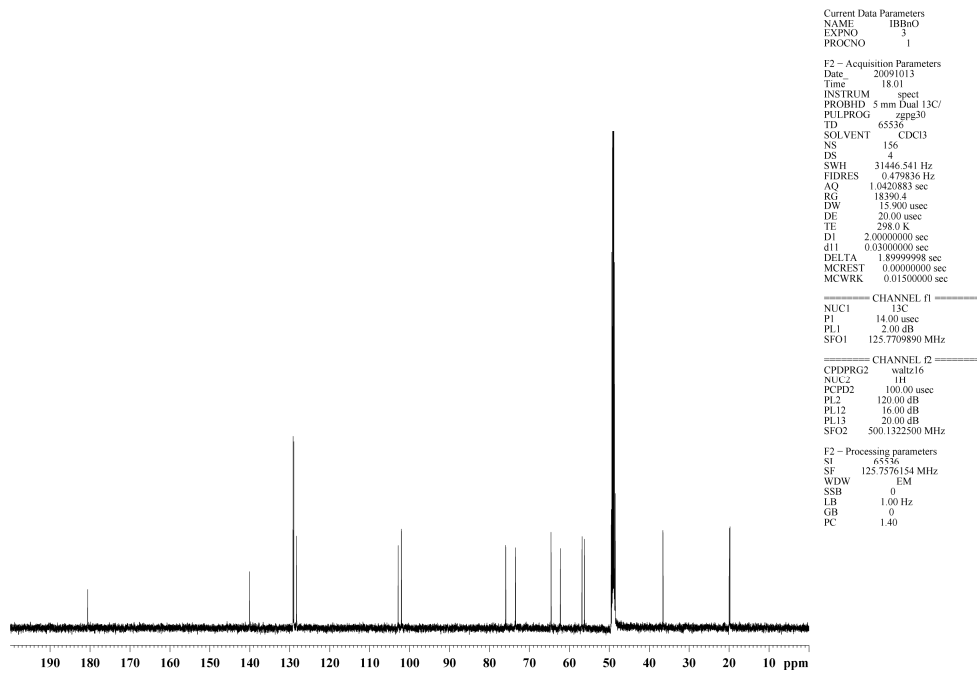
¹H NMR of 17.



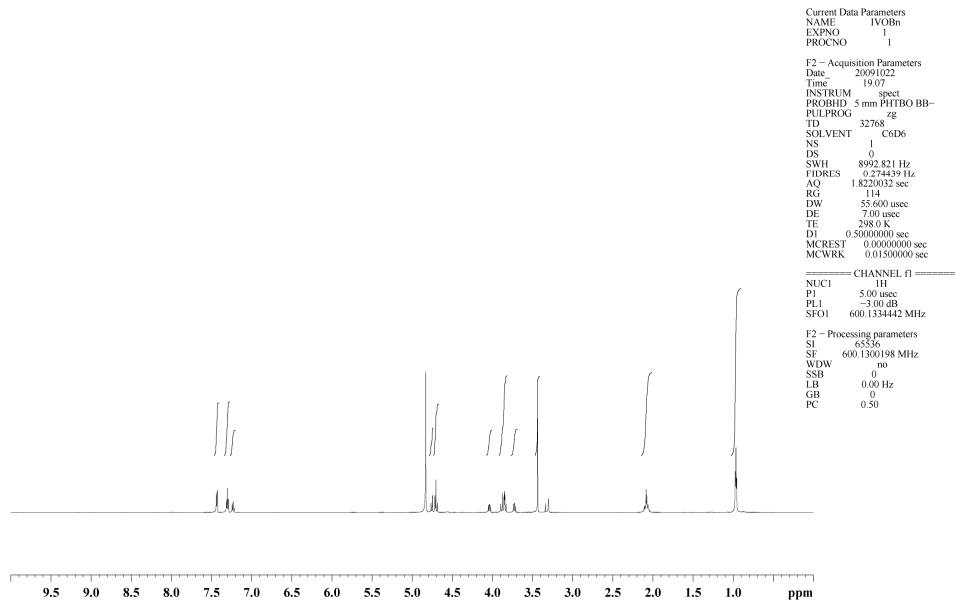
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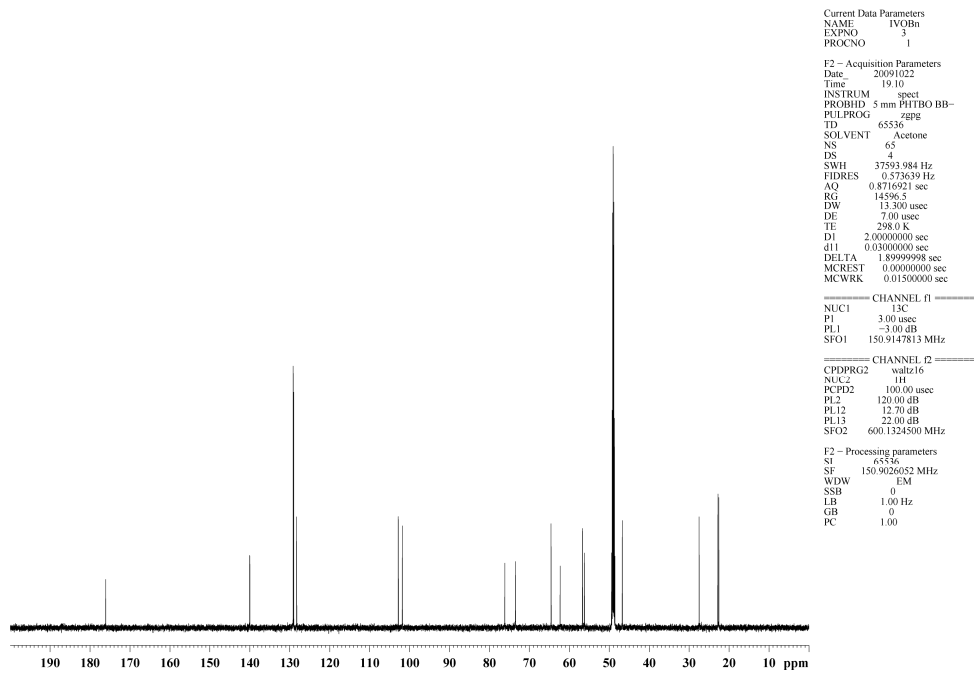
^1H NMR of **18**.



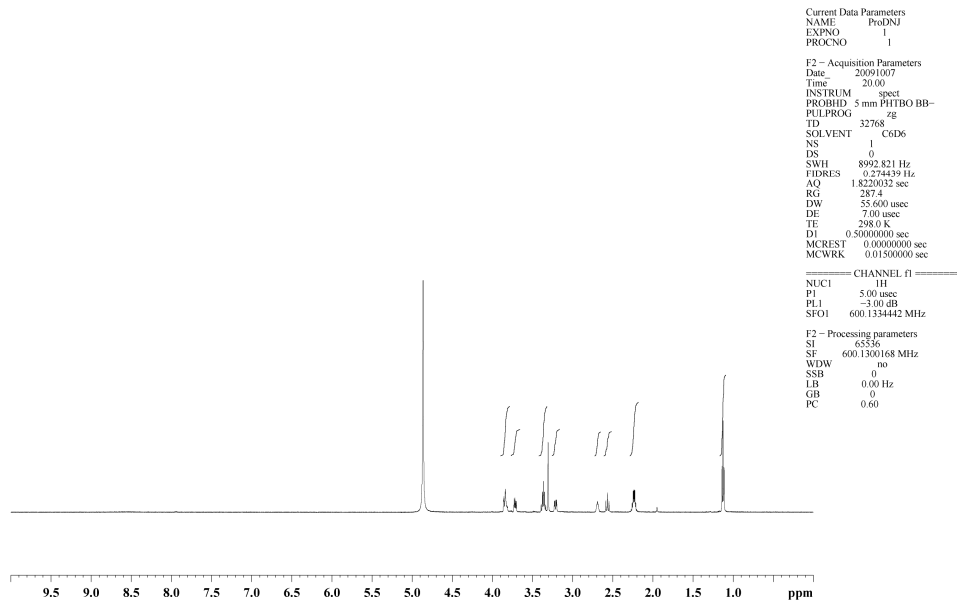
^{13}C NMR of **18**.



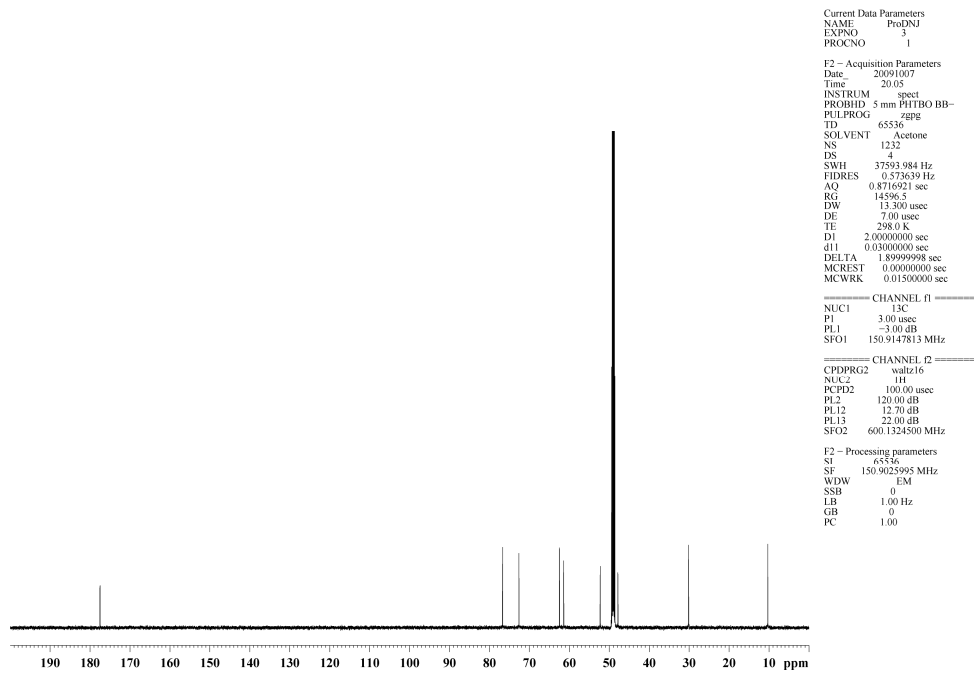
^1H NMR of **19**.



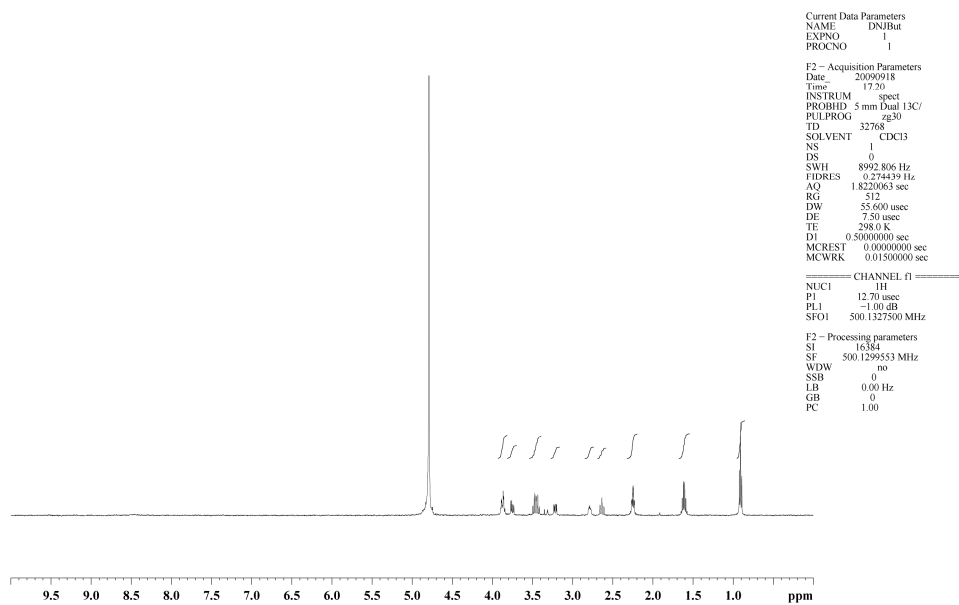
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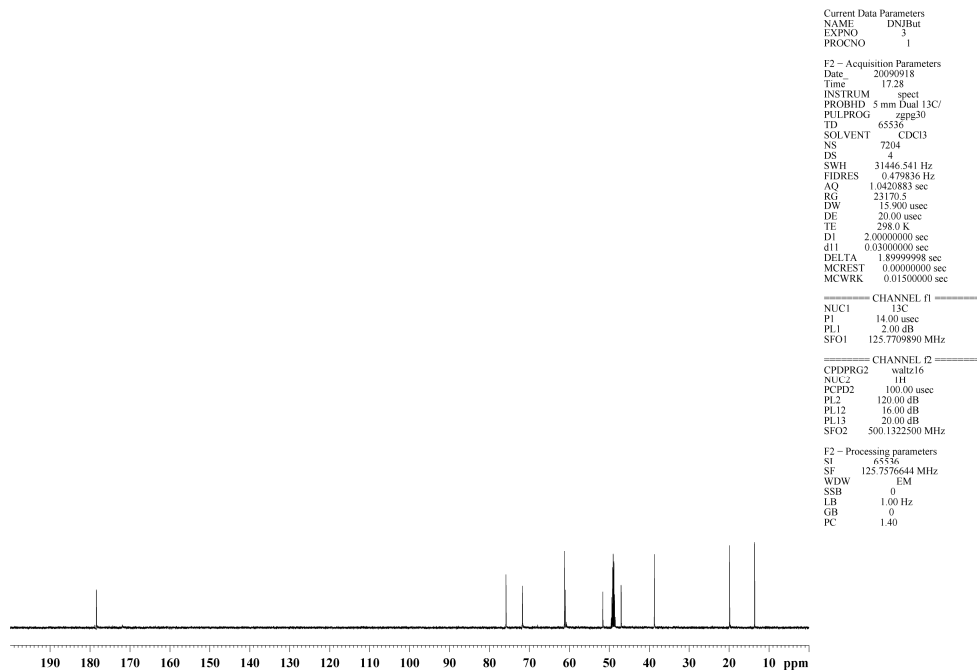
^1H NMR of **20**.



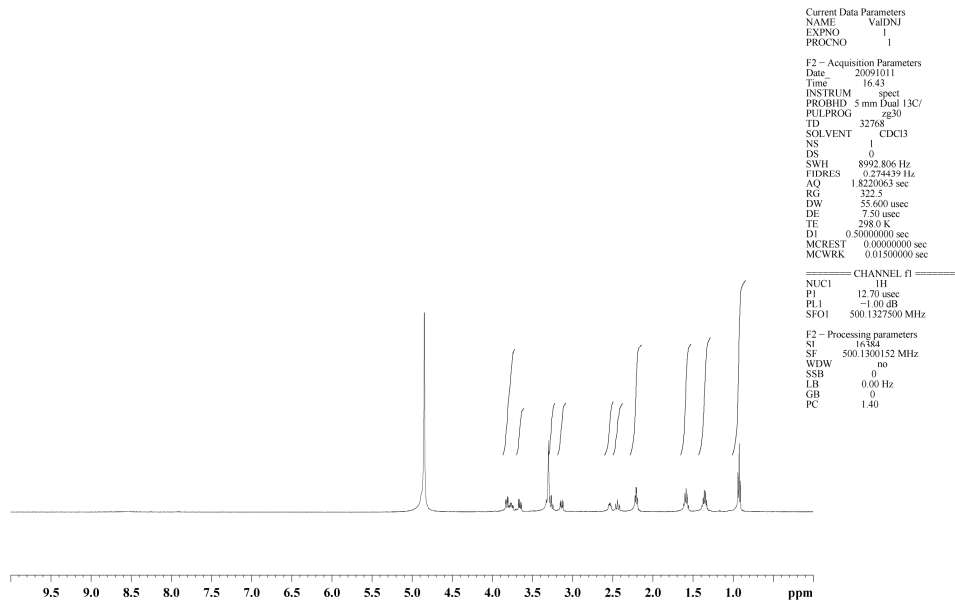
^{13}C NMR of **20**.



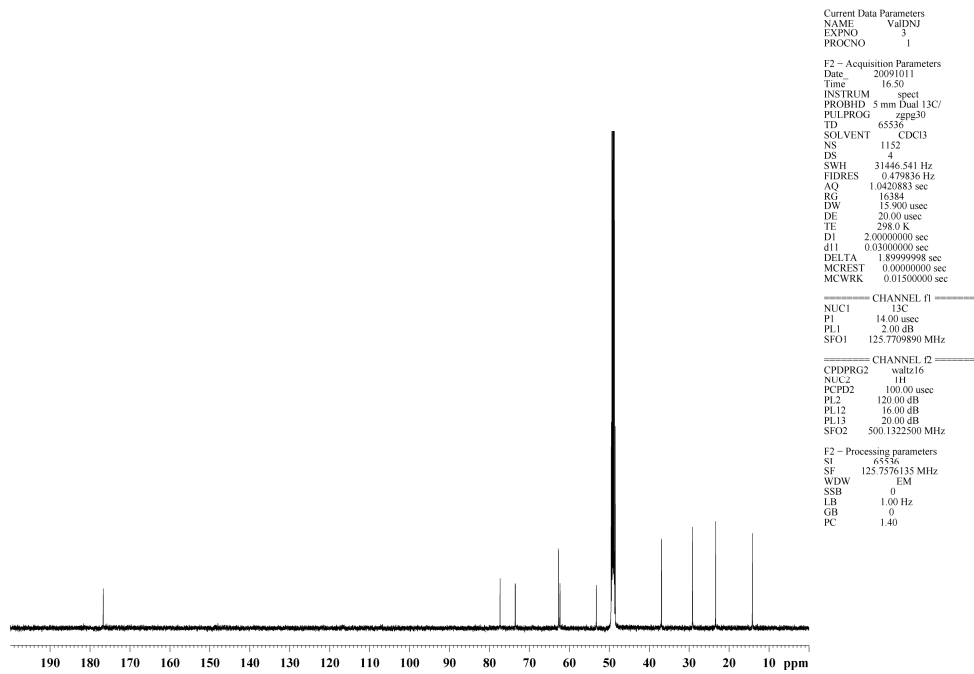
^1H NMR of **21**.



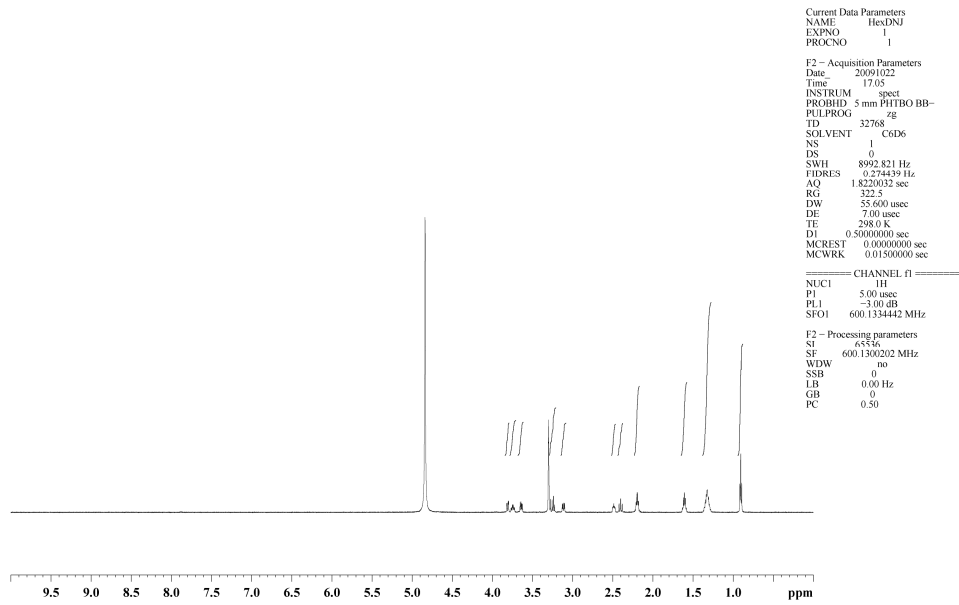
^{13}C NMR of **21**.



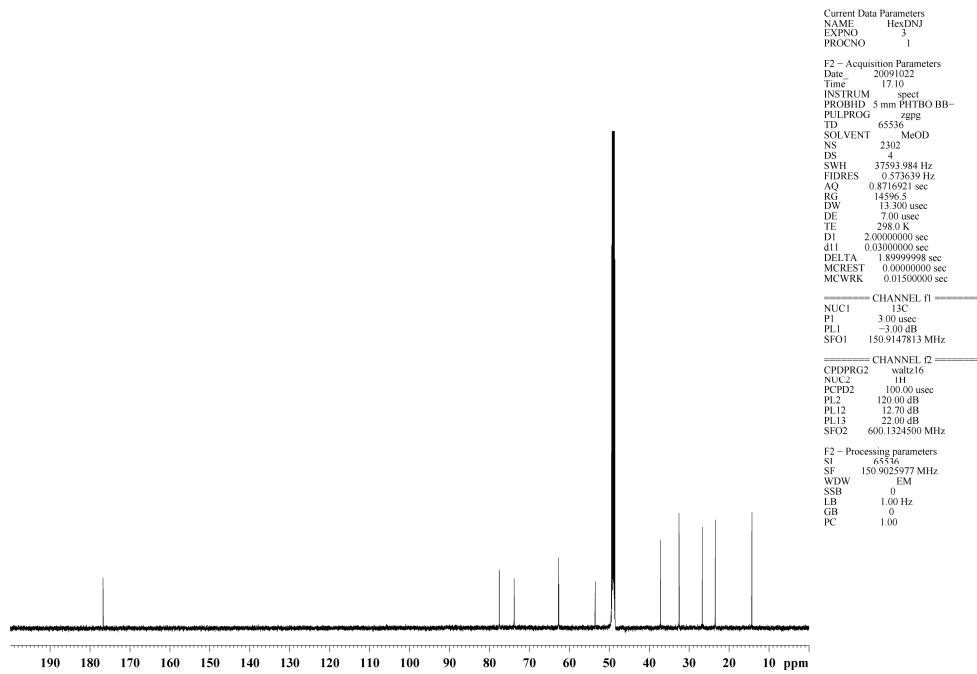
^1H NMR of **22**.



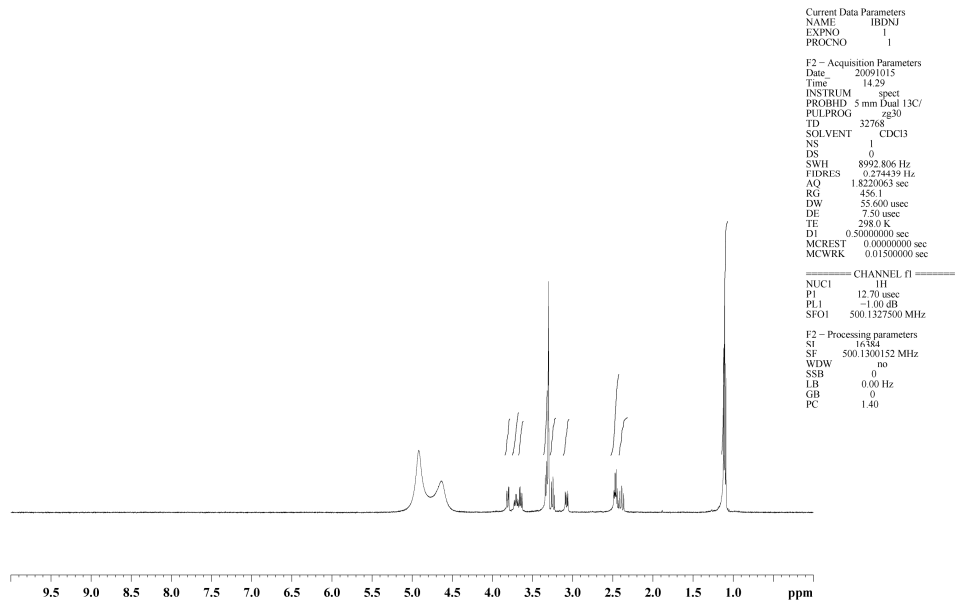
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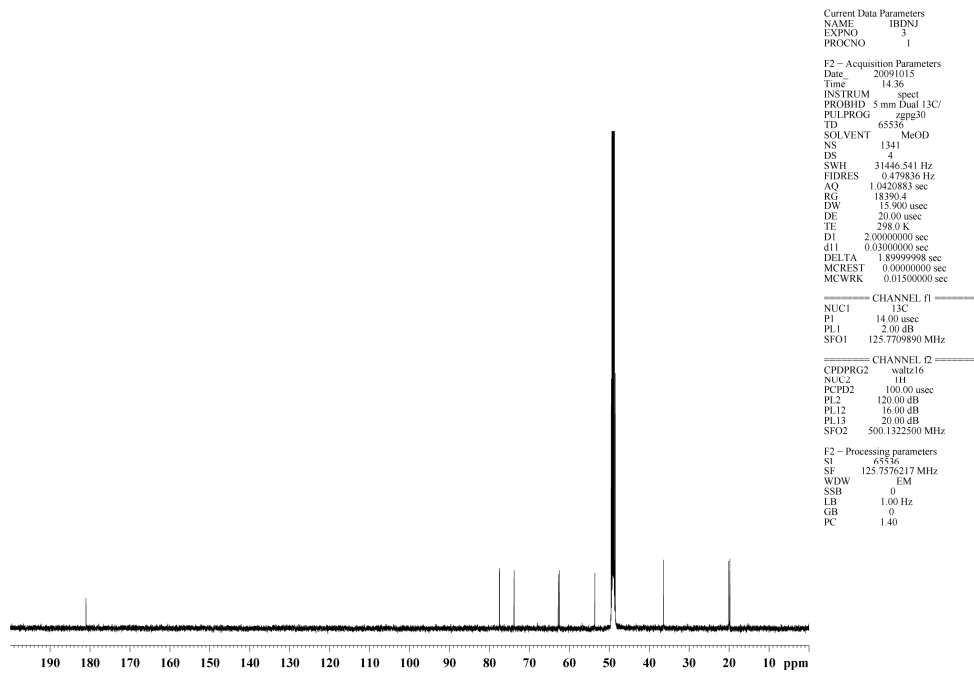
^1H NMR of **23**.



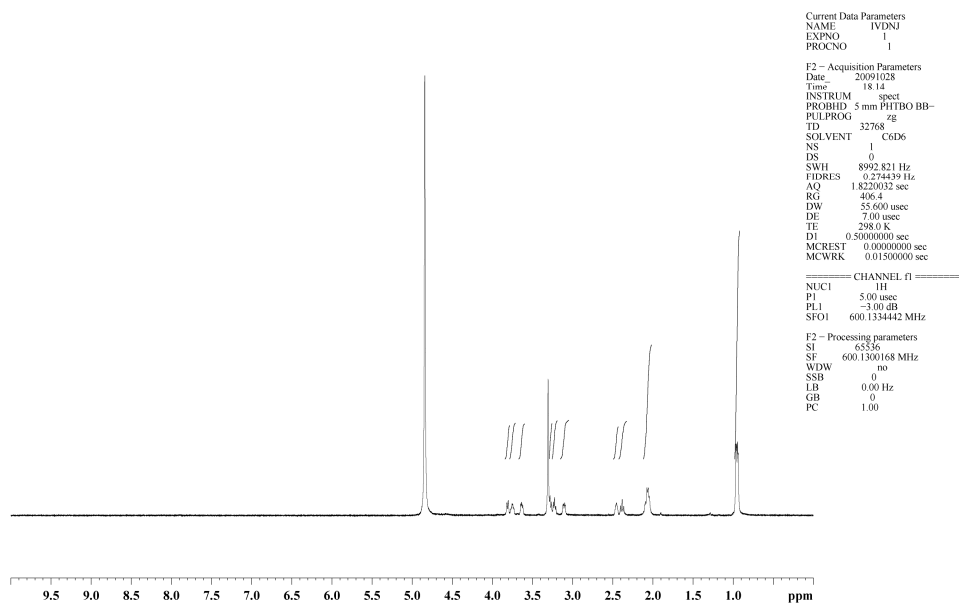
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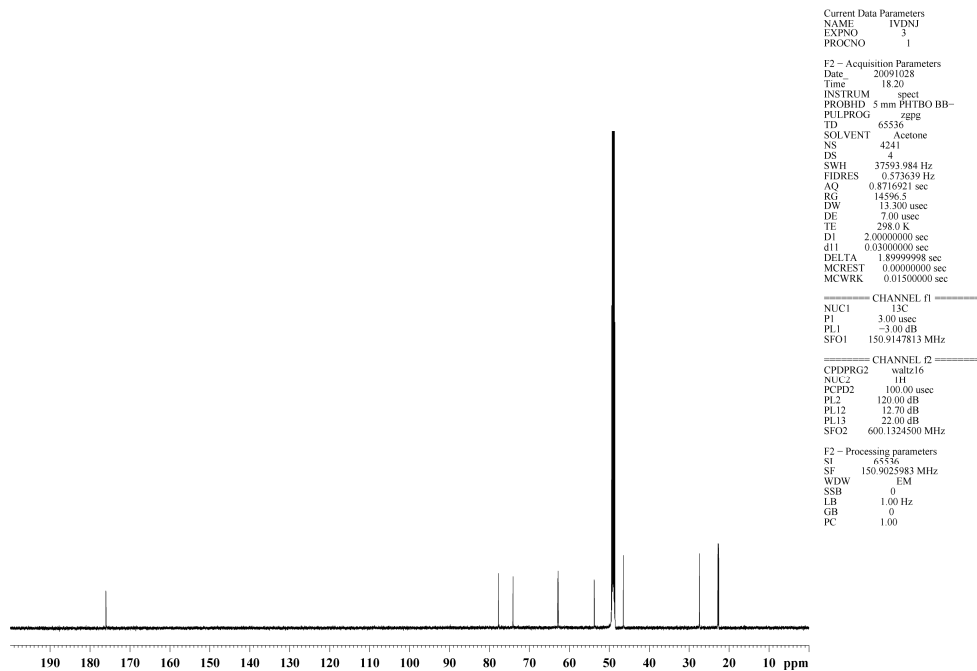
¹H NMR of 24.



¹³C NMR of 24.



^1H NMR of **25**.



^{13}C NMR of **25**.