

Supporting Information

Metal-Free Tandem Approach to Structurally Diverse N-Heterocycles: Synthesis of 1,2,4-Oxadiazoles and Pyrimidinones

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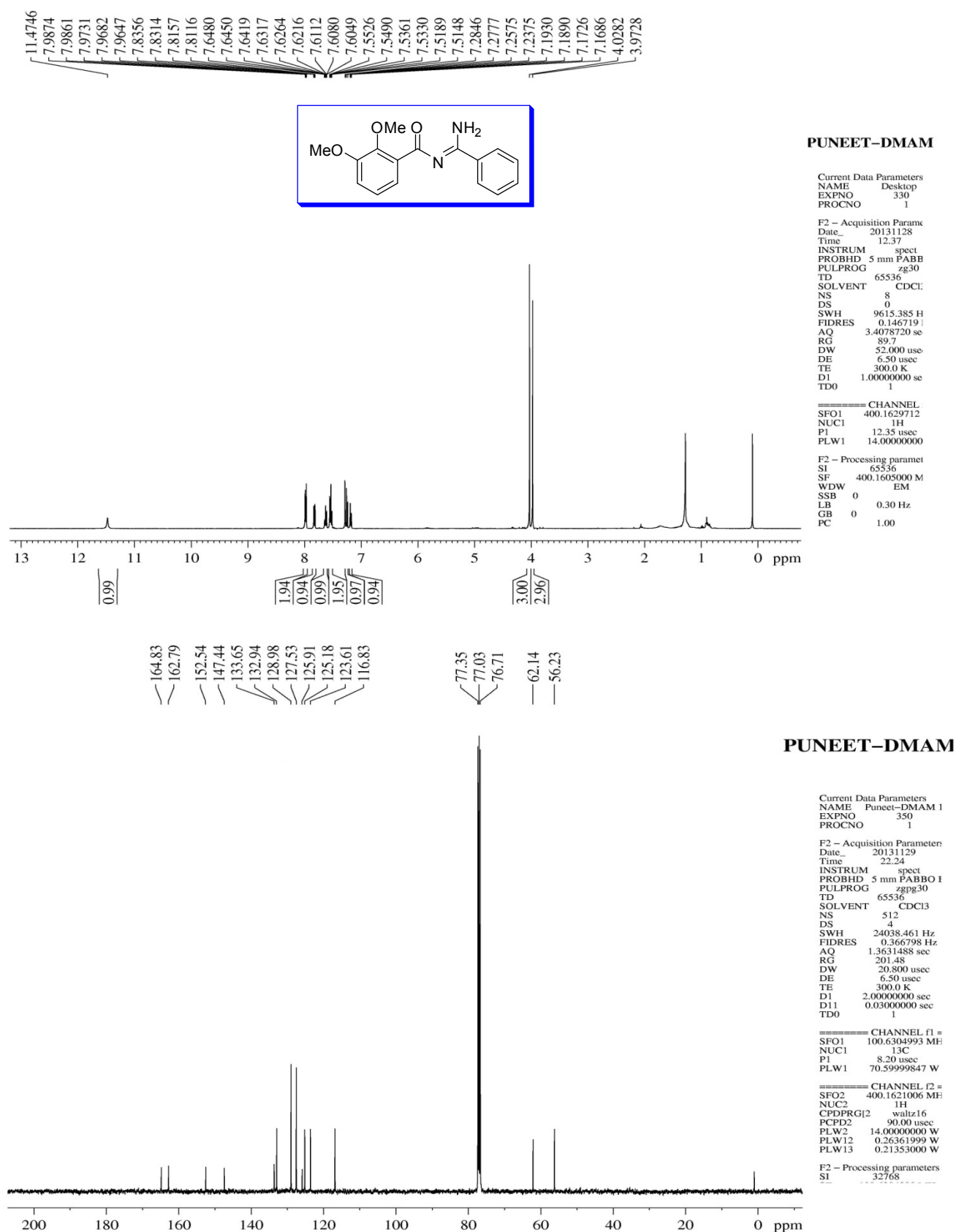


Figure 1: ¹H and ¹³C Spectra of Acyl amidine

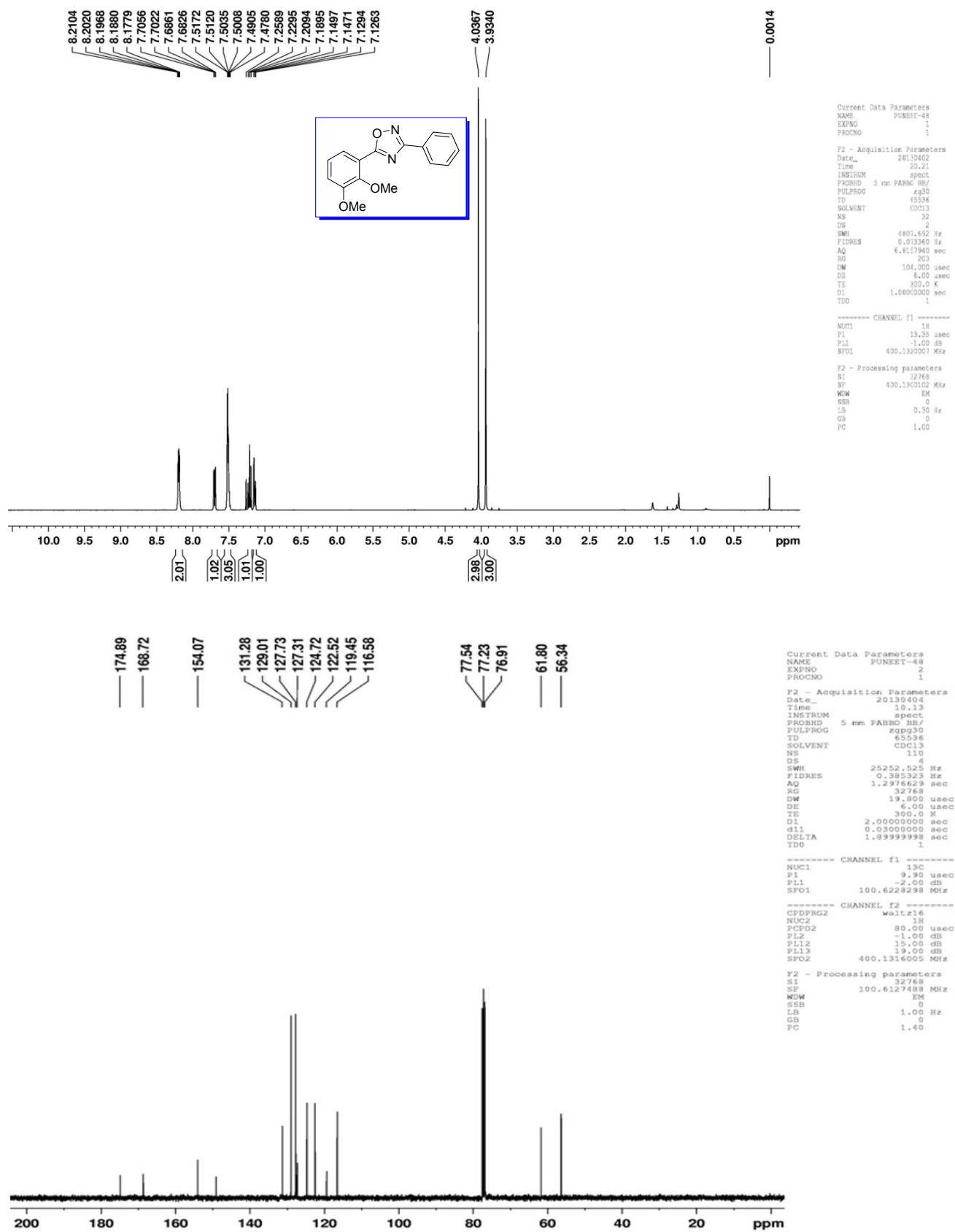


Figure 2: ¹H and ¹³C Spectra of compound 3a

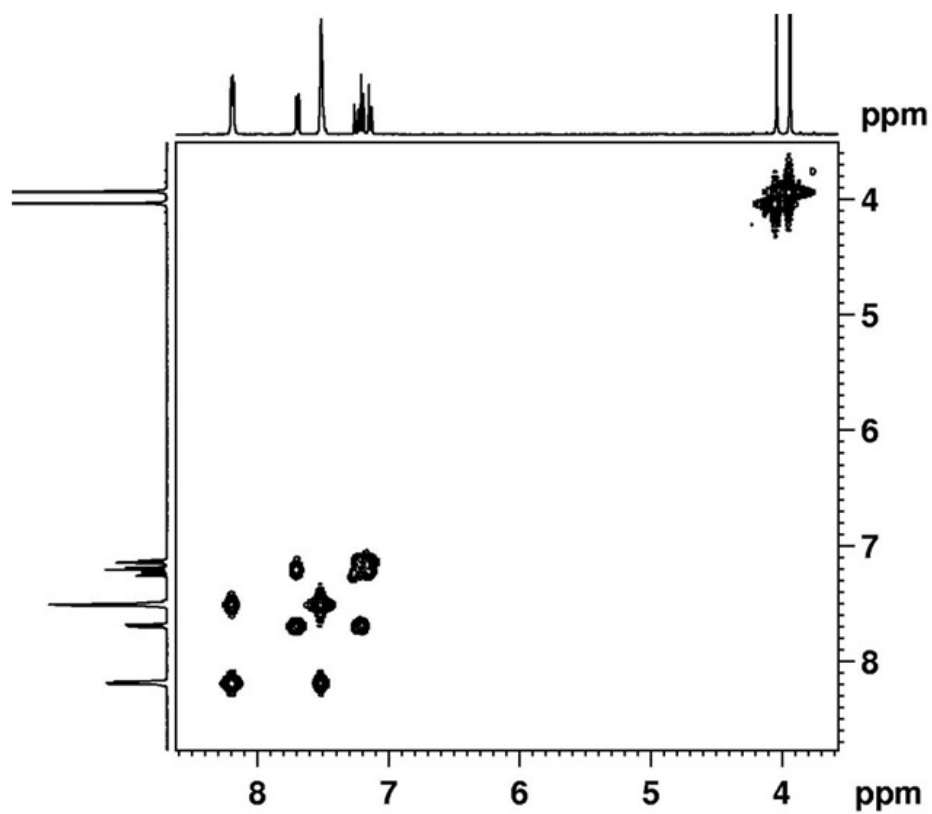


Figure 3: COSY spectrum of compound 3a

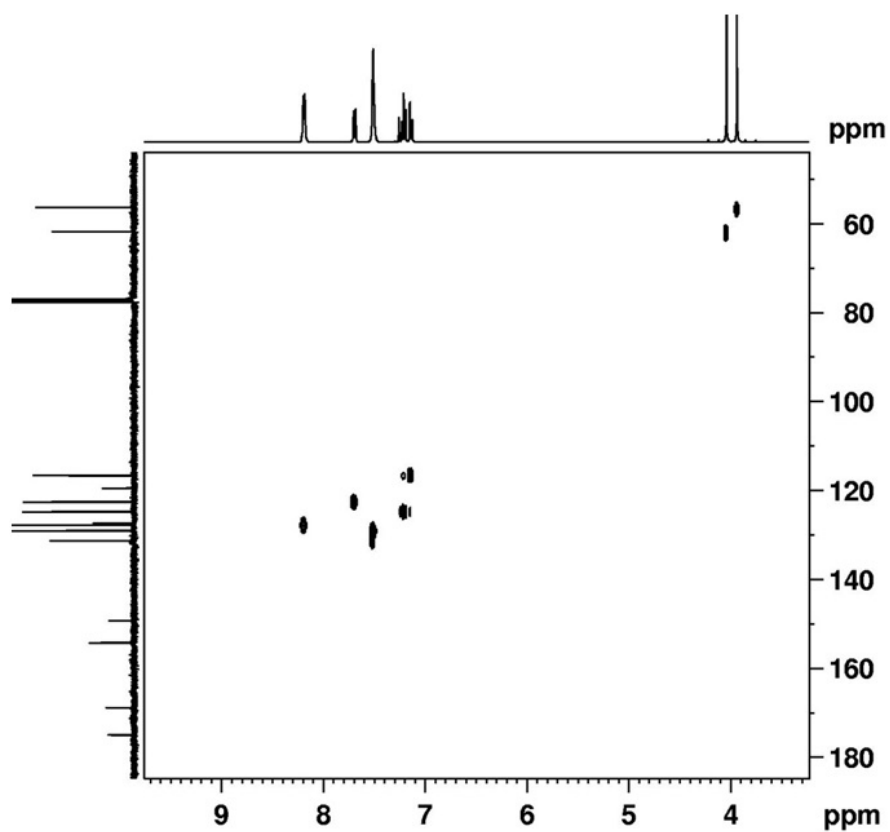


Figure 4: HSQC spectrum of compound 3a

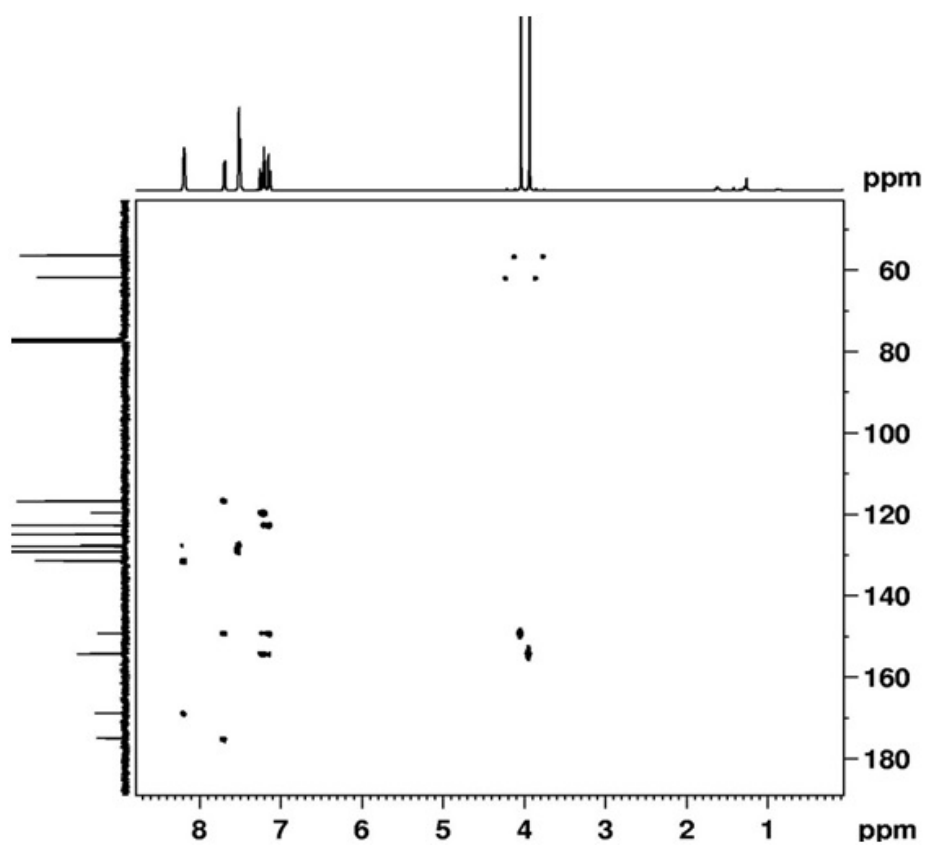
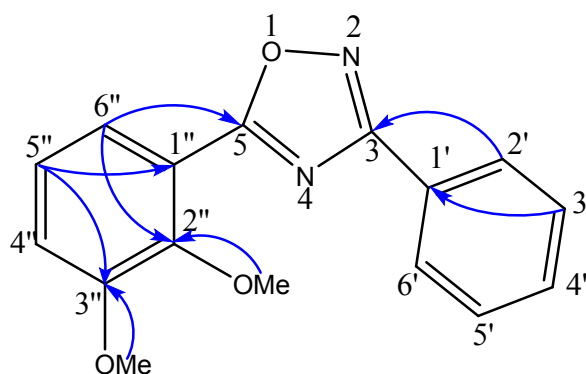


Figure 5: HMBC spectrum of compound 3a

Important HMBC correlations of 3a



Carbon position	¹³ C Chemical shift (ppm)	¹ H Chemical shift (ppm)
C-3	168.7	-
C-5	174.8	-

C-1'	127.3	-
C-2', C-6'	127.4	8.19 (m)
C-3', C-5'	129.0	7.51(m)
C-4'	131.2	7.49 (m)
C-1''	119.4	-
C-2''	149.1	-
C-3''	154.0	-
C-4''	116.6	7.12 (dd, $J_1 = 8.0$ Hz, $J_2 = 1.2$ Hz)
C-5''	124.7	7.20 (t, $J = 8.0$ Hz)
C-6''	122.5	7.68 (dd, $J_1 = 7.8$ Hz, $J_2 = 1.6$ Hz)
C-2''-OMe	61.8	4.03 (s)
C-3''-OMe	56.3	3.93 (s)

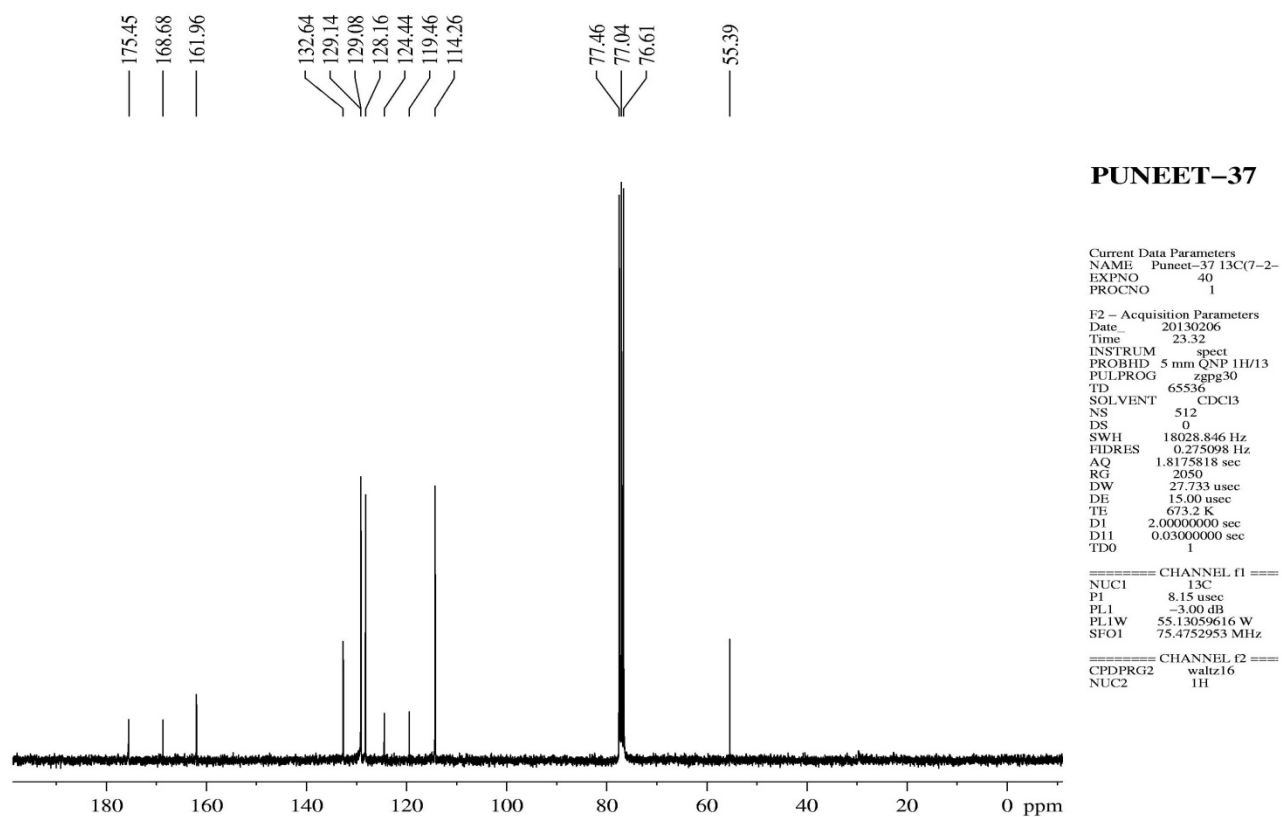
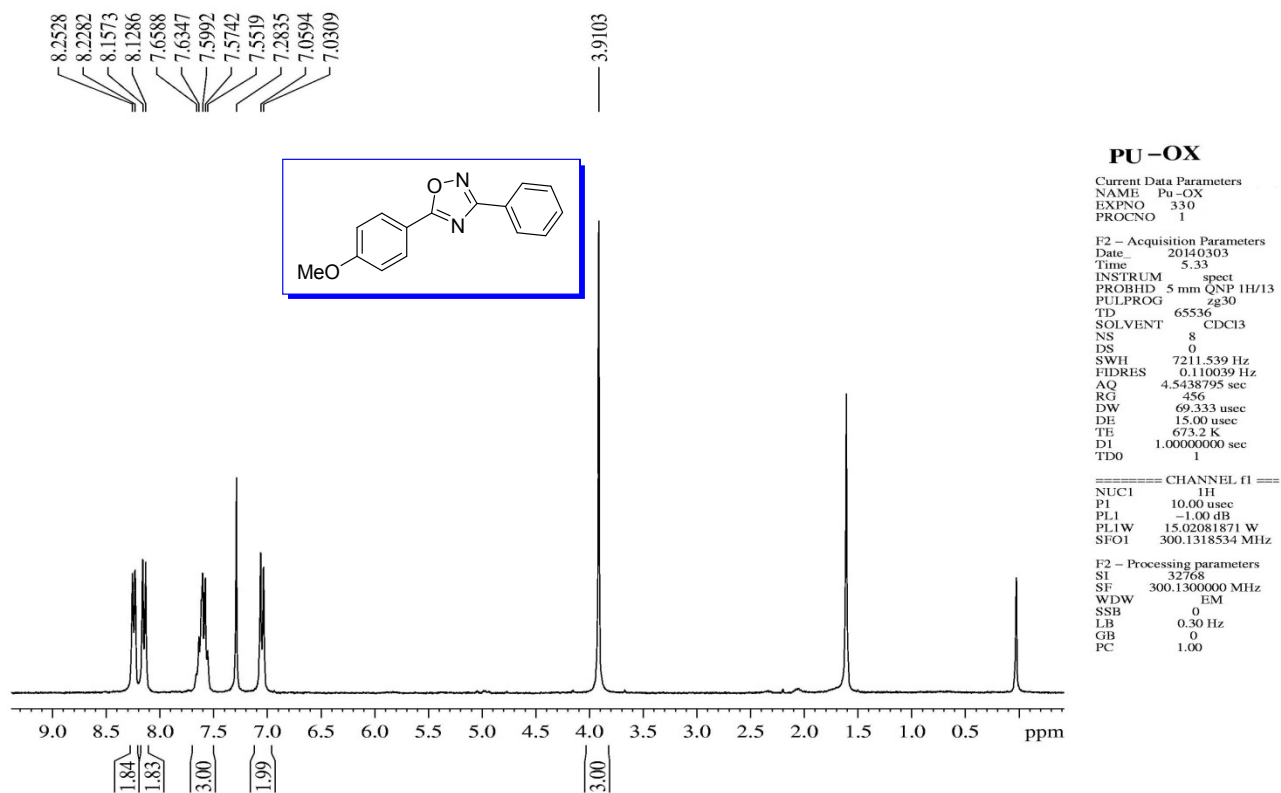


Figure 6: ^1H and ^{13}C Spectra of compound 3b

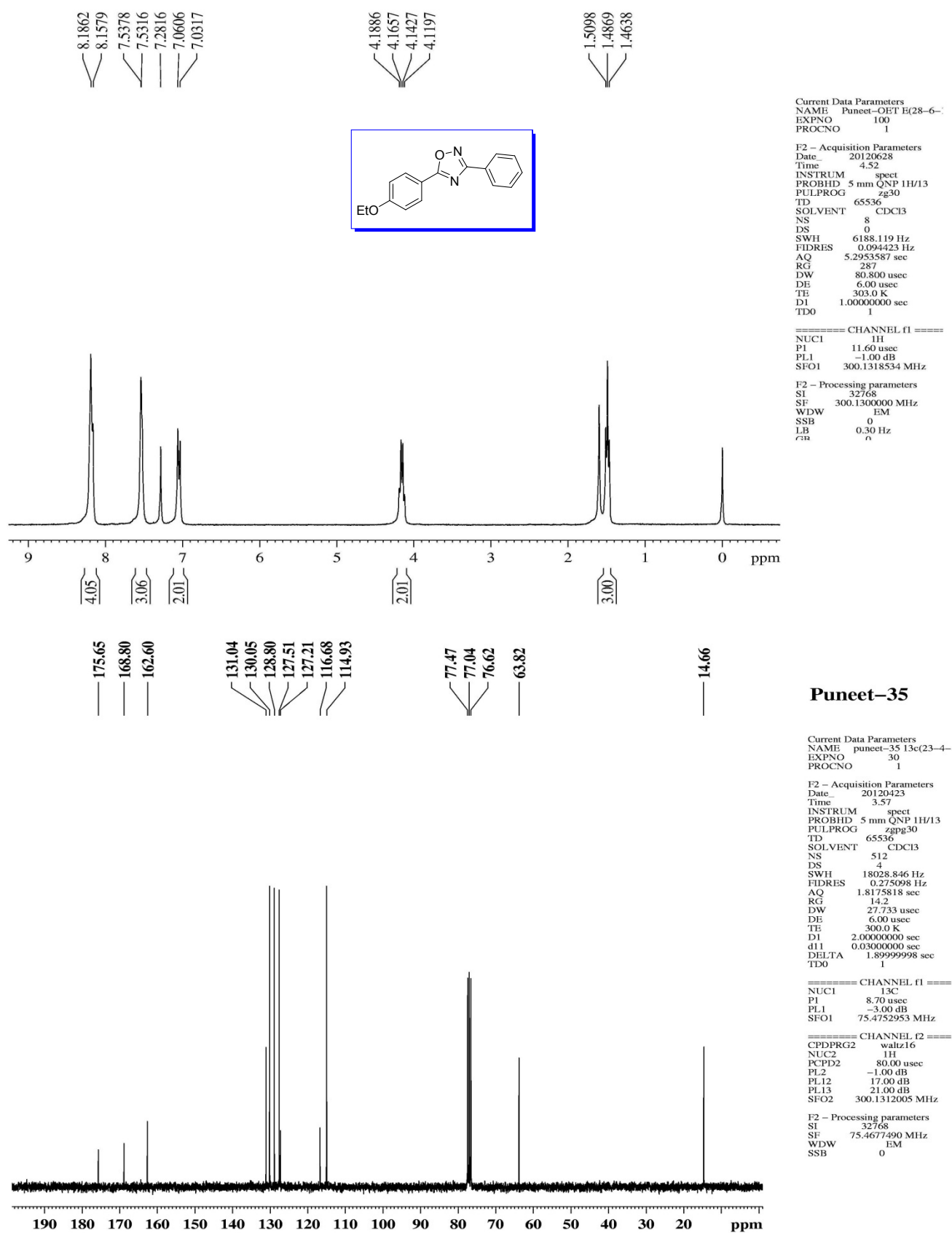


Figure 7: ^1H and ^{13}C Spectra of compound 3c

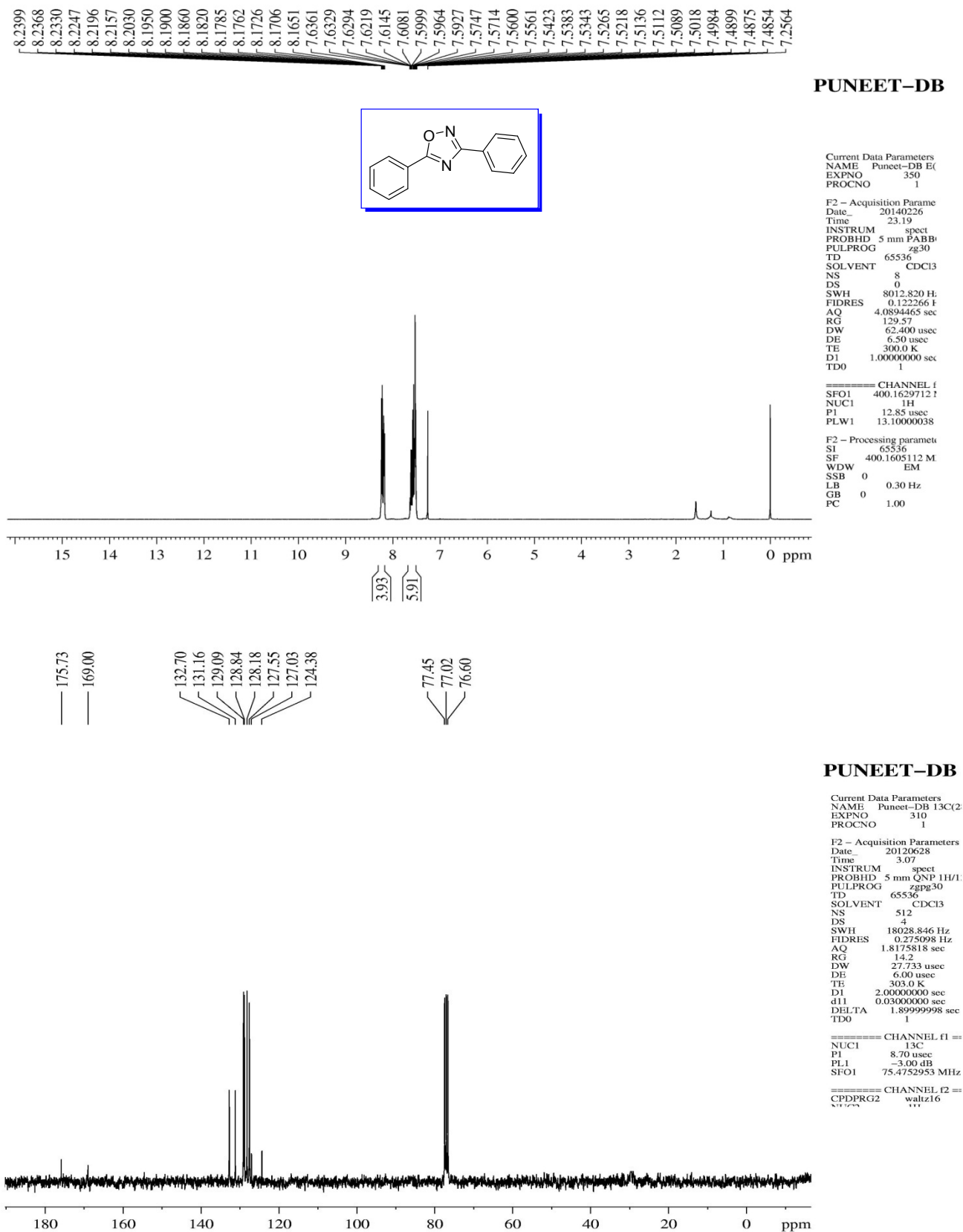
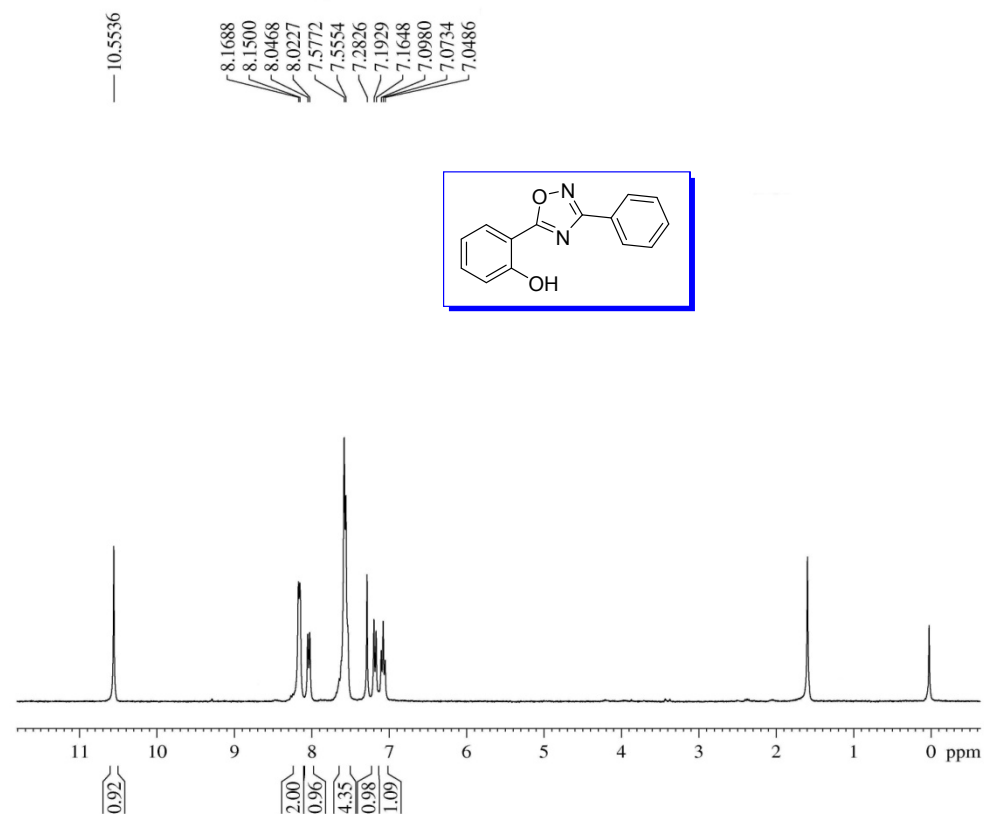


Figure 8: ^1H and ^{13}C Spectra of compound 3d



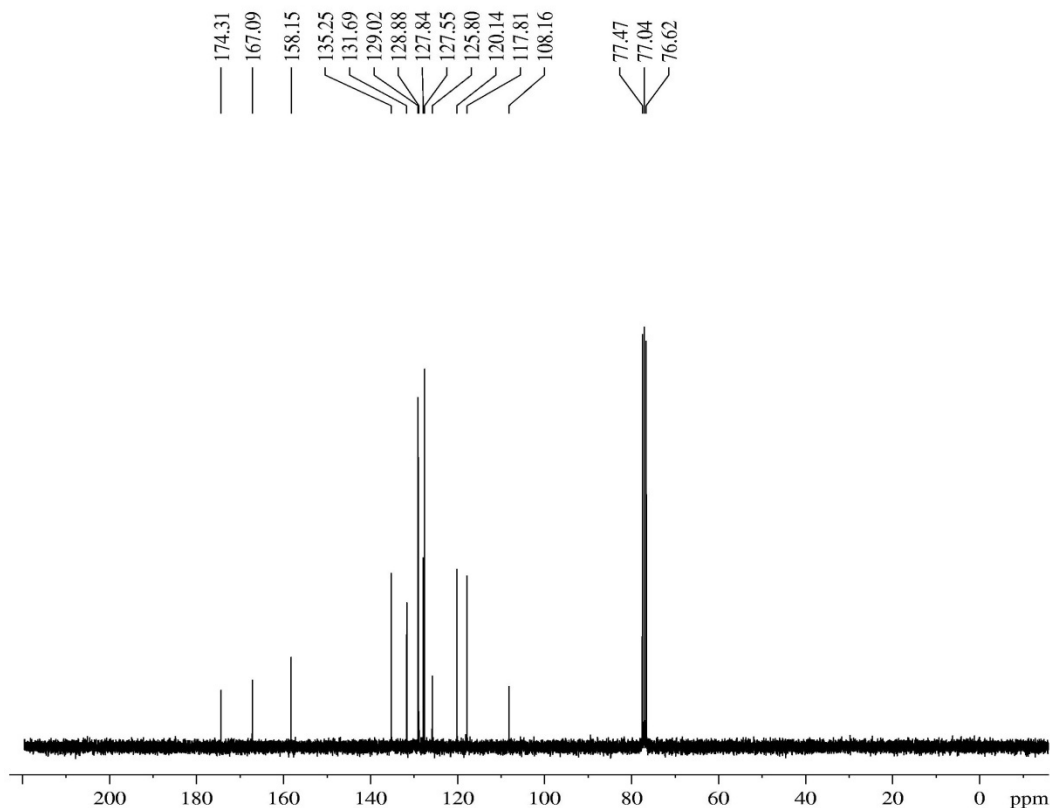
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FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 256
DW 80.800 usec
DE 6.00 usec
TE 297.5 K
D1 1.00000000 sec
TD0 1

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PL1 -1.00 dB
SFO1 300.1318534 MHz

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GB 0
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FIDRES 0.275098 Hz
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DW 27.733 usec
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TE 673.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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SFO1 75.4752953 MHz

===== CHANNEL f2 =====
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PCPD2 80.00 usec
PL2 -1.00 dB
PL12 17.06 dB
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PL13W 0.00477406 W

Figure 9: ^1H and ^{13}C Spectra of compound 3e

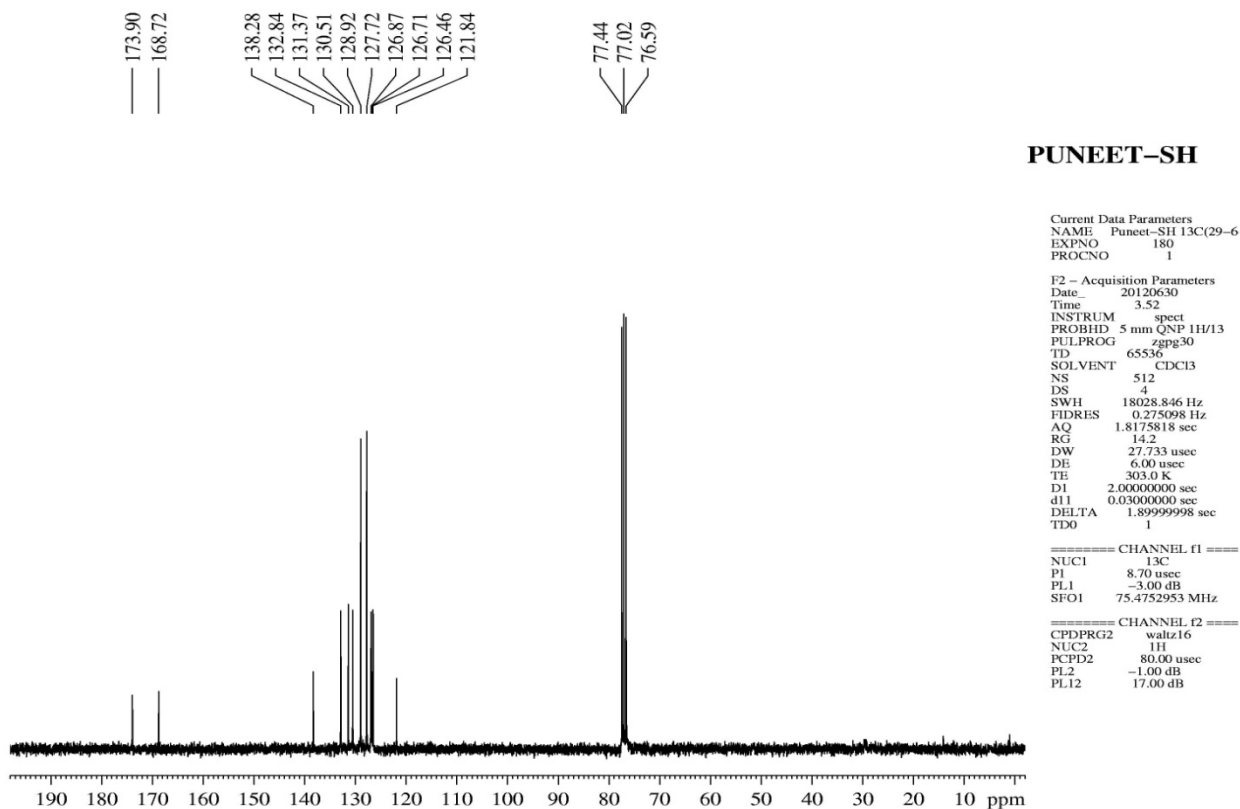
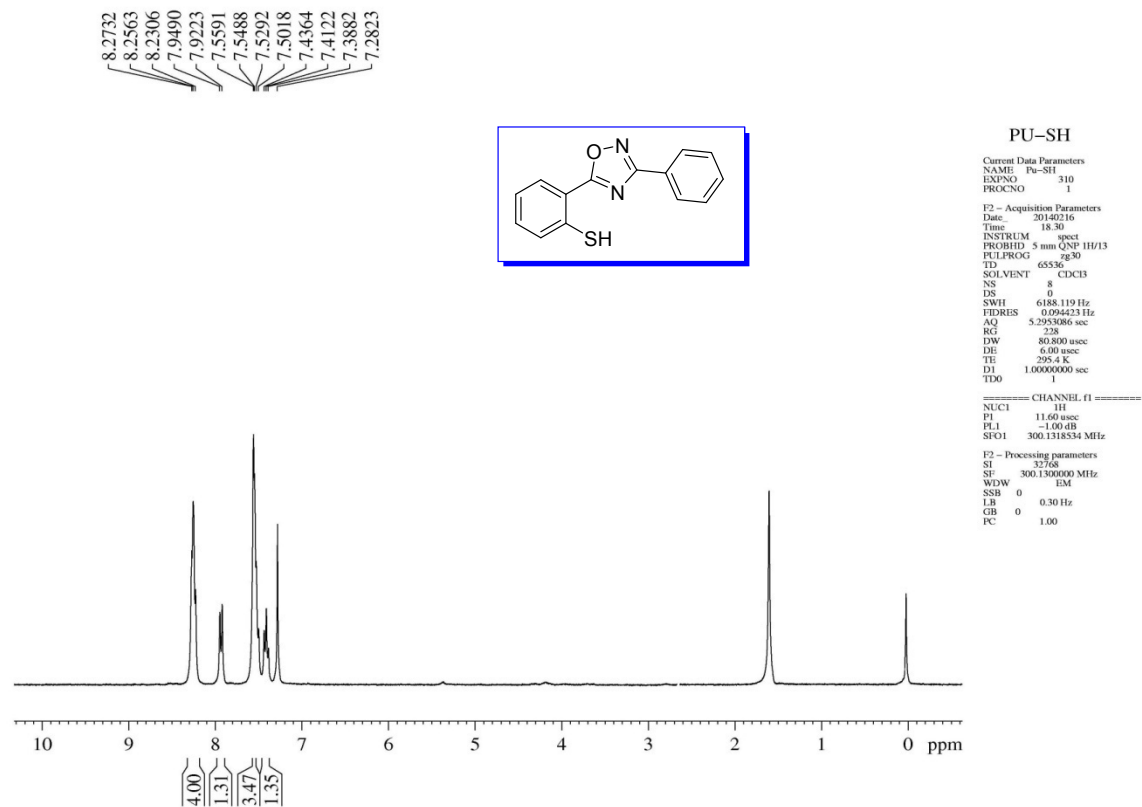


Figure 10: ¹H and ¹³C Spectra of compound 3f

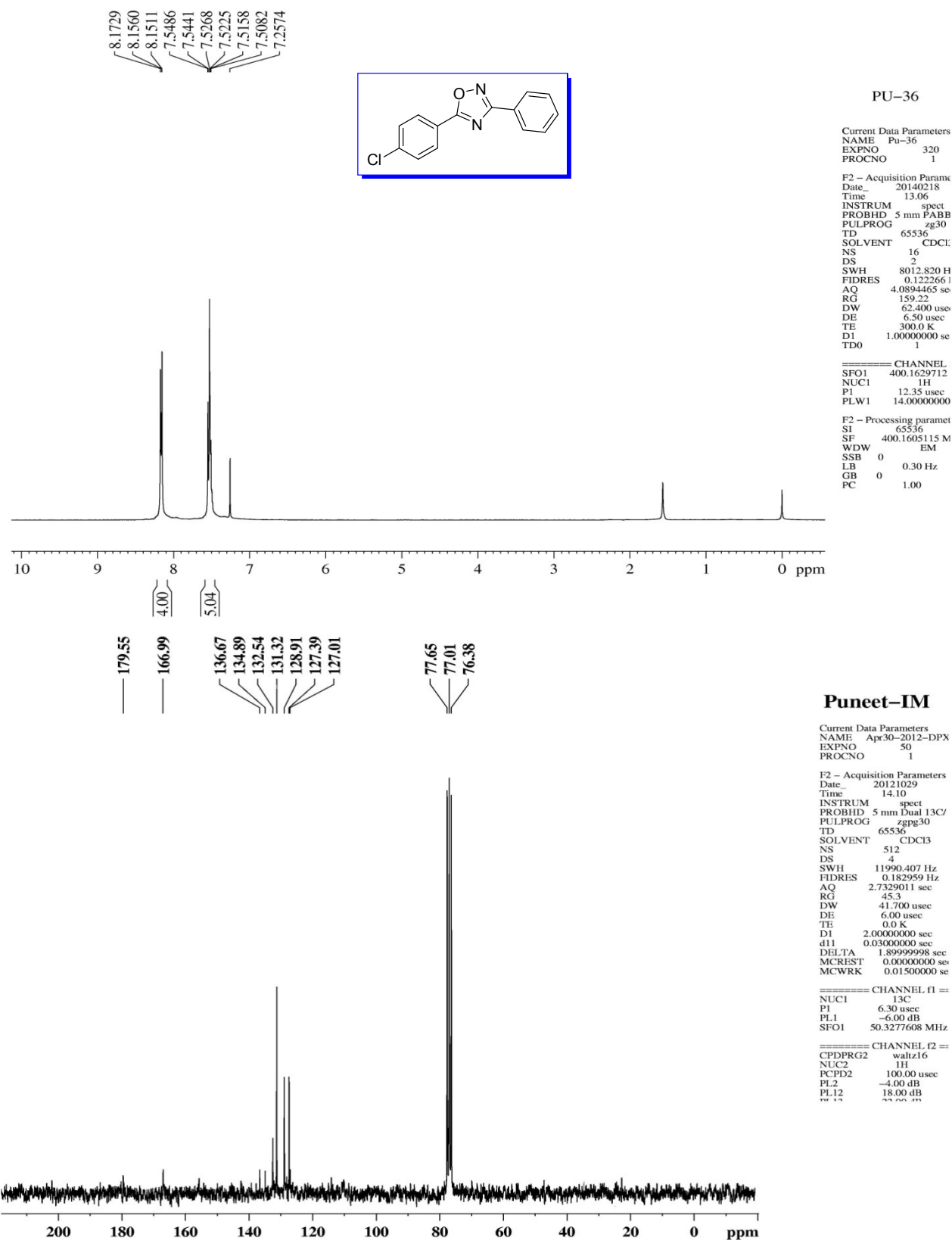


Figure11: ¹H and ¹³C Spectra of compound 3g

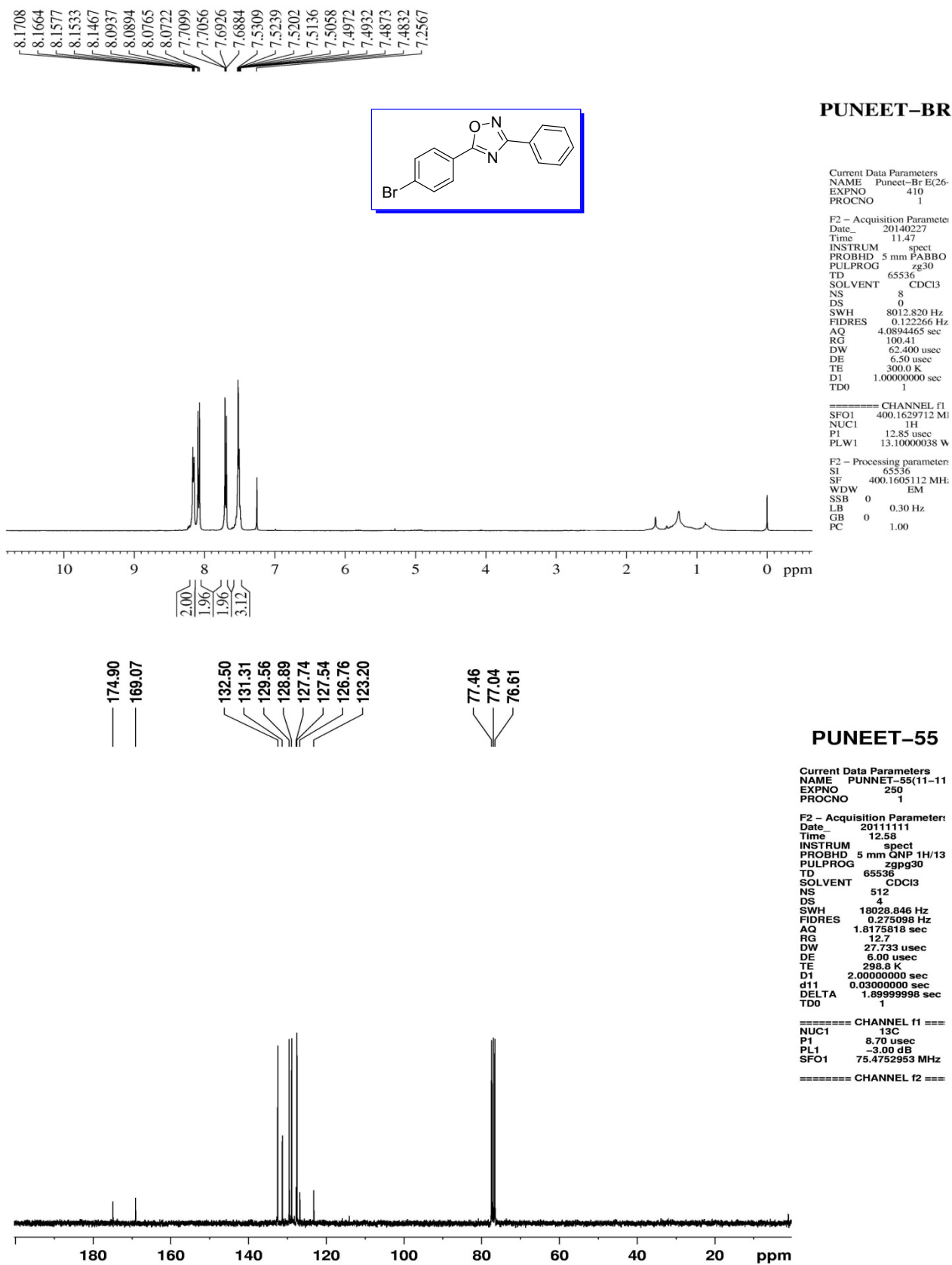


Figure 12: ^1H and ^{13}C Spectra of compound 3h

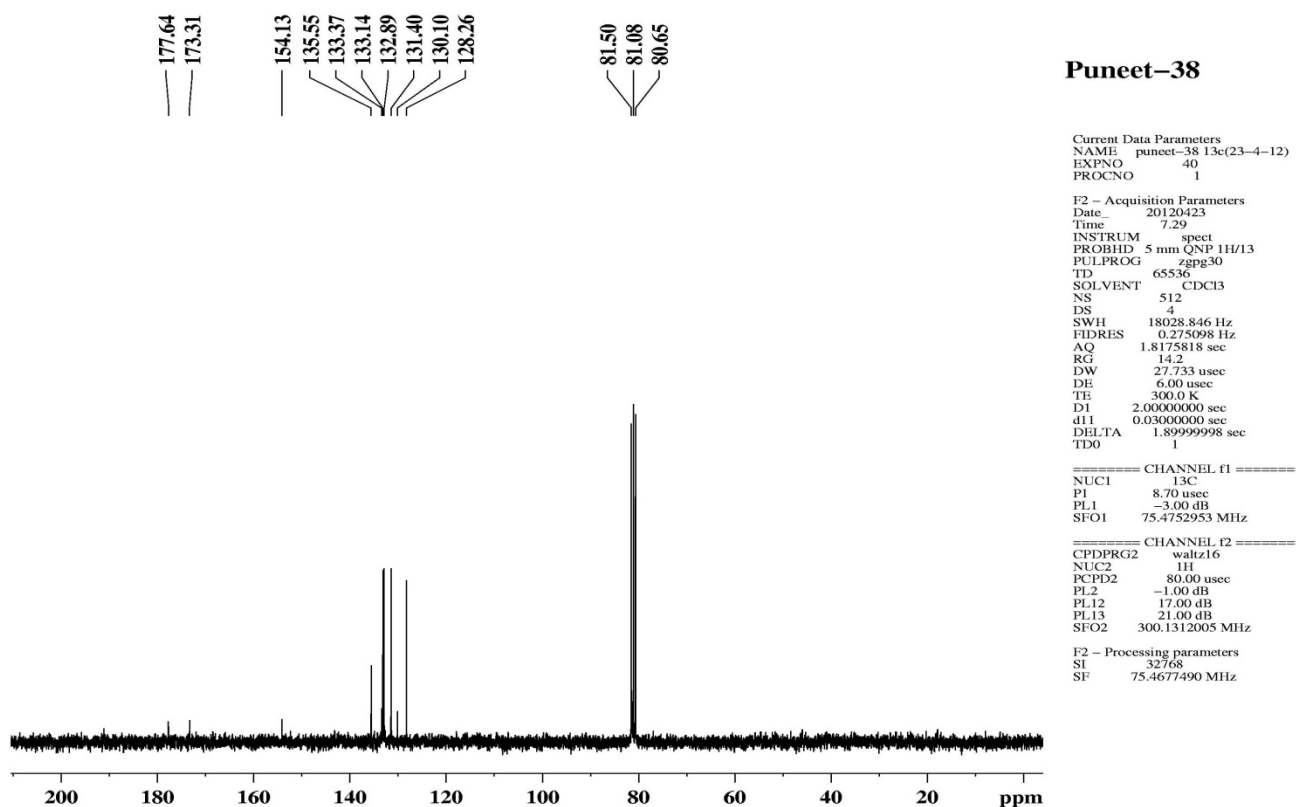
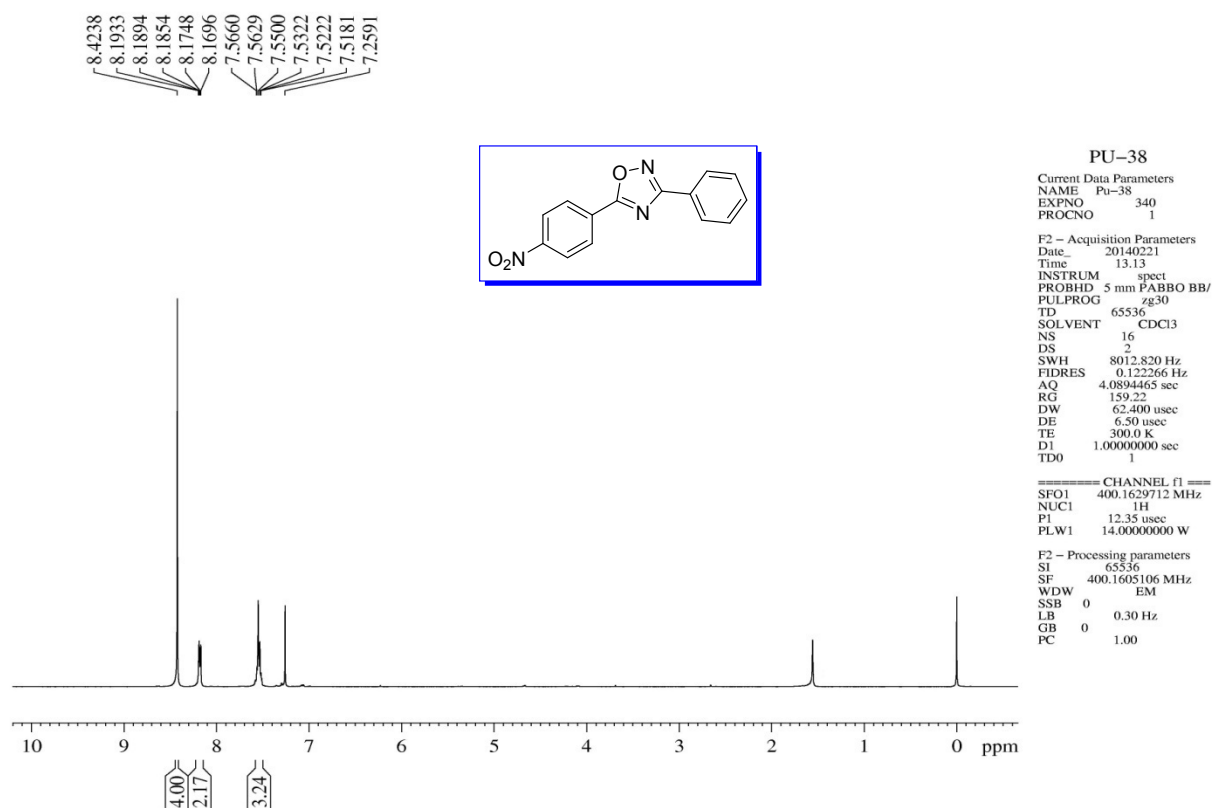


Figure 13: ^1H and ^{13}C Spectra of compound 3i

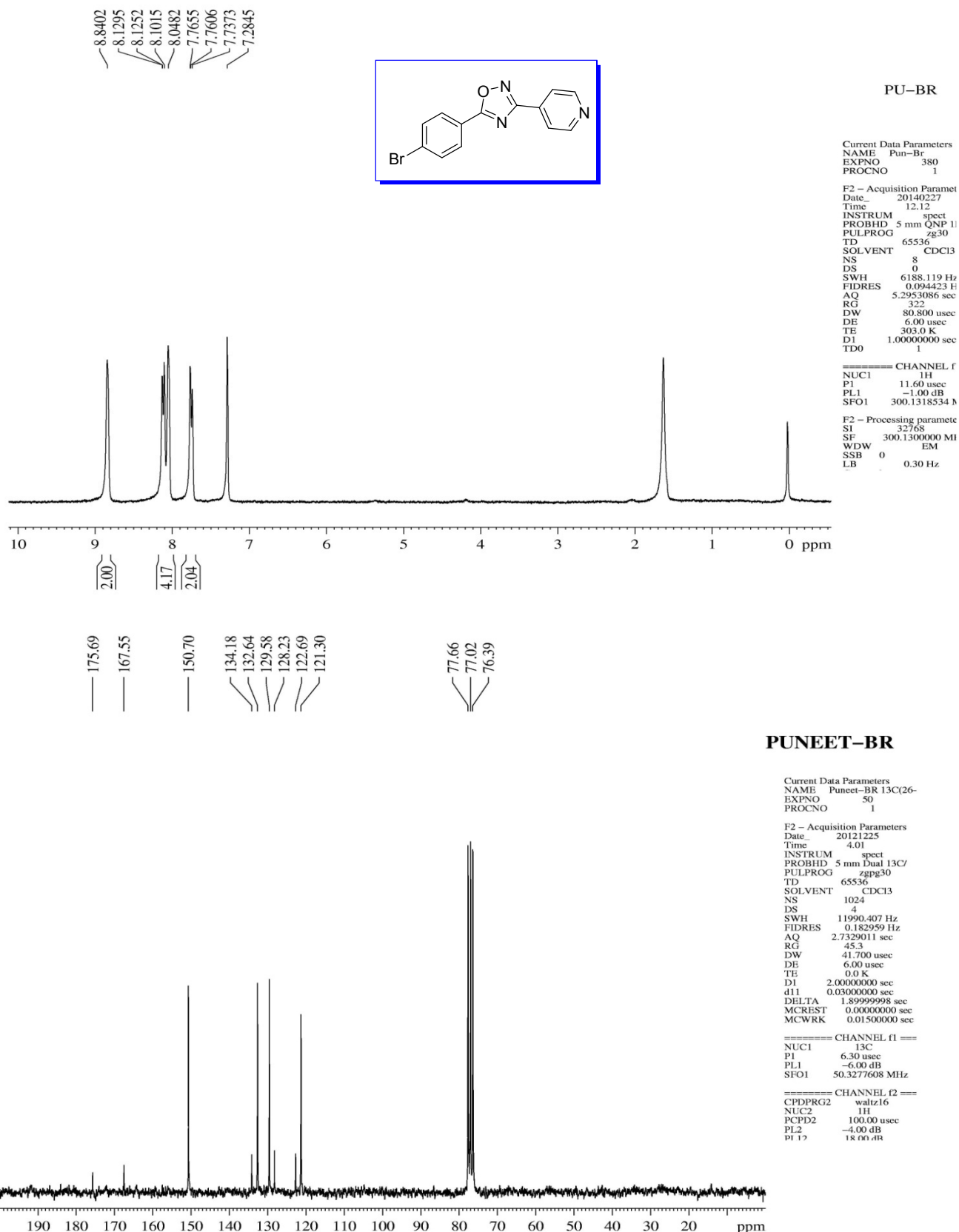


Figure 14: ^1H and ^{13}C Spectra of compound 3j

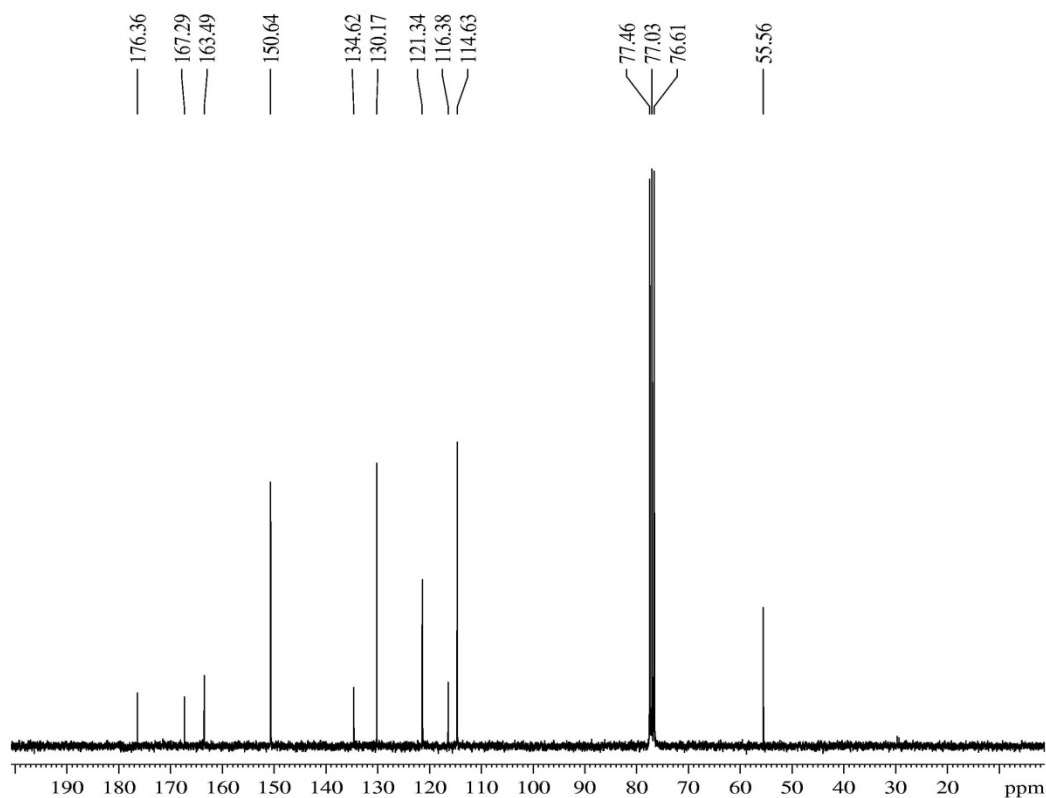
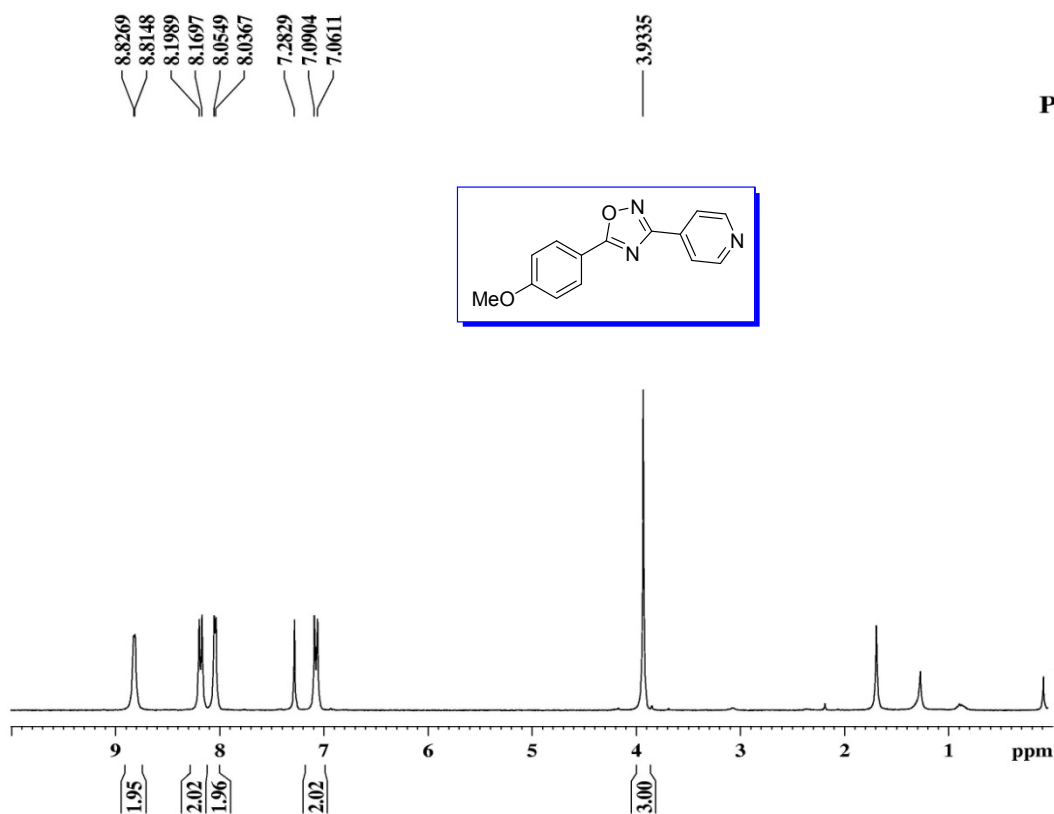


Figure 15: ¹H and ¹³C Spectra of compound 3k

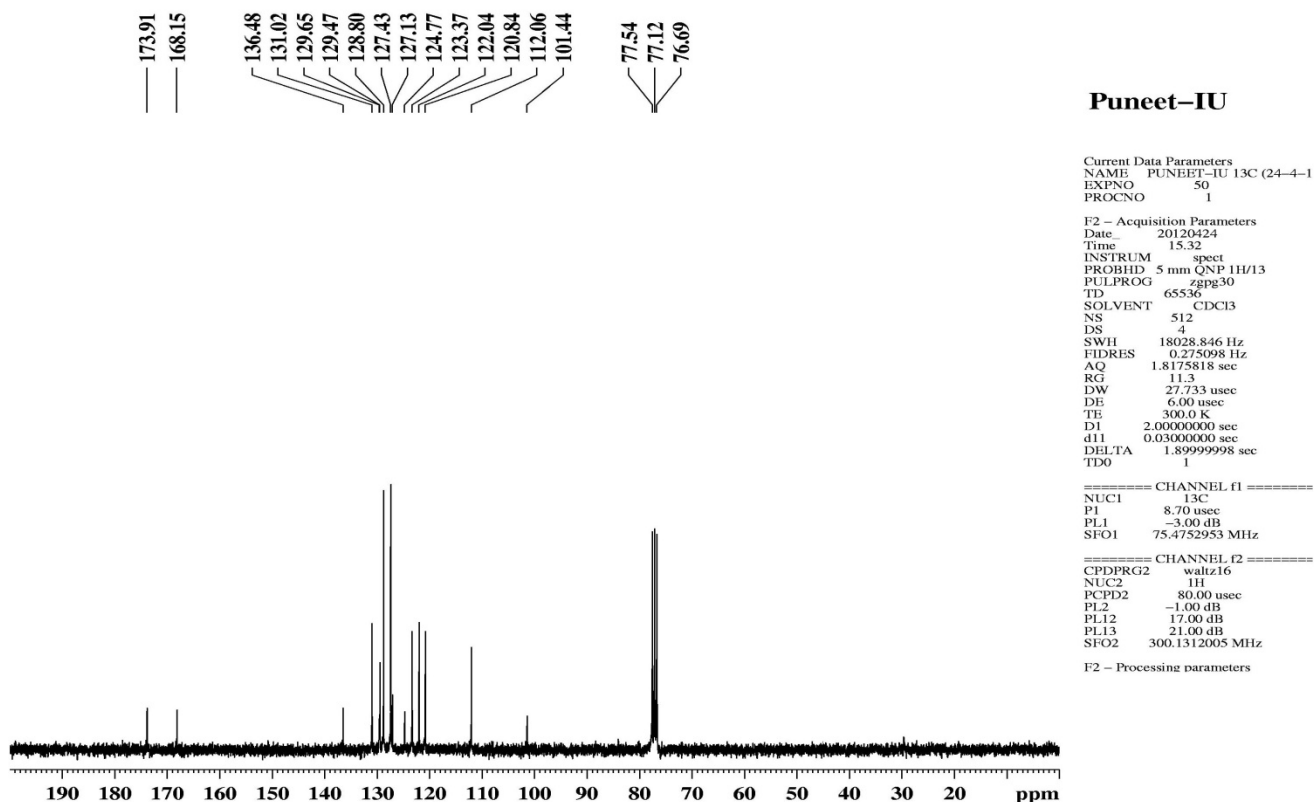
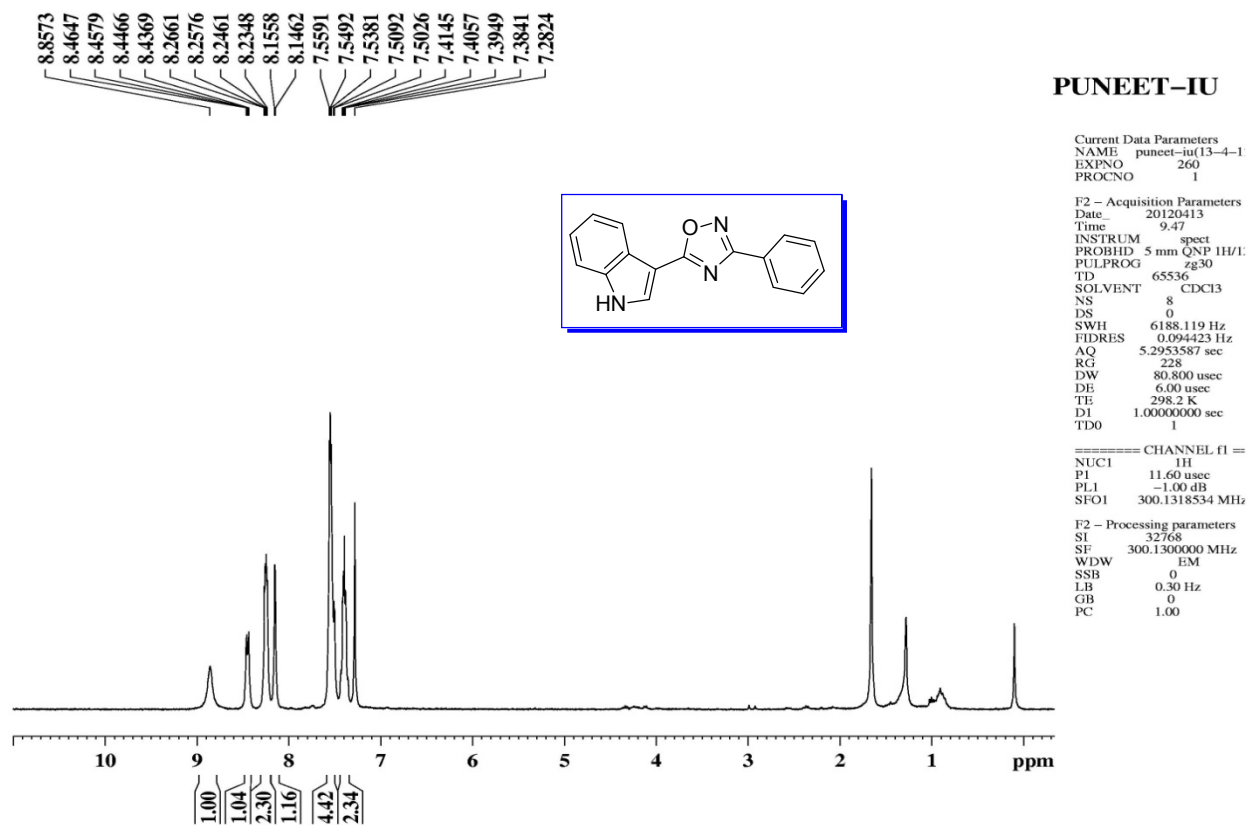


Figure 16: ¹H and ¹³C Spectra of compound 31

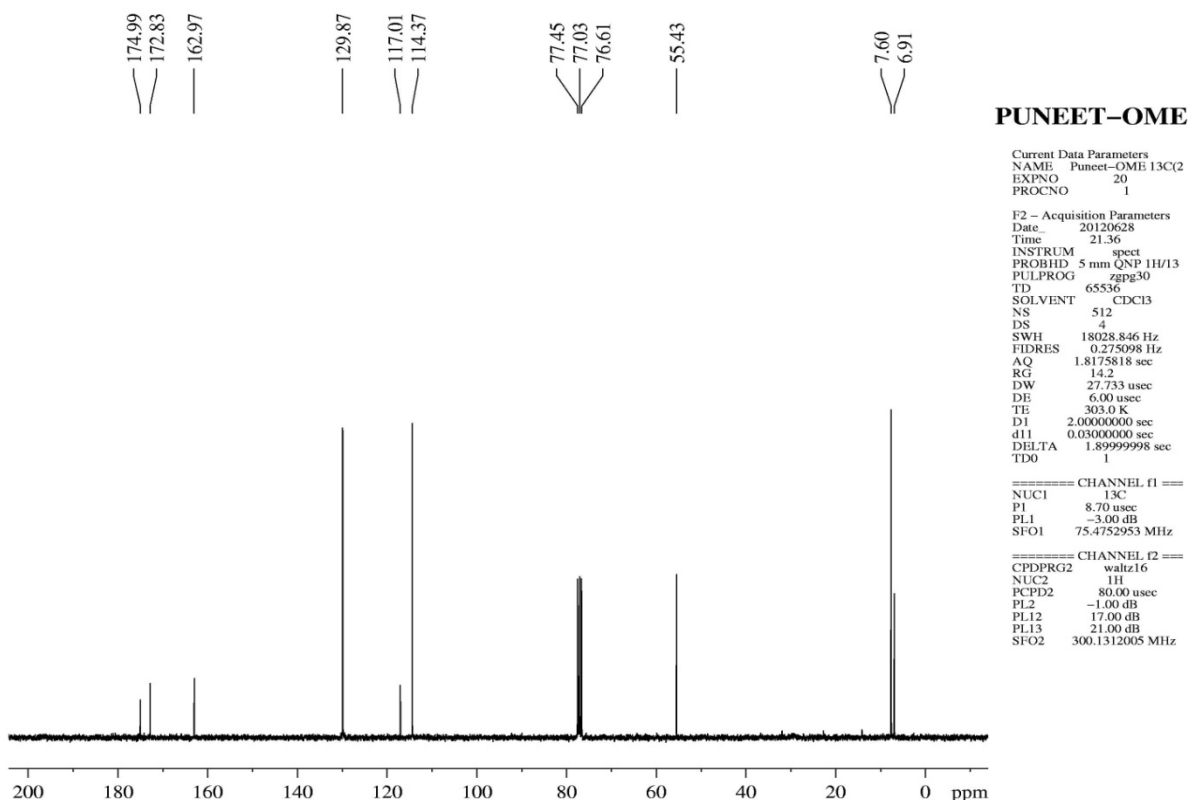
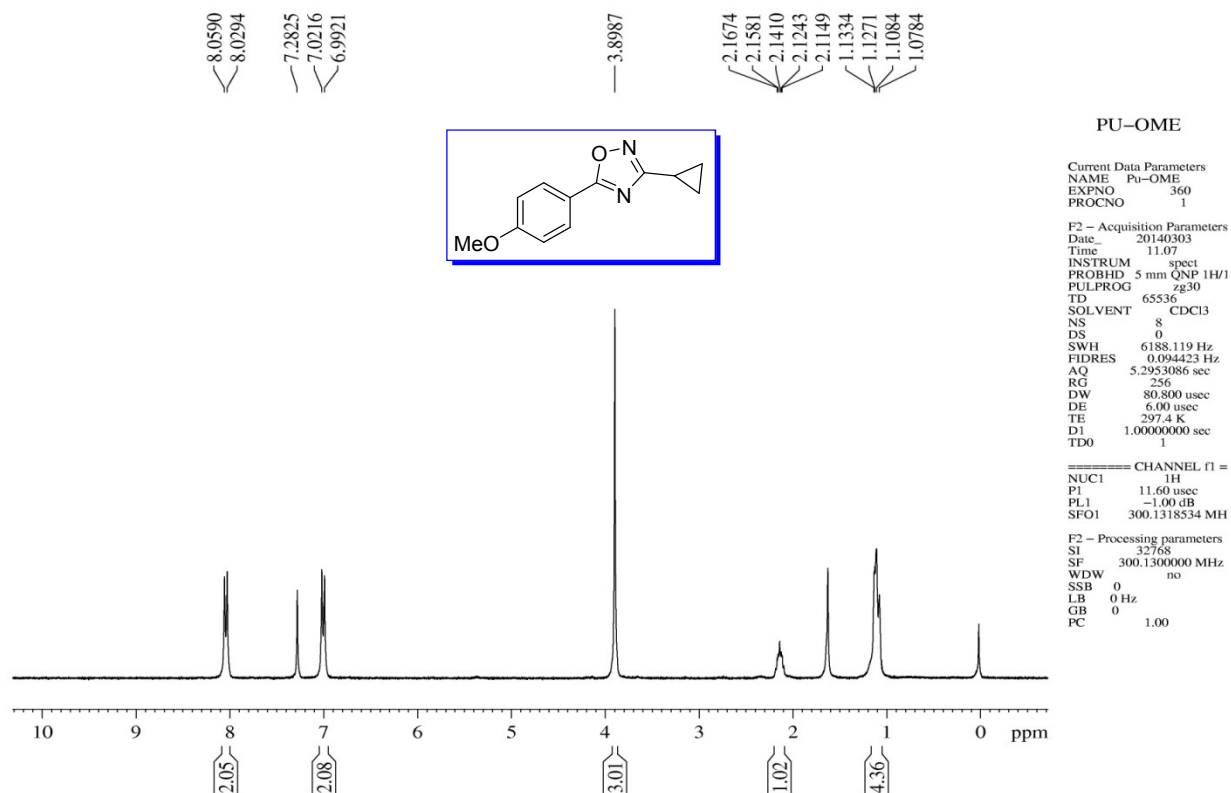
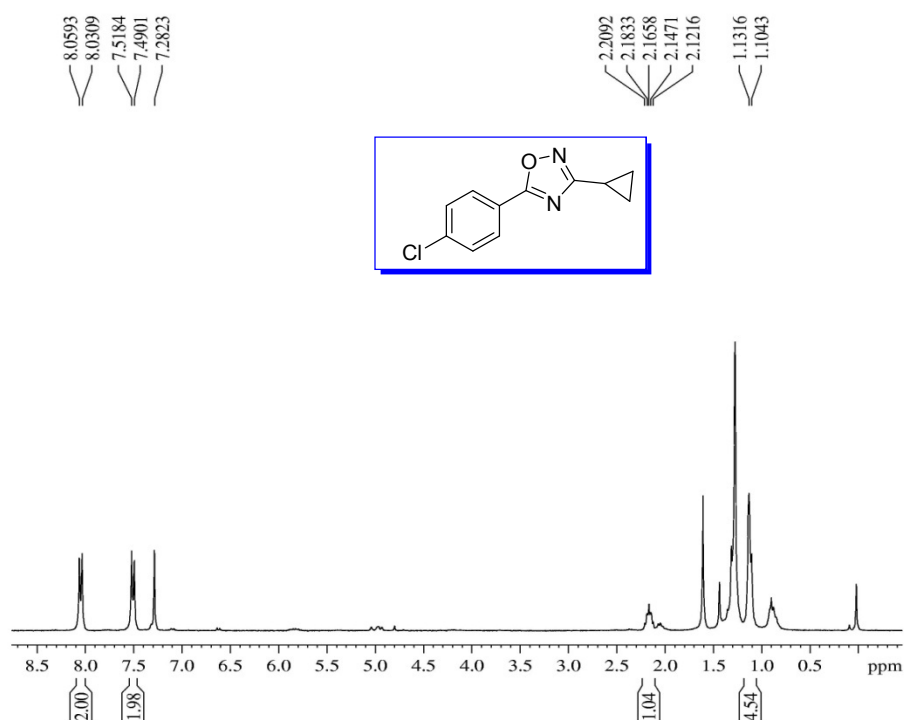
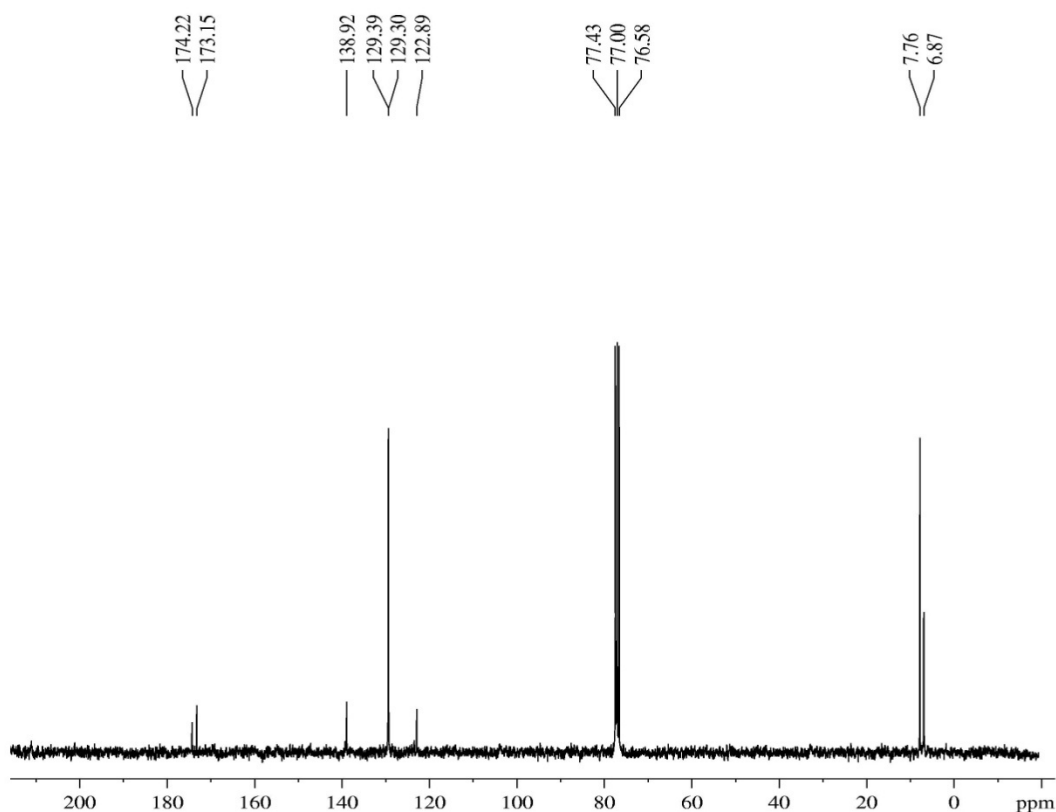


Figure 17: ^1H and ^{13}C Spectra of compound 3m



PUNEET-CL

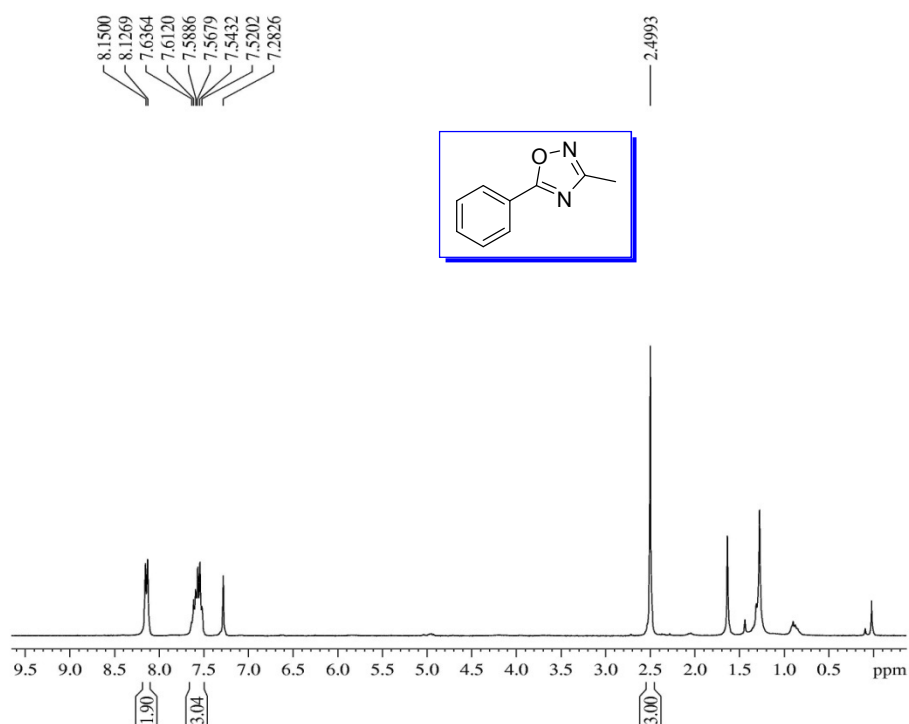
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 FIDRES 0.094423 Hz
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 DE 6.00 usec
 TE 297.5 K
 D1 1.00000000 sec
 TDO 1
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 WDW EM
 SSB 0
 GB 0



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 FIDRES 0.275098 Hz
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 RG 14.2
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 DE 6.00 usec
 TE 303.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
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 PL1 -3.00 dB
 SFO1 75.4752953 MHz
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Figure 18: ¹H and ¹³C Spectra of compound 3n



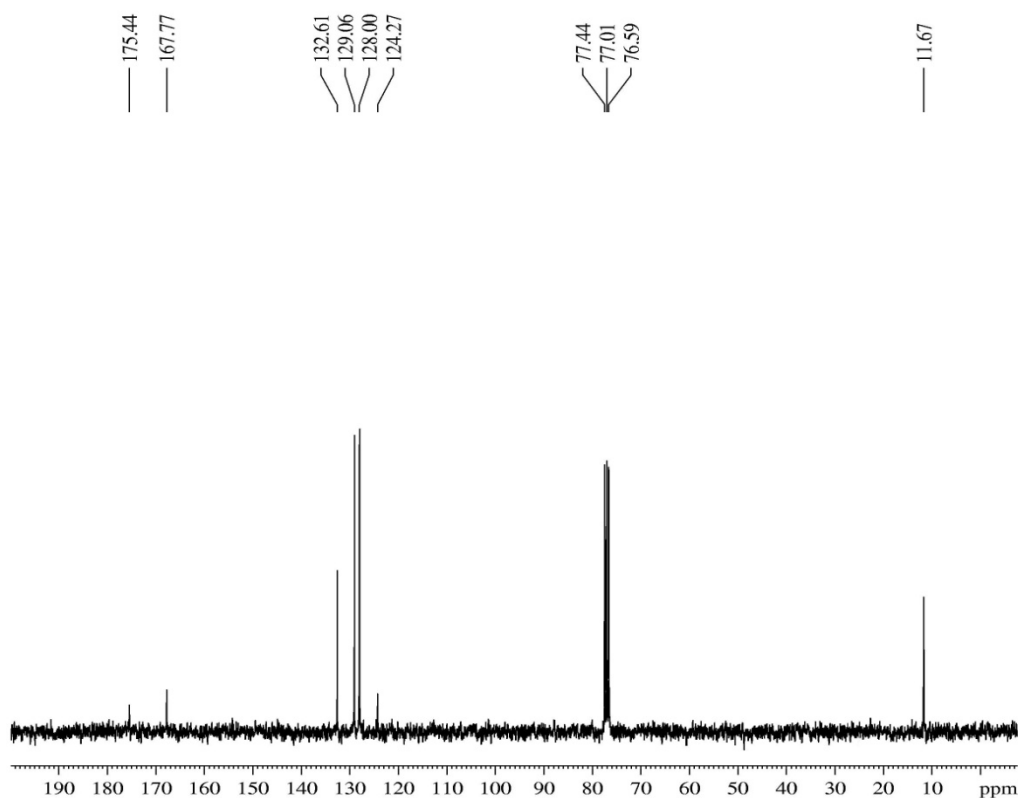
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TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 256
DW 80.800 usec
DE 6.00 usec
TE 297.5 K
D1 1.00000000 sec
TD0

===== CHANNEL f1 =====
NUC1 1H
P1 11.60 usec
PL1 -1.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz



PUNEET-AB

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PROCNO 1

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SOLVENT CDCl3
NS 512
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 14.2
DW 27.733 usec
DE 6.00 usec
TE 303.0 K
D1 2.00000000 sec
d11 0.05000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
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P1 8.70 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 17.00 dB
PL13 21.00 dB

Figure 19: ¹H and ¹³C Spectra of compound 3o

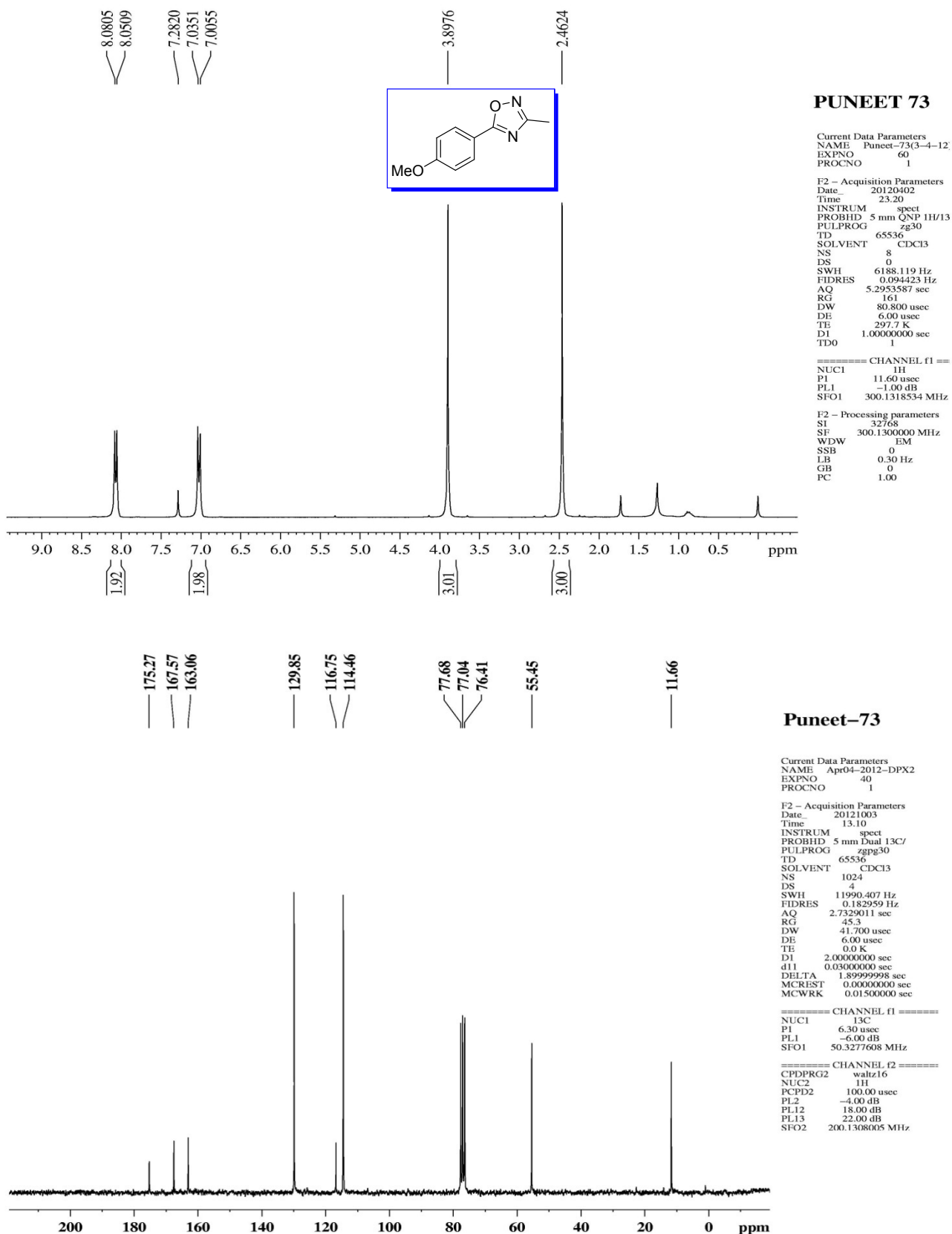


Figure 20: ¹H and ¹³C Spectra of compound 3p

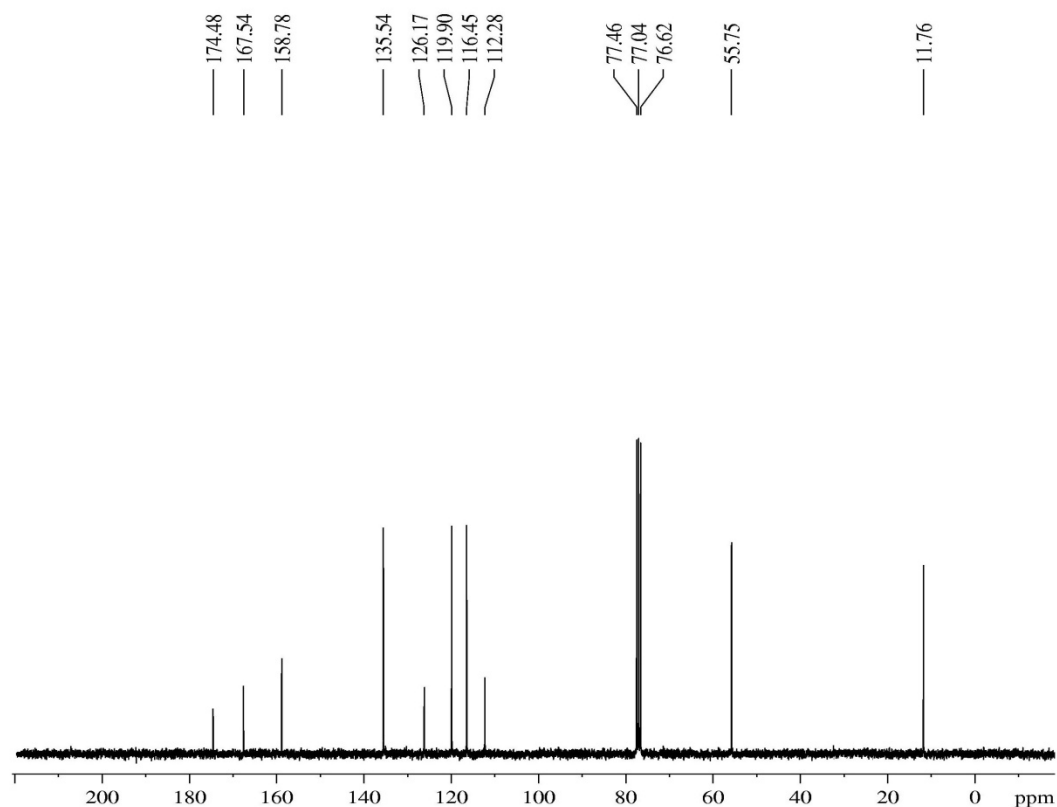
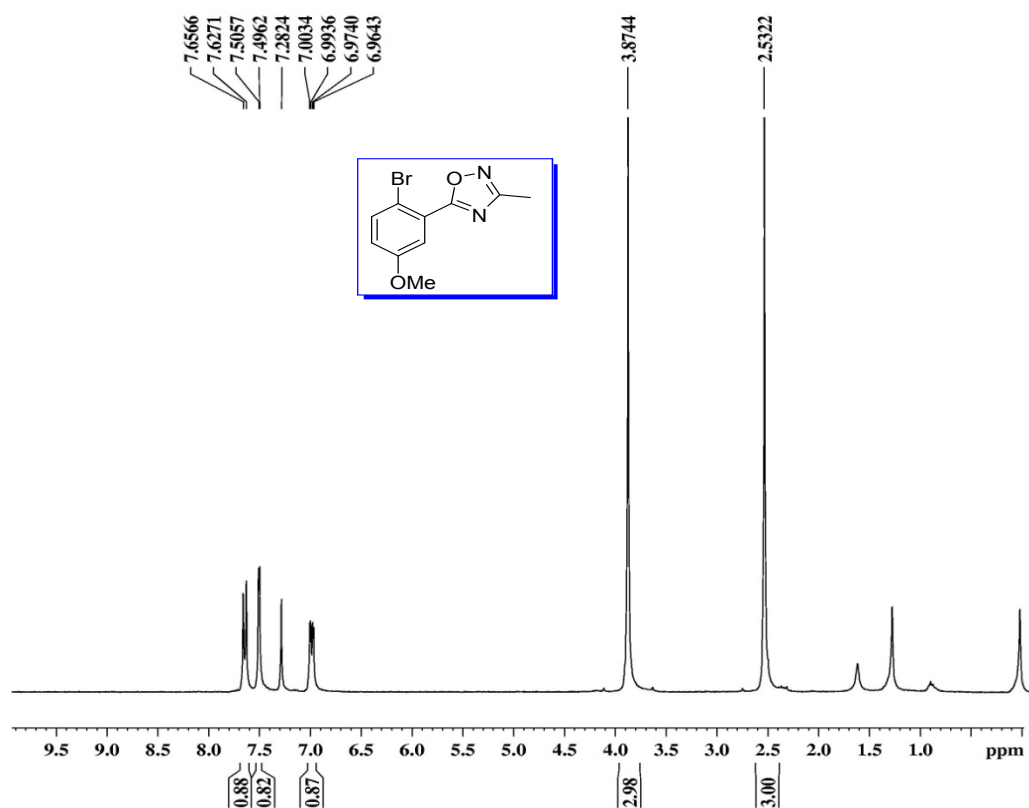


Figure 21: ^1H and ^{13}C Spectra of compound 3q

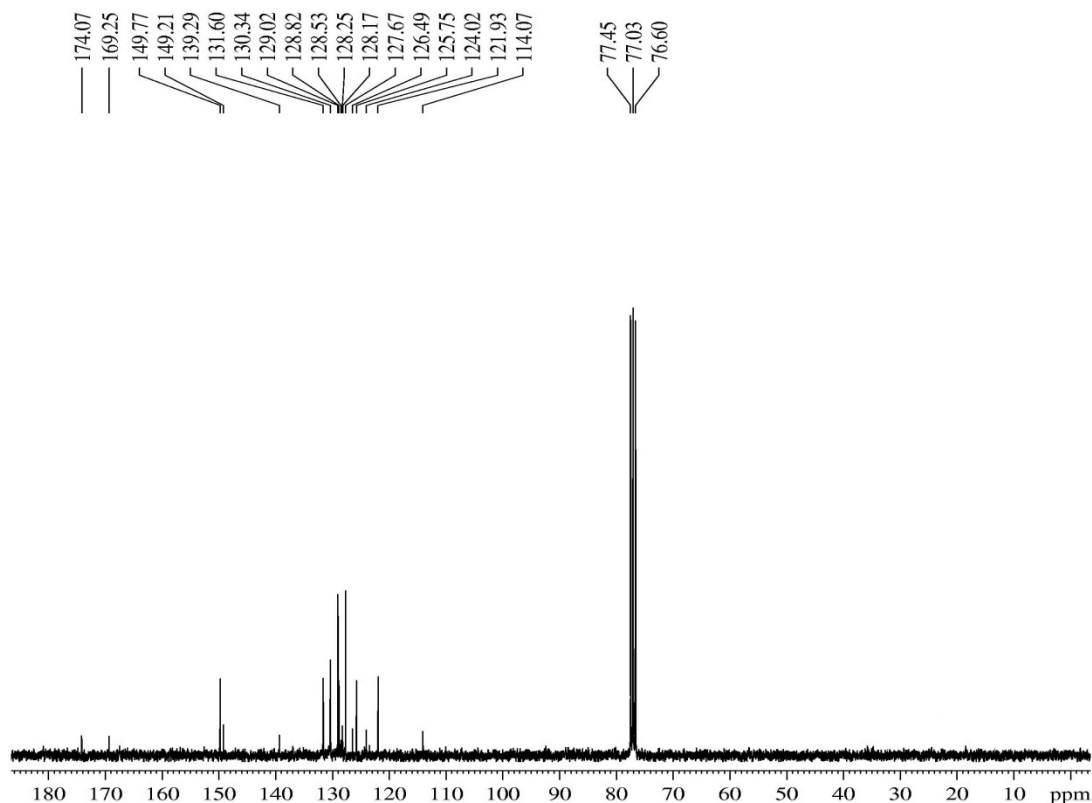
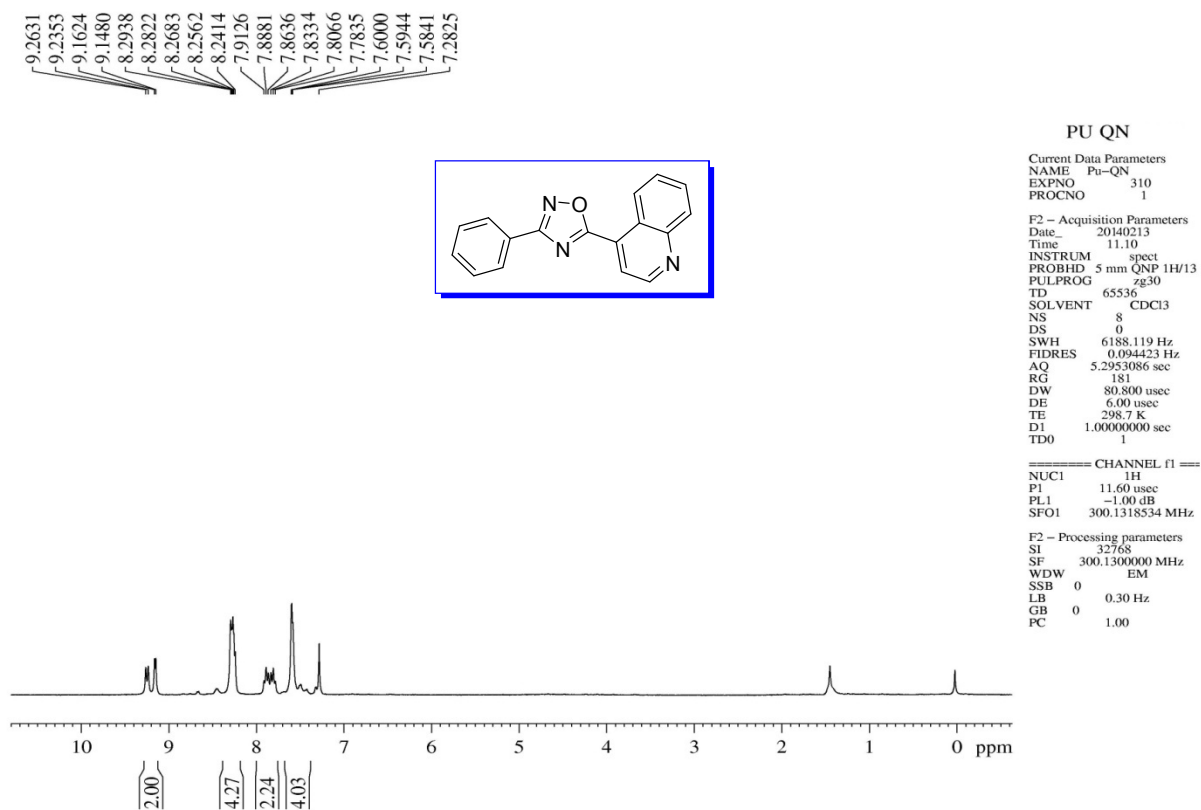
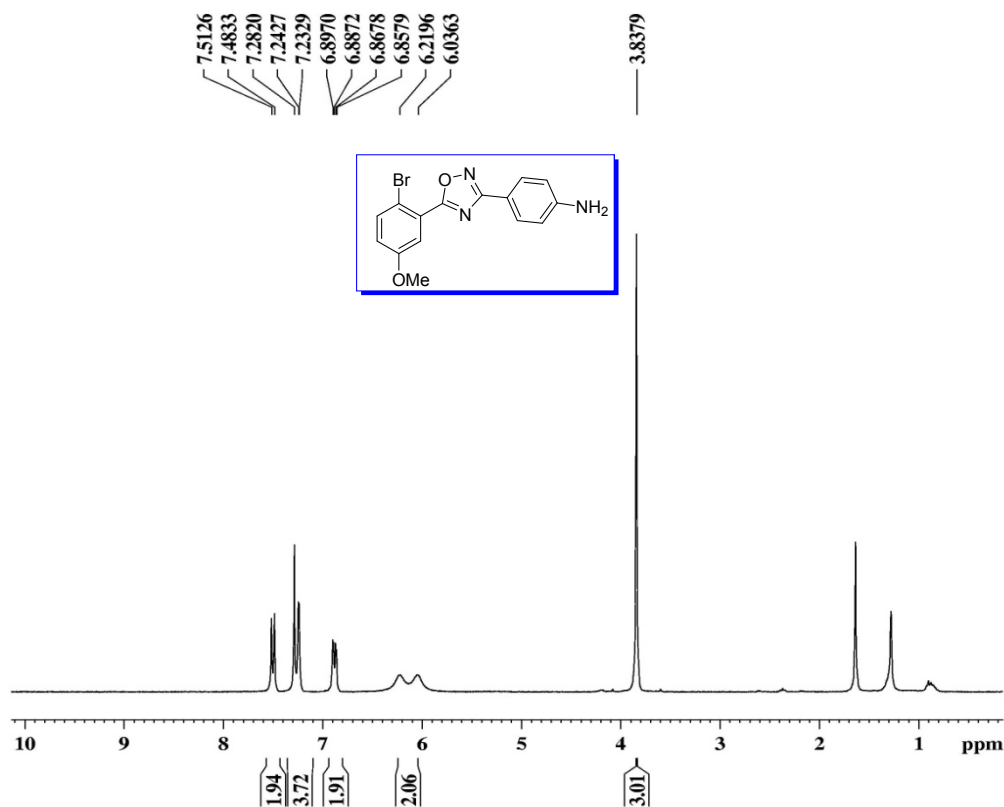


Figure 22: ^1H and ^{13}C Spectra of compound 3r



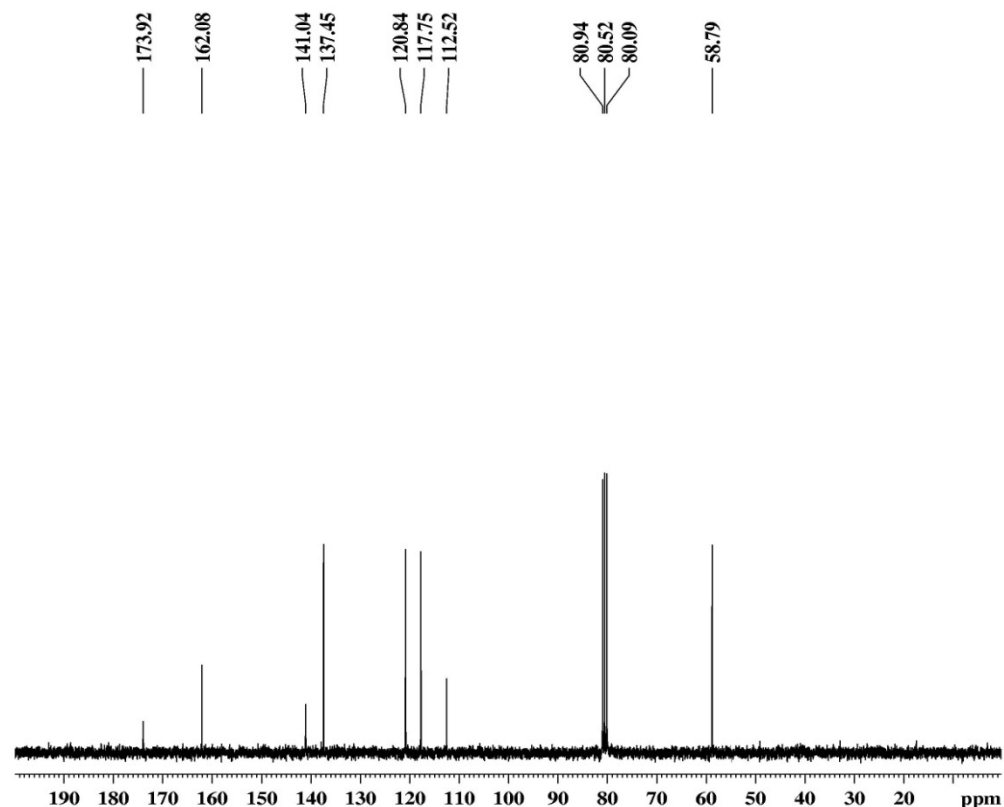
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FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 256
DW 80.800 usec
DE 6.00 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1

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P1 11.60 usec
PL1 -1.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
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SF 300.1300000 MHz
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SSB 0



PUNEET-74

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AQ 1.8175818 sec
RG 11.3
DW 27.733 usec
DE 6.00 usec
TE 298.8 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.70 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
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PL12 17.00 dB
PL13 21.00 dB
SFO2 300.1312005 MHz

Figure 23: ¹H and ¹³C Spectra of compound 3s

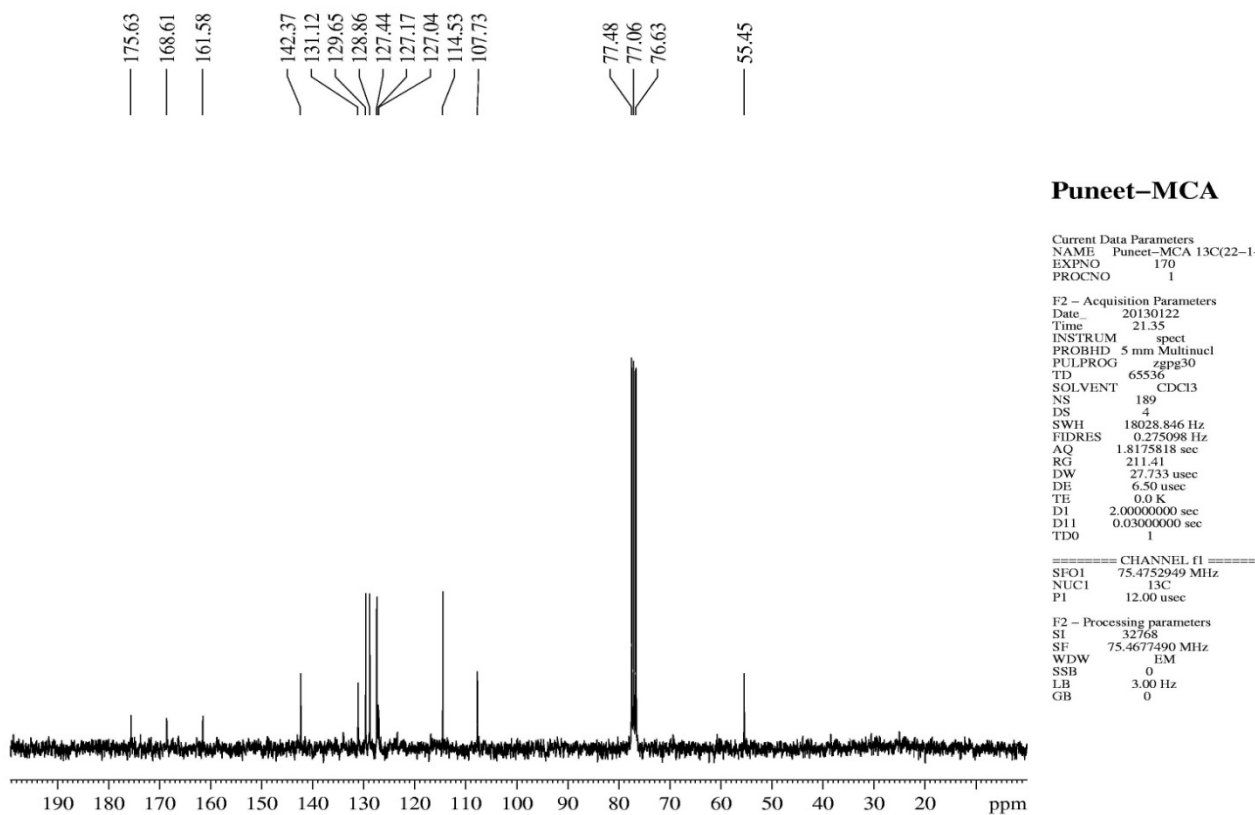
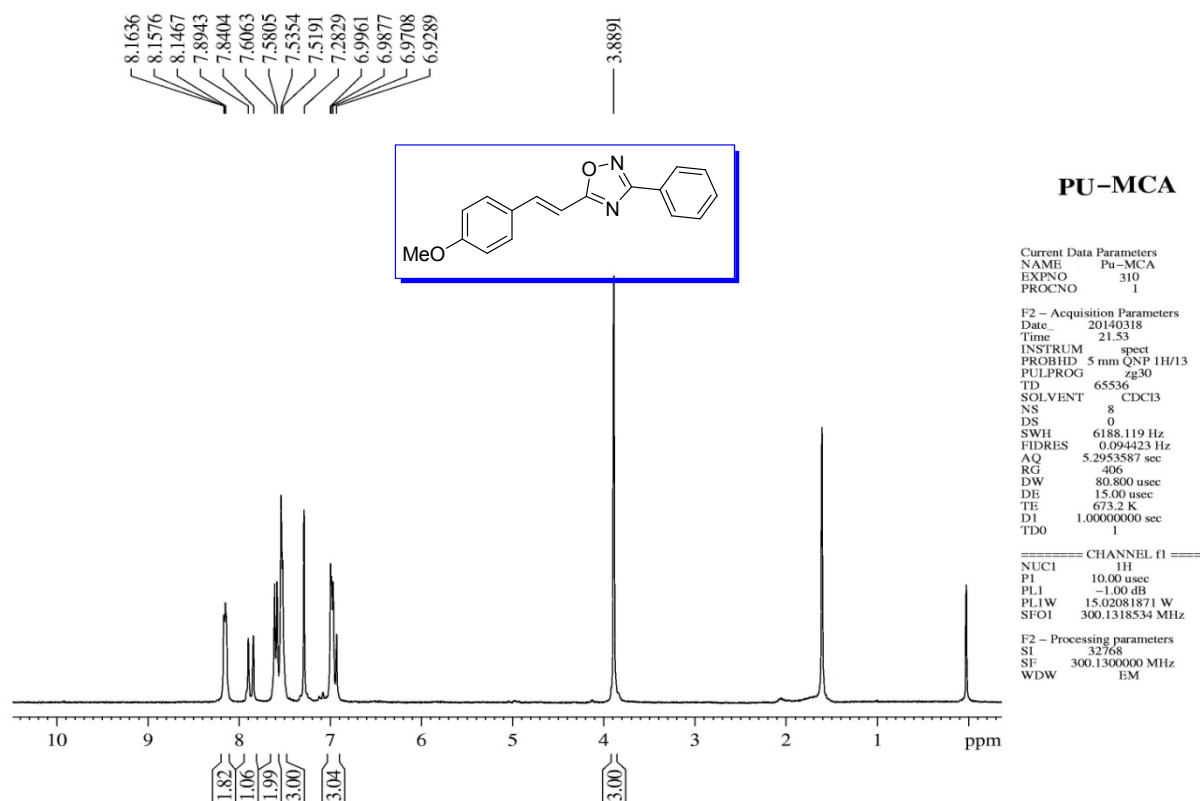


Figure 24: ¹H and ¹³C Spectra of compound 3t

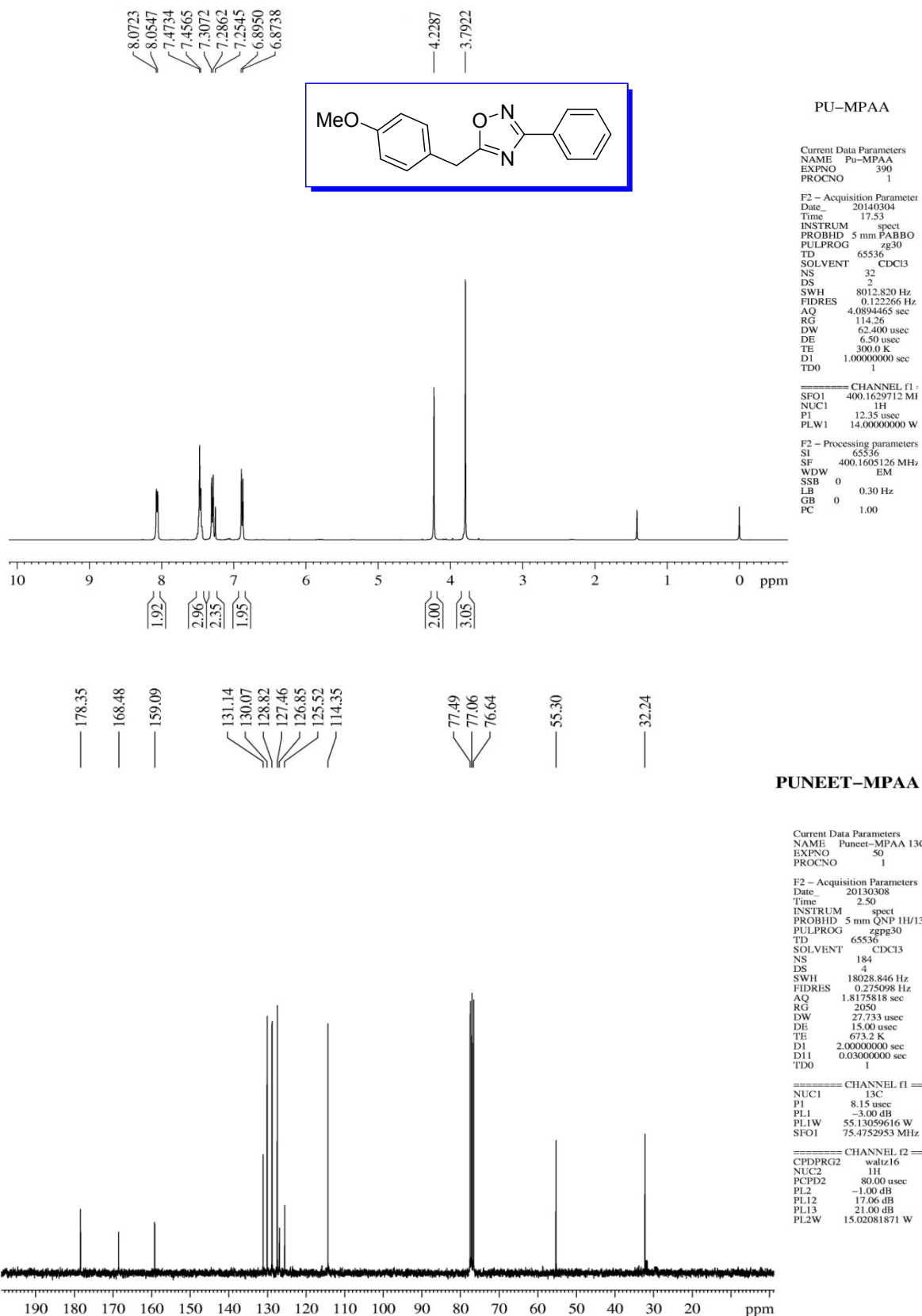


Figure 25: ^1H and ^{13}C Spectra of compound 3u

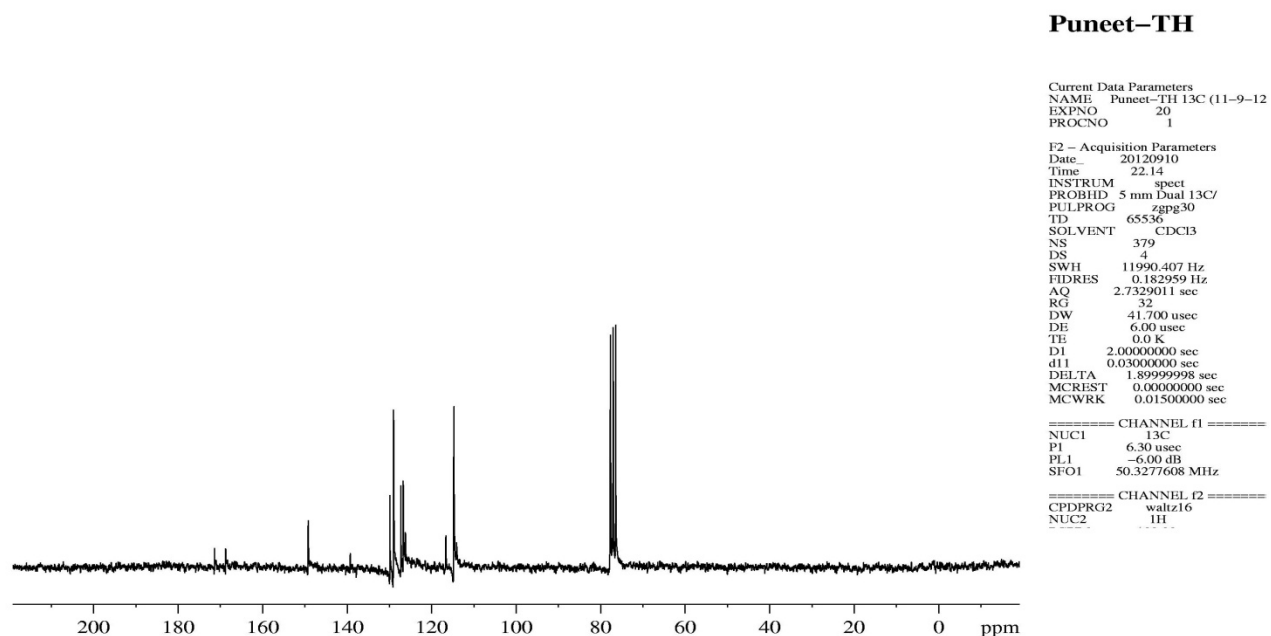
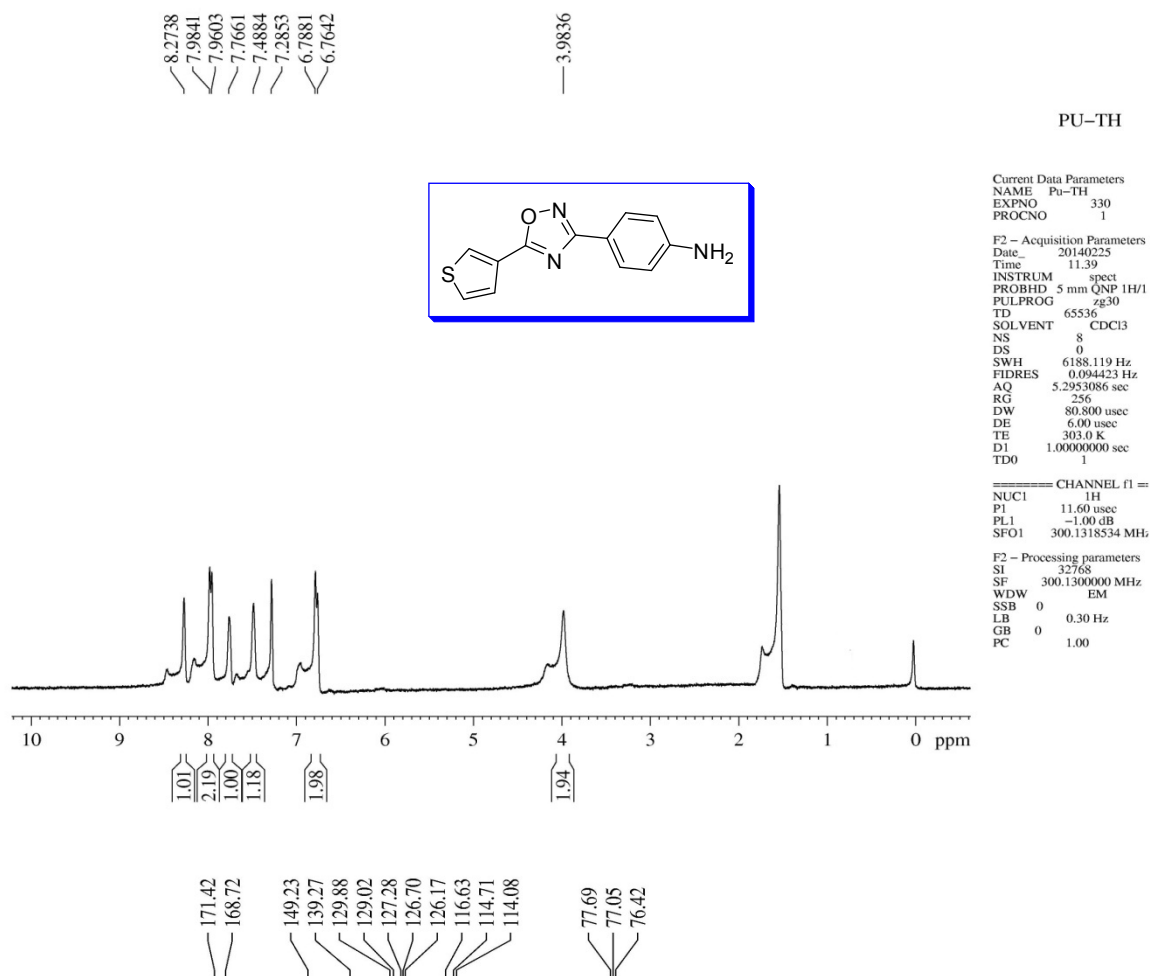


Figure 26: ¹H and ¹³C Spectra of compound 3v

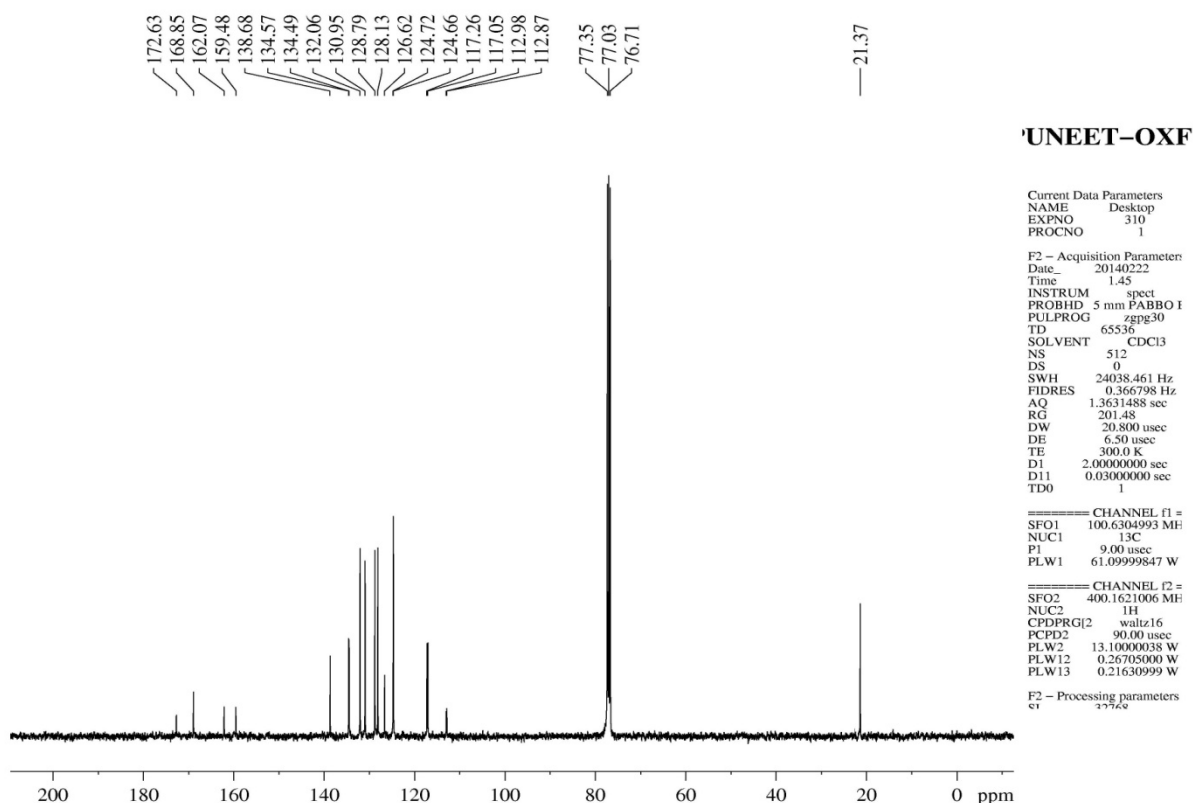
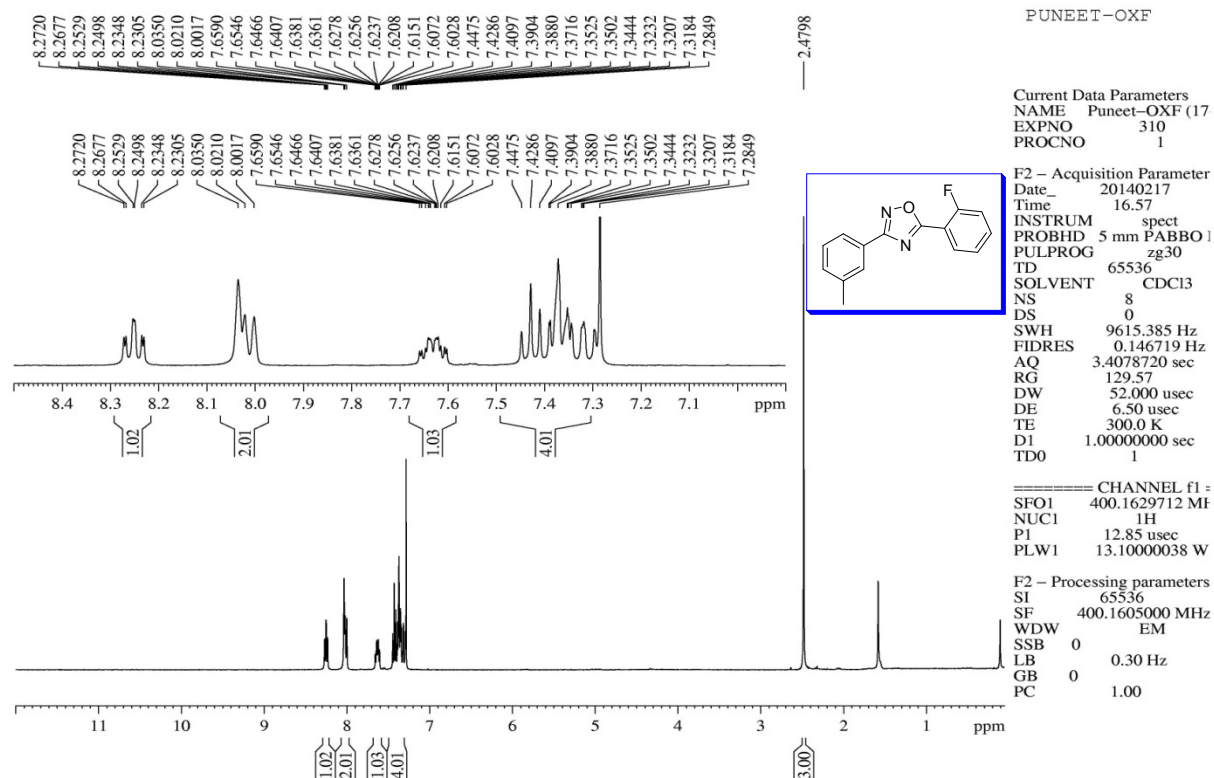


Figure 27: ^1H and ^{13}C Spectra of compound 3w

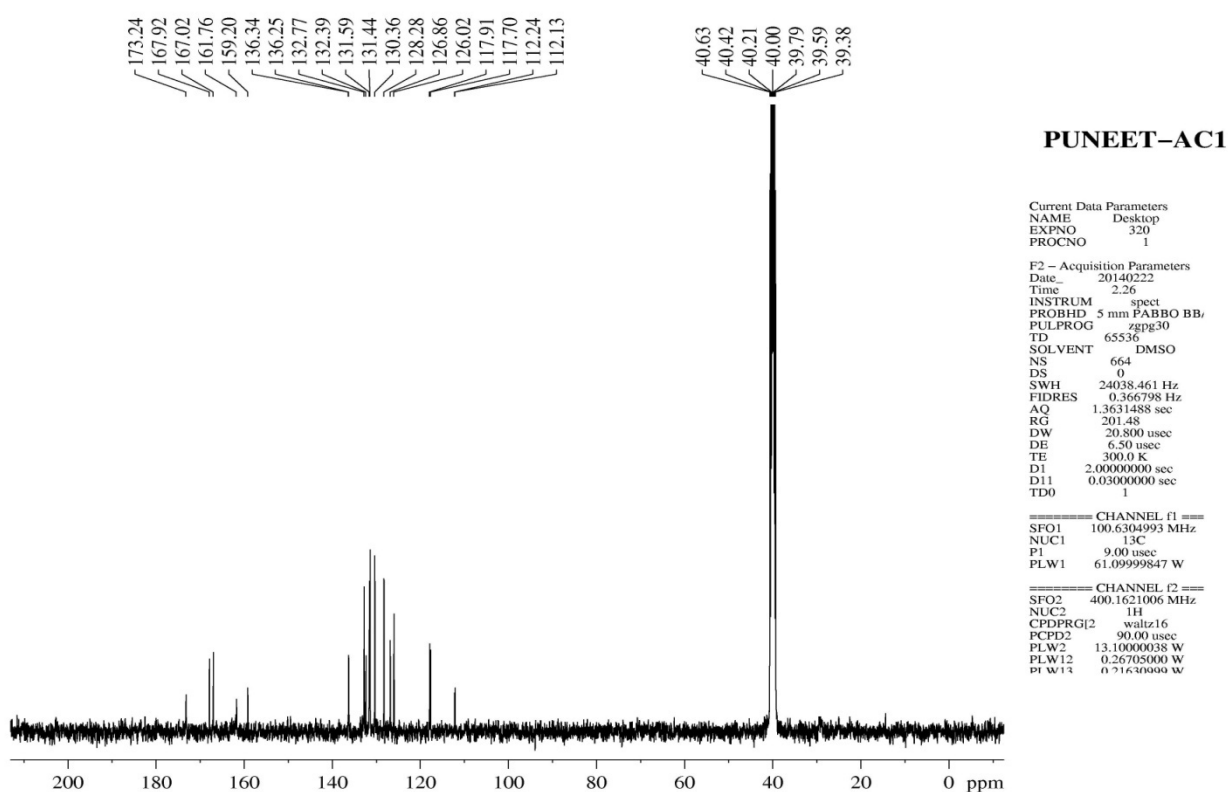
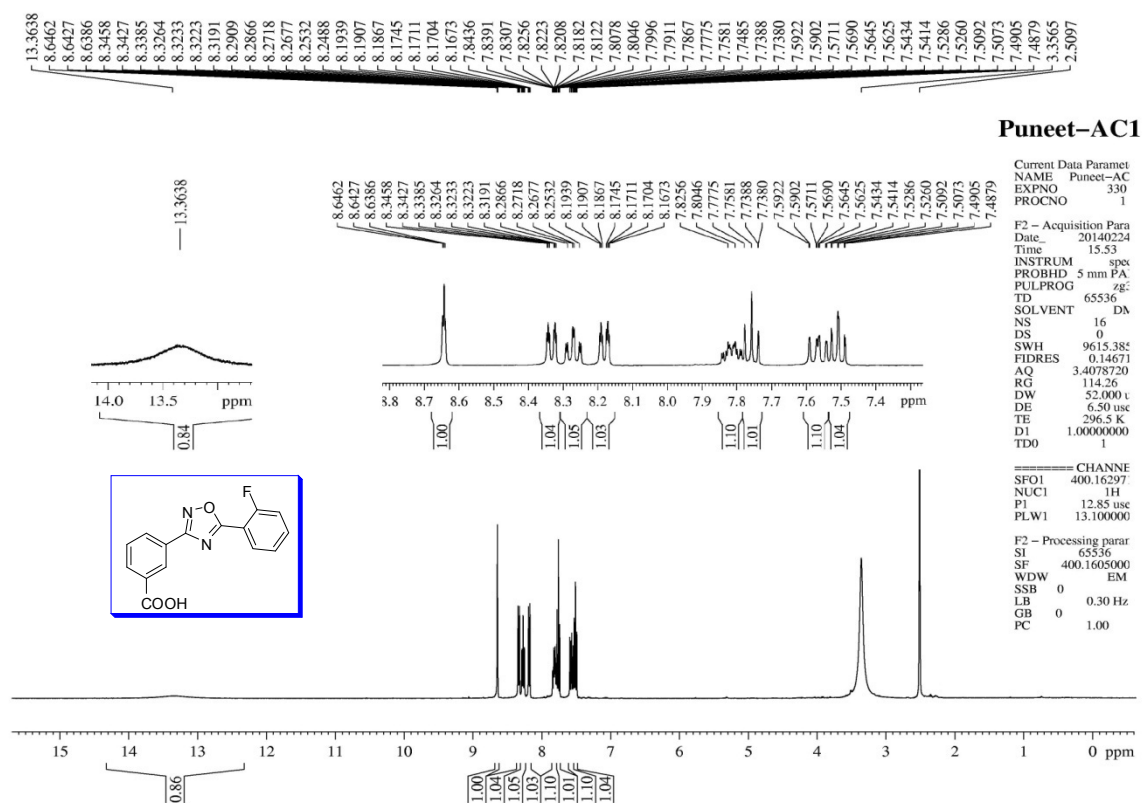


Figure 28: ^1H and ^{13}C Spectra of compound 3x

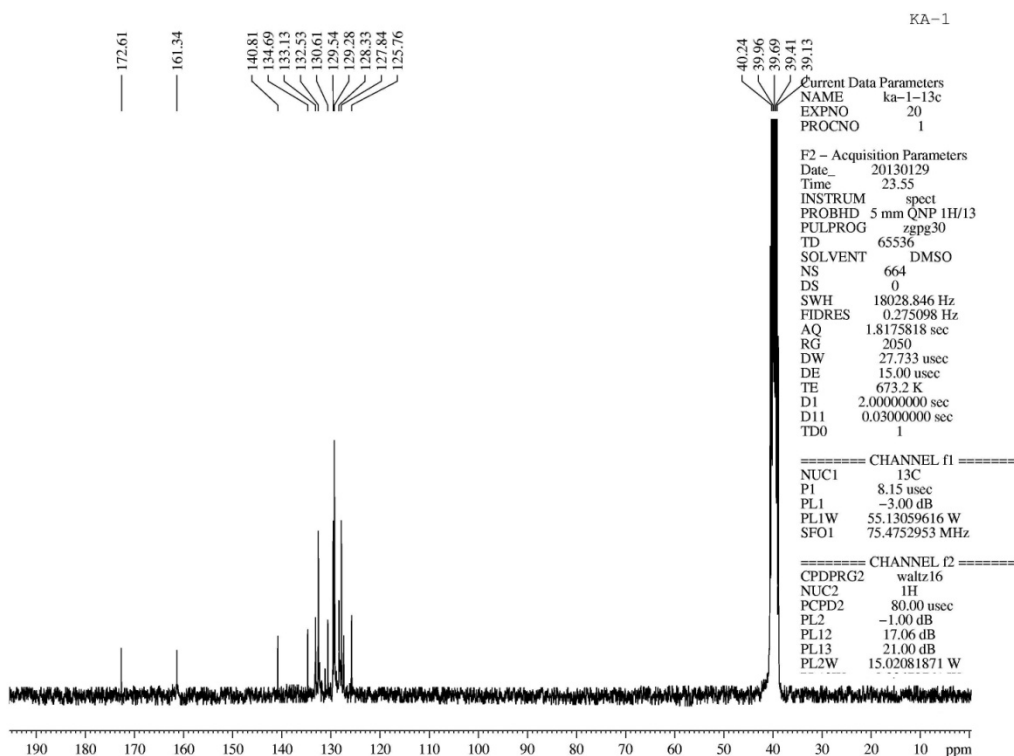
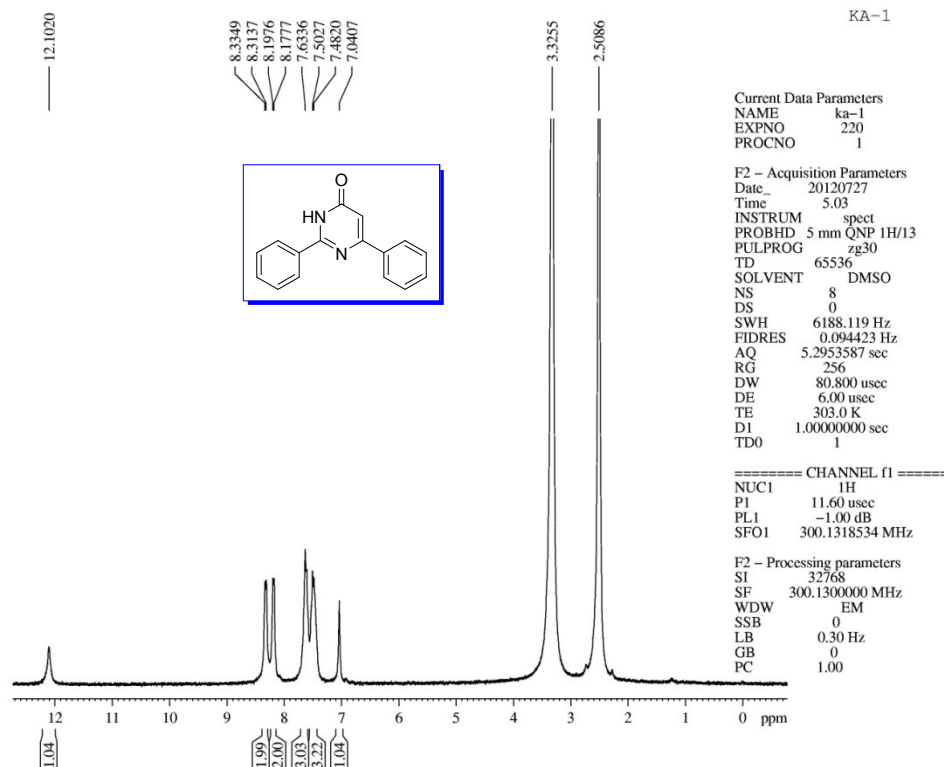


Figure 29: ^1H and ^{13}C Spectra of compound 5a

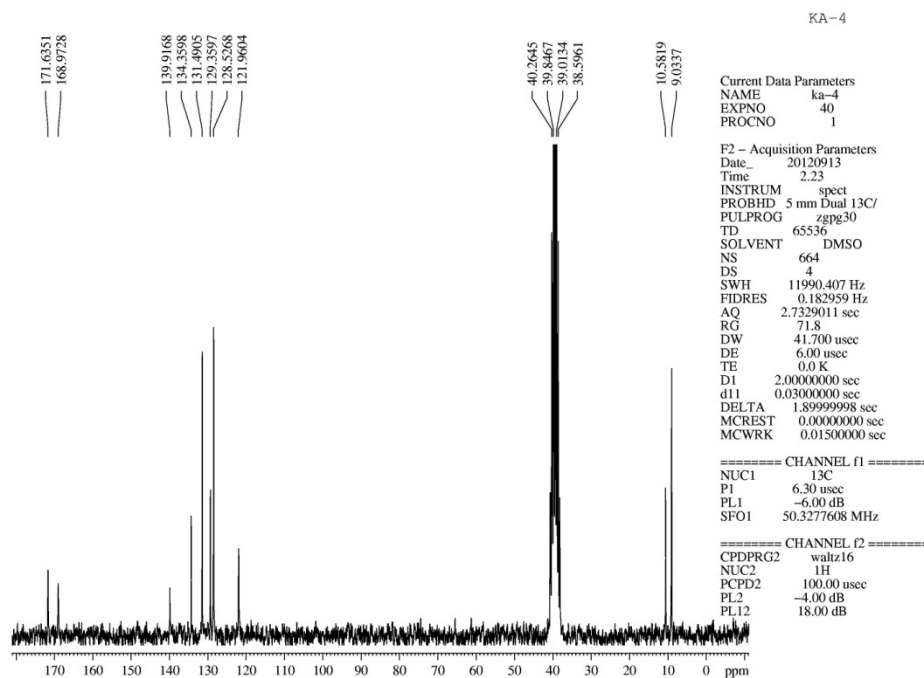
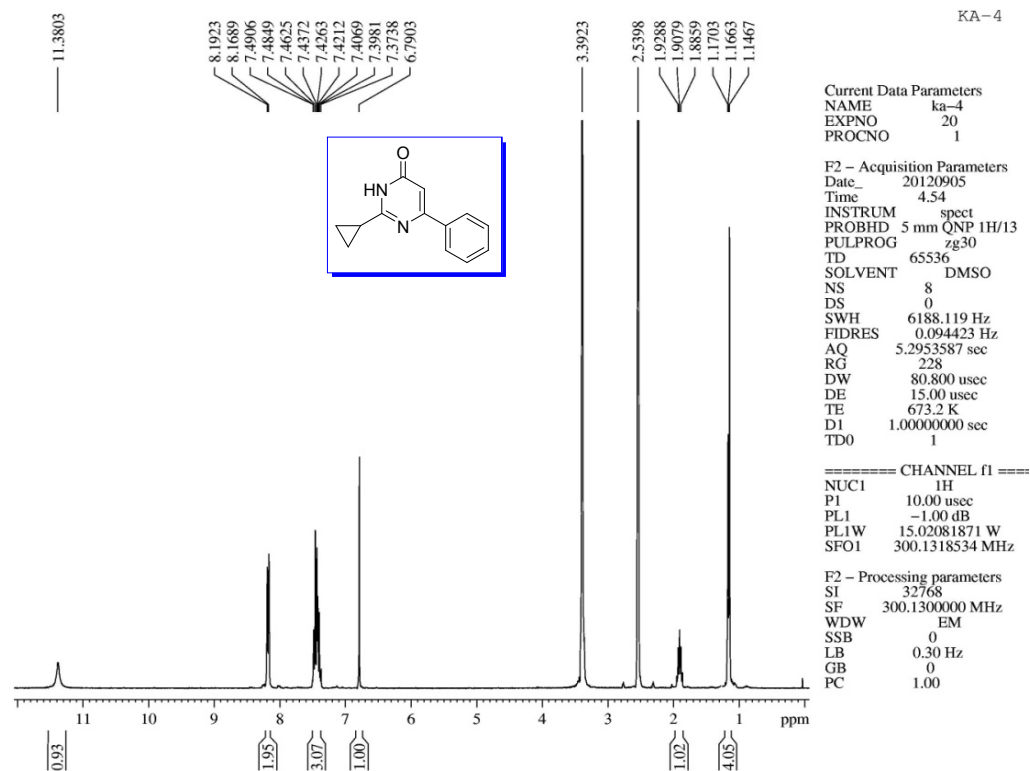


Figure 30: ^1H and ^{13}C Spectra of compound 5b

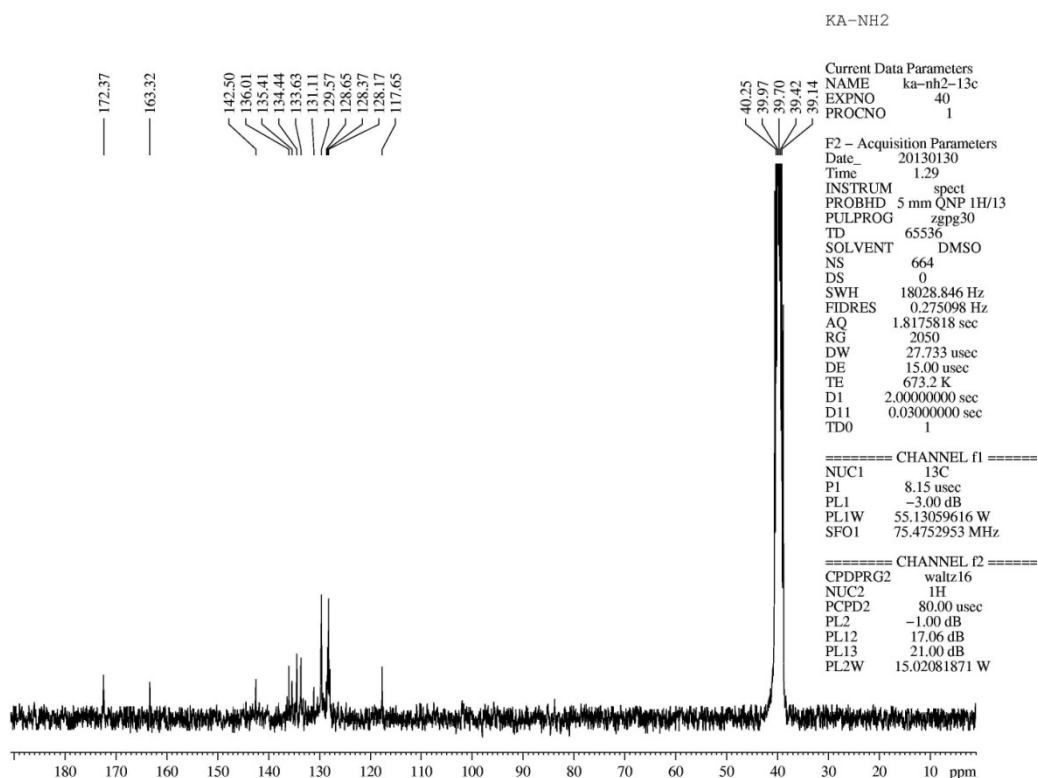
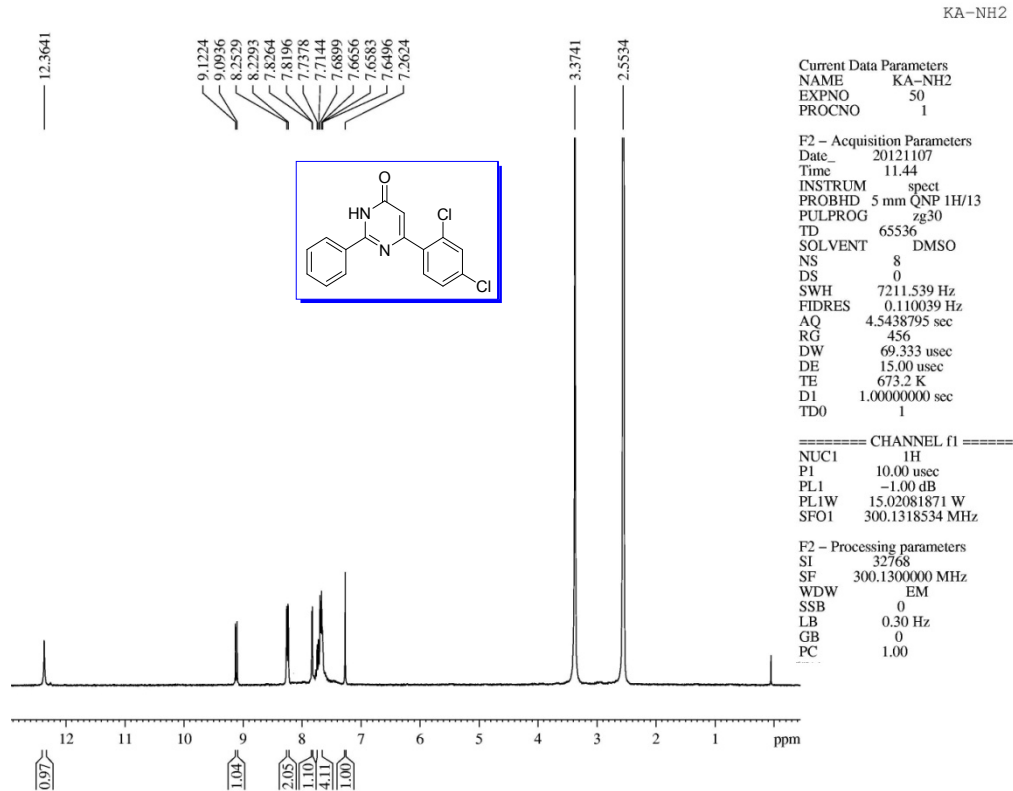


Figure 31: ^1H and ^{13}C Spectra of compound 5c

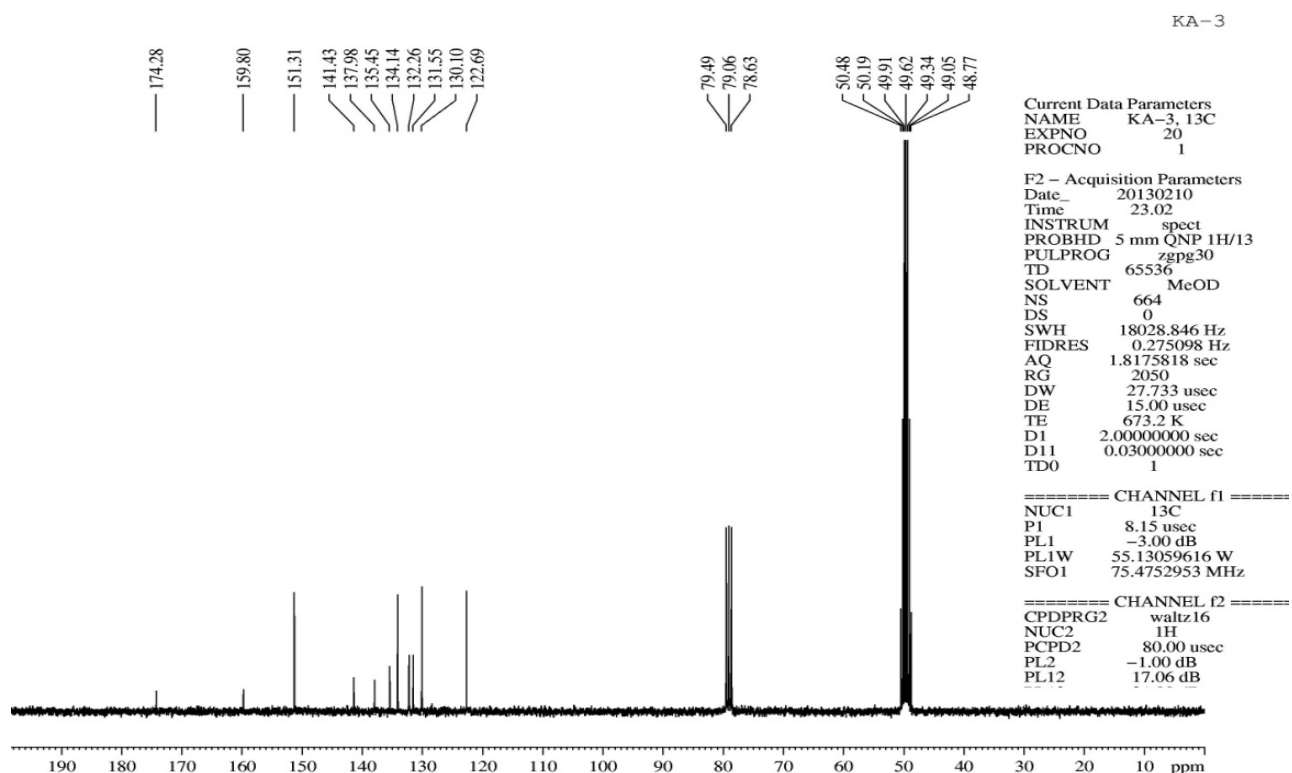
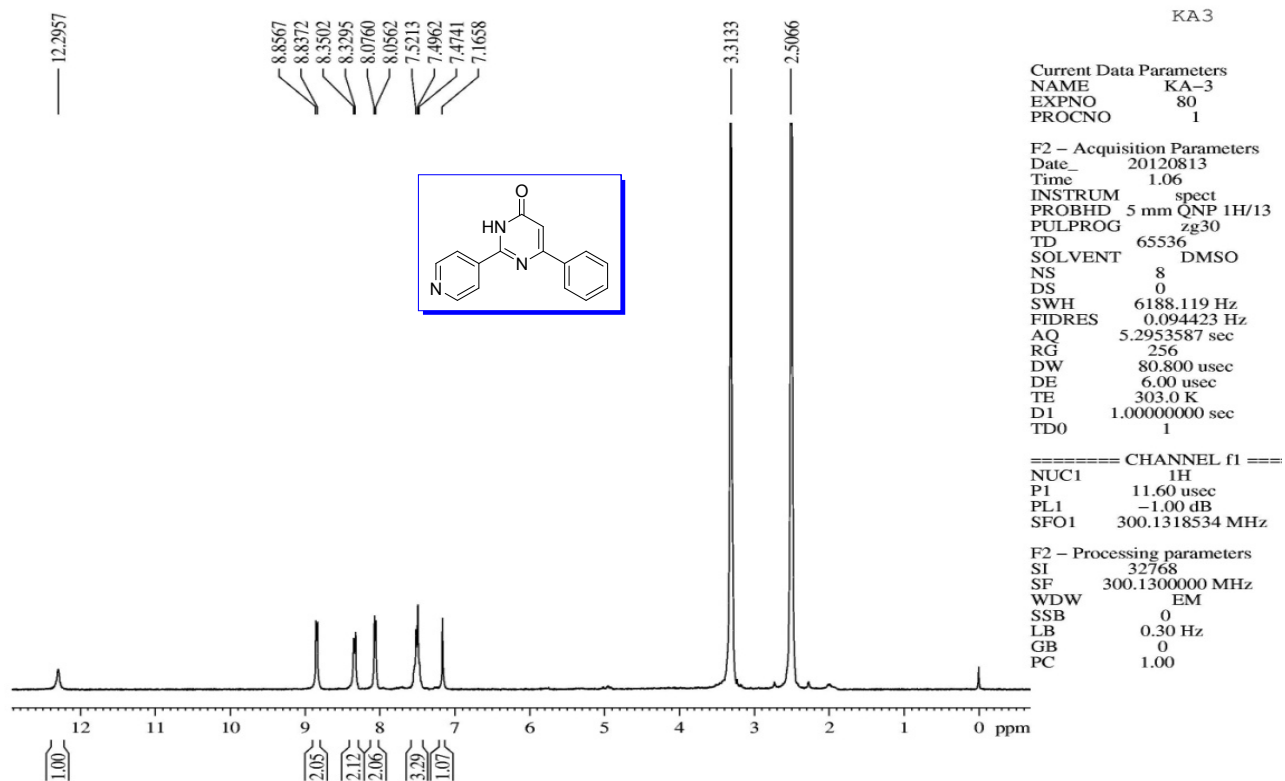


Figure 32: ^1H and ^{13}C Spectra of compound 5d

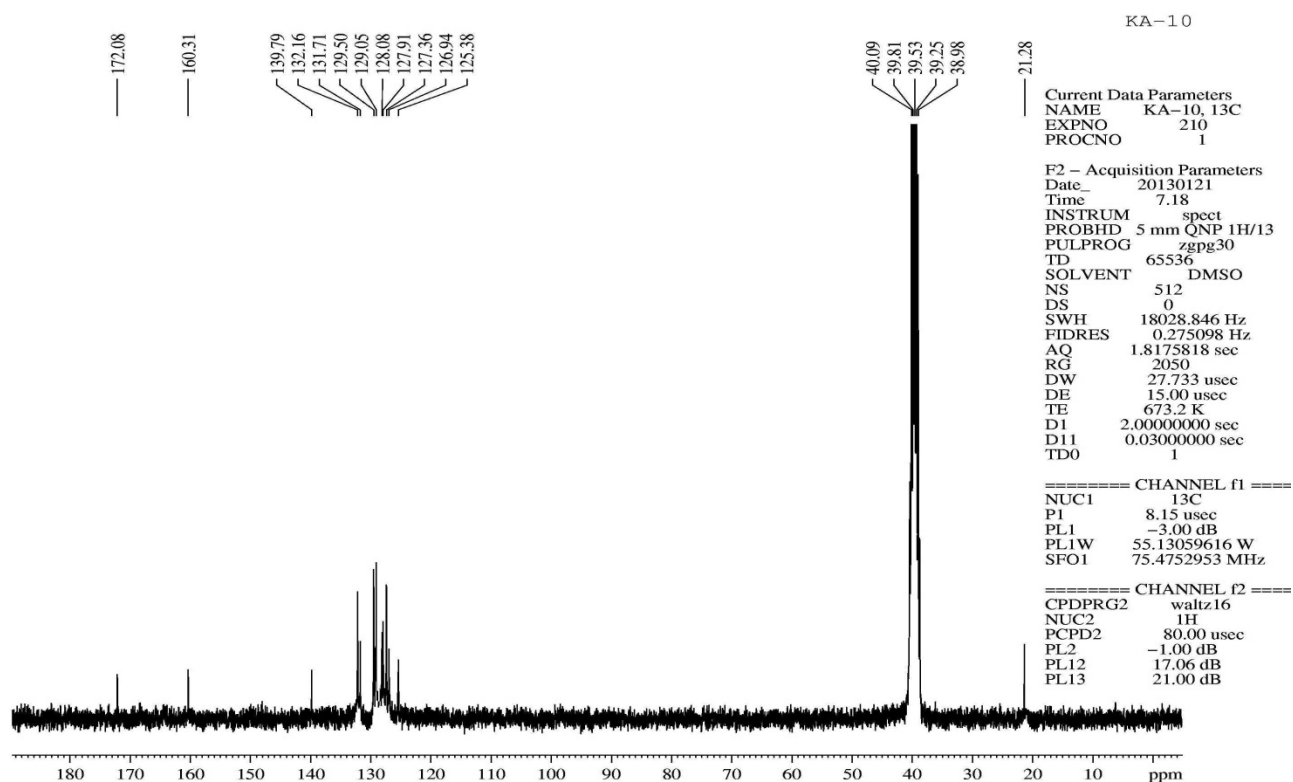
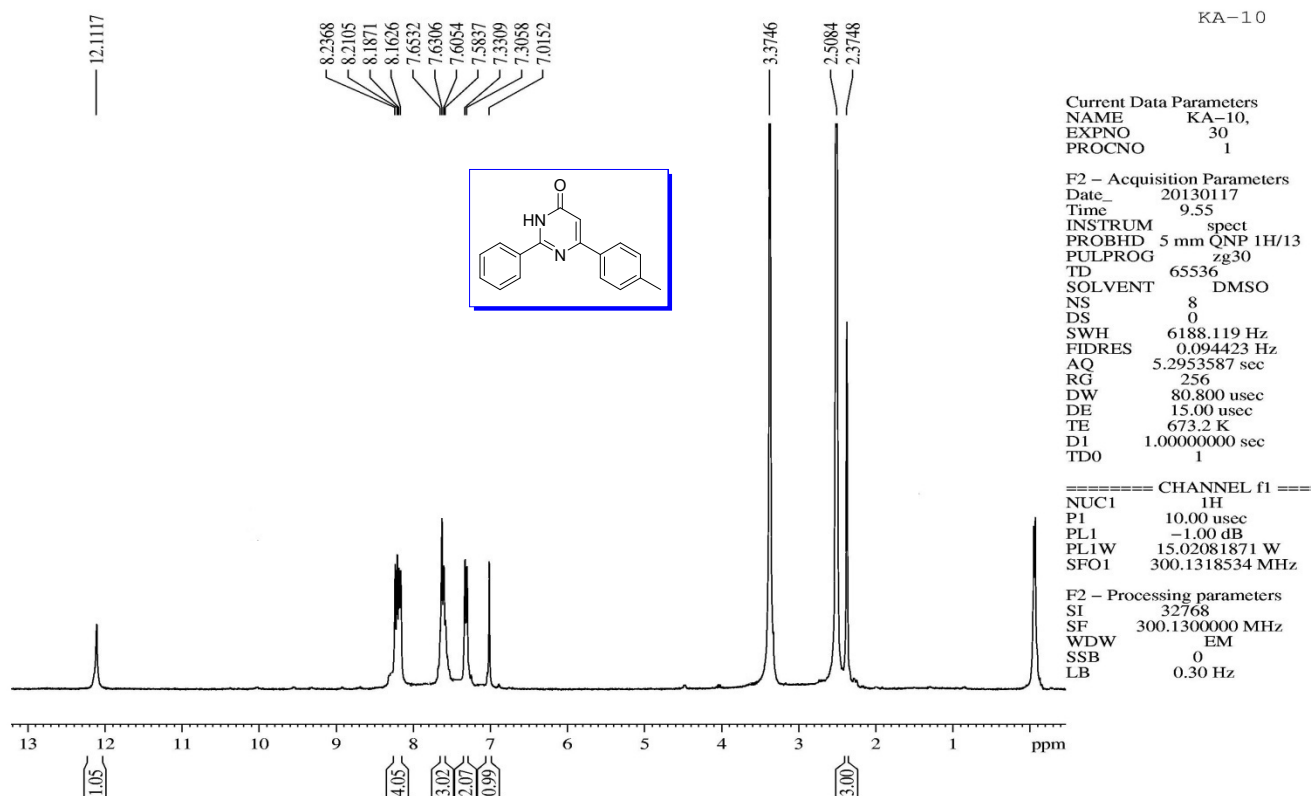


Figure 33: ^1H and ^{13}C Spectra of compound 5e

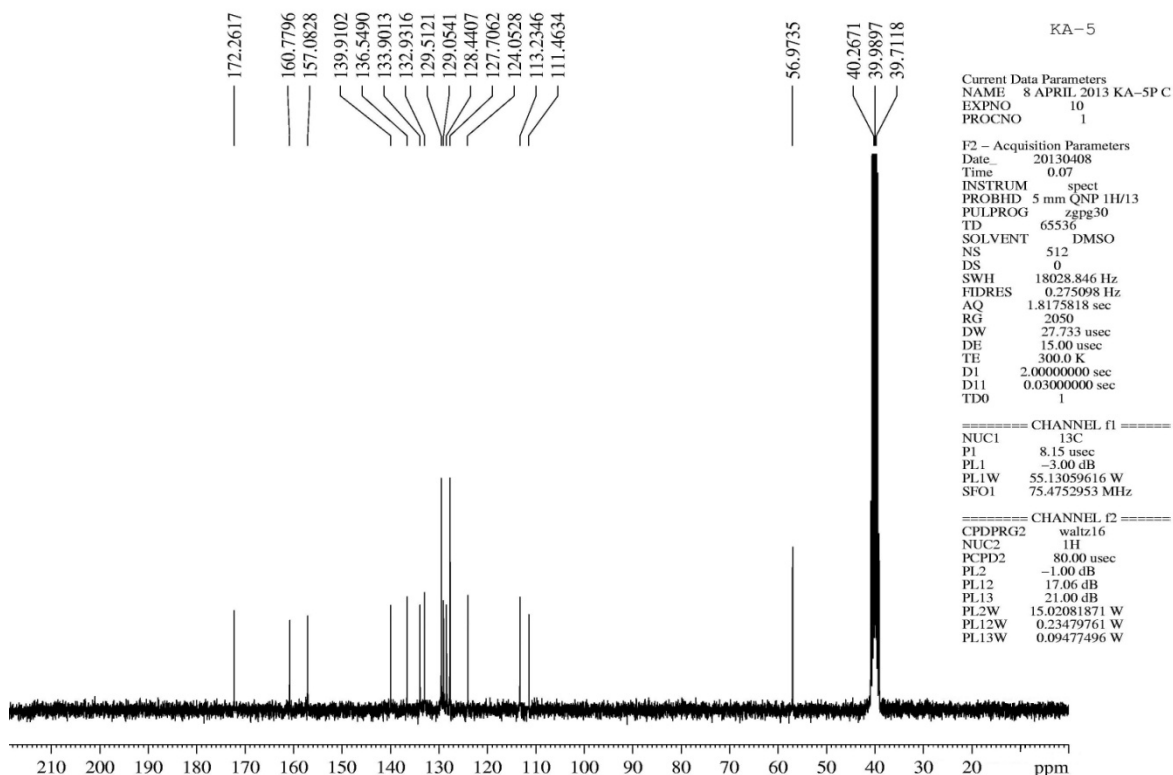
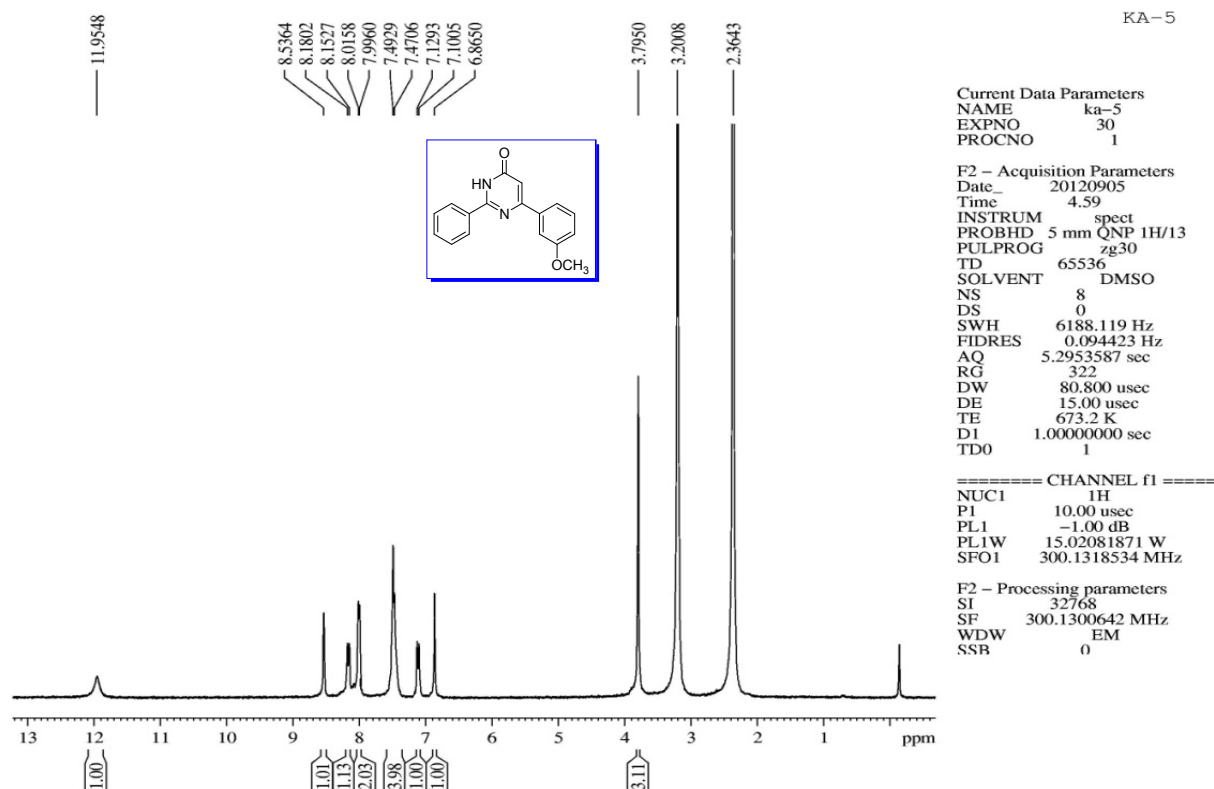


Figure 34: ¹H and ¹³C Spectra of compound 5f

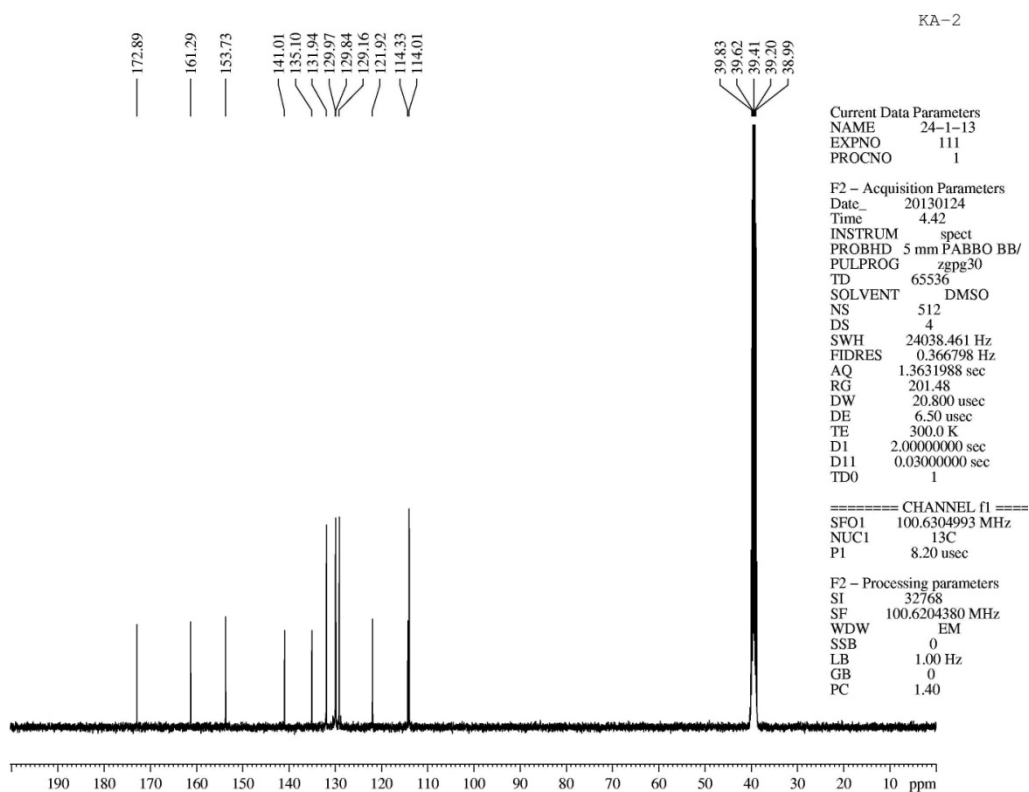
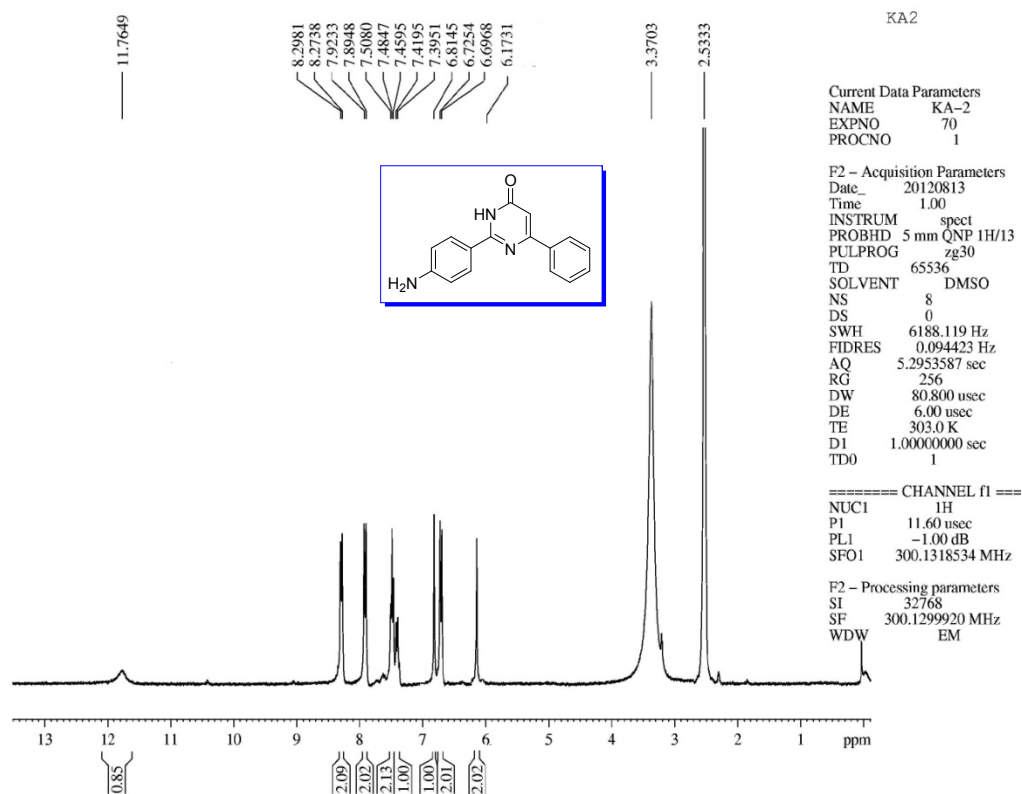


Figure 35: ^1H and ^{13}C Spectra of compound 5g

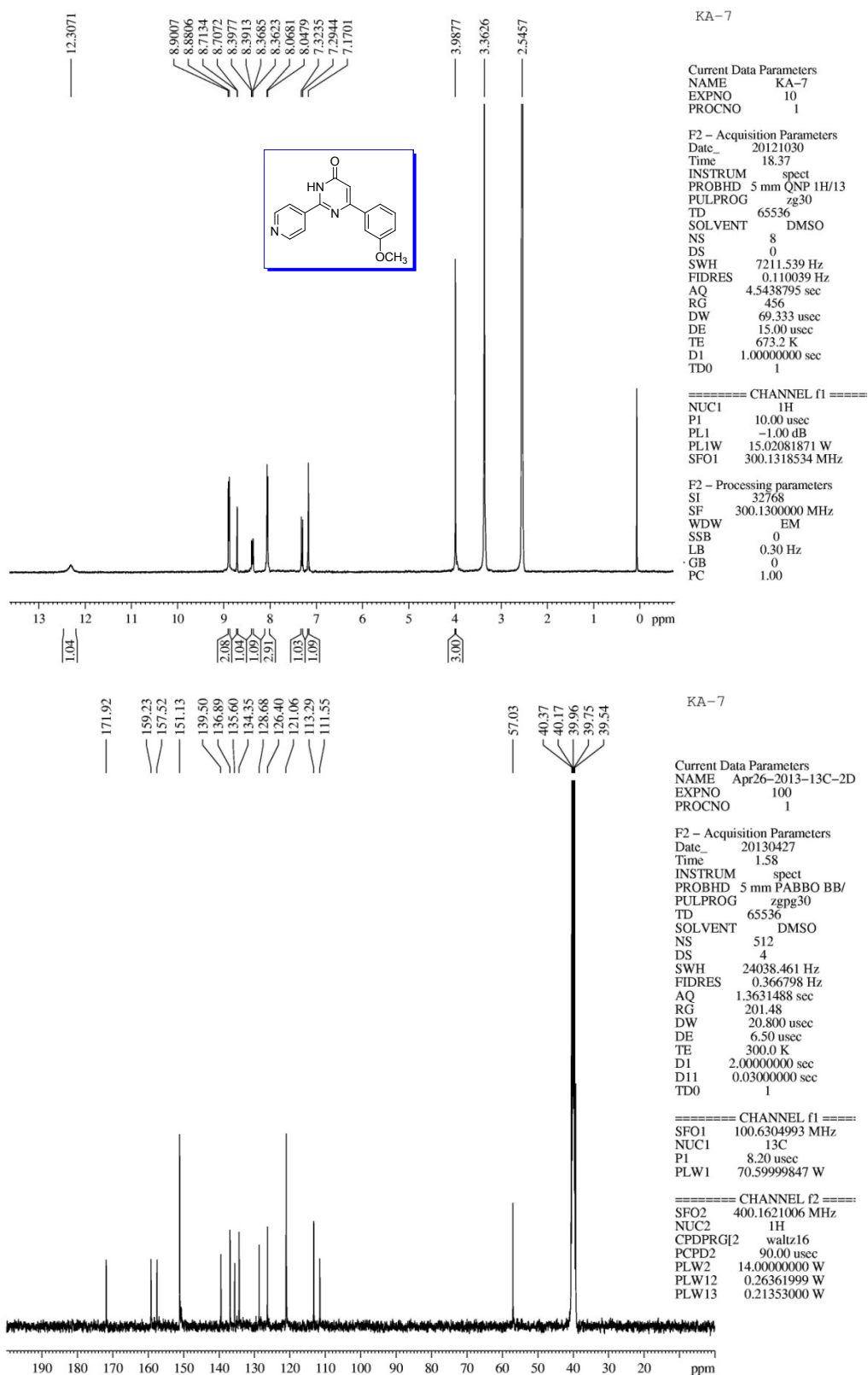


Figure 36: ¹H and ¹³C Spectra of compound 5h

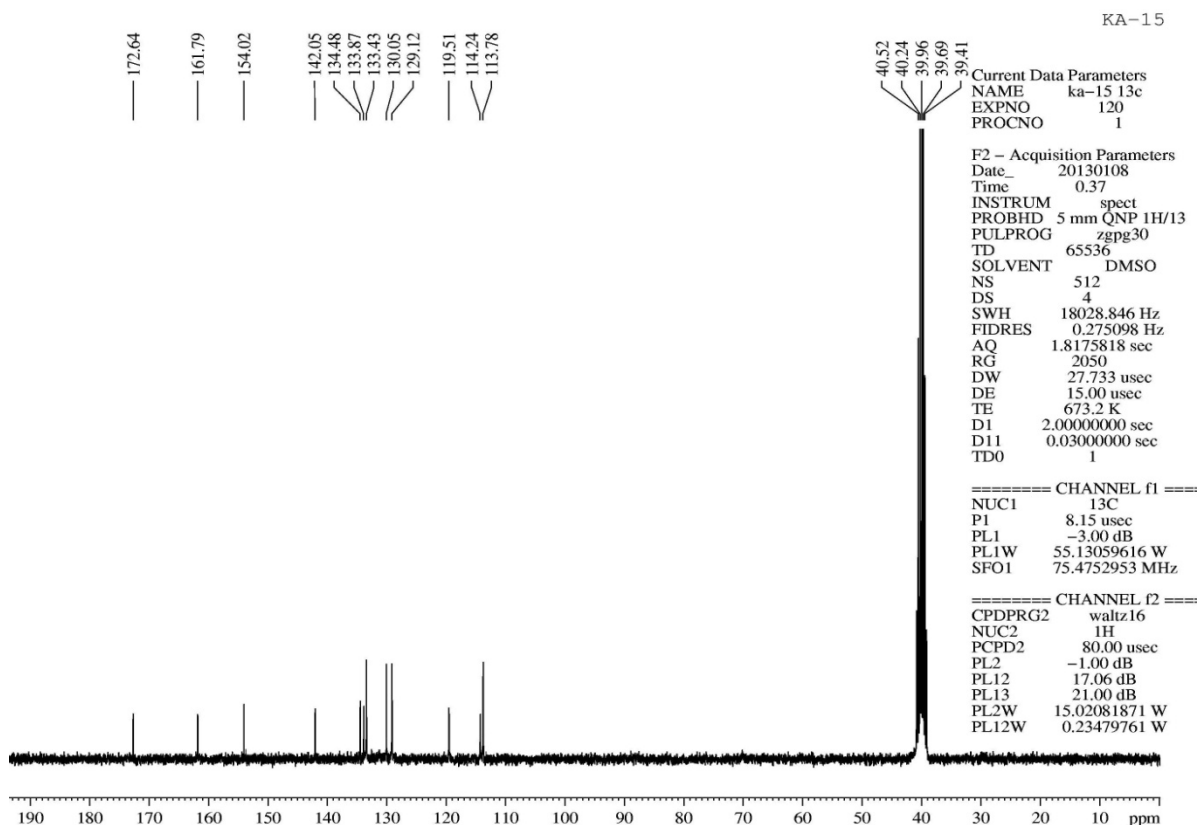
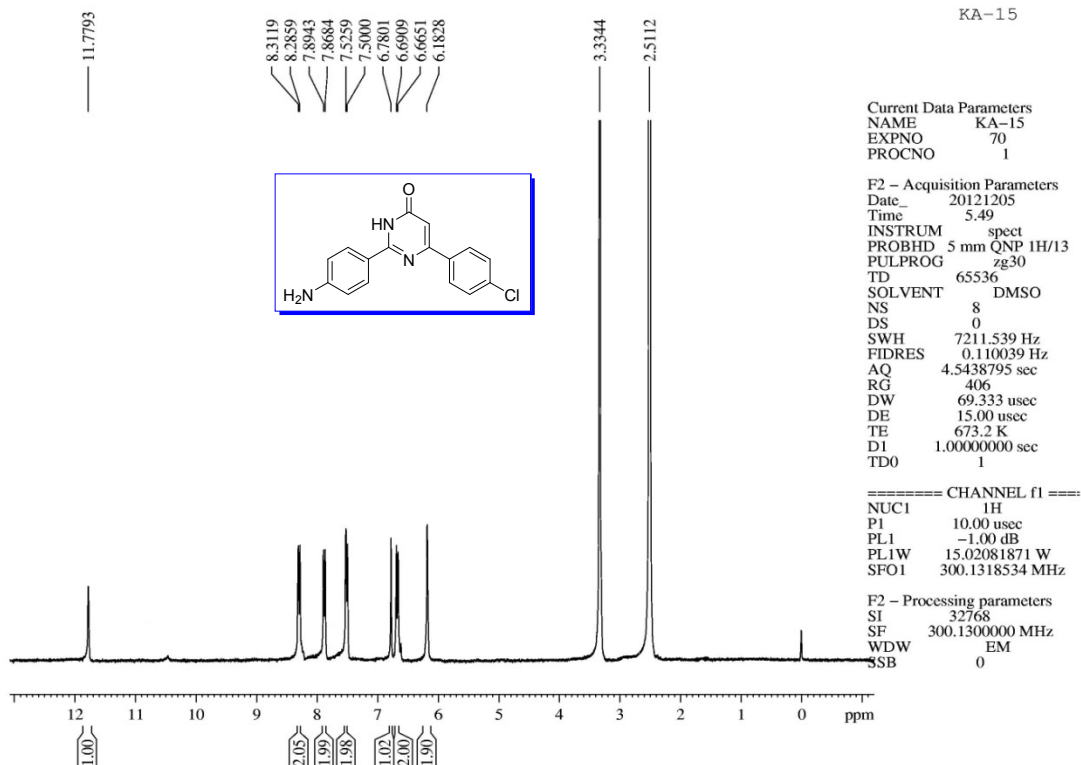


Figure 37: ^1H and ^{13}C Spectra of compound 5i

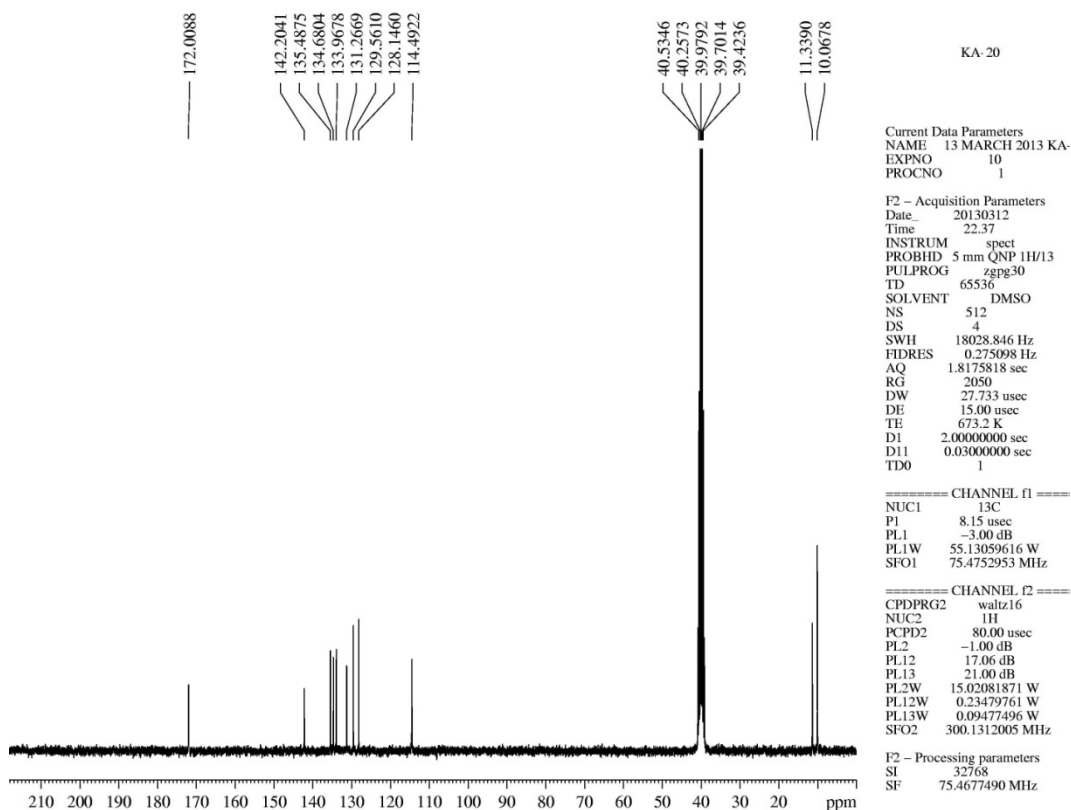
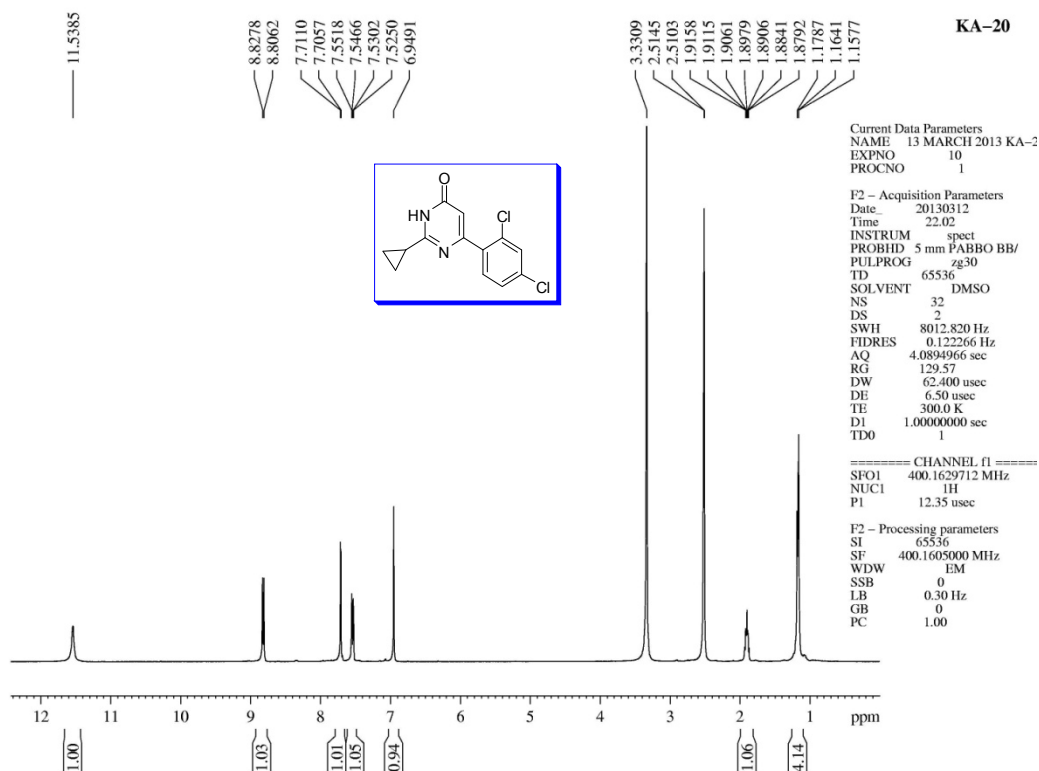


Figure 38: ^1H and ^{13}C Spectra of compound 5j

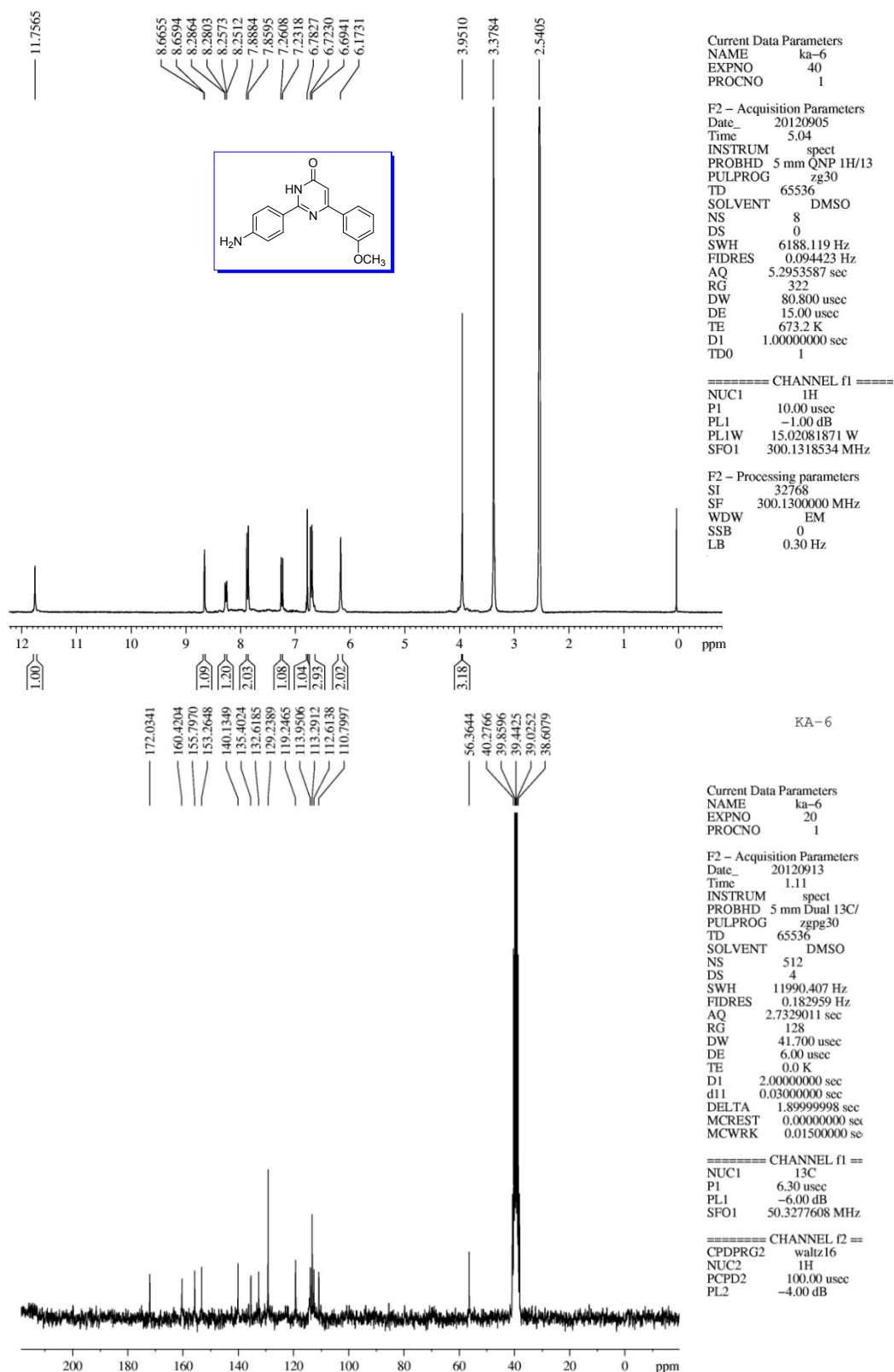


Figure 39: ¹H and ¹³C Spectra of compound 5k

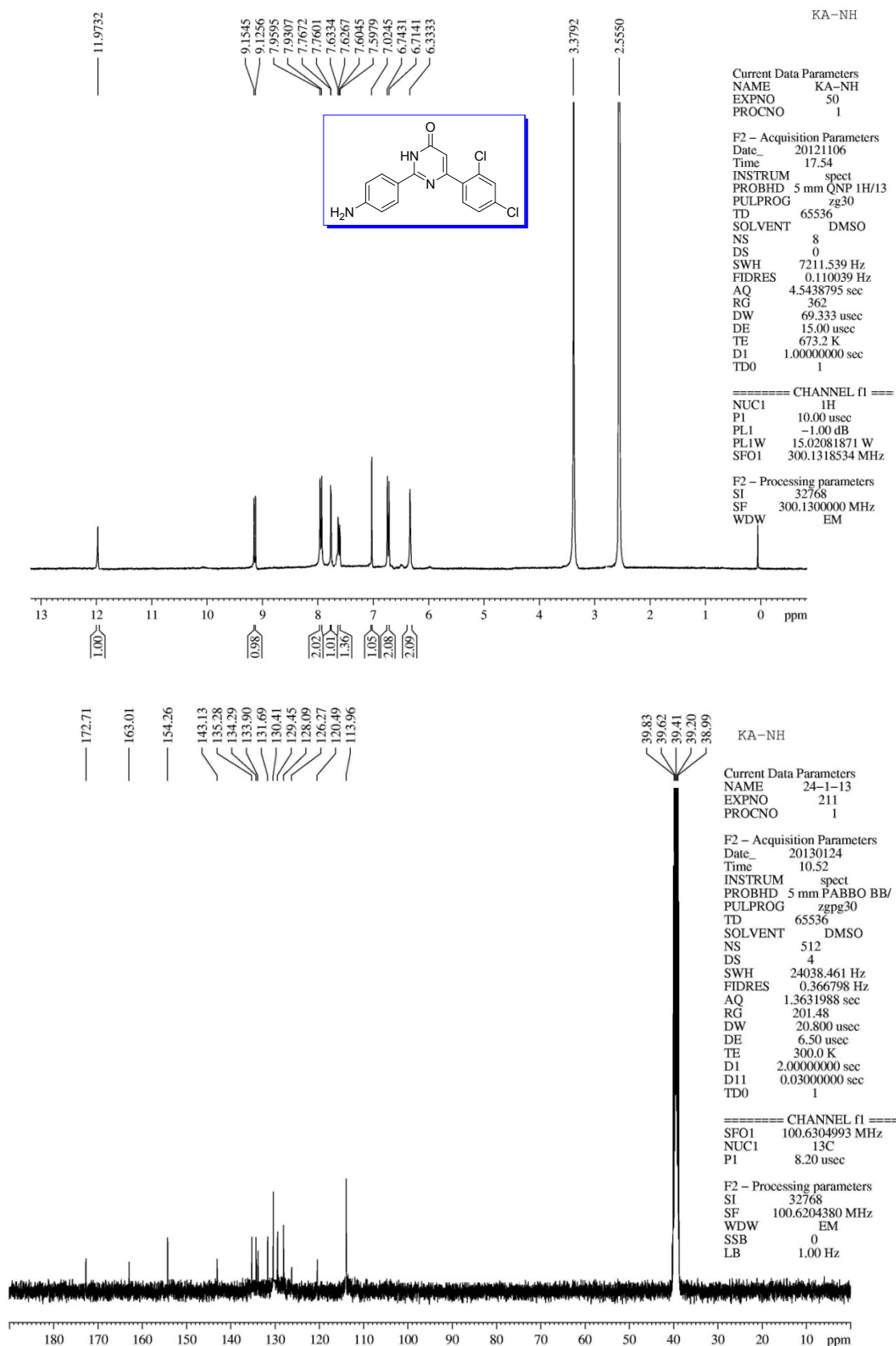


Figure 40: ^1H and ^{13}C Spectra of compound 5l

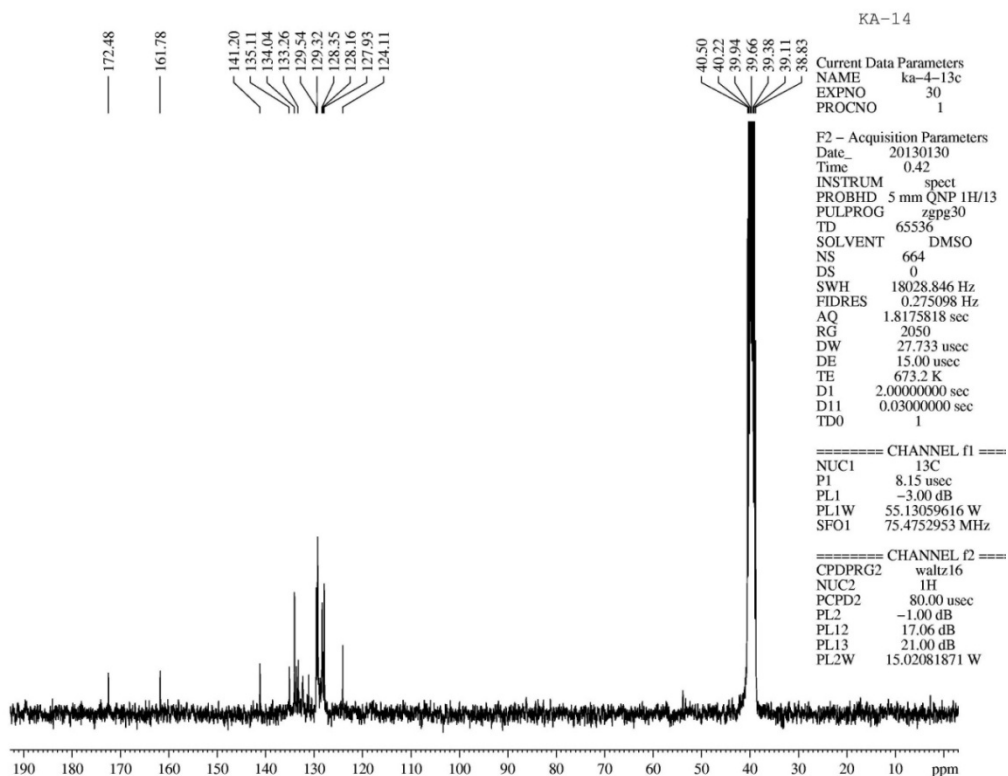
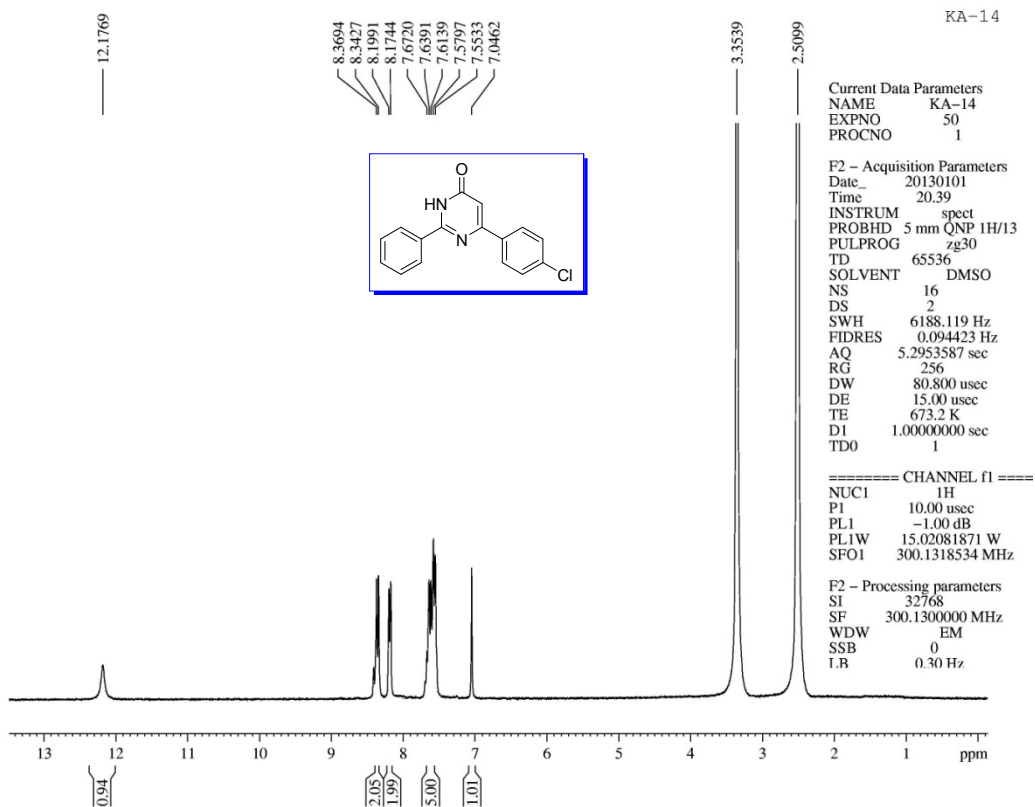


Figure 41: ^1H and ^{13}C Spectra of compound 5m

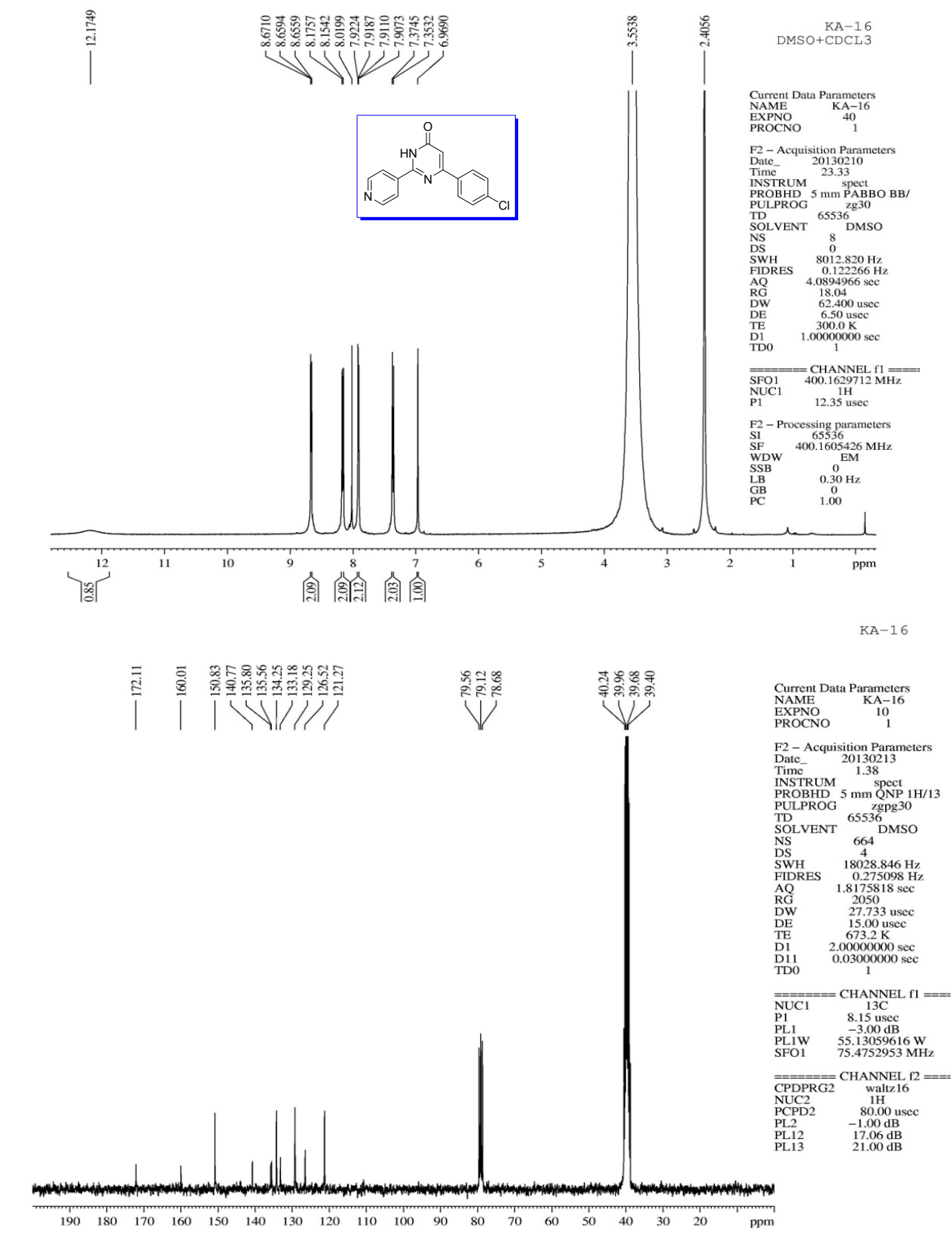


Figure 42: ¹H and ¹³C Spectra of compound 5n

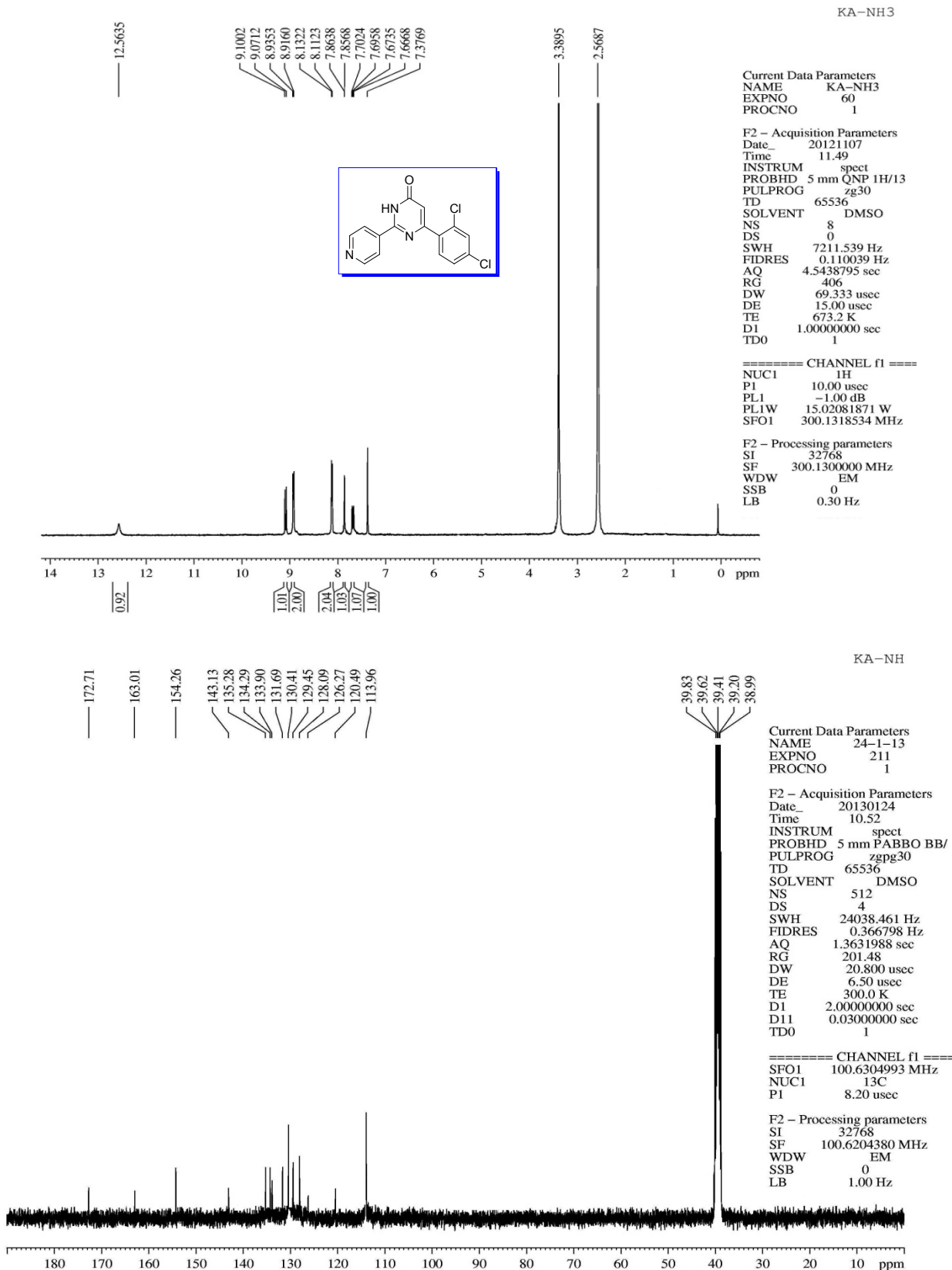


Figure 43: ^1H and ^{13}C Spectra of compound 50

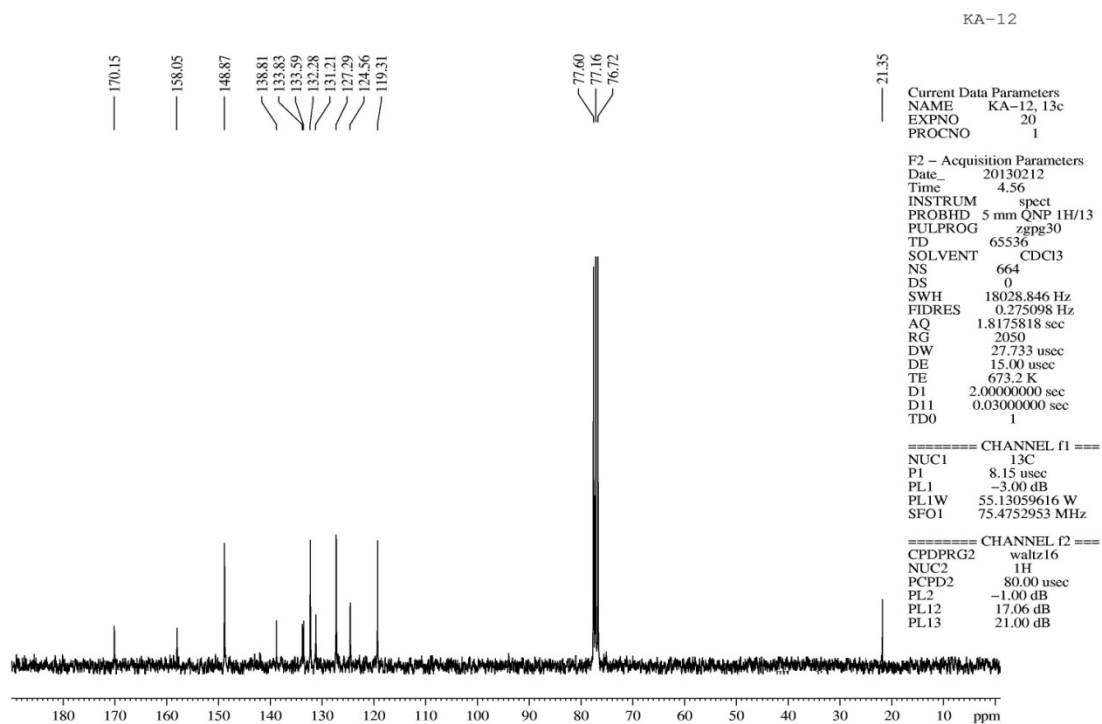
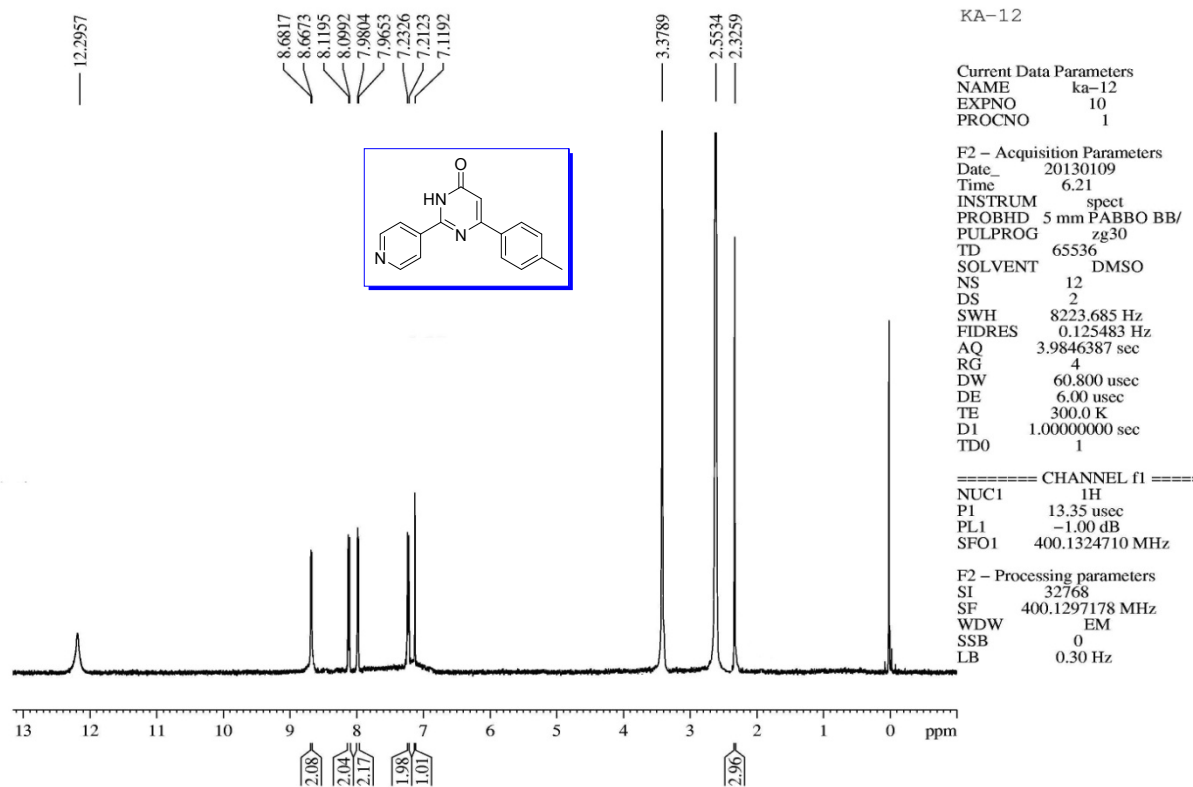


Figure 44: ^1H and ^{13}C Spectra of compound 5p

