

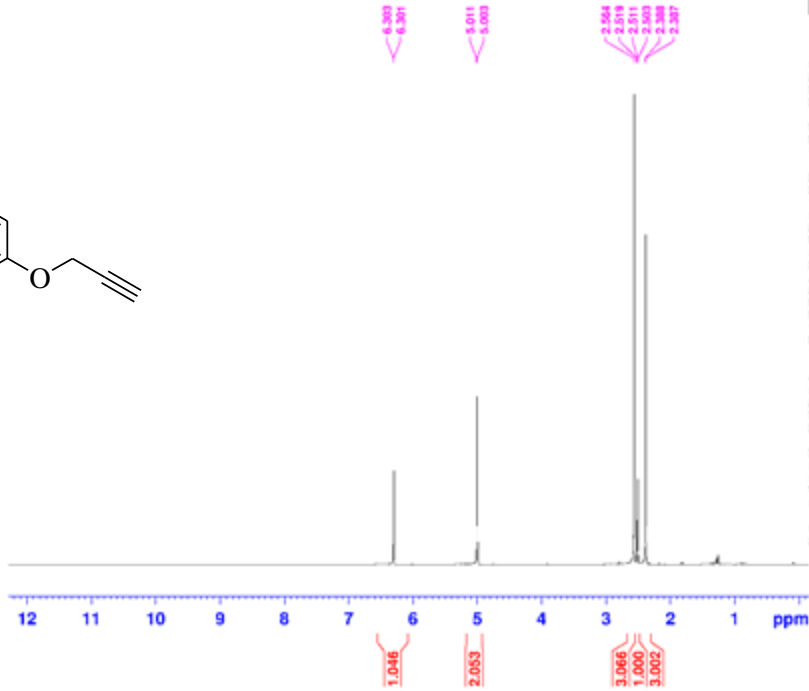
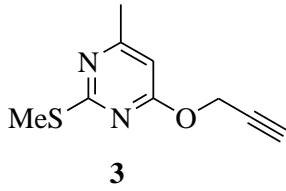
# **Sonogashira coupling reactions: Synthesis of 4-substituted-6-methyl-2-(methylthio)pyrimidines catalyzed by Pd-Cu**

Fatemeh Rezaeimanesh, Mohammad Bakherad, Hossein N. Isfahani

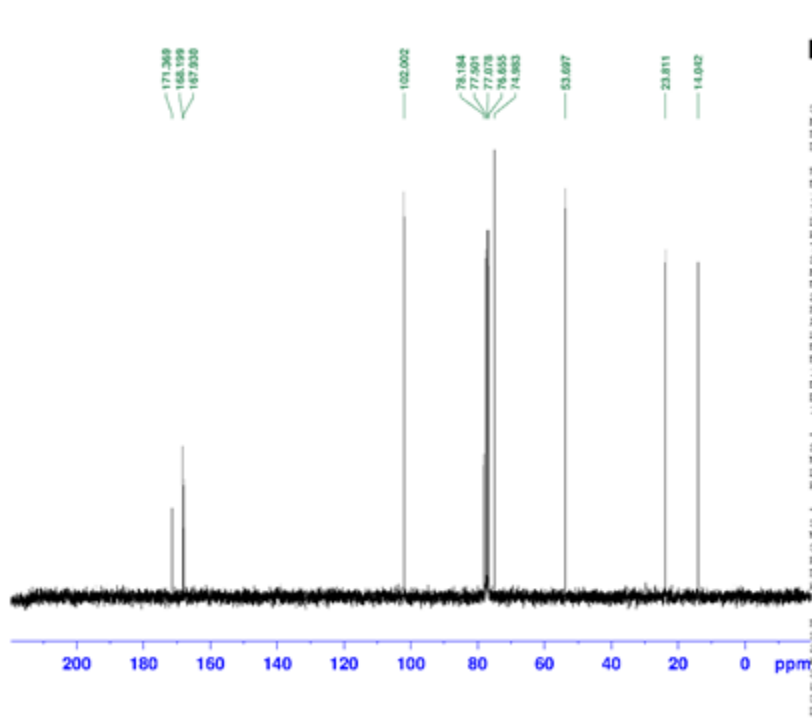
## **Supplementary information**

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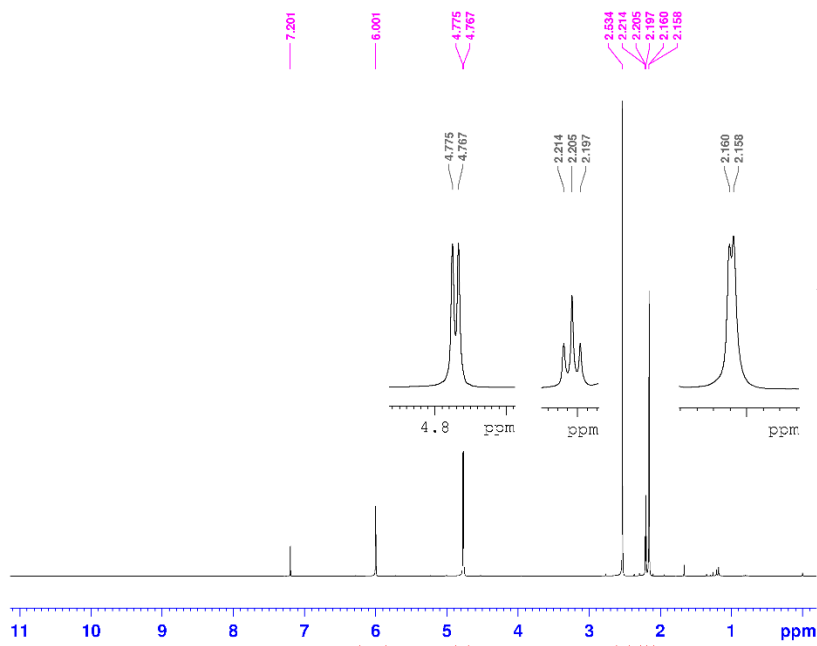
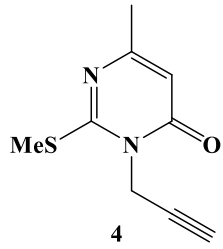
Copies of  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectrum of products **3**, **4**, **6a**, **6b**, **6c**, **6d**, **6e**, **6f**, **6g**



Current Data Parameters  
 NAME Feb08-2018-amz  
 EXPNO 21  
 PROCNO 1  
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 Time 16.10  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6009.615 Kz  
 FREQS 0.091699 MHz  
 AQ 5.4523952 sec  
 SFO 113.32  
 FM 83.700 MHz  
 FE 6.50 MHz  
 LC 295.8 K  
 E1 1.0000000 sec  
 D0 1  
 ----- CHANNEL f1 -----  
 SFO1 300.811876 MHz  
 NUC1 13  
 P1 19.00 MHz  
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 F2 - Processing parameters  
 S1 65536  
 SF 300.8100000 MHz  
 WM 1M  
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 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME Feb08-2018-amz  
 EXPNO 22  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20180708  
 Time 16.20  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 140  
 DS 4  
 SWH 18115.941 Kz  
 FREQS 0.276427 MHz  
 AQ 1.8087935 sec  
 SFO 202  
 FM 27.600 MHz  
 FE 6.50 MHz  
 LC 296.4 K  
 E1 2.0000000 sec  
 E11 0.0300000 sec  
 D0 1  
 ----- CHANNEL f1 -----  
 SFO1 75.5462982 MHz  
 NUC1 13C  
 P1 16.00 MHz  
 PLW1 0.4000000 M  
 ----- CHANNEL f2 -----  
 SFO2 300.8117032 MHz  
 NUC2 1H  
 CFEPRG2 waltz16  
 PCPD2 90.00 MHz  
 PLW2 0.4000000 M  
 PLW3 0.7778000 M  
 PLW4 0.743999999 M  
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 SF 300.8117032 MHz  
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 SSB 0  
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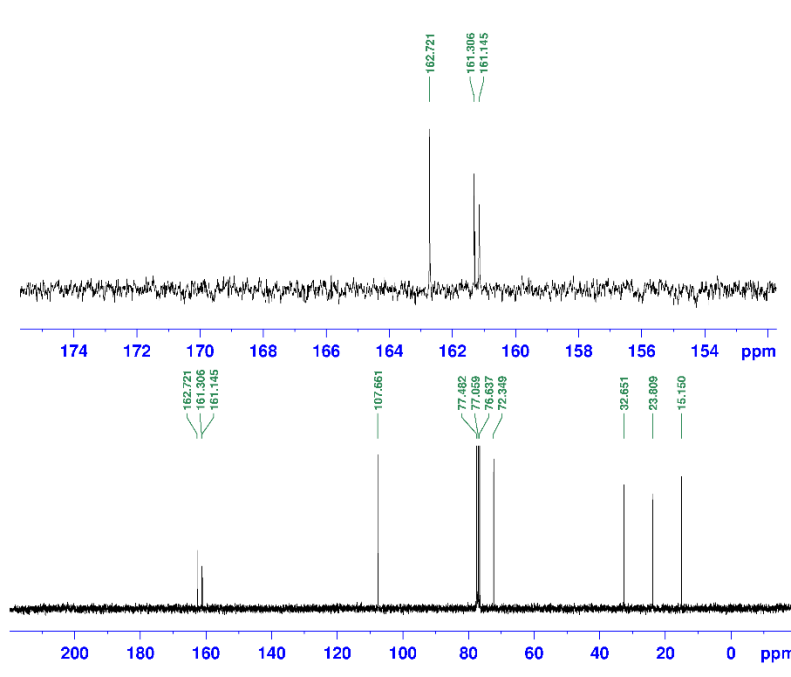


Current Data Parameters  
 NAME Feb08-2018-nmr  
 EXPNO 23  
 PROCNO 1

F2 - Acquisition Parameters  
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 PROBHD 5 mm F4BBO BB  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SMH 6009.615 Hz  
 FIDRES 0.091699 Hz  
 AQ 5.452992 sec  
 RG 181.36  
 TM 83.700 usec  
 DE 6.50 usec  
 TE 295.9 K  
 D1 1.00000000 sec  
 TD0 1

----- CHANNEL f1 -----  
 SFO1 303.8118576 MHz  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 6.40000010 W

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 SF 303.8100295 MHz  
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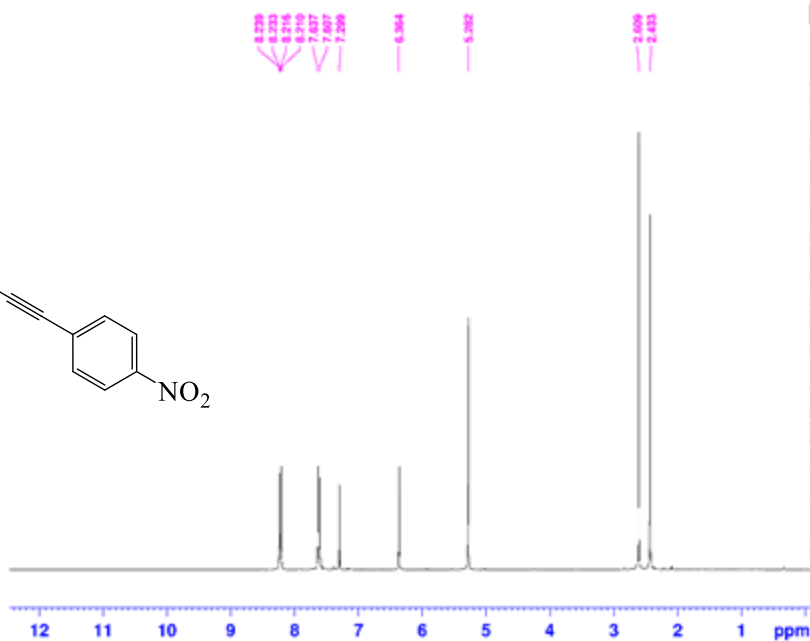
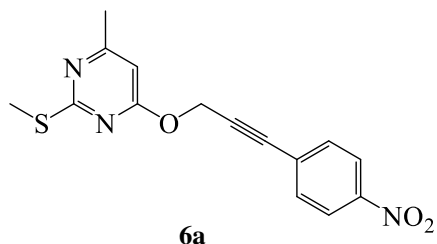
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 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 256  
 DS 4  
 SWE 18115.941 Hz  
 FIDRES 0.276427 Hz  
 AQ 1.8087935 sec  
 RG 202  
 TM 27.600 usec  
 DE 6.50 usec  
 TE 296.5 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

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 SFO1 75.6462982 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 30.00000000 W

----- CHANNEL #2 -----  
 SFO2 306.8112032 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 DM2 6.40000010 W  
 PLW2 0.17778000 W  
 PLW13 0.14399999 W

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 SI 32768  
 SF 75.6387350 MHz  
 MDW EM  
 SSB 0  
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 GB 0  
 PC 1.40

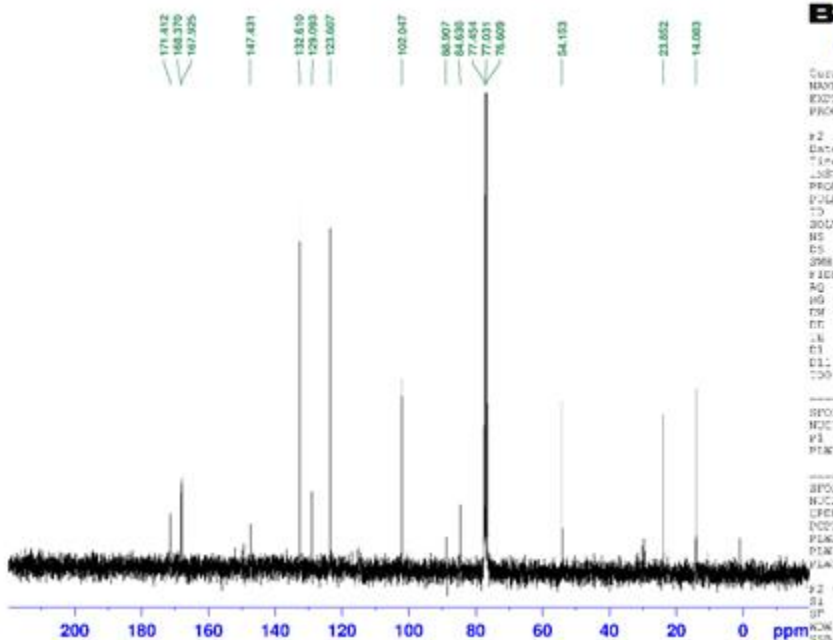


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 PROGRAM 5 mm PABBO 7H-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SFR 8009.615 Kz  
 FIDRES 0.391499 Hz  
 AQ 5.4525952 sec  
 RG 302  
 TR 83.203 msec  
 DE 6.50 msec  
 TE 297.3 K  
 D1 1.00000000 sec  
 D0 1

----- CHANNEL f1 -----  
 SFO1 300.8118576 MHz  
 NUC1 13  
 P1 15.00 usec  
 PLW1 6.40000010 W

#2 - Processing parameters  
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 SF 300.8100000 MHz  
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 LB 0  
 GB 0 6.30 Hz  
 PC 1.00



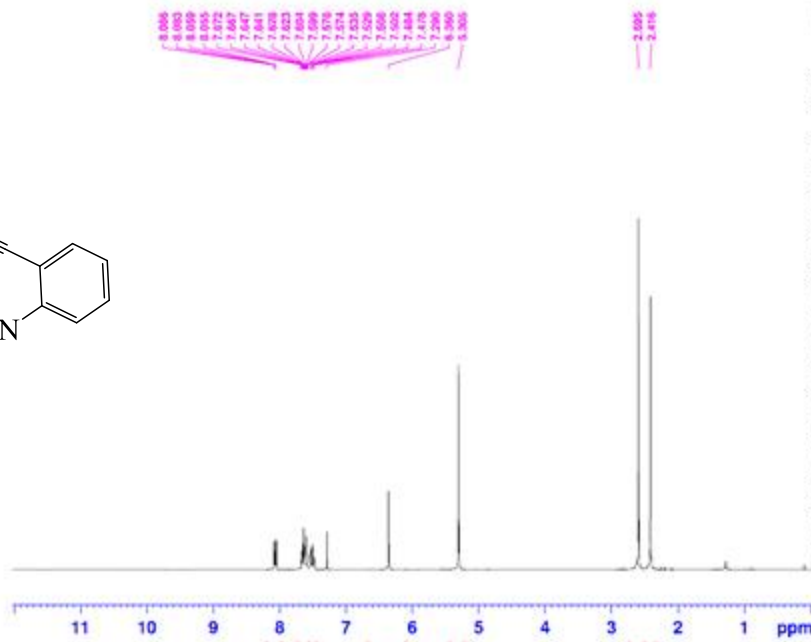
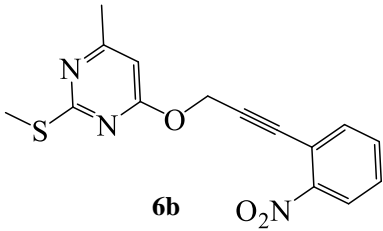
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 PROGRAM 5 mm PABBO 7H-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SFR 18115.941 Kz  
 FIDRES 0.276427 Hz  
 AQ 1.8087935 sec  
 RG 302  
 TR 37.603 msec  
 DE 6.50 msec  
 TE 298.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 D0 1

----- CHANNEL f1 -----  
 SFO1 75.6462982 MHz  
 NUC1 13C  
 P1 16.00 usec  
 PLW1 30.00000000 W

----- CHANNEL f2 -----  
 SFO2 300.8112032 MHz  
 NUC2 13  
 CPDPRG12 waltz16  
 NS252 95.00 usec  
 PLW2 6.40000010 W  
 PLW12 0.77780000 W  
 PLW13 0.47999999 W

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 PC 1.00

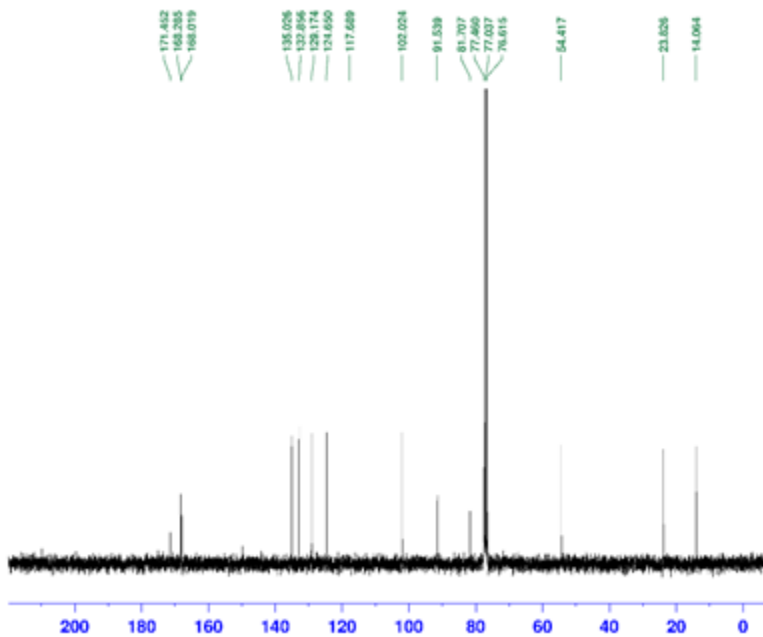


Current Data Parameters  
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 PROCNO 1

F2 Acquisition Parameters  
 Date\_ 20180526  
 Time 13.07  
 \_INSTNAM spect  
 PROGRAM 5 mm PANGO M-  
 PULPROG zgpg30  
 TD 65536  
 SFO1 300.135063  
 SOLVENT CDCl3  
 NS 68  
 DS 2  
 SWH 609.415 Hz  
 FIDRES 0.391690 Hz  
 AQ 5.4575957 sec  
 RG 262  
 FM 85.700 usec  
 DT 6.50 usec  
 DE 297.5 K  
 F1 1.00000000 sec  
 DQ 1

----- CHANNEL f1 -----  
 SFO1 300.135063 MHz  
 NUC1 13  
 P1 15.00 usec  
 PL1 6.40000000 W

F2 - Processing parameters  
 ST 65536  
 SF 300.135063 MHz  
 KCM EM  
 SSB 0  
 LB 6.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME Jun0-2018-nmr  
 EXPNO 6  
 PROCNO 1

F2 Acquisition Parameters  
 Date\_ 20180607  
 Time 17.02  
 \_INSTNAM spect  
 PROGRAM 5 mm PANGO M-  
 PULPROG zgpg30  
 TD 65536  
 SFO1 300.135063  
 SOLVENT CDCl3  
 NS 4  
 DS 4  
 SWH 18115.941 Hz  
 FIDRES 0.276427 Hz  
 AQ 1.8087935 sec  
 RG 262  
 FM 27.600 usec  
 DT 6.50 usec  
 DE 298.9 K  
 F1 2.00000000 sec  
 F11 0.03000000 sec  
 DQ 1

----- CHANNEL f1 -----  
 SFO1 75.6462982 MHz  
 NUC1 13C  
 P1 16.00 usec  
 PL1 30.00000000 W

----- CHANNEL f2 -----  
 SFO2 300.135063 MHz  
 NUC2 13  
 CFEPRG12 waltz16  
 DCCD2 96.00 usec  
 PL12 6.40000000 W  
 PL13 0.77780000 W  
 PL14 0.43999999 W

F2 - Processing parameters  
 SI 32768  
 SF 75.6387350 MHz  
 KCM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

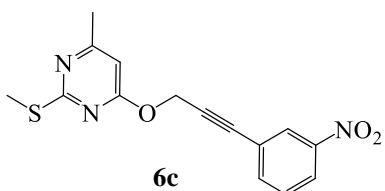
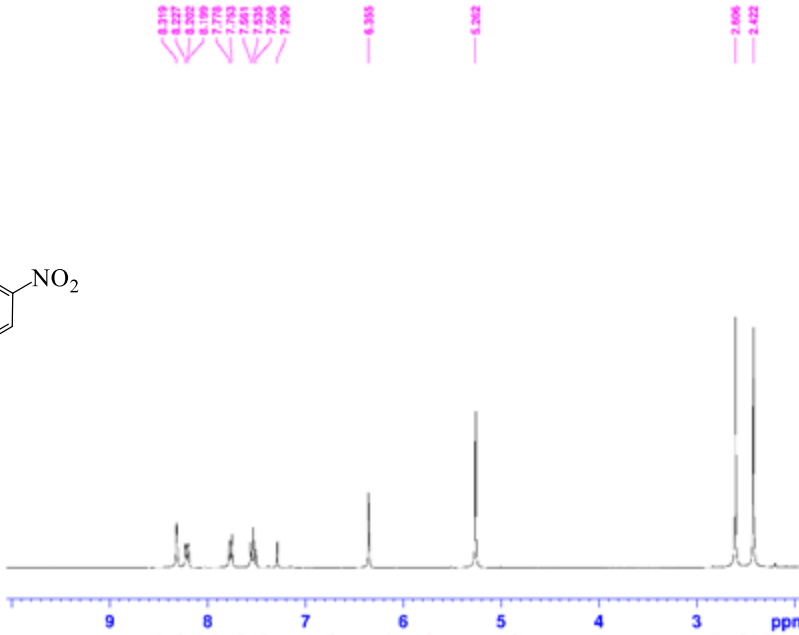


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NAME: Jun02-2018-nar  
EX290: 21  
PROCNO: 1

F2 Acquisition Parameters  
Date\_: 20180602  
Time: 14.05  
INSTRUM: spect  
PROBHD: 5 mm PABBO 90-  
PULPROG: zgpg30  
TD: 65536  
SOLVENT: CDCl3  
NS: 64  
DS: 2  
SWH: 8009.615 Kz  
FIDRES: 0.091699 Kz  
AQ: 9.4839903 sec  
RG: 158.22  
EM: 83.200 uVcc  
DE: 6.50 uVcc  
LB: 296.2 K  
EI: 1.00000000 sec  
CO: 1

===== CHANNEL f1 =====  
NUC1: 13  
P1: 15.00 uVcc  
PLW1: 6.40000010 W

F2 - Processing parameters  
SI: 55036  
SF: 300.9100029 MHz  
WDW: EM  
SSB: 0  
LB: 6.30 Kz  
GB: 0  
PC: 1.00



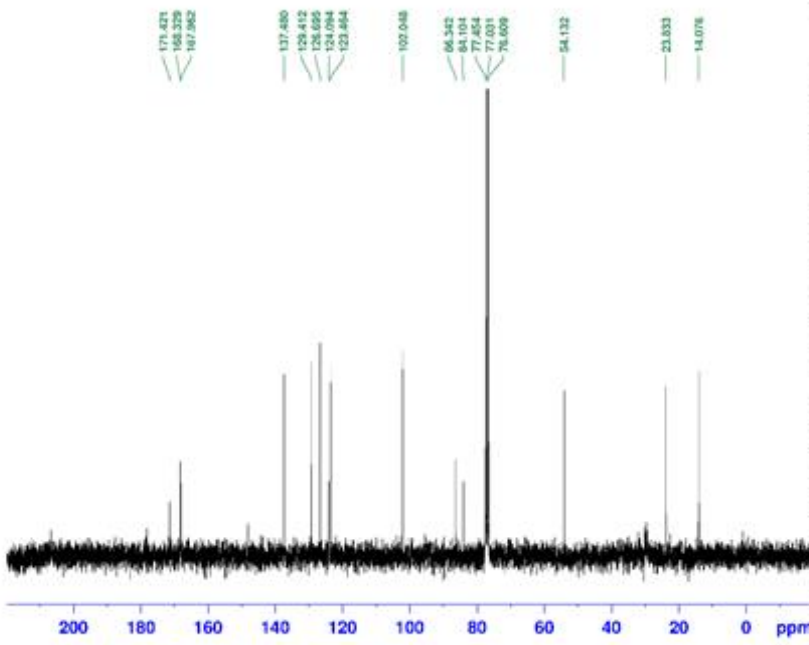
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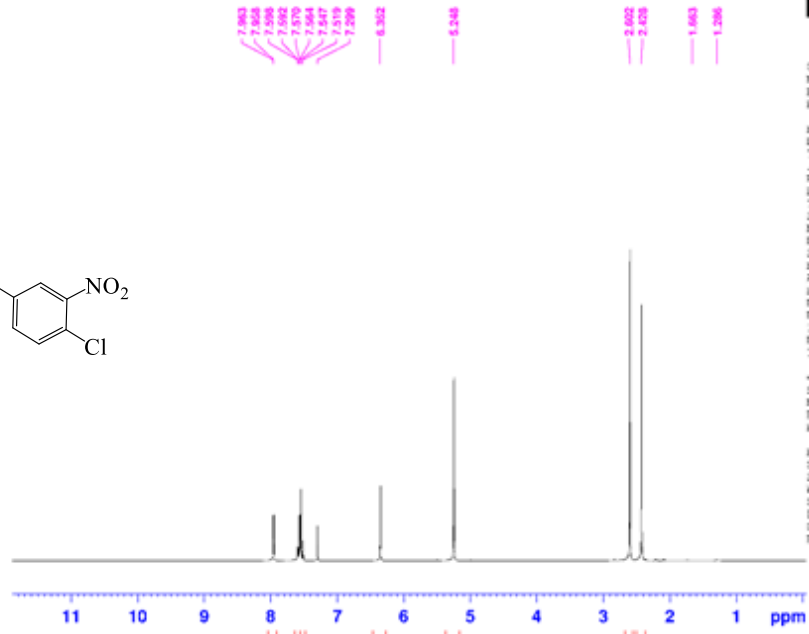
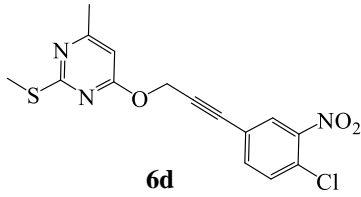
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Date\_: 20180605  
Time: 16.31  
INSTRUM: spect  
PROBHD: 5 mm PABBO 90-  
PULPROG: zgpg30  
TD: 65536  
SOLVENT: CDCl3  
NS: 320  
DS: 4  
SWH: 18115.961 Kz  
FIDRES: 0.276427 Kz  
AQ: 1.6087935 sec  
RG: 262  
EM: 27.400 uVcc  
DE: 6.50 uVcc  
LB: 362.2 K  
EI: 3.00000000 sec  
D11: 0.03000000 sec  
CO: 1

===== CHANNEL f1 =====  
NUC1: 13C  
P1: 16.00 uVcc  
PLW1: 30.00000000 W

===== CHANNEL f2 =====  
NUC2: 13C  
P2PRG2: waltz16  
DCCD2: 96.00 uVcc  
PLW2: 6.40000010 W  
PLW12: 0.77780000 W  
PLW13: 0.14399999 W

F2 - Processing parameters  
SI: 32768  
SF: 99.6261300 MHz  
WDW: EM  
SSB: 0  
LB: 1.00 Kz  
GB: 0  
PC: 1.00



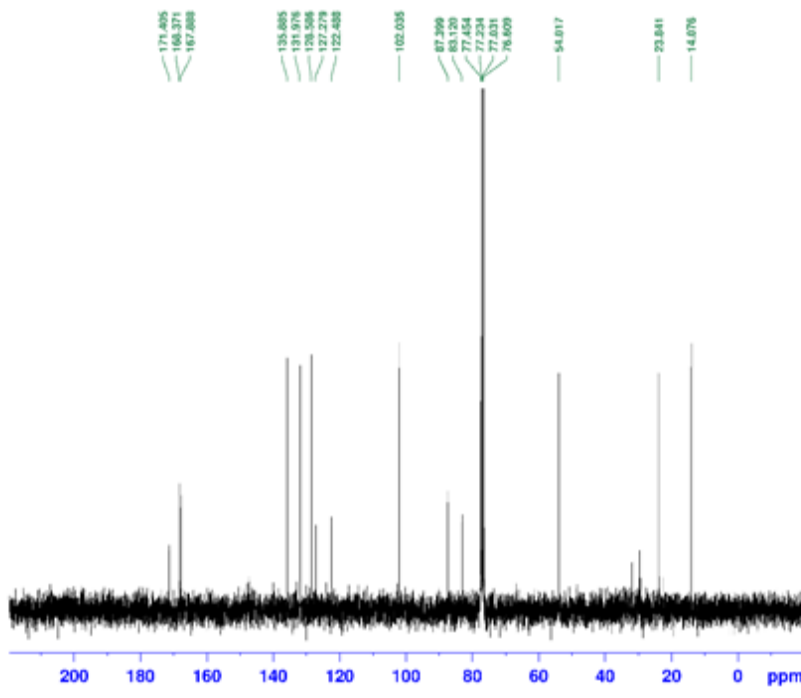


Current Data Parameters  
 NAME May20-2018-nmr  
 EXNO 21  
 PROCNO 1

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 Time 11.39  
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 PRGRM 5 mm PABBO 7H-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 56  
 DS 2  
 SFR 509.615 Hz  
 FIDRES 0.391699 Hz  
 AQ 5.4525952 sec  
 RG 262  
 TM 83.203 sec  
 DE 6.50 usec  
 TE 297.4 K  
 LB 1.0000000 sec  
 CO 1

----- CHANNEL f1 -----  
 NUC1 13C  
 P1 15.00 usec  
 PL1 6.40000010 W

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 KW EM  
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 LB 6.30 Hz  
 GB 0  
 PC 1.40



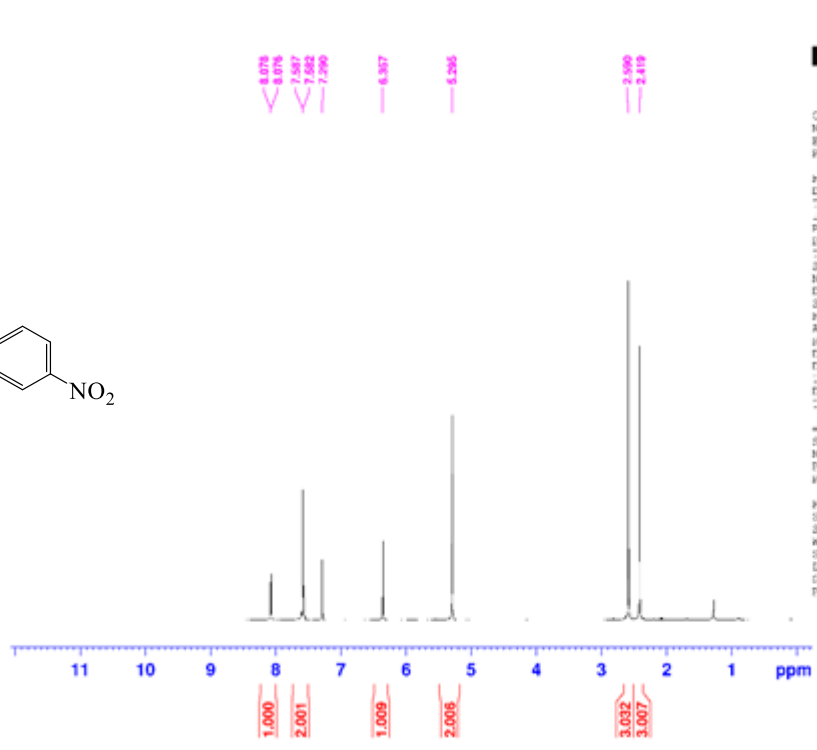
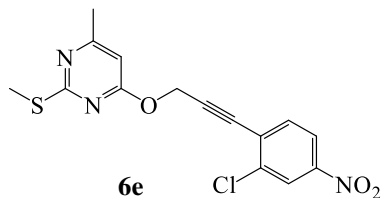
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 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
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 DS 4  
 SFR 18115.941 Hz  
 FIDRES 0.276427 Hz  
 AQ 1.8087935 sec  
 RG 262  
 TM 27.403 sec  
 DE 6.50 usec  
 TE 299.8 K  
 LB 2.0000000 sec  
 CO 0.0300000 sec  
 PC 1

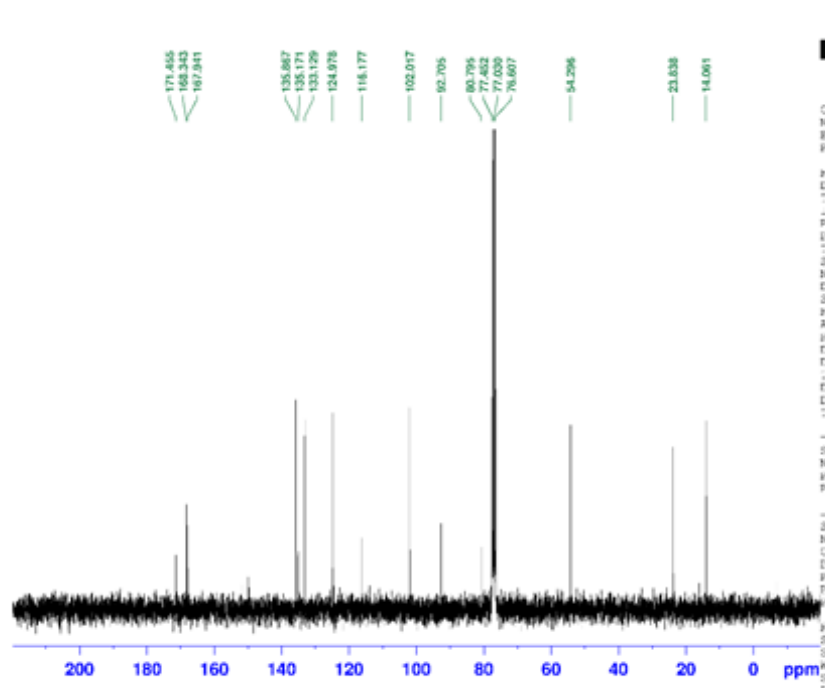
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 P1 15.00 usec  
 PL1 30.00000000 W

----- CHANNEL f2 -----  
 NUC2 13C  
 P2 15.00 usec  
 PL2 6.40000010 W  
 PL12 0.7778000 W  
 PL13 0.4399999 W

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 KW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

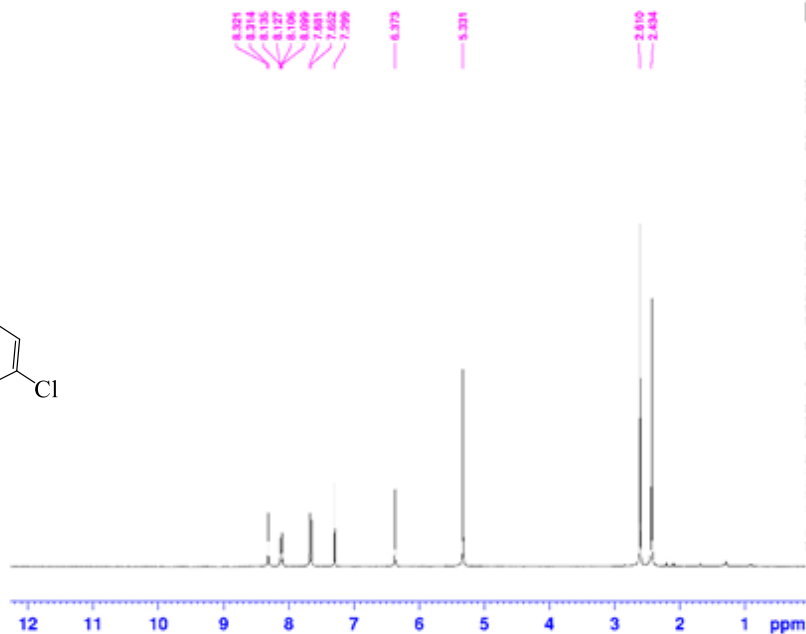
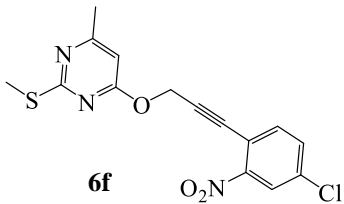


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 EXPO 25  
 PROCNO 1  
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 INSTRUM spect  
 PROBRD 5 mm PABBO 7H-  
 PULPROG zg30  
 TO 50036  
 SOLVENT CDCl3  
 NS 72  
 DS 2  
 SFO1 300.815 MHz  
 FIDRES 0.381699 Hz  
 AQ 5.4525952 sec  
 RG 262  
 FM 83.200 kHz  
 DE 6.50 kHz  
 LE 297.4 K  
 D1 1.0000000 sec  
 TD0 1  
 ----- CHANNEL f1 -----  
 SFO1 300.8118576 MHz  
 NUC1 13  
 P1 15.00 usec  
 PL1 6.4000000 W  
 F2 - Processing parameters  
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 SF 300.8100000 MHz  
 KW 1M  
 SS 0  
 LB 0 6.30 Hz  
 GB 0  
 PC 1.00



**BRUKER**  
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 NAME Jun07-2018-nmr  
 EXPO 8  
 PROCNO 1  
 F2 Acquisition Parameters  
 Date\_ 20180607  
 Time 17.36  
 INSTRUM spect  
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 PULPROG zgpg30  
 TO 50036  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SFO1 101.625 MHz  
 FIDRES 0.276427 Hz  
 AQ 1.8087935 sec  
 RG 262  
 FM 27.600 kHz  
 DE 6.50 kHz  
 LE 298.7 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1  
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 SFO1 75.6462982 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PL1 30.0000000 W  
 ----- CHANNEL f2 -----  
 SFO2 300.8112032 MHz  
 NUC2 13  
 CPDPRG2 waltz16  
 DDD2 96.00 usec  
 PL12 6.4000000 W  
 PL13 0.7778000 W  
 PL14 0.4339999 W  
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 KW 1M  
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 LB 0 1.00 Hz  
 GB 0  
 PC 1.00





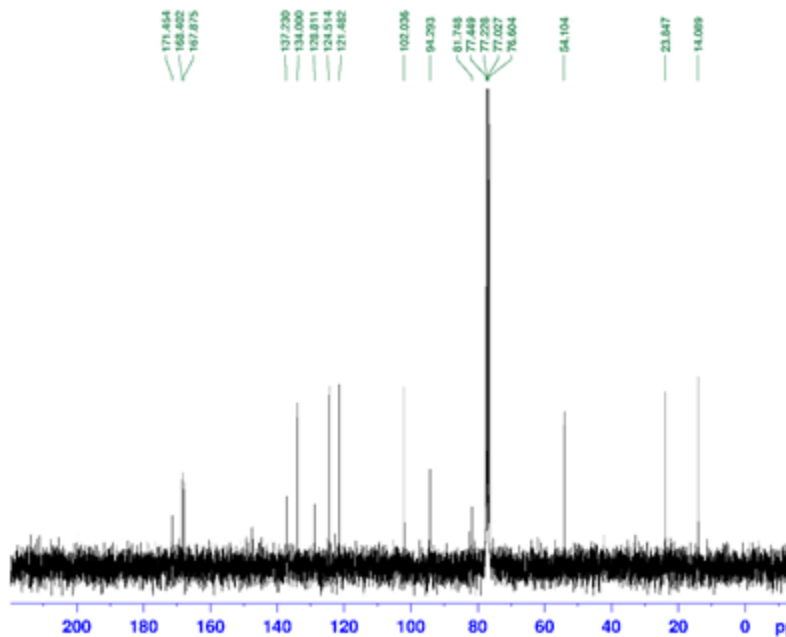
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 PROCNO 1

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 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1324  
 DS 4  
 SFR 18115.961 Kz  
 FIDRES 0.276427 Hz  
 AQ 1.8087935 sec  
 RG 262  
 FM 27.400 uHz  
 DE 6.50 uHz  
 LB 299.2 K  
 D1 2.00000000 sec  
 D2 0.03000000 sec  
 D3 1

----- CHANNEL f1 -----  
 SFO1 75.6462982 MHz  
 NUC1 13C  
 P1 16.00 uHz  
 PLW1 30.00000000 W

----- CHANNEL f2 -----  
 SFO2 300.8112032 MHz  
 NUC2 1H  
 CPDPRG2 wa:tr16  
 DCD2 96.00 uHz  
 PLW2 6.40000010 W  
 PLW12 0.17780000 W  
 PLW13 0.14399999 W

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 SF 75.6367350 MHz  
 KW 128  
 SSB 0  
 LB 1.00 Kz  
 GB 0  
 PC 1.00



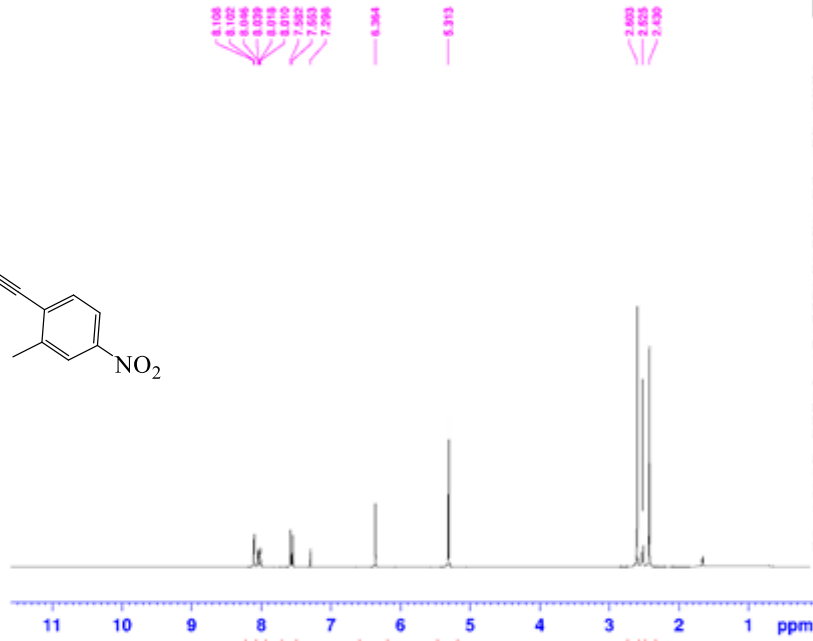
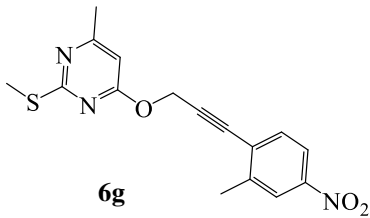
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F2 - Acquisition Parameters  
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 PROBRD 5 mm FATHO 7H-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1324  
 DS 4  
 SFR 18115.961 Kz  
 FIDRES 0.276427 Hz  
 AQ 1.8087935 sec  
 RG 262  
 FM 27.400 uHz  
 DE 6.50 uHz  
 LB 299.2 K  
 D1 2.00000000 sec  
 D2 0.03000000 sec  
 D3 1

----- CHANNEL f1 -----  
 SFO1 75.6462982 MHz  
 NUC1 13C  
 P1 16.00 uHz  
 PLW1 30.00000000 W

----- CHANNEL f2 -----  
 SFO2 300.8112032 MHz  
 NUC2 1H  
 CPDPRG2 wa:tr16  
 DCD2 96.00 uHz  
 PLW2 6.40000010 W  
 PLW12 0.17780000 W  
 PLW13 0.14399999 W

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 SF 75.6367350 MHz  
 KW 128  
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 LB 1.00 Kz  
 GB 0  
 PC 1.00

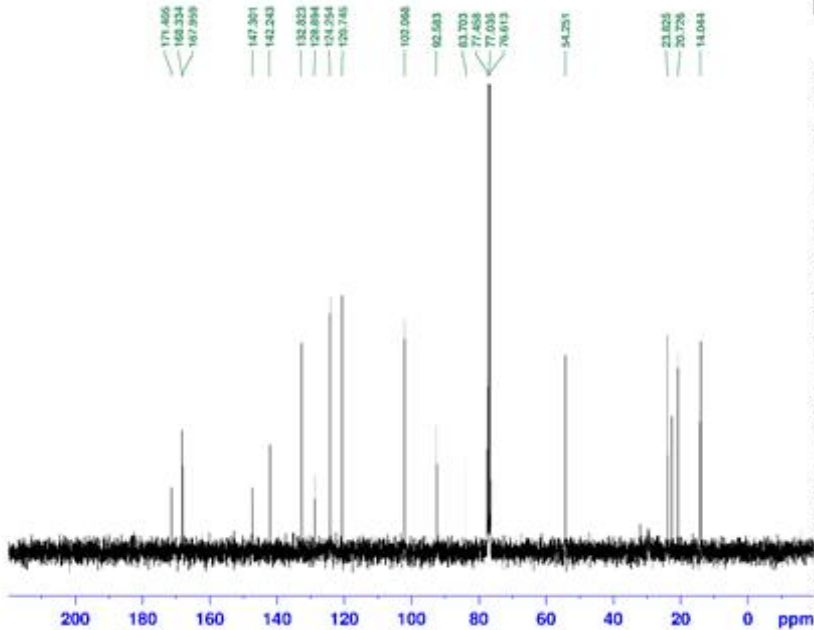


Current Data Parameters  
 NAME May20-2018-nmr  
 EXPTNO 21  
 PROCNO 1

F2 Acquisition Parameters  
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 Time 17.13  
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 PULPROG zgpg30  
 TD 65536  
 SOLVENT cdcl3  
 NS 102  
 DS 2  
 SWH 809.615 Kz  
 FIDRES 0.091699 Kz  
 AQ 9.453993 sec  
 RG 127.27  
 DW 83.203 usec  
 DE 6.50 usec  
 EK 297.3 K  
 D1 1.00000000 sec  
 D20 1

===== CHANNEL f1 =====  
 SFO1 300.811876 Mhz  
 NUC1 13  
 P1 15.00 usec  
 PLW1 6.40000010 W

F2 - Processing parameters  
 SI 65536  
 SF 300.810000 Mhz  
 KW 128  
 SSB 0  
 LB 0.33 Kz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME Jun07-2018-nmr  
 EXPTNO 1  
 PROCNO 1

F2 Acquisition Parameters  
 Date\_ 20180607  
 Time 9.35  
 INSTRUM spect  
 PROBRM 5 mm F400 NQ-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT cdcl3  
 NS 124  
 DS 4  
 SWH 801.591 Kz  
 FIDRES 0.276427 Kz  
 AQ 1.6981935 sec  
 RG 262  
 DW 27.403 usec  
 DE 6.50 usec  
 EK 303.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 D20 1

===== CHANNEL f1 =====  
 SFO1 75.5462982 Mhz  
 NUC1 13C  
 P1 16.00 usec  
 PLW1 30.00000000 W

===== CHANNEL f2 =====  
 SFO2 300.8112032 Mhz  
 NUC2 13  
 P2PRG12 wa-zz16  
 NUC3 9C  
 PLW2 6.40000010 W  
 PLW12 0.77780000 W  
 PLW13 0.43999999 W

F2 - Processing parameters  
 SI 32768  
 SF 75.5387350 Mhz  
 KW 128  
 SSB 0  
 LB 1.00 Kz  
 GB 0  
 PC 1.40