

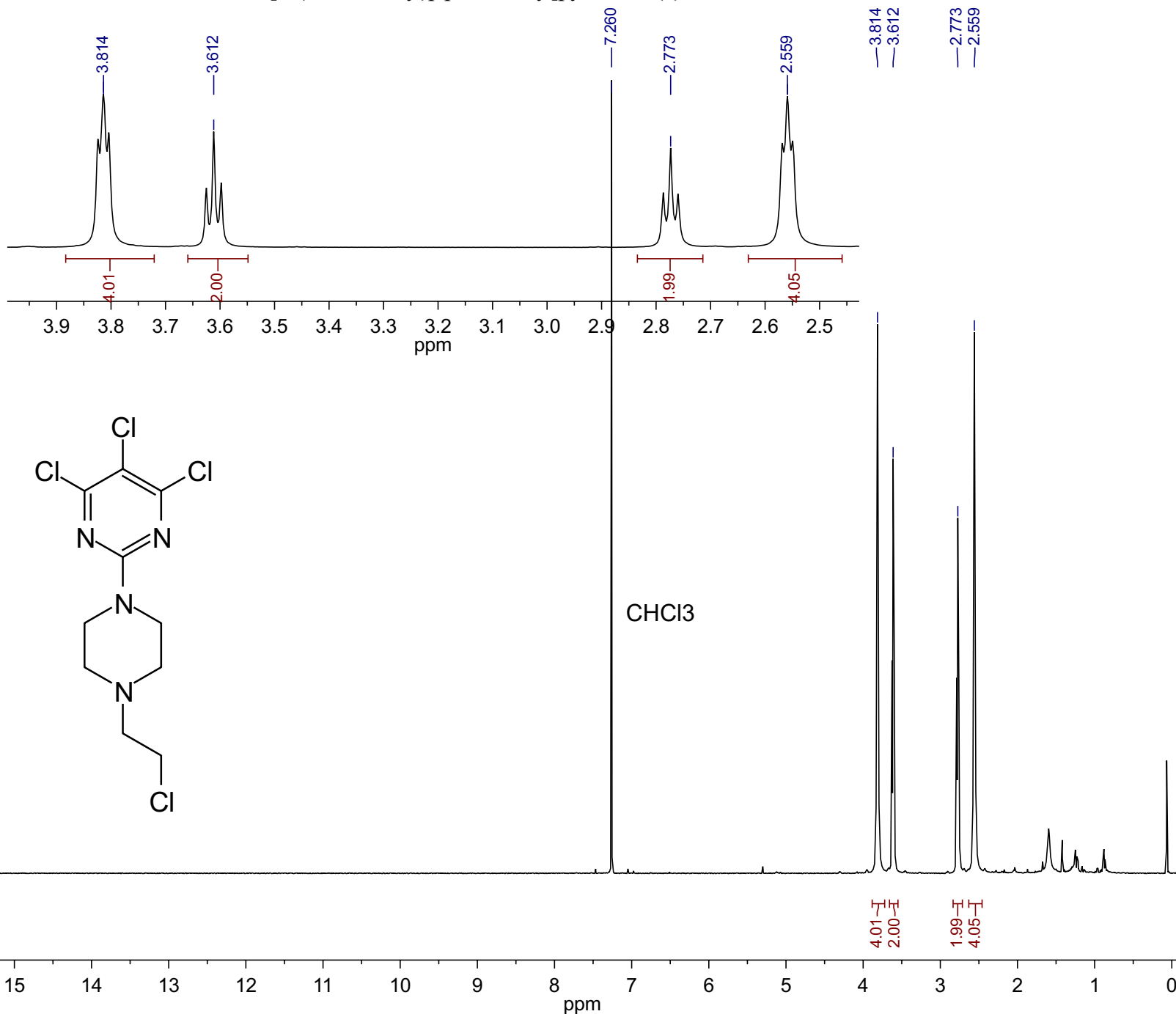
## **Supporting Information**

### **Reactions of polychlorinated pyrimidines with DABCO**

Andreas S. Kalogirou\* and Panayiotis A. Koutentis

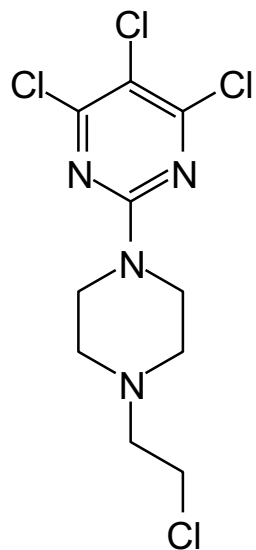
## **$^1\text{H}$ and $^{13}\text{C}$ NMR Spectra of new compounds**

<sup>1</sup>H NMR of 2,4,5-trichloro-6-[4-(2-chloroethyl)piperazin-1-yl]pyrimidine (5).



Current Data Parameters	
NAME	Kalogirou
EXPNO	249
PROCNO	1
F2 - Acquisition Parameters	
Date_	20170127
Time	15.13
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCI3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2767999 sec
RG	161
DW	50.000 usec
DE	6.50 usec
TE	294.7 K
D1	1.00000000 sec
TD0	1
===== CHANNEL f1	
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SFO1	500.0361158 MHz
NUC1	1H
P1	12.00 usec
PLW1	14.50000000 W
F2 - Processing parameters	
SI	65536
SF	500.0330400 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

<sup>13</sup>C NMR of 2,4,5-trichloro-6-[4-(2-chloroethyl)piperazin-1-yl]pyrimidine (5).



159.230  
157.195

113.071

77.000

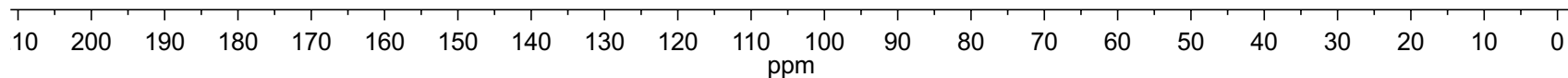
59.631

52.661

44.007

40.782

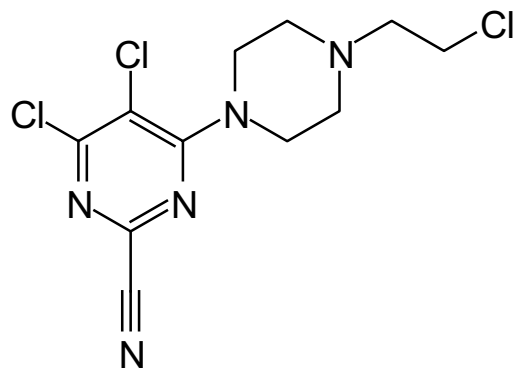
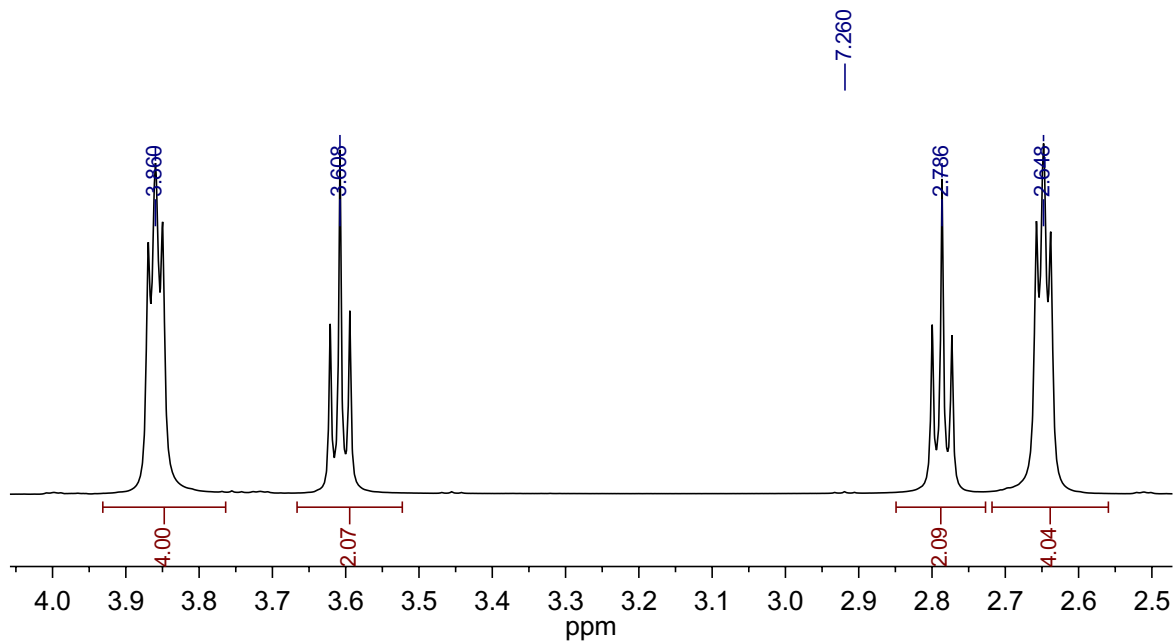
CDCI3



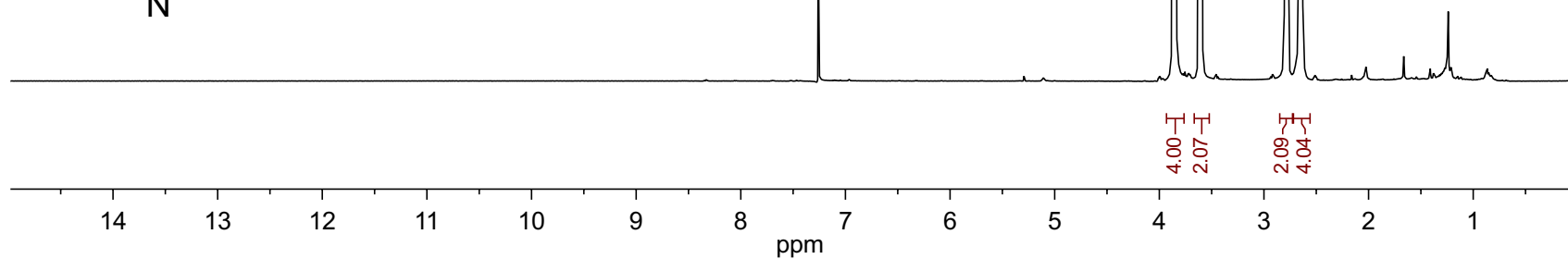
Current Data Parameters

NAME Kalogirou  
EXPNO 256  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20170205  
Time 21.18  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG jmod  
TD 65536  
SOLVENT CDCl3  
NS 13824  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010048 sec  
RG 2050  
DW 16.800 usec  
DE 6.50 usec  
TE 295.9 K  
CNST2 145.000000  
CNST11 1.000000  
D1 2.00000000 sec  
D20 0.00689655 sec  
TD0 1  
===== CHANNEL f1 =====  
SFO1 125.7459782 MHz  
NUC1 13C  
P1 9.00 usec  
P2 18.00 usec  
PLW1 133.00000000 W  
===== CHANNEL f2 =====  
SFO2 500.0350280 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 80.00 usec  
PLW2 14.50000000 W  
PLW12 0.32624999 W  
F2 - Processing parameters  
SI 32768  
SF 125.7334089 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

<sup>1</sup>H NMR of 4,5-dichloro-6-[4-(2-chloroethyl)piperazin-1-yl]pyrimidine-2-carbonitrile (6).



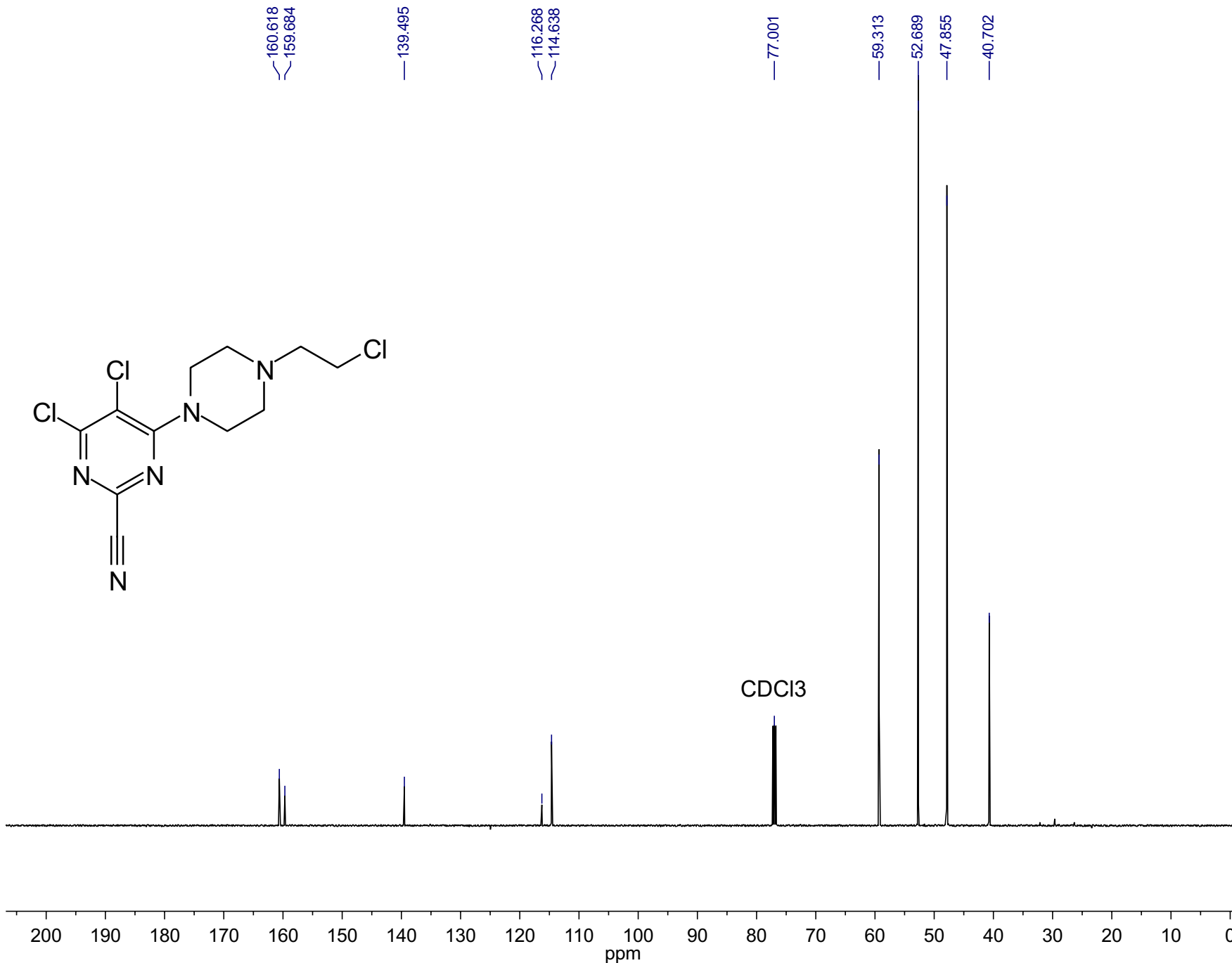
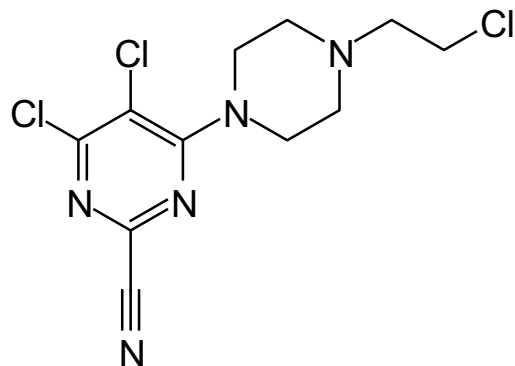
CHCl<sub>3</sub>



Current Data Parameters

NAME	Kalogirou
EXPNO	253
PROCNO	1
F2 - Acquisition Parameters	
Date_	20170203
Time	13.31
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCB
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2767999 sec
RG	71.8
DW	50.000 usec
DE	6.50 usec
TE	295.3 K
D1	1.00000000 sec
TD0	1
===== CHANNEL f1 =====	
SFO1	500.0361158 MHz
NUC1	1H
P1	12.00 usec
PLW1	14.50000000 W
F2 - Processing parameters	
SI	65536
SF	500.0330401 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

<sup>13</sup>C NMR of 4,5-dichloro-6-[4-(2-chloroethyl)piperazin-1-yl]pyrimidine-2-carbonitrile (**6**).



Current Data Parameters

NAME Kalogirou  
EXPNO 254  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20170203  
Time 16.01  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG jmod  
TD 65536  
SOLVENT CDCl3  
NS 2816  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010048 sec  
RG 2050  
DW 16.800 usec  
DE 6.50 usec  
TE 296.9 K  
CNST2 145.000000  
CNST11 1.000000  
D1 2.00000000 sec  
D20 0.00689655 sec  
TD0 1  
===== CHANNEL f1 =====  
SFO1 125.7459782 MHz  
NUC1 13C  
P1 9.00 usec  
P2 18.00 usec  
PLW1 133.00000000 W  
===== CHANNEL f2 =====  
SFO2 500.0350280 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 80.00 usec  
PLW2 14.50000000 W  
PLW12 0.32624999 W  
F2 - Processing parameters  
SI 32768  
SF 125.7334135 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40