

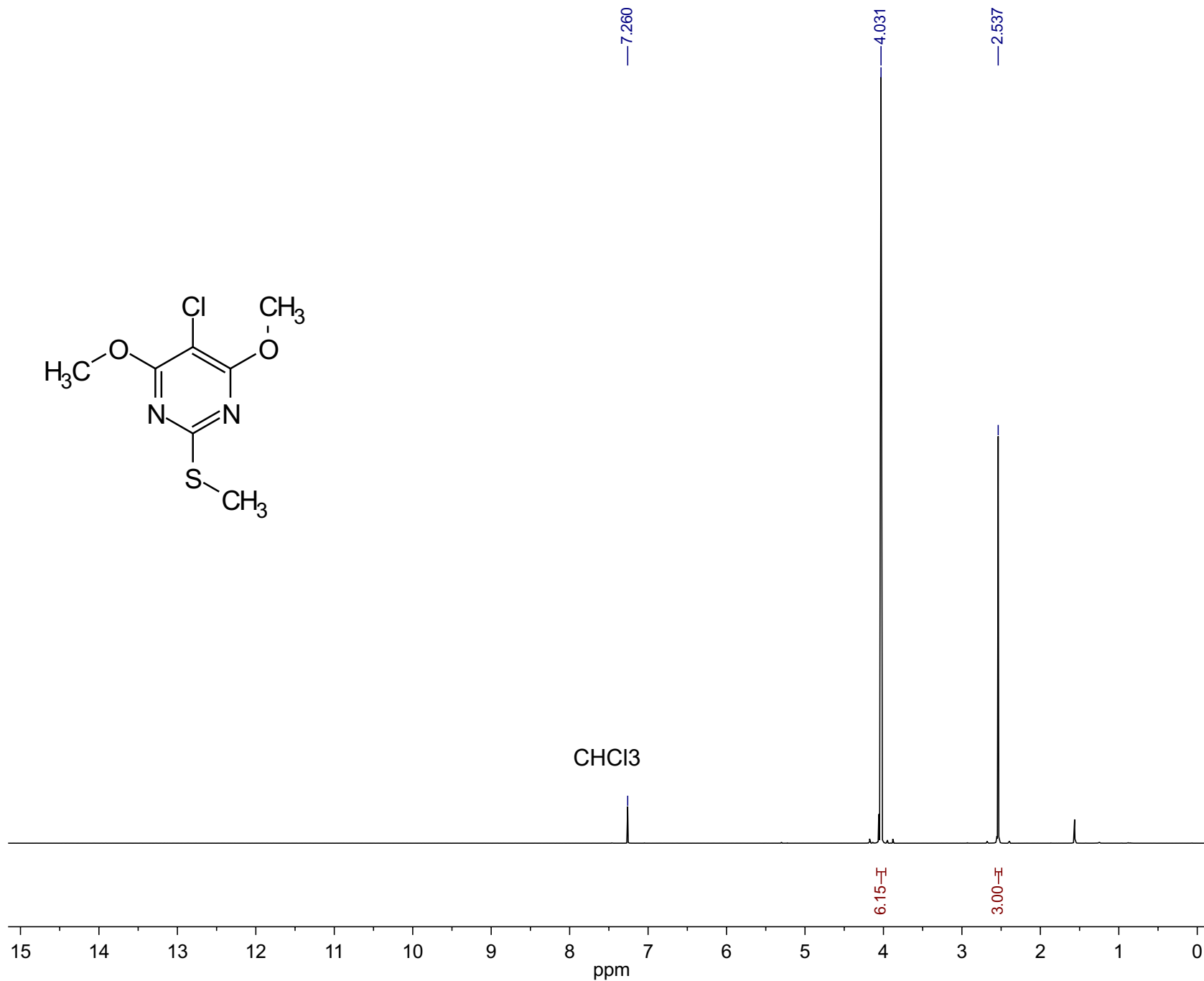
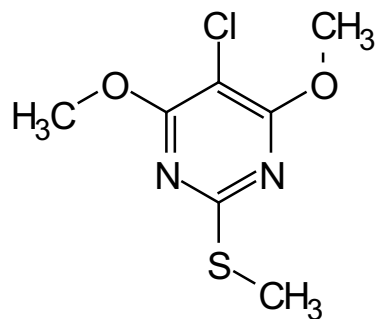
## **Supporting Information**

### **Synthesis of 2-cyanopyrimidines**

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 5-chloro-4,6-dimethoxy-2-(methylthio)pyrimidine (16)

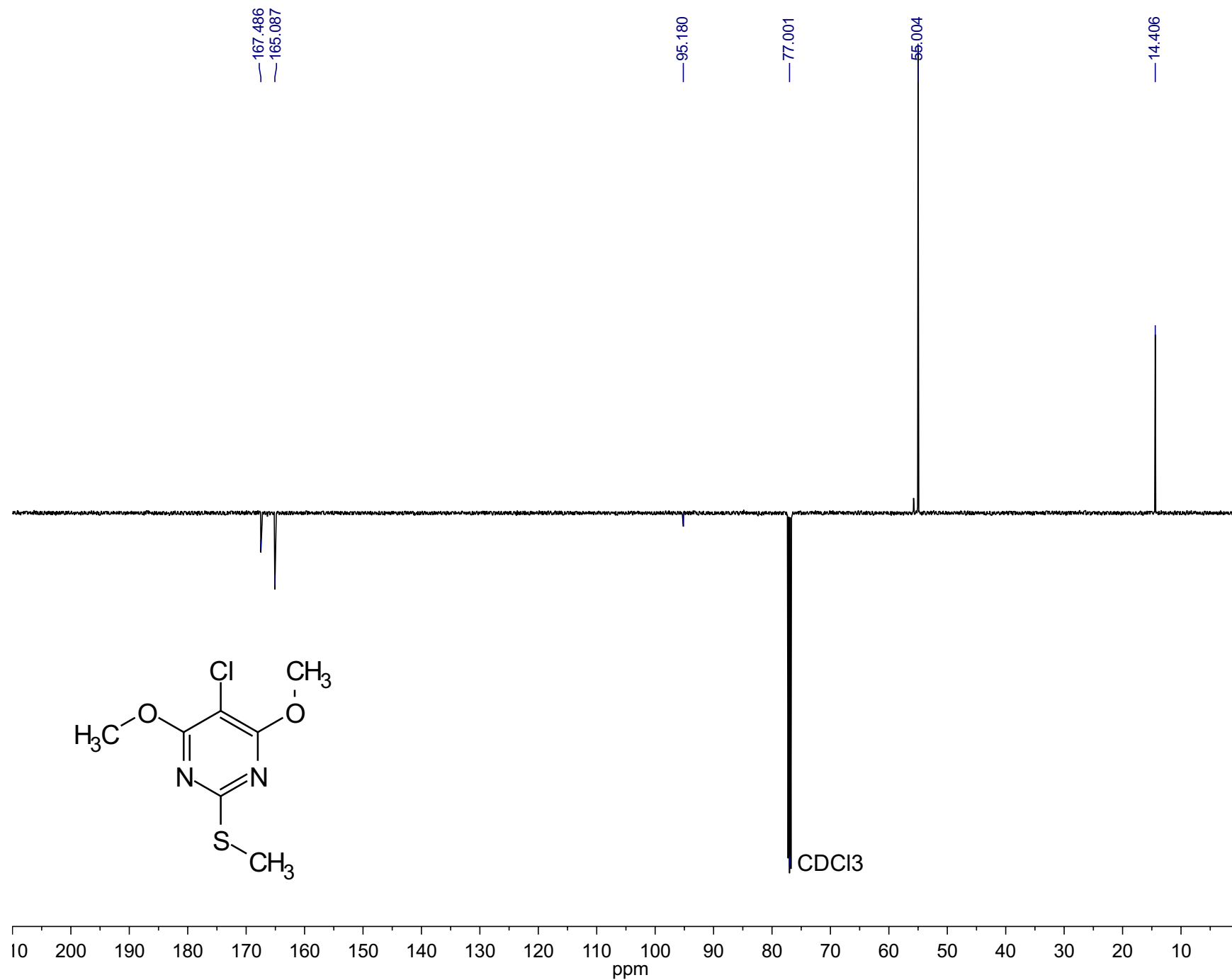


Current Data Parameters  
NAME Kalogirou  
EXPNO 224  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20161224  
Time 21.04  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 128  
DW 50.000 usec  
DE 6.50 usec  
TE 294.8 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

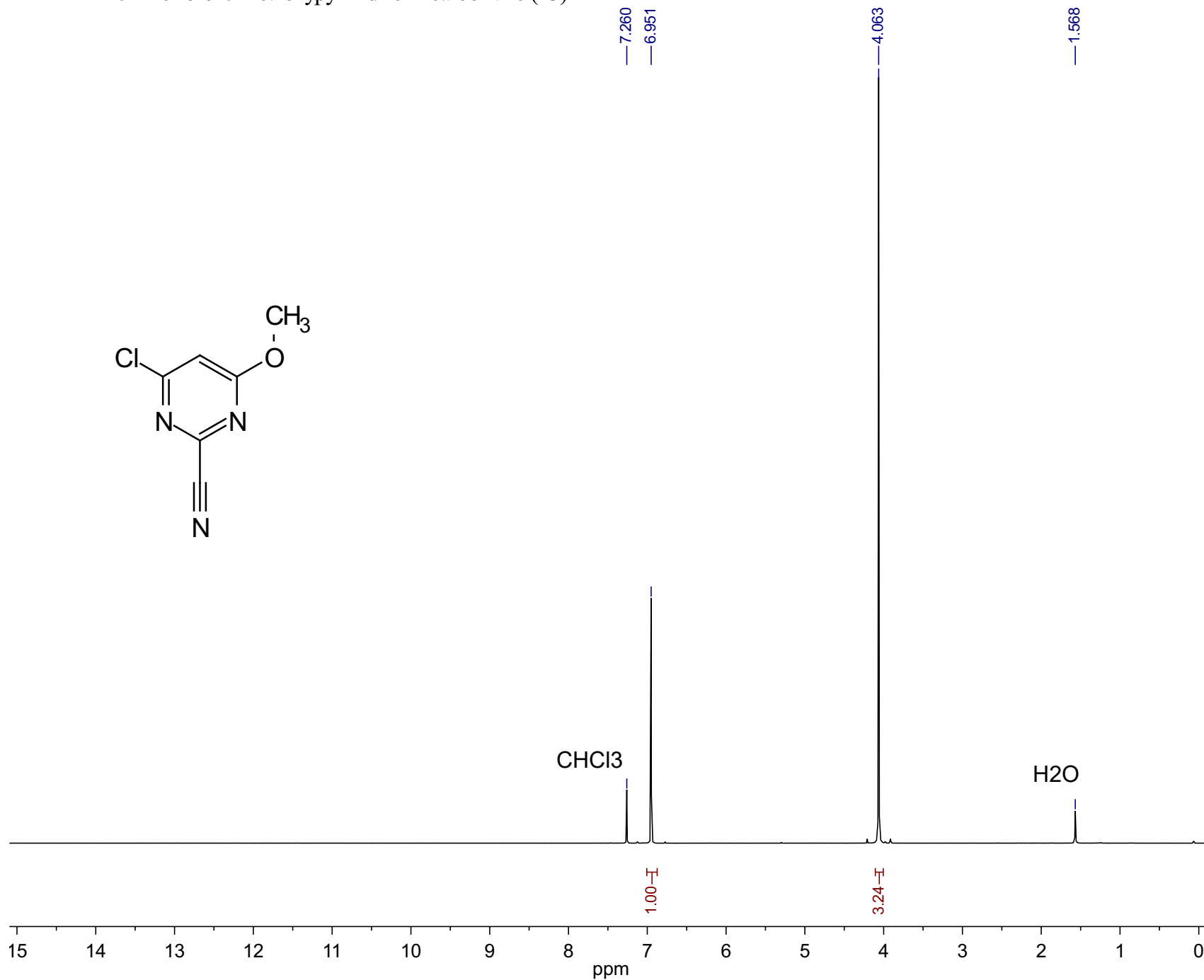
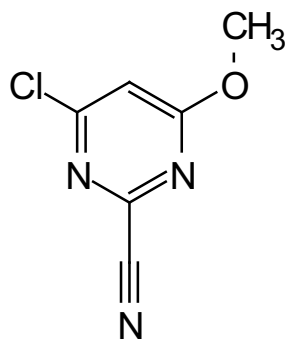
F2 - Processing parameters  
SI 65536  
SF 500.0330398 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

<sup>13</sup>C NMR of 5-chloro-4,6-dimethoxy-2-(methylthio)pyrimidine (16)



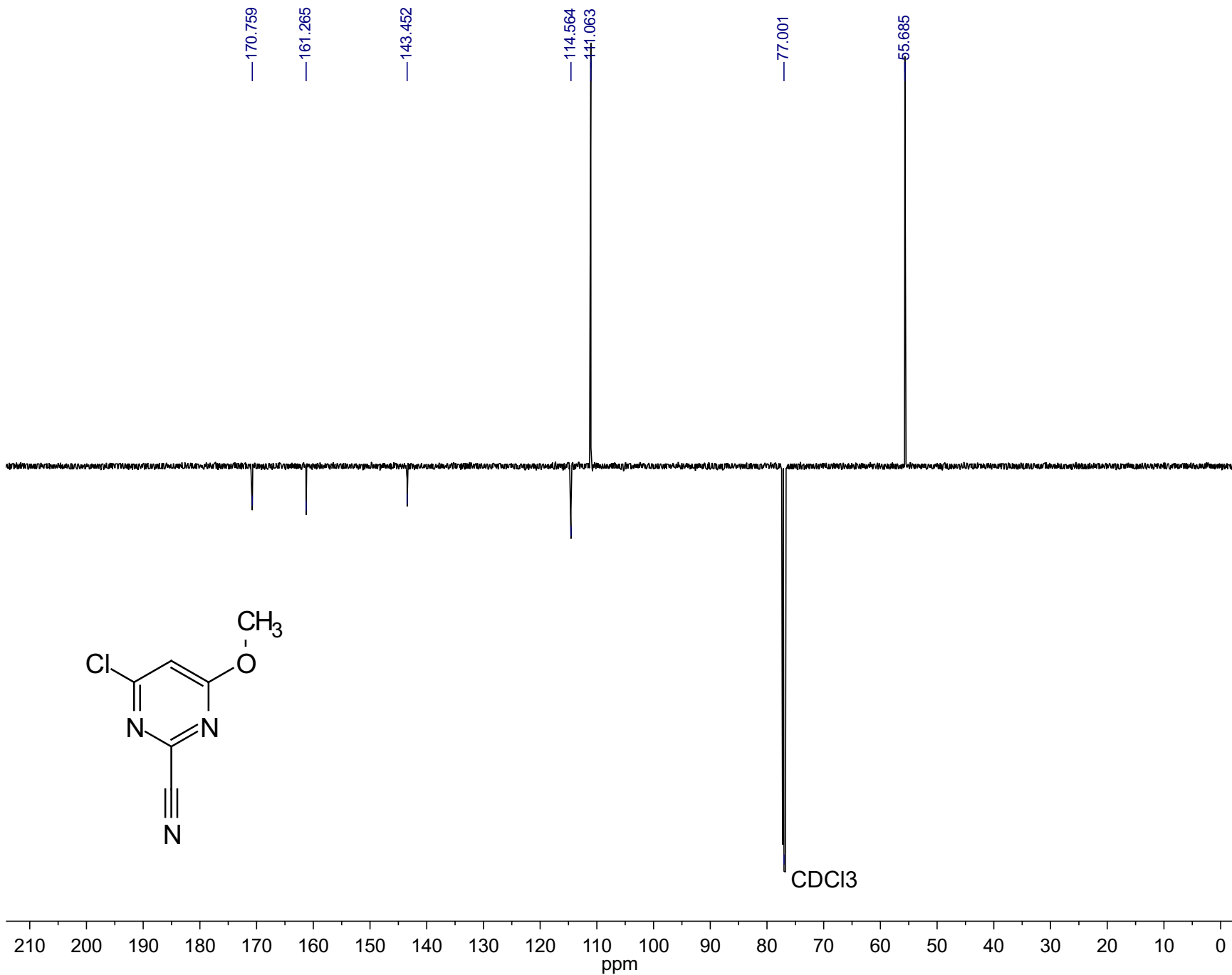
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NAME	Kalogirou
EXPNO	225
PROCNO	1
F2 - Acquisition Parameters	
Date_	20161225
Time	6.10
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	jmod
TD	65536
SOLVENT	CDCl3
NS	10240
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010048 sec
RG	2050
DW	16.800 usec
DE	6.50 usec
TE	298.3 K
CNST2	145.0000000
CNST11	1.0000000
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
CPDPRG[2]	waltz16
PCPD2	80.00 usec
PLW2	14.50000000 W
PLW12	0.32624999 W
F2 - Processing parameters	
SI	32768
SF	125.7334082 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

<sup>1</sup>H NMR of 4-chloro-6-methoxypyrimidine-2-carbonitrile (**13**)



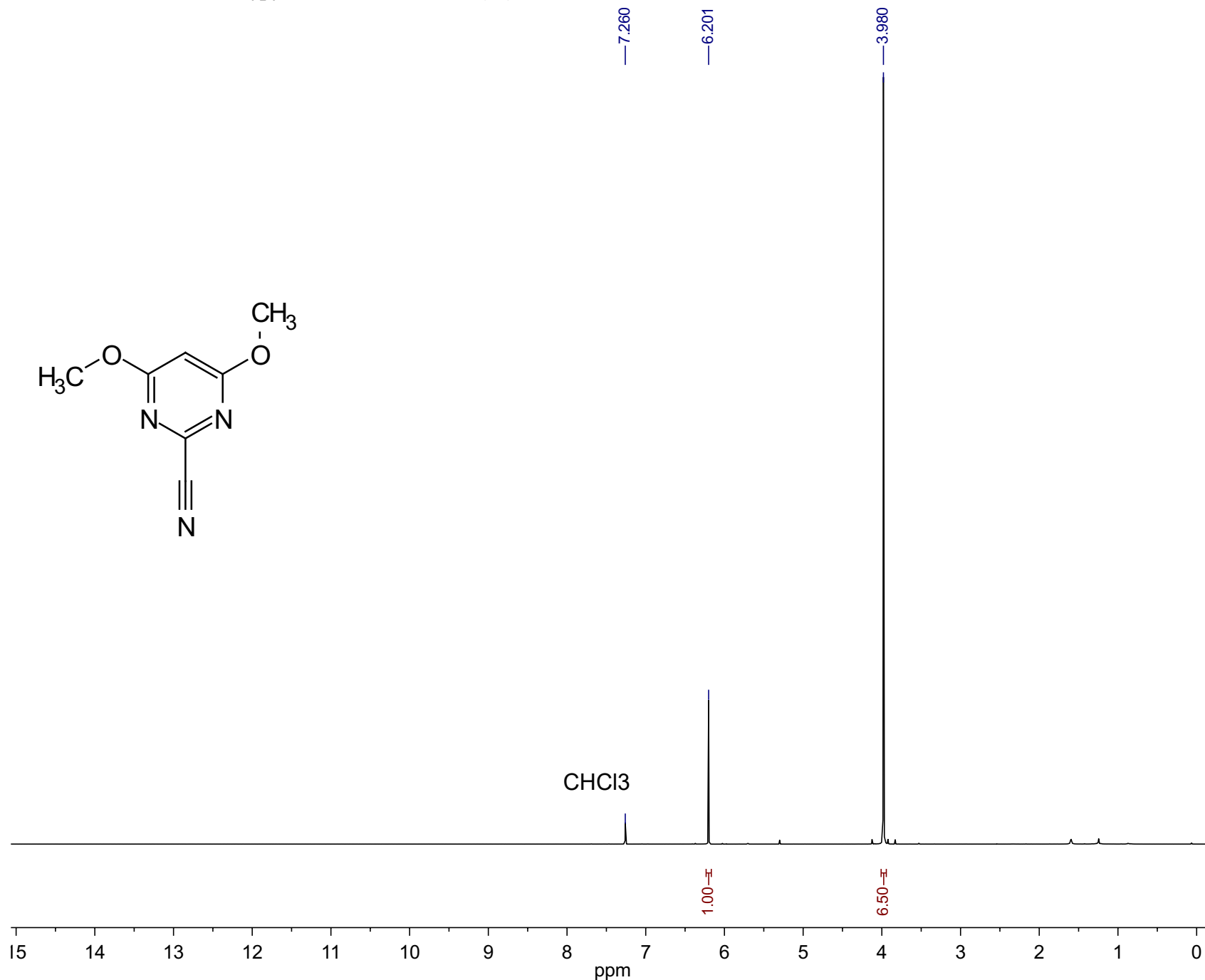
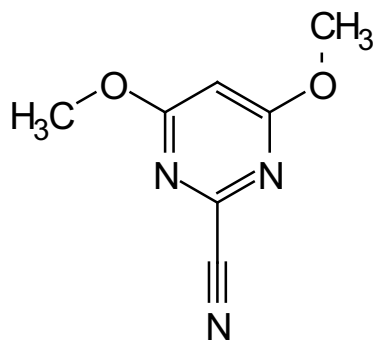
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NAME Kalogirou  
EXPNO 235  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20170102  
Time 16.54  
INSTRUM spect  
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PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 161  
DW 50.000 usec  
DE 6.50 usec  
TE 294.9 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 500.0330402 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

<sup>13</sup>C NMR of 4-chloro-6-methoxypyrimidine-2-carbonitrile (**13**)



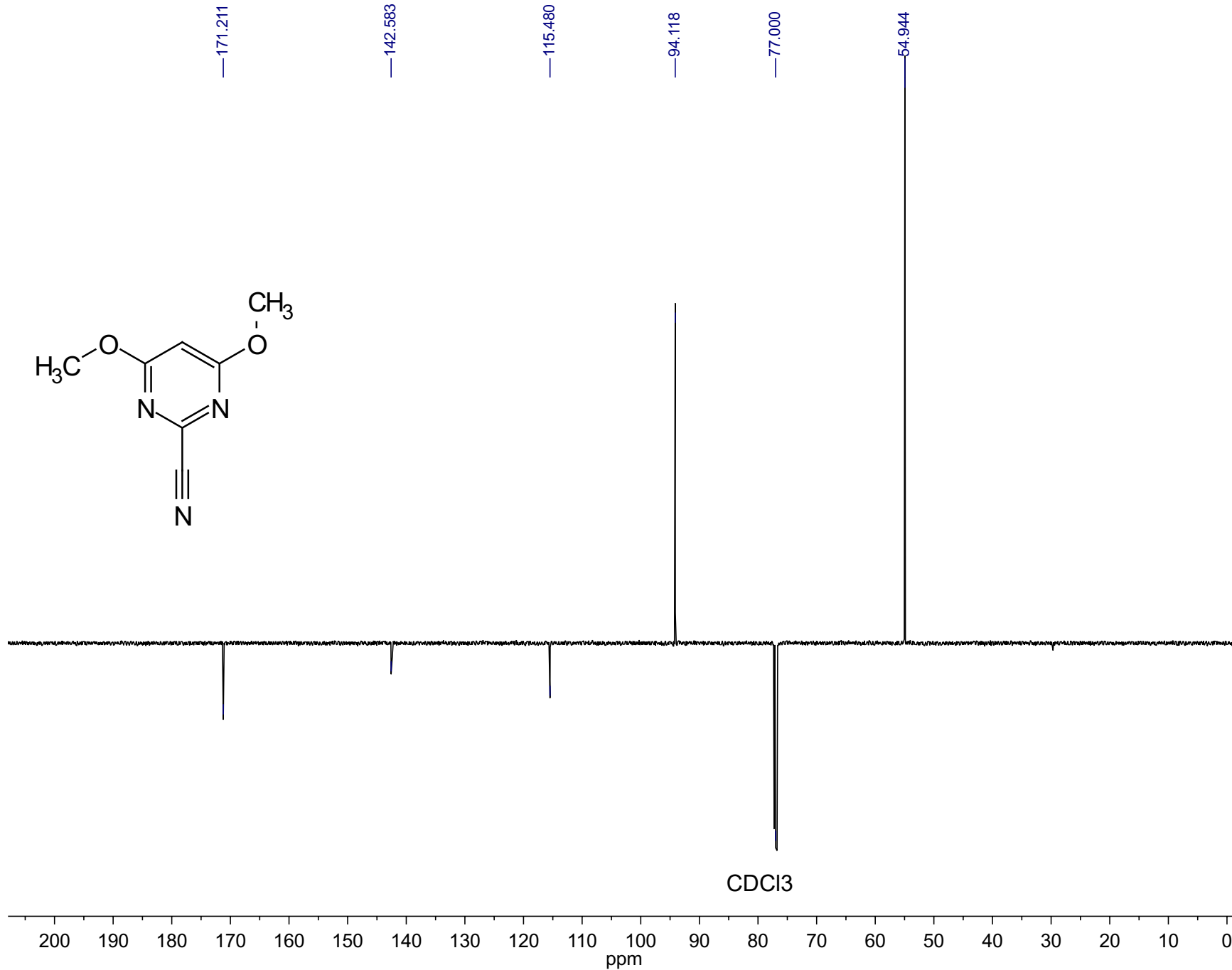
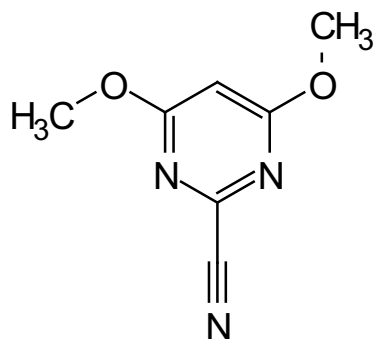
Current Data Parameters  
NAME Kalogirou  
EXPNO 236  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20170102  
Time 18.03  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG jmod  
TD 65536  
SOLVENT CDCl3  
NS 3389  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010048 sec  
RG 2050  
DW 16.800 usec  
DE 6.50 usec  
TE 296.2 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  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 14.50000000 W  
PLW12 0.32624999 W  
F2 - Processing parameters  
SI 32768  
SF 125.7334092 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

<sup>1</sup>H NMR of 4,6-dimethoxypyrimidine-2-carbonitrile (**12**)



Current Data Parameters  
NAME Kalogirou  
EXPNO 215  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20161208  
Time 12.10  
INSTRUM spect  
PROBHD 5 mm PABBO  
BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 114  
DW 50.000 usec  
DE 6.50 usec  
TE 295.2 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 500.0330402 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

<sup>13</sup>C NMR of 4,6-dimethoxypyrimidine-2-carbonitrile (**12**)

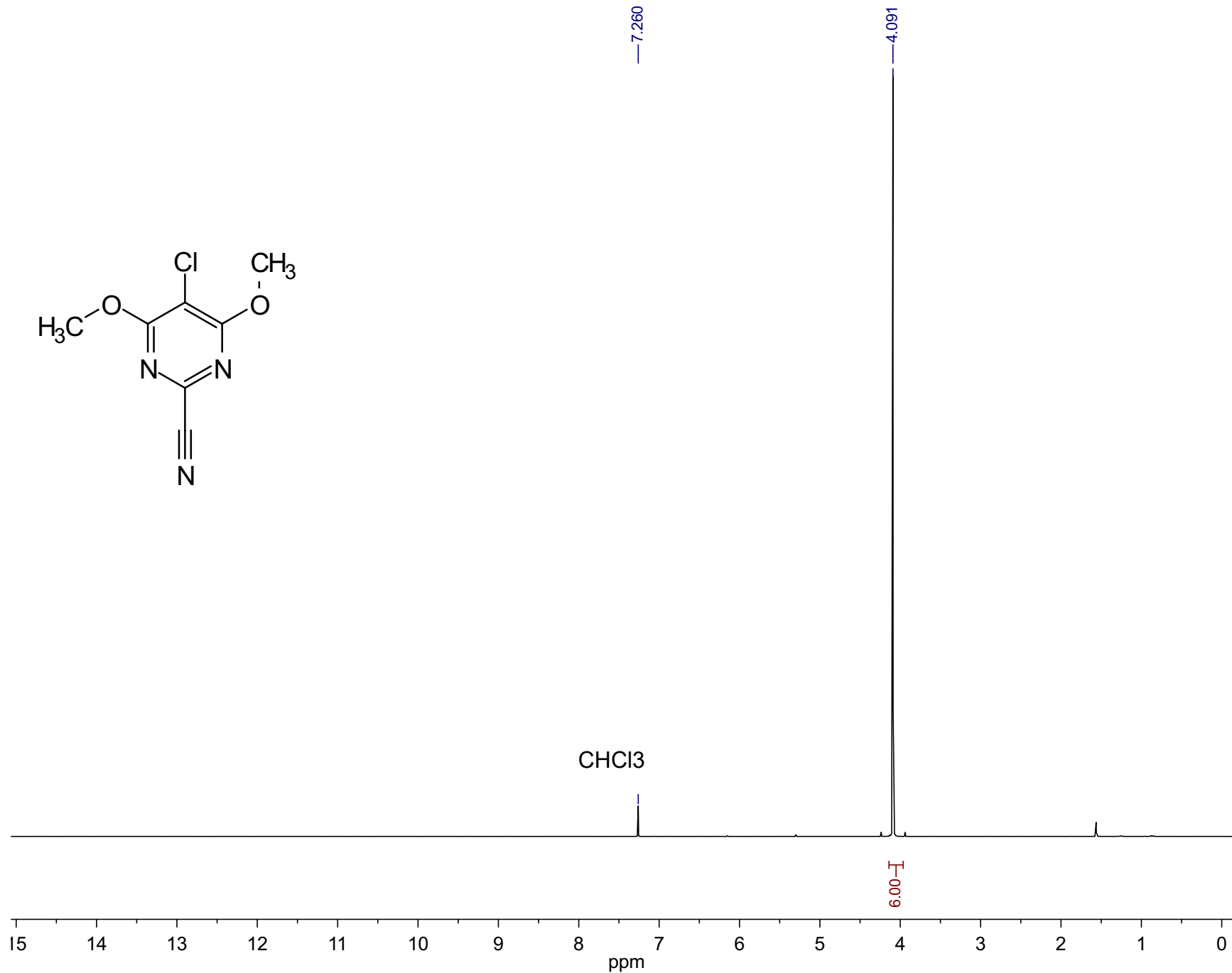
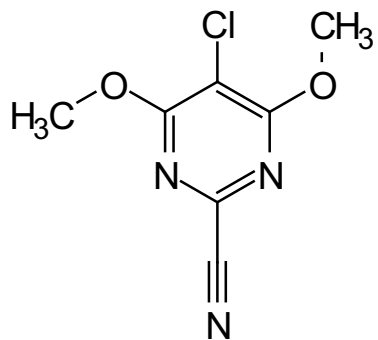


Current Data Parameters

NAME	Kalogirou
EXPNO	216
PROCNO	1
F2 - Acquisition Parameters	
Date_	20161208
Time	14.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	jmod
TD	65536
SOLVENT	CDCl <sub>3</sub>
NS	2048
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	296.4 K
CNST2	145.0000000
CNST11	1.0000000
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	125.7334096 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



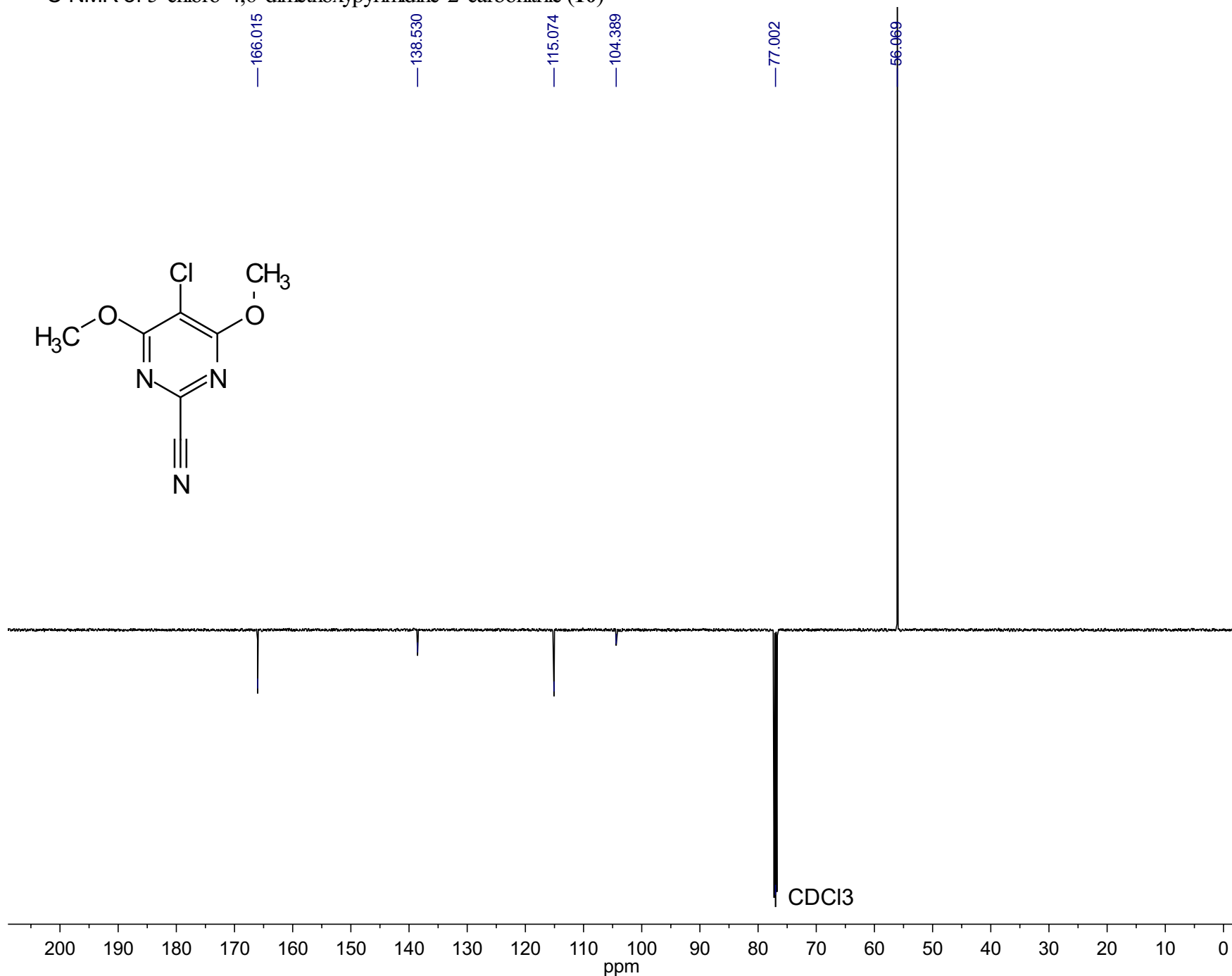
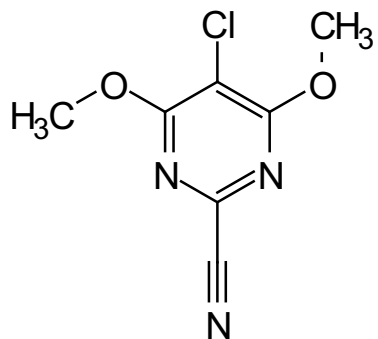
<sup>1</sup>H NMR of 5-chloro-4,6-dimethoxypyrimidine-2-carbonitrile (**10**)



Current Data Parameters

NAME Kalogirou  
EXPNO 217  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20161210  
Time 13.42  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 144  
DW 50.000 usec  
DE 6.50 usec  
TE 294.5 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 500.0330399 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

<sup>13</sup>C NMR of 5-chloro-4,6-dimethoxypyrimidine-2-carbonitrile (**10**)



Current Data Parameters	
NAME	Kalogirou
EXPNO	218
PROCNO	1
F2 - Acquisition Parameters	
Date_	20161210
Time	20.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	jmod
TD	65536
SOLVENT	CDCl3
NS	7168
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	296.1 K
CNST2	145.0000000
CNST11	1.0000000
D1	2.0000000 sec
D20	0.00689655 sec
TD0	1
===== CHANNEL f1 =====	
SFO1	125.7459782 MHz
NUC1	13C
P1	9.00 usec
P2	18.00 usec
PLW1	133.0000000 W
===== CHANNEL f2 =====	
SFO2	500.0350280 MHz
NUC2	1H
CPDPRG[2]	waltz16
PCPD2	80.00 usec
PLW2	14.5000000 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