

Supplementary Material

Synthesis of 4,5,6-trichloropyrimidine-2-carbonitrile from 4,6-dichloro-2-(methylthio)pyrimidine

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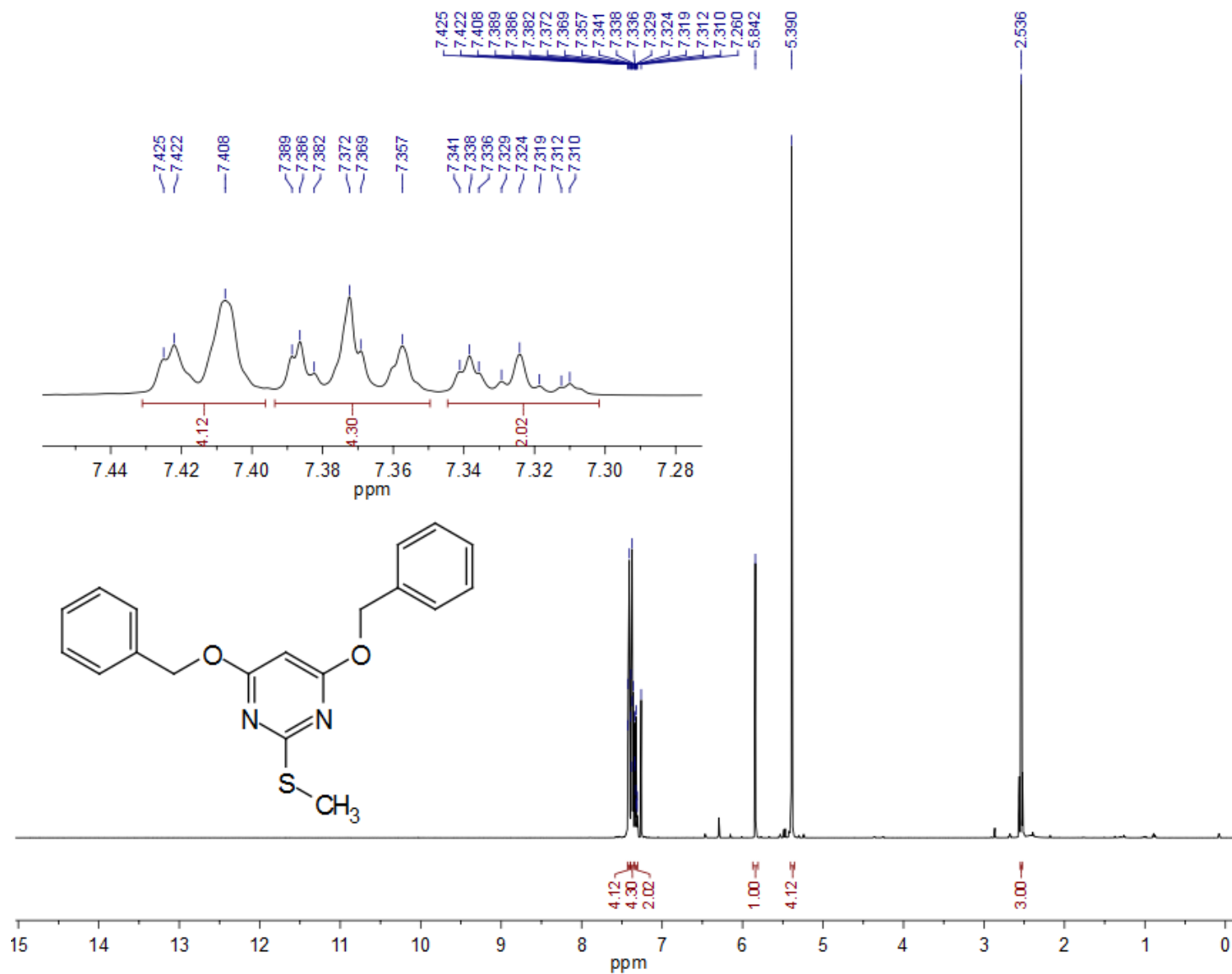
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¹H NMR of 4,6-bis(benzyloxy)-2-(methylthio)pyrimidine (**14**)

Current Data Parameters

NAME Kalogirou
EXPNO 267
PROCNO 1

F2 - Acquisition Parameters

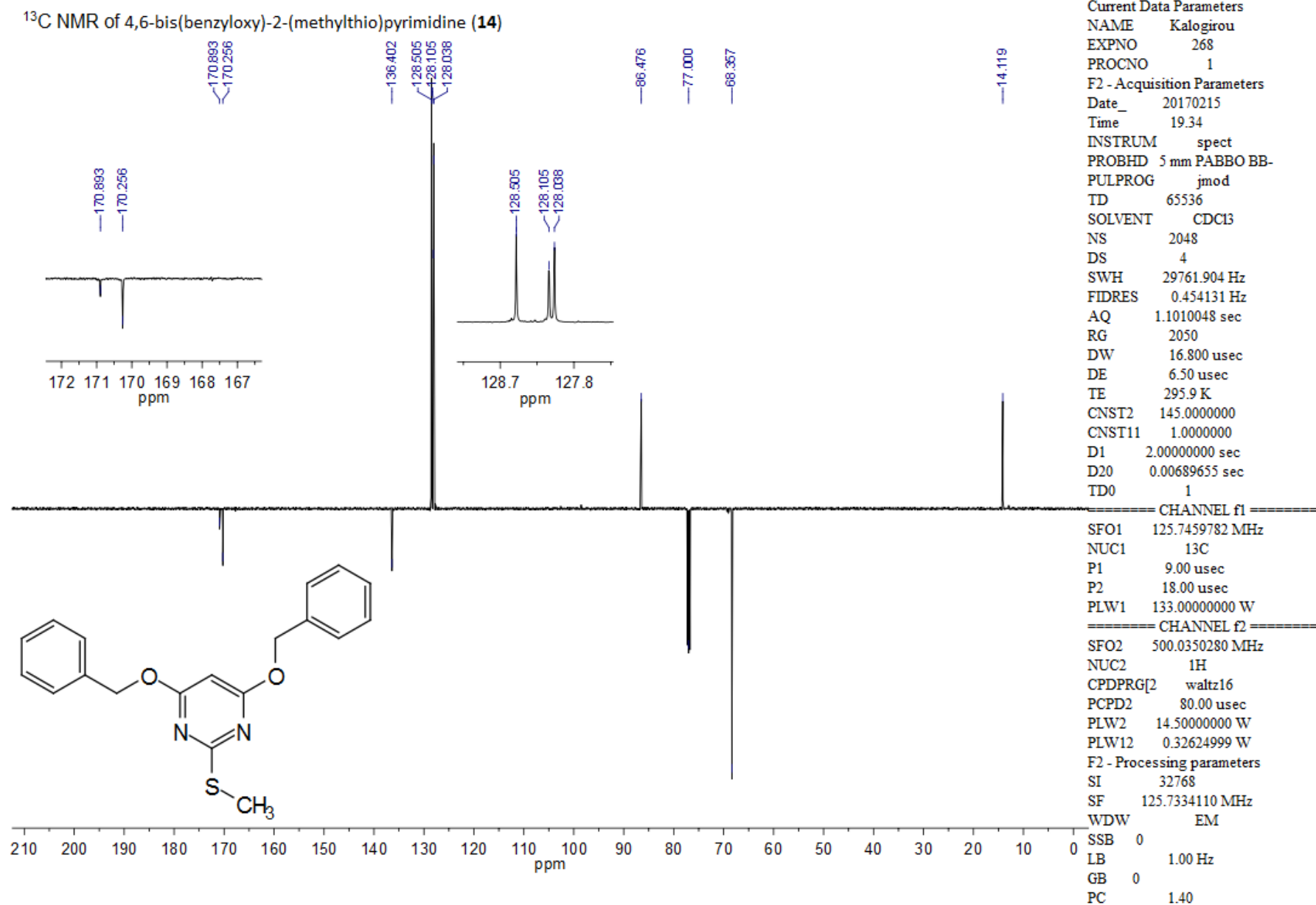
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TD0 1

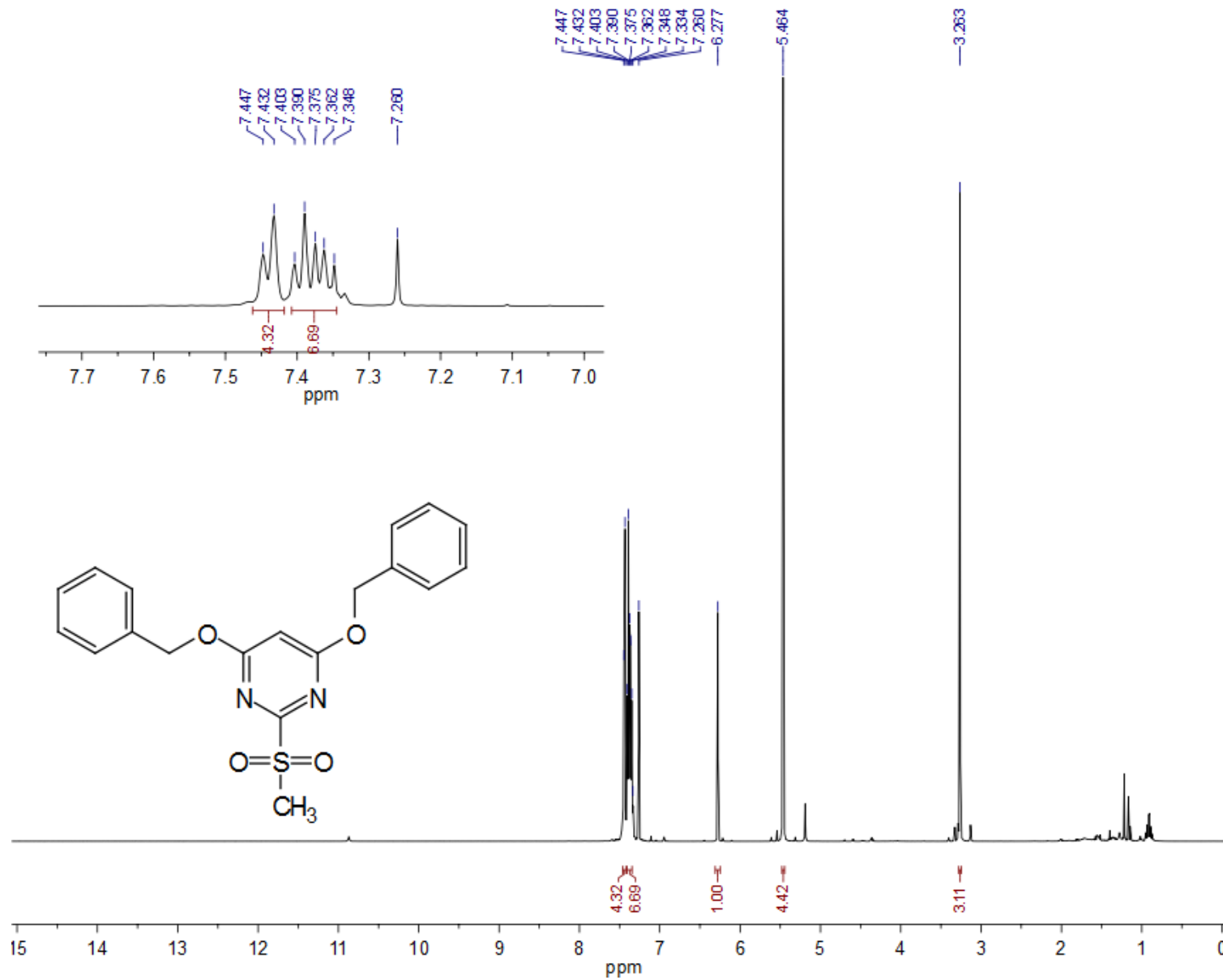
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PLW1 14.50000000 W

F2 - Processing parameters

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WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H NMR of 4,6-bis(benzyloxy)-2-(methylsulfonyl)pyrimidine (**15**)

Current Data Parameters

NAME Kalogirou
EXPNO 271
PROCNO 1

F2 - Acquisition Parameters

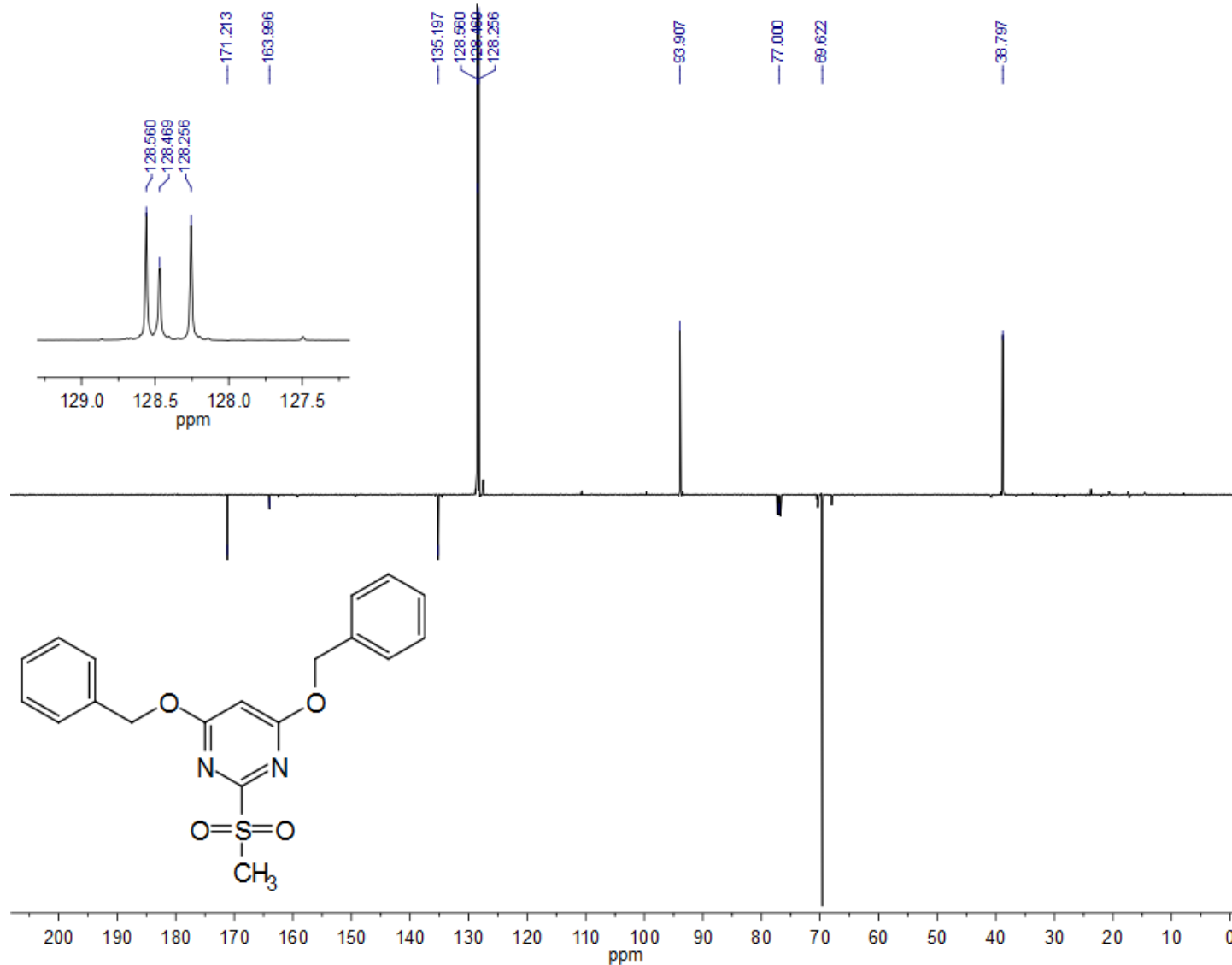
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TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 32
DW 50.000 usec
DE 6.50 usec
TE 294.5 K
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PLW1 14.50000000 W

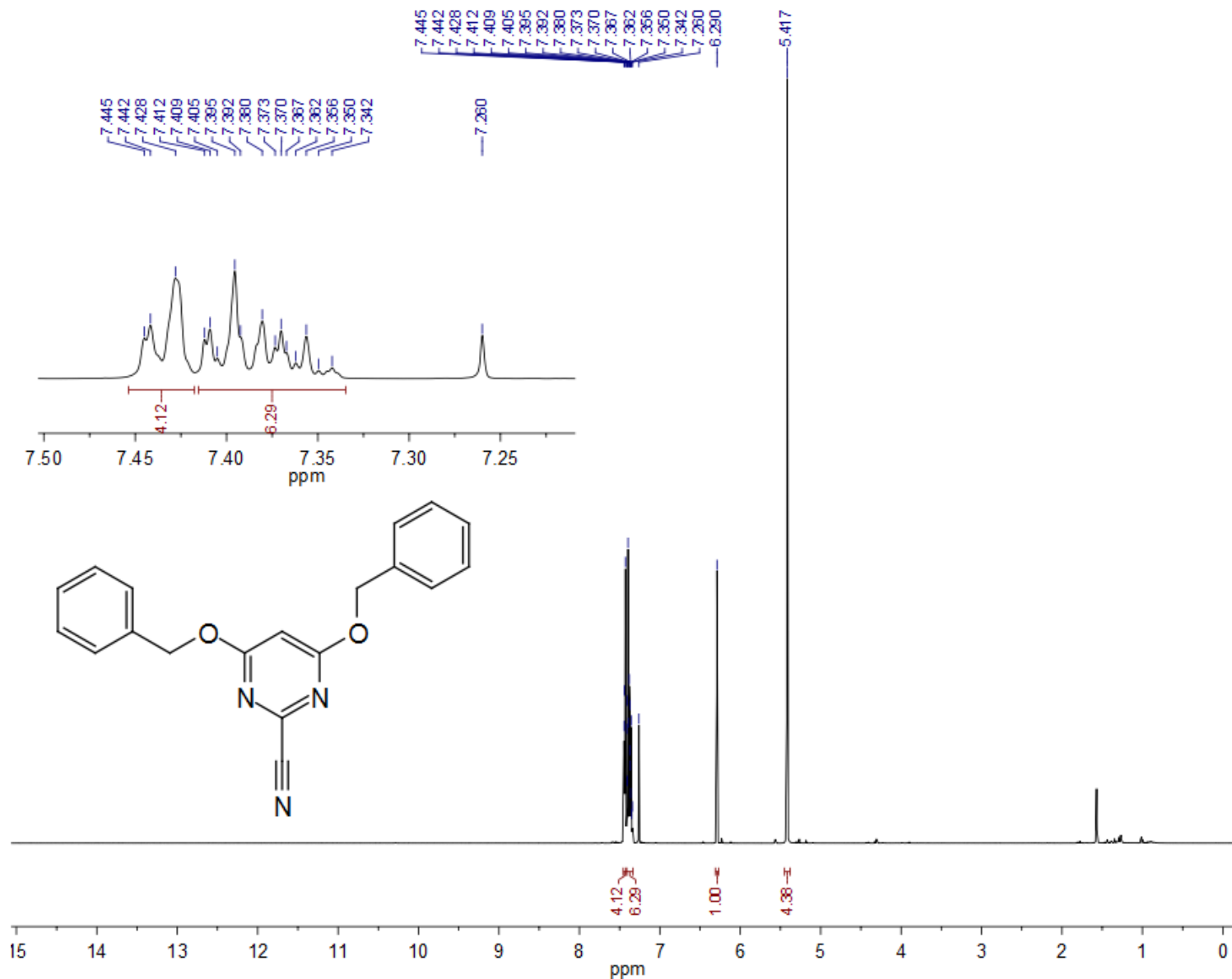
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LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of 4,6-bis(benzyloxy)-2-(methylsulfonyl)pyrimidine (**15**)

Current Data Parameters

NAME	Kalogirou
EXPNO	272
PROCNO	1
F2 - Acquisition Parameters	
Date_	20170306
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PROBHD	5 mm PABBO BB-
PULPROG	jmod
TD	65536
SOLVENT	CDCl3
NS	1792
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
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D20	0.00689655 sec
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P1	9.00 usec
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NUC2	1H
CPDPRG[2]	waltz16
PCPD2	80.00 usec
PLW2	14.50000000 W
PLW12	0.32624999 W
F2 - Processing parameters	
SI	32768
SF	125.7334234 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

¹H NMR of 4,6-bis(benzyloxy)pyrimidine-2-carbonitrile (**16**)

Current Data Parameters

NAME Kalogirou
EXPNO 273
PROCNO 1

F2 - Acquisition Parameters

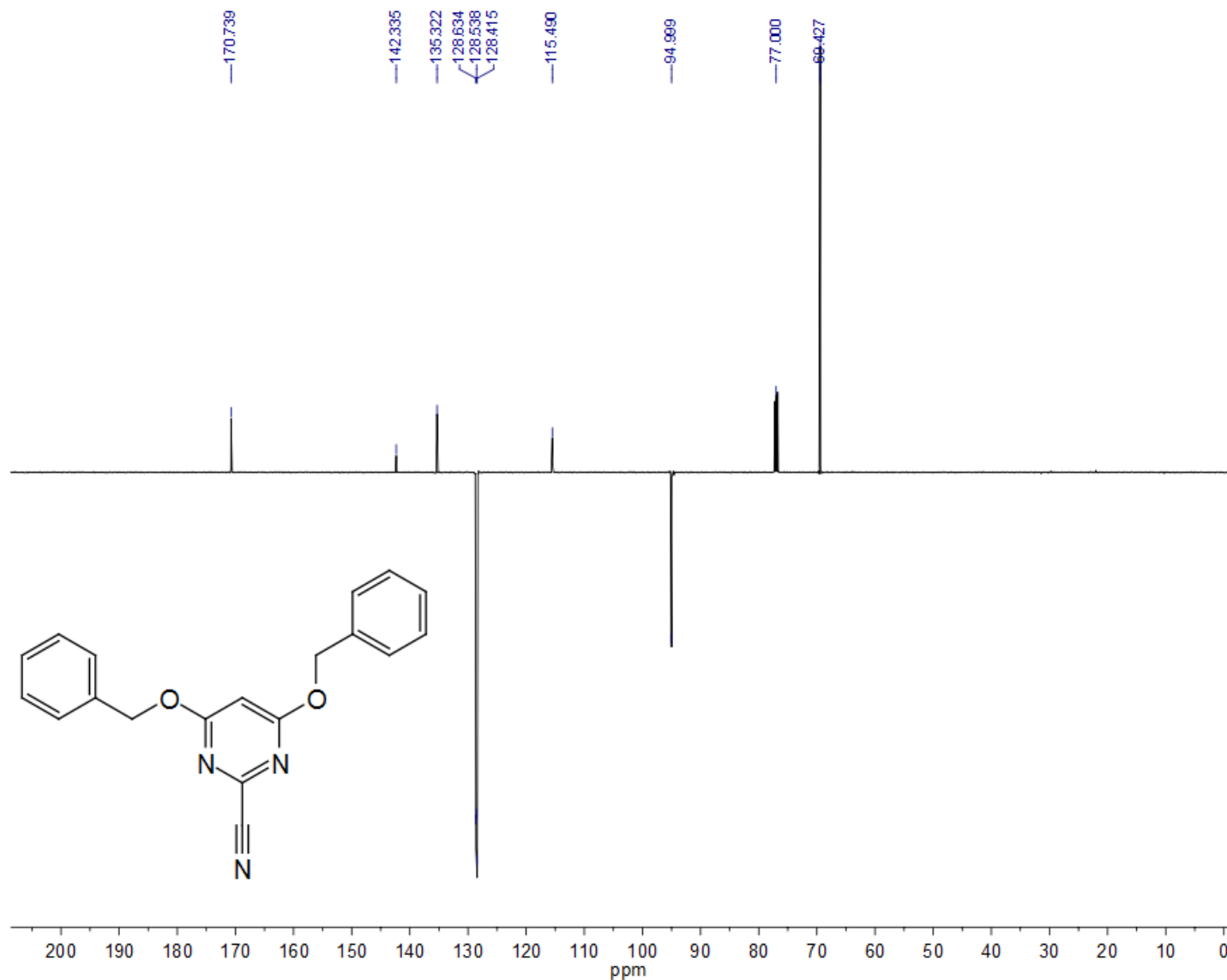
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PULPROG zg30
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SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 90.5
DW 50.000 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1

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PLW1 14.50000000 W

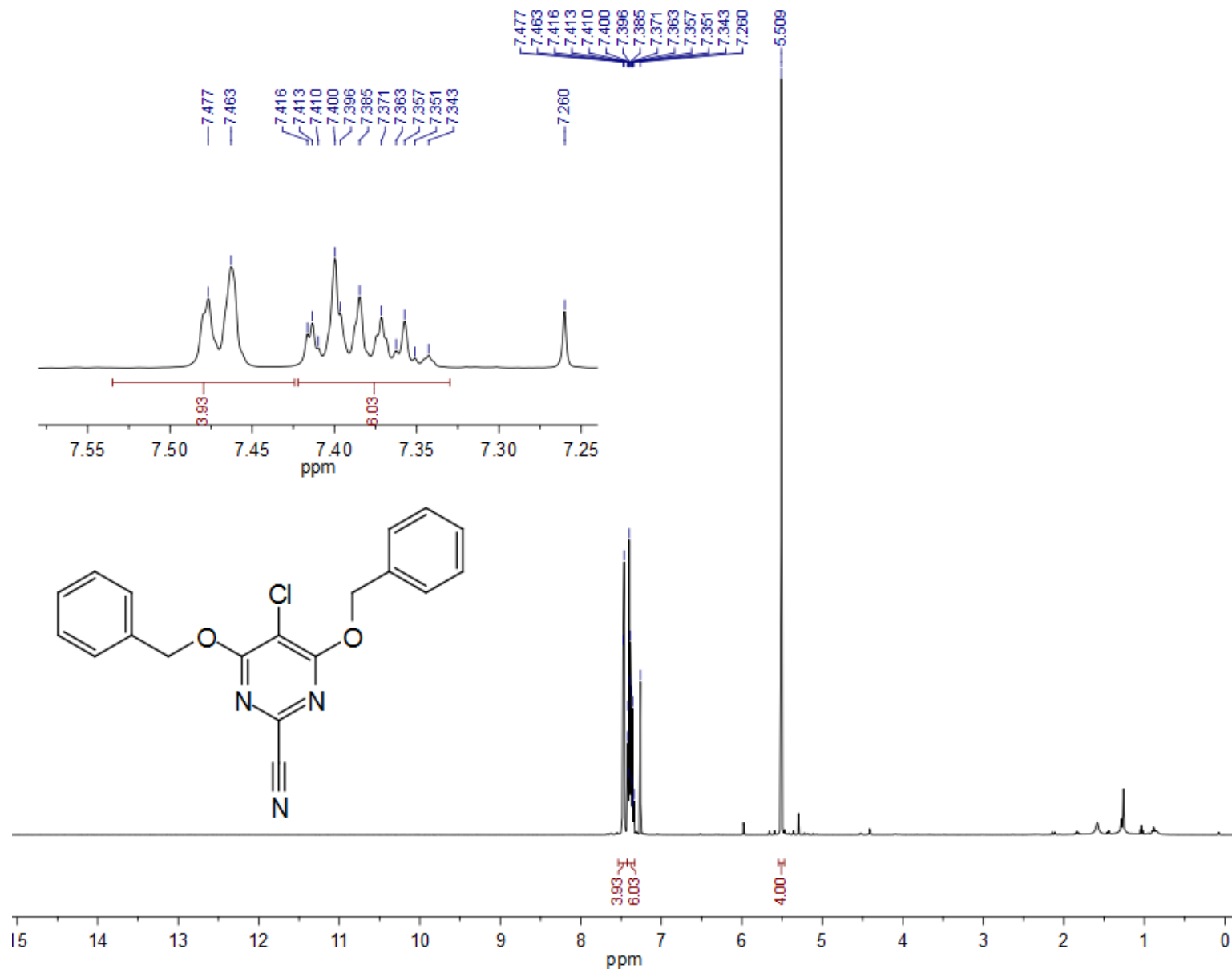
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SSB 0
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PC 1.00

¹³C NMR of 4,6-bis(benzyloxy)pyrimidine-2-carbonitrile (**16**)

Current Data Parameters

NAME	Kalogirou
EXPNO	274
PROCNO	1
F2 - Acquisition Parameters	
Date_	20170309
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INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	jmod
TD	65536
SOLVENT	CDC13
NS	7680
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	297.2 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	125.7334107 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

¹H NMR of 4,6-bis(benzyloxy)-5-chloropyrimidine-2-carbonitrile (**17**)

Current Data Parameters

NAME Kalogirou
EXPNO 275
PROCNO 1

F2 - Acquisition Parameters

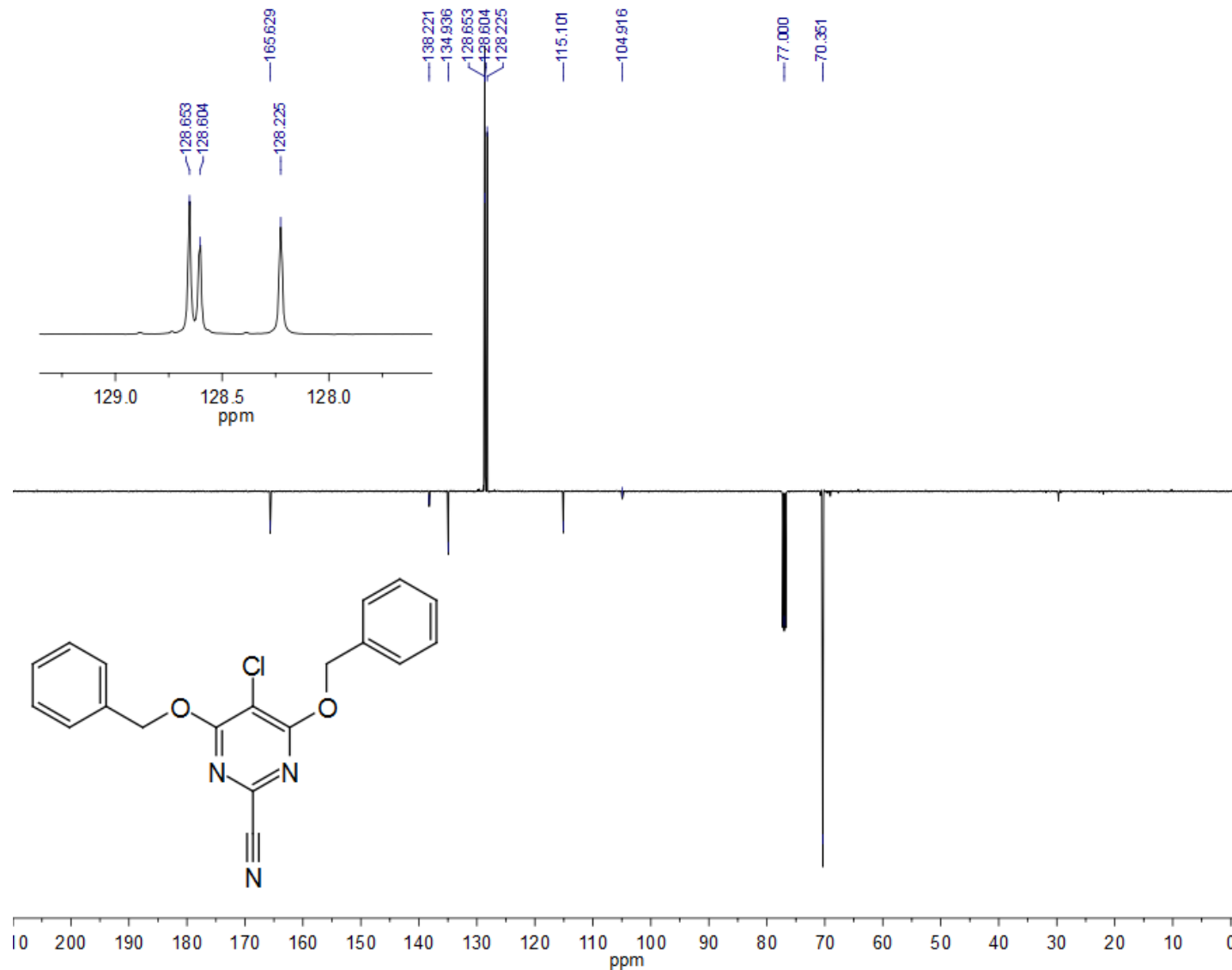
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 114
DW 50.000 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====

SFO1 500.0361158 MHz
NUC1 1H
P1 12.00 usec
PLW1 14.50000000 W

F2 - Processing parameters

SI 65536
SF 500.0330403 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of 4,6-bis(benzyloxy)-5-chloropyrimidine-2-carbonitrile (**17**)

Current Data Parameters

NAME	Kalogirou
EXPNO	276
PROCNO	1
F2 - Acquisition Parameters	
Date_	20170314
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INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	jmod
TD	65536
SOLVENT	CDCl3
NS	14848
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	297.1 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	125.7334098 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40