

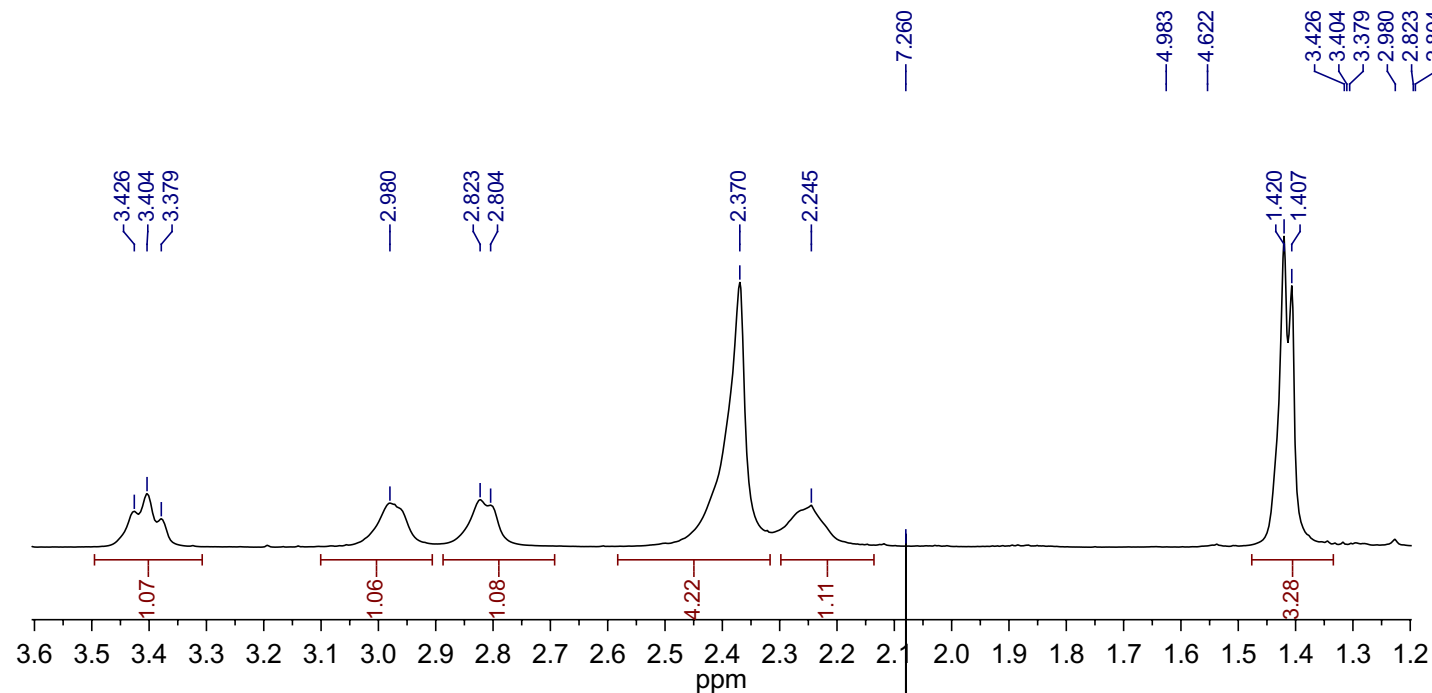
Supporting Information

Synthesis of (*R*) and (*S*)-3-chloro-5-(2,4-dimethylpiperazin-1-yl)-4*H*-1,2,6-thiadiazin-4-one

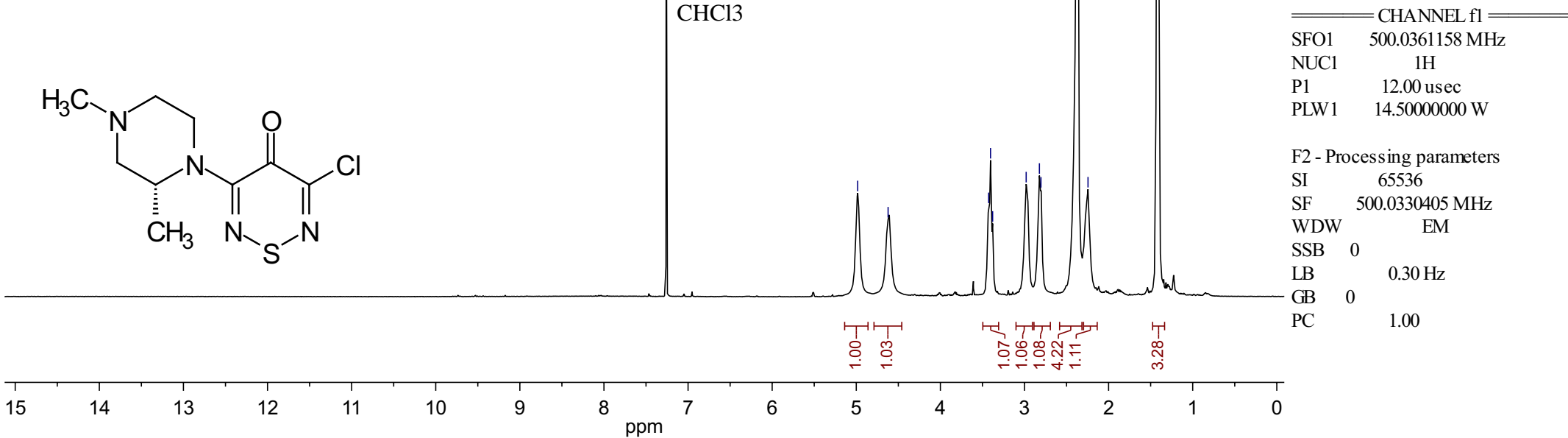
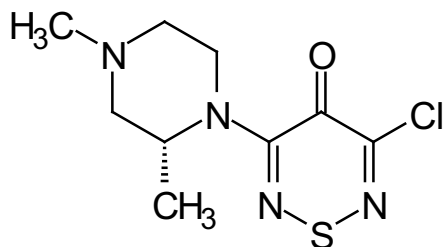
Andreas S. Kalogirou, Christopher R. M. Asquith and Panayiotis A. Koutentis

^1H and ^{13}C NMR Spectra of new compounds

¹H-NMR of (R)-3-chloro-5-(2,4-dimethylpiperazin-1-yl)-4H-1,2,6-thiadiazin-4-one (6a)



CHCl3



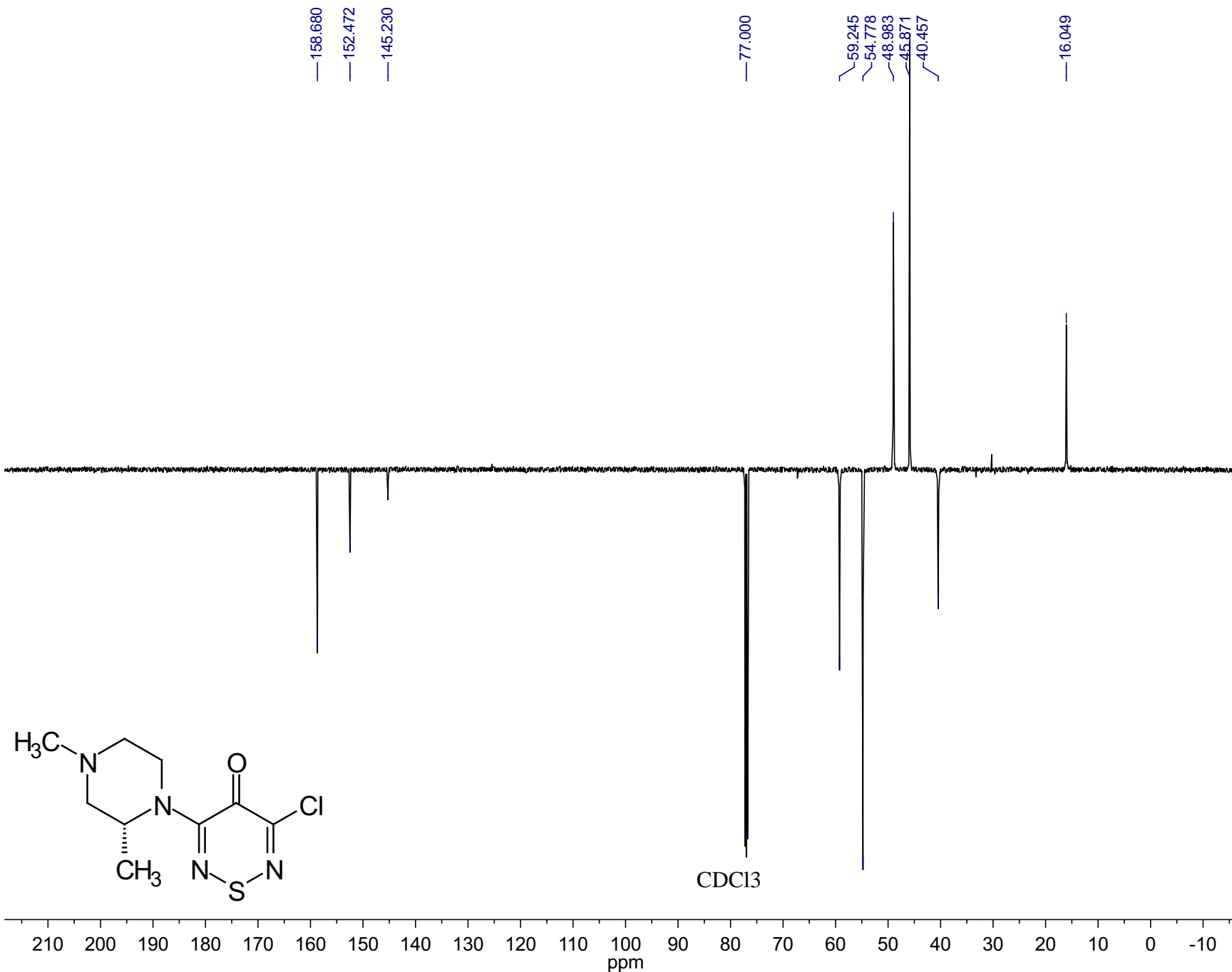
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NAME Kalogirou
EXPNO 768
PROCNO 1

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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 71.8
DW 50.000 usec
DE 6.50 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
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NUC1 1H
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PLW1 14.50000000 W

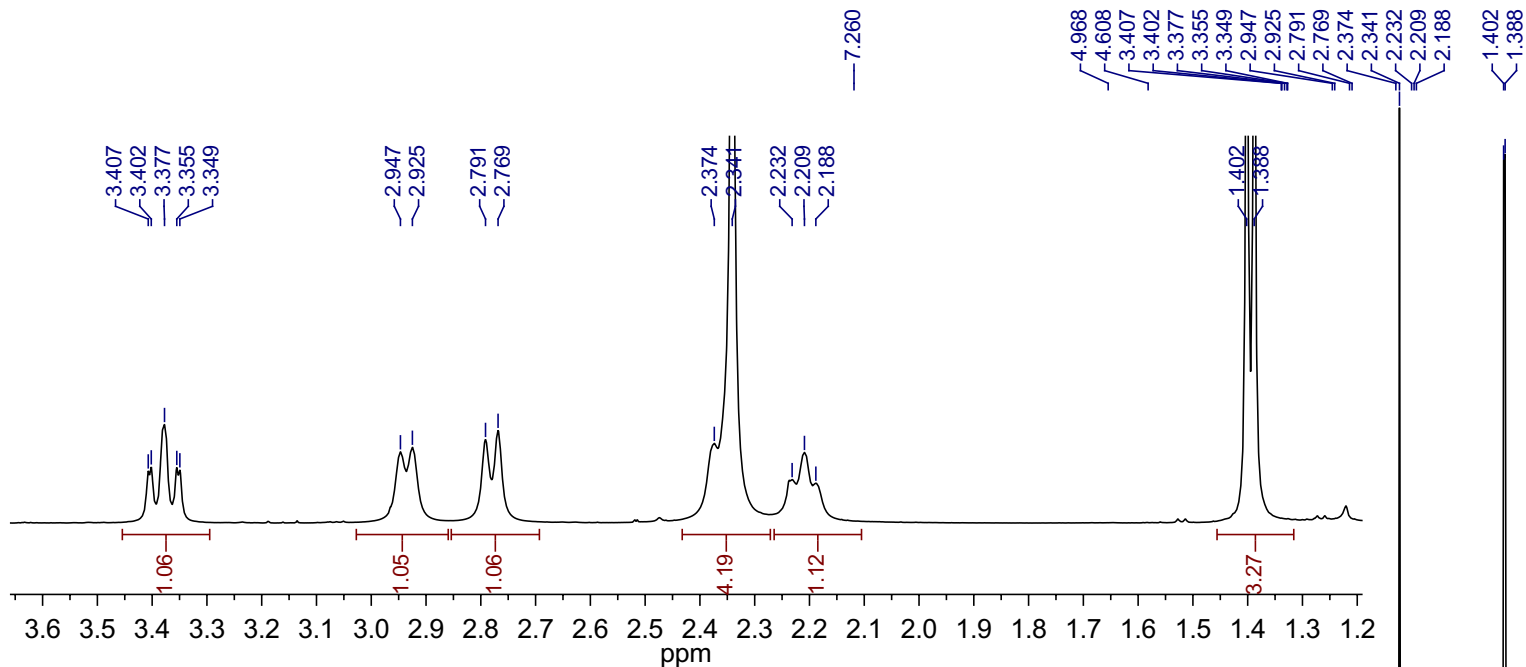
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WDW EM
SSB 0
LB 0.30 Hz
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¹³C-NMR of (*R*)-3-chloro-5-(2,4-dimethylpiperazin-1-yl)-4*H*-1,2,6-thiadiazin-4-one (**6a**)



Current Data Parameters	
NAME	Kalogirou
EXPNO	769
PROCNO	1
F2 - Acquisition Parameters	
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PULPROG	jmod
TD	65536
SOLVENT	CDCl3
NS	5000
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010048 sec
RG	1820
DW	16.800 usec
DE	6.50 usec
TE	296.1 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	9.20 usec
P2	18.40 usec
PLW1	140.00000000 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	125.7334137 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

¹H-NMR of (S)-3-chloro-5-(2,4-dimethylpiperazin-1-yl)-4H-1,2,6-thiadiazin-4-one (6b)



Current Data Parameters

NAME Kalogirou
EXPNO 822
PROCNO 1

F2 - Acquisition Parameters

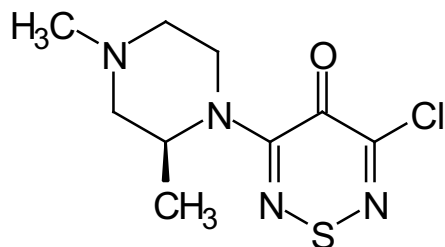
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Time 14.33
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 57
DW 50.000 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
TD0 1

CHANNEL f1

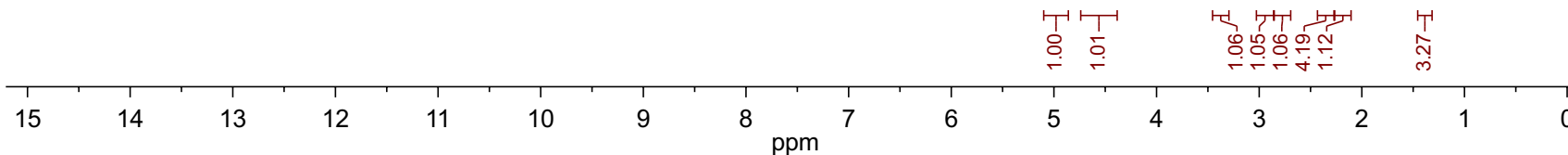
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NUC1 1H
P1 12.00 usec
PLW1 14.50000000 W

F2 - Processing parameters

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SF 500.0330405 MHz
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SSB 0
LB 0.30 Hz
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PC 1.00

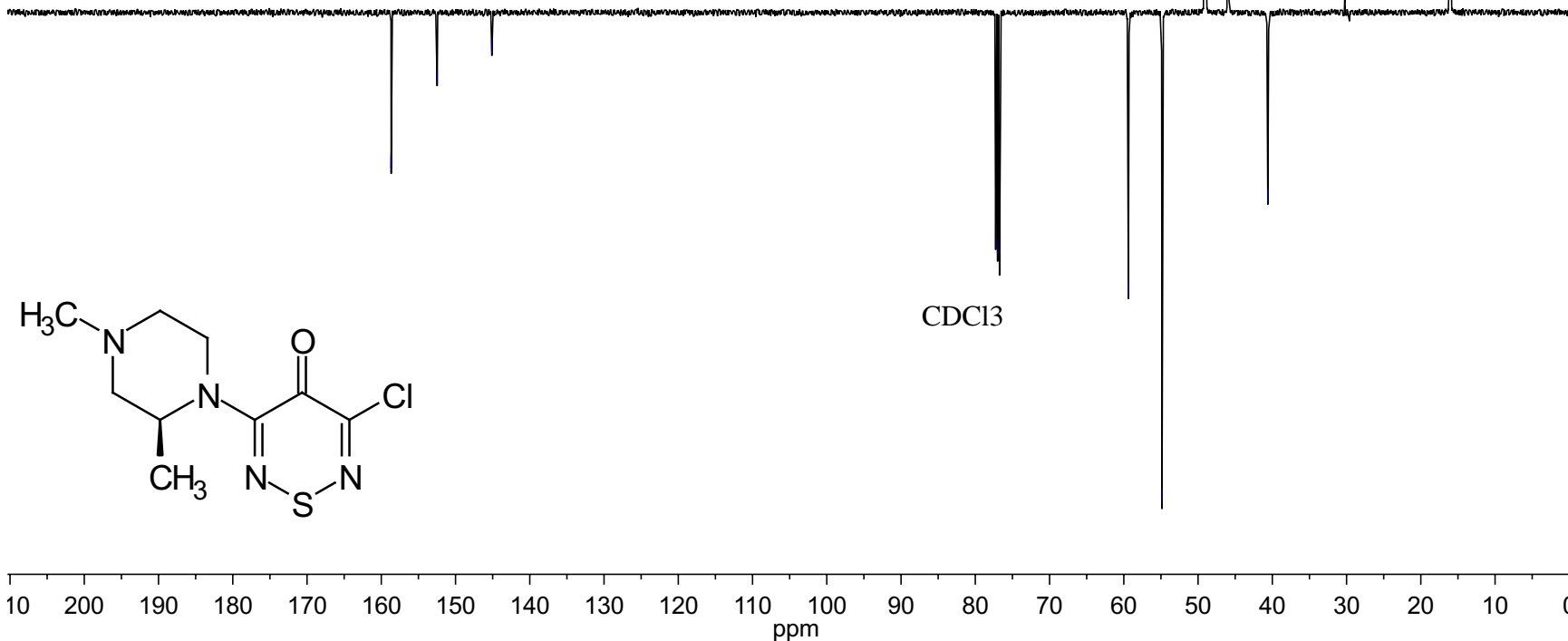


CHCl3



¹³C-NMR of (*S*)-3-chloro-5-(2,4-dimethylpiperazin-1-yl)-4*H*-1,2,6-thiadiazin-4-one (**6b**)

158.669
152.474
145.111
77.000
59.376
54.854
49.060
45.950
40.603
16.036



CDCl₃

Current Data Parameters

NAME Kalogirou
EXPNO 821
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200416
Time 13.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl₃
NS 1401
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 295.3 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 9.20 usec
P2 18.40 usec
PLW1 140.00000000 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 125.7334152 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40