

## **3-(1,3-Benzothiazol-2-ylsulfanyl)-1,2,6-thiadiazinones: surrogates for 3-halo-1,2,6-thiadiazinones**

**Andreas S. Kalogirou<sup>1\*</sup>, Panayiotis A. Koutentis<sup>2</sup>**

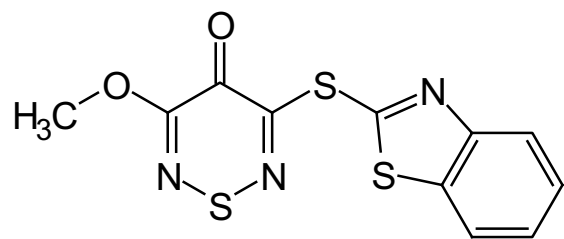
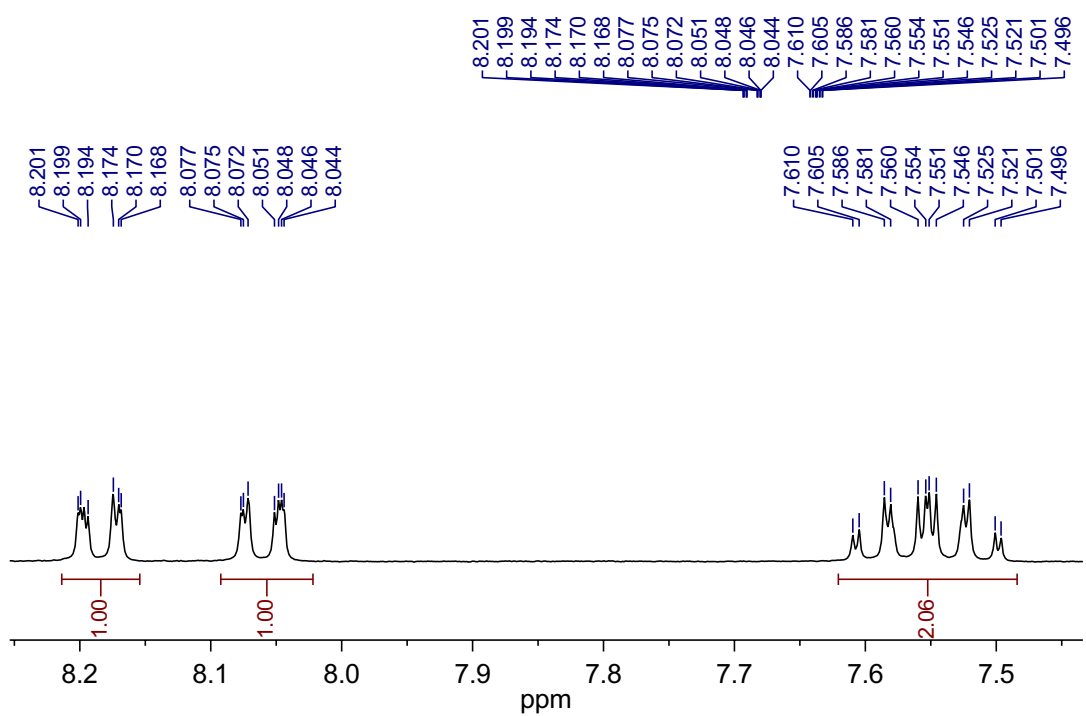
<sup>1</sup> *Department of Life Sciences, School of Sciences, European University Cyprus,  
6 Diogenis St., Engomi, P. O. Box 22006, 1516 Nicosia, Cyprus; e-mail: A.Kalogirou@euc.ac.cy*

<sup>2</sup> *Department of Chemistry, University of Cyprus,  
P. O. Box 20537, 1678 Nicosia, Cyprus; e-mail: koutenti@ucy.ac.cy*

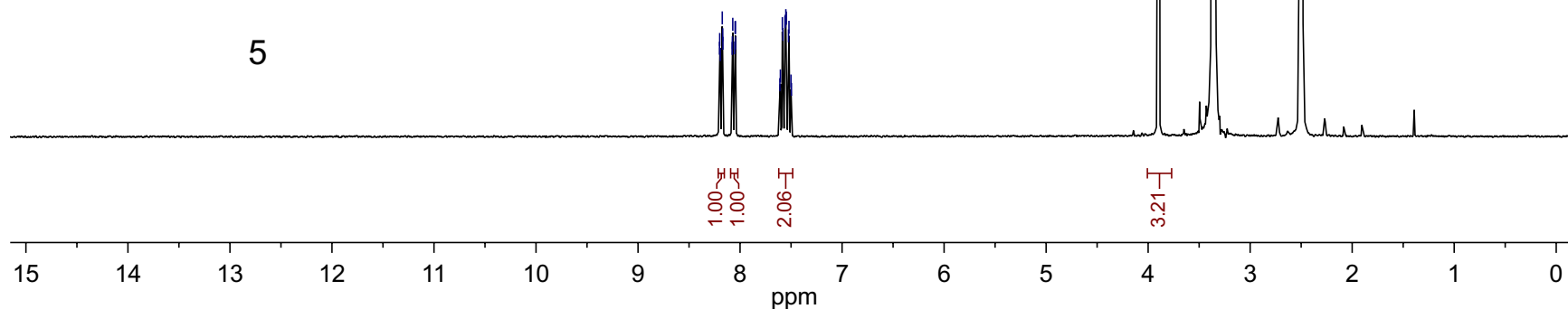
## **SUPPLEMENTARY INFORMATION**

**<sup>1</sup>H and <sup>13</sup>C NMR Spectra of all new compounds**

<sup>1</sup>H NMR of 3-(benzo[*d*]thiazol-2-ylthio)-5-methoxy-4*H*-1,2,6-thiadiazin-4-one (**5**)



**5**



Current Data Parameters

NAME Andreas  
EXPNO 422  
PROCNO 1

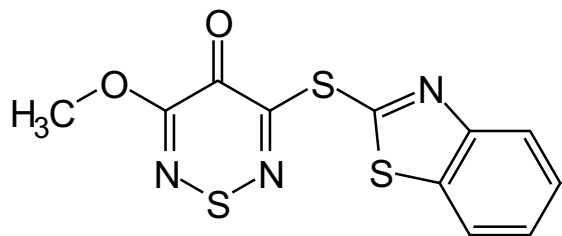
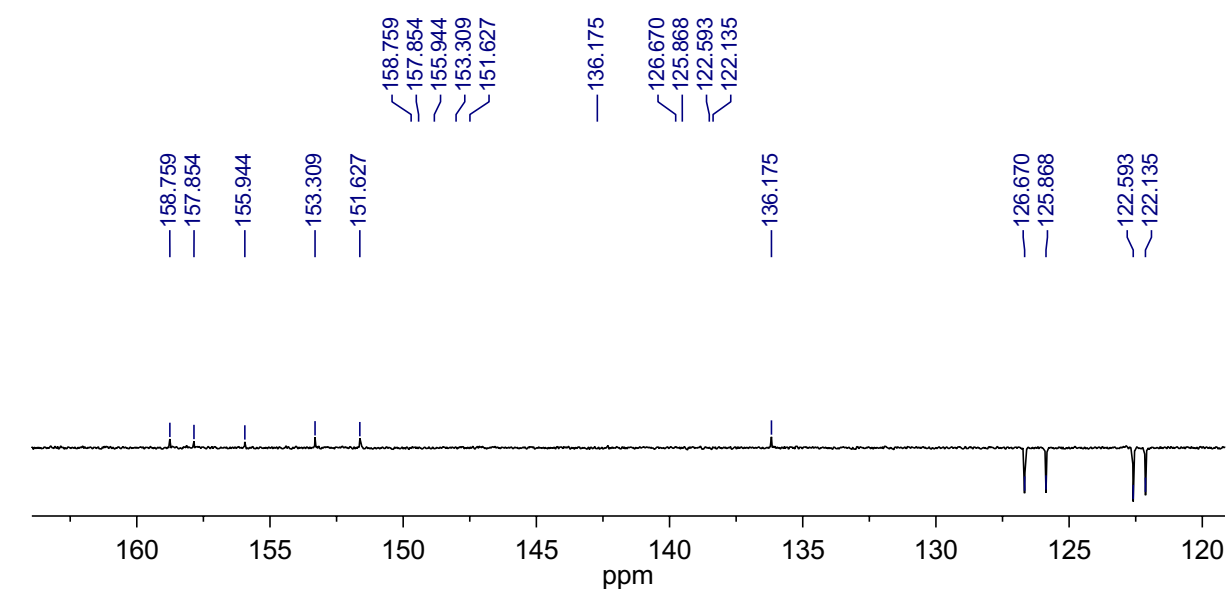
F2 - Acquisition Parameters

Date\_ 20220111  
Time 18.01 h  
INSTRUM spect  
PROBHD Z104275\_0375 (zg30)  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 6009.615 Hz  
FIDRES 0.183399 Hz  
AQ 5.4525952 sec  
RG 201.81  
DW 83.200 usec  
DE 6.50 usec  
TE 294.2 K  
D1 1.00000000 sec  
TD0 1  
SFO1 300.1318533 MHz  
NUC1 1H  
P1 14.00 usec  
PLW1 8.19999981 W

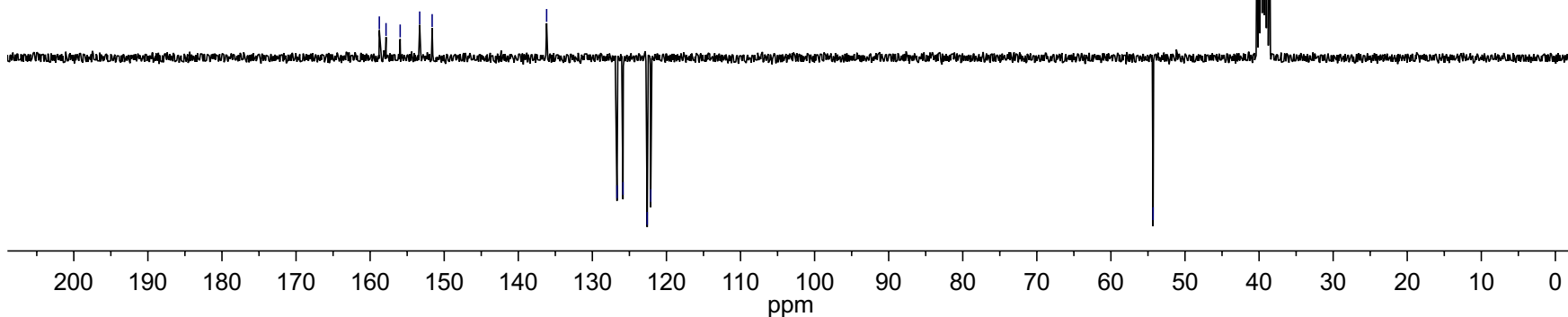
F2 - Processing parameters

SI 65536  
SF 300.1300024 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

<sup>13</sup>C NMR of 3-(benzo[d]thiazol-2-ylthio)-5-methoxy-4*H*-1,2,6-thiadiazin-4-one (**5**)

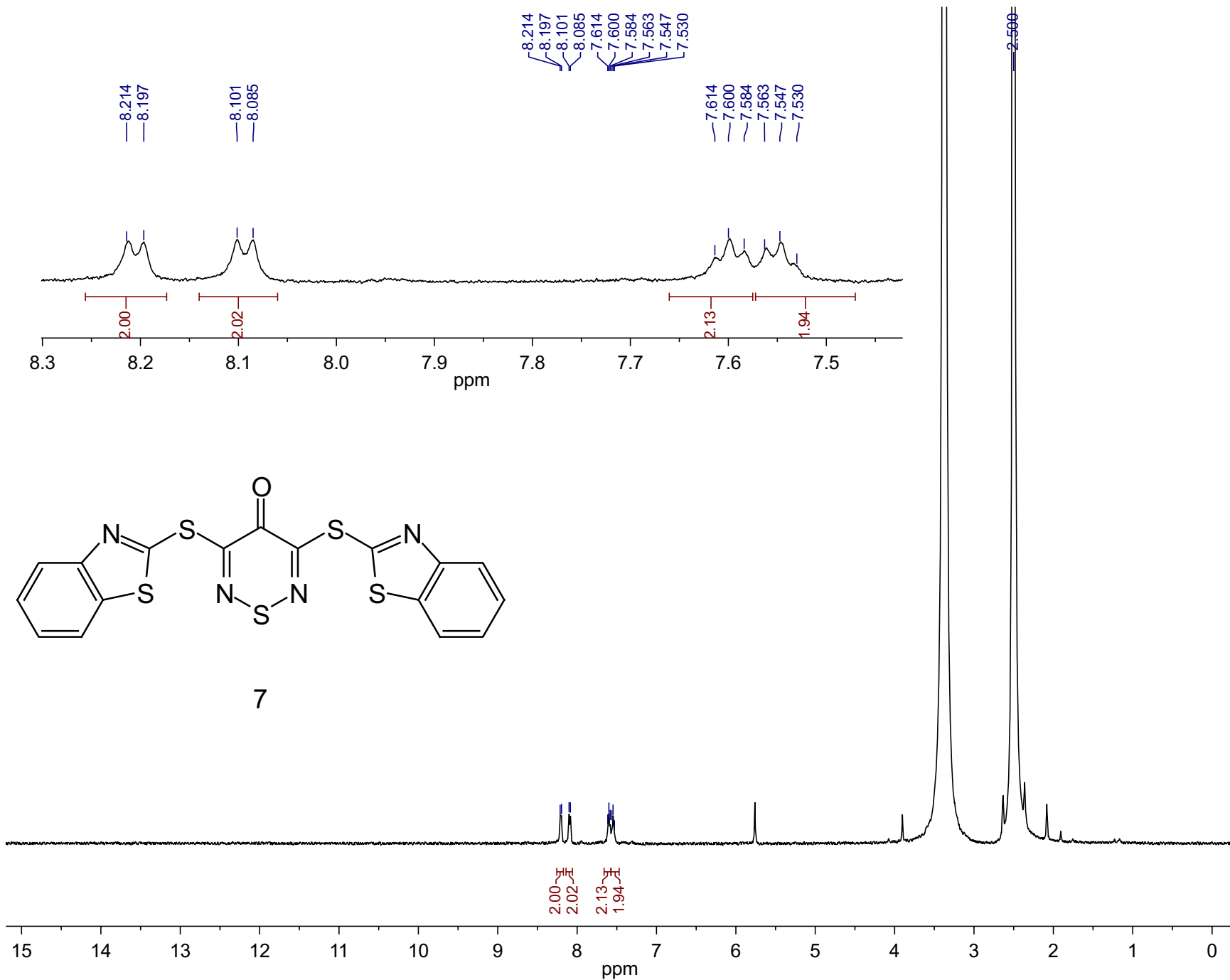


**5**



Current Data Parameters	
NAME	Andreas
EXPNO	423
PROCNO	1
F2 - Acquisition Parameters	
Date_	20220112
Time	14.10 h
INSTRUM	spect
PROBHD	Z104275_0375 (
PULPROG	jmod
TD	65536
SOLVENT	DMSO
NS	18719
DS	4
SWH	18115.941 Hz
FIDRES	0.552855 Hz
AQ	1.8087935 sec
RG	201.81
DW	27.600 usec
DE	6.50 usec
TE	295.1 K
CNST2	145.000000
CNST11	1.000000
D1	2.0000000 sec
D20	0.00689655 sec
TD0	1
SFO1	75.4752953 MHz
NUC1	13C
P1	10.00 usec
P2	20.00 usec
PLW1	41.00000000 W
SFO2	300.1312005 MHz
NUC2	1H
CPDPRG[2	waltz16
PCPD2	80.00 usec
PLW2	8.19999981 W
PLW12	0.25112000 W
F2 - Processing parameters	
SI	32768
SF	75.4677890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

<sup>1</sup>H NMR of 3,5-bis(benzo[d]thiazol-2-ylthio)-4*H*-1,2,6-thiadiazin-4-one (**7**).



Current Data Parameters

NAME Kalogirou  
 EXPNO 1129  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20211231  
 Time 10.24  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 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 291.0 K  
 D1 1.0000000 sec  
 TD0 1

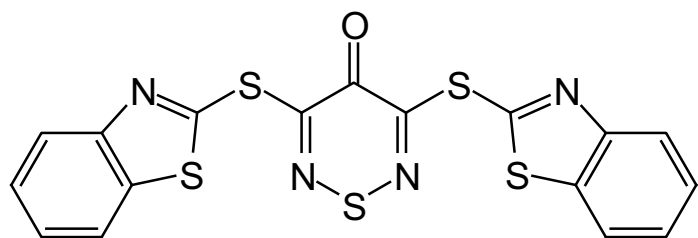
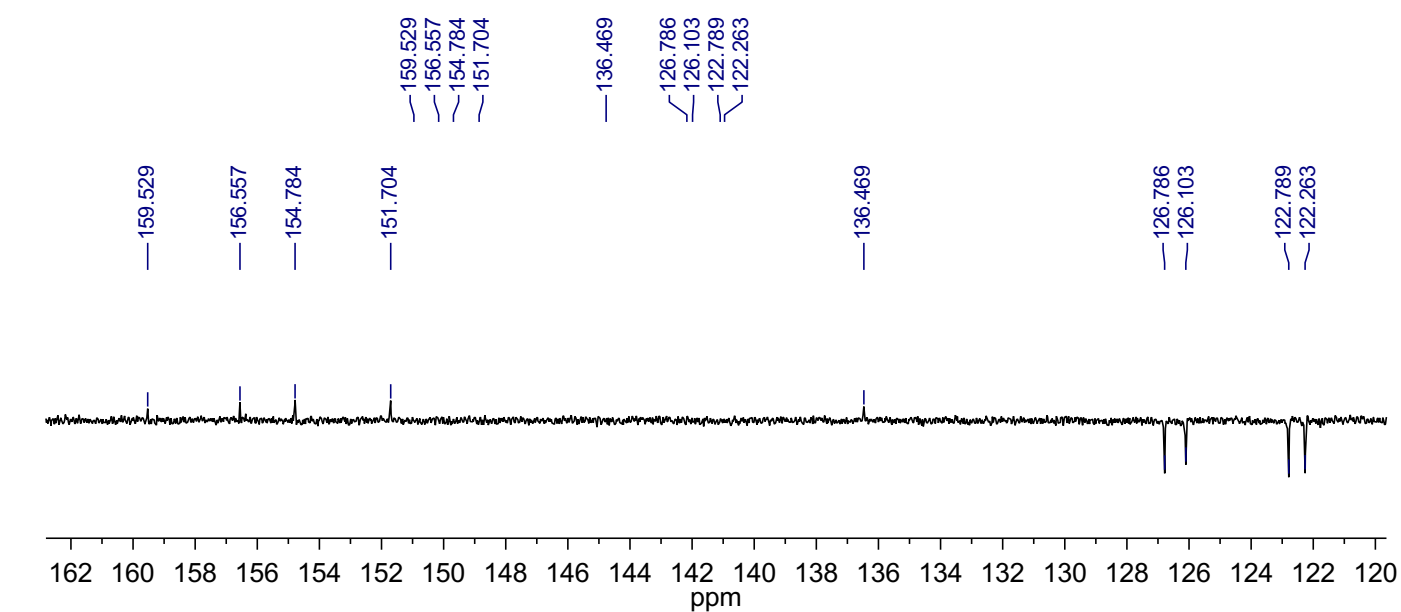
==== CHANNEL f1

SFO1 500.0361158 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 14.5000000 W

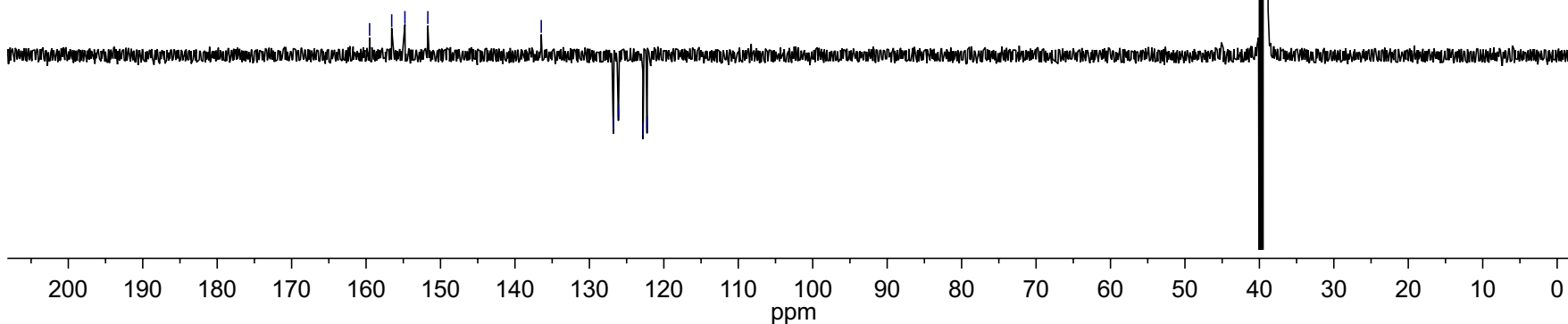
F2 - Processing parameters

SI 65536  
 SF 500.0330279 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

<sup>13</sup>C NMR of 3,5-bis(benzo[d]thiazol-2-ylthio)-4H-1,2,6-thiadiazin-4-one (**7**).



**7**



Current Data Parameters	
NAME	Kalogirou
EXPNO	1130
PROCNO	1
F2 - Acquisition Parameters	
Date_	20211231
Time	10.38
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	jmod
TD	65536
SOLVENT	DMSO
NS	81657
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	292.2 K
CNST2	145.000000
CNST11	1.000000
D1	2.0000000 sec
D20	0.00689655 sec
TD0	1
===== CHANNEL f1 =====	
SFO1	125.7459782 MHz
NUC1	13C
P1	9.20 usec
P2	18.40 usec
PLW1	140.0000000 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	125.7334687 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40































