

## Supporting Information for

### Synthesis of Hybrid Molecules with Imidazole-1,3,4-thiadiazole Core and Evaluation of Biological Activity on *Trypanosoma cruzi* and *Leishmania donovani*

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Ecuador

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Caracas 1058-A, Venezuela

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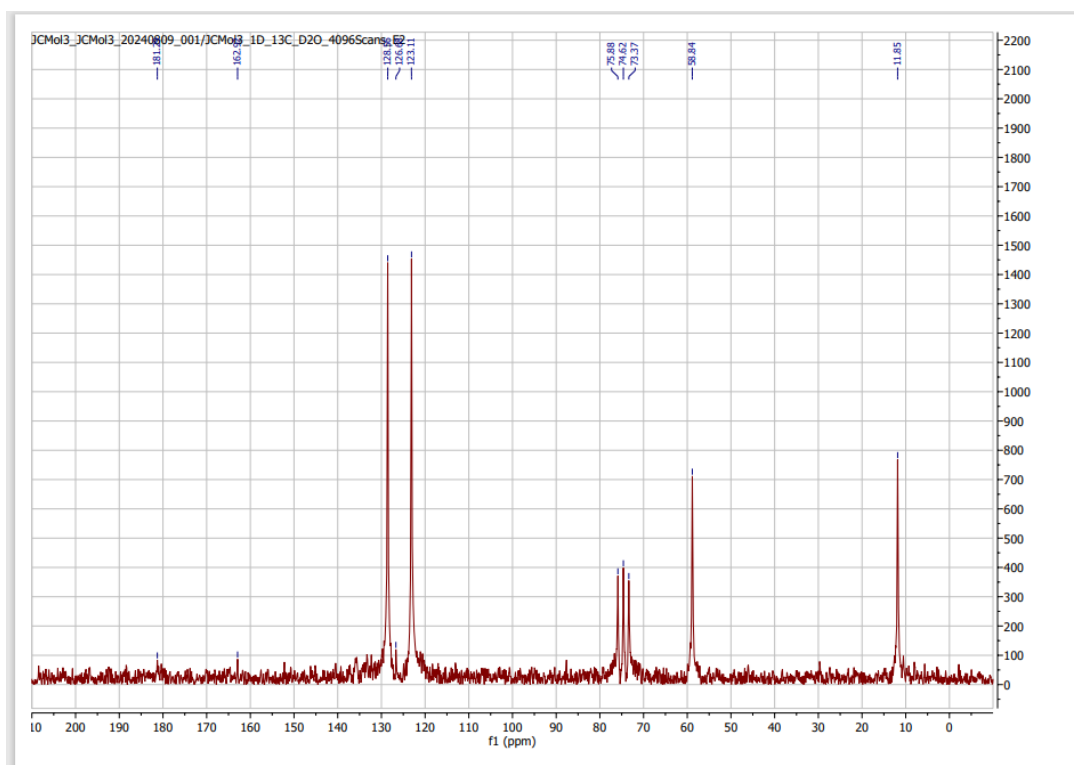
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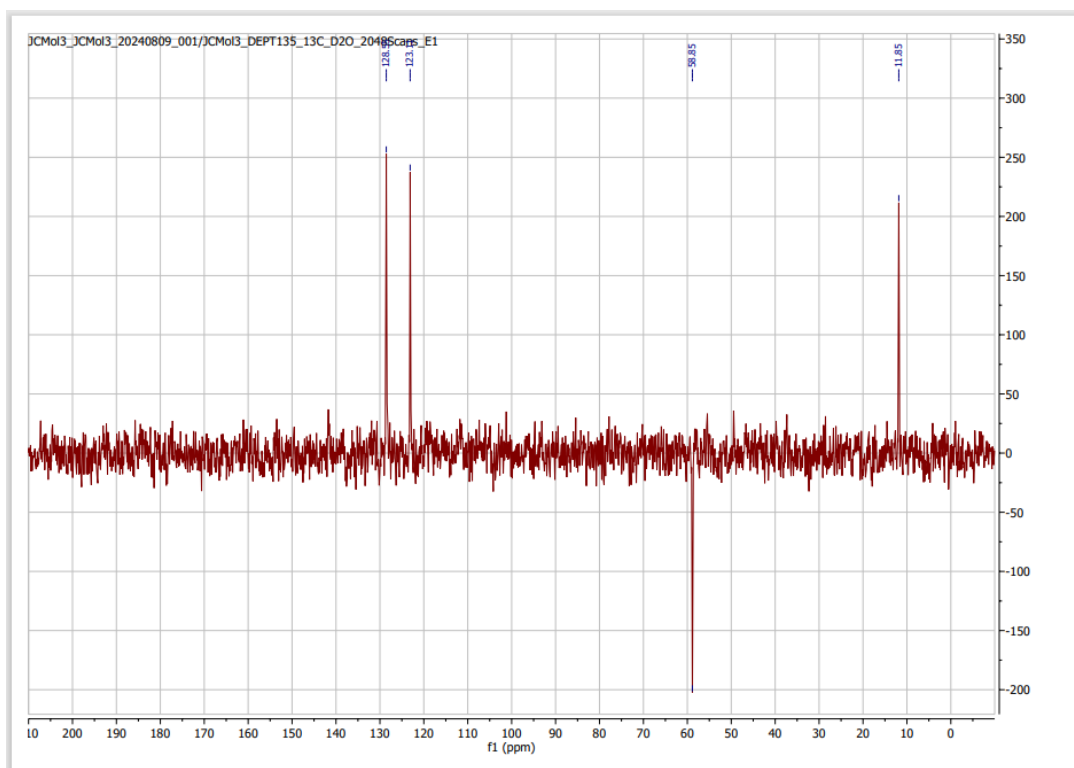
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S2

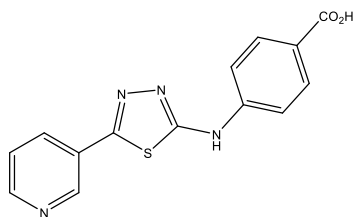




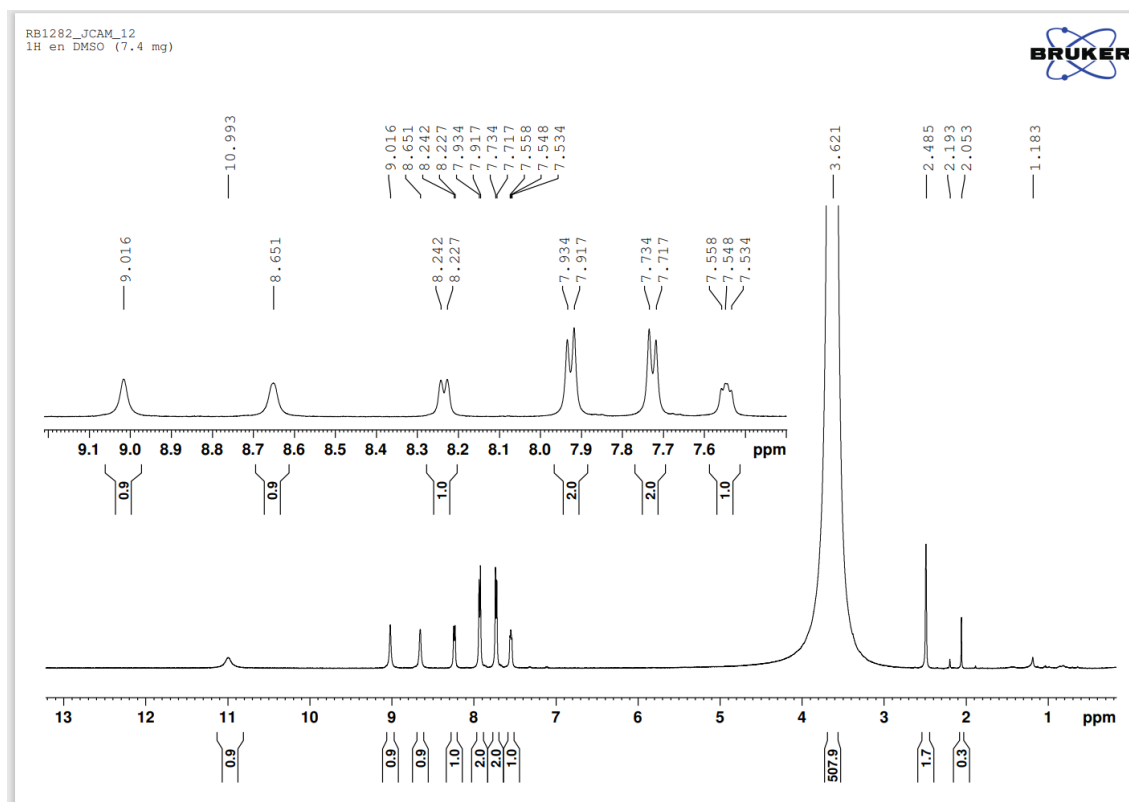
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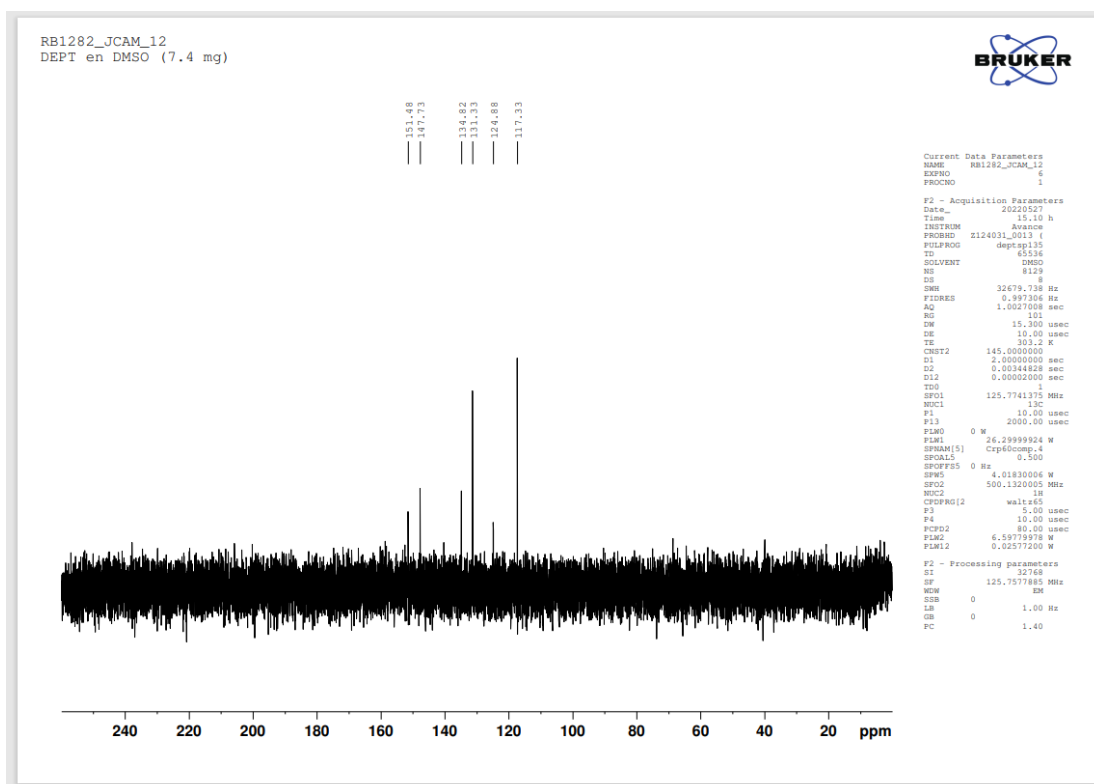
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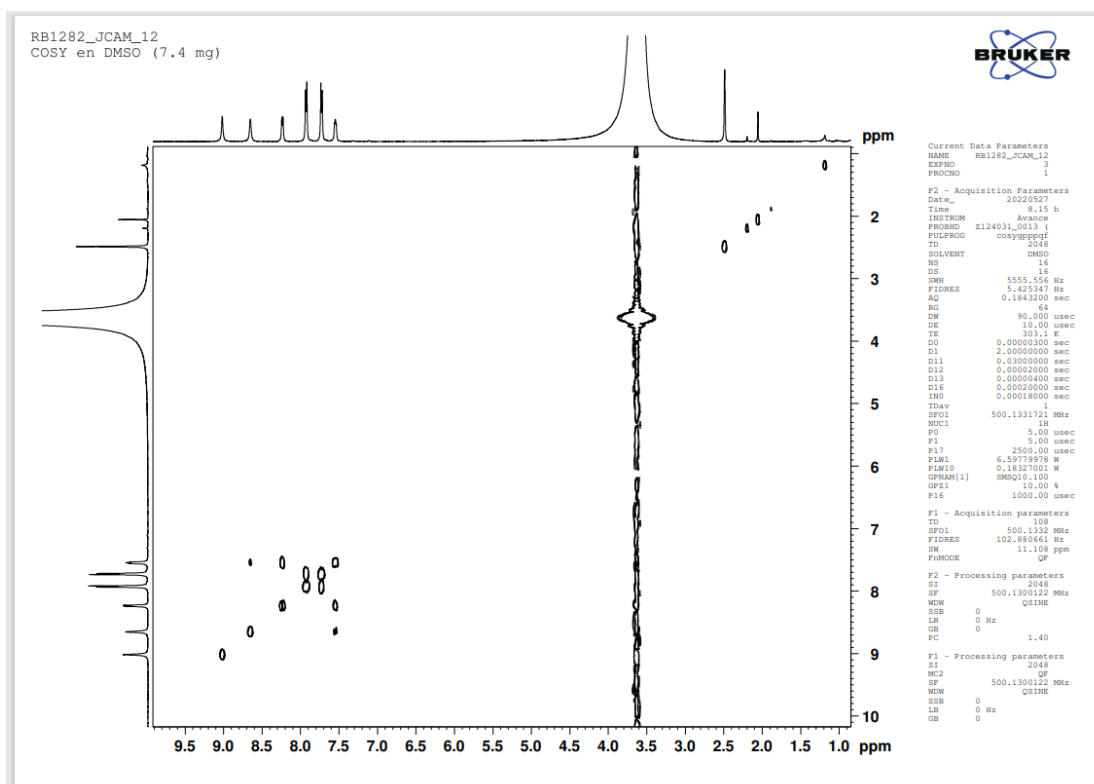
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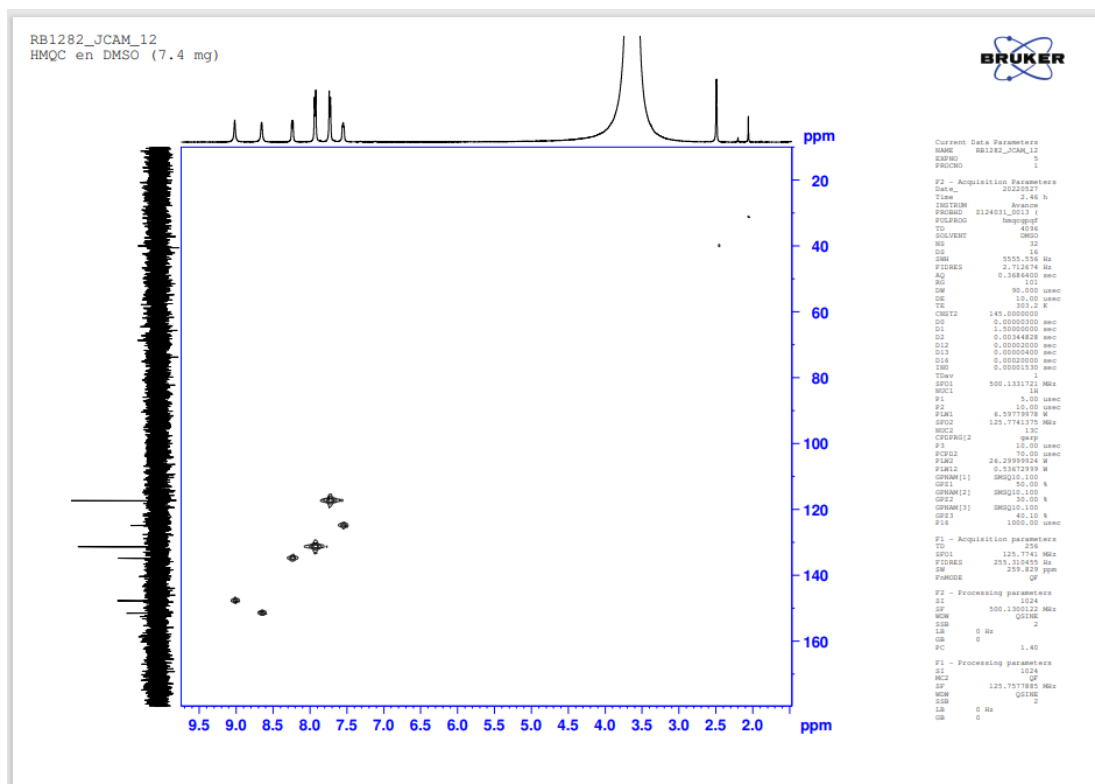


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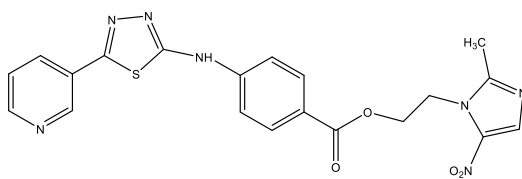
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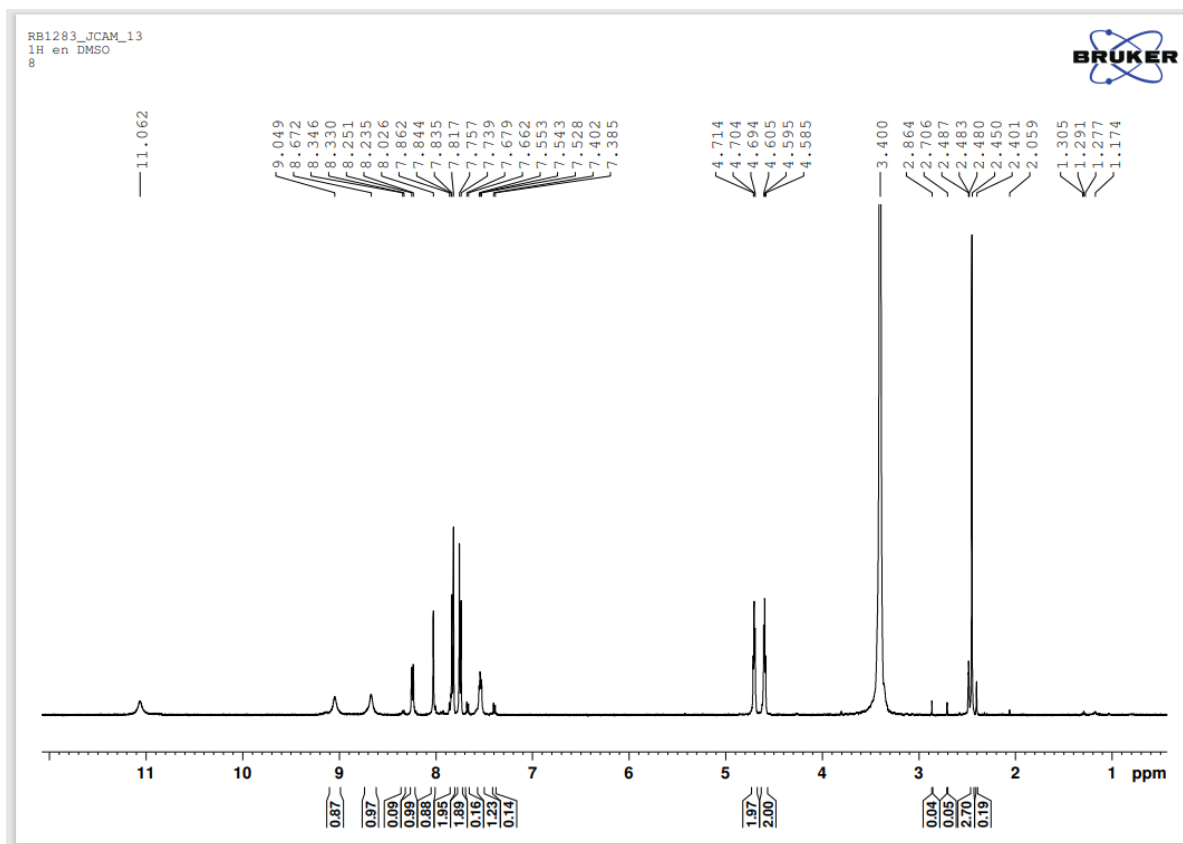




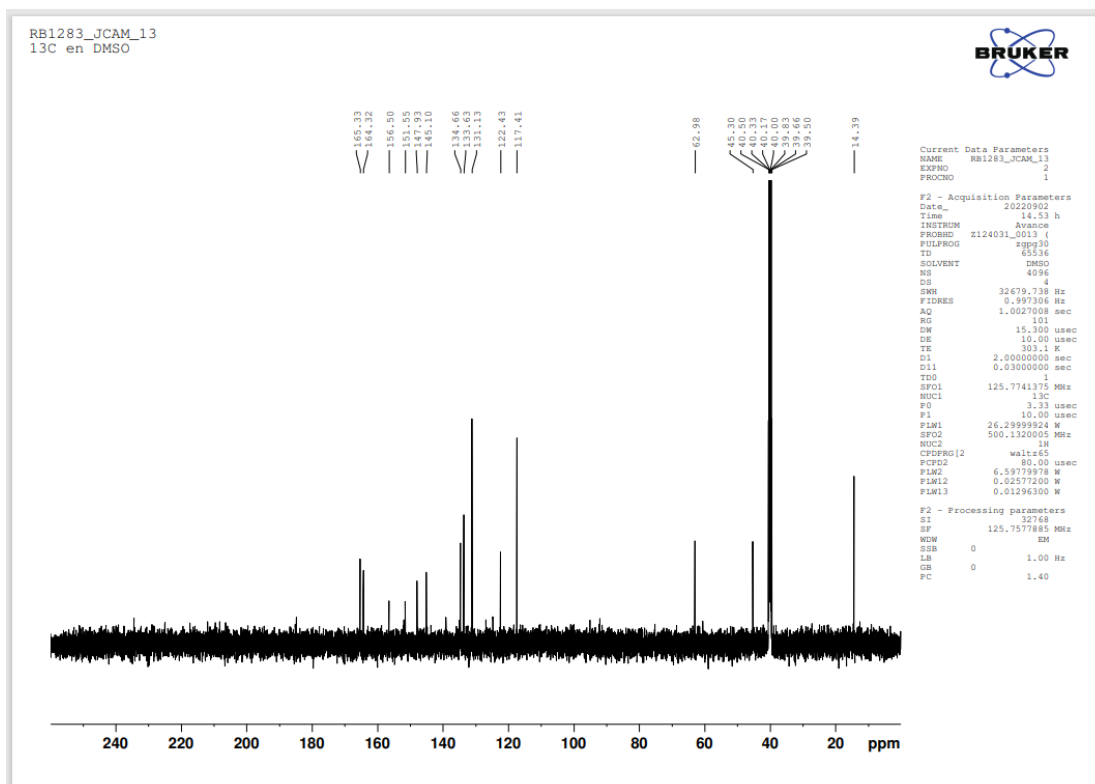
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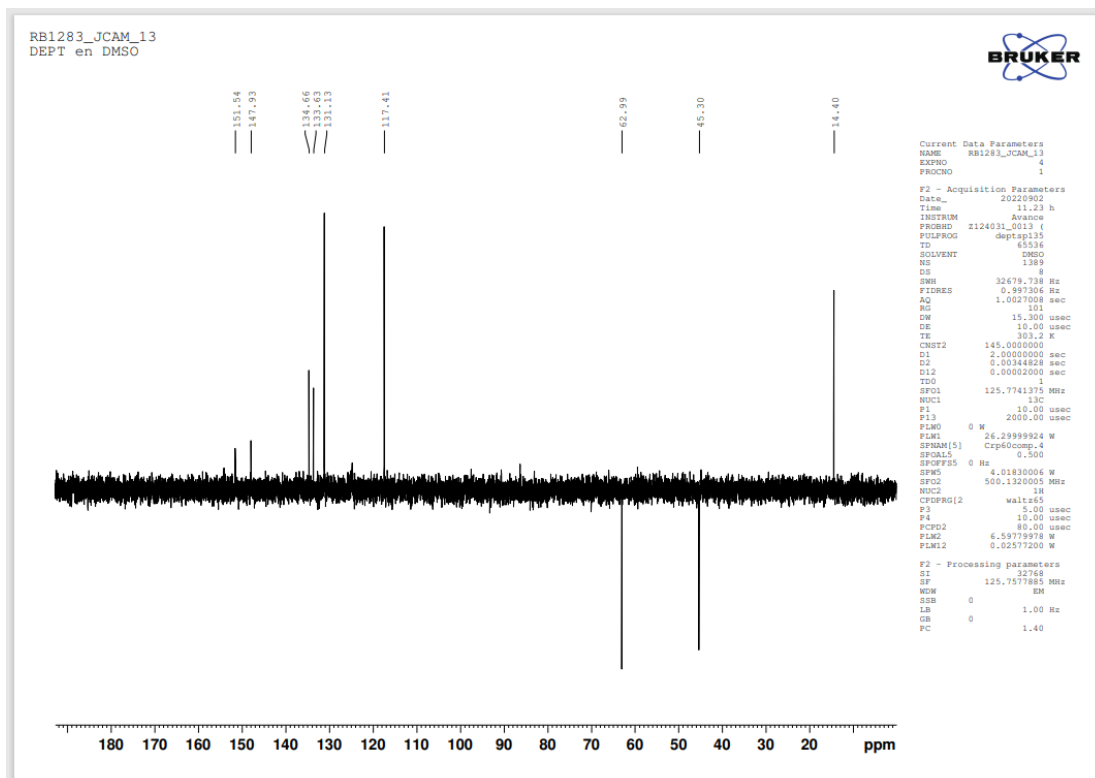
**13**



S9



S10



RB1283\_JCAM\_13  
HMOC en DMSO

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EXPNO 4  
PROCNO 1

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SOLVENT DMSO  
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DS 16  
SWH 5555.516 Hz  
FIDRES 2.712474 Hz  
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RG 320  
DW 90.000 usec  
DE 19.00 usec  
TE 303.1 K  
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D2 0.00344828 sec  
D12 0.00000000 sec  
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D18 0.00000000 sec  
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TM0 1  
TH0 500.133351 MHz  
NUC1 13  
P1 5.00 usec  
P2 15.00 usec  
PL1 6.59779978 Hz  
PL2 125.7741379 MHz  
NUC2 13C  
CPCPRG2 gapp  
P3 15.00 usec  
PCPD2 70.00 usec  
PL12 0.53872999 Hz  
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CPCPRG12 SMOQ10, 150  
CPCPRG13 SMOQ10, 150  
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PL12 0.53872999 Hz  
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CPCPRG15 SMOQ10, 150  
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CPCPRG18 SMOQ10, 150  
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PC 1.40  
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SF 125.7741 MHz  
WDW EM  
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GB 0  
PC 1.40

RB1283\_JCAM\_13  
HMBC en DMSO

BRUKER

Current Data Parameters  
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PROCNO 1

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SWH 4250.000 Hz  
F2RES 3.191718 Hz  
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RG 101  
SW 80.000 usec  
DE 10.00 usec  
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CHST2 145.000000  
CHST3 18.000000  
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D1 1.5000000 sec  
D2 0.0034482 sec  
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D14 0.0002000 sec  
DM 0.0001130 sec  
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SFO2 125.7741375 MHz  
NUC2 13C  
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P14 1000.00 usec

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GB 0  
PC 1.40

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WDW 0  
SSB 0  
LB 0 Hz  
GB 0

CCOC(=O)c1ccc(NC(=S)NNC(=O)c2ccc(Cl)cc2)cc1

RB1287\_JCAM\_17  
1H en DMSO  
6.1 mg

BRUKER

— 10.665

— 9.928

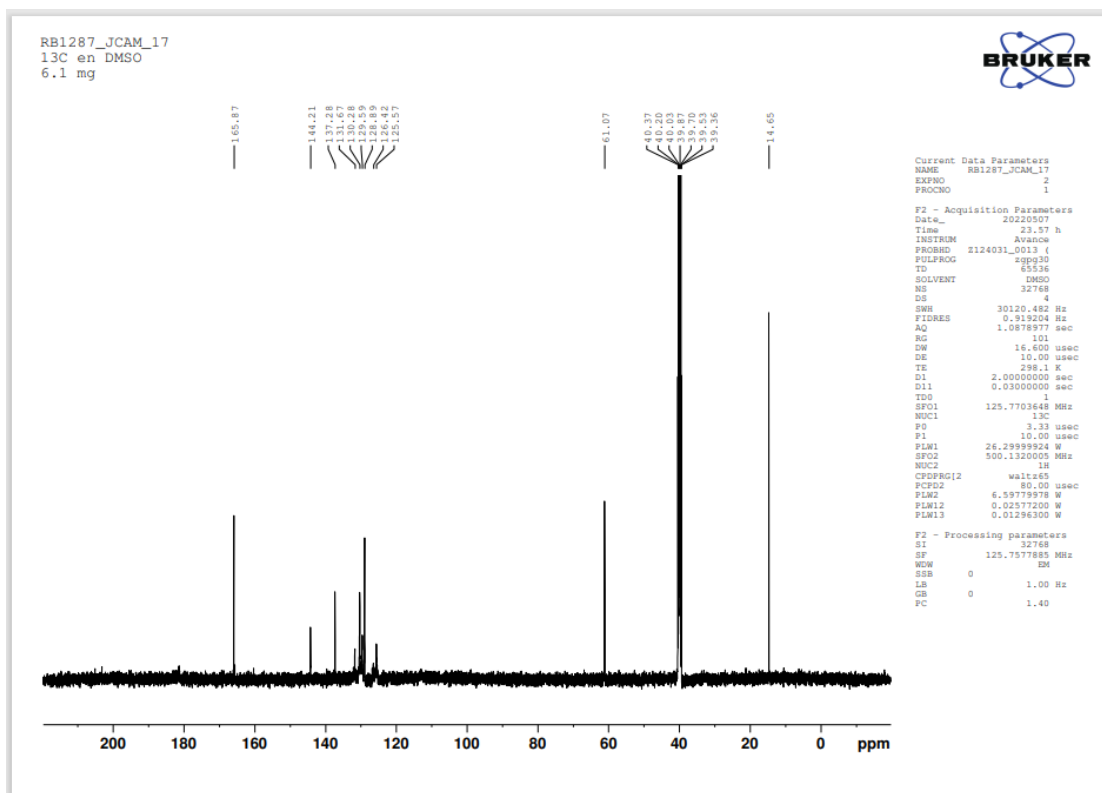
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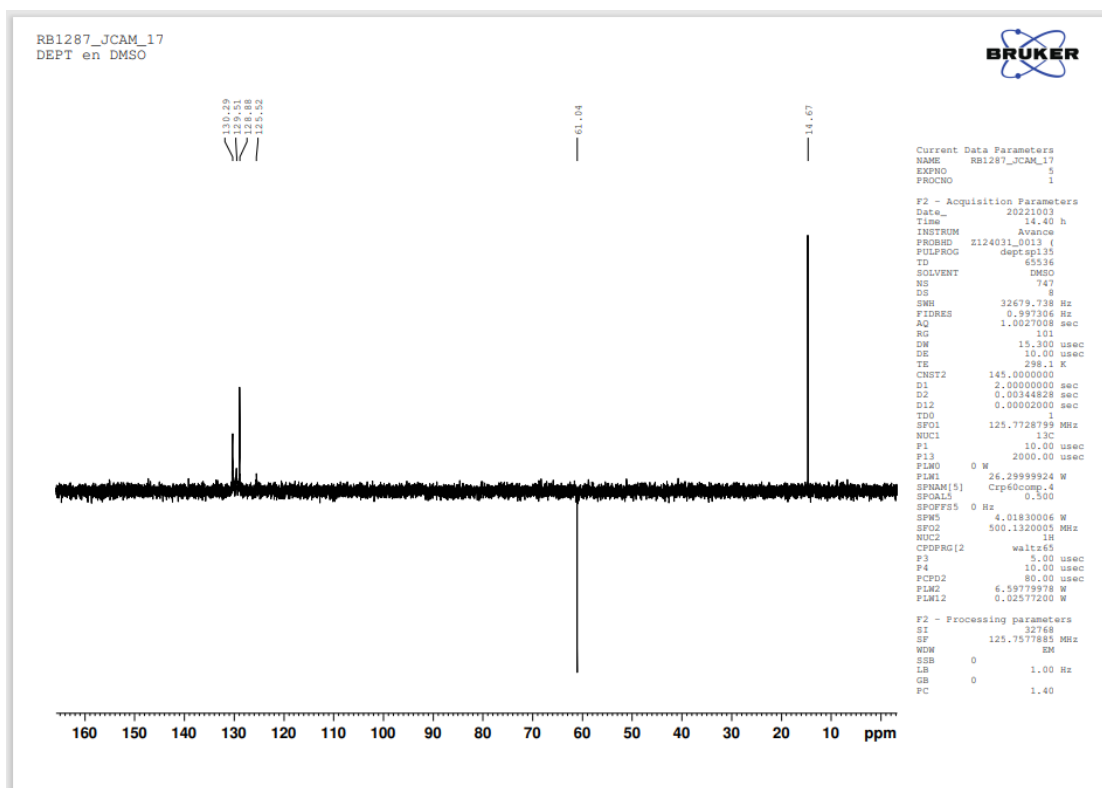
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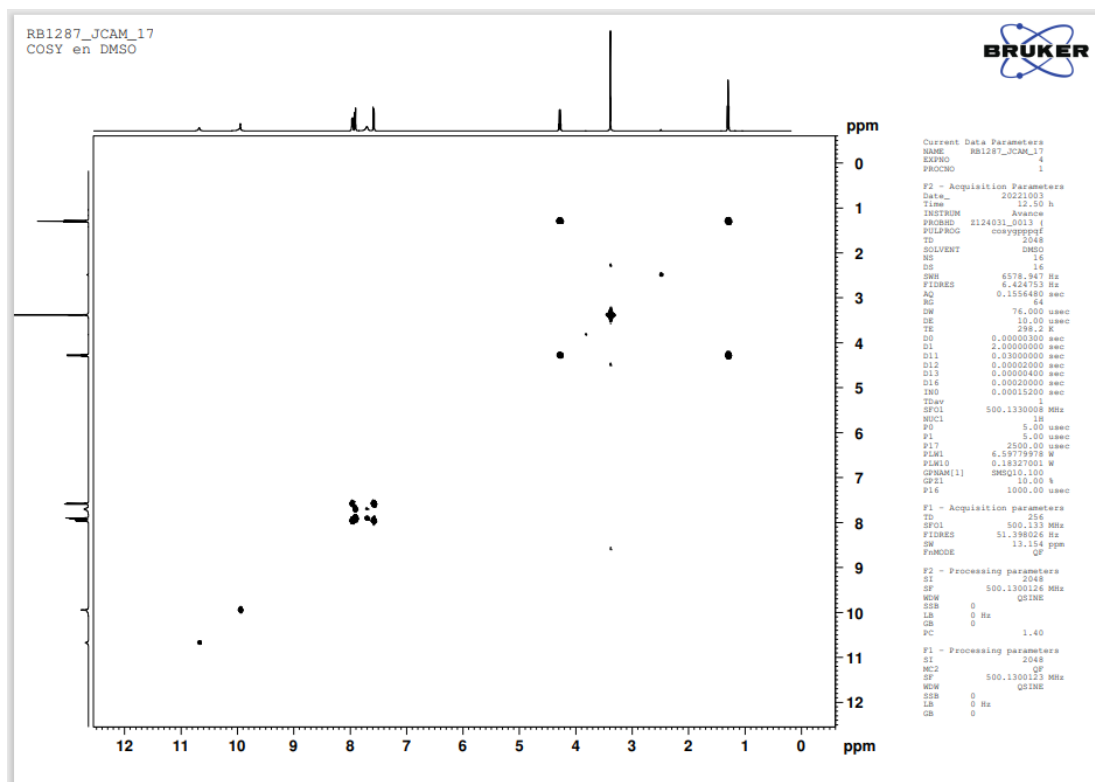
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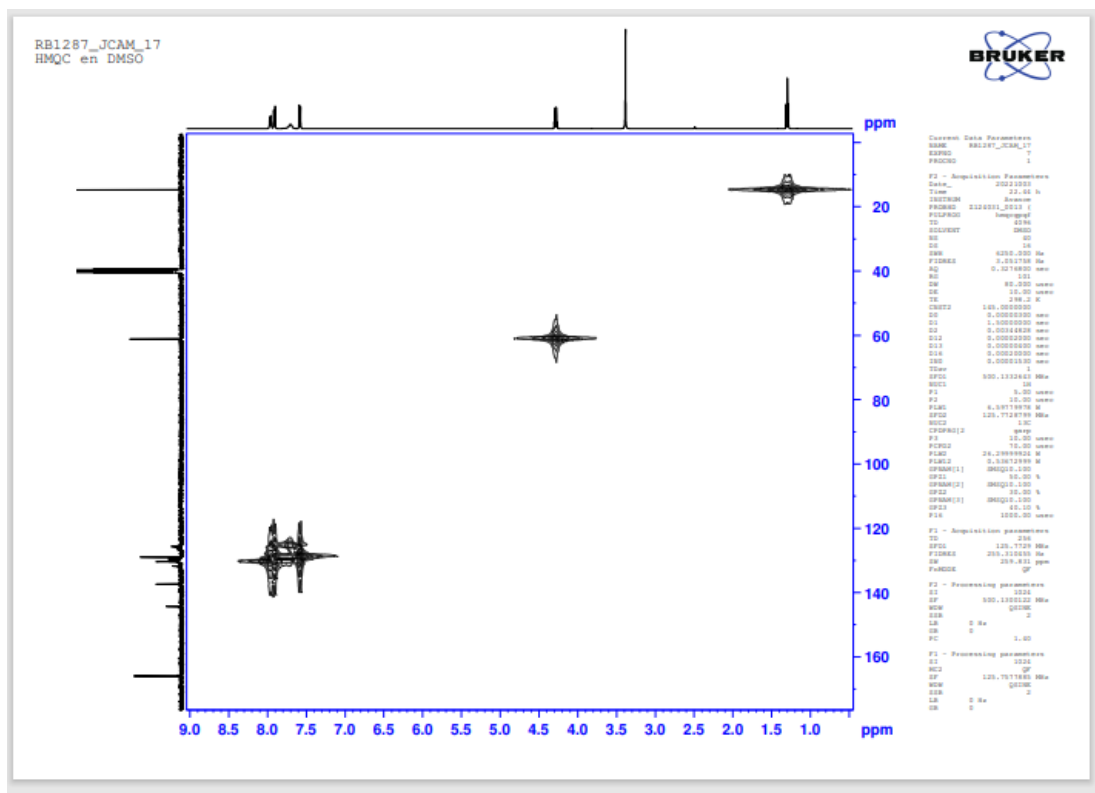
S15



S16



S17



RB1287\_JCAM\_17  
HMBC en DMSO

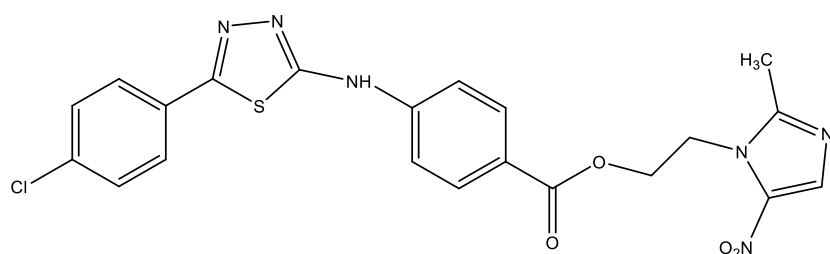
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PROCNO 1

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SOLVENT DMSO  
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DPR1 14  
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DPR3 129.7728789 MHz  
SOL2 1.00  
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F4RES 26.23899804 Hz  
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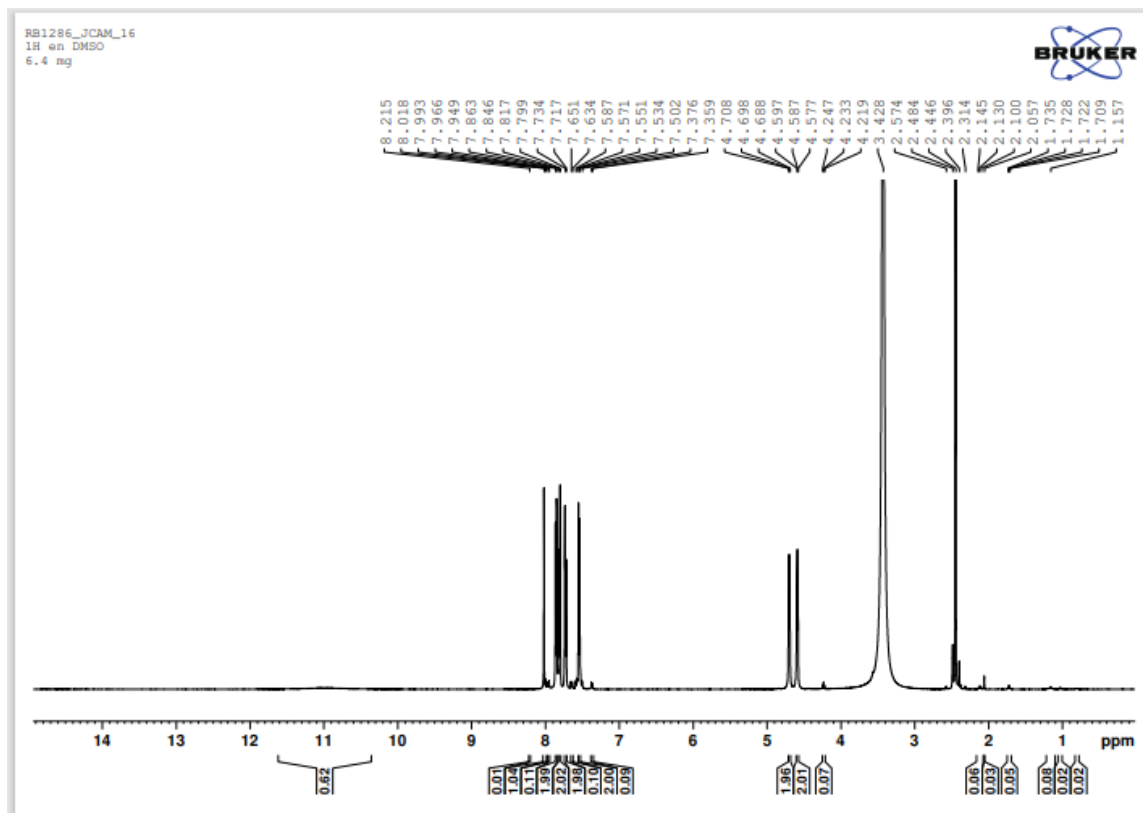
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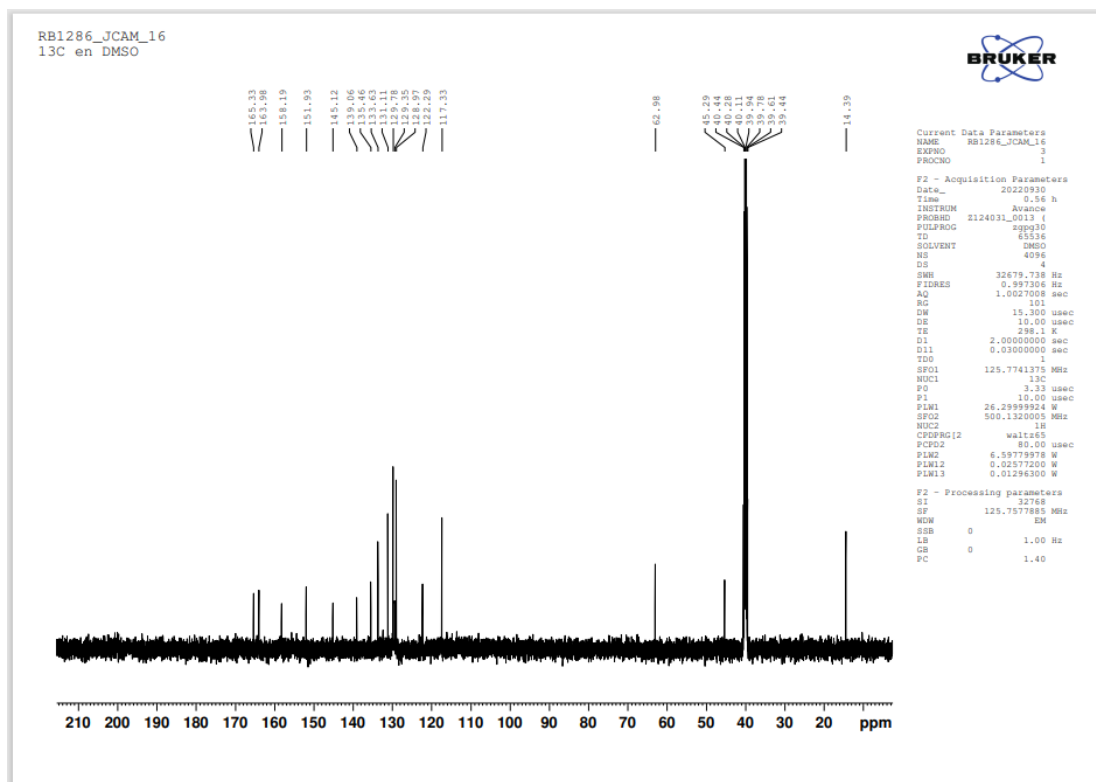
S19

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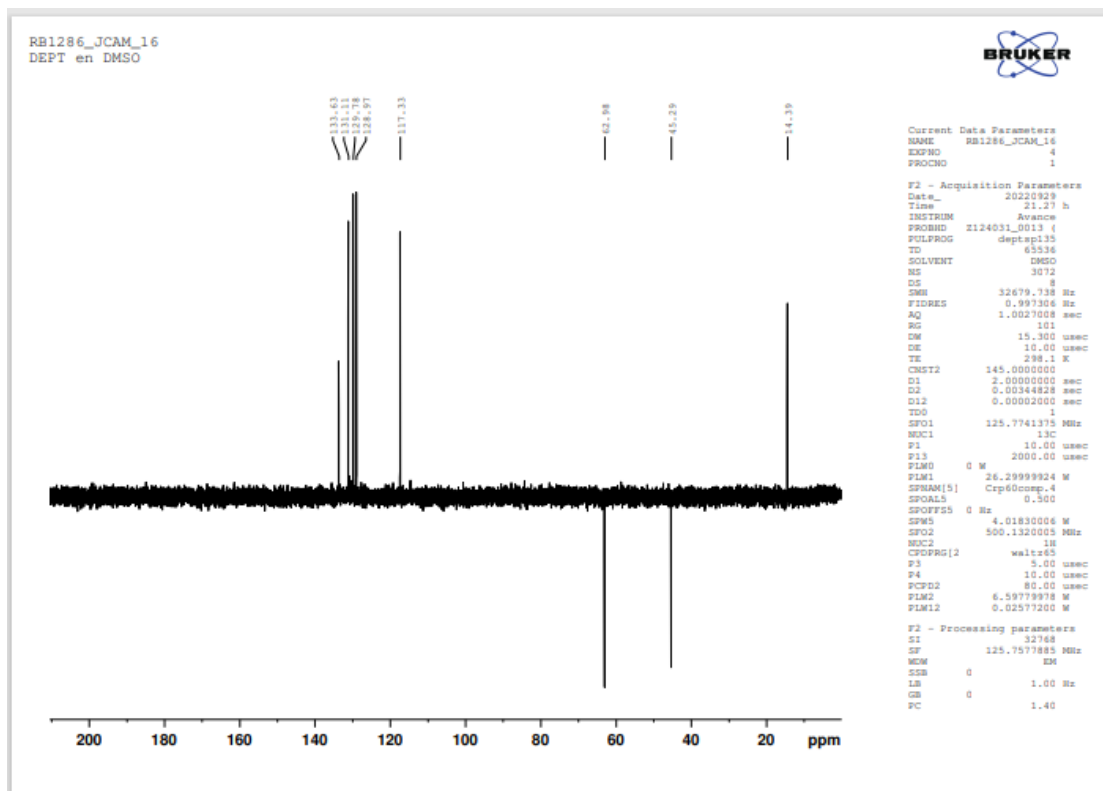




S20



S21



RB1286\_JCAM\_16  
COSY en DMSO

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PROCNO 1

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RB1286\_JCAM\_16  
HMQC en DMSO

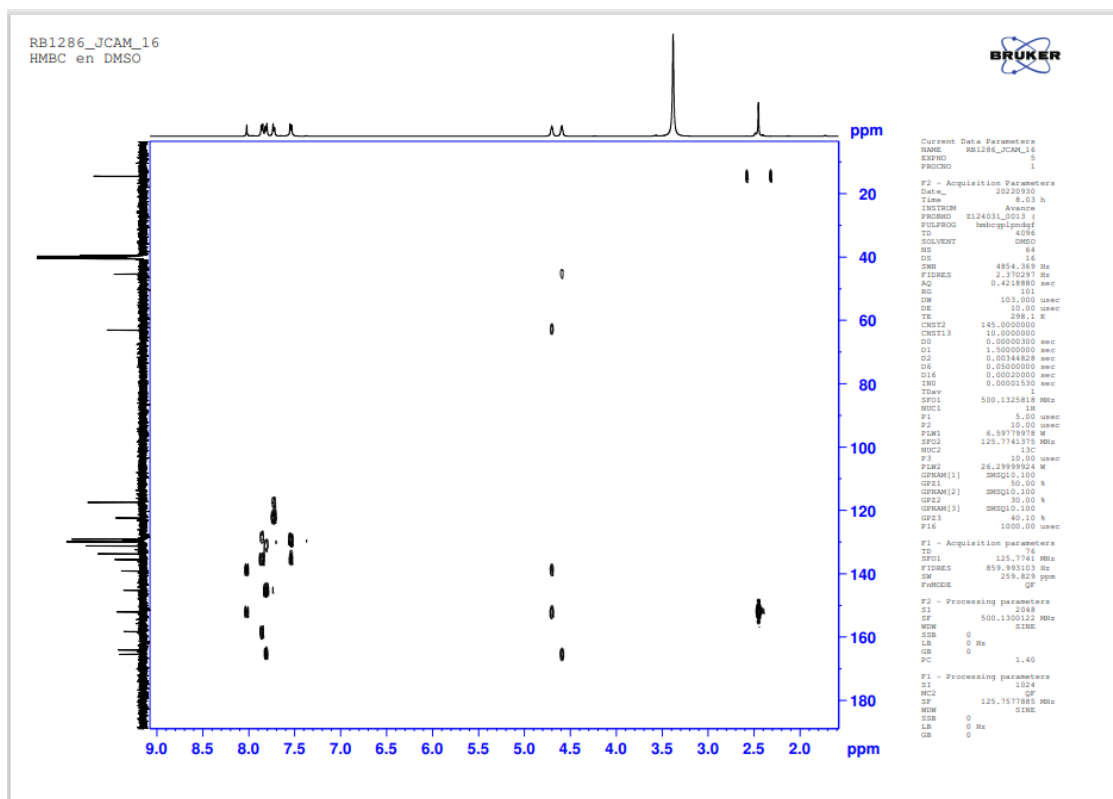
Current Data Parameters  
NAME RB1286\_JCAM\_16  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20220910  
Time 9.21 h  
INSTRUM spect  
PROBHD BBO4001-0013 (1  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 12  
DS 14  
SWH 4854.265 Hz  
F2RES 2.376257 Hz  
AQ 0.4218880 sec  
RG 501  
SW 107.000 usec  
ZC 15.00 usec  
TE 298.2 K  
CH22 145.000000 MHz  
G1 0.00002000 MHz  
G2 0.00002000 MHz  
G3 0.00002000 MHz  
G4 0.00002000 MHz  
G5 0.00002000 MHz  
G6 0.00002000 MHz  
G7 0.00002000 MHz  
G8 0.00002000 MHz  
G9 0.00002000 MHz  
TDav 500.1325815 MHz  
MPC1 10  
P1 10.00 usec  
P2 10.00 usec  
PL1 6.7577978 W  
PL2 125.7741375 MHz  
NUC1 13C  
CPDPRG2 jmg  
P3 15.00 usec  
PCPD 75.00 usec  
PL12 26.29999024 W  
PL12 0.5367999 W  
CPDPRG2 jmg  
G1 50.00 V  
G2 50.00 V  
G3 50.00 V  
G4 50.00 V  
G5 50.00 V  
G6 50.00 V  
G7 50.00 V  
G8 50.00 V  
G9 50.00 V  
P18 1000.00 usec

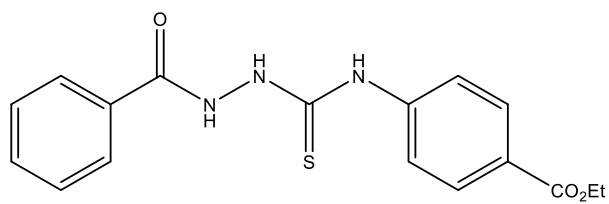
F1 - Acquisition parameters  
TD 65536  
SFO1 125.7741375 MHz  
F2RES 2.376257 Hz  
SW 4854.265 Hz  
PULPROG zgpg30

F2 - Processing parameters  
SI 1024  
SF 500.1301222 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

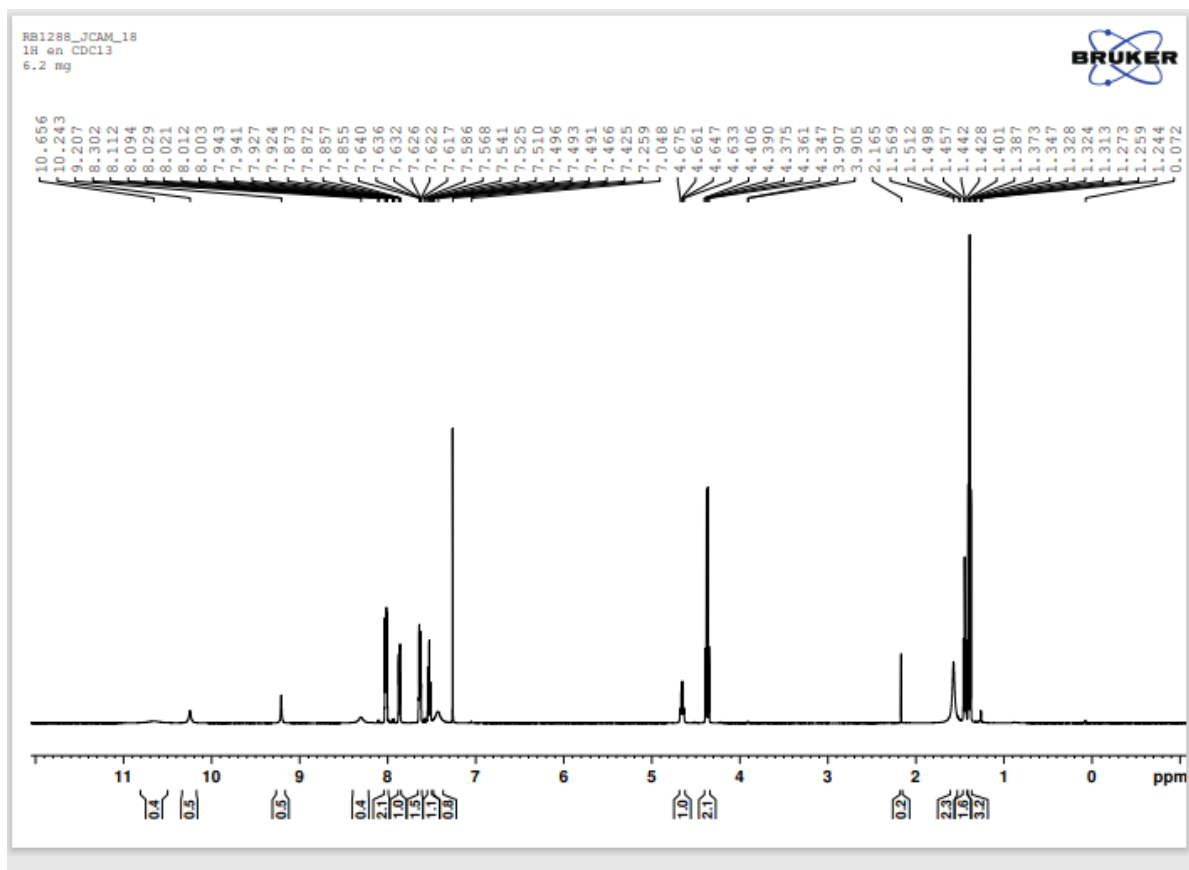
F1 - Processing parameters  
SI 1024  
SF 500.1301222 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0



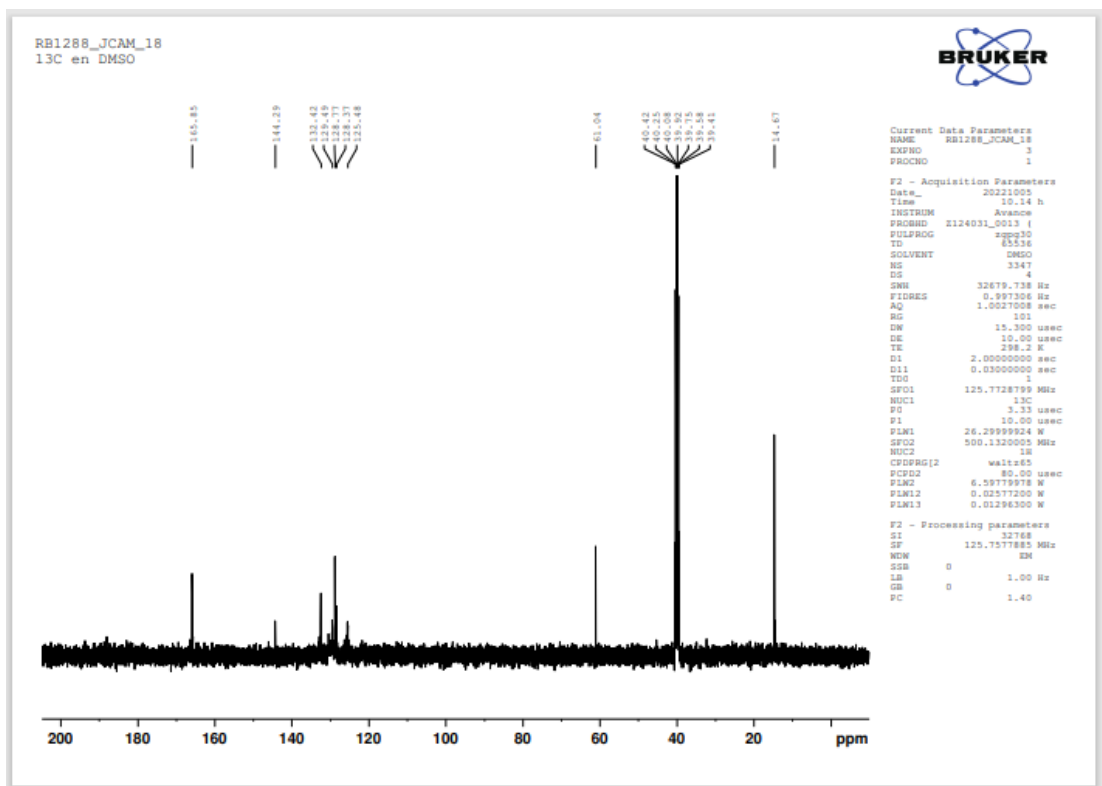
S25



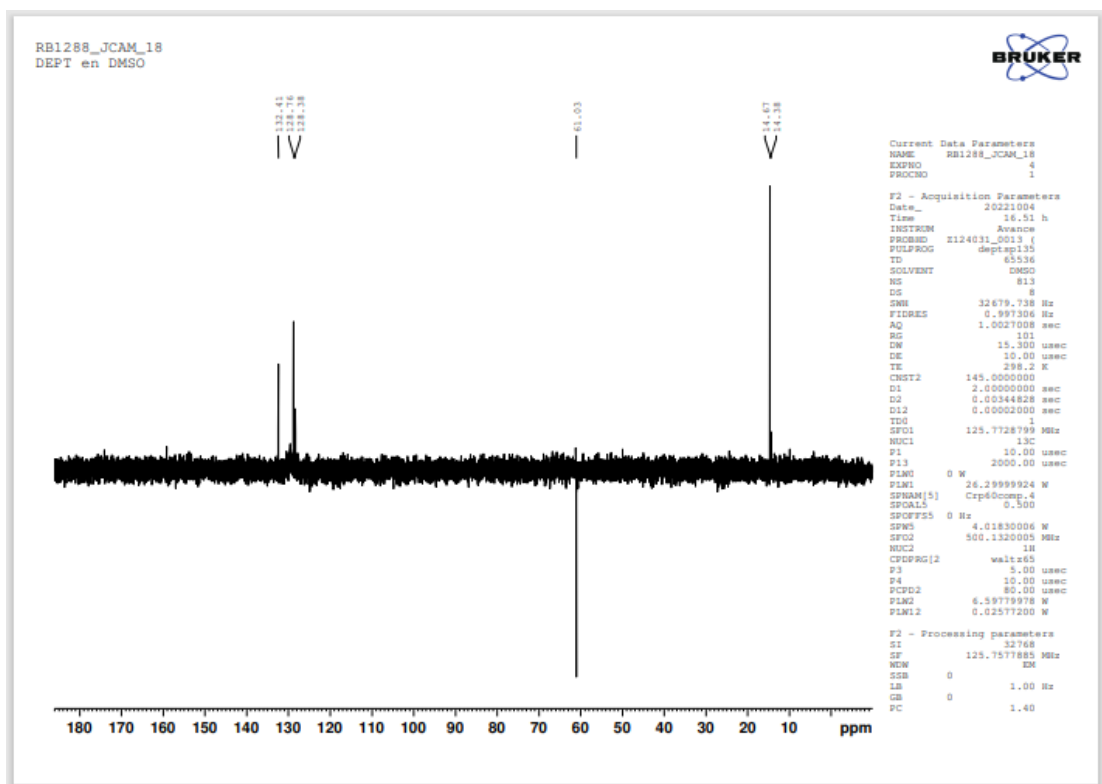
8



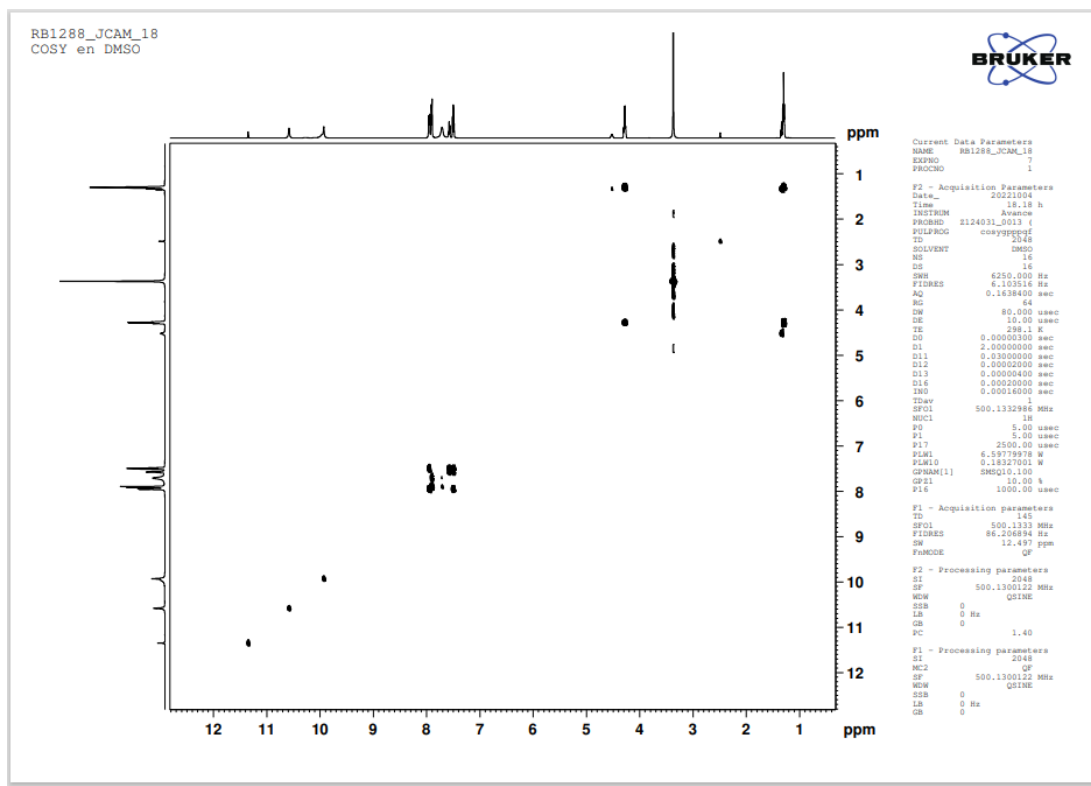
S26



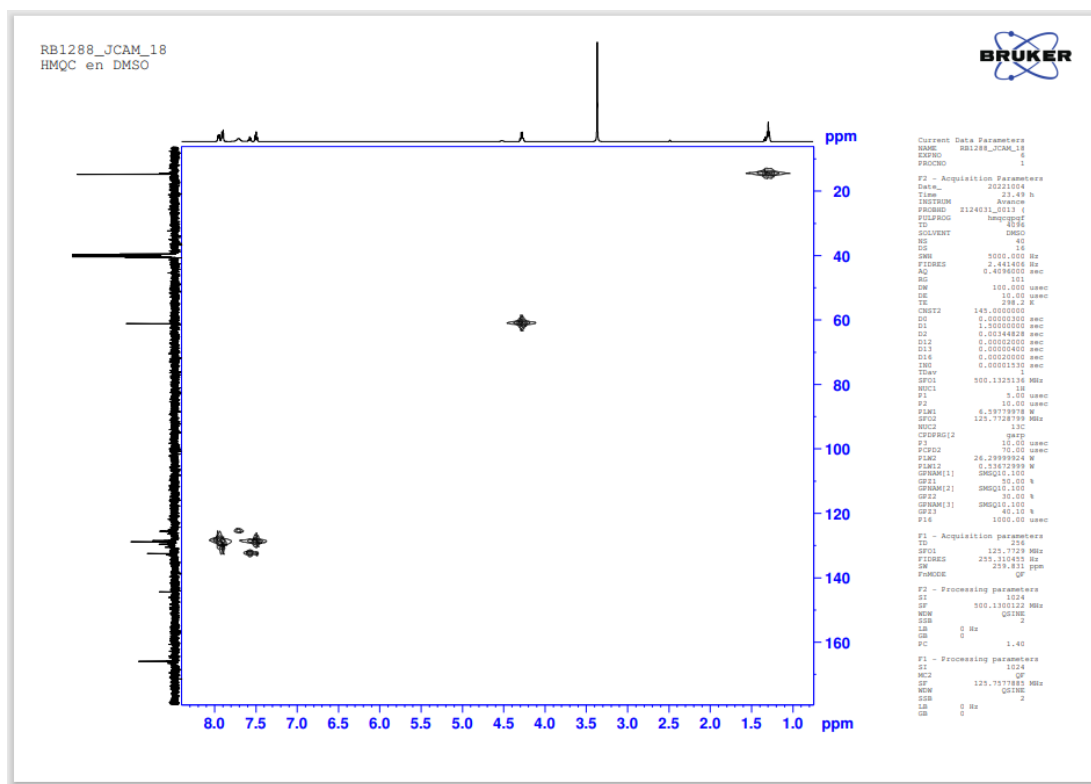
S27



S28



S29





Cc1cnc(CCNc2nc3ccccc3s2)cc1[N+](=O)[O-]

RB1289\_7CAM\_19  
 1H en DMSO (8.1 mg)

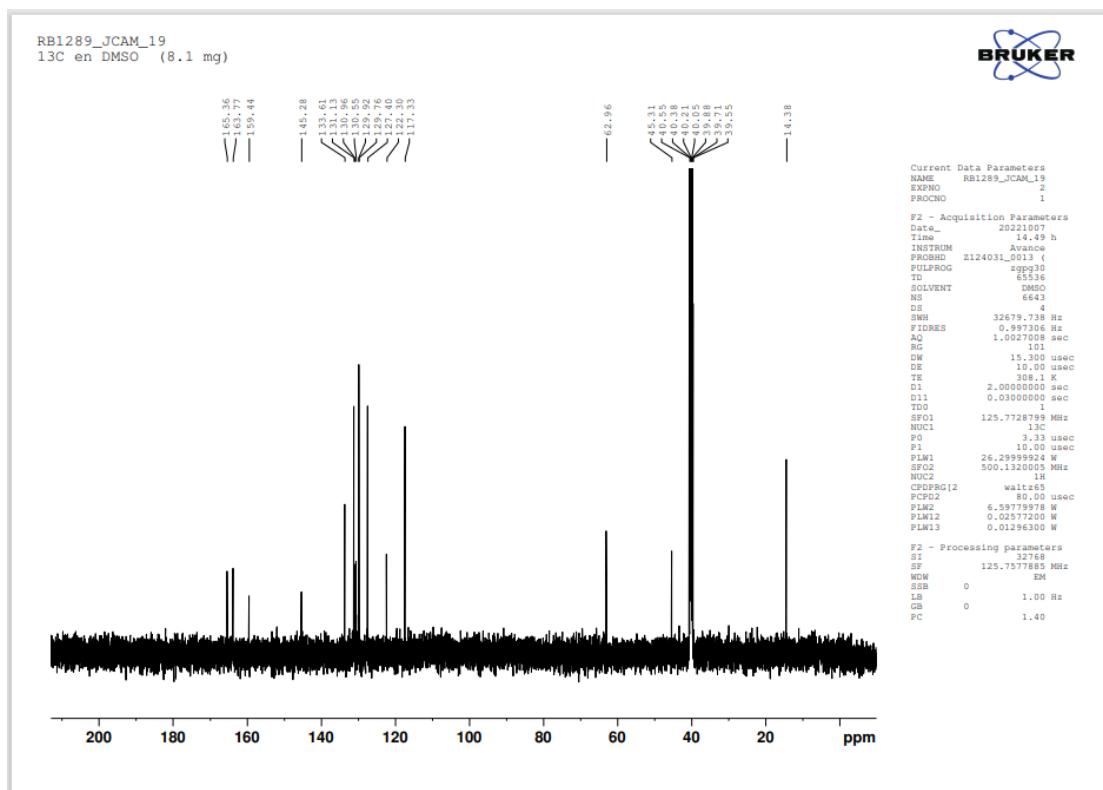
10.932  
 8.043  
 8.020  
 7.999  
 7.966  
 7.957  
 7.952  
 7.947  
 7.940  
 7.873  
 7.868  
 7.858  
 7.854  
 7.843  
 7.826  
 7.789  
 7.772  
 7.759  
 7.742  
 7.669  
 7.652  
 7.641  
 7.531  
 7.523  
 7.520  
 7.513  
 7.508  
 7.502  
 7.499  
 7.494  
 7.483  
 7.410  
 7.392  
 7.123  
 7.105  
 6.723  
 6.357  
 6.353  
 6.323  
 4.723  
 4.713  
 4.702  
 4.626  
 4.612  
 4.602  
 4.592  
 3.847  
 3.843  
 3.813  
 3.793  
 3.301  
 2.870  
 2.714  
 2.487  
 2.484  
 2.480  
 2.456  
 2.437  
 2.408  
 2.065  
 1.330  
 1.316  
 1.302  
 1.288  
 1.201

0.4  
 0.5  
 1.1  
 1.0  
 1.8  
 0.7  
 1.9  
 3  
 1.4

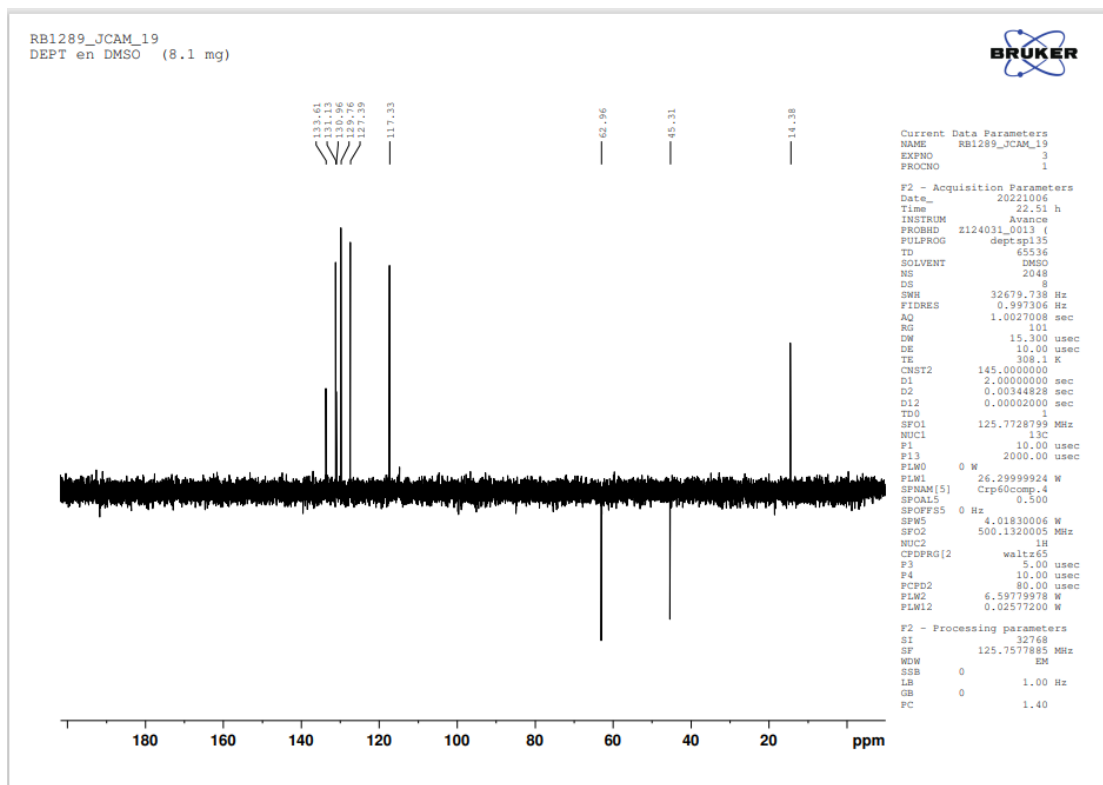
ppm



S32



S33



RB1289\_JCAM\_19  
COSY en DMSO (8.1 mg)

Current Data Parameters  
NAME RB1289\_JCAM\_19  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221006  
Time 21.07 h  
INSTRUM Avance  
PROBHD 124031\_5013 1  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 4  
SWH 5882.253 Hz  
FIDRES 0.1744860 Hz  
AQ 0.1745000 sec  
RG 64  
SW 85.000 MHz  
DE 10.00 MHz  
TE 300.2 K  
D0 0.0000000 sec  
D1 2.0000000 sec  
D11 0.1200000 sec  
D12 0.0000000 sec  
D13 0.0000000 sec  
D14 0.0000000 sec  
DRO 0.0001760 sec  
TD0V  
SFO1 500.133222 MHz  
NUC1 1H  
P1 5.00 MHz  
P17 2500.00 MHz  
PL1 6.59779978 W  
PL12 0.1632700 W  
GPRAM[1] DMG10.100 V  
GPR1 10.00 V  
P1A 1000.00 MHz

F1 - Acquisition parameters  
TD 256  
SFO1 500.1331 MHz  
FIDRES 61.958461 Hz  
SW 11.740 ppm  
FAMODE QP

F2 - Processing parameters  
SI 2048  
SF 500.130122 MHz  
WDW QDMC  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 2048  
SF 500.130122 MHz  
WDW QDMC  
SSB 0  
LB 0 Hz  
GB 0

RB1289\_JCAM\_19  
HMQC en DMSO (8.1 mg)

Current Data Parameters  
NAME RB1289\_JCAM\_19  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221007  
Time 3:14 h  
INSTRUM Avance  
PROBHD 2124012\_2012 (4  
PULPROG zgpg30  
TD 4836  
SOLVENT DMSO  
NS 32  
DS 16  
SWH 5000.000 Hz  
FIDRES 2.441406 Hz  
AQ 0.4294000 sec  
RG 101  
DM 100.000 usec  
DE 10.00 usec  
TE 300.2 K

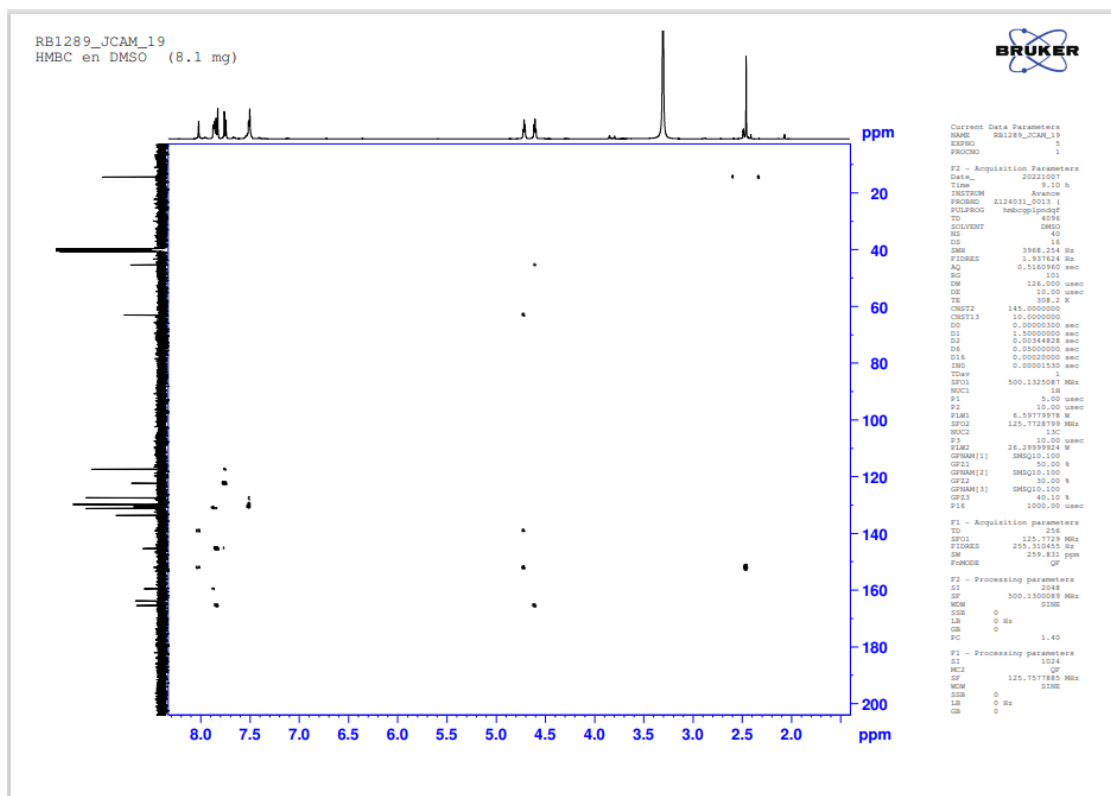
CHGT2 145.0000000  
G0 0.00000000 sec  
D0 1.50000000 sec  
D1 0.00144428 sec  
D12 0.00002000 sec  
D13 0.00000000 sec  
D16 0.00020000 sec  
DMS 0.00010130 sec

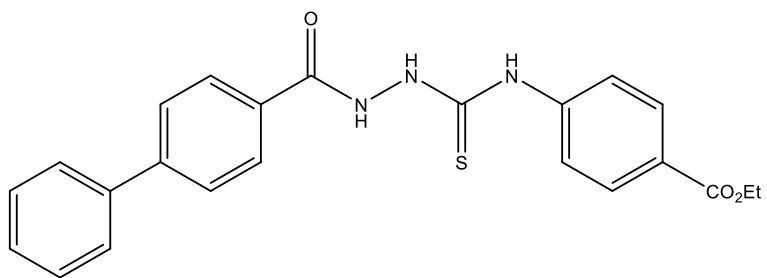
TDsv 500.1325134 MHz  
SFO1 500.1325134 MHz  
NUC1 13C  
P1 5.00 usec  
P2 10.00 usec  
PLM1 6.9377978 W  
SFO2 125.7728789 MHz  
NUC2 13C  
CHPFG2 90.00 Hz  
P3 10.00 usec  
PLM2 26.29999924 W  
PLM3 0.54872999 W  
GPMW(1) 0MSQ10.100 s  
GPMW(2) 0MSQ10.100 s  
GPMW(3) 0MSQ10.100 s  
GPMW(4) 0MSQ10.100 s  
GPMW(5) 0MSQ10.100 s  
P14 1000.00 usec

F2 - Acquisition parameters  
TD 614  
FIDRES 125.7729 MHz  
FIDRES 235.11045 Hz  
SW 239.811 ppm  
PULPROG zgpg30

F2 - Processing parameters  
SI 1024  
SF 500.1300122 MHz  
GFM 2  
RG 0 Hz  
LB 0  
PC 1.40

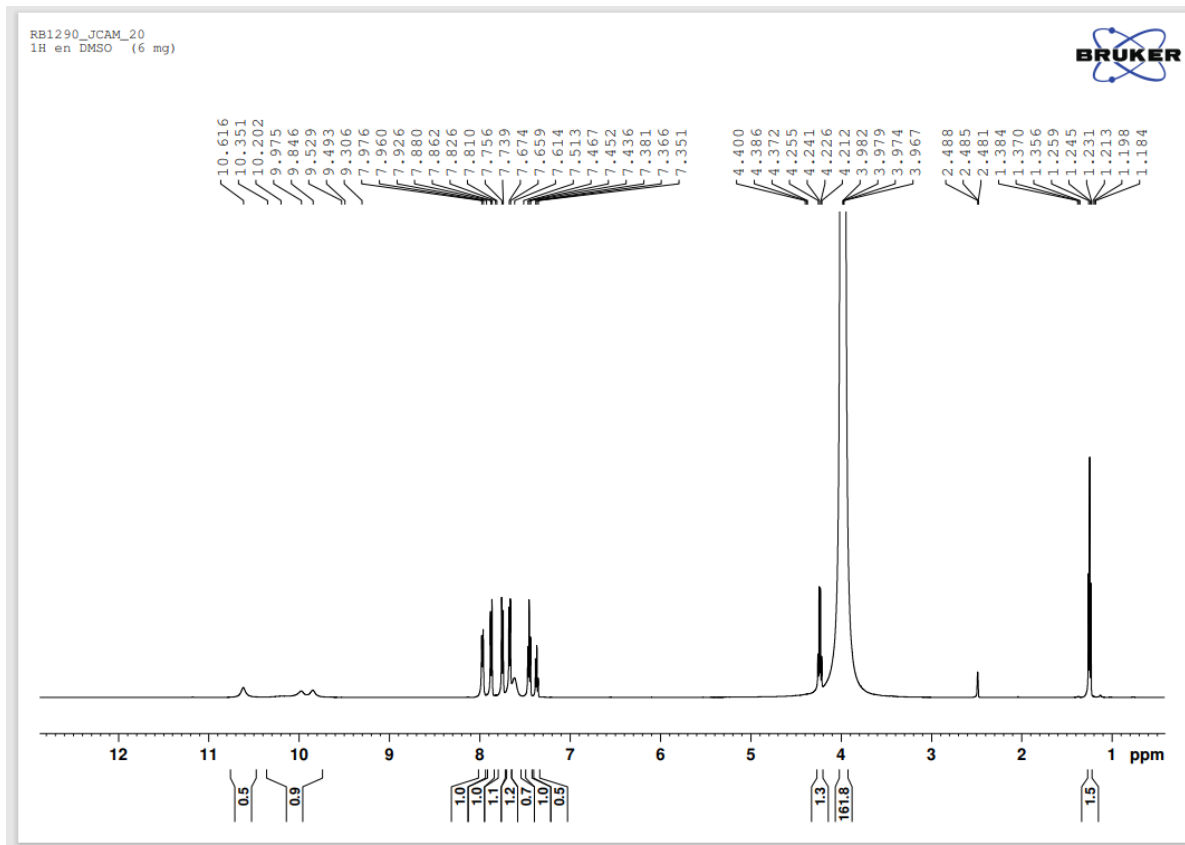
F1 - Processing parameters  
SI 1024  
SF 125.7577885 MHz  
GFM 2  
RG 0 Hz  
LB 0  
PC 0



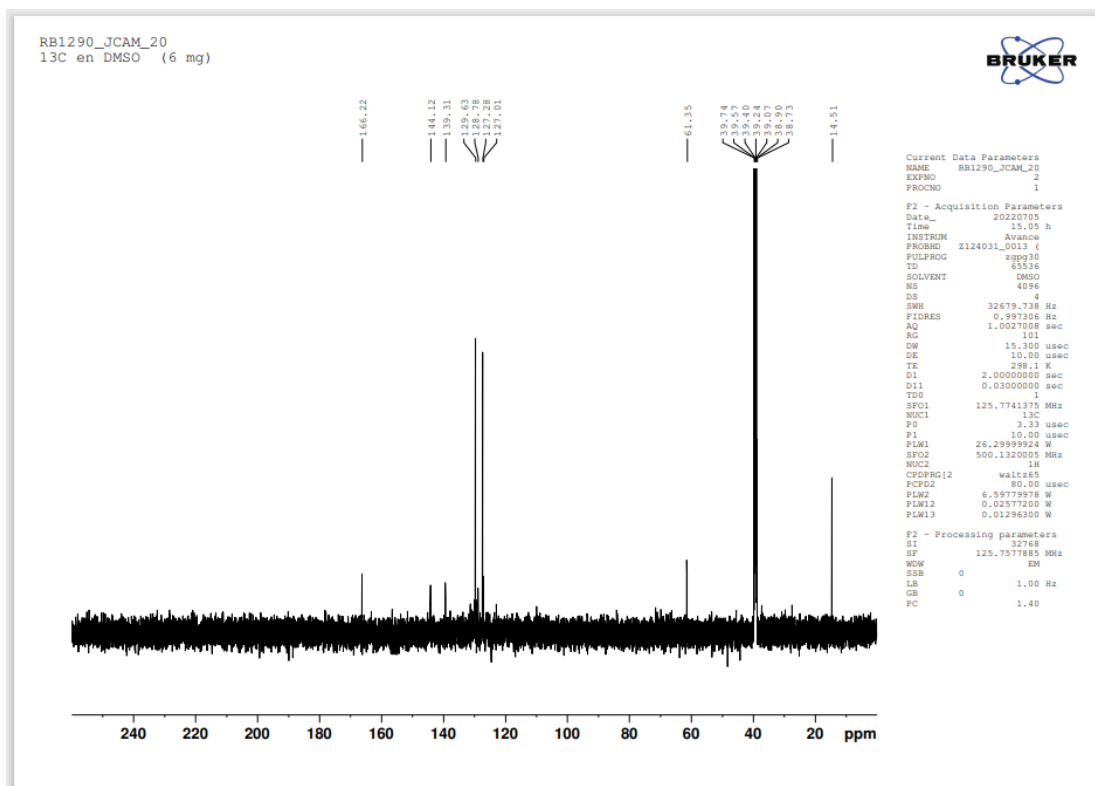


S37

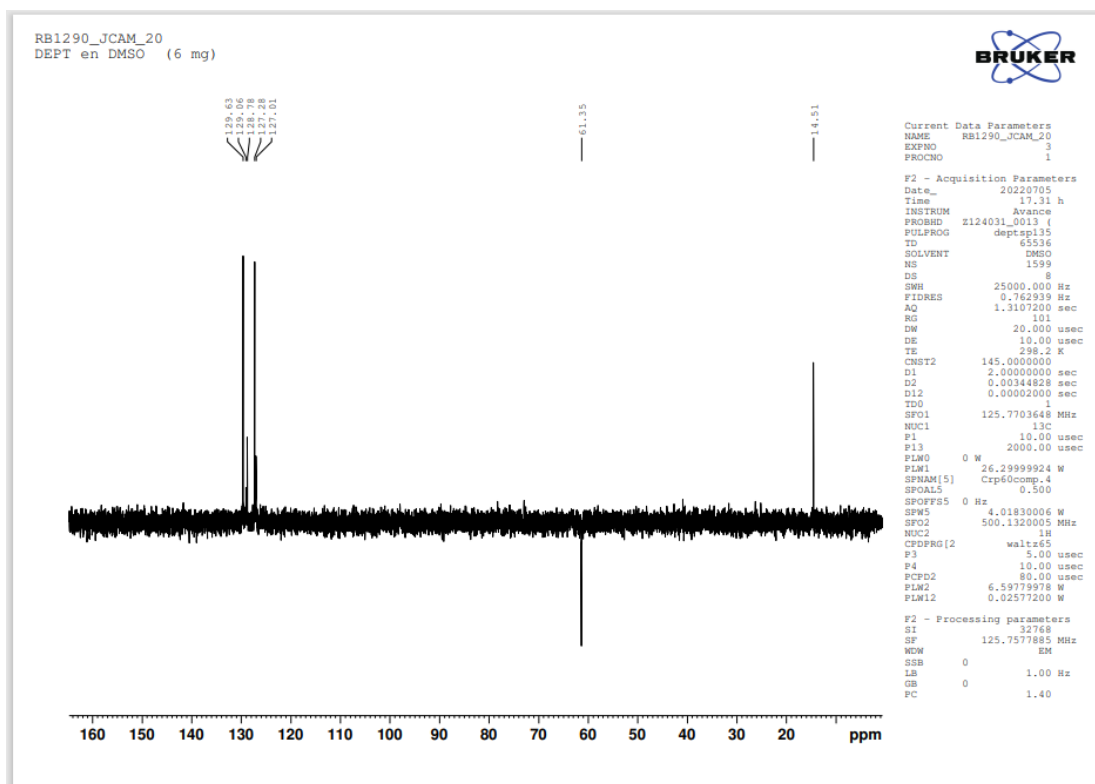
9



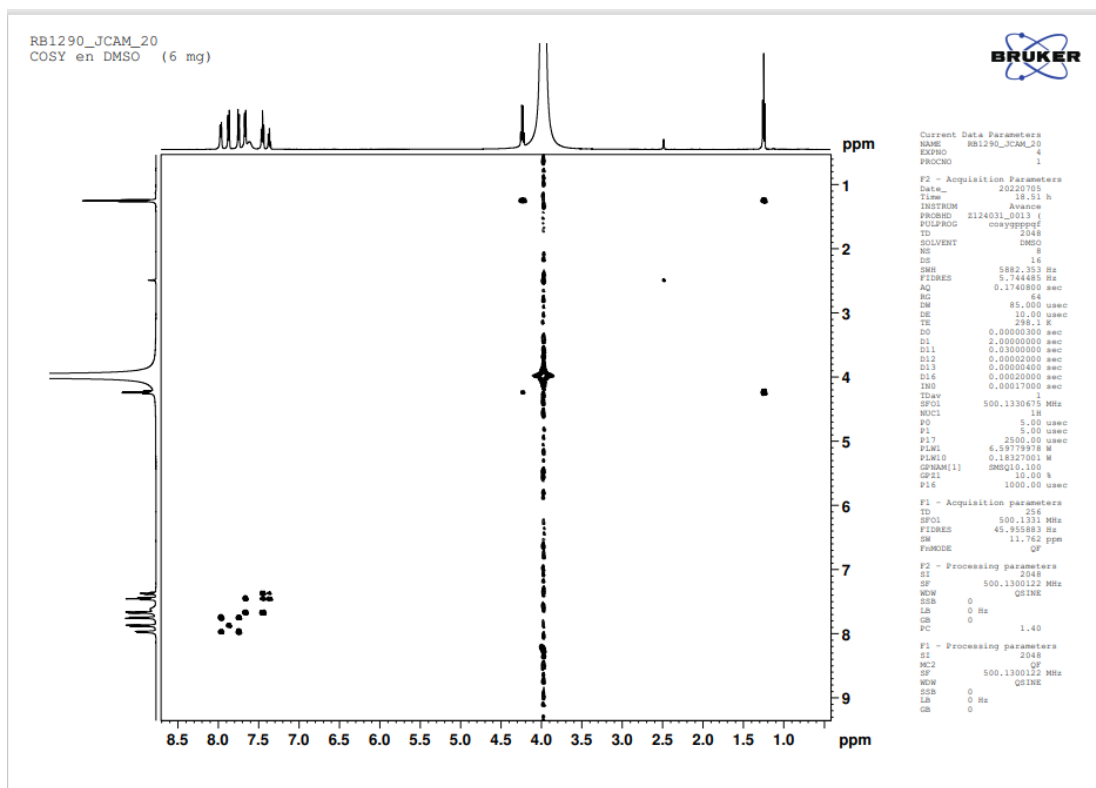
S38



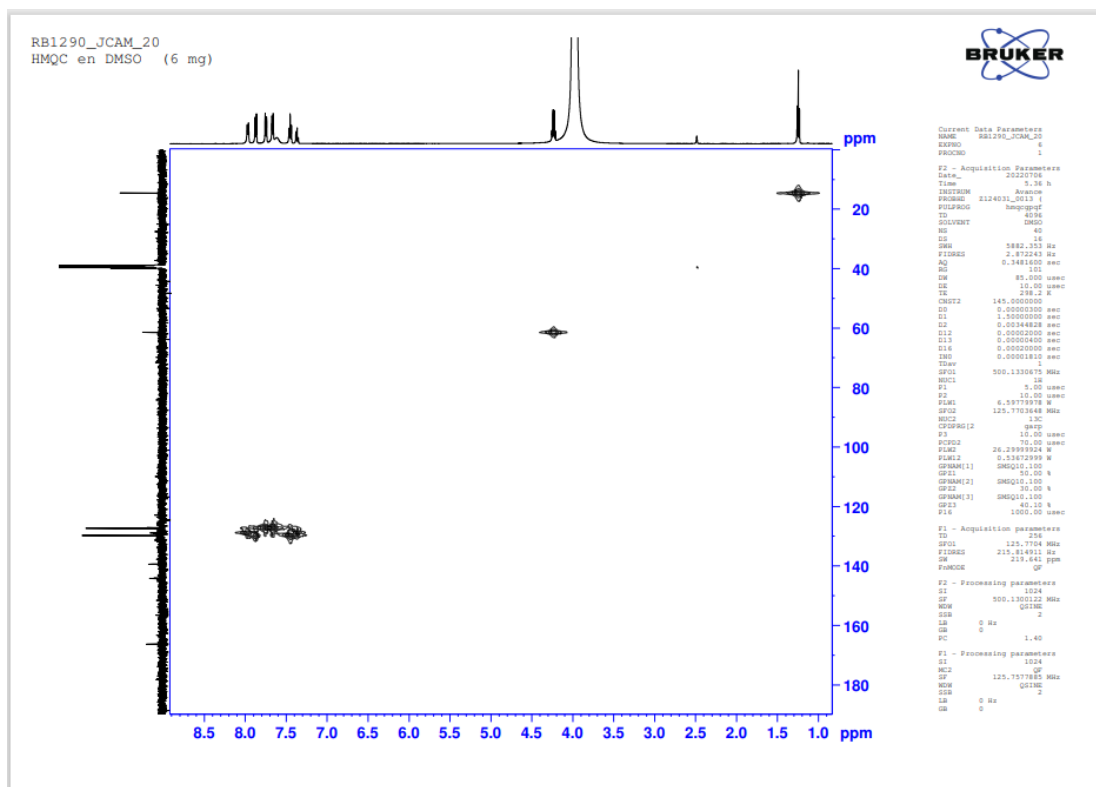
S39

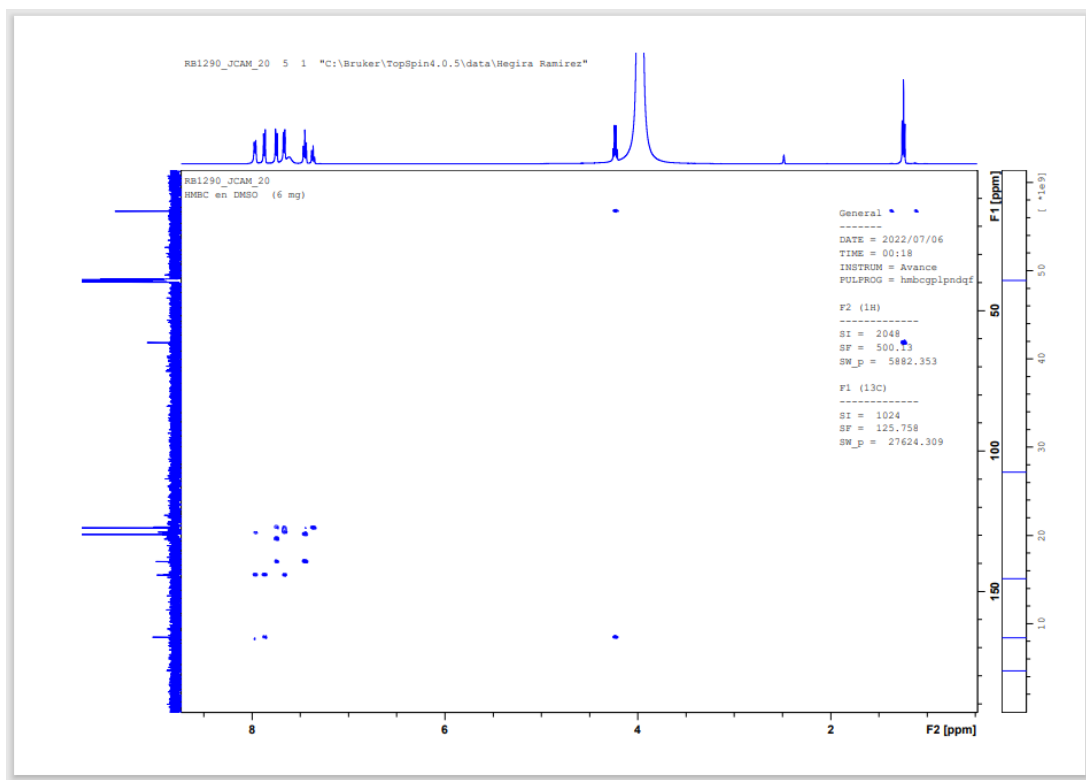


S40

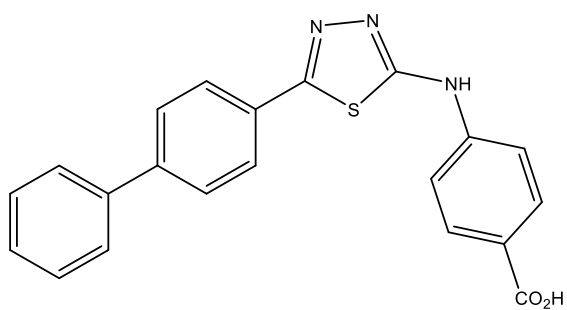


S41

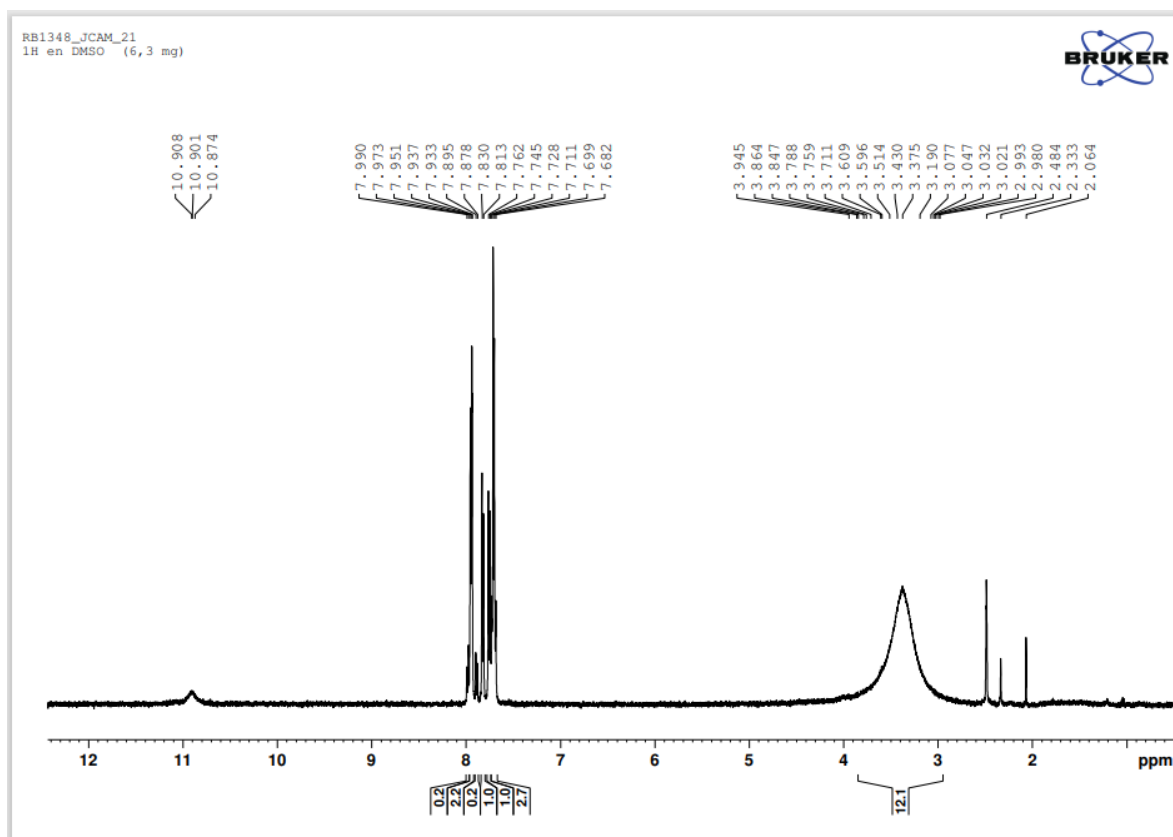




S43

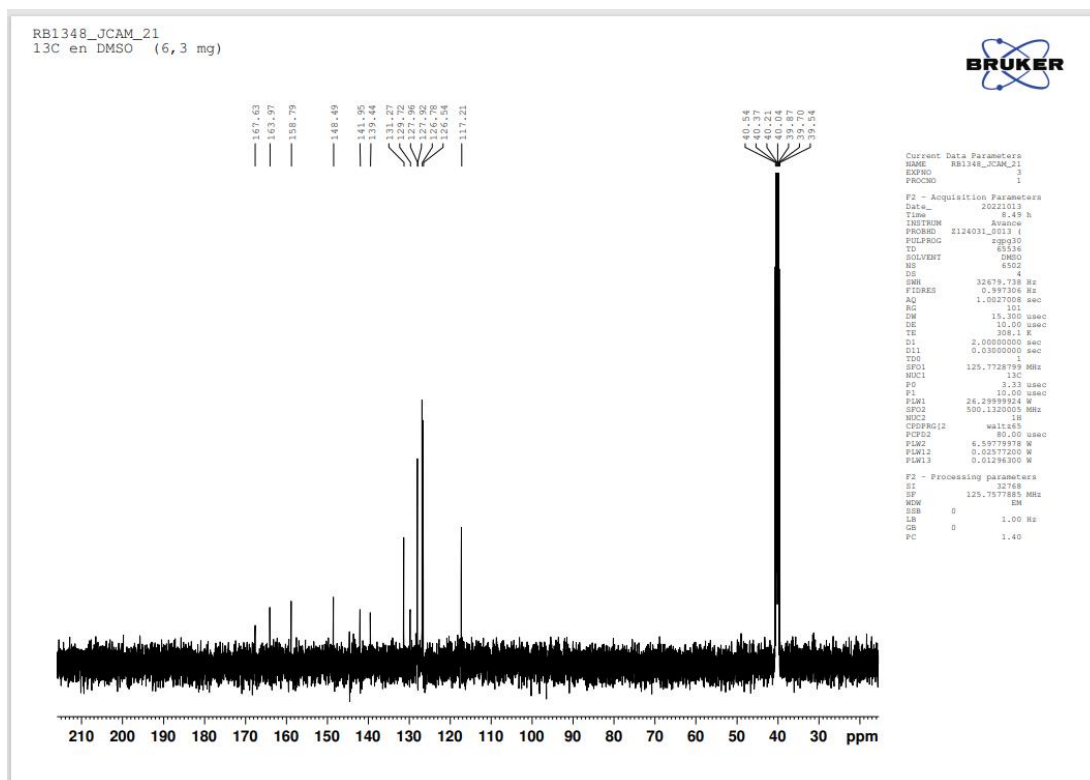


15

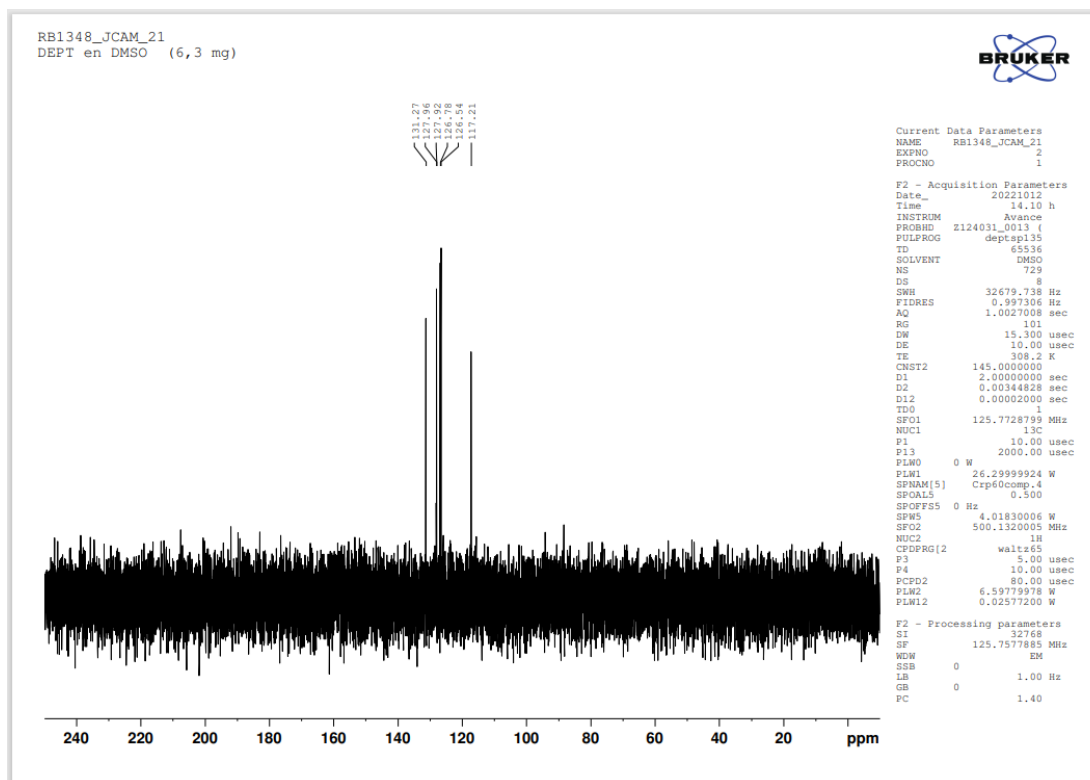




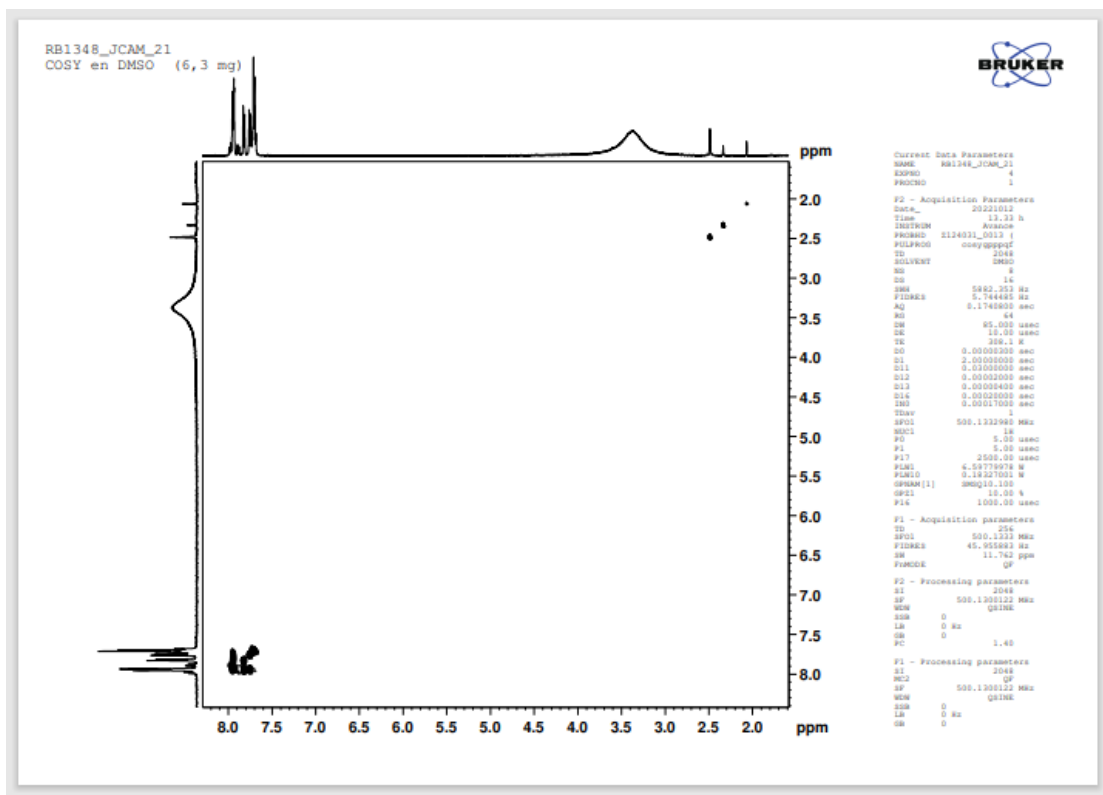
S44



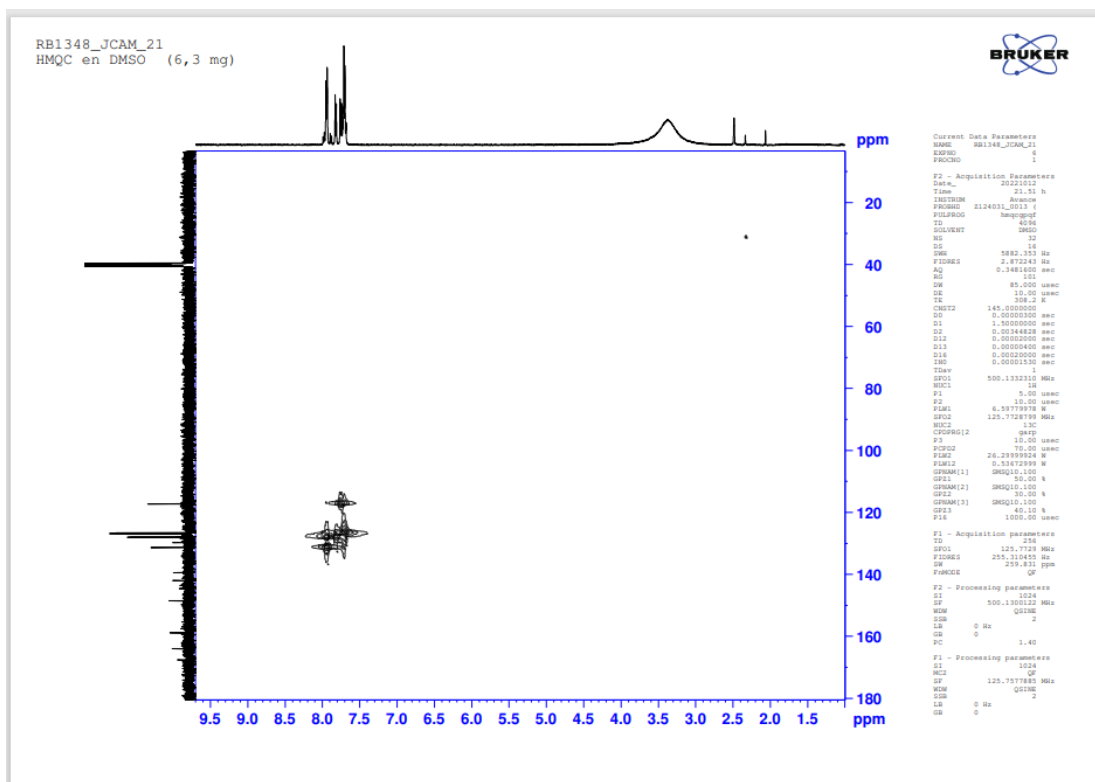
S45



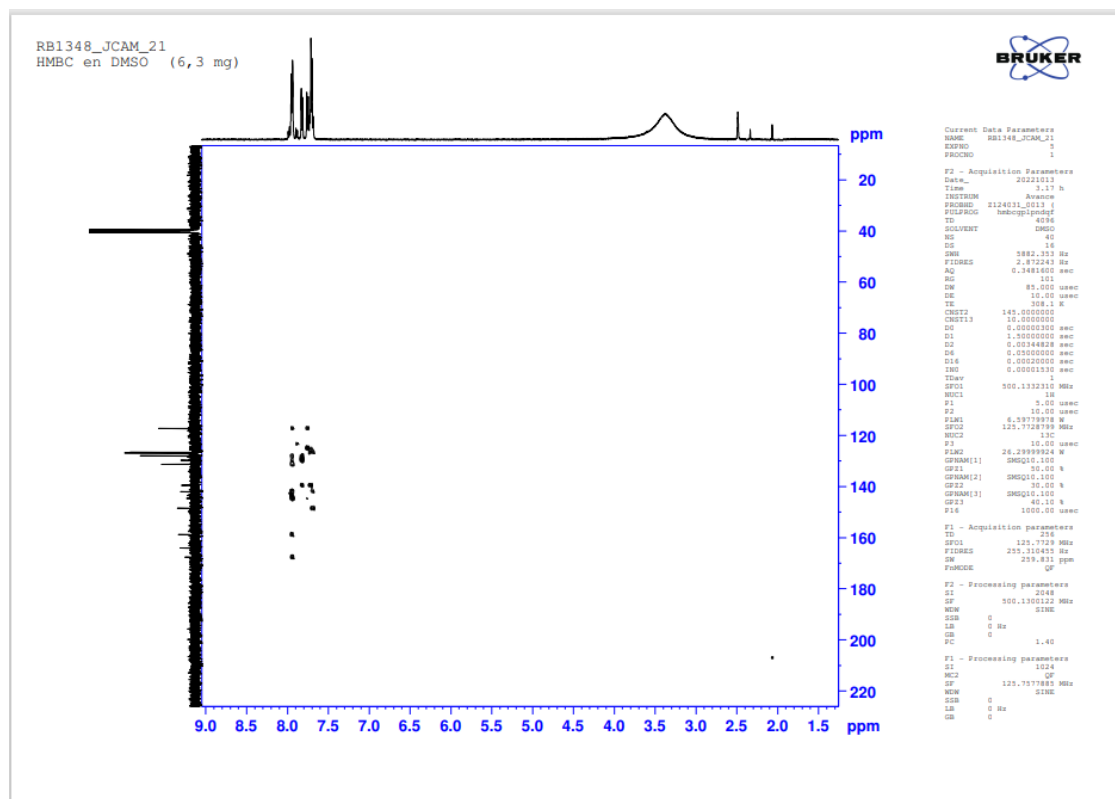
S46



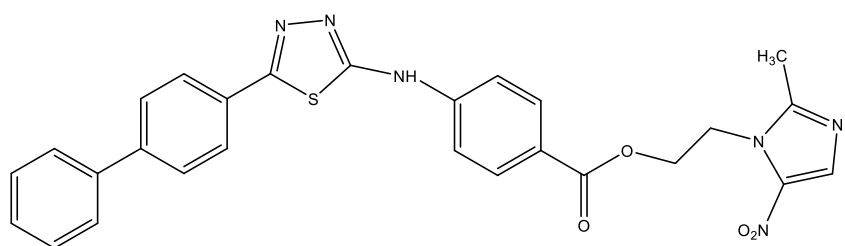
S47



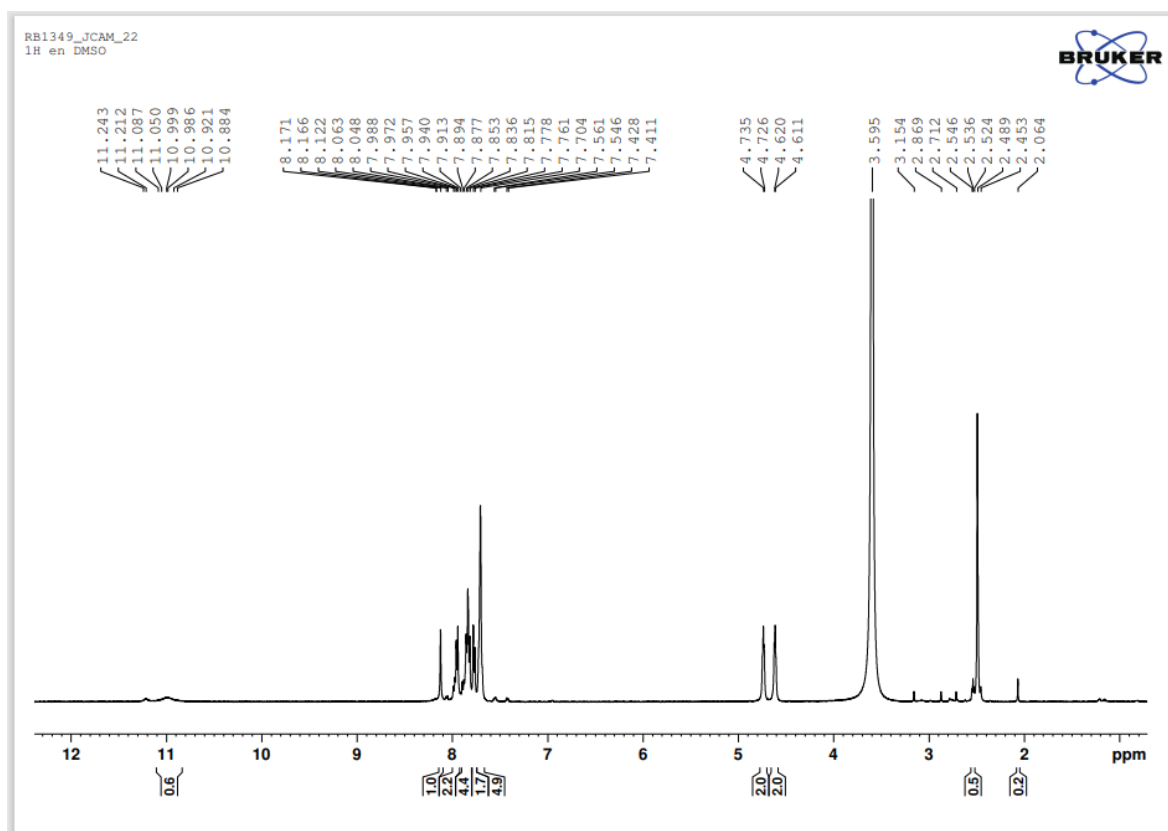
S48



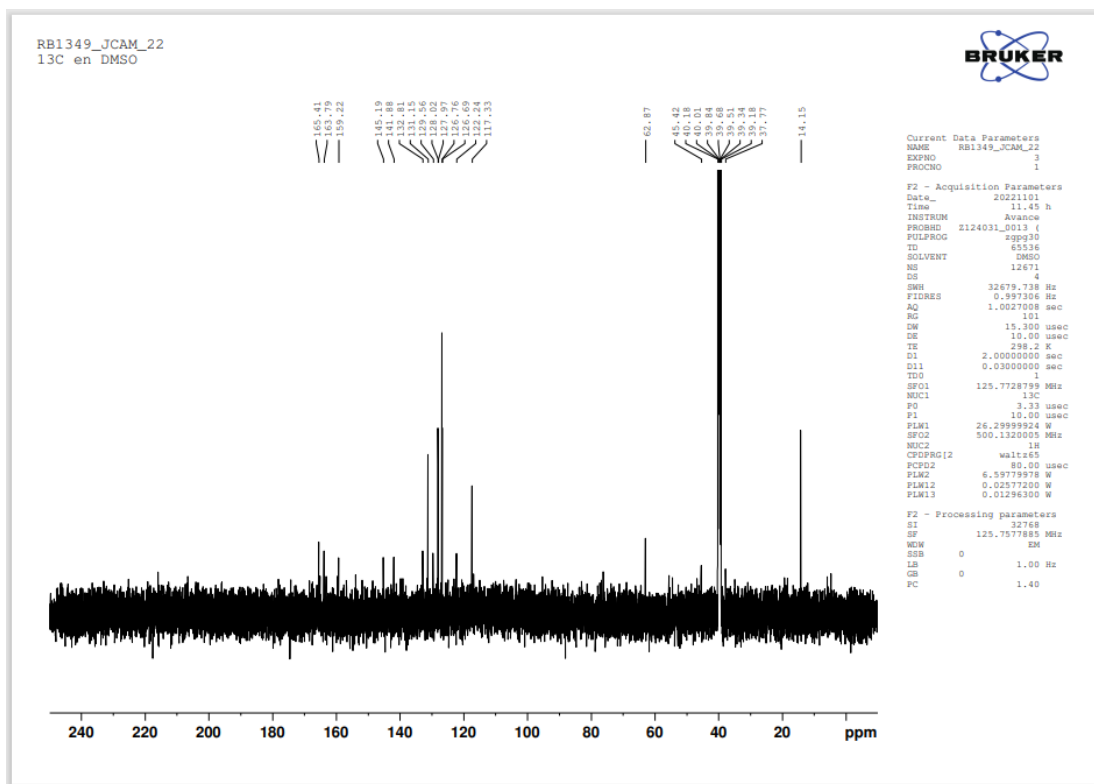
S49



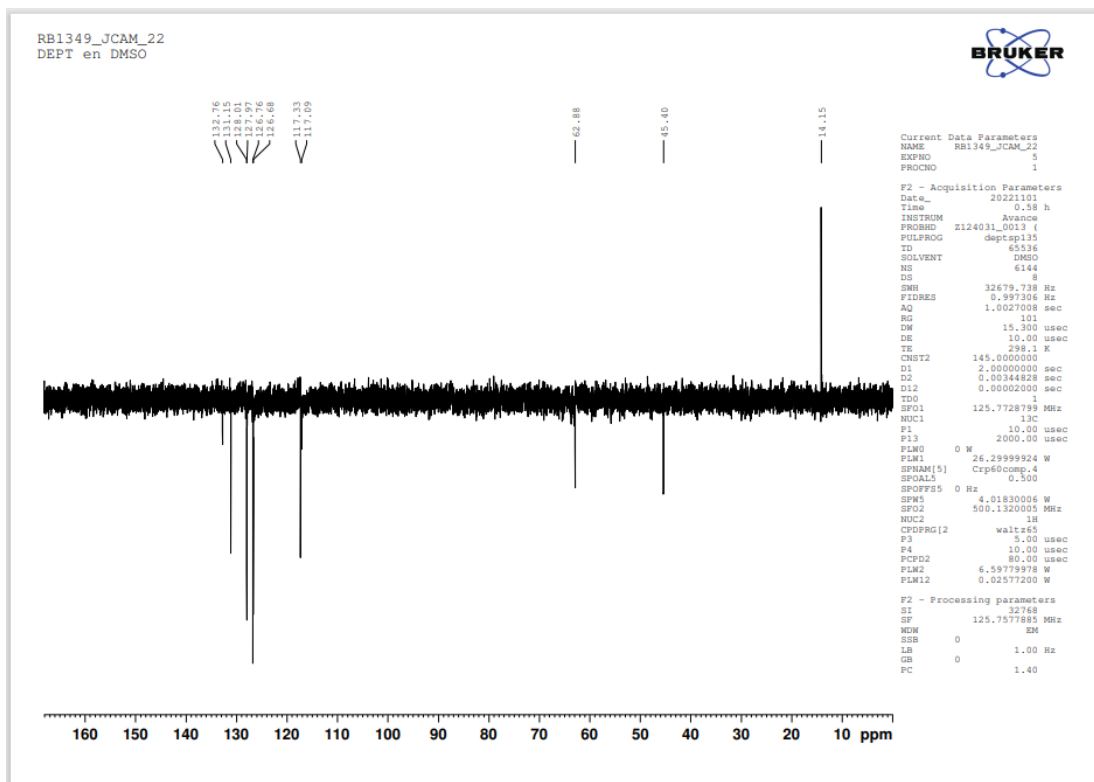
22



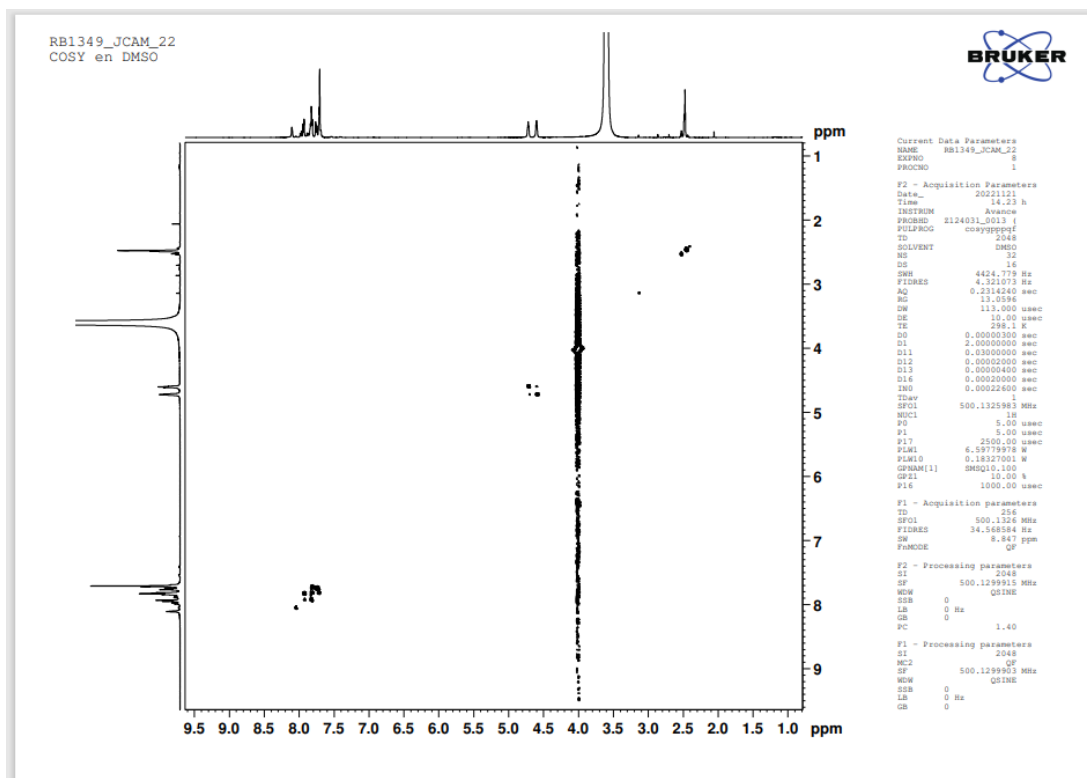
S50



S51



S52



S53

