

New Benzimidazole-1,2,4-Triazole Hybrid Compounds: Synthesis, Anticandidal Activity and Cytotoxicity Evaluation

Hülya Karaca Gençer , Ulviye Acar Çevik, Serkan Levent, Begüm Nurpelin Sağlık, Büşra Korkut, Yusuf Özkay, Sinem Ilgın, Yusuf Öztürk

Spectra for the most active compounds 5w and 5ad.

DOPNALAB

Item	Value
Acquired Date&Time	26.01.2017 11:24:21
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\Serkan\tu serisi\tu-431.ispd
Spectrum name	tu-431
Sample name	tu-43
Sample ID	
Option	
Comment	
No. of Scans	10
Resolution	4 [cm-1]
Apodization	Happ-Genzel

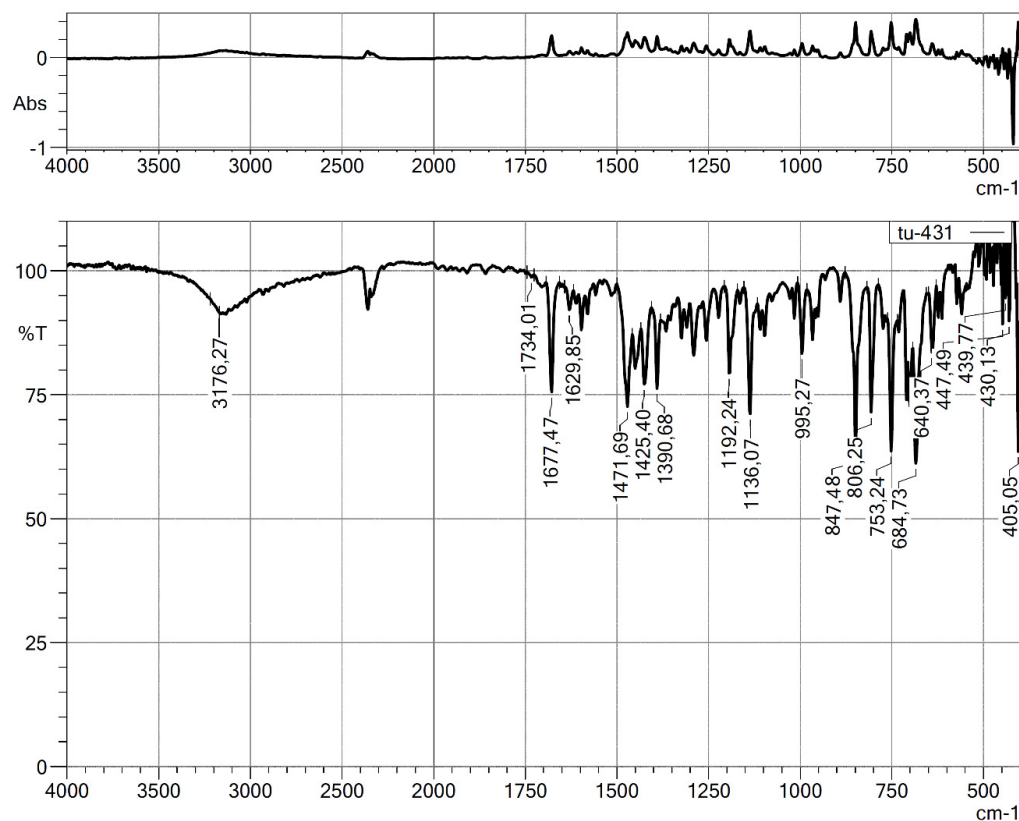


Figure SI-1. IR spectra of compound 5w.

Data File: C:\LabSolutions\Data\Analiz\lac\ TU-43_61.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	17	19	O	2	1	3	Cl	1	0	3	H
C	4	22	40	F	1	0	2	Br	1	0	1	
N	3	5	6	S	2	1	1					

Error Margin (ppm): 5

DBE Range: 17.0 - 30.0

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: yes

Use MSn Info: no

Max Isotopes: 3

Isotope RI (%): 1.00

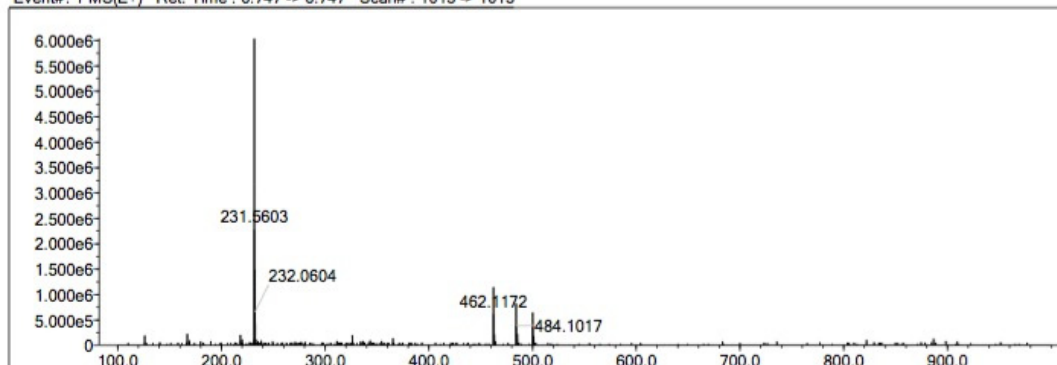
Isotope Res: 10000

MSn Iso RI (%): 10.00

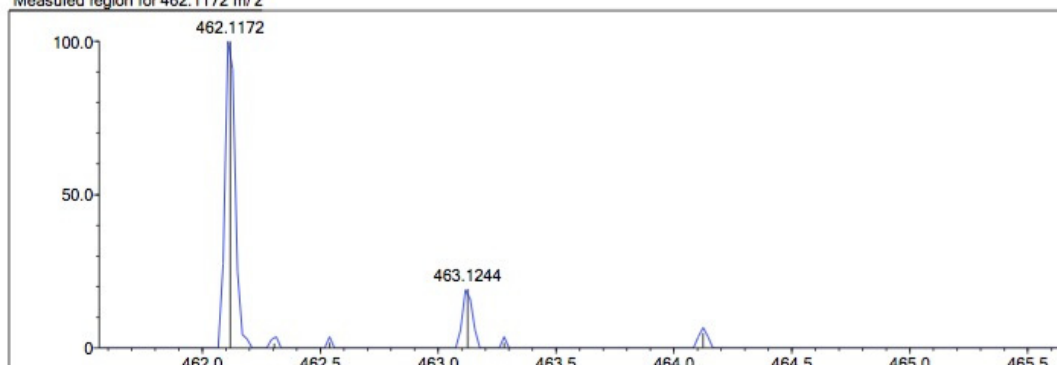
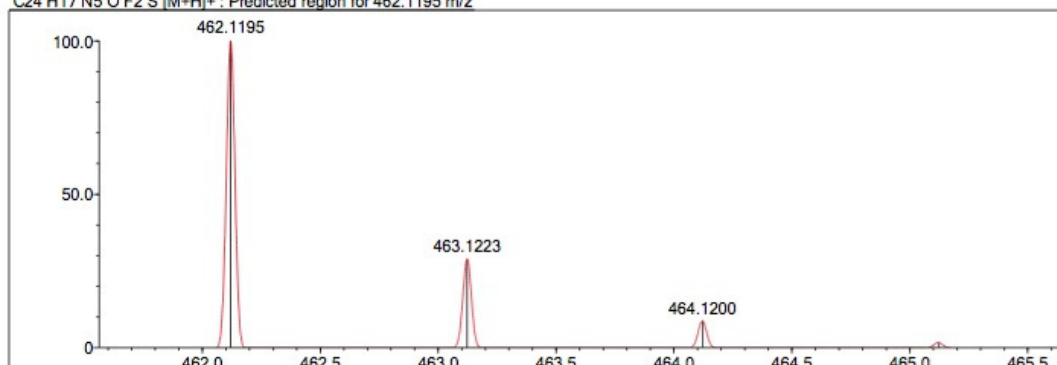
MSn Logic Mode: AND

Max Results: 500

Event#: 1 MS(E+) Ret. Time : 6.747 -> 6.747 Scan# : 1013 -> 1013



Measured region for 462.1172 m/z

C24 H17 N5 O F2 S [M+H]⁺: Predicted region for 462.1195 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	58.68	C24 H17 N5 O F2 S	[M+H] ⁺	462.1172	462.1195	-2.3	-4.98	65.17	18.0

Figure SI-2. HRMS spectra of compound **5w**.

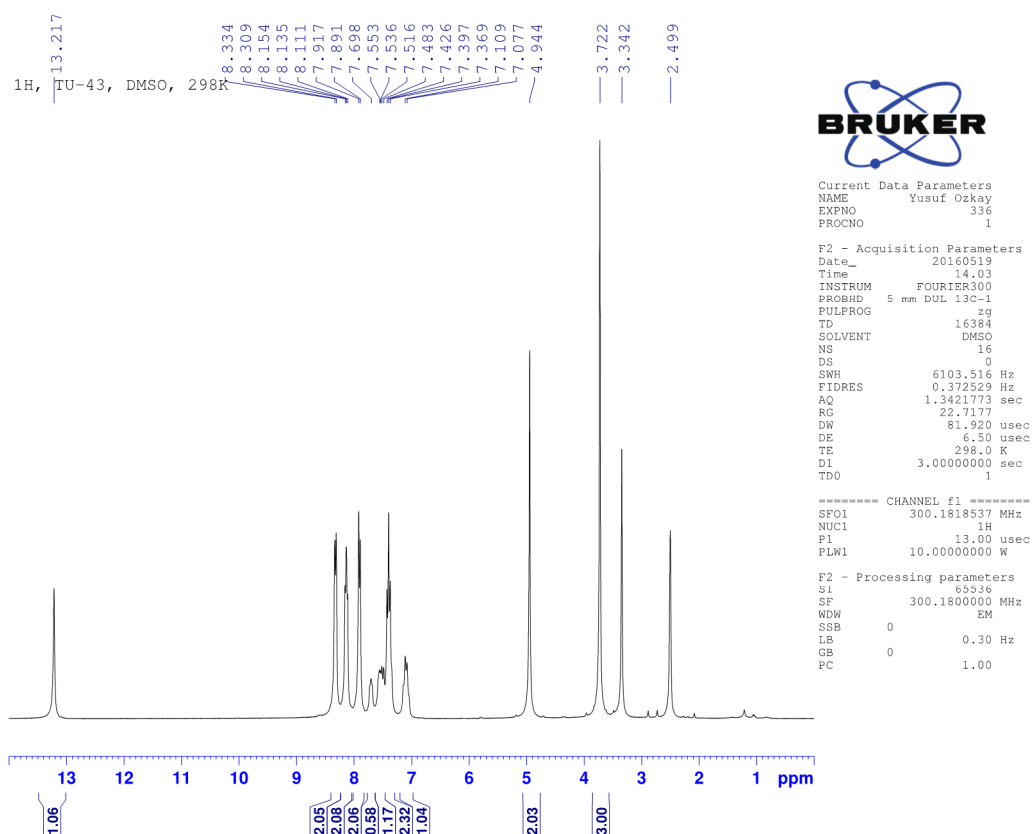


Figure SI-3. ¹H-NMR spectrum of compound **5w**.

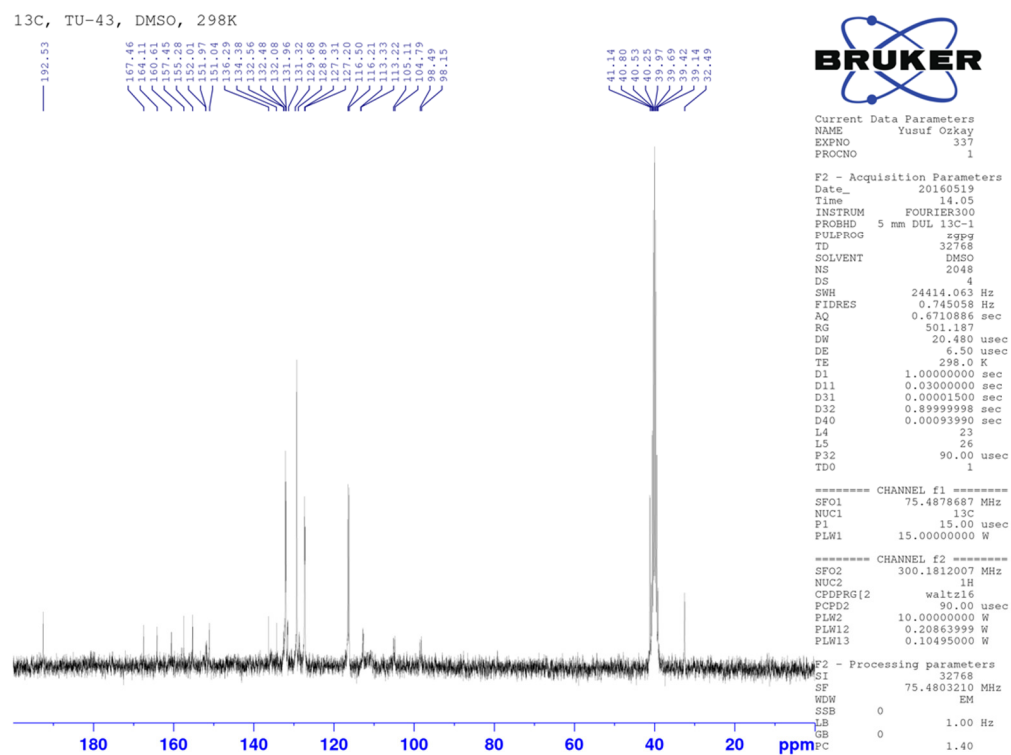


Figure SI-4. ¹³C-NMR spectra of compound **5w**.

DOPNALAB

Item	Value
Acquired Date&Time	26.01.2017 11:45:58
Acquired by	System Administrator
Filename	C:\Users\dopnalab\Desktop\Serkan\tu serisi\tu-561.ispd
Spectrum name	tu-561
Sample name	tu-56
Sample ID	
Option	
Comment	
No. of Scans	10
Resolution	4 [cm-1]
Apodization	Happ-Genzel

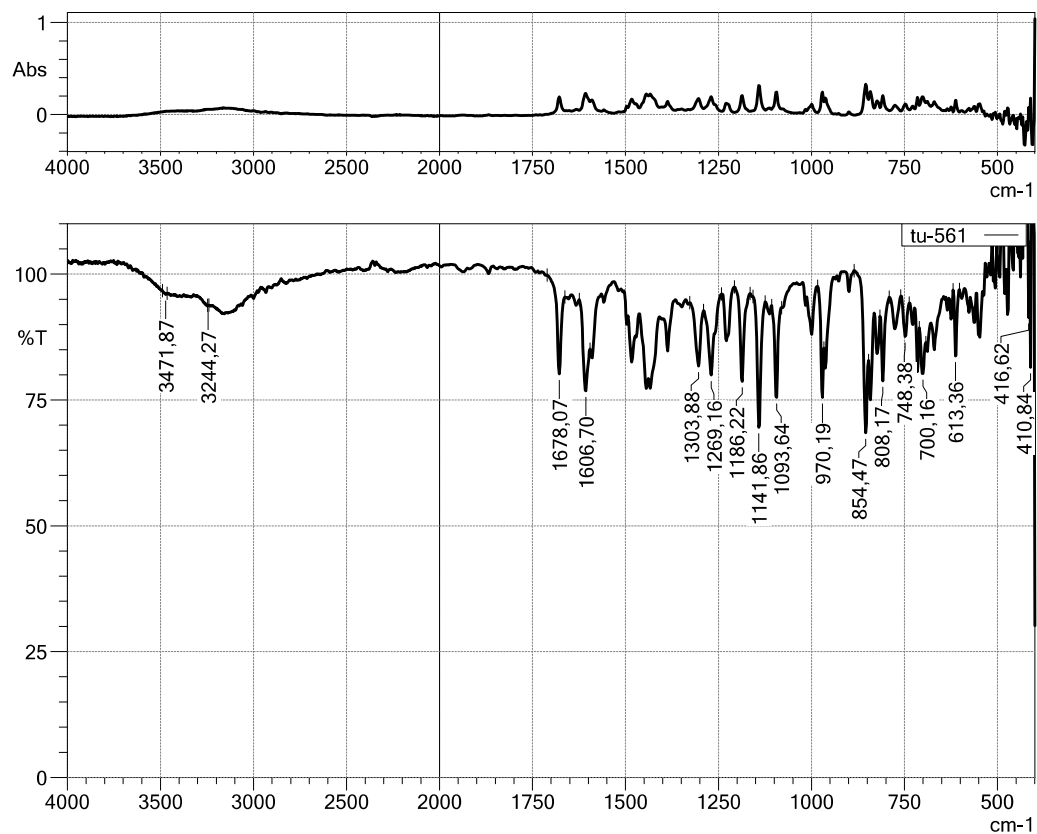


Figure SI-5. IR spectra of compound **5ad**.

Data File: C:\LabSolutions\Data\Analiz\aac\ TU-56_77.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	15	25	O	2	1	3	Cl	1	0	3	H
C	4	22	40	F	1	0	3	Br	1	0	1	
N	3	5	6	S	2	1	1					

Error Margin (ppm): 5

DBE Range: 17.0 - 21.0

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: yes

Use MSn Info: no

Max Isotopes: 3

Isotope RI (%): 1.00

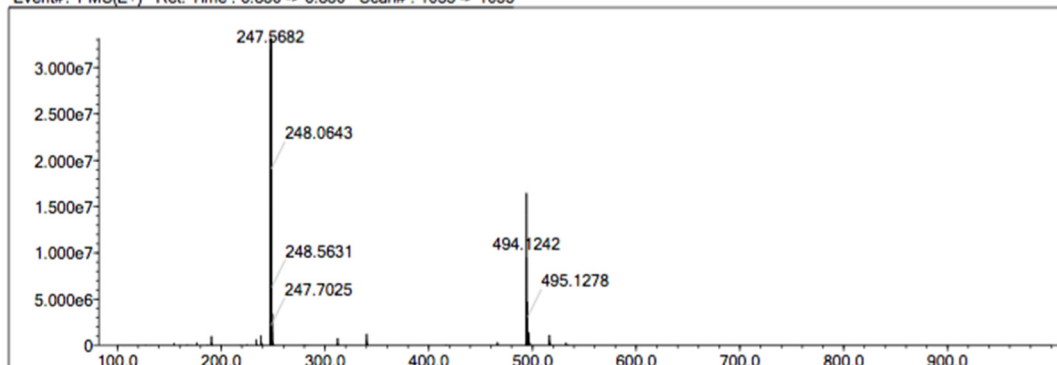
Isotope Res: 10000

MSn Iso RI (%): 10.00

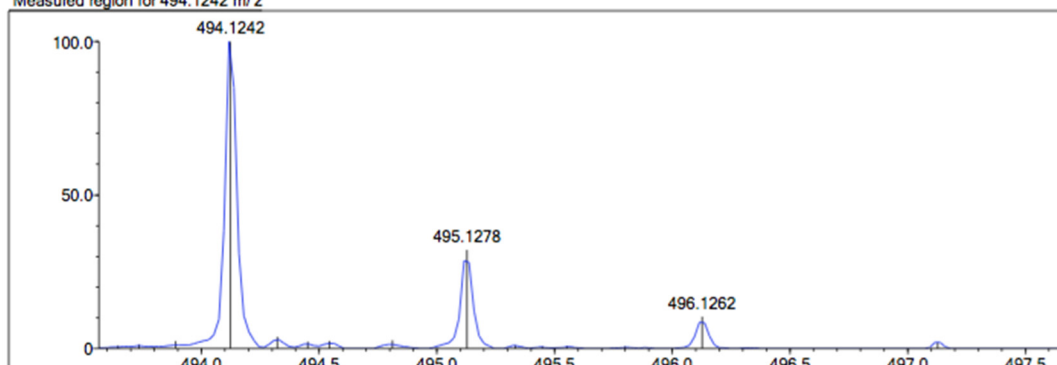
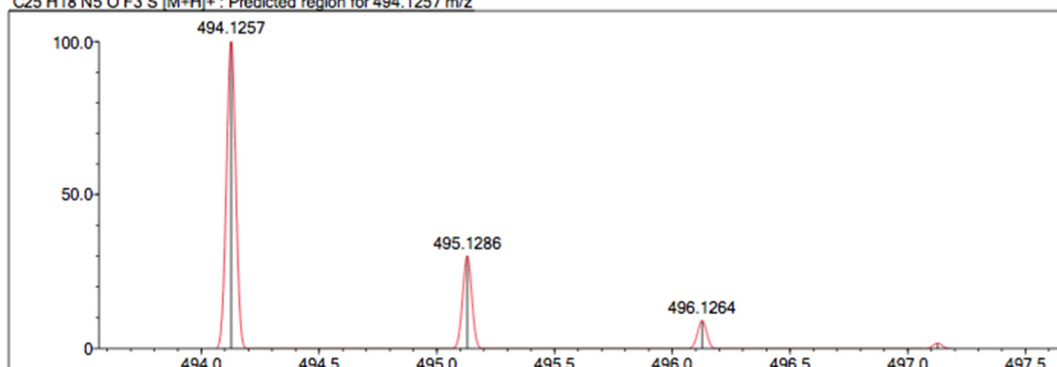
MSn Logic Mode: AND

Max Results: 500

Event#: 1 MS(E+) Ret. Time : 6.880 -> 6.880 Scan# : 1033 -> 1033



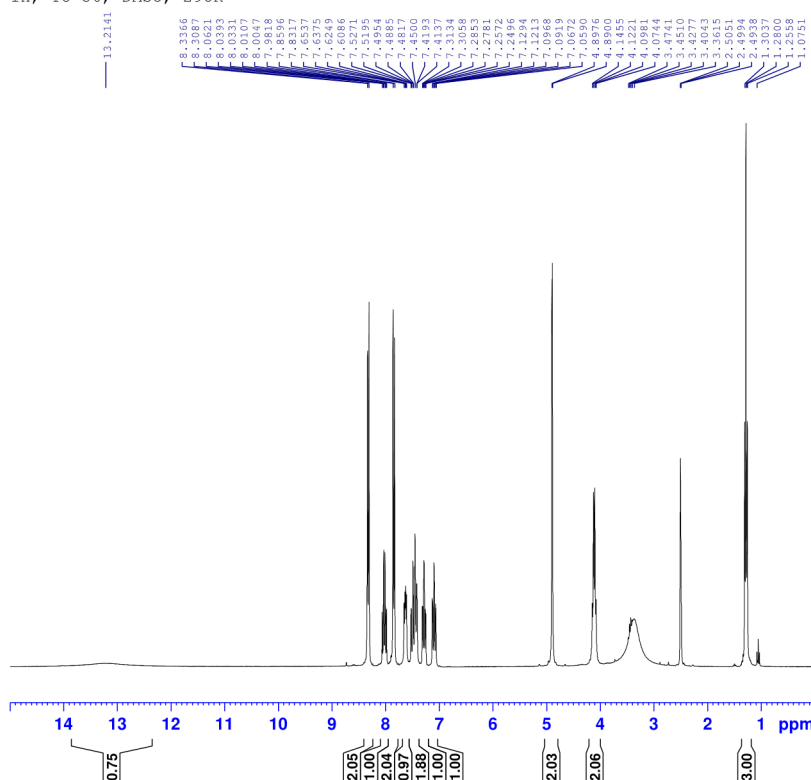
Measured region for 494.1242 m/z

C25 H18 N5 O F3 S [M+H]⁺ : Predicted region for 494.1257 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	84.53	C25 H18 N5 O F3 S	[M+H] ⁺	494.1242	494.1257	-1.5	-3.04	89.07	18.0

Figure SI-6. HRMS spectra of compound **5ad**.

¹H, TU-56, DMSO, 298K



Current Data Parameters
NAME Yusuf Ozkay
EXPNO 360
PROCNO 1

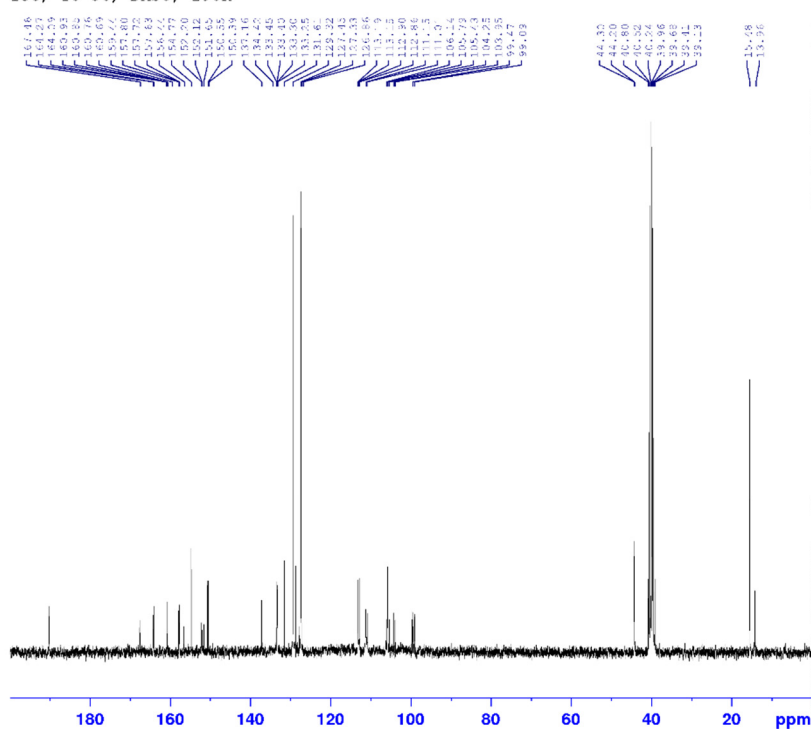
F2 - Acquisition Parameters
Date_ 20160521
Time 14.05
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg
TD 16384
SOLVENT DMSO
NS 16
DS 0
SWH 6103.516 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 17.162
DW 81.920 usec
DE 6.50 usec
TE 297.9 K
D1 3.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1818537 MHz
NUC1 ¹H
P1 13.00 usec
PLW1 10.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1800000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure SI-7. ¹H-NMR spectrum of compound **5ad**.

¹³C, TU-56, DMSO, 298K



Current Data Parameters
NAME Yusuf Ozkay
EXPNO 361
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160521
Time 4.07
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 7648
DS 0
SWH 24414.063 Hz
FIDRES 0.745358 Hz
AQ 0.6710386 sec
RG 501.87
DW 20.480 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
D11 0.30000000 sec
D12 0.30001500 sec
D32 0.89999998 sec
D40 0.00033990 sec
L4 23
L5 25
P32 90.00 usec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4878687 MHz
NUC1 ¹³C
P1 15.00 usec
PLW1 15.00000000 W

===== CHANNEL f2 =====
SFO2 300.1812007 MHz
NUC2 ¹H
TD0RG[2] 8816.6
FIDRES 0.30000000 sec
P1 10.00000000 W
PLW2 0.20863999 W
PLW3 0.10495000 W

F2 - Processing parameters
SI 32768
SF 75.4803210 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure SI-8. ¹³C-NMR spectra of compound **5ad**.