

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

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

DOPNALAB

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Acquired Date&Time	26.01.2017 11:24:21
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Sample name	tu-43
Sample ID	
Option	
Comment	
No. of Scans	10
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Apodization	Happ-Genzel

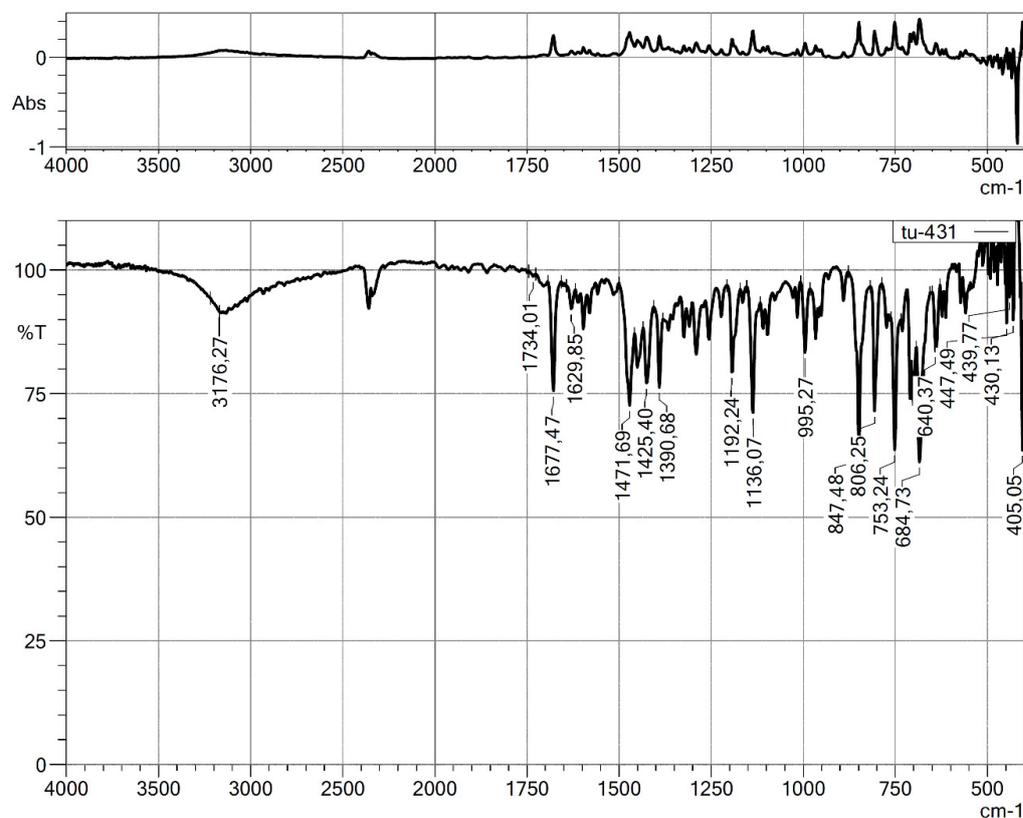


Figure SI-1. IR spectra of compound 5w.

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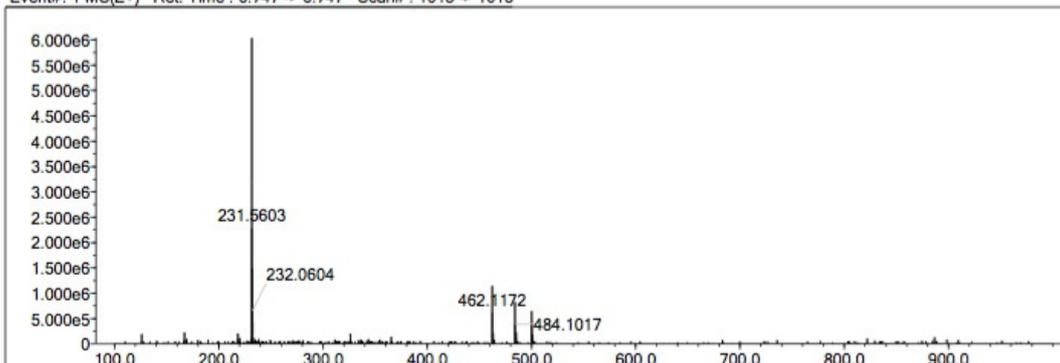
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H	1	17	19	O	2	1	3	Cl	1	0	3	H
C	4	22	40	F	1	0	2	Br	1	0	1	
N	3	5	6	S	2	1	1					

Error Margin (ppm): 5
 HC Ratio: unlimited
 Max Isotopes: 3
 MSn Iso RI (%): 10.00

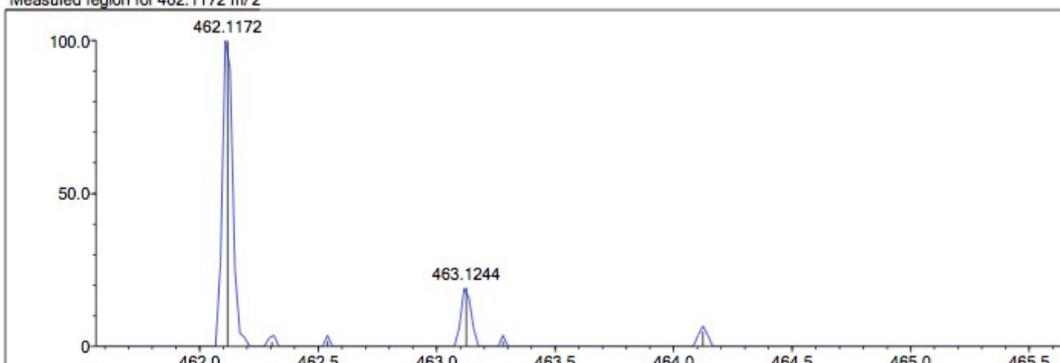
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Electron Ions: both
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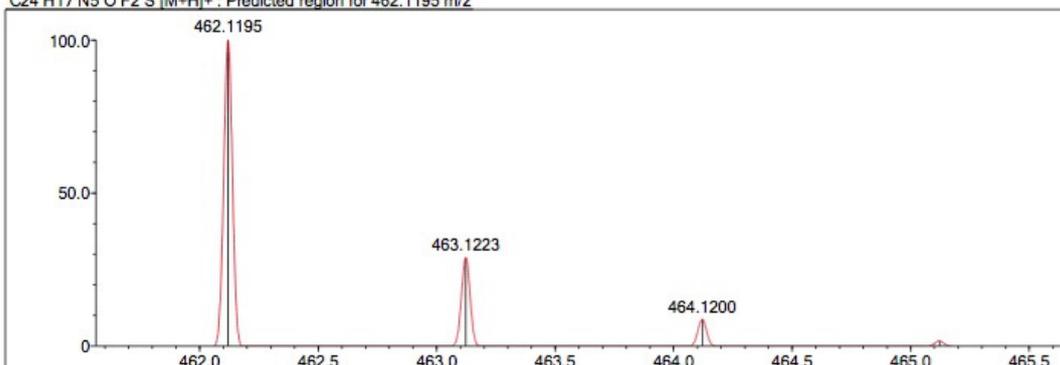
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Measured region for 462.1172 m/z



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.

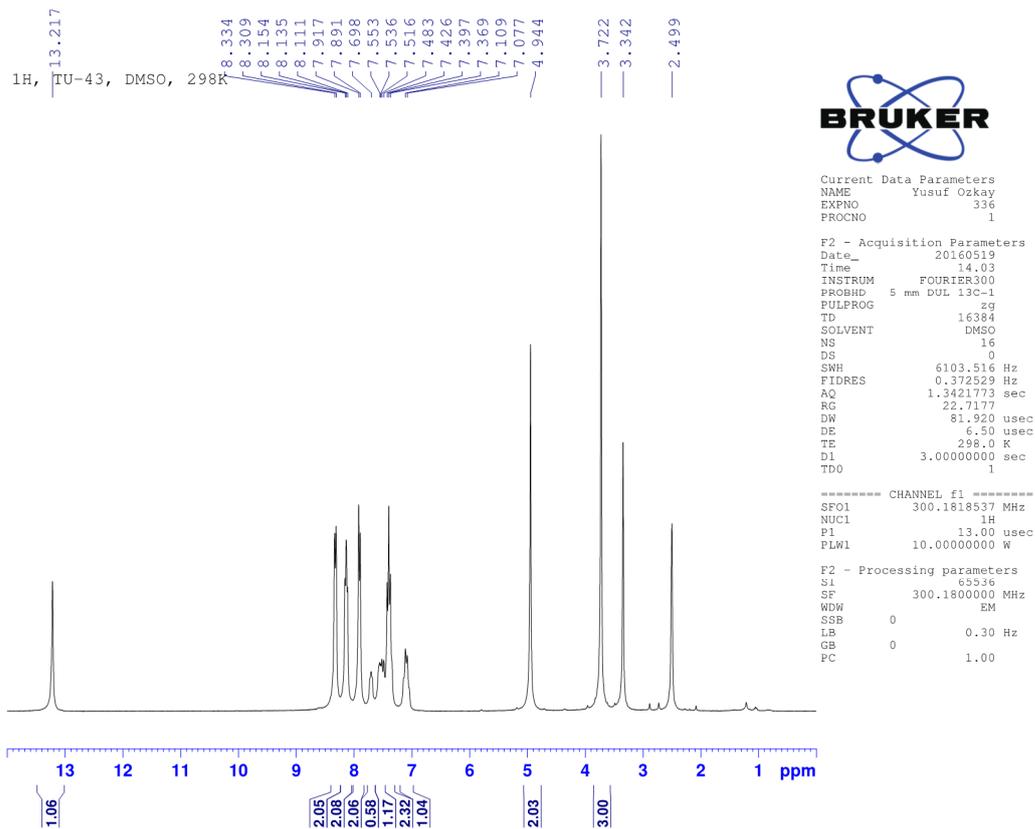


Figure SI-3. ¹H-NMR spectrum of compound 5w.

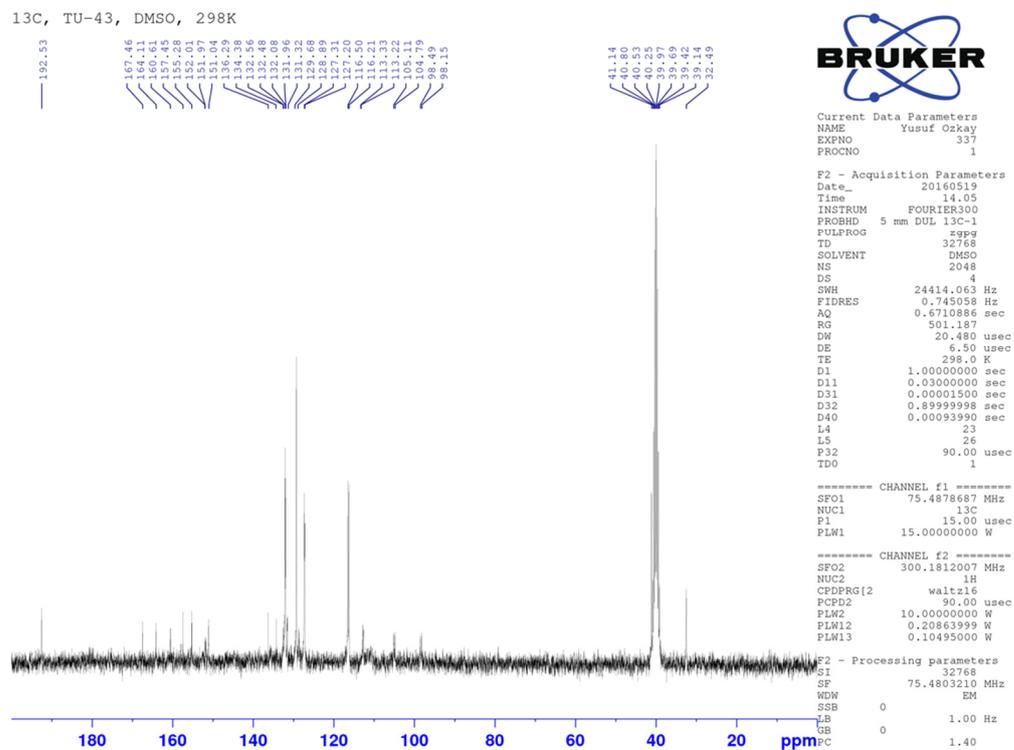


Figure SI-4. ¹³C-NMR spectra of compound 5w.

DOPNALAB

Item	Value
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Sample ID	
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Resolution	4 [cm-1]
Apodization	Happ-Genzel

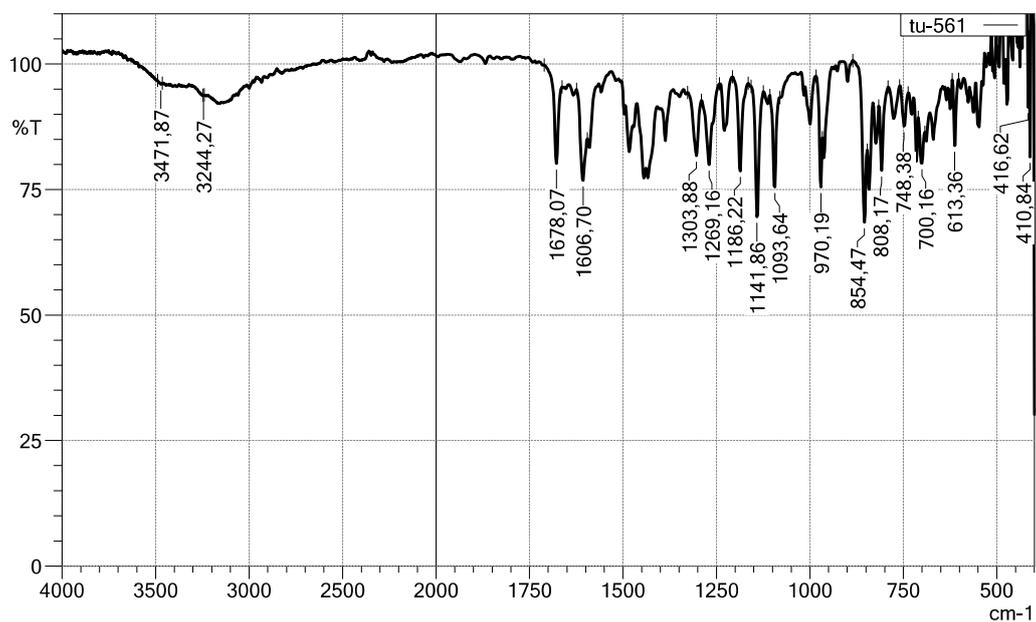
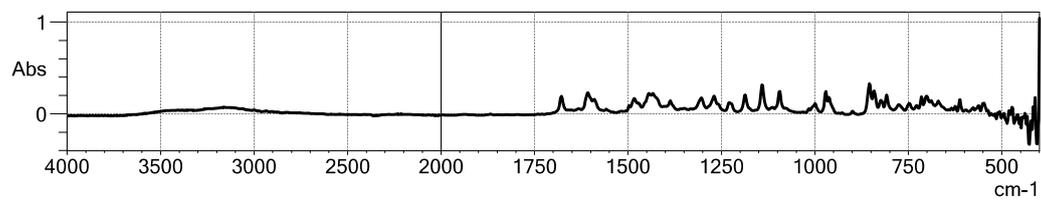


Figure SI-5. IR spectra of compound **5ad**.

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

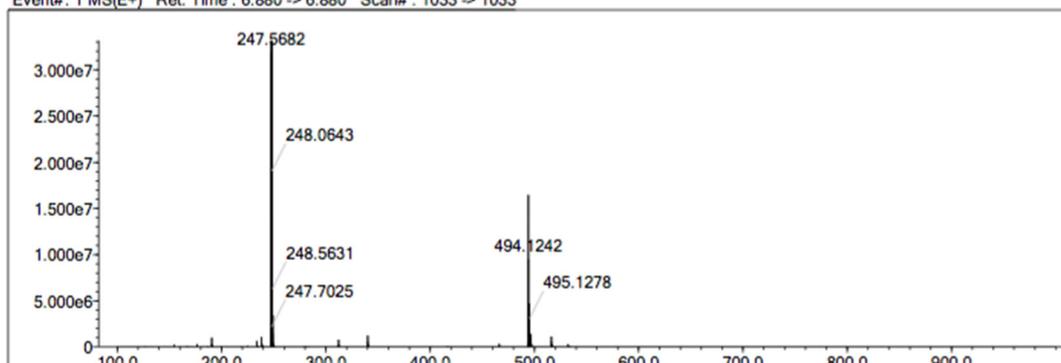
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H	1	15	25	O	2	1	3	Cl	1	0	3	H
C	4	22	40	F	1	0	3	Br	1	0	1	
N	3	5	6	S	2	1	1					

Error Margin (ppm): 5
 HC Ratio: unlimited
 Max Isotopes: 3
 MSn Iso RI (%): 10.00

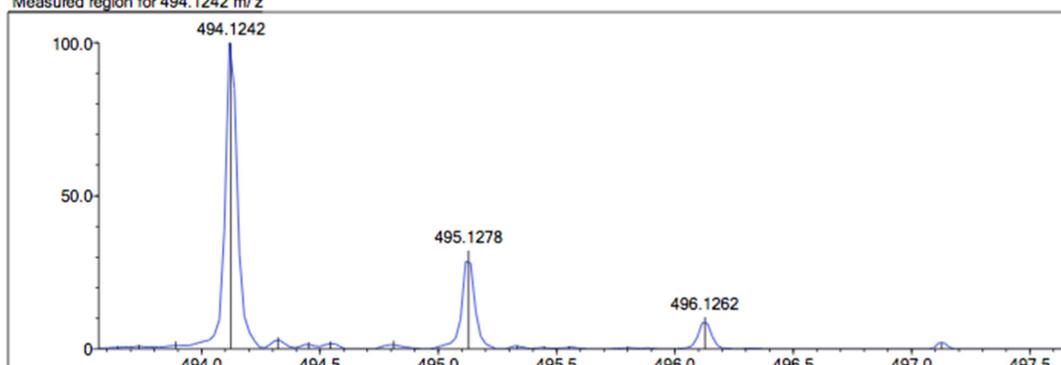
DBE Range: 17.0 - 21.0
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 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
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 Max Results: 500

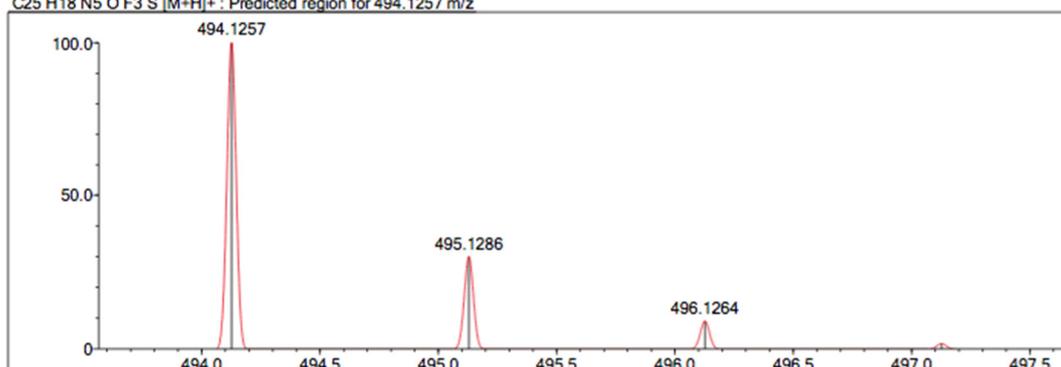
Event#: 1 MS(E+) Ret. Time : 6.880 -> 6.880 Scan# : 1033 -> 1033



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

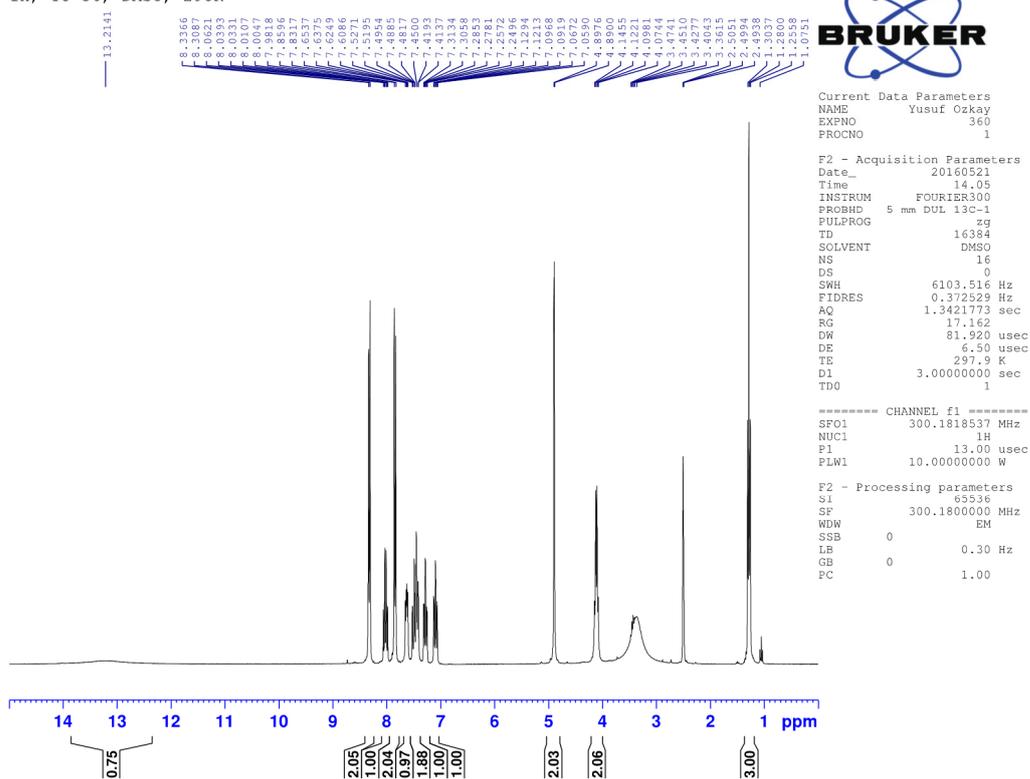


Figure SI-7. ¹H-NMR spectrum of compound 5ad.

¹³C, TU-56, DMSO, 298K

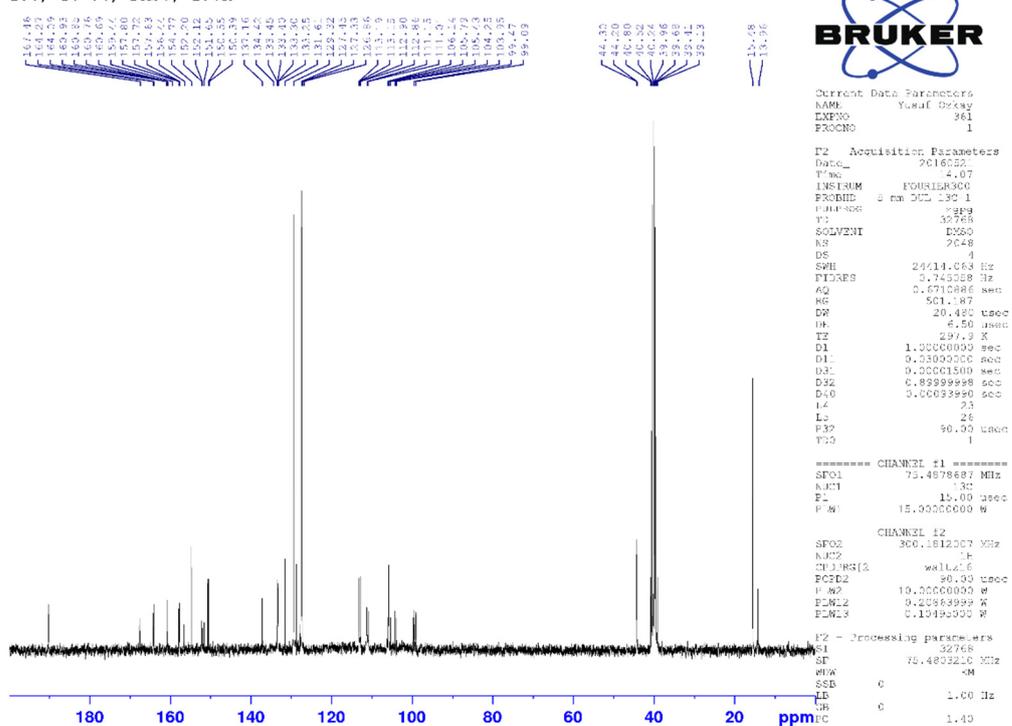


Figure SI-8. ¹³C-NMR spectra of compound 5ad.