

Supporting Information

Design, synthesis, biological assessment, and *In Silico* ADME prediction of some new 2-(4-(methyl sulfonyl) phenyl) benzimidazoles as selective cyclooxygenase-2 inhibitors

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1. General Information:

Melting points were detected by Tomas-Hoover capillary melting apparatus without any correction. All solvents, chemical, and reagent supplied from Aldrich chemical company (Milwaukee, WI), and El Nasr pharmaceutical chemical companies, Cairo, Egypt. Infrared (IR) spectra was monitored as films on KBr discs using Shimadzu FT-IR 8400S spectrophotometer and values were presented as cm^{-1} . Purity of the synthesized compounds, and Reaction's progress were checked by using precoated thin layer chromatography (TLC) silica gel plates 60F254 with thickness of 0.25 supplied from MERCK, Darmstadt, Germany. UV λ_{max} was used to monitor reaction process. ^{13}C NMR and ^1H NMR spectra were carried out on a Bruker avance III 400 MHz spectrophotometer, faculty of pharmacy, Benisuef University and Mansoura University, Egypt in dimethyl sulfoxide (DMSO-d_6) or D_2O as a solvent. Chemical shift was estimated in ppm on δ scale and J (Coupling constant) was estimated in Hertz. Microanalysis for C, H, and N were performed on perkin-Elmer 2400 analyzer (perkin-Elmer, Norwalk, CT. USA) at the regional center for mycology and Biotechnology, Al-azhar University, Egypt. All results were with in $\pm 0.4\%$ of the theoretical values.

Table

Compd. No	¹ H-NMR(ppm)				S1: ¹ H- NMR chemic al shifts and the ratios of peak intensit ies of selecte d peaks in compo
	N=CH ₃ (Ratio %)	N-CH ₂ (Ratio %) ^a	N=CH (Ratio %)	CONH(Ratio %)	
11a	-	5.14, 5.62 (26:74)	8.12, 8.28 (74:26)	11.83, 12.01 (74:26)	
11b	-	5.13, 5.62 (26:74)	8.12, 8.26 (74:26)	11.88, 12.07 (74:26)	
11c	-	5.11, 5.58 (26:74)	8.10, 8.12 (74:26)	11.60, 11.99 (74:26)	
11d	-	5.13, 5.62 (26:74)	8.11, 8.26 (74:26)	11.84, 12.03 (74:26)	
11e	-	5.11, 5.64 (26:74)	8.13, 8.20 (74:26)	11.83, 11.98 (74:26)	
11f	-	5.61, 5.63 (23:77)	8.12, 8.27 (77:23)	11.91, 12.10 (77:23)	
11g	-	5.14, 5.51 (24:76)	8.06, 8.25 (76:24)	11.70, 11.82 (76:24)	
11h	-	5.16, 5.65 (25:75)	8.12, 8.26 (75:25)	11.81, 12.01 (75:25)	
11i	-	5.24, 5.67 (23:77)	8.11, 8.26 (77:23)	11.80, 12.01 (77:23)	
11j	-	5.48, 5.58 (22:78)	8.13, 8.27 (78:22)	11.10, 12.09 (78:24)	
11k	-	5.58, 5.49 (31:69)	8.10, 8.25 (69:31)	11.86, 12.05 (69:31)	
11l	-	5.24, 5.56 (29:71)	8.10, 8.26 (71:29)	11.78, 12.02 (71:29)	
12a	2.37, 2.26 (77:23)	5.28, 5.64 (23:77)	-	10.98, 11.08 (23:77)	
12b	2.29, 2.50 (69:31)	5.24, 5.59 (31:69)	-	11.09, 12.02 (31:69)	
12c	2.29, 2.35 (77:23)	5.28, 5.57 (23:77)	-	10.94, 11.07 (31:69)	
12d	2.25, 2.23 (78:22)	4.93, 5.69 (22:78)	-	10.99, 11.18 (22:78)	
12f	2.47, 2.56 (62:38)	5.26, 6.64 (38:62)	-	11.07, 11.12 (38:62)	

unds

^a)Approximate ratio as determined from peak integration.

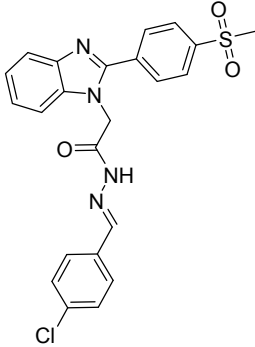
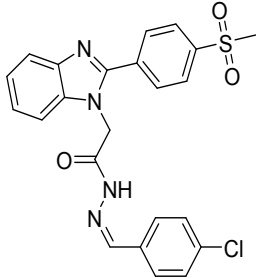
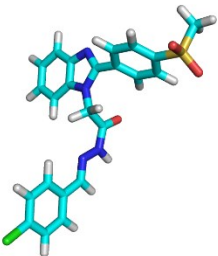
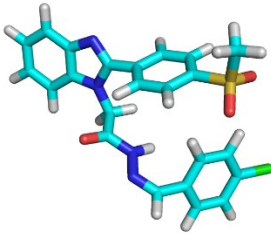
Isomer	E isomer	Z isomer
2D	 <p>(<i>E</i>)-<i>N'</i>-(4-chlorobenzylidene)-2-(2-(4-(methylsulfonyl)phenyl)-1<i>H</i>-benzo[d]imidazol-1-yl)acetohydrazide</p>	 <p>(<i>Z</i>)-<i>N'</i>-(4-chlorobenzylidene)-2-(2-(4-(methylsulfonyl)phenyl)-1<i>H</i>-benzo[d]imidazol-1-yl)acetohydrazide</p>
3D Minimized		
Total Energy	96.170	112.180
E_{Str} (bond stretch energy)	4.955	4.934
E_{Ang} (bond angle bend energy)	10.320	10.884
E_{Stb} (stretch-bend energy)	0.276	0.354
E_{Oop} (out-of-plane energy)	0.084	0.107
E_{Tor} (torsion energy)	3.631	12.570
E_{Vdw} (van der Waals energy)	53.254	49.306
E_{Ele} (electrostatics energy)	23.650	34.026

Table S2: The values of the total energies of E and Z isomers of compound 11b^a

$$^a \text{ Total energy} = E_{\text{Str}} + E_{\text{Ang}} + E_{\text{Stb}} + E_{\text{Oop}} + E_{\text{Tor}} + E_{\text{Vdw}} + E_{\text{Ele}}$$

Table S3: Ulcer index, ulcer number, and preventive index of the most potent AI Compounds and relative ulcerogenicity to reference drugs indomethacin and celecoxib.

Group Name	Ulcer index (mm)			Ulcer number			Preventive Index (%) % to normal control
	Mean	% to Indomethacin	% to Celecoxib	Mean	% to Indomethacin	% to Celecoxib	
Normal Control	0	0	0	0	0	0	100
Indomethacin (Ulcer Control)	13	100	371.4	8	100	200	
Celecoxib	3.5	26.9	100	4	50	100	73.0
11b	0.83	6.3	23.7	1	12.5	25	93.5
12d	1	7.6	28.5	0.33	4.1	8.2	92.3
11k	4.5	34.6	128.5	2.67	33.3	66.7	65.3

Compound	Affinity Kcal/mol	Distance (in Å) from main residue		Functional Group	Interaction
Celecoxib	-17.6675	3.76	Ser353	Diazole ring	pi-H
		2.84	Arg120	-SO ₂ NH ₂ -	H-acceptor
11b	-16.9546	4.09	Ala527	Diazole ring	pi-H
		3.26	Arg120	-SO ₂ CH ₃	H-acceptor
12b	-15.3202	4.04	Ala527	Diazole ring	pi-H

Table S4: Data of molecular modeling for test compounds, and Celecoxib obtained by docking in COX-2(PDB ID: 1CX2) active site.

		3.18	Ser353	=N-NH	H-acceptor	
		3.28	Arg120	-SO ₂ CH ₃	H-acceptor	
11c	-13.3881	4.36	Gly526	Ph-ring	pi-H	
		3.26	Arg120	-SO ₂ CH ₃	H-acceptor	
11f	-12.5111	3.27	Arg120	-SO ₂ CH ₃	H-acceptor	
11g	-12.1350	3.32	Arg120	-SO ₂ CH ₃	H-acceptor	
12d	-16.0124	4.03	Ala527	Diazole ring	pi-H	
		3.29	Arg120	-SO ₂ CH ₃	H-acceptor	
11j	-13.4163	3.75	Ala527	Diazole ring	pi-H	
		3.31	Arg120	-SO ₂ CH ₃ -	H-acceptor	
11k	-16.1407	4.17	Gly526	Benzo-moiety	pi-H	
		3.99	Ala527	Diazole ring	pi-H	
		3.30	Ser353	=N-NH	H-acceptor	Table
		3.29	Arg120	-SO ₂ CH ₃	H-acceptor	

S5: Physicochemical properties and lipophilicity of the most active compounds predicted by swissADME software.

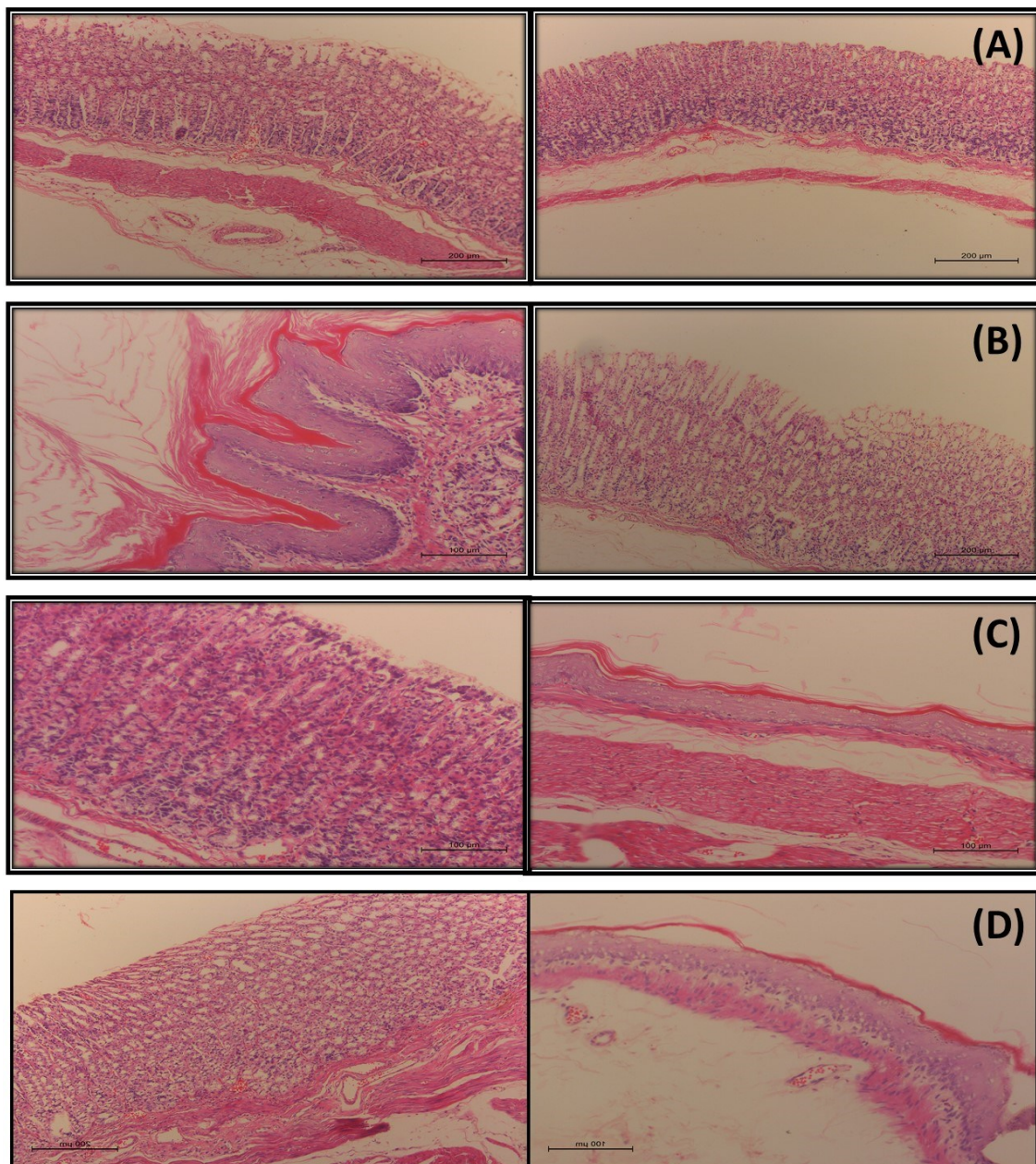
Code	Lipophilicity consensus log P	M.W ^a g/mol	Rot. bond	Physicochemical properties				%ABS ^d
				H-bond acc.	H-bond don.	MR ^b	TPSA ^c (Å ²)	
11a	3.24	432.49	7	5	1	120.31	101.80	73.879
11b	3.81	466.94	7	5	1	125.32	101.80	73.879
11c	3.29	462.52	8	6	1	126.80	111.02	70.6981
11d	3.57	450.49	7	6	1	120.27	101.80	73.879
11f	4.37	501.38	7	5	1	130.33	101.80	73.879
11g	3.83	496.97	8	6	1	131.81	111.03	70.6947
11h	4.15	484.93	7	6	1	125.28	101.80	73.879
11j	4.16	481.97	7	5	1	139.29	101.80	73.879
11k	3.61	476.55	8	6	1	131.77	111.03	70.6947
11l	3.94	464.51	7	6	1	125.24	101.80	73.879
12a	3.58	446.52	7	5	1	125.12	101.80	73.879
12b	4.06	480.97	7	5	1	130.13	101.80	73.879
12d	4.64	515.42	7	5	1	135.41	104.80	72.844
12f	4.45	494.99	7	5	1	135.10	101.80	73.879

Abbreviation: ^aMW, molecular weight; ^bMR, molar refractivity; ^cTPSA, topological polar surface; ^d%ABS: percentage of absorption

Property		Compounds				
		celecoxib	11b	11k	12b	12d
Absorption	Water solubility (log mol/L)	-3.61	-2.893	-2.894	-2.893	-2.894
	Caco2 permeability (log Papp in 10 ⁻⁶ cm/s)	1.067	0.795	0.725	0.743	0.642
	Intestinal absorption (% Absorbed)	93.126	97.683	93.231	98.485	99.577
	Skin Permeability (log Kp)	-2.755	-2.735	-2.735	-2.735	-2.735
	P-glycoprotein substrate	yes	Yes	Yes	Yes	Yes
	P-glycoprotein I inhibitor	no	Yes	Yes	Yes	Yes
	P-glycoprotein II inhibitor	yes	Yes	Yes	Yes	Yes
Distribution	VDss (human) (log L/kg)	0.095	-0.297	-0.412	-0.304	-0.322
	Fraction unbound (Fu)	0.125	0.212	0.203	0.207	0.198
	BBB permeability (log BB)	-0.952	-0.373	-0.474	-0.371	-0.594
	CNS permeability (log PS)	-2.086	-2.169	-2.374	-2.083	-1.963
Metabolism	CYP3A4 substrate	yes	Yes	Yes	Yes	Yes
	CYP2C19 inhibitor	Yes	Yes	Yes	Yes	Yes

Table S6: ADME data of the target synthesized compounds predicted using pkCSM software.

	CYP2C9 inhibitor	Yes	Yes	Yes	Yes	Yes
	CYP3A4 inhibitor	No	Yes	Yes	Yes	Yes
Excretion	Total Clearance (log ml/min/kg)	0.472	0.528	0.614	0.518	0.45
	Renal OCT2 substrate	Yes	Yes	Yes	Yes	Yes
	Max. tolerated dose (log mg/kg/day)	0.163	-0.232	-0.271	-0.26	-0.282
	hERG I inhibitor	No	No	No	Yes	No
	hERG II inhibitor	No	Yes	Yes	Yes	Yes
	Hepatotoxicity	Yes	No	No	No	No
	Skin Sensitisation	No	No	No	No	No
	<i>T.Pyriformis</i> toxicity(log ug/L)	0.429	0.285	0.285	0.285	0.285
	Minnow toxicity (log mM)	0.658	-1.695	-1.878	-2.167	-2.746



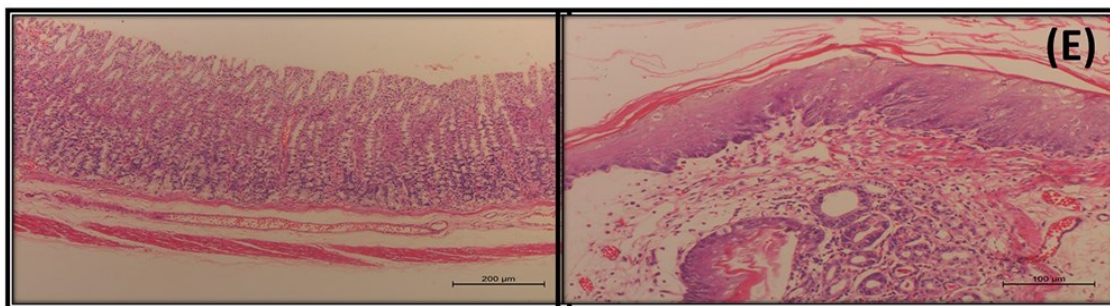


Figure. S1: Histopathological examination of gastric mucosa (A) for negative control group (B) for indomethacin (C) for celecoxib (D) for compounds **11b** and **12d** (E) for compound **11k**.

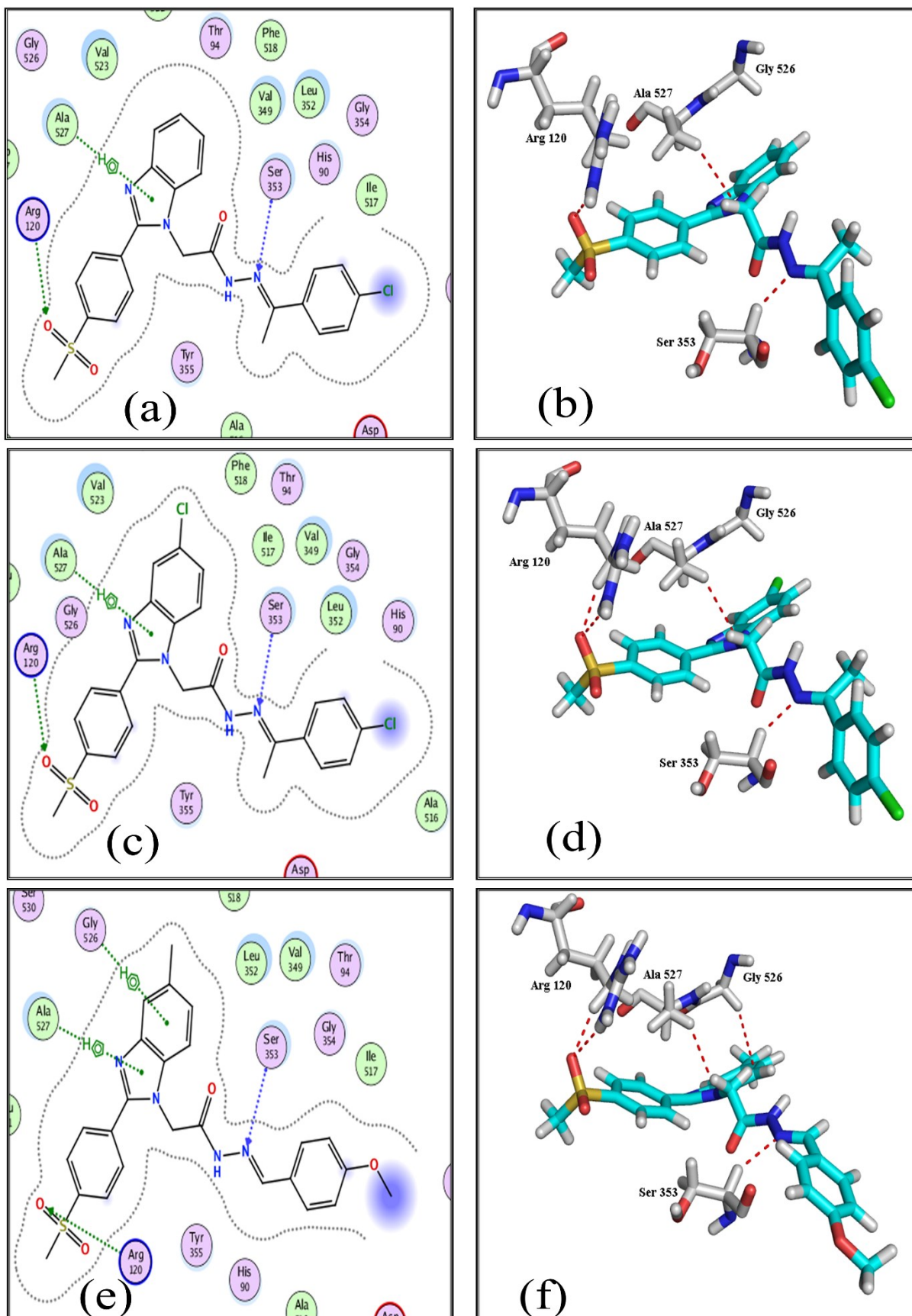
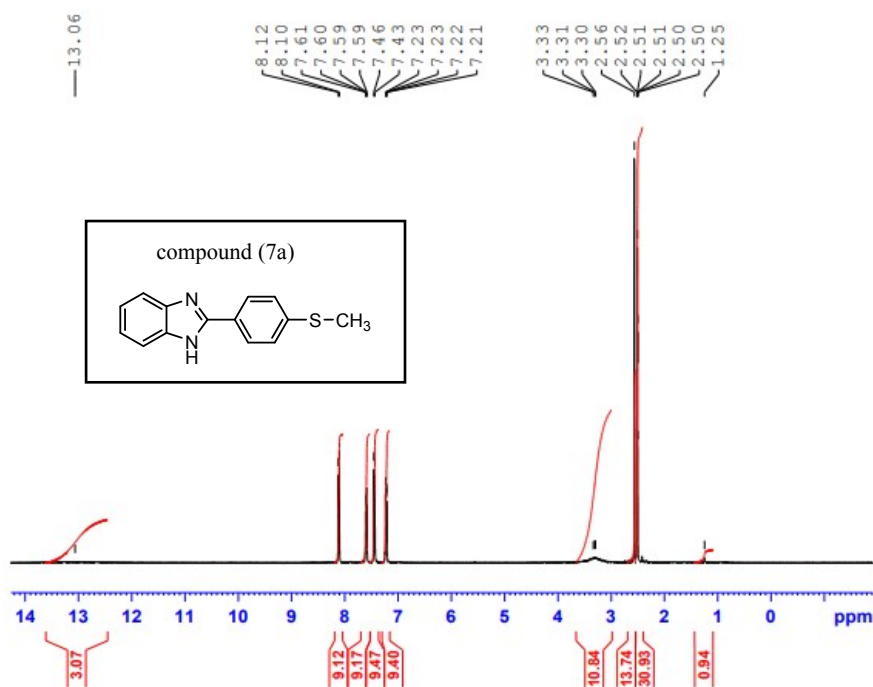


Figure S2: 2D and 3D interaction of compound 12b (a) and (b) compound 12d (c) and (d) compound 11k (e) and (f)

1. ¹H Spectra of 7a:

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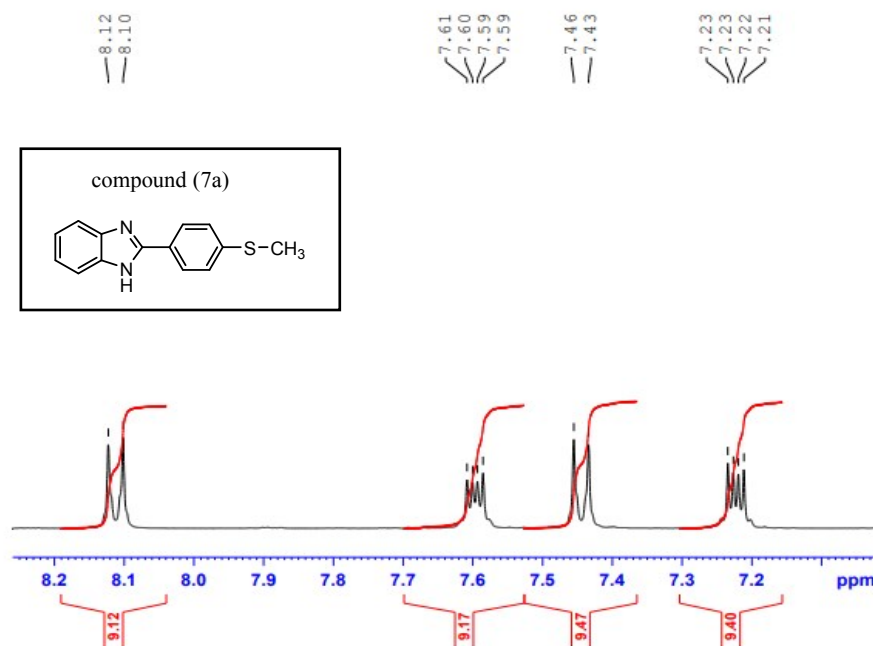
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Act
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A-1
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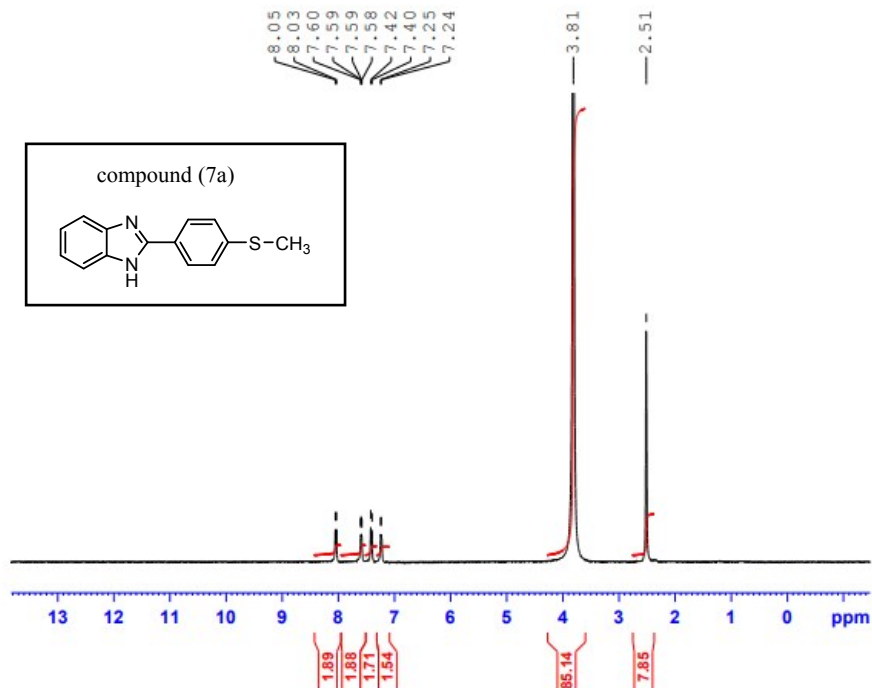
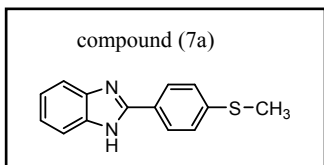
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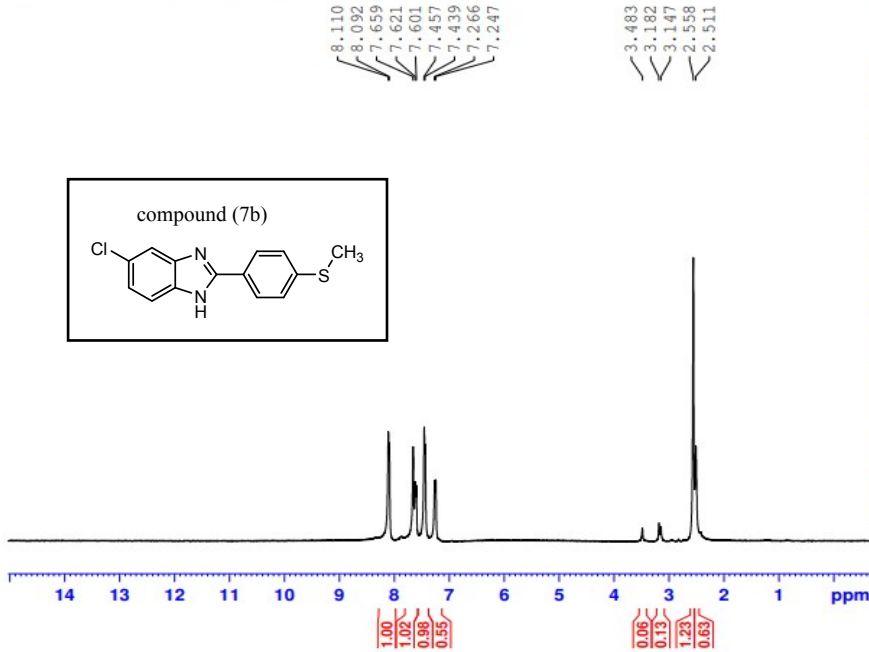
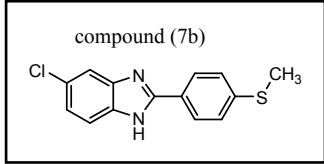
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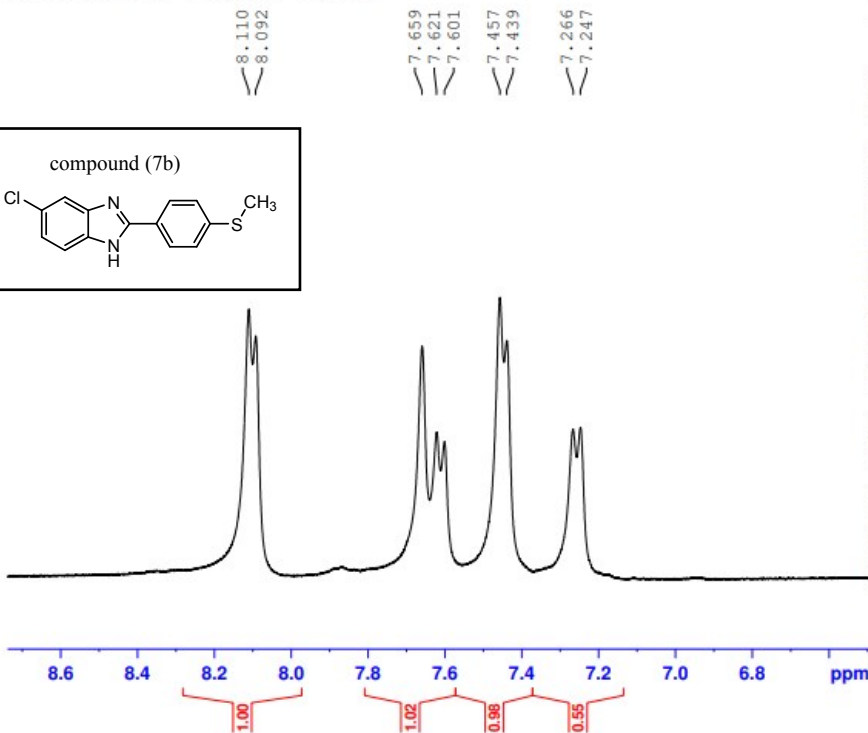
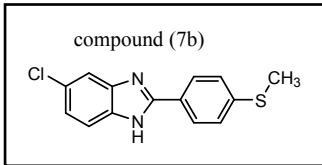
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Active
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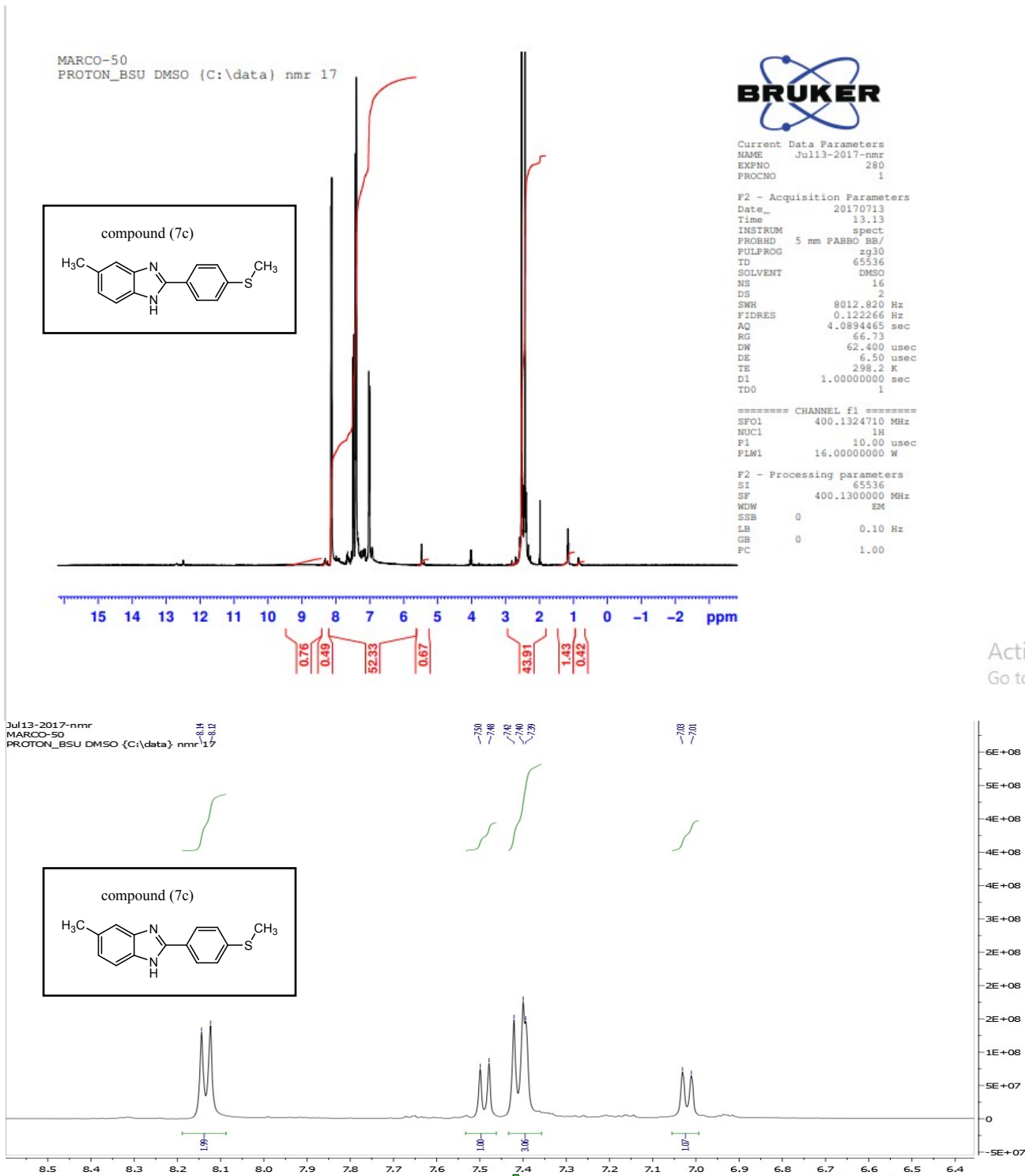
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 DE 6.50 usec
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 TDO 1

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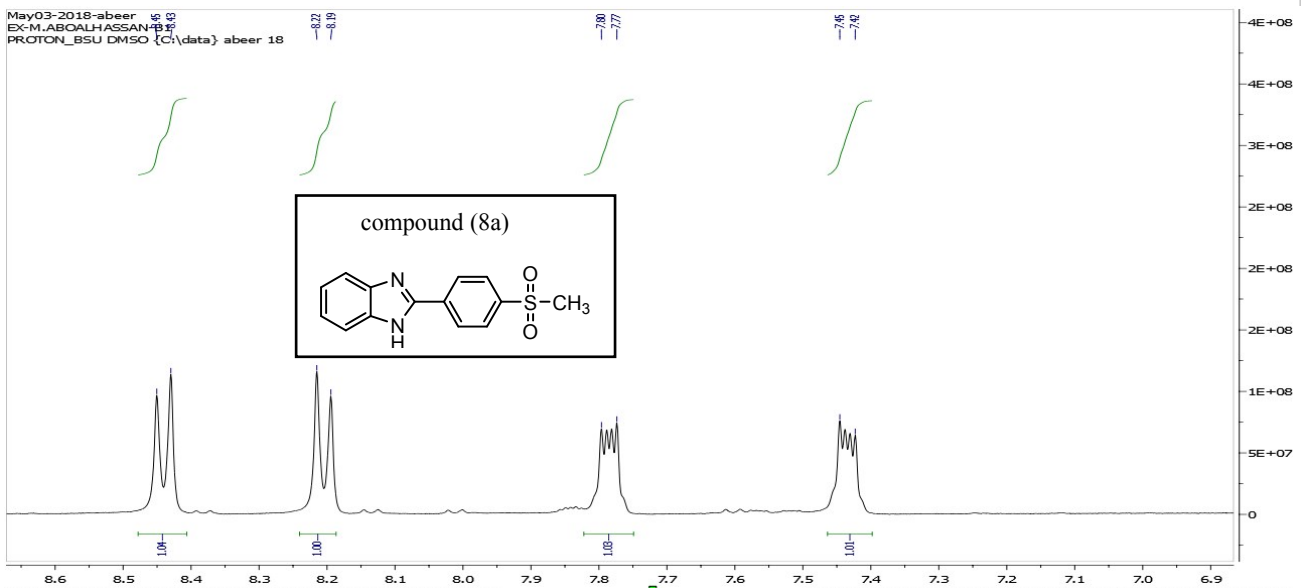
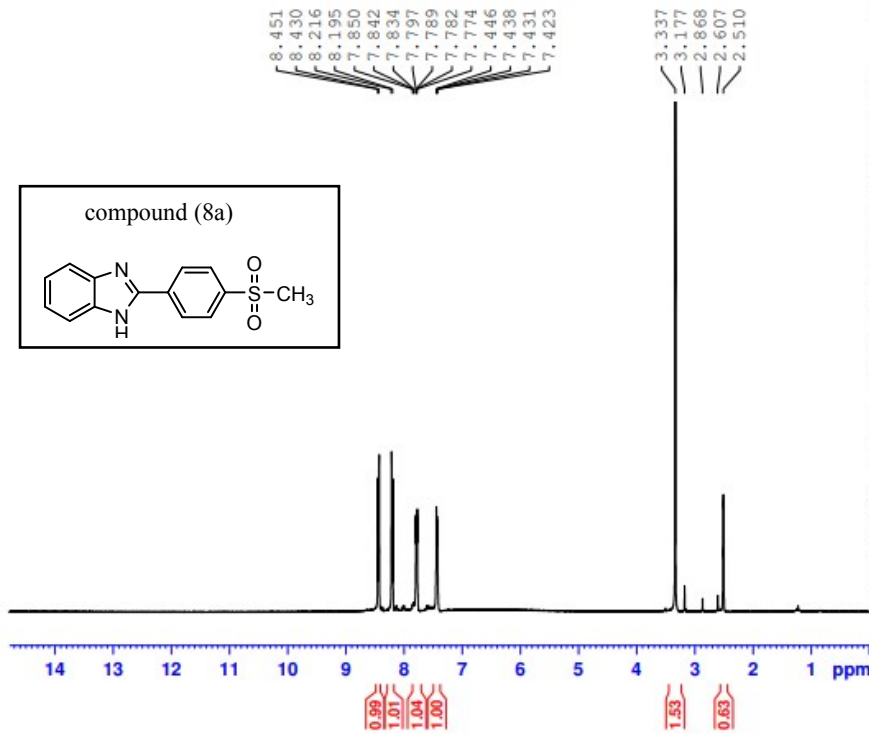
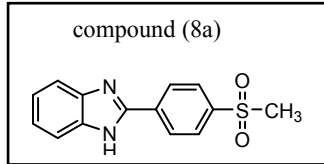
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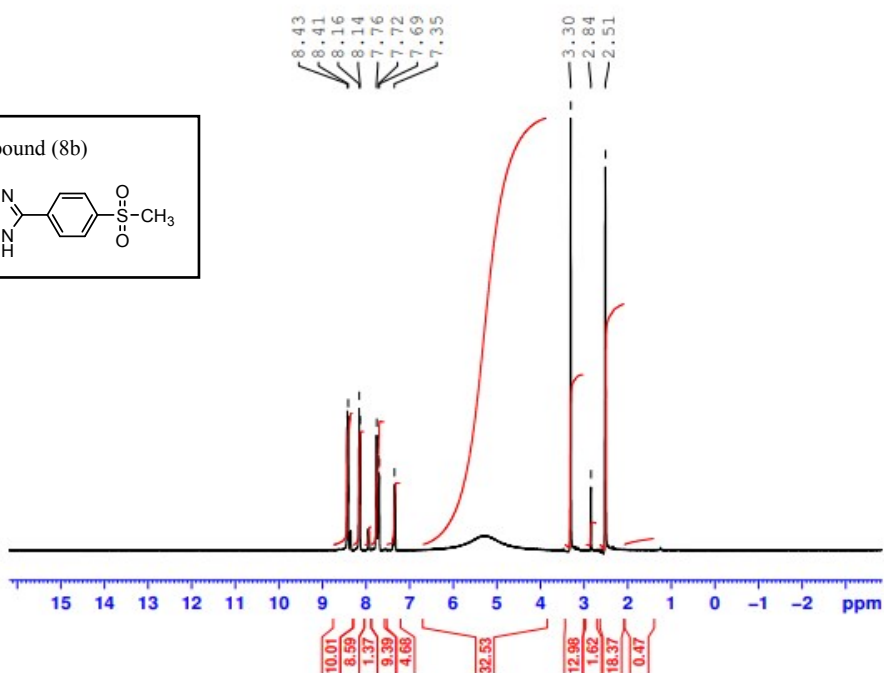
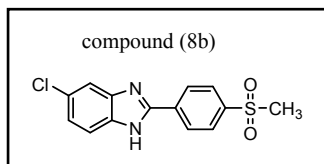
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EX-M.ABOALHASSAN-B1
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5. ¹H Spectra of 8b:

B-2
proton_su DMSO (C:\nmr-data) Student 20



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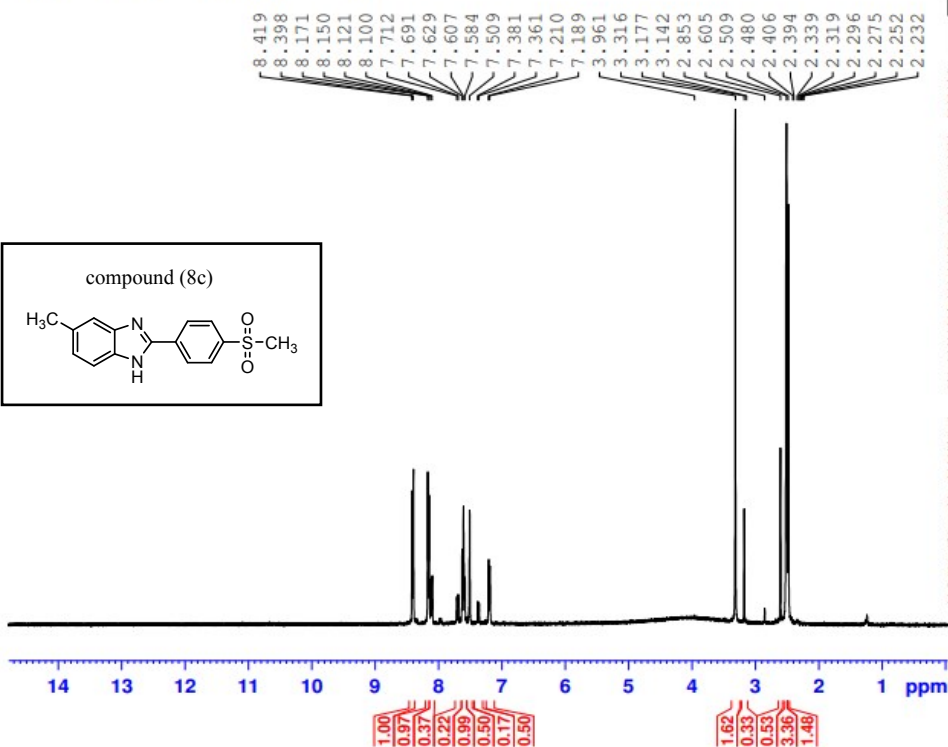
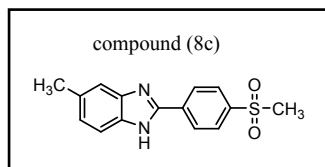
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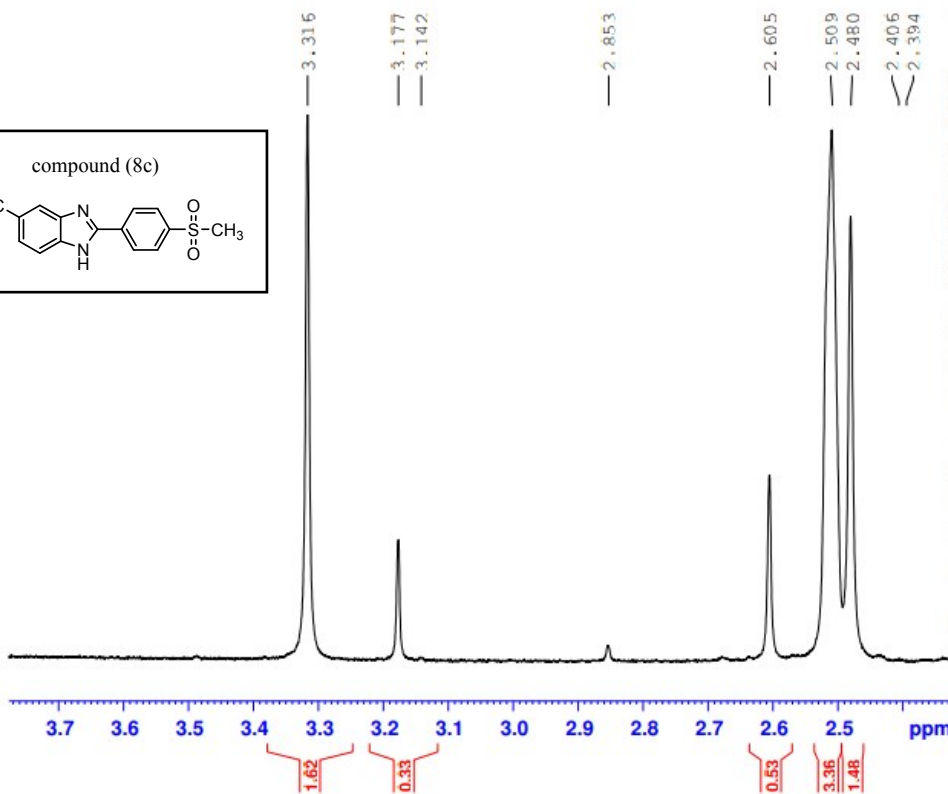
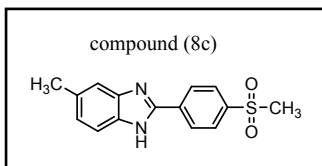
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 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
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ex-m.aboalhassan-B3
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 NAME May03-2018-abeer
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180503
 Time 9.33
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

ex-m.aboalhassan-B3
PROTON_BSU DMSO (C:\data) abeer 17

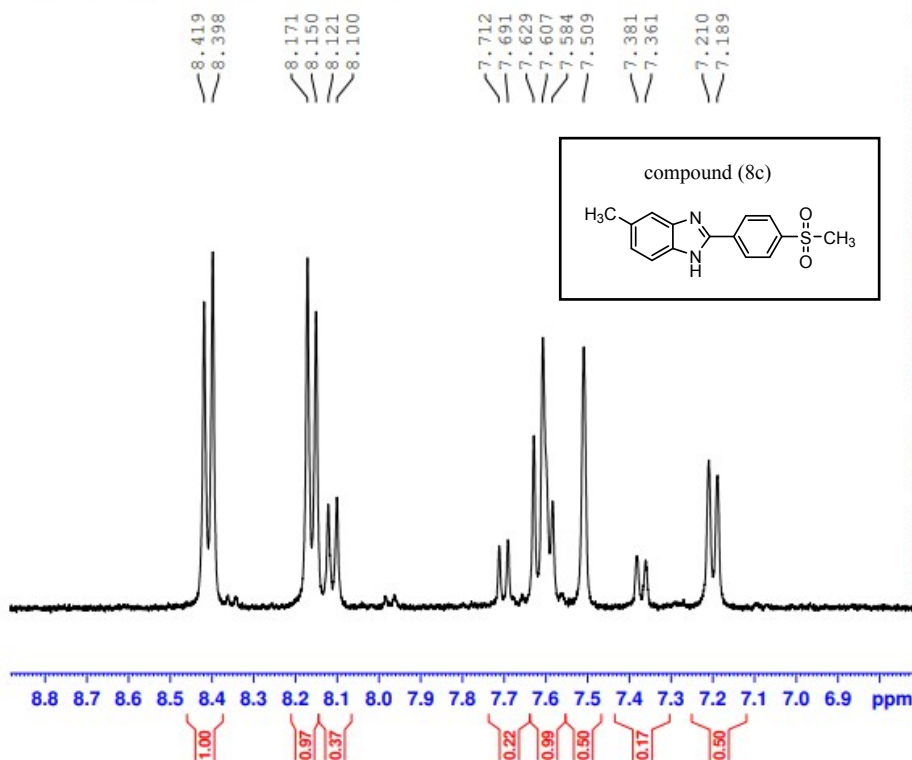
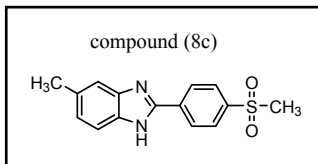


Current Data Parameters
NAME May03-2018-abeer
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180503
Time 9.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DM 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

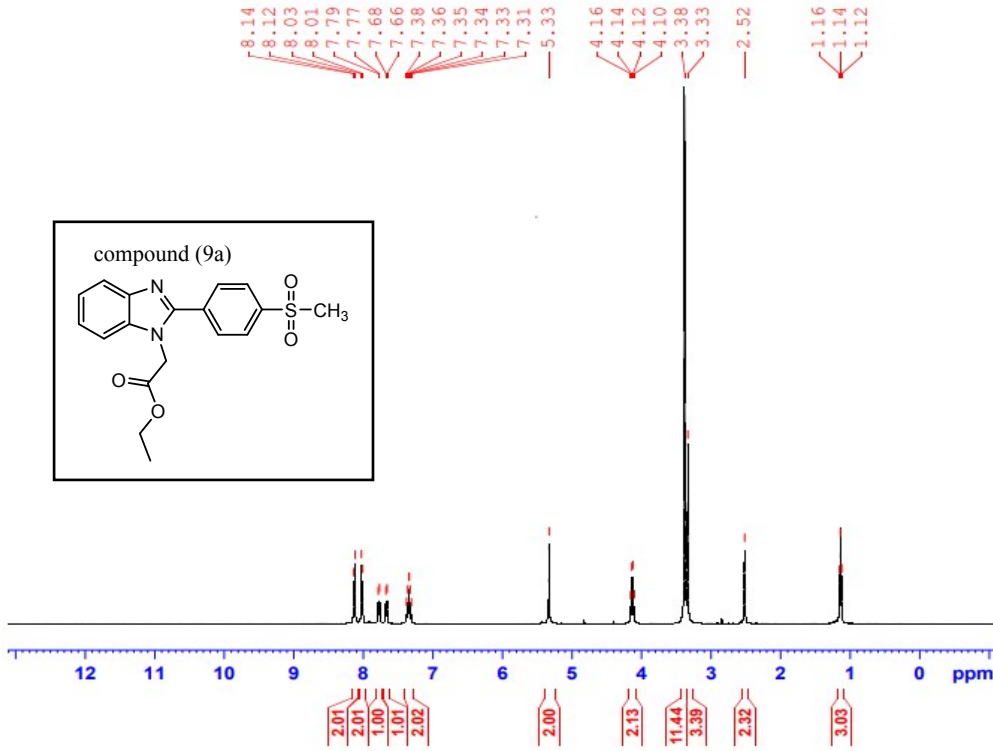
==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



7. ¹H and ¹³C NMR Spectra of 9a:

Martha Moheb-C1-AS-proton



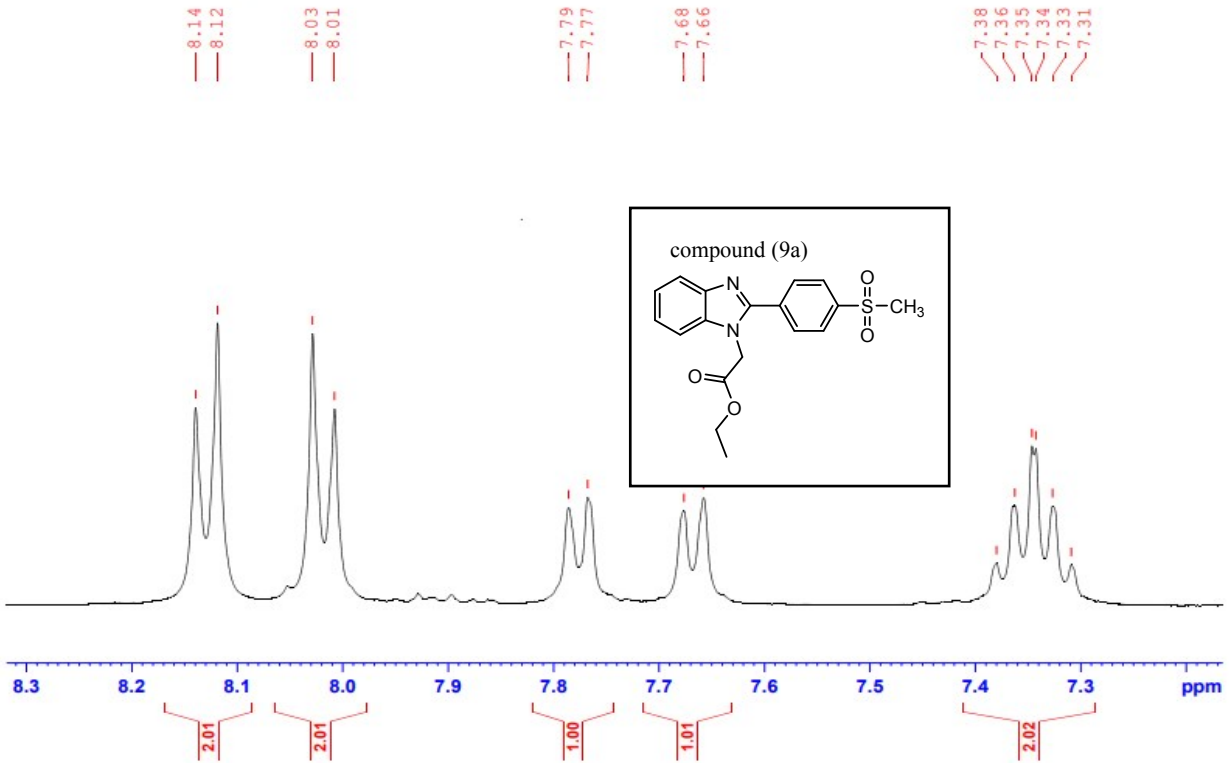
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Current Data Parameters
NAME      Martha Moheb-C1-AS-pi
EXPNO    10
PROCNO   1

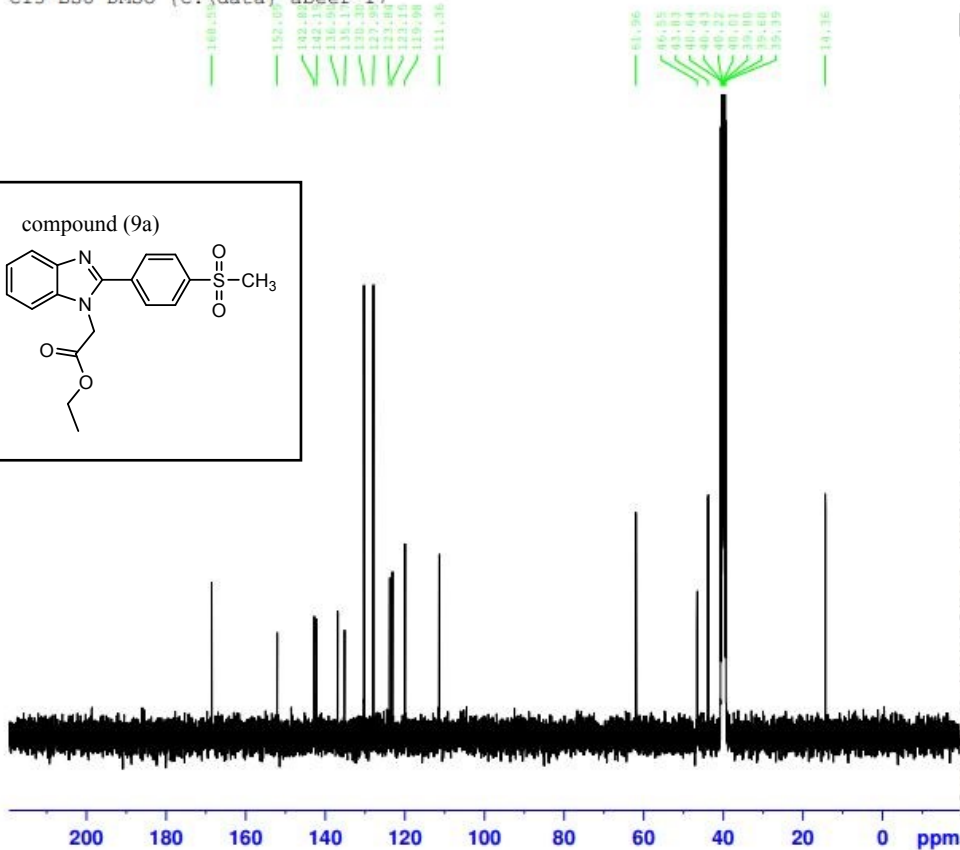
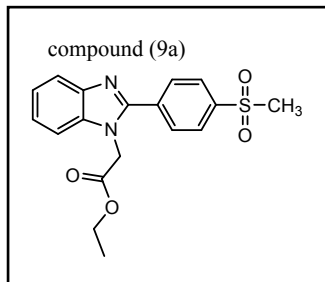
F2 - Acquisition Parameters
Date_    20190915
Time     11.47 h
INSTRUM  spect
PROBHD   zgpg30
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.244932 Hz
AQ        4.0894465 sec
RG        158.72
SQ        62.400 usec
DE        6.50 usec
TE        292.6 K
D1        1.00000000 sec
TDO       1
SFO1      400.2024712 MHz
NUC1      1H
P1        13.50 usec
PLM1      13.00000000 W

F2 - Processing parameters
SI        65536
SF        400.2000000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

Martha Moheb-C1-AS-proton



MOHAMED-9A
C13-BSU DMSO (C:\data) aber 17



Current Data Parameters
NAME Jul11-2021-abeer
EXPNO 110
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210711
Time 23.16
INSTRUM spect
PROBHD 5 mm F4BBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

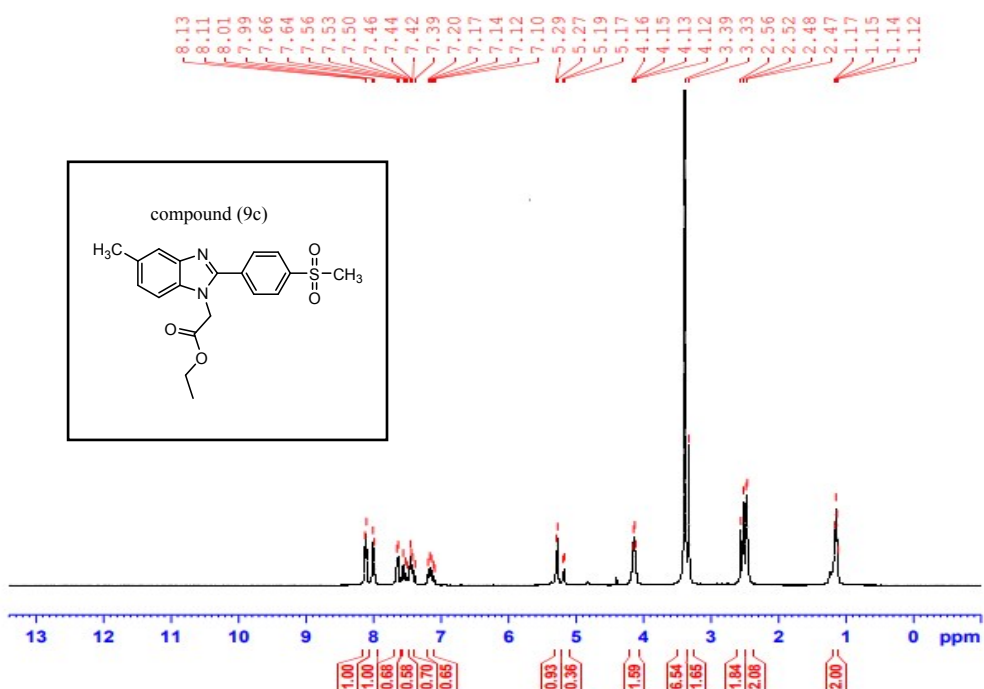
===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 66.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W
PLW13 0.17640001 W

F2 - Processing parameters
SI 131072
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

9. ¹H and ¹³C NMR Spectra of 9c:

Martha Moheb-C3-AS-proton

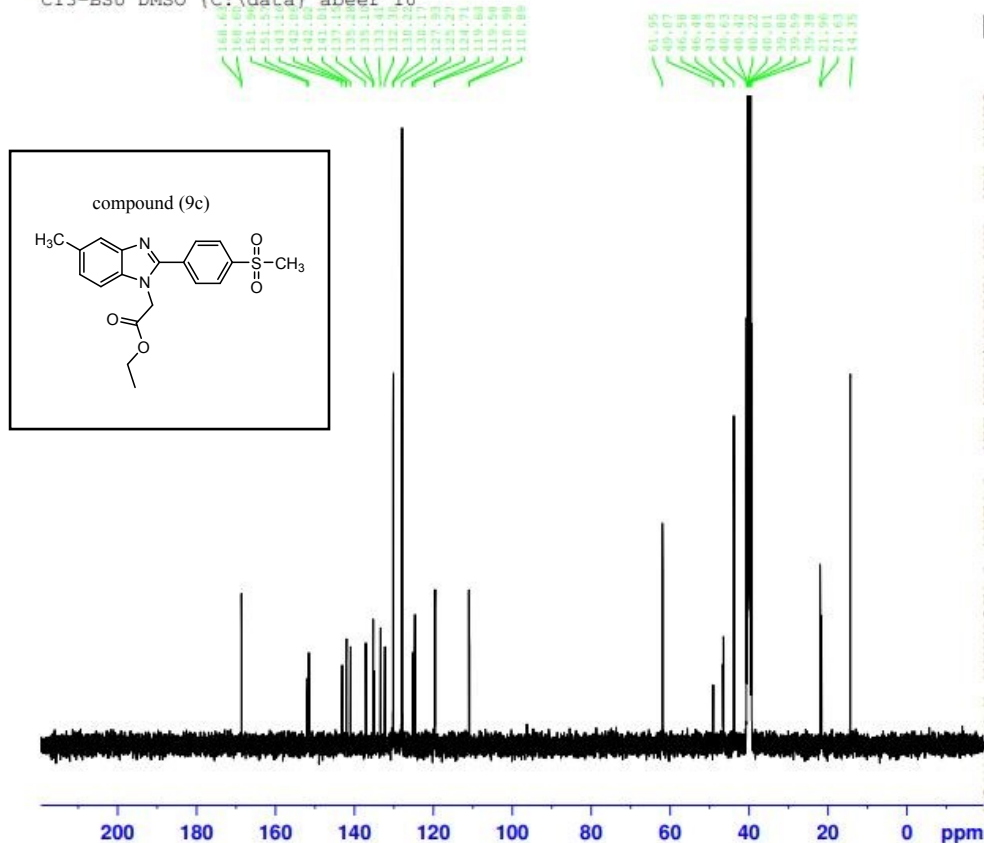


Current Data Parameters
 NAME Martha Moheb-c3-AS-proton
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190915
 Time 11.57 h
 INSTRUM spect
 PROBHD z108618_0945 ()
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0884483 sec
 RG 120.93
 DW 62.400 usec
 DE 6.50 usec
 TE 292.6 K
 D1 1.00000000 sec
 TDO 1
 SFO1 400.2024712 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 13.0000000 W

F2 - Processing parameters
 SI 65536
 SF 400.2000000 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

MOHAMED-9C
 C13-BSU DMSO (C:\data) abeer 10



Current Data Parameters
 NAME Jul12-2021-abeer
 EXPNO 160
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210713
 Time 2.43
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 4000
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 205.44
 DW 20.800 usec
 DE 6.50 usec
 TE 299.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

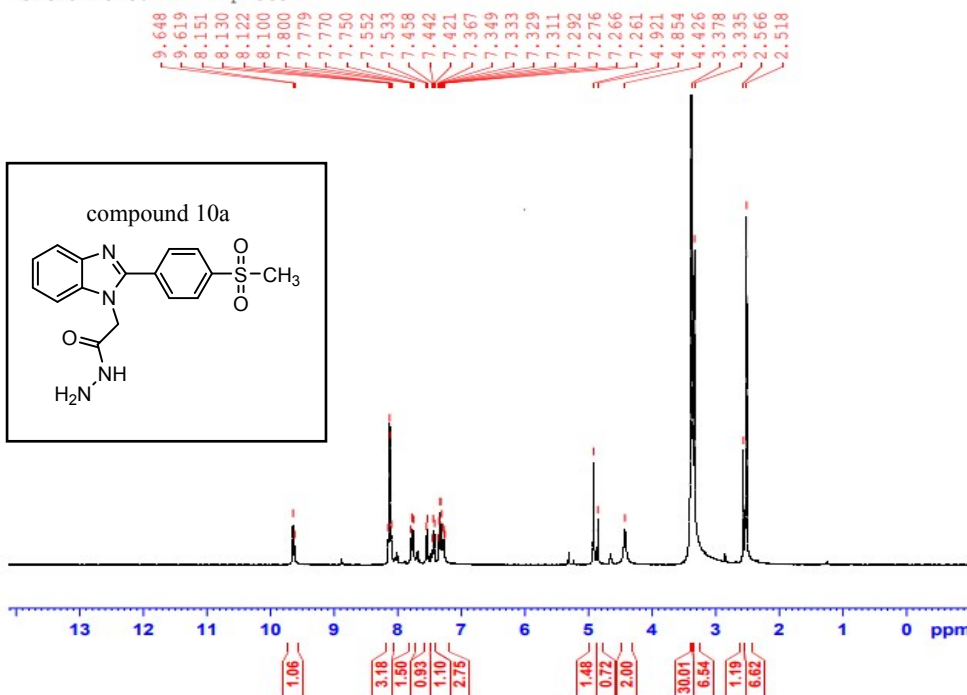
===== CHANNEL f1 =====
 SFO1 100.6228293 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 66.00000000 W

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.21777999 W
 PLW13 0.17640001 W

F2 - Processing parameters
 SI 131072
 SF 100.6127690 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

10. ¹H and ¹³C NMR Spectra of 10a:

Martha Moheb-El-WH-proton

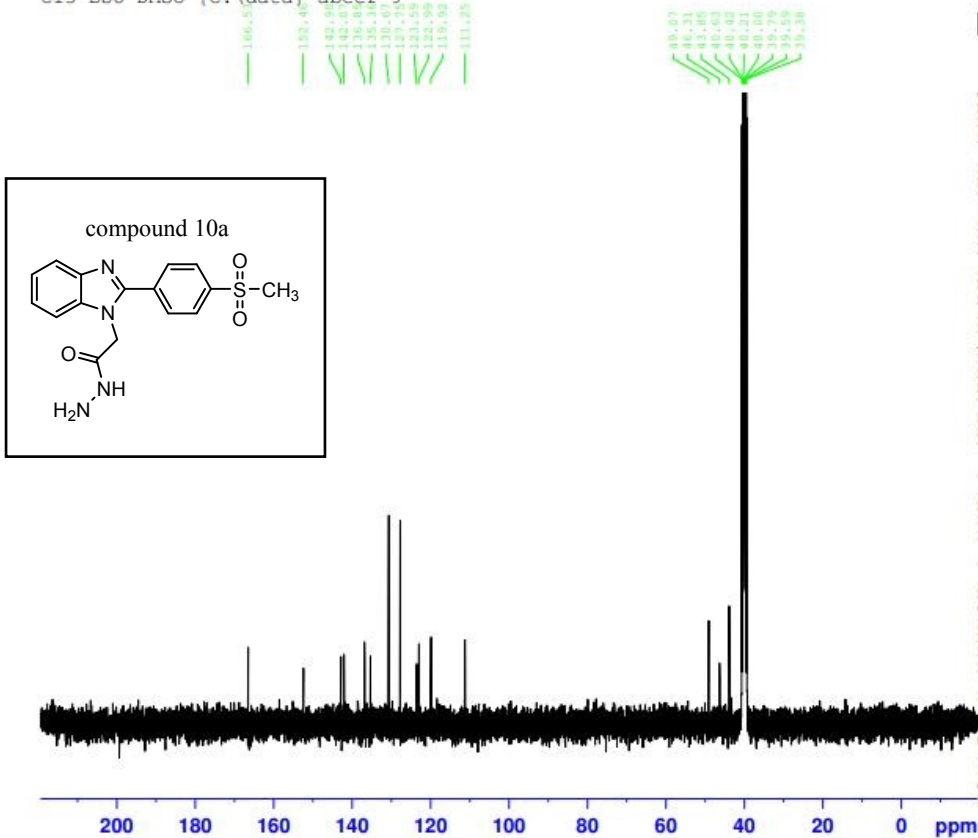


Current Data Parameters
 NAME Martha Moheb-El-WH-proton
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180930
 Time 11.14 h
 INSTRUM spect
 PROBHD z108618_0945 (4
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 197.77
 DW 62.400 usec
 DE 6.50 usec
 TE 299.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.2024712 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 13.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.2000000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

MOHAMED-10A
 C13-BSU DMSO (C:\data) abeer 9



Current Data Parameters
 NAME Jul12-2021-abeer
 EXPNO 150
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210712
 Time 22.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 4000
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 205.44
 DW 20.800 usec
 DE 6.50 usec
 TE 299.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6228293 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 66.00000000 W

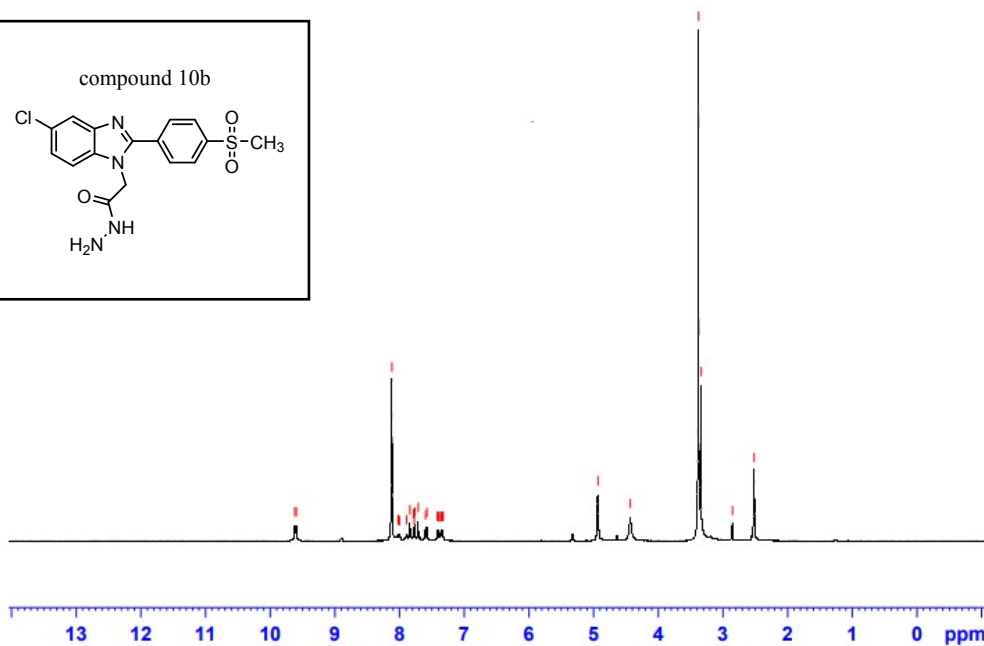
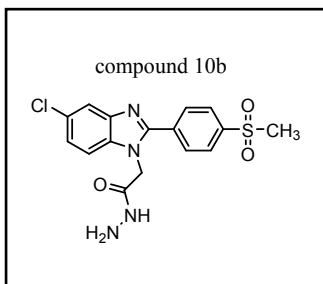
===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.21777999 W
 PLW13 0.17640001 W

F2 - Processing parameters
 SI 131072
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

11. ¹H and ¹³C NMR Spectra of 10b:

Martha Moheb-E2-WH-proton

9.620
9.596
8.118
8.025
8.019
8.003
7.892
7.839
7.785
7.773
7.763
7.712
7.601
7.579
7.413
7.409
7.391
7.388
7.353
7.349
7.331
7.328
4.933
4.431
3.378
3.338
2.852
2.518



Current Data Parameters
NAME Martha Moheb-E2-WH-proton
EXPNO 10
PROCNO 1

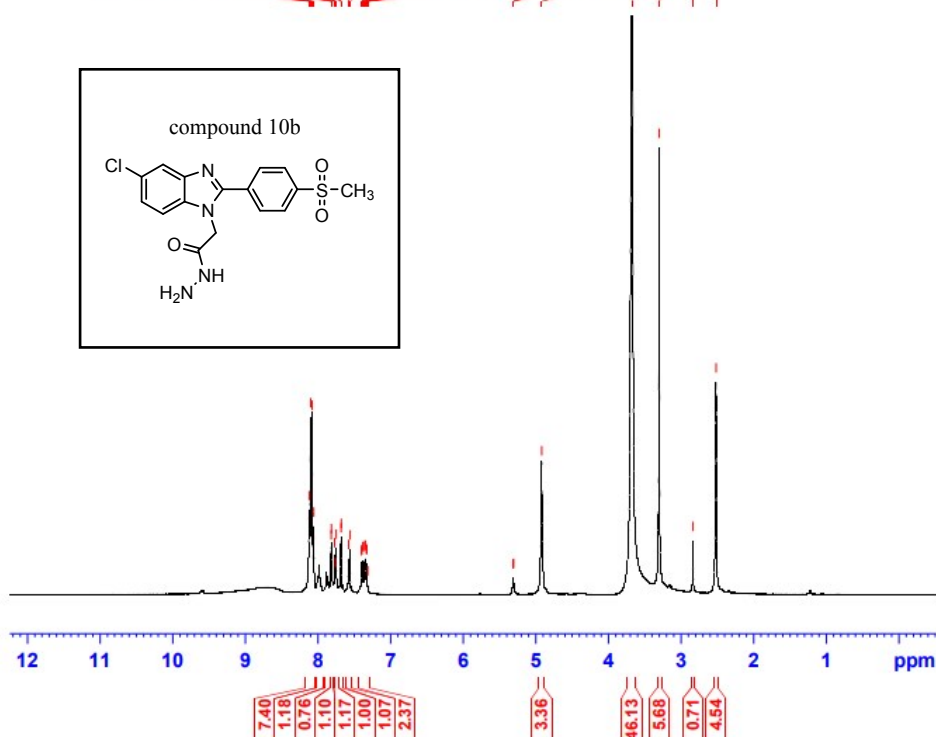
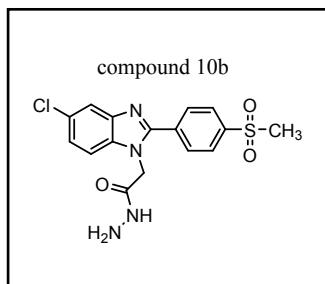
F2 - Acquisition Parameters
Date_ 20190930
Time_ 11:19 h
INSTRUM spect
PROBHD Z108618_0945 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 176.72
DW 62.400 usec
DE 6.50 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2024712 MHz
NUC1 1H
P1 13.50 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Activa
Go to S

Martha Moheb-E2-D2O-D

8.121
8.100
8.080
8.058
7.819
7.814
7.771
7.760
7.749
7.682
7.678
7.579
7.558
7.402
7.397
7.380
7.376
7.354
7.350
7.332
7.328
7.313
5.314
5.307
4.919
3.678
3.302
2.836
2.519



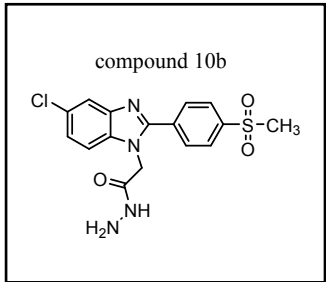
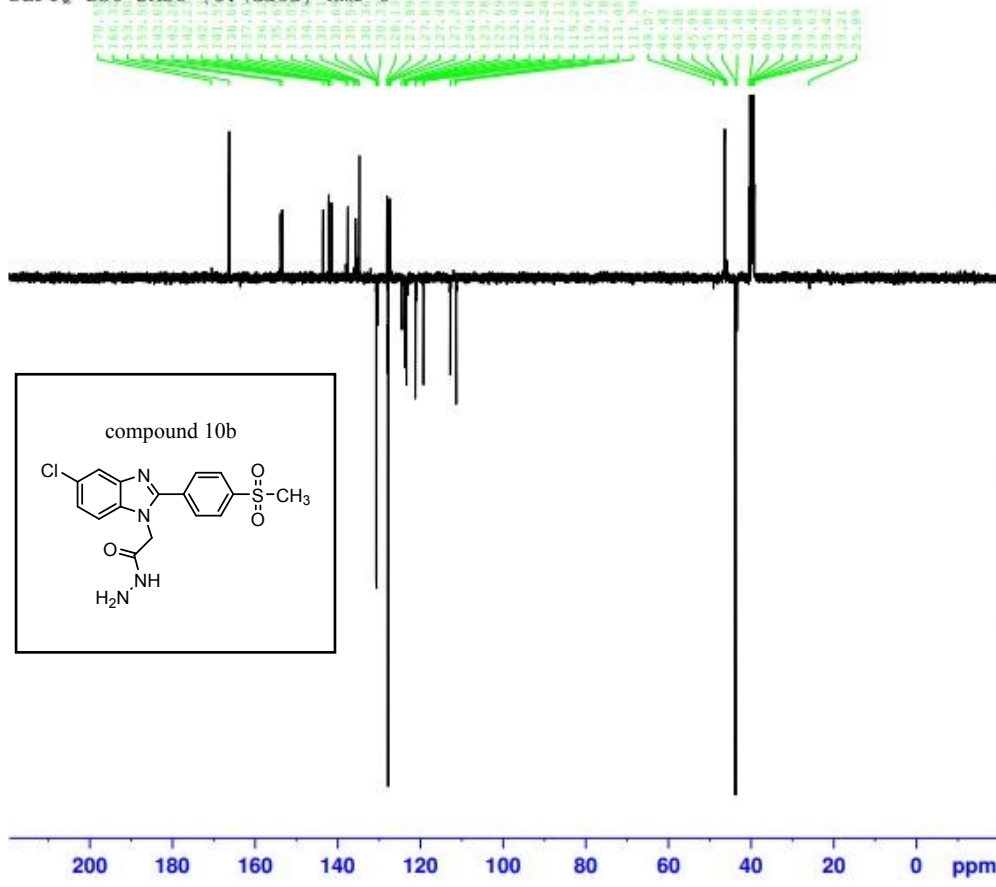
Current Data Parameters
NAME Martha Moheb-E2-D2O
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191001
Time_ 3:08 h
INSTRUM spect
PROBHD Z108618_0945 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 135.42
DW 62.400 usec
DE 6.50 usec
TE 292.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.2024712 MHz
NUC1 13C
P1 13.50 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Activa
Go to

AHMED S-29
 DEPTQ-BSU DMSO (C:\data) nmr_8



Current Data Parameters
 NAME Jun24-2017-nmr
 EXPNO 160
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170625
 Time 0.06
 INSTRUM spect
 PULPROG 3 == PABPO 2B/
 DCLPROG dephcpgppp
 TD 65536
 SOLVENT DMSO
 NS 4000
 DS 4
 SWS 24038.461 Hz
 FIDRES 0.366738 Hz
 AQ 1.3631488 sec
 RG 205.44
 DW 20.800 usec
 DE 6.50 usec
 TE 295.7 K
 CMT2 145.000000
 CMT12 1.5000000
 D1 2.0000000 sec
 D2 0.00344828 sec
 D12 0.00000000 sec
 D18 0.00020000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6228303 MHz
 NUC1 13C
 P1 10.00 usec
 P13 2000.00 usec
 PLW0 0 W
 P1M1 68.0000000 W
 SFOALS 0 Hz
 SFOFFS 0 Hz
 SFR3 10.08399843 W

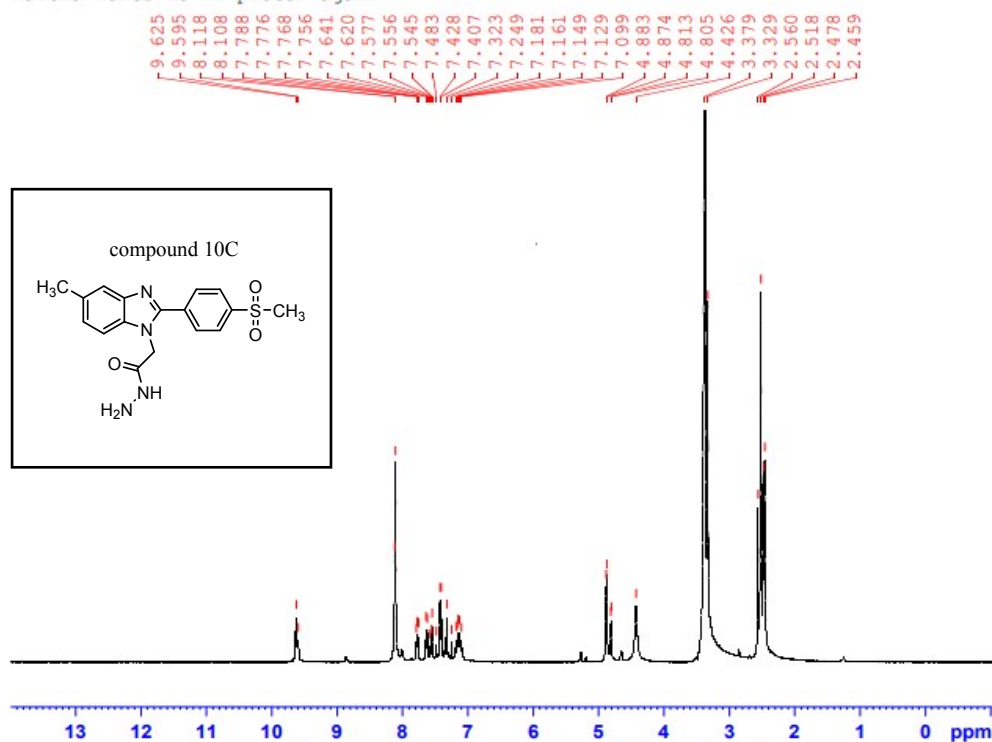
===== CHANNEL f2 =====
 SFO2 400.1313791 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PC 11.75 usec
 P3 10.50 usec
 P4 21.00 usec
 PCPD2 90.00 usec
 PLW2 16.0000000 W
 PLW12 0.21777999 W

===== GRADIENT CHANNEL1 =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPNAM[3] SMSQ10.100
 GP21 31.00 %
 GP22 31.00 %
 GP23 31.00 %
 P16 1000.00 usec

F2 - Processing parameters
 SI 32768
 SF 100.6127490 MHz
 WCW RM
 SGB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

12. ¹H and ¹³C NMR Spectra of 10c:

Martha Moheb-E3-WH-proton again



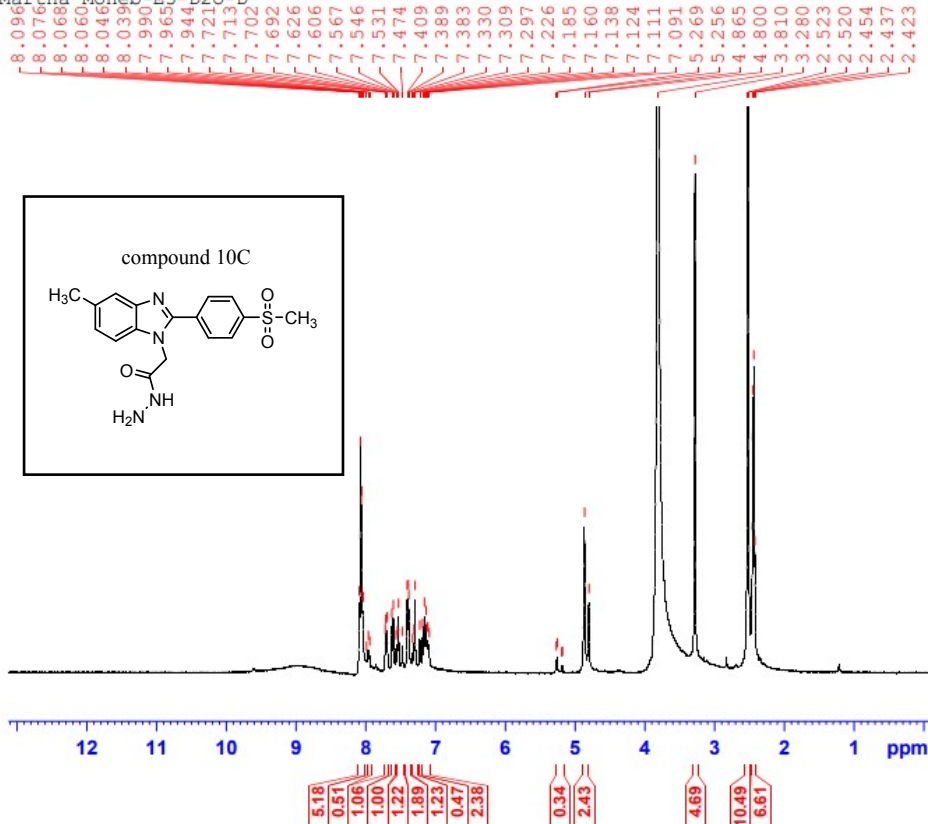
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Current Data Parameters
NAME      Martha Moheb-E3-WH-proton again
EXPNO    10
PROCNO   1

F2 - Acquisition Parameters
Date_    20190930
Time     12.22 h
INSTRUM spect
PROBHD   Z108618_0945 (
PULPROG zg30
TD       65536
SOLVENT  DMSO
NS       16
DS       2
SWH      8012.820 Hz
FIDRES   0.244532 Hz
AQ       4.0894465 sec
RG       176.72
SW       62.400 usec
DE       6.30 usec
TE       292.9 K
D1       1.00000000 sec
TD0      1
SFO1     400.2024712 MHz
NUC1     1H
P1       13.50 usec
PLW1     13.00000000 W

F2 - Processing parameters
SI       65536
SF       400.2000000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```

Martha Moheb-E3-D2O-D



```

Current Data Parameters
NAME      Martha Moheb-E3-D2O-
EXPNO    10
PROCNO   1

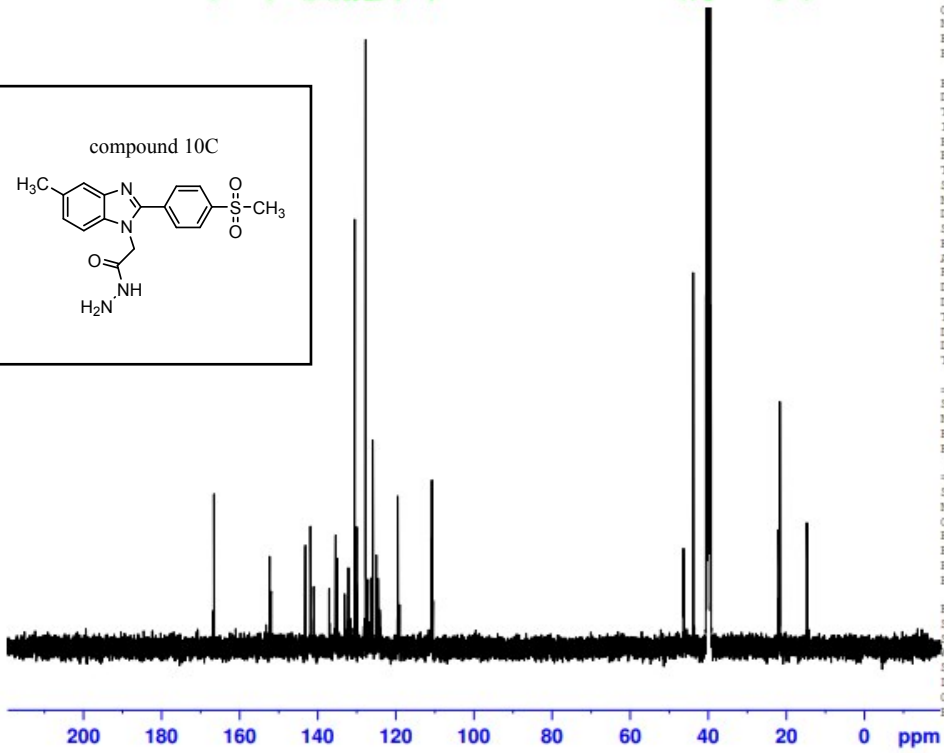
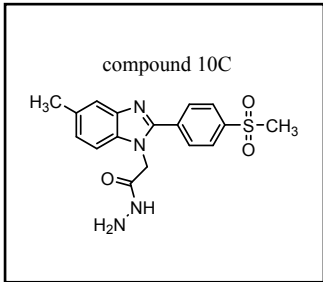
F2 - Acquisition Parameters
Date_    20191001
Time     3.12 h
INSTRUM spect
PROBHD   Z108618_0945 (
PULPROG zg30
TD       65536
SOLVENT  DMSO
NS       16
DS       2
SWH      8012.820 Hz
FIDRES   0.244532 Hz
AQ       4.0894465 sec
RG       158.72
DW       62.400 usec
DE       6.50 usec
TE       292.9 K
D1       1.00000000 sec
TD0      1
SFO1     400.2024712 MHz
NUC1     1H
P1       13.50 usec
PLW1     13.00000000 W

F2 - Processing parameters
SI       65536
SF       400.2000000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```

MARCO-53
C13-BSU DMSO (C:\data) nmr 1



166.8630
166.8630
166.8630
152.7190
151.9190
149.2720
141.8110
141.8110
137.7740
137.7740
135.0130
135.0130
133.1330
132.7790
132.7790
131.6180
131.6180
130.9130
130.9130
129.0130
128.0130
127.9180
127.9180
127.1180
126.8180
126.8180
125.9180
125.9180
125.0130
124.9130
124.9130
124.3130
124.3130
124.1230
124.1230
119.1170
119.1170
118.0130
118.0130
116.8130
116.8130
116.4930
116.4930
116.5230
86.3330
86.2230
83.8630
80.3730
80.3730
80.1630
79.9530
79.7430
79.5330
79.3330
21.0930
21.0630
21.0630
21.6530
14.7730
14.7730



Current Data Parameters
NAME Jul13-2017-nmr
EXPNO 360
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170714
Time 7.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 66.00000000 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltr16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W
PLW13 0.17640001 W

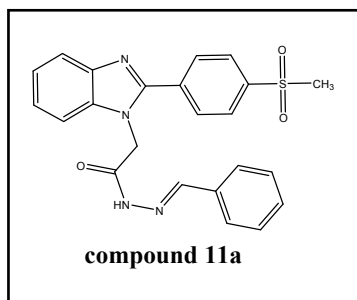
F2 - Processing parameters
SI 131072
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

13. ¹H and ¹³C NMR Spectra of 11a:

MOHAMEDA-2
 PROTON_BSU DMSO {C:\data} nmr 6

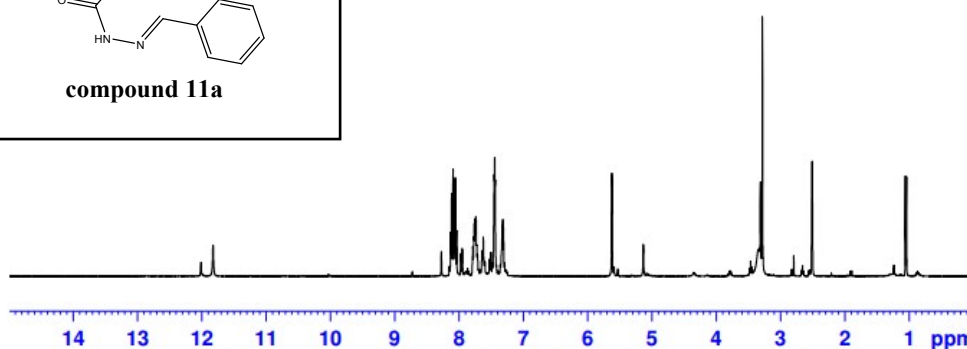


12.016
 11.828
 8.276
 8.130
 8.116
 8.094
 8.073
 8.060
 8.039
 7.971
 7.952
 7.786
 7.770
 7.762
 7.751
 7.741
 7.737
 7.727
 7.716
 7.647
 7.642
 7.634
 7.625
 7.524
 7.505
 7.453
 7.446
 7.440
 7.334
 7.329
 7.320
 7.311
 5.623
 5.136
 3.466
 3.346
 3.324
 3.312
 2.795
 2.509



Current Data Parameters
 NAME Dec13-2016-nmr
 EXPNO 80
 PROCNO 1

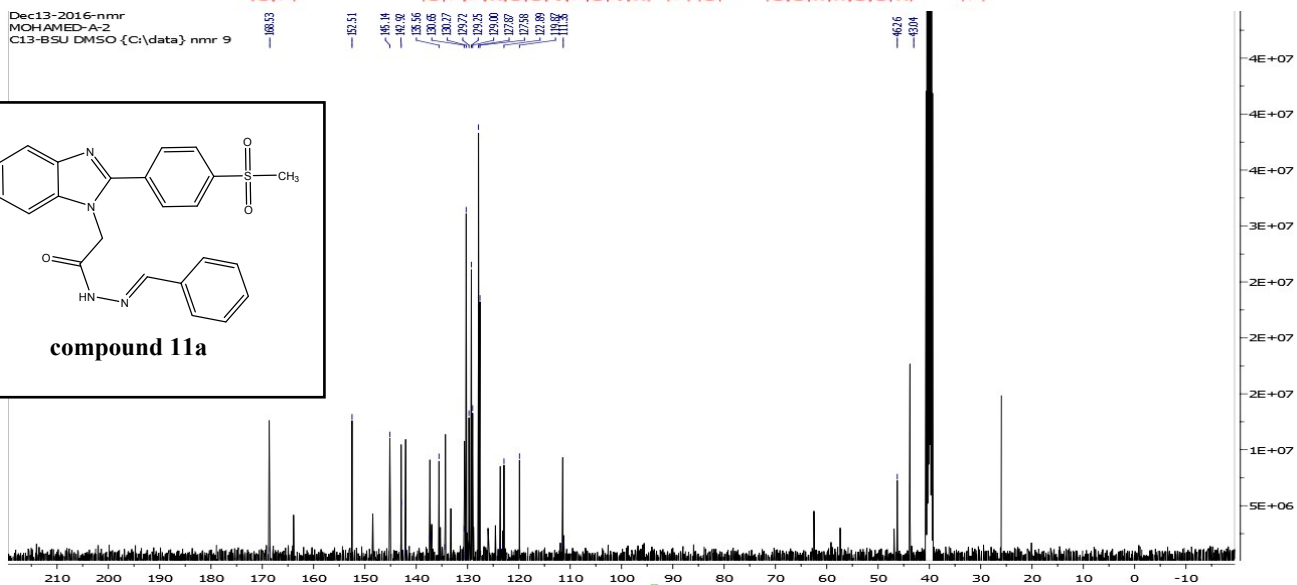
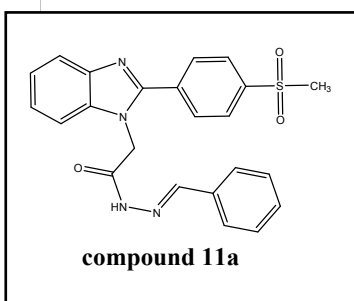
F2 - Acquisition Parameters
 Date_ 20161213
 Time 9.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 299.1 K
 D1 1.00000000 sec
 TD0 1



----- CHANNEL f1 -----
 SF01 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

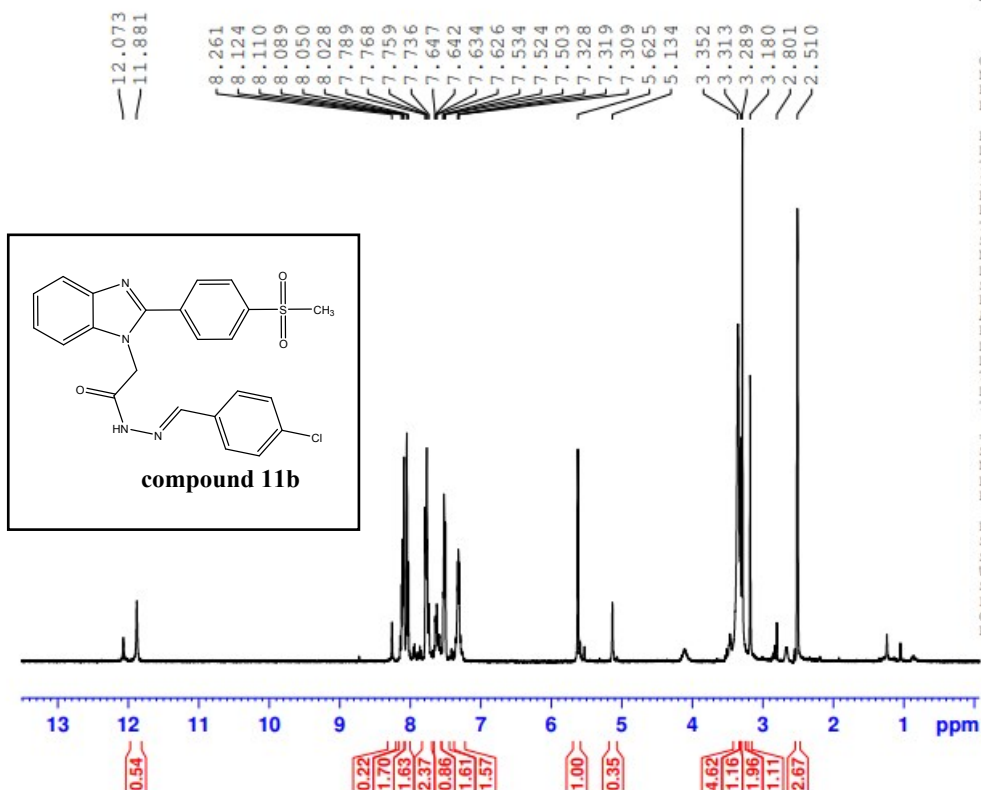
F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

Dec13-2016-nmr
 MOHAMED-A2
 C13-BSU DMSO {C:\data} nmr 9



14. ¹H and NOESY Spectra of 11b:

AHMED S-1H
 PROTON_BSU DMSO {C:\data} abeer 11

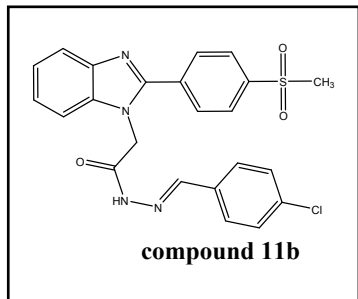


Current Data Parameters
 NAME Jun03-2018-abeer
 EXPNO 180
 PROCNO 1

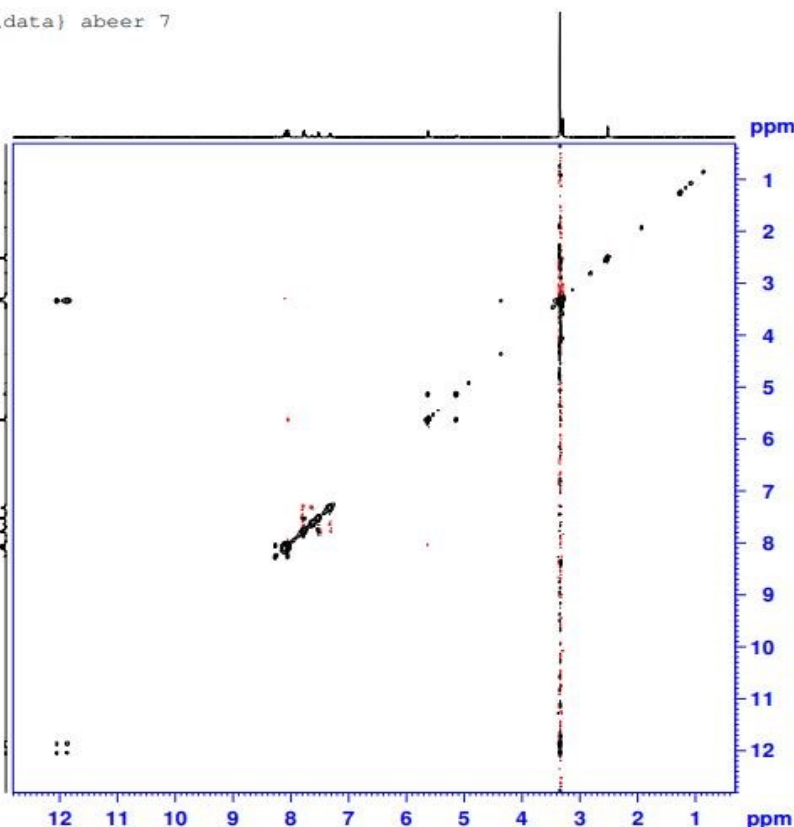
F2 - Acquisition Parameters
 Date_ 20180603
 Time 12.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.089465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



MOHAMED-11B
 NOESY DMSO {C:\data} abeer 7



Current Data Parameters
 NAME Jul14-2021-abeer
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210714
 Time 15.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG noesygpgphpp
 TD 2048
 SOLVENT DMSO
 NS 8
 DS 32
 SWH 5000.000 Hz
 FIDRES 2.441406 Hz
 AQ 0.2048000 sec
 RG 66.73
 DW 100.000 usec
 DE 6.50 usec
 TE 299.1 K
 D0 0.00008727 sec
 D1 1.07263505 sec
 D8 0.30000001 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 D16 0.00020000 sec
 IN0 0.00020000 sec

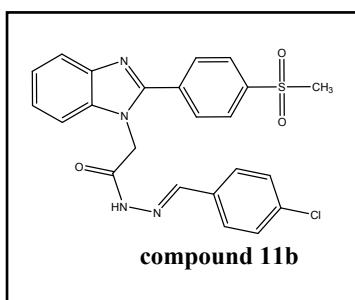
===== CHANNEL f1 =====
 SF01 400.1326244 MHz
 NUC1 1H
 P1 10.00 usec
 P2 20.00 usec
 P17 2500.00 usec
 PLW1 16.00000000 W
 PLW0 2.36689997 W

===== GRADIENT CHANNEL =====
 GPPHM[1] SMSQ10.100
 GPC1 40.00 Hz
 F16 1000.00 usec

F1 - Acquisition parameters
 TD 256
 SF01 400.1326 MHz
 FIDRES 19.531250 Hz
 SW 12.496 ppm
 FWH00K States=TPP1

F2 - Processing parameters
 SI 1024
 SF 400.1300000 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 NUC2 States=TPP1
 SF 400.1300000 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0



15. ¹H and ¹³C NMR Spectra of 11c:

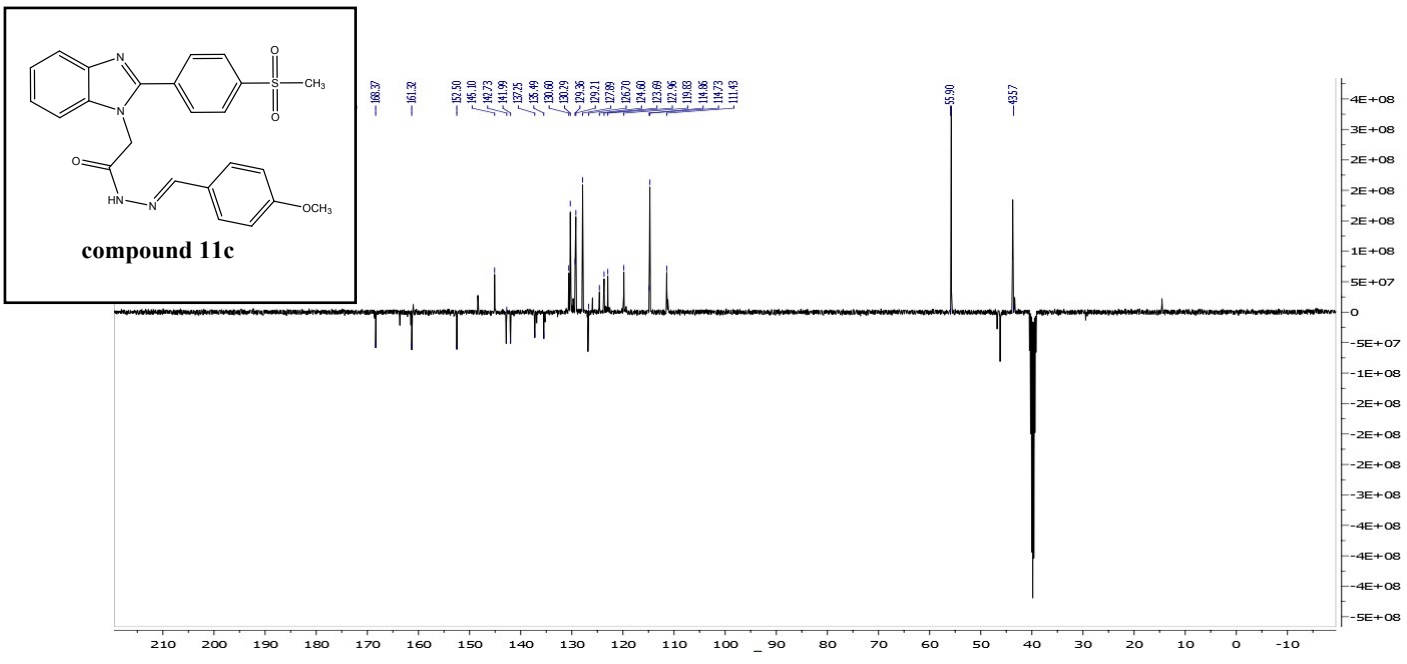
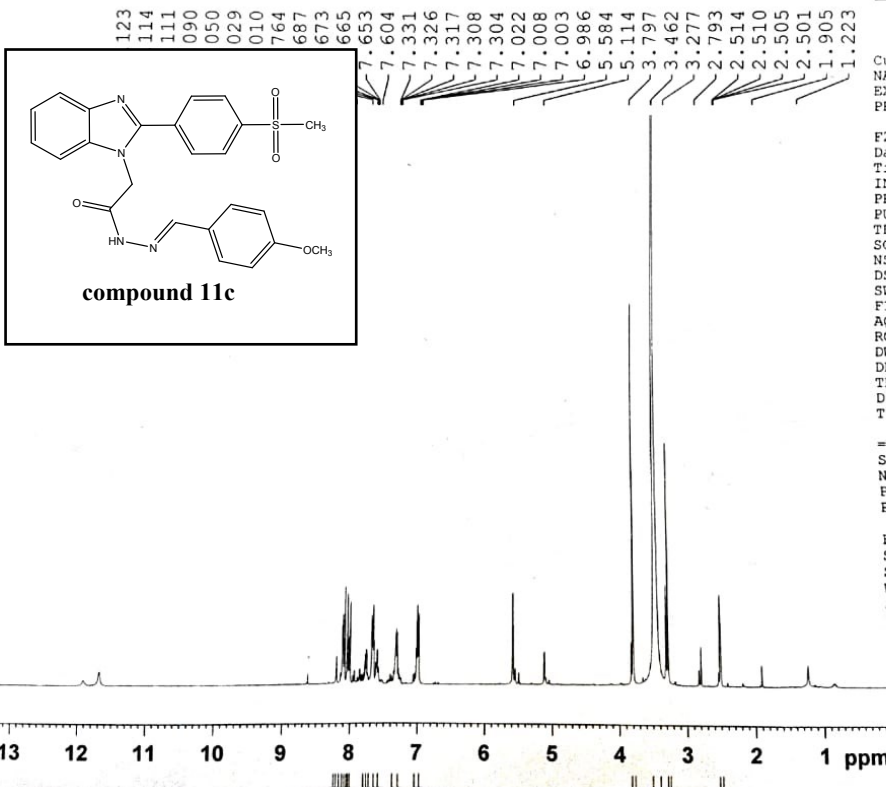


Current Data Parameters
 NAME Jun15-2017-nmr
 EXPNO 30
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170617
 Time_ 3.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 91.28
 DW 62.400 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TDO 1

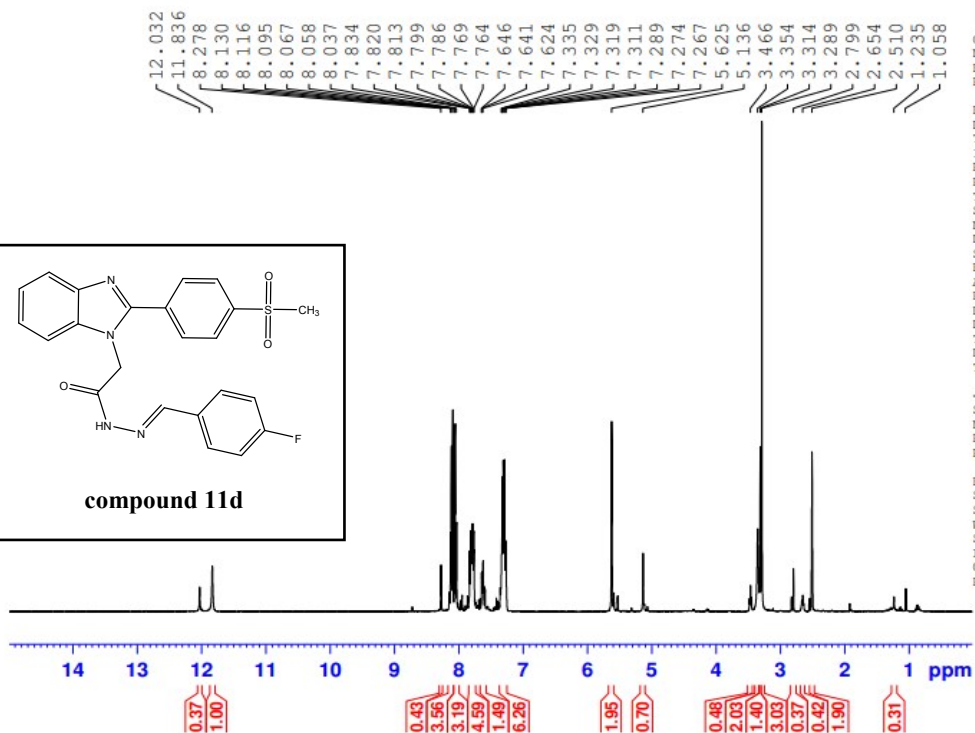
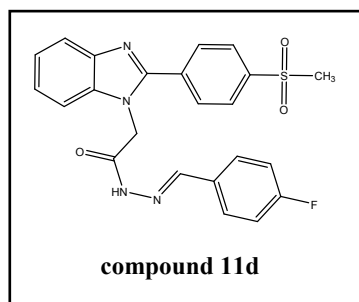
===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



16. ¹H and ¹³C NMR Spectra of 11d:

MOHAMEDA-8
PROTON_BSU DMSO {C:\data} nmr 5

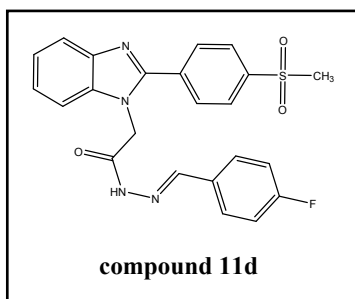


Current Data Parameters
NAME Dec13-2016-nmr
EXPNO 70
PROCNO 1

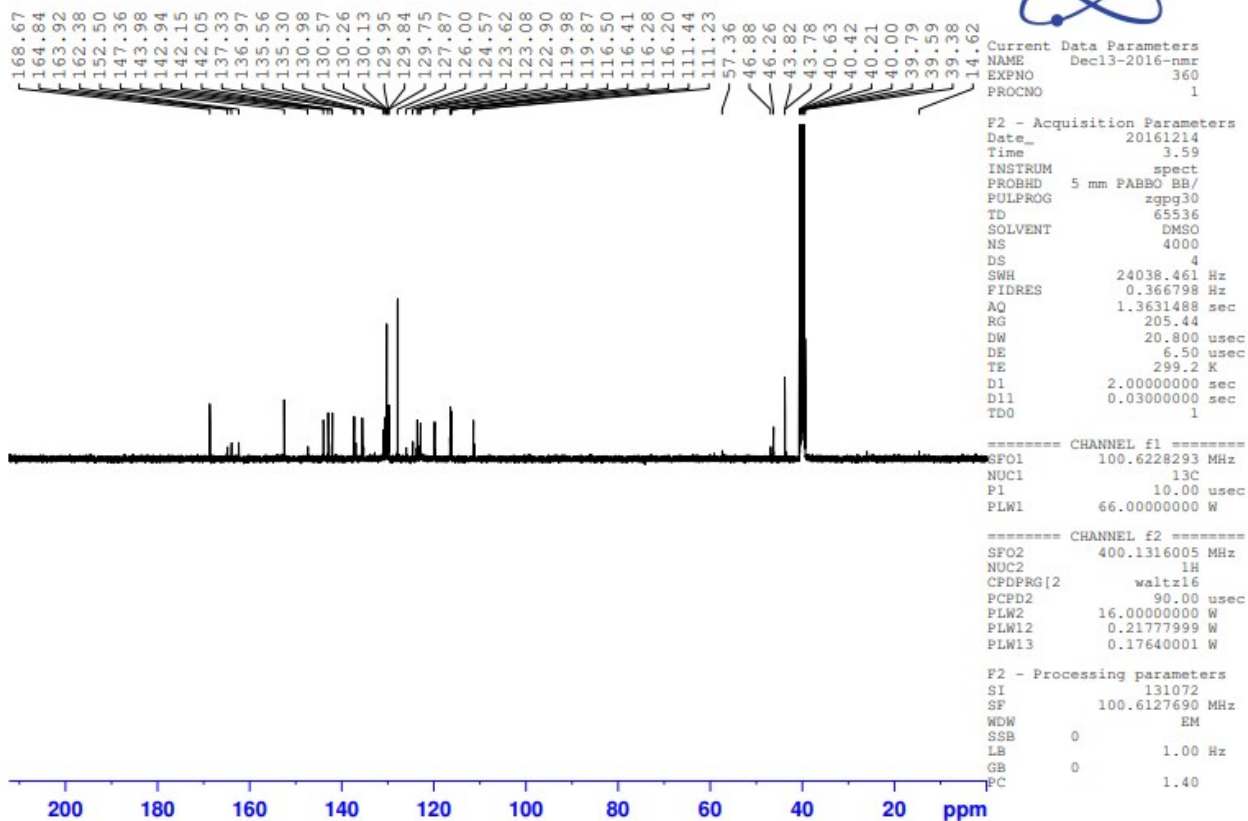
F2 - Acquisition Parameters
Date_ 20161213
Time 9.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 299.1 K
D1 1.0000000 sec
TD0 1

CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

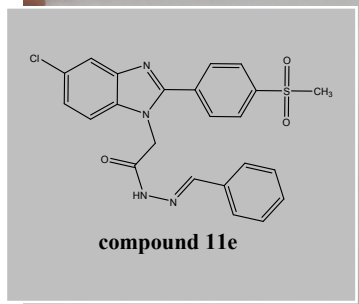
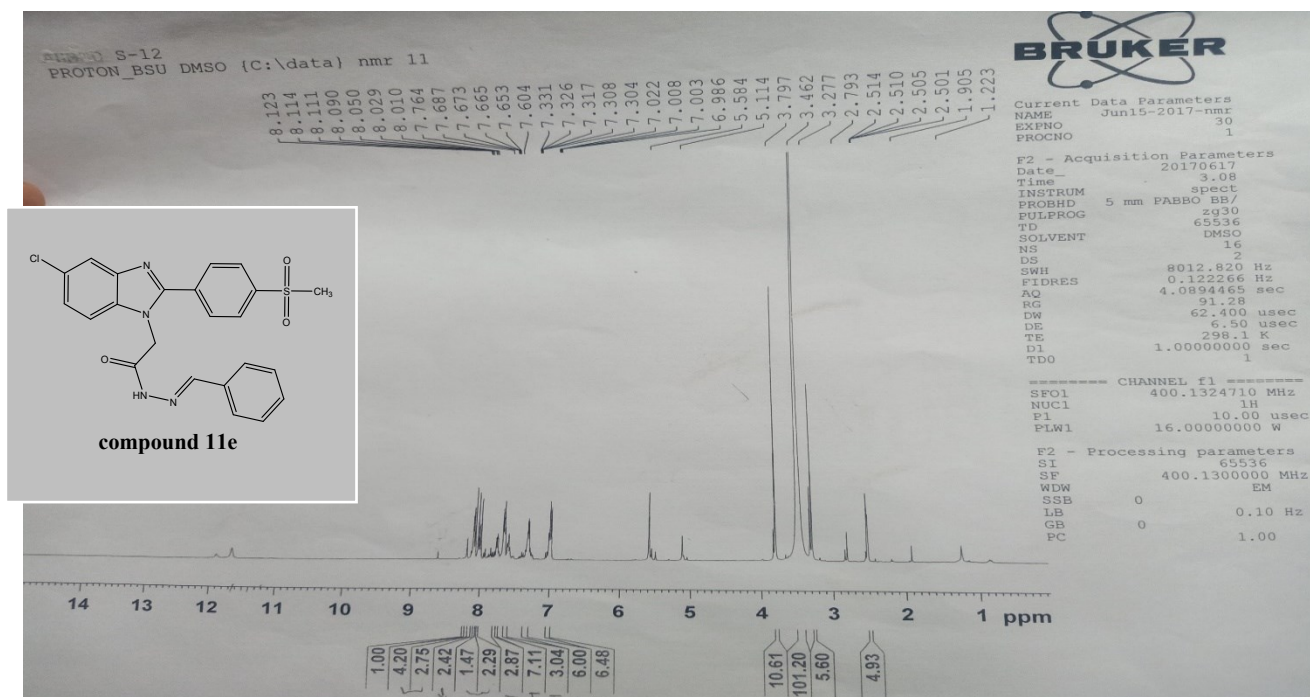
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



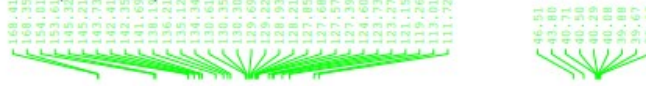
MOHAMED-A-8
C13-BSU DMSO (C:\data) nmr 10



17. ¹H and ¹³C NMR Spectra of 11e:

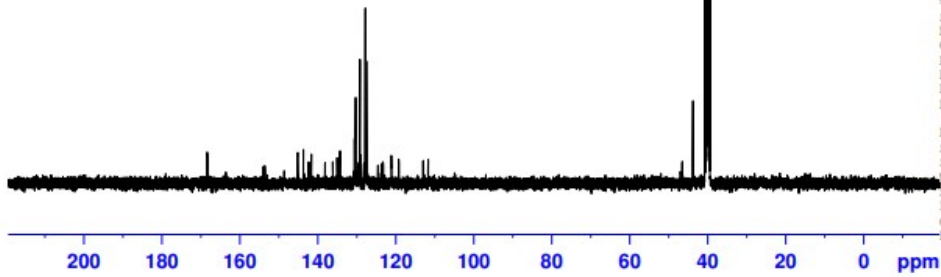
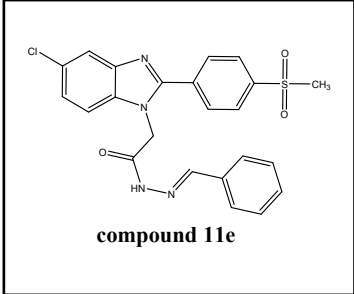


FEBY-CL2
C13-BSU DMSO (C:\data) nmr 20



Current Data Parameters
NAME Feb05-2017-nmr
EXPNO 120
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170206
Time 10.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 313.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

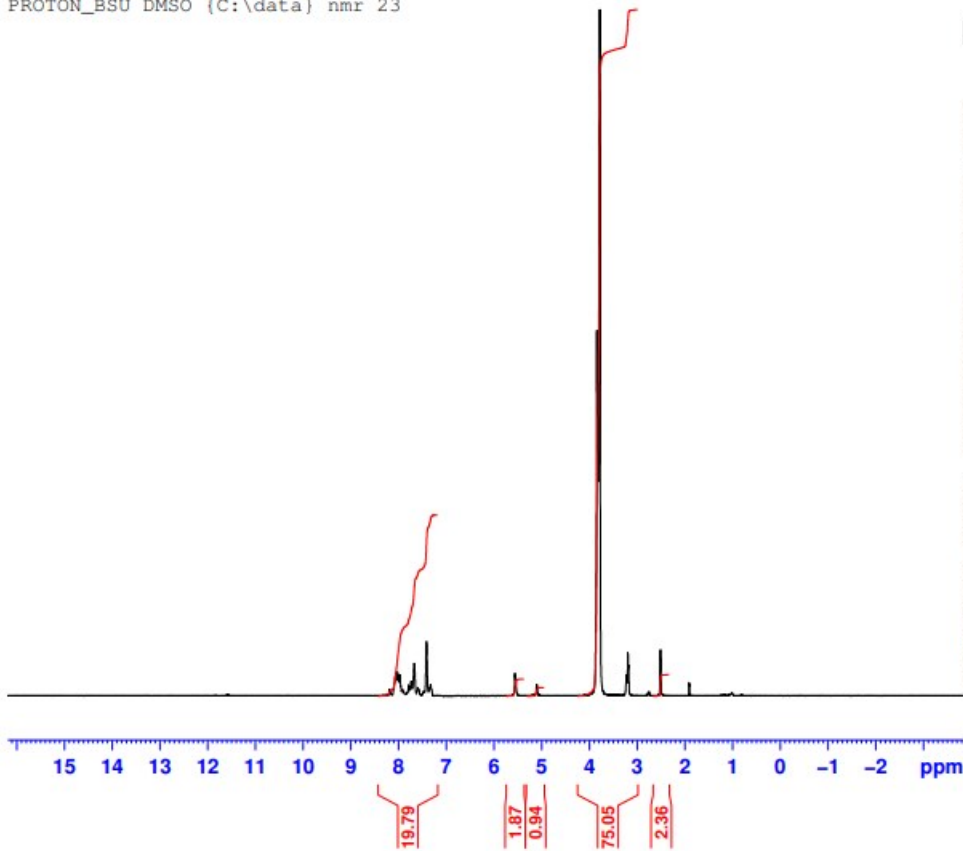


===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 66.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW3 0.21777999 W
PLW13 0.17640001 W

F2 - Processing parameters
SI 131072
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

FEBY-CL2-D20
PROTON_BSU DMSO (C:\data) nmr 23



Current Data Parameters
NAME Feb06-2017-nmr
EXPNO 30
PROCNO 1

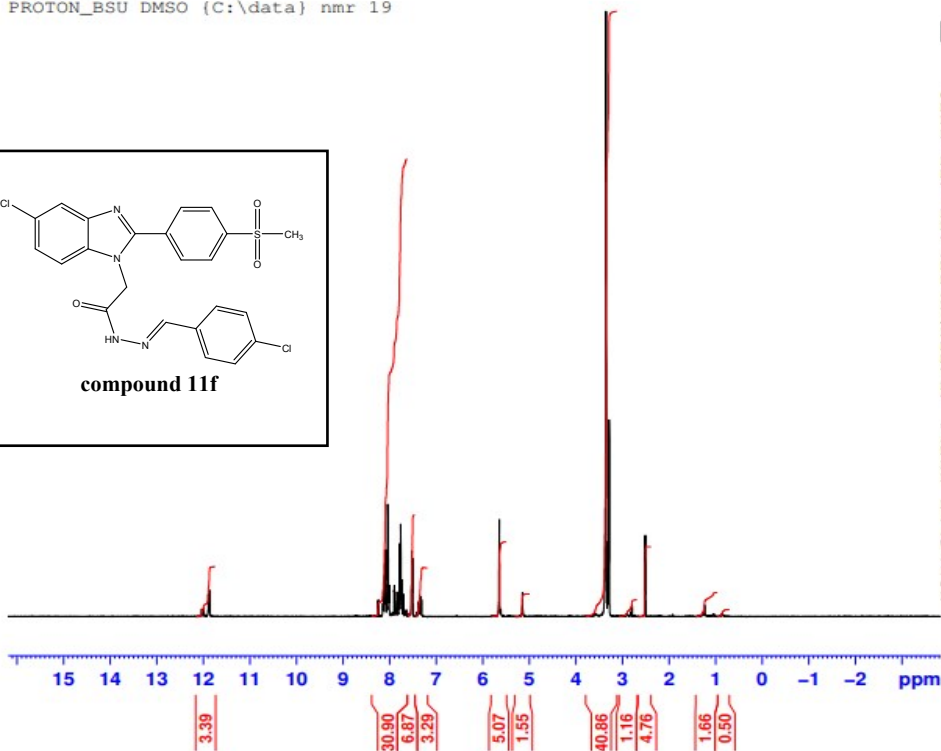
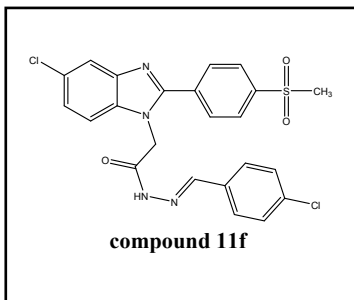
F2 - Acquisition Parameters
Date_ 20170206
Time 11.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 102.37
DW 62.400 usec
DE 6.50 usec
TE 313.2 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

18. ¹H and ¹³C NMR Spectra of 11f:

MARCO-CL10
 PROTON_BSU DMSO (C:\data) nmr 19



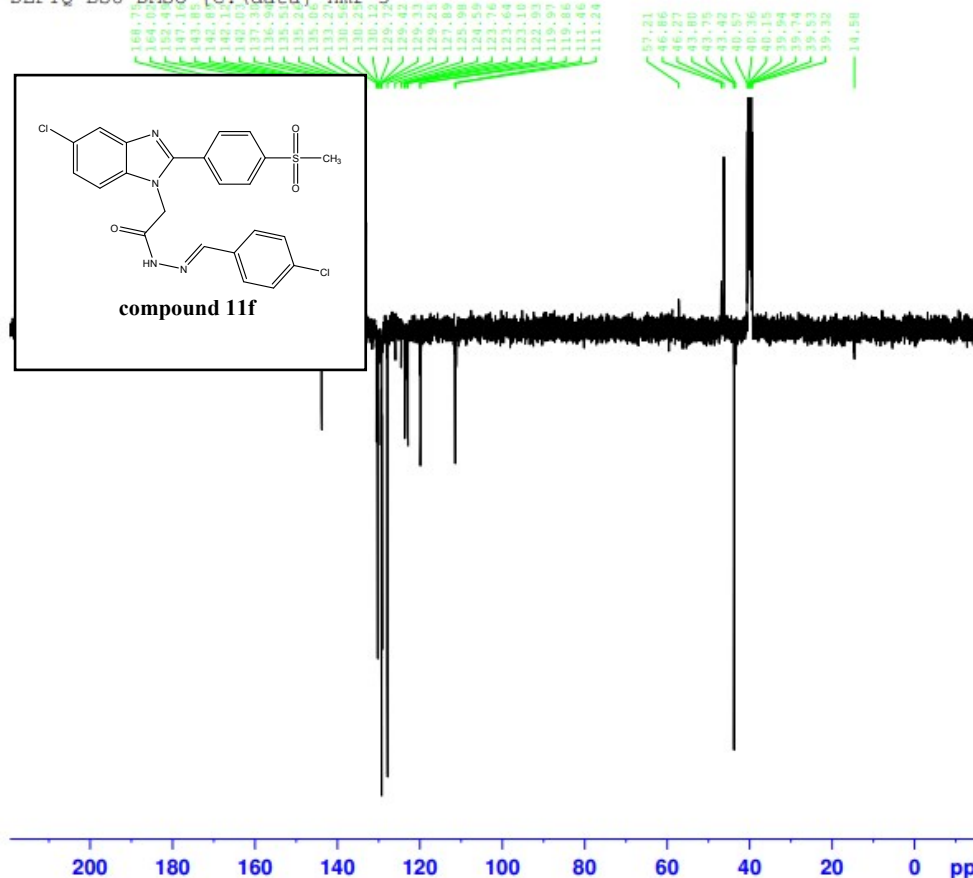
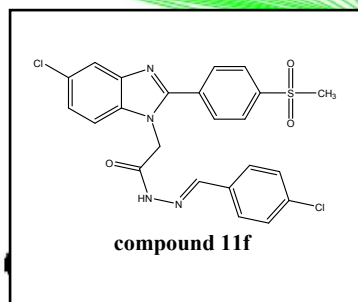
Current Data Parameters
 NAME Mar11-2017-nmr
 EXPNO 270
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170311
 Time 17.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 SF01 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.0000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

MARCO-10
DEPTQ-BSU DMSO (C:\data) nmr 3



Current Data Parameters
NAME Apr13-2017-nmr
EXPNO 40
PROCNO 1

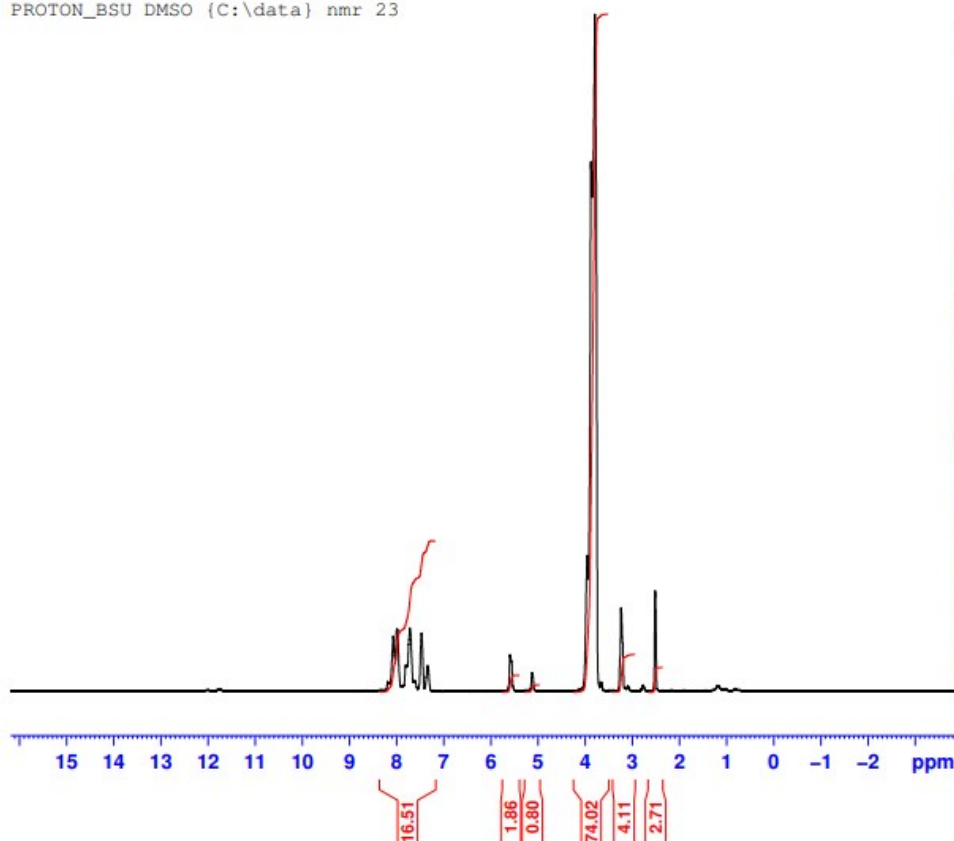
F2 - Acquisition Parameters
Date_ 20170414
Time 11.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.343188 sec
RG 205.44
DM 20.800 usec
DE 6.50 usec
TE 296.2 K
CHST2 145.000000
CHST12 1.500000
D3 2.0000000 sec
D2 0.00344828 sec
D12 0.00020000 sec
D16 0.00020000 sec
TD0 3

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
PL1 2000.00 usec
PLW1 0 W
SFO2 400.132797 MHz
NUC2 1H
CFPRG(2) waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.0000000 W
PLW12 0.21771999 W

===== GRADIENT CHANNEL =====
GPRAM[1] SMC10.100
GPRAM[2] SMC10.100
GPRAM[3] SMC10.100
GPI1 31.00 %
GPI2 31.00 %
GPI3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

MARCO-CL10-D20
PROTON_BSU DMSO (C:\data) nmr 23



Current Data Parameters
NAME Mar18-2017-nmr
EXPNO 60
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170318
Time 13.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 91.28
DM 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

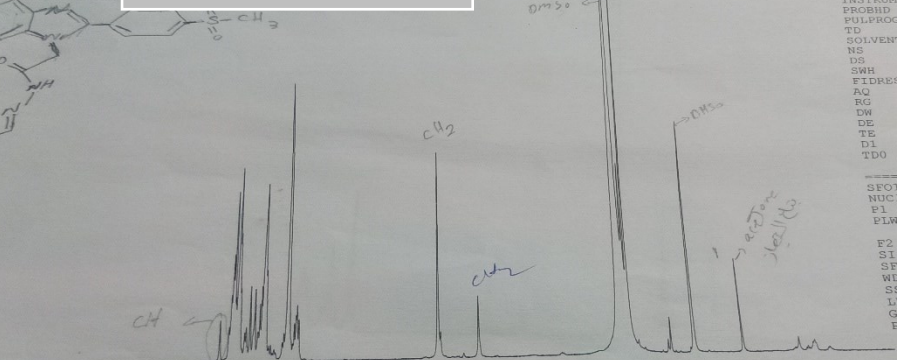
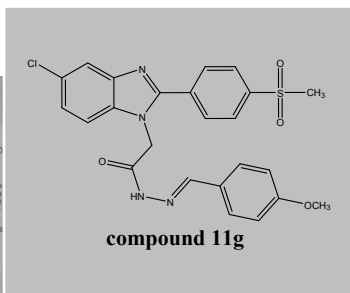
===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.0000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

19. ¹H and ¹³C NMR Spectra of 11g:

-CL2
ON_BSU DMSO

8.257
8.151
8.130



Current Data Parameters
NAME Jan29-2017-nmr
EXPNO 220
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170125
Time 17.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.830 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
RW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1

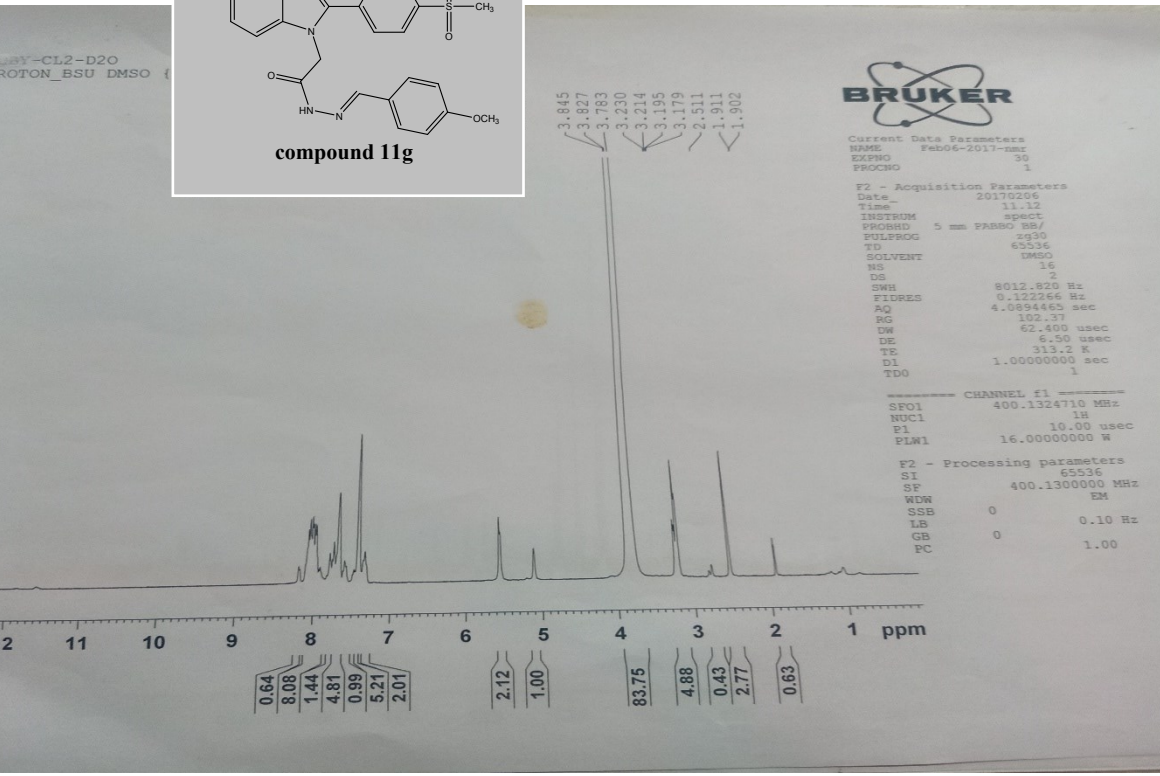
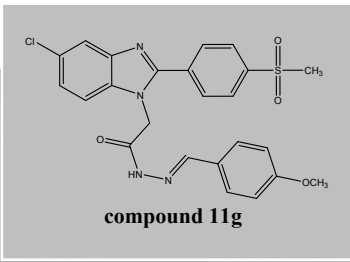
==== CHANNEL f1 =====

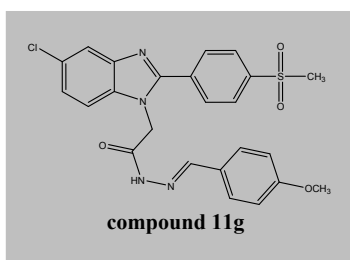
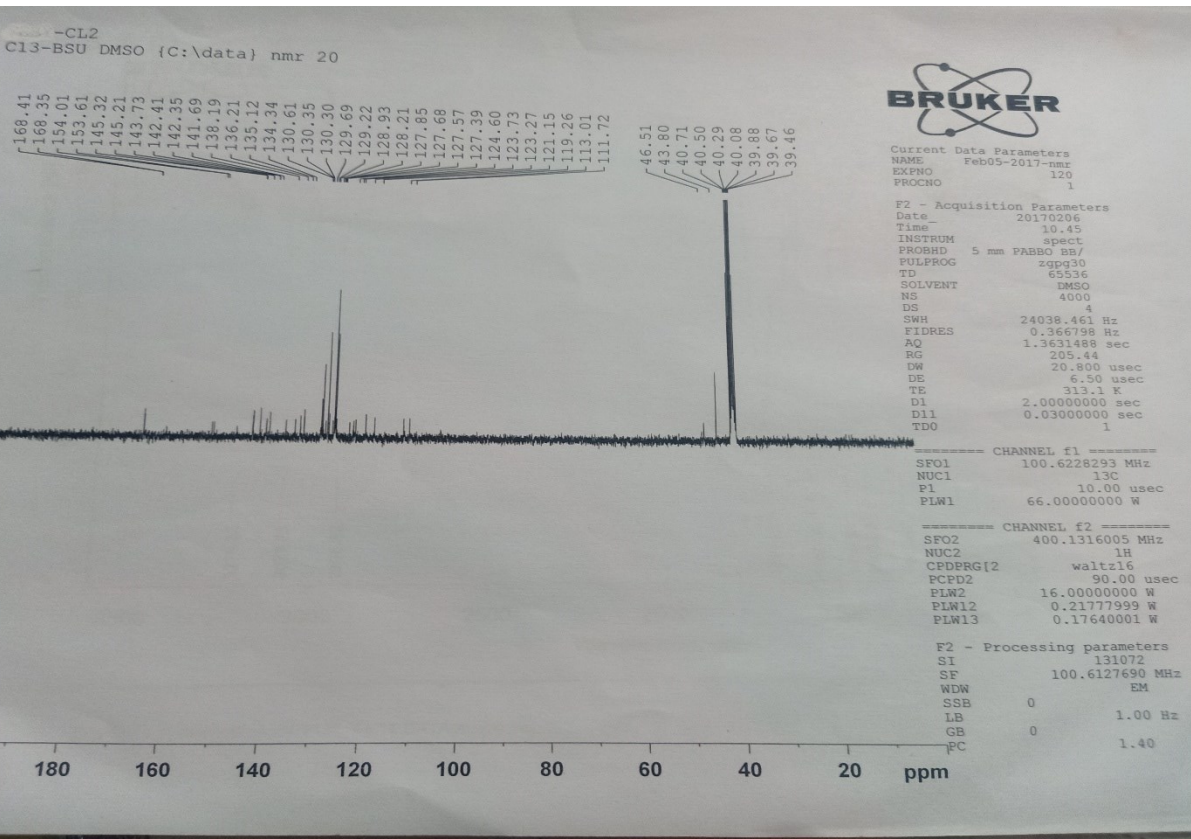
SE01 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

10 9 8 7 6 5 4 3 2 1 ppm

0.33 3.11 3.32 1.53 4.38 4.16 1.28 2.10 0.65 14.31 1.93 3.37 2.27 0.50

...-CL2-D2O
...OTON_BSU DMSO





20. ¹H and ¹³C NMR Spectra of 11h:

MARCO-CL8
PROTON_BSU DMSO [C:\data] nmr 4

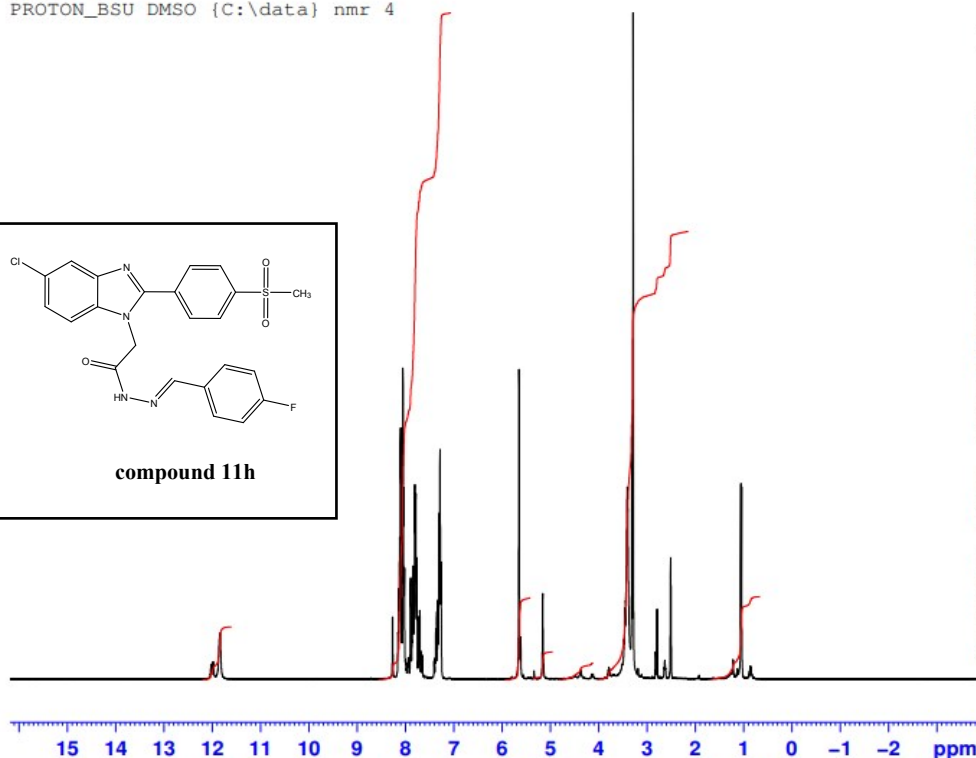
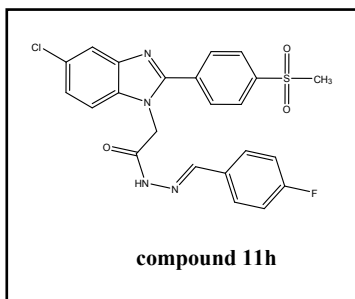


Current Data Parameters
NAME Mar11-2017-nmr
EXPNO 120
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170311
Time 16.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 91.28
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



MARCO-CL-8
C13-BSU DMSO [C:\data] nmr 10



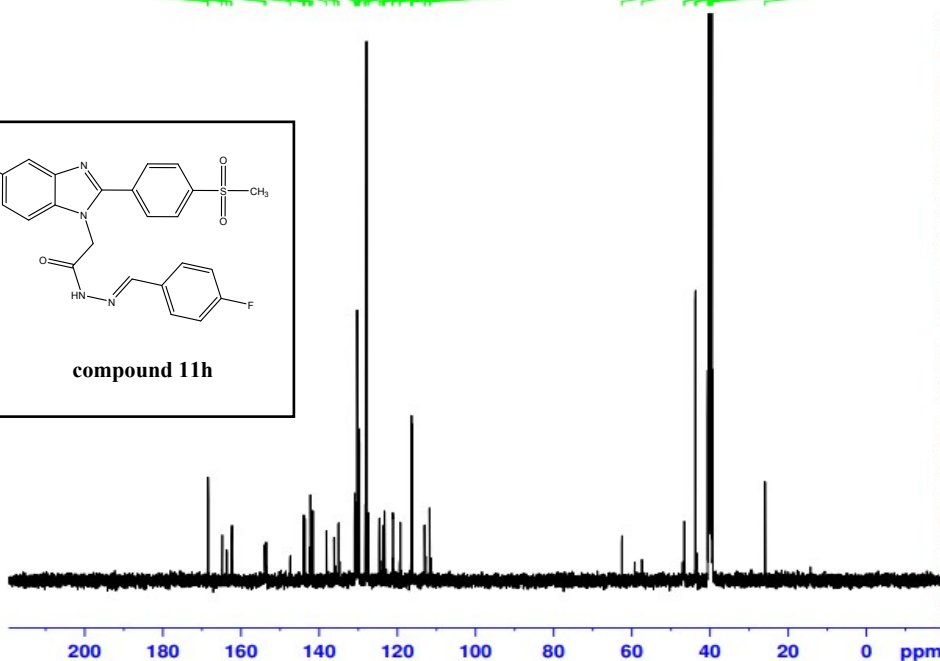
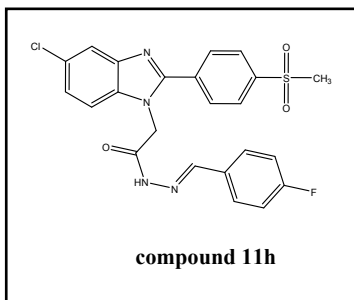
Current Data Parameters
NAME Mar16-2017-nmr
EXPNO 150
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170316
Time 22.21
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

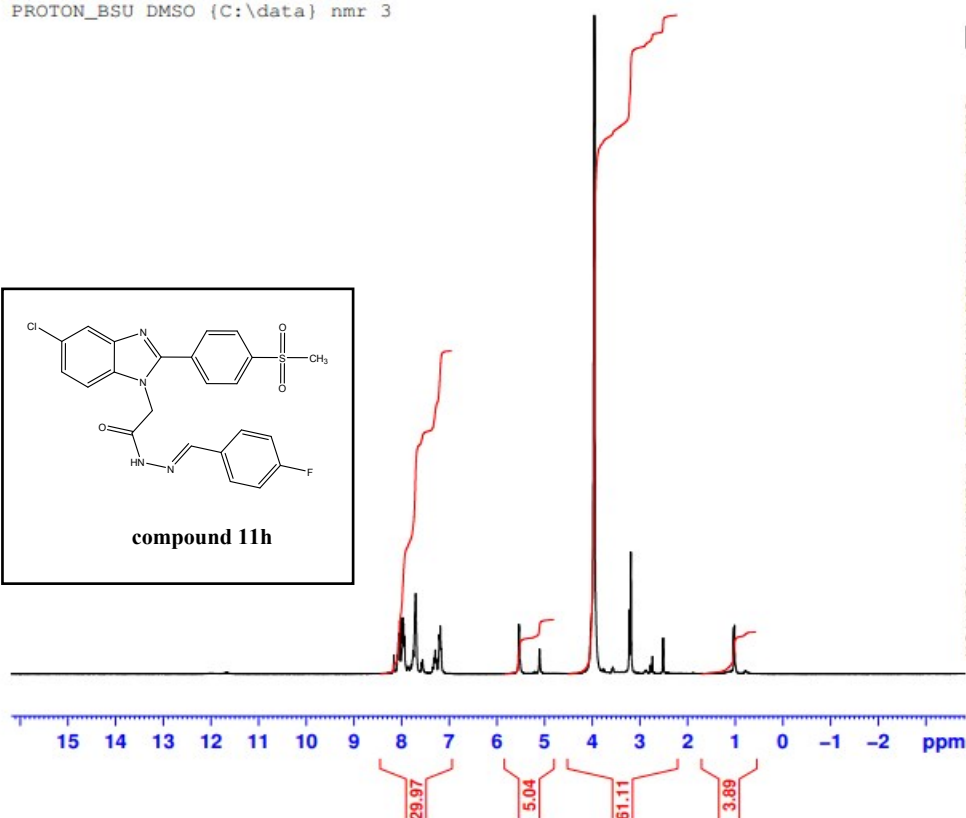
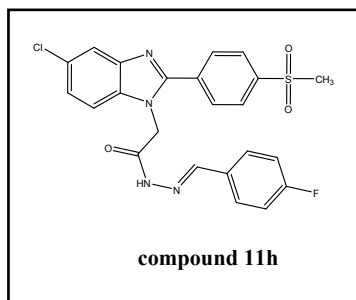
----- CHANNEL f1 -----
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 66.00000000 W

----- CHANNEL f2 -----
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W
PLW13 0.17640001 W

F2 - Processing parameters
SI 131072
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



MARCO-CL8-D20
PROTON_BSU DMSO (C:\data) nmr 3



Current Data Parameters
NAME Mar18-2017-nmr
EXPNO 100
PROCNO 1

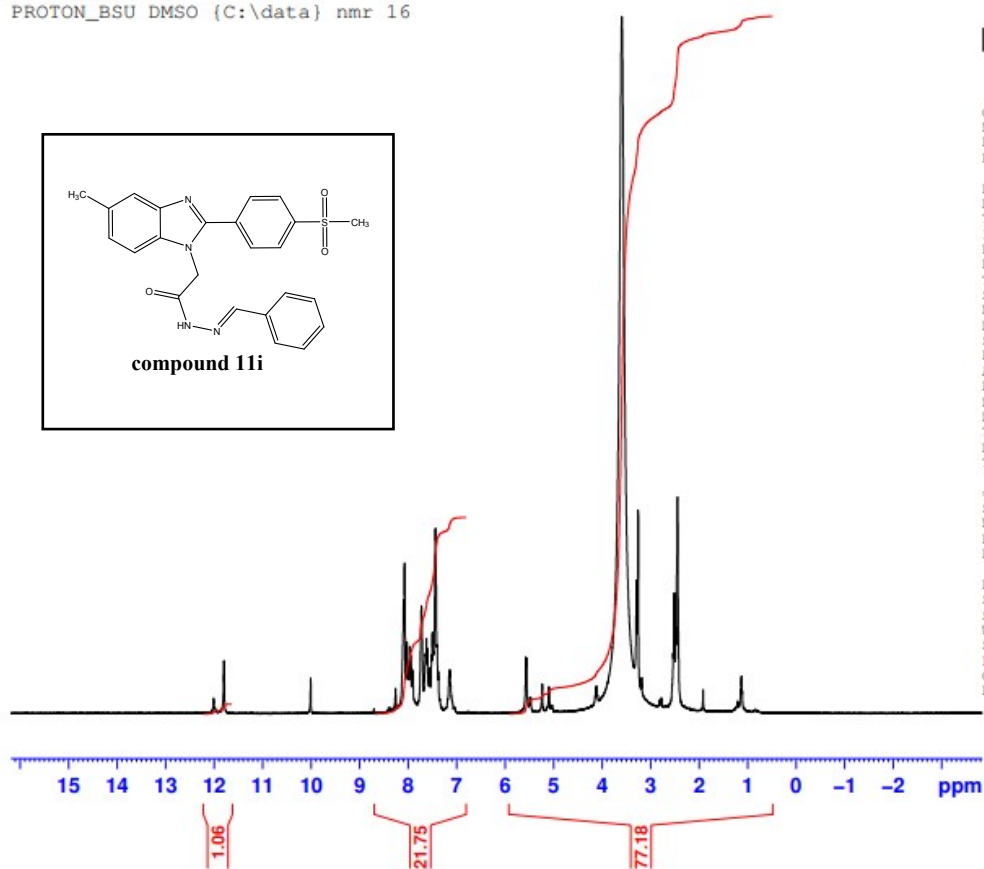
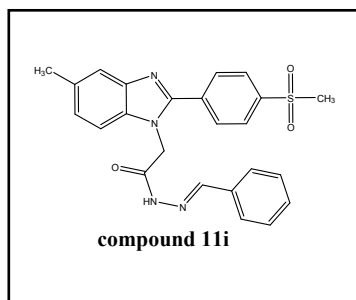
F2 - Acquisition Parameters
Date_ 20170318
Time 14.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 91.28
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.0000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

21. ¹H Spectra of 11i:

AHMED S-M2
PROTON_BSU DMSO (C:\data) nmr 16



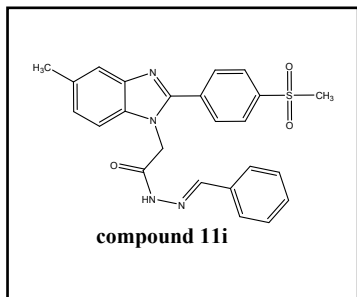
Current Data Parameters
NAME Jul19-2017-nmr
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170719
Time 14.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 74.78
DW 62.400 usec
DE 6.50 usec
TE 298.3 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.0000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

AHMED S - M2 (D2O)
PROTON_BSU DMSO {C:\data} nmr 8

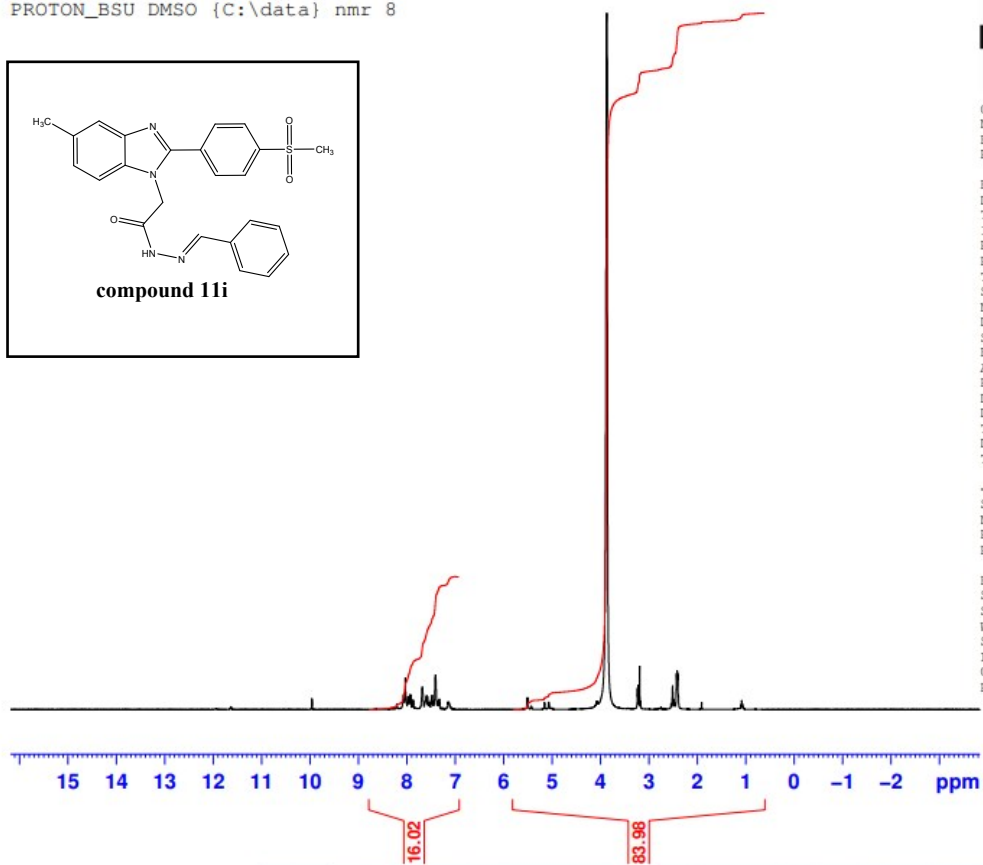


Current Data Parameters
NAME Jul29-2017-nmr
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170729
Time 12.19
INSTRUM spect
FROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 66.73
DW 62.400 usec
DE 6.50 usec
TE 306.9 K
D1 1.00000000 sec
TD0 1

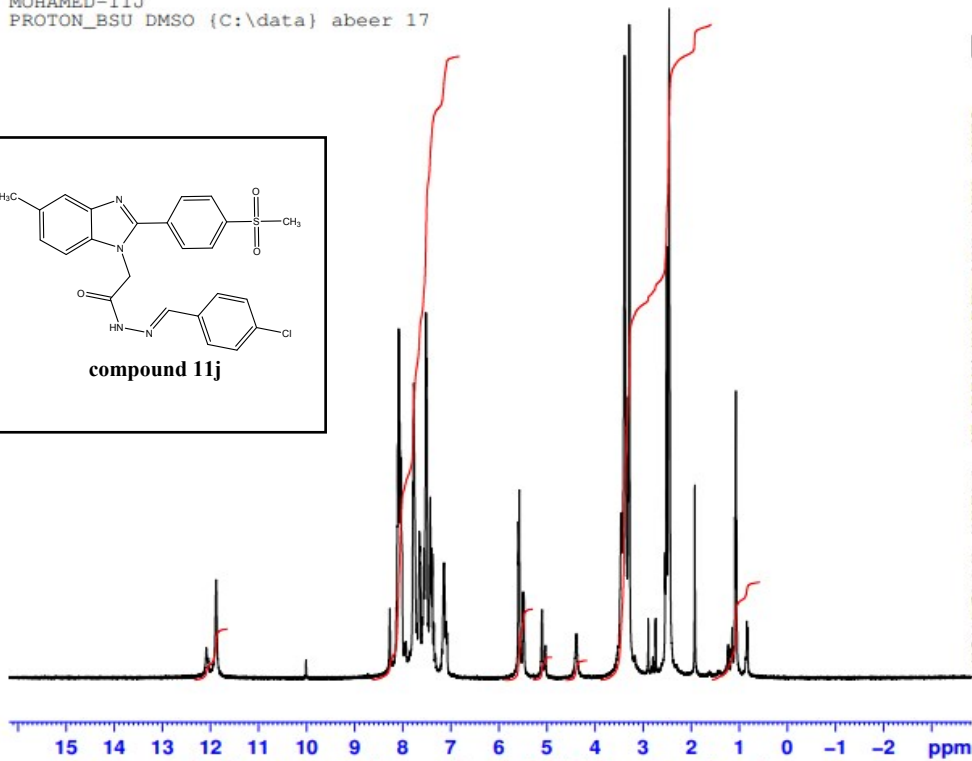
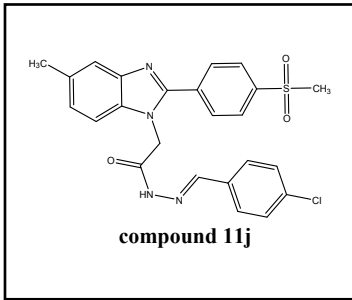
----- CHANNEL f1 -----
SF01 400.1324710 MHz
NUC1 1H
F1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



22. ¹H and ¹³C NMR Spectra of 11j:

MOHAMED-11J
PROTON_BSUS DMSO {C:\data} abeer 17



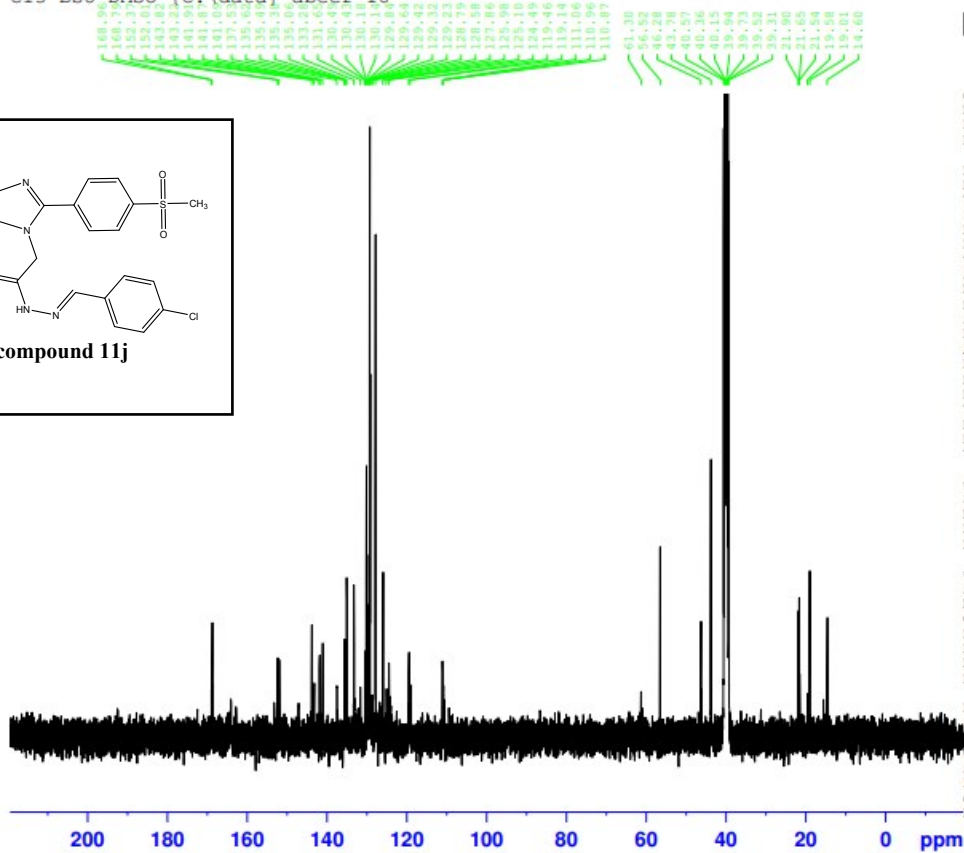
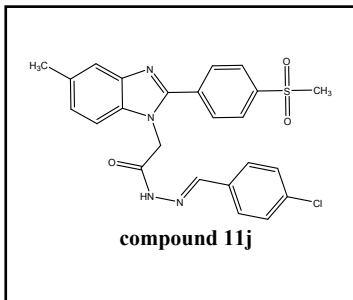
Current Data Parameters
NAME Apr05-2021-abeer
EXPNO 90
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210405
Time 10.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 296.7 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.0000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

MOHAMED-11J
C13-BSUS DMSO {C:\data} abeer 18



Current Data Parameters
NAME Apr08-2021-abeer
EXPNO 170
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210409
Time 10.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 297.5 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

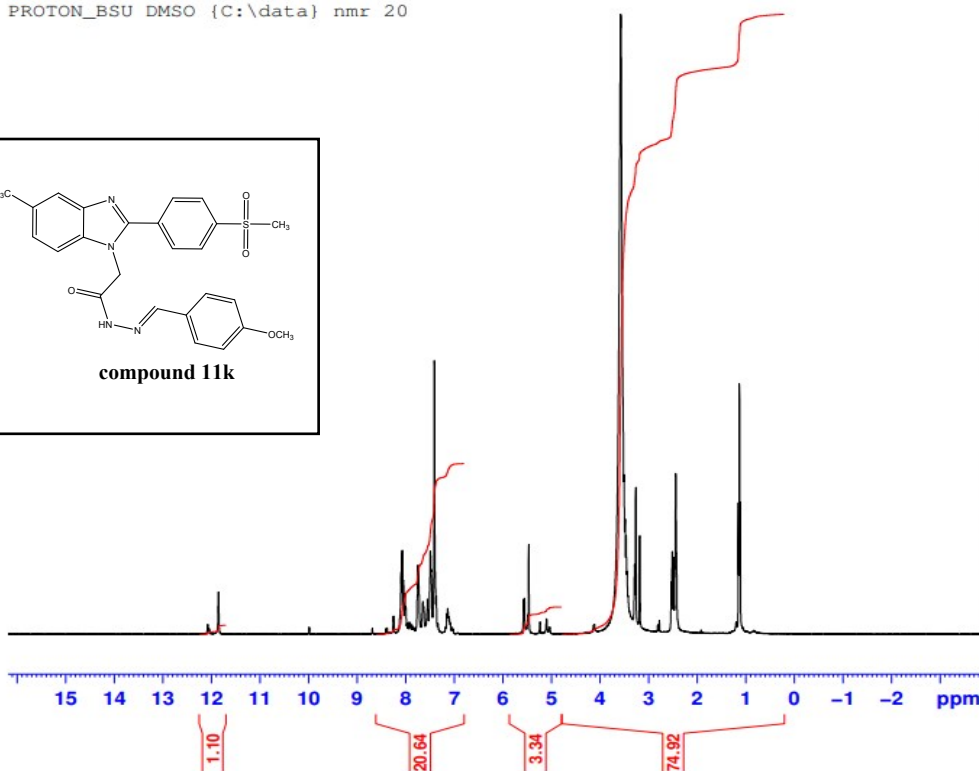
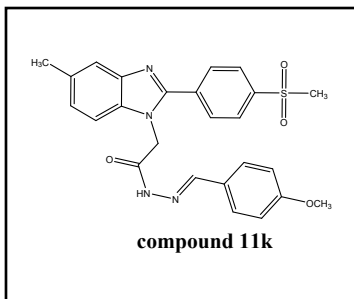
===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 66.0000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.0000000 W
PLW12 0.21777999 W
PLW13 0.17640001 W

F2 - Processing parameters
SI 131072
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

23. ¹H Spectra of 11k:

PROTON_BSU DMSO {C:\data} nmr 20



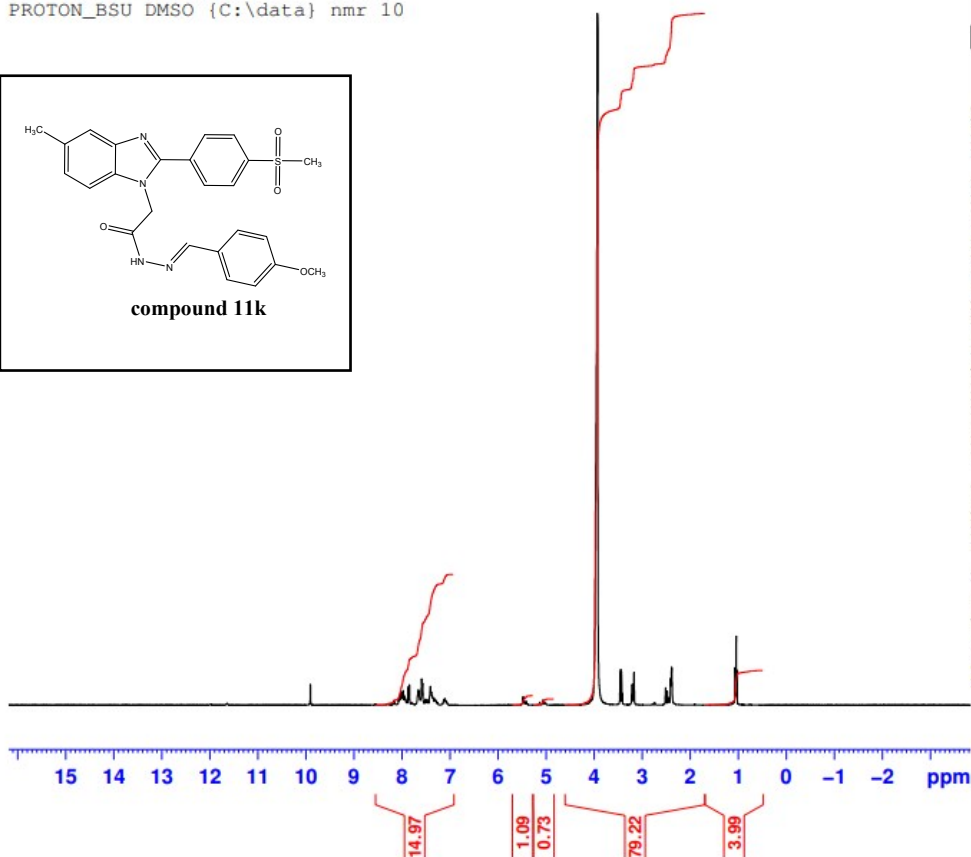
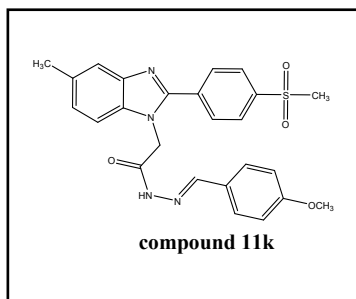
Current Data Parameters
 NAME Jul19-2017-nmr
 EXPNO 70
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170719
 Time 15.18
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 74.78
 DW 62.400 usec
 DE 6.50 usec
 TE 298.9 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

AHMED S - M10 (D2O)
 PROTON_BSU DMSO {C:\data} nmr 10



Current Data Parameters
 NAME Jul29-2017-nmr
 EXPNO 50
 PROCNO 1

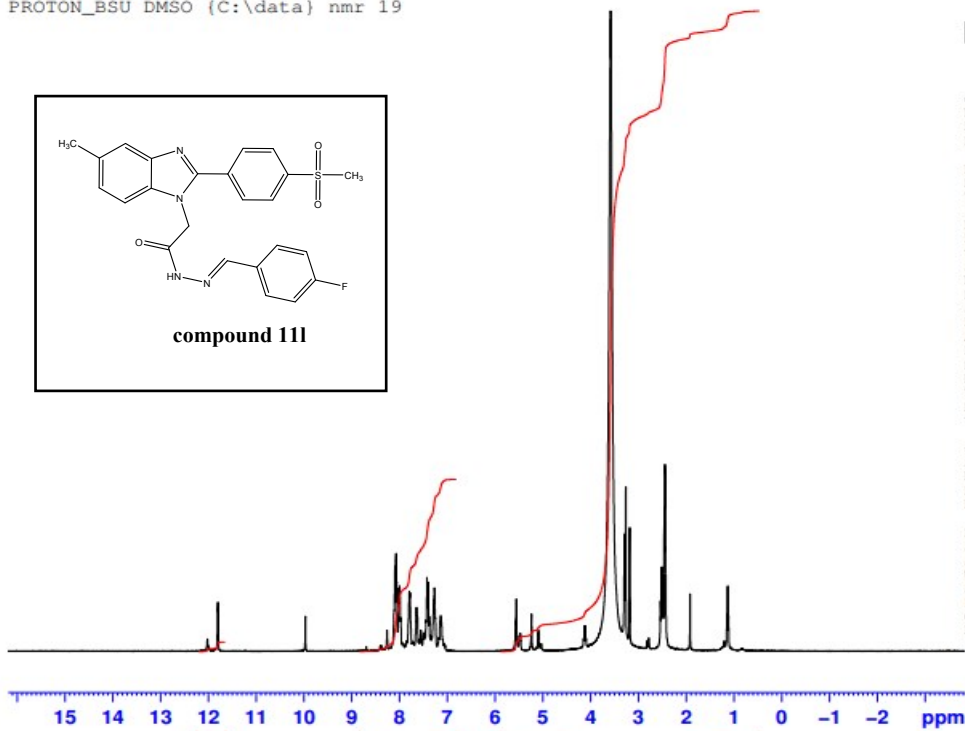
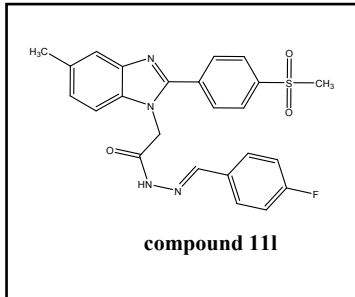
F2 - Acquisition Parameters
 Date_ 20170729
 Time 12.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 66.73
 DW 62.400 usec
 DE 6.50 usec
 TE 308.0 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

24. ¹H and ¹³C NMR Spectra of 111:

AHMED S-M 8
PROTON_BSU DMSO {C:\data} nmr 19



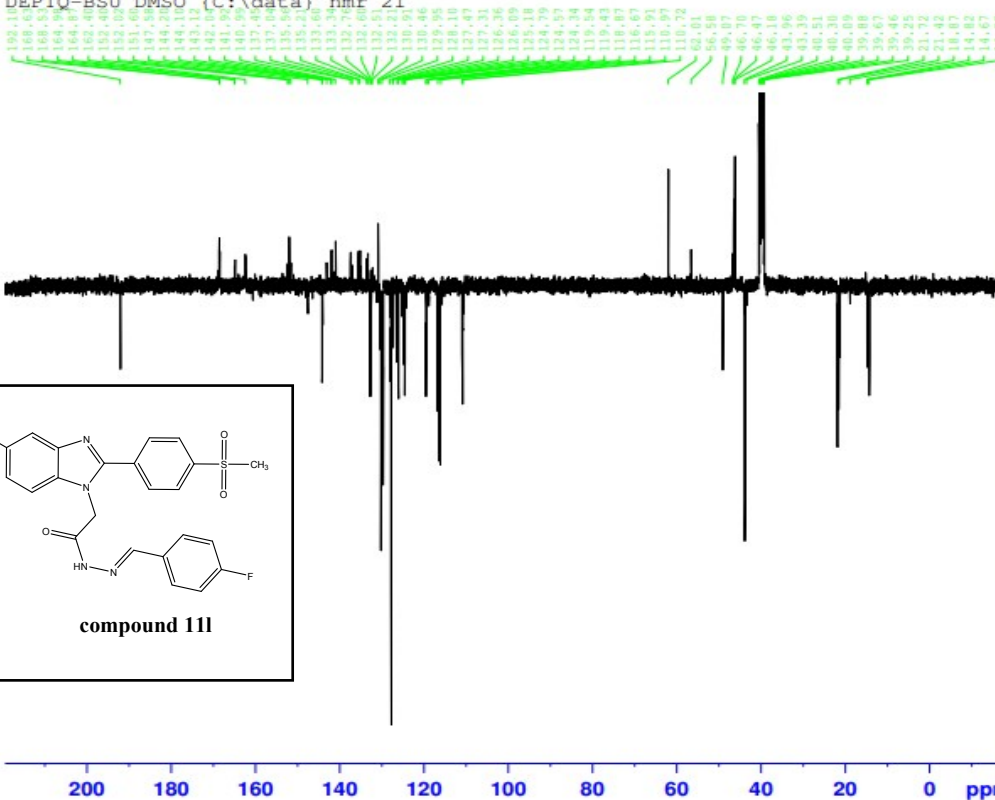
Current Data Parameters
NAME Jul19-2017-nmr
EXPNO 60
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170719
Time 15.14
INSTRUM spect
PROBHD 5 mm FAPBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 74.78
DW 62.400 usec
DE 6.50 usec
TE 298.9 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.0000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

AHMED S- M8
DEPTQ-BSU DMSO {C:\data} nmr 21



Current Data Parameters
NAME Jul19-2017-nmr
EXPNO 30
PROCNO 1

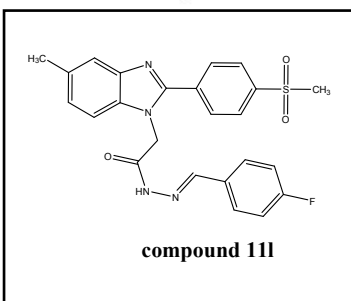
F2 - Acquisition Parameters
Date_ 20170731
Time 22.26
INSTRUM spect
PROBHD 5 mm FAPBO BB/
PULPROG deptq002
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.448 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 313.1 K
CMST2 145.000000
CMST12 1.300000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
PLW1 2000.00 usec
PLW2 0 W
PLW3 66.0000000 W
SFOFF5 Ccpd0comp. 4
SFOFF5 0 Hz
SFOFF5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG2 waltz16
P2 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.0000000 W
PLW12 0.21177999 W

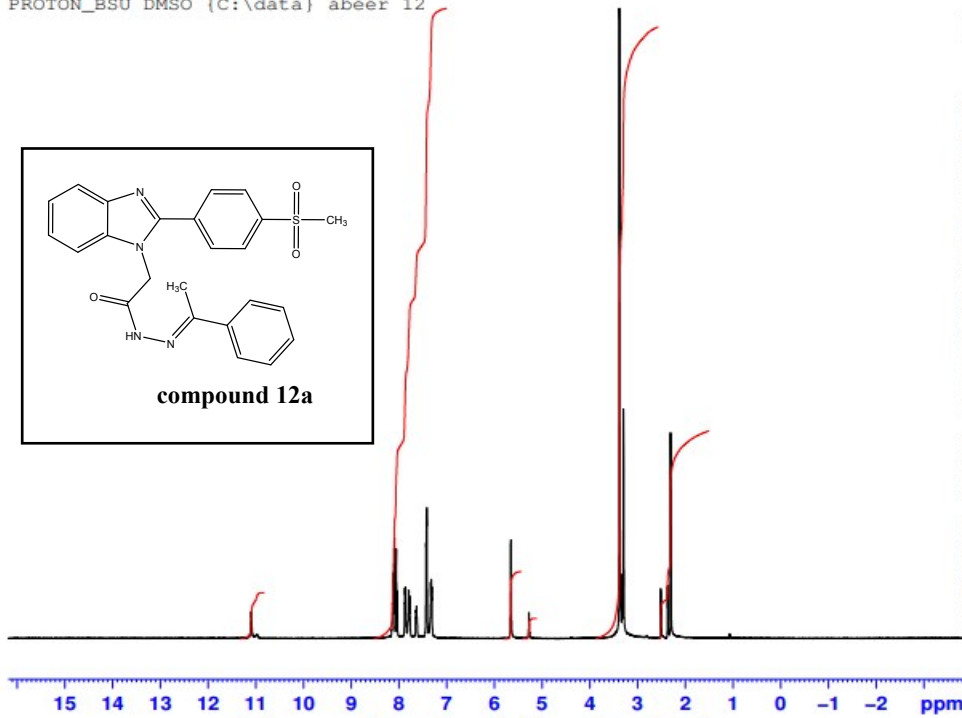
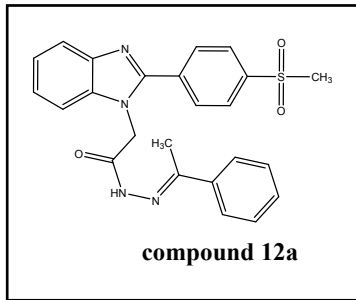
===== GRADIENT CHANNEL =====
GPNAM[1] SREG0.100
GPNAM[2] SREG0.100
GPNAM[3] SREG0.100
GPE1 31.00 %
GPE2 31.00 %
GPE3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.40



25. ¹H and ¹³C NMR Spectra of 12a:

MOHAMED-12a
 PROTON_BSU DMSO {C:\data} abeer 12



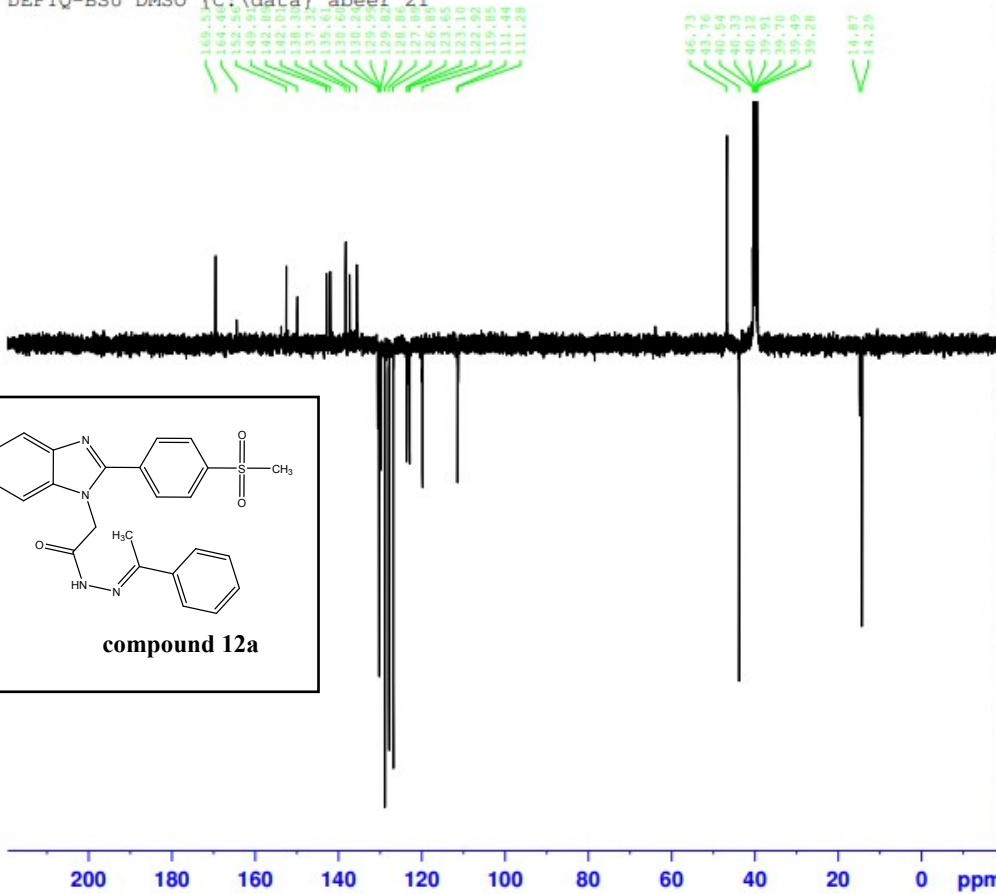
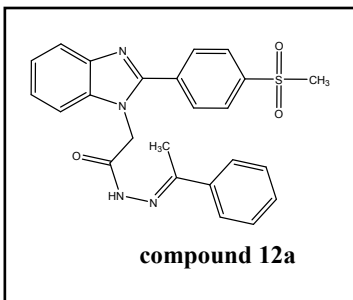
Current Data Parameters
 NAME Apr06-2021-abeer
 EXPNO 60
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210406
 Time 9.44
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 296.6 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

MOHAMED-12a
 DEPTQ-BSU DMSO {C:\data} abeer 21



Current Data Parameters
 NAME April-2021-abeer
 EXPNO 50
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210411
 Time 9.34
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG deptq
 TD 65536
 SOLVENT DMSO
 NS 4000
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.136798 Hz
 AQ 1.3431488 sec
 RG 205.44
 DW 20.800 usec
 DE 6.50 usec
 TE 297.1 K
 INST2 145.000000
 CHST12 1.500000
 D1 2.0000000 sec
 D2 0.00344828 sec
 D12 0.0002000 sec
 D16 0.0002000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6228303 MHz
 NUC1 13C
 P1 10.00 usec
 PL13 2000.00 usec
 PLW1 0 W
 PLW1 66.00000000 W
 SPNAM(5) Crp40comp.4
 SFOAL5 0.500
 SFOFT55 0 Hz
 SPW5 10.08399963 W

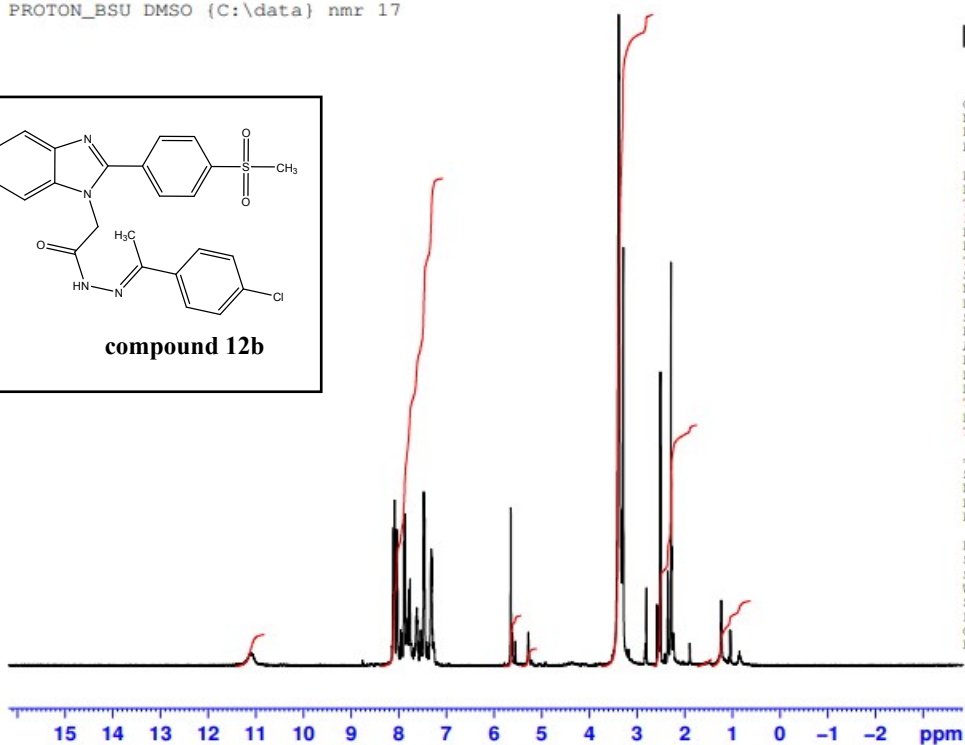
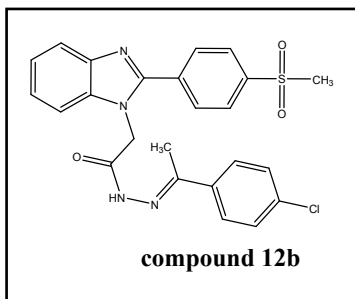
===== CHANNEL f2 =====
 SFO2 400.1321797 MHz
 NUC2 1H
 CPDPRG2 waltz16
 P0 15.75 usec
 P3 10.50 usec
 P4 21.00 usec
 PCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
 GPNAM[1] SMCQ10.100
 GPNAM[2] SMCQ10.100
 GPNAM[3] SMCQ10.100
 GPZ1 31.00 %
 GPZ2 31.00 %
 GPZ3 31.00 %
 P16 1000.00 usec

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 MCM RM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

26. ¹H and ¹³C NMR Spectra of 12b:

AHMED-1A
PROTON_BSU DMSO {C:\data} nmr 17



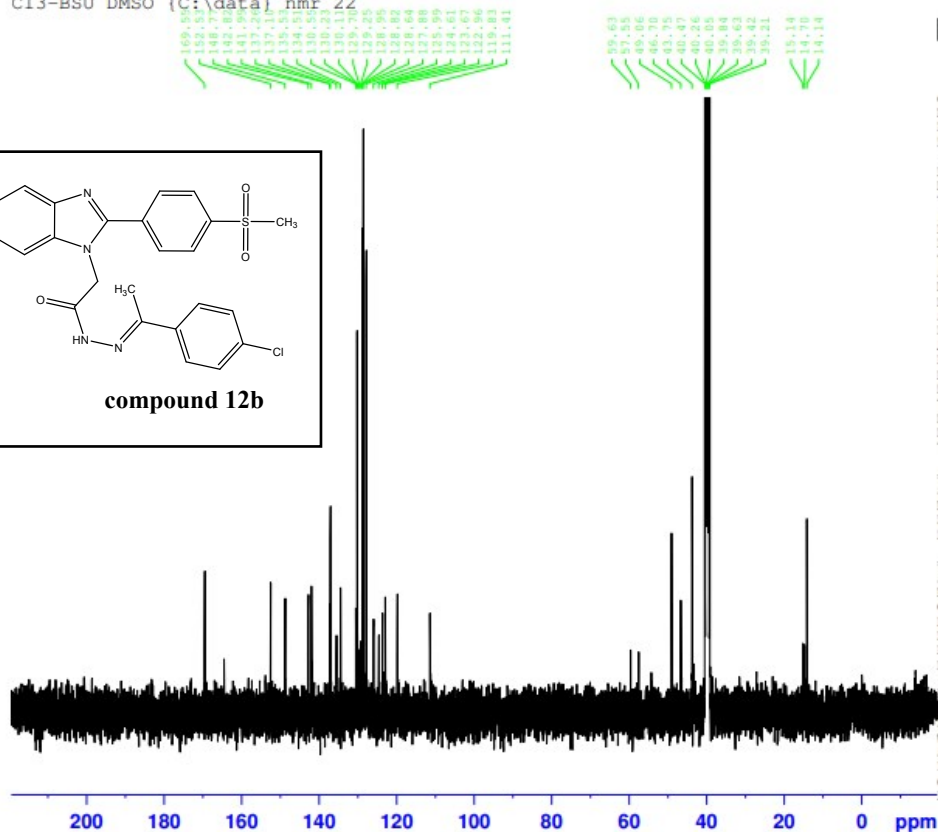
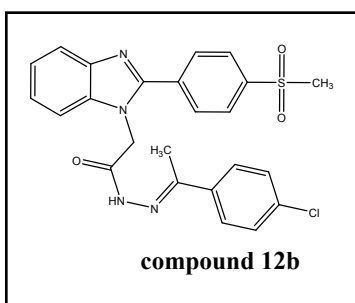
Current Data Parameters
NAME Jan25-2017-nmr
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170125
Time 16.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.0000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

AHMED S-1A
C13-BSU DMSO {C:\data} nmr 22



Current Data Parameters
NAME Feb22-2017-nmr
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170222
Time 13.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

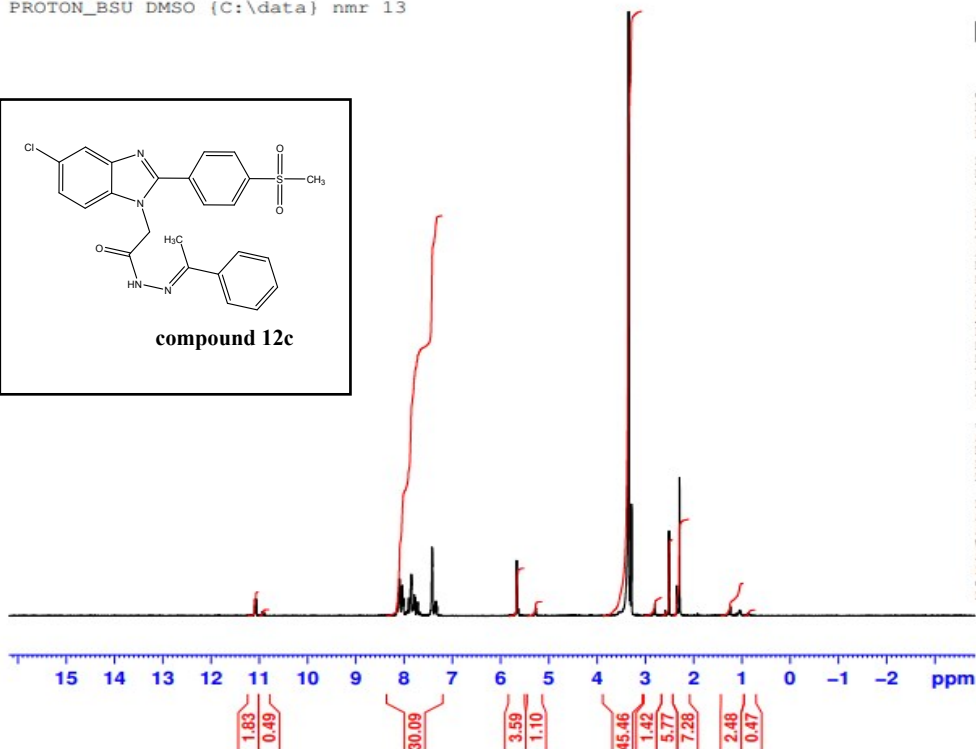
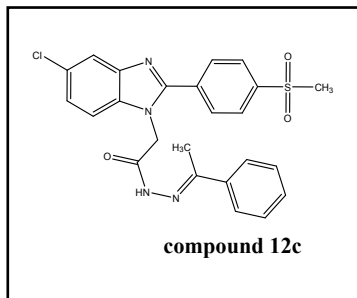
===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 66.0000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CFDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.0000000 W
PLW12 0.2177999 W
PLW13 0.17640001 W

F2 - Processing parameters
SI 131072
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

27. ¹H and ¹³C NMR Spectra of 12c:

MARCO-CL3
PROTON_BSU DMSO {C:\data} nmr 13



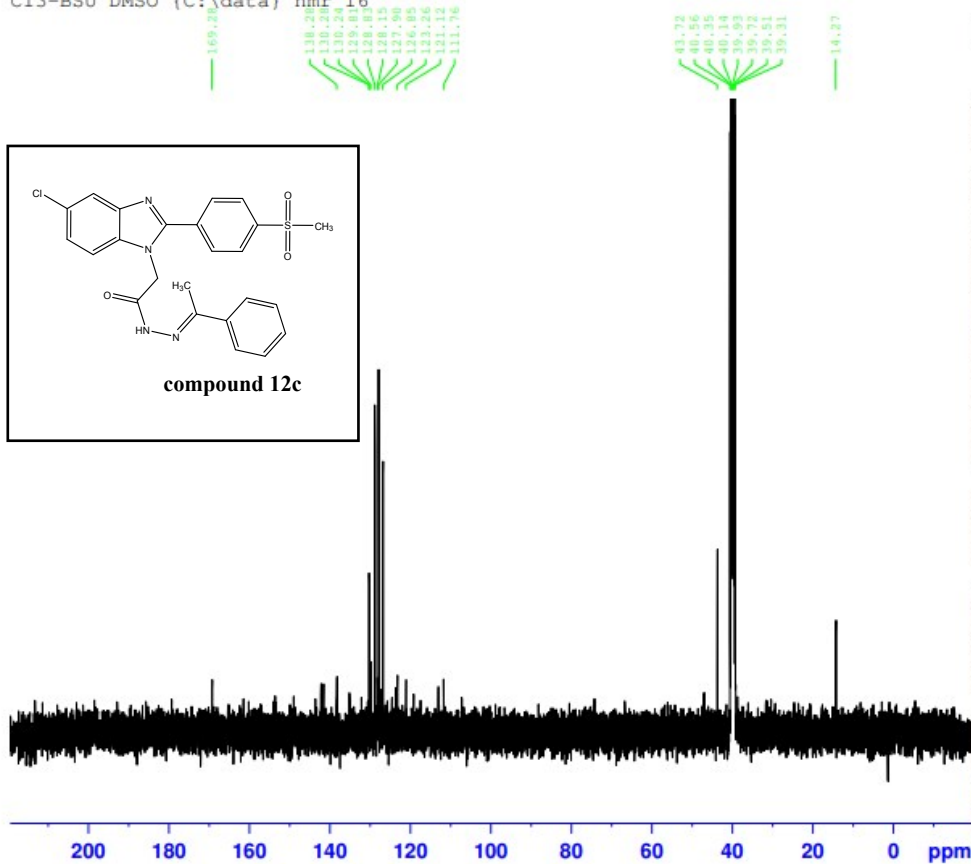
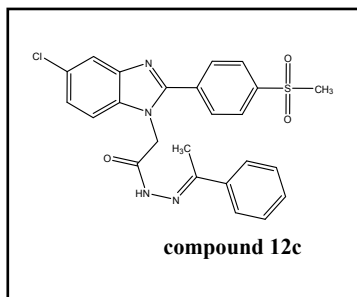
Current Data Parameters
NAME Mar11-2017-nmr
EXPNO 210
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170311
Time 16.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.0000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

MARCO-CL3
C13-BSU DMSO {C:\data} nmr 16



Current Data Parameters
NAME Mar16-2017-nmr
EXPNO 210
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170317
Time 21.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 66.0000000 W

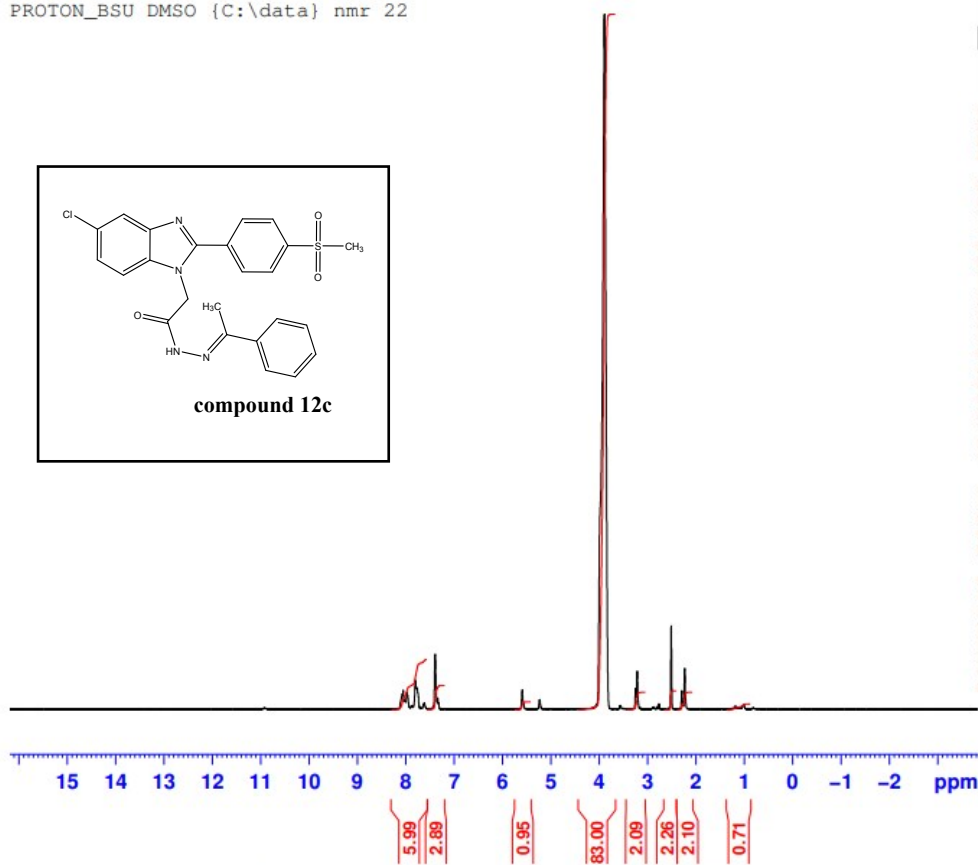
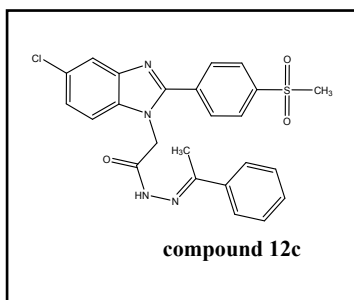
===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.0000000 W
PLW12 0.2177999 W
PLW13 0.17640001 W

F2 - Processing parameters
SI 131072
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME Mar18-2017-nmr
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170318
Time 13.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 91.28
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

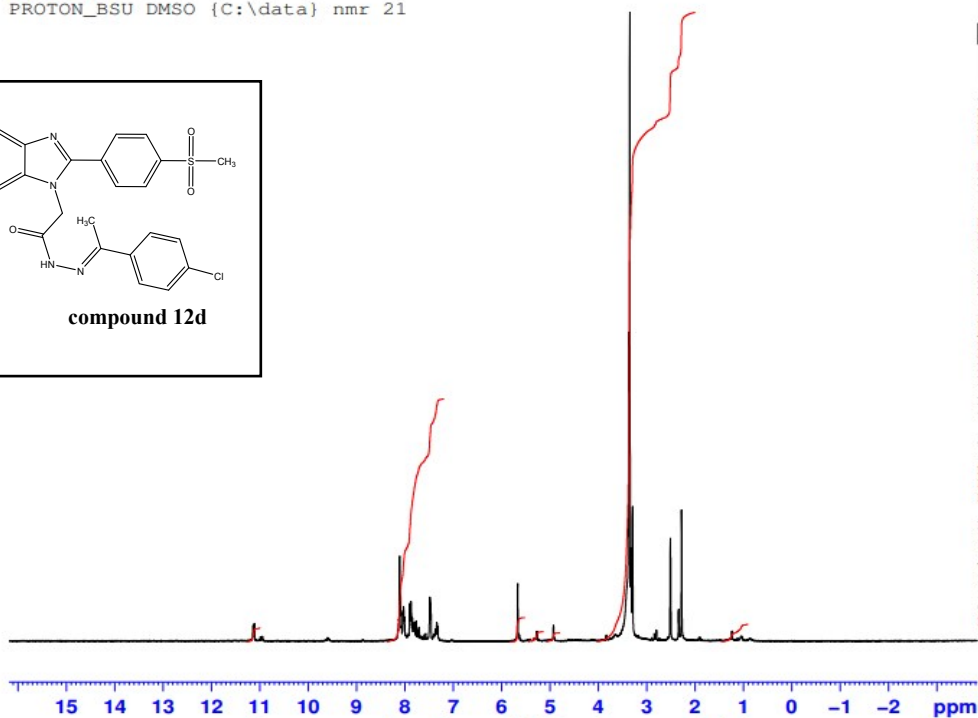
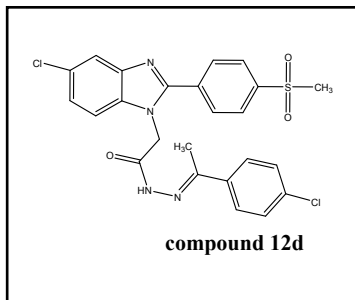


----- CHANNEL f1 -----
SF01 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

28. ¹H and ¹³C NMR Spectra of 12d:

MARCO-CL1
PROTON_BSU DMSO {C:\data} nmr 21



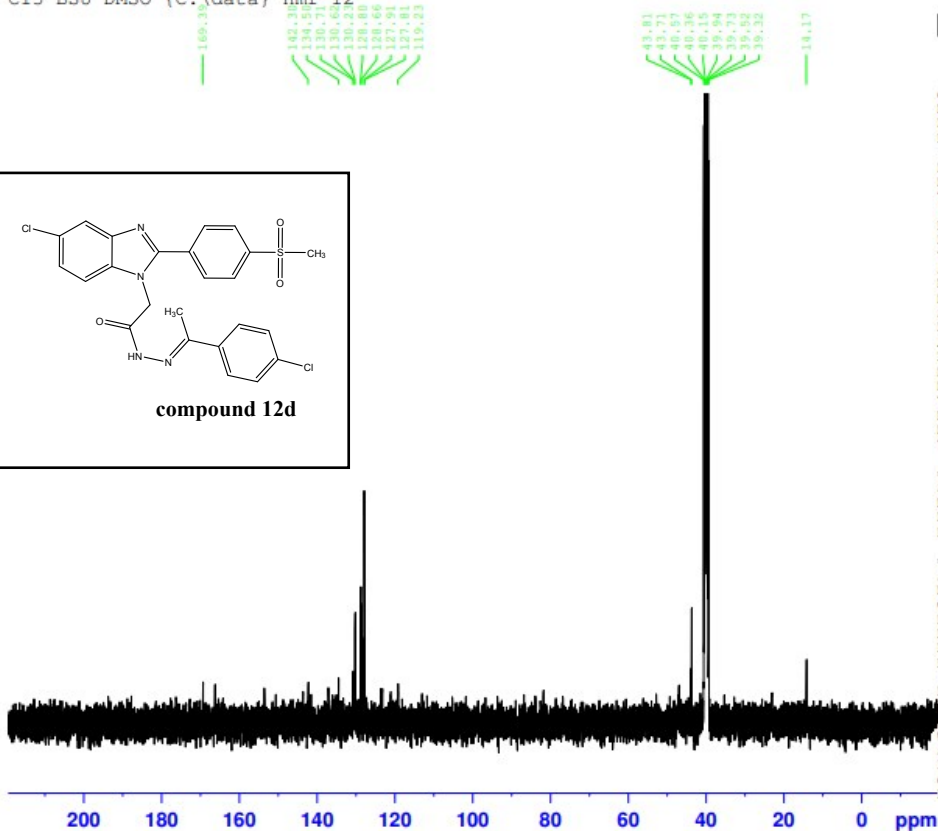
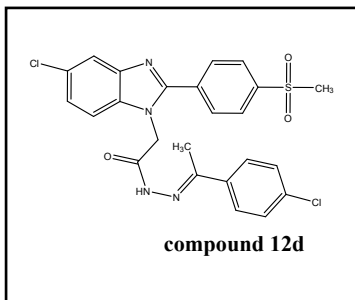
Current Data Parameters
NAME Mar11-2017-nmr
EXPNO 290
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170311
Time 17.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
RG 147.93
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DE 62.400 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

MARCO-CL1
C13-BSU DMSO {C:\data} nmr 12



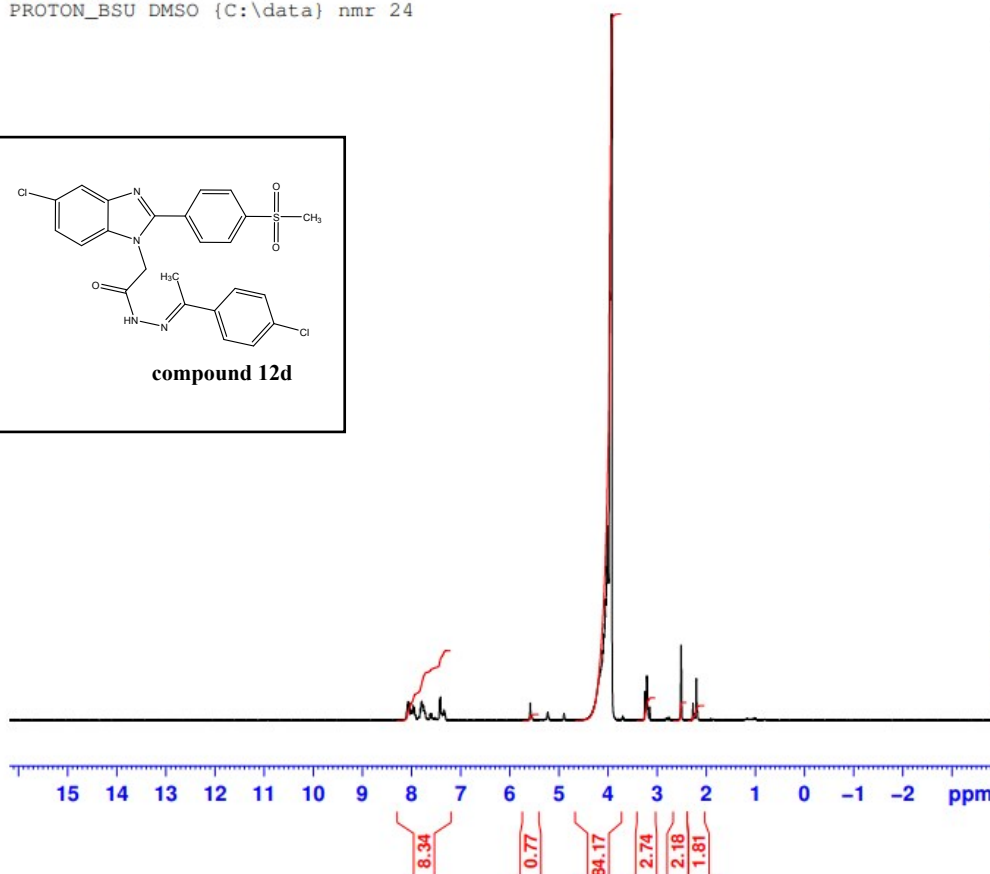
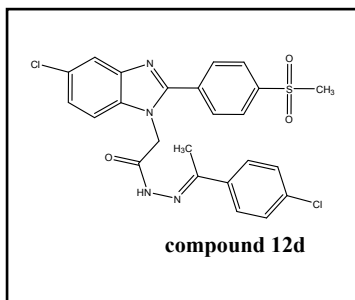
Current Data Parameters
NAME Mar16-2017-nmr
EXPNO 170
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170317
Time 6.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DE 20.800 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 66.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W
PLW13 0.17640001 W

F2 - Processing parameters
SI 131072
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME Marl8-2017-nmr
EXPNO 70
PROCNO 1

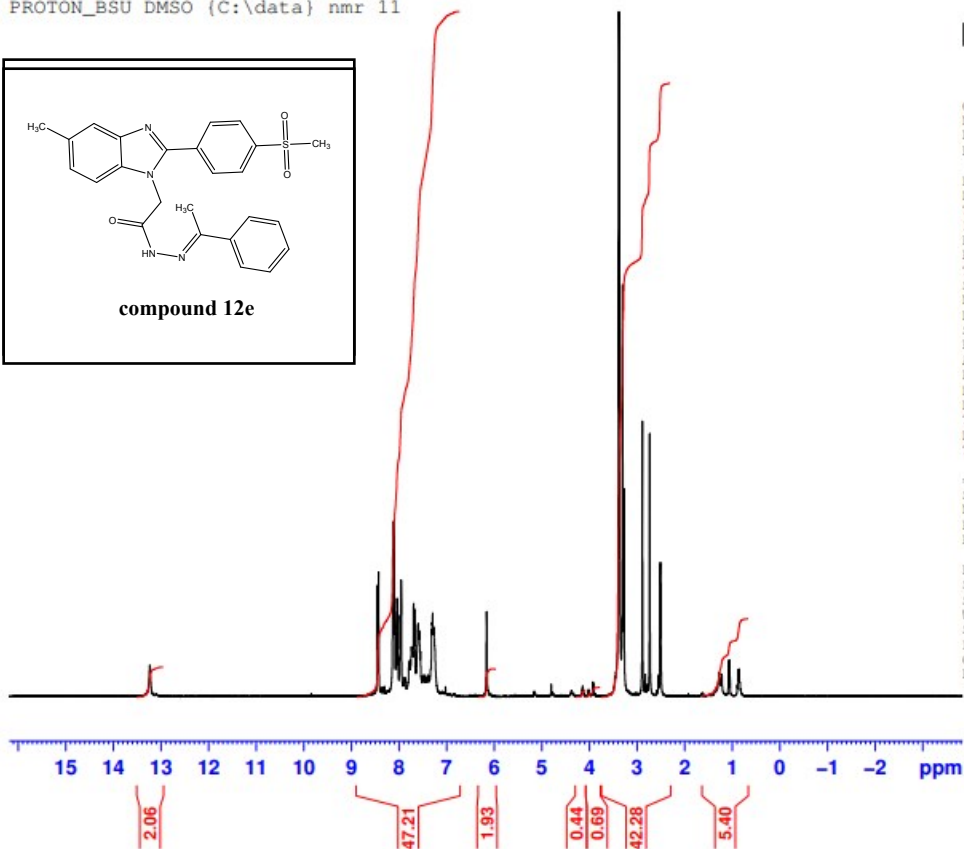
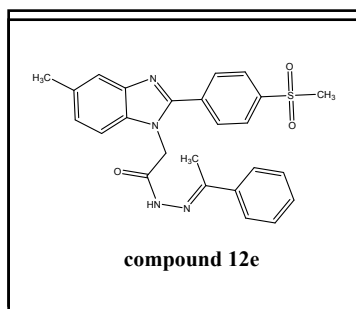
F2 - Acquisition Parameters
Date_ 20170318
Time 14.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 91.28
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

29. ¹H and ¹³C NMR Spectra of 12e:

JOHN-34
PROTON_BSU DMSO {C:\data} nmr 11



Current Data Parameters
NAME Marl8-2017-nmr
EXPNO 180
PROCNO 1

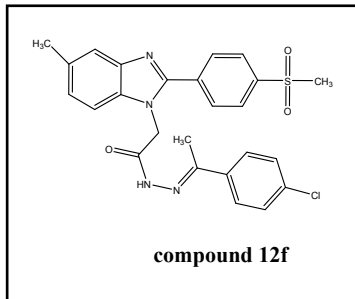
F2 - Acquisition Parameters
Date_ 20170318
Time 17.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 102.37
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

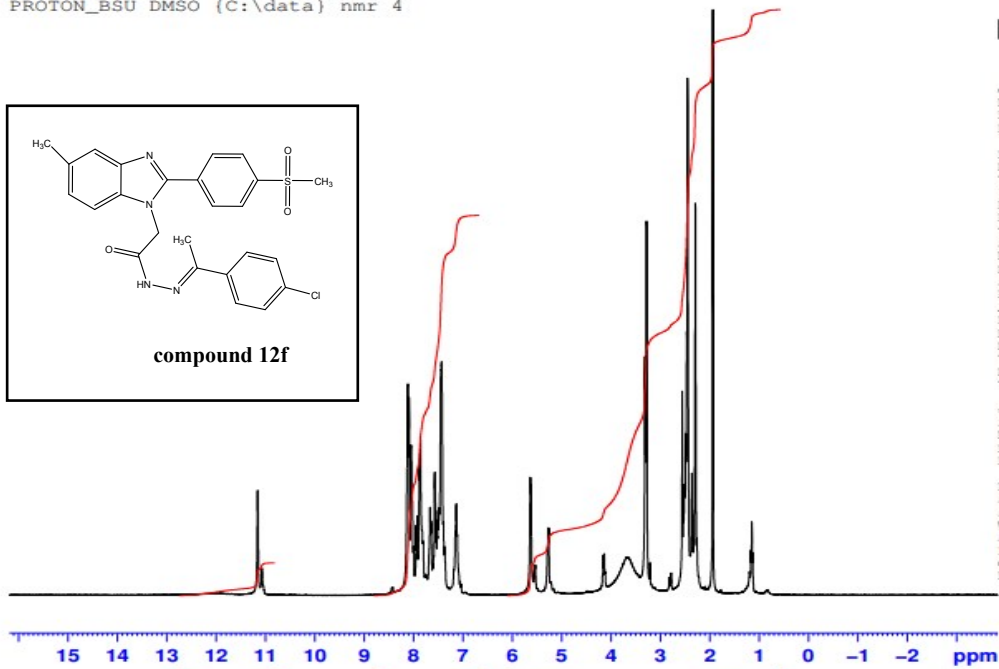
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

30. ¹H and ¹³C NMR Spectra of 12f:

MARCO-ME1
PROTON_BSU DMSO (C:\data) nmr 4



compound 12f



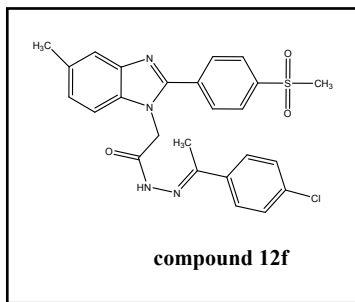
Current Data Parameters
NAME Jul23-2017-nmr
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170723
Time 11.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 51.15
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.0000000 sec
TDO 1

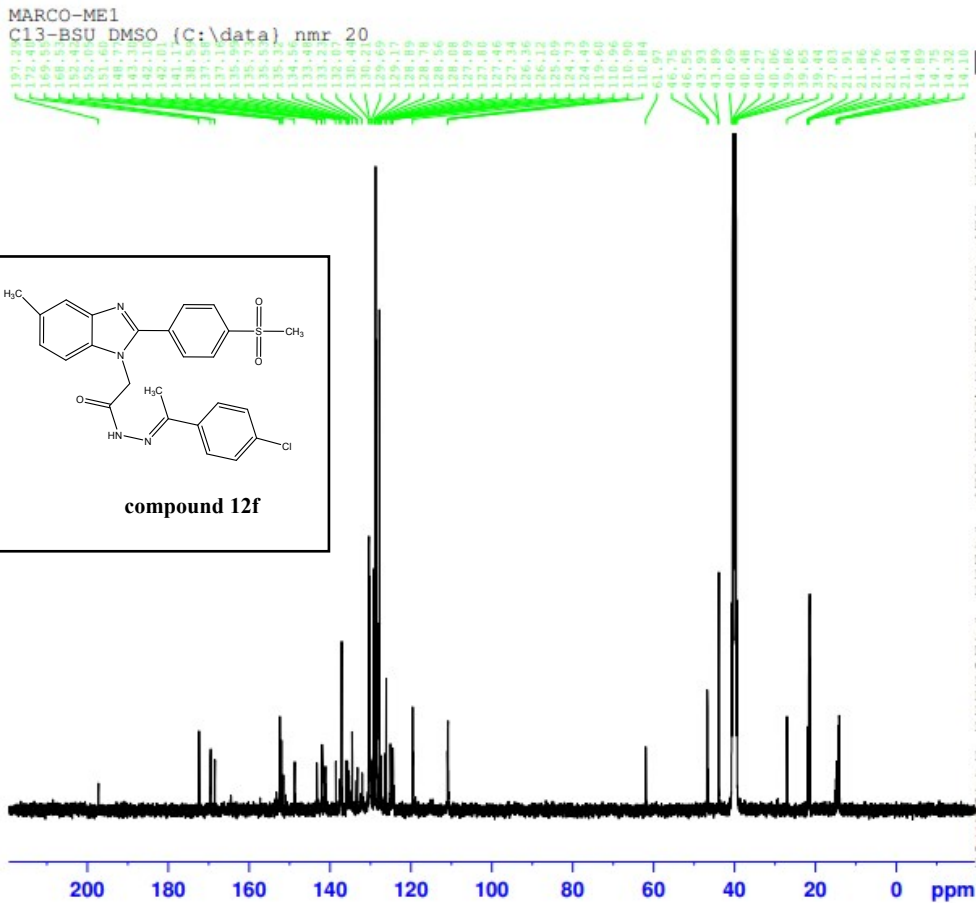
==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.0000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

MARCO-ME1
C13-BSU DMSO (C:\data) nmr 20



compound 12f



Current Data Parameters
NAME Jul23-2017-nmr
EXPNO 200
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170724
Time 7.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 313.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 66.0000000 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 16.0000000 W
PLW12 0.2177999 W
PLW13 0.17640001 W

F2 - Processing parameters
SI 131072
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

MARCO-ME1-D2O
PROTON_BSU DMSO (C:\data) nmr 7



Current Data Parameters
NAME Jul25-2017-nmr
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170725
Time 13.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 56.51
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SF01 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

