

Supplementary Data

Antiurease screening of alkyl chain linked thiourea derivatives: In vitro biological activities, molecular docking and dynamic simulations studies

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Muhammad Muddassar, PhD

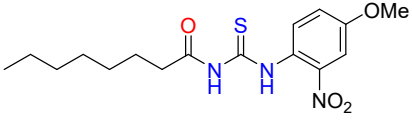
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Abdul Hameed, PhD

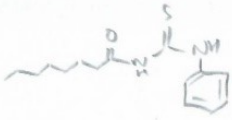
abdul_hameed8@hotmail.com

---12.439
---11.581

731
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344
329
322



SANA/DR, ABDUL HAMEED/SI-1-12//
ICCBS, U.O. K/1H

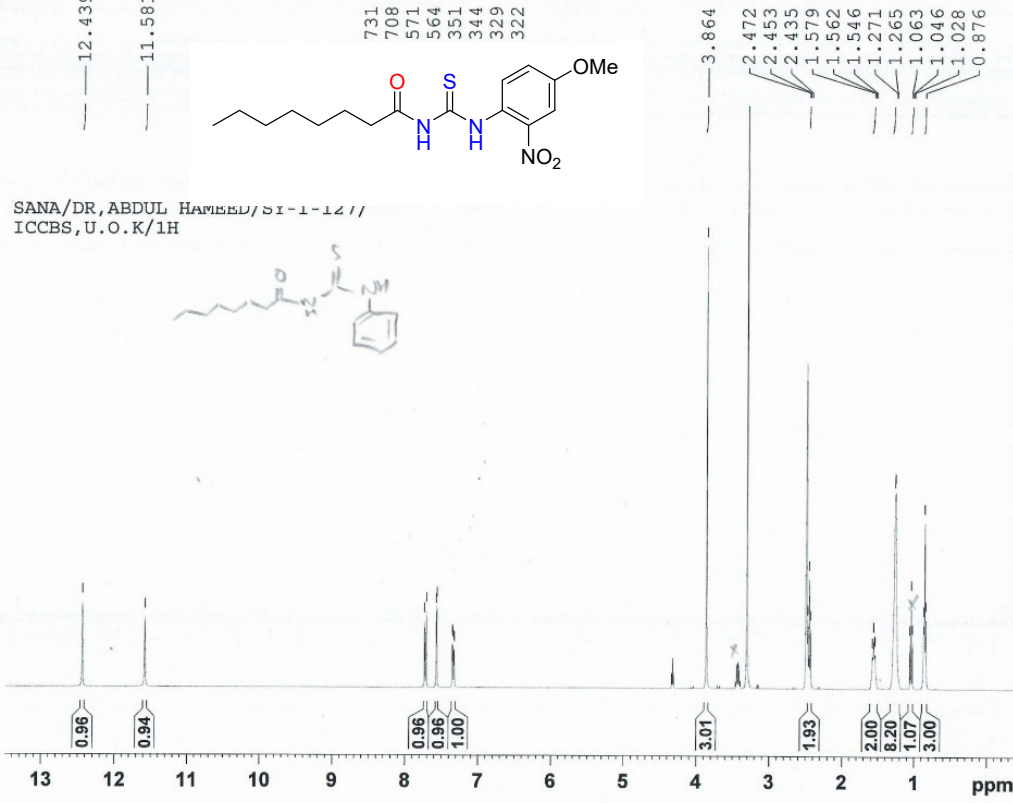


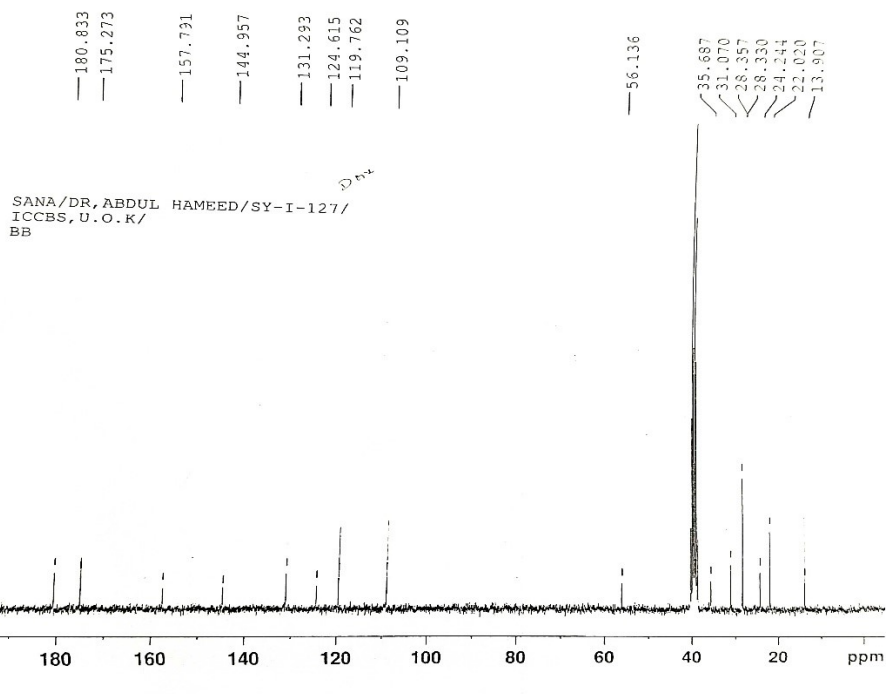
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TD 32768
SOLVENT DMSO
NS 64
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FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 322.5
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DE 6.50 usec
TE 300.0 K
D1 2.0000000 sec
TDO 1

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SFO1 400.1332010 MHz

F2 - Processing parameters
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GB 0
PC 1.00





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PULPROG zgpg
TE 300K
SOLVENT DMF
NS 1519
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FIDRES 0.350197 Hz
AQ 0.7037583 sec
RG 1024
EQ 16.12
DQ 47.703 usec
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TE 300.2 K
D1 1.00000000 sec
D11 0.00000000 sec
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PL1 0 dB
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SFO1 101.626125 MHz

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NUC2 1H
FPCP2 30.00 usec
PL2 0 dB
PL12 16.12 dB
PL13 17.00 dB
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PL1XW 0.1781132 W
PL1YW 0.1782212 W
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PS - Processing parameters
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Fig-S1: ¹H- and ¹³C-NMR Spectra of (3a)

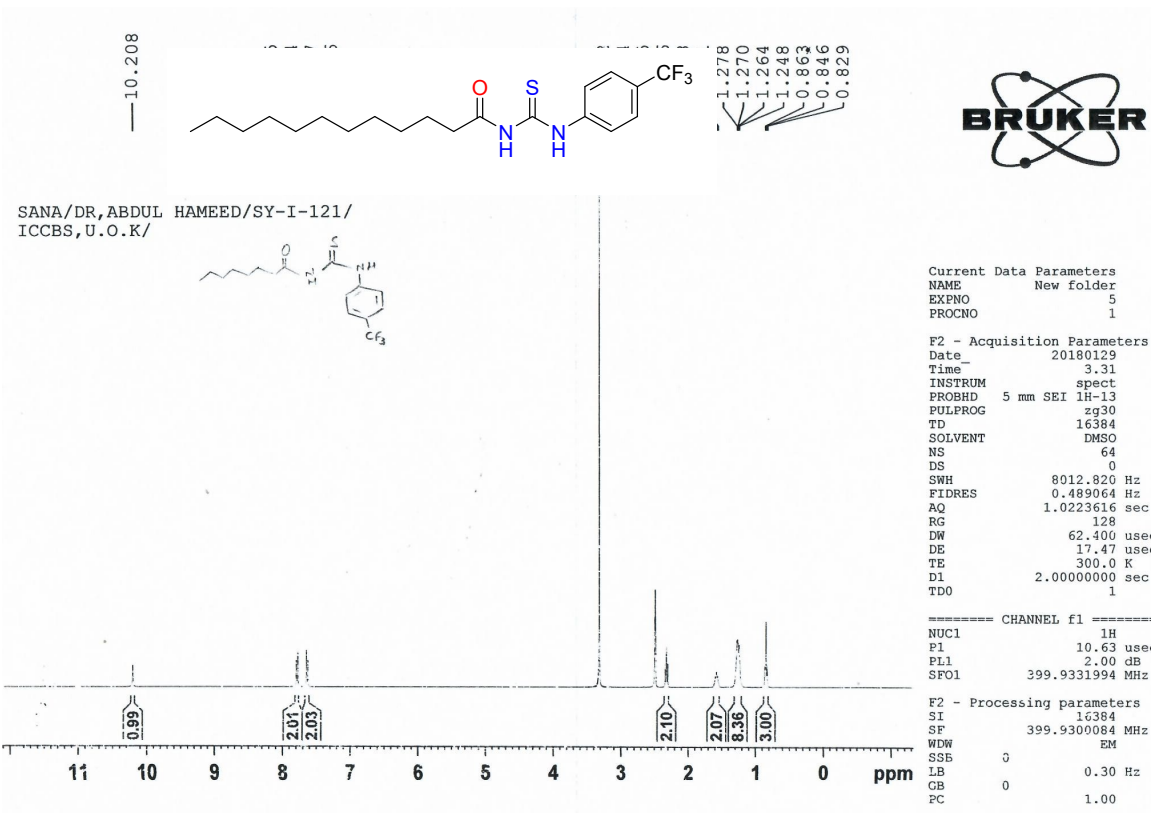
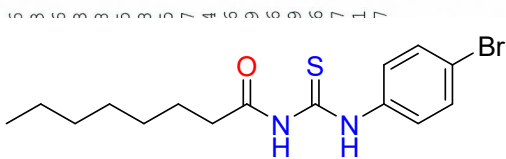


Fig-S2: ¹H-NMR Spectrum of (3b)

—12.411

—11.586

ANA/DR, ABDUL HAMEI
CCBS, U.O.K/1H



2.465
2.447
1.579
1.562
1.545
1.268
1.262
0.874

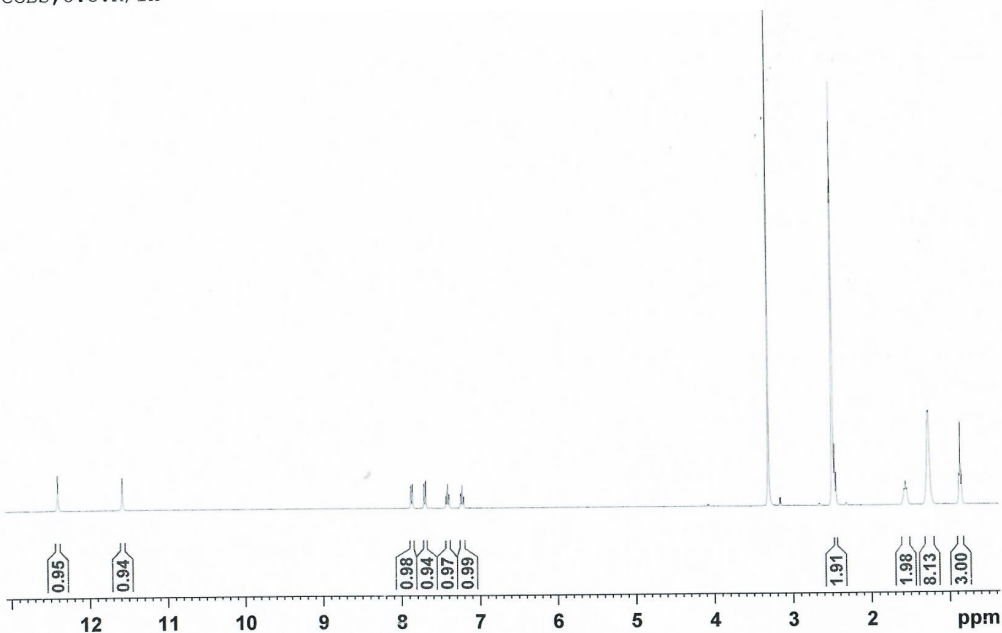


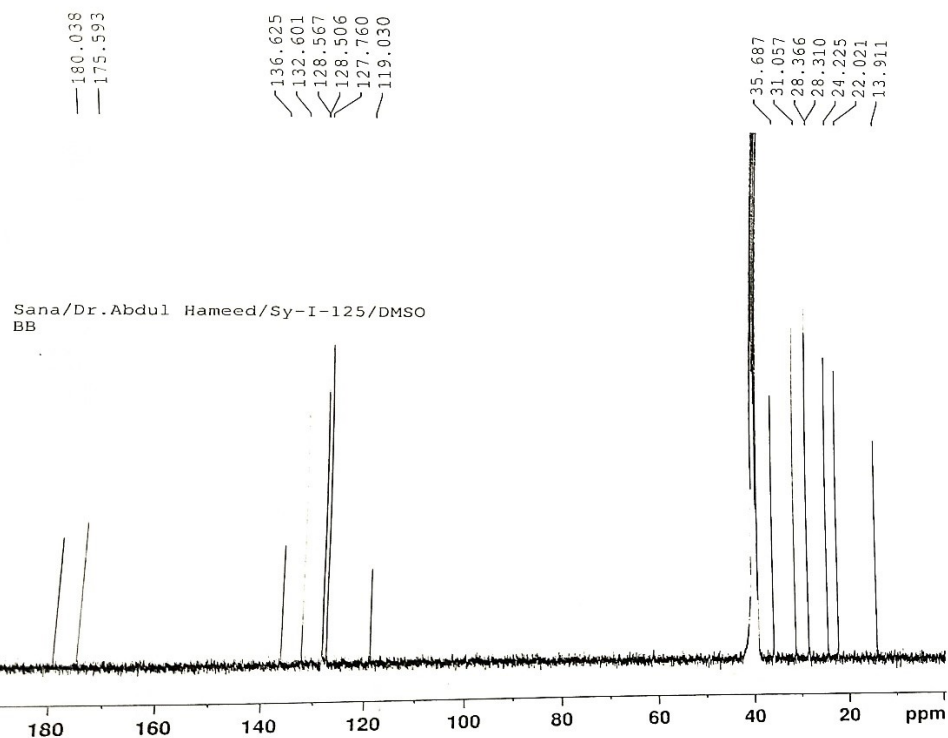
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PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 0
SWH 9012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 322.5
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 2.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.40 usec
PL1 0 dB
SFO1 400.1332010 MHz

F2 - Processing parameters
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SF 400.130065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





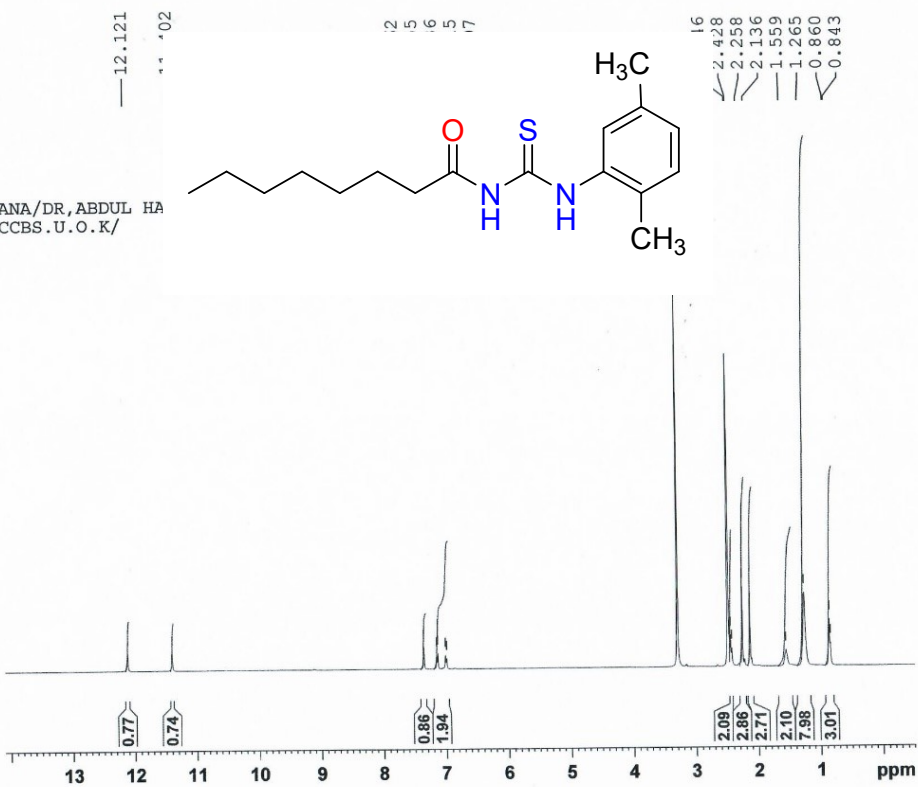
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 PULPROG zgpg
 TD 32768
 SOLVENT DMSO
 NS 20400
 DS 4
 SWH 24028.461 Hz
 FIDRES 1.467191 Hz
 AQ 0.6815744 sec
 RG 196.51
 DW 20.800 usec
 DE 6.50 usec
 TE 299.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 20
 SFO1 100.6605511 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 56.16659982 W
 SFO2 400.2816011 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 8.31400013 W
 PLW12 0.23388711 W
 PLW13 0.11722420 W

F2 - Processing parameters
 SI 32768
 SF 100.6505364 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Fig-3: ¹H- and ¹³C-NMR Spectra of (3c)

SANA/DR, ABDUL HA
ICCBS.U.O.K/



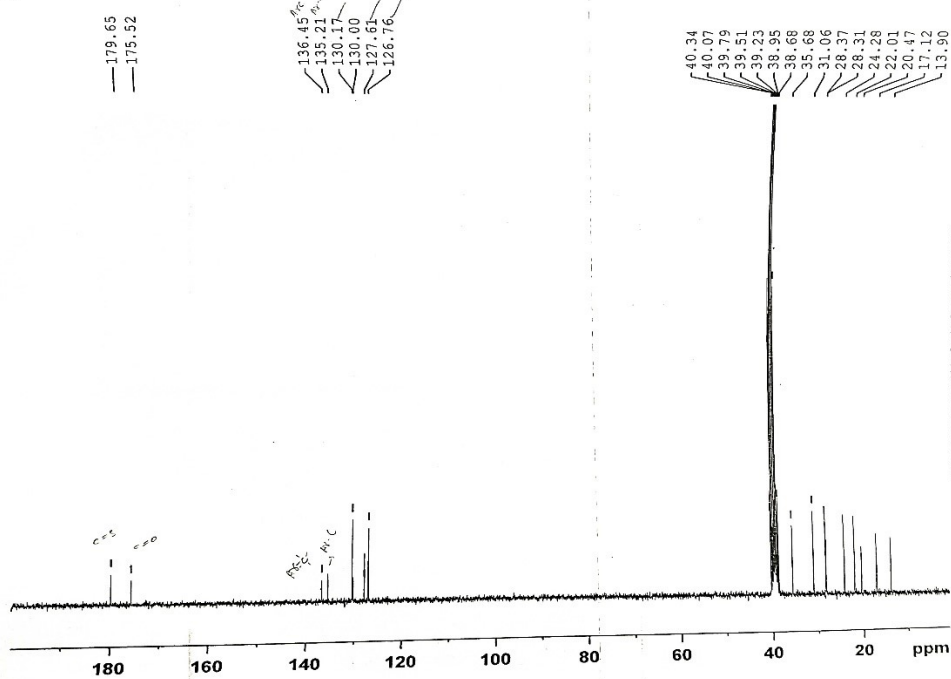
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PROCNO 1

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PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 456.1
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
DL 2.0000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 8.40 usec
PL1 0 dB
SFO1 400.1332010 MHz

F2 - Processing parameters
SI 16384
SF 400.130065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Sana / Dr. Abdul Hameed / SY-I-117 / DMSO
BB



AVANCE NEO
300 MHz
Lab # 108

Current Data Parameters
NAME Aug20-18
EXPNO 1
PROCNO 1

F2 - Acquisition Parameter
Date_ 20180821
Time_ 3.33 h
INSTRUM Avance Neo 300
PROBHD Z8284_0948 (PH)
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 16384
DS 8
SWH 17857.143 Hz
FIDRES 1.089913 Hz
AQ 0.9175040 sec
RG 4.6975
DW 28.000 usec
DE 12.00 usec
TE 300.0 K
D1 1.50000000 sec
D11 0.03000000 sec
TDO 16
SEO1 75.4764278 MHz
NUC1 13C
P1 10.00 usec
PLW1 53.07400131 W
SEO2 300.1312005 MHz
NUC2 1H
CPDPRG2 waltz65
PCPD2 90.00 usec
PLW2 8.72920036 W
PLW12 0.24247989 W
PLW13 0.121196000 W

F2 - Processing parameters
SI 16384
SF 75.4677860 MHz
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SSB 0 1.00 Hz
LB 0
GB 0
PC 1.20

Fig-S4: ¹H- and ¹³C-NMR Spectra of (3d)

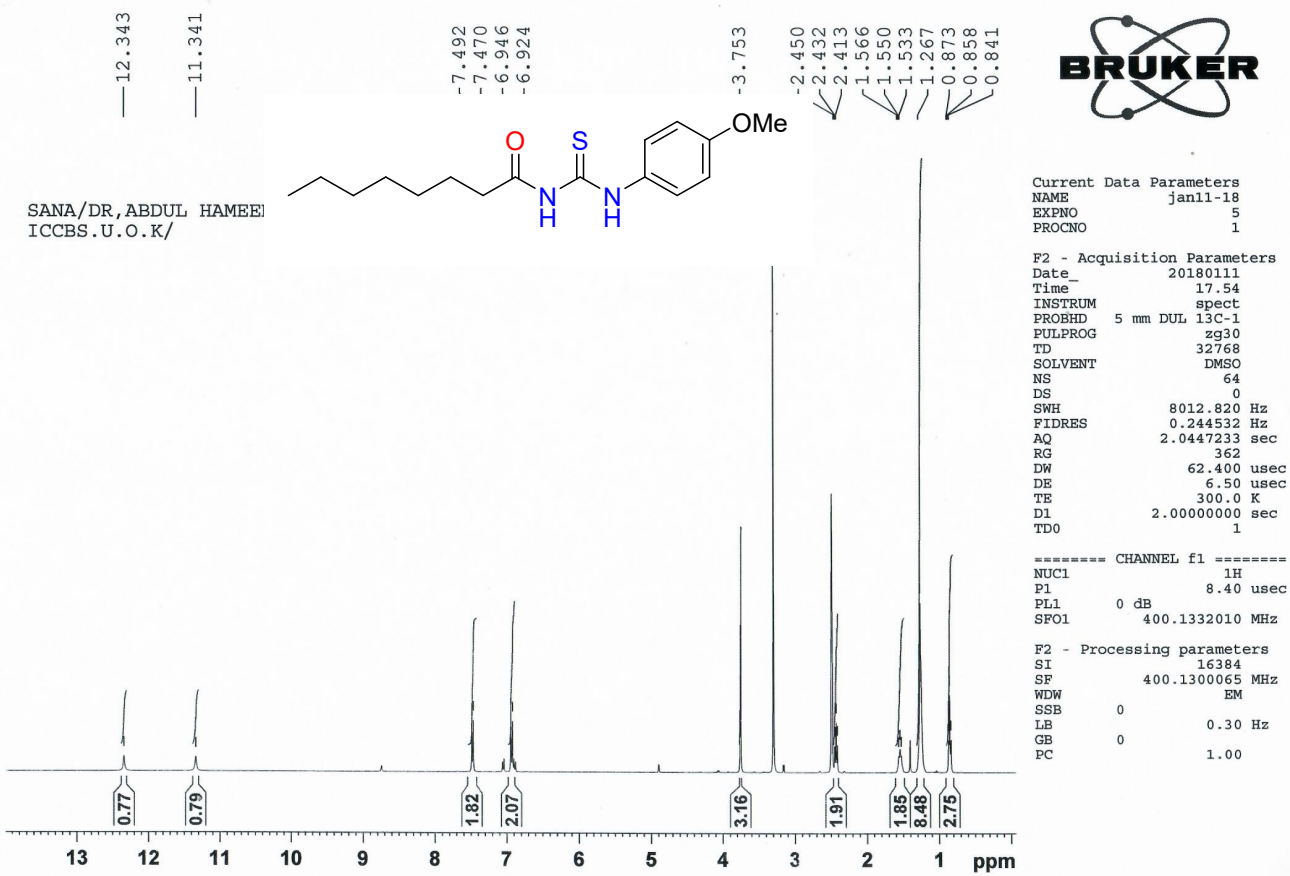
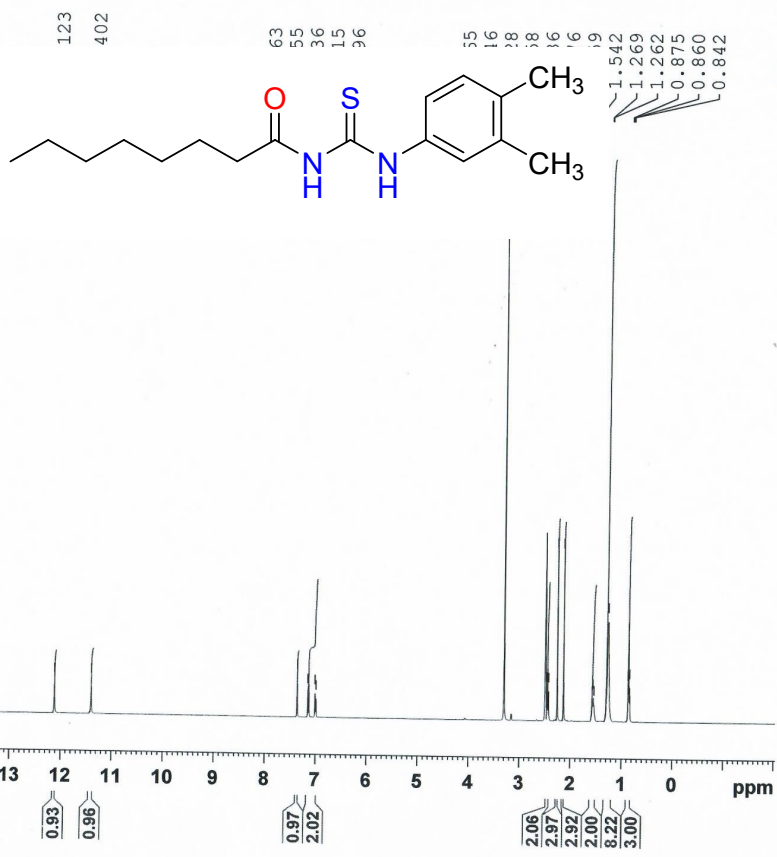


Fig-S5: ¹H-Spectrum of (3e)

SANA/DR, ABDUL HAM
ICCBS . U . O . K /



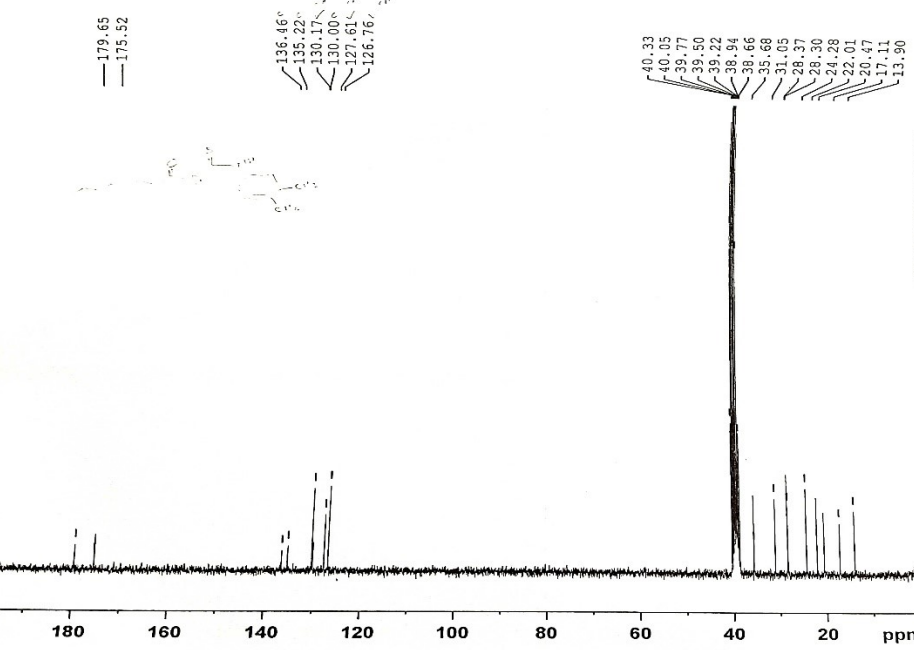
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PROCNO 1

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PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 362
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 8.40 usec
PL1 0 dB
SFO1 400.1332010 MHz

F2 - Processing parameters
SI 16384
SF 400.130065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

/ Dr. Abdul Hameed / SY-I-109 / DMSO



AVANCE NEO
300 MHz
Lab # 108

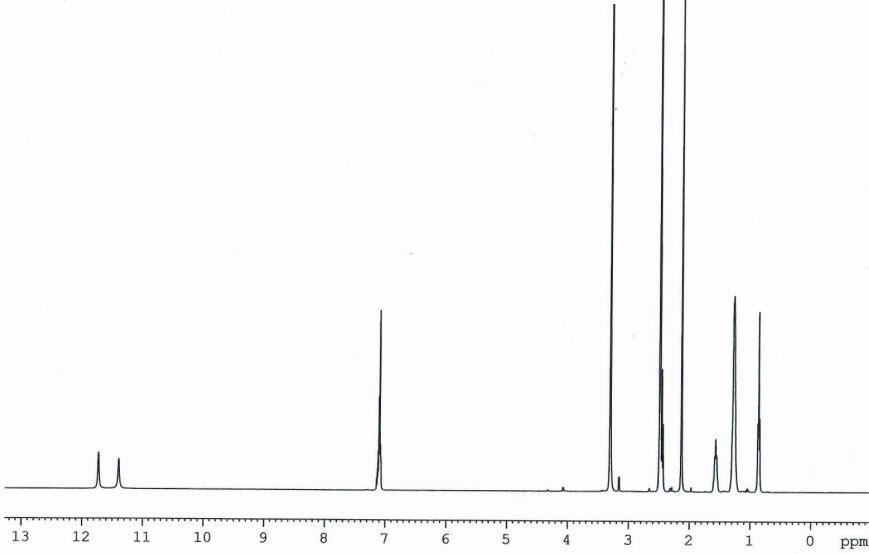
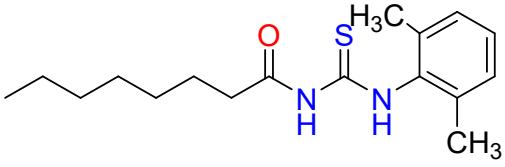
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EXPNO 1
PROCNO 1

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PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 18432
DS 8
SWH 17857.143 Hz
FIDRES 1.089913 Hz
AQ 0.915948 sec
RG 4.6875
DE 28.000 usec
TE 32.00 usec
TE 300.0 K
D1 1.50000000 sec
D11 0.03000000 sec
TDO 18
SFO1 75.4764278 MHz
NUC1 13C
P1 10.00 usec
PLW1 53.07400131 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 90.00 usec
PLW2 8.72920036 W
PLW12 0.24247999 W
PLW13 0.12196000 W

F2 - Processing parameters
SI 16384
SF 75.4677860 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.20

Fig-S6: ¹H- and ¹³C-NMR Spectra of (3f)

SANA/D
ICCBS.



AVANCE 400
LAB NO 117

NAME Dec22-17
EXPNO 4
PROCNO 1
Date_ 20171222
Time 12.25
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 362
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.40 usec
PL1 0.00 dB
SFO1 400.1332010 MHz
SI 16384
SF 400.1300065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
EC 1.00

Sana / Dr. Abdul Hameed / SY-I-107 / DMSO
BB

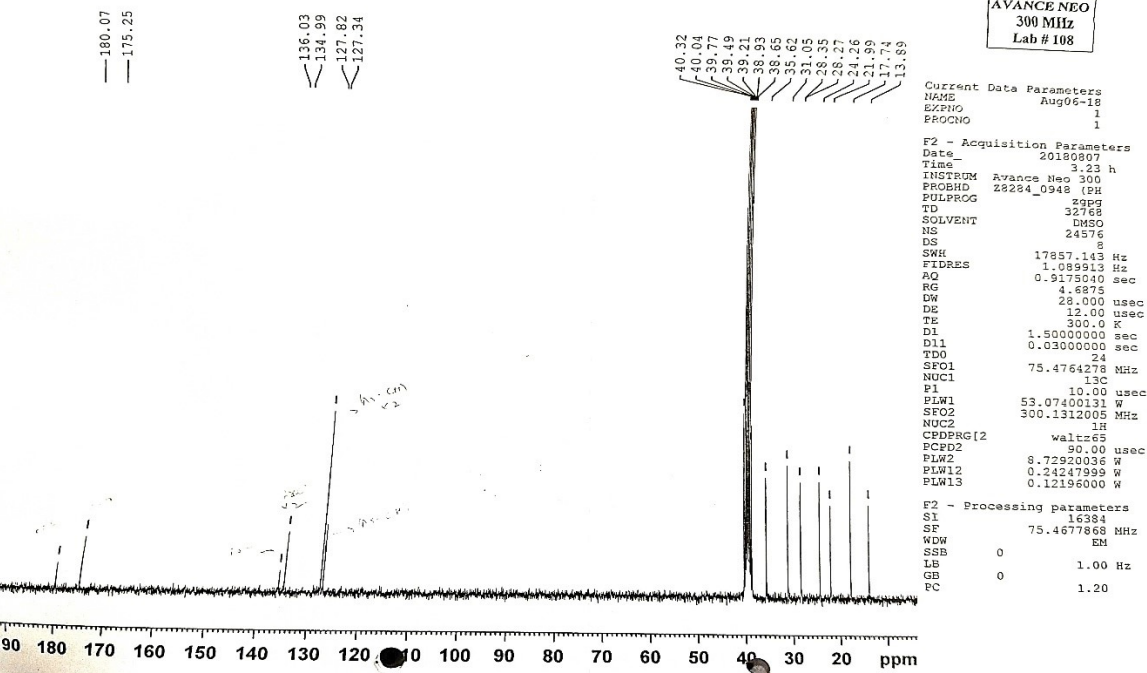
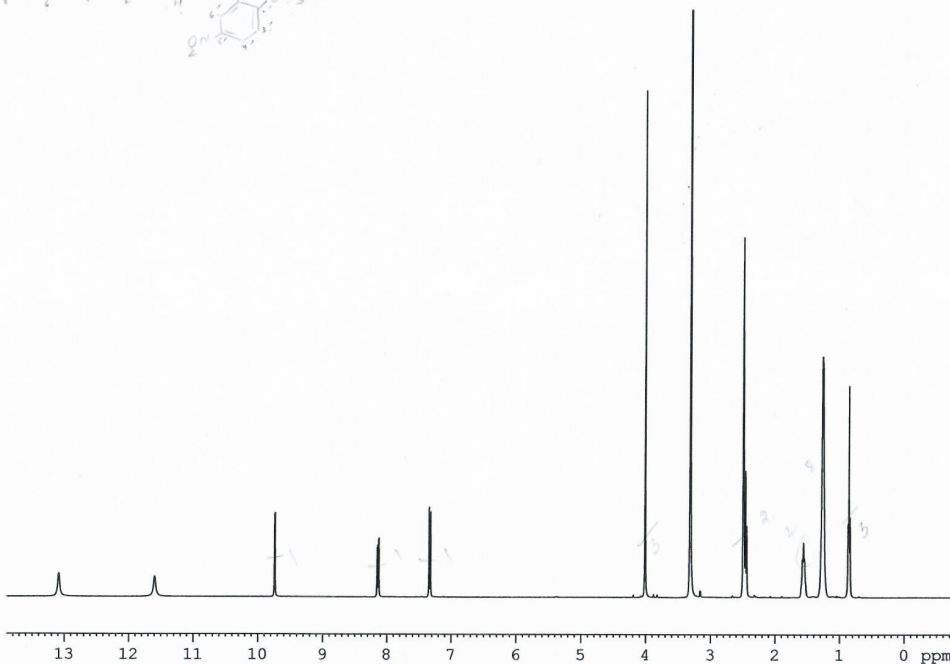
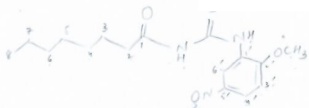
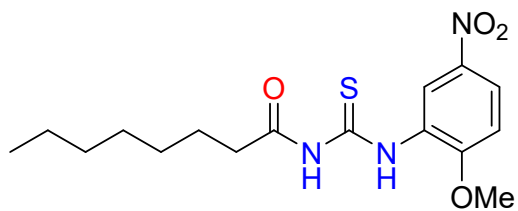


Fig-S7: ¹H- and ¹³C-NMR Spectra of (3g)

SANA/DR, ABDUL H
ICCBS.U.O.K/



AVANCE 400
LAB NO 117

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EXPNO 1
PROCNO 1
Date_ 20171214
Time 11.52
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 256
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.40 usec
PL1 0.00 dB
SF01 400.1332010 MHz
SI 16384
SF 400.1300065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

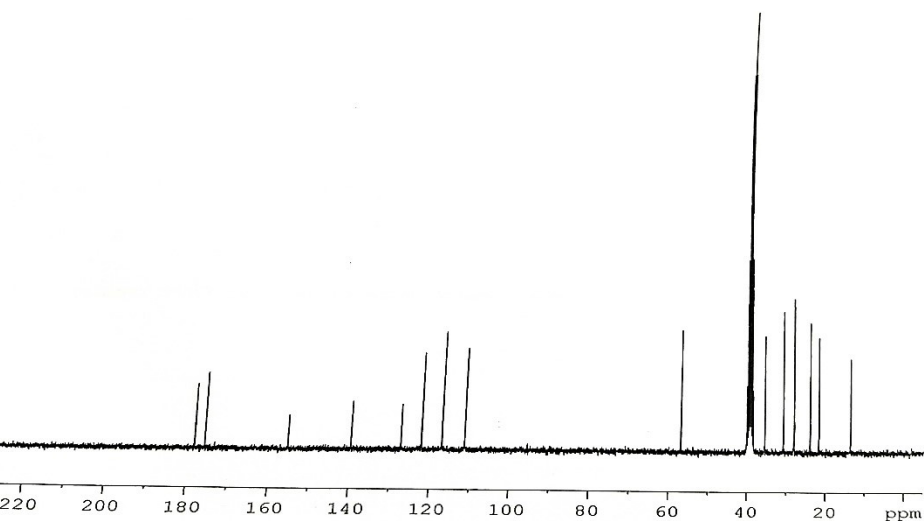
SANA/DR, ABDUL HAMEED/SY-I-99/
ICCBS, U.O.K/
BB

AVANCE AV - III
300 MHz, LAB # 116

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Time          19.48
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PULPROG       zgpg
TD            32768
SOLVENT       DMSO
NS            2738
DS            2
SWH           18028.946 Hz
FIDRES        0.350197 Hz
AQ            0.9089159 sec
RG            48.2
DW            27.723 usec
DE            6.50 usec
TE            300.0 K
D1            2.0000000 sec
D11           0.0300000 sec
TDO           18

----- CHANNEL f1 -----
NUC1          13C
P1            12.00 usec
PL1           0.00 dB
PL1W          28.88669395 W
SFO1          75.4764278 MHz

----- CHANNEL f2 -----
CPDPRG2       waltz16
NUC2          1H
PCPD2         1H
PCPD2         80.00 usec
PL2           0.00 dB
PL12          16.12 dB
PL13          17.00 dB
PL2W          13.16229485 W
PL12W         0.32161123 W
PL13W         0.26262212 W
SFO2          300.1315007 MHz
SI            16384
SF            75.4677950 MHz
WDW           EM
SBB           0
IS            1.00 Hz
GB            0
PC            1.00
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—178.148
—175.653

—155.321

—139.682

—127.293

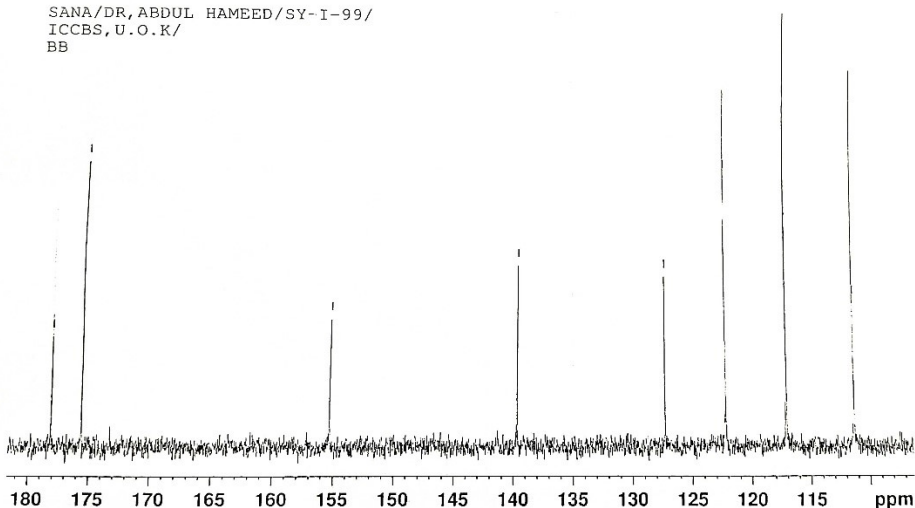
—122.197

—117.053

—111.327



SANA/DR, ABDUL HAMEED/SY-I-99/
ICCBS, U.O.K/
BB



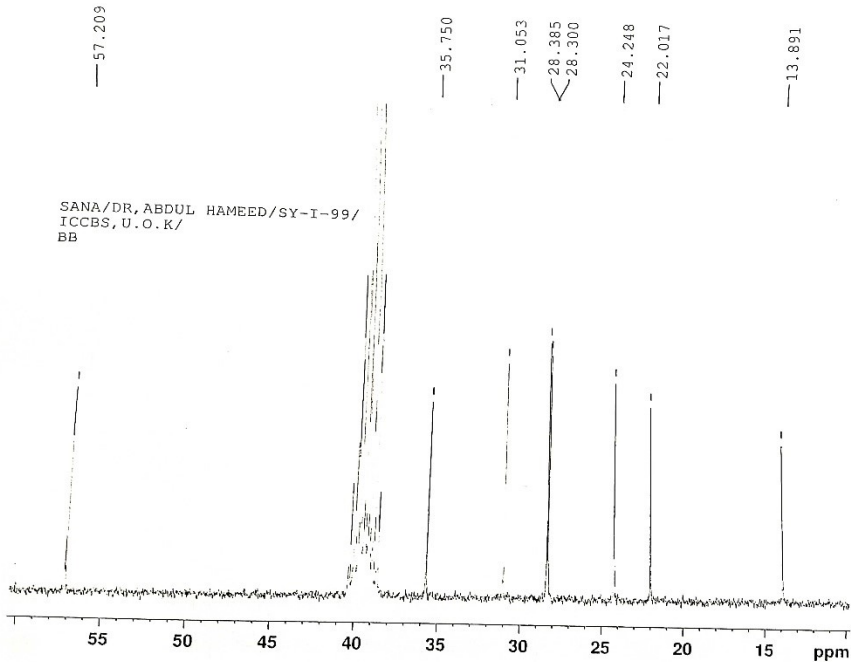
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PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 2735
DS 2
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FIDRES 0.230177 Hz
AQ 0.2987050 sec
RG 48.2
DW 27.733 usec
DE 6.50 usec
TE 300.2 K
E1 2.00000000 sec
E11 0.03000000 sec
TDO 18

===== CHANNEL #1 =====
NUC1 13C
P1 12.00 usec
PL1 0 dB
PL1W 28.88669295 W
SFO1 75.4764278 MHz

===== CHANNEL #2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 50.00 usec
PL2 0 dB
PL12 16.12 dB
PL13 17.00 dB
PL2W 12.16228485 W
PL12W 0.32161123 W
PL13W 0.26262212 W
SFO2 300.1315007 MHz

F2 - Processing parameters
S1 16384
SF 75.4677850 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



Current Data Parameters
NAME MAY-11-13 SY-I-99 C13
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180511
Time_ 1.48
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 32768
TS 0.000
SOLVENT DMSO
NS 2738
DS 2
SWH 18028.846 Hz
FIDRES 0.556177 Hz
AQ 0.9087659 sec
RG 45.2
DM 27.733 usec
DE 6.50 usec
TE 300.0 K
U1 2.0000000 sec
C11 0.0300000 sec
TD0 38

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NUC1 13C
P1 12.00 usec
PL1 0 dB
PL1W 28.8866935 W
SFO1 75.4764278 MHz

==== CHANNEL f2 =====
CDEPRG2 waitc16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL2 16.12 dB
PL3 17.00 dB
PL2W 13.16228485 W
PL2W 0.32181123 W
PL3W 0.2626212 W
SFO2 300.1315007 MHz

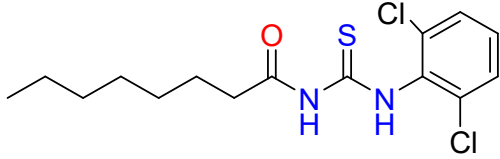
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S1 16384
SF 75.4677850 MHz
EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Fig-S8: ¹H- and ¹³C-NMR Spectra of (3h)

11.864
11.626

7.541
7.521
7.388
7.368
7.347

2.464
2.446
1.583
1.566
1.549
1.279
1.269
0.875
0.859
0.841



SANA/DR,ABDU
298K / 1H

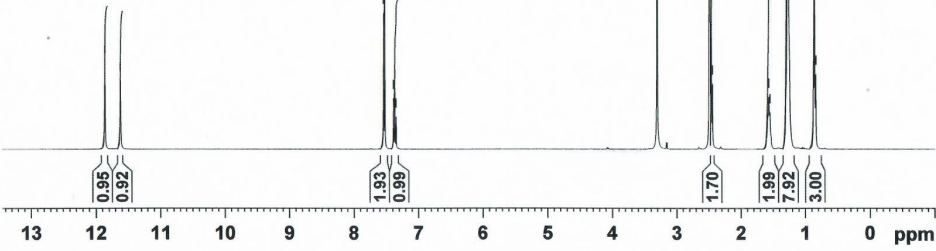


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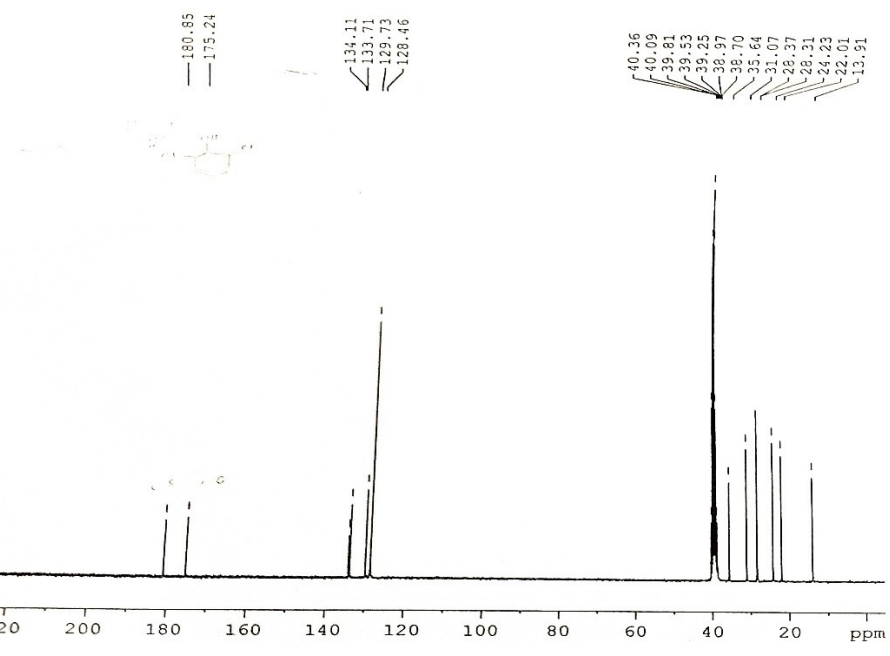
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PULPROG zg30
TD 32768
SOLVENT DMSO
NS 64
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 574.7
DW 62.400 usec
DE 17.47 usec
TE 300.0 K
D1 2.0000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 10.63 usec
PL1 2.00 dB
SFO1 400.0332002 MHz

F2 - Processing parameters
SI 32768
SF 400.0300043 MHz
WDW EM
SSB 0
LB 0.80 Hz
GB 0
PC 1.00



ANA/DR, ABDUL HAMEED/SY-I-957
 CCBS, U.O.K/
 B



AVANCE AV - III
 300 MHz, LAB # 116

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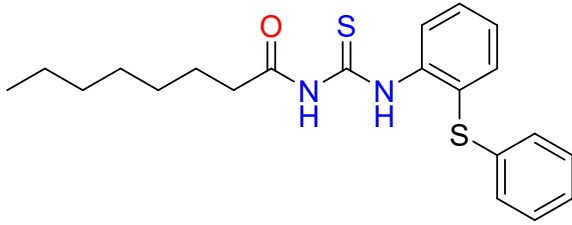
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PROCNO        1
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Time         17.15
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PULPROG       zgpg30
TD            32768
SOLVENT       DMSO
NS            18432
DS            2
SWH           18028.846 Hz
FIDRES        0.550197 Hz
AQ            0.9088159 sec
RG            45.2
DW            27.733 usec
DE            6.50 usec
TE            300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           18

----- CHANNEL f1 -----
NUC1          13C
P1            12.00 usec
PL1           0.00 dB
PL1W         28.88669395 W
SFO1         75.4764278 MHz

----- CHANNEL f2 -----
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2           0.00 dB
PL12         16.12 dB
PL13         17.00 dB
PL2W         13.16228485 W
PL12W        0.32161123 W
PL13W        0.26262212 W
SFO2         300.1315007 MHz
SI            16384
SF           75.4677850 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.00
  
```

Fig-S9: ¹H- and ¹³C-NMR Spectra of (3i)

SANA/DR,
ICCBS, U.



1.529
1.512
1.496
1.243
0.867
0.850
0.833

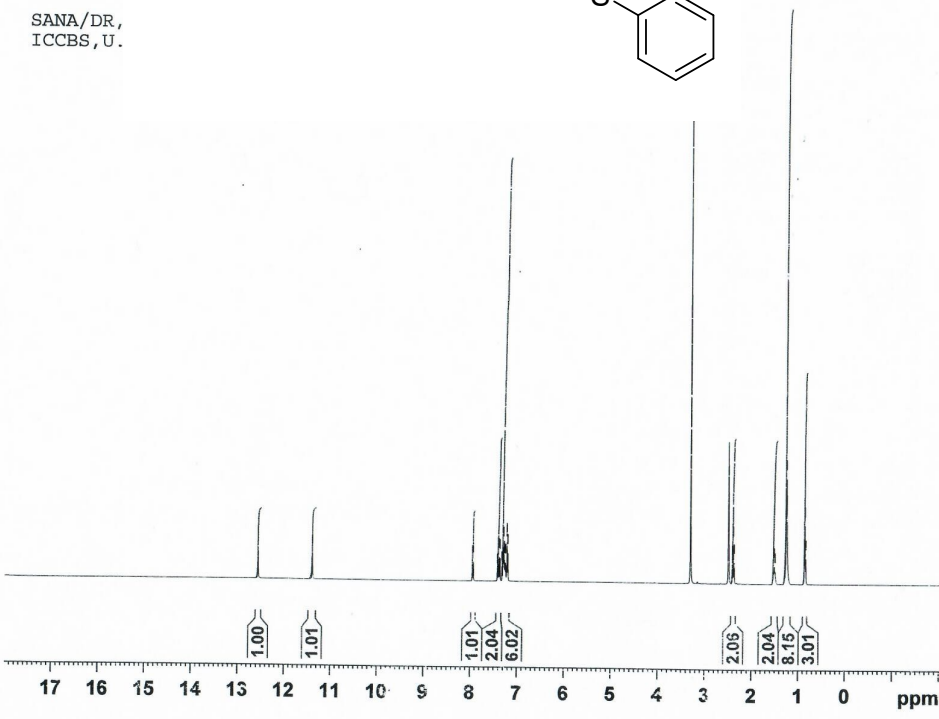


Current Data Parameters
NAME NOV 1ST 2017
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171101
Time 16.57
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 64
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 322.5
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 8.40 usec
PL1 0 dB
SFO1 400.1332010 MHz

F2 - Processing parameters
SI 16384
SF 400.1300065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



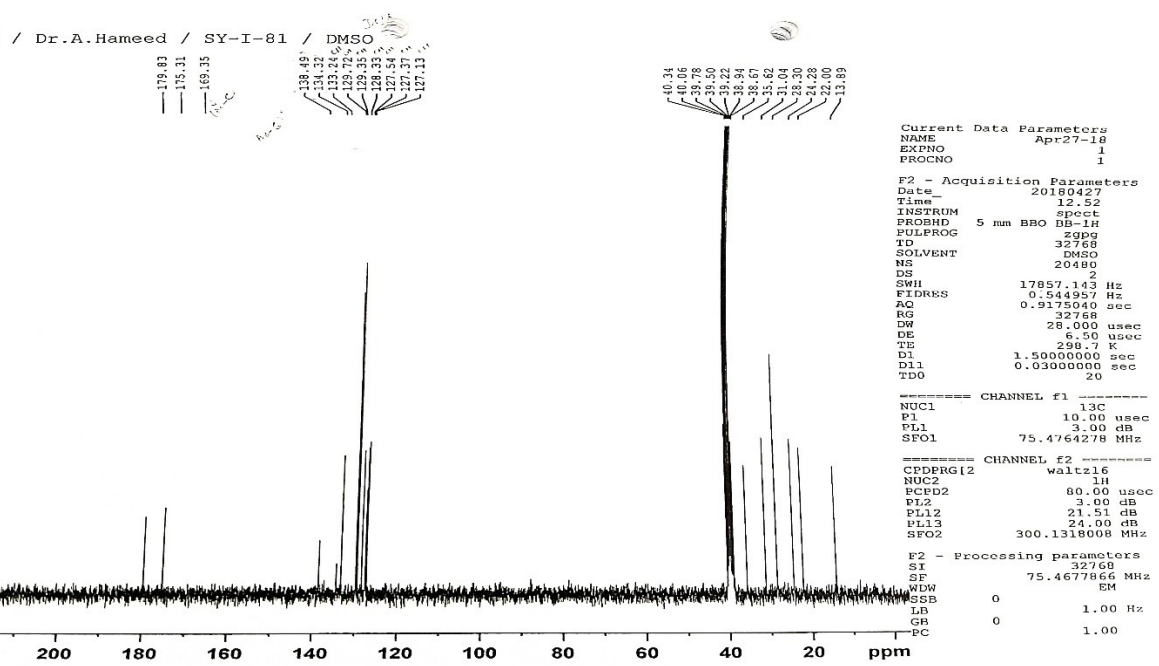


Fig-S10: ¹H- and ¹³C-NMR Spectra of (3j)

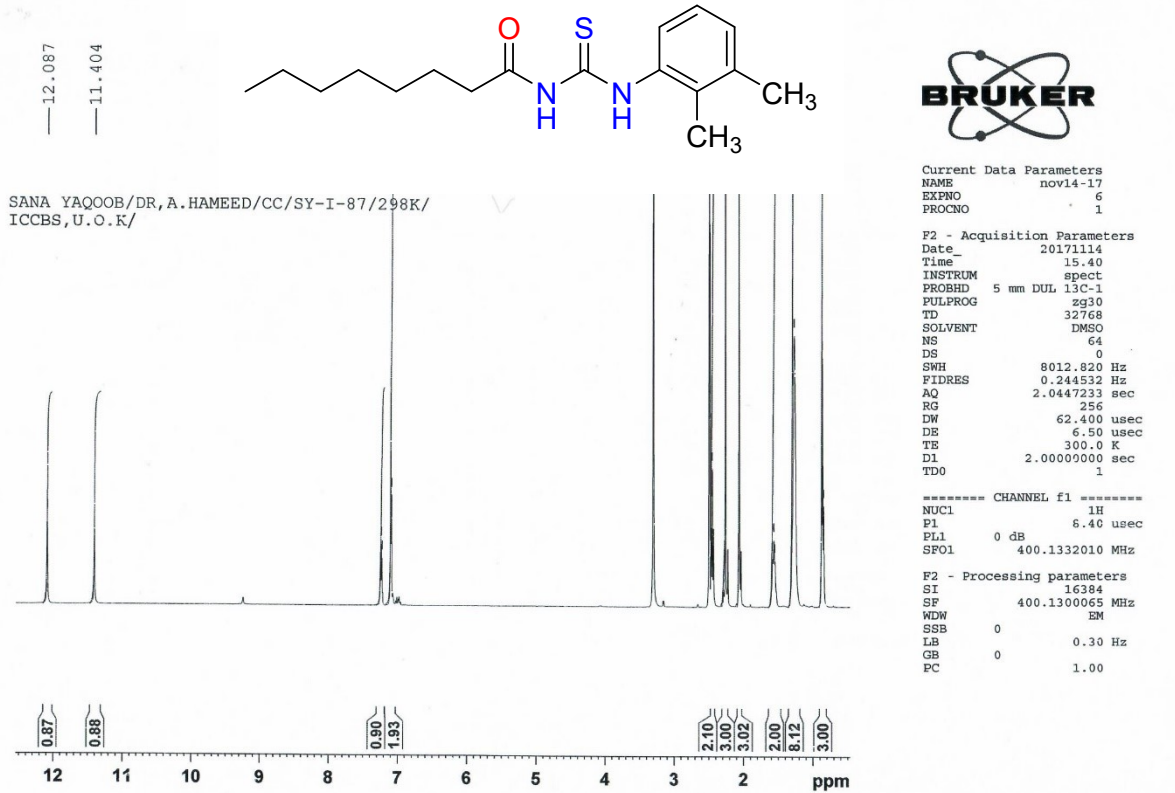
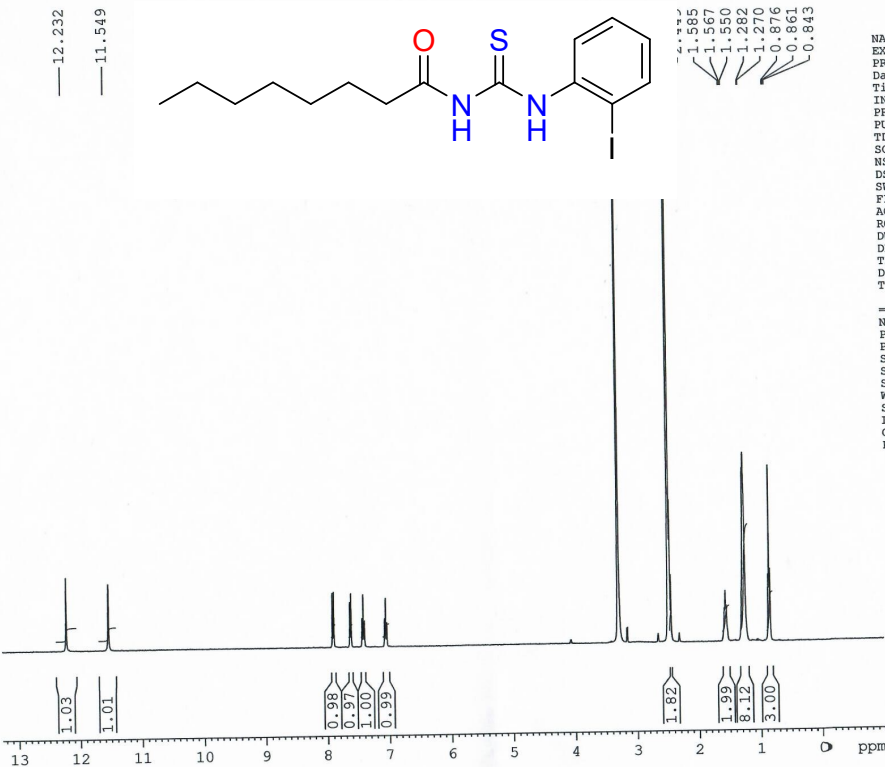


Fig-S11: ¹H-NMR Spectrum of (3k)

SANA/DR, ABDUL HAMMED/SY-I-65/
ICCBS, U.O.K/

AVANCE 400
LAB NO 117



NAME aug24-17
EXPNO 4
PROCNO 1
Date 20170824
Time 12.29
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 64
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 512
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
DI 2.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.40 usec
PL1 0.00 dB
SFO1 400.1332010 MHz
SI 16384
SF 400.1300065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

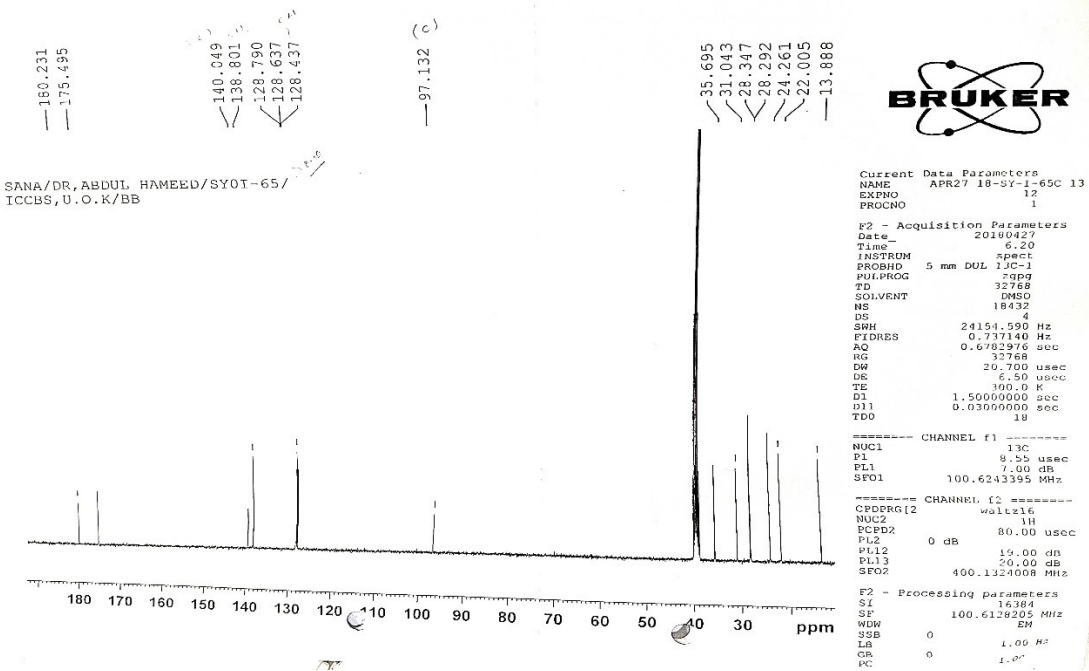


Fig-S12: ¹H- and ¹³C-NMR Spectra of (31)

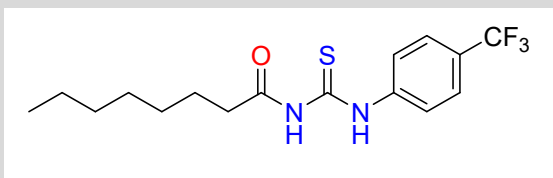
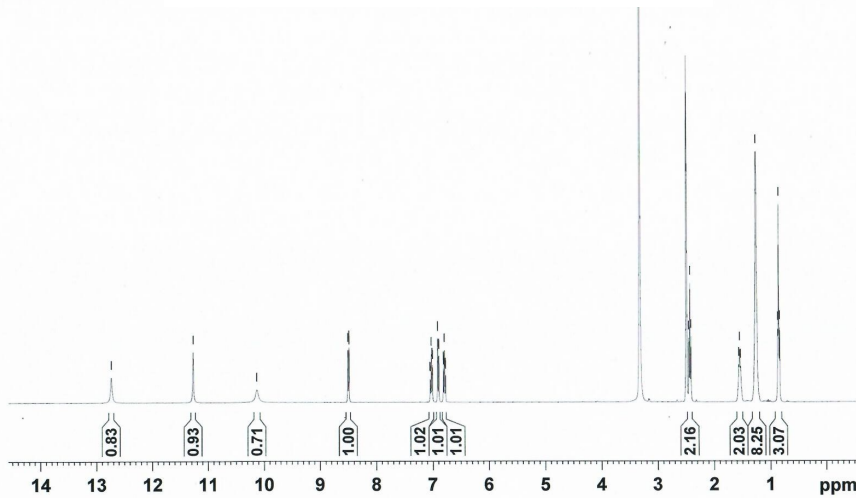
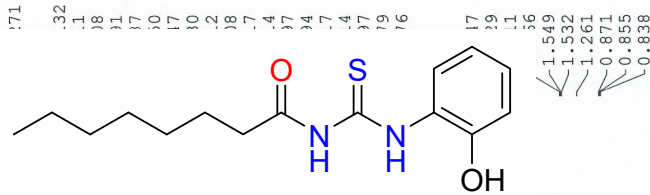


Fig-S 13: ¹H-NMR Spectrum of (3m)

SANA/DR, ABDUL HAJ
ICCBS, U.O. K/1H

12.736



Curf 5678
NAME 1
EXPRO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20180314
Time 4.07
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 228.1
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.40 usec
PL1 0 dB
SFO1 400.1332010 MHz

F2 - Processing parameters
SI 16384
SF 400.1300065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00

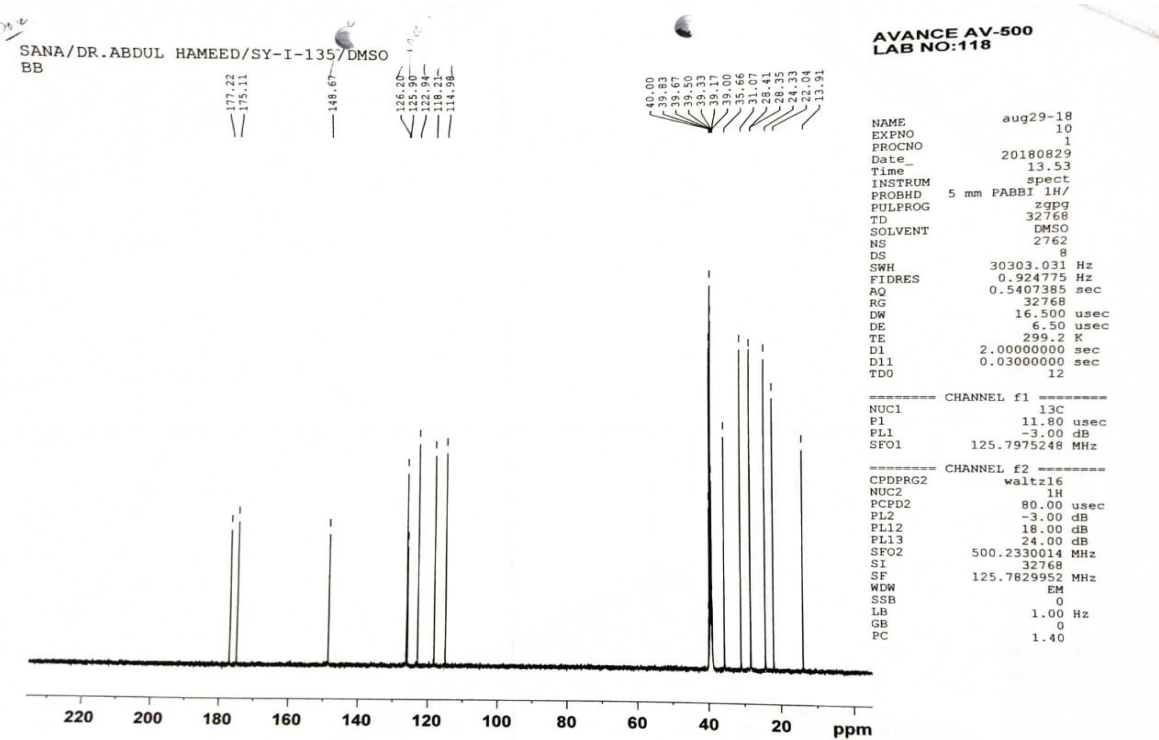


Fig-S14: ^1H - and ^{13}C -NMR Spectra of (3n)

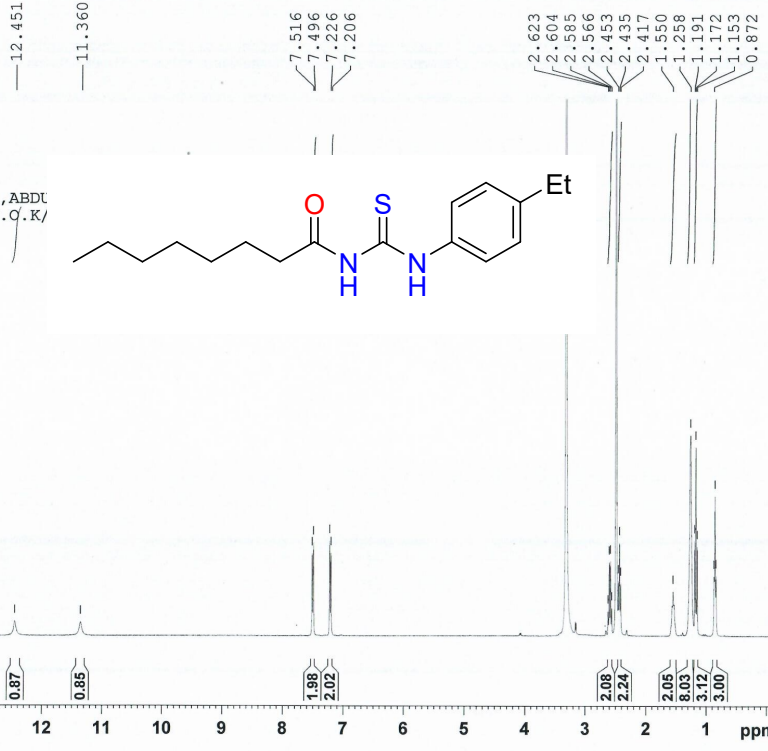


Current Data Parameters
NAME 5678
EXPNO 2
PROCNO 1

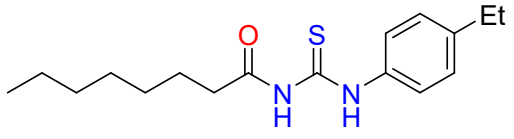
F2 - Acquisition Parameters
Date_ 20180314
Time 4.15
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 64
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 322.5
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 2.0000000 sec
TDO 1

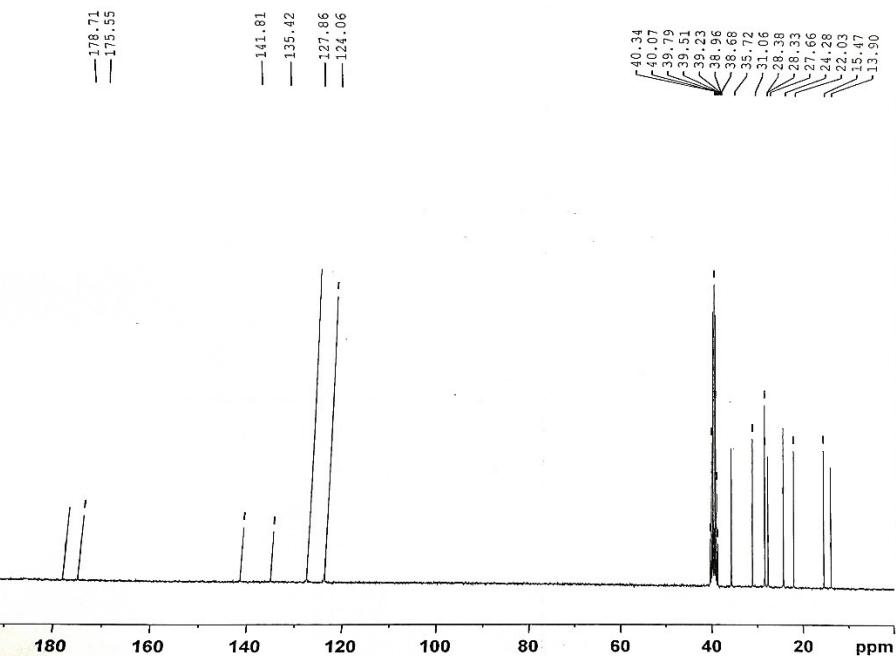
==== CHANNEL f1 =====
NUC1 1H
P1 8.40 usec
PL1 0 dB
SFOL 400.1322010 MHz

F2 - Processing parameters
SI 16384
SF 400.130065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



SANA/DR, ABDU
ICCBS, U.C.K/





AVANCE NEO
300 MHz
Lab # 108

Current Data Parameters
 NAME Aug28-18
 EXPNO 1
 PROCNO 1

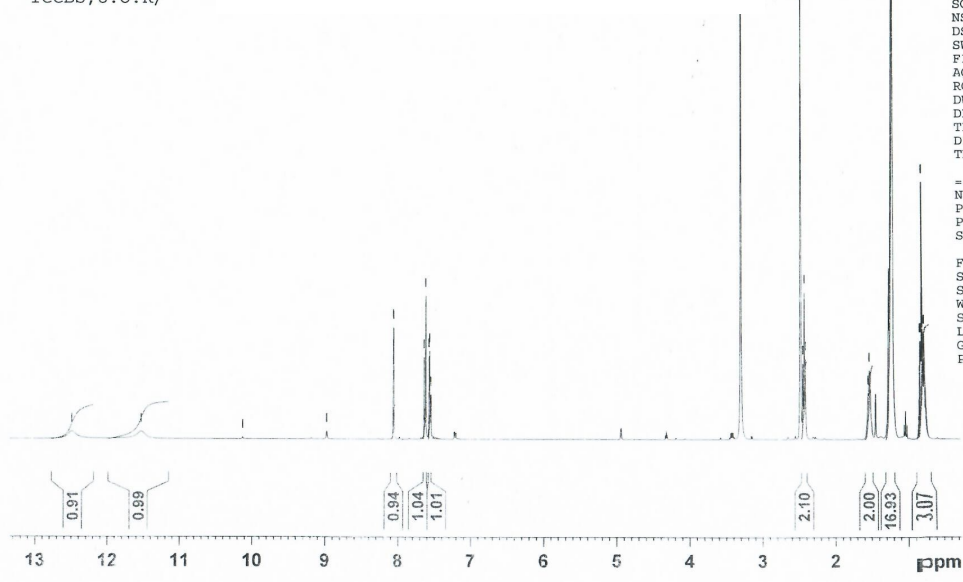
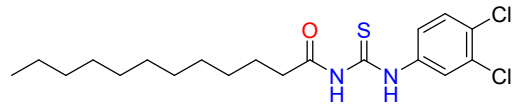
F2 - Acquisition Parameters
 Date_ 20180829
 Time_ 2.18 h
 INSTRUM Avance Neo 300
 PROBHD Z8264_0948 1H
 PULPROG zgpg
 TD 32768
 SOLVENT DMSO
 NS 16384
 DS 8
 SWH 17857.143 Hz
 FIDRES 1.089913 Hz
 AQ 0.9175040 sec
 RG 4.6875
 DW 28.000 usec
 DE 12.00 usec
 TE 300.0 K
 D1 1.50000000 sec
 D11 0.03000000 sec
 TDO 16
 SFO1 75.4764278 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 53.07400131 W
 SFO2 500.1312005 MHz
 NUC2 1H
 CPDPRG2 waltz65
 FCPDZ 90.00 usec
 PLW2 8.72920036 W
 PLW12 0.24247999 W
 PLW13 0.12196000 W

F2 - Processing parameters
 SI 16384
 SF 75.4677860 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.20

Fig-S15: ¹H- and ¹³C-NMR Spectra of (30)

—12.491
 —11.531
 10.130

SANA/DR, ABDUL HAM
 ICCBS, U.O.K/



2.455
 2.437
 2.419
 1.560
 1.543
 1.527
 1.232
 0.855



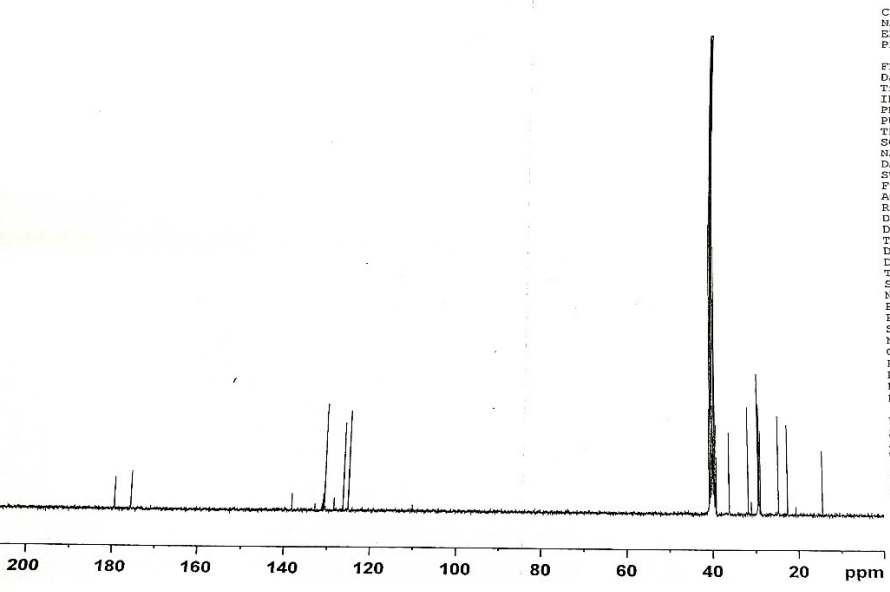
Cur
 NAME
 EXPR
 PROC...

F2 - Acquisition Parameters
 Date_ 20170925
 Time_ 12.32
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 128
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 256
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.40 usec
 PL1 0 dB
 SF01 400.1332010 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300065 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 FC 1.00

AVANCE NEO
300 MHz
Lab # 108



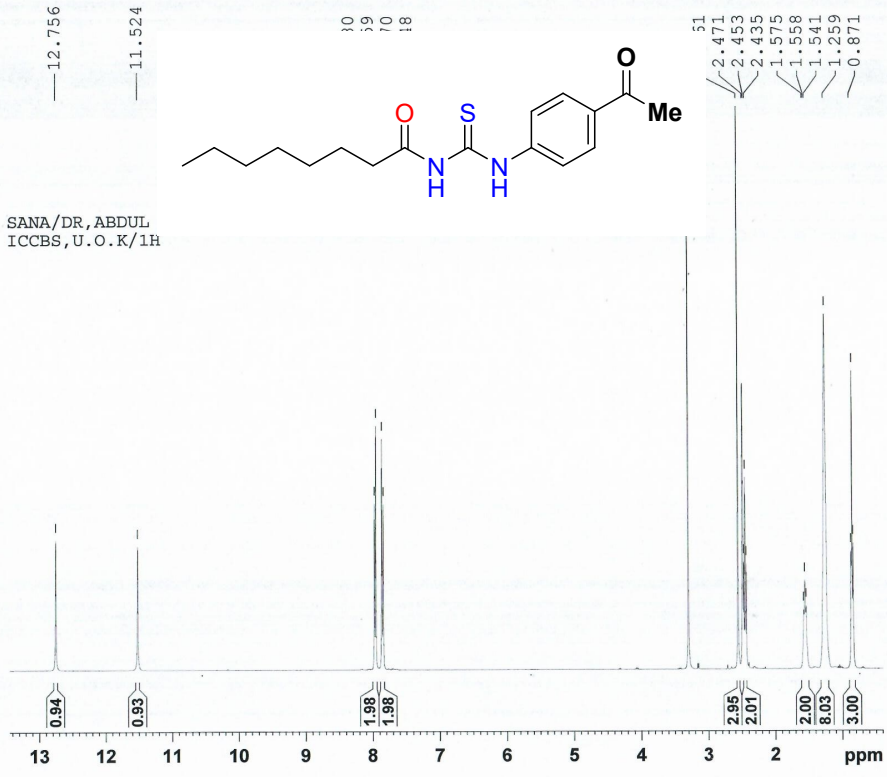
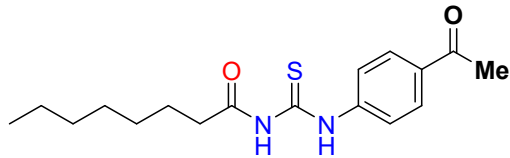
Current Data Parameters
NAME July24-18
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180725
Time 12.52 h
INSTRUM Avance Neo 300
PROBHD Z8284_0948 (PH
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 30720
DS 8
SWH 17857.143 Hz
FIDRES 1.089911 Hz
AQ 0.9175040 sec
RG 4.6875
DW 28.000 usec
DE 12.00 usec
TE 300.0 K
D1 1.5000000 sec
D11 0.0300000 sec
TDO 30
SFO1 75.4764278 MHz
NUC1 13C
P1 10.00 usec
PLW1 53.07400131 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPDZ 90.00 usec
PLW2 8.72920036 W
PLW12 0.24247999 W
PLW13 0.12196000 W

F2 - Processing parameters
SI 16384
SF 75.4677547 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.20

Fig-S16: ¹H- and ¹³C-NMR Spectra of (3p)

SANA/DR, ABDUL
 ICCBS, U.O.K/1H



Current Data Parameters
 NAME 5678
 EXPNO 7
 PROCNO 1

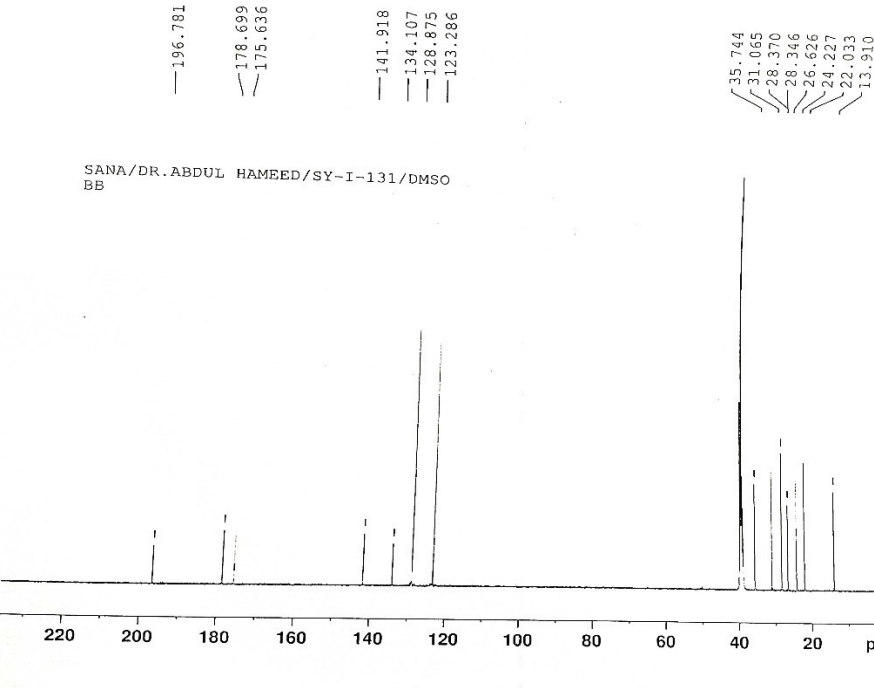
F2 - Acquisition Parameters
 Date_ 20180309
 Time 3.48
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 32
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 181
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.40 usec
 PL1 0 dB
 SFO1 400.1332010 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300065 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



SANA/DR.ABDUL HAMEED/SY-I-131/DMSO
BB



Current Data Parameters
NAME SY1-131
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180830
Time 7.22
INSTRUM spect
PROBHD 5 mm FABBI 1H/
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 18432
DS 8
SWH 30303.031 Hz
FIDRES 0.924775 Hz
AQ 0.506700 sec
RG 32768
DW 16.500 usec
DE 6.50 usec
IE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TDD 18

----- CHANNEL f1 -----
NUC1 13C
P1 11.80 usec
PL1 -3.00 dB
SFO1 125.7975248 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 24.00 dB
SFO2 500.2350014 MHz

F2 - Processing parameters
SI 32768
SF 125.7829954 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig-S17: ¹H- and ¹³C-NMR Spectra of (3q)