

## Synthesis of novel coumarin-hydrazone hybrids as $\alpha$ -glucosidase inhibitors and their molecular docking studies

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Munawwarah, Kingdom of Saudi Arabia*

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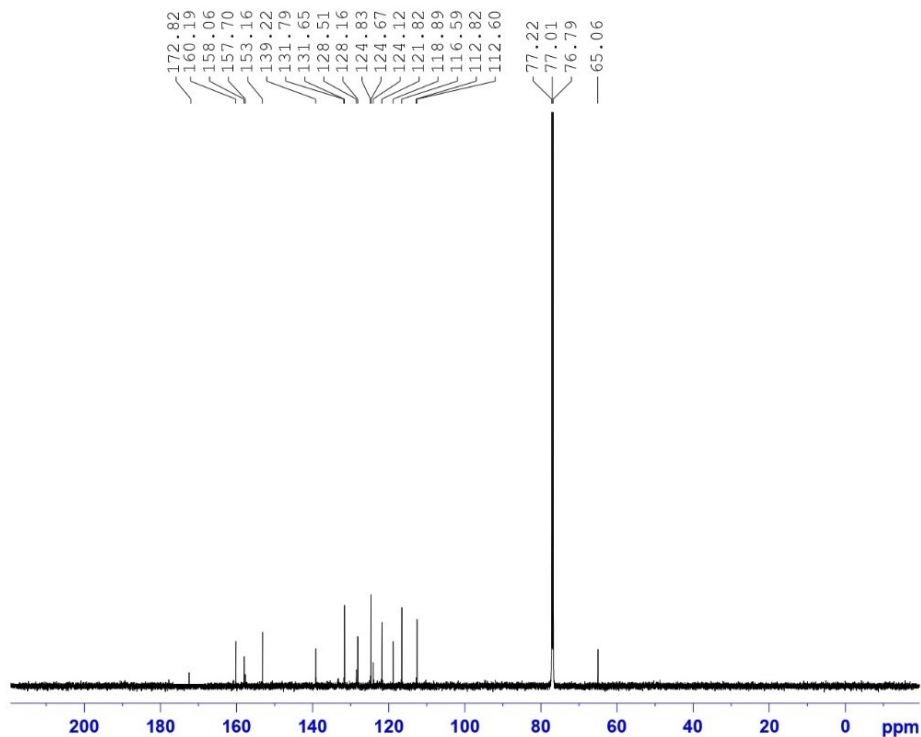
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# $^1\text{H}$ -NMR and $^{13}\text{C}$ -NMR Spectra of 7a

Dr. Ajmal / Bu-2 / CDCl<sub>3</sub>  
C13CPD



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PROCNO    1

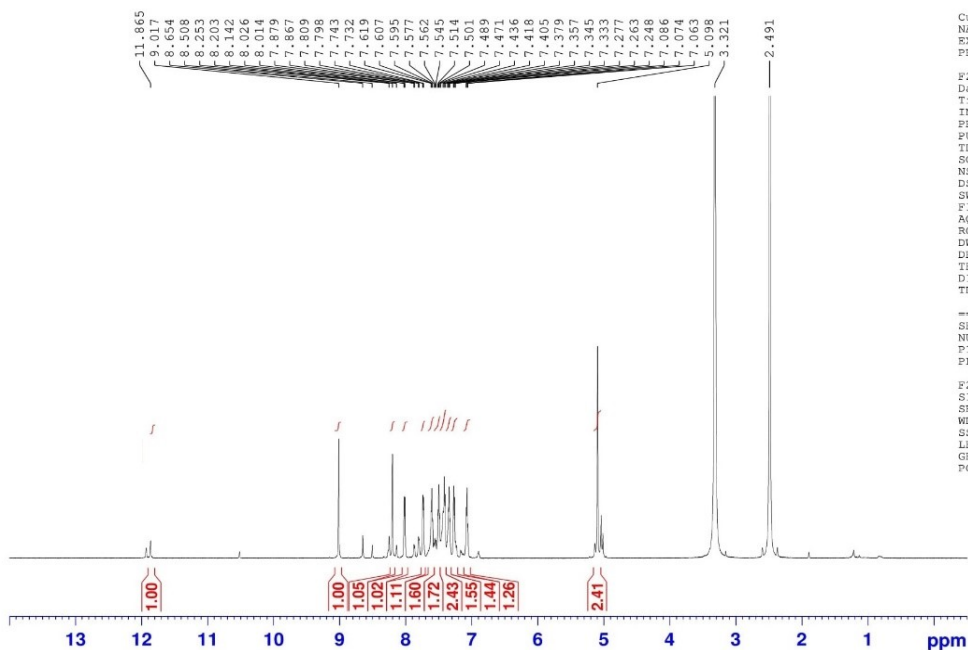
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RG         195.2
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DE         6.50 usec
TE         298.1 K
D1         2.00000000 sec
D11        0.03000000 sec
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NUC1       13C
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PLW1       83.00000000 W

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NUC2       1H
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PLW13     0.23874999 W

F2 - Processing parameters
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Dr. Ajmal/Bu-2/DMSO  
PROTON



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EXPNO 71  
PROCNO 1

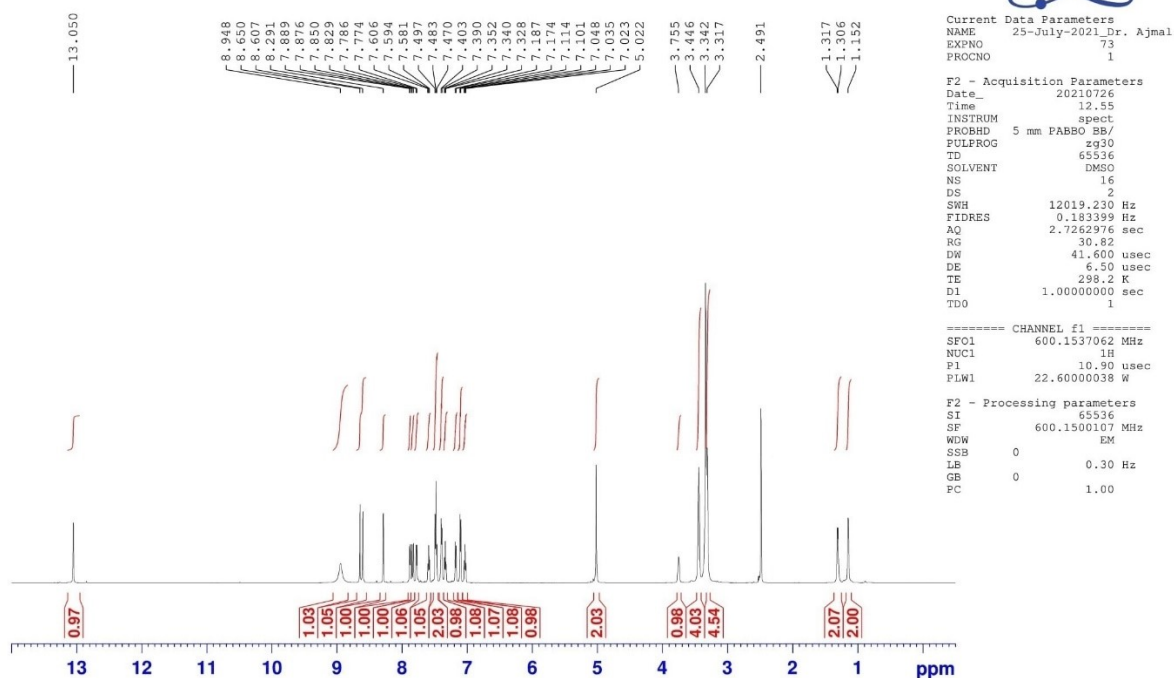
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TE 298.2 K  
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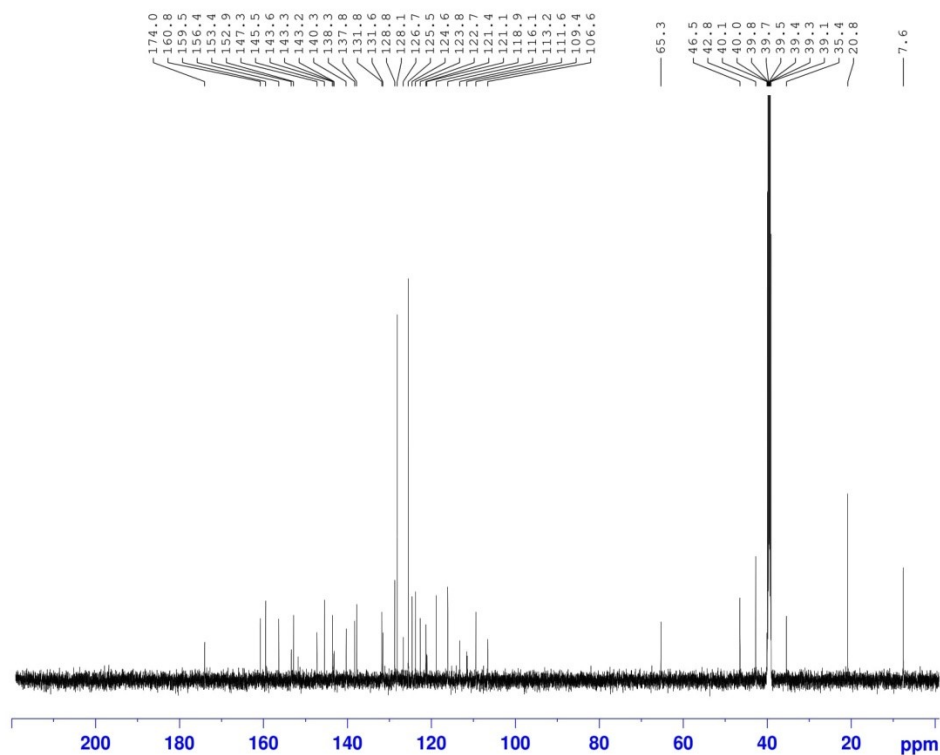
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# <sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of 7b

Dr. Ajmal/Bu-3/DMSO  
PROTON



Dr. Ajmal/Bu-3/DMSO  
C13CPD



Current Data Parameters  
NAME 25-July-2021\_Dr. Ajmal  
EXPNO 74  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210726  
Time 12.57  
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PULPROG zgpg30  
TD 32768  
SOLVENT DMSO  
NS 256  
DS 4  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
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DE 6.50 usec  
TE 298.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

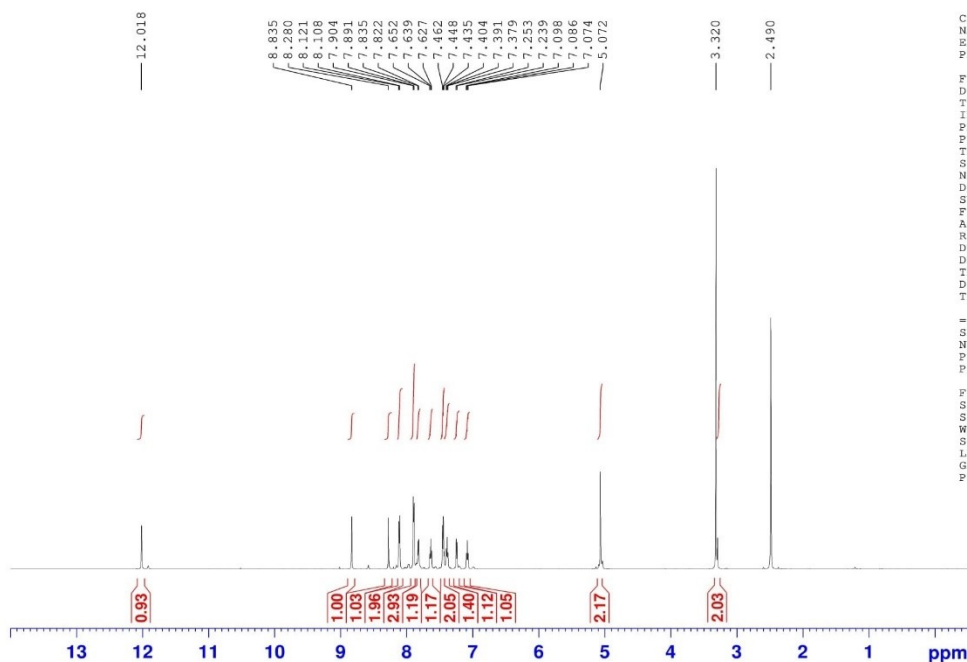
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PLW13 0.25874999 W

F2 - Processing parameters  
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**$^1\text{H}$ -NMR and  $^{13}\text{C}$ -NMR Spectra of 7c**

Dr. Ajmal/Bu-4/DMSO  
PROTON



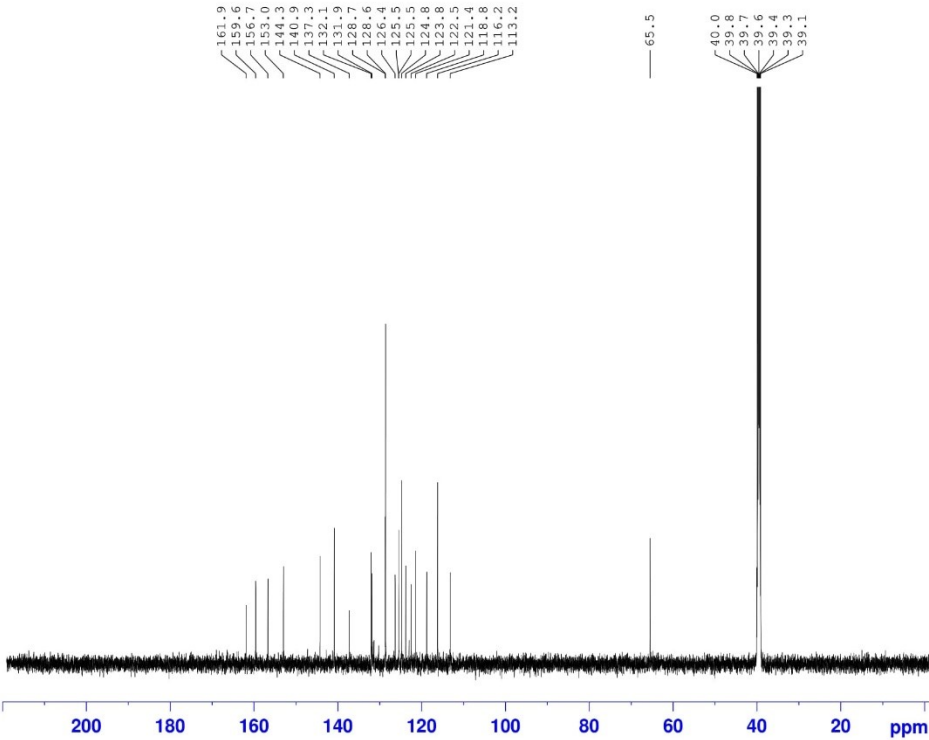
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EXPNO 89  
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SOLVENT DMSO  
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DS 2  
SWH 12019.230 Hz  
FIDRES 0.183399 Hz  
AQ 2.7262976 sec  
RG 86.85  
DW 41.600 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1

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NUC1 1H  
P1 10.90 usec  
PLW1 22.60000038 W

F2 - Processing parameters  
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WDW EM  
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GB 0  
PC 1.00

Dr. Ajmal/Bu-4/DMSO  
C13CPD



Current Data Parameters  
NAME 25-July-2021\_Dr. Ajmal  
EXPNO 90  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210726  
Time 16.18  
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PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT DMSO  
NS 1024  
DS 4  
SWH 36057.693 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 195.2  
DW 13.867 usec  
DE 6.50 usec  
TE 298.2 K  
D1 2.00000000 sec  
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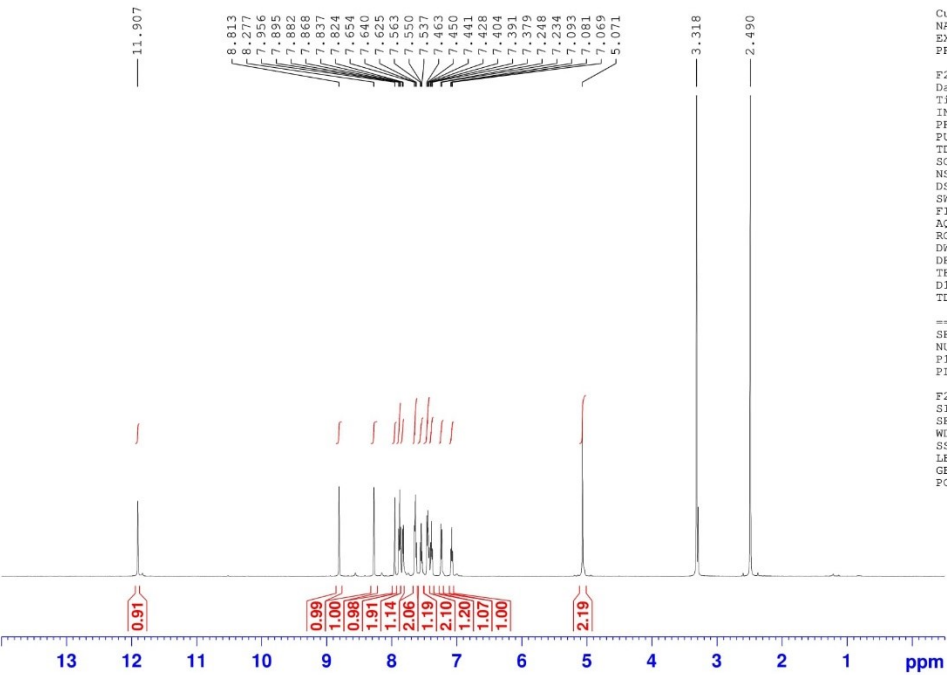
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PLW12 0.52806002 W  
PLW13 0.25874999 W

F2 - Processing parameters  
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SF 150.9079041 MHz  
WDW EM  
SSB 0  
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## **$^1\text{H}$ -NMR and $^{13}\text{C}$ -NMR Spectra of 7d**



Dr. Ajmal/Bu-7/DMSO  
PROTON



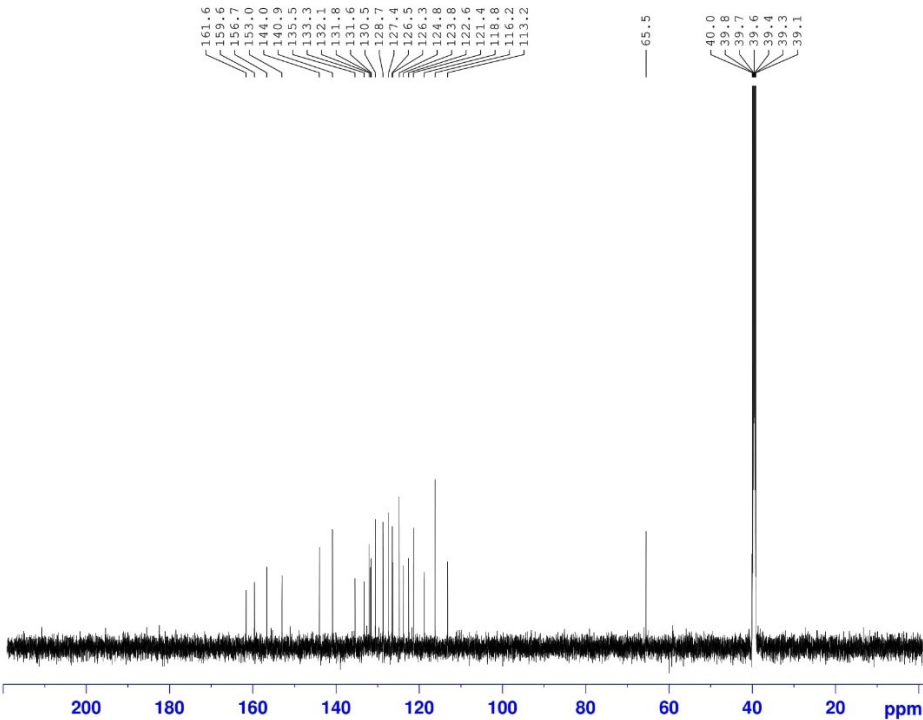
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PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.183399 Hz  
AQ 2.7262976 sec  
RG 86.85  
DW 41.600 usec  
DE 6.50 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SF01 600.1537062 MHz  
NUC1 1H  
P1 10.90 usec  
PLW1 22.60000038 W

F2 - Processing parameters  
SI 65536  
SF 600.1500107 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Dr. Ajmal/Bu-7/DMSO  
C13CPD



Current Data Parameters  
NAME 25-July-2021\_Dr. Ajmal  
EXPNO 62  
PROCNO 1

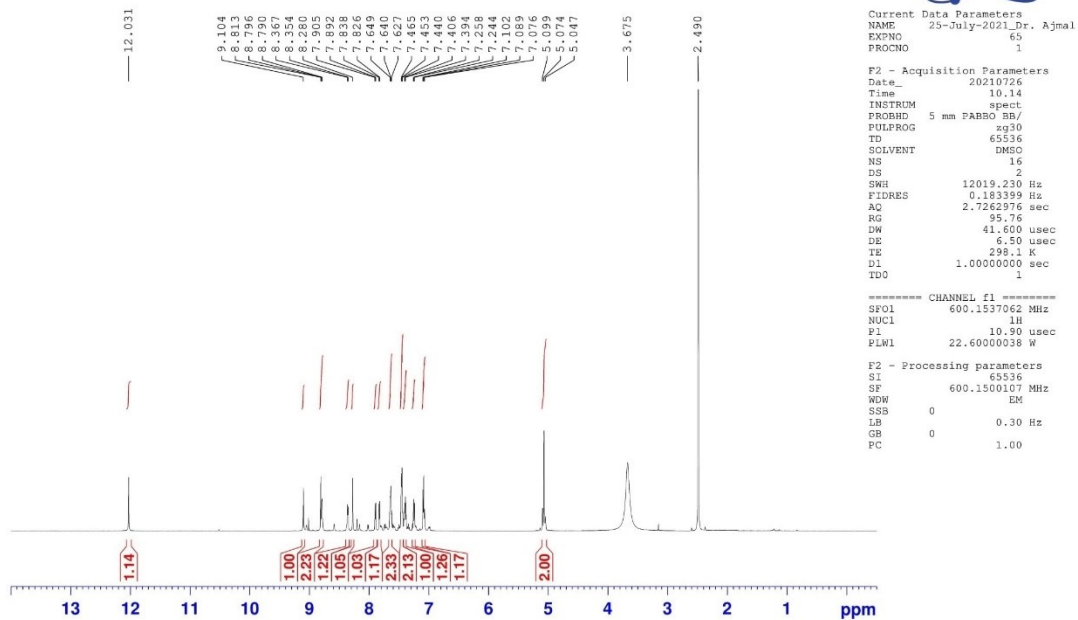
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SOLVENT DMSO  
NS 512  
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SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543823 sec  
RG 195.2  
DW 13.867 usec  
DE 6.50 usec  
TE 298.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
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NUC1 13C  
P1 11.60 usec  
PLW1 83.00000000 W

===== CHANNEL f2 =====  
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NUC2 1H  
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PCPD2 70.00 usec  
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PLW12 0.52806002 W  
PLW13 0.25874999 W

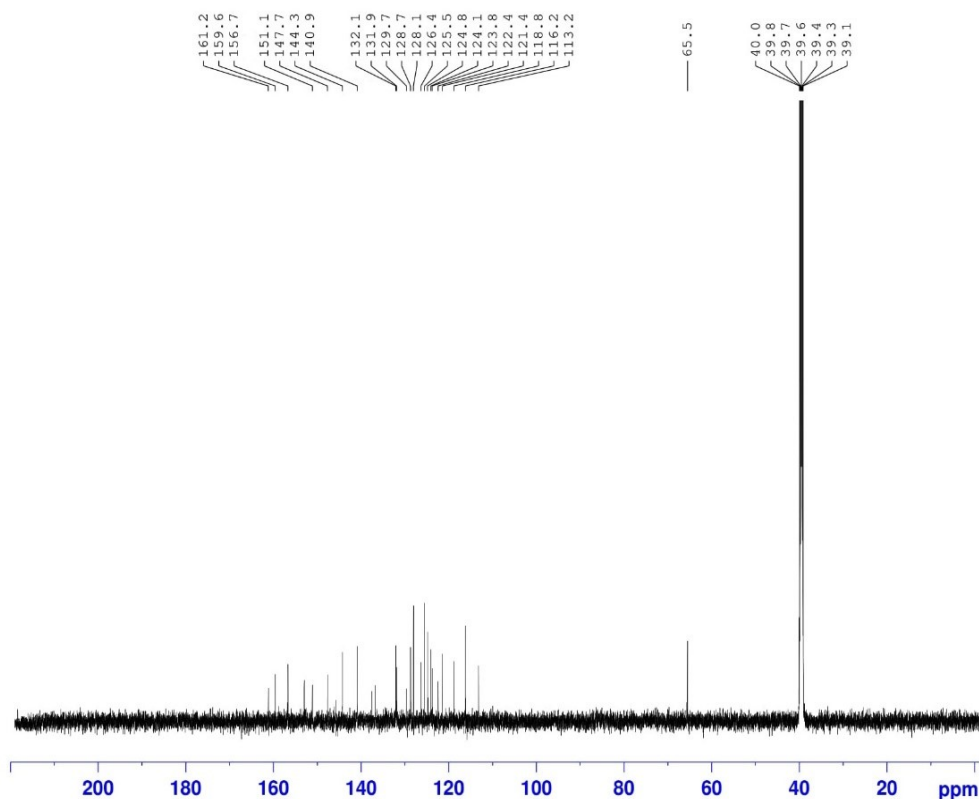
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PC 1.40

Dr. Ajmal/Bu-8/DMSO  
PROTON



**$^1\text{H}$ -NMR and  $^{13}\text{C}$ -NMR Spectra of 7e**

Dr. Ajmal/Bu-8/DMSO  
C13CPD



Current Data Parameters  
NAME 25-July-2021-Dr. Ajmal  
EXPNO 66  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210726  
Time 10.21  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT DMSO  
NS 1024  
DS 4  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 195.2  
DW 13.867 usec  
DE 6.50 usec  
TE 298.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

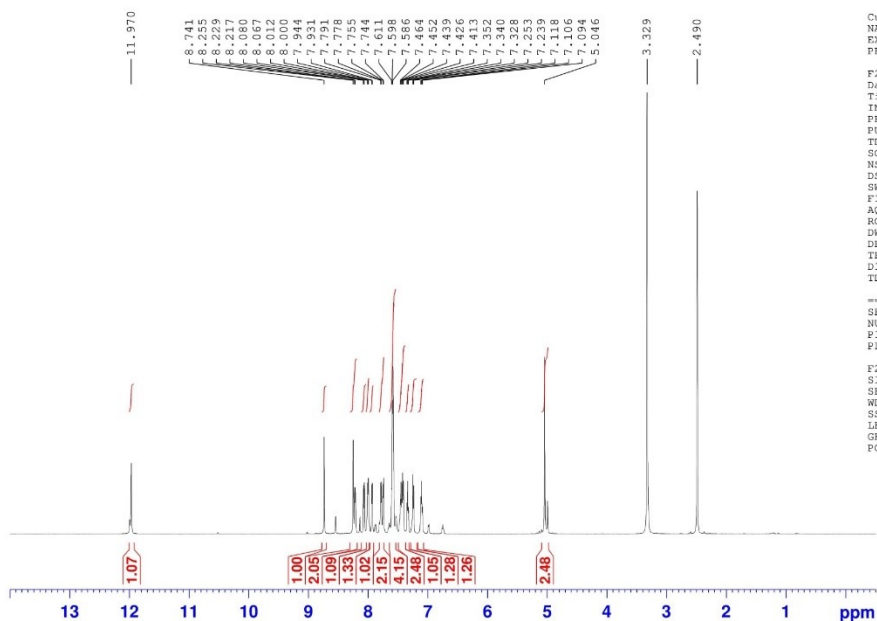
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===== CHANNEL f2 =====  
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NUC2 1H  
CPDPRG2 waltz16  
PCPD2 70.00 usec  
PLW2 22.60000038 W  
PLW12 0.52806002 W  
PLW13 0.25874999 W

F2 - Processing parameters  
SI 32768  
SF 150.9079041 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

## $^1\text{H}$ -NMR and $^{13}\text{C}$ -NMR Spectra of 7f

Dr. Ajmal/Bu-11/DMSO  
PROTON



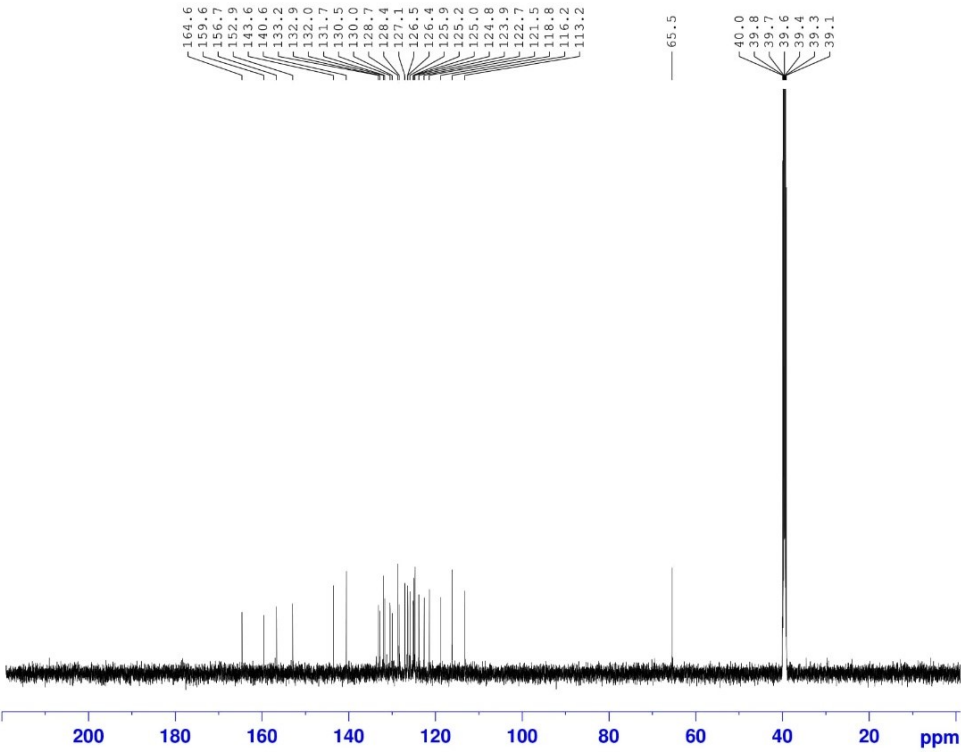
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EXPNO 77  
PROCNO 1

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PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.183399 Hz  
AQ 2.7262976 sec  
RG 70.11  
DW 41.600 usec  
DE 6.50 usec  
TE 298.2 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SF01 600.1537062 MHz  
NUC1 1H  
P1 10.90 usec  
PLW1 22.60000038 W

F2 - Processing parameters  
SI 65536  
SF 600.1500107 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Dr. Ajmal/Bu-11/DMSO  
C13CPD



Current Data Parameters  
NAME 25-July-2021\_Dr. Ajmal  
EXPNO 78  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210726  
Time 13.25  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT DMSO  
NS 271  
DS 4  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
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DE 6.50 usec  
TE 298.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

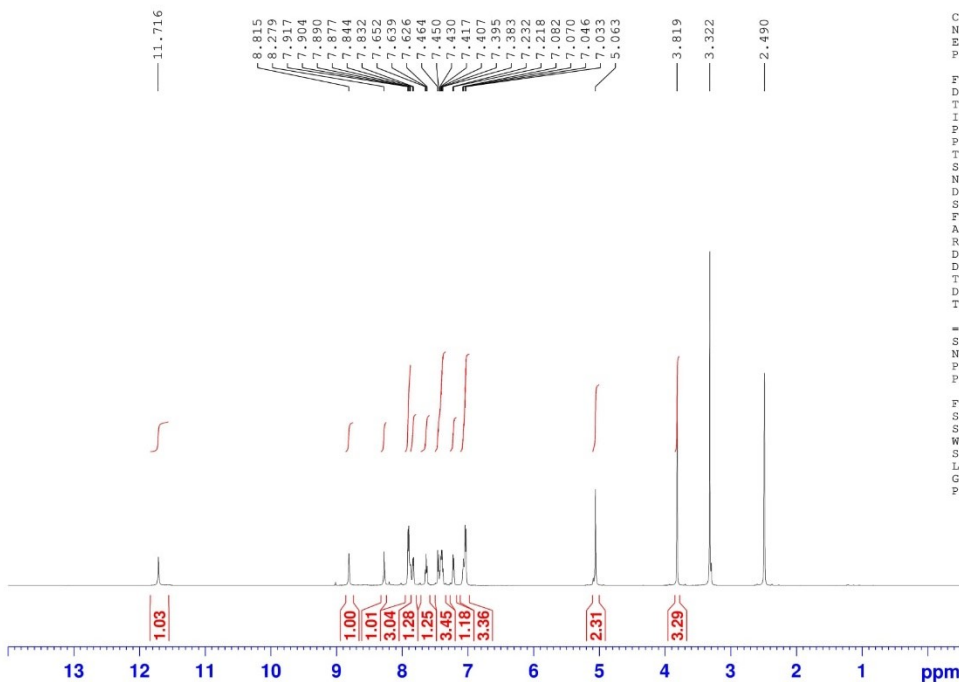
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NUC2 1H  
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PCPD2 70.00 usec  
PLW2 22.60000038 W  
PLW12 0.52806002 W  
PLW13 0.25874999 W

F2 - Processing parameters  
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SF 150.9079041 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
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**<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of 7g**

Dr. Ajmal/Bu-12/DMSO  
PROTON



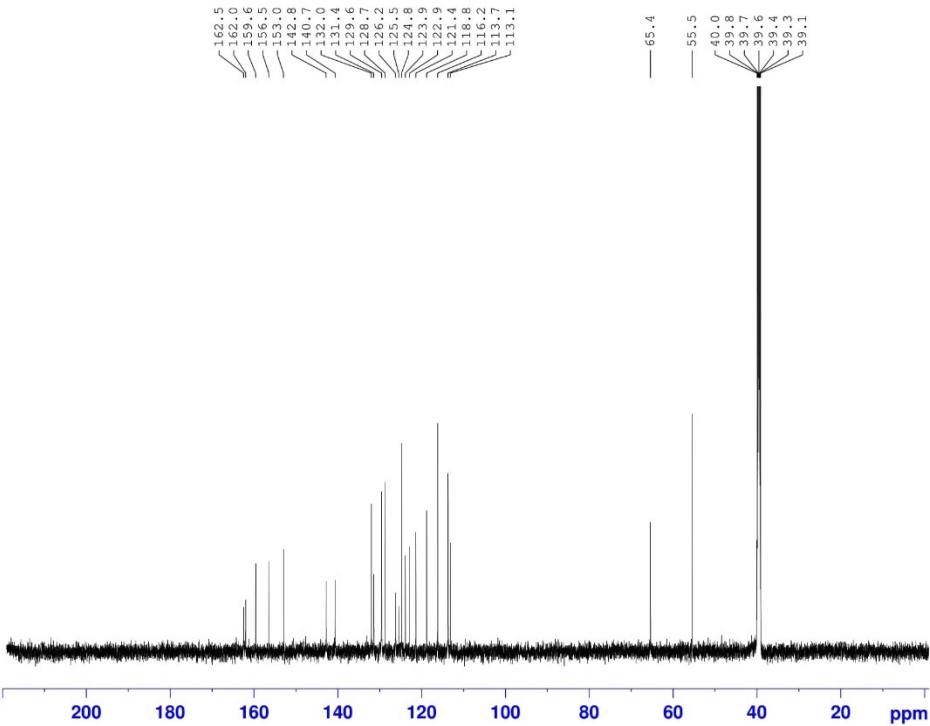
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EXPNO 81  
PROCNO 1

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SOLVENT DMSO  
NS 16  
DS 2  
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FIDRES 0.183399 Hz  
AQ 2.7262976 sec  
RG 76.79  
DW 41.600 usec  
DE 6.50 usec  
TE 298.2 K  
D1 1.00000000 sec  
TD0 1

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NUC1 1H  
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PLW1 22.60000038 W

F2 - Processing parameters  
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SF 600.1500107 MHz  
WDW EM  
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PC 1.00

Dr. Ajmal/Bu-12/DMSO  
C13CPD



Current Data Parameters  
NAME 23-July-2021 Dr. Ajmal  
EXPNO 82  
PROCNO 1

F2 - Acquisition Parameters  
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INSTRUM spect  
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SOLVENT DMSO  
NS 1024  
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FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
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DE 6.50 usec  
TE 298.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

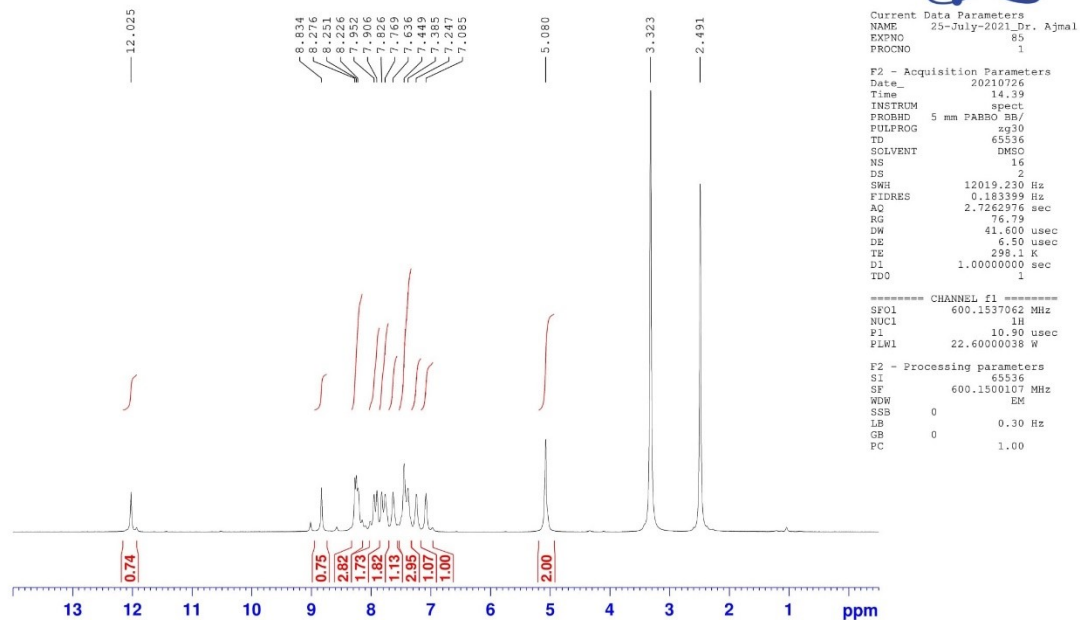
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NUC2 1H  
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PCPD2 70.00 usec  
PLW2 22.60000038 W  
PLW12 0.52806002 W  
PLW13 0.25874999 W

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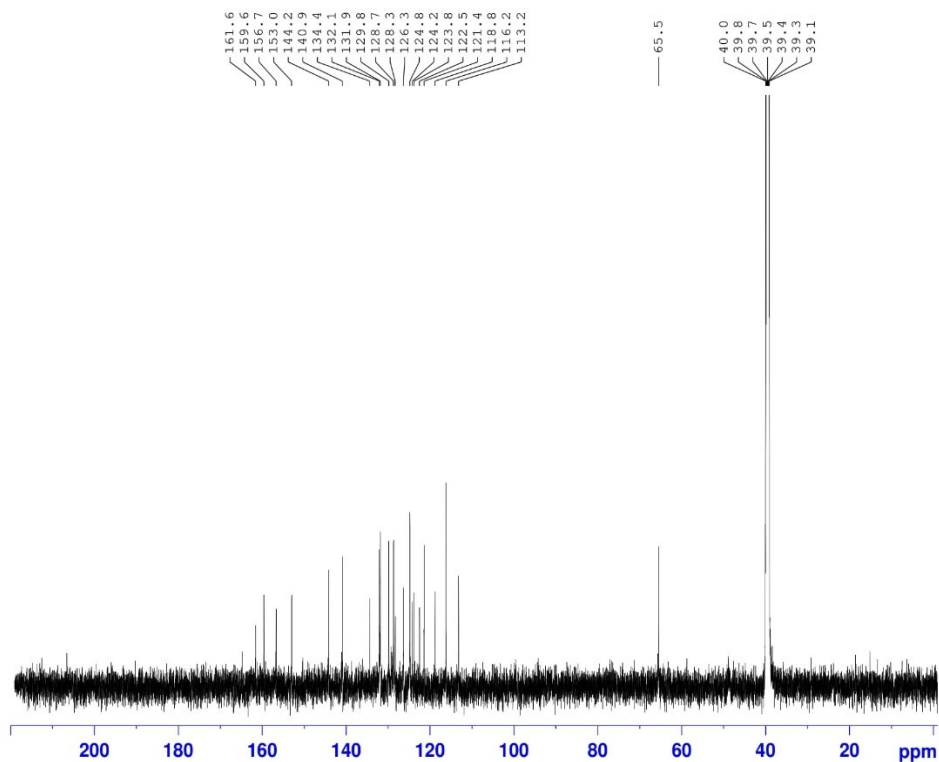
# $^1\text{H}$ -NMR and $^{13}\text{C}$ -NMR Spectra of 7h

Dr. Ajmal/Bu-13/DMSO  
PROTON





Dr. Ajmal/Bu-13/DMSO  
C13CPD



```

Current Data Parameters
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EXPNO     86
PROCNO    1

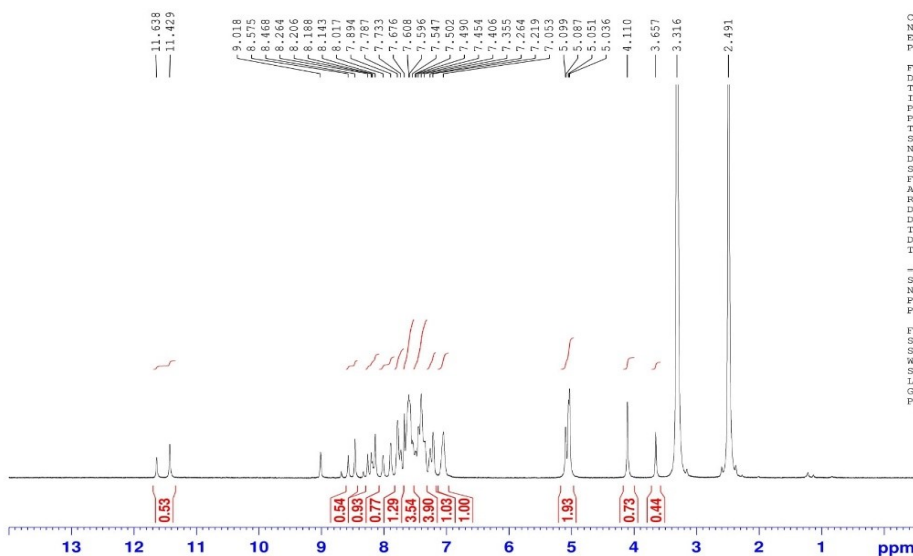
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SOLVENT   DMSO
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DS         4
SWH        36057.691 Hz
FIDRES     1.100393 Hz
AQ         0.4543829 sec
RG         195.2
DN         13.867 usec
DE         6.50 usec
TE         298.1 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

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NUC1       13C
P1         11.60 usec
PLW1       83.00000000 W

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NUC2       1H
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PCPD2      70.00 usec
PLW2       22.60000038 W
PLW12      0.52805002 W
PLW13      0.25874999 W

F2 - Processing parameters
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WDW        EM
SSB        0
LB         1.00 Hz
GB         0
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Dr. Ajmal/Bu-14/DMSO  
PROTON



Current Data Parameters  
NAME 25-July-2021.Dr. Ajmal  
EXPNO 69  
PROCNO 1

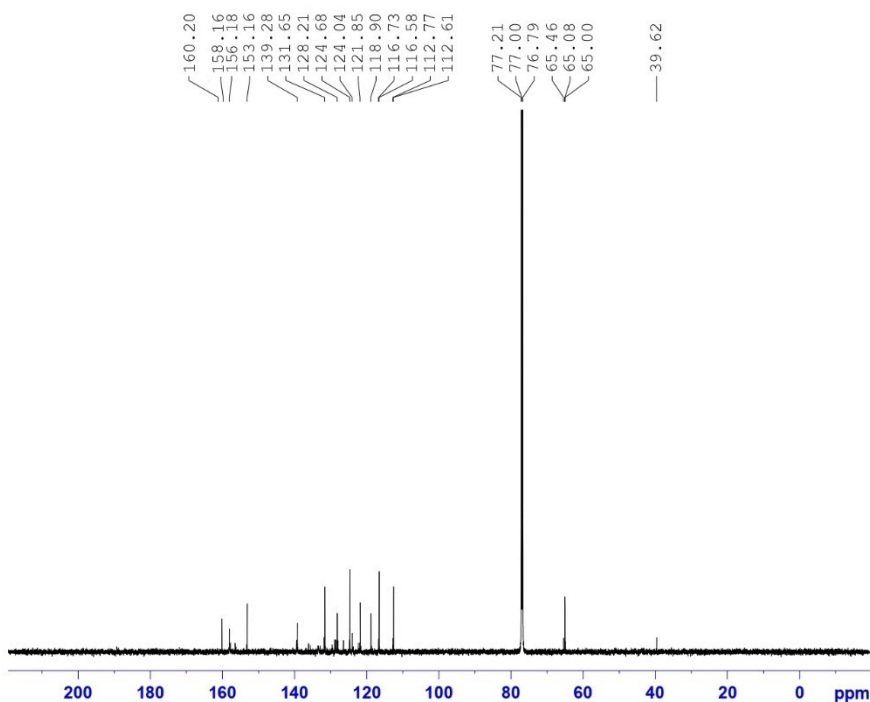
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TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.183339 Hz  
AQ 2.7262976 sec  
RG 76.79  
DW 41.600 usec  
DE 6.50 usec  
TE 298.2 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 600.1537062 MHz  
NUC1 1H  
P1 10.90 usec  
PLW1 22.60000038 W

F2 - Processing parameters  
SI 65536  
SF 600.1500107 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

## <sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of 7i

Dr. Ajmal / Bu-14 / CDCl<sub>3</sub>  
C13CPD



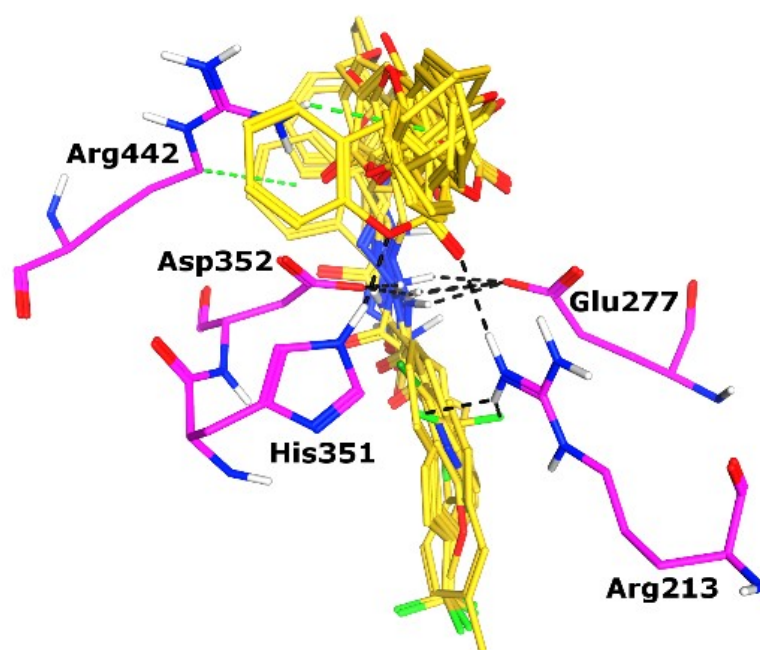
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TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 10240  
DS 4  
SWH 36057.691 Hz  
FIDRES 0.550197 Hz  
AQ 0.9087659 sec  
RG 191.2  
DW 13.867 usec  
DE 6.50 usec  
TE 298.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 150.9229276 MHz  
NUC1 13C  
P1 11.60 usec  
PLN1 83.00000000 W

===== CHANNEL f2 =====  
SFO2 600.1524006 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 70.00 usec  
PLN2 22.60000038 W  
PLN12 0.52806002 W  
PLN13 0.25874999 W

F2 - Processing parameters  
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SF 150.9078399 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



**Figure S1.** The docked conformations of all the compounds (presented in yellow sticks) are shown in the active site of  $\alpha$ -glucosidase. The binding residues in the active site are presented in magenta sticks, H-bonds and hydrophobic bonds are depicted in black and green dotted lines, respectively.