

Novel C-2 Symmetric Molecules as α -Glucosidase and α -Amylase Inhibitors: Design, Synthesis, Kinetic Evaluation, Molecular Docking and Pharmacokinetics

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Supplementary data

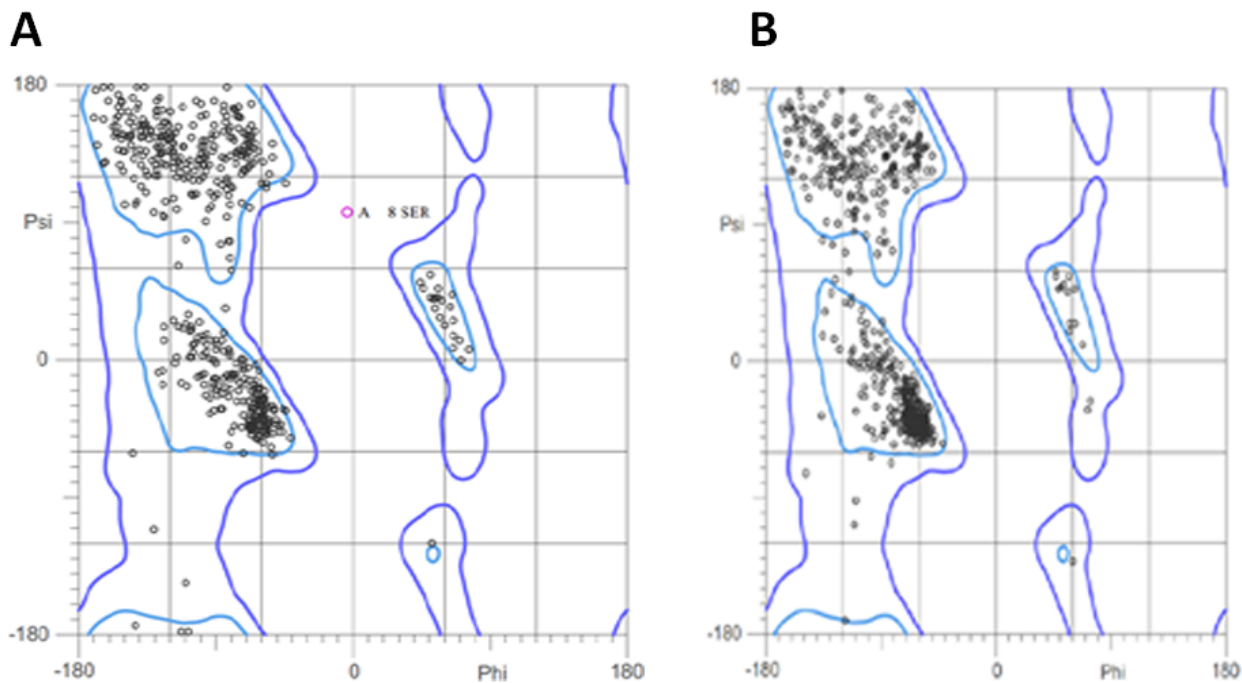


Figure. S1. Ramachandran graphs of α -amylase (A) and α -glucosidase (B)

Docking Energy value equation

$$\Delta G_{binding} = \Delta G_{gauss} + \Delta G_{repulsion} + \Delta G_{hbond} + \Delta G_{hydrophobic} + \Delta G_{tors} \quad (i)$$

Here, ΔG_{gauss} : attractive term for dispersion of two gaussian functions, $\Delta G_{repulsion}$: square of the distance if closer than a threshold value, ΔG_{hbond} : ramp function - also used for interactions with metal ions, $\Delta G_{hydrophobic}$: ramp function, ΔG_{tors} : proportional to the number of rotatable bonds.

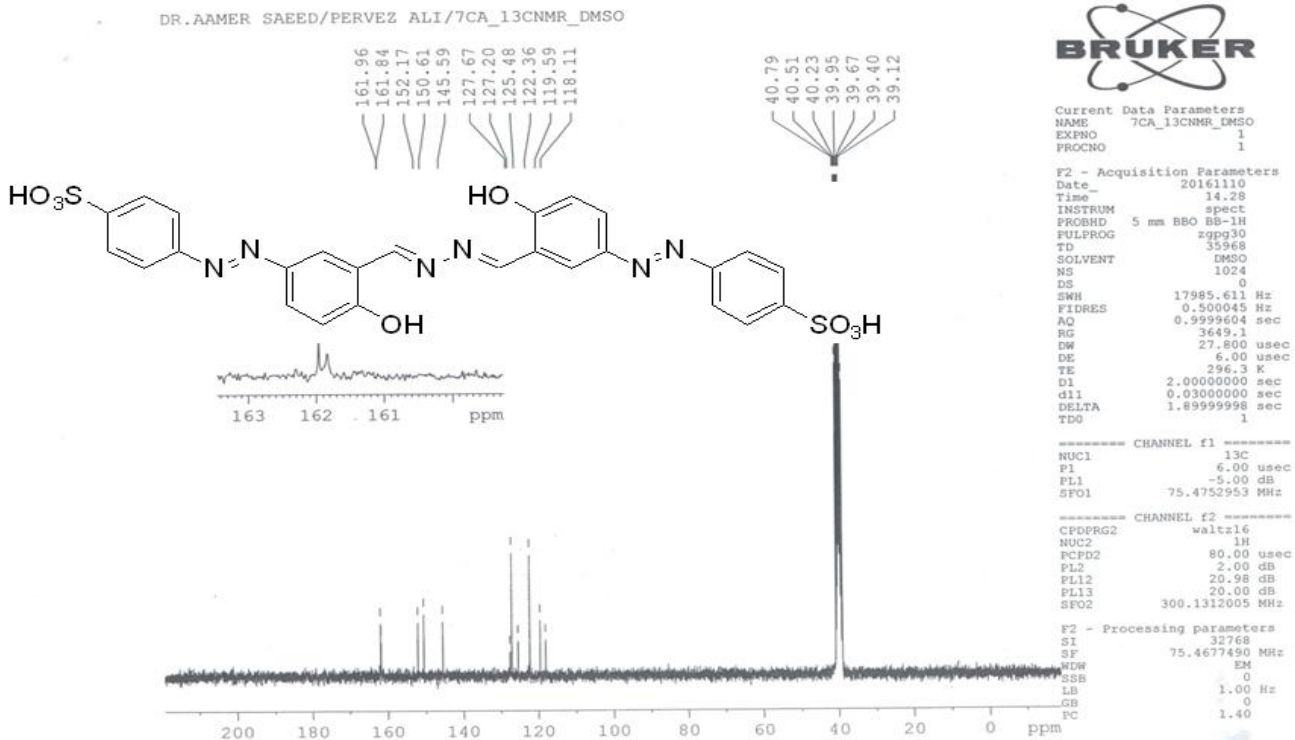
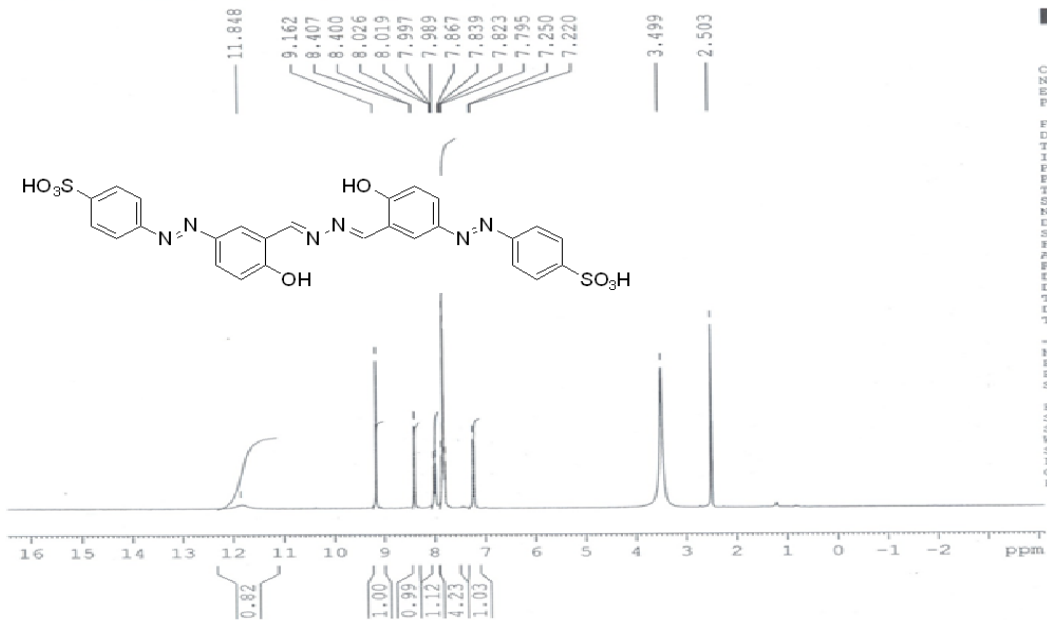


Figure -S2 ^{13}C NMR spectrum of (**5f**)

DR.AAMER SAEED/PERVEZ ALI/7CA_1HNMR_DMSO



Current Data Parameters
NAME 7CA_1HNMR_DMSO
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161110
Time 14.45
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 6172.839 Hz
FIDRES 0.094199 Hz
AQ 5.3084660 sec
RG 406.4
EM 81.000 usec
DE 6.00 usec
TE 295.9 K
D1 1.0000000 sec
TDO 1

CHANNEL f1
NUC1 1H
P1 9.00 usec
PL1 2.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
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SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure -S3 ¹H NMR spectrum of (5f)

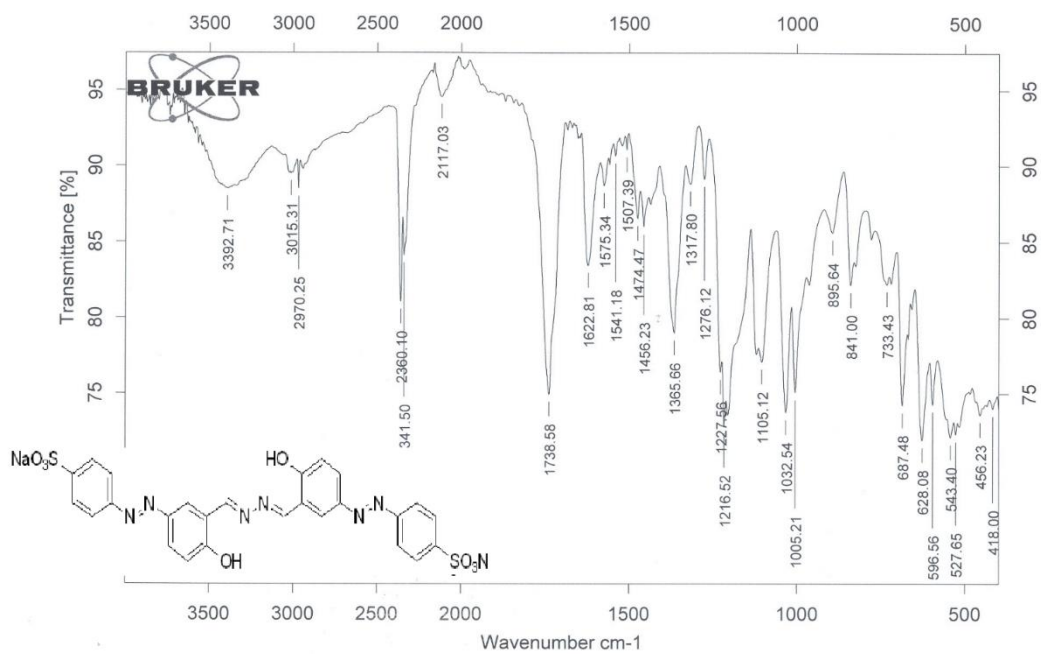


Figure S4. FT-IR spectrum of **5f**