

**Copper-Vit B<sub>3</sub> MOF preparation, characterization and catalytic evaluation in one-pot synthesis of benzoxanthenones with docking validation as anti *H-pylori***

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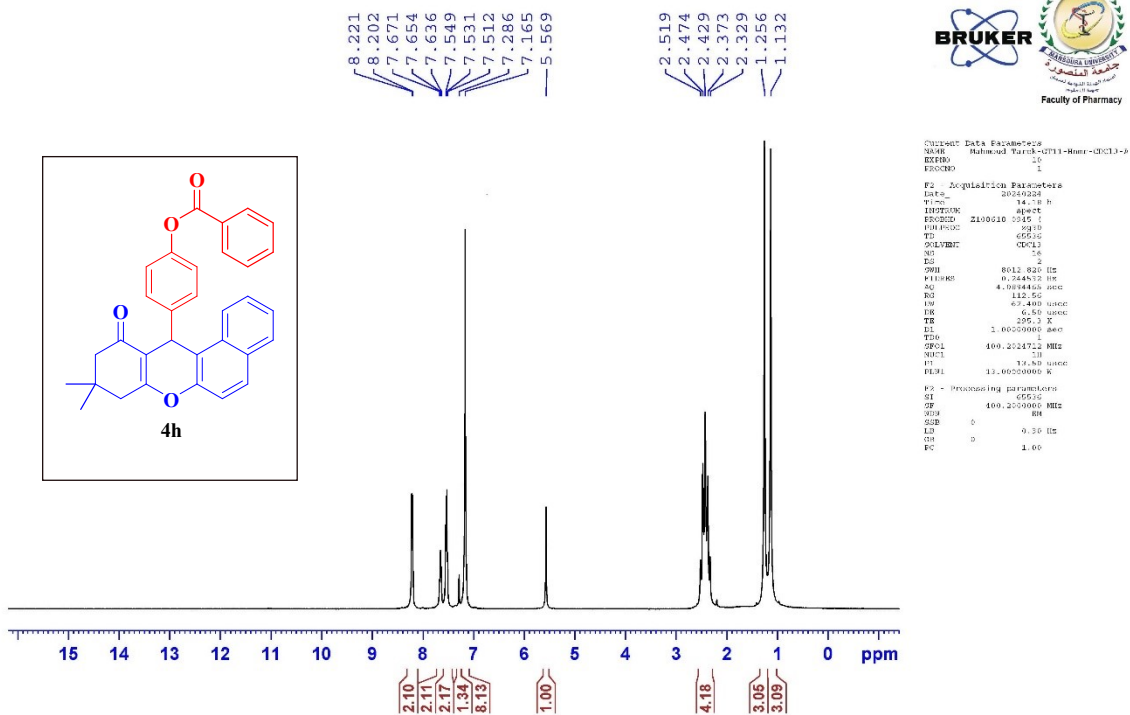
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(**T.K.Khatab**)

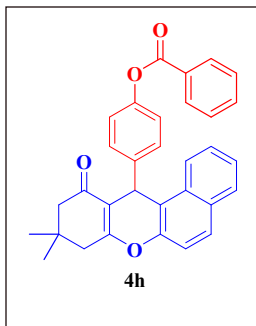
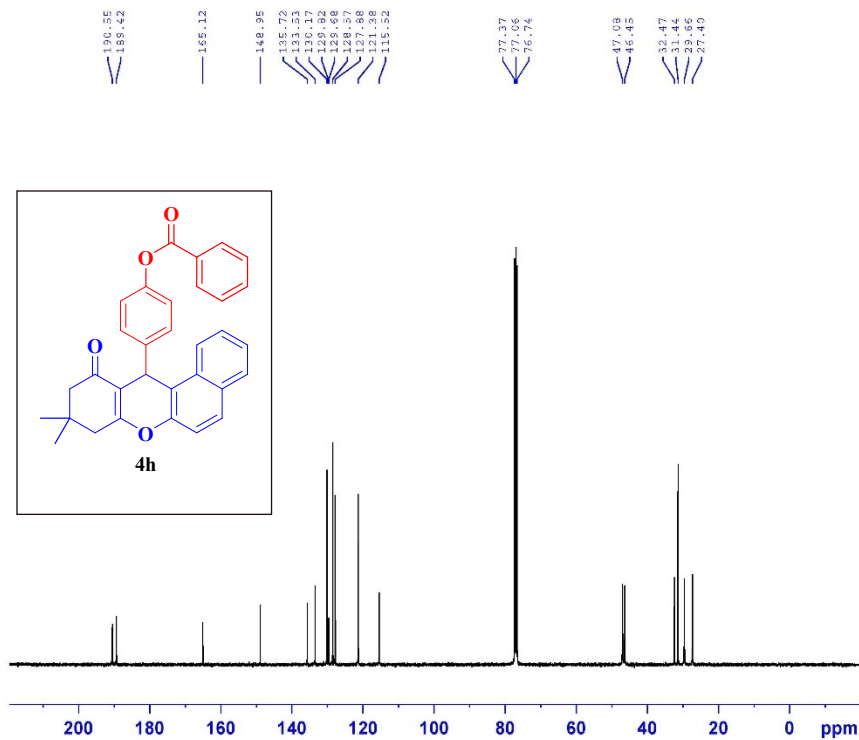
## Experimental

All melting points were evaluated using electric Gallenkamp (Germany) apparatus. The <sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectra were run on a Bruker Avance III spectrophotometer at 400 and 100 MHz, respectively. The elemental microanalytical data were measured at the Microanalytical Unit, Cairo University on Vario, Elementar apparatus (Shimadzu). TLC was used to monitor the reaction mixtures using silica gel-coated plates and irradiation with UV-Lamp for visualization. The solvents and reagents were purchased from sigma Aldrich and fluka companies.



<sup>1</sup>H NMR spectrum of compound 4h

Mahmoud Tarek-GT11-CNMR-AF



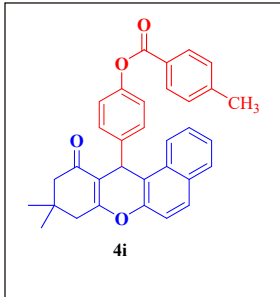
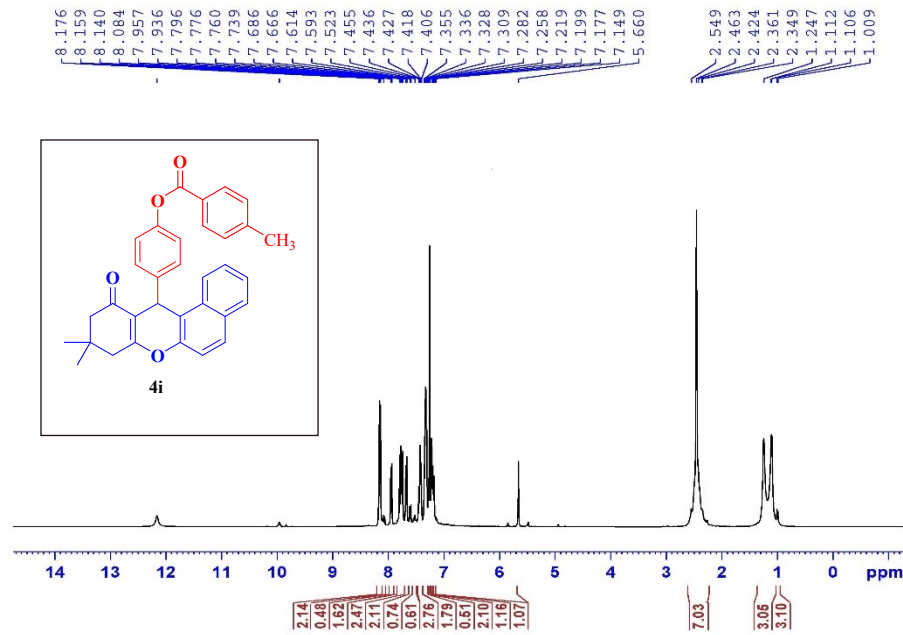
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SOLVENT CDCL3  
NS 2000  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 1.3631488 sec  
RG 197.77  
DW 20.800 usec  
DR 6.50 usec  
TE 296.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1  
SFO1 100.6404331 MHz  
NUC1 13C  
P1 10.00 usec  
PLA1 47.00000000 W  
SFO2 400.2016008 MHz  
NUC2 1H  
CPDPRG2 waltz16  
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PLA12 0.29249999 W  
PLA13 0.14713000 W

F2 - Processing parameters  
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GB 0  
PC 1.40

<sup>13</sup>C NMR spectrum of compound 4h

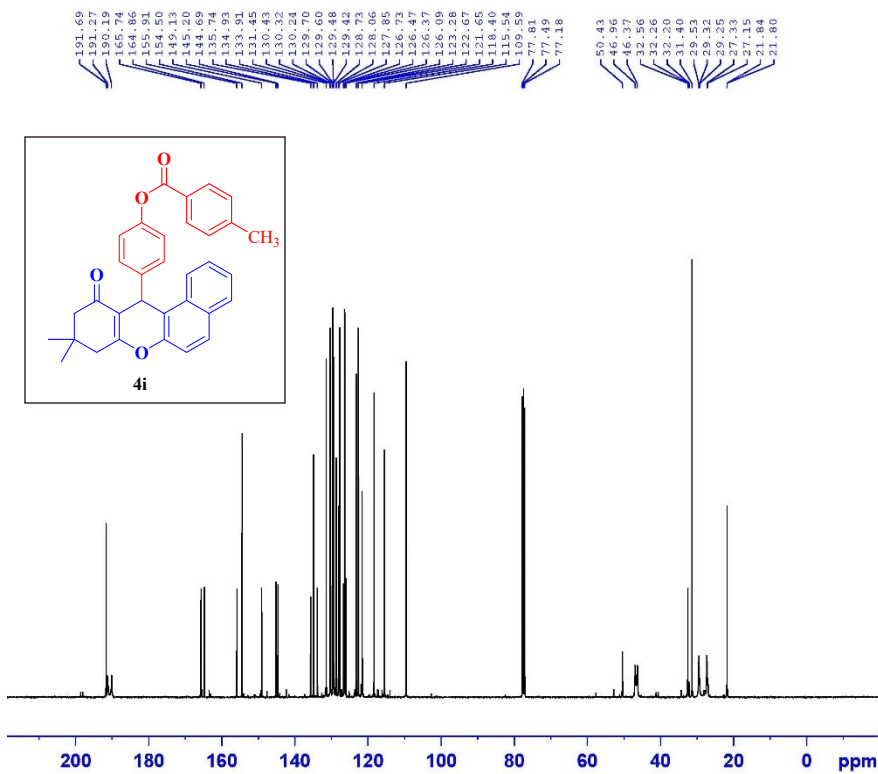
Gehad Ibrahim-GT12-Re-CDCL3-HNMR-EA



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<sup>1</sup>H NMR spectrum of compound 4i



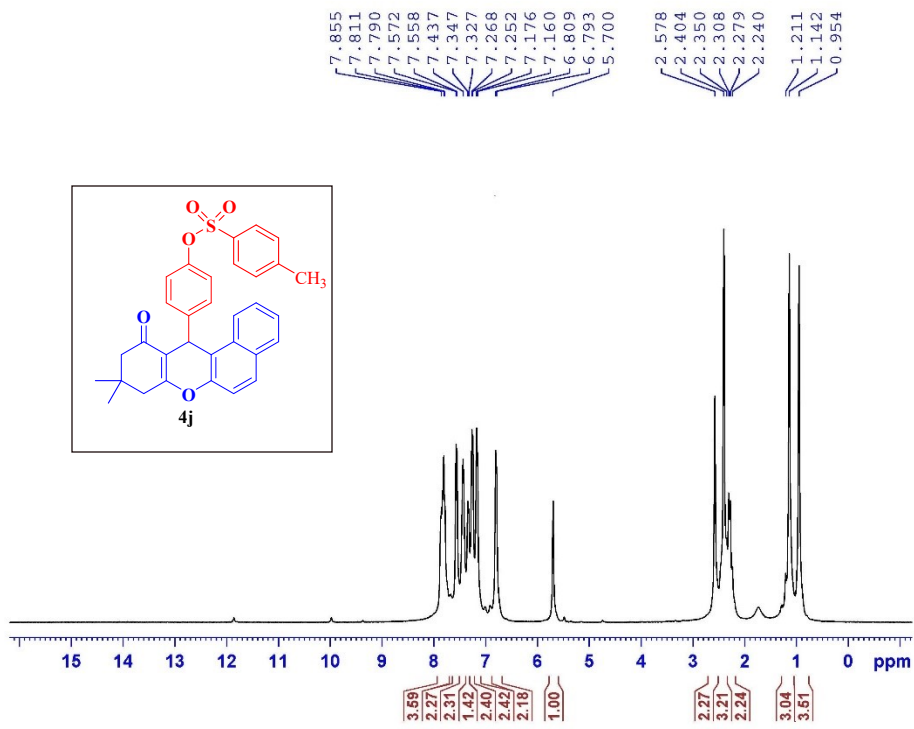
<sup>13</sup>C NMR spectrum of compound 4i



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 D11 0.03000000 sec  
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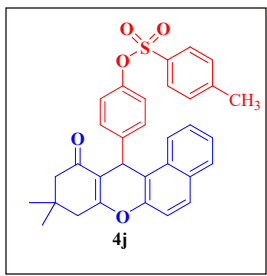
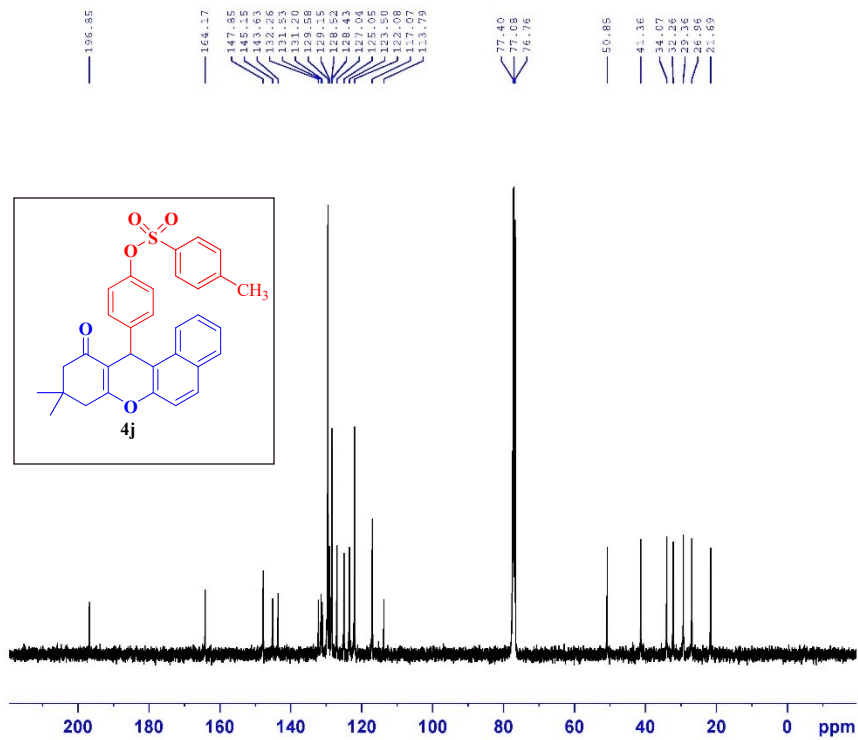


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**<sup>1</sup>H NMR spectrum of compound 4j**



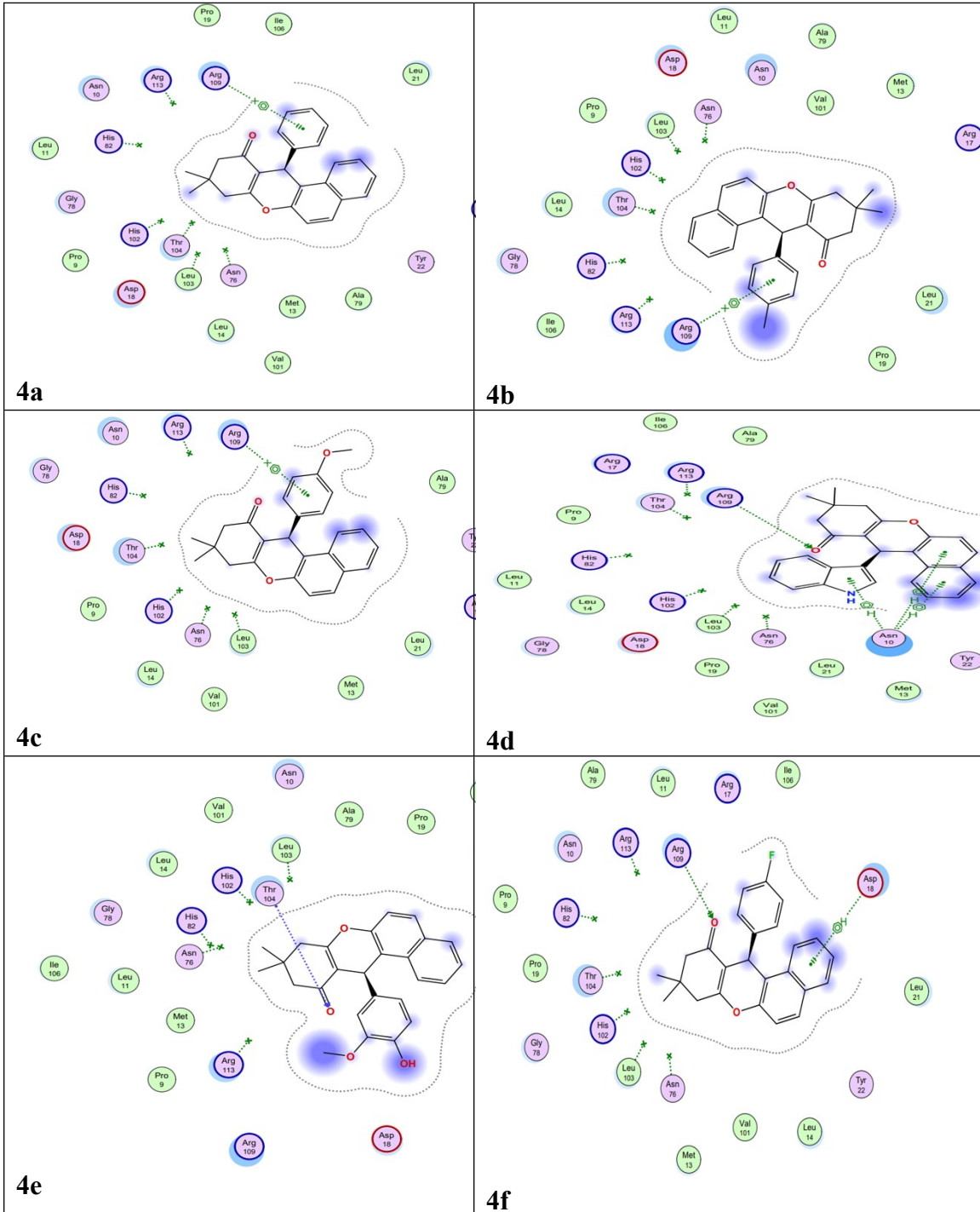
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 RG 197.77  
 DW 20.600 usec  
 DE 6.50 usec  
 TX 296.4 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1  
 SF01 100.6104331 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLM1 47.0000000 W  
 SF02 100.2016008 MHz  
 NUC2 1H  
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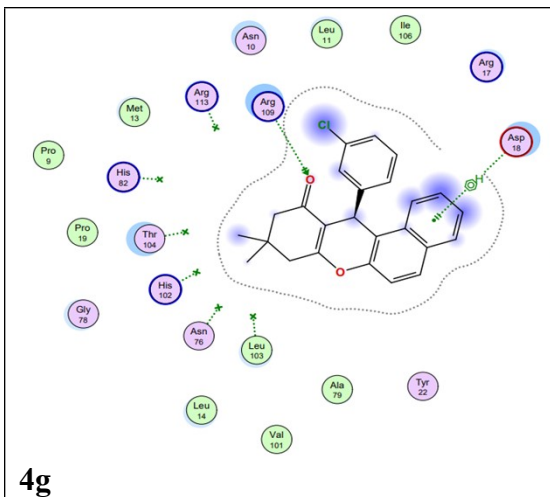
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<sup>13</sup>C NMR spectrum of compound 4j

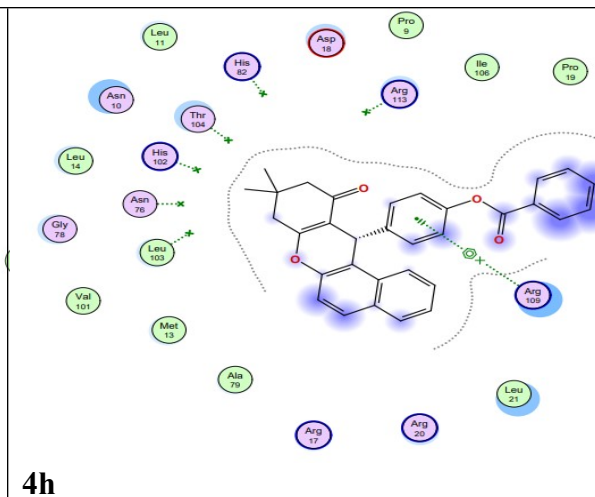
2D interaction between the prepared ligands and “*Helicobacter pylori* Type II dehydroquinase”



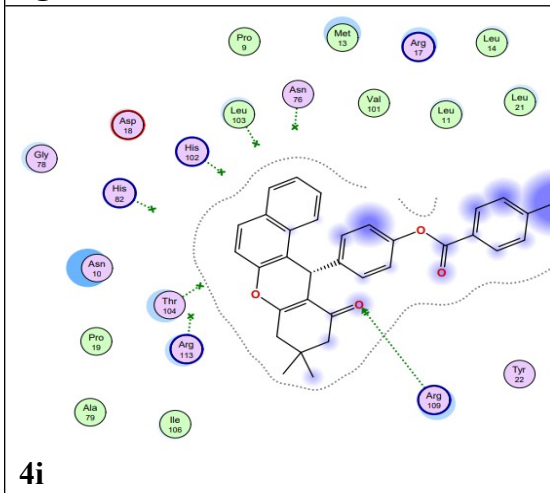




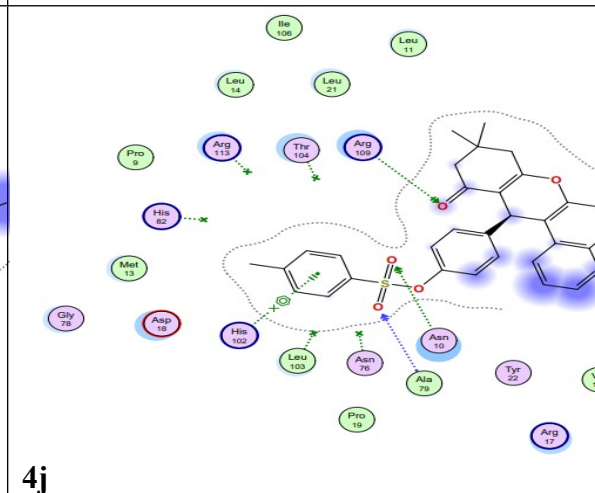
4g



4h



4i



4j