

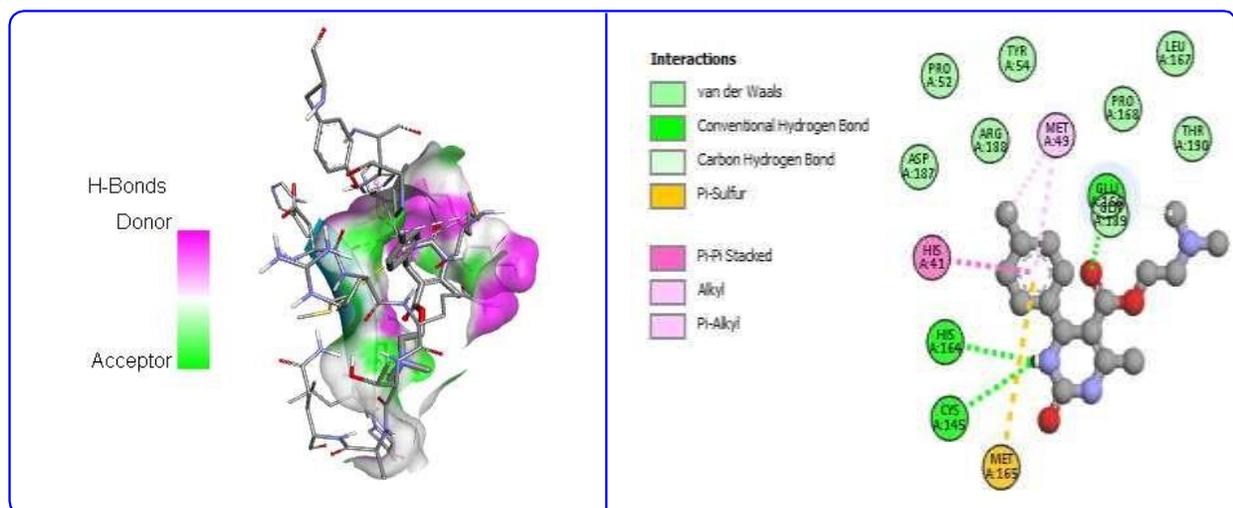
SUPPORTING INFORMATION

CuFe₂O₄ Magnetic Nanoparticles as Heterogeneous Catalysts for Synthesis of Dihydropyrimidinones as Inhibitors of SARS-CoV-2 Surface Proteins – Insights from Molecular Docking Studies

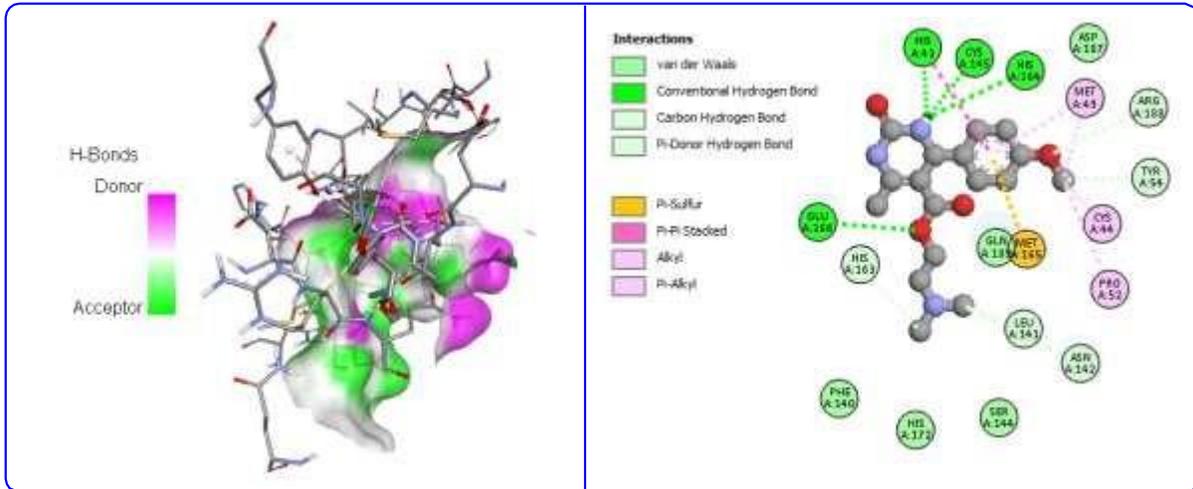
1. Molecular Docking Studies:

The crystal structure of COVID-19 main protease at 2.16 Å resolution (PDB: 6LU7), Pre-fusion spike glycoprotein with single receptor binding domain at 3.46 Å resolution (PDB: 6VSB) and the crystal structure of papain-like protease of SARS CoV-2 at 2.7 Å resolution (PDB: 6W9C) were retrieved from the Protein Data Bank. Molecular docking studies were carried out using the Autodock Vina 4.2 program and Discovery Studio Visualizer. The obtained results through molecular docking studies of 13 potential ligands with three different proteins of SARS-CoV-2 in different models of ligand–protein interactions with particular binding affinity (docking score) were summarized as follows:

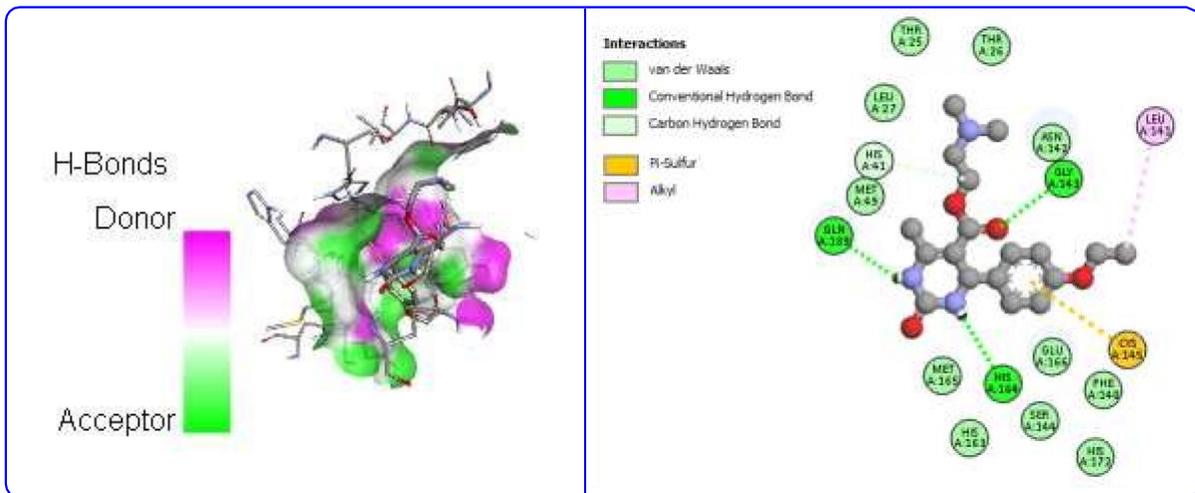
Docking results of 13 different ligands with COVID-19 main protease at 2.16 Å resolution (PDB: 6LU7)



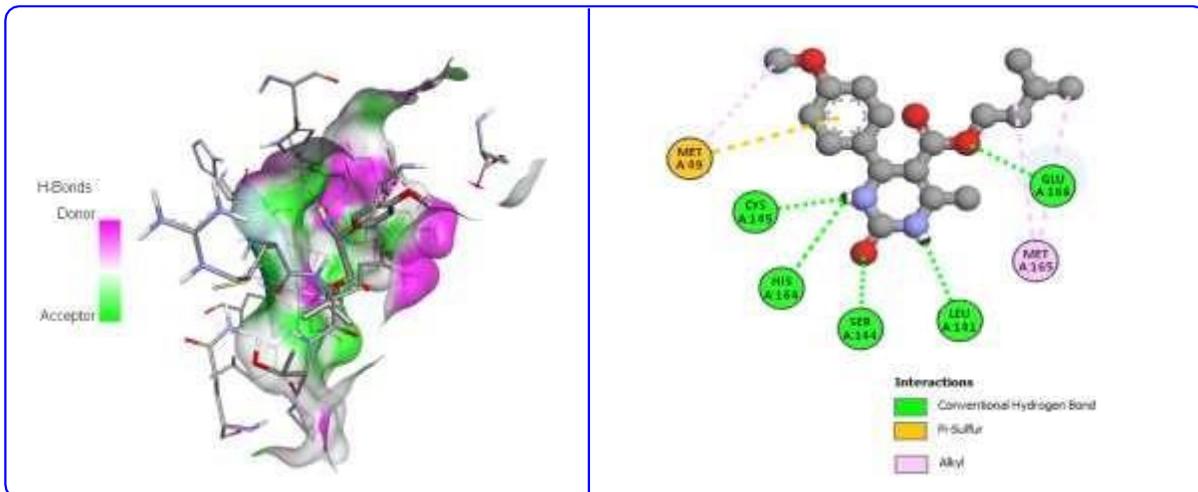
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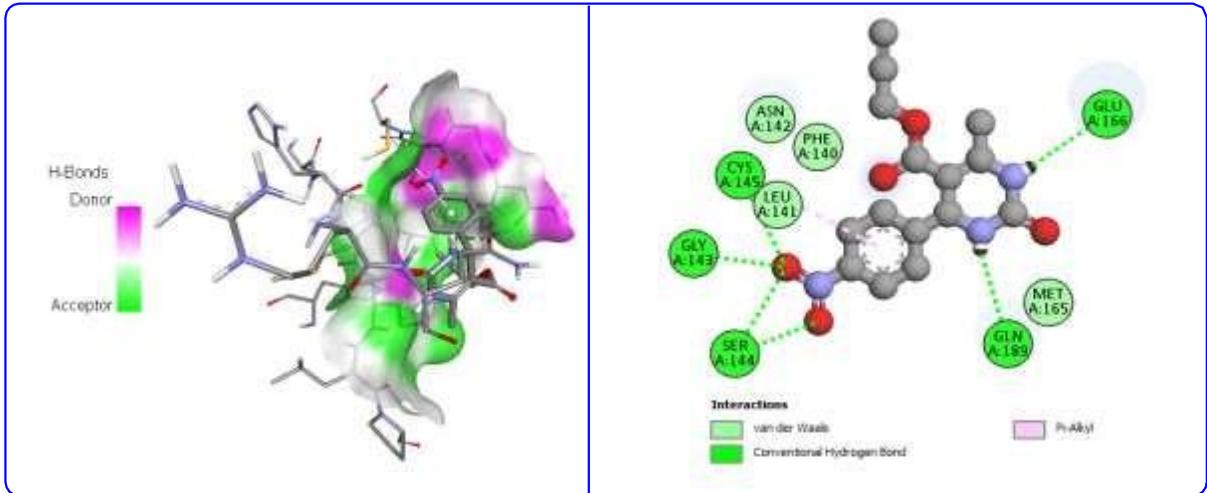
DHPM 2



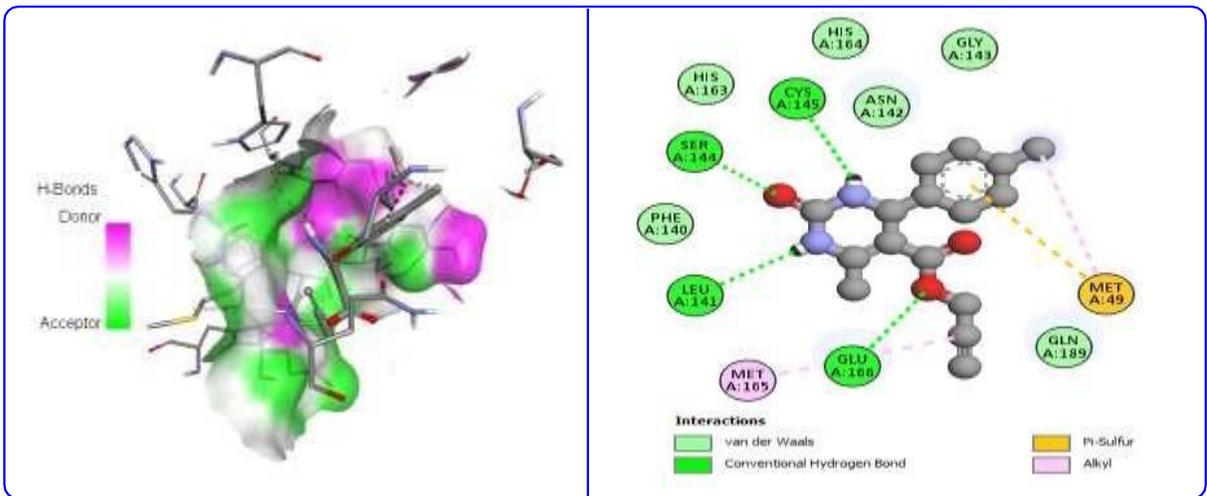
DHPM 3



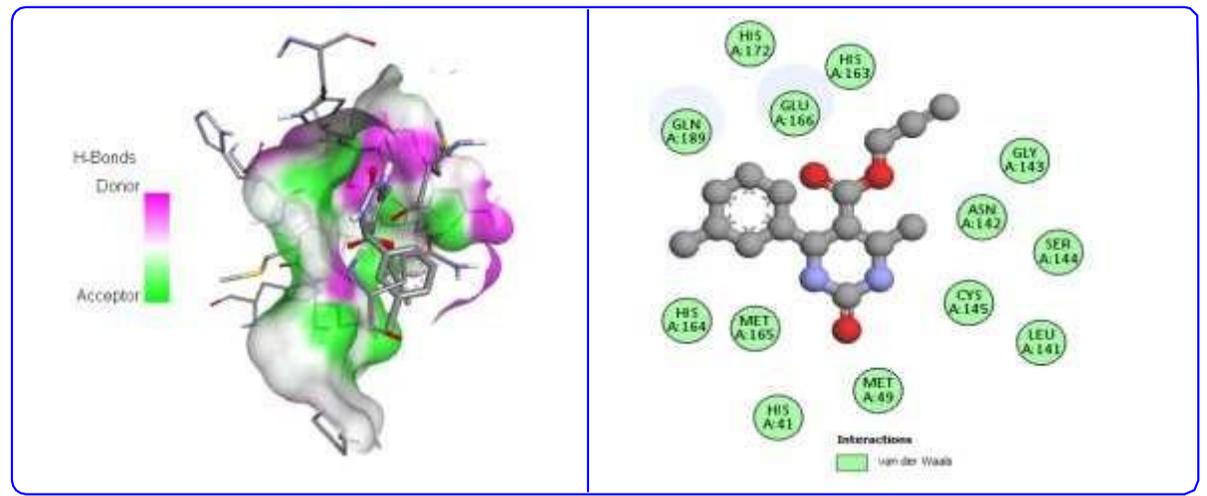
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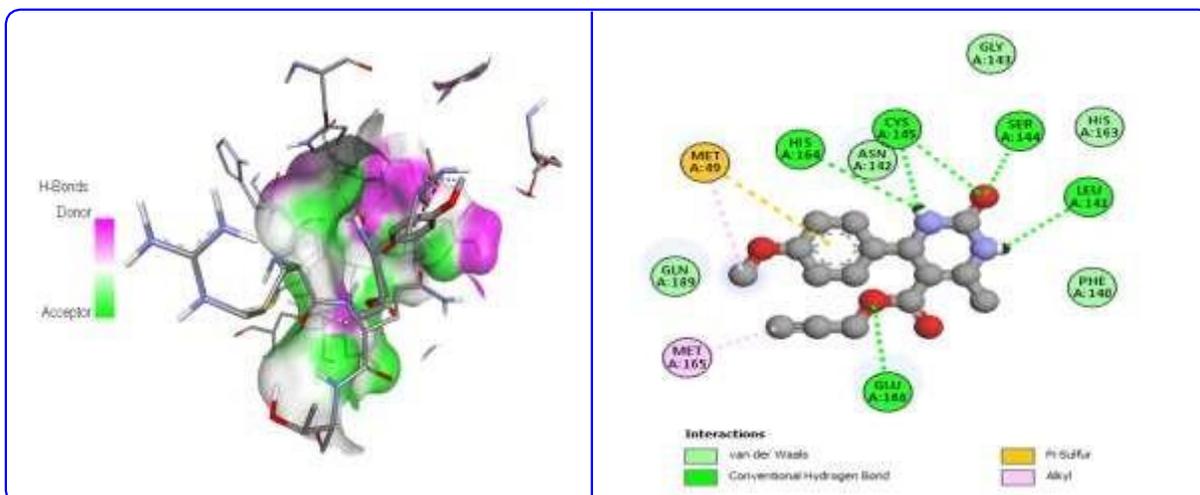
DHPM 5



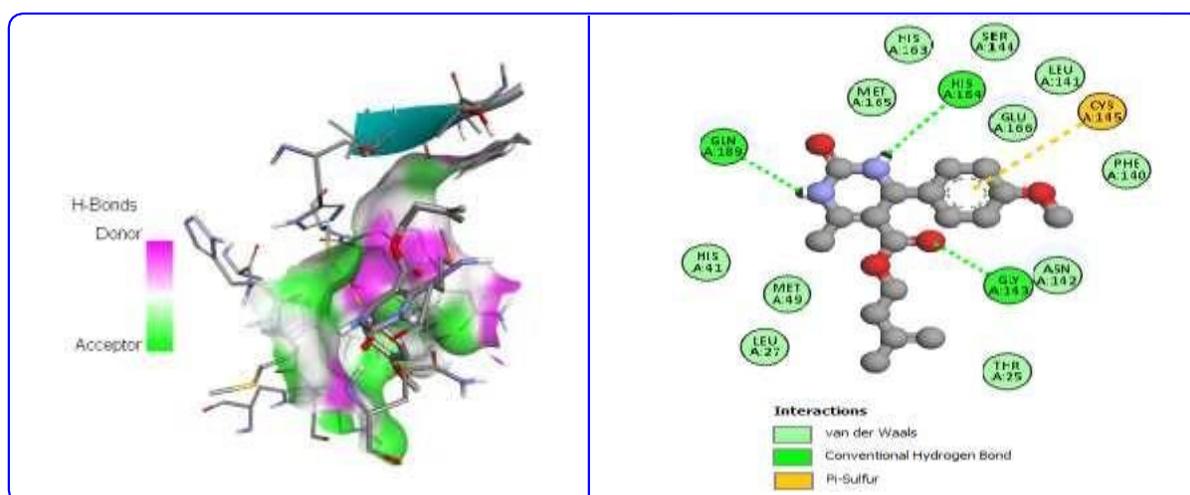
DHPM 6



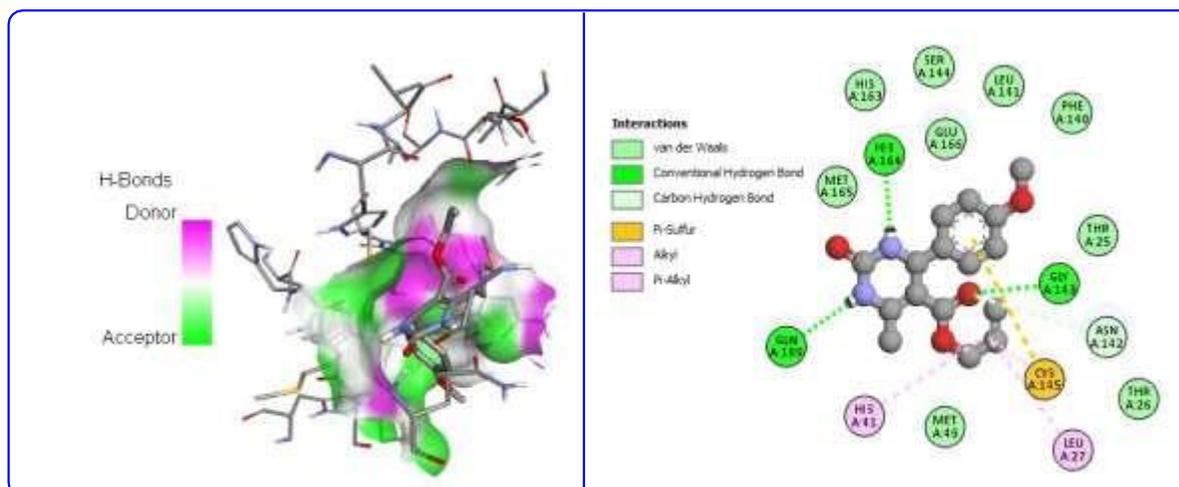
DHPM 7



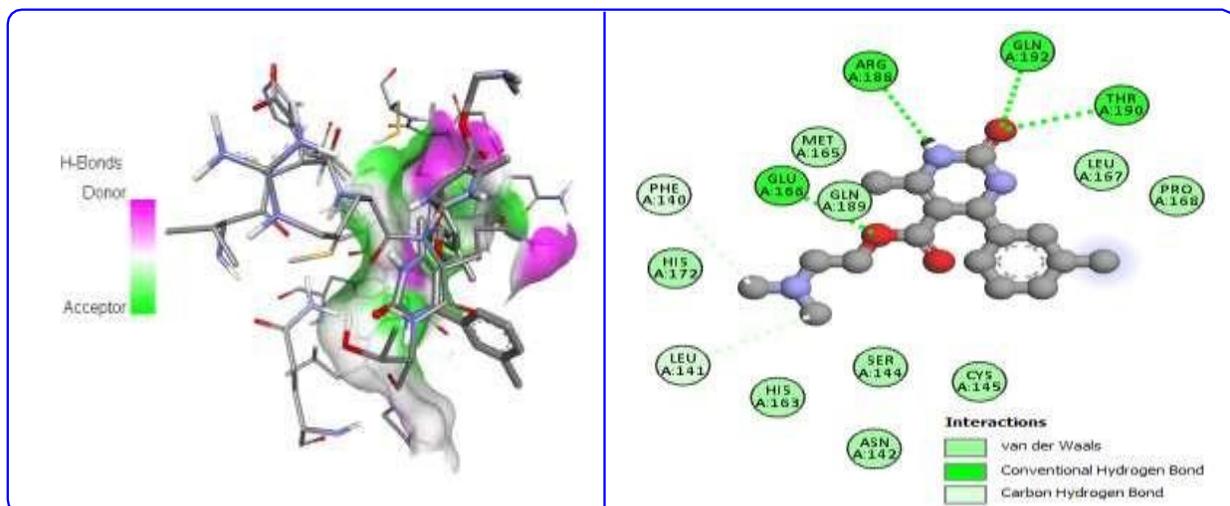
DHPM 8



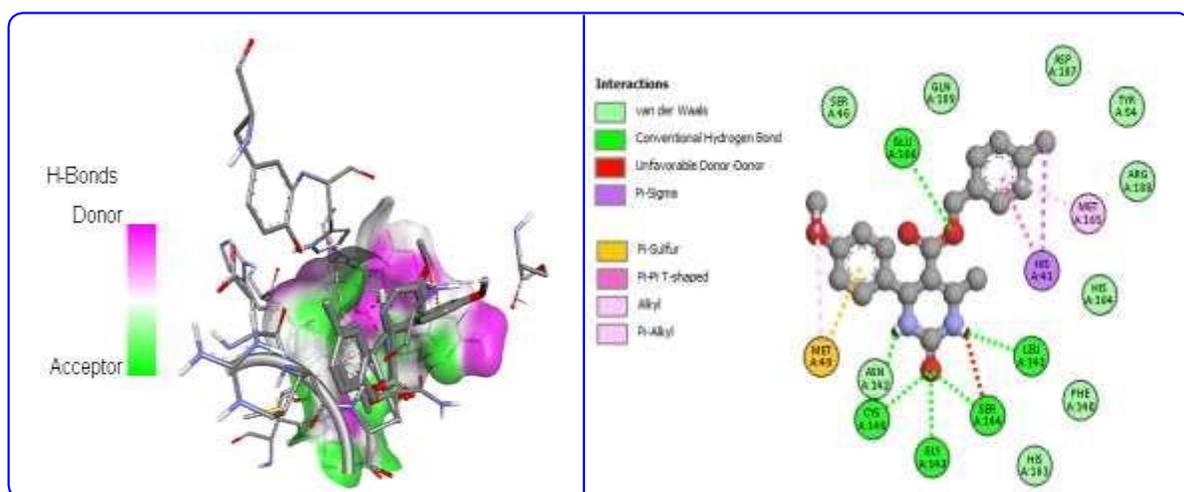
DHPM 9



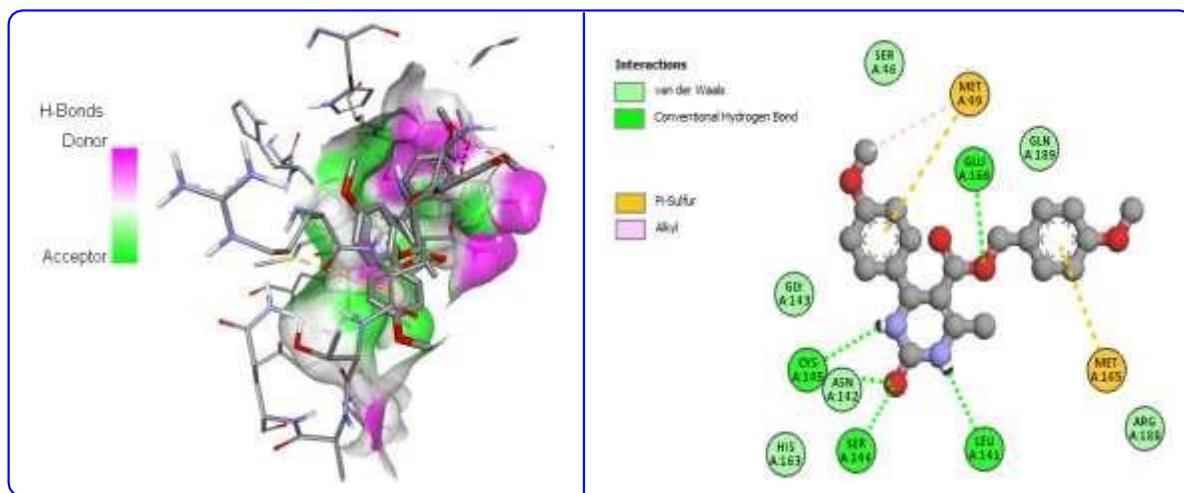
DHPM 10



DHPM 11

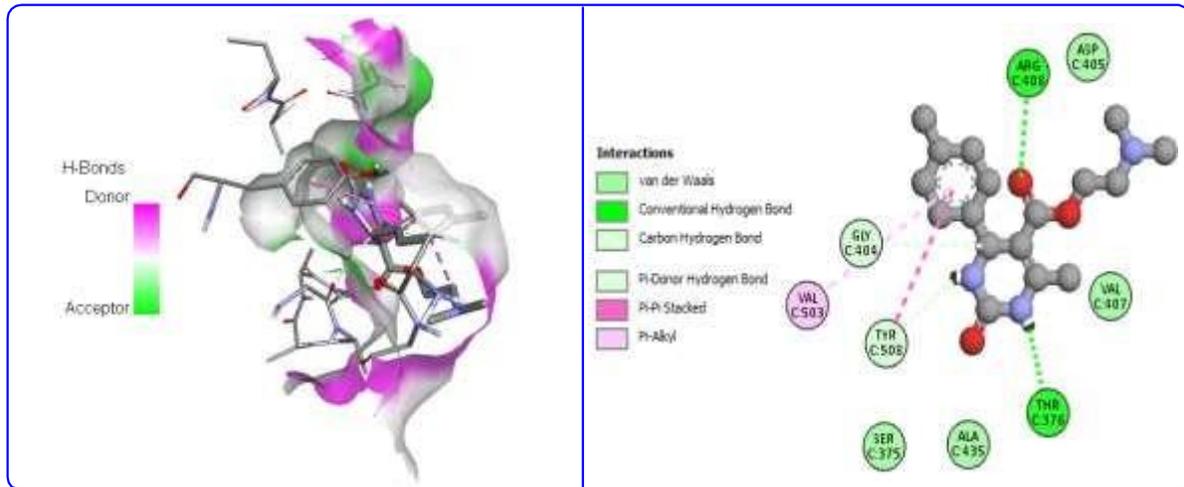


DHPM 12

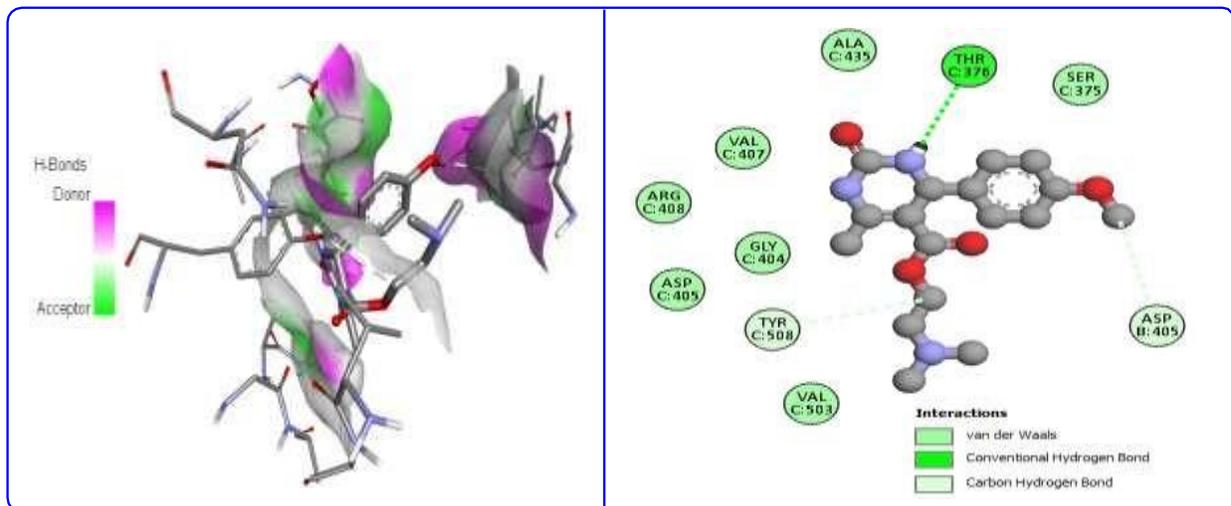


DHPM 13

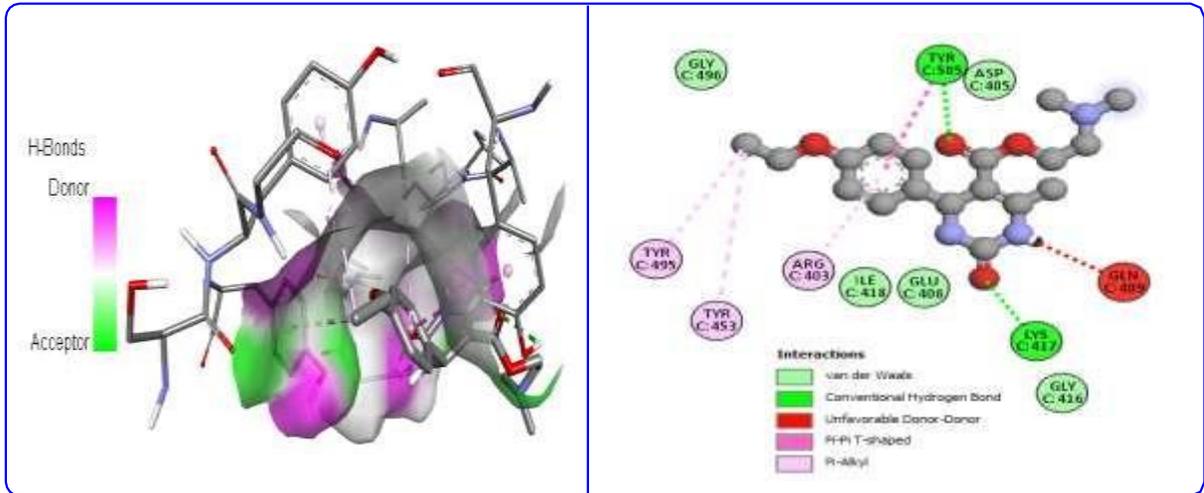
Docking results of 13 different ligands with Pre-fusion spike glycoprotein with single receptor binding domain at 3.46 Å resolution (PDB: 6VSB)



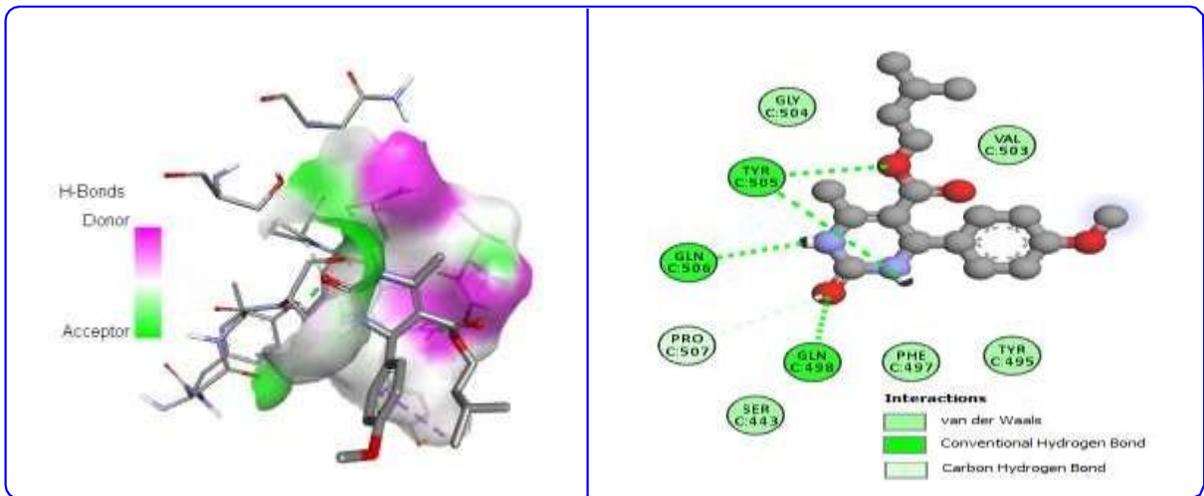
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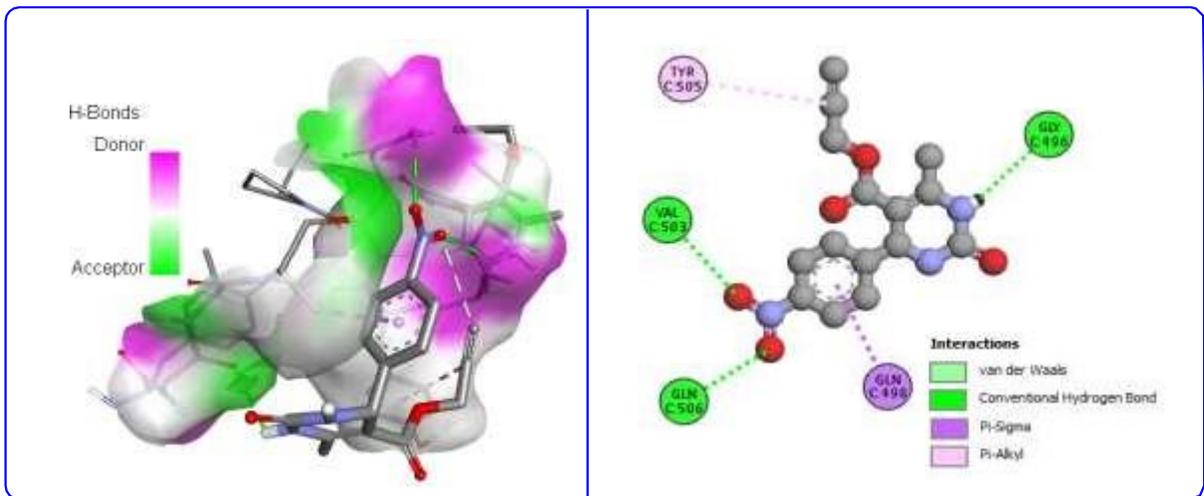
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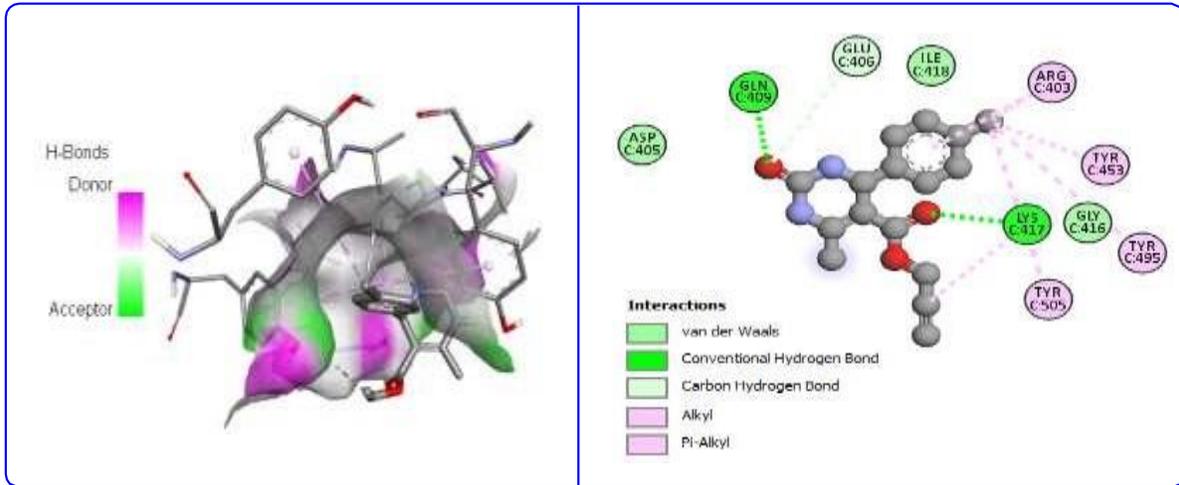
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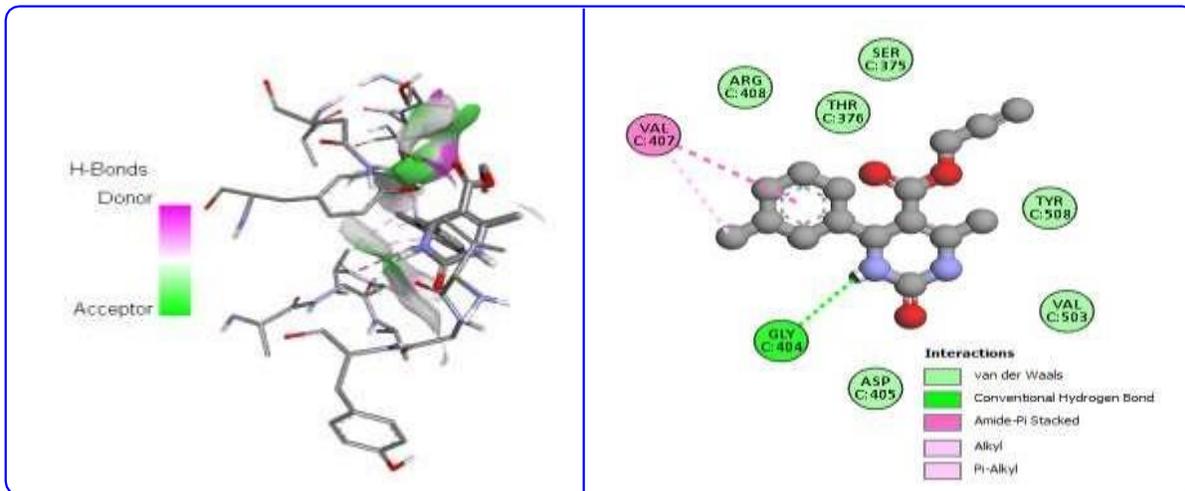
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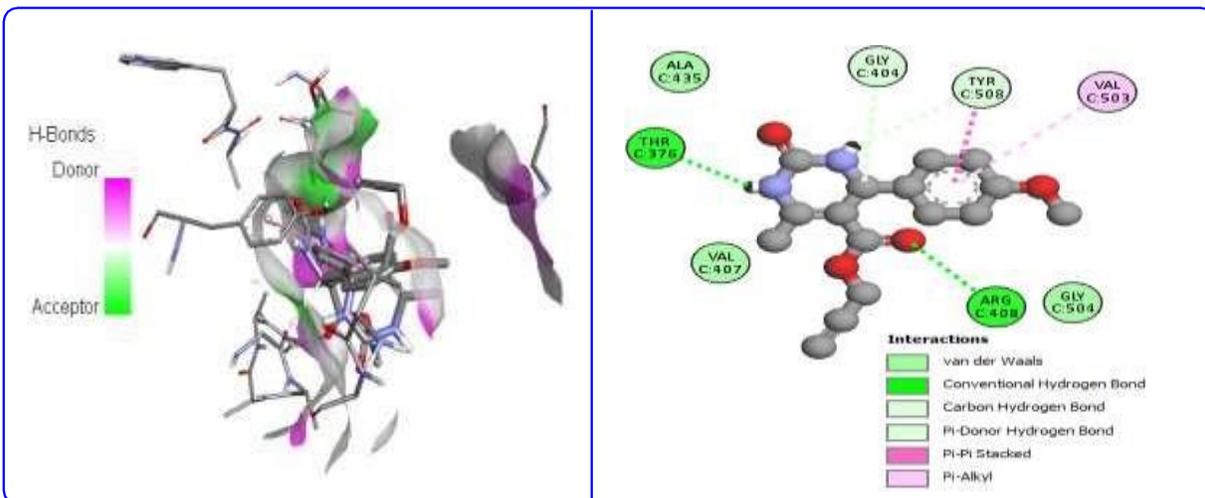
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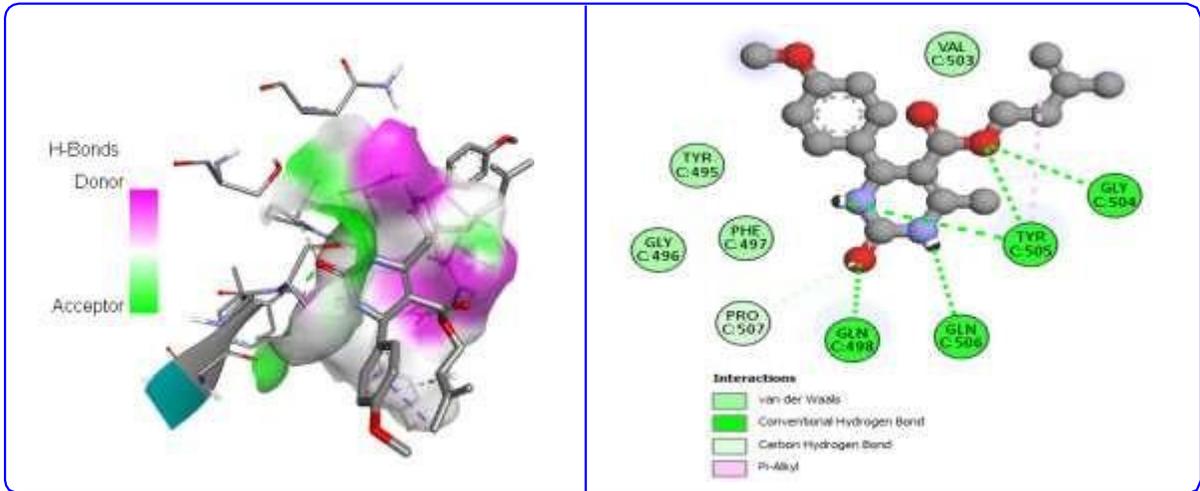
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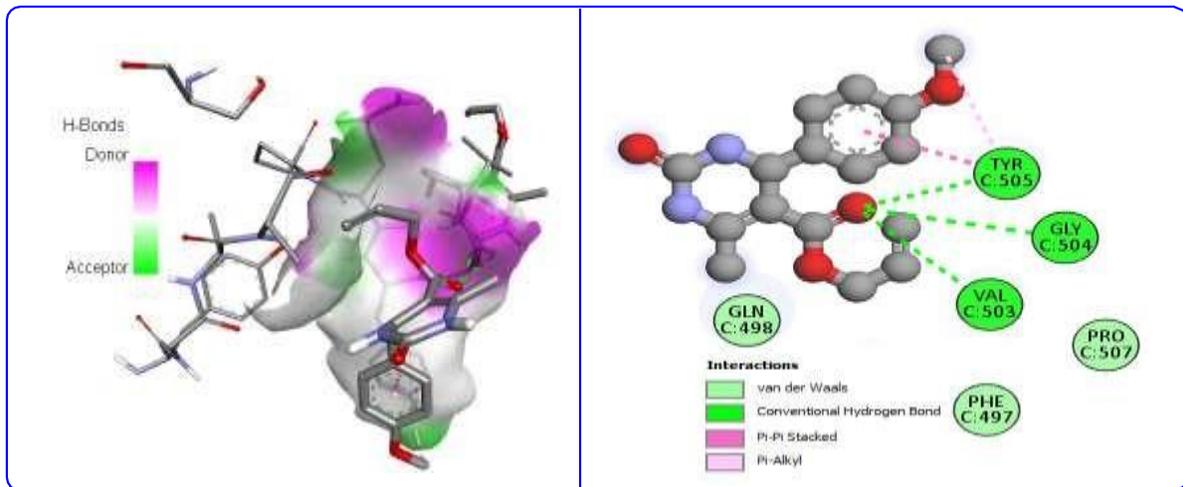
DHPM 7



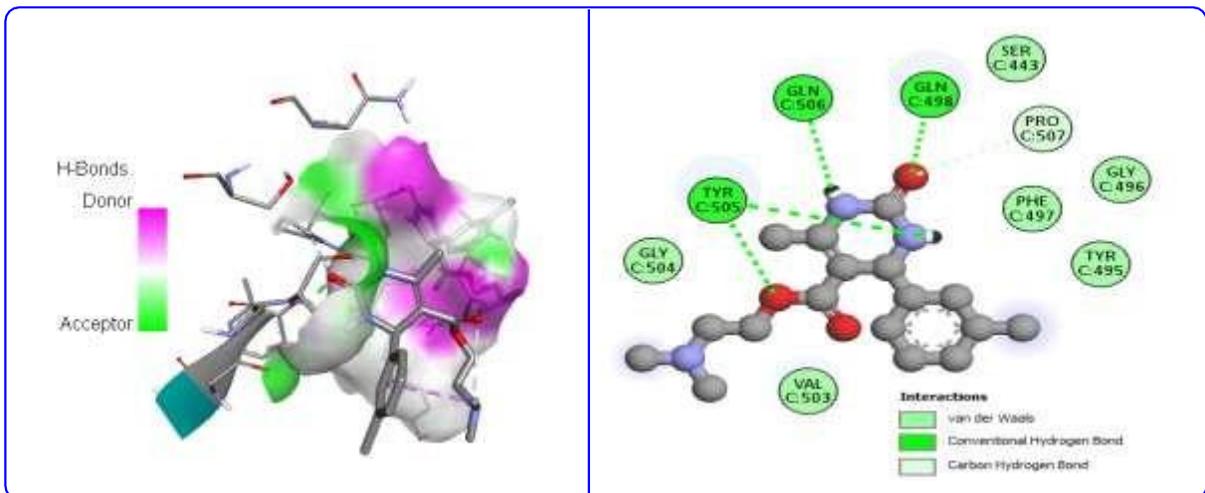
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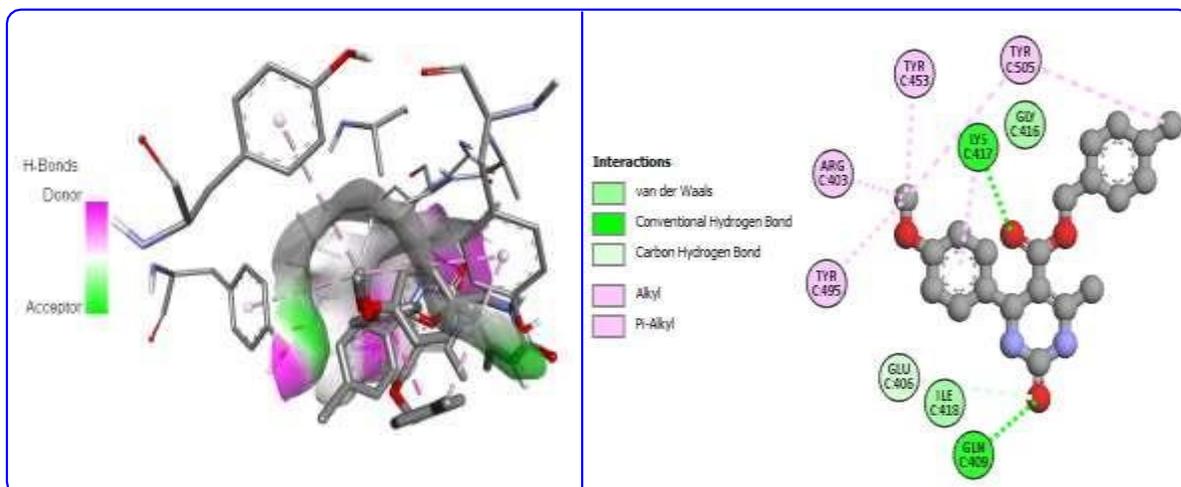
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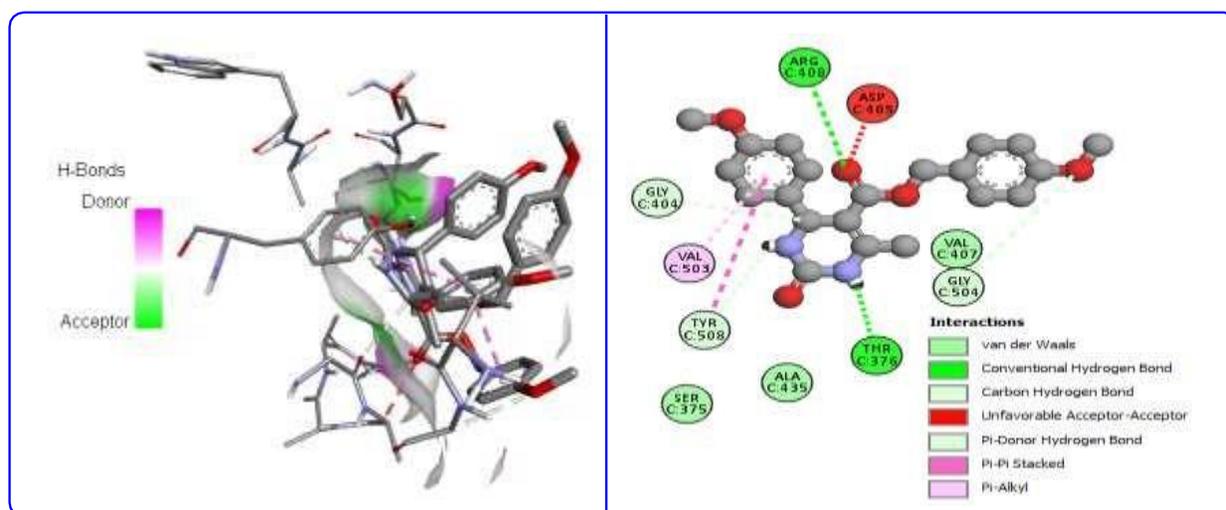
DHPM 10



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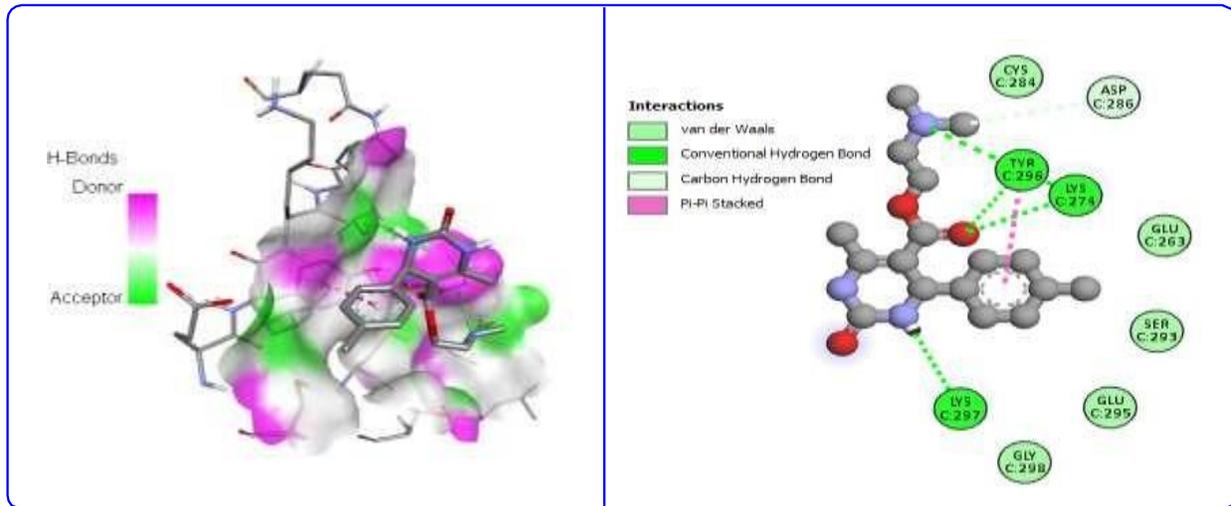


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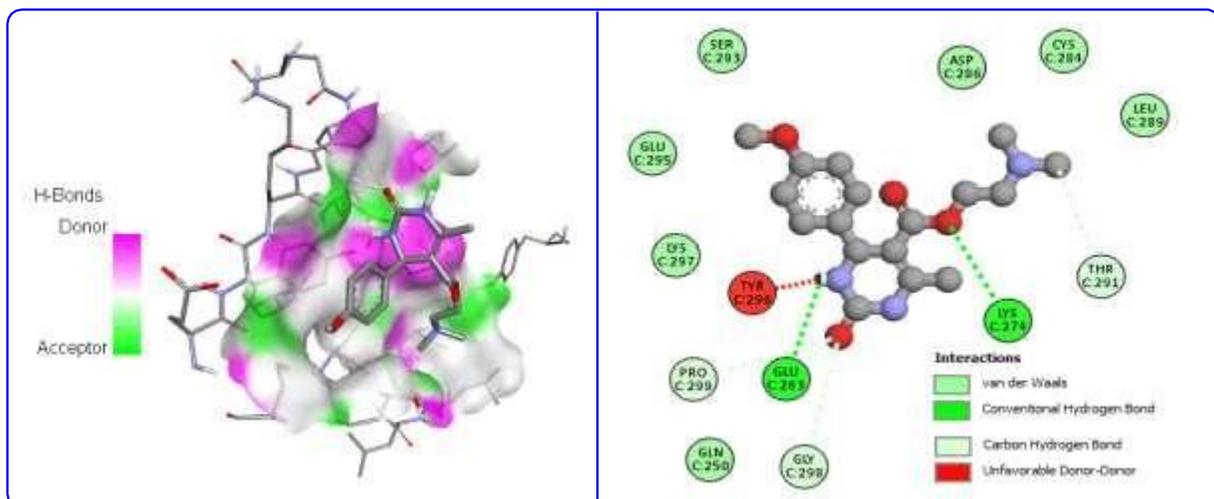


DHPM 13

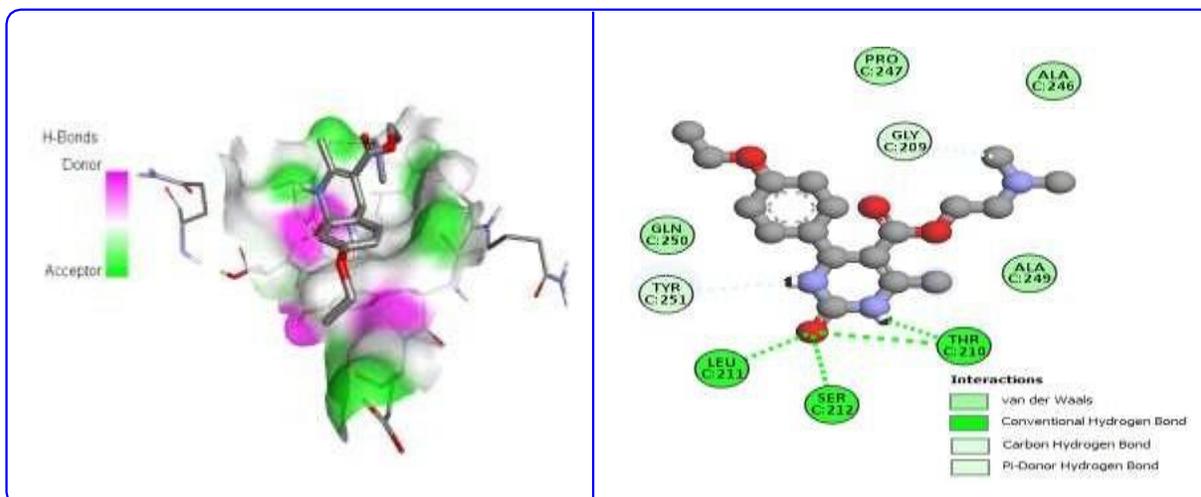
Docking results of 13 different ligands with papain-like protease of SARS CoV-2 at 2.7 Å resolution (PDB: 6W9C)



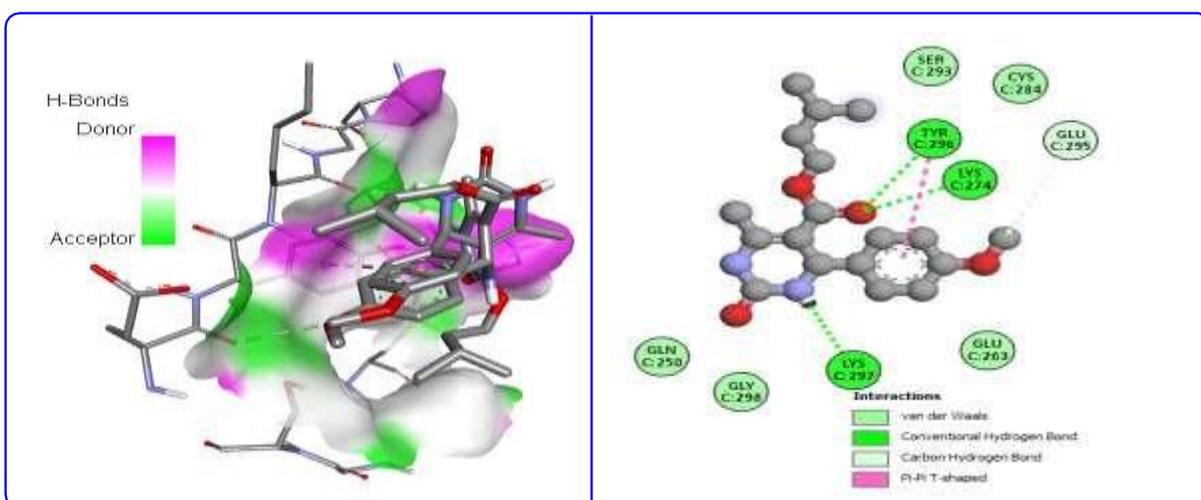
DHPM 1



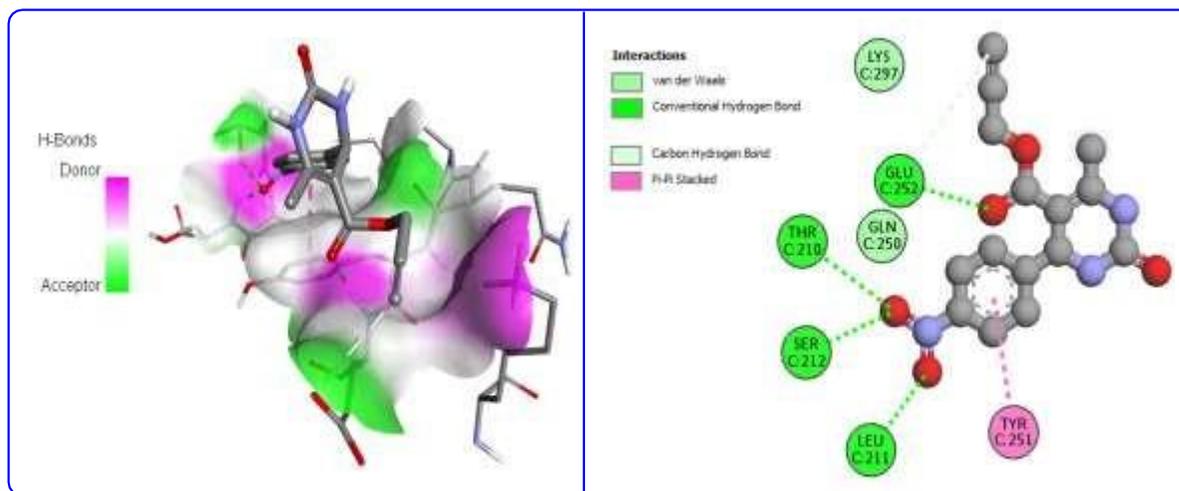
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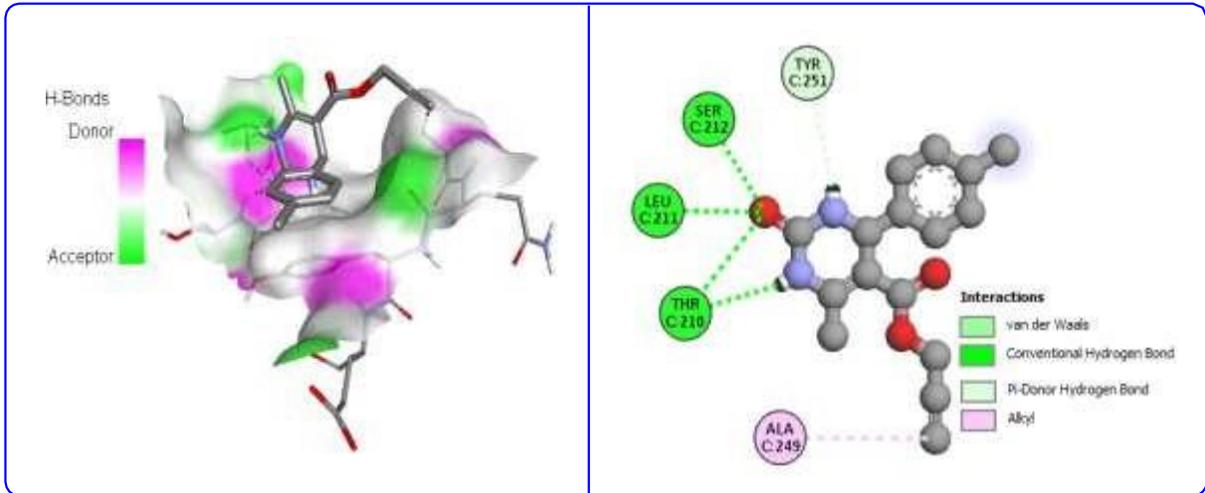
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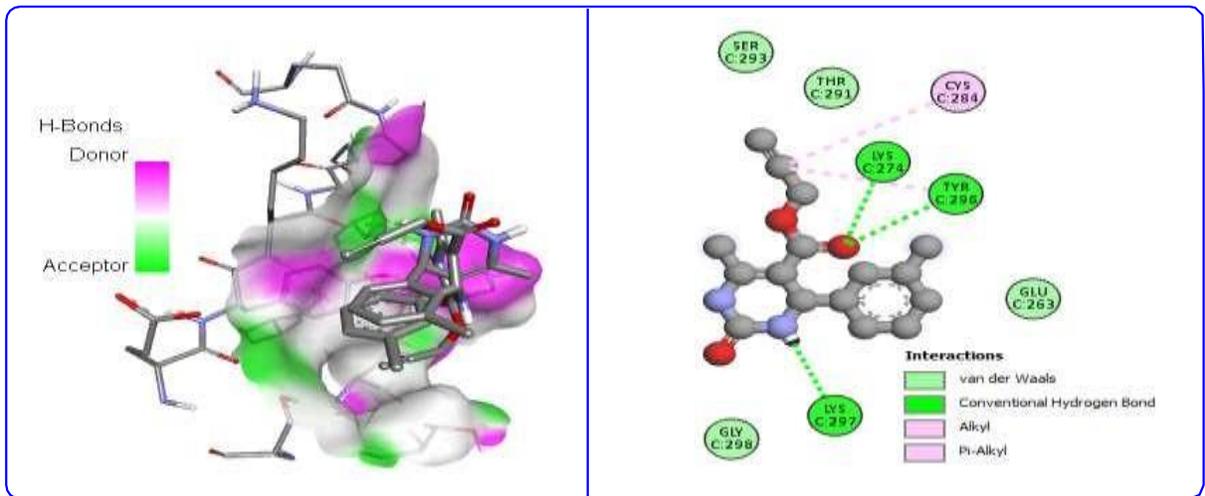
DHPM 4



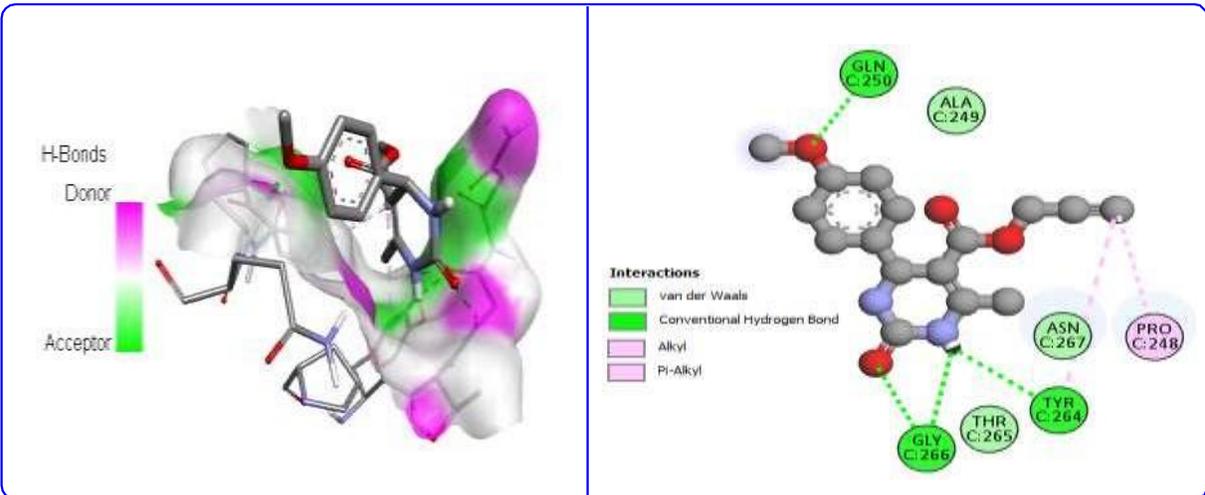
DHPM 5



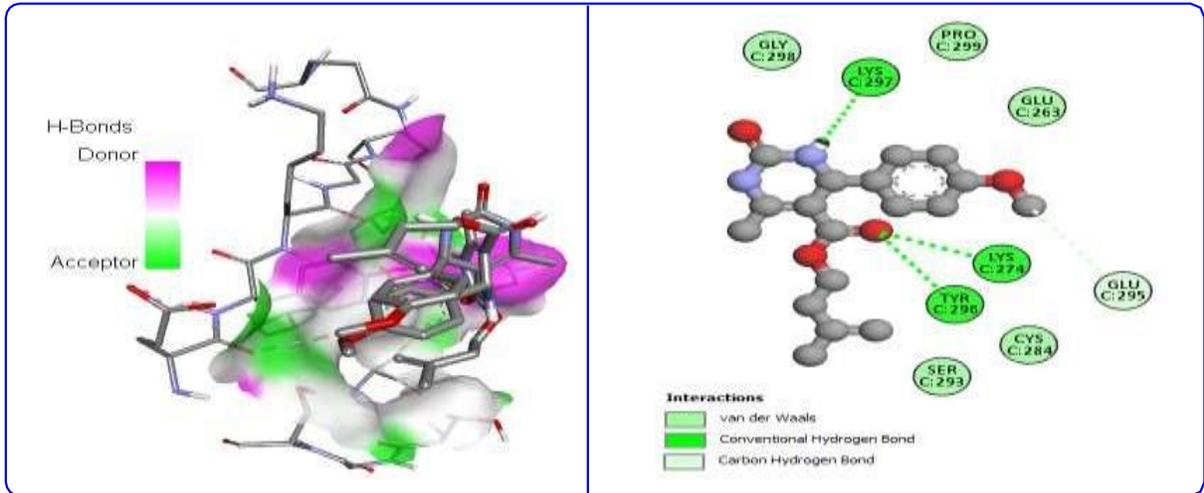
DHPM 6



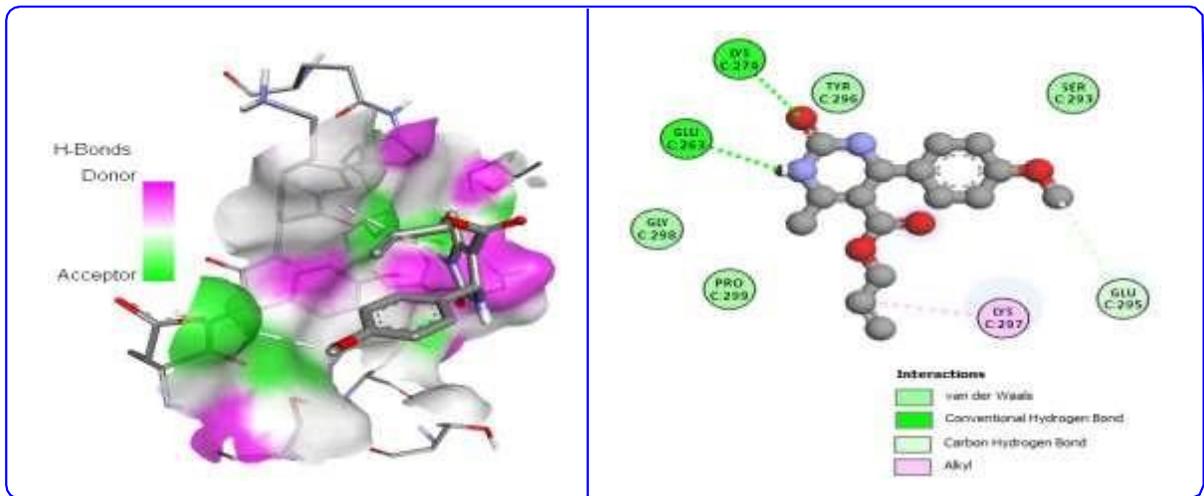
DHPM 7



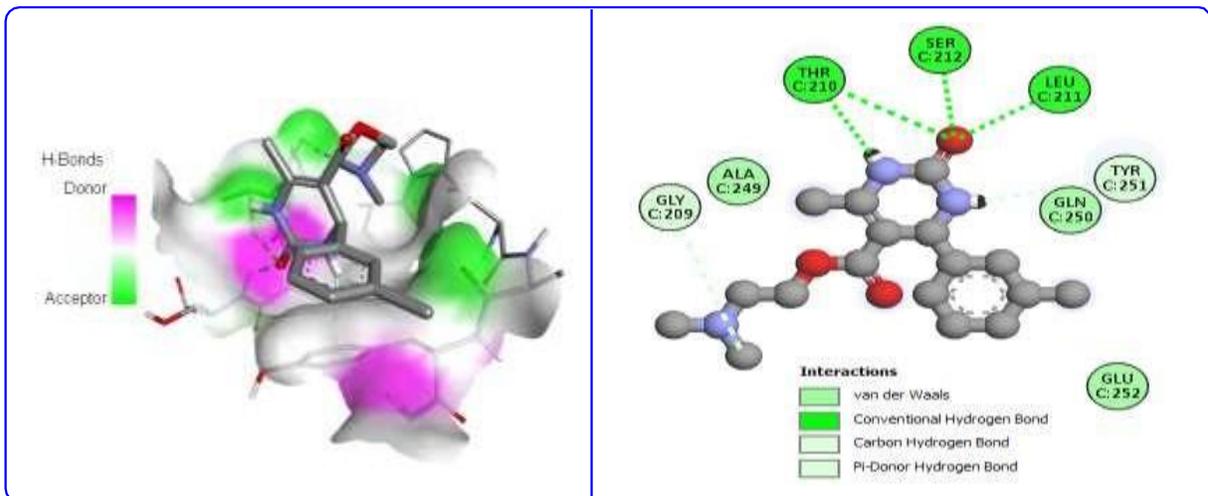
DHPM 8



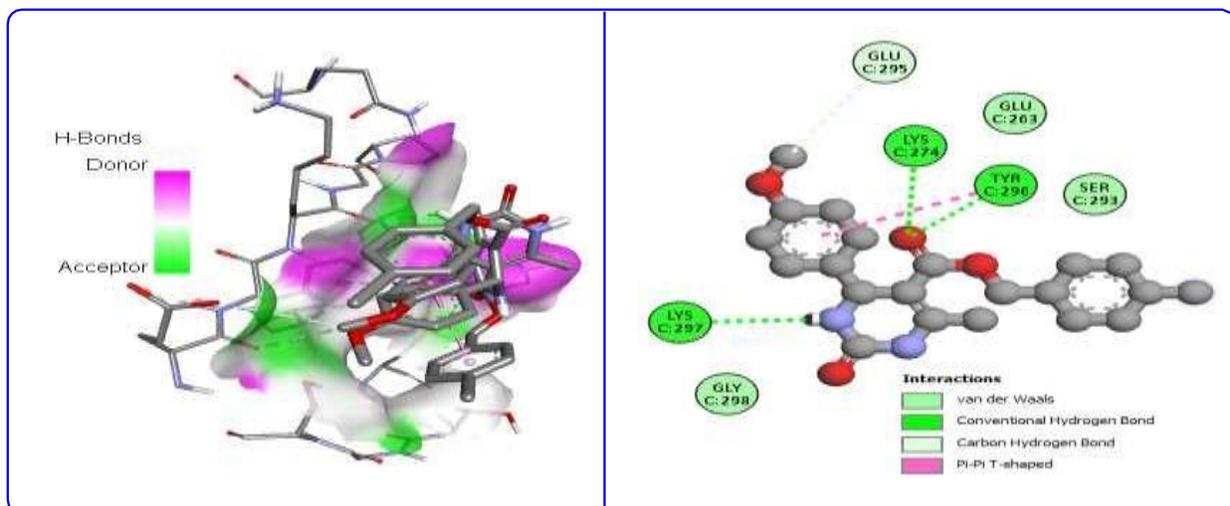
DHPM 9



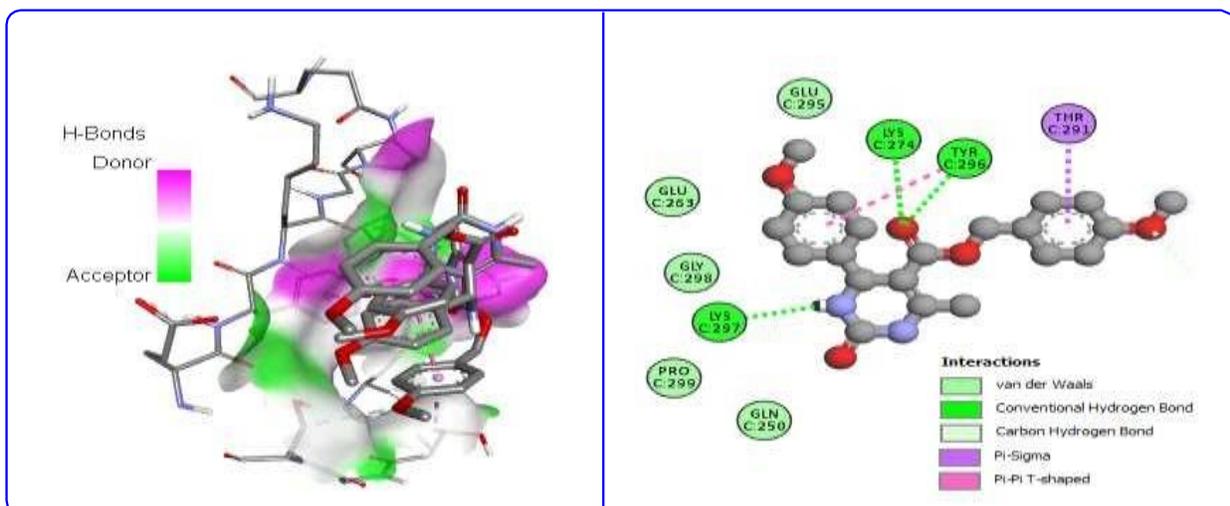
DHPM 10



DHPM 11



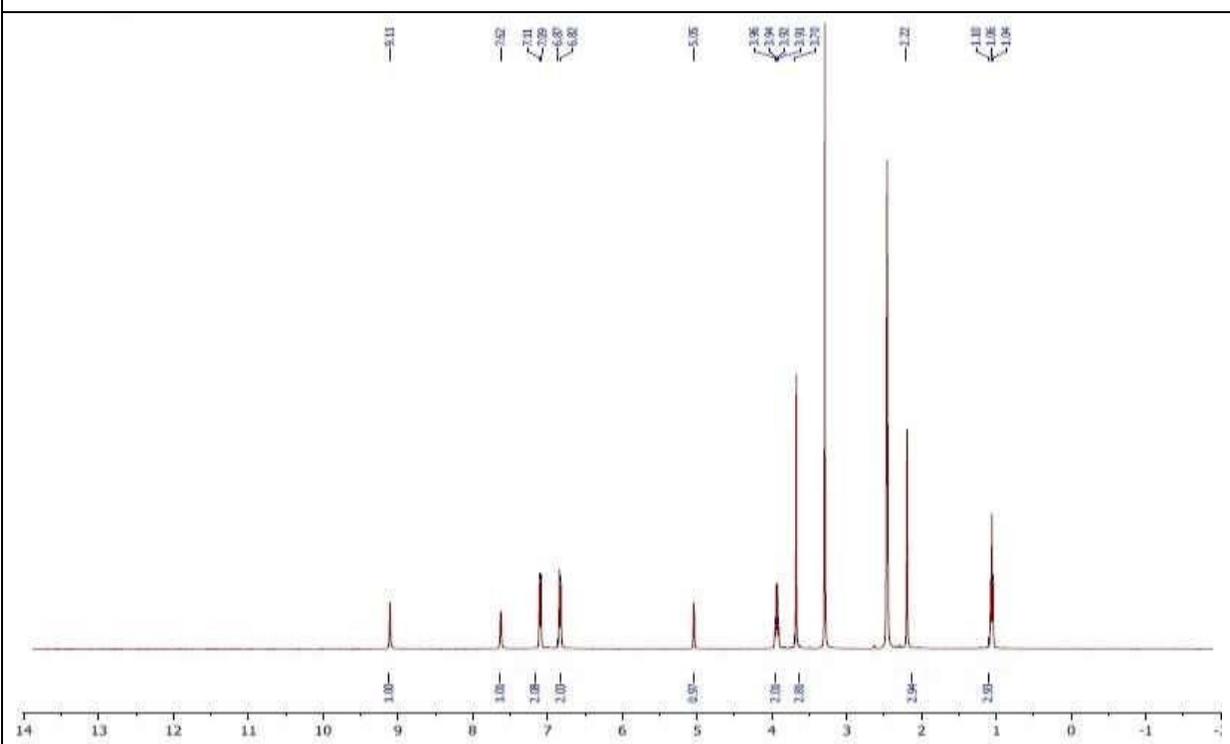
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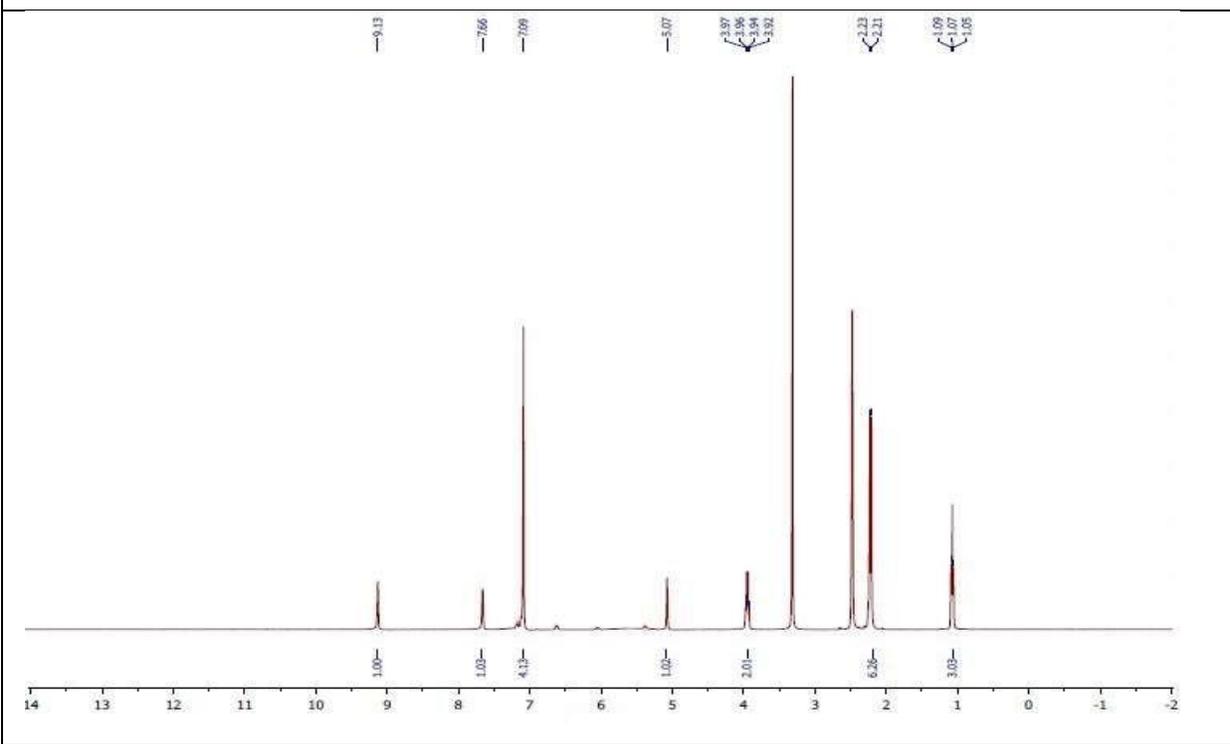
DHPM 13

1. Spectral data (¹HNMR) of some representative compounds:

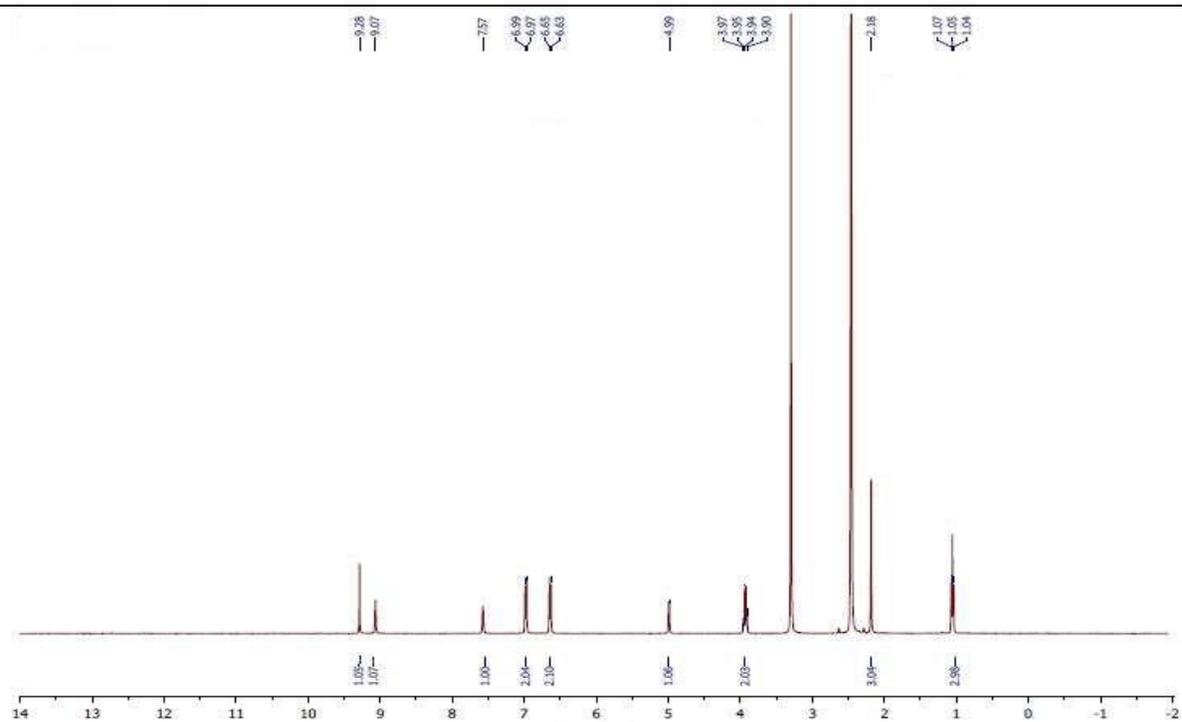
Ethyl 4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (DHPM16)



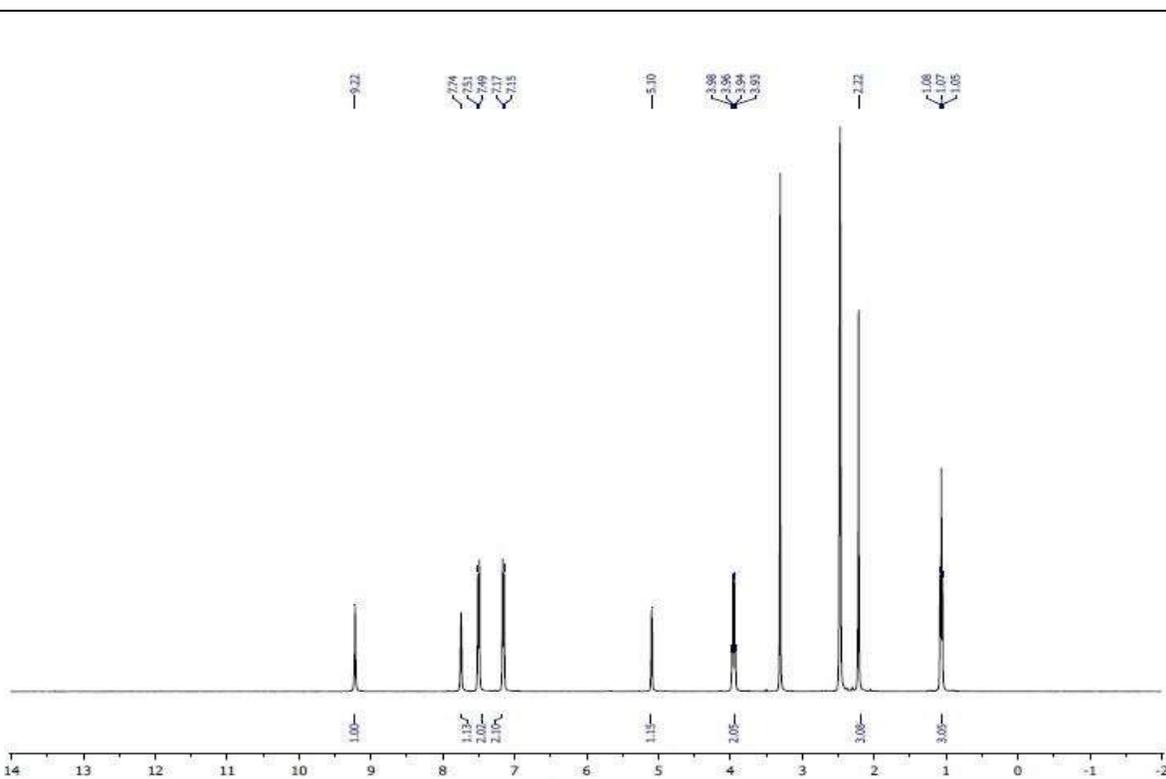
Ethyl 4-(4-methylphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (DHPM17)



Ethyl 4-(4-hydroxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (DHPM19)



Ethyl 4-(4-bromophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (DHPM21)



Methyl 4-(4-fluorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (DHPM36)

