

Electronic Supporting information

**Synthesis of new Nilutamide-pyrazole derivatives as VEGFR-2  
targeting anti-prostate cancer agents**

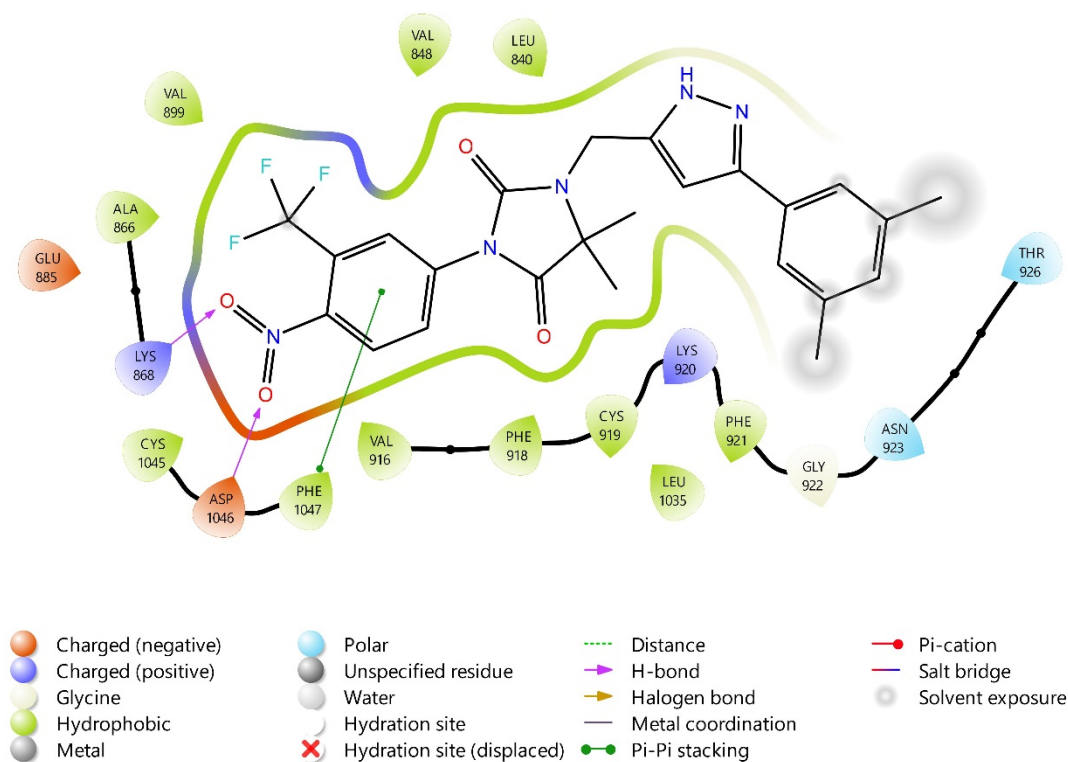
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Moinabad, (M), Rang Reddy (D), Hyderabad, Telangana, India.*

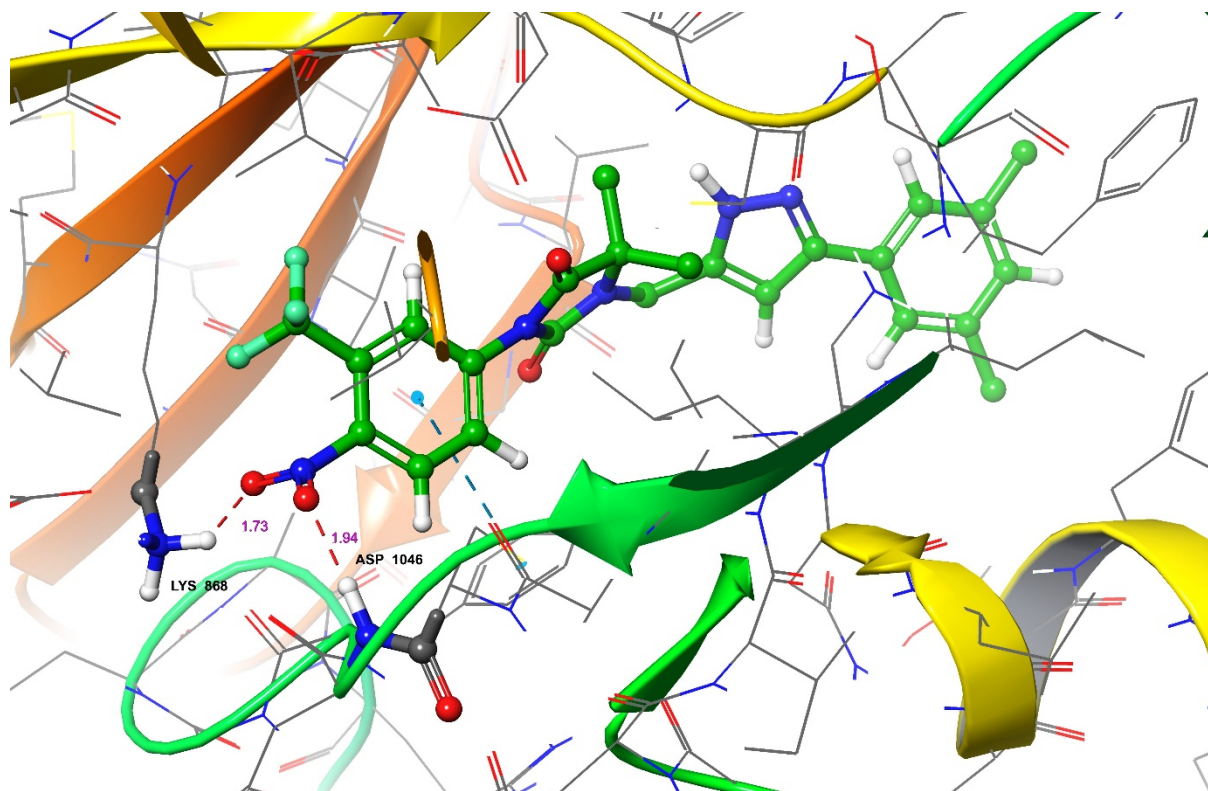
<sup>[b]</sup>*R.B.V.R.R Womens College, Narayanaguda, Hyderabad, Telangana, India.*

<sup>[c]</sup>*Department of Chemistry, Satavahana University, Karimnagar, Telangana, India.*

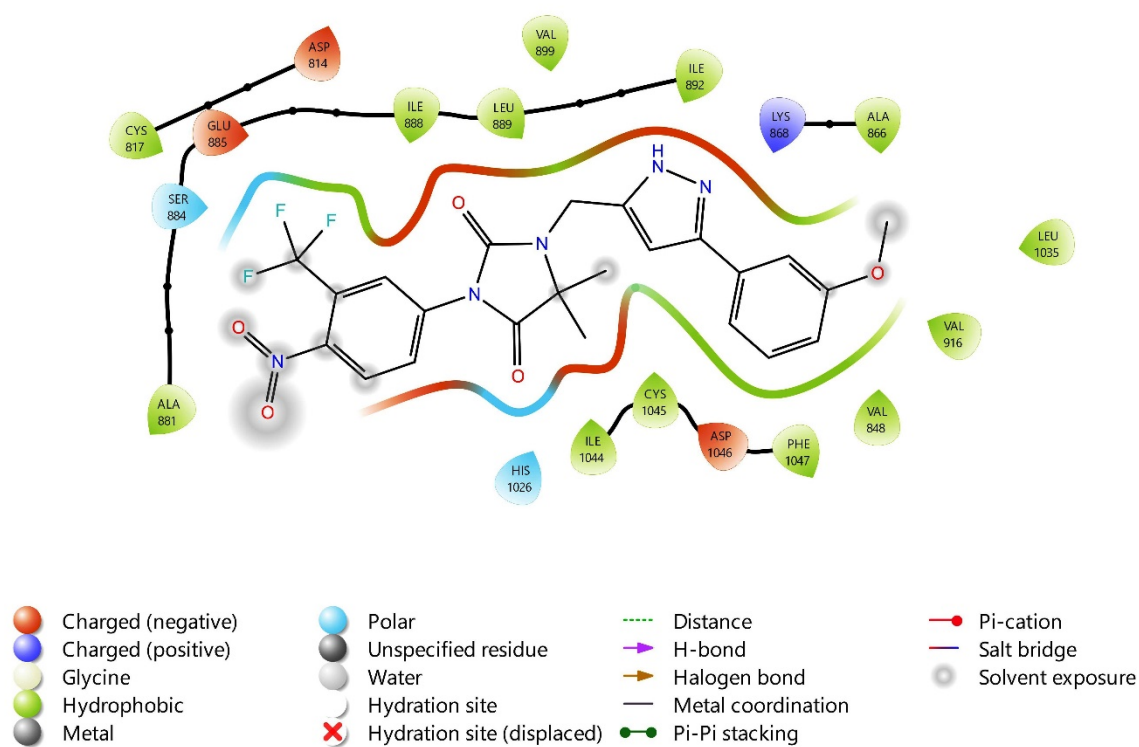
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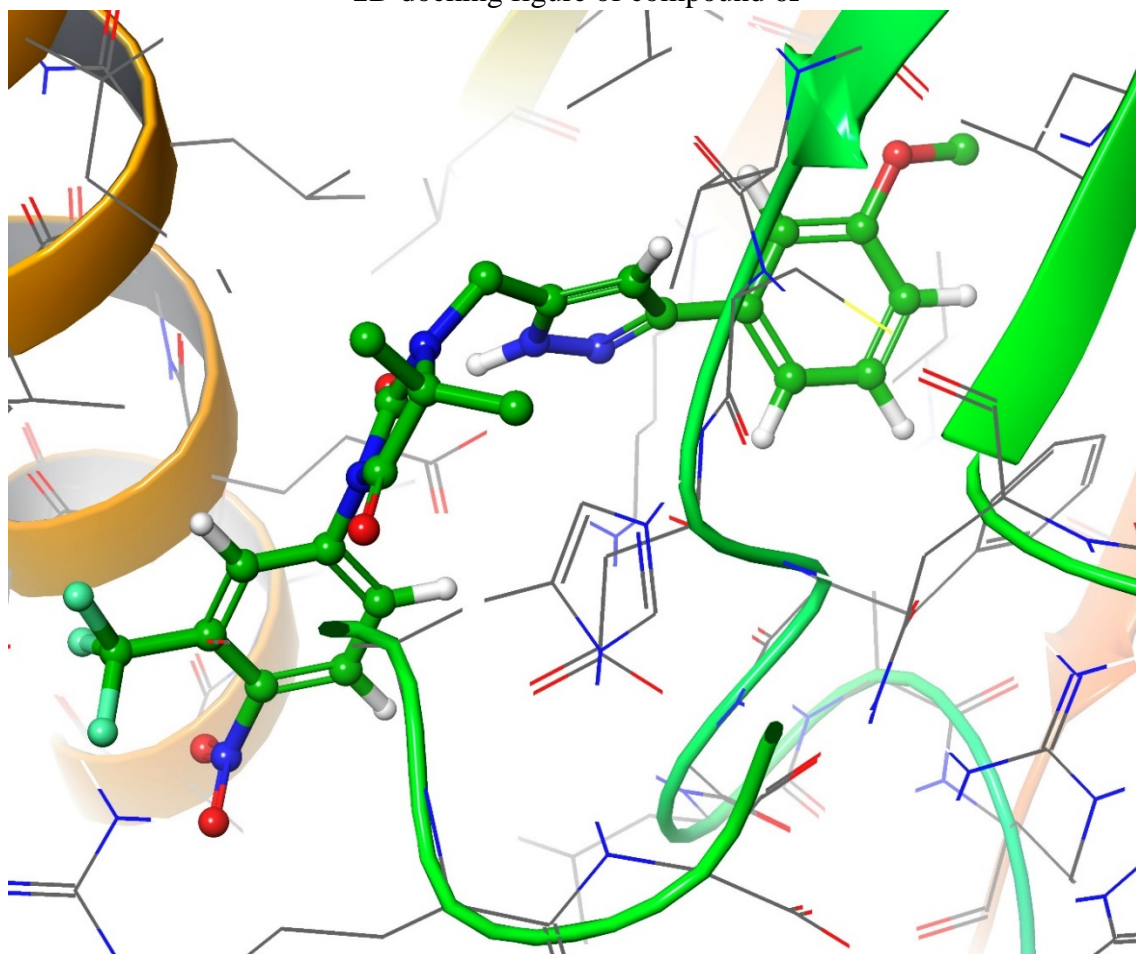
2D docking figure of compound **6d**



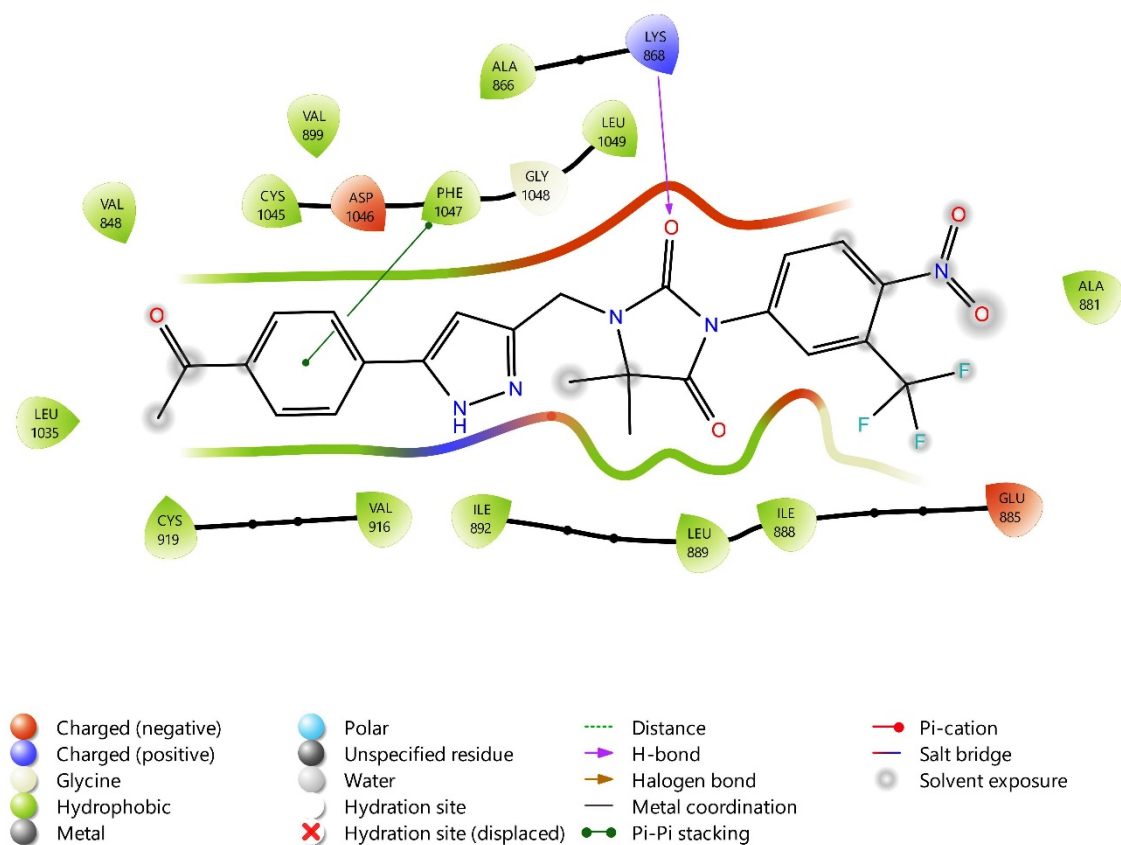
3D docking figure of compound **6d**



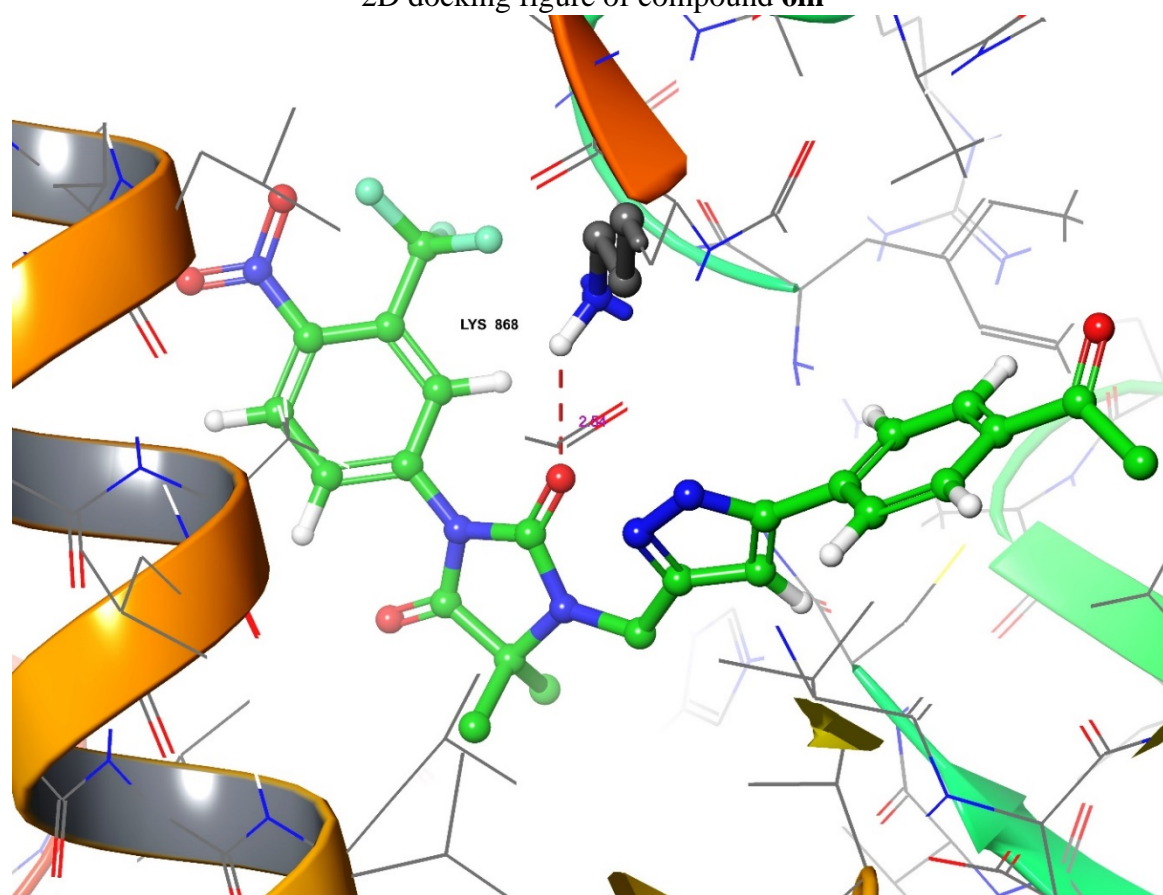
2D docking figure of compound **6f**



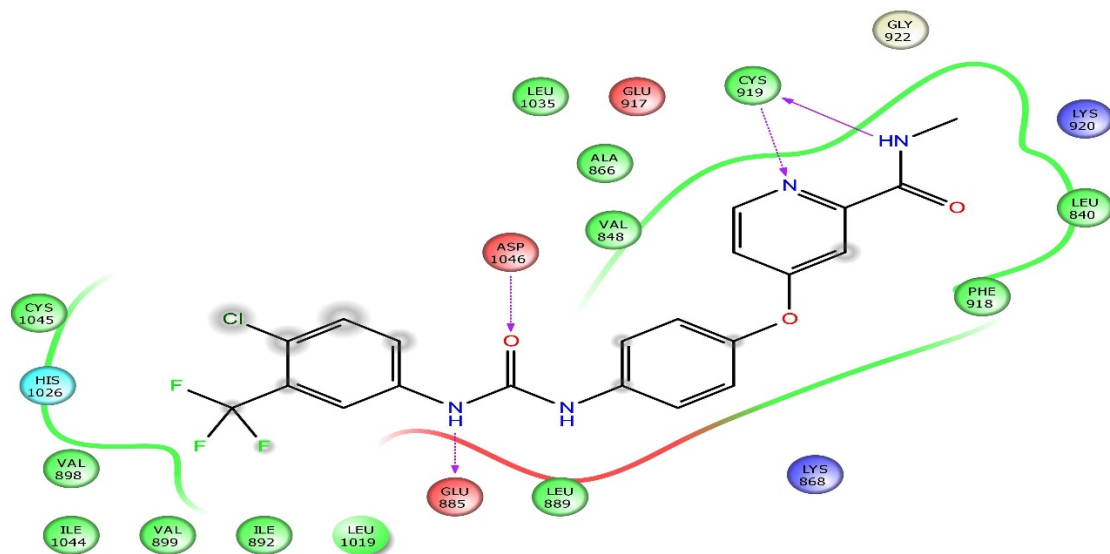
3D docking figure of compound **6f**



2D docking figure of compound **6m**

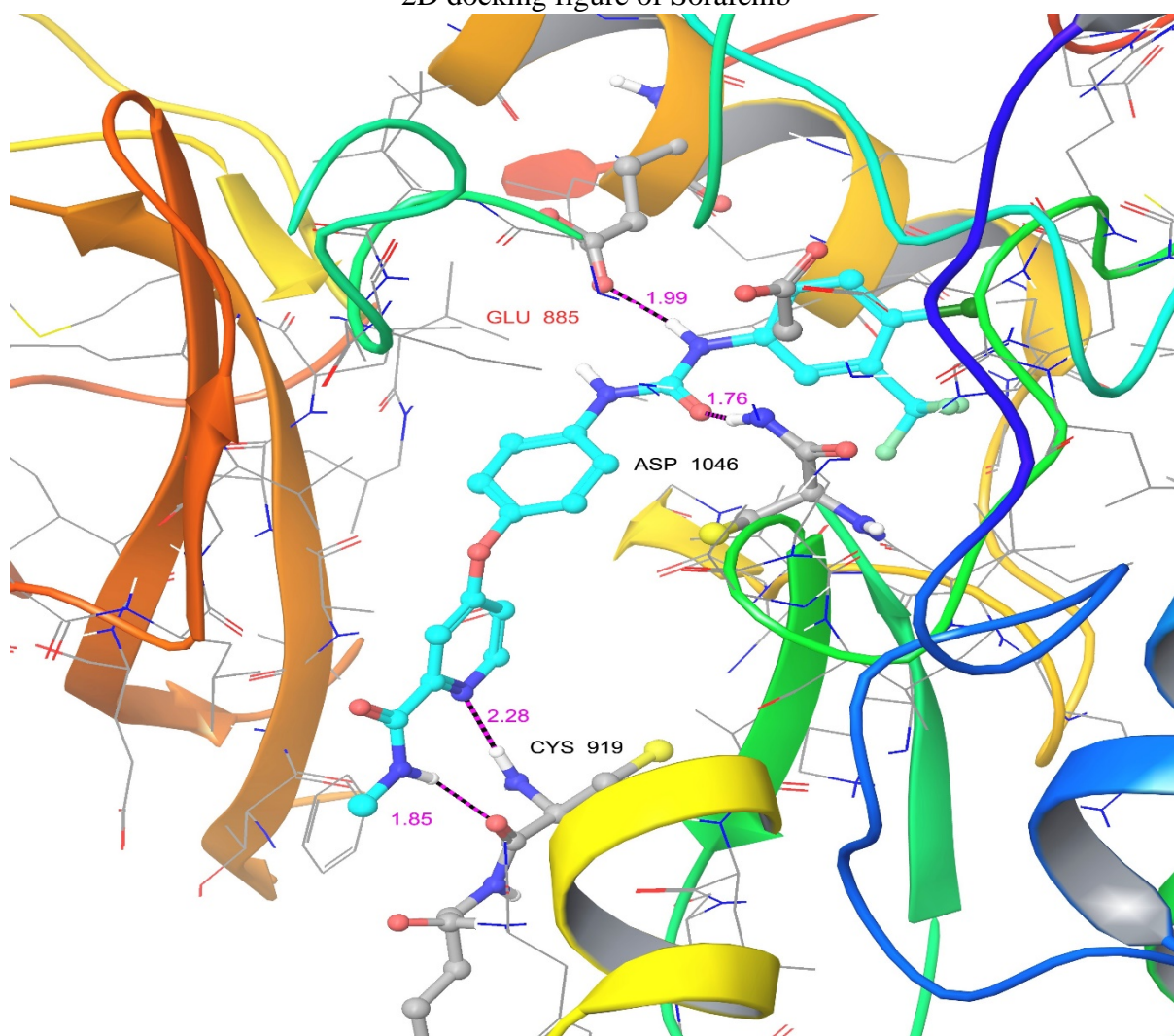


3D docking figure of compound **6m**

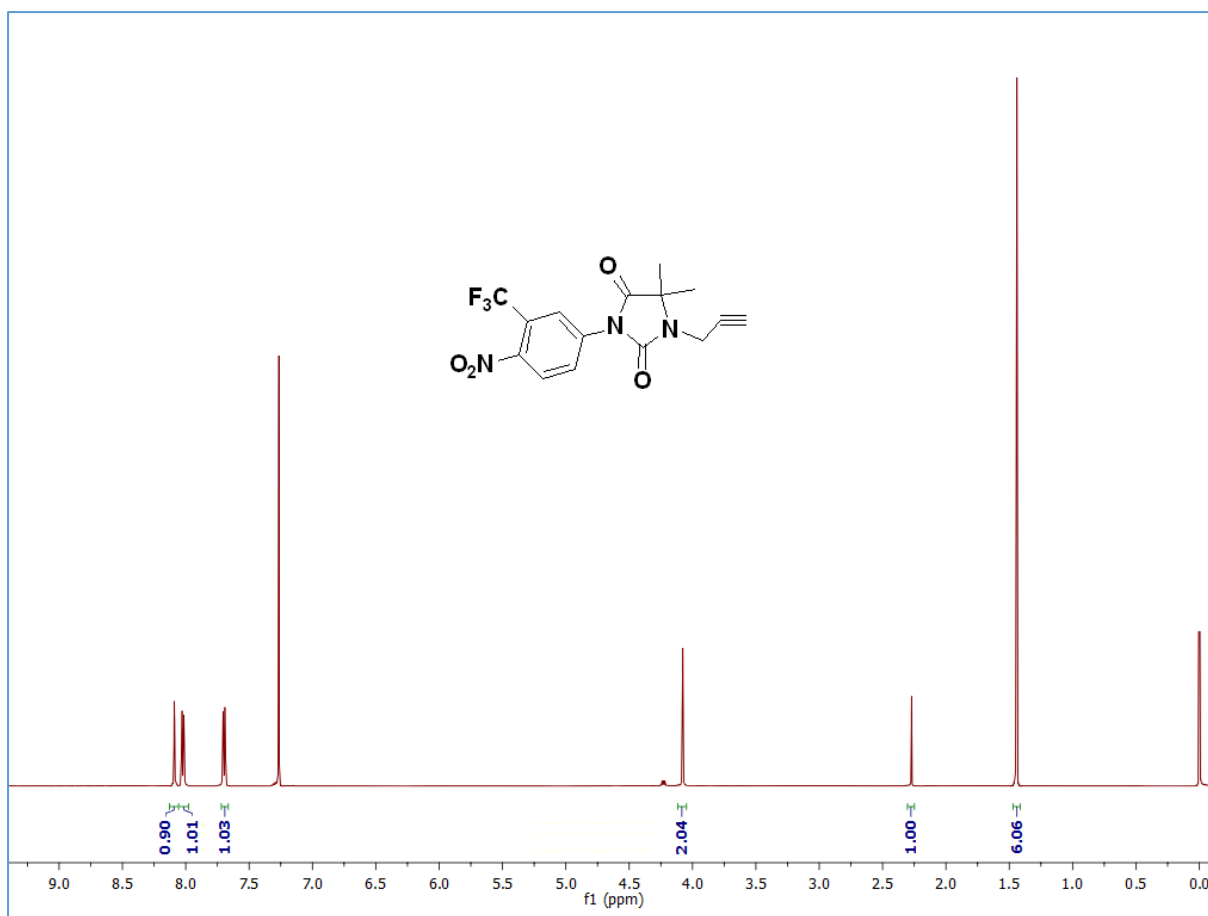


- |  |   |   |
|--|---|---|
| <span style="color: red;">●</span> Charged (negative)  | <span style="color: grey;">●</span> Water                   | <span style="color: purple;">---</span> H-bond (side chain) |
| <span style="color: blue;">●</span> Charged (positive) | <span style="color: orange;">●</span> Hydration site        | <span style="color: black;">---</span> Metal coordination   |
| <span style="color: green;">●</span> Polar             | <span style="color: red;">●</span> Displaced hydration site | <span style="color: black;">---</span> Salt Bridge          |
| <span style="color: yellow;">●</span> Hydrophobic      | <span style="color: black;">---</span> n-π stacking         | <span style="color: black;">---</span> Solvent exposure     |
| <span style="color: grey;">●</span> Glycine            | <span style="color: red;">---</span> π-cation               |   |
| <span style="color: grey;">●</span> Metal              | <span style="color: purple;">---</span> H-bond (backbone)   |   |

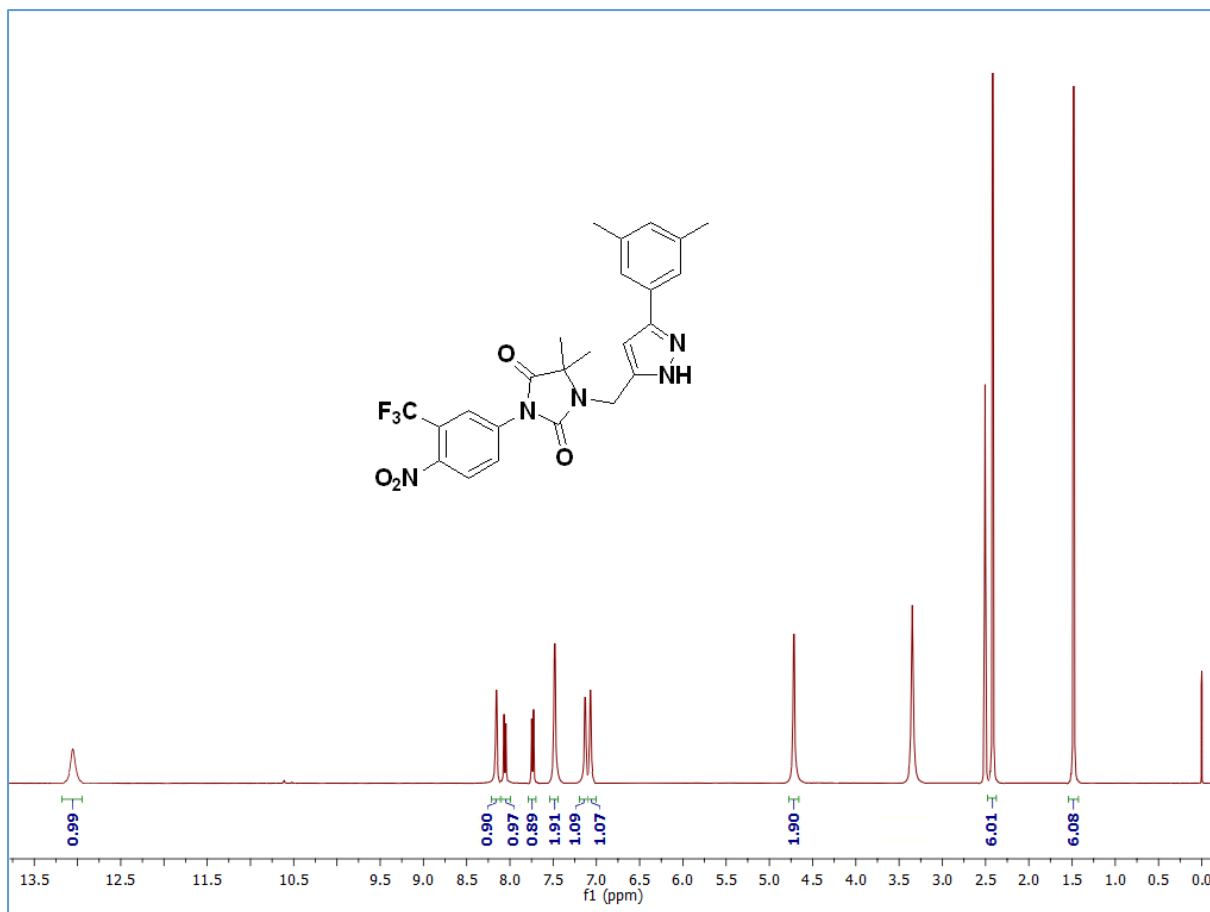
2D docking figure of Sorafenib



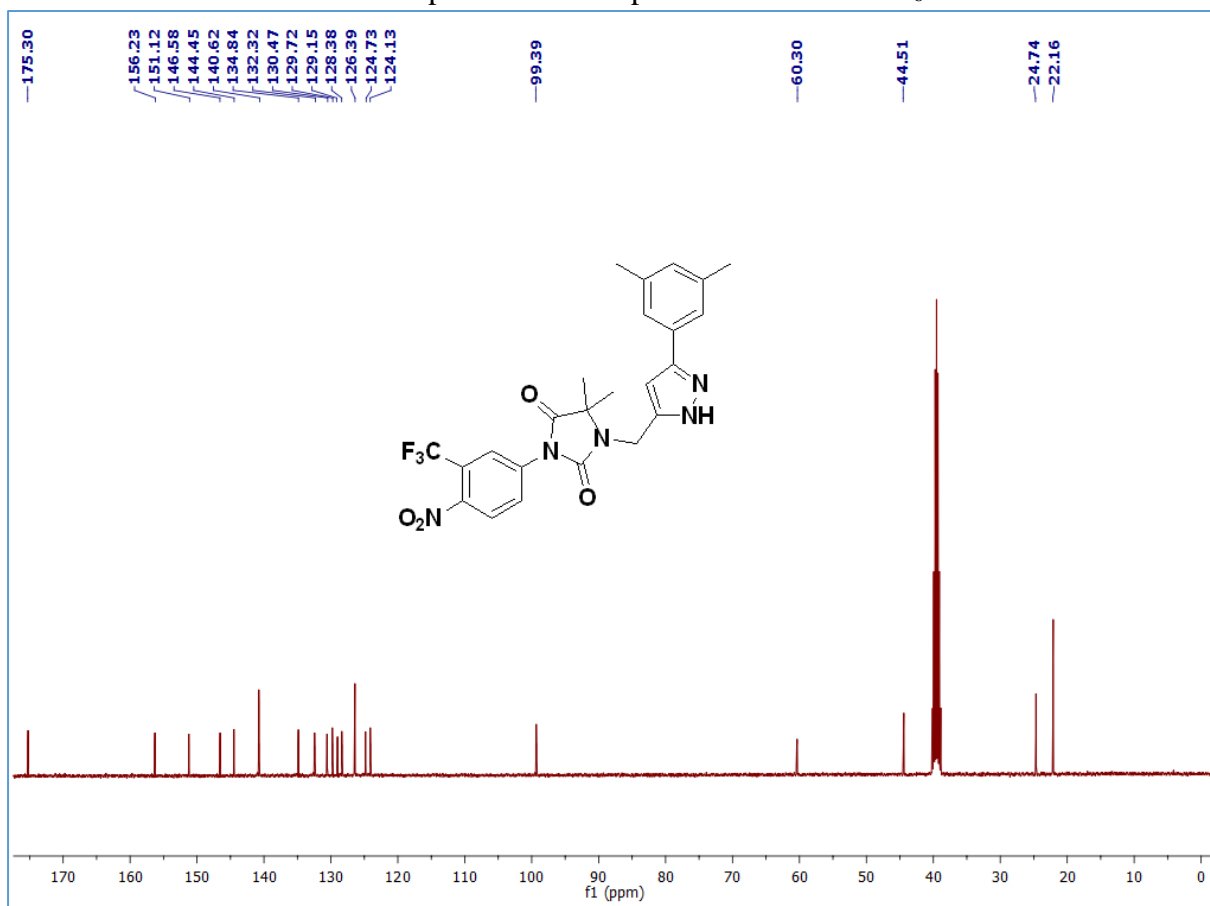
3D docking figure of Sorafenib



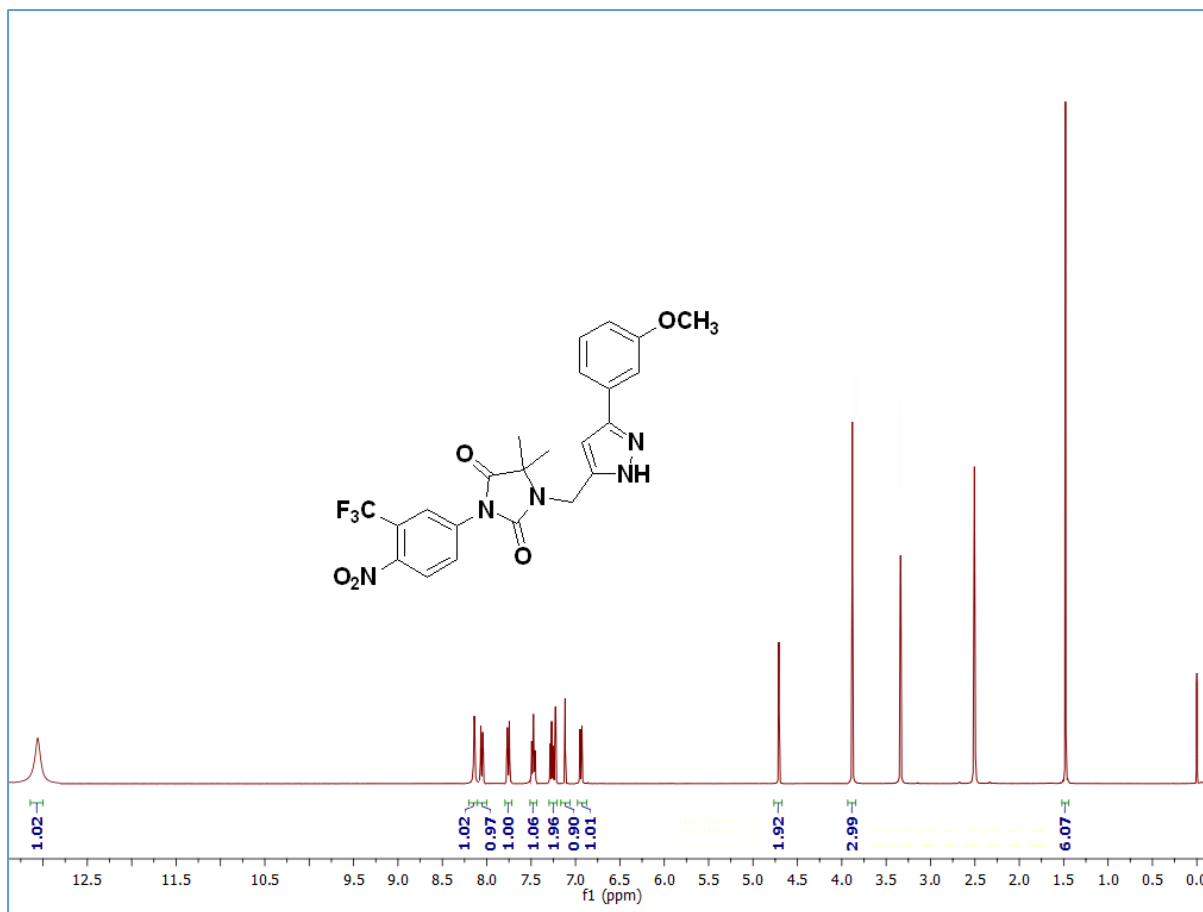
<sup>1</sup>H NMR spectrum of intermediate **3** in CDCl<sub>3</sub>



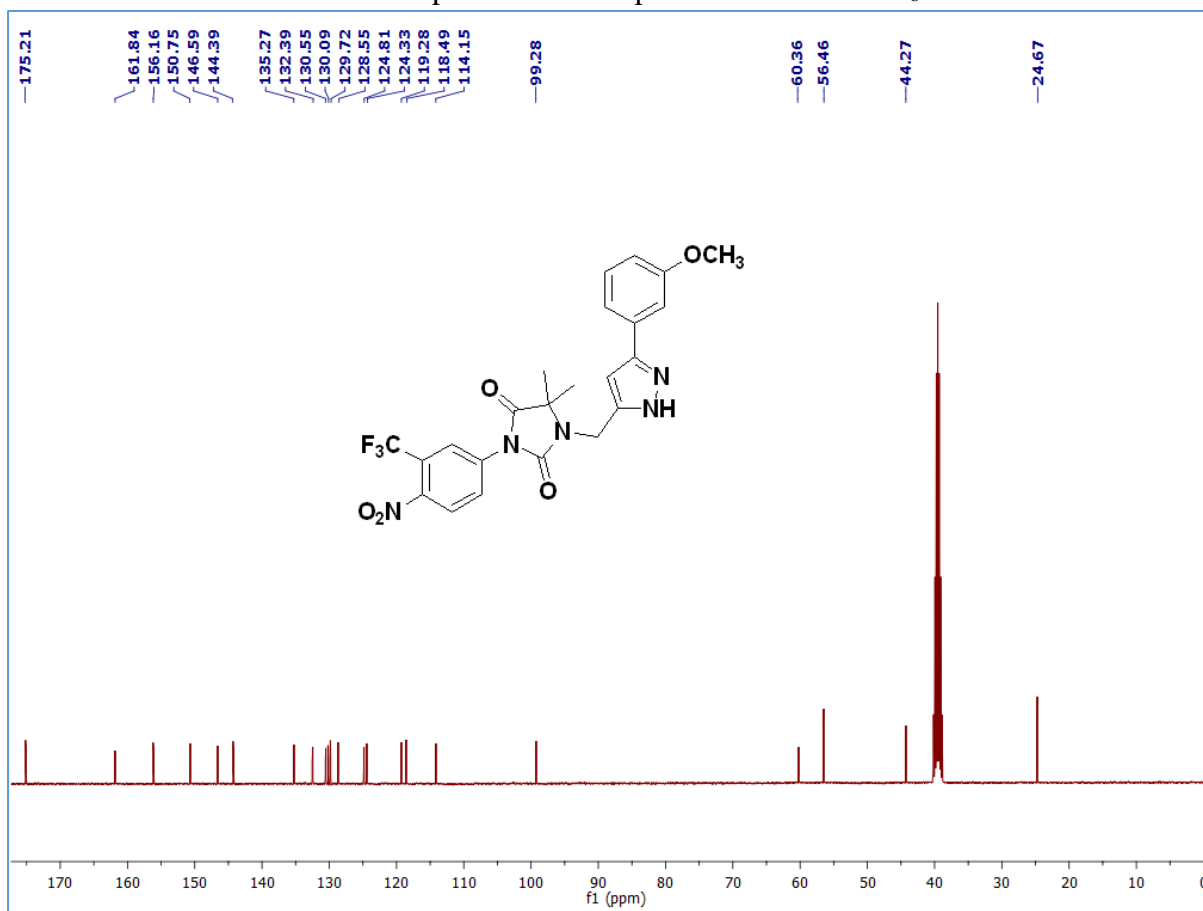
<sup>1</sup>H NMR spectrum of compound **6d** in DMSO-d<sub>6</sub>



<sup>13</sup>C NMR spectrum of compound **6d** in DMSO-d<sub>6</sub>

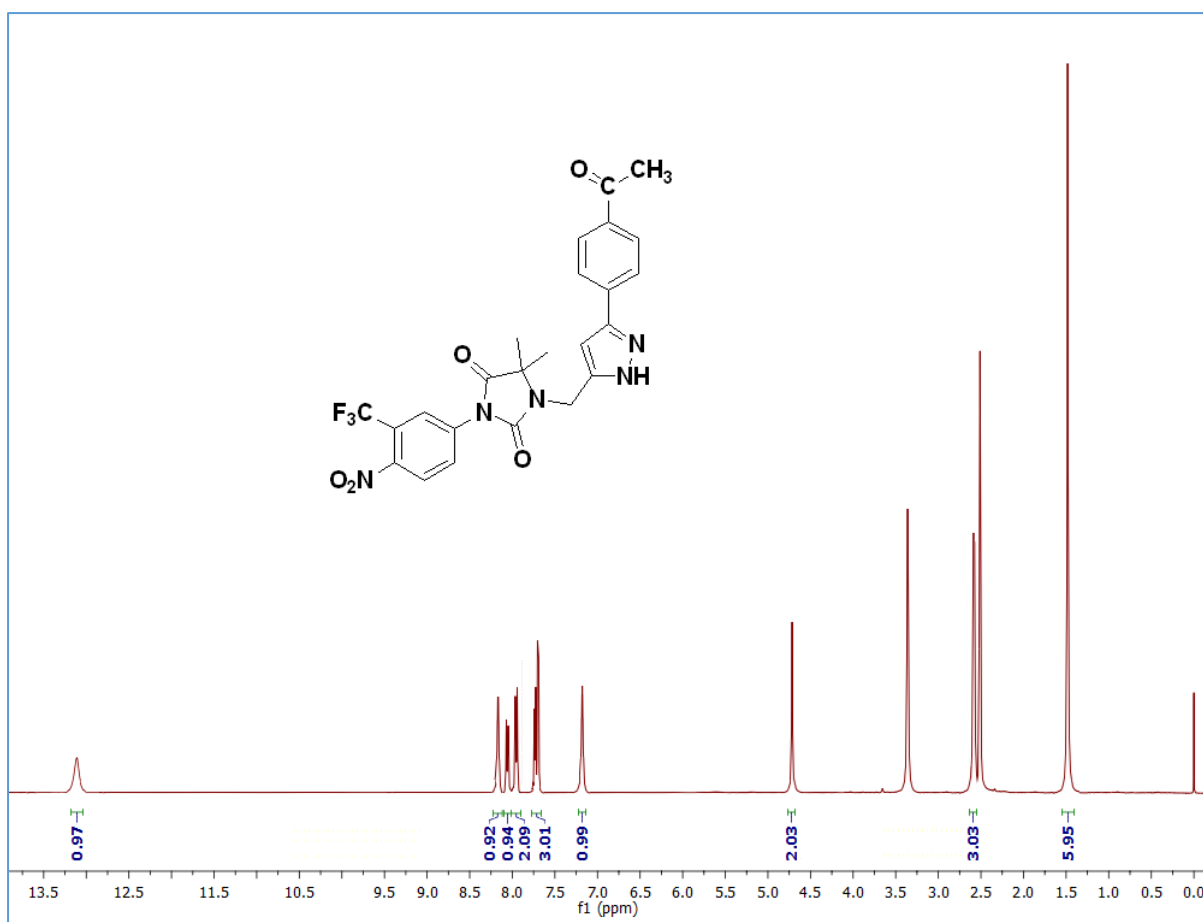


<sup>1</sup>H NMR spectrum of compound **6f** in DMSO-d<sub>6</sub>

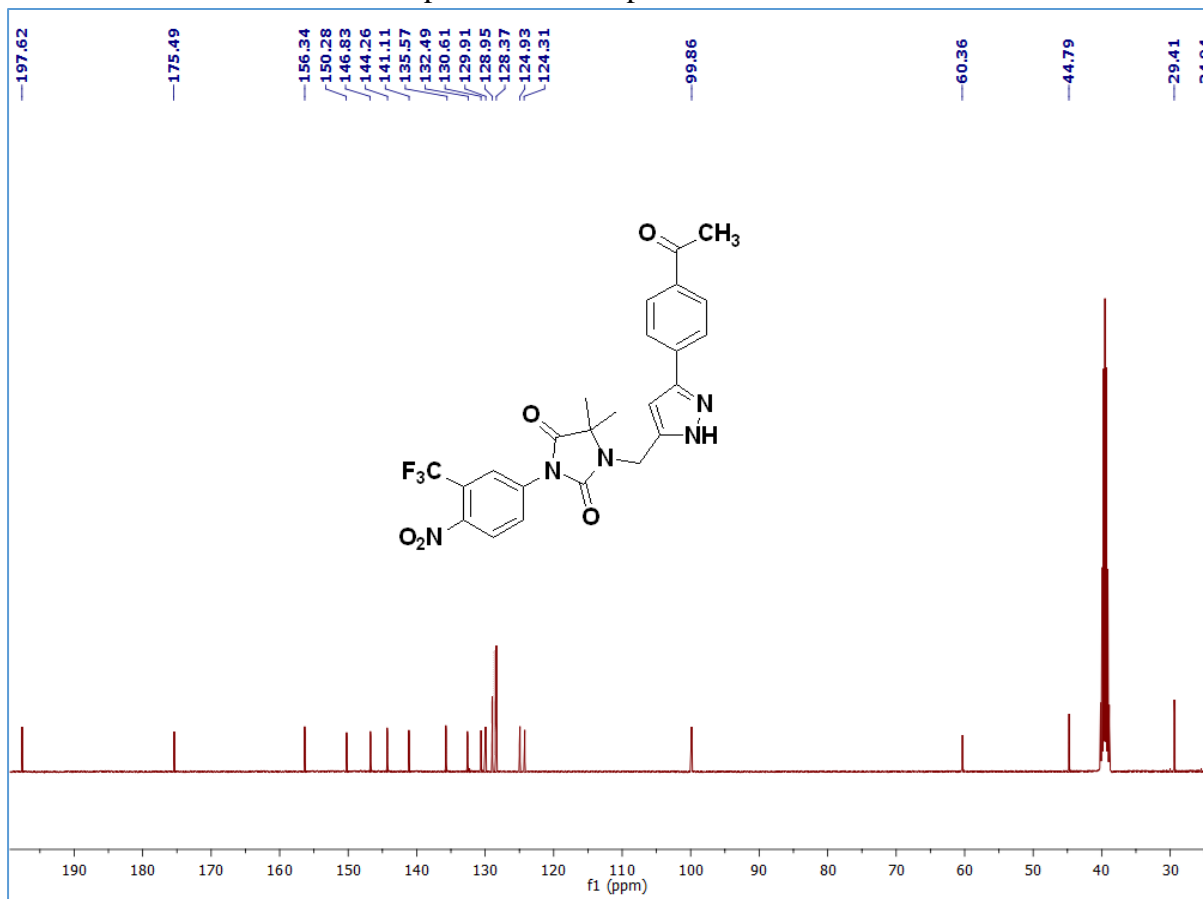


<sup>13</sup>C NMR spectrum of compound **6f** in DMSO-d<sub>6</sub>





<sup>1</sup>H NMR spectrum of compound **6m** in DMSO-d<sub>6</sub>



<sup>13</sup>C NMR spectrum of compound **6m** in DMSO-d<sub>6</sub>