# Supplementary: Development of a Fingerprint-Based Scoring Function for the Prediction of the Binding Mode of Carbonic Anhydrase II Inhibitors

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## Table of Contents

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**Figure S1.** Fingerprint analysis of the interaction between 5-[(phenylsulfonyl)amino]-1,3,4-thiadiazole-2-sulfonamide and CAII (PDB code 3DBU).

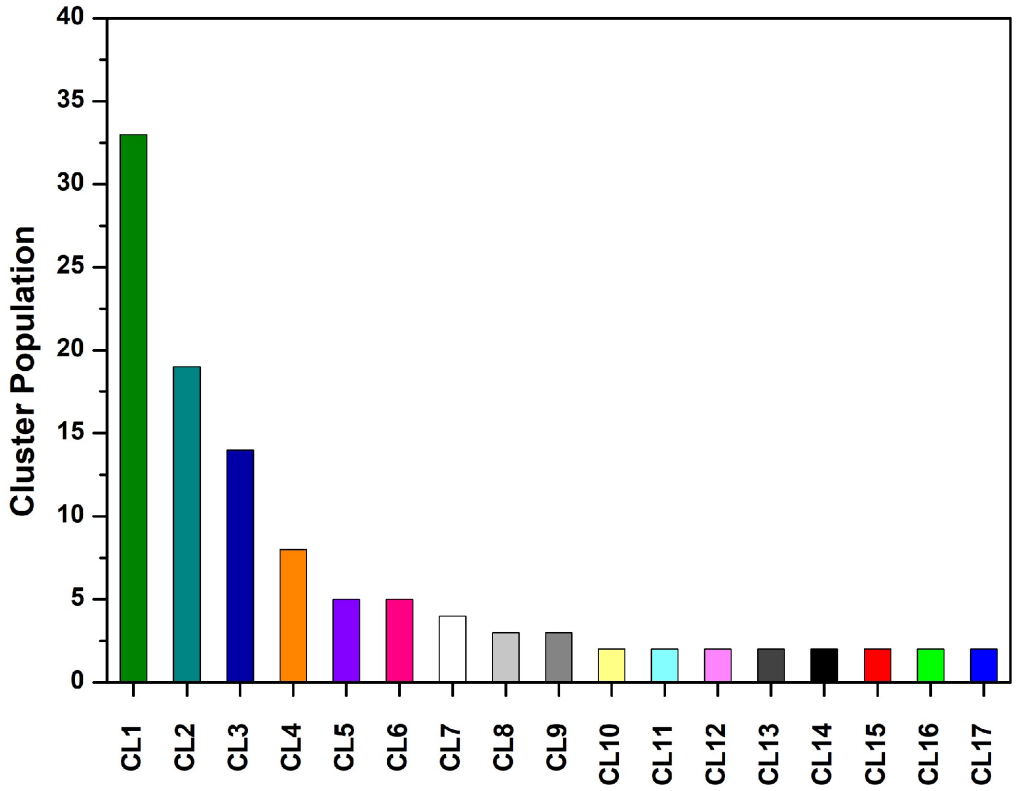


**Figure S2.** Similarity analysis of the deposited ligand-CAII X-ray complexes on the basis of the Tc-IFP score.

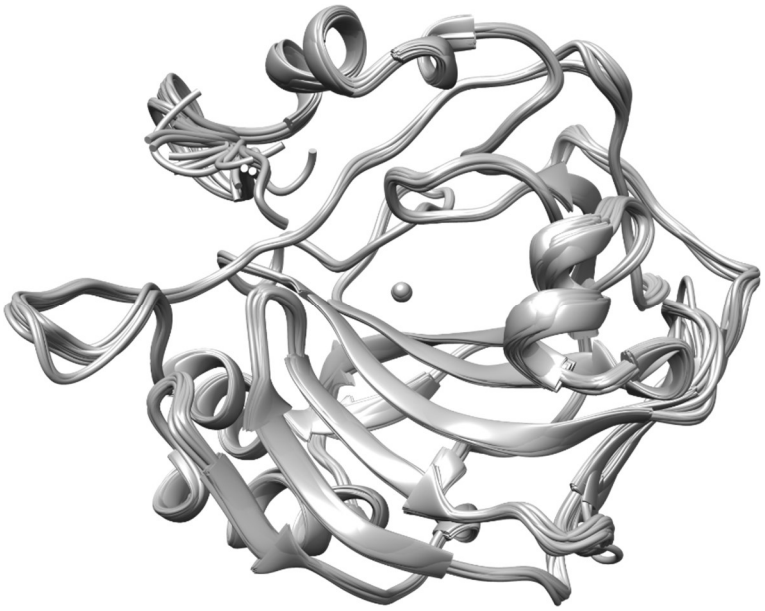

**Figure S3.** Superimposition of the 127 CAII X-ray structures.

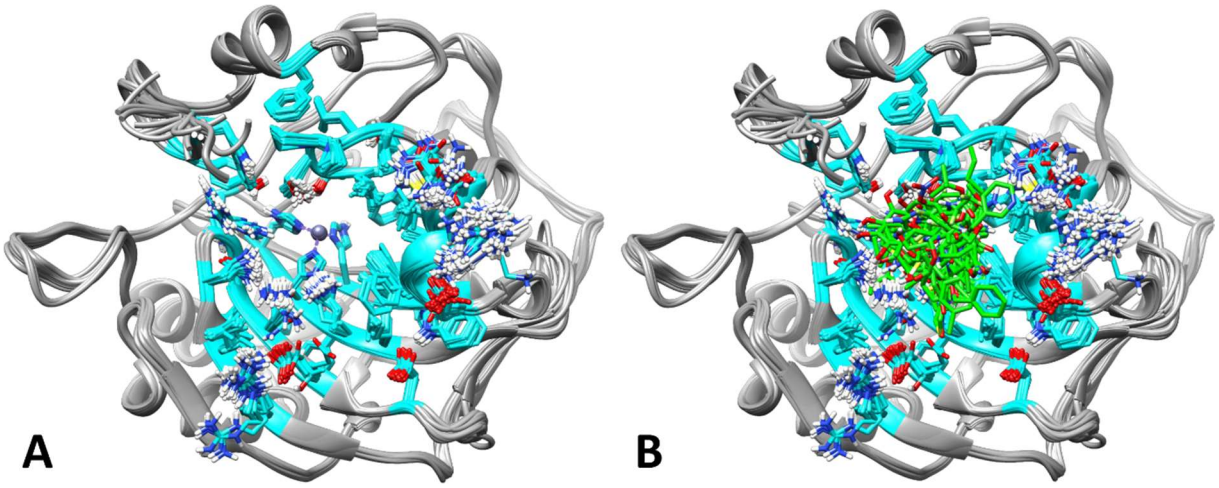


**Figure S4.** Protein binding site mapped by the CAII-rIFP. (A) The 44 residues of the 127 CAII X-ray structures whose interactions are mapped by the CAII-rIFP are showed in cyan sticks, while the co-crystallized ligands are hidden. (B) The 127 co-crystallized ligands are also shown in green sticks.

**Table S1.** Structure and interactions of the 127 ligands co-crystallized with CAII.

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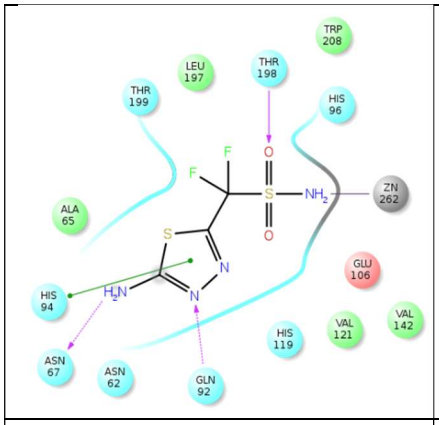
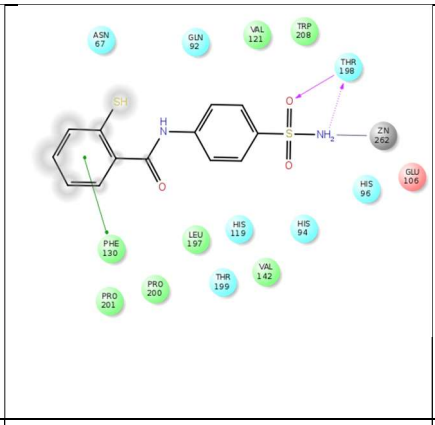
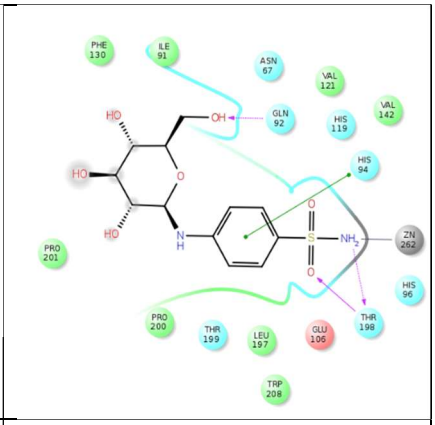
|  |  |  |
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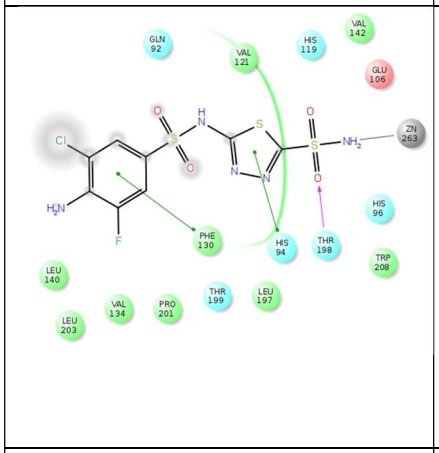
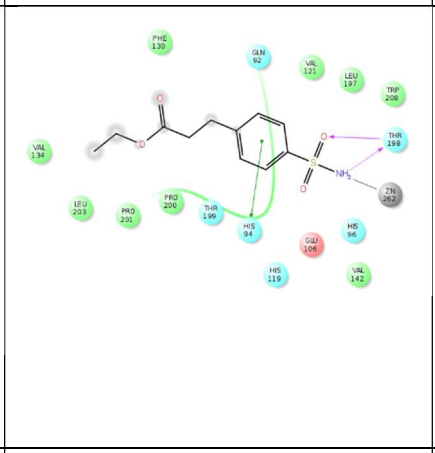
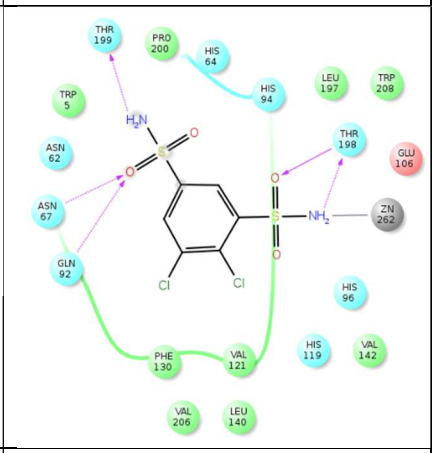
|  |  |  |
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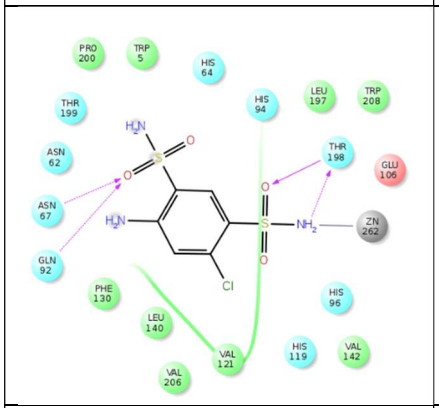
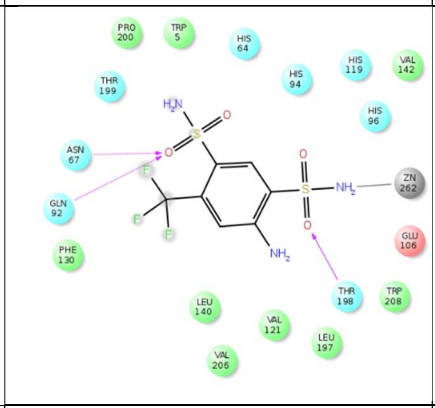
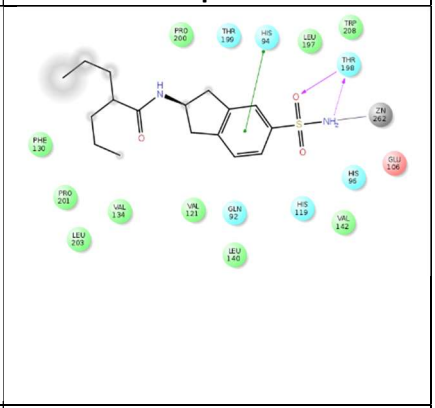
|  |  |  |
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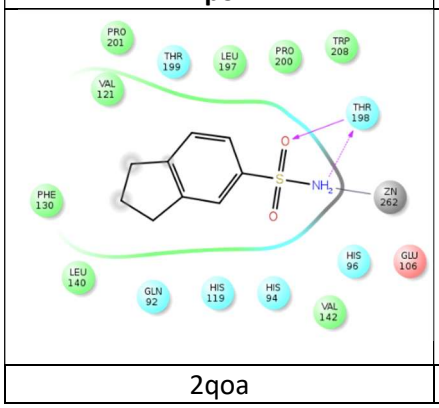
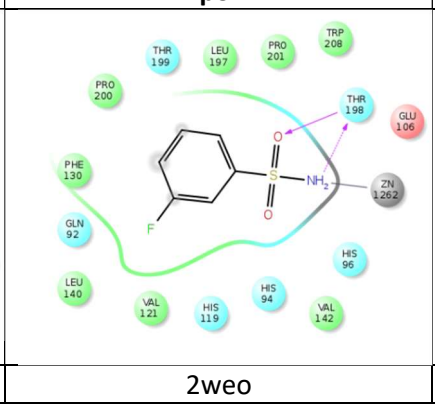
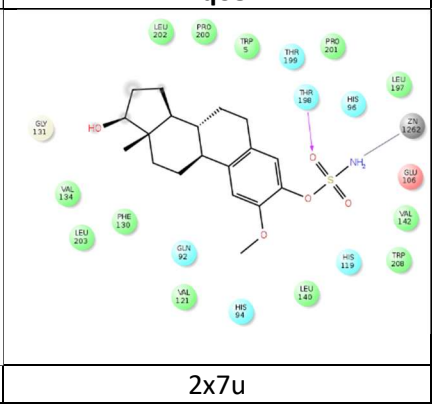
|  |  |  |
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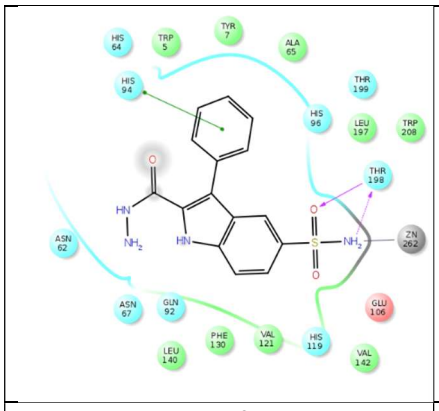
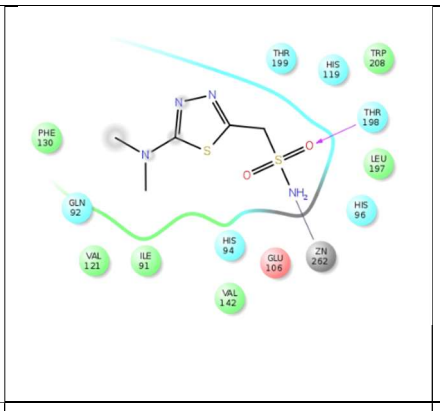
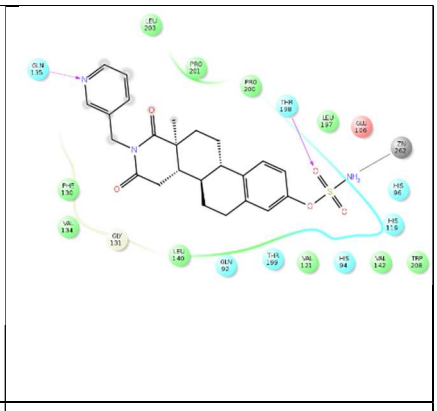
|  |  |  |
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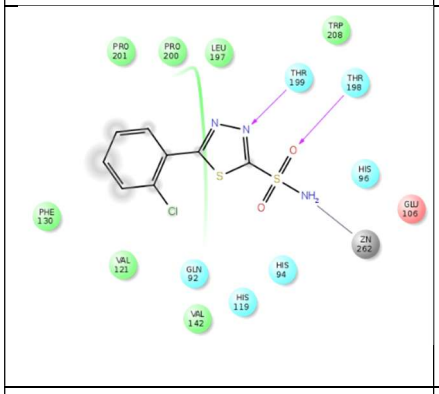
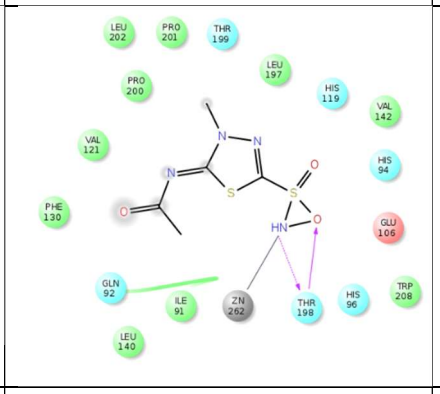
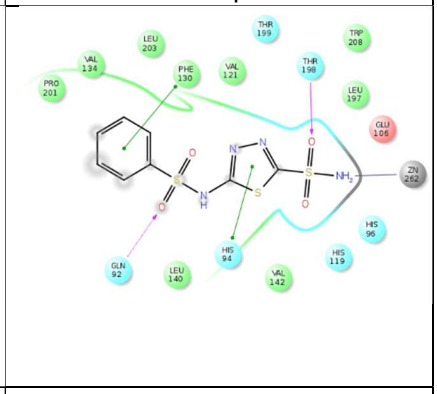
|  |  |  |
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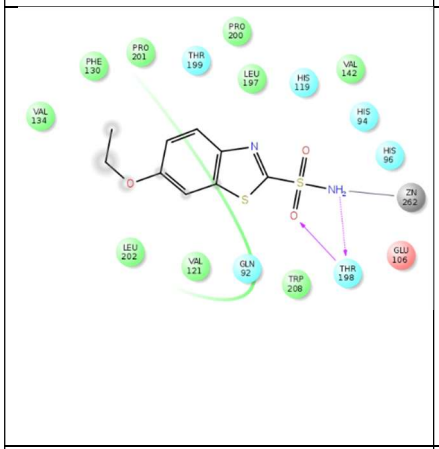
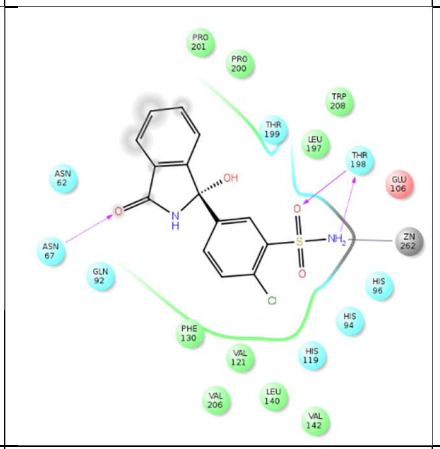
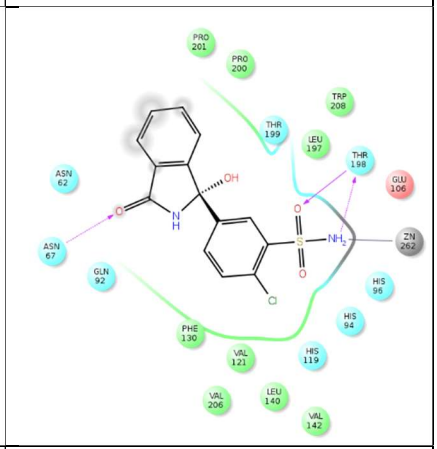
|  |  |  |
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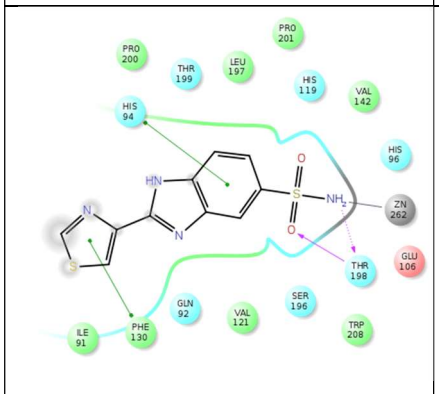
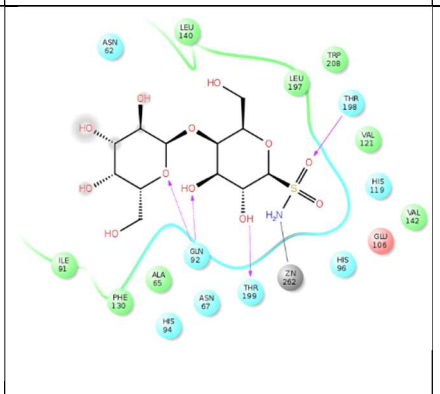
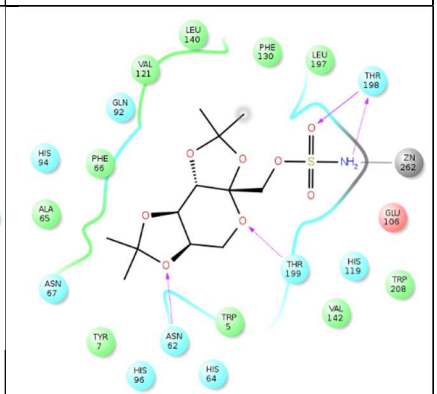
|  |  |  |
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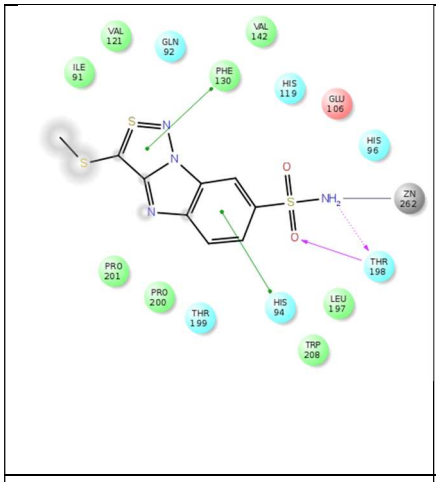
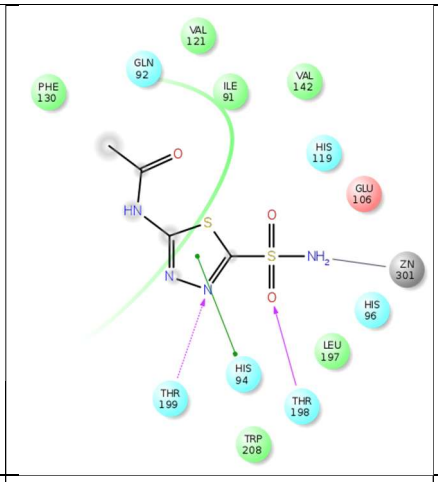
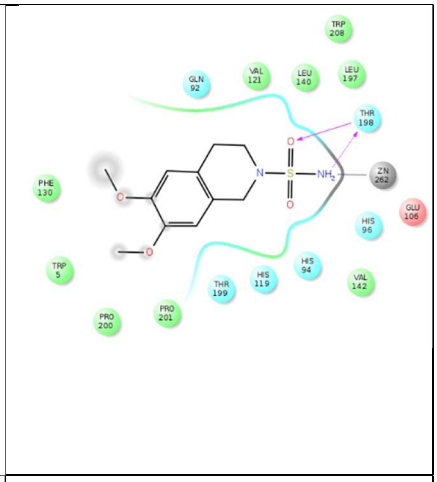
|  |  |  |
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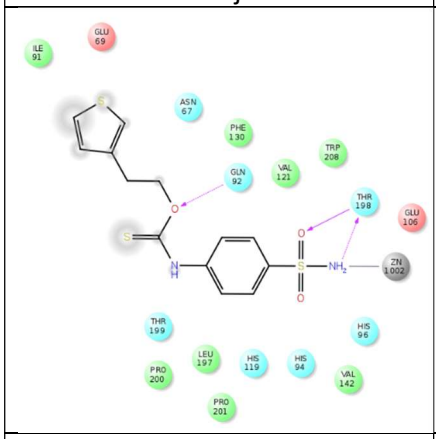
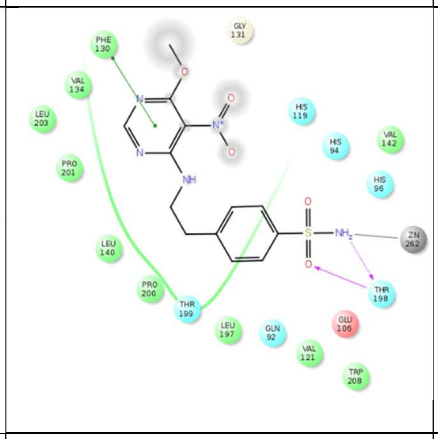
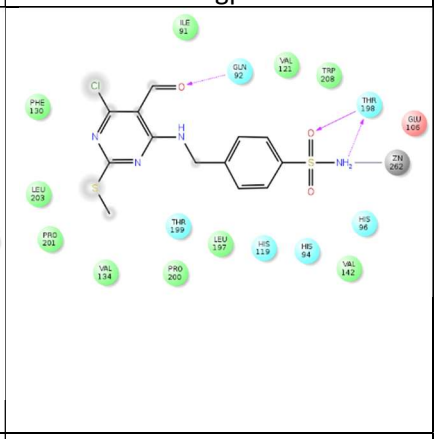
|  |  |  |
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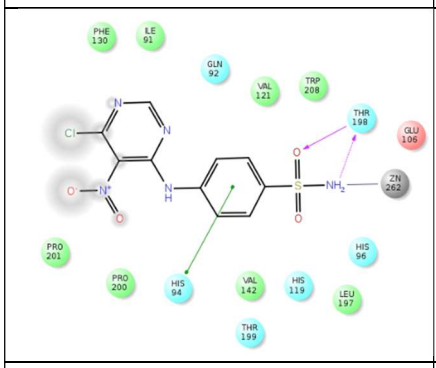
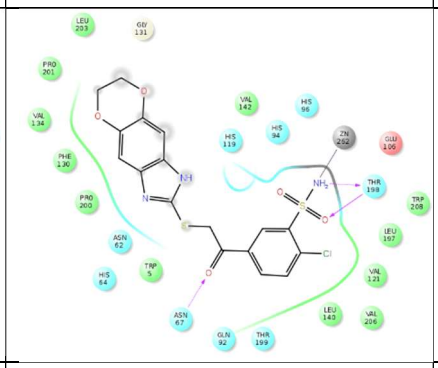
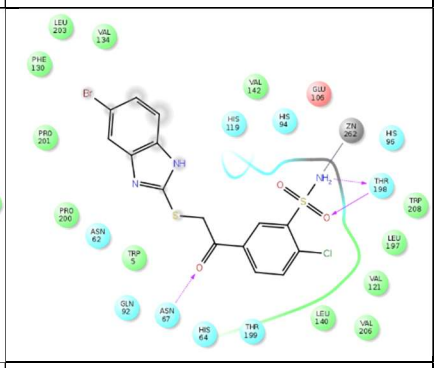
|  |  |  |
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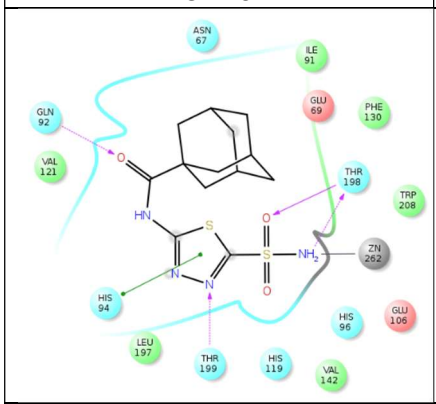
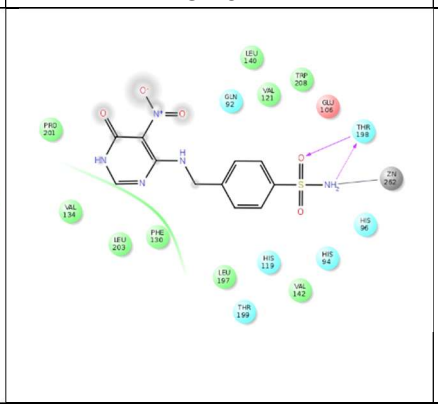
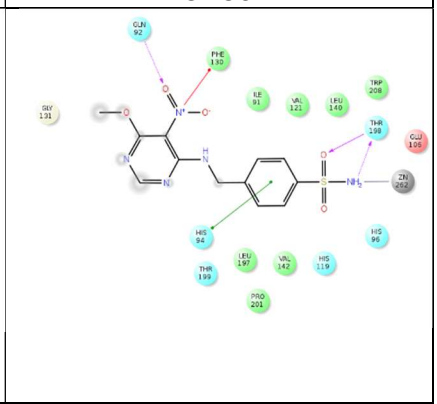
|  |  |  |
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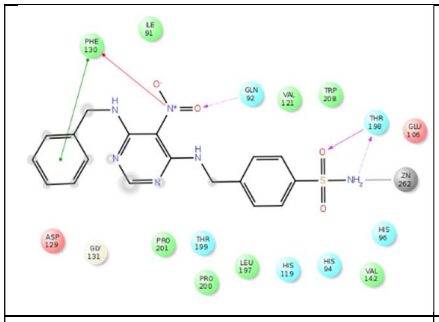
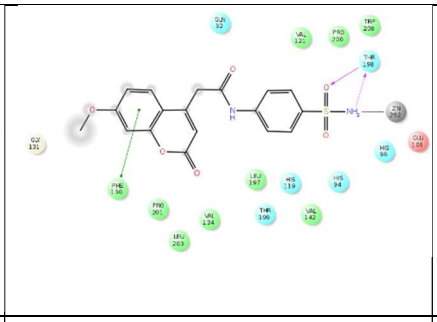
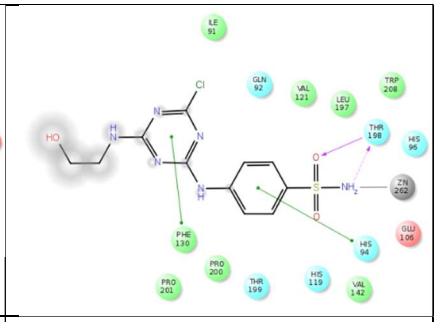
|  |  |  |
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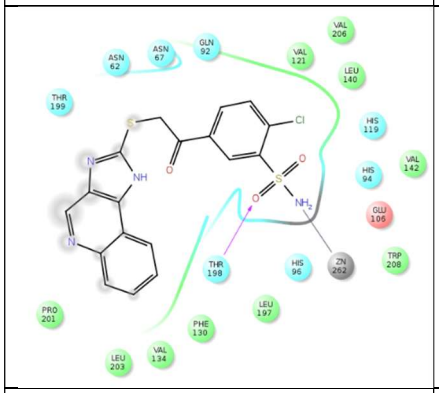
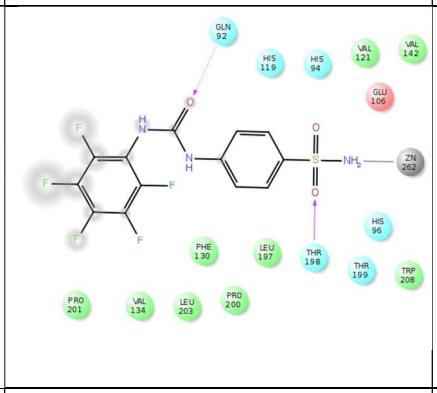
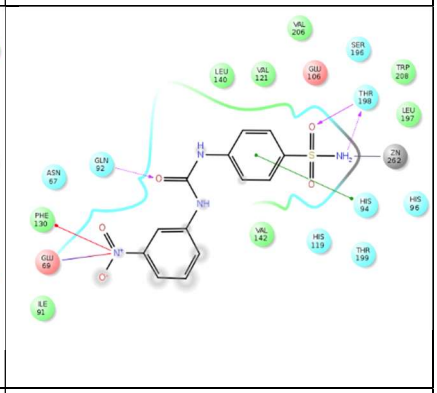
|  |  |  |
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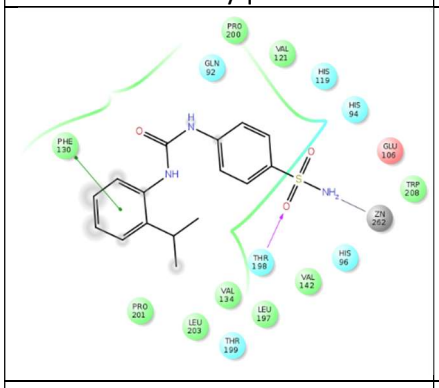
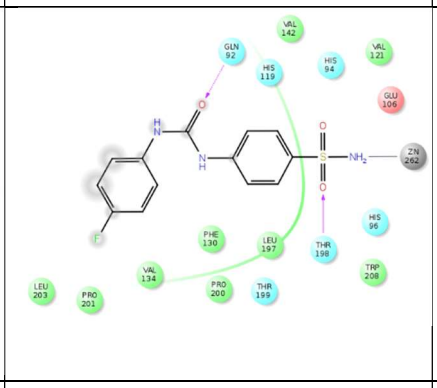
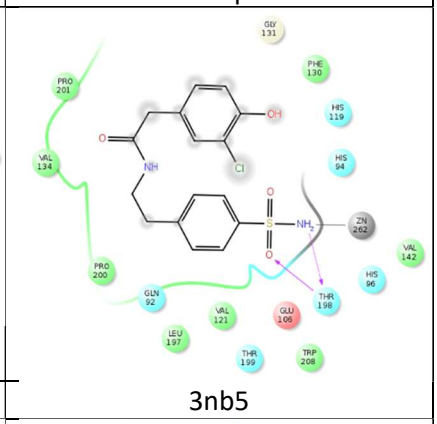
|  |  |  |
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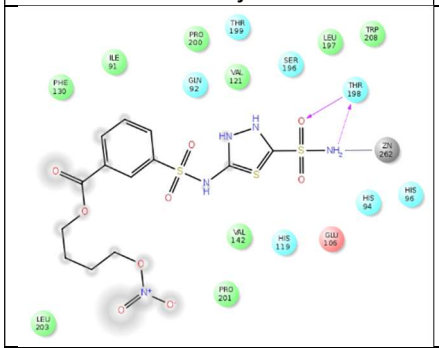
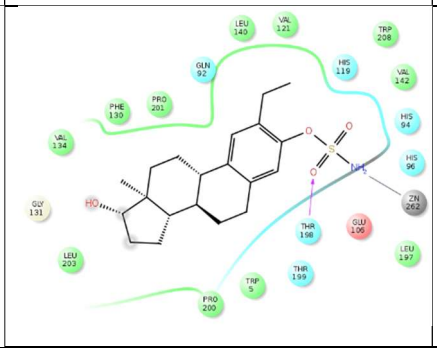
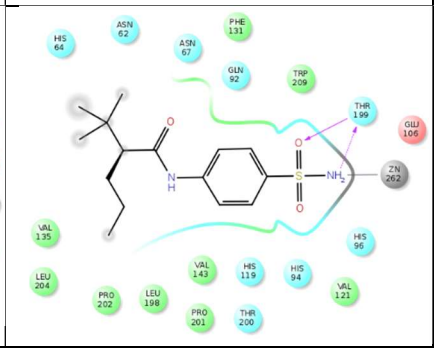
|  |  |  |
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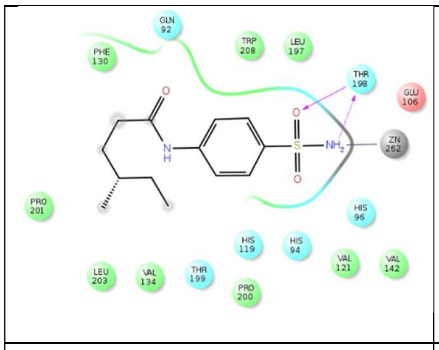
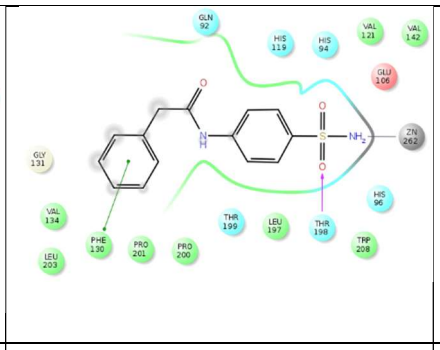
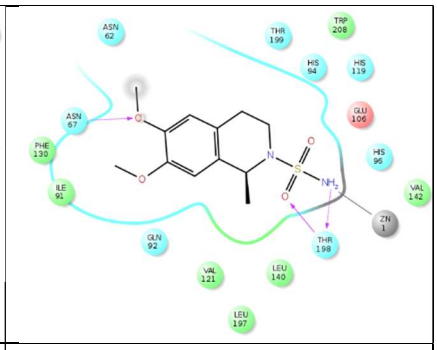
|  |  |  |
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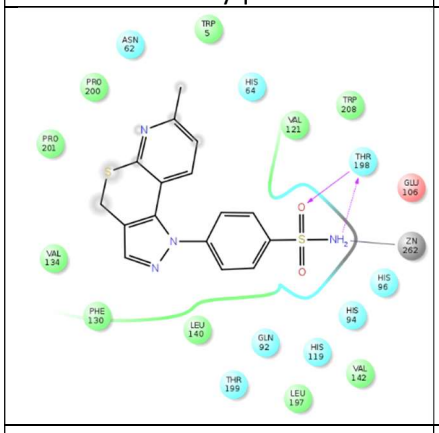
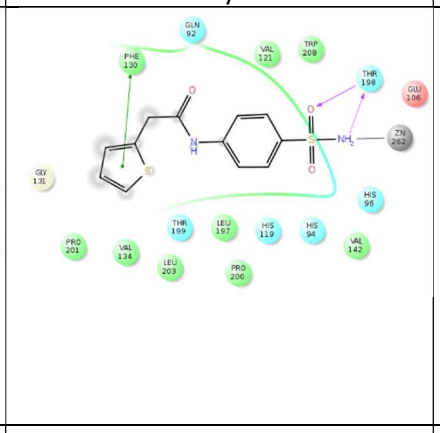
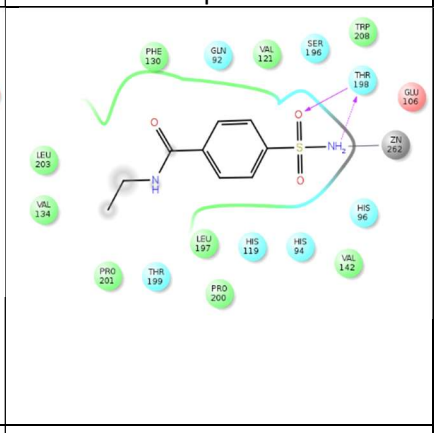
|  |  |  |
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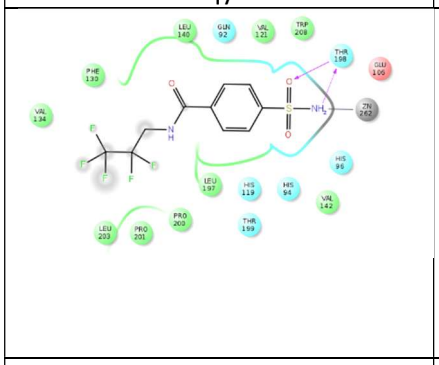
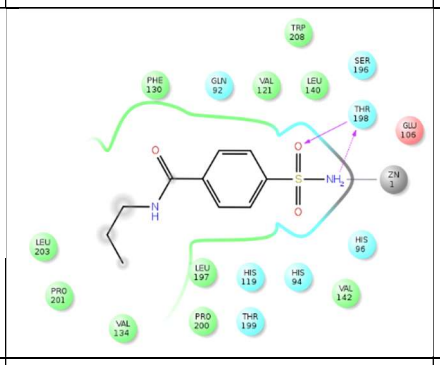
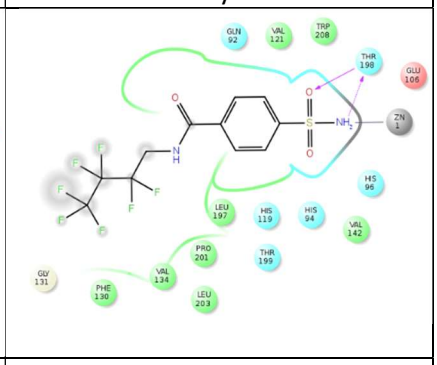
|  |  |  |
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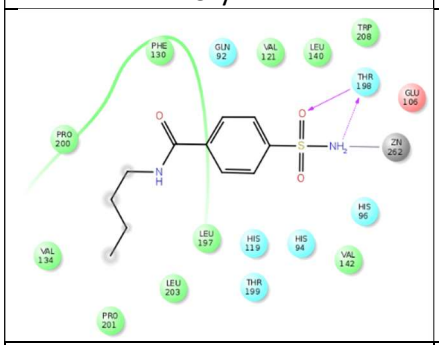
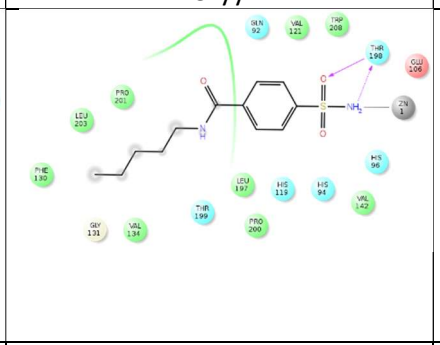
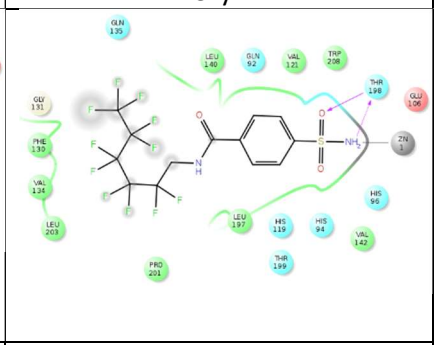
|  |  |  |
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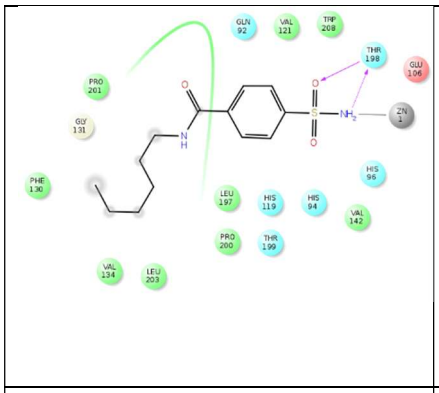
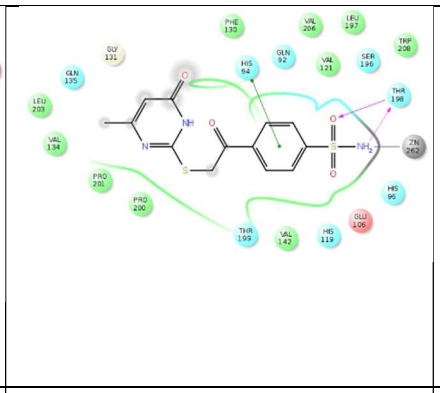
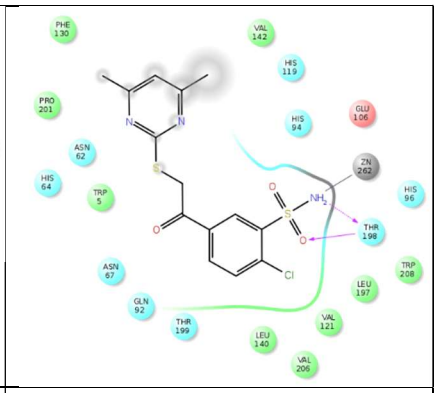
|  |  |  |
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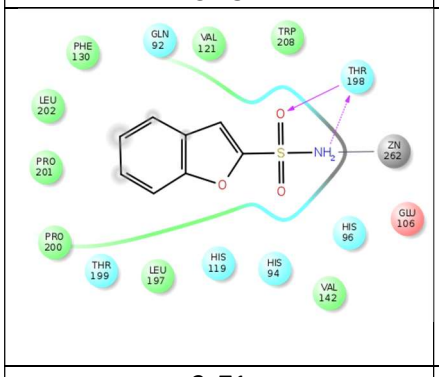
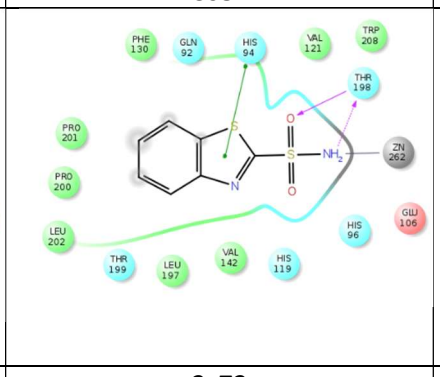
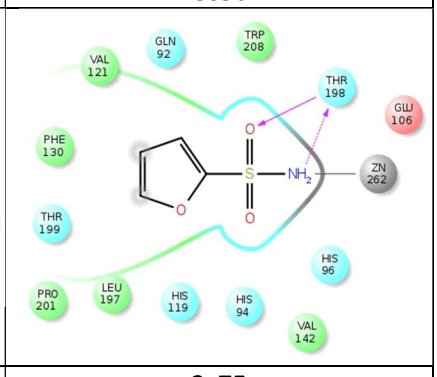
|  |  |  |
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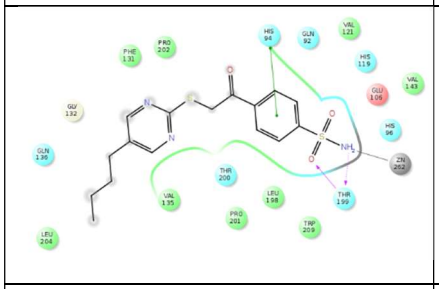
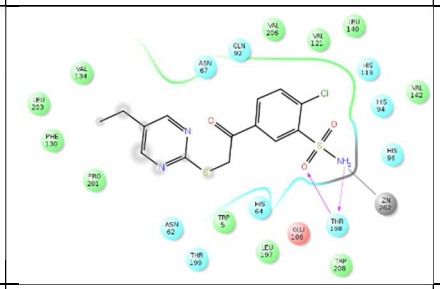
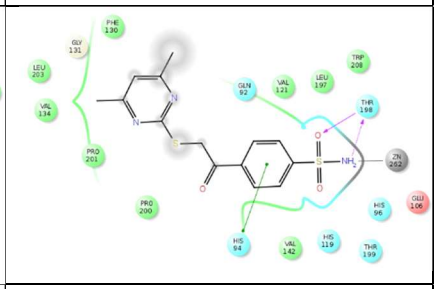
|  |  |  |
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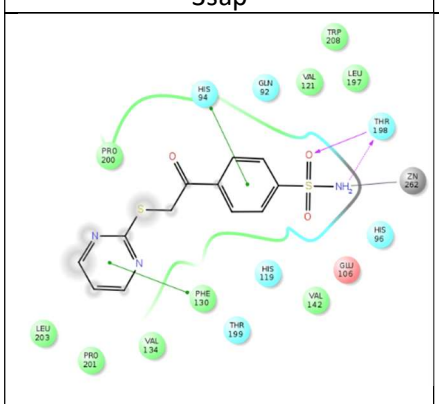
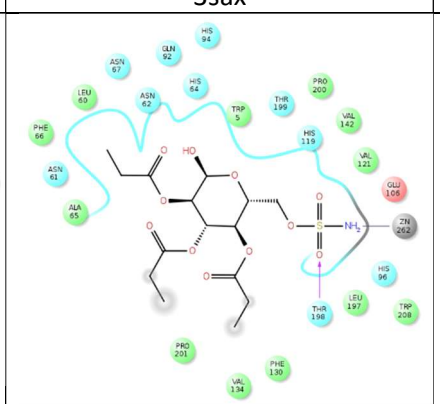
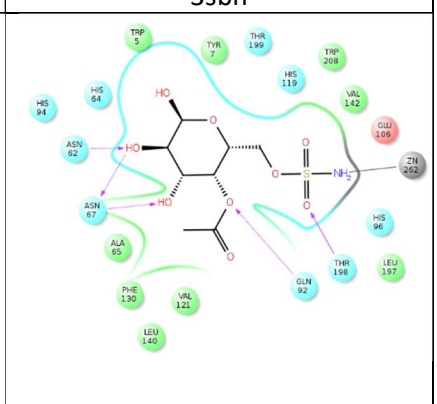
|  |  |  |
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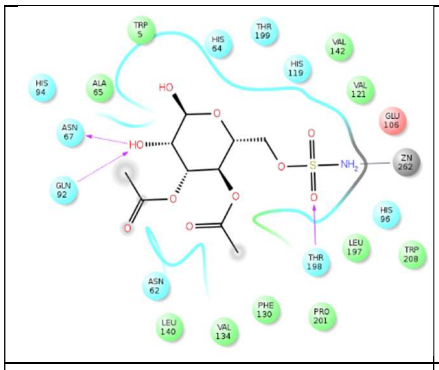
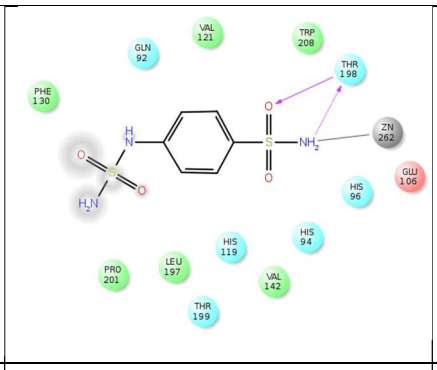
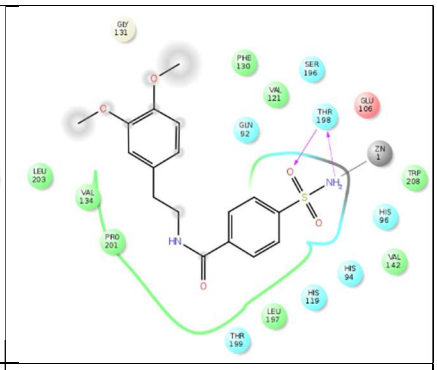
|  |  |  |
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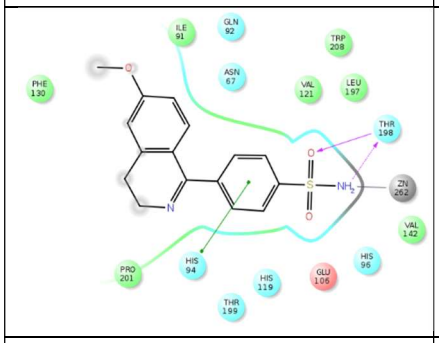
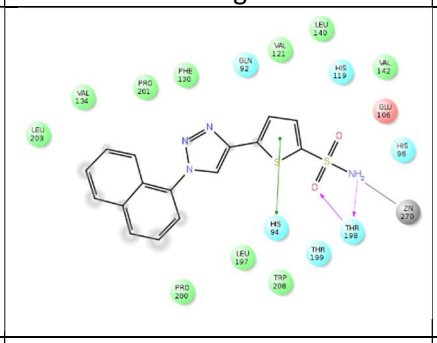
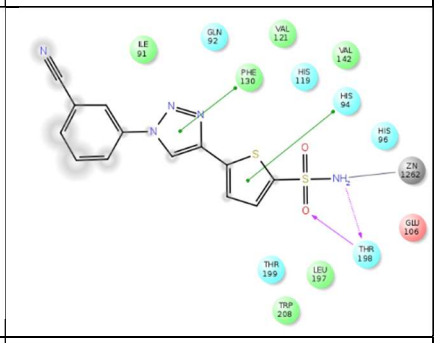
|  |  |  |
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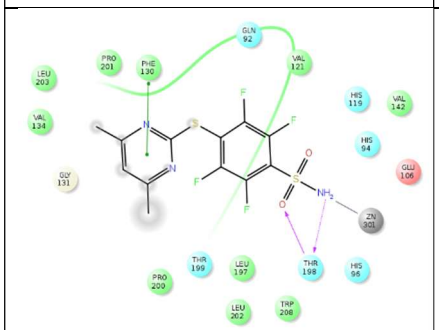
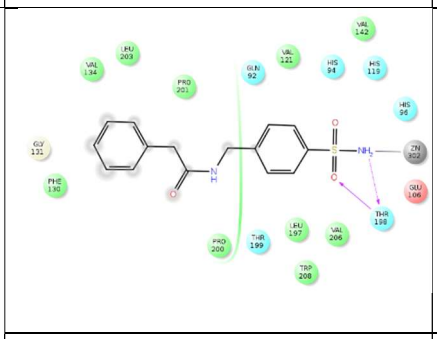
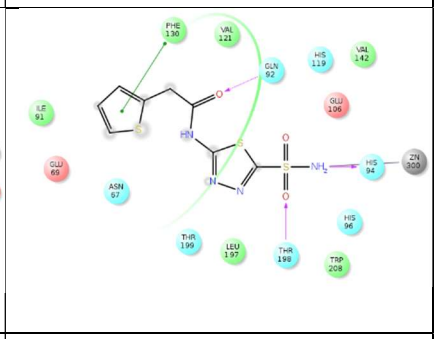
|  |  |  |
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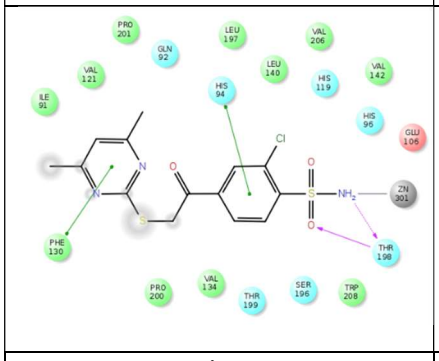
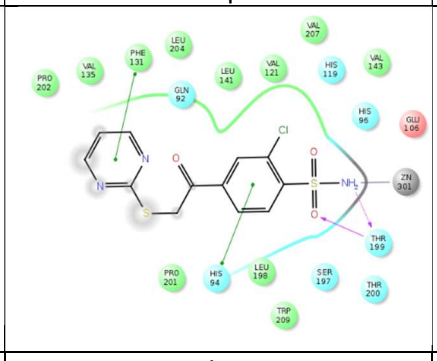
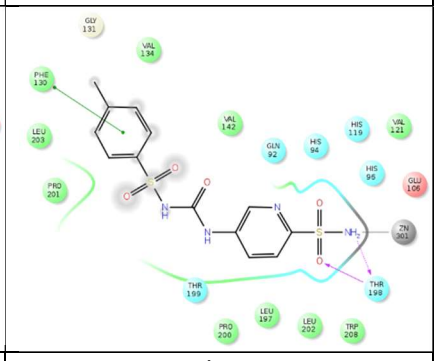
|  |  |  |
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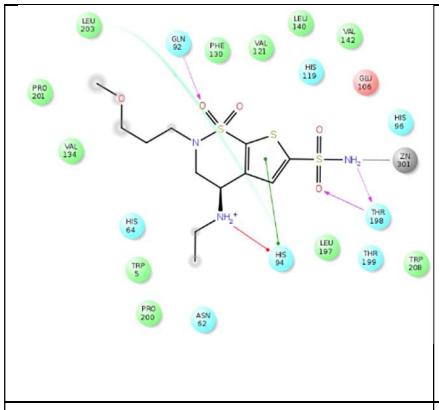
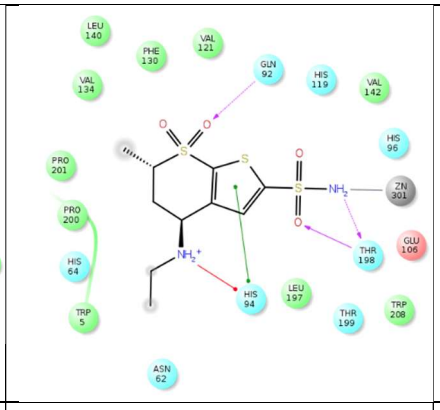
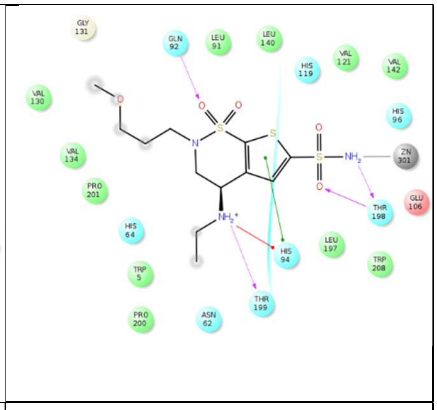
|  |  |  |
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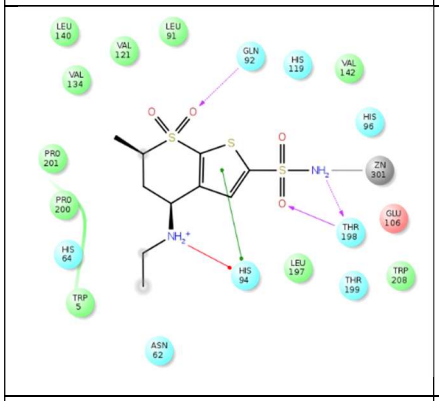
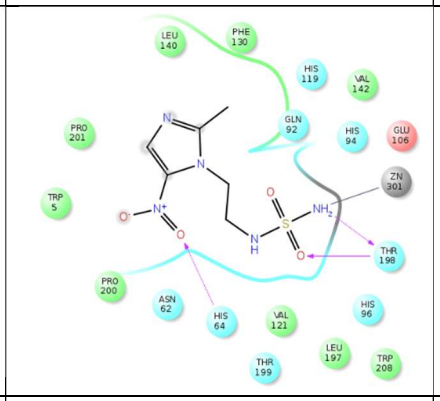
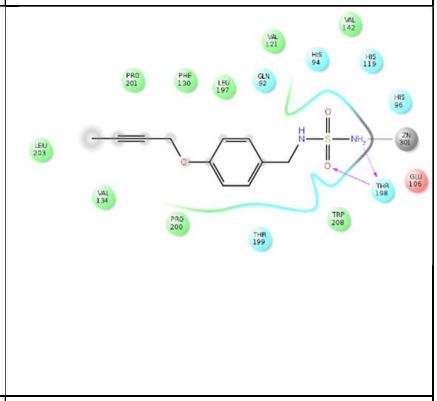
|  |  |  |
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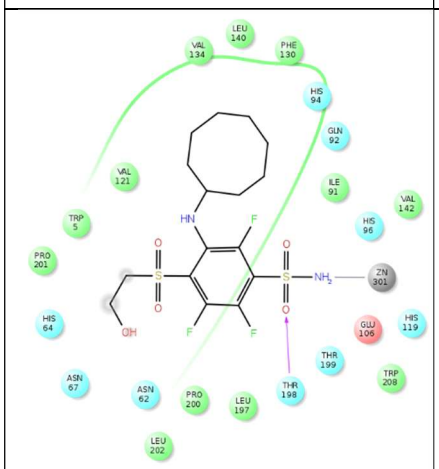
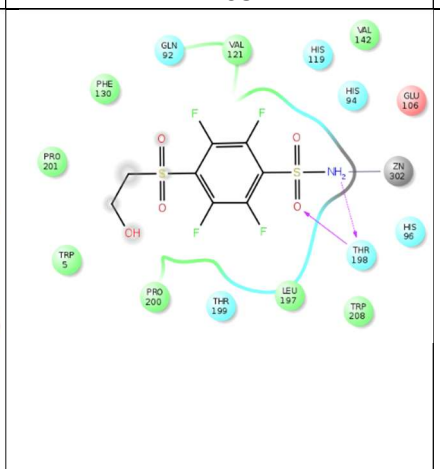
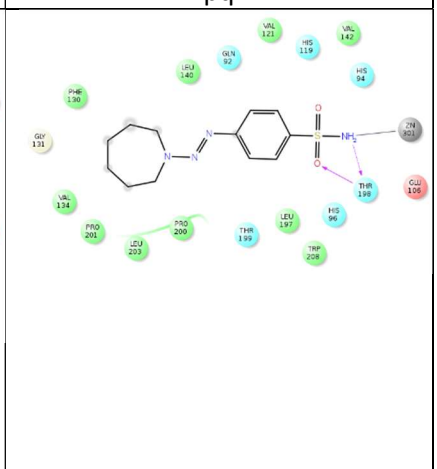
|  |  |  |
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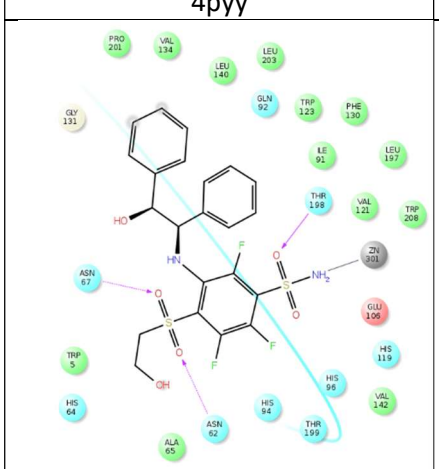
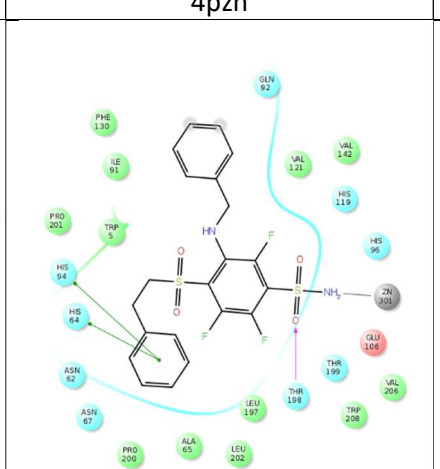
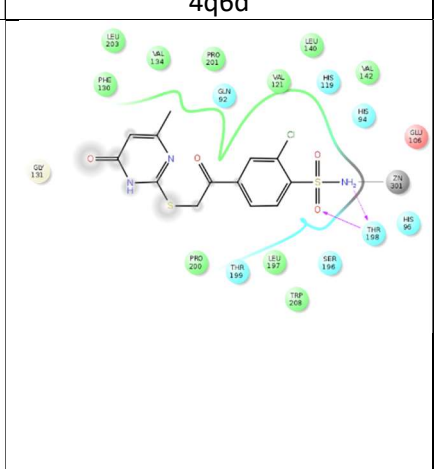
|  |  |  |
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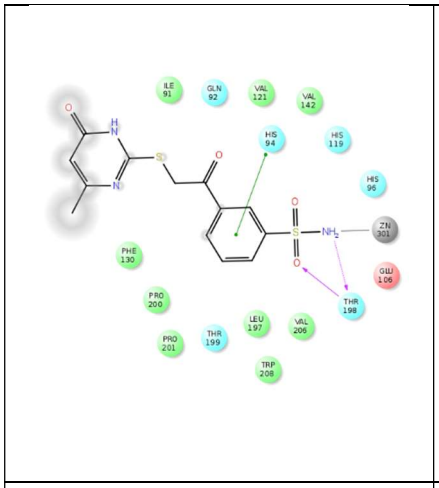
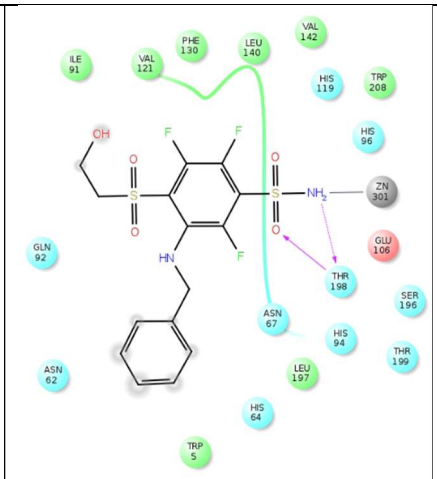
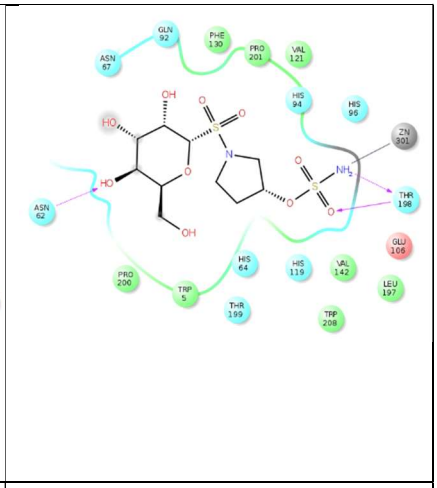
|  |  |  |
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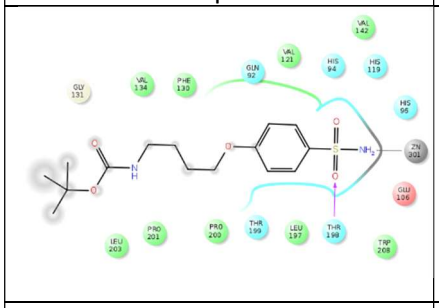
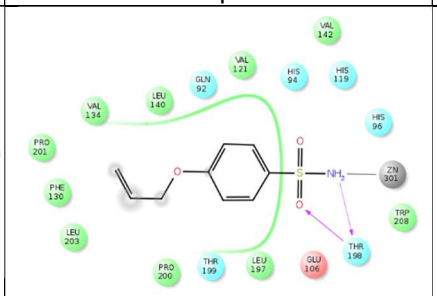
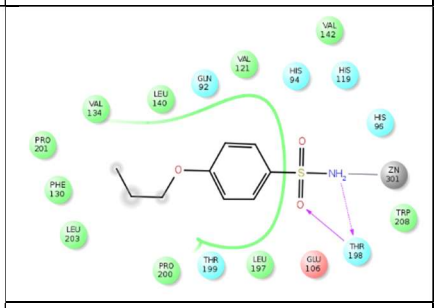
|  |  |  |
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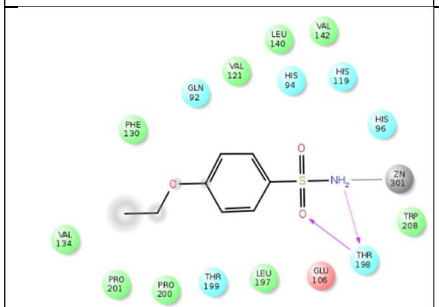
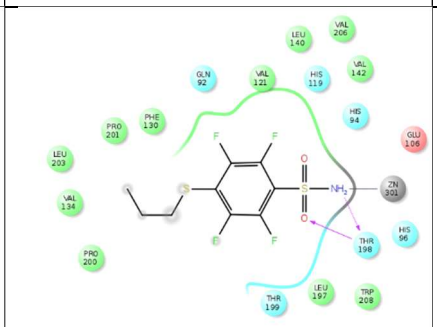
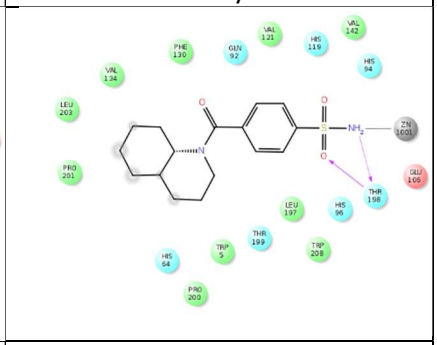
|  |  |  |
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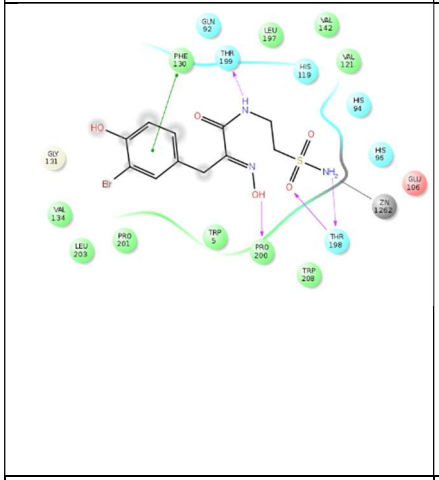
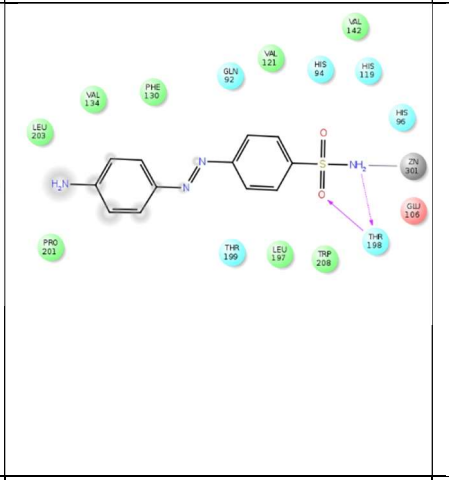
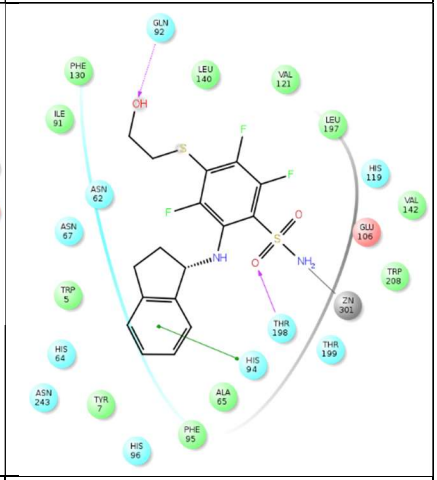
|  |  |  |
| 5a6h | 5byi | 5doh |

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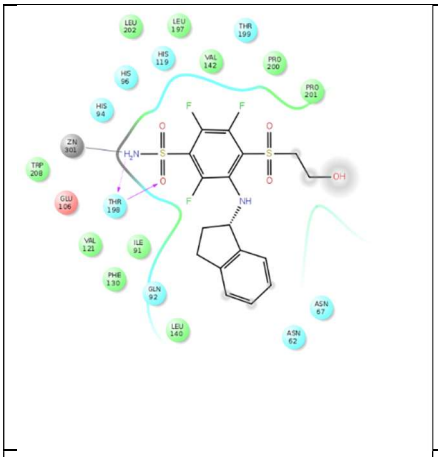
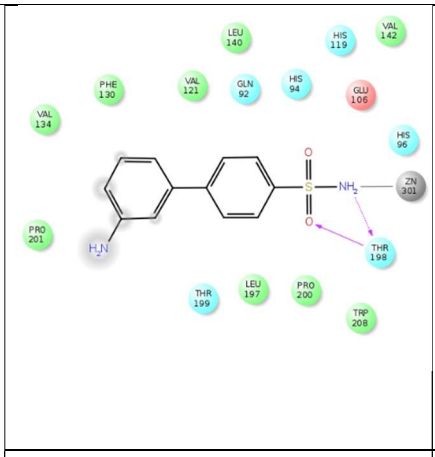
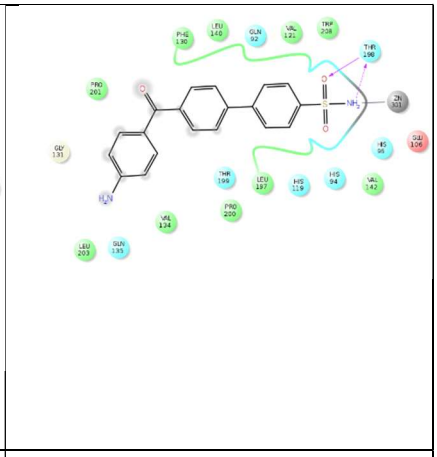
|  |  |  |
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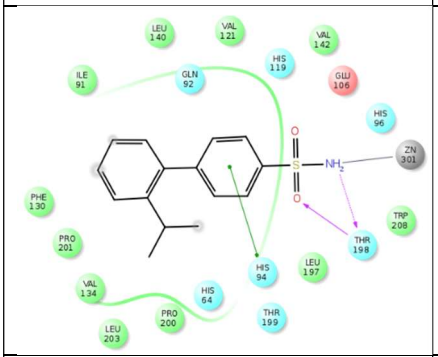
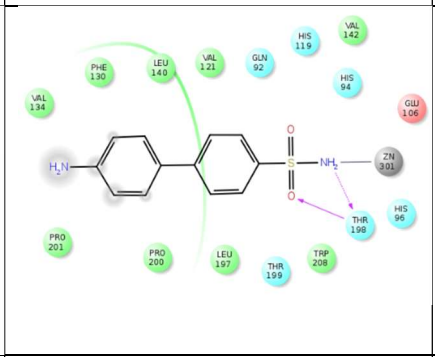
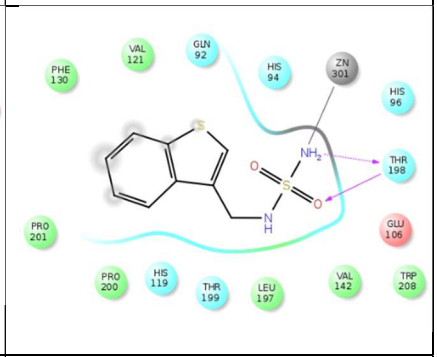
|  |  |  |
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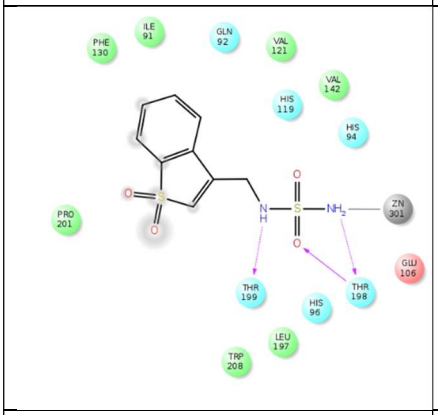
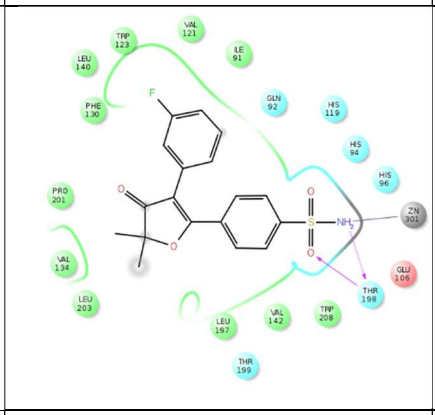
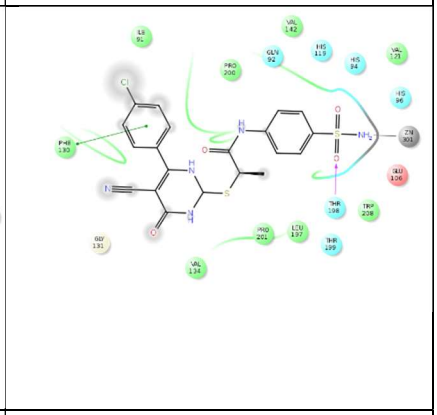
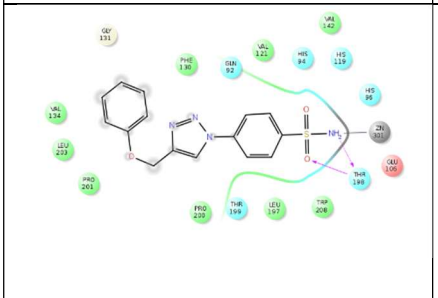
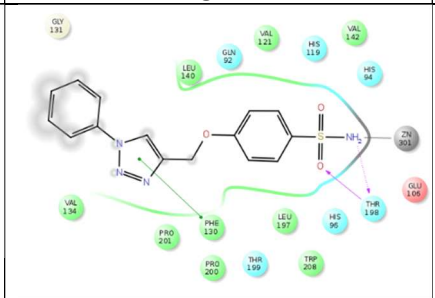
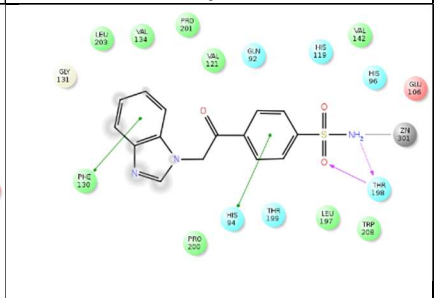
|  |  |  |
| 5fdi | 5gmn | 5j8z |
|  |  |  |
| 5jlq | 5ljt | 5ll4 |

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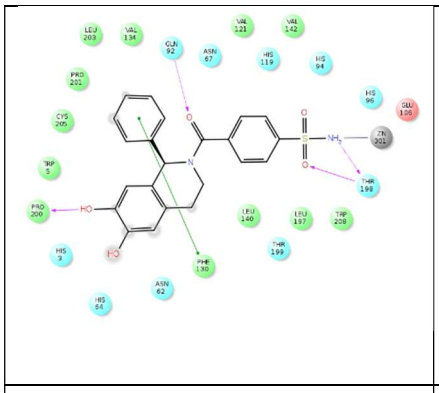
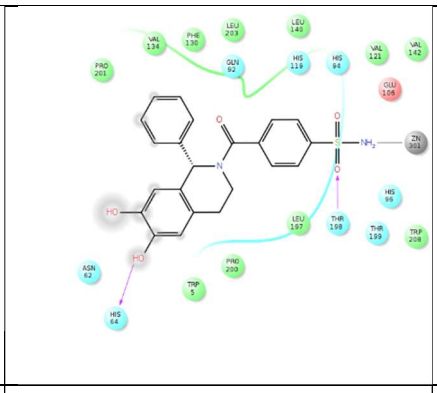
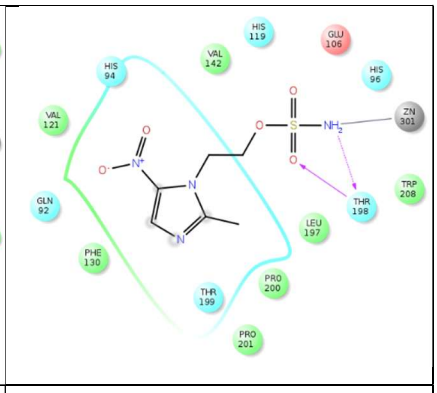
|---|---|---|
|  |  |  |
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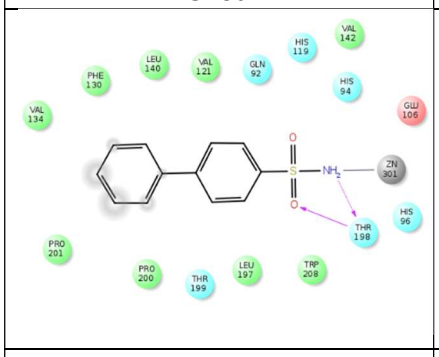
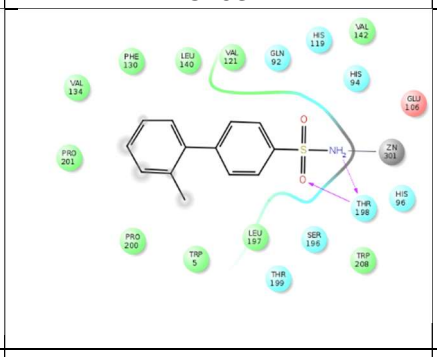
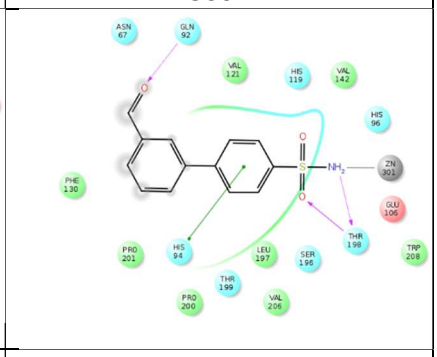
|  |  |  |
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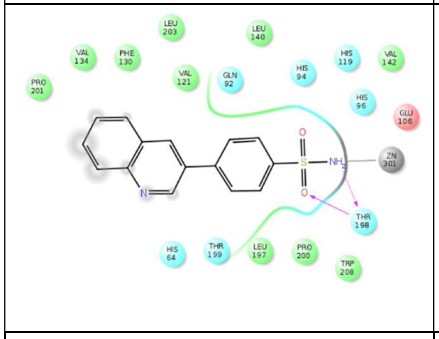
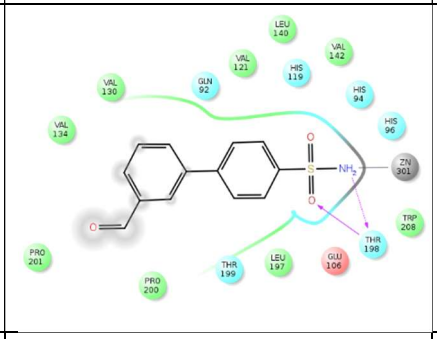
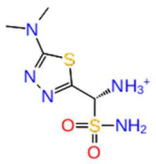
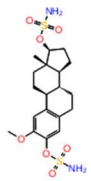
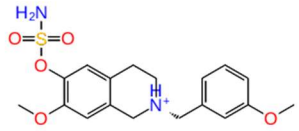
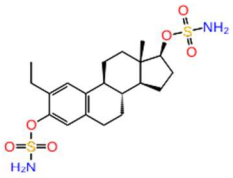
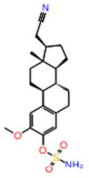
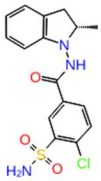
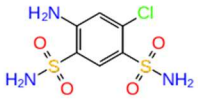
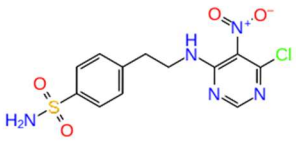
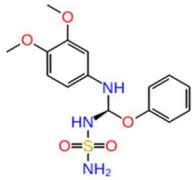
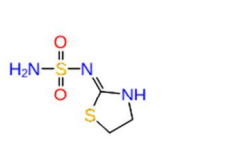
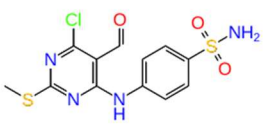
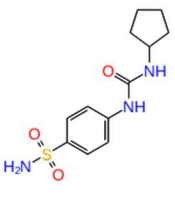
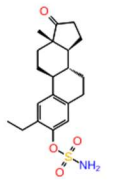
|  |  | |
| 5sz3 | 5sz6 | |

**Table S2**. Structures of the 70 ligands used as a first external test set.

| | | |
|---|---|---|
|  |  |  |
| **2eu2** | **2gd8** | **2h15** |
|  |  |  |
| **2qp6** | **2wd2** | **2weg** |
|  |  |  |
| **2weh** | **2x7t** | **3bet** |
|  |  |  |
| **3bl1** | **3hkn** | **3kig** |
|  |  |  |
| **3l14** | **3m2n** | **3m2x** |
|  |  |  |
| **3m04** | **3m14** | **3m98** |
|  |  |  |
| **3mho** | **3mzc** | **3oku** |

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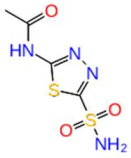
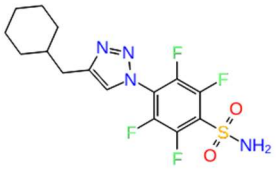
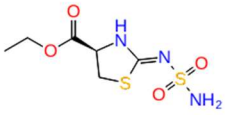
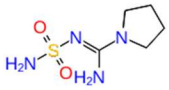
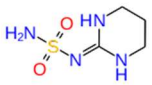
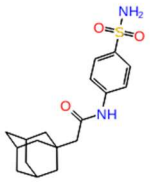
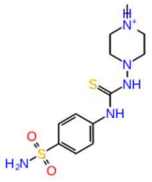
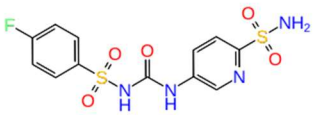
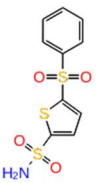
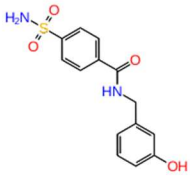
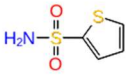
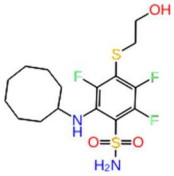
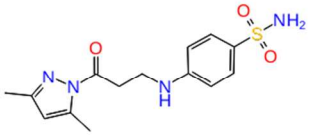
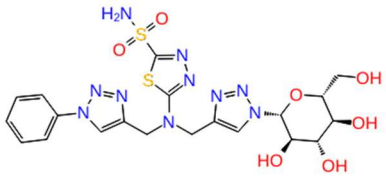
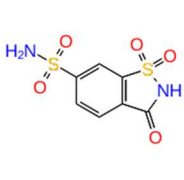
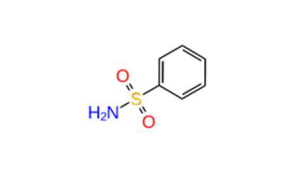
|---|---|---|
|  |  |  |
| **3s76** | **3v2m** | **4dz7** |
|  |  |  |
| **4dz9** | **4fpt** | **4frc** |
|  |  |  |
| **4fu5** | **4fvn** | **4fvo** |
|  |  |  |
| **4ilx** | **4ito** | **4kuw** |
|  |  |  |
| **4lhi** | **4mty** | **4n0x** |
|  |  |  |
| **4pyx** | **4q6e** | **4rfd** |
|  |  |  |
| **4rn4** | **4xe1** | **4yx4** |

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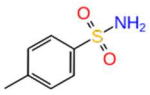
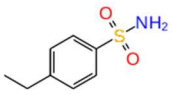
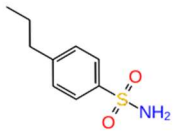
|  |  |  |
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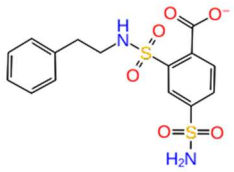
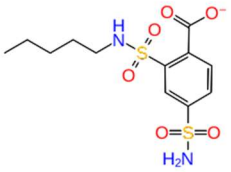
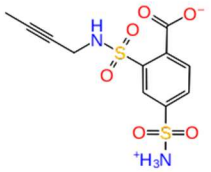
|  |  |  |
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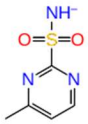
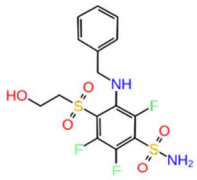
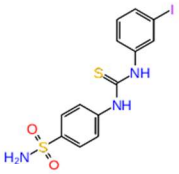
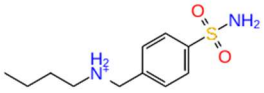
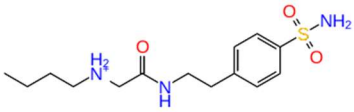
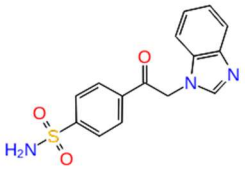
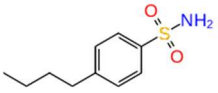
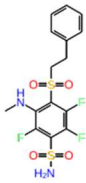
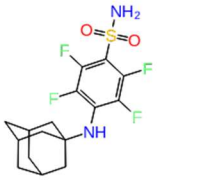
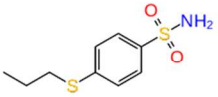
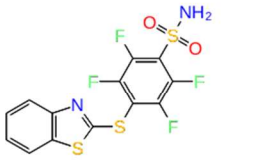
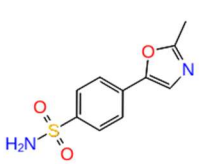
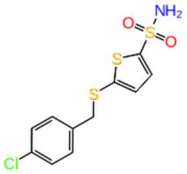
|  |  |  |
| **5eh5** | **5ehe** | **5eij** |
|  |  |  |
| **5ekh** | **5ekj** | **5ll4** |
|  |  |  |
| **5ll8** | **5llc** | **5lle** |
|  |  |  |
| **5llg** | **5llh** | **5mjn** |
|  |  |  |
| **5nea** | **5nee** | **5nx0** |

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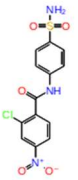
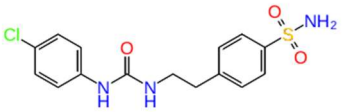
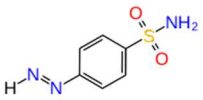
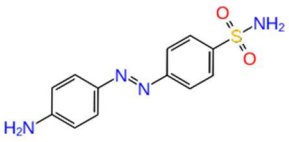
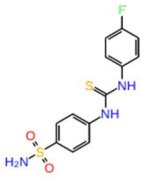
|---|---|---|
|  |  |  |
| **5nxg** | **5ny3** | **5t71** |
|  |  |  |
| **5t74** | **5t75** | **5tfx** |
|  | | |
| **5uln** | | |

**Table S3.** Structures of the 15 ligands used as additional external test set.

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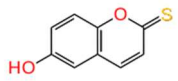
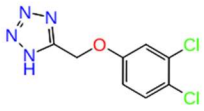
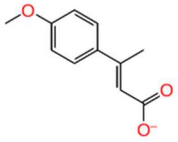
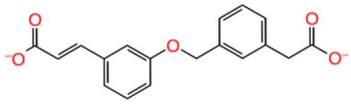
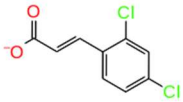
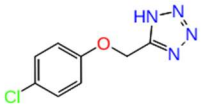
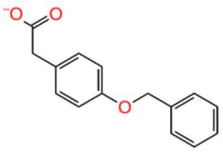
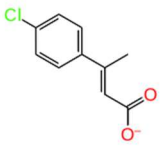
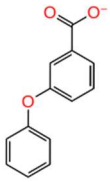
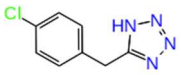
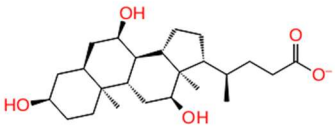
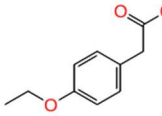
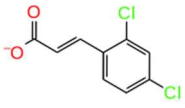
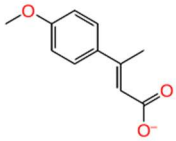
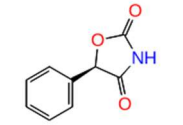
|  |  |  |
| **4wl4** | **5eh7** | **5eh8** |
|  |  |  |
| **5ehv** | **5ehw** | **5flo** |
|  |  |  |
| **5flq** | **5fls** | **5flt** |
|  |  |  |
| **5fng** | **4pxx** | **5fnj** |
|  |  |  |
| **5fnk** | **5fnm** | **5txy** |