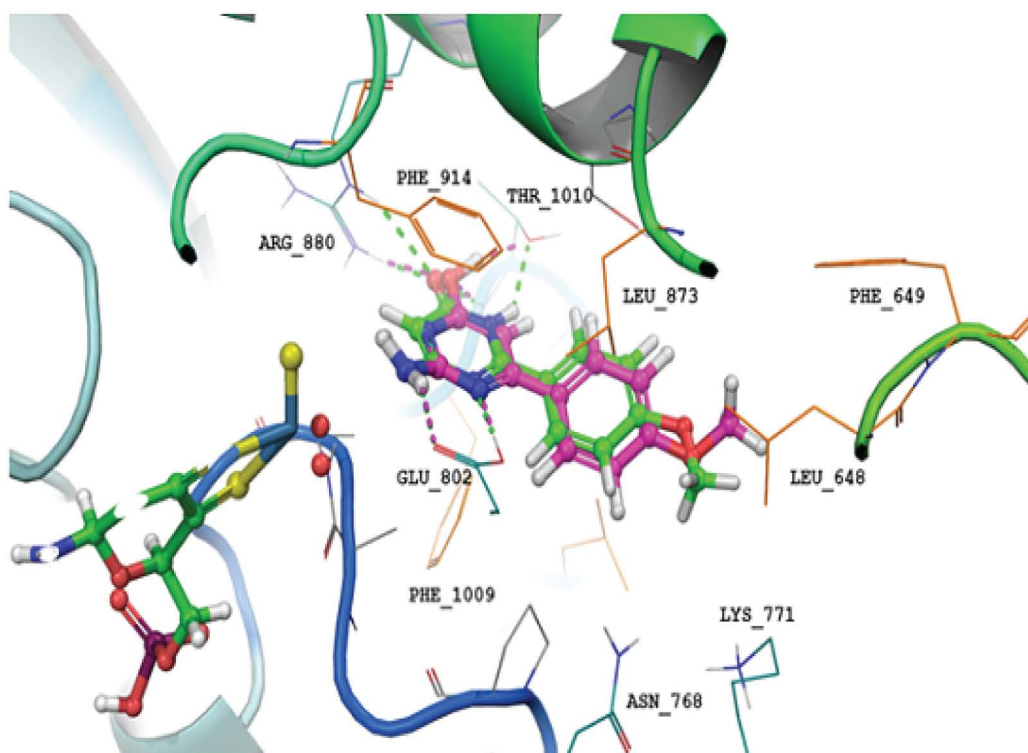


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Smriti Khanna et al., Discriminating between active and inactive compounds using binding energy calculations – a case study

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