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Molecular Dynamics based screening for Cag A protein: Using *Quercus brantii* extract substances as lead-like

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Statement of the Problem: Gastric cancer is among the fifth common malignancy and third cause of cancer related mortality worldwide (approximately 700000 victims registered each year). *Helicobacter pylori*, that has been closely related to gastric ulcers and adenocarcinoma, infects nearly more than 50% of the entire human population based on presence or absence of CagA gene-encoded CagA protein, *H. pylori* divided into 2 strains: CagA positive and CagA negative. Currently, it has been demonstrated that CagA positive strain directly effects on gastric cancer incidence, so that *H. pylori* infection may lead to gastric cancer if it is getting chronic. But due to antibiotics resistance module which revealed by *H. pylori* strains, significance of discovering new generation of antibiotics is certainly tangible.

Methodology & Theoretical: In this study *Quercus brantii* as an Iranian aborigine, which rich extract called Shookeh has been obtained from it, used whereas leading like compound to inhibit specifically Cag A protein. Since utilization of GC MASS technique for analysis Shookeh, Furfural was identified as the most abundant compound. The structure of Cag A protein with PDB ID 4IRV used for expectancy of binding affinity between the protein and Furfural by PyRx autodock vina software. Whereof the aim of this study is to present an efficient drug-like substance we respectively engineered furfural by Hyperchem software and make carbon nano tube around substance by SAMSON software to making an improved inhibitor for Cag A protein.

Conclusion & Significance: Molecular docking analysis indicates -4.3 kcal/mol for binding affinity and pharmacokinetic analysis by using FAFDrugs4 server does not predict any oral toxicity for furfural. After engineering the substance binding affinity reduces up to -6.8 kcal/mol with no oral toxicity even with carbon nanotube.

Recent Publications

- HATAKEYAMA, Masanori (2017) Structure and function of *Helicobacter pylori* CagA, the first-identified bacterial protein involved in human cancer. Proceedings of the Japan Academy, Series B
- Lai, Chih-Ho et al (2011) *Helicobacter pylori* CagA-mediated IL-8 induction in gastric epithelial cells is cholesterol-dependent and requires the C-terminal tyrosine phosphorylation-containing domain. FEMS microbiology letters.
- Mishra, Ajay Kumar (2013) Nanomedicine for drug delivery and therapeutics, John Wiley & Sons.
- Shrivastava, Arpit Kumar et al (2017) Insilico identification and validation of a novel hypothetical protein in *Cryptosporidium hominis* and virtual screening of inhibitors as therapeutics. Parasitology research.
- Murata-Kamiya, Naoko (2010) Helicobacter pylori exploits host membrane phosphatidylserine for delivery, localization and pathophysiological action of the CagA oncoprotein. Cell host & microbe

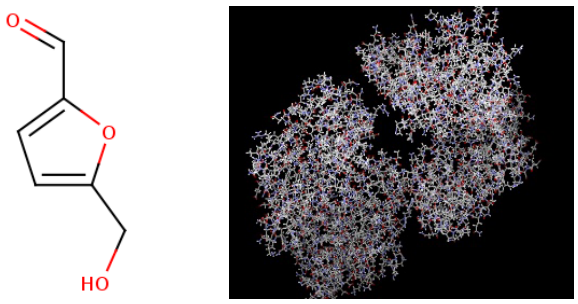

Figure 1: *Furfural substance obtained from pubchem NCBI and 3D structure of Cag A protein*

Biography

Fatemeh Khoddam is currently working as a faculty of Biological Sciences in the Department of Microbiology at Islamic Azad University, Iran.

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