J Appl Bioinforma Comput Biol 2019, Volume: 8
DOI: 10.4172/2329-9533-C1-009

Insight from structural interactions of curcumin biotransformed compounds and conventional drugs to N-terminal residues of CagA protein of Helicobacter pylori for suppression of oncogenic activities

Akhileshwar Kumar Srivastava
Banaras Hindu University, India

The oncoprotein cytotoxic associated gene A (CagA) of Helicobacter pylori leads for the development of gastric cancer. Conventional drugs like clarithromycin, amoxicillin, pantoprazole, and metronidazole are used against *H. pylori* infection. The chemopreventive role of curcumin against oncogenic activities of *H. pylori* is still a major scientific challenge with several reasons such as its low bioavailability related to curcumin biotransformation via either conjugation or reduction. The curcumin (CUR) is metabolized into curcumin glucuronidase (CUR-GLR) and curcumin sulphate (CUR-SUL) after oral administration and dihydroxycurcumin, tetrahydrocurcumin, and hexahydrocurcumin (HHC) are formed through intraperitoneal administration. The current study emphasized to assess the interactive potential of curcumin biotransformed and conventional drugs with CagA oncoprotein. All lead compounds were screened using Lipinski's rule of five and the druglikeness property for assessment of pharmacological properties. The molecular docking was conducted using PatchDock and Firedock online server. The obtained structure from docking was visualized through software Discovery client 4.5. The results obtained from FireDock, the binding energy (-36.37 kcal/mol) of curcumin was higher than amoxicillin (-34.78 kcal/mol), pantoprazole (-34.08 kcal/mol), and metronidazole (-25.12 kcal/mol), except for clarithromycin (-51.06 kcal/mol) whereas metabolized CUR-GLR (54.55 kcal/mol) had highest binding affinity with CagA. The current study based on virtual profiling of compounds suggested that the curcumin and its biotransformed compounds similar to conventional drugs could act as anticancerous agents against CagA+ *H. pylori* infection.

akhileshwar.kumar2@gmail.com