Abstract

Quassinoids are the naturally available plant extracts which exhibit a wide range of biological activities, that include anti malarial, anti amoebic, anti tumor properties etc. The present experiment aims to exploit the antitumor properties of the quassinoids. 68 quassinoid analogues were designed and were docked with hDHFR (human dihydrofolate reductase) a potential cancer target. The docking results showed compound 33 to be the best ligand for DHFR.

References

- Melanie J. O'Neill, Dorothy H. Bray, Peter Boardman, J. David Phillipson, David
- Dihydrofolate Reductase October 2002 Molecule of the Month by David Goodsell/10. 2210/rcbs/pdb.

Index Terms
Computer Science  Bio-informatics

Keywords
Quassinoids  quassinoid ligands  quassinoids analogues  anti tumor  DHFR