

COMPUTATIONAL
CHEMISTRY AND DRUG
DESIGNING
CHITRANI MEDHI
GAUHATI UNIVERSITY

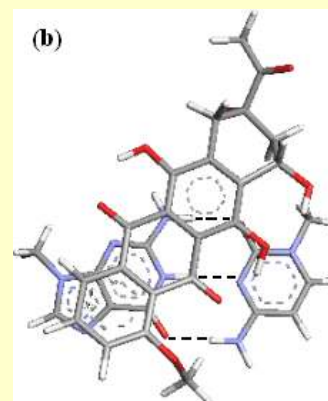
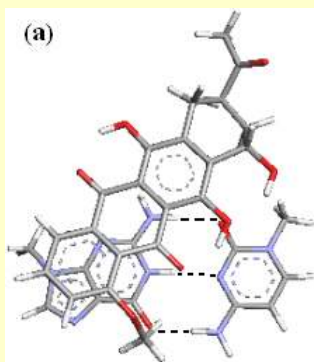
DNA AND DRUG INTERACTION

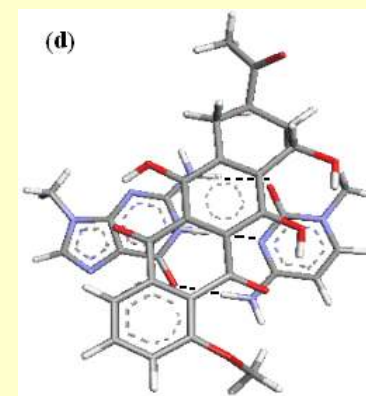
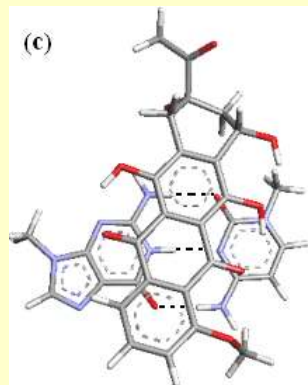
- Anticancer drug, daunomycin acquires unique preference for GC or CG rich triplets of DNA.
- It has less affinity for AT sequence compared to GC sequence.
- Assessment of DNA binding ability of this drug is important.
- Stacking interaction between the aromatic rings with the purine and pyrimidine rings of base pairs.

Tricyclic to tetracyclic chromophore in intercalation

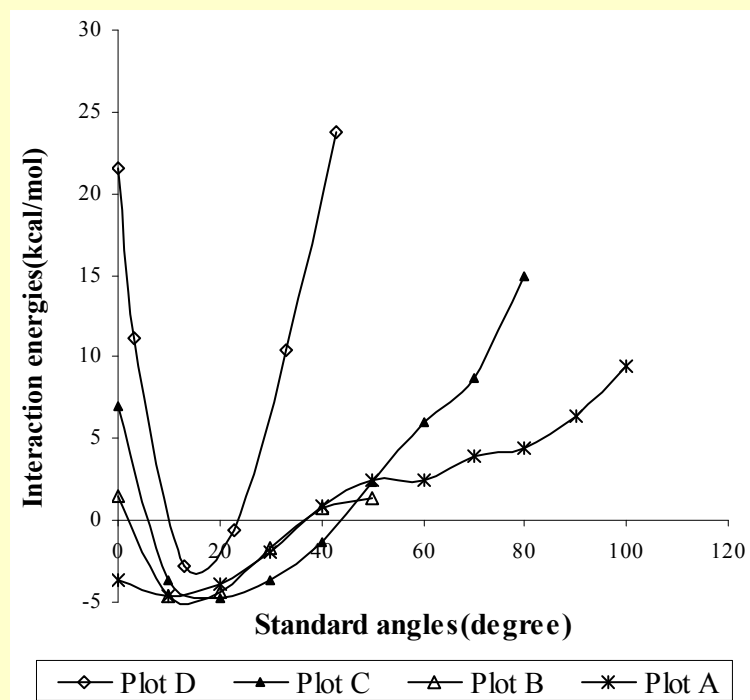
- Steric effect results lack of accessibility of tetracyclic ring within GC sequences. Daunomycin has been known as an intercalating drug.
- Stacking stabilization is the core factor for stabilizing the DNA binding.
- What is the advantage of tetracyclic chromophore as intercalator from tricyclic intercalative drugs

Interaction between chromophore and base pair.

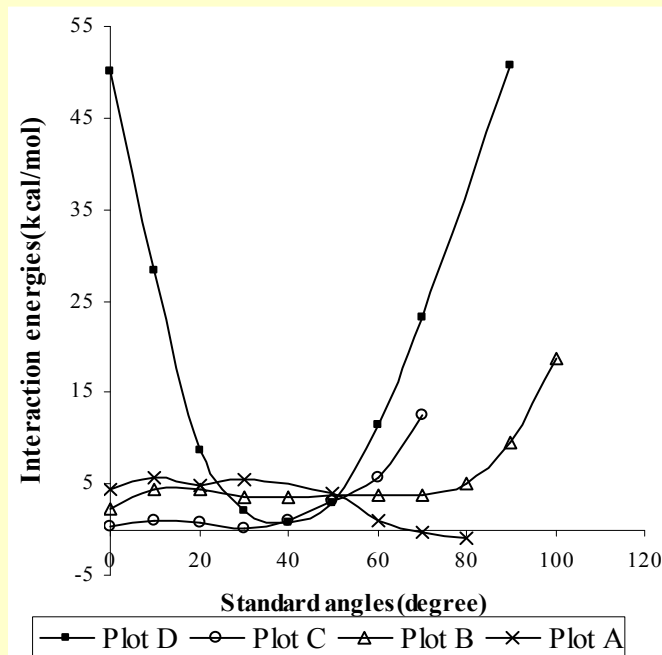




Minor grooves of GC base pair

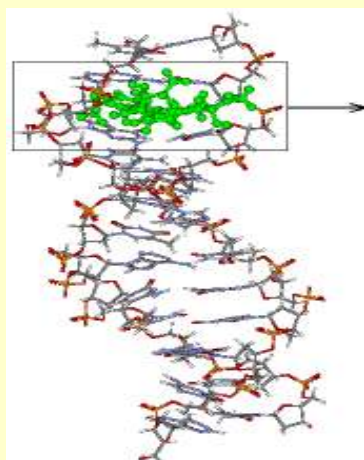


Major grooves of GC base pair



Minimised structure of intercalated daunomycin within dG-dC

Workshop on Developing Applications on GARUDA-DAG07



GARUDA Partner Presentations

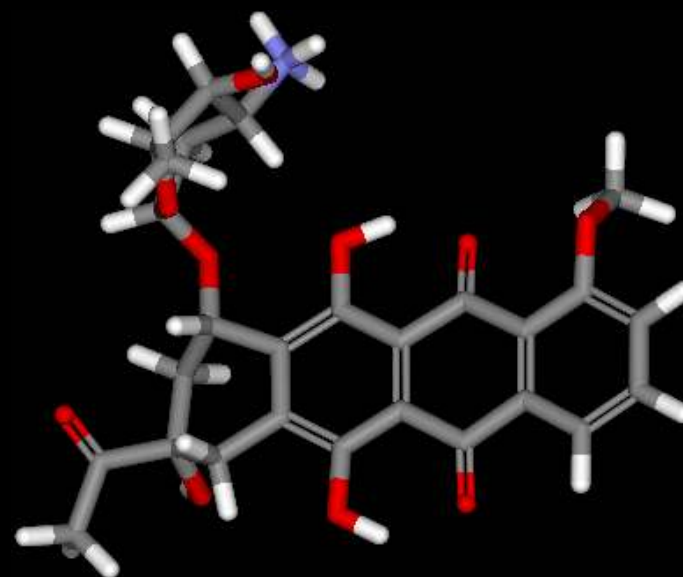
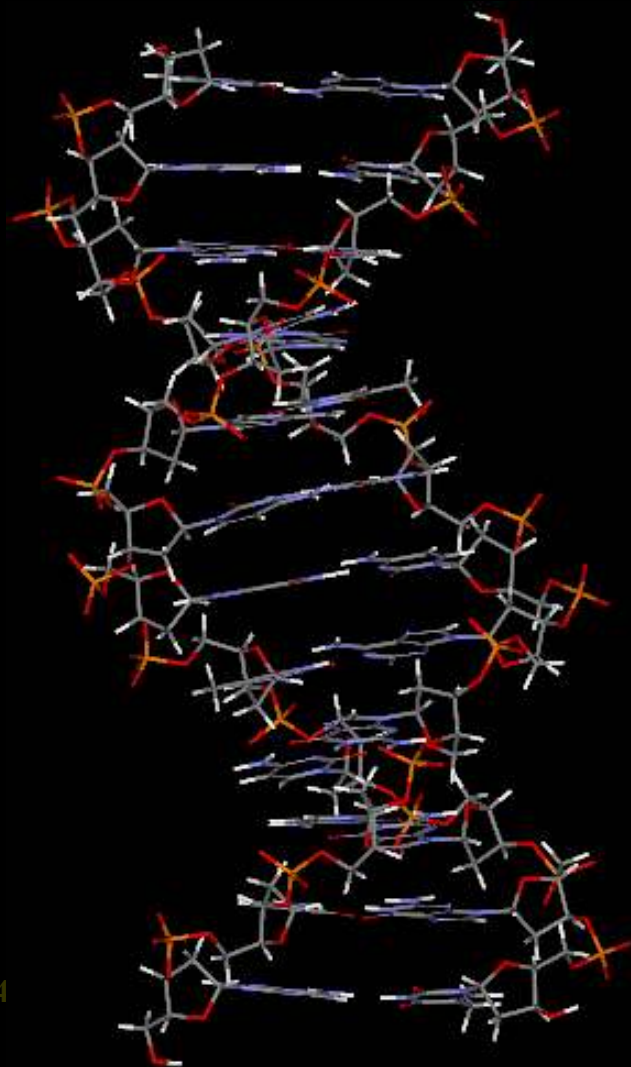
4th - 6th Oct 20 07

DAG07, JNU, Delhi

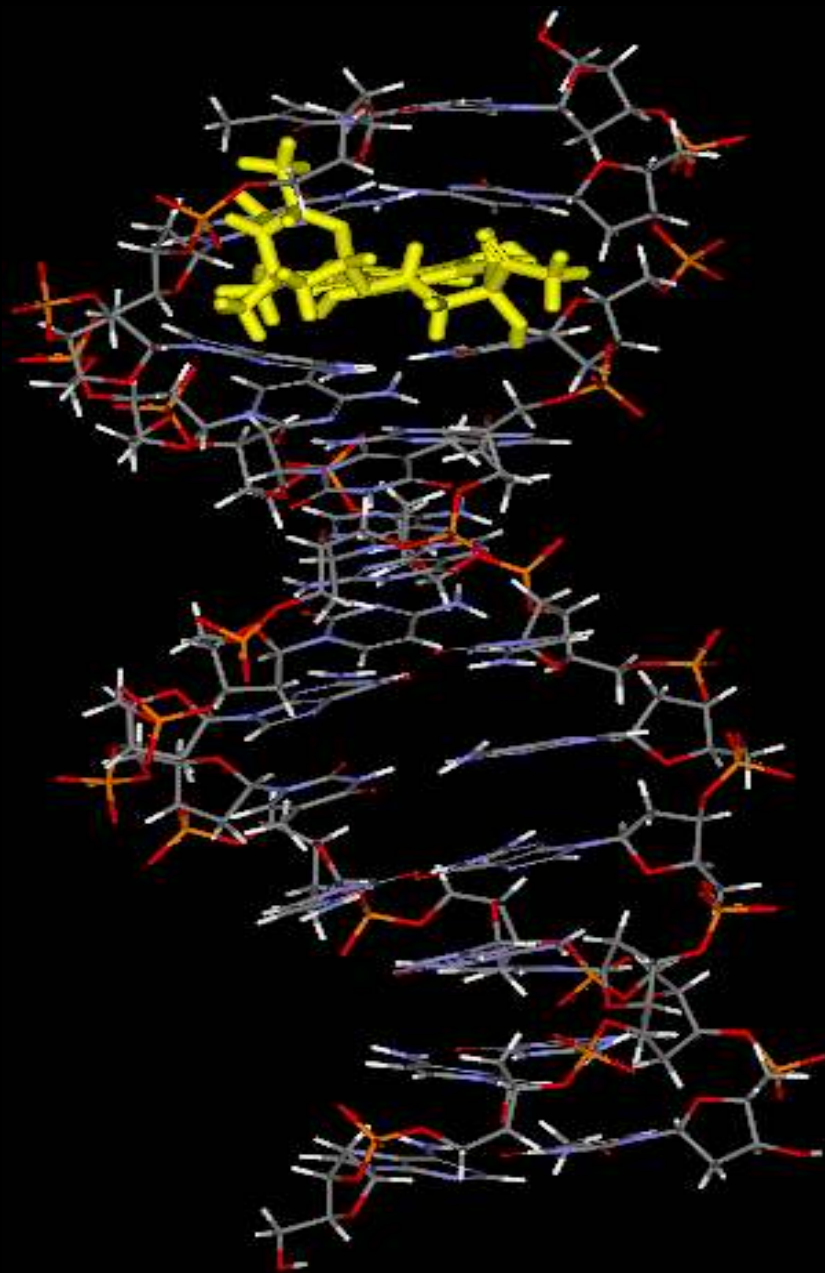
COMPUTATIONAL CHEMISTRY AND
DRUG DESIGNING

8

Drug and DNA before intercalation

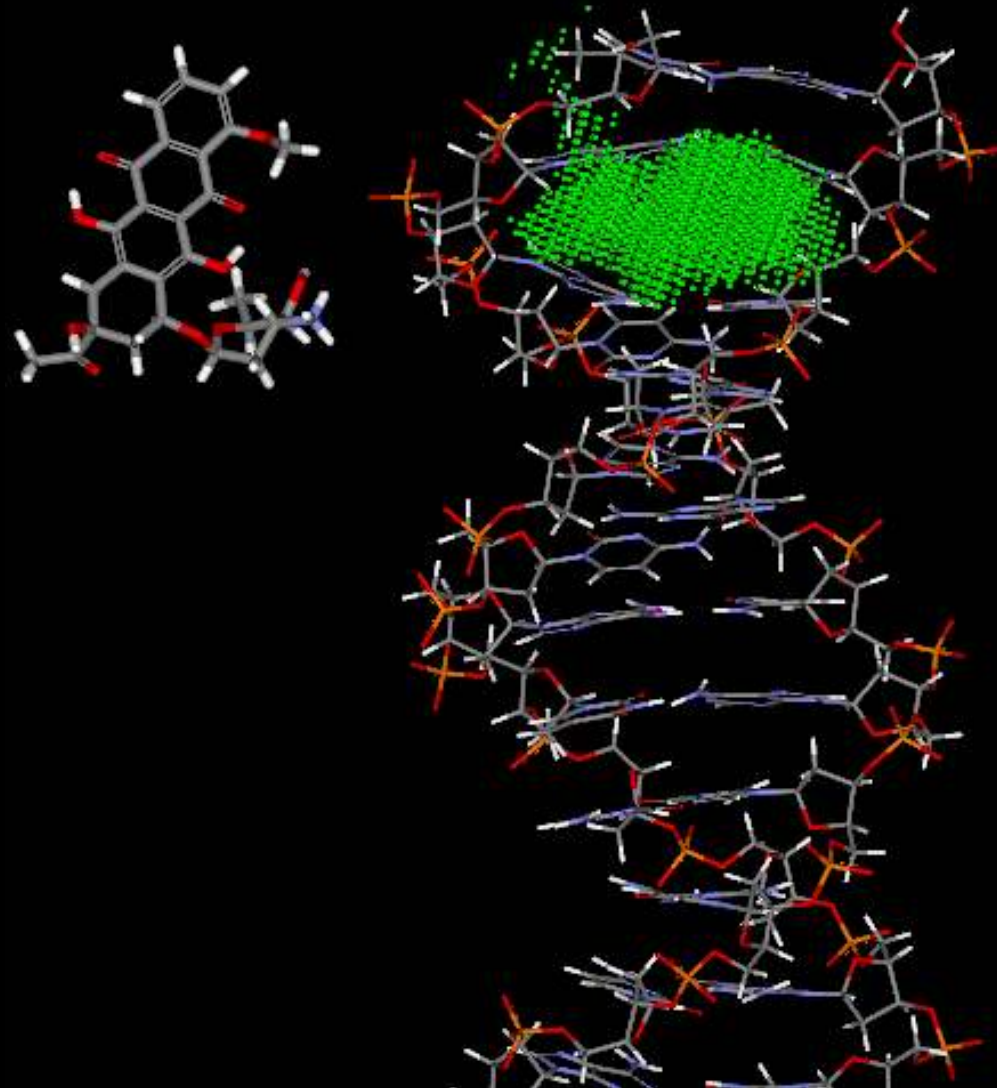


Drug- DNA interaction after minimization



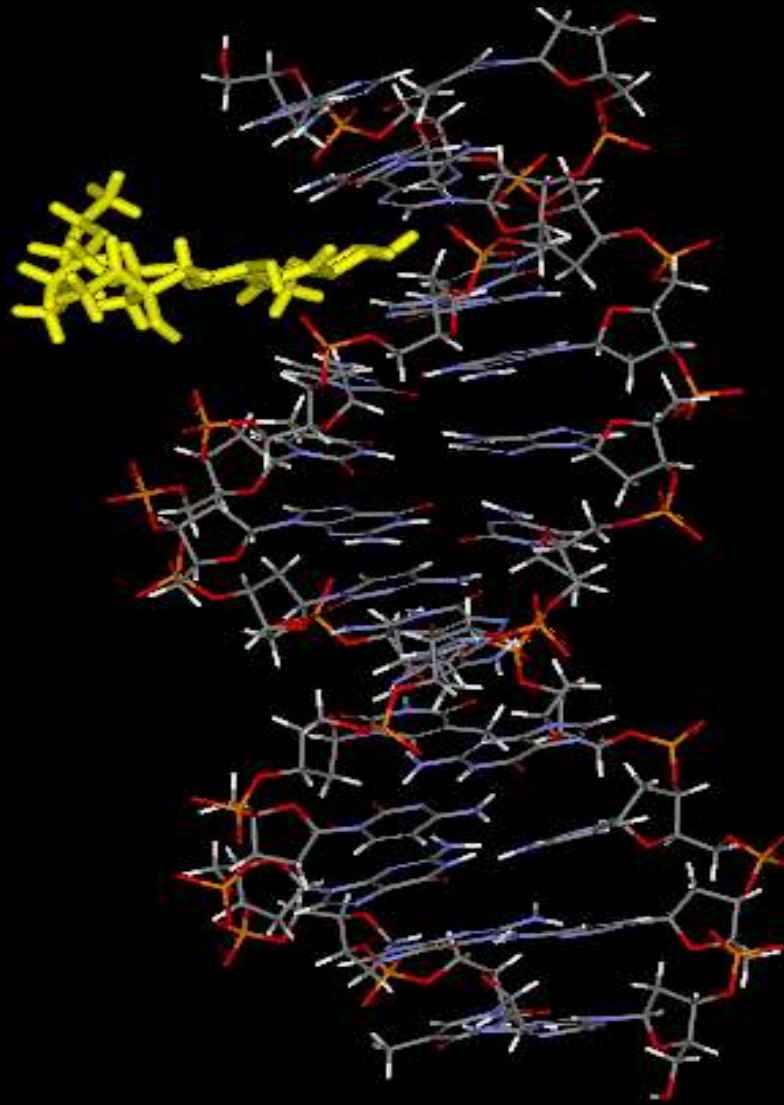
4th - 6th Oct 20 07

Binding site on DNA with respect to Drug



4th - 6th Oct 20 07

Drug after Docking



4th - 6th Oct 20 07