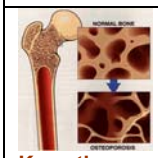
RESEARCH ACTIVITIES

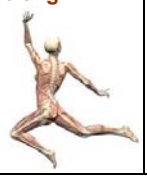
- **Some Significant Research contributions of our group in the area of Medicinal chemistry and Green Chemistry**

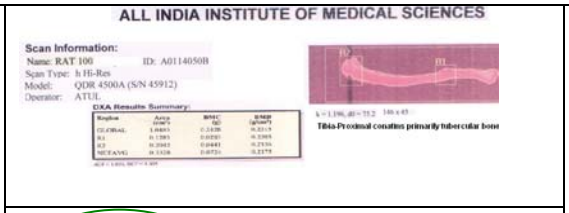
Medicinal chemistry

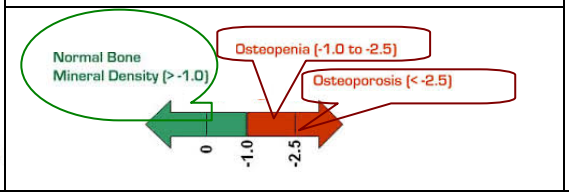
- We have Design and synthesize a **novel chemical Entities CDRI-99/373** (**CENTHANK**) **An Anti-osteoporosis drug candidate and is currently in Phase–I Clinical Trials.**
  CENTHANK is a **First in Class Drug** with RANKL modulating activity.
  CSIR-CDRI Web Page displaying all New drug developed by CDRI http://www.cdriindia.org/newdrugs.htm



Keep the Skeleton Strong



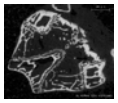




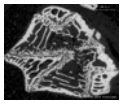
Synthesis: CENTHANK CDRI-99/373 : One-pot synthetic methodology

MICRO-CT Analysis of femur head after 6 month treatment of CENTHANK-CDRI-99/373

Sham+Veh



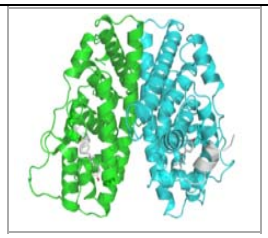
OVx+Veh



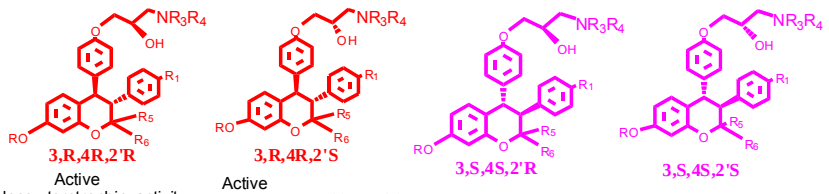
OVx+Centhank

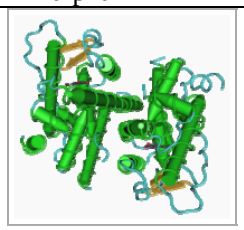
For details : Web Link: http://www.cdriindia.org/cdr99373.htm (CSIR-CDRI Web Page displaying details of CDRI compound 99/373 developed by CDRI).

- We have designed and synthesized Selective estrogen receptor modulators, which have been showing very promising (CDRI- S-001-80 and S-004-1001) and **anticancer breast activity**. Patents have been granted.. **The compound have three chiral centers so we have synthesized all the eight possible enantiomers and** evaluated them for anti-fertility and anti cancer activity. Some of the compounds showing better anti-fertility profile than Centchroman. Further studies are in progress
  Web Link: http://www.cdriindia.org/Site/anualreport.pdf

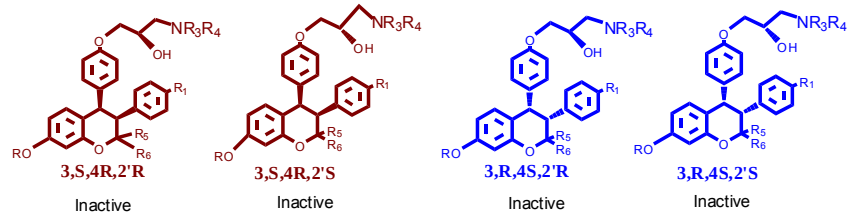


ER-alpha

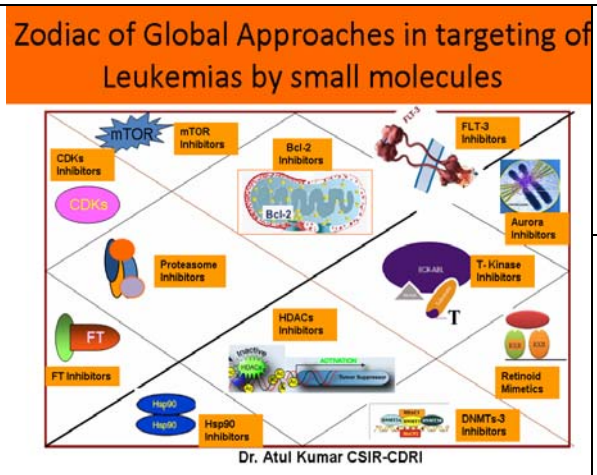


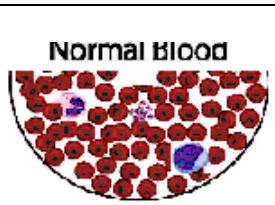


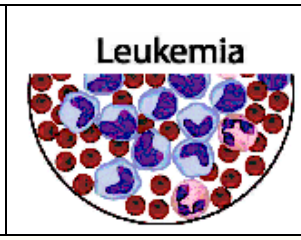
ER-beta

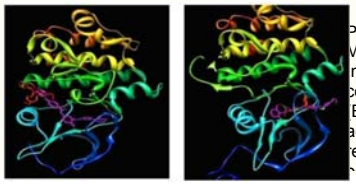


- We have design and synthesized a new chemical entity (CDRI-S-009-1235) exhibiting promising **anti-leukemia activity**. Patent has been filed. Further research work is in progress



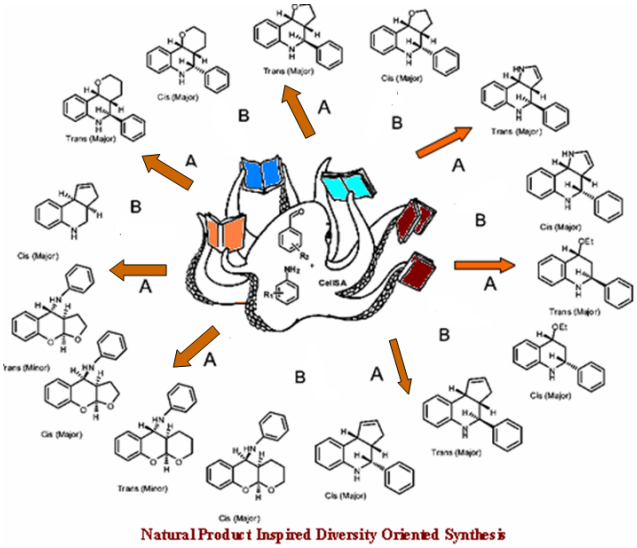




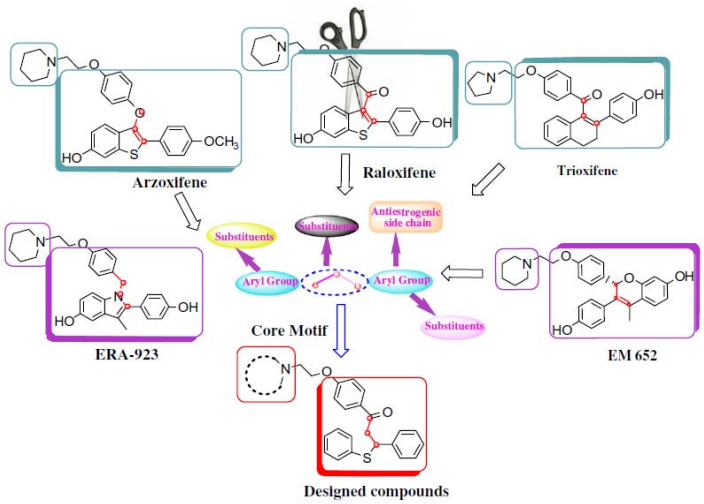


Proposed binding mode of MND (RED), Imatinib (A. matinib- Pink, ABL – inactive confirmation) and Dasatinib B. Dasatinib - Pink, ABL active confi) with surrounding esidues in the ATP-binding

- **Natural product inspired Diversity oriented synthesis using green chemistry protocol: Natural Product Inspired Diversity Oriented Synthesis of Tetrahydroquinoline Scaffolds as Antitubercular agent,**



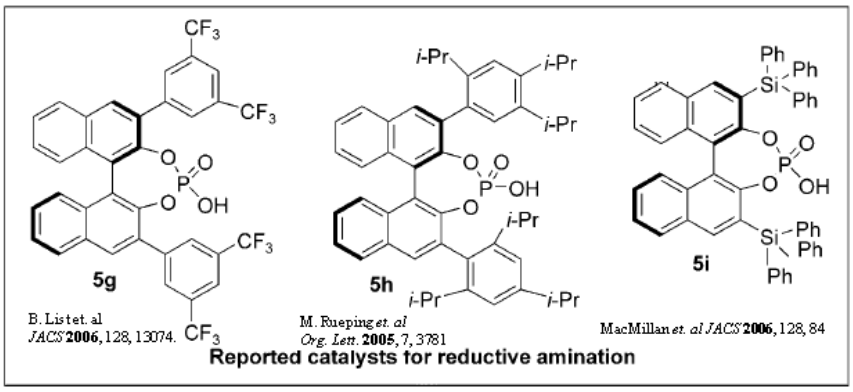
- **Design and synthesis of 1,3-biarylsulfanyl derivatives as new anti-breast cancer agents**

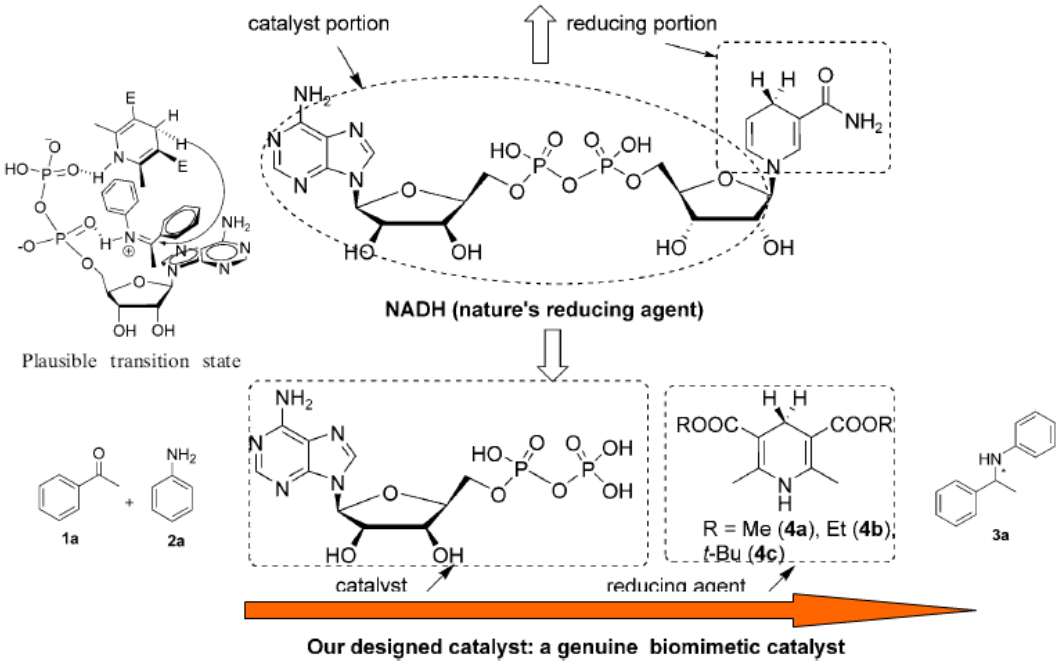


GREEN CHEMISTRY lab

- Development **of First Single Nucleotide organic reaction: "Single Nucleotide Catalysed Biomimetic reductive Amination reaction** *Advanced Synthesis and Catalyst 2010,* **352** (13): 2227–2232, doi:10.1002/adsc.201000178,http://onlinelibrary.wiley.com/doi/10.1002/adsc.201000178/abstract

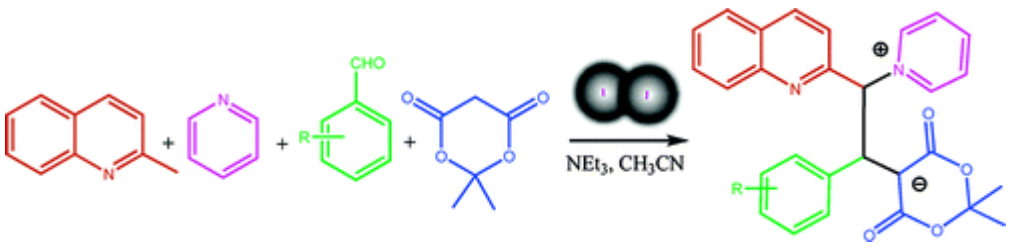
We have successfully developed a single nucleotide (adenosine 5′-diphosphate)-catalyzed enantioselective direct reductive amination of aldehydes and ketones using a Hantzsch ester as reducing agent. The process is a simple, efficient and a real mimic of the NADH reduction approach for the synthesis of structurally diverse amines. This reaction is the first report demonstrating the ability of a single nucleotide as catalyst and one of the most genuine biomimetic reactions of organic chemistry.



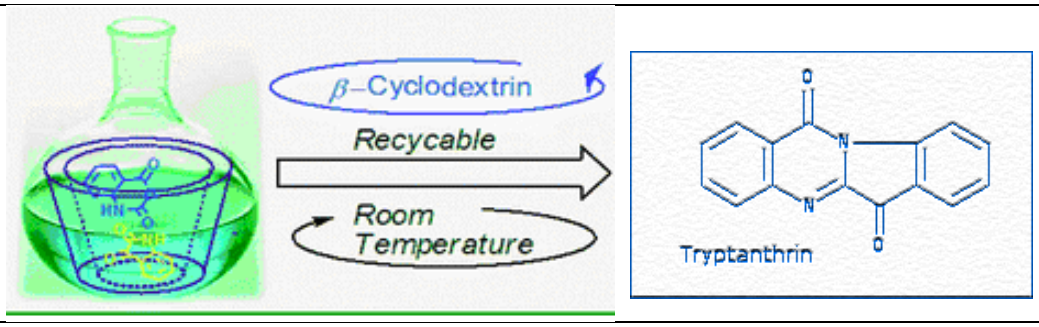


- **Synthesis of New Class of Alkyl Azarene Pyridinium Zwitterions via Iodine Mediated sp^3 C–H Bond Activation** **Organic Letters, 2011**, *13* (24), pp 6366–6369

An efficient and conceptually different approach toward C–H bond activation by using iodine mediated sp^3 C–H functionalization for the synthesis of alkyl azaarene pyridinium zwitterions is described. This work has the interesting distinction of being the first synthesis of a new class of alkyl azaarene pyridinium zwitterion via transition-metal-free sp^3 C–H bond activation of an alkyl azaarene.

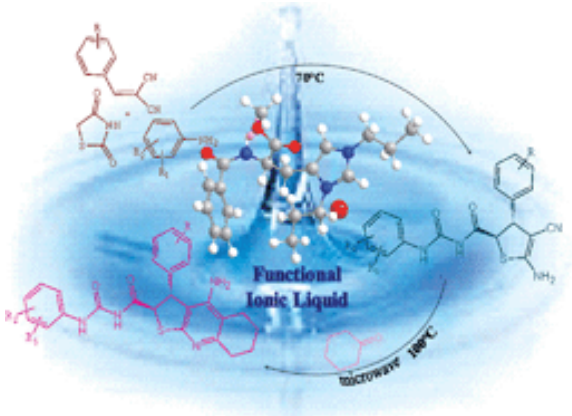


- Developed green synthesis of bioactive Natural product **Tryptanthrin**. β-Cyclodextrin catalysed synthesis of tryptanthrin in water **Green Chemistry** 2011, **13**, 51



- Introduced a **new strategy for organic synthesis** utilizing Functional Ionic Liquid and **named as Functional Ionic Liquid Mediated Synthesis (FILMS) Green Chemistry** 2011, 13, 2459, DOI: 10.109/c1gc15410a

Natural amino acid-based functional ionic liquid [Bz-His(n-propyl)$_2$-OMe$^+$Br$^-$] promoted diastereoselective synthesis of dihydrothiophenes is described. Further this functional ionic liquid was efficiently utilized to form tacrine derivatives from dihydrothiophenes using microwave irradiation. The functional ionic liquid exhibits organocatalytic as well as medium engineering capability, thus we named this synthetic protocol functional ionic liquid mediated synthesis (FILMS).



- **Cascade [4+1] annulation Green Chemistry via greener nitrogen ylide in water: Synthesis of bicyclic and tricyclic fused dihydrofuran *Green Chemistry.* 2012 14, 3269-3272. DOI: 10.1039/C2GC36276G**

A novel imidazolium ylide activated [4 + 1] annulation approach is described for the diastereoselective synthesis of bicyclic and tricyclic fused dihydrofurans in water. This cascade annulation presumably proceeds *via* a Michael reaction triggered zwitterion enolate followed by concomitant intramolecular cyclization. The methodology has distinction of being the first report on imidazolium ylide mediated [4 + 1] annulation in water as a unified greener approach involving an *in situ* base regeneration system and an alternative to pyridine ylide.