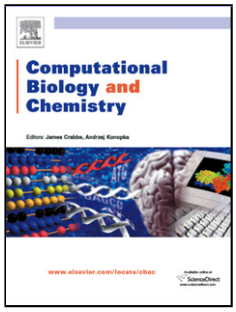

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Computer-aided Drug Design and Virtual Screening of Targeted Combinatorial Libraries of Mixed-Ligand Transition Metal Complexes of 2-butanone thiosemicarbazone

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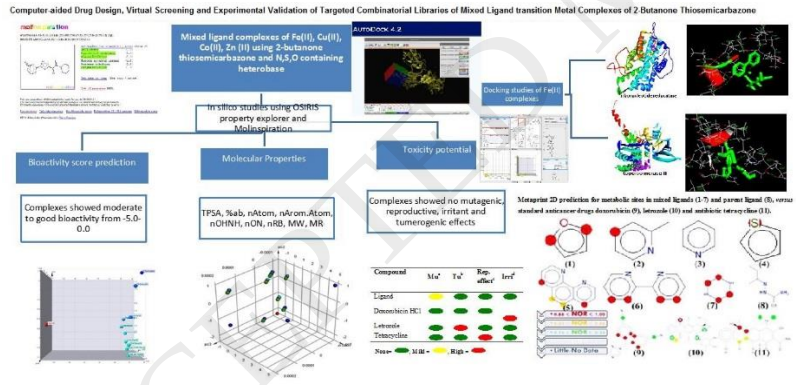
GRAPHICAL ABSTRACT



HIGHLIGHTS

- The study deals with in silico evaluation of mixed ligand transition metal complexes
- Drug likeliness, toxicity and bioactivity score were predicted by different softwares
- Multivariate data were analysed by Principal Component Analysis in OSIRIS software
- Docking results yielded best scores with bipyridine and 1,10 phenanthroline
- Drug likeliness and oral bioavailability were tested on several known filters
- All complexes exhibited promising medicinal properties with no toxic effects