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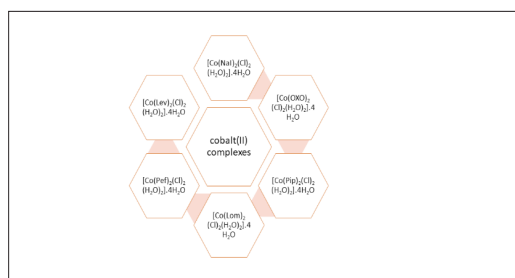
## CHEMISTRY IN DRUG DISCOVERY &amp; DESIGNING

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## Synthesis, spectroscopic, thermal, biological, morphological and molecular docking studies of the different quinolone drugs and their cobalt(II) complexes

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New six cobalt(II) complexes 1-6 with four generation of quinolone drugs (nalidixic acid (Nal), oxolonic acid (Oxo), pipemidic acid (Pip), lomefloxacin (Lom), pefloxacin mesylate (Pef) and levofloxacin (Lev)) have been synthesized in methanol medium and the general formula was designed as  $[\text{Co}(\text{L})_2(\text{Cl})_2(\text{H}_2\text{O})_2] \cdot 4\text{H}_2\text{O}$  (L=Nal (1), Oxo (2), Pip (3), Lom (4), Pef (5) and Lev (6)). The Co(III) complexes were identified using micro-analytical, FT-IR spectroscopy, conductance data, effective magnetic moments, electronic UV-vis spectra and thermal analyses. The six quinolone drug chelates acts as uni-dentate via nitrogen atom of pyridone/piperazyl moiety. Electronic spectroscopic tools are in agreement with an octahedral geometrical structure. Thermal degradation analyses TG-DTG in nitrogen gas environmental are discussed the number and location of water molecules. The thermal decomposition process is completely in 3-4 steps, that the first step is responsible to loss of four uncoordinated water molecules. The stabilities of Co(II) complex 1-6 were studied dependent on activations of energy E, entropy  $\Delta S$ , enthalpy  $\Delta H$  and Gibbs free energy  $\Delta G$  that have been estimated using Coats-Redfern and Horowitz-Metzger non-isothermal methods. Molecular docking was used to predict the binding between some quinolone drugs with the receptor of breast cancer mutant 3hb5-oxidoreductase. The structural view of the synthesized cobalt(II)-quinolone nanoparticles has been documented with the help of transmission electron microscope (TEM). The synthesized metal chelates have been screened *in vitro* antibacterial activity against bacteria, Gram-positive (*Staphylococcus aureus*) and Gram-negative (*Escherichia coli*) and two strains of fungus (*Aspergillus flavus* and *Candida albicans*). The cobalt(II) chelates were shown to possess more antibacterial activity than the free chelates.



## Recent Publications

1. Refat M S, Al-Saif F A (2015) Synthesis, spectral, thermal, and antimicrobial studies of transition metal complexes of atorvastatin calcium as a lipid-lowering agent. *Journal of Thermal Analysis and Calorimetry*; 120(1): 863-878.
2. Foziah A Al-Saif (2014) Spectroscopic Elucidation, Conductivity and Activation Thermodynamic Parameters Studies on Pt(IV), Au(III) and Pd(II) 1,5-Dimethyl-2-phenyl-4-[(thiophen-2-ylmethylene)-amino]-1,2-dihydro-pyrazol-3-one Schiff Base Complexes. *Int. J. Electrochem. Sci.*; 9: 398-417.

## References

1. A Debnath, N K Mogha, T D Masram (2015) Metal Complex of the First-Generation Quinolone Antimicrobial Drug Nalidixic Acid: Structure and Its Biological Evaluation. *Appl. Biochem. Biotechnology*; 175(5): 2659.
2. M N Patel, D S Gandhi, P A Parmar (2012) Effect of substituent of terpyridines on the DNA-interaction of polypyridyl ruthenium(II). *Inorg. Chem. Commun.*; 15: 248.
3. J L Hobman, L C Crossman (2014) Bacterial antimicrobial metal ion resistance. *J. Med. Microbiology*; 64: 471-497.

## Biography

Foziah Ali Al-Saif is an Associate Professor of Inorganic Chemistry, Department of Chemistry, Faculty of Science, Princess Nourah bint Abdulrahman University, Kingdom of Saudi Arabia. She has variety of experience after years of work in research, teaching and administration of university. Her research area is metal-drug interaction. She has participated in three projects funded by Princess Nourah bint Abdulrahman University and presently she is working as Principle Investigator of research group named Chemistry of Metal-drug Complexes and its Biological Applications.

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