

**Design, synthesis, and physicochemical properties of  
 ternary Nd(III) systems with flavonoids.  
 Relevance to human health.**

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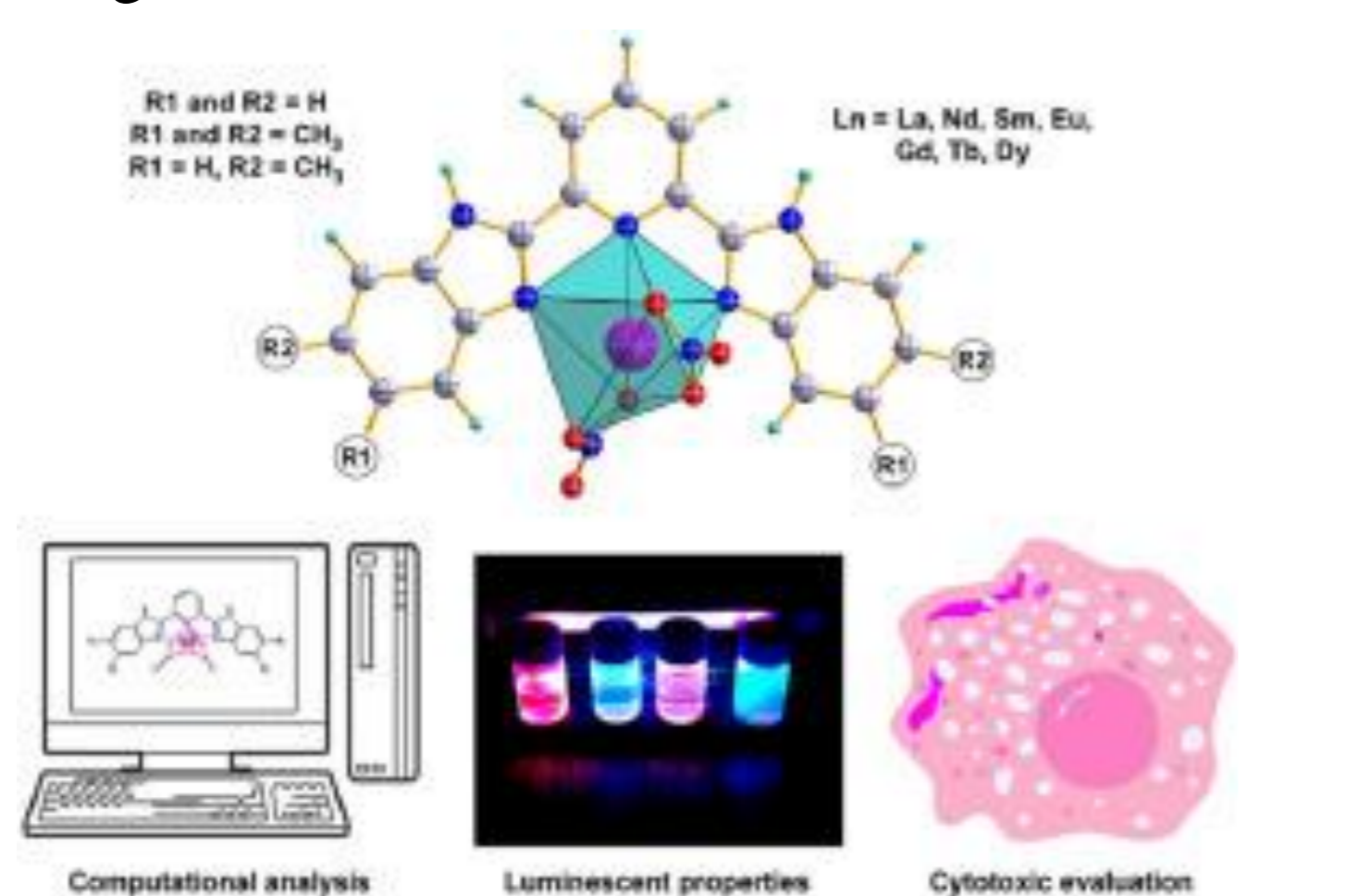
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**Abstract:** Our Lab initiated an exploration into combinations of Nd(III) systems and flavonoids to discover viable therapeutic profiles and improved pharmacological functions compared to the original substances. The selection of the lanthanide metal Neodymium is based on its magnetic and cytotoxic properties. Chrysin was chosen as the flavonoid to use due to its anti-inflammatory, anti-tumor, and antiviral properties. Strictly adhering to literature protocols, a ternary Neodymium-Chrysin-Phenanthroline complex was successfully synthesized, isolated, and its physicochemical properties were evaluated.

• Introduction

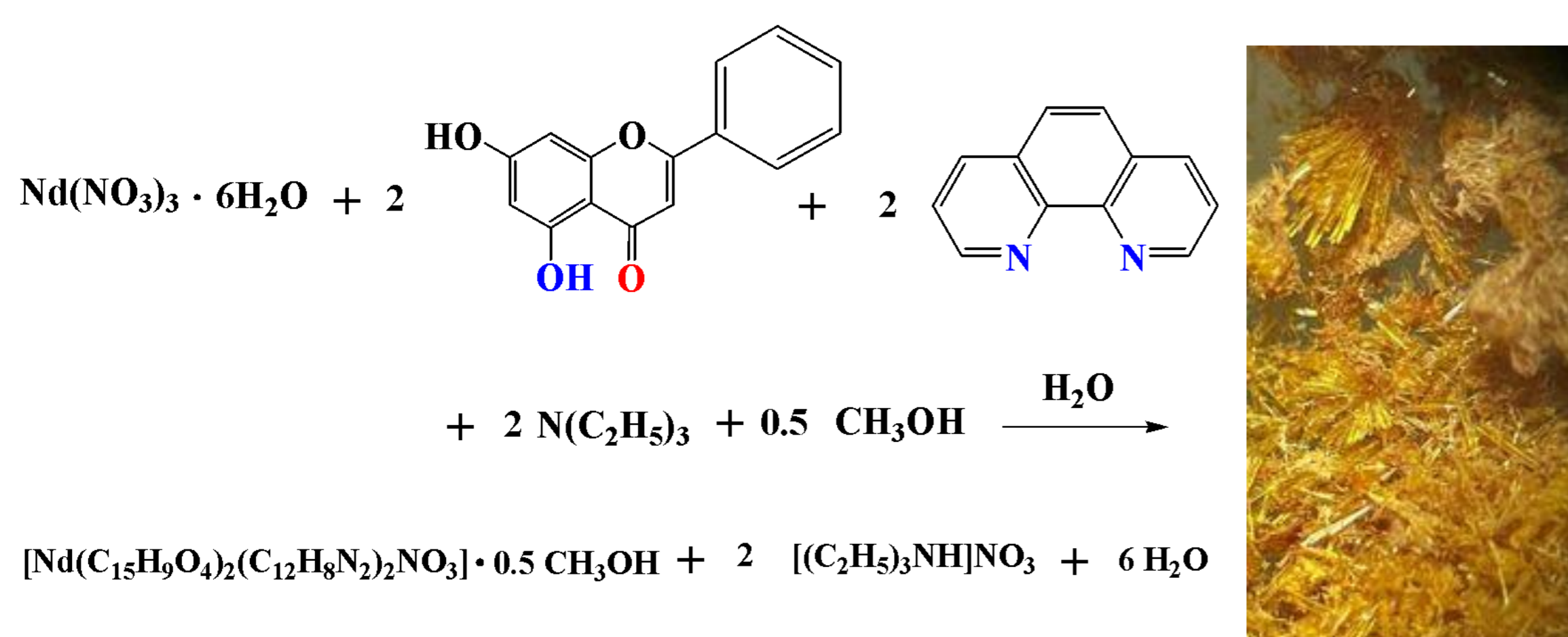
Metallodrugs are medicinal compounds composed of at least one metallic element and have been demonstrated to possess anti-cancer, antibacterial, and antiviral properties. Therapeutic and diagnostic applications have already been established for introducing metallic ions into the human biological system.<sup>1</sup> Metallodrugs that incorporate flavonoids tend to exhibit increased biological activity when compared to the naked ligands. Nowadays, the synthesis of coordination complexes based on lanthanides(III) (**Fig. 1**) is constantly gaining ground due to their particular photophysical properties. In the biological sciences, applications of lanthanide(III) complexes are limitless and include optical contrast agents for fluorescence microscopy, luminescent probes for immunoassays, and optical sensors to quantify biomolecules, amongst others. Lanthanide(III) ions, such as europium(III), terbium(III), neodymium(III), and ytterbium(III) are extensively utilized for these purposes due to their unique spectroscopic properties, including large Stokes shifts, narrow emission bands, and long luminescence lifetimes.<sup>2,3</sup>



**Fig. 1:** Lanthanide(III)-organic ligand complex

• Materials and method

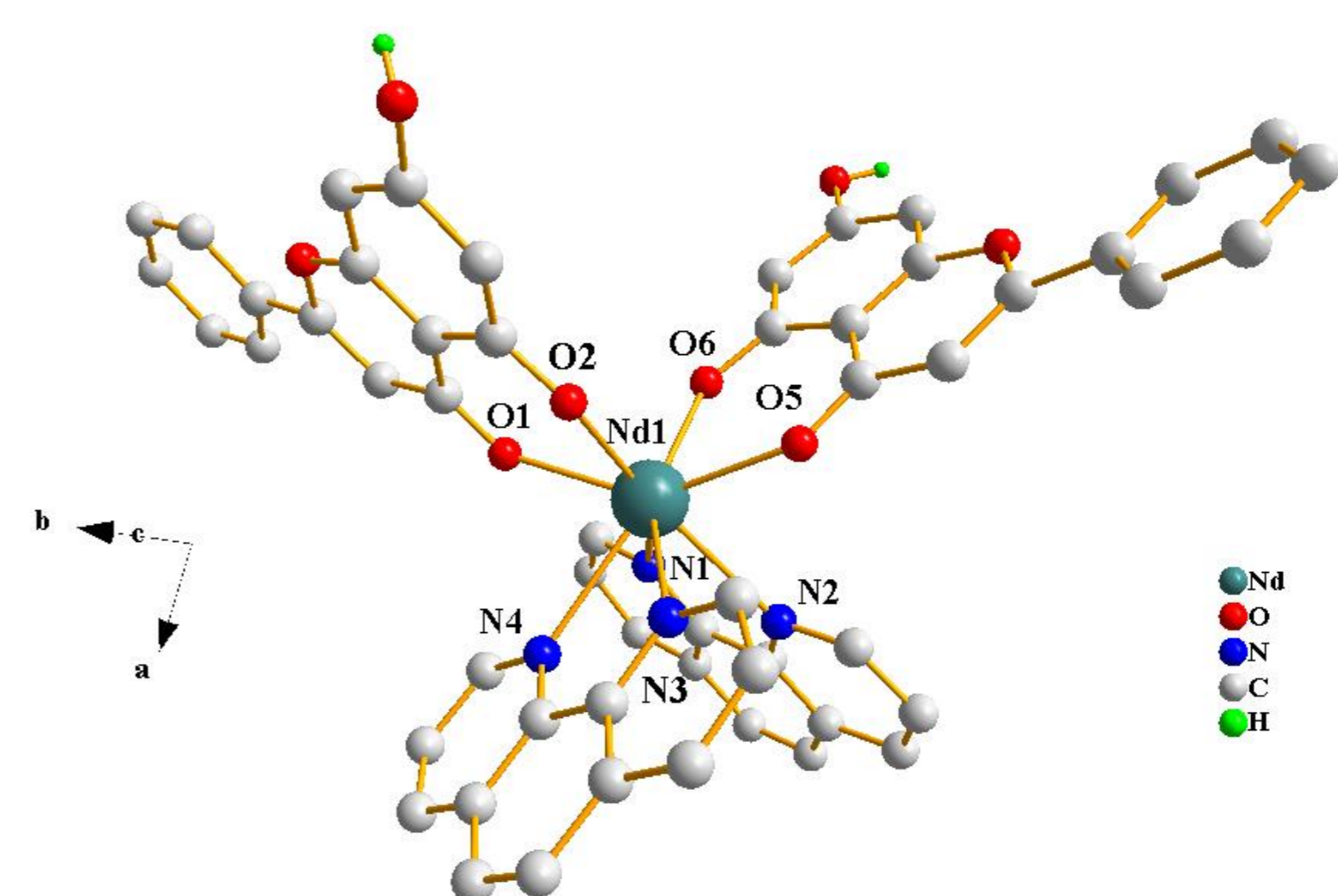
**Synthesis of Nd-Chr-Phen**



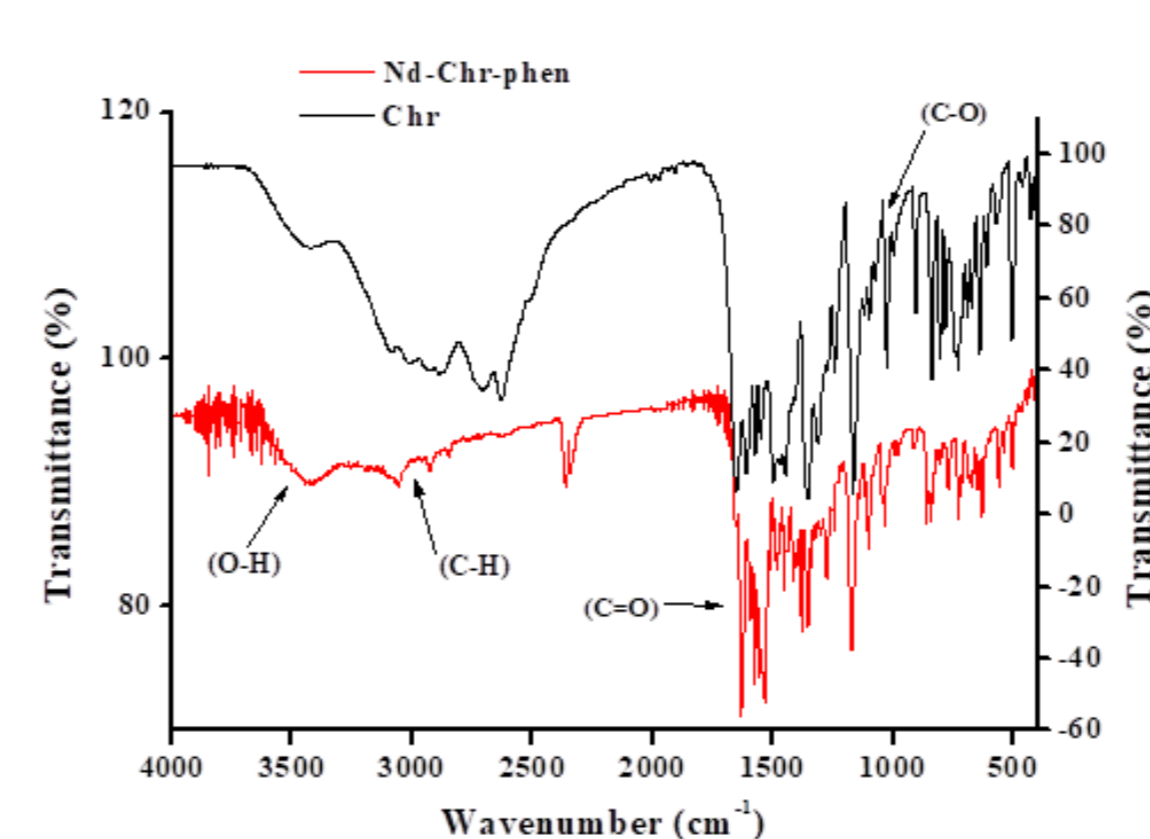
• Results and discussion

The desired ternary complex assembly is formed by two chrysin and two phenanthroline molecules binding a neodymium ion. The yield of the reaction is 38%. Fourier transform infrared spectroscopy (FT-IR) shows a shift at 1640 cm<sup>-1</sup>, which indicates weakening of the C=O bond of the Chrysin molecule. Furthermore, the intensity of both luminescence diagrams decreases from the initial ligand to the metal organic complex. This phenomenon can be attributed to the Chelation Enhancement of Quenching effect (CHEQ). Moreover, the Nd-Chr-Phen complex assembly shows enhanced UV-Vis behavior, compared to the parent ligands.

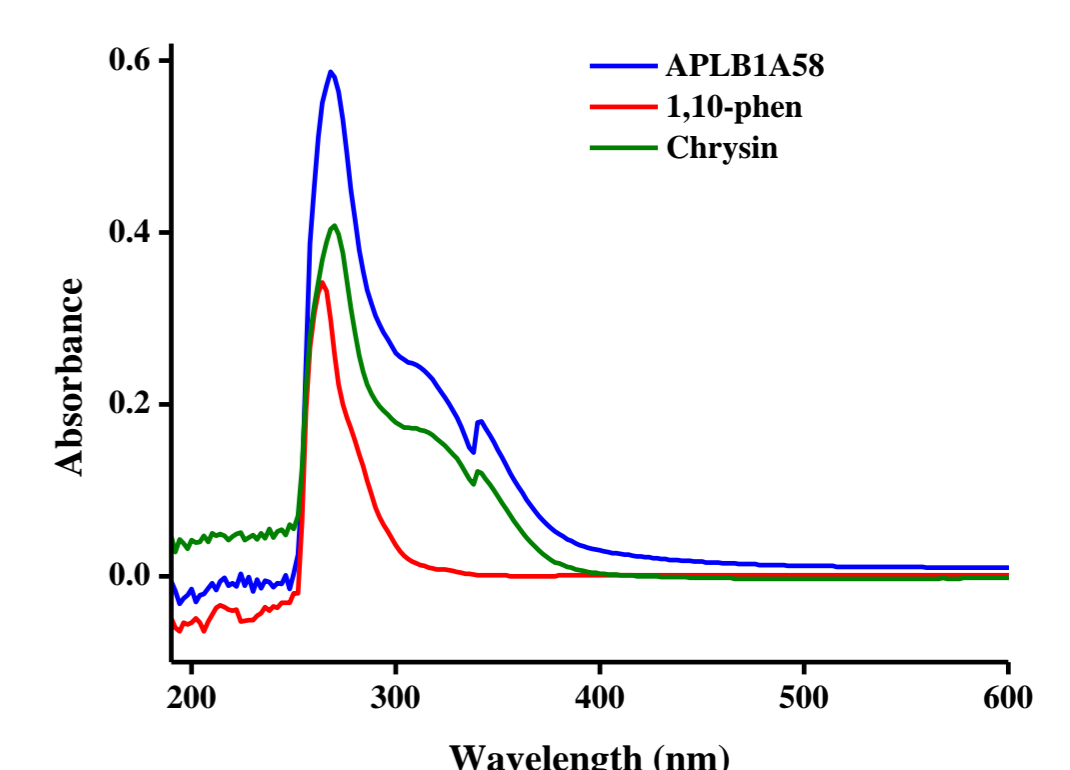
**X-ray crystal structure**



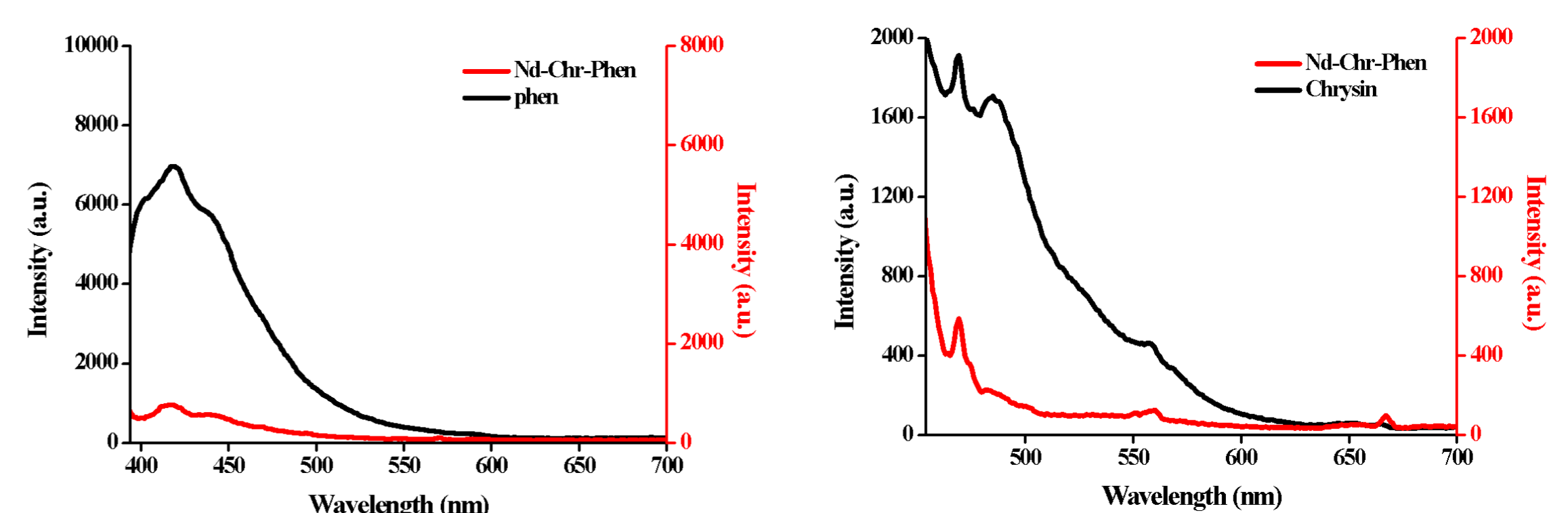
**Comparison of FT-IR spectra**



**Comparison of UV-Visible spectra**



**Luminescence spectrum compared to Chr and phen**



• Conclusions

- ❖ The ternary system of Nd-Chr-phen has been designed and synthesized in a molar ratio of 1:1:1 in methanol.
- ❖ Two Chrysin and two phenanthroline moieties have been bound to Nd(III) metal center.
- ❖ The complex is soluble in DMSO at a concentration of 10<sup>-4</sup>, thus providing a solvent medium of the study of its properties.
- ❖ The electronic and vibrational properties of the Nd-Chr-phen assembly are consistent with the X-ray crystal structure, suggesting unique features for further exploitation.

• Literature

1. S. Cotton, J. Harrowfield, Encyclopedia of Inorganic and Bioinorganic Chemistry 1<sup>st</sup> Edition (2012) John Wiley & Sons.
2. X. Wang, H. Chang, J. Xie, B. Zhao, B. Liu, S. Xu, W. Pei, N. Ren, L. Huang, W. Huang, Coord. Chem. Rev. 273-274 (2014) 201-212.
3. J.C.G. Bünzli, J. Lumin., 170 (3) (2016) 866-878.