Synthesis, structural characterization and biological activity evaluation of novel Cu(II) complexes with 3-(trifluoromethyl)-phenylthiourea derivatives

Oral Presentation
Date of presentation
Time of presentation

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Copper complexes with organic ligands are widely studied due to their potential bioactive properties. Among them, Cu(II) complexes with 1,3-disubstituted thiourea derivatives were designed and studied by our research group[1-4]. We are looking for compounds that can be used as anticancer chemotherapeutics as well as antimicrobial drugs. In this presentation, the synthesis and structure-activity relationship studies of novel complexes with 3-(trifluoromethyl)phenylthiourea moiety will be presented.

The novel compounds were obtained by the reaction of copper(II) chloride with thiourea derivatives. The synthesis path was proposed (see Fig. 1). To determine the molecular structure of complexes **Cu1-Cu5** in their powder form the following measurements were used: ATR-IR, UV-Vis, EPR and synchrotron-based techniques (XAFS), as well as theoretical calculations performed at the DFT level.

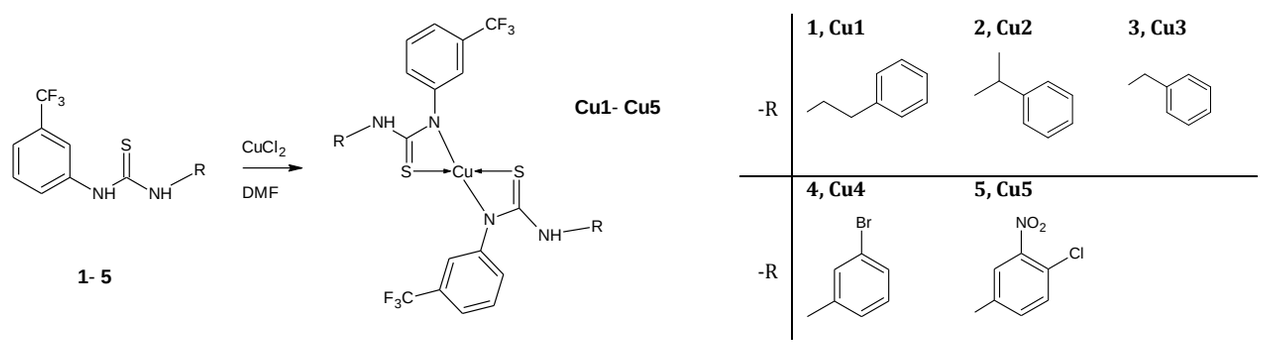

Fig. 1 Synthesis path of studied complexes.

The XAFS measurements were performed at Cu K edge at Elettra synchrotron. For all complexes two S and two N atoms were identified in the first coordination sphere (see Fig. 1). The second copper cation was identified in the second coordination sphere for **Cu4** and **Cu5**. The EXAFS data allows us to build structural models that were refined by DFT calculations and verified by XANES analysis. Moreover, the biological activity of novel compounds has been evaluated.

Acknowledgements: This project was partially supported by PLGrid infrastructure.

References

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