Synthesis, physicochemical characterisation, and bio-activity of new pyrazole with transitional metals

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Abstract This research aims to synthesise new pyrazole-based complex compounds with selected transition metals using metal ions in correlation with ligand-metal structures, structurally characterise them, and check for their bio-activity on phytopathogenic fungus. The design of the newly synthesised compounds is to be confirmed based on physicochemical characterisations. Some prepared compounds will be evaluated for their in vitro activity on different fungi.

1 Problem definition, background, research methodology and our progress

The issue of protection of fruit trees, flowers, and olives in Montenegro against selected fungal pathogens has gained the particular attention of the Montenegrin scientific and research public.

Therefore, finding new chemical compounds that can treat many fungal infections has become a challenge to our society. Our research focuses on already recognisable pyrazoles and their various derivatives as antifungal agents [1,2,3,4,5].

Four different pyrazole ligands: (3-(hydroxyphenyl)-1Hpyrazole-5 carboxylic acid (L1); 3-3nitrophenyl-1-Hpyrazole (L2); 3-4-(chlorophenyl-1Hpyrazole) (L3); 4-Bromo-3-nitro-1Hpyrazole-5-carboxylic acid (L4) and available salts of the following metals Zn, Cu, Co, Ni, Fe, Mn, Cd, and Hg will be used as bases on our synthesis.

The novelty of our research of the previous database is that the mentioned pyrazole derivatives will be used for the first time in synthetic procedures.

These initial activities of synthesis of potential active substances of fungicides precede the structural characterisation and determination of the biological effectiveness of the synthesized chemical compounds.

Therefore, our workflow is organised into three parts: synthesis, physicochemical characterisation, and bio-activity study. Thus far, all the materials have been prepared for the first stage of our work – synthesis.

A part of the physicochemical characterisations of FTIR, UV-VIS, conductivity, and magnetic measurements will take place in the Laboratory of the Faculty of Metallurgy Technology, University of Montenegro, while the XRD and XRF characterisations will be carried out in the Laboratory Institute for Medicines and Medical Devices of Montenegro and Faculty of Chemistry and Chemical Engineering, University of Maribor.
A Sanitary Laboratory at the Faculty of Biotechnology, University of Montenegro, is available to determine the fungicidal effect of newly synthesised complex compounds.

2 Future works and Conclusions

The aforementioned first stage of our work should be finalised during September, with the possible addition of new syntheses in the later stages. The second phase, physicochemical characterisation, is planned to be completed until June 2023 and will consist of characterisations via XRD, XRF, IR, UV/VIS, CHNO/S, and other instrumental and analytical analyses, while the final phase should be concluded in September 2023.

The current knowledge on the fungicide effects on the overall ecosystem is fragmentary but still sufficient to point to the need to conduct overall biological research with the aim of registering new chemicals and potential active fungicide substances.

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