

Editorial

It is a pleasure to announce the last issue of this 2022 year. Opens this issue a brief review showing recent phytochemical studies involving *T. orientalis* and *T. occidentalis*, as well as 40 constituents isolated from these species. Plants from Thuja genus in traditional medicine are used to treat cough, skin allergies, and asthma, and in Brazil are also used in the ornamentation of urban areas. Different parts of these plants displayed insecticidal, antitumor, and antioxidant activities, e.g., the essential oil of the leaves are constituted by monoterpenes and sesquiterpenes, with the flavonoids being the main substances found that have relevant biological activities. Computational chemistry is routinely used for the qualitative and quantitative evaluation of substances in almost every field of chemistry as in drug discovery/design activities. These tools were applied to study the effect of several substituents in the 1-(2-hydroxyethyl)-2-methyl-5-nitroimidazole, a powerful antibacterial and antiparasitic used alongside other drugs against *Helicobacter pylori* infection and on the interactions with the target nitroreductase RdxA protein. In the sequence, X-ray single-crystal crystallography was used to solve the structure of a coordination polymer having the formula $[\text{Cd}(\text{BTC})(\text{H}_2\text{O})_2]_n$. Furthermore, the complex's stability and overall reactivity were theoretically examined. The electron distribution in the complex's HOMO is concentrated in a small area, with no electrons distributed over the metallic center. Consequently, the electrons in the complex's LUMO were dispersed equally. The ADMET studies showed that the examined complex has important biological uses, notably for the treatment of microbial diseases. Closes this issue a theoretical study about the effects of addition of thiophene, bridged phenyl-thiophene, thia-tetra-azacyclopenta-naphthalene, benzo-bis-thiadiazole and pyrido(3,4-b)pyrazine to 9-(4-octyloxyphenyl)-2,7-divinylcabazole on the internal reorganization energies, electronic affinity and ionization potential. These compounds were characterized by their charge exchange potentials, donor-acceptor, which can be applied in energy conversion devices such as photovoltaic cells.

The editorial team of Eclética Química would like to gently tanks the enormous effort of all authors, reviewers and collaborators that made possible to conclude this year with highly promise results.

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