

MS35-P11 | STRUCTURAL AND COMPUTATIONAL STUDY OF QUINOLINE-BASED CHALCOGENSEMICARBAZONES

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Chalcogensemicarbazones are condensation products between semicarbazide and its sulphur and selenium isosters with carbonyl compounds with a broad spectrum of biological activities [1-3]. In this work the X-ray structural investigation of library of six chalcogensemicarbazones has been complemented with computational study of their global and local reactive properties, within the framework of density functional theory (DFT). Among other information, DFT calculations helped us to locate the most reactive sites of studied molecules and to identify their sensitivity towards the oxidation. Investigated compounds have been also checked for their optoelectronic properties, due to the fact that they share certain structural similarity with molecules that have exhibited potentially important properties for the area of organic electronics. Pharmacokinetic properties have been assessed by the analysis of frequently employed drug likeness parameters.

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- [1] Calcaterra, V., et al., Phenolic thio- and selenosemicarbazones as multi-target drugs. *Eur J Med Chem*, 2015. 94: p. 63-72.
- [2] Todorovic, T.R., et al., (Chalcogen)semicarbazones and their cobalt complexes differentiate HL-60 myeloid leukaemia cells and are cytotoxic towards tumor cell lines. *MedChemComm*, 2017. 8(1): p. 103-111.
- [3] Filipović, N.R., et al., Pro-apoptotic and pro-differentiation induction by 8-quinolinecarboxaldehyde selenosemicarbazone and its Co(III) complex in human cancer cell lines. *MedChemComm*, 2016. 7(8): p. 1604-1616.