



संशोधन केन्द्र  
CSIR  
भारत का नवाचार इंजन  
The Innovation Engine of India

Indian Journal of Chemistry  
Vol. 64, January 2025, pp. 43-53  
DOI: 10.56042/ijc.v64i1.14056

निःशुल्क  
NISP  
सीएसआईआर-जिज्ञेष्णु

# Synthesis, spectral characterization, DFT calculations and investigation of anticancer properties of carbothioamide and metal ( $\text{Fe}^{\text{II}}$ and $\text{Cr}^{\text{III}}$ ) complexes

Elif Güney<sup>a</sup>, Koray Sayin\*<sup>a</sup> & Hayreddin Gezegen<sup>b</sup>

<sup>a</sup>Sivas Cumhuriyet University, Faculty of Science, Department of Chemistry 58140 Sivas, Türkiye

<sup>b</sup>Sivas Cumhuriyet University, Faculty of Health Science, Department of Nutrition and Dietetics 58140 Sivas, Türkiye  
E-mail: krysayin@gmail.com, ksayin@cumhuriyet.edu.tr

Received 29 September 2024; accepted (revised) 27 December 2024

Schiff base and its metal complexes have a broad application in areas such as medicine, pharmacy, cosmetics, agriculture, plastic industry, dyestuff production, etc. Recently, the anticancer activities of these compounds have been investigated, and it is a matter of curiosity how the effectiveness changes with complexation. 2-(1-(2-Hydroxyphenyl) ethylidene) hydrazine-1-carbothioamide (HL) and its metal ( $\text{Fe}^{\text{II}}$  and  $\text{Cr}^{\text{III}}$ ) complexes have been synthesized and investigated computationally and experimentally. In the calculations, B3LYP-D3/6-31+G(d) for HL and B3LYP-D3/6-31+G(d)(LANL2DZ) for metal complexes have been used. Anticancer properties of these complexes have been investigated against three different cell lines which are breast cancer (MCF-7), colorectal cancer (HT-29) and gastric cancer (SNU-16). XTT test has been used in the cell viability assays. It is found that the studied compounds are active against breast cancer and  $\text{Fe}(\text{II})$  complex has shown the best activity. Structural properties of compound have been examined computationally and experimentally. Electronic properties of the studied compounds (for HL) have been investigated by Hirshfeld surface analyses and MEP maps. Anticancer properties of studied compounds have been investigated by cell viability assays. It is found that synthesized compounds are only active against breast cell line, MCF-7. The best compound is found as  $[\text{FeL}_2]$  due to the fact that its  $\text{IC}_{50}$  has been calculated as 1.62  $\mu\text{M}$ .

**Keywords:** Carbothioamide, Metal complex, DFT, Hirshfeld surface analysis, Anticancer properties