HALIDE SUBSTITUTED BIS(DIBENZOYLMETHANOATO) VANADIUM(IV) COMPLEXES AS POTENTIAL ANTICANCER AGENTS

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Aside the well-known noble metal-based compounds like cisplatin or NAMI-A, Lewis acidic metal-based complexes gained recent interest as anti-cancer drugs. Vanadium is a promising candidate due to its rich redox chemistry, flexible coordination modes and biocompatibility.[1] Over the past decades, several vanadium compounds (bearing e.g. *O*-/*N*-donor ligands) have been developed and tested against various cancer cell lines with low micromolar activity.[2-4]

A derivative of vanadyl acetylacetonate, vanadyl bis(1,3-diphenyl-1,3-propanedionato) (Figure 1, **1**) has raised our interest due to its superior activity towards multiple cancer cell lines like MCF7 (breast) and MIA PaCa-2 (pancreatic) when compared to cisplatin.[3, 5] Previous studies have already shown possible modes of action like interaction with DNA and proteins or formation of reactive oxygen species (ROS). However, the speciation of the compound *in-vitro* and influences of electronic effects have not been studied until now.

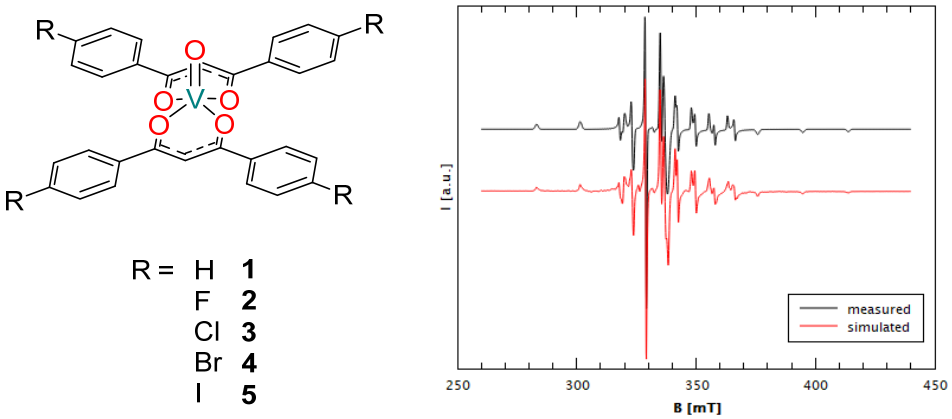

Figure 1: (left) Structure of the investigated compounds and (right) an EPR spectrum and its simulation of the lead compound 1 (1 mM in THF, 153 K, X-band EPR).

A series of halide substituted derivatives of the lead compound **1** (Figure 1) are synthesised and characterised. The influence of the substituents on the electronic structure is assessed using EPR, IR and cyclic voltammetry and their biological activity is tested against multiple cell lines. A library of EPR parameters of adducts with fragments of selected amino acids is presented for future identification using whole-cell EPR.

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[3] Sergi, B., *et al., ChemMedChem*, **2021**, *16*, 2402.

[4] Scalese, G., *et al., J. Inorg. Biochem.*, **2017**, *175*, 154.

[5] Mohamadi, M., *et al., RSC Advances*, **2015**, *5*, 101063.