Electronic Supplementary Information

New Journal of Chemistry

Synthesis, structural and thermal characterization, reactivity assessment by DFT computations and biological evaluation of a hydrazone derivative and its coordination compounds with Co(III), Ni(II), Cu(II) and Zn(II)

B. Barta Holló,[a] J. Magyari,[a] S. Armaković,[b] G. A. Bogdanović,[c] M. V. Rodić,[a] S. J. Armaković,[a] J. Molnár,d G. Spengler[d], V. M. Leovac,[a] K. Mészáros Szécsényi[a]

[a]University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, 21000, Novi Sad, Serbia; [b]University of Novi Sad, Faculty of Sciences, Department of Physics, Trg Dositeja Obradovića 4, 21000, Novi Sad, Serbia; [c]"Vinča" Institute of Nuclear Sciences, Laboratory of Theoretical Physics and Condensed Matter Physics, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia; [d]University of Szeged, Faculty of Medicine, Department of Medical Microbiology and Immunobiology, Szeged, Hungary, H-6720 Szeged, Dóm tér 10

The influence of DMSO solvent to the geometries of proposed complexes has been also investigated through DFT calculations. In this work solvent effects are taken into account using a self-consistent reaction field method employing standard Poisson-Boltzmann solver [1-2], as implemented in Jaguar program. Figure S1 contains geometries of complexes **2** and **3** with the DMSO solvent effects used for the geometrical optimizations. Results concerning the complex **4**, the one based on the Zn atom, have not been included in the Figure S1 because geometrical optimizations with the solvent effects resulted in unreasonable geometries with lots of imaginary frequencies indicating molecular geometry that is not in ground state, most probably as a result of the unfavorable square-planar coordination geometry around the Zn atom. According to the geometries presented in Figure S1 can be seen that although solvent significantly rotated the pyridazine moiety around the N–N bond, the complexes preserved their square-planar coordination geometry in solution. These results are in the accordance with the observation that the colors of the resulting solutions are very similar to that of the crystals.

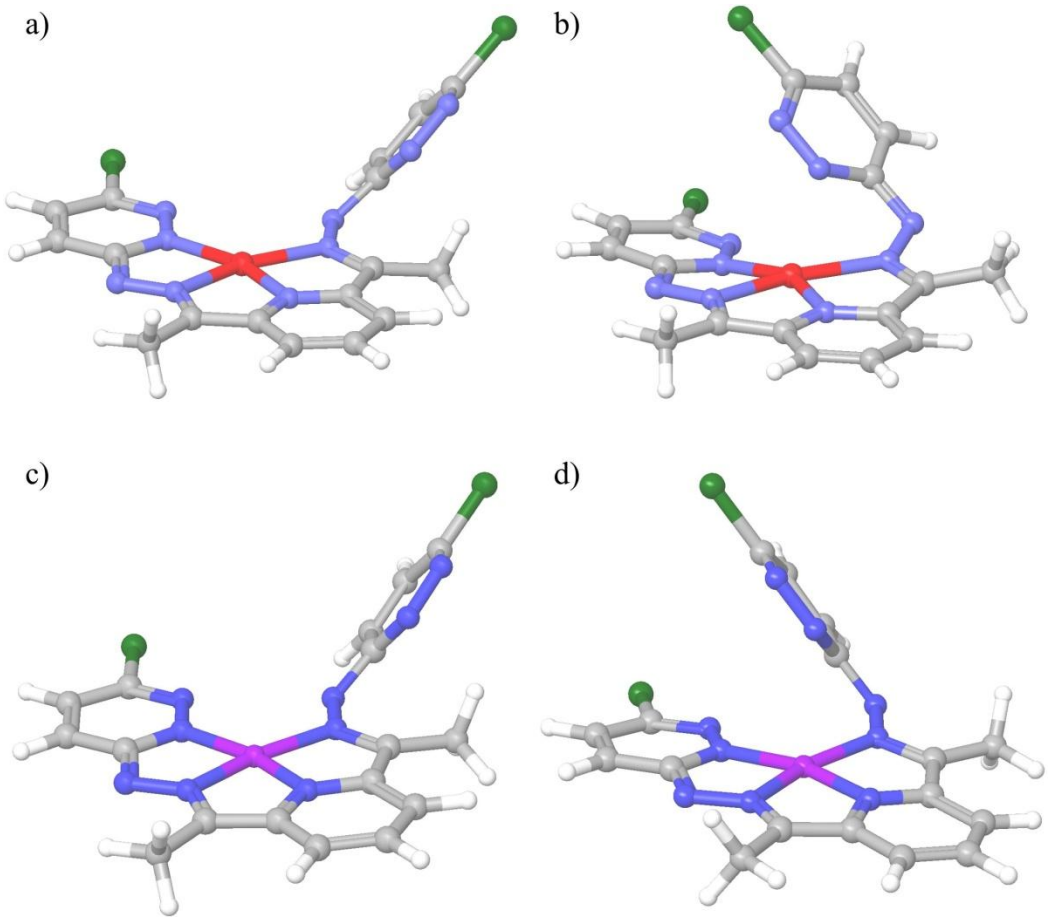

Figure S1. Molecular geometries of complexes **2** and **3**: a) and c) without solvent effects and b) and d) with solvent effects of DMSO

1. Tannor, D.J., B. Marten, R. Murphy, R.A. Friesner, D. Sitkoff, A. Nicholls, B. Honig, M. Ringnalda, and W.A. Goddard III, *Accurate first principles calculation of molecular charge distributions and solvation energies from ab initio quantum mechanics and continuum dielectric theory.* Journal of the American Chemical Society,Vol. **116**, (1994), 11875-11882.
2. Marten, B., K. Kim, C. Cortis, R.A. Friesner, R.B. Murphy, M.N. Ringnalda, D. Sitkoff, and B. Honig, *New model for calculation of solvation free energies: correction of self-consistent reaction field continuum dielectric theory for short-range hydrogen-bonding effects.* The Journal of Physical Chemistry,Vol. **100**, (1996), 11775-11788.