

Supervisor's assessment report of the Ph.D. thesis of RNDr. Martin Srnec

Thesis: *Catalytic and Electronic Properties of Redox-Active Metalloenzymes and Transition-Metal Complexes: Insight from Computational Chemistry*

Supervisor: Mgr. Lubomír Rulíšek, CSc.

Martin began to work in my group as a Ph.D. student on the title thesis in 2005. From the very first moment, I found him a highly motivated and hardworking person with a very strong background in physical, theoretical, and quantum chemistry. Martin has begun to develop this knowledge already during his university studies (finishing all exams with the mark "excellent") and by his previous work on the master thesis under the supervision of Prof. Rudolf Zahradník (in 2002-2005).

As can be inferred from the title of his thesis, Martin is involved in a challenging area of theoretical bioinorganic chemistry. The main focus was on three important enzymatic systems: superoxide dismutases, multi-copper oxidases and desaturases. His work mostly involved a highly demanding task of unravelling reaction mechanisms of these enzymes by means of computational chemistry. This task is non-trivial due to the fact that all of these systems contain open-shell metal ions with multiple spin states available, spin-orbit coupling and other effects that must be treated by fairly advanced methodology. Martin has carried out his job with a high level of diligence and expertise which is well documented by publishing the results in high-quality journals, such as *J. Am. Chem. Soc.*, *J. Phys. Chem. B*, or *Faraday Discuss.* Up to date, he has authored or co-authored fourteen research articles including one manuscript in the late stage of its preparation. Concomitantly, he has been, during his short stay at Stanford University with Prof. Edward I. Solomon, involved in the experimental (spectroscopic) studies of diiron Δ^9 desaturase, which again shows his deep interest in the studied problem. Martin has also been very active in presenting his work to an international scientific audience at several international conferences (either as a speaker or presenting a poster).

Last but not least, I should mention that since 2006 Martin has been responsible for teaching MSc. students at the Faculty of Sciences, Charles University (conducting exercises in *Chemical Structure*).

Without any doubt, I rate him in the top 10% of Ph.D. students I got acquainted with or supervised and it is my great pleasure to recommend his Ph.D. thesis as the material and RNDr. Martin Srnec as the candidate for obtaining Ph.D. degree.