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ODDĚLENÍ MOLEKULOVÉHO MODELOVÁNÍ
DEPARTMENT OF MOLECULAR MODELING

Filip Zimandl: Conformational Study of a Flexibility of the Fluorescence Dye QSY 21

Supervisor's Review of the bachelor thesis

Filip was working in my computational lab for three weeks. During his presence he shown a big interest about the studied topics and his knowledge and skills were greatly improved during his stay. He managed to handle the main quantum chemical packages like Turbomole and Gaussian as well in the end of his stay he was also capable to write the scripts and programs which make life computational chemist easier. The thesis is clearly written at the acceptable language level. My only criticism concerns the fact that although the all data had been calculated till January, the major part of the thesis was being written just in last few days before the deadline. At the end I must conclude that Filip's work is an integral part of the paper, which was recently accepted for publication in highly impacted journal *Phys. Chem. Chem. Phys.* I strongly recommend Filip Zimandl's work for the defense.

Prague , May 31st 2010



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