ZB-9, Wydział Chemii Uniwersytetu Wrocławskiego
Aleksander Filarowski

Prace opublikowane w 2011 zawierające podziękowania dla WCSS

1. **Jezierska-Mazzarello A.**, Panek J. J., Vuilleumier R., Koll A., Ciccotti G. Direct observation of the substitution effects on the hydrogen bridge dynamics in selected Schiff bases—A comparative molecular dynamics study. J. Chem. Phys., 2011, 134, 034308, 1-10. ImpF: **2.92**.
2. Panek J. J., Mazzarello R., Novič M., **Jezierska-Mazzarello A.** Impact of mercury(II) on proteinase K catalytic center: investigations via classical and Born-Oppenheimer molecular dynamics. Mol. Divers., 2011, 15, 215-226. ImpF: **3.72**.
3. Ryng S., Zimecki M., **Jezierska-Mazzarello A.**, Panek J. J., Mączyński M., Głowiak T., Sawka-Dobrowolska W., Koll A. A complex study of 5-amino-3-methyl-4-[2-(5-amino-1,3,4-oxadiazolo)]-isoxazole monohydrate: A new low-molecular-weight immune response modifier. J. Mol. Struct., 2011, 999, 60-67. ImpF: **1.59**.
4. Minovski N., **Jezierska-Mazzarello A.**, Vračko M., Šolmajer T. Investigation of 6-fluoroquinolones activity against *Mycobacterium tuberculosis* using theoretical molecular descriptors : a case study. Cent. Eur. J. Chem., 2011, 9, 855-866. ImpF: **0.99**.
5. Panek J. J., **Jezierska-Mazzarello A.**, Koll A., Dovbeshko G., Fesenko O. p-nitrobenzoic acid adsorption on nanostructured gold surfaces investigated by combined experimental and computational approaches. ChemPhysChem, 2011, 12, 2485-2495. ImpF: **3.33**.
6. **Majerz I.**, Olovsson I. Influence of proton transfer degree on the potential energy surface for two very short hydrogen bonds. Acta Chim. Slov., 2011, 58, 379-384. ImpF: **1.01**.
7. **Majerz I.**, Dziembowska T. Geometric aspects of aromaticity : interrelations between intramolecular hydrogen bonds, steric effects and π-electron delocalisation in nitroanilines. Eur. J. Org. Chem., 2011, 280-286. ImpF: **3.2**.
8. Tang S., **Majerz I.**, Caminati W. Sizing the Ubbelohde effect : the rotational spectrum of a *tert*-butylalcohol dimer. Phys. Chem., Chem. Phys., 2011, 13, 9137-9139. ImpF: **3.45**.
9. **Majerz I.** The influence of potassium cation on a strong OHO hydrogen bond. Org. Biomol. Chem., 2011, 9, 1466-1473. ImpF: **3.45**.
10. **Majerz I.**, Gutmann M. J. Mechanism of proton transfer in the strong OHN intermolecular hydrogen bond. RSC Advances, 2011, 1, 219-228. ImpF: 0.
11. Majewska P., **Rospenk M.**, Czarnik-Matusewicz B., **Sobczyk L**. Correlation between structure and shape of the polarized infrared absorption spectra of 4-chloro-2'-hydroxy-4'-alkoxyazobenzenes. J. Phys. Chem. B., 2011, 115, 2728-2736. ImpF: **3.6**.
12. Pawlukojć A., Sawka-Dobrowolska W., Bator G., **Sobczyk L.**, Grech E., Nowicka-Scheibe J. The structure and vibrational spectra of the 2,5-dimethylpyrazine (2,5-DMP) 1: 1 adduct with 2,5-dichloro-3,6-dihydroxy-p-benzoquinone (CLA). Chem. Phys., 2011, 380, 34-39. ImpF: **2.01**.
13. Kuduk-Jaworska J., Chojnacki H., **Jański** J. Non-empirical quantum chemical studies on electron transfer reactions in *trans*- and *cis*-diamminedichloroplatinum(II) complexes. J. Mol. Model., 2011, 17, 2411-2421. ImpF: **1.87**.
14. Grzegorzek J., **Filarowski A.**, Mielke Z. The photoinduced isomerization and its implication in the photo-dynamical processes in two simple Schiff bases isolated in solid argon. Phys. Chem., Chem. Phys., 2011, 13, 16596-16605. ImpF: **3.45**.

Sumaryczny ImpF = 34.69

Tematy badań realizowanych w 2011 roku:

Tematyka realizowanych badań obejmowała kierunki badań:
teoretyczna charakterystyka wiązań wodorowych,
potencjałów na przeniesienie protonu w mostku wodorowym,
przepisanie pasm w widmie podczerwonym,
wpływu efektów sterycznych i indukcyjnych na dynamikę mostków wodorowych,
wpływu metali na własności katalityczne proteinazy K,
układów posiadających aktywność biologiczną – analiza struktury elektronowej i parametrów geometrycznych,
oddziaływanie ligandów z powierzchnią metali.

Tematy badań na rok 2012 - 2013:

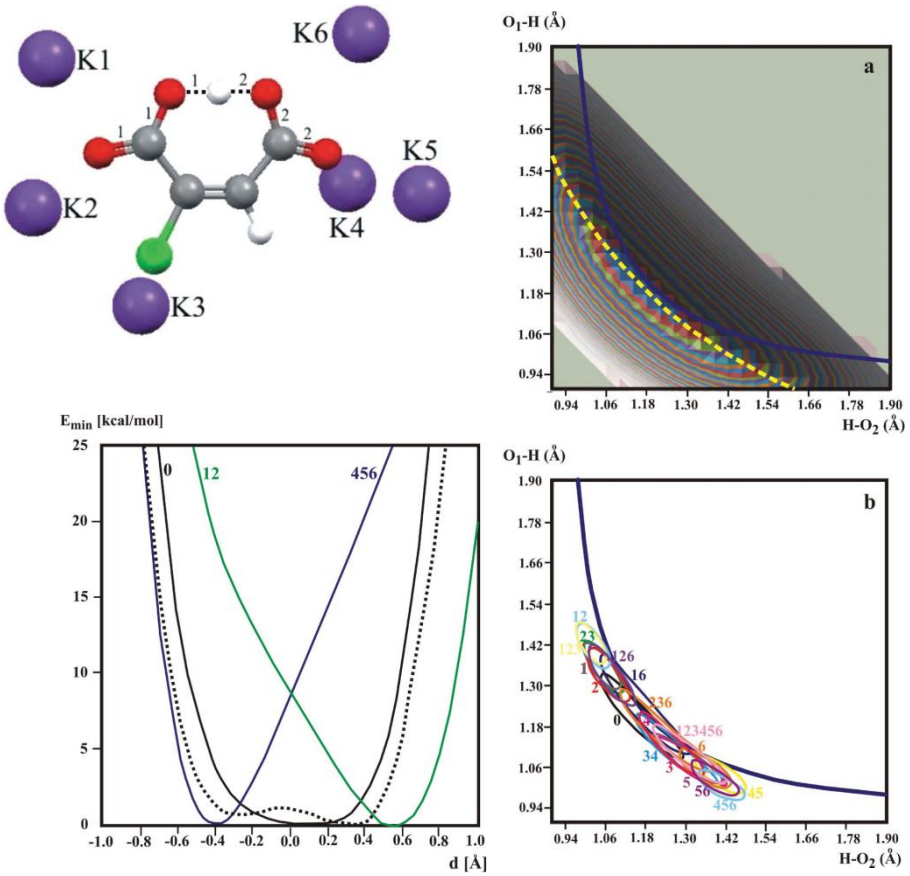
Badanie układów zawierających pierścienie skondensowane metodami dynamiki molekularnej.
Badania wpływu mutacji i obecności ligandów na ludzkie enzymy z grupy transferaz – badania metodami dynamiki molekularnej z polem siłowym klasycznym oraz *ab initio*.
Badanie potencjałów adiabatycznych i nie adiabatycznych na ruch protonu w mostku wodorowym.
Badanie wpływu podstawników na cykliczne wiązania wodorowe metodami ab initio, DFT i CPMD.
Obliczenie parametrów spektroskopowych stanów wzbudzonych metodą TD-DFT.
Badanie równowagi tautomerycznej z stanie podstawowym i wzbudzonym metodami chemii kwantowej.

Planowane współprace:

Profesor Marjana Novič, National Institute of Chemistry, Słowenia
Profesorowie M. Van der Auweraer i N. Boens, KUL, Leuven, Belgia.

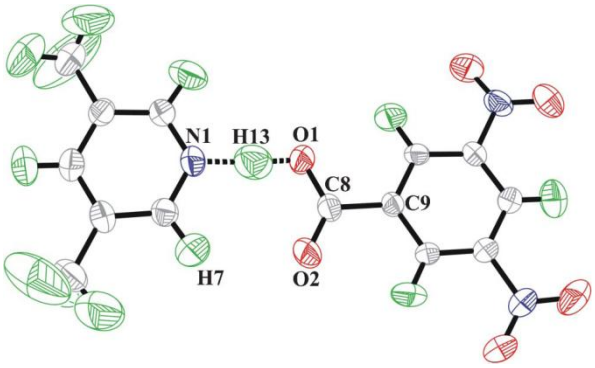
Wpływ kationu na silne wiązanie wodorowe.

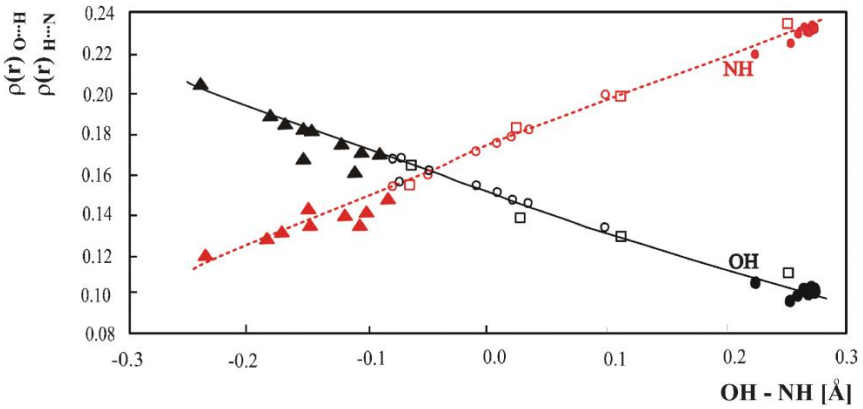
DFT

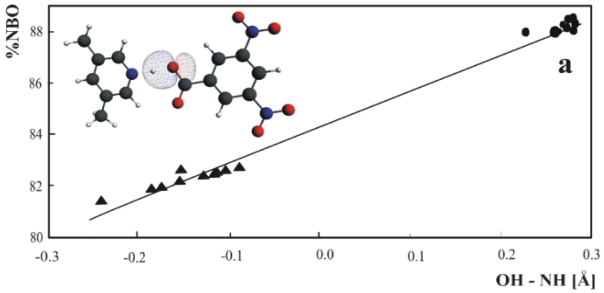


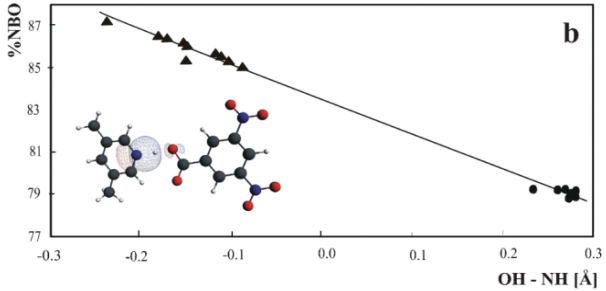
Majerz I. The influence of potassium cation on a strong OHO hydrogen bond. Org. Biomol. Chem., 2011, 9, 1466-1473.

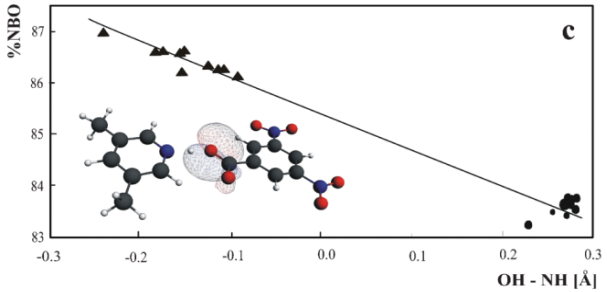
AIM

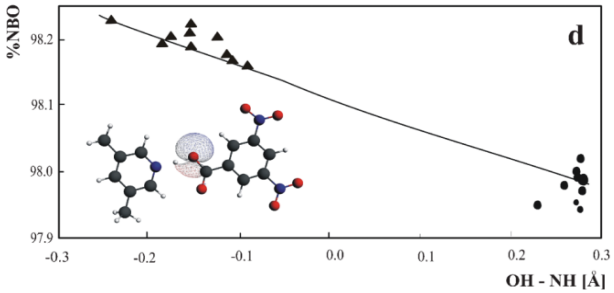








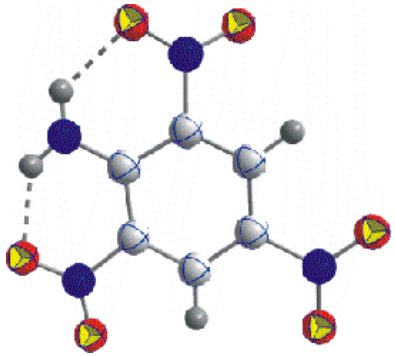


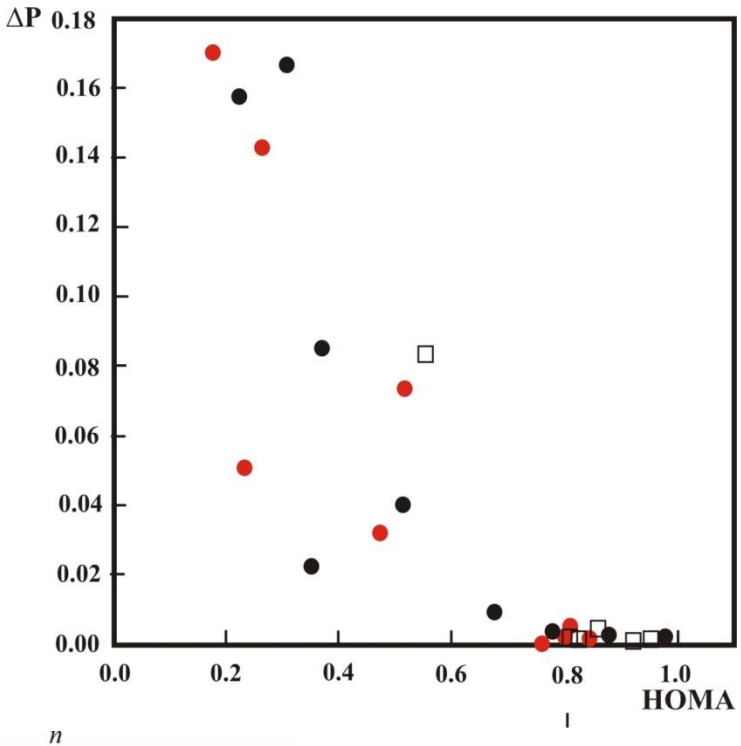


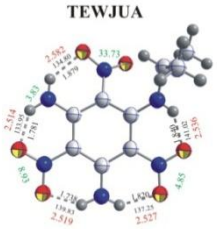
Majerz I., Gutmann M. J. Mechanism of proton transfer in the strong OHN intermolecular hydrogen bond. RSC Advances, 2011, 1, 219-228.

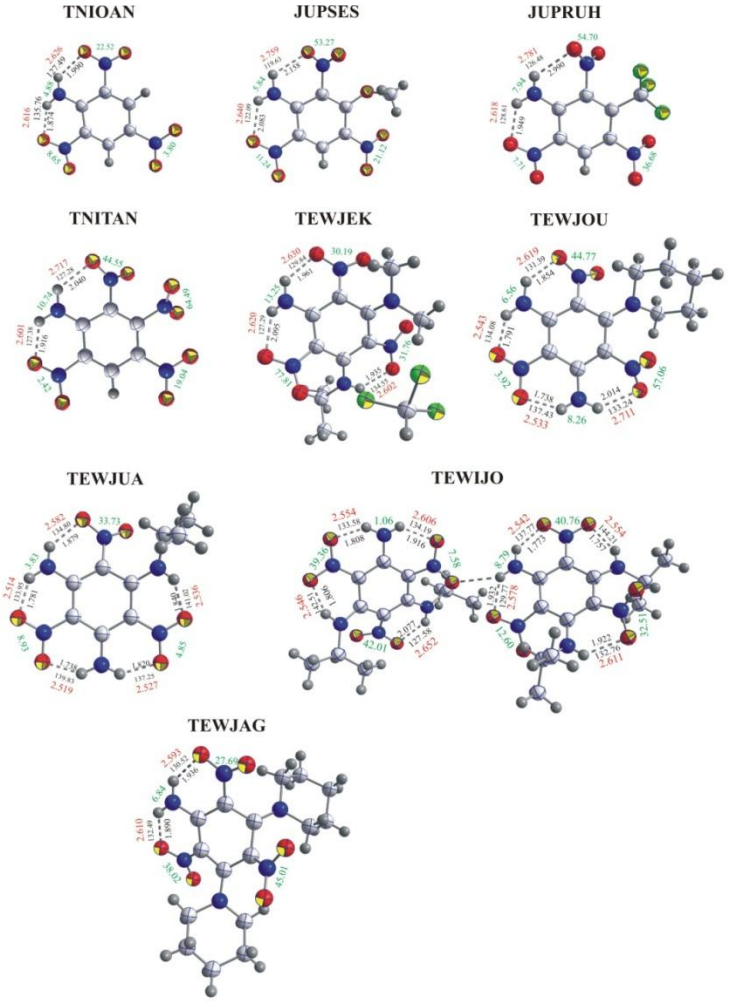
%NBO – stopień delokalizacji

DFT



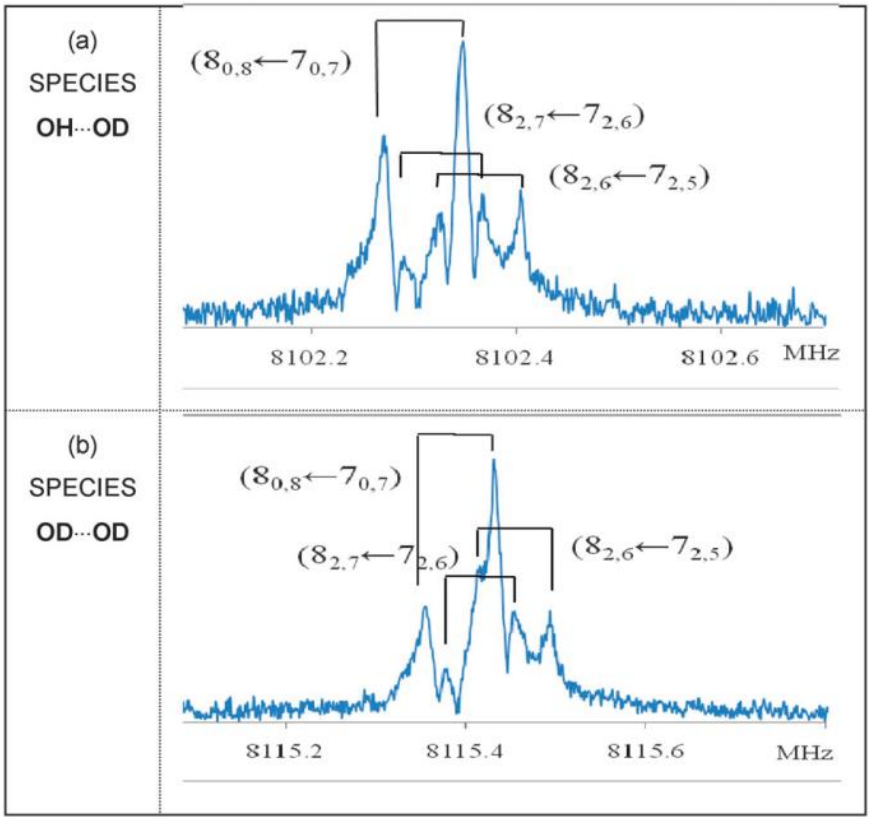


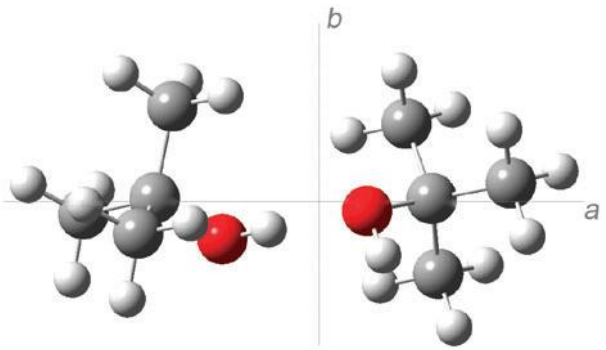




$$\mathrm{HOMA} = 1 - \alpha/n \sum^{n} (R_{opt} - R_{ij})^2 \qquad \Delta P = \Sigma(\mathrm{dC})^2$$

Majerz I., Dziembowska T. Geometric aspects of aromaticity : interrelations between intramolecular hydrogen bonds, steric effects and π-electron delocalisation in nitroanilines. Eur. J. Org. Chem., 2011, 280-286.

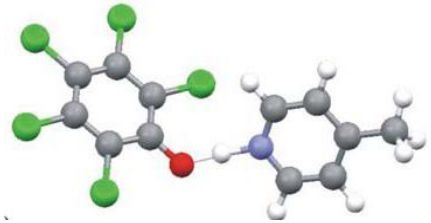


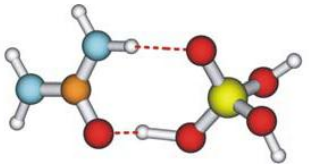


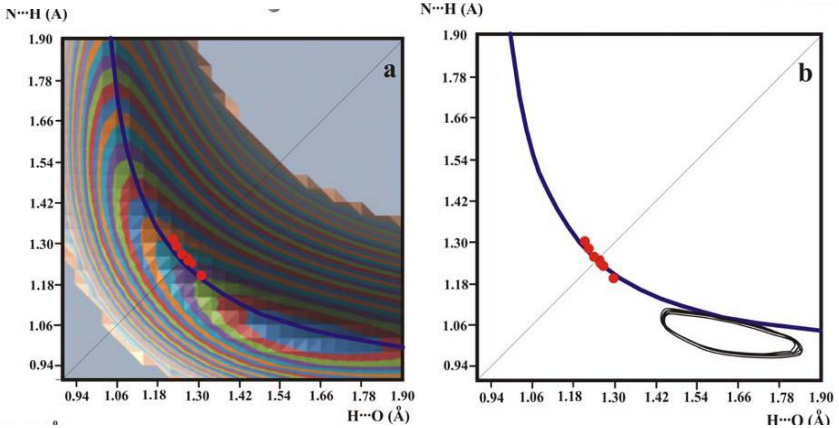
Tang S., **Majerz I.**, Caminati W. Sizing the Ubbelohde effect : the rotational spectrum of a *tert*-butylalcohol dimer. Phys. Chem., Chem. Phys., 2011, 13, 9137-9139.

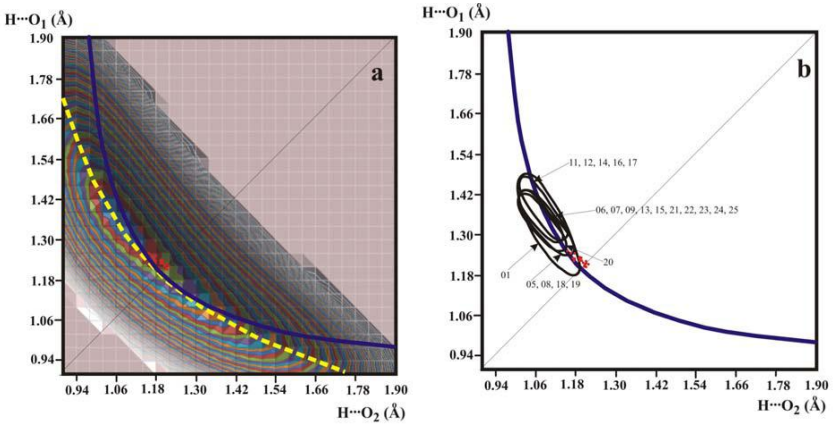
Influence of Proton Transfer Degree on the Potential Energy Surface for Two Very Short Hydrogen Bonds.

Irena Majerz, Ivar Olovsson
Acta Chim. Slov. 2011, 58, 379-384

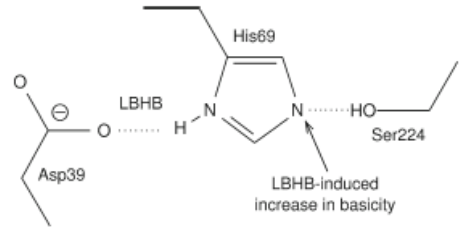


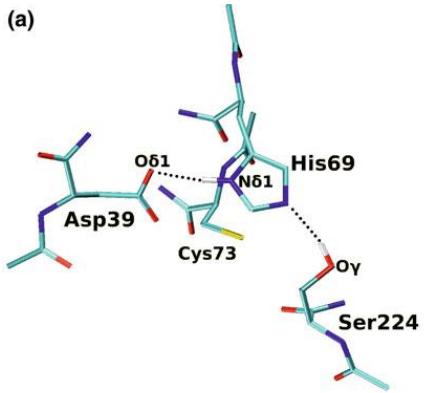


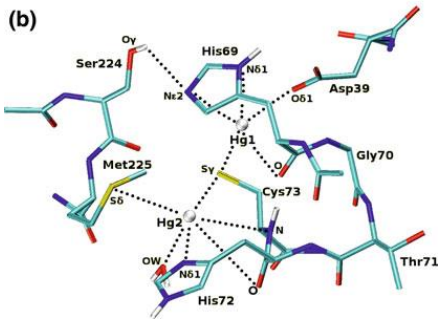


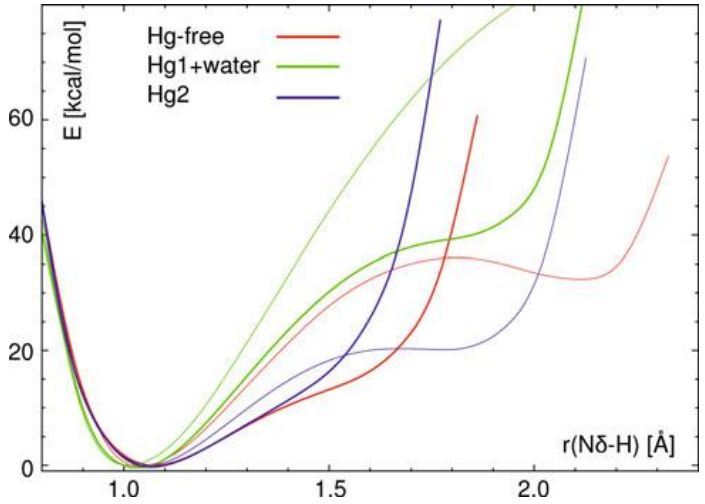


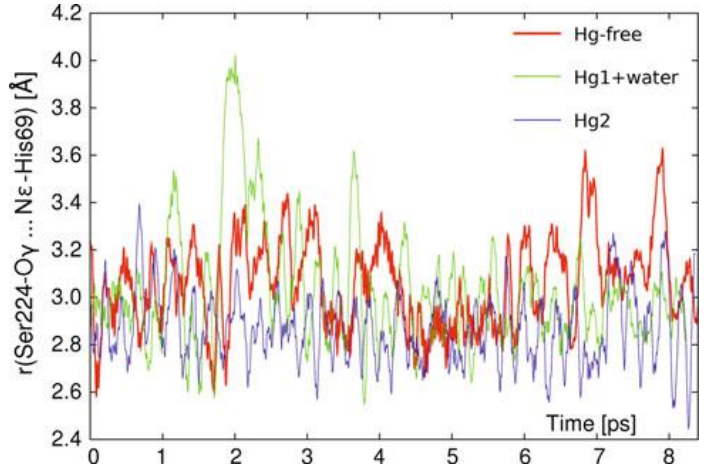
Born-Oppenheimer (DFT) molecular dynamics





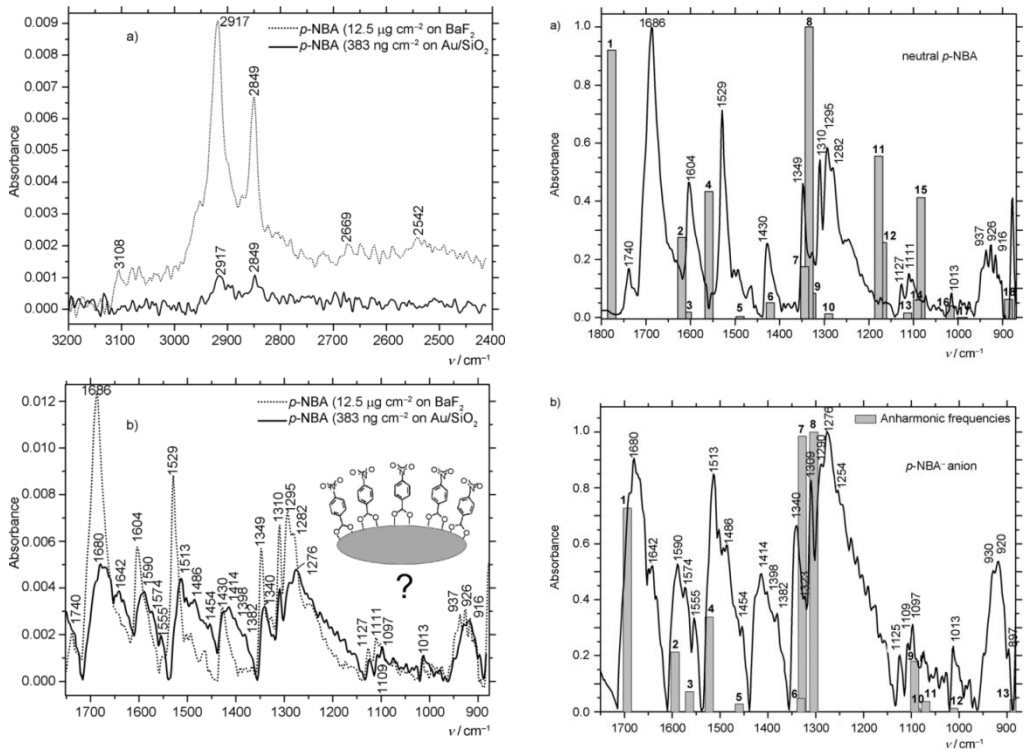






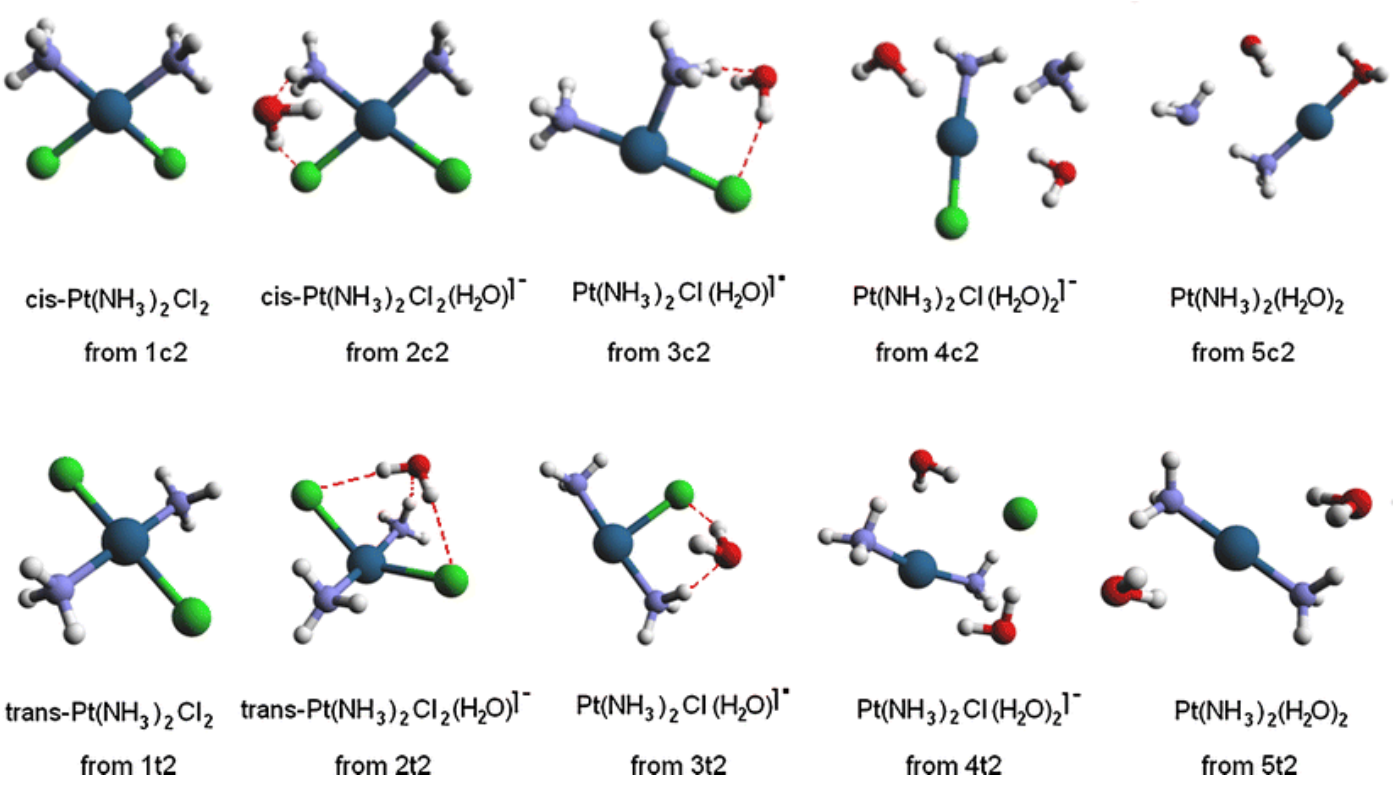
Centrum aktywne proteinazy zatrute jonem rtęci.

Panek J. J., Mazzarello R., Novič M., **Jezierska-Mazzarello A.** Impact of mercury(II) on proteinase K catalytic center: investigations via classical and Born-Oppenheimer molecular dynamics. Mol. Divers., 2011, 15, 215-226.



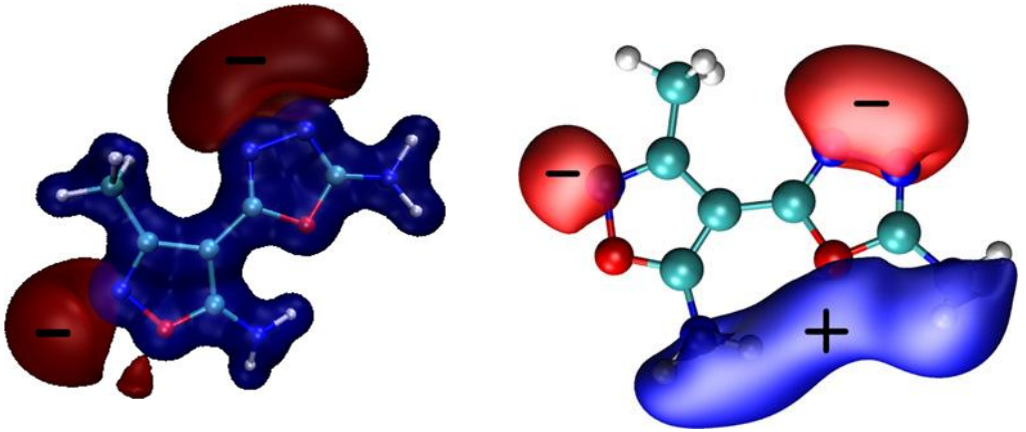
Kwas p-nitro benzoesowy osadzony na złocie

Panek J. J., **Jezierska-Mazzarello A.**, Koll A., Dovbeshko G., Fesenko O. p-nitrobenzoic acid adsorption on nanostructured gold surfaces investigated by combined experimental and computational approaches. ChemPhysChem, 2011, 12, 2485-2495.

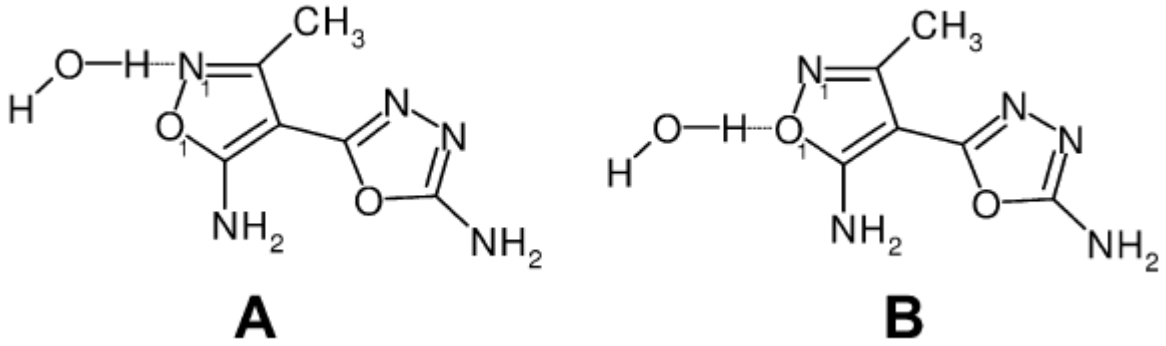


The description of the Pt atom the quasi-relativistic Stuttgart–Dresden pseudopotentials (MWB-60) were utilised. The original platinum valence basis set was augmented by a set of diffuse functions: as=0.0075, ap=0.013 and ad=0.025; and polarisation functions: af=0.98.

Kuduk-Jaworska J., Chojnacki H., **Jański** J. Non-empirical quantum chemical studies on electron transfer reactions in *trans*- and *cis*-diamminedichloroplatinum(II) complexes. J. Mol. Model., 2011, 17, 2411-2421.



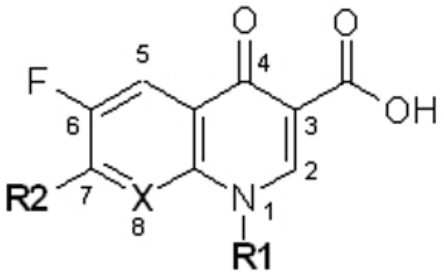
Obliczenia potencjałów elektrostatycznych



The electrostatic potential distribution around molecule of 5-amino-3-methyl-4-[2-(5-amino-1,3,4-oxadiazolo)]-isoxazole calculated in the gas phase. The minus sign indicates 0.04 a.u. isosurface, while the transparent areas denote + 0.30 a.u. ESP isosurface

Ryng S., Zimecki M., **Jezierska-Mazzarello A.**, Panek J. J., Mączyński M., Głowiak T., Sawka-Dobrowolska W., Koll A. A complex study of 5-amino-3-methyl-4-[2-(5-amino-1,3,4-oxadiazolo)]-isoxazole monohydrate: A new low-molecular-weight immune response modifier. J. Mol. Struct., 2011, 999, 60-67.

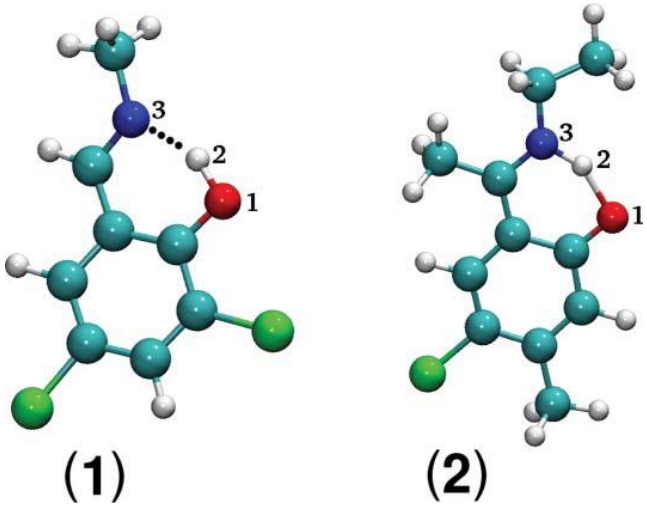
QSAR - Quantitative Structure Activity Relationship

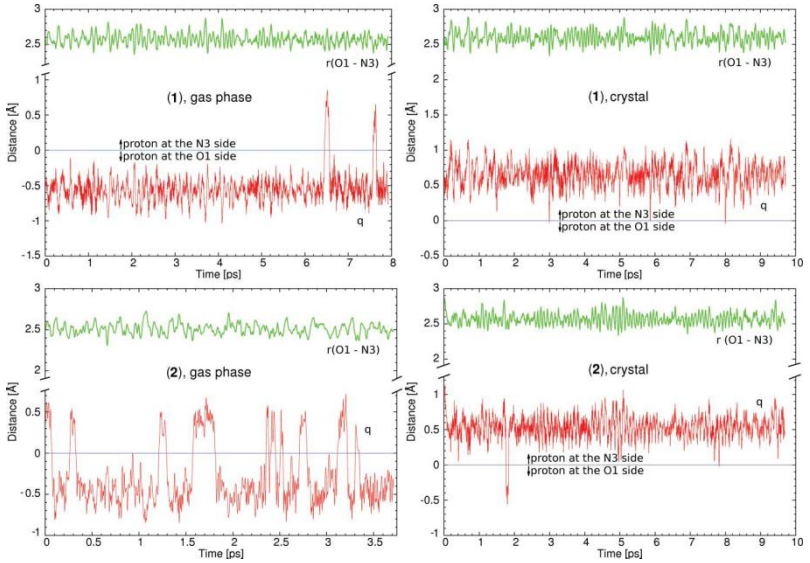


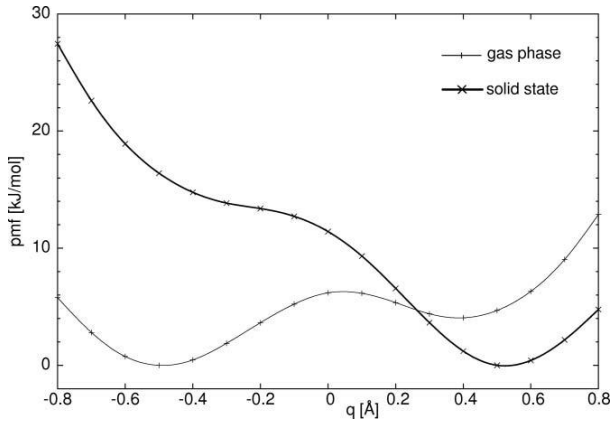
R1 = usually cyclopropyl
R2 = heterosystem
X = N, C

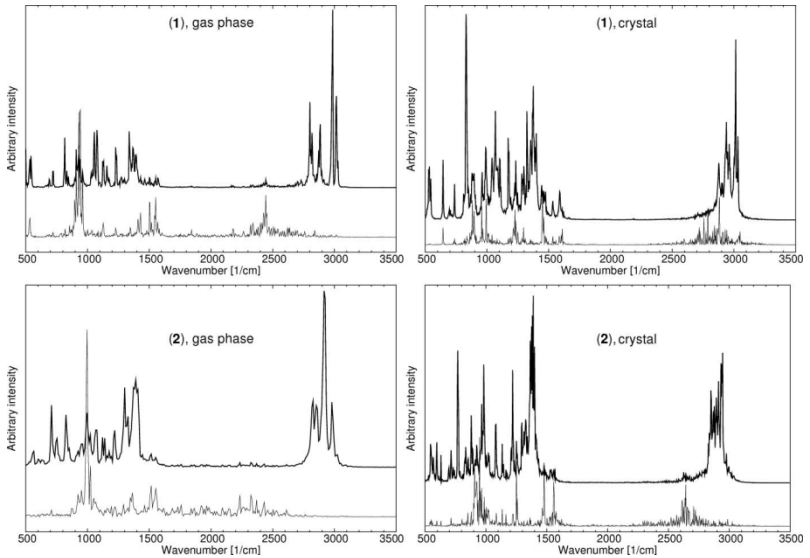
Fluoroquinolones

Minovski N., **Jezierska-Mazzarello A.**, Vračko M., Šolmajer T. Investigation of 6-fluoroquinolones activity against *Mycobacterium tuberculosis* using theoretical molecular descriptors : a case study. Cent. Eur. J. Chem., 2011, 9, 855-866



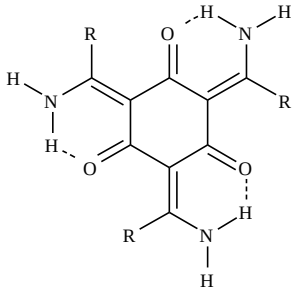




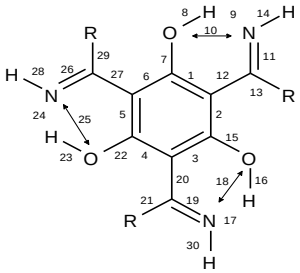


Jezierska-Mazzarello A., Panek J. J., Vuilleumier R., Koll A., Ciccotti G. Direct observation of the substitution effects on the hydrogen bridge dynamics in selected Schiff bases—A comparative molecular dynamics study. J. Chem. Phys., 2011, 134, 034308, 1-10.

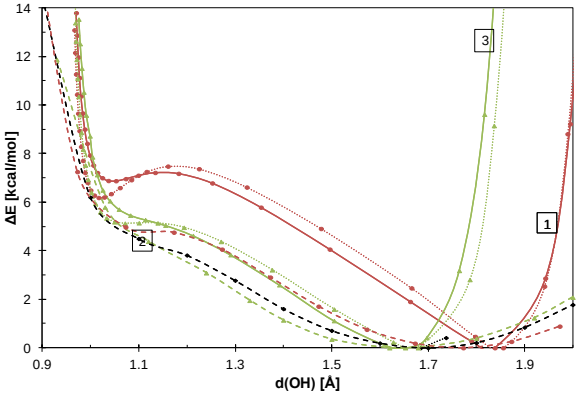
Analiza konformacyjna, B3LYP



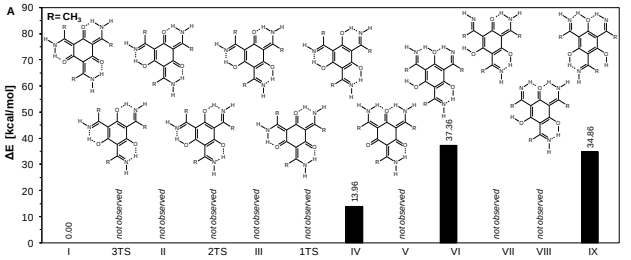
Keto-enamine

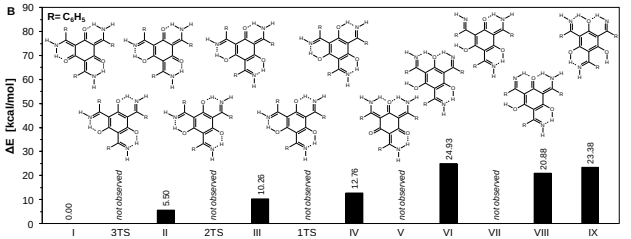


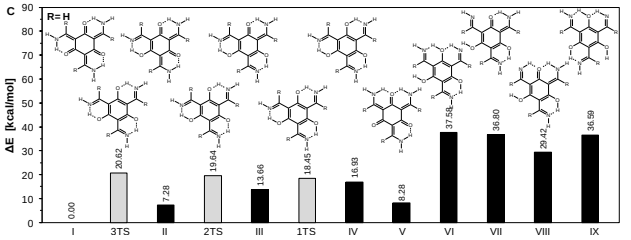
Enol-imine



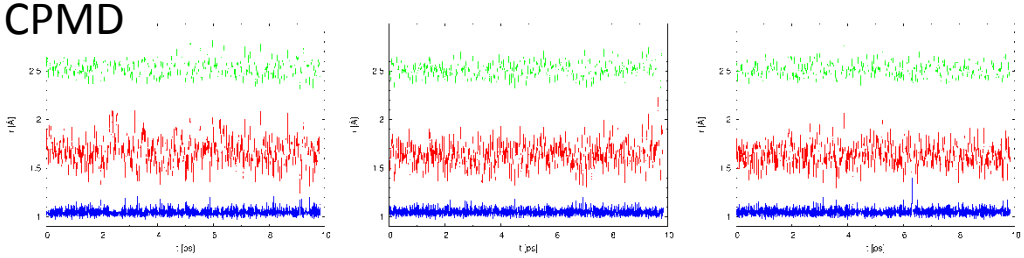
PES; CPMD, MP2 i B3LYP

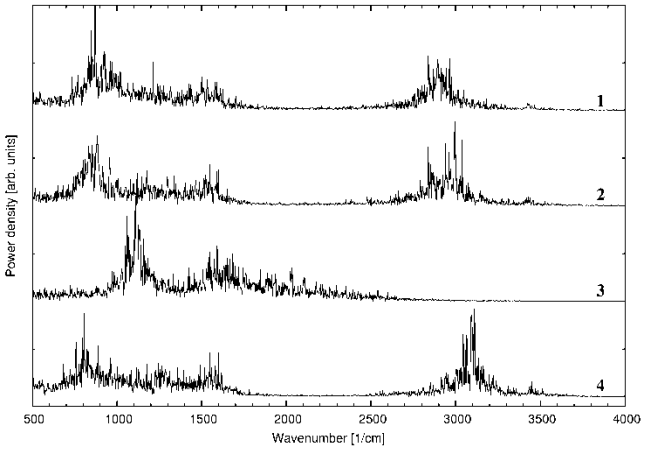




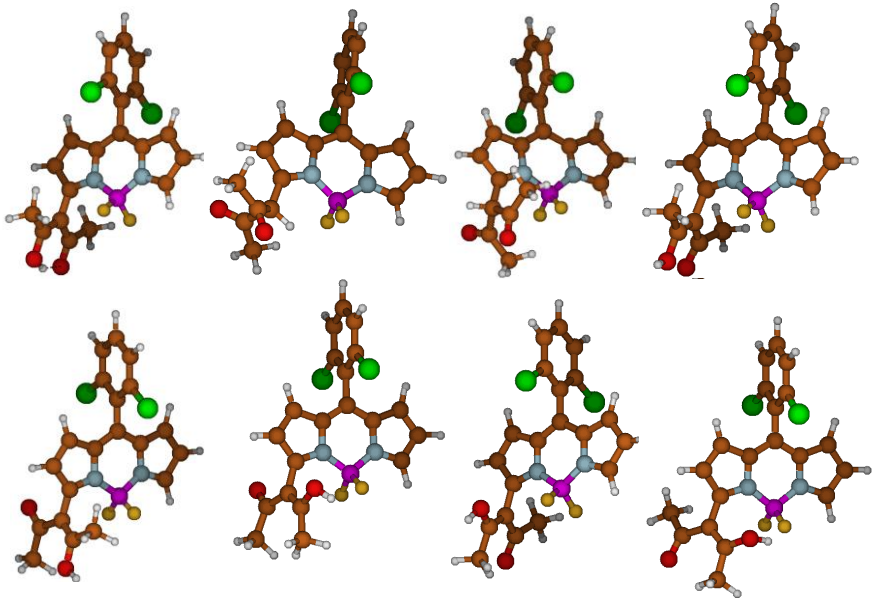


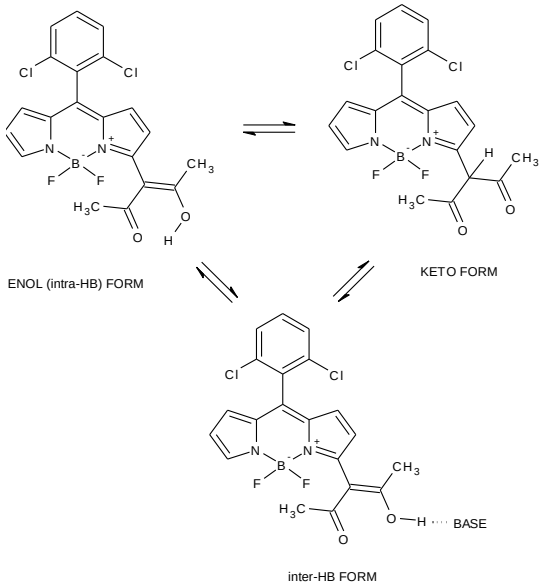
CPMD





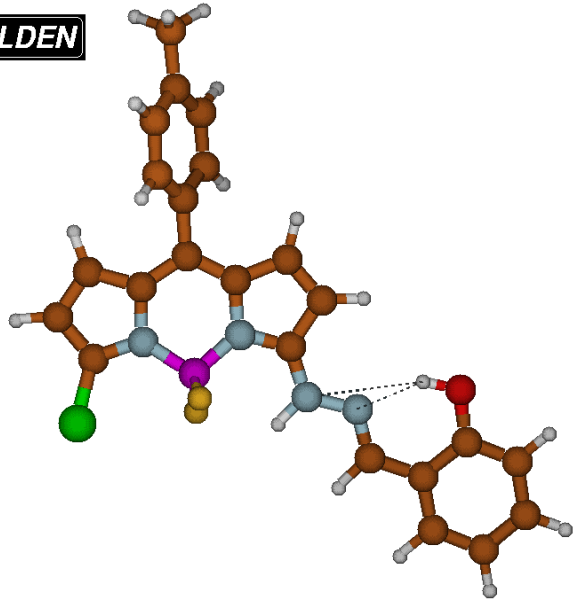
A. Jezierska, A. Martyniak, J. Panek, A. Filarowski J. Phys. Chem.





DFT, TD-DFT

MOLDEN



P. Lipkowski, A. Martyniak, M. Lopatkova, A. Kochel, J. Molisho Ngongo, N. Boens, W. Dehaen, M. Van der Auweraer, A. Filarowski J. Phys. Chem. A; PCCP.

Dziękuję za uwagę