JCTC Journal of Chemical Theory and Computation

Article

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Exploring Relative Thermodynamic Stabilities of Formic Acid and Formamide Dimers – Role of Low-Frequency Hydrogen-Bond Vibrations

Michael A. Cato, Jr.,[†] D. Majumdar,*[,†] Szczepan Roszak,*[,‡] and Jerzy Leszczynski*[,†]

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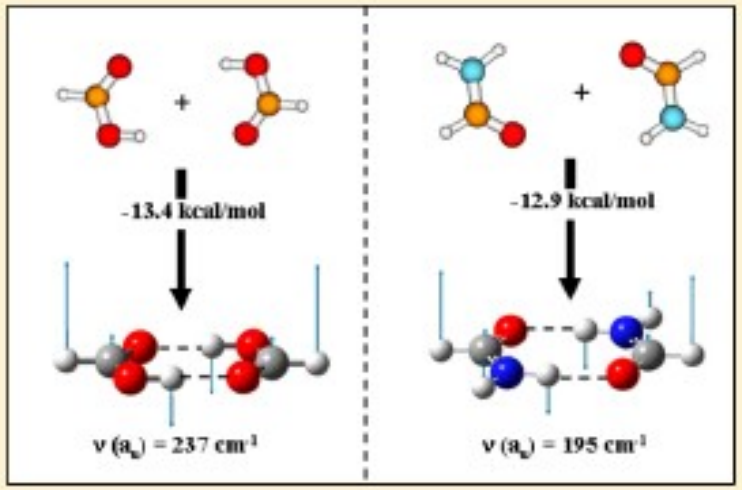
W pracy badano korelacje pomiędzy stabilizacją termodynamiczną dimerów kwasu mrówkowego i formamidu a niskoczęstościowymi drganiami oscylacyjnymi wiązań wodorowych. Wykonano zaawansowane (z uwzględnieniem anharmoniczności) obliczenia kwantowo-chemiczne osiągając dobrą zgodność z dostępnymi wynikami eksperymentalnymi. Znaleziono korelację pomiędzy energiami wiązań a wysoko i niskoczęstościowymi modami drgań oscylacyjnych



THE JOURNAL OF PHYSICAL CHEMISTRY A

Article

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Role of the Multipolar Electrostatic Interaction Energy Components in Strong and Weak Cation−π Interactions

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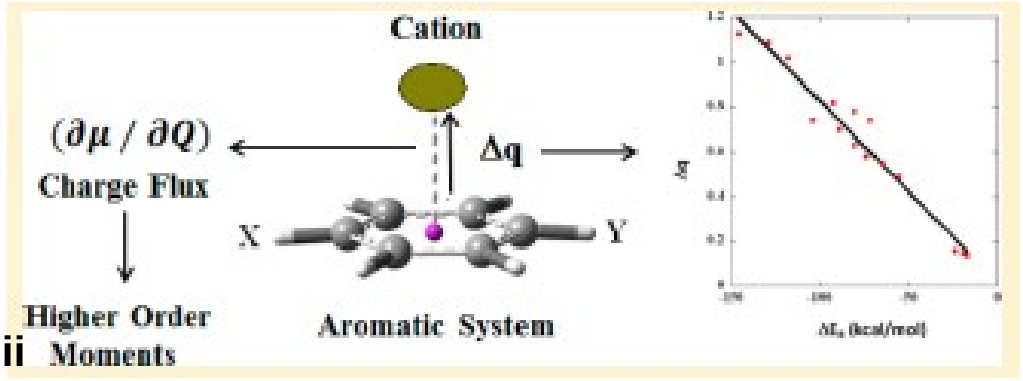


W pracy zaprezentowano rezultaty mocnych i słabych kompleksów charakteryzowanych jako oddziaływania kation-π. Wykonano dekompozycję energii oddziaływań ze szczególnym uwzględnieniem multipolowych oddziaływań elektrostatycznych. Dodatkowo wykonano analizę modów drgań elektrostatycznych odpowiedzialnych za formowanie się kompleksów.

J Mol Model (2013) 19:4209–4214
DOI 10.1007/s00894-013-1841-9

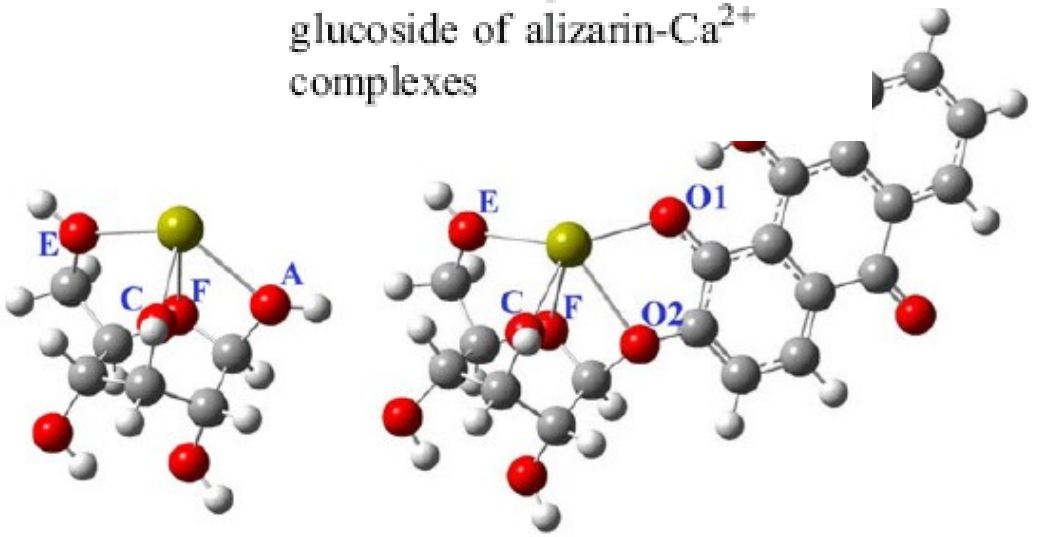
ORIGINAL PAPER

Theoretical studies of structure, energetics and properties of Ca^{2+} complexes with alizarin glucoside

Dariusz Toczek · Karolina Kubas · Michał Turek · Szczepan Roszak · Roman Gancarz

Badania teoretyczne kompleksow jonów metali z cukrami zostały wykonane jako uzupełnienie eksperymentalnych badań nad kamienicą nerkową. Właściwości utworzonych kompleksów (struktura, energia oddziaływań) są cenną wskazówką dla poszukiwania procedur kontrolowania poziomu jomów metali w organiźmie.

Fig. 2 The structure of the most stable **a** glucose-Ca^{2+} **b** glucoside of alizarin-Ca^{2+} complexes



Optical Materials 35 (2013) 1004–1012

Contents lists available at SciVerse ScienceDirect

Optical Materials

journal homepage: www.elsevier.com/locate/optmat

Oscillatory polarons generation by near IR and spin induced chirality studies in optically nonlinear 1,3-dinitrobenzene crystal

M. Magdalena Szostak [a,*], Henryk Chojnacki [a,1], Katarzyna Piela [a], Ewa Bidzińska [b], Krystyna Dyrek [b]

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[b] Faculty of Chemistry, Jagiellonian University, ul. Ingardena 3, PL-30-060 Kraków, Poland

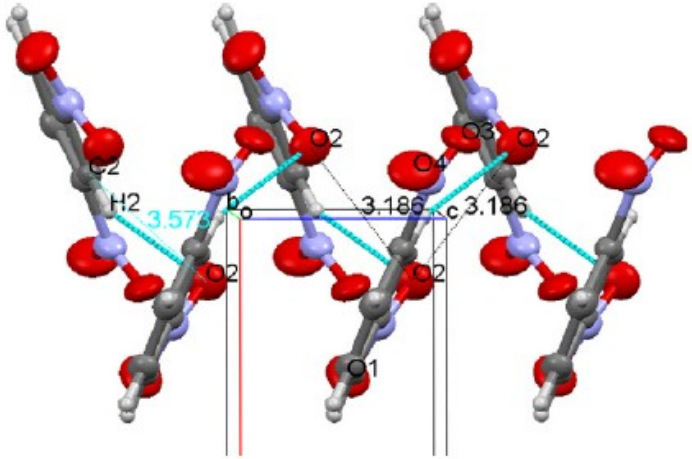

Fig. 1. Projection along the crystallographic *c* axis of the *m*DNB molecules forming hypothetical helix. Structural data was taken from Ref. [11].

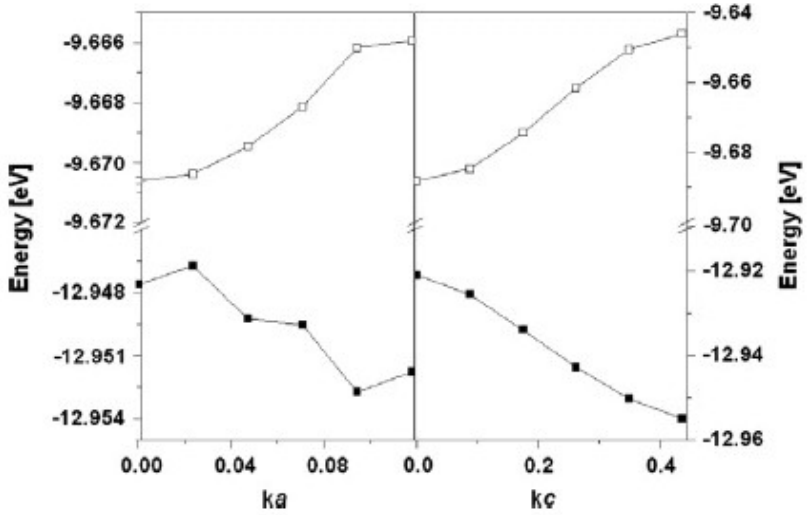

Fig. 9. Theoretical band structure calculated for whole unit cell of *m*DNB. The lines are only guides for eyes.

Journal of Molecular Structure 1033 (2013) 91–97

Contents lists available at SciVerse ScienceDirect

Journal of Molecular Structure

journal homepage: www.elsevier.com/locate/molstruc

Molecular motions contributions to optical nonlinearity of *N*-benzyl-2-methyl-4-nitroaniline studied by temperature-dependent FT-IR, ^{1}H NMR spectroscopy and DFT calculations

Katarzyna Piela [a], Krystyna Hołderna-Natkaniec [b], Mikołaj Baranowski [b], Tomasz Misiaszek [a], Jan Baran [c], M. Magdalena Szostak [a,*]

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[b] Faculty of Physics, Adam Mickiewicz University, Umultowska 85, 61-614 Poznań, Poland
[c] Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okólna 2, 50-422 Wroclaw, Poland

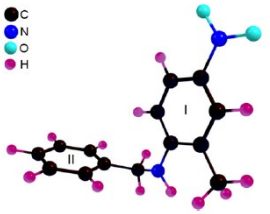


Fig. 1. The BNA L-shaped molecule geometry taken from crystallographic data [17] used in DFT calculations and benzene rings numbering. The angle between tri-(I)

Table 1
Activation energy, E_a (kJ/mol) and correlation time, τ_c (s) values of chosen groups rotations in BNA orthorhombic crystal estimated from FT-IR, ^{1}H NMR measurements and DFT calculations.

	ν (cm^{-1})	E_a (kJ/mol)			τ (s)	
		FT-IR	^{1}H NMR	DFT	FT-IR	^{1}H NMR
–CH_3			12.7 ± 0.6	10.75		2.08×10^{-14}
–CH_2	$\nu_{as}(CH_2)$ (2909 cm^{-1})	11.09 ± 0.12			8.92×10^{-12}	
–NO_2	$\nu_{as}(NO_2)$ (1535 cm^{-1})	9.61 ± 0.18		28.07	4.90×10^{-12}	
	$\nu_s(NO_2)$ (1320 cm^{-1})	9.07 ± 0.24			3.94×10^{-12}	
–NH	ν(NH) (3395 cm^{-1})	10.68 ± 0.08			7.56×10^{-12}	

Journal of COMPUTATIONAL CHEMISTRY WWW.C-CHEM.ORG RAPID COMMUNICATION

Low-Cost Prediction of Relative Stabilities of Hydrogen-Bonded Complexes from Atomic Multipole Moments for Overly Short Intermolecular Distances

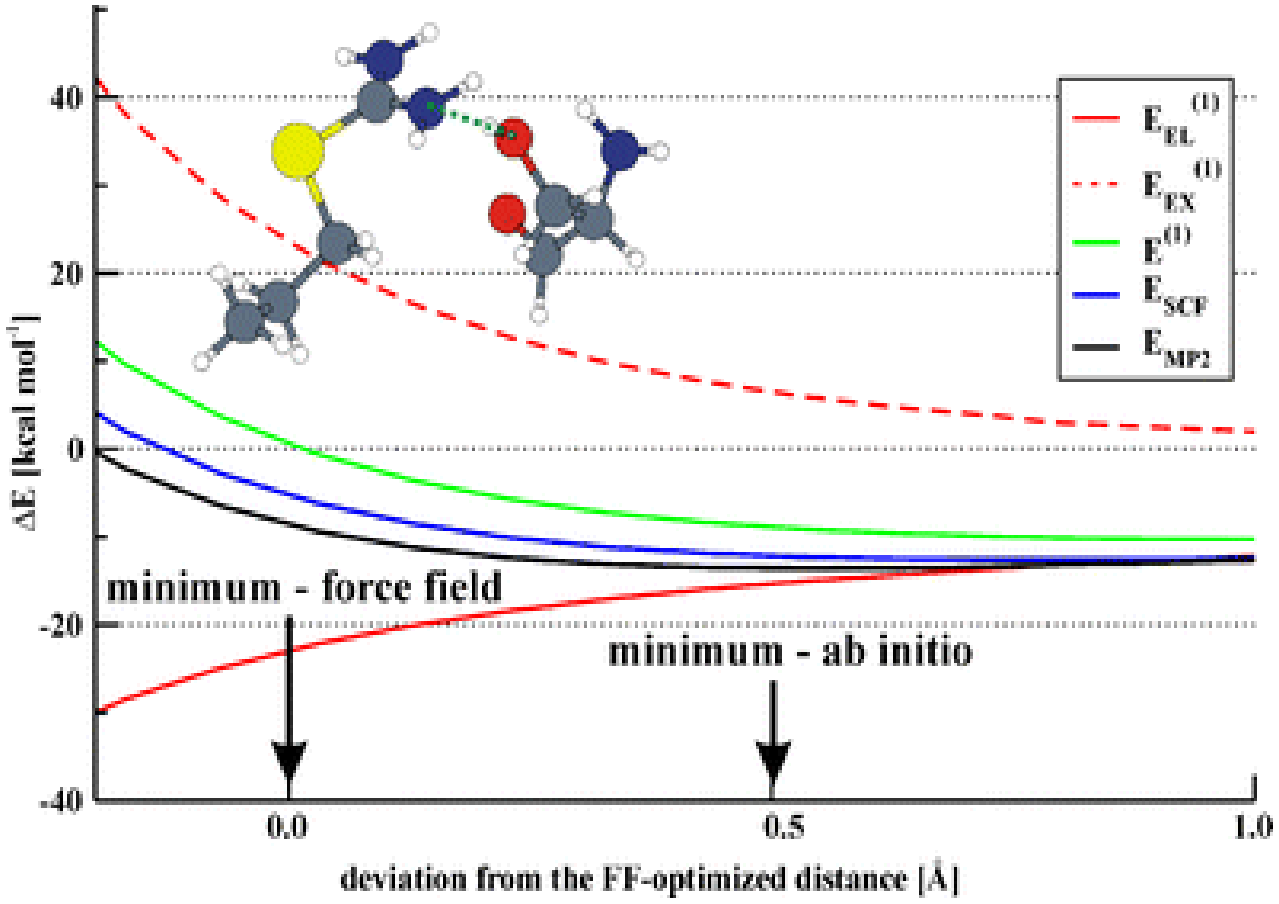
Wiktor Beker,[a] Karol M. Langner,[b] Edyta Dyguda-Kazimierowicz,[a] Mikołaj Feliks,[c] and W. Andrzej Sokalski[a]*

The relative stability of biologically relevant, hydrogen bonded complexes with shortened distances can be assessed at low cost by the electrostatic multipole term alone more successfully than by *ab initio* methods. These results imply that atomic multipole moments may help improve ligand–receptor ranking predictions, particularly in cases where accurate structural data are not available.

DOI: 10.1002/jcc.23326

Wykazano, ze człon elektrostatycznych oddziaływań multipolowych pozwala na przewidywanie względnych stabilności kompleksów z wiązaniem wodorowym w sytuacjach gdy nieznana jest dokładna struktura badanych układów.

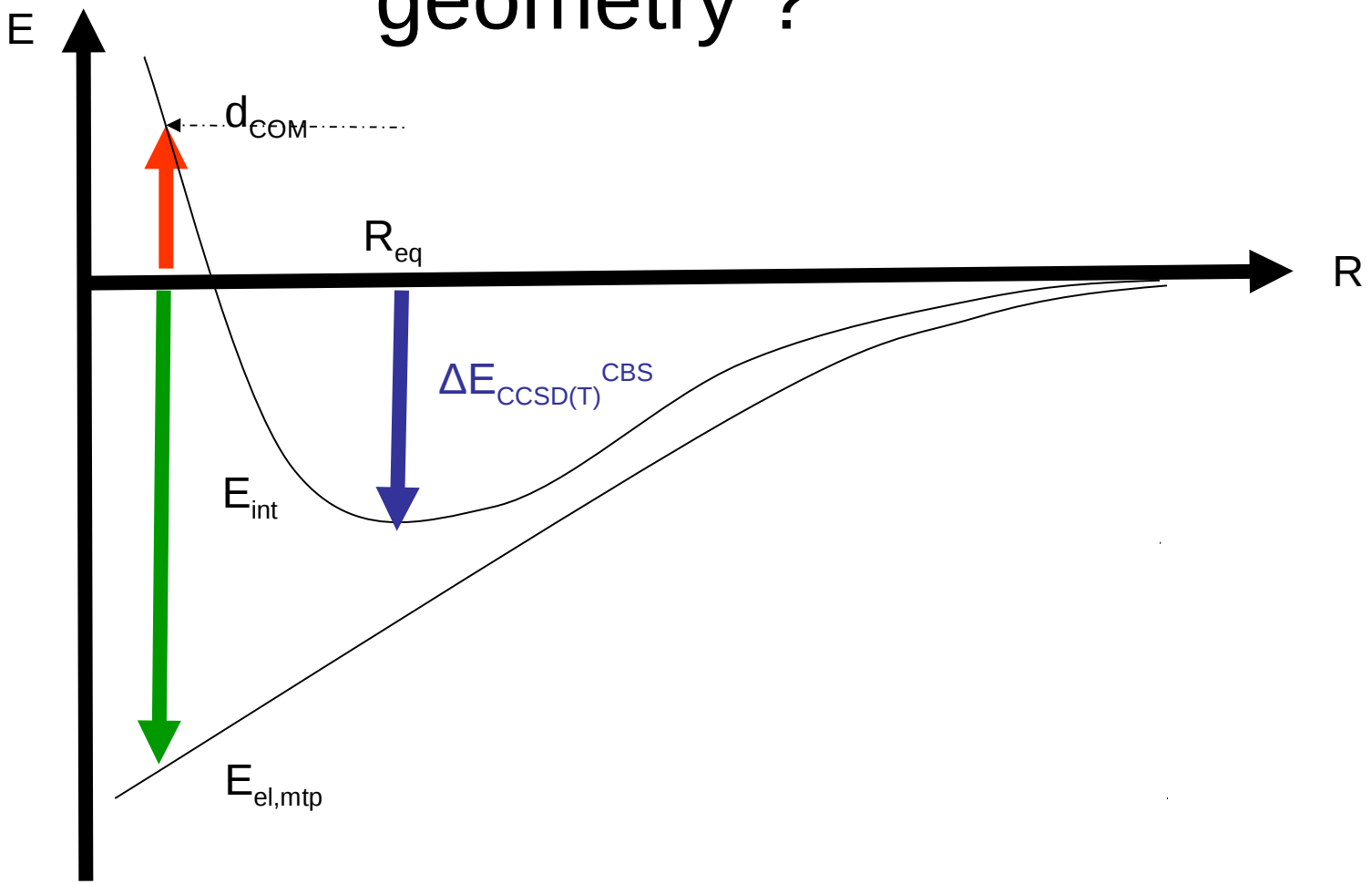
Binding energy terms for the Cbz-*S*ArgP(OPh)2 inhibitor and Ser190 interaction. (R. Grzywa et al., J.Mol.Mod., 13, 677 (2007)



Inaccurate enzyme-ligand contacts (in Angstroms) predicted by force field calculations (short contacts in red)

INHIBITOR #	SER 190		GLY 219	
	Force field	MP2	Force field	MP2
1	2.88	3.08	1.56	2.06
2	3.11	2.70	2.08	1.98
3	1.84	2.40	1.62	2.02
4	2.53	3.00	1.62	2.02
5	3.19	2.80	2.02	2.32

Which term calculated at shortened intermolecular distances can be best predictor of relative stability at equilibrium geometry ?



CORRECT PREDICIONS OF RELATIVE STABILITIES BY ELECTROSTATIC MULTIPOLE TERM FOR TRAINING SET OF 23 HB COMPLEXES (Hobza et al., JCTC,7,2427(2011)

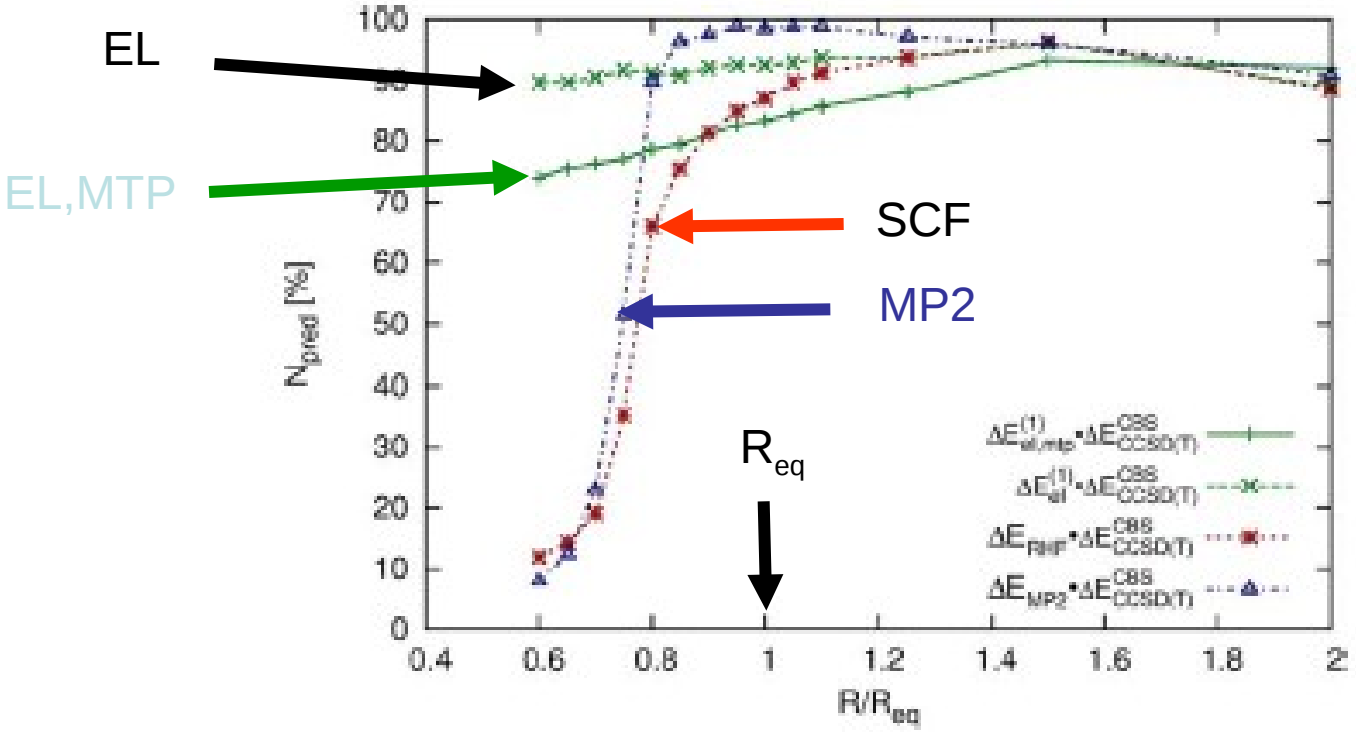


Figure 2. Success rate N_{pred} of predicting the relative stability of dimer pairs at equilibrium geometry for the subset of 23 hydrogen bonded complexes, using several approximate methods and as a function of the factor R/R_{eq} scaling the shortest intermolecular contact.

THE JOURNAL OF PHYSICAL CHEMISTRY B

Article

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Nonempirical Energetic Analysis of Reactivity and Covalent Inhibition of Fatty Acid Amide Hydrolase

Ewa I. Chudyk,[†] Edyta Dyguda-Kazimierowicz,[‡] Karol M. Langner,[‡,∥] W. Andrzej Sokalski,*[,‡] Alessio Lodola,[§] Marco Mor,[§] Jitnapa Sirirak,[†] and Adrian J. Mulholland*[,†]

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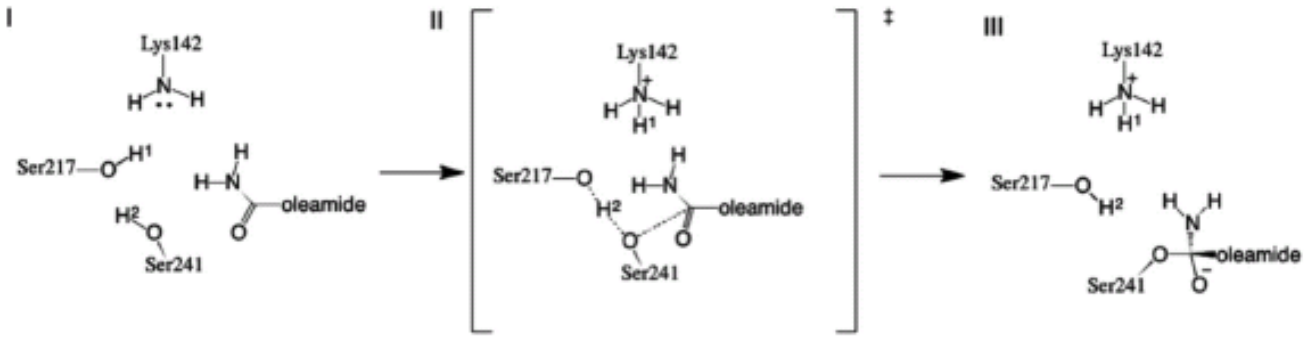


Figure 1. Proposed mechanism of FAAH acylation[23,16] proceeds from the Michaelis complex (I) through the transition state (II) up to the tetrahedral intermediate (III). In the reactant state, both catalytic serines (Ser217 and 241) are protonated, while Lys142 is neutral. A second proton transfer involving H^2 accompanies the first, Ser217-assisted one. The highest energy configuration is attained in QM/MM calculations[17] when H^2 is almost equidistant between Ser241 and Ser217 and the oleamide is halfway to Ser241. The tetrahedral intermediate is formed subsequently.

- **Przeanalizowano fizyczną naturę oddziaływań w centrum aktywnym hydrolazy amidów kwasów tłuszczowych. Wyniki wskazują na szczególną rolę treoniny 236, seryny 218 oraz jednej z cząsteczek wody i są zgodne z przeprowadzoną analizą sekwencji 42 pokrewnych enzymów .**

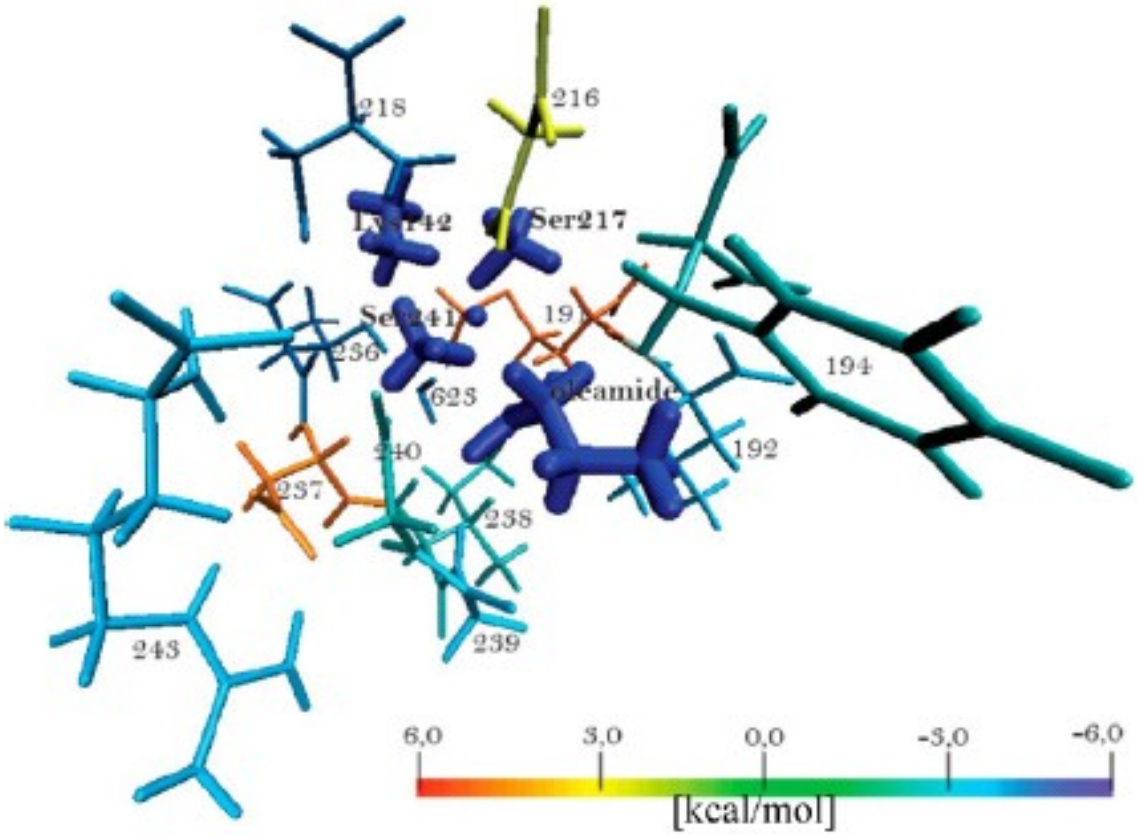


Figure 4. Structure of the FAAH active site at the transition state for the reactive conformation D of oleamide acylation. The coloring scheme applied to active site components reflects their contribution to differential transition-state stabilization (blue colors represent stabilizing and yellow to red represent destabilizing effects). The reaction center subsystem, including the Lys142-Ser217-Ser241 triad, is shown as a dark-blue thick stick

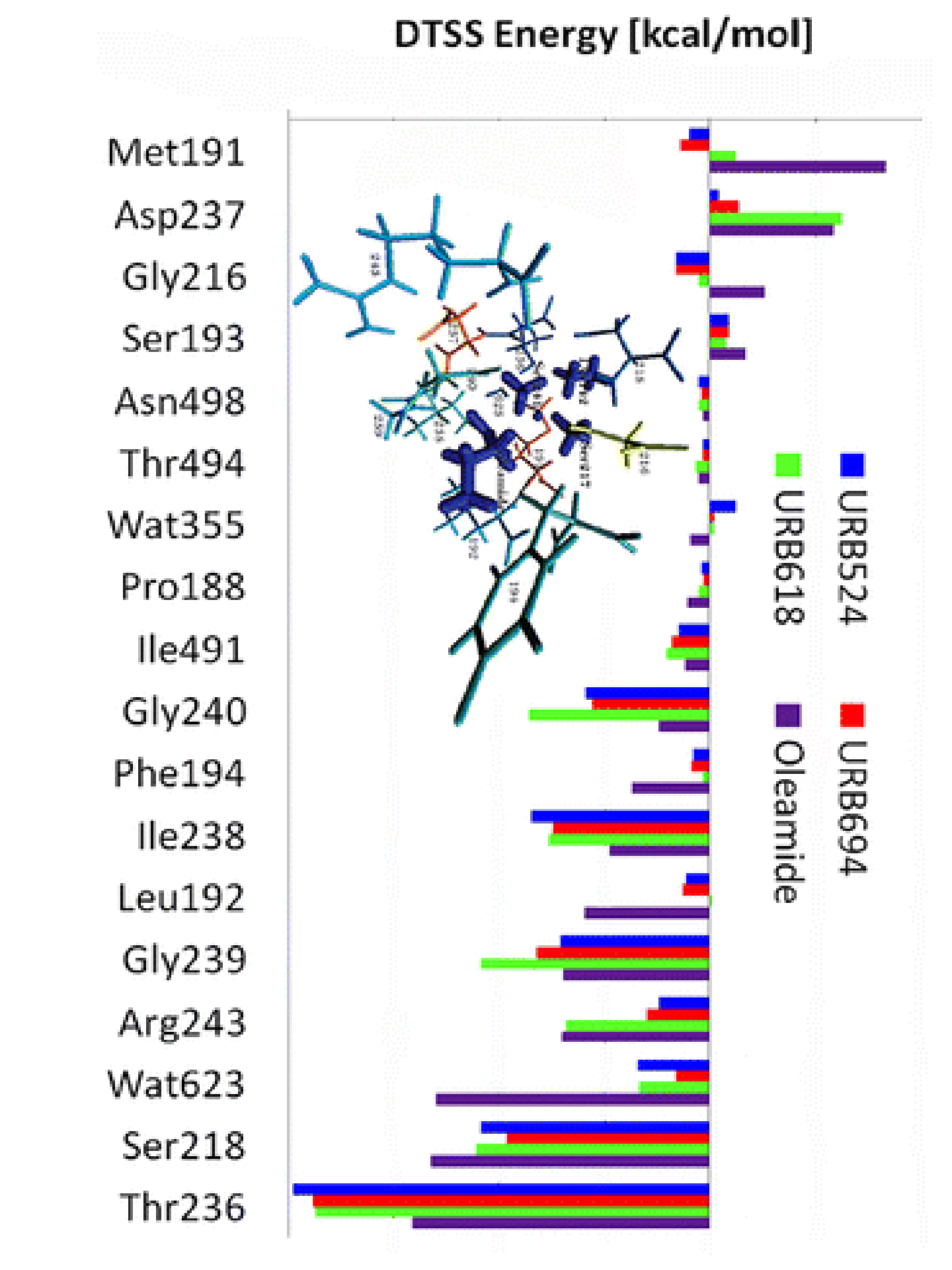

DTSS Energy [kcal/mol]
Met191
Asp237
Gly216
Ser193
Asn498
Thr494
Wat355
Pro188
Ile491
Gly240
Phe194
Ile238
Leu192
Gly239
Arg243
Wat623
Ser218
Thr236
URB524
URB694
URB618
Oleamide

Table 2. Interaction Energies between the FAAH-Oleamide Reaction Model and Its Enzymatic Environment at Various Levels of Theory, As Defined by Equation 2[a]

	sum of pairwise interactions				supermolecule environment			
	Δ_{EL}	Δ_{HL}	Δ_{SCF}	Δ_{MP2}	Δ_{EL}	Δ_{HL}	Δ_{SCF}	Δ_{MP2}
substrate	−64.7	18.6	−3.2	−25.4	−68.4	11.9	−12.0	−34.9
transition state	−88.0	9.3	−24.2	−46.5	−92.1	1.9	−34.9	−58.4
DTSS	−23.3	−9.3	−21.0	−21.1	−23.7	-10.0	−22.9	−23.5

[a]Polarization effects among residues are largely responsible for the differences between the left (pair-wise interactions between single residues) and the right (interactions for the entire active site model) sides of the Table. All values are in kilocalories per mole. The counterpoise correction was applied throughout, although basis set extension effects due to different basis set sizes of the pair-wise and supermolecule models were not considered. This may be responsible for minor DTSS differences observed between the two models.

dx.doi.org/10.1021/jp401834v | J. Phys. Chem. B 2013, 117, 6656−6666

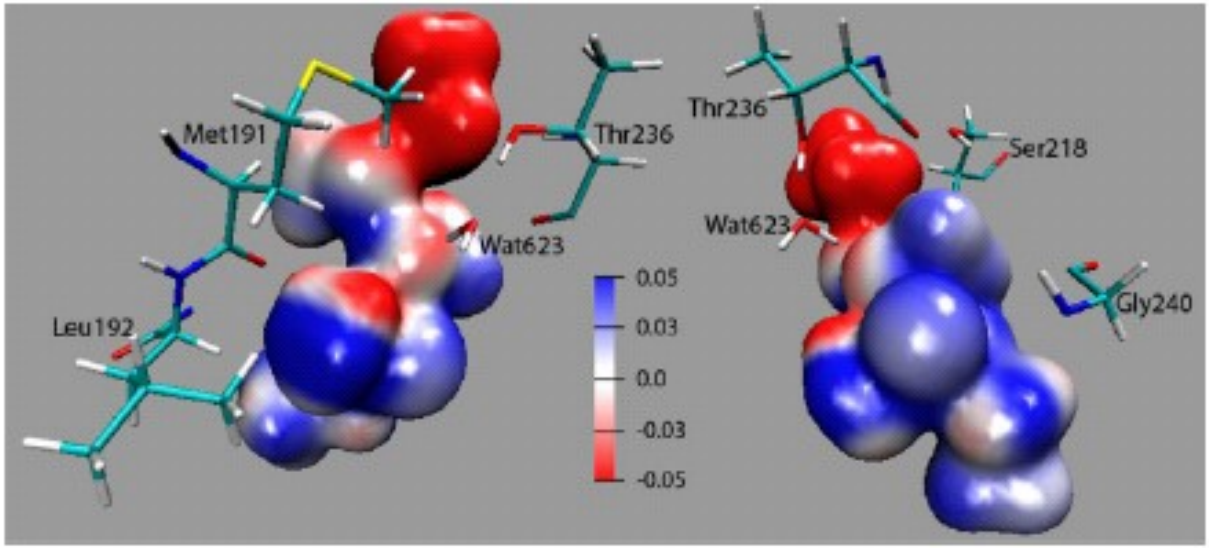
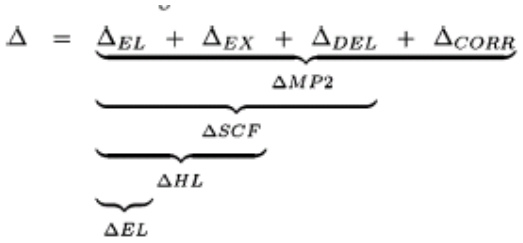


Figure 8. Catalytic field (differential electrostatic potential in au) mapped onto the electronic isodensity surface of 0.01 au around the reaction center of conformation D (the catalytic triad Lys142- Ser217-Ser241 and oleamide up to C4). Selected catalytic residues identified by DTSS analysis are also shown for context.

Differential transition state stabilisation energies (in [kcal/mole] for FAAH active site residues at different theory levels

Residue	ΔEL,M1	ΔEL1	ΔHL	ΔSCF	ΔE(MP2)
asp237	4,102	4,135	4,306	3,342	3,599
gly216	3,84	4,321	3,589	3,746	2,952
met191	2,091	2,62	0,021	1,465	1,024
ser218	0,82	1,068	0,375	-0,028	-0,126
pro188	0,082	0,446	-0,259	-0,224	-0,276
tip355	-0,306	-0,305	-0,305	-0,307	-0,295
thr494	-0,355	-0,353	-0,353	-0,376	-0,365
asn498	-0,387	-0,387	-0,387	-0,421	-0,398
ile491	0,053	0,314	-0,728	-0,647	-0,456
phe194	-0,417	-0,032	-1,918	-1,8	-0,947
ser193	-1,571	-1,216	-2,219	-2,126	-1,451
gly240	-2,078	-2,408	-1,507	-2,022	-1,771
leu192	-1,264	-1,076	-1,43	-1,992	-2,046
arg243	-4,316	-4,316	-4,316	-4,402	-4,194
thr236	-3,79	-3,916	-1,661	-4,073	-4,464
tip623	-4,346	-6,566	-3,315	-4,475	-4,486
ile238	-5,952	-10,197	0,625	-4,833	-4,73
gly239	-5,604	-5,284	-2,51	-5,183	-5,348
SUM	**-19,398**	**-23,152**	**-11,992**	**-24,356**	**-23,778**
CC	0,987	0,932	0,787	0,990	1,000



MP2 results correlate very well with SCF, HL, El and multipolar electrostatic theory levels

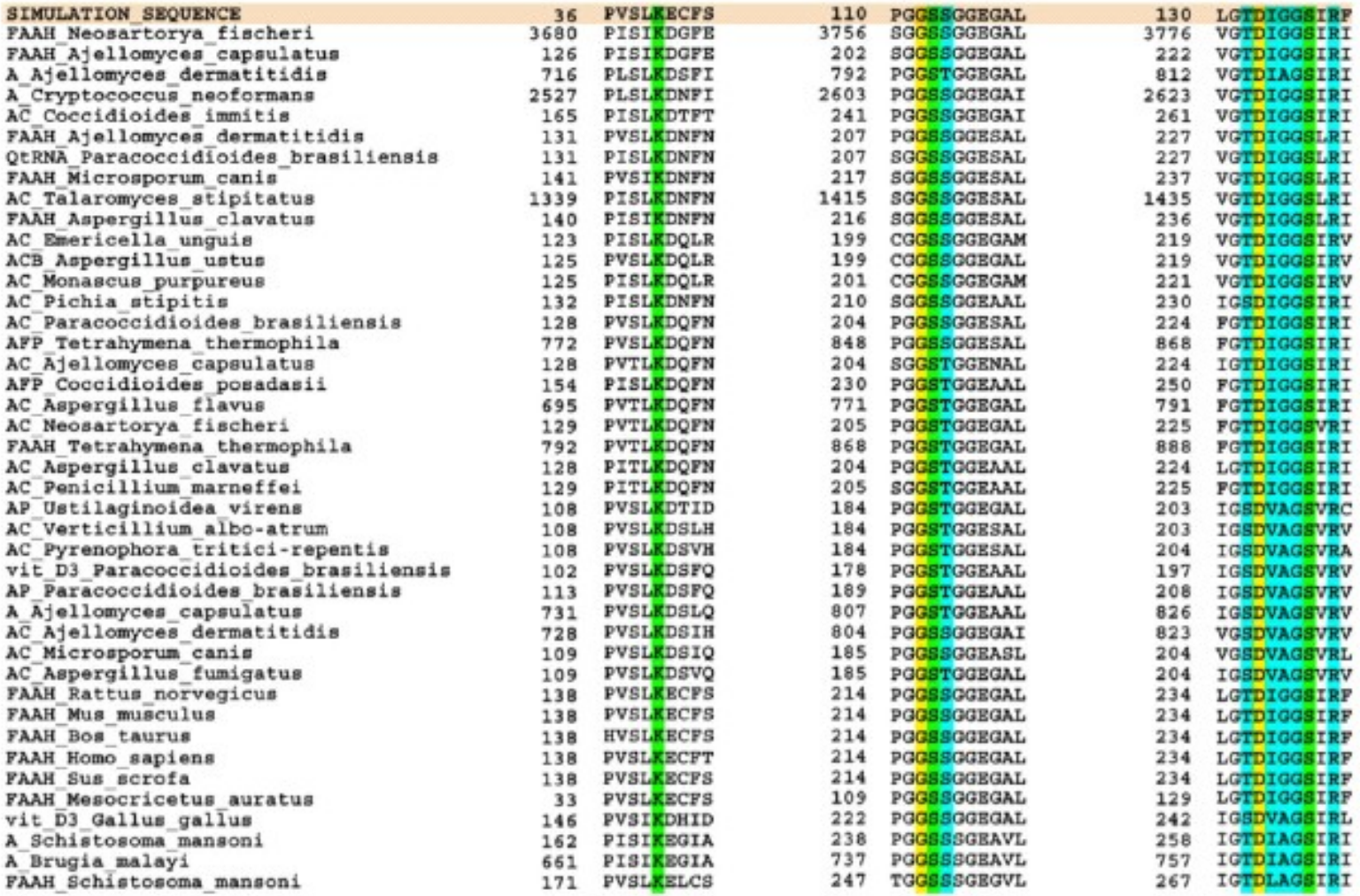


Figure 9. Multiple sequence alignment in the proximity of the catalytic triad (Lys142-Ser217-Ser241 residues shown in green) from the amidase signature family. Some of the most important residues that stabilize (Ser218, Thr236, Ile238, Gly239, Gly240, Arg243) or destabilize (Gly216, Asp237) the transition state are shown in blue and yellow, respectively. Abbreviations: vit_D3 – vitamin D3 hydroxylase-associated protein; QtRNA, glutamyl-tRNA(gln) amidotransferase; FAAH, fatty acid amide hydrolase; AC, acetamidase; AP, amidase protein; A, amidase; AFP, amidase family protein; and ACB, acetamidase-B. Residues in all sequences are numbered according to the first deposited FAAH amino acid sequence of *Rattus norvegicus* (the common rat).

THE JOURNAL OF PHYSICAL CHEMISTRY C

Article

dx.doi.org/10.1021/jp402414n | J. Phys. Chem. C 2013, 117, 10809−10817

Theoretical Study on Physicochemical Aspects of a Single Molecular Junction: Application to the Bases of ssDNA

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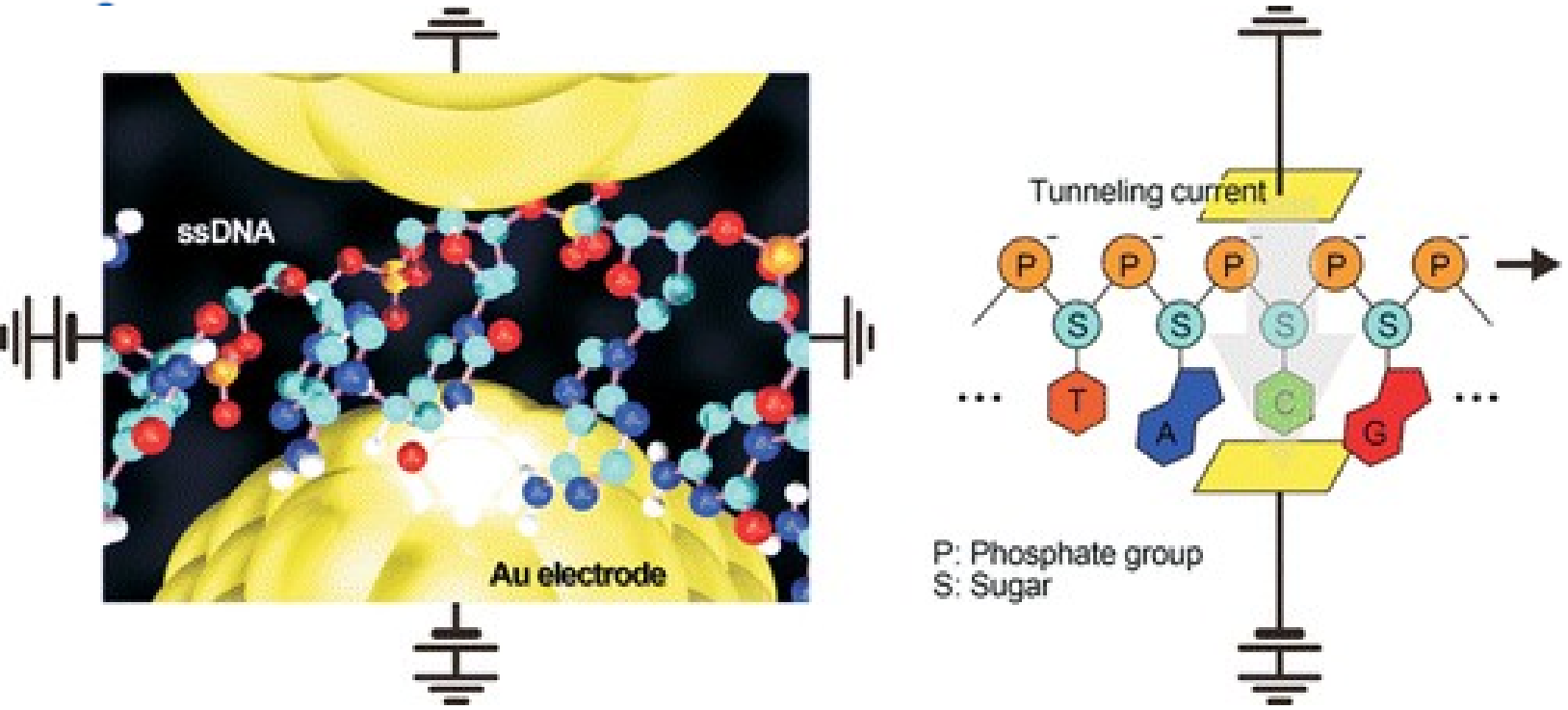
Department of Mechanical Science and Bioengineering, Graduate School of Engineering Science, Osaka University, 1-3 Machikaneyama, Toyonaka, Osaka 560-8531, Japan



Opracowano nieempiryczny model przewodnictwa w nanodetektorze mogącym służyć do odczytywania sekwencji kwasu nukleinowego

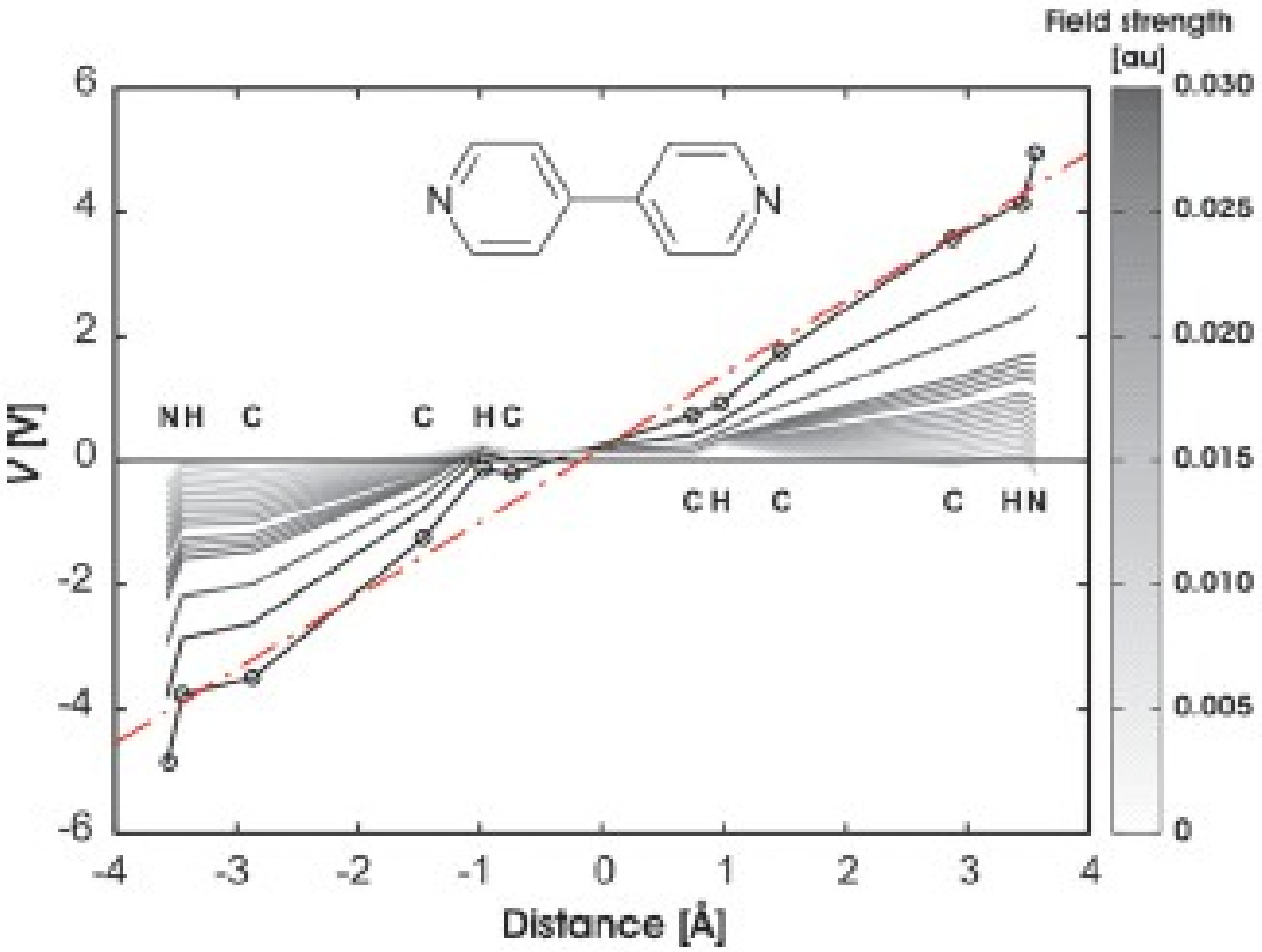


Figure 2. Potential drop on atoms across the BPY molecule in order with respect to the uniform electric field direction. The color gradient corresponds to the electric field strength. The linear regression ($V = 1.19x$) of the potential drop for the largest field is shown with a broken line.

JCTC Journal of Chemical Theory and Computation

Article

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dx.doi.org/10.1021/ct400423u | J. Chem. Theory Comput. 2013, 9, 4915−4927

Geometries and Vertical Excitation Energies in Retinal Analogues Resolved at the CASPT2 Level of Theory: Critical Assessment of the Performance of CASSCF, CC2, and DFT Methods

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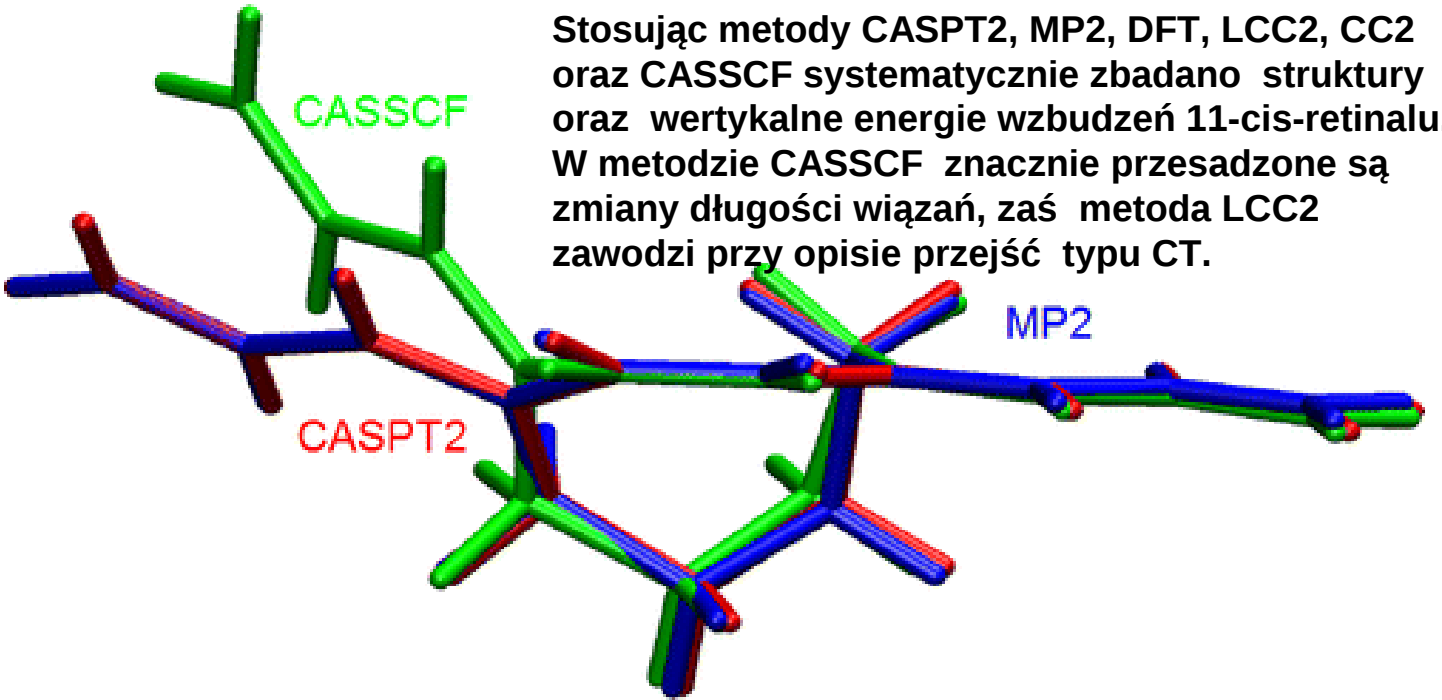
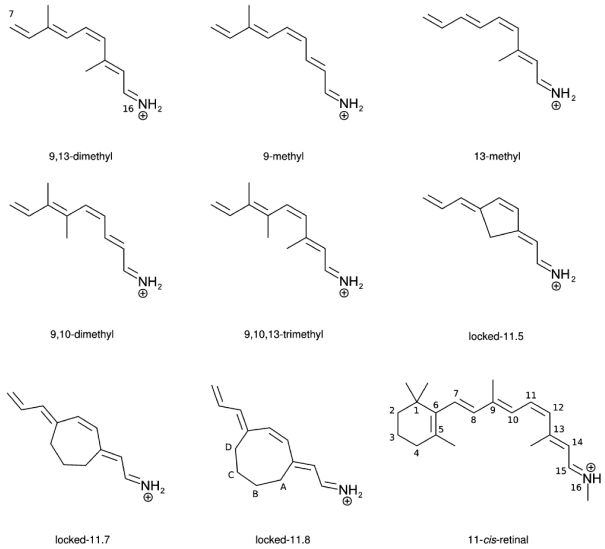
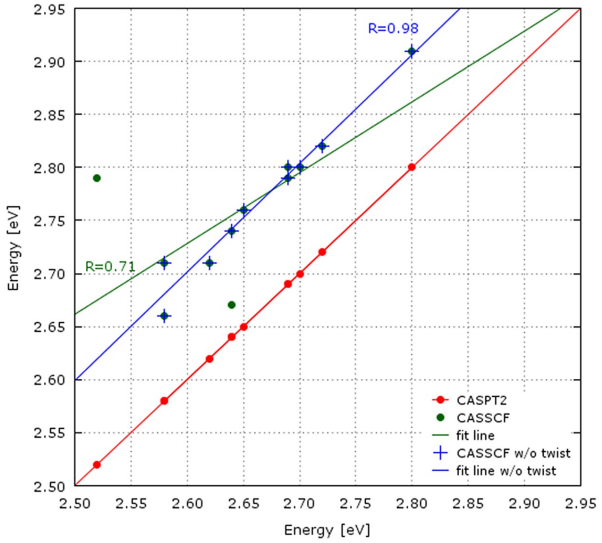
Wroclaw University of Technology, Institute of Physical & Theoretical Chemistry, Wyb. Wyspianskiego 27, 50-370 Wroclaw, Poland



Stosując metody CASPT2, MP2, DFT, LCC2, CC2 oraz CASSCF systematycznie zbadano struktury oraz wertykalne energie wzbudzeń 11-cis-retinalu. W metodzie CASSCF znacznie przesadzone są zmiany długości wiązań, zaś metoda LCC2 zawodzi przy opisie przejść typu CT.

Spectral properties of retinal analogues resolved at CASPT2 level of theory





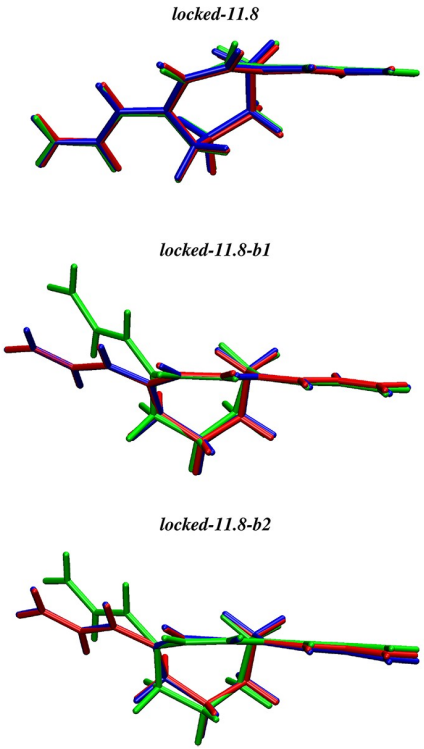


Figure 3. Superposition of *locked-11.8* conformer structures obtained at the CASPT2/ANO-L-VDZP (in blue), CASSCF/ANO-L-VDZP (in green), and MP2/cc-pVTZ (in red) levels of theory.

Biochimie 95 (2013) 1640–1649

Contents lists available at SciVerse ScienceDirect

Biochimie

journal homepage: www.elsevier.com/locate/biochi

Research paper

Toward very potent, non-covalent organophosphonate inhibitors of cathepsin C and related enzymes by 2-amino-1-hydroxy-alkanephosphonates dipeptides

Marcin Drąg [a,*], Ewa Wieczerzak [b], Małgorzata Pawełczak [c], Łukasz Berlicki [a], Zbigniew Grzonka [b], Paweł Kafarski [a]

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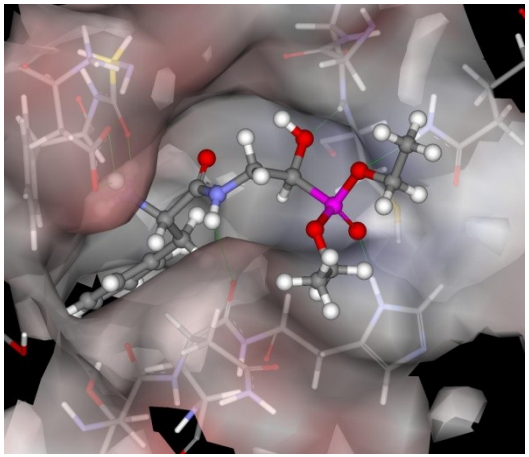
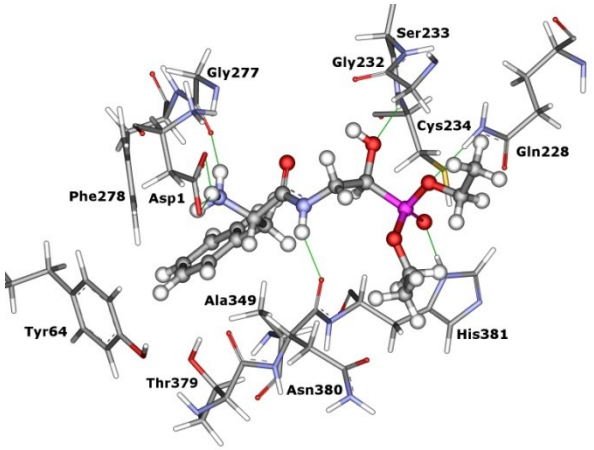
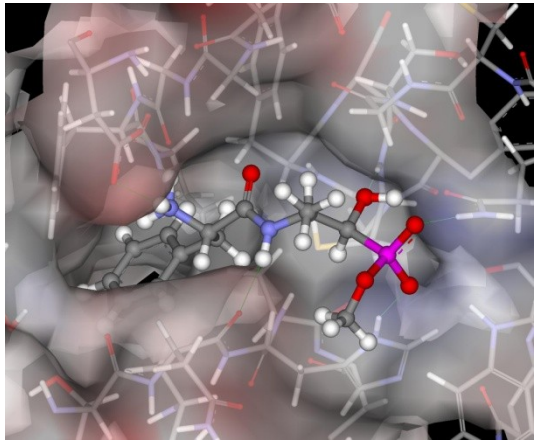
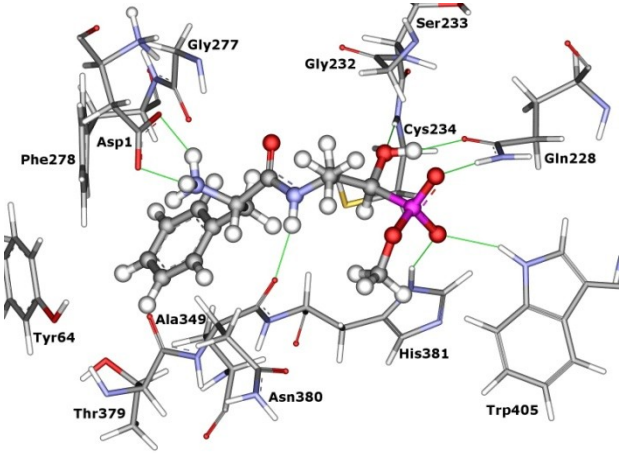
Zsyntezowano i zbadano doświadczalnie aktywność 17 inhibitorów katepsyny. Stosując pakiet oprogramowania Accelrys ustalono, że istotnym elementem wiążącym się w centrum aktywnym jako analog stanu przejściowego jest grupa hydroksymetylowa a nie fosfonowa.

Inhibitory katepsyny C









Drąg, M.; Wieczerzak, E.; Pawełczak, M.; Berlicki, Ł.; Grzonka, Z.; Kafarski, P. Toward very potent, non-covalent organophosphonate inhibitors of cathepsin C and related enzymes by 2-amino-1-hydroxy-alkanephosphonates dipeptides. *Biochemie* **2013**, *95*, 1640 - 1649.

J Biol Inorg Chem (2013) 18:391–399
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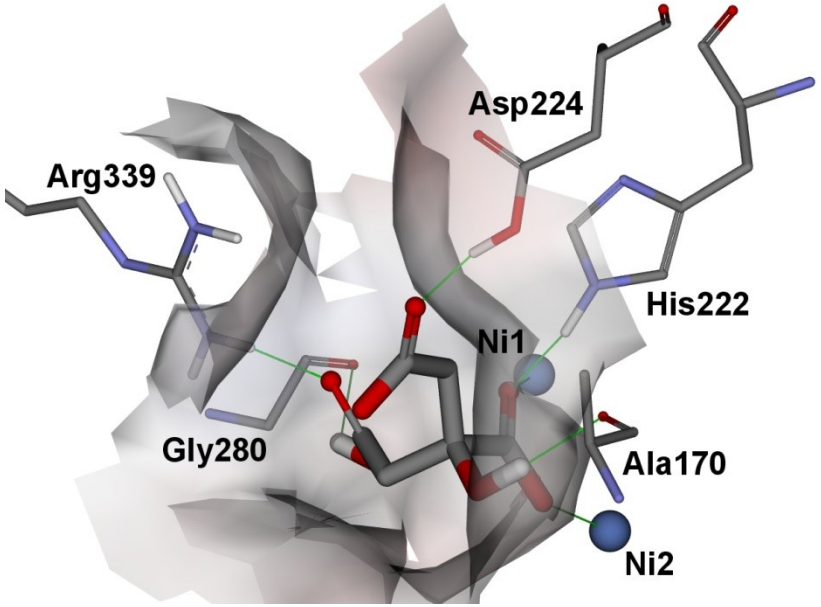
ORIGINAL PAPER

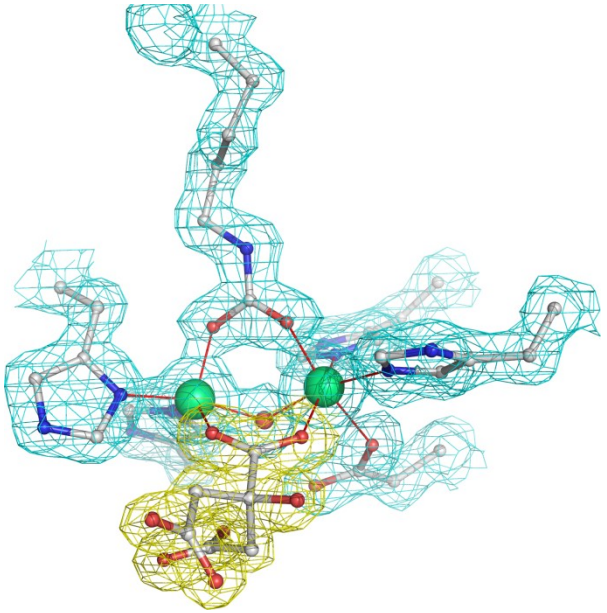
The crystal structure of *Sporosarcina pasteurii* urease in a complex with citrate provides new hints for inhibitor design

Stefano Benini · Paulina Kosikowska · Michele Cianci · Luca Mazzei · Antonio Gonzalez Vara · Łukasz Berlicki · Stefano Ciurli

Stosujac metodę dyfrakcji rentgenowskiej wyznaczono strukturę kompleksu ureazy z cytrynianem. Stosując oprogramowanie Discovery Studio opracowano szczegółowy model wiązania liganda w centrum aktywnym.

Analiza sposobu wiązania cytrynianu do bakteryjnej ureazy





Benini, S.; Kosikowska, P.; Cianci, M.; Mazzei, L.; Vara, A. G.; Berlicki, Ł.; Ciurli, S. The crystal structure of Sporosarcina pasteurii urease in a complex with citrate provides new hints for inhibitor design. *J. Biol. Inorg. Chem.* **2013**, *18*, 391 - 399.

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Research paper

An integrated approach to the ligand binding specificity of *Neisseria meningitidis* M1 alanine aminopeptidase by fluorogenic substrate profiling, inhibitory studies and molecular modeling☆

Ewelina Węglarz-Tomczak [a], Marcin Poręba [a], Anna Byzia [a], Łukasz Berlicki [a], Bogusław Nocek [b], Rory Mulligan [b], Andrzej Joachimiak [b], Marcin Drąg [a], Artur Mucha [a,*]

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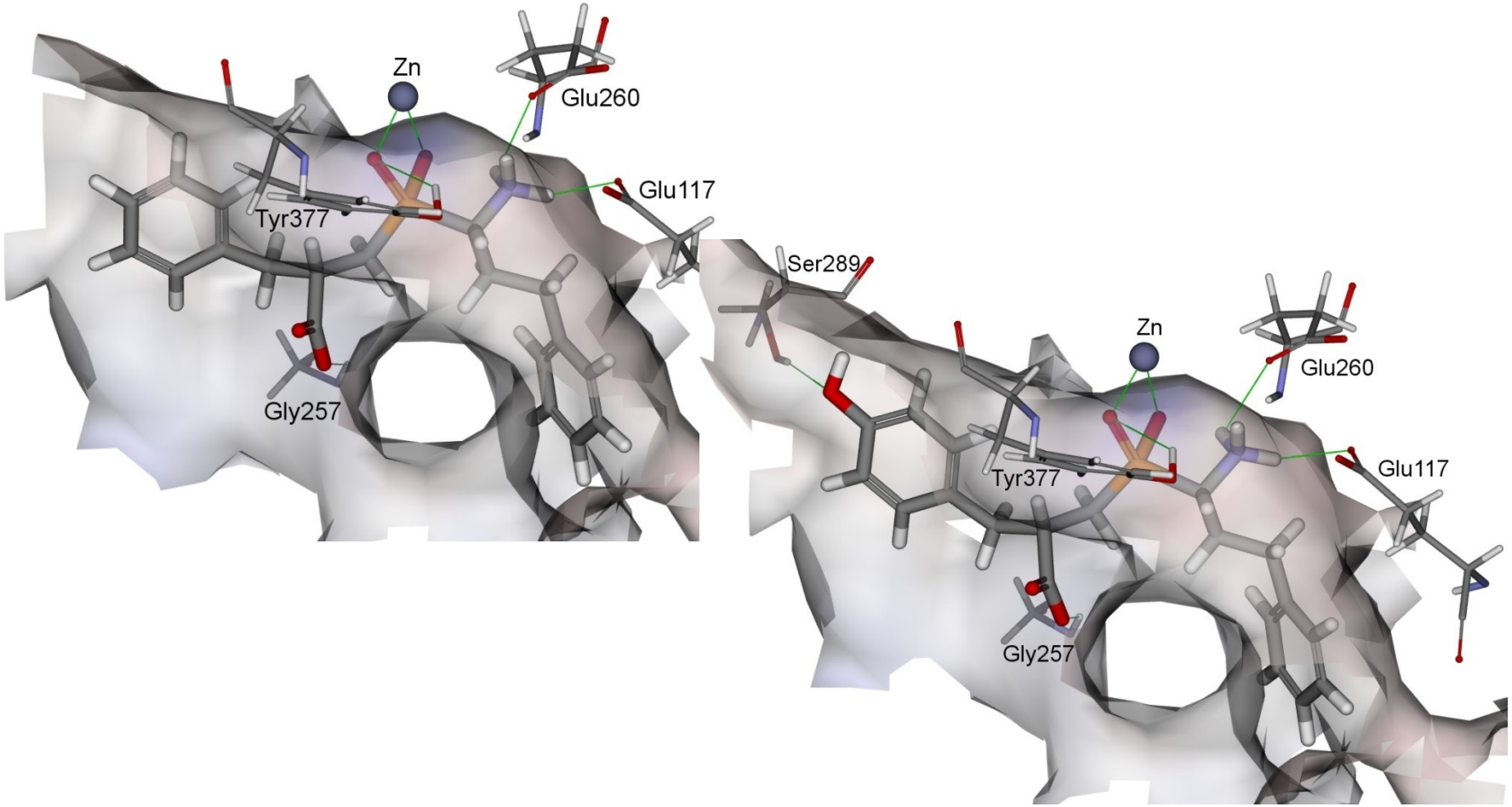
[b] *The Midwest Center for Structural Genomics, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439, USA*

Stosując oprogramowanie Discovery Studio przeanalizowano możliwości wiązania organofosforowych inhibitorów przez aminopeptydazę alaninową.

Inhibitory APN



Węglarz-Tomczak, E.; Poręba, M.; Byzia, A.; Berlicki, Ł.; Nocek, B.; Mulligan, R.; Joachimiak, A.; Drąg, M.; Mucha, A. An integrated approach to the ligand binding specificity of Neisseria meningitidis M1 alanine aminopeptidase by fluorogenic substrate profiling, inhibitory studies and molecular modeling. *Biochimie* **2013**, *95*, 419 - 428.

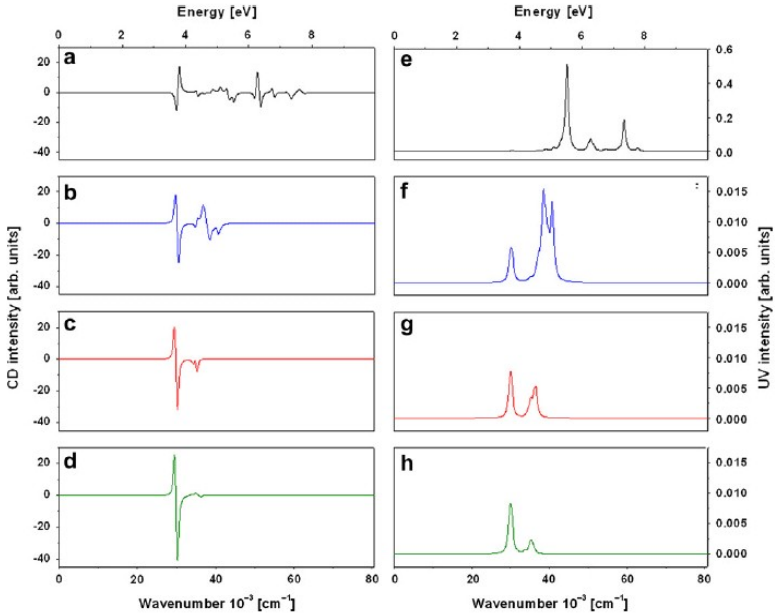


Fig. 7. Theoretical CD spectra of *m*DNB: (a) for neutral molecule monomer, (b) dimer, (c) trimer, (d) tetramer, and corresponding UV–Vis spectra (e–h), all along hypothetical helix shown in Fig. 1.

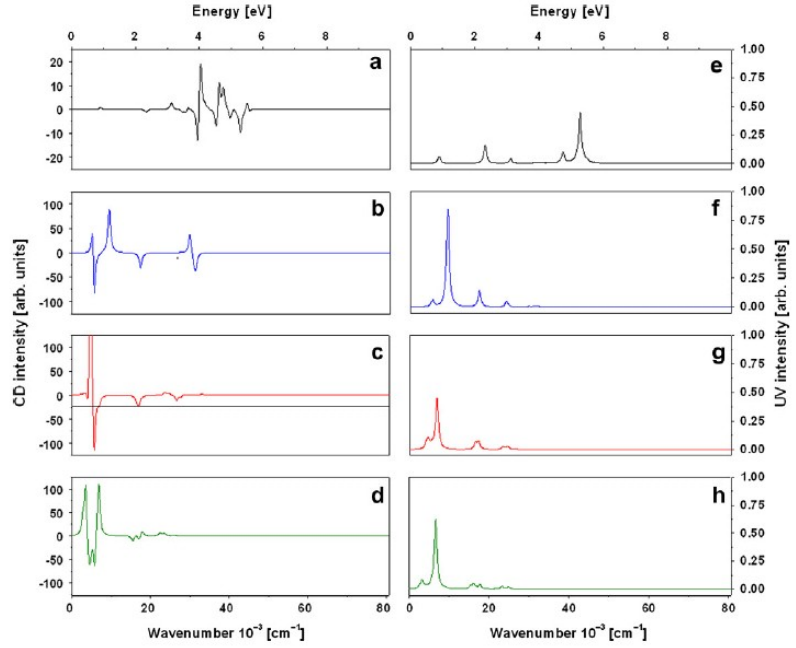


Fig. 8. Theoretical CD (a–d) and UV–Vis –NIR (e–h) spectra of *m*DNB: for radical anion monomer, charged dimer, charged trimer, and charged tetramer, respectively, all along hypothetical helix shown in Fig. 1.

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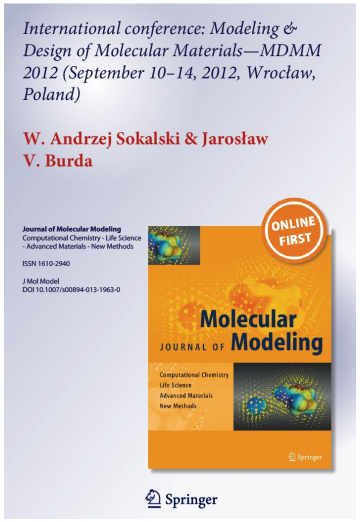

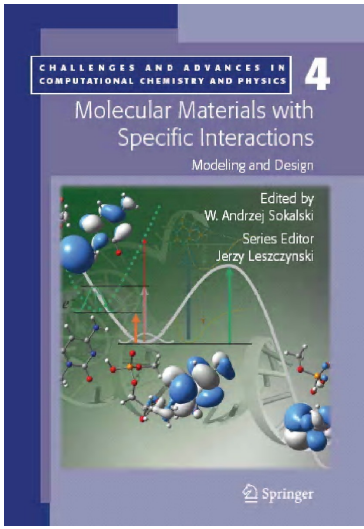

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