



## ACADEMIC TEACHER PROFESSIONAL EXPERIENCE

### DOCTORAL SCHOOL OF WROCLAW UNIVERSITY OF SCIENCE AND TECHNOLOGY

#### 1. Basic information

Name, surname:	W. Andrzej Sokalski
Grade / Title:	Professor
Scientific discipline	nauki chemiczne / chemical sciences
Faculty:	W3 Wydział Chemiczny / Faculty of Chemistry
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#### 2. Publication record

*Up to 10 most important papers published over the period of previous 10 years.*

No.	Description (authors, publication title, journal / conference, DOI)	Publication year
1.	Paweł Kędzierski; Martyna Moskal; W. Andrzej Sokalski, Catalytic Fields as a Tool to Analyze Enzyme Reaction Mechanism Variants and Reaction Steps, Journal of Physical Chemistry B, DOI: 10.1021/acs.jpcc.1c05256	2021
2.	Wiktor Beker, W. Andrzej Sokalski, Bottom-Up Nonempirical Approach To Reducing Search Space in Enzyme Design Guided by Catalytic Fields, J.Chem.Theor.Comp., <a href="https://doi.org/10.1021/acs.jctc.0c00139">https://doi.org/10.1021/acs.jctc.0c00139</a>	2020
3.	Paweł Kędzierski, Maria Zaczekowska, W. Andrzej Sokalski, Extreme Catalytic Power of Ketosteroid Isomerase Related to the Reversal of Proton Dislocations in Hydrogen-Bond Network, J.Phys.Chem. B, <a href="https://doi.org/10.1021/acs.jpcc.0c01489">https://doi.org/10.1021/acs.jpcc.0c01489</a>	2020
4.	Martyna Chojnacka, Mikołaj Feliks, Wiktor Beker, W. Andrzej Sokalski, Predicting substituent effects on activation energy changes by static catalytic fields, Journal of Molecular Modeling, DOI: 10.1007/s00894-017-3559-6	2018
5.	Sławomir J. Grabowski; W. Andrzej Sokalski, Are Various $\sigma$ -Hole Bonds Steered by the Same Mechanisms?, ChemPhysChem, DOI: 10.1002/cphc.201700224	2017
6.	Wiktor Beker; Marc W. van der Kamp; Adrian J. Mulholland; W. Andrzej Sokalski, Rapid Estimation of Catalytic Efficiency by Cumulative Atomic Multipole Moments: Application to Ketosteroid Isomerase Mutants, J.Chem.Theor.Comp, <a href="https://doi.org/10.1021/acs.jctc.6b01131">https://doi.org/10.1021/acs.jctc.6b01131</a>	2017
7.	Langner, K.M.; Beker, W.L.; Dyguda-Kazimierowicz, E.; Sokalski, W.A., Tracking molecular charge distribution along reaction paths with atomic multipole moments, Struct.Chem., DOI: 10.1007/s11224-016-0741-x	2016
8.	Konieczny, J.K.; Sokalski, W.A., Universal short-range ab initio atom-atom potentials for interaction energy contributions with an optimal repulsion functional form, J.Mol.Model., DOI: 10.1007/s00894-015-2729-7	2015
9.	Dyguda-Kazimierowicz, E.; Roszak, S.; Sokalski, W.A., Alkaline hydrolysis of organophosphorus pesticides: The dependence of the reaction mechanism	2014



	on the incoming group conformation, J.Phys.Chem.B, DOI: 10.1021/jp503382j	
10.	Giedroyć-Piasecka, W.; Dyguda-Kazimierowicz, E.; Beker, W.; Mor, M.; Lodola, A.; Sokalski, W.A., Physical nature of fatty acid amide hydrolase interactions with its inhibitors: Testing a simple nonempirical scoring model, J.Phys.Chem. B, DOI: 10.1021/jp5059287	2014

### 3. Projects and grants

List of the most important 5 projects/grants with basic description including: title, source(s) of funding, name of the call, role in the project (e.g., principal investigator).

1.	Role in the project (e.g., principal investigator, work package leader, etc.)	Principal Investigator
	Project title	Catalytic fields as the tool for theoretical analysis and design of biocatalysts
	Sources of funding	NCN
	Name of the call	OPUS 17
	Implementation period	2017-2023
2.	Role in the project (e.g., principal investigator, work package leader, etc.)	Work package leader
	Project title	Applications of new modeling techniques aiding rational design of inhibitors, biocatalysts or molecular switches
	Sources of funding	POIG
	Name of the call	EIT+
	Implementation period	2009-2012
3.	Role in the project (e.g., principal investigator, work package leader, etc.)	Principal Investigator
	Project title	European Reintegration Grant LIGDES
	Sources of funding	European Union
	Name of the call	MERG -CT-2004-516486
	Implementation period	2006-2008
4.	Role in the project (e.g., principal investigator, work package leader, etc.)	Principal Investigator
	Project title	Chemical Materials and Computational Modeling Program
	Sources of funding	US GOVERNMENT
	Name of the call	W912HZ-04-2-002
	Implementation period	2005-2008
5.	Role in the project (e.g., principal investigator, work package leader, etc.)	Principal Investigator
	Project title	Development of Scientific and Didactic Potential of Young Research Staff at Wrocław University of Science and Technology
	Sources of funding	NCBR
	Name of the call	POKL 04.01.01-00-125/09-01
	Implementation period	2010-2014



#### 4. International experience

*Brief description of international cooperation and experience (e.g., research stays, cooperation with foreign entities, coordination or participation in international projects or programmes, keynote speeches and presentations delivered at renowned international conferences, visiting professor stays, invited lectures).*

No.	Description	Year(s)
1.	The Johns Hopkins University, Baltimore, MD, USA	1979-1990
2.	Roswell Memorial Cancer Institute, Buffalo, NY, USA	1990-1992
3.	Visiting Professor at P & M Curie University Paris VI, France	1995
4.	Jackson State University, Jackson, MS, USA	2000-2006
5.	Visiting Professor at Universite de Bourgogne, Dijon, France	2001
6.	Visiting Professor at Kyoto University, Japan	2008
7.	Visiting Professor of Chinese Academy of Science, Shanghai, Beijing, Dalian	2013

#### 5. Experience in teaching doctoral students

*Brief description of experience in teaching doctoral students (e.g., courses in doctoral schools and PhD studies, summer/winter schools for doctoral students, tutorials, trainings, etc.).*

No.	Description	Year(s)
1.	Retrieval of Scientific and Technical Information	1995-2018
2.	Research Skills	2019 --
3.	Lecturing at NSF Workshops "Modeling Biomolecules" in Jackson, MS, USA	2006-2007

#### 6. List of supervised doctoral students

*List of all supervised doctoral students that defended the PhD including: name of the student, dissertation title, year of awarding PhD.*

No.	Name, surname	Dissertation title	Year of awarding PhD
1.	Krzysztof Strasburger	Quantum Chemical Studies of Bound Positron States in Atomic and Molecular Systems	1996
2.	Paweł Kędzierski	Investigation of the Nature of Interactions in Enzyme Active Centers	2000
3.	Paweł Dziekoński	Investigation of the Physical Nature of Catalytic Effects and Modeling of Optimal Catalytic Fields	2003
4.	Borys Szefczyk	Theoretical Methods for Investigation of Catalytic and Inhibitory Activity of Enzymes for Chorismate Mutase and Phenylalanine Ammonialyase	2005
5.	Edyta Dyguda	Modeling of Enzymatic Inhibition and Catalysis within the Framework of the Theory of Intermolecular Interactions	2009
6.	Karol M. Langner	Nonempirical methods in the analysis and electrostatic modelling of biomolecule interactions	2010



7.	Wiktorija Jedwabny	The Analysis of Interactions in Protein Binding Sites as a Tool Aiding Inhibitory Activity Prediction	2016
8.	Wiktor Beker	Methods of Analysis of Catalytic Activity and Catalyst Design based on the Theory of Intermolecular Interactions	2017
9.	Jan Konieczny	Modeling of Ionic Liquid Properties with empirical and Nonempirical Potential Functions	2019

## 7. Prizes and awards

*The most important national and international prizes and awards related to research, development and teaching activities.*

No.	Description	Year
1.	Minister of Science and Education Prize	1977,1980,1985, 2006
2.	Docento Discimus	2010
3.	Prof. Trzebiatowski Scientific Prize	2015
4.	Medal of Polish Education Committee	2016

## 8. Other significant achievements

*Information on other significant achievements related to research, development and teaching activities.*

Senior Editor of Journal of Molecular Modeling (Springer-Nature),  
Editorial Board Member of Computational Biology & Chemistry (Elsevier)  
and Wiadomości Chemiczne (PTCh)  
Organizer of Computational Chemistry (1997) and Bioinformatics (2009) MSc Eng programs  
Supervisor of Doctoral Studies at 13 Departments at WUST 2002-2023,  
Organizer of 8 international conferences Modeling & Design of Molecular Materials 2004-2018