

Curriculum vitae: Dr. David M. Smith

PERSONAL: Born April 22, 1973, Dubbo Australia. Married, Three children.
Holder of Croatian and Australian citizenships.

**CURRENT STATUS**

- 03.18-: Director General of the Ruđer Bošković Institute (RBI) in Zagreb, Croatia. The Institute has 11 Divisions and over 850 employees.

PREVIOUS WORK EXPERIENCE

- 03.16-03.18.: Divisional Head and Senior Scientist, Division of Physical Chemistry, Ruđer Bošković Institute (RBI) in Zagreb, Croatia. The Division has 6 research laboratories and 75 employees.
- 04.16-10.16: Special Advisor to the Croatian Minister for Science, Education and Sports, in the area of Research and Development.
- 10.09-01.14: Assistant Director for International Collaboration and Projects at the Ruđer Bošković Institute (RBI).
- 10.09-12.17: Visiting Professor at the Excellence Cluster: "Engineering of Advanced Materials" (EAM) and the Center for Computational Chemistry (CCC) at the Friedrich-Alexander-University (FAU) of Erlangen-Nuremberg, Germany.
- 02.14-02.16: Senior Scientist (equivalent to Full Professor) in the Division of Organic Chemistry and Biochemistry (DOCB) at RBI in Zagreb, Croatia.
- 10.08-02.16: Group leader of the Group for Quantum Organic Chemistry (GQOC) in DOCB, RBI. The group grew from 6 and 16 members during this period.
- 02.08-02.14: Senior Research Associate (equivalent to Associate Professor), DOCB, RBI
- 03.04-02.08: Research Associate (equivalent to Assistant Professor), DOCB, RBI.
- 10.01-02.04: Postdoctoral Fellow in the group of Prof. Hendrik Zipse at the Department of Chemistry, Ludwig-Maximilians-University (LMU), Munich, Germany.
- 04.00-08.01: Postdoctoral Researcher in the group of Prof. Zvonimir Maksić, DOCB, RBI.

EDUCATION

- 01.96-03.00: PhD at the Research School of Chemistry (RSC), Australian National University (ANU), Canberra, Australia; Supervisor Prof. Leo Radom; Thesis: Theoretical Studies of Coenzyme-B₁₂-Dependent Reactions.
- 03.95-11.95: Awarded first class honors [BSc(Hons)] in Chemistry from the ANU Department of Chemistry; Supervisor Prof. Gad Fischer; Thesis: An Ab initio study of the electronic spectrum of the triazine molecules.
- 04.91-11.94: Bachelor of Science (BSc) and Bachelor of Economics (BEC), ANU.

ADDITIONAL MOBILITY

- 01.14-09.14: Sabbatical stay at EAM-FAU, Erlangen, Germany.
- 10.08-12.08; 04.08-05.08; 02.05-05.05: Visiting Fellowships at the School of Chemistry, University of Sydney, Sydney, Australia.
- 02.03-05.03: Visiting Fellowship - RSC, ANU, Canberra, Australia.
- 05.97-07.97: Partnerships for Excellence: British Council Postgraduate Bursary to collaborate with Professor Bernard Golding at the Department of Chemistry, University of Newcastle upon Tyne, England.

FELLOWSHIPS, SCHOLARSHIPS, AWARDS AND DONATIONS

- 11.08: Recipient of the 2008 Lavoslav (Leopold) Ružička Award of the Croatian Chemical Society for Young Scientists.
- 01.05: Recipient of an equipment donation from the Alexander von Humboldt (AvH) Foundation in the form of a computer cluster valued at 20,000 EUR.
- 04.04-04.05: Return Fellowship for Research Fellows of the AvH Foundation in Central and Eastern Europe to be carried out at the RBI.

- 11.03–02.04: DFG (German Research Organization) Funded Postdoctoral Fellowship to work at the Department of Chemistry, LMU, Munich, Germany.
- 03.02–10.03: AvH postdoctoral fellowship carried out at LMU Munich, Germany.
- 04.01: Winner of the Dean's Prize for the best PhD thesis in 2000 at RSC, ANU.
- 05.97–07.97: British Council Postgraduate Bursary (see above).
- 01.96–09.99: Australian Postgraduate Award for PhD students.
- 03.95–11.95: RSC Honors year Scholarship for talented students.
- 12.94-03.95: RSC Summer Research Scholarship.

RESEARCH AND OTHER PROJECTS

- 07.15–10.16: Principle investigator of the project funded by a European Social Fund program for Research Scholarships for the Professional Development of Young Researchers and Postdocs, entitled *Network for Professional Development Network for Young Scientists in Interdisciplinary Research of Innovative Surfaces and Materials (MIPoMat)* and valued at 2 000 000 HRK.
- 01.15–12.19: Principle investigator of a Career Development Project for Young Researchers – The Training of New Doctors of Science funded by the Croatian Science Foundation (CSF) and valued at 480 000 HRK.
- 07.14–12.18: Principle investigator of a Research Project funded by the Croatian Science Foundation (CSF), entitled *Computational Solutions in the Life Science: The Importance of Molecular Flexibility* and valued at 900 000 HRK.
- 10.13–10.15: Coworker for a project within the Research Cooperability, Crossing Borders Programme, entitled *Time resolved photoelectron spectroscopy as a probe for ultrafast excited state dynamics*, funded by the Unity through Knowledge Fund (UKF) and valued at 185 000 EUR.
- 07.13–01.17: Leader of the Management Work Package of a project within the Seventh Framework Programme, entitled *Enhancement of the Innovation Potential in SEE through New Molecular Solutions in Research and Development - InnoMol (FP7- REGPOT-2012-2013-1)* valued at 4.7 million EUR.
- 10.10–10.13: Joint principle investigator of a project within the Research Group Linkage Programme, entitled *Computational Life Sciences on Open Shell Intermediates*, funded by the Alexander von Humboldt Foundation (AvH) and valued at 50 000 EUR.
- 04.07–04.10: Coordinator of a successfully completed project within the Sixth Framework Programme (FP6), entitled *Reinforcement of the Centre for Computational Solutions in the Life Sciences (EU-FP6-043749-ReCompSoLS)*, funded by the European Commission and valued at 380 000 EUR.
- 01.07–12.13: Principle investigator of the project entitled *Computational Studies of Protein Structure and Function (098-0982933-2937)*, funded by the Croatian Ministry of Science, Education and Sport (MSES) and valued at 90 000 HRK per year.
- 04.05–12.06: Principle investigator of the successfully completed project: *Computational Studies of Protein Structure and Function (0098151)*, funded by MSES and valued at 30 000 HRK per year.

SUPERVISION

- 01.15–: Supervisor of the PhD students: Marko Hanževački, Nataša Vučemilović-Alagić and Robert Stepić within the Integrated Graduate School (IGS) "Advanced Materials and Processes" of the EAM at the FAU of Erlangen-Nuremberg, Germany.
- 11.15 –: Supervisor of Dr. Christian R. Wick, a postdoctoral researcher employed on a Croatian Science Foundation project at the RBI
- 05.10–04.16: Supervisor of Zlatko Brkljača's and Zoran Miličević's PhD theses, within IGS, EAM, FAU, Germany.
- 05.09–11.09: Host for Dr. Gregory M. Sandala, a postdoctoral fellow financed by the Croatian Science Foundation, through its "Brain Gain" programme.
- 06.07–07.13: Supervisor of Karmen Čondić-Jurkić's doctoral thesis, within IGS, EAM, FAU, Germany.
- 03.09–09.09: Supervisor of Zlatko Brkljača's diploma thesis, completed at the Faculty of Chemistry (FC) at the University of Zagreb (UniZg), Croatia. Mark: Excellent.

- 02.09–06.09: Supervisor of Zoran Miličević's diploma thesis, FC, UniZg Mark: Excellent.
- 10.05–06.06: Supervisor of Karmen Čondić-Jurkić's diploma, FC, UniZg Mark: Excellent.
- 03.05–11.05: Co-Supervisor of Daniel Miller's diploma, Department of Chemistry (DC), University of Sydney (USyd), Australia. Mark: Excellent.

REFEREEING

- Frequent expert reviewer in journals including: *Angew. Chemie*; *J. Am. Chem. Soc.*; *Chem. Eur. J.*; *J. Chem. Theory Comput.*; *Chem. Sci.*; *J. Comput. Chem.*; *J. Org. Chem.*; *J. Phys. Chem. Lett.*; *PhysChemChemPhys*; *Soft Matter*; *Langmuir*; *Comput. Theor. Chem.*; *J. Chem. Phys.*; *Int. J. Quant. Chem.*; *Mol. Simul.*; *J. Mol. Mod.*; *J. Phys. Org. Chem.*; *Adv. Syn. Cat.*; and *Chirality*.

TEACHING

- 10.11-: Lecturer for the course in Computational Chemistry given as part of the postgraduate study program in Medicinal Chemistry at the University of Rijeka.
- 09.07 & 09.09: Presenter of "hands-on" practical computational sessions in Molecular Dynamics and QM/MM Calculations at conferences in Opatija and Primošten.
- 03.95–10.98: Teaching assistant for Chemistry A11 (introductory course for first-year undergraduate students), Department of Chemistry, Australian National University.
- 03.9 –10.97: Personal tutor for numerous high school students in the areas of Chemistry, Mathematics, Physics, and Economics.

COMMITTEES, BOARDS AND WORK GROUPS

- 11.15-03.18: Chairman of the Committee for collaboration between RBI and its spin-off company: RMC.
- 02.15-03.18: Member of the Managing Board of RMC.
- 02.15-10.15: Member of the Croatian Science Foundation's Expert Panel for Chemistry.
- 05.12-: Representative of the Ruder Bošković Institute in EARTO.
- 05.12-: Member of EARTO's Expert Working Group for Horizon 2020.
- 02.12-06.15: Member of the Expert Panel for the National Science Awards in the Field of Natural Sciences.
- 04.11-: Member of the Steering Committee for Preparation of Structural projects at RBI.
- 03.11-: Member of the Committee for Monitoring Croatian Participation in EU-FP.
- 05.10-: Member of the Committee for the Thematic Evaluation of the RBI.
- 01.10-: Coordinator of the Committee for Strategic International Projects at the RBI.

INVITED LECTURES AT INTERNATIONAL CONFERENCES AND INSTITUTIONS

- 35 keynote and invited lectures at conferences including:
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| 09.17. | WATOC2017 (Eleventh Triennial Congress) in Munich, Germany. |
| 07.16 | ICPOC23 (23rd IUPAC Conference on Physical Organic Chemistry), Sydney, Australia. |
| 12.15. | Pacificchem 2015 in Honolulu, Hawaii, USA. |
| 06.14. | CSC2014 (97th Canadian Chemistry Conference), Vancouver, Canada. |
| 04.12 | SEB-2012 (3rd Inaugural Symposium on Enzymes & Biocatalysis-2012) in Xi'an, China |
| 07.11. | WATOC2011 (Ninth Triennial Congress) in Santiago de Compostela, Spain. |
| 12.10. | Pacificchem 2010 in Honolulu, Hawaii, USA. |
| 09.10. | CtB2010 (Chemistry towards Biology), Primošten, Croatia. |
| 06.10. | From Solid State to Biophysics V, Cavtat, Dubrovnik, Croatia. |
| 02.10. | The 24th Molecular Modelling Workshop, Erlangen, Germany. |
| 09.09. | ICCMSE 2009 (7th Conference of Comput. Methods in Sci. and Eng.), Rhodes, Greece. |
| 08.09. | Gordon Research Conference on Vitamin B ₁₂ and Cophins, Oxford, UK. |
| 09.08. | TACC2008 (Theory and Applications of Comp. Chem. 2008) in Shanghai, China. |
| 09.08. | WATOC2008 (Eighth Triennial Congress) in Sydney, Australia. |

- Invited lectures at numerous international institutions, including the:
 - University of Western Australia and Curtin University, Perth, Australia
 - Australian National University, Canberra, Australia
 - National Institute of Chemistry, Ljubljana, Slovenia;
 - Department of Chemistry, University of Newcastle upon Tyne, UK;
 - Department of Microbiology, Phillips University, Marburg, Germany;
 - Department of Chemistry, LMU, Munich, Germany; and
 - Department of Chemistry, University of Sydney Australia.,
 - Department of Chemistry, University of California, Los Angeles, USA.

ORGANIZATION OF CONFERENCES AND WORKSHOPS

Co-organizer of the following conferences and workshops:

- 06.14: Symposium within the 97th Canadian Chemistry Conference, Vancouver, Canada
 09.13: Summer School on Open Shell Intermediates, Primošten, Croatia (within AvH project)
 06.13: EARTO Annual Conference in Dubrovnik, Croatia
 03.12: Winter School on Open Shell Intermediates, Munich, Germany (within AvH project)
 09.09: The 3rd Adriatic Meeting on Computational Solutions in the Life Sciences, Primošten, Croatia (FP6 & ESF)
 09.07: The 2nd Opatija Meeting on Computational Solutions in the Life Sciences, Opatija, Croatia (FP6 & AvH)

MEMBERSHIPS IN SCIENTIFIC ORGANIZATIONS

Currently a member of the:

- American Chemical Society (ACS),
- Croatian Chemical Society (HKD) and the
- World Association of Theoretically Oriented Chemists (WATOC).

OVERVIEW OF PUBLICATION TRACK RECORD AND SELECTED PUBLICATIONS

Number of articles in journals listed in WoS	60
Number of articles in Q1 (IF ₂₀₁₅ , JCR)	46
Cumulative impact factor (IF ₂₀₁₅ , JCR)	442
Average impact factor (IF ₂₀₁₅ , JCR)	7.5
Number of citations (WoS 03.19/Research Gate)	1466/1549
Sum of Times Cited without self-citations (WoS 03.19)	1328
h-index (WoS/Research Gate)	20/21

5 Selected papers:

1. Bucher*, D.; Sandala*, G. M.; Durbeej, B.; Radom*, L.; **Smith*, D. M.** *J. Am. Chem. Soc.* **134** (2012), 1591-1599. The Elusive 5'-Deoxyadenosyl Radical in Coenzyme-B₁₂-Mediated Reactions.
2. Brkljača, Z.; Čondić-Jurkić, K.; Smith*, A.-S.; **Smith*, D. M.** *J. Chem. Theory Comput.* **8** (2012), 1694–05. Calculation of a CD Spectrum of a Peptide from its Conformational Phase Space: The Case of Met-enkephalin and Its Unnatural Analogue.
3. Dragičević, I.; Barić*, D.; Kovačević, B.; Golding, B. T.; **Smith*, D. M.** *Chem. Eur. J.* **21** (2015), 6132-6143. Non-enzymatic Ribonucleotide Reduction in the Prebiotic Context.
4. Kovačević, B.; Barić, D.; Babić, D.; Bilić, L.; Hanževački, M.; Sandala, G. M.; Radom, L.; **Smith*, D. M.** *J. Am. Chem. Soc.* **140** (2018), 8487-8496. Computational Tale of Two Enzymes: Glycerol Dehydration With or Without B₁₂.
5. Stepić, R.; Wick, C. R.; Strobel, V.; Berger, D.; Vučemilović-Alagić, N.; Haumann, M.; Wasserscheid, P.; Smith, A.-S.; **Smith*, D. M.** *Angew. Chem. Int. Ed. Eng.* **58**, (2019), 741-745 (Inside Cover). Mechanism of the Water–Gas Shift Reaction Catalyzed by Efficient Ruthenium Based Catalysts: A Computational and Experimental Study.