

ALEKSANDR B. SAHAKYAN, PHD

PLACE AND DATE OF BIRTH: Yerevan, 1987
ADDRESS: Centre for Computational Biology,
Weatherall Institute of Molecular Medicine,
Radcliffe Department of Medicine,
John Radcliffe Hospital, University of Oxford,
Headington, Oxford, OX3 9DS, United Kingdom.
EMAILS: aleksandr.sahakyan@imm.ox.ac.uk
aleksahak@cantab.net
HOME PAGE: <http://www.atgcdynamics.org>

RESEARCH INTERESTS

My research targets genomics and genome dynamics through the development of highly quantitative methods for defining the structure and dynamics of (epi)genome, gene regulatory pathways, involved macromolecules and their interaction networks. I am interested in combining computational biology, advanced predictive modelling (a.k.a machine learning), computational chemistry (QM, MD) and experimental biophysical techniques to reach a new level of precision in systems biology at both genome and proteome levels. Other interests span the origin of life research, prebiotic pathway exploration and weak intermolecular forces.

●Machine Learning ●Advanced Biological Sequence Analysis and Functional (Gen/Prote)omics ●Biomolecular Structure and Dynamics ●Quantum Mechanical Calculations and Molecular Modeling ●Molecular Dynamics Simulations ●NMR of Bio- and Small Molecules ●UV/Vis/CD Optical Spectroscopy ●Nucleic Acids ●Proteins ●Origin of Life

Bullet colours encode the research technique/area for labelling the publication and presentation list in this CV.

RECENT EMPLOYMENT

SEP. 2017 - PRESENT Principal Investigator / Group Head,
Centre for Computational Biology,
Weatherall Institute of Molecular Medicine,
Radcliffe Department of Medicine,
John Radcliffe Hospital, University of Oxford,
Headington, Oxford, OX3 9DS, United Kingdom.

DEC. 2013 - SEP. 2017 Research Fellow,
Department of Chemistry, University of Cambridge,
and Cancer Research UK Cambridge Institute.
“Computational Genomics and Structural
Systems Biology of (Epi)Genome”
Advisor: Prof. Sir Shankar BALASUBRAMANIAN, FRS, FMedSci.

EDUCATION

OCT. 2009 - MAY 2012 Ph.D. in Chemistry (Theoretical and Biological),
Department of Chemistry, University of Cambridge.
“Extending the Boundaries of Deciphering
Biomolecular Structure and Dynamics Using NMR
Chemical Shifts” | Advisor: Prof. Michele VENDRUSCOLO
THE DISSERTATION CAN BE FOUND AT:
<http://www.dspace.cam.ac.uk/handle/1810/243642>

- OCT. 2008 - AUG. 2009 M.Phil. in Computational Biology, Department of Applied Mathematics and Theoretical Physics, University of Cambridge.
Graduated with distinction and Director's award.
- SEP. 2003 - JUN. 2008 B.Sc. & M.Sc. in Pharmaceutical Sciences, Faculty of Pharmacy, Yerevan State Medical University.
Graduated with summa cum laude distinction.

PAST EMPLOYMENT AND RESEARCH VISITS

- OCT. 2012 - OCT. 2015 Schlumberger Interdisciplinary Research Fellow, Darwin College, University of Cambridge.
- OCT. 2012 - DEC. 2013 Department of Chemistry, University of Cambridge.
"Computational Structural Biology"
Post-doctoral research associate | Advisor: Prof. Michele VENDRUSCOLO
- APR. 2005 - SEP. 2008 Molecule Structure Research Centre, National Academy of Sciences, Yerevan, Armenia.
Research assistant | Advisors: Dr. Aleksan SHAHKHATUNI and Dr. Henrik PANOSYAN
- 9 APR. - 7 MAY 2007 Ad Bax Group, Section of Biophysical NMR Spectroscopy, National Institutes of Health (NIH), NIDDK, LCP, Bethesda MD, USA.
Supported by US CRDF grant.
- SEP. 2003 - APR. 2005 Laboratory of Porphyrines, Department of Pharmaceutical Chemistry, Yerevan State Medical University, Yerevan, Armenia.
Contractor | Advisor: Dr. Robert GHAZARYAN

COURSES AND SUMMER SCHOOLS

- 16-19 AUG. 2010 Writing Skills Summer School, CMS, University of Cambridge, Cambridge, UK.
- 18-27 JUL. 2010 CCP5 Summer School, "Methods in Molecular Simulation", Queens University Belfast, Belfast, Northern Ireland, UK.
- 2-9 SEP. 2009 FEBS practical course "Structure, Folding and Dynamics of Proteins and Their Complexes", Budapest, Hungary.
- 19-30 JUL. 2007 Course on "Biophysics and the Challenges of Emerging Threats", International School of Biological Magnetic Resonance, Erice, Sicily.
- 4-14 JUL. 2006 Course on "Protein Folding and Drug Design", International School of Physics "Enrico Fermi", Varenna, Lake Como, Italy.

AWARDS

- APR. 2012 Darwin College Schlumberger Interdisciplinary Research Fellowship
- SEP. 2009 Director's award, Department of Applied Mathematics and Theoretical Physics, University of Cambridge.
*For the outstanding performance in MPhil studies.
(Computational Biology)*
- 28 JUL. 2009 FEBS (Federation of European Biochemical Societies) YTF grant to attend the "Structure, Folding and Dynamics of Proteins and their Complexes" practical course. Budapest, Hungary.
- 29 JUN. 2009 Herchel Smith PhD Studentship.
- 11 SEP. 2008 University of Cambridge, Darwin College bursary award.
- 15 AUG. 2008 Cambridge Overseas Trust, Shell Centenary Scholarship for the MPhil Course in Computational Biology.
- 7 JUL. 2007 16th ISMAR travel stipend (not taken) to attend the 16th ISMAR conference. Kenting, Taiwan.
- 20 MAY 2007 NATO ASI (Advanced Science Institute) award to attend the International School on Biological Magnetic Resonance. Erice, Sicily.
- 27 FEB. 2007 48th ENC (Experimental NMR Conference) student stipend.
- DEC. 2006 Best student award from Yerevan State Medical University.
- 12 SEP. 2006 SMASH 2006 student/post-doc stipend to attend Small Molecule NMR Conference.
- 31 JUL. 2006 Travel grant award from National Foundation of Science and Advanced Technologies in Armenia (NFSAT TGP2006/05).
- 17 MAY 2006 Scholarship grant from Italian Physical Society to attend Enrico Fermi International School of Physics for "Protein Folding and Drug Design" Summer Course. Varenna (Lake Como), Italy.
- MAR. 2006 - SEP. 2008 Participant in CRDF Collaborative Research Grant, Project num.: ARB2-2834-YE-06.
- JAN. 2006 - JAN. 2007 Participant in ANSEF Research Grant, Project num.: 05-PS-chemorg-0823-306.
- 20 DEC. 2005 First place in Students' Scientific Olympiad on Biochemistry.
- SEP. 2005 - JUN. 2008 Highest nominal scholarship (after Mkhitar Heratsi) of the Yerevan State Medical University.
Granted 1 year earlier than the normal practice in YSMU.

- 17 SEP. 2005 Diploma for the best report in Students' Scientific Conference Dedicated to the Anniversary of YSMU.
- 22 JUL. 2004 YSMU Foreign Language Department certificate for outstanding performance in Latin course.
- 25 DEC. 2003 Diploma from the Ministry of Science and Education of the Republic of Armenia for distinctive academic achievements.
- 2-10 MAY 2003 Bronze medal in 37th International Mendeleevian Olympiad on Chemistry. Moscow, Russia.
- 2-10 MAY 2002 3-rd scale diploma in the same 36th Olympiad. Almati, Kazakhstan.
- 1999 - 2003 4 - First scale, 3 - second scale and 2 - third scale diploma from various Armenian Science Olympiads.

PUBLICATIONS

Sahakyan A. B., Chambers V. S., Marsico G., Santner T., Di Antonio M., Balasubramanian S. "Machine Learning Model for Sequence-Driven DNA G-Quadruplex Formation", *Sci. Rep.*, 7, 14535, 2017. <http://dx.doi.org/10.1038/s41598-017-14017-4> ● ● ● ● ● ● ● ●

Sahakyan A. B., Murat P., Mayer, C., Balasubramanian S. "G-quadruplex Structures within the 3'-UTR of LINE-1 Elements Stimulate Retrotransposition", *Nature Str. Mol. Biol.*, 24, 243-247, 2017. <http://dx.doi.org/10.1038/nsmb.3367> ● ● ● ● ● ● ● ●

Sahakyan A. B., Balasubramanian S. "Single Genome Retrieval of Context-Dependent Variability in Mutation Rates for Human Germline", *BMC Genomics*, 18, 81, 2017. <http://dx.doi.org/10.1186/s12864-016-3440-5> ● ● ● ● ● ● ● ●

Kwok C. K., Marsico G., **Sahakyan A. B.**, Chambers V. S., Balasubramanian S. "rG4-seq Reveals Widespread Formation of G-Quadruplex Structures in the Human Transcriptome", *Nature Methods*, 13, 841-844, 2016. <http://dx.doi.org/10.1038/nmeth.3965> ● ● ● ● ● ● ● ● I have performed the rG4 evolutionary conservational analysis across 68 species, reflected in Figure 3 and Methods.

Kwok C. K., **Sahakyan A. B.**, Balasubramanian S. "Structural Analysis Using SHALiPE to Reveal RNA G-Quadruplex Formation in Human Precursor MicroRNA", *Angew. Chem. Int. Ed.*, 55, 8958-8961, 2016. <http://dx.doi.org/10.1002/anie.201603562> ● ● ● ● ● ● ● ●

Sahakyan A. B. and Balasubramanian S. "Long Genes and Genes with Multiple Splice Variants are Enriched in Pathways Linked to Cancer and Other Multigenic Diseases", *BMC Genomics*, 17, 225, 2016. <http://dx.doi.org/10.1186/s12864-016-2582-9> ● ● ● ● ● ● ● ●

Sahakyan A. B. and Balasubramanian S. "Core Variability in Substitution Rates and the Basal Characteristics of the Human Genome", *bioRxiv*, 10 August, 2015. <http://dx.doi.org/10.1101/024257> ● ● ● ● ● ● ● ●

Hardisty R. E., Kawasaki F., **Sahakyan A. B.**, Balasubramanian S. "Selective Chemical Labeling of Natural T Modifications in DNA", *J. Am. Chem. Soc.*, 137, 9270-9272, 2015. <http://dx.doi.org/10.1021/jacs.5b03730> ● ● ● ● ● ● ● ●

Shahkhatuni A. A., Shahkhatuni A. G., Minasyan N. S., Panosyan H. A., **Sahakyan A. B.** "Revealing the Specific Solute-Solvent Interactions via the Measurements of the NMR Spin-Spin Coupling Constants", *J. Mol. Struct.*, 1083, 175-178, 2015. <http://dx.doi.org/10.1016/j.molstruc.2014.11.058> ● ● ● ● ● ● ● ●

Camilloni C., **Sahakyan A. B.**, Holliday M. J., Isern N. G., Zhang F., Eisenmesser E. Z., Vendruscolo M. "Cyclophilin A Catalyzes Proline Isomerization by an Electrostatic Handle Mechanism", *Proc. Natl. Acad. Sci. U. S. A.*, 111, 10203-10208, 2014. <http://dx.doi.org/10.1073/pnas.1404220111> ●●●●●

Fu B., **Sahakyan A. B.**, Camilloni C., Tartaglia G. G., Paci E., Caflisch A., Vendruscolo M., Cavalli A. "ALMOST: an All Atom Molecular Simulation Toolkit for Protein Structure Determination", *J. Comput. Chem.*, 35, 1101-1105, 2014. <http://dx.doi.org/10.1002/jcc.23588> ●●●●●

Kannan A., Camilloni C., **Sahakyan A. B.**, Cavalli A., Vendruscolo M. "A Conformational Ensemble Derived Using NMR Methyl Chemical Shifts Reveals a Mechanical Clamping Transition that Gates the Binding of the HU Protein to DNA", *J. Am. Chem. Soc.*, 136, 2204-2207, 2014. <http://dx.doi.org/10.1021/ja4105396> ●●●●●

Suardiaz R., **Sahakyan A. B.**, Vendruscolo M. "A Geometrical Parametrisation of C1'- C5' RNA Ribose Chemical Shifts Calculated by Density Functional Theory", *J. Chem. Phys.*, 139, 034101, 2013. <http://dx.doi.org/10.1063/1.4811498> ●●●●●

Sahakyan A. B. and Vendruscolo M. "Analysis of Ring Current and Electric Field Effects on the Chemical Shifts of RNA Bases", *J. Phys. Chem. B*, 117, 1989-1998, 2013. <http://dx.doi.org/10.1021/jp3057306> ●●●●●

Sahakyan A. B. "Computational Studies of Dielectric Permittivity Effects on Chemical Shifts of Alanine Dipeptide", *Chem. Phys. Lett.*, 547, 66-72, 2012. <http://dx.doi.org/10.1016/j.cpllett.2012.07.069> ●●●●●

Shahkhatuni A. A., **Sahakyan A. B.**, Shahkhatuni A. G., Mamayan S. S., Panosyan H. A. "Correlation of $^1J_{CH}$ Spin-Spin Coupling Constants and Their Solvent Sensitivities", *Chem. Phys. Lett.*, 542, 56-61, 2012. <http://dx.doi.org/10.1016/j.cpllett.2012.06.010> ●●●●●

Sahakyan A. B., Cavalli A., Vranken W. F., Vendruscolo M. "Protein Structure Validation Using Side-Chain Chemical Shifts", *J. Phys. Chem. B*, 116, 4754-4759, 2012. <http://dx.doi.org/10.1021/jp2122054> ●●●●●

Sahakyan A. B., Vranken W. F., Cavalli A., Vendruscolo M. "Using Side-Chain Aromatic Proton Chemical Shifts for a Quantitative Analysis of Protein Structures", *Angew. Chem. Int. Ed.*, 50, 9620-9623, 2011. <http://dx.doi.org/10.1002/anie.201101641> ●●●●●

Sahakyan A. B., Vranken W. F., Cavalli A., Vendruscolo M. "Structure-Based Prediction of Methyl Chemical Shifts in Proteins", *J. Biomol. NMR*, 50, 331-346, 2011. <http://dx.doi.org/10.1007/s10858-011-9524-2> ●●●●●

Sahakyan A. B., Shahkhatuni A. G., Shahkhatuni A. A., Panosyan H. A. "Electric Field Effects on One-Bond Indirect Spin-Spin Coupling Constants and Possible Biomolecular Perspectives", *J. Phys. Chem. A*, 112, 3576-3586, 2008. <http://dx.doi.org/10.1021/jp800670y> ●●●●●

Sahakyan A. B., Shahkhatuni A. G., Shahkhatuni A. A., Panosyan H. A. "Torsion Sensitivity in NMR of Aligned Molecules: Study on Various Substituted Biphenyls", *Magn. Reson. Chem.*, 46, 144-149, 2008. <http://dx.doi.org/10.1002/mrc.2142> ●●●●●

Sahakyan A. B., Shahkhatuni A. A., Shahkhatuni A. G., Panosyan H. A. "Dielectric Permittivity and Temperature Effects on Spin-Spin Couplings Studied on Acetonitrile", *Magn. Reson. Chem.*, 46, 63-68, 2008. <http://dx.doi.org/10.1002/mrc.2137> ●●●●●

Shahkhatuni A. A., Shahkhatuni A. G., Panosyan H. A., **Sahakyan A. B.**, Byeon I. -J., Gronenborn A. M. "Assessment of Solvent Effects: Do Weak Alignment Media Affect the Structure of the Solute?", *Magn. Reson. Chem.*, 45, 557-563, 2007. <http://dx.doi.org/10.1002/mrc.2004> ●●●●●

GENERAL IT SKILLS

LANGUAGES AND ENVIRONMENT R, Fortran 95/03, Bash scripting, R markdown, Shiny, Python, Docker, Caret, TensorFlow, TeX/LaTeX, Linux/Unix, OSX.

MAJOR STRENGTHS High performance computing,
Advanced *Big Data* analysis,
Machine learning,
Multidisciplinary approach to problems
Education and publishable professional experience in computing,
theoretical and applied chemistry and biology.

PROFESSIONAL SERVICES

MANUSCRIPT REVIEWER *Nucl. Acids Res.*, *BMC Genomics*, *ChemPhysChem*,
J. Phys. Chem. B, *Comp. Mat. Sci.*, *Mol. Inform.*,
Chem. Phys. Lett.

TEACHING

OCT. 2009 - MAR. 2010 Part IB Theoretical Chemistry seminar demonstrator,
Department of Chemistry, University of Cambridge.

OCT. 2005 - MAR. 2008 Separate advanced lectures on drug design,
Department of Pharmaceutical Chemistry, Yerevan State
Medical University.