Mgr. David Jakubec

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Current position

2015–now *PhD student*, Bioinformatics group (Dr. Vondrášek), Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic

Past experience

2017 (3 months) *Visiting scientist*, Sequence families team (Dr. Finn), European Bioinformatics Institute (EMBL-EBI), Hinxton, Cambridgeshire, United Kingdom

2013–2015 *Master's student*, Bioinformatics group (Dr. Vondrášek), Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic

Skills & interests

Language skills: Slovak (*native speaker*); Czech (*native speaker*); English (*fluent; FCE certificate, level C1*); German (*basic*)

General computing & programming skills: GNU/Linux OS & Unix shell (*proficient*); Python (with NumPy, SciPy, Matplotlib scientific stack; *proficient*); web development (HTML/CSS/ JavaScript; *intermediate*); LATEX (*intermediate*); high-performance computing

Professional & scientific skills: molecular modeling (*PyMOL, VMD*); molecular dynamics simulations, free energy calculations (*GROMACS*); hidden Markov model applications (*HMMER*); biological database mining (*UniProt, Pfam, Protein Data Bank*); microscale thermophoresis (*intermediate*); standard biochemical laboratory techniques (*weighting, pipetting, solution preparation*)

Education

2015–now PHD program Modeling of Chemical Properties of Nano- and Biostructures (*ongoing*), Faculty of Science, Charles University, Prague, Czech Republic

2013–2015 MASTER's degree in Modeling of Chemical Properties of Nano- and Biostructures (*graduation with honors*), Faculty of Science, Charles University, Prague, Czech Republic

2010–2013 BACHELOR's degree in Molecular Biology and Biochemistry of Organisms (*graduation with honors*), Faculty of Science, Charles University, Prague, Czech Republic

Grants

2017–2020   Assessment of accuracy and efficiency of theoretical free energy calculation methods: application to protein–DNA interactions, Charles University Grant Agency project no. 1048317

Awards

2015   Third place in Students' science conference, University of Chemistry and Technology, Prague

2014   First place in Students' science conference, University of Chemistry and Technology, Prague

Conference & workshop participation

2019   *Workshop* Best practices in programming 2019, Basel, Switzerland

2018   *Poster* EMBL Conference: From Functional Genomics to Systems Biology, Heidelberg, Germany

2018   *Poster* German Conference on Bioinformatics, Vienna, Austria

2018   *Presentation* National bioinformatic conference ENBIK 2018, Bystřice nad Pernštejnem, Czech Republic

2018   *Flash talk* ELIXIR All Hands meeting, Berlin, Germany

2018   *Poster* Prague Protein Spring 2018, Prague, Czech Republic

2018   *Presentation* XV Discussions in Structural Molecular Biology, Nové Hrady, Czech Republic

2017   Gene Regulation by the Numbers: Quantitative Approaches to Study Transcription, Mainz, Germany

2016   *Poster* National bioinformatic conference ENBIK 2016, Loučeň, Czech Republic

2016   *Poster* Prague Protein Spring 2016, Prague, Czech Republic

2015   *Presentation* Students' science conference, University of Chemistry and Technology, Prague, Czech Republic

2015   *Presentation* XIII Discussions in Structural Molecular Biology, Nové Hrady, Czech Republic

2014   *Presentation* Students' science conference, University of Chemistry and Technology, Prague, Czech Republic

2014   *Poster* Second Protein–Protein Interactions conference, Boston, USA

2014   *Poster* National bioinformatic conference ENBIK 2014, Kouty na Vysočině, Czech Republic

2014   Prague Protein Spring 2014, Prague, Czech Republic

Publications

2020   Faltejsková,K., Jakubec,D. and Vondrášek,J. (2020) Hydrophobic Amino Acids as Universal Elements of Protein-Induced DNA Structure Deformation. *Int. J. Mol. Sci.*, **21**, 3986.

2020   Škerle,J., Humpolíčková,J., Johnson,N., Rampírová,P., Poláchová,E., Fliegl,M., Dohnálek,J., Suchánková,A., Jakubec,D. and Strisovsky,K. (2020) Membrane Protein Dimerization in Cell-Derived Lipid Membranes Measured by FRET with MC Simulations. *Biophys. J.*, **118**, 1861–1875.

2020 Jakubec,D. and Vondrášek,J. (2020) Efficient Estimation of Absolute Binding Free Energy for a Homeodomain–DNA Complex from Nonequilibrium Pulling Simulations. *J. Chem. Theory Comput.*, **16**, 2034–2041.

2019 Jakubec,D. and Vondrášek,J. (2019) Can All-Atom Molecular Dynamics Simulations Quantitatively Describe Homeodomain–DNA Binding Equilibria? *J. Chem. Theory Comput.*, **15**, 2635–2648.

2019 Jakubec,D., Vondrášek,J. and Finn,R.D. (2019) 3DPatch: fast 3D structure visualization with residue conservation. *Bioinformatics*, **35**, 332–334.

2018 Jakubec,D., Kratochvíl,M., Vymětal,J. and Vondrášek,J. (2018) Widespread evolutionary crosstalk among protein domains in the context of multi-domain proteins. *PLoS One*, **13**, e0203085.

2017 Galgonek,J., Vymětal,J., Jakubec,D. and Vondrášek,J. (2017) Amino Acid Interaction (INTAA) web server. *Nucleic Acids Res.*, **45**, W388–W392.

2017 Stasyuk,O.A., Jakubec,D., Vondrášek,J. and Hobza,P. (2017) Noncovalent Interactions in Specific Recognition Motifs of Protein–DNA Complexes. *J. Chem. Theory Comput.*, **13**, 877–885.

2016 Jakubec,D., Laskowski,R.A. and Vondrášek,J. (2016) Sequence-Specific Recognition of DNA by Proteins: Binding Motifs Discovered Using a Novel Statistical/Computational Analysis. *PLoS One*, **11**, e0158704.

2015 Hostaš,J., Jakubec,D., Laskowski,R.A., Gnanasekaran,R., Řezáč,J., Vondrášek,J. and Hobza,P. (2015) Representative Amino Acid Side-Chain Interactions in Protein-DNA Complexes: A Comparison of Highly Accurate Correlated *Ab Initio* Quantum Mechanical Calculations and Efficient Approaches for Applications to Large Systems. *J. Chem. Theory Comput.*, **11**, 4086–4092.

2015 Jakubec,D., Hostaš,J., Laskowski,R.A., Hobza,P. and Vondrášek,J. (2015) Large-Scale Quantitative Assessment of Binding Preferences in Protein-Nucleic Acid Complexes. *J. Chem. Theory Comput.*, **11**, 1939–1948.

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