

# Computational Approaches to Understanding and Engineering Enzyme Catalysis

25–29 September 2023 | Zagreb, Croatia

The University of Zagreb, The Faculty of Science, Department of Chemistry  
Horvatovac 102a, Zagreb, Croatia



**HDBMB** 

The logo for HDBMB (High-Throughput Database of Biomolecular Modeling). The text 'HDBMB' is in large blue capital letters. To the right is a blue graphic element consisting of a stylized DNA double helix or ribbon structure.

Day	Time	Lectures	Tutorials/Demonstrations	Poster Session
25 September 2023 Monday	<b>Chairs: Aleksandra Maršavelski and Tomica Hrenar</b>			
	9:00-9:50 <b>REGISTRATION</b>			
	9:50-10:10 <b>Opening words</b>			
	10:10-11:00	<b>Professor Dame Janet Thornton</b>  Computational Enzymology - Enzyme Reactions and active sites in 1D, 2D and 3D		
	11:00-11:10	<b>Q&amp;A</b>		
	11:10-12:00	<b>Professor Ita Gruič-Sovulj</b>  Pre-steady and steady state kinetics of enzyme catalysed reactions		
	12:00-12:10	<b>Q&amp;A</b>		
	12:10-13:30 <b>Lunch Break</b>			
	13:30-14:20	<b>Professor Kenneth A. Johnson</b>  KinTek Explorer software: explore key kinetic concepts		
	14:20-14:30	<b>Q&amp;A</b>		
	14:30-16:30		<b>Dr. Deepti Gupta</b>  Tutorial on using PDBe and PDBe-KB tools	
	16:30-16:45 <b>Coffee Break</b>			
	16:45-18:00			<b>2-minute (2-slide) presentation</b>
	18:00-19:00			<b>Poster presentation</b>
26 September 2023 Tuesday	<b>Chairs: Outi Lampela, Tiila-Riikka Kiema and Rikkert Wierenga</b>			
	9:30-10:20	<b>Assistant Professor Tina Perica</b>  Allosteric pathways in protein function		
	10:20-10:30	<b>Q&amp;A</b>		
	10:30-11:20	<b>Professor Chris Oostenbrink</b>  Molecular dynamics simulation as a tool in protein engineering		
	11:20-11:30	<b>Q&amp;A</b>		
	11:30-13:00 <b>Lunch Break</b>			
	13:00-15:00		<b>Professor Chris Oostenbrink</b>  Tutorial on MD simulations	
	15:00-16:30		<b>Professor Chris Oostenbrink</b>	

			Tutorial on MD simulations; Analysis of Protein Conformational Changes	
	<b>16:30-17:00 Coffee Break and discussion</b>			
	17:00-18:30		<b>Professor Chris Oostenbrink</b>  Analysis of Protein Conformational Changes	
	<b>Chairs: Outi Lampela, Tiila-Riikka Kiema and Rikkert Wierenga</b>			
<b>27 September 2023 Wednesday</b>	9:00-9:50		<b>Research Assistant Profesor Ajasja Ljubetič</b>  Demo/Lecture - <i>De novo</i> protein design using Rosetta and deep learning methods	
	9:50-10:00		<b>Q&amp;A</b>	
	10:00-10:20	<b>Prof. Antonio Díaz Quintana,</b> FEBS-MIC, FEBS opportunities for scientists in molecular life sciences		
	10:20-12:30		<b>Research Assistant Profesor Ajasja Ljubetič</b>  Tutorial - <i>De novo</i> protein design using Rosetta and deep learning methods	
	<b>12:30-14:00 Lunch Break</b>			
	14:00-17:30		<b>Research Assistant Professor Ajasja Ljubetič</b>  Tutorial - <i>De novo</i> protein design using Rosetta and deep learning methods	
	<b>17:30-18:00 Coffee Break</b>			
	18:00-18:50	<b>On-line lecture Professor David Baker</b>  Design of new protein functions using deep learning		
	18:50-19:00	<b>Q&amp;A</b>		
	<b>19:00 Departure</b>			
<b>20:00 Social event, Dinner in town, Johann Franck, Trg bana Josipa Jelačića 9, Zagreb</b>				
<b>28 September 2023 Thursday</b>	<b>Chairs: Outi Lampela, Tiila-Riikka Kiema and Rikkert Wierenga</b>			
	9:30-10:20	<b>Dr. Marc Van der Kamp</b>  The use of (QM/MM) biomolecular simulation to understand enzyme- catalyzed reactions: activity and selectivity		
	10:20-10:30	<b>Q&amp;A</b>		
	10:30-11:20	<b>Prof. Jernej Stare</b>		

		Reaction Pathway Sampling by Empirical Valence Bond Simulation		
	11:20-11:30	<b>Q&amp;A</b>		
	<b>11:30-13:00 Lunch Break</b>			
	13:00-13:50	<b>Professor Jiri Damborsky</b>  Computational tools for designing and engineering enzymes		
	13:50-14:00	<b>Q&amp;A</b>		
	14:00-15:30		<b>Professor Jiri Damborsky/ Mgr. David Bednář, Ph.D.</b>  Engineering Protein Stability (FireProt; FireProt <sup>ASR</sup> and FireProt <sup>DB</sup> )	
	15:30-17:30		<b>Professor Jiri Damborsky/ Mgr. David Bednář, Ph.D.</b>  Identification of Enzyme Tunnels and Ligand Pathways - Caver Web and CaverDock;  Identification of Hot Spots and Design of Smart Libraries - HotSpot Wizard	
	<b>17:30-18:00 Coffee Break</b>			
	18:00-19:00	<b>Q&amp;A session on all tutorials and lectures during the course</b>		
	<b>Chair: Aleksandra Maršavelski</b>			
<b>29 September 2023 Friday</b>	9:30-10:20	<b>Professor Per-Olof Syrén</b>  Novel enzyme engineering strategies for applications in biopolymer science		
	10:20-10:30	<b>Q&amp;A</b>		
	10:30-11:20	<b>Professor Donald Hilvert</b>  Designing proteins with customized catalytic properties		
	11:20-11:30	<b>Q&amp;A</b>		
	11:30-12:00	<b>The Best Presentation and FEBS Open Bio Poster Prize Award Concluding remarks Aleksandra Maršavelski and Rikkert Wierenga</b>		
	<b>Lunch and Departure</b>			

All lectures will be in A1 Amphitheatre Lecture Rooms and demonstrations/tutorials will be in P2, The Faculty of Science, Department of Chemistry, Horvatovac 102a, Zagreb, Croatia