

9th Annual European Molecular Computational Summer School
for Life Science Students
University of Szeged, Hungary, EU

12 May-27 June 2014

Each topic represents a lecture that varies between 2 and 4 hours and starts at 10 o'clock.

<i>Date</i>	<i>Lecturer</i>	<i>Lecture</i>	<i>Practice</i>
Mon. 12 May	Andras Varró	Greetings (11:00)	Setup of the students' PC (all of us)
	Béla Viskolcz	Exposition of the Projects	
	Imre G. Csizmadia	Introduction remarks	
Tue. 13 May	Methos L. Müller	Basics of Computational Informatics	Literature Search in Online Library (BF)
Wed. 14 May	Imre G. Csizmadia	Chemistry as an Excursion on Potential Energy Surfaces (PES)	Practical introduction to Mendeley (BJ&AR)
Thur. 15 May	Imre G. Csizmadia	Critical Points (CP) on the PES	Practical introduction to ChemOffice software (MSZ&GK)
Fri. 16 May	Imre G. Csizmadia	Gradients and Hessians of the PES	Practical introduction to Origin software (MSZ)
<i>Quantum Chemical Background</i>			
Mon. 19 May	Imre G. Csizmadia	Introduction to First Principles Calculations I. Hartree-Fock Methods	My first Gaussian input (BV&BF&MSZ)
Tue. 20 May	Béla Viskolcz	Introduction to First Principles Calculations II. Basis Sets	Study of the Basis set effect(BV&BF&MSZ)
Wed. 21 May	Imre G. Csizmadia	Electron Correlation Methods	Method dependence of the PES(BV&BF&MSZ)
Thur. 22 May	Béla Viskolcz	Density Functional Theory and Its Applications	Project work
Fri. 23 May	Béla Viskolcz	Ab initio calculations in practice I.: Optimizations	Project work
Mon. 26 May	Enrique Gómez Bengoa	Applications of Density Functional Theory in chemical catalysis	Project work
Tue. 27 May	Michael Owen	Ab initio calculations in practice II.: Scan	Project work
Wed. 28 May	Béla Viskolcz	Ab initio calculations in practice III.: Normal mode analysis	Project work
Thur. 29 May	Milán Szőri	Statistical Thermodynamics: from Molecule to Ensemble	Project work
Fri. 30 May	Milán Szőri	Application of Hess's law to calculation of the heat of formation	Project work
Mon. 2 June	Béla Viskolcz	Project work	Project work
<i>Molecular Structure</i>			
Tue. 3 June	Svend Jensen	Searching for Transition States	Project work
Wed. 4 June	Milán Szőri	Project work	Project work
Thur. 5 June	Balázs Jójárt	Introduction to Force Fields I.	Optimizations with AMBER force field
Fri. 6 June	Balázs Jójárt	Introduction to Docking	Force Field Calculations
<i>Reaction Mechanisms</i>			
Mon. 9 June	Pentecost		
Tue. 10 June		Working on Poster Presentation	Working on Poster Presentation
Wed. 11 June	Zoltán Mucsi	Reaction Mechanisms by Molecular Computations	Project work
Thur. 12 June	Zoltán Mucsi	Systems Chemistry	Project work
<i>Macromolecules Modeling and Molecular Dynamics</i>			
Fri. 13 June	David Setiadi	TBA	Working on Poster Presentation
Mon. 16 June		Working on Poster Presentation	Working on Poster Presentation
Tue. 17 June	Balázs Jójárt	Protein Structures and Databases	

<i>3rd Annual Central European Visegrad Symposium (Czech Republic)</i>			
Wed. 18 June		Attendance at Symposium	
Thur. 19 June			
Fri. 20 June			
<i>Practical Applications</i>			
Mon. 23 June	Szilárd Fejér	Modeling Viral Interactions	Project work
Tue. 24 June	Szilárd Fejér	Folding of Nucleic acids	Project work
Wed. 25 June	Béla Viskolcz	Free Radicals in Oxidation Processes and Oxidative Stress	Working on Final Report
Thur. 26 June	Imre Jákli	Toroidal representation of Conformational PES	Working on Final Report
Fri. 27 June	Zoltan Mucsi	The Art of Drug Design	Working on Final Report

Participating Lecturers Listed in Alphabetical Order According to First Name

	Lecturers	University
	Balázs Jójárt	University of Szeged (Hungary)
2	Béla Viskolcz	University of Szeged (Hungary)
3	David Setiadi	University of New York (USA)
4	Enrique Gómez Bengoa	University of the Basque Country (Spain)
5	Imre G. Csizmadia	University of Toronto (Canada)
7	Imre Jakli	Eötvös Loránd University (Hungary)
8	László Müller	University of Szeged (Hungary)
9	Michael C. Owen	Forschungszentrum Jülich (Germany)
10	Milán Szőri	University of Szeged (Hungary)
11	Svend Jensen	Aarhus University (Denmark)
12	Szilárd Fejér	University of Szeged (Hungary)
13	Zoltán Mucsi	Budapest University of Technology and Economics (Hungary)