General information

University of Miskolc, Hungary, from Sunday, May 15 - July 1, 2016 (7 weeks)
The University of Miskolc is the largest university in Northern Hungary. As part of the program with the Drug Discovery Research Center, students will attend lectures given by international researchers and participate in a laboratory component. Students will be guided and supervised through the practical components, where lecture material will be expanded on. The skills learned will later be used for data collection in individual projects. Each student will be responsible for construction of input, submitting calculations to the computer system, and data collection/analysis. This program will be comprised of students from North America and Europe.
As part of this program for 2016, students will take part in a research symposium.

CHM396Y0 – Research Topic Abroad
Course credit for research or field studies abroad under the supervision of a faculty member.

Prerequisite
At least 8.5 FCEs and no more than 14.0 FCEs including at least 1.5 FCEs in 2nd year chemistry courses, or permission of the instructor.

Recommended Preparation
Knowledge of introductory physical chemistry (e. g. CHM220H or equivalent) is highly valuable, as is any previous experience with computational chemistry software or visualization software. A basic knowledge of organic chemistry is expected (e.g. CHM247H or equivalent).
Research skills and chemistry journal literacy are advantageous to successful project completion. Having taken CHM299 will also be beneficial.
This is a Science course; BR=5.

Eligibility and Selection Criteria
This program is open to all science students who have completed at least 8.5 credits by the time the program begins. Participants must have completed courses in Chemistry or related science disciplines or have permission from the instructor.
• Students should be interested in using computational chemistry software or visualization software.
• Applicants may be invited for an interview.

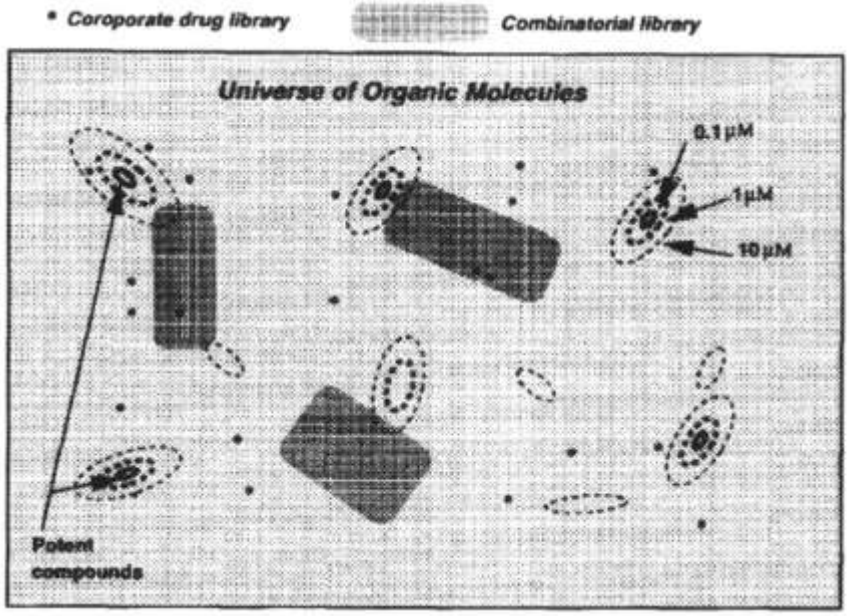
Living Costs
The approximate cost of living in Miskolc for the period of the program is CAD $1300, which includes accommodation and meals.

Entry Requirements for Visitors to Hungary
All students are responsible for making sure that they have the necessary travel documents to enter Hungary as visitors.
At of the time of publication (December 2013), Canadian citizens only require a passport valid for at least six months beyond their return date to enter Hungary as a visitor. Citizens of other countries may have other requirements. Information on entry requirements is available from the embassy of Hungary:
• Hungary, Embassy of the Republic of Hungary in
Ottawa. www.mfagov.hufkulkepviselet/CA/en
Note: Hungary is party to the Schengen Agreement, to students who do need a visa to enter they should only need to obtain one Schengen visa. For further information, please contact the embassy above. If applying for the Schengen visa, you should apply through the Hungarian embassy. Hungary is the primary destination for this program.

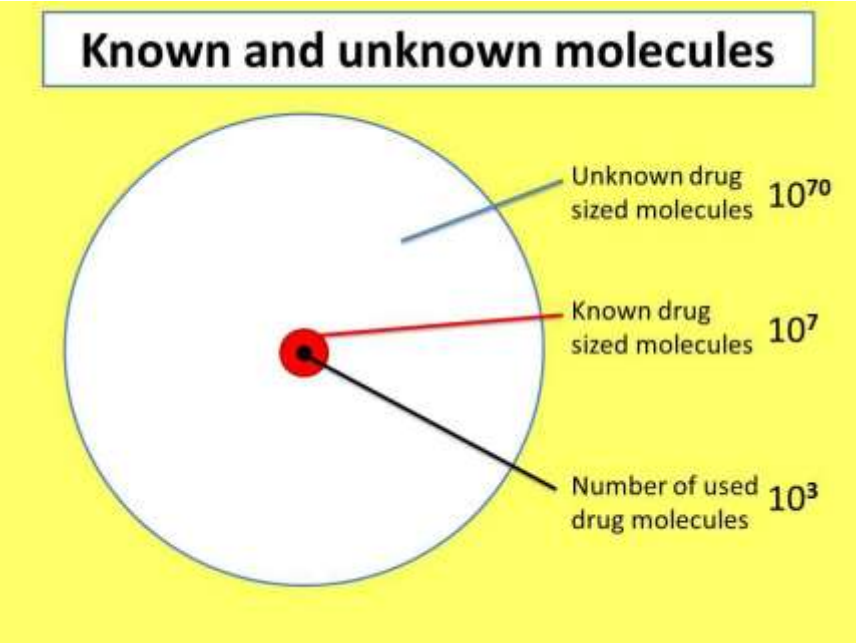
Historic Predicament
(I. G. Csizmadia)

Similar to the Industrial Revolution marked by the establishment of the first safe and successful steam power plant over 300 years ago, the invention of digital computers has led to a new Scientific Revolution within in our present lifetime. The significance of the computer is visible in all aspects of today's society, however the field of chemistry and pharmaceutical industry in particular, are experiencing the most dramatic change at present as a result. This

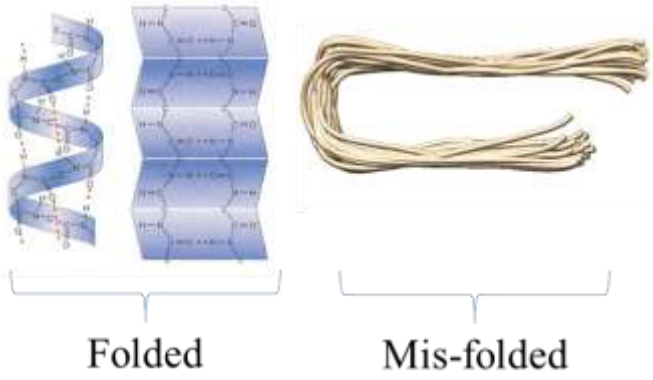
change implies that within the present Scientific Revolution which is still in the midst of unfolding, there is a significant dominance of a Molecular Revolution which will change drug discovery research just as dramatically.
Some time ago, the situation was illustrated by the following schematic figure.



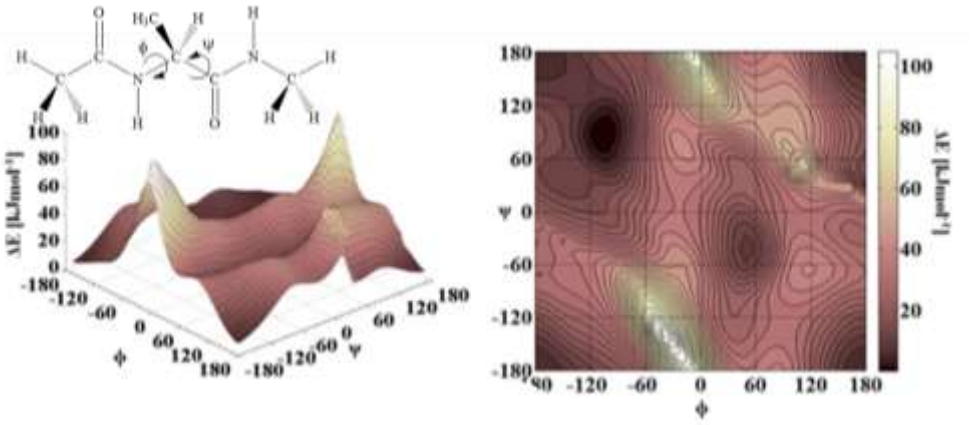
The above figure demonstrates the fact that most of the potential drug molecules are located somewhere else where we do our research. The innacuracy of such a figure, however, lies in the unexplored area, labelled as Universe of Organic Molecules, which is considerably larger than illustrated.
The following schematic figure, however, demonstrates this misproportion more accurately and illustates the number of drug-sized molecules left unknown today, more accurately 63 orders of magnitude larger (10^{70} / 10^{7} = 10^{63}) than the currently known drug database. Because only ten million (10^{7}) drug-sized organic molecules were discovered by the human race in the past two centuries, it isn't unreasonable to suggest that it would require an significantly long time to discover the other 10^{63} molecules by traditional drug discovery techniques and strategies.



Fortunately, with computational methods, this process of drug discovery may be achieved faster with the use of High Performance Computers (HPC) and big-data storage facilities. Such *in silico* research would lead to the discovery of "lead-structures" which could then be synthesized and subjected to *in vitro* and *in vivo* testing for use in pharmaceutical research.
Another research topic of interest for students studying the Life Sciences may be folded and misfolded polypeptides. Misfolded peptides are the causes of multiple neurodegenerative diseases. These include Alzheimer's disease, Parkinson's disease, Amyloidosis, and ALS.



Each amino acid residue within these misfolded polypeptide sequences can be represented as a potential energy surface.



The purpose of the CHM396Y1 Science Abroad program is to expose undergraduate students to this novel way of thinking in terms of drug research design, as well as allow them the opportunity to develop the computational skills required to the carry out similar research projects in their future scientific careers.

Participating lecturers

Lecturer	University/Institute
Anita Rágyanszki	University of Miskolc, Miskolc, Hungary
Béla Fiser	University of the Basque Country, San Sebastián, Spain
Béla Viskolcz	University of Miskolc, Miskolc, Hungary
Eszter P. Faragó	TEVA Pharmaceutical Ltd., Debrecen Hungary
Imre G. Csizmadia	University of Toronto, Toronto Canada
Imre Jákli	Eötvös Loránd University, Budapest, Hungary
John J. Villar	University of the Philippines Diliman, Quezon City, Philippines
Michael C. Owen	Forschungszentrum Jülich, Jülich, Germany
Michelle Sahai	University of Roehampton, London, UK
Milán Szőri	University of Szeged, Szeged, Hungary
Ödön Farkas	Eötvös Loránd University, Budapest, Hungary
Svend K. Jensen	Aarhus University, Aarhus, Denmark
Szilárd Fejér	University of Szeged, Szeged, Hungary
Zoltán Mucsi	Budapest University of Technology and Economics, Budapest, Hungary

Program

Sunday 15 May	Arrival & Accommodations		
Monday 16 May	Sight-Seeing Tour		
Date	**Lecturer**	**Lecture (starting at 10 a.m.)**	**Seminar (starting at 2 p.m.)**
Tuesday 17 May	Béla Viskolcz	Opening ceremonies (starting at 9 a.m.)	Introduction to organic chemistry
Wednesday 18 May	Imre G. Csizmadia	Introduction to physical chemistry	Introduction to literature searches
Thursday 19 May	Imre G. Csizmadia	Introduction to quantum chemistry I	Practical introduction to ChemOffice software
Friday 20 May	Anita Rágyanszki	Introduction to quantum chemical computations	Project work
Monday 23 May	Michael C. Owen	Potential energy surfaces calculations	Project work
Tuesday 24 May	Michael C. Owen	Introduction to free radical formation	Study of the Basis set effect
Wednesday 25 May	Anita Rágyanszki	Conformational networks	Project work
Thursday 26 May	John J. Villar	Mathematical background	Practical introduction to Matlab software
Friday 27 May	John J. Villar	Mathematical analysis of PES	Project work
Monday 30 May	Szilárd Fejér	Energy Landscapes of Self-assembling Systems	Project work
Tuesday 31 May	Szilárd Fejér	Computational Modelling of Viruses	Project work
Wednesday 1 June	Béla Fiser	Introduction to Force Fields	Project work
Thusrday 2 June	Béla Fiser	Introduction to Molecular Dynamics	Optimizations with AMBER force field
Friday 3 June	Eszter P. Faragó	TBA	MM/MD Calculations
Monday 6 June	TBA	TBA	MM/MD Calculations
Tuesday 7 June	János J. Szórád	TBA	MM/MD Calculations
Wednesday	Zoltán Mucsi	Introduction to	Project work

8 June		Pharmaceuticals	
Thursday 9 June	Svend K. Jensen	Determination of transition states and activation energies	Project work
Firday 10 June	Svend K. Jensen	TBA	Project work
Monday 13 June	TBA	TBA	Project work
Tuesday 14 June	TBA	TBA	Project work
Wednesday 15 June	Milán Szőri	TBA	Deadline to finish Posters
Thursday 16 June	Milán Szőri	TBA	Preparation for Poster Presentation
Friday 17 June	Milán Szőri	TBA	-
Saturday 18 June			
Sunday 19 June	6th Visegrad Symposium on Structural Systems Biology		
Monday 20 June	6th Visegrad Symposium on Structural Systems Biology		
Tuesday 21 June	6th Visegrad Symposium on Structural Systems Biology		
Wednesday 22 June			
Thursday 23 June	Imre Jákli	TBA	Project work
Friday 24 June	Ödön Farkas	Strategies of Geometry Optimizations	Project work
Monday 27 June	Béla Viskolcz	Molecular Aging	Project work
Tuesday 28 June	Final Report Preparation		
Wednesday 29 June	Final Report Preparation		
Thursday 30 June	Final Report Preparation		
Friday 1 July	Deadline to submit final report; Farewell Party		