Program of the ECO Summer School 2012, in Verona, Italy , 11 - 15 June 2012

SUNDAY, 10 JUNE		
Arrivals		Hotel Marco Polo (Hall)
18:00 - 20:00	Registration	
MONDAY, 11 JUNE		
09:00 - 09:30	**Welcome and Introduction by the Organizer**	Hotel Marco Polo (Floor -1)
Practical Lessons		
09:30 - 13:00	**QSAR: from molecular structure to models**	
	Andrea Mauri, Davide Ballabio, University of Milano Bicocca, Italy	
	Alberto Manganaro, KODE Srl, Pisa, Italy	
09:30 - 10:30	Preparation of toxicological data	
10:30 - 11:00	**Coffee break**	
11:00 - 12:00	Molecular representation: formats and matching	
12:00 - 13:00	Retrieval of experimental toxicological data	
13:00 - 14:30	**Lunch Break** (Restaurant at Hotel Mastino)	
Practical Lessons		Hotel Marco Polo (Floor -1)
14:30 - 18:30	**How to build a QSAR model**	
14:30 - 15:00	Introduction to molecular descriptors	
	Roberto Todeschini and Viviana Consonni, University of Milano Bicocca, Italy	
15:00 - 16.00	Calculation and screening of molecular descriptors by means of Dragon software	
	Andrea Mauri, University of Milano Bicocca, Italy	
16:00 - 16:30	**Coffee break**	
16:30 - 17:30	QSAR Modelling: how to build a predictive model	
	Davide Ballabio, University of Milano Bicocca, Italy	
17:30 - 18:30	Applying existing QSAR models: practical examples on VEGA platform	
	Alberto Manganaro, KODE Srl, Pisa, Italy	
TUESDAY, 12 JUNE		
Practical Lessons		Hotel Marco Polo (Floor -1)
09:00 - 12:45	**The QSAR toolbox**	
	Emiel Rorije, Dutch National Institute for Public Health and the Environment, The Netherlands	
09:00 - 09:45	Introduction to the OECD QSAR Toolbox, Read Across and Category approaches	
09:45 - 10:30	Demonstration of two examples of using the QSAR Toolbox (acute fish toxicity and BCF)	
10:30 - 11:00	**Coffee break**	
11:00 - 12:45	Interactive session using the toolbox	
13:00 - 14:00	**Lunch Break** (Restaurant at Hotel Mastino)	
14:00 - 15:20	**Fellows presentations** (10 min each) - *Chair: Karl-Werner Schramm*	otel Marco Polo (Floor -1)
	Valentina Zingarelli, Helmholtz-Zentrum München	
	Katarzyna Odziomek, Linneuniversitetet	
	Matteo Cassotti, Helmholtz-Zentrum München	
	Chris Eckstein, Universiteit Leiden	
	Jacques Ehret, Universiteit Leiden	
	Evanthia Giagloglou, Università degli Studi di Milano Bicocca	
	Tine Ringsted, Università degli Studi di Milano Bicocca	
15:20 - 15:50	**Coffee break**	
15:50 - 17:00	**Fellows presentations** (10 min each) - *Chair: Willie Peijnenburg*	
	Martina Perisa, Hochschule Fresenius	

	Pantelis Sopasakis, Helmholtz-Zentrum München	H
	Ioana Oprisiu, Helmholtz-Zentrum München	
	Inge van Driezum, Hochschule Fresenius	
	Swapnil Chavan, Linneuniversitetet	
	Ian Ken Dimzon, Hochschule Fresenius	
17:15 - 19:00	**General Assembly** *only for ECO project leaders and manager*	
19:30 - 20:30	**Cocktail Party** (Restaurant at Hotel Mastino)	
WEDNESDAY, 13 JUNE		
09:00 - 09:40	**Fellows presentations** (10 min each) - *Chair: Josè Maria Navas*	Hotel Marco Polo (Floor -1)
	Lan Song, Universiteit Leiden	
	Oleksandra Ieromina, Universiteit Leiden	
	Isabel O'Connor, Radboud Universiteit Nijmegen	
Scientific Excursion		
09:45 - 12:30	**Visit to APTUIT Medicine Research Center**	
09:45	Departure in front of Hotel Mastino	
09:45 - 10:00	Bus ride	
10:00 - 10:15	Introduction to Aptuit Research Center, *Dr. Alfonso Pozzan*	
	Note: all of the participants must have their identity card / passport	
10:15 - 10:30	Visit to biological laboratories	
10:40 - 12:00	Visit to chemical laboratories, *Dr. Alfonso Pozzan*	
	- Chemical development lab, kilo-lab, pilot plant, *Dr. P.Westerduin*	
	- Pharmaceutical development lab, *Dr. M. Galvan*	
12:30 - 22:00	**Scientific trip to Venice lagoon**	
12:30	Departure from Aptuit Medicine Research Center	
12:30 - 14:30	**Light meal during the bus ride**	
14:30	Estimated arrival in Venezia (Tronchetto)	
14:30 - 19:30	Free time for Venice tour	
20:00	Departure from Tronchetto	
20:30	Stop for dinner at Autogrill near Padova	
22:00	Arrival in Verona	
THURSDAY, 14 JUNE		
09:00 - 09:30	**Welcome by the President of IAMC (R. Todeschini) and the Coordinator of the ECO project (I. Tetko)**	Palazzo Castelvecchio Conference Hall
Theoretical Lessons		
09:30 - 13:00	**Chemoinformatics and mathematical methods for modelling** - *Chair: Roberto Todeschini*	
09:30 - 10:15	Sparse statistical methods: theory, applications, software	
	Peter Filzmoser, Vienna University of Technology, Austria	
10:15 - 10:45	Combining chemo-bio-informatics and experimental methods in transmembrane protein structure resolution	
	Marjana Novic, University of Ljubljana, Slovenia	
10:45 - 11:15	**Coffee break**	
11:15 - 12:15	New artificial adaptive systems for intelligent data mining	
	Massimo Buscema, SEMEION (Italy) and University of Colorado (CO)	
12:15- 13:00	Evaluation of empirical models for calibration and classification	
	Kurt Varmuza, Vienna University of Technology , Austria	
13:00 - 14:00	**Lunch Break** (Palazzo Castelvecchio - Giardino del Pozzo)	
Theoretical Lessons		
14:00 - 17:10	**Chemoinformatics and mathematical methods for modelling** - *Chair: Edward Kirby*	
14.00 - 14:30	Computer classification, design and search of organic reactions	
	Nikolay Zefirov, Moscow State University, Russia	
14.30 - 15:00	An integral equation approach to chemical and photophysical kinetics	
	Mario Nuno Berberan-Santos, Technical University of Lisbon, Portugal	
15:00 - 15:30	Graphical Bioinformatics	

	Milan Randic, Drake University (IA) and University of Ljubljana, Slovenia	Palazzo Castelvecchio Conference Hall
15:30 - 16:00	**Coffee break**	
16:00 - 16:25	AutoGraphiX-3: a new computer environment for studying graph theory	
	Gilles Caporossi, HEC Montreal, Quebec, Canada	
16:25 - 16:50	Bounds and relations involving betweenness centrality in some families of graphs	
	Snjezana Majstorovic, University of Osijek, Croatia	
16:50 - 17:10	Polybenzenes and relared nanostructures	
	Mircea Diudea, "Babes-Bolyai" University, Cluj, Romania	
17:10 - 18:30	**Fellows' presentations (10 min each)** - *Chair: Igor Tetko*	
	Alessandra Pirovano, Radboud Universiteit Nijmegen	
	Ahmed Abdelaziz, Helmholtz Zentrum München	
	Rajesh Rathore, Helmholtz Zentrum München	
	Mona Connolly, Instituto Nacional de Investigacion y Tecnologia Agraria y Alimentaria	
	Tobias Lammel, Instituto Nacional de Investigacion y Tecnologia Agraria y Alimentaria	
	Kamel Mansouri, Università degli Studi di Milano Bicocca	
	Faizan Sahigara, Università degli Studi di Milano Bicocca	
21:00	**Gala Dinner** (Palazzo Castelvecchio restaurant)	
FRIDAY, 15 JUNE		
Theoretical Lessons		Palazzo Castelvecchio Conference Hall
09:00 - 12:45	**Graph theory and topological indices** - *Chair: Milan Randic*	
09:00 - 09:45	The Topological Index Deluge	
	Ivan Gutman, University of Kragujevac, Serbia	
09:45 - 10:15	On DNA Graph and its Application to DNA Fragment Assembly	
	Ali Iranmanesh, Tarbiat Modares University, Tehran, Iran	
10:15 - 10:35	Recent Results on Bipartite Edge and Vertex Frustration of Molecular Graphs	
	Ali Reza Ashrafi, University of Kashan, Iran	
10:35 - 11:00	**Coffee break**	
11:00 - 11:30	Prediction of stability constants of coordination compounds from their connectivity indices	
	Nenad Raos, Institute for Medical Research and Occupational Health, Croatia	
11:30 - 12:00	Interpolation Method and Topological Indices	
	Sandi Klavzar, University of Ljubljana and University of Maribor, Zagreb, Slovenia	
12:00 - 12:45	Molecules in silico	
	Adalbert Kerber, University of Bayreuth, Germany	
13:00 - 14:00	**Lunch Break** (Palazzo Castelvecchio - Giardino del Pozzo)	
Theoretical Lessons		Palazzo Castelvecchio Conference Hall
14:00 - 15:30	**Graph theory and topological indices** - *Chair: Nikolay Zefirov*	
14.00 - 14:30	Some New Applications of Graph Eigenvalues and Spectral Moments	
	Jorge Galvez, University of Valencia, Spain	
14:30 - 14:50	Integral eigenvalues of Cayley graphs	
	Bojan Mohar, University of Ljubljana, Slovenia	
14.50 - 15:10	Graphs and Thermodynamics	
	Lionello Pogliani, University of Calabria, Italy	
15:10 - 15:30	Design of bivalent ligands as neuroprotective and anti-cancer compounds	
	Vladimir Palyulin, Lomonosov Moscow State University, Russia	
15:30	Closure	