Centrum Studiów Zaawansowanych
Politechniki Warszawskiej
Pl. Politechniki 1, 00-661 Warszawa, tel./fax +48 22 234 6003 (6002), www.csz.pw.edu.pl

Chematica: An automatic chemist for the 21st century

Bartosz A. Grzybowski
K. Burgess Professor of Physical Chemistry and Chemical Systems Engineering
Director of the DoE Non-Equilibrium Research Center
Northwestern University,
Department of Chemistry and
Depertment of Chemical and Biological Engineering
Evanston, USA.
www: dysa.northwestern.edu or www.nerc.northwestern.edu
email:grzybor@northwestern.edu

Abstract: The millions of reactions performed and compounds synthesized by organic chemists over the past two centuries connect to form a network larger than the metabolic networks of higher organisms and rivaling the complexity of the World Wide Web. Despite its apparent randomness, the network of chemistry has a well-defined, modular architecture and evolves in time according to trends that have not changed since the inception of the discipline, thus projecting into chemistry's future. Analysis of organic chemistry using the tools of graph theory, linguistics and machine learning enables the optimization of chemical syntheses including predictions of how unknown molecules can be efficiently made. All of these capabilities are embodied in a unified software environment called *Chematica*. *Chematica* plans synthesis of life-saving drugs, dyes and pigments, complex natural products and any other molecule one wishes to make in a matter of seconds vs. weeks to months by human experts. *Chematica* is the Deep Blue of chemistry, constantly self-learning and improving. It is already being deployed in and used by the American and E.U. chemical industries and also by several national security/intelligence agencies (in the context of chemical warfare prevention). Please come see the live demo of *Chematica* at the TOPTECHNIKA lecture!

Key References:

1. B.A. Grzybowski, K.J.M. Bishop, B. Kowalczyk, C.E. Wilmer The wired universe of organic chemistry *Nature Chemistry* 1, 31 (2009).
2. K.J.M. Bishop, R. Klajn & B.A. Grzybowski The core and most useful molecules in organic chemistry *Angew. Chem. Int. Ed.*, 45, 5348 (2006).
3. M. Fialkowski, K.J.M. Bishop, V. Chubukov, C.J. Campbell & B.A. Grzybowski, The architecture and evolution of organic chemistry, *Angew. Chem. Int. Ed.*, 44, 7263 (2005)
4. C.M. Gothard, S. Soh, N.A. Gothard, B. Kowalczyk, Y. Wei. B. Baytekin, B.A. Grzybowski Rewiring Chemistry: Algorithmic Discovery and Experimental Validation of One-Pot Reactions in the Network of Organic Chemistry. *Angew. Chem. Int. Ed.* 51, 7922 (2012).
5. M. Kowalik, C.M. Gothard, A.M. Drews, N.A. Gothard, A. Wieckiewicz, P.E. Fuller, B.A. Grzybowski, K.J.M. Bishop Parallel Optimization of Synthetic Pathways within the Network of Organic Chemistry. *Angew. Chem. Int. Ed.* 51, 7928 (2012).
6. P.E. Fuller, C.M. Gothard, N.A. Gothard, A. Wieckiewicz, B.A. Grzybowski Chemical Network Algorithms for the Risk Assessment and Management of Chemical Threats. *Angew. Chem. Int. Ed.* 51, 7933 (2012).