Can computer think like a chemist - synthetic planning with Chematica

Prof. Bartosz A. Grzybowski

Distinguished Professor of Chemistry and IBS Group Leader, UNIST, South Korea

When new compounds are to be made, there are billions of billions of potential retrosyntheses that one needs to consider – such numbers are certainly beyond the cognition of a human, but within the reach for modern computers. Mathematically, these synthetic possibilities form a giant network whose complexity substantially exceeds that of the World Wide Web. Analysis of this network using expert chemical knowledge, graph theory, artificial intelligence and even linguistics enabled us to create Chematica -- the software platform that uses all this information to predict de novo synthetic pathways. Chematica knows tens of thousands of chemical rules with which it explores billions of possible reaction combinations, ultimately selecting optimal synthetic pathways. In doing so, Chematica suggests protection groups, navigates around reactivity conflicts, strategizes several steps ahead, etc. In my talk, I will show how Chematica designed syntheses of non-trivial targets that were later confirmed in both academic and industrial laboratories, offering substantial savings in terms of time and cost.