Organic Synthesizability

An examination of a strictly mathematical representation of the organic chemical synthesis

Dr. Luca Ermanni

October 17, 2015

A fundamental question of the organic chemical synthesis can be expressed in the following way:

> Given any notion of organic synthesis, finitely many arbitrary starting organic compounds and a final one, is there a synthesis of the final compound from the starting compounds?

Here a notion of synthesis has to be considered fully determined by finitely many (chemically correct) reaction step rules, in the sense that a synthesis is a sequence generated by the application of the rules to its elements.

Written differently, given any finite set of reaction step rules, finitely many arbitrary starting organic compounds and a final one, is there an organic reaction that carries a left side constituted by compounds that are all among the initial ones into a right side containing the final compound, having a mechanism whose steps are all correct with respect to the given rules?

This question would be certainly answered, once for all, if there would be an effective procedure that answers it. Therefore the question now is:

Does such a procedure exist or not?

Since organic compounds, reaction steps, reactions, synthesis,etc. are not mathematical entities and are therefore subject to the typical ambiguities and unclarities of the ordinary concepts, it has been, first of all, necessary to mathematically represent these entities. Once this was done, the question, whether there is the procedure or not, could be approached mathematically and conclusively answered in this work.

This answer allowed to determine, for some additional model-theoretical and logical problem, whether they are decidable or not.

The mathematical representations of the finite sets of reaction step rules have been shown to coincide with a model-theoretical concept, putting organic reactions in a perspective different from the usual one.