



COMPUTATIONAL BIOLOGY WEBINAR @ IMSc

THE CHEMICAL SPACE AND ITS THREE STATISTICAL REGIMES

DR. GUILLERMO RESTREPO
MPI FOR MATHEMATICS IN THE SCIENCES LEIPZIG

THURSDAY, 6 AUGUST 2020, 3 PM IST

Exploring the chemical space, spanned by all chemical species, is at the core of chemical activity. Records of how the space is expanded through chemical reactions exist in more than 200 years of scientific publications, now available in electronic databases. Despite its importance, very little is known about this exploration throughout history and about the driving forces affecting it. Here we show, by analysing millions of reactions stored in Reaxys® database, that the exploration is marked by three regimes and by social and scientific factors. The first regime was dominated by volatile inorganic production and ended about 1860, when structural theory gave place to a century of guided production, the organic regime. After 1980 began the least volatile regime, the current organometallic one. We found a stable 4.4% annual growth rate of production of new compounds not affected in the long run neither by World Wars nor by the introduction of new theories. However, World Wars have delayed production. Moreover, we found that chemists have been conservative in the selection of their starting materials but have been historically motivated to unveil new compounds of the space.

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