Intuition-Enabled Machine Learning Beats the Competition When Joint Human-Robot Teams Perform Inorganic Chemical Experiments

Leroy Cronin, Vasilios Duros, Jonathan Grizou, Abhishek Sharma, Hessam Mehr, Andrius Bubliauskas, Przemyslaw Frei, Haralampos N. Miras

Submitted date: 13/02/2019 • Posted date: 13/02/2019
Licence: CC BY-NC-ND 4.0

Citation information: Cronin, Leroy; Duros, Vasilios; Grizou, Jonathan; Sharma, Abhishek; Mehr, Hessam; Bubliauskas, Andrius; et al. (2019): Intuition-Enabled Machine Learning Beats the Competition When Joint Human-Robot Teams Perform Inorganic Chemical Experiments. ChemRxiv. Preprint.

Traditionally, chemists have relied on years of training and accumulated experience in order to discover new molecules. But the space of possible molecules so vast, only a limited exploration with the traditional methods can be ever possible. This means that many opportunities for the discovery of interesting phenomena have been missed, and in addition, the inherent variability of these phenomena can make them difficult to control and understand. The current state-of-the-art is moving towards the development of automated and eventually fully autonomous systems coupled with in-line analytics and decision-making algorithms. Yet even these, despite the substantial progress achieved recently, still cannot easily tackle large combinatorial spaces as they are limited by the lack of high-quality data. Herein, we explore the utility of active learning methods for exploring the chemical space by comparing collaboration between human experimenters with an algorithm-based search, against their performance individually to probe the self-assembly and crystallization of the polyoxometalate cluster $Na_6[Mo_{120}Ce_6O_{366}H_{12}(H_2O)_{78}]-200H_2O \ (1)$ We show that the robot-human teams are able to increase the prediction accuracy to 75.6±1.8%, from 71.8±0.3% with the algorithm alone and 66.3±1.8% from only the human experimenters demonstrating that human-robot teams beat robots or humans working alone.
| Other files |
|-------------|
| preprint-.pdf (6.23 MiB) | view on ChemRxiv » download file |