ORGANIC: Computer Assisted Molecular Design

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With rising Research & Development costs and the average time of taking a new material/drug to market sitting at around 20 years, both industry and academia are searching for ways to cut down on development times. In the field of Drug Discovery, inverse design is a common approach. Given a target and certain characteristics of the desired drug, the goal is to create a molecule that meets the criteria. Recent developments in machine learning such as Generative Adversarial Networks have shown promise to help solve inverse problems.

We collaborated with the Alan Aspuru-Guzik's group at Harvard on their ORGANIC (Objective-Reinforced Generative Adversarial Network for Inverse-design Chemistry) program, which aims to improve navigation through chemical space. Throughout this summer, I improved documentation of the code and created guides for basic features of the program. I also finished some partially implemented features, such as giving an estimate for how well the compound will dissolve in water. Another feature I wrote was a data visualisation suite that tracks standard metrics used in machine learning while concurrently sampling batches of molecules.