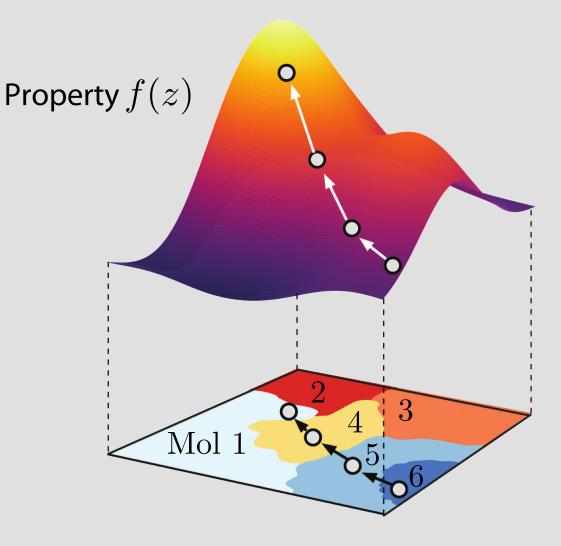
## **Bayesian optimization**



Optimize property like effectiveness against cancer.

## While **True**:

- Find maximum of acquisition function
- 2. Perform trials on new molecule

Rafael Gómez-Bombarelli et. al. https://arxiv.org/abs/1610.02415

