# Day 27: Generative Models for Scientific Applications

## Project: Drug Molecule Generation with VAE

### About

- Author: Victor Basu
- Source: Keras.io
- Generate molecules for drug discovery using VAEs
- The model generates new molecules - open ended spaces of chemical compounds

#### Components of the model:

- **Encoder**: converts the discrete representation of a molecule into a real-valued continuous vector
- **Decoder**: converts these continuous vectors back to discrete molecule representations
- **Predictor**: estimates chemical properties from the latent continuous vector representation of the molecule

### Steps:

- Setup
- Dataset
- Hyperparameters
- Generating Training Set
- Build the Encoder & Decoder
- Build the Sampling Layer
- Train the model
- Inference

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