Encoding-decoding

Train VAE on SMILES:

Any point reconstructs valid molecule

c1ccccc1

Discrete Structure
SMILES

ENCODER
Neural Network

CONTINUOUS MOLECULAR
REPRESENTATION
Latent Space

DECODER
Neural Network

c1ccccc1

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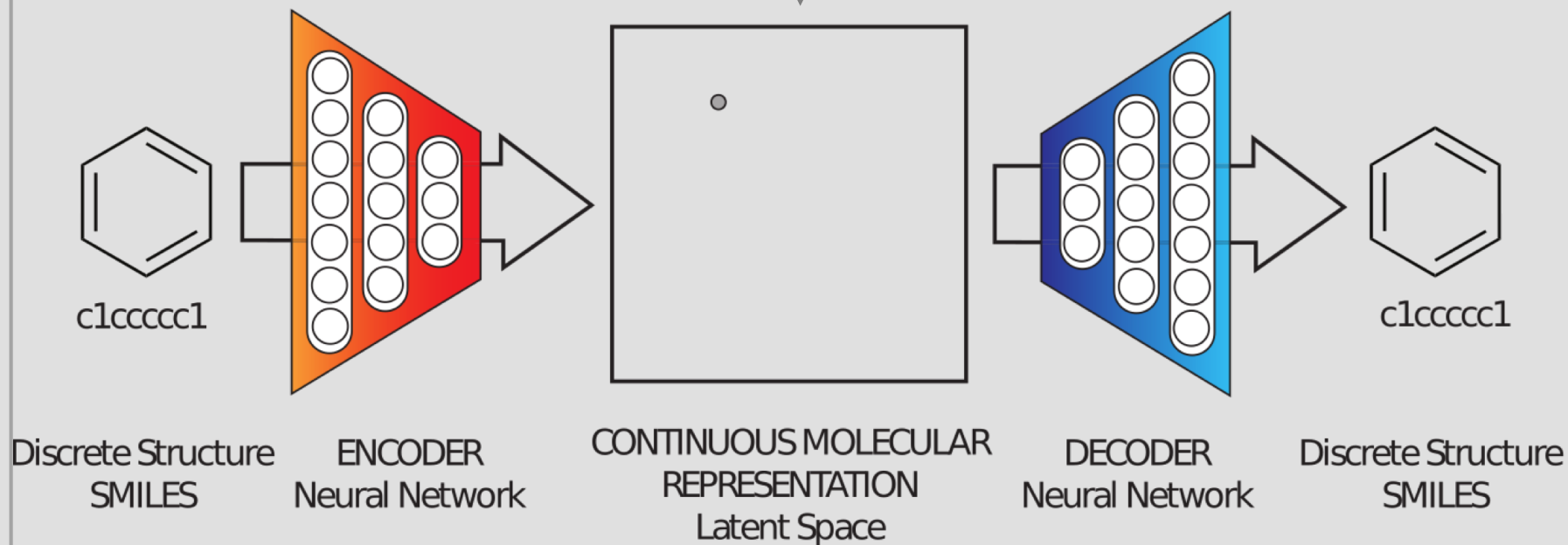
Rafael Gómez-Bombarelli et. al. https://arxiv.org/abs/1610.02415