Title of the Presentation

Hongming Chen

Guangzhou Laboratory, No. 9 XingDaoHuanBei Road, Guangzhou International Bio Island, Guangzhou 510005, Guangdong Province, China
chen_hongming@gzlab.ac.nc

De novo molecular design plays an important role in drug discovery. In this talk, two novel AI generative models, Tree-Invent and EC-Conf, were introduced. Tree-Invent was proposed to integrate topological constraints in the generation of molecular graph. In this model, a molecular graph is represented as a multi-fork topological tree in which ring system, non-ring atom and chemical bond are regarded as ring node, single node and edge respectively. Combining with reinforcement learning, Tree-Invent model could efficiently explore targeted chemical space. Moreover, due to incorporation of topology constraints in the methodology, Tree-Invent model is flexible enough to be used in versatile molecule design settings such as scaffold decoration, scaffold hopping and linker generation.

Secondly, an equivariant consistency model (EC-Conf) was proposed as a fast diffusion method for low-energy conformation generation. In EC-Conf, a modified SE (3)-equivariant transformer model was directly used to encode the Cartesian molecular conformations and a highly efficient consistency diffusion process was carried out to generate molecular conformations. It was demonstrated that, with only one sampling step, it can already achieve comparable quality to other diffusion-based models running with thousands denoising steps. The performance of EC-Conf is evaluated on both GEOM-QM9 and GEOM-Drugs sets. Our results demonstrate that the efficiency of EC-Conf for learning the distribution of low energy molecular conformation is at least two magnitudes higher than current SOTA diffusion models.