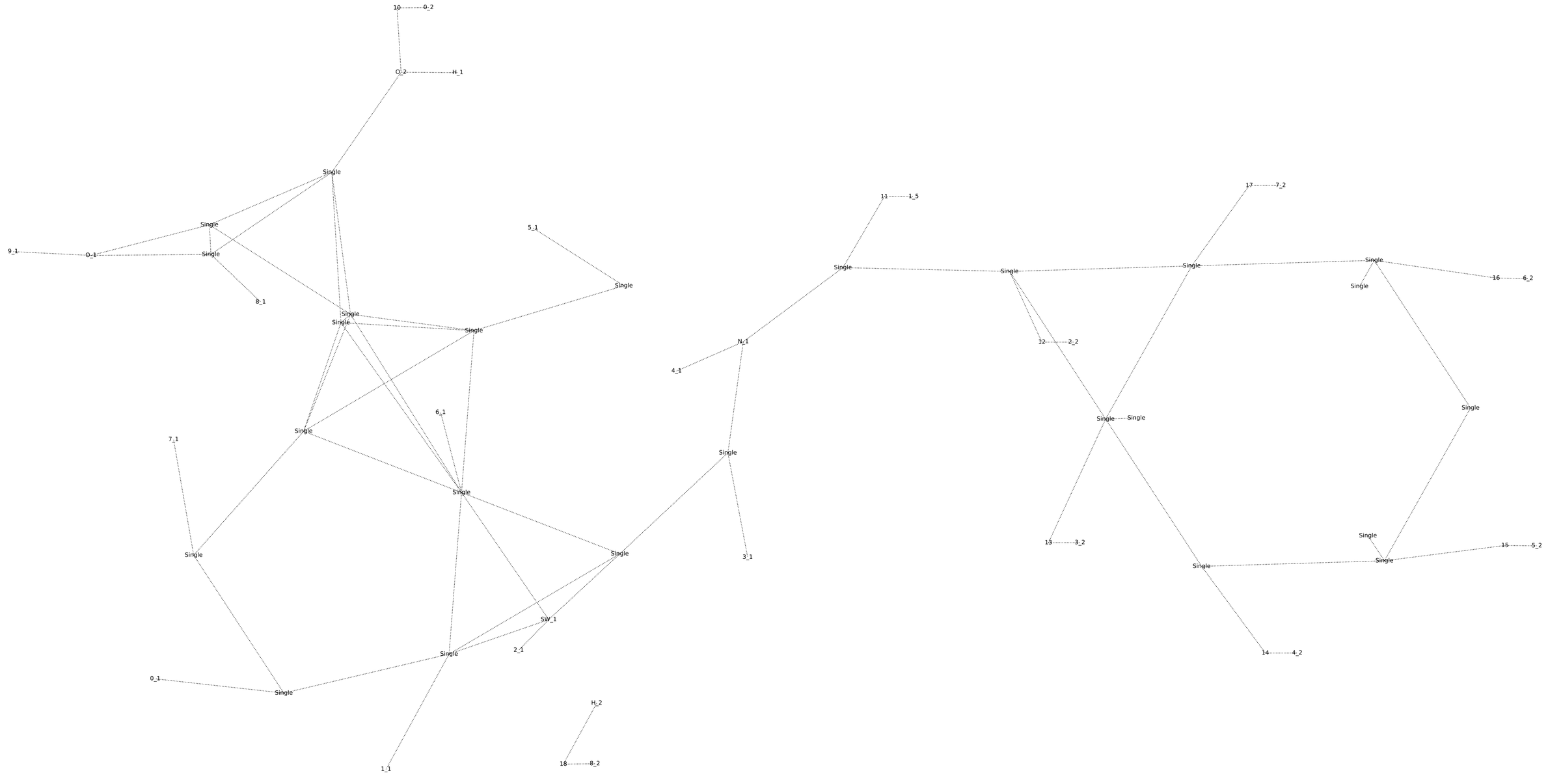1515515_rdkit