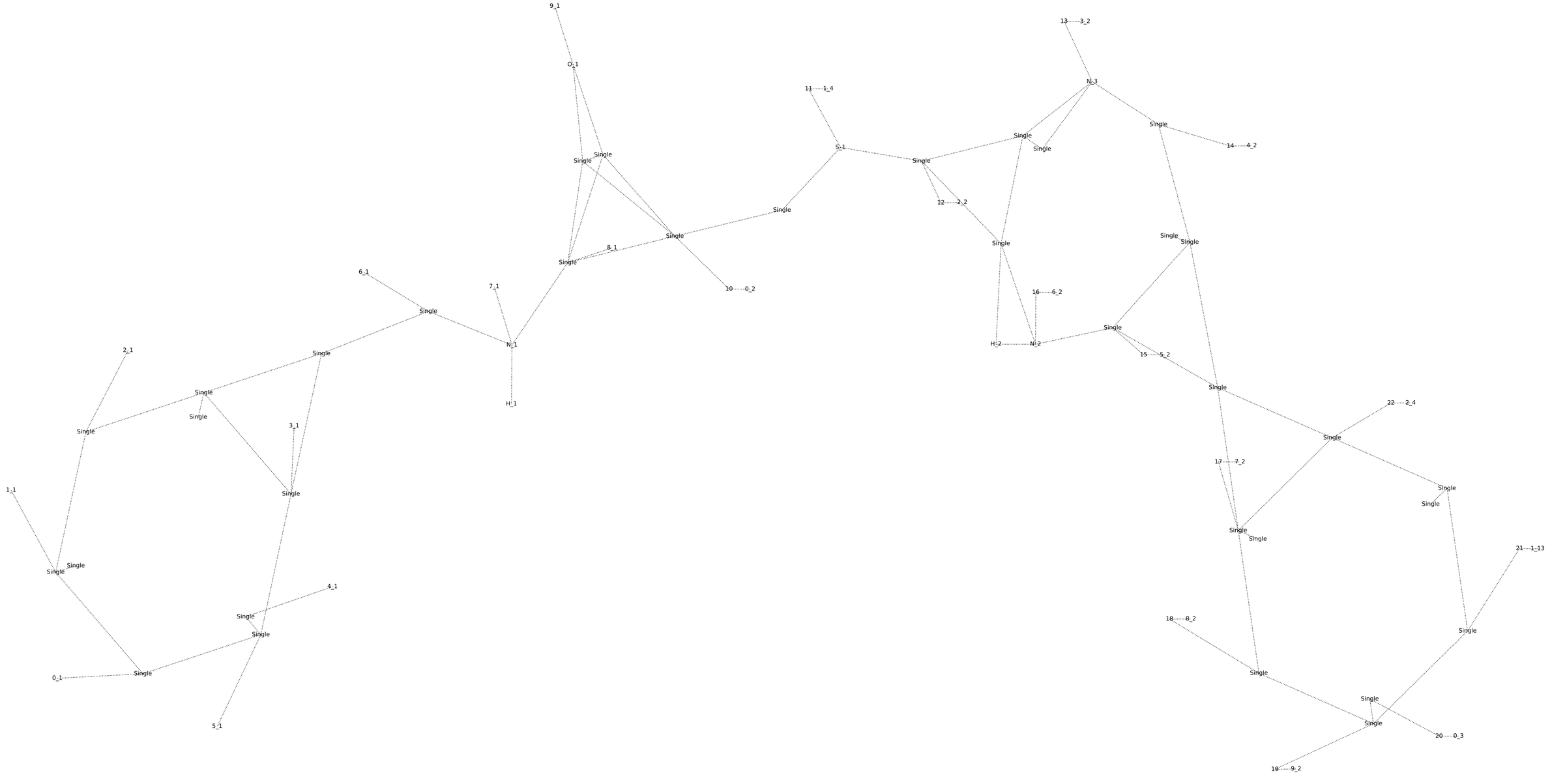4223819_rdkit