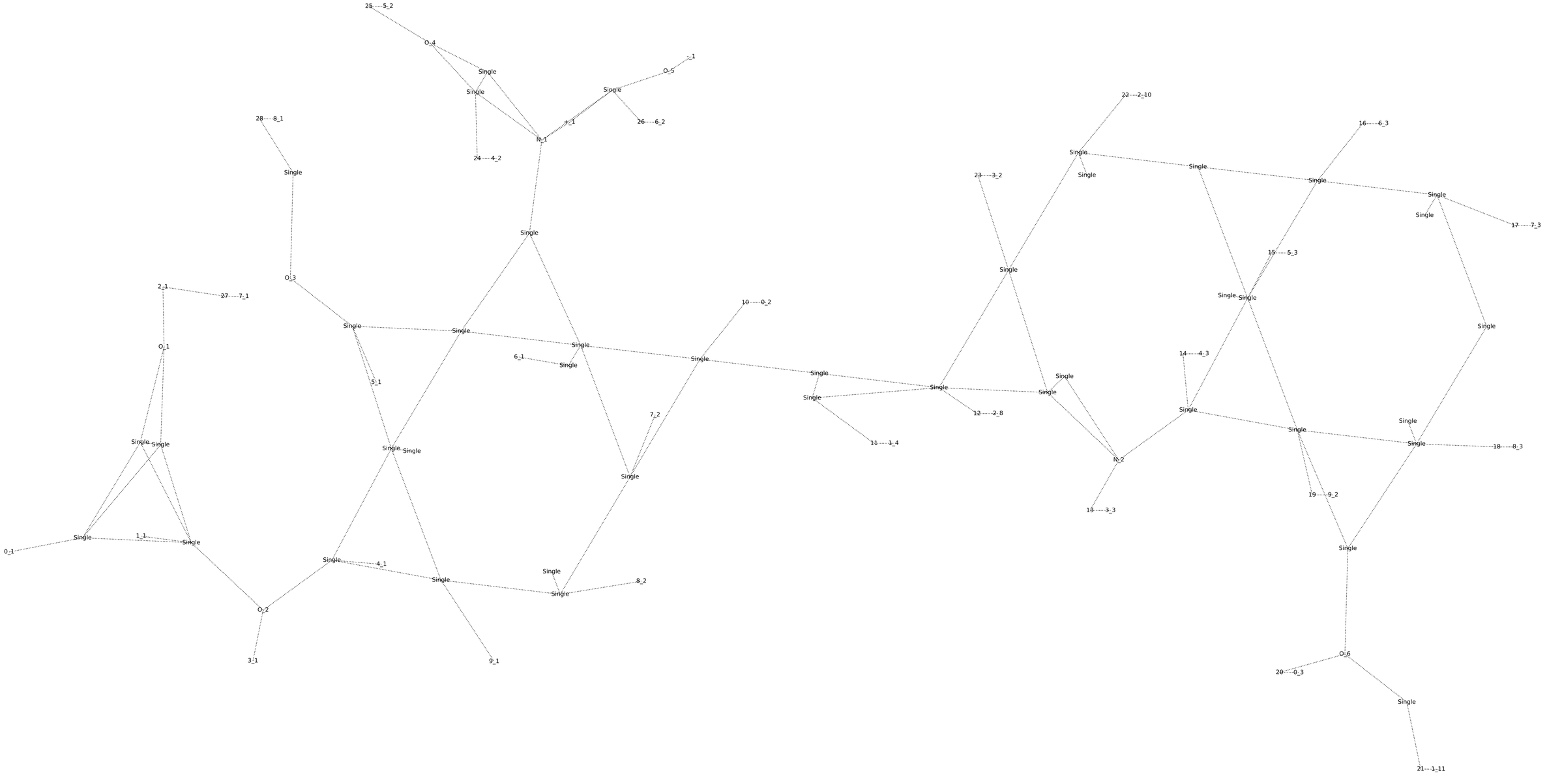5739019_rdkit