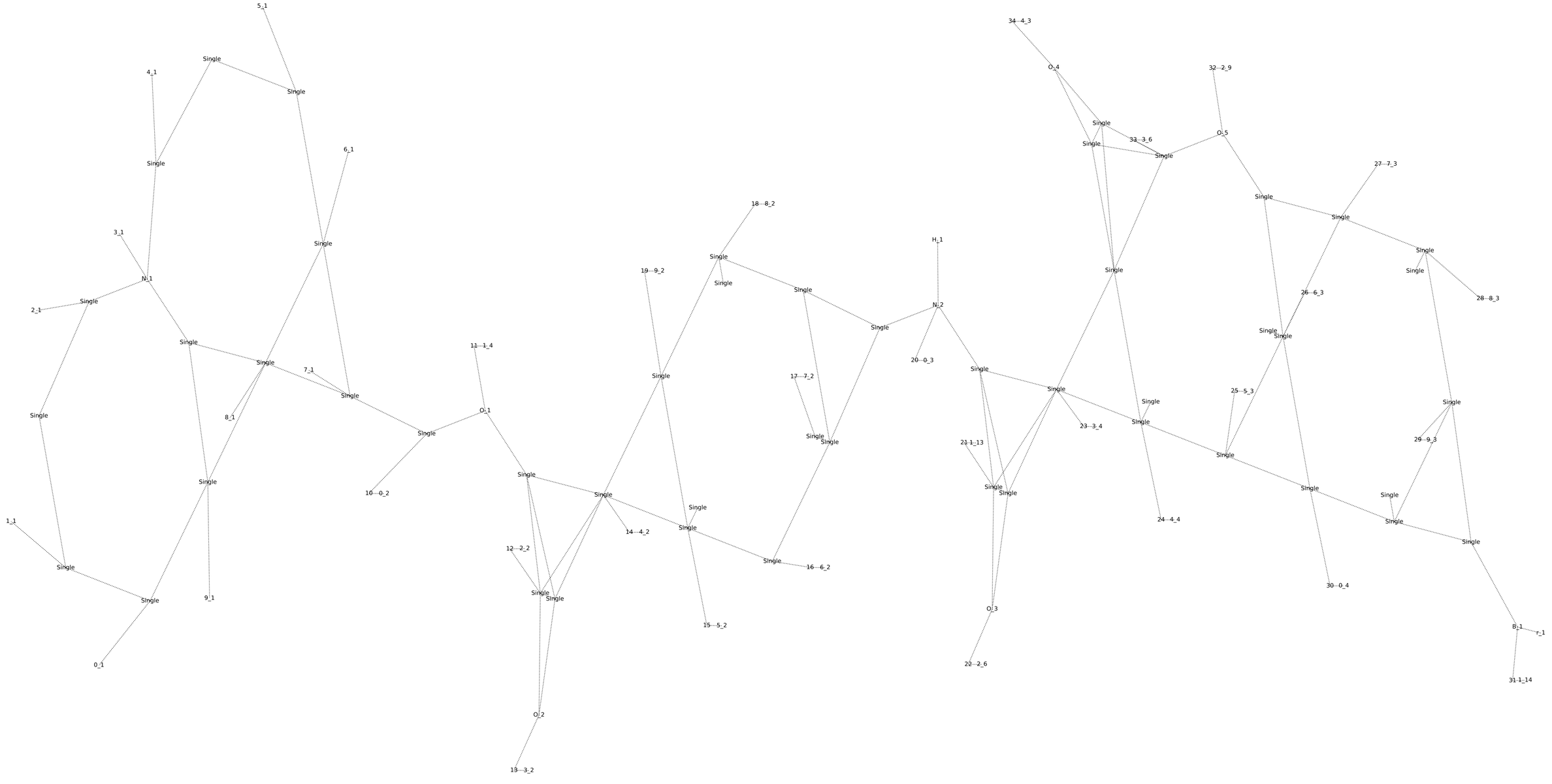3468557_rdkit