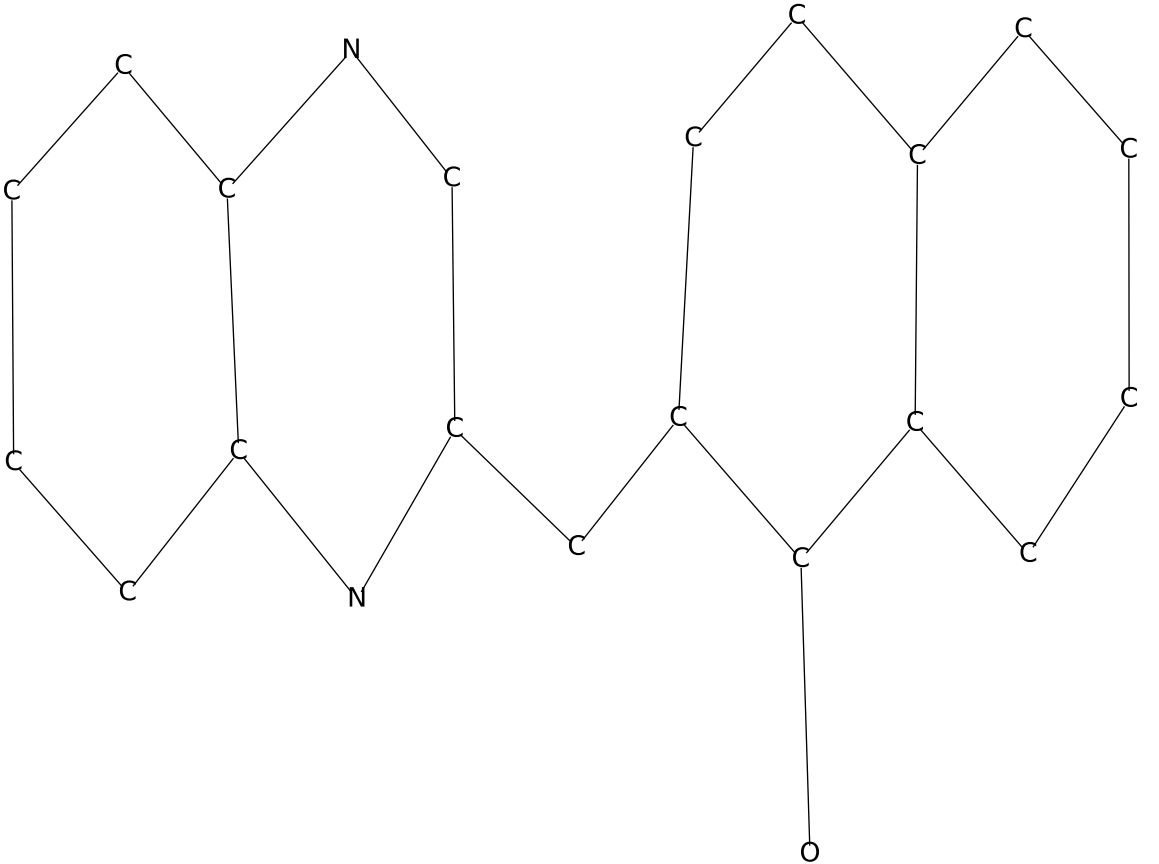9028188_rdkit_chemical