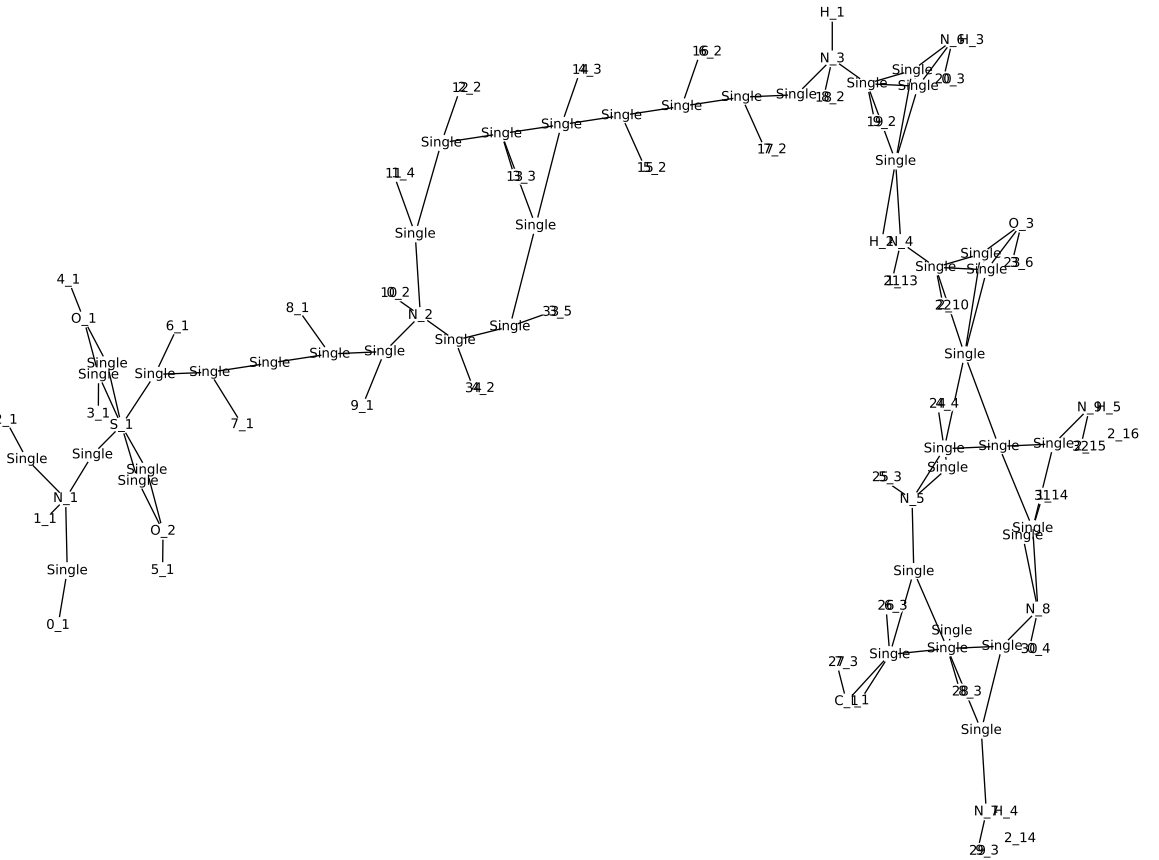US07317013-20080108-C00053_rdkit