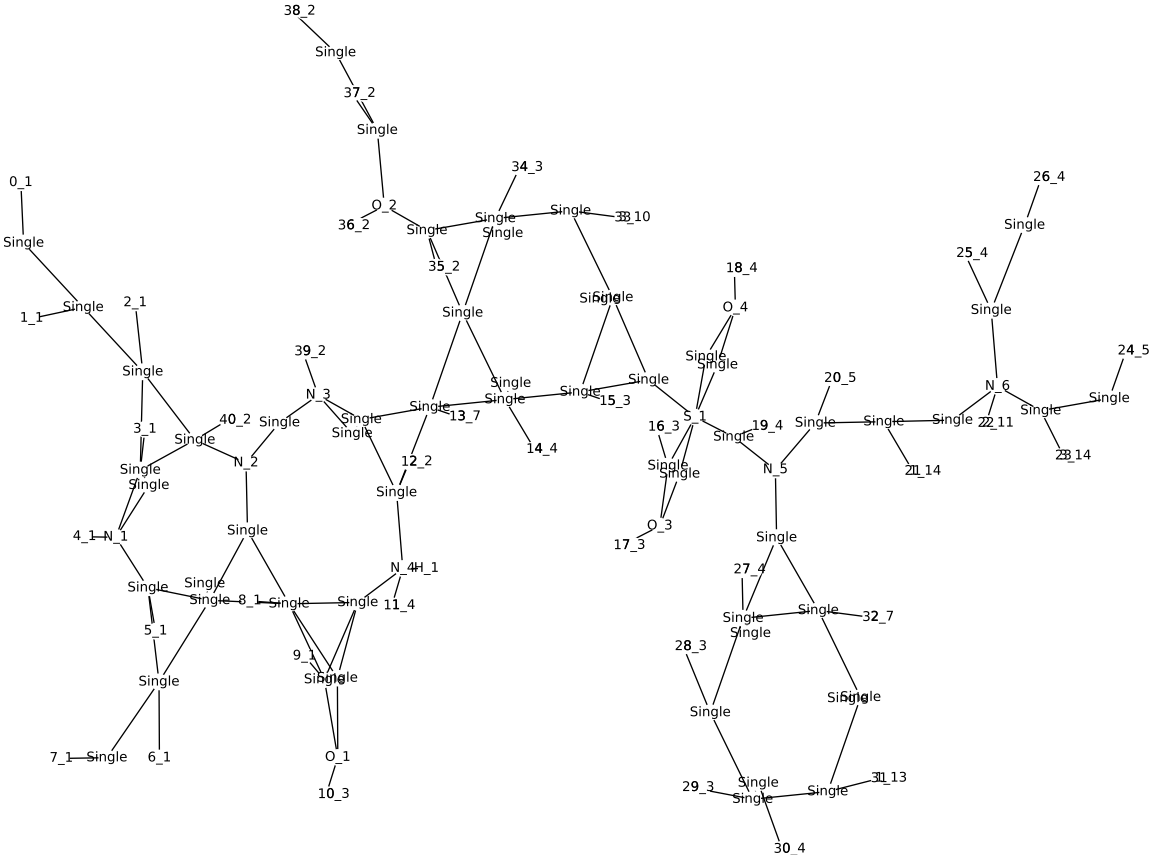US07314871-20080101-C00317_rdkit