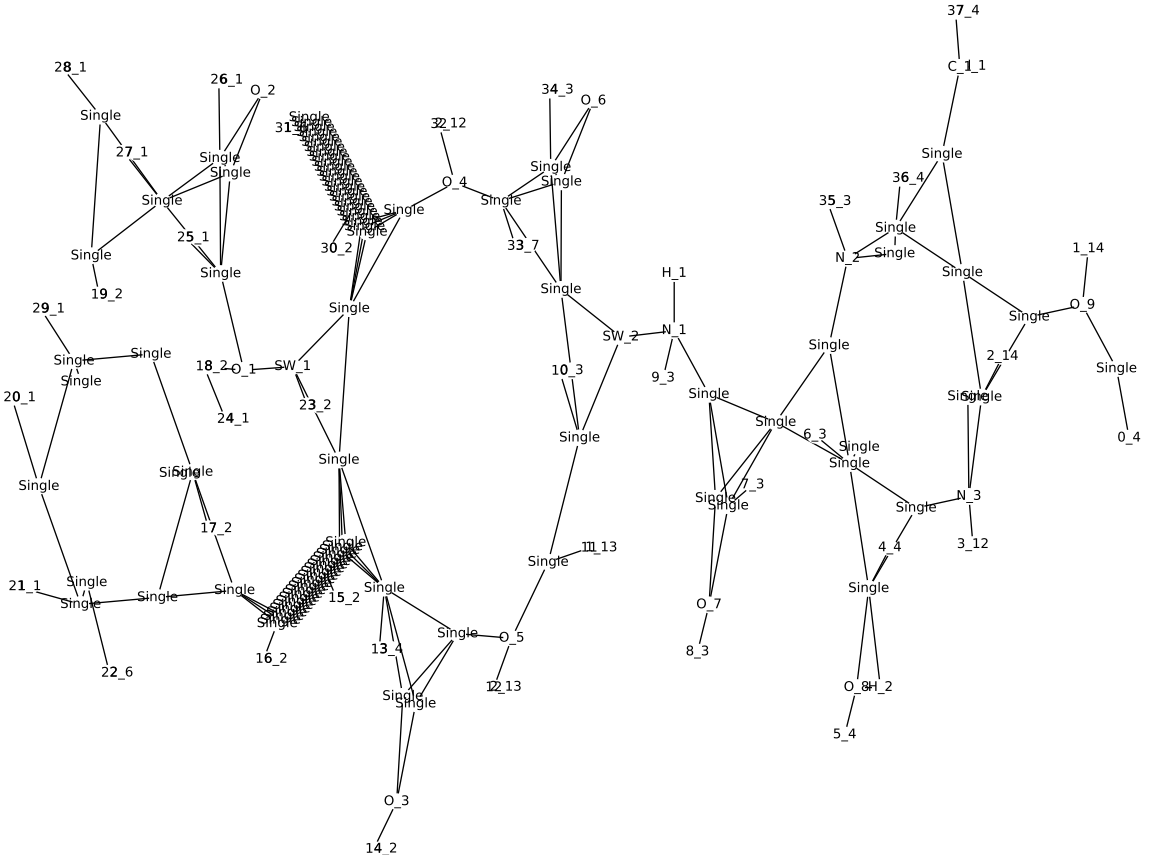USRE039991-20080101-C00429_rdkit