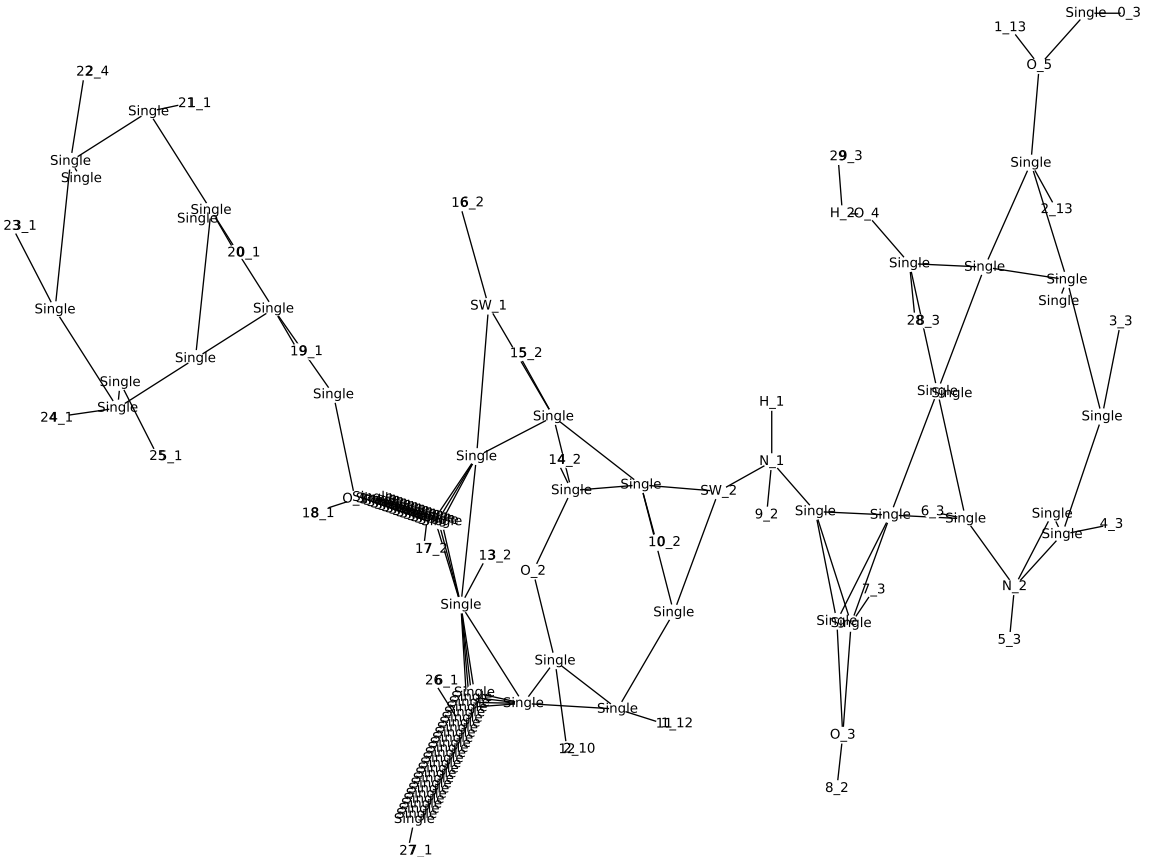USRE039991-20080101-C00216_rdkit