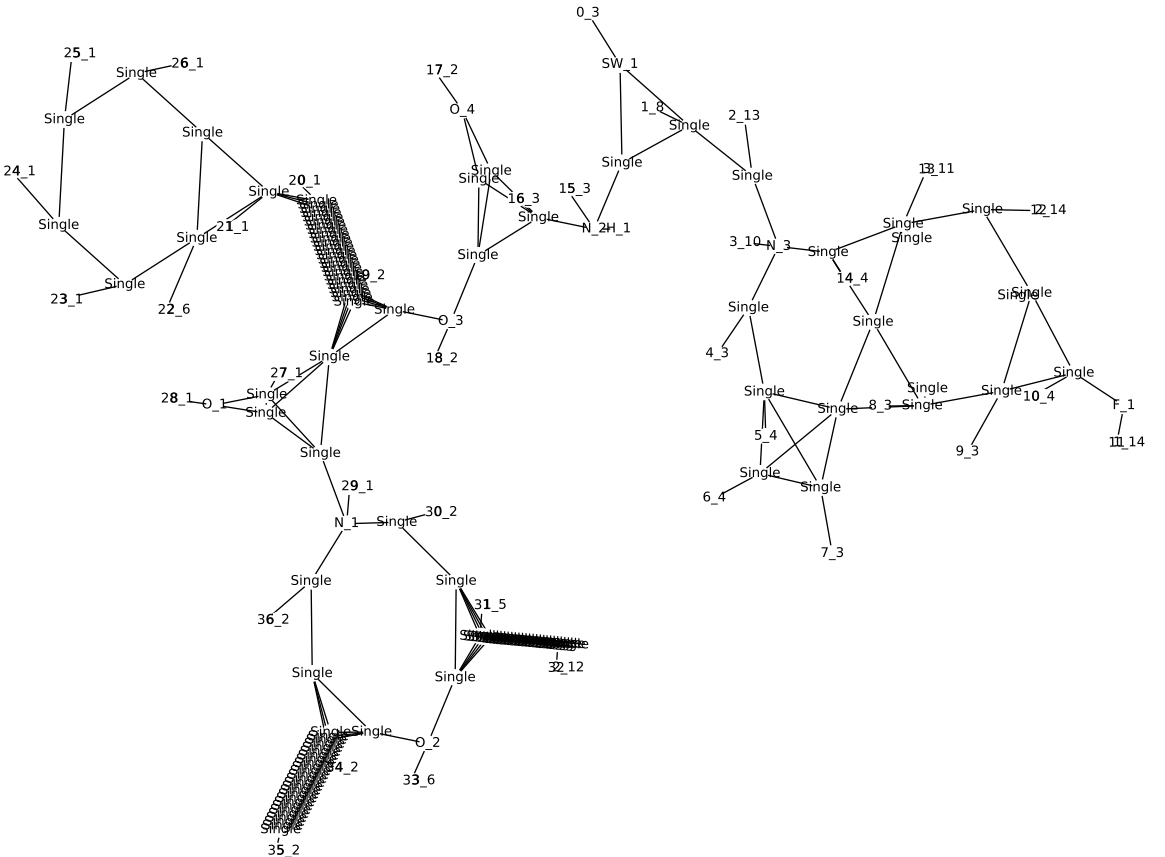US07314872-20080101-C00114_rdkit