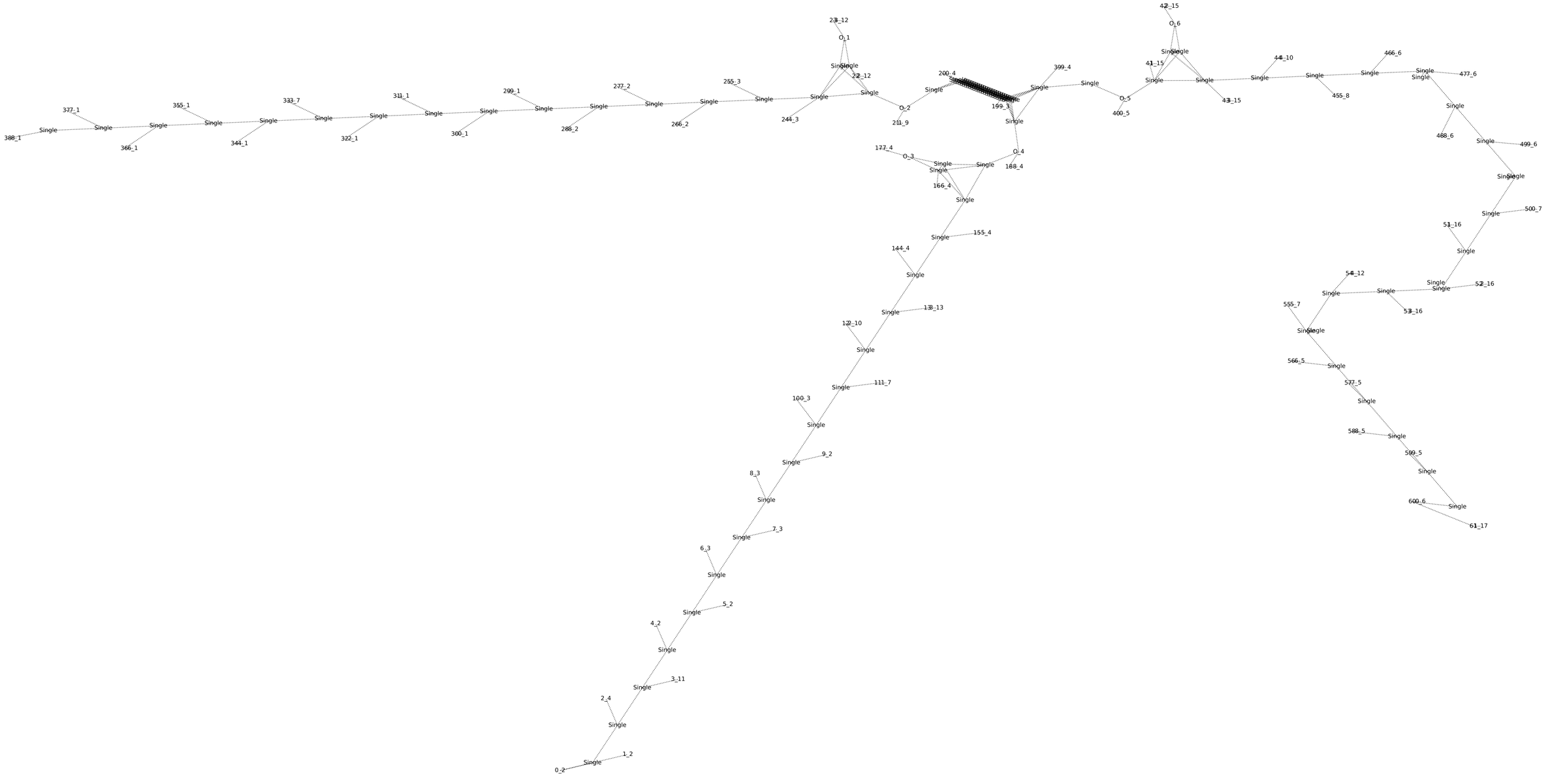9544178_rdkit