

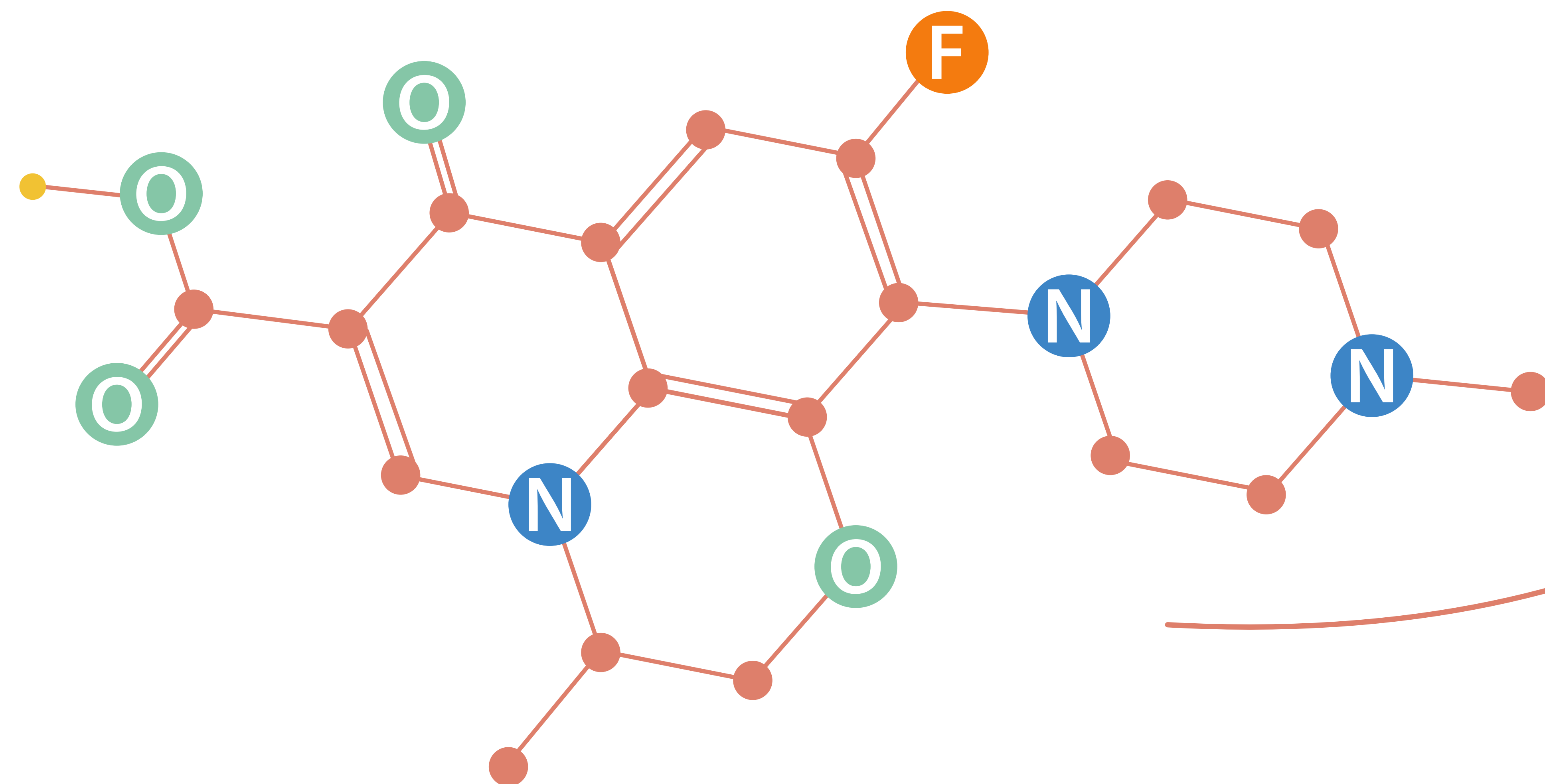
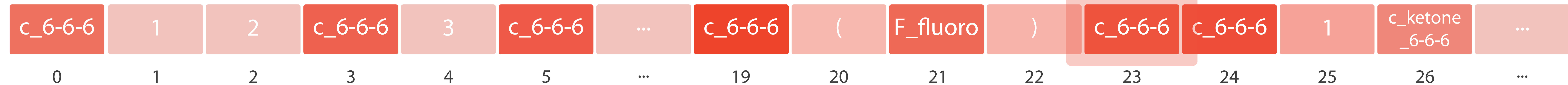
c_6-6-6 1 2 c_6-6-6 3 c_6-6-6 (N_tertiary_amine_6 4 C_6 C_6 N_tertiary_amine_6 ... c_6-6-6 n_tertiary_amine_6-6-6 2 C_tertiary_carbon_6-6-6 (C_alkyl) C_6-6-6 O_ether_6-6-6

FG-enhanced SMILES indexing

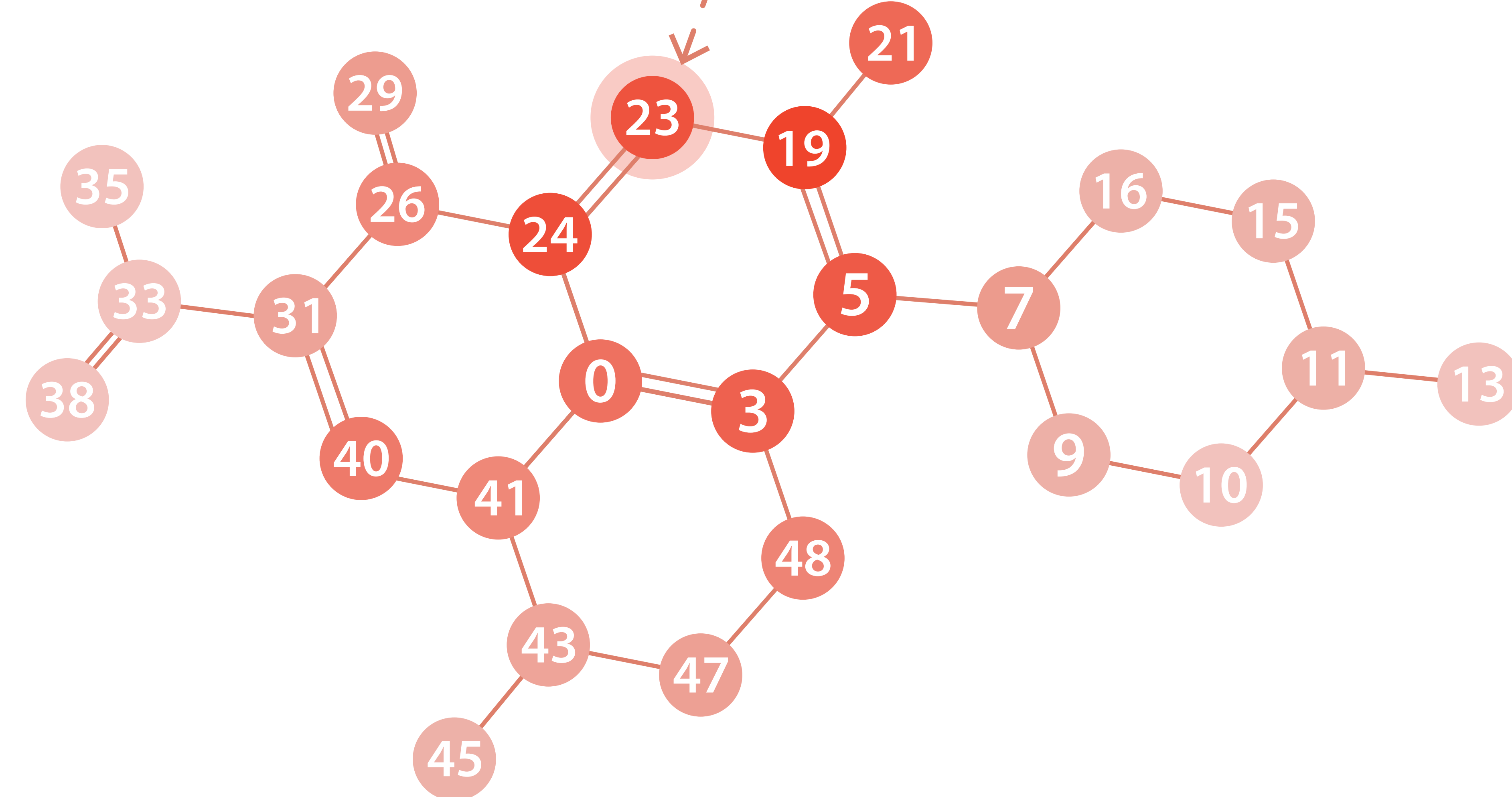


query atom

Attention map



Molecular graph



Molecular graph with attention map

