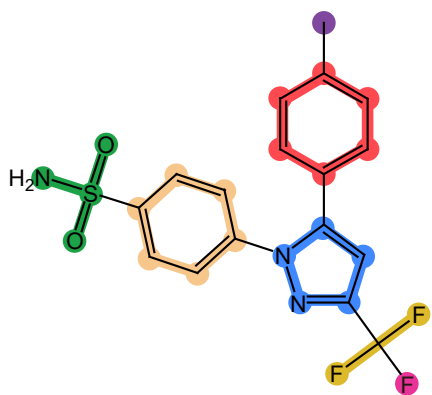


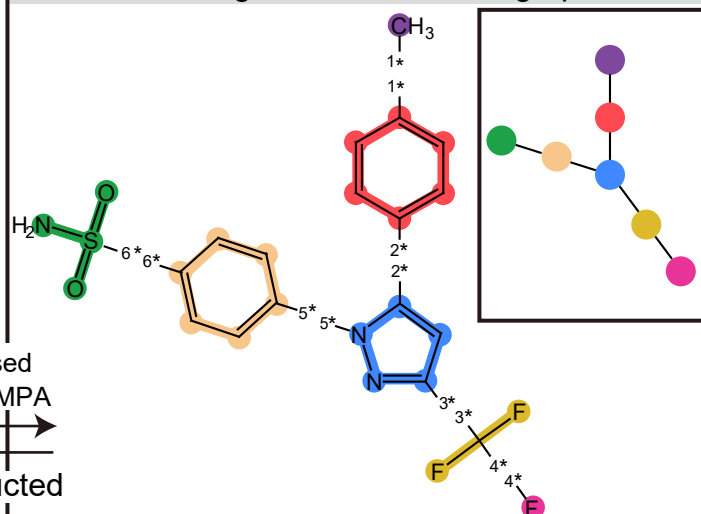
SMILES: CC1=CC=C(C=C1)C2=CC(=NN2C3=CC=C(C=C3)S(=O)(=O)N)C(F)(F)F

Represented $\longleftrightarrow$ Reconstructed

Molecular structural graph



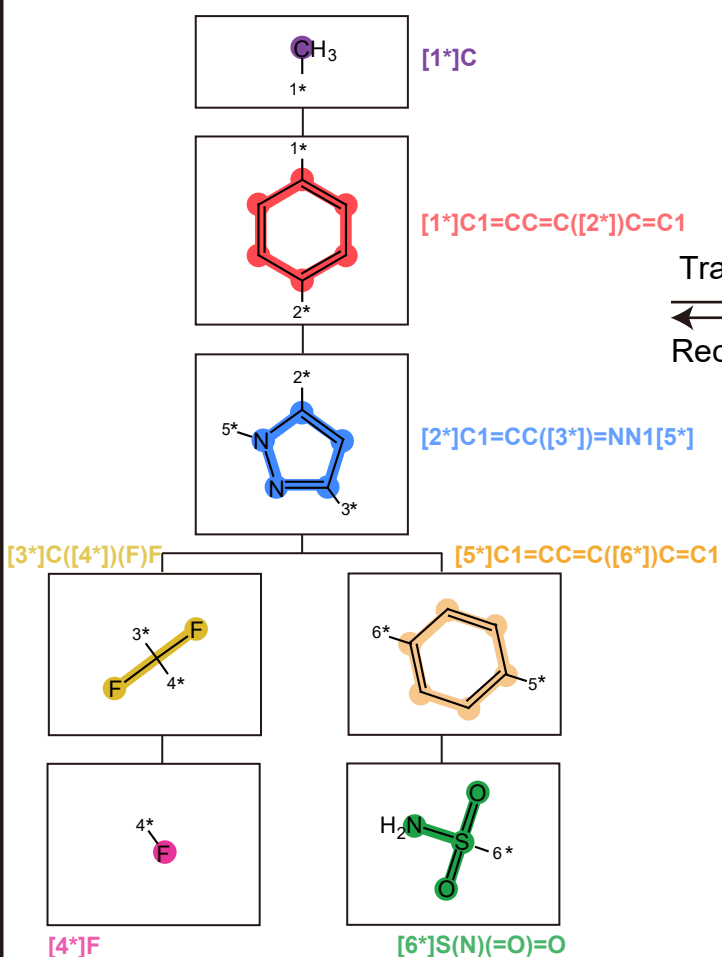
Fragmented molecular graph



Decomposed
based on MMPA
 $\longleftrightarrow$
Reconstructed

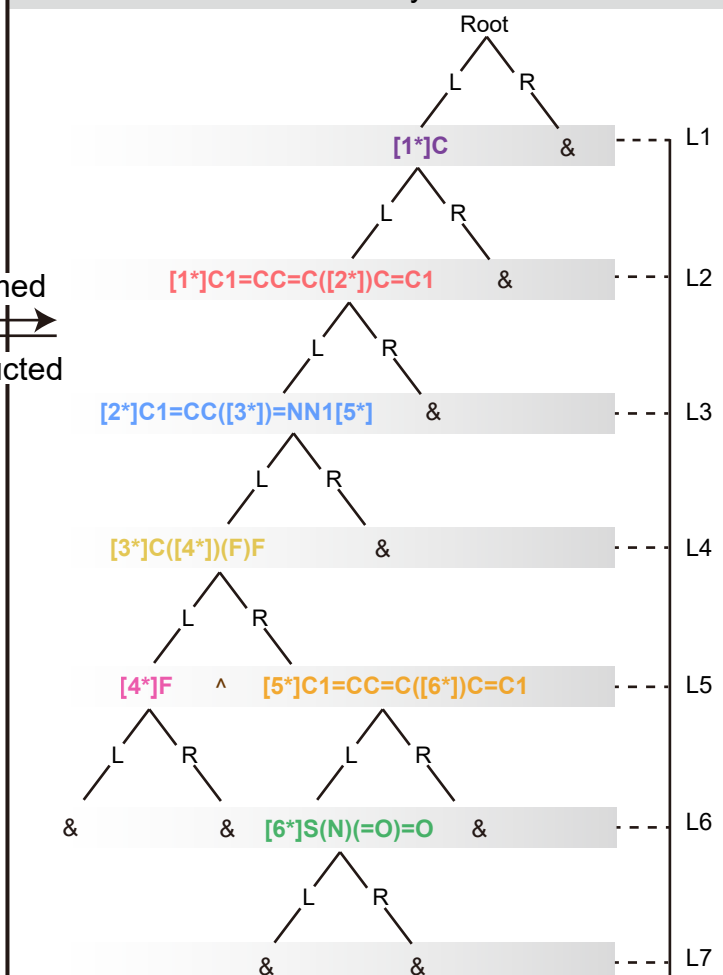
Transformed $\longleftrightarrow$ Reconstructed

Acyclic Molecular Tree



Transformed
 $\longleftrightarrow$
Reconstructed

Full Binary Tree



Reconstructed $\uparrow$

Read out
based on BFS $\downarrow$

t-SMILES strings

t-SMILES (TSID) : [1*]C&[1*]C1=CC=C([2*])C=C1&[2*]C1=CC([3*])=NN1[5*]&[3*]C([4*])(F)F&[4*]F^
[5*]C1=CC=C([6*])C=C1&&[6*]S(N)(=O)=O&&&

t-SMILES (TSDY) : *C&*C1=CC=C(*)C=C1&*C1=CC(*)=NN1* &*C(*) (F)F &*F^*C1=CC=C(*)C=C1&&
*S(N)(=O)=O&&&