

Task: for each row, adjust the center molecule such that it is chemically 'in the middle' of ligand A and B.
For ease of interpretation, perturbed atoms/bonds in ligand A/B are indicated in red.

Index/target/pert_name	Ligand A	Intermediate (adjust)	Ligand B
1: TYK2 - ejm_54~ejm_31			
2: TYK2 - ejm_42~ejm_44			
3: TYK2 - ejm_44~ejm_31			
4: TYK2 - jmc_27~ejm_54			
5: TYK2 - ejm_43~ejm_47			
6: TYK2 - ejm_49~ejm_45			
7: TNKS2 - 5p~5m			
8: TNKS2 - 1b~3a			
9: TNKS2 - 1a~8a			
10: EG5 - CHEMBL1084678~CHEMBL1085666			
11: EG5 - CHEMBL1077227~CHEMBL1096002			
12: EG5 - CHEMBL1082249~CHEMBL1085666			
13: GALECTIN - 07_ligOH~05_ligOEt			
14: CATS - 165~132			
15: CATS - 29~141			
16: JNK1 - 18635-1~18636-1			
17: JNK1 - 18627-1~18625-1			
18: JNK1 - 18634-1~18659-1			
19: JNK1 - 18634-1~18659-1			