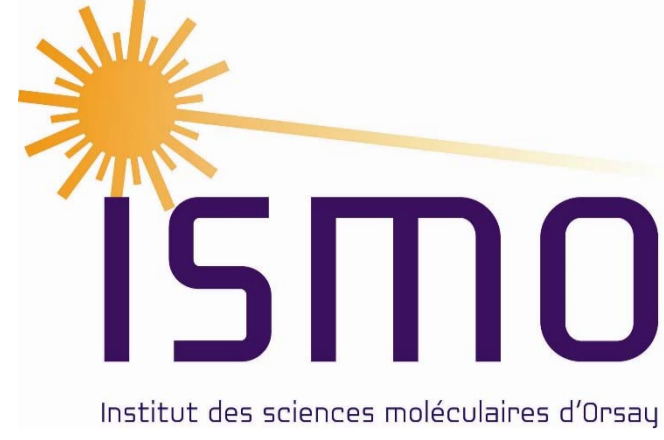


# Chirality effects in the structure of several Diketopiperazine



## Diketopiperazine

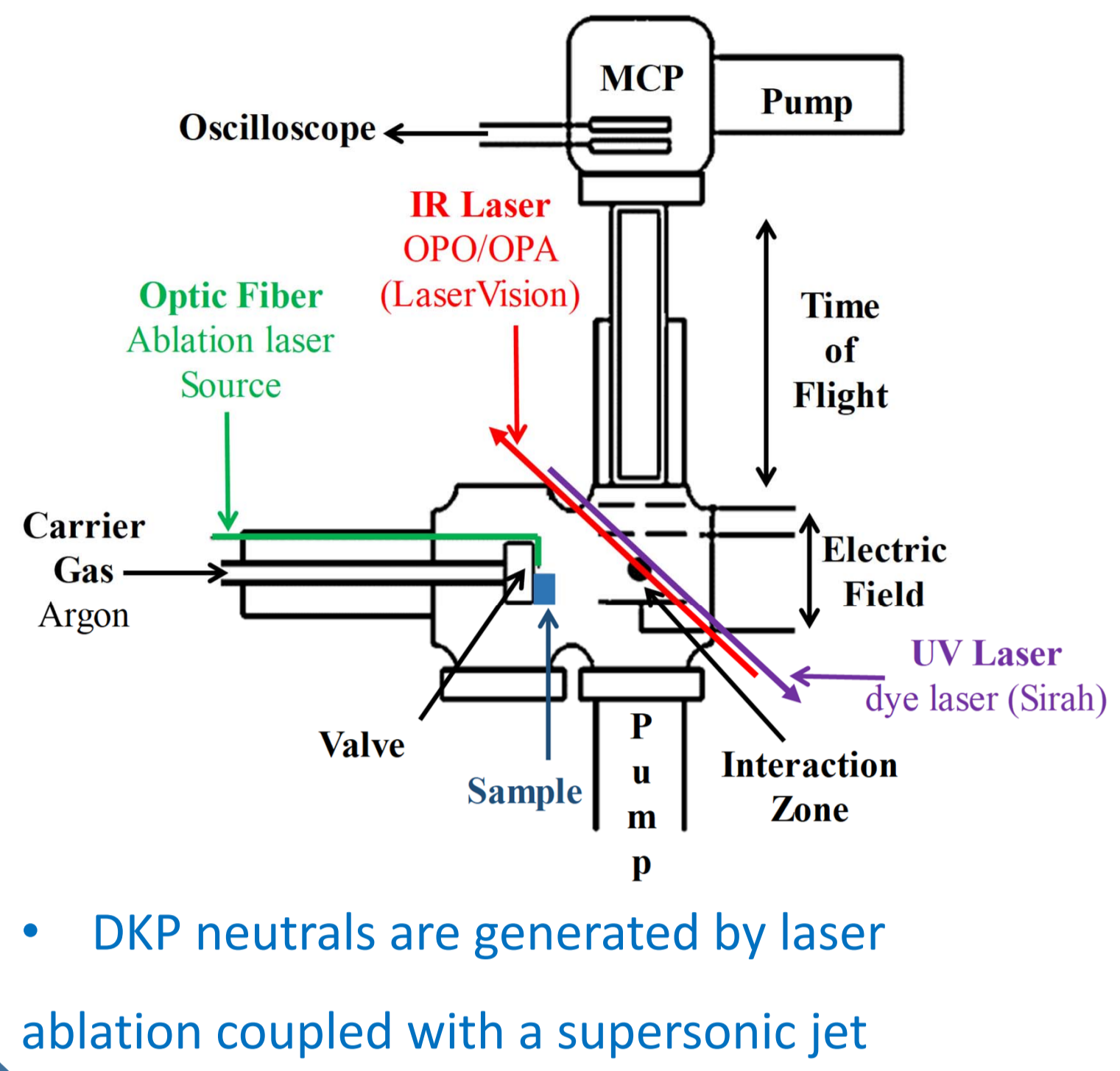


Comprendre le monde, construire l'avenir®

Ariel Francis Perez-Mellor, Ivan Alata, Feriel Ben Nasr, Valéria Lepère, Katia Le Barbu-Debus, Anne Zehnacker-Rentien

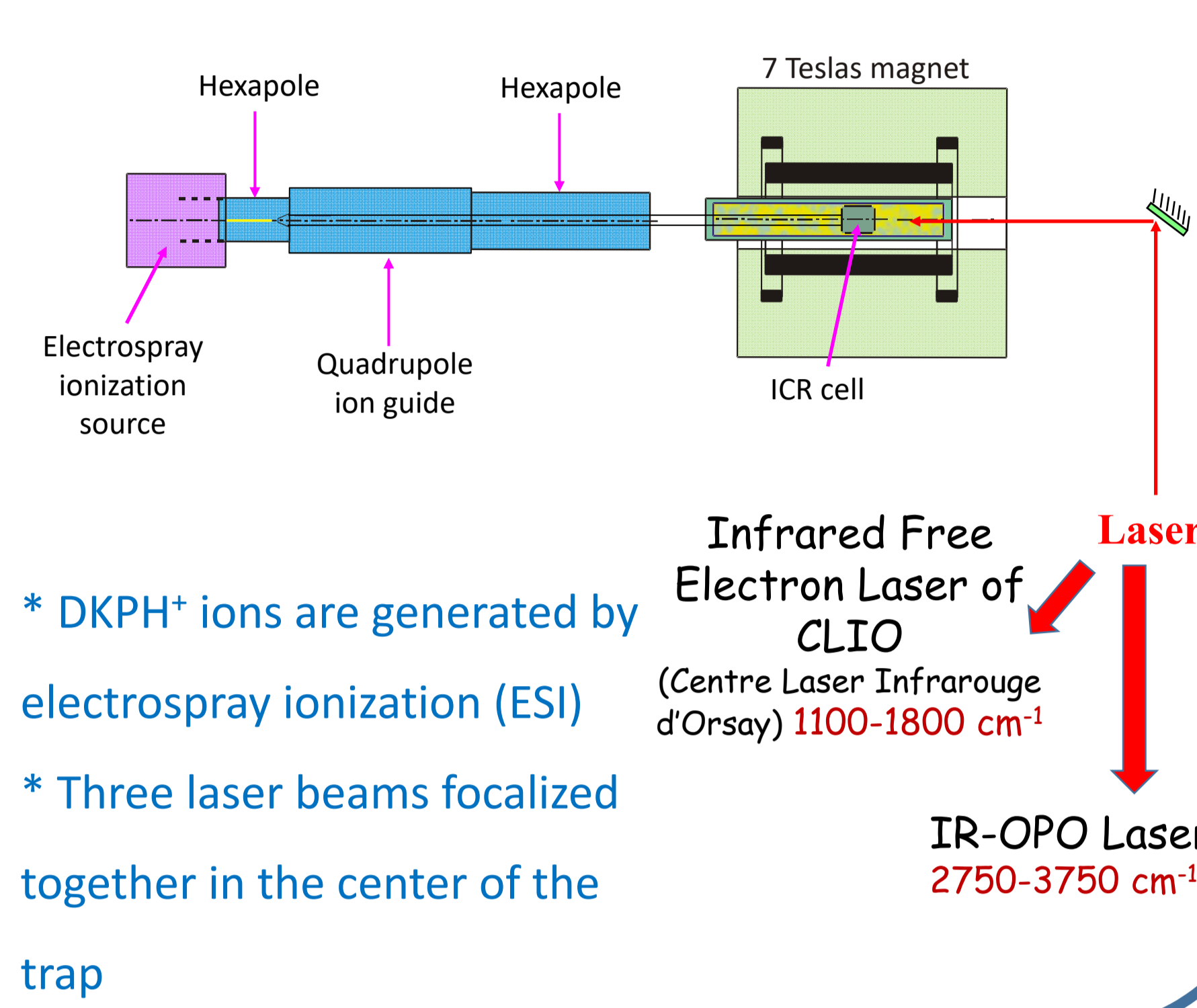
Institut des Sciences Moléculaires d'Orsay ISMO, UMR8214, CNRS, Univ. Paris-Sud, Univ Paris-Saclay, Orsay (France)

### Neutral DKP



- DKP neutrals are generated by laser ablation coupled with a supersonic jet

### Ions DKPH<sup>+</sup>

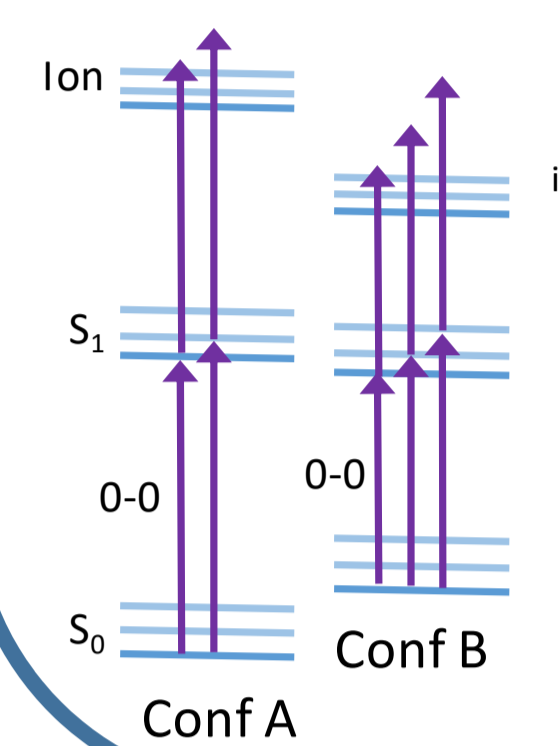


- \* DKPH<sup>+</sup> ions are generated by electrospray ionization (ESI)
- \* Three laser beams focalized together in the center of the trap

### Spectroscopy techniques

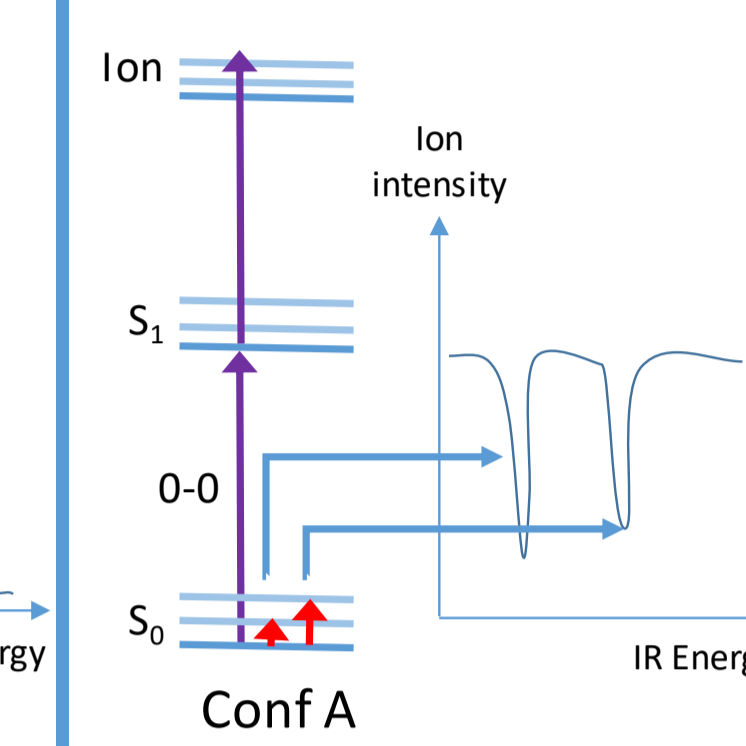
#### RE2PI

Identification of several conformers

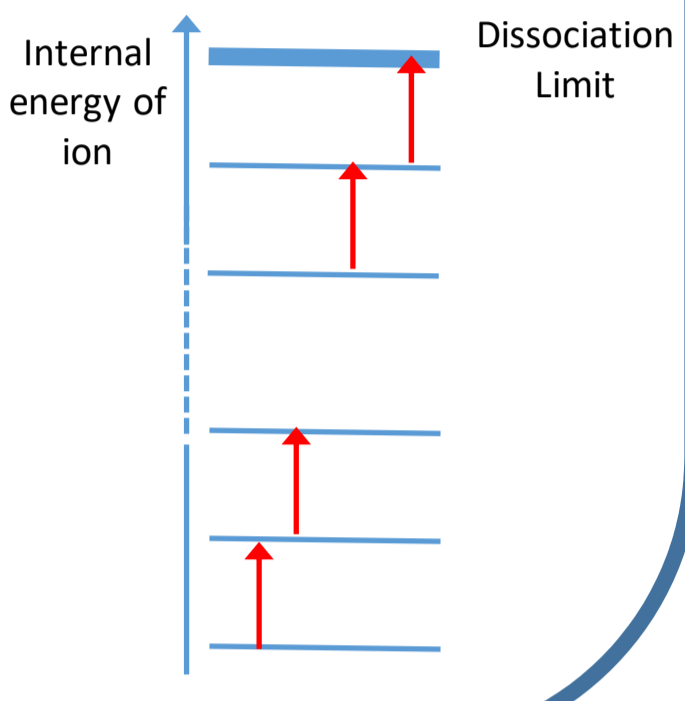


#### Resonant ion-dip infrared

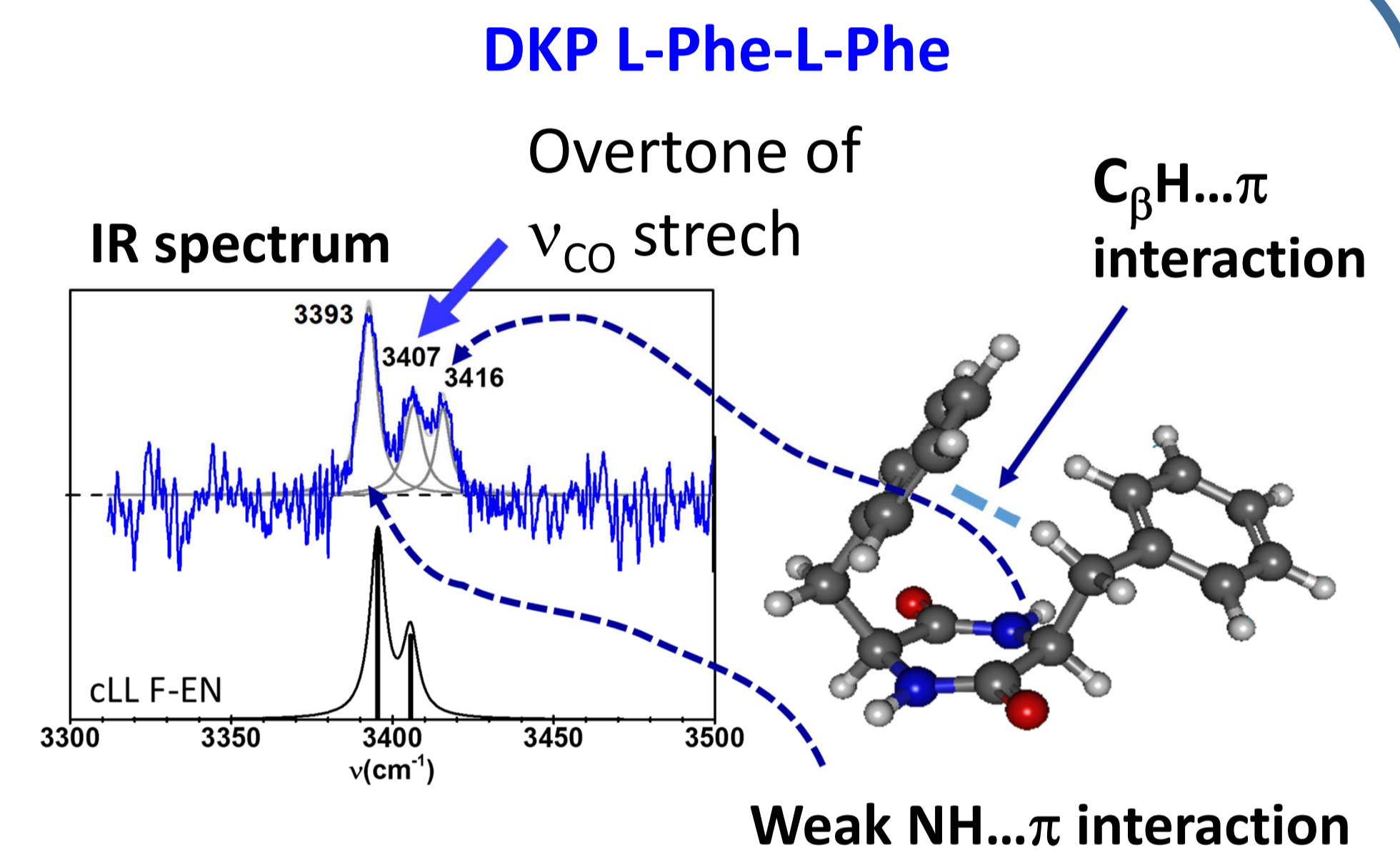
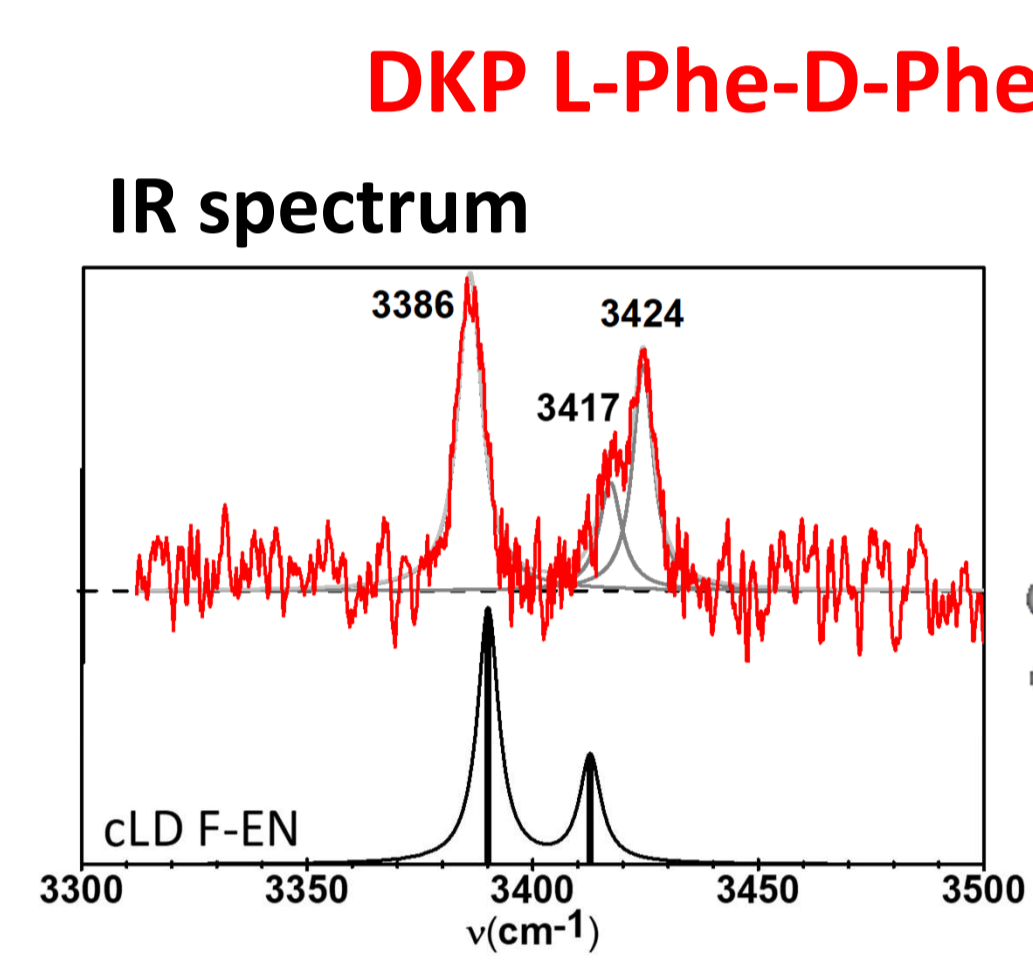
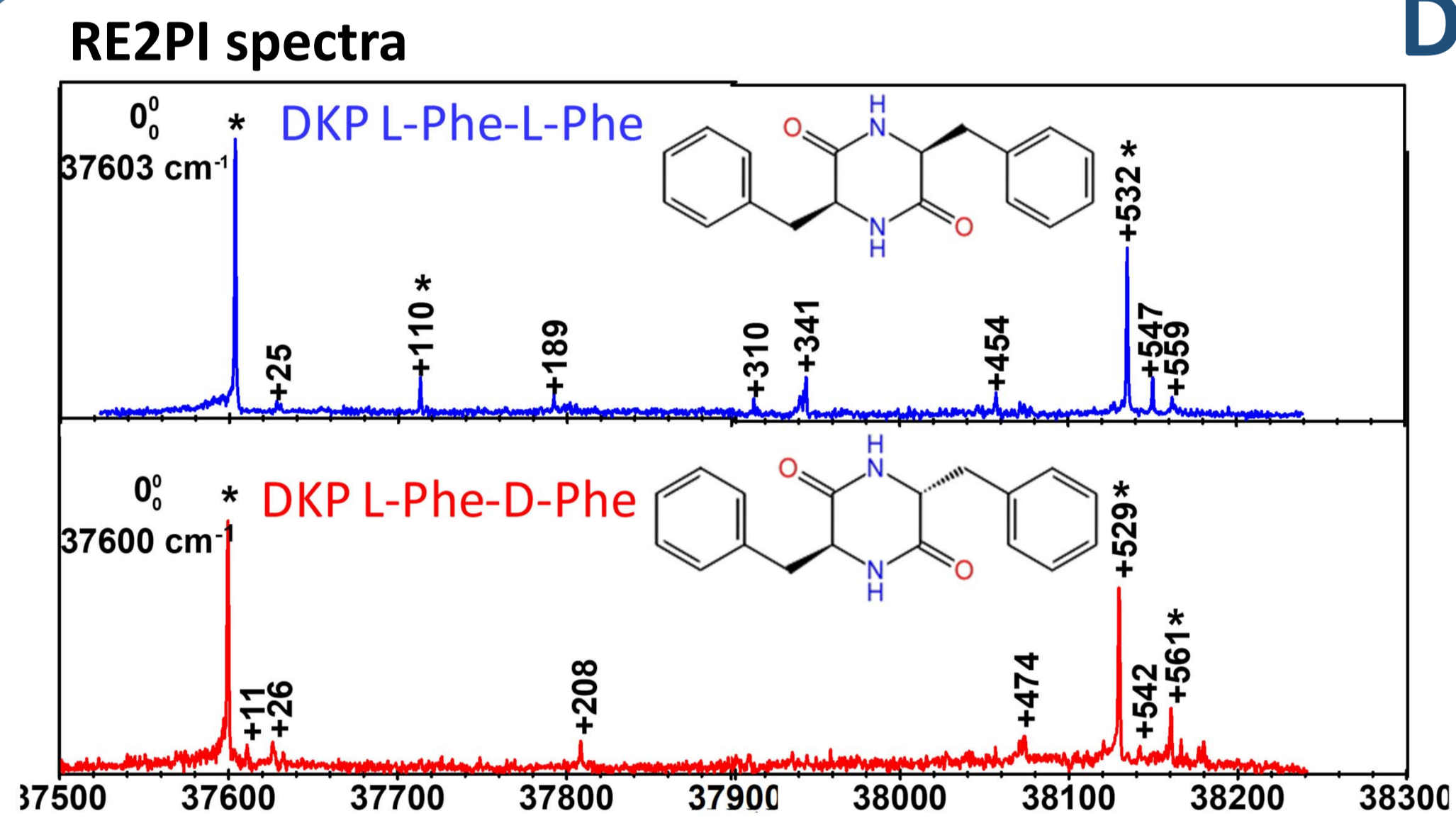
Identification of vibrational modes of molecule in OH or NH region



#### IRMPD



### DKP Phenylalanine-Phenylalanine



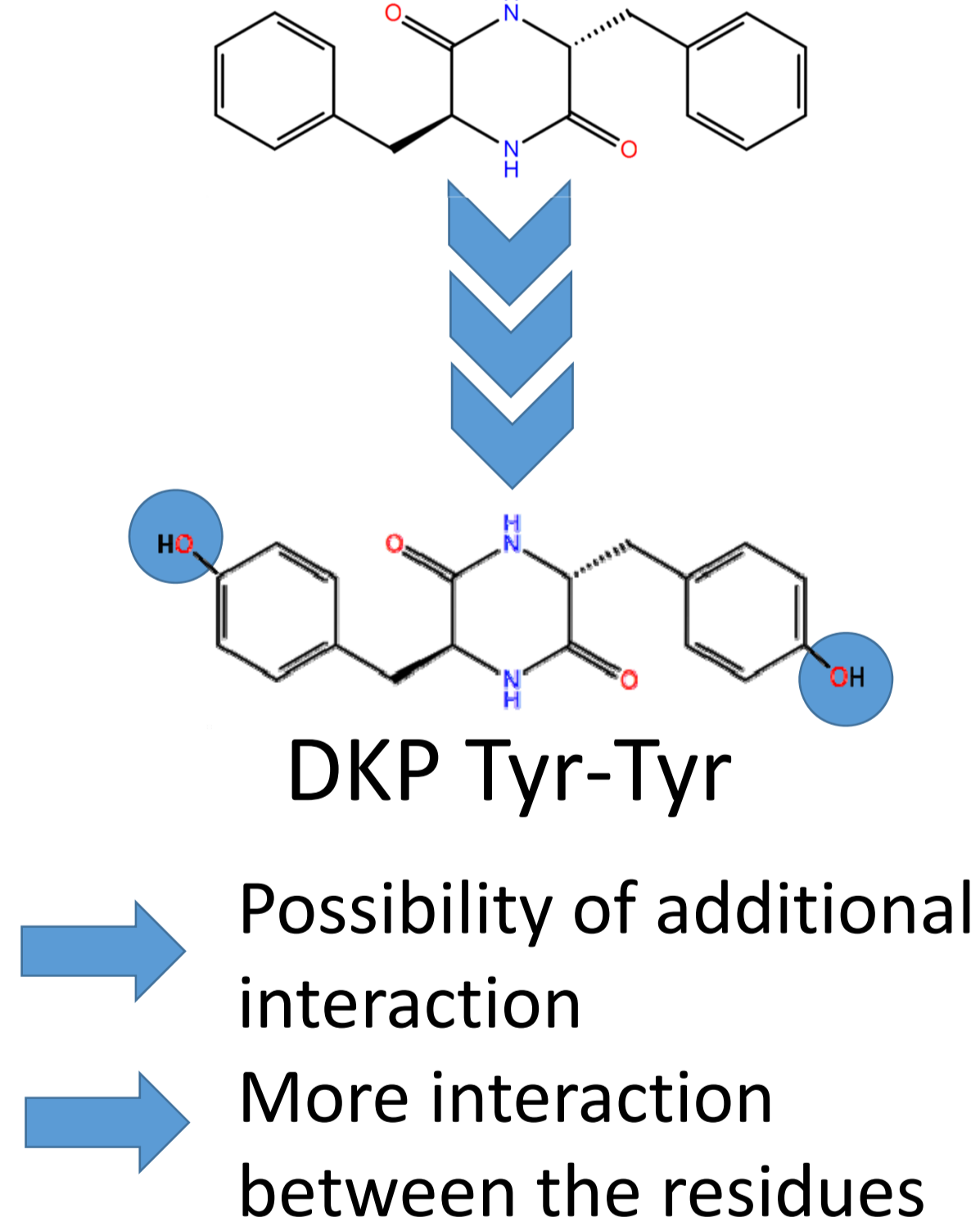
Almost no chiral discrimination  
Same vibronic pattern  
Same Herzberg-Teller coupling

What we learn: two similar structures, few chirality effects

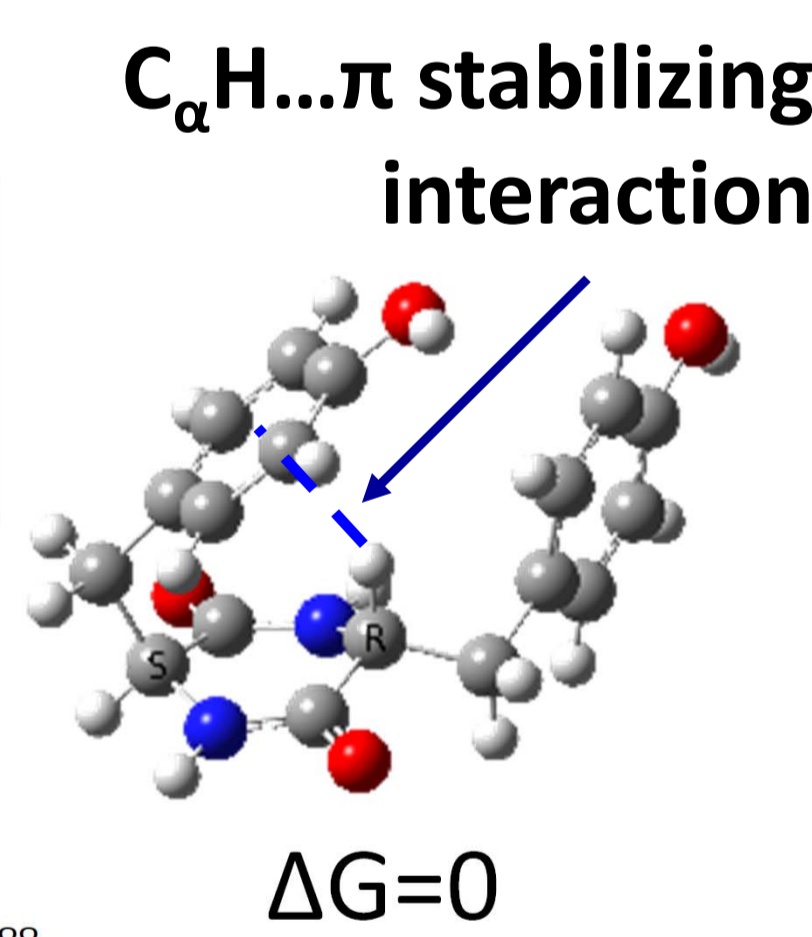
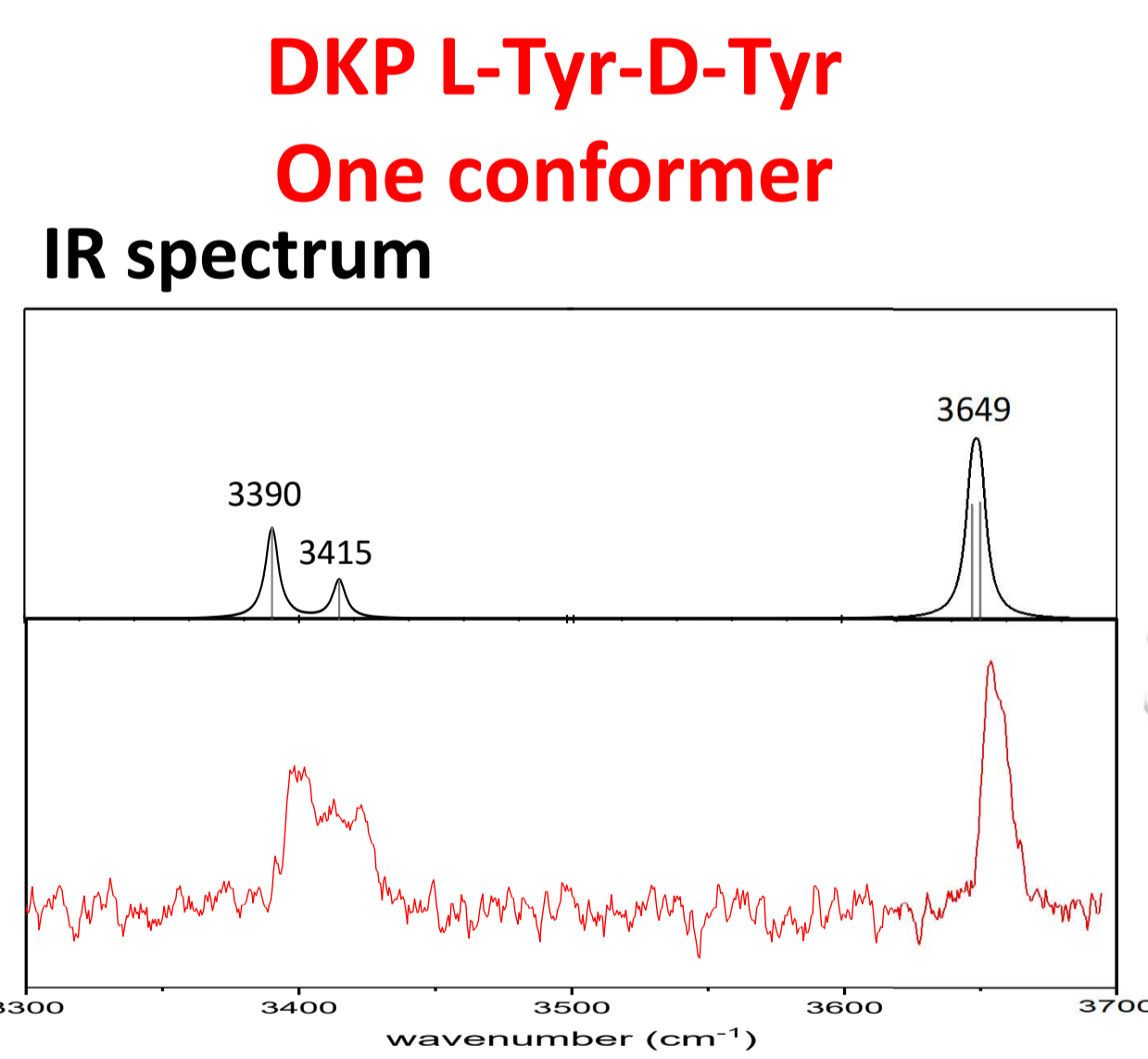
### DKP Phe-Phe

### DKP Tyrosine-Tyrosine

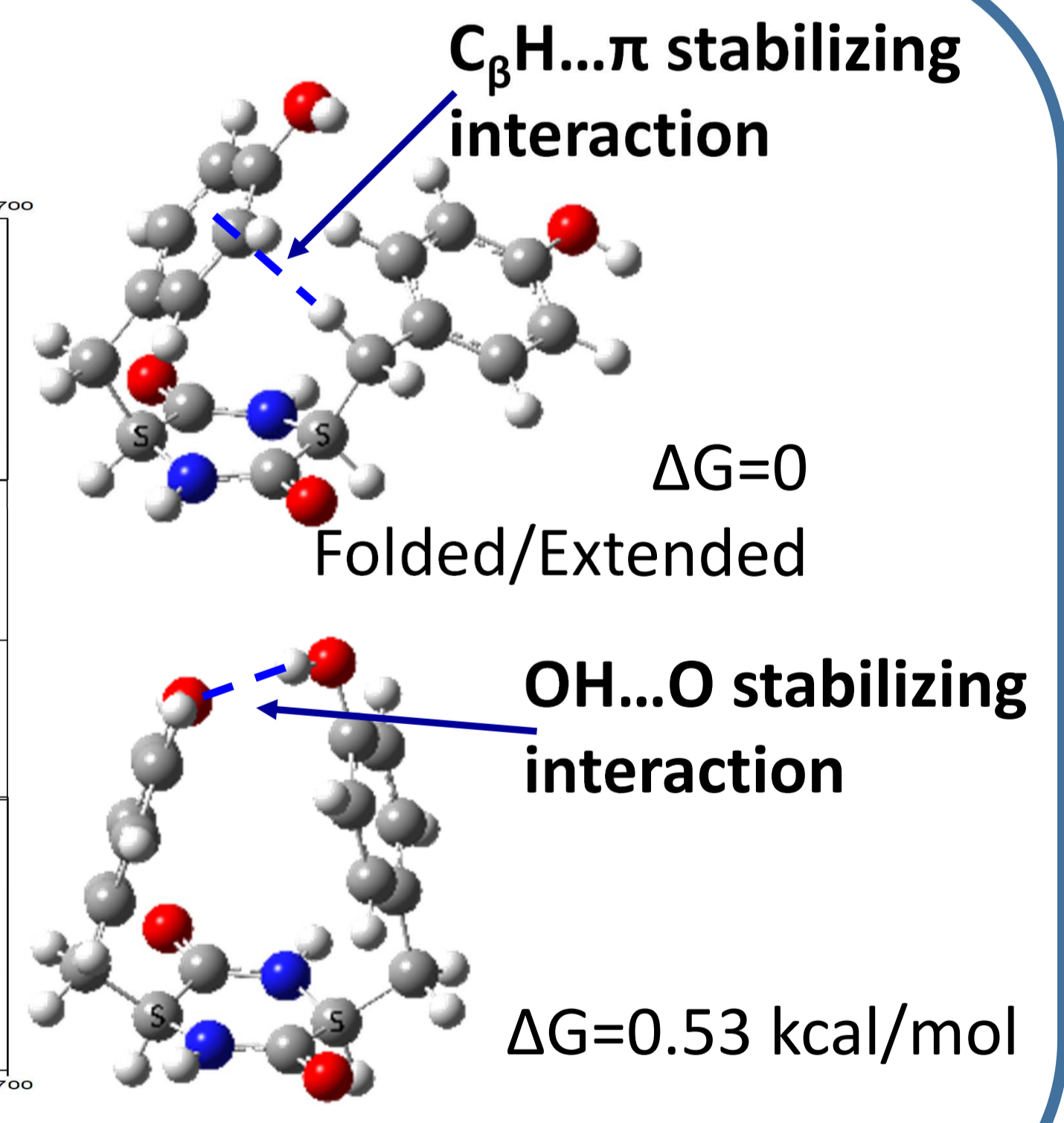
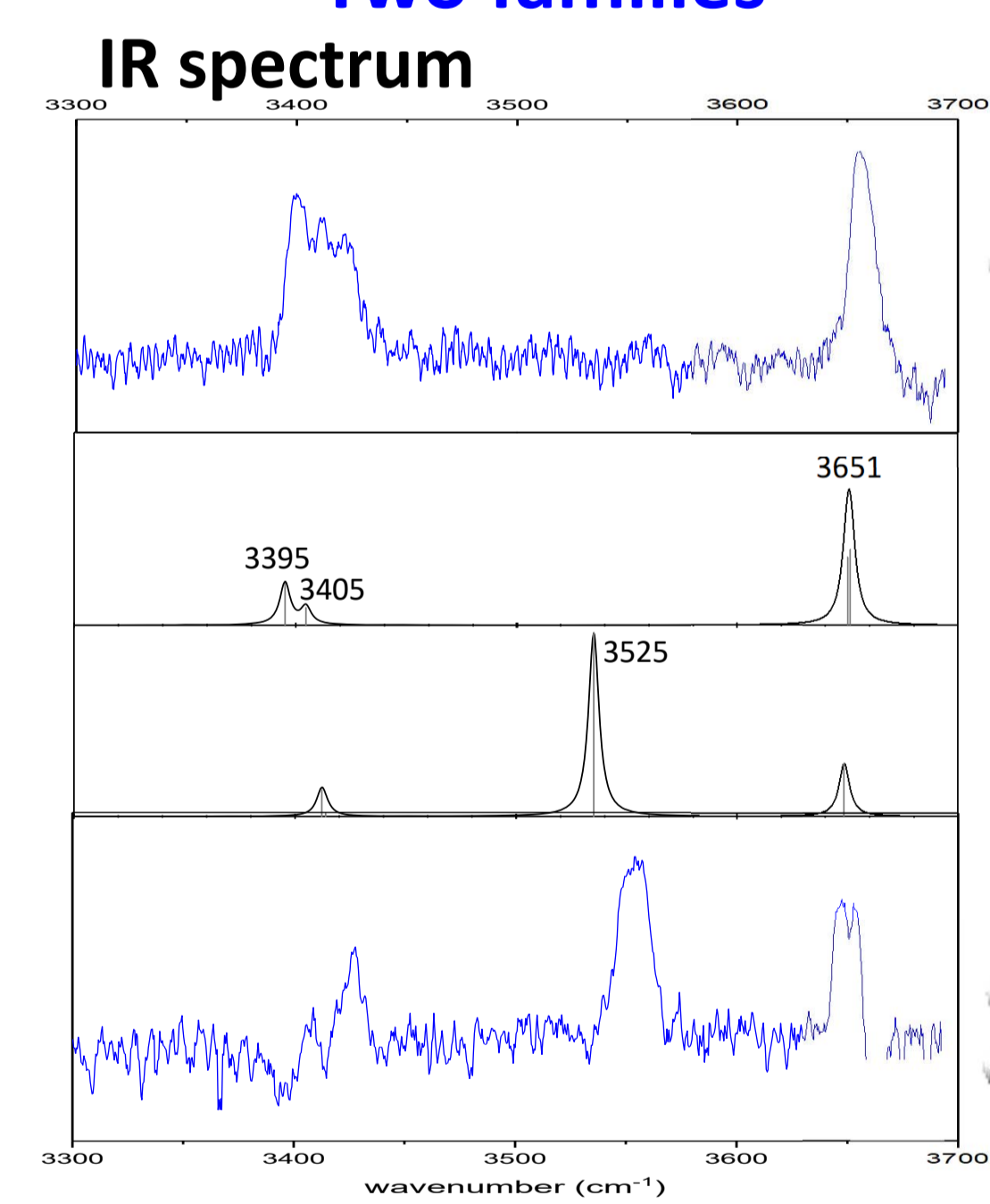
### DKP L-Tyr-L-Tyr Two families



Possibility of additional interaction  
More interaction between the residues



ΔG=0

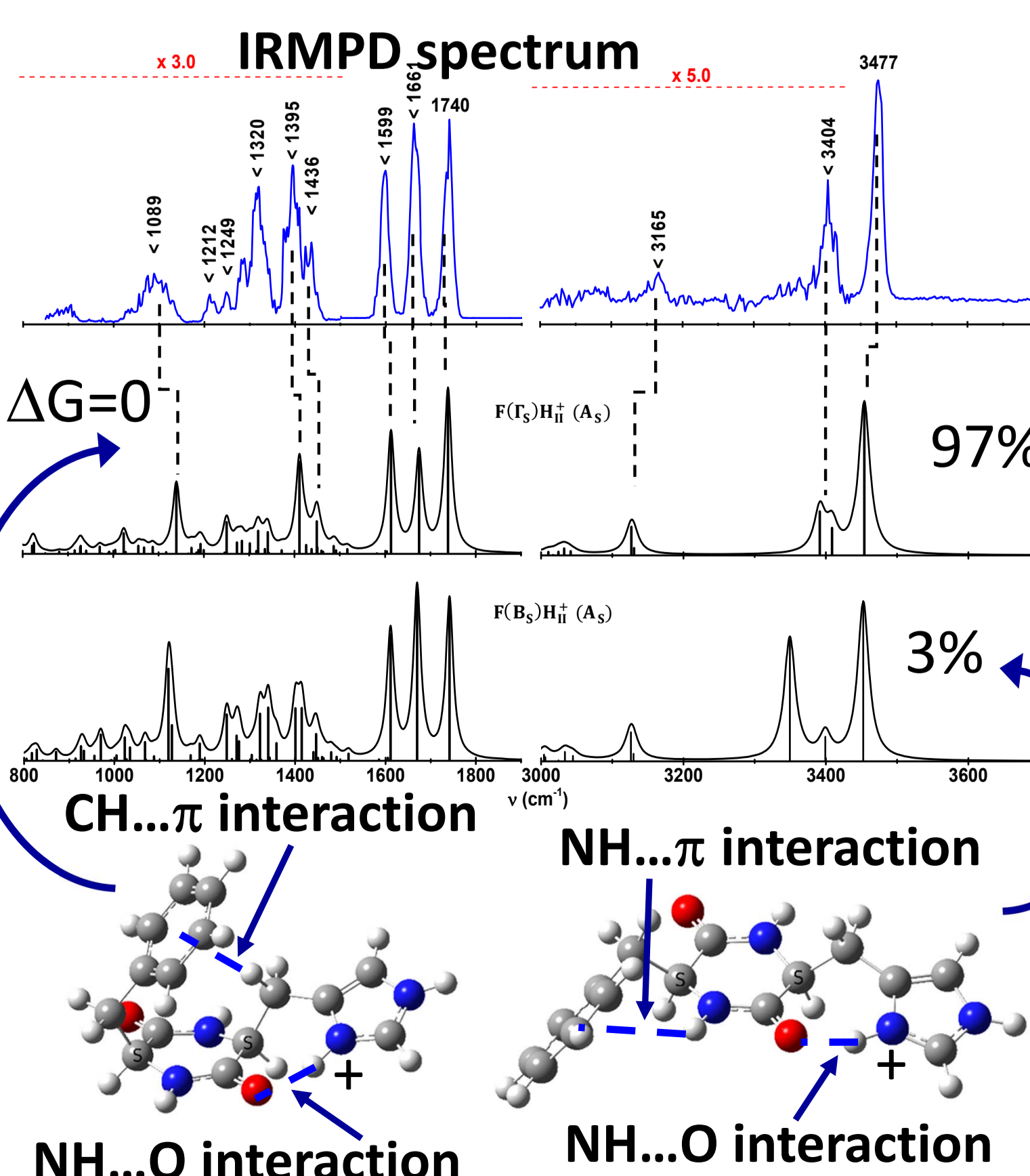
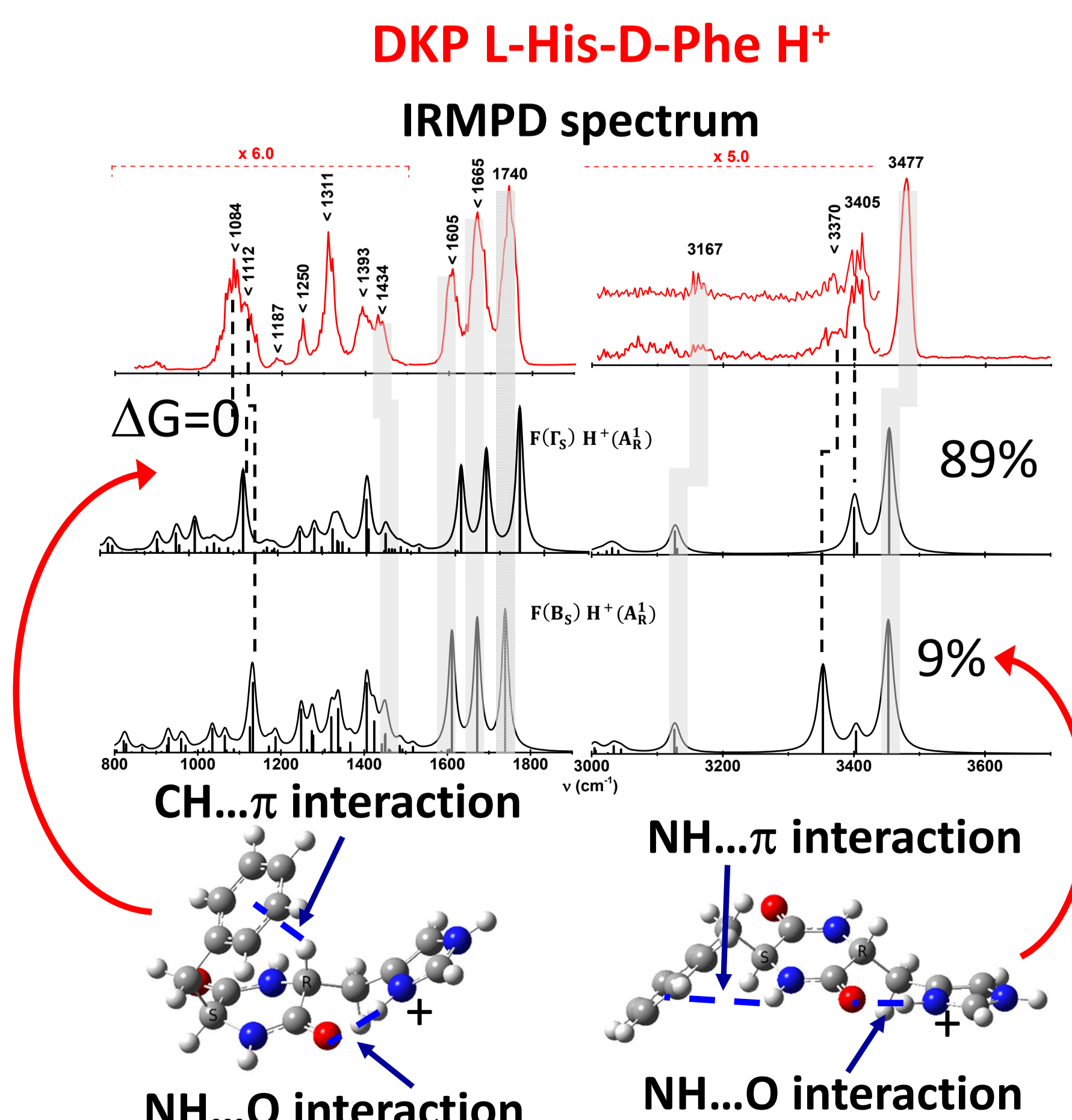
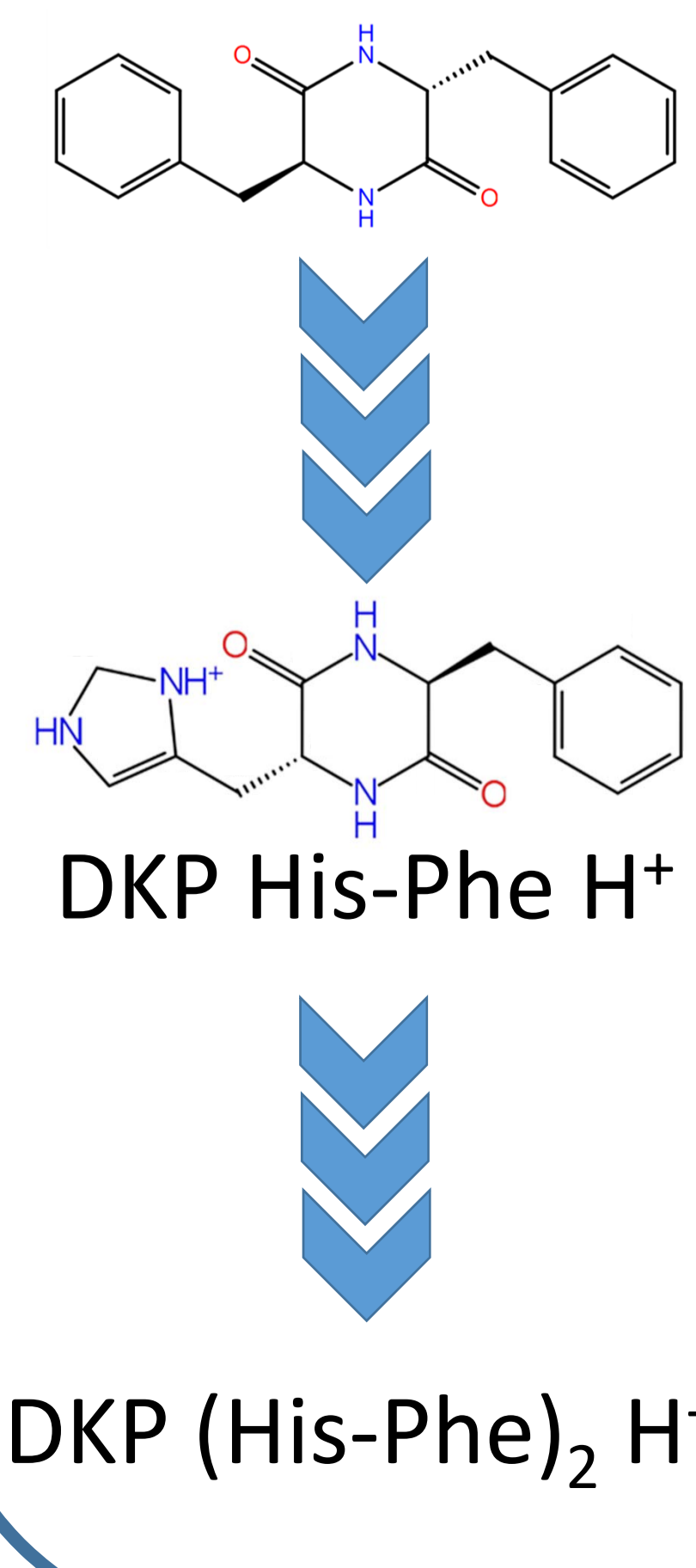


What we learn: « Proper » interaction between the two residues increases chirality effects

### DKP Phe-Phe

### DKP Histidine-Phenylalanine H<sup>+</sup>

### DKP (L-His-D-Phe)<sub>2</sub> H<sup>+</sup> vs DKP (L-His-L-Phe)<sub>2</sub> H<sup>+</sup>



Calculation in progress...  
What we learn: weak chirality effects for monomers, but strong chiral recognition for dimers