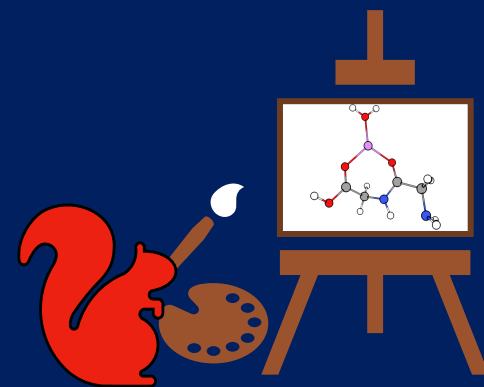


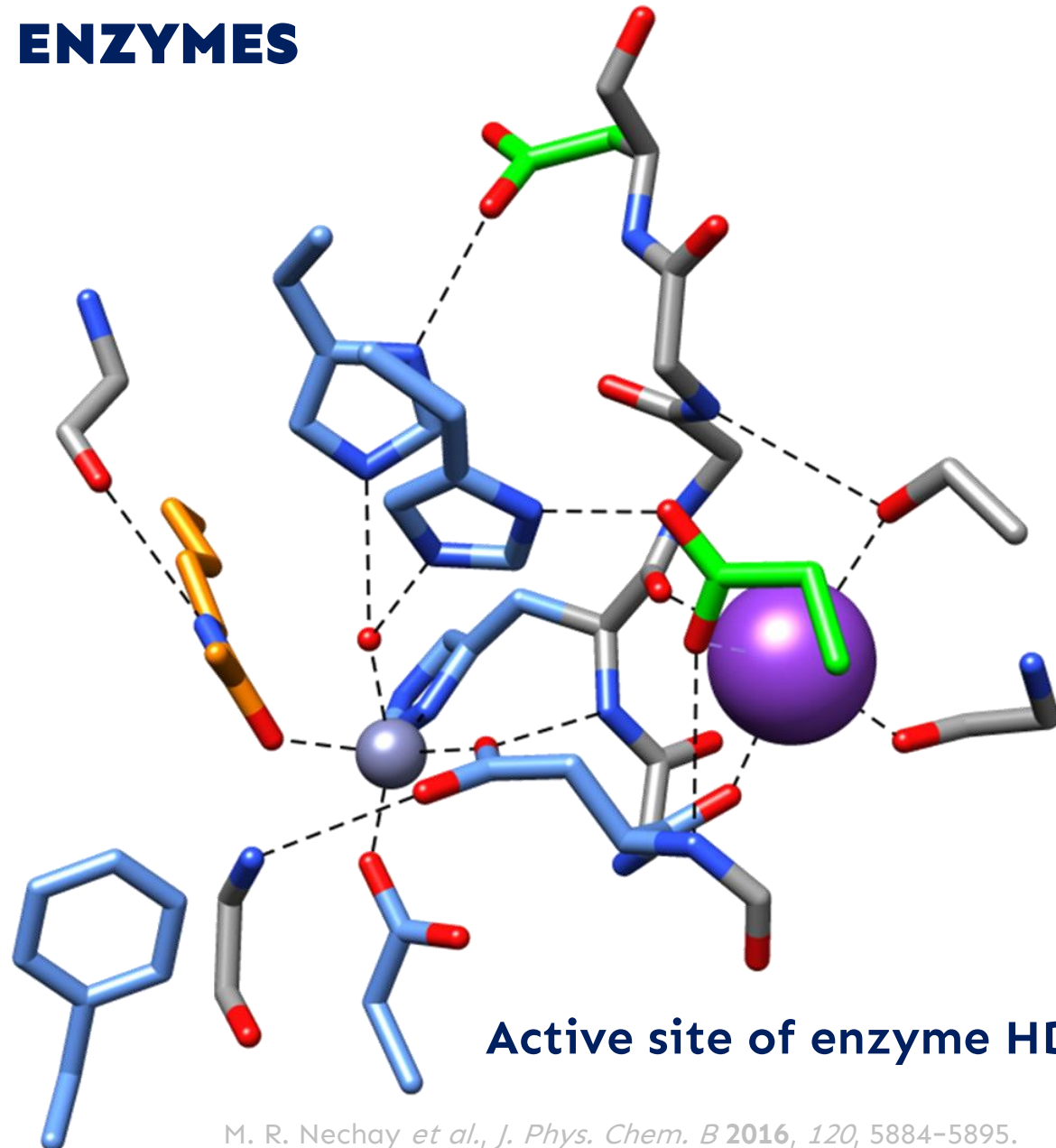
# AN ELECTRIC AFFAIR: THE IMPACT OF SOLVATION ON THE STRUCTURE OF METAL ION-PEPTIDE COMPLEXES

Katharina A. E. Meyer, E. Garand



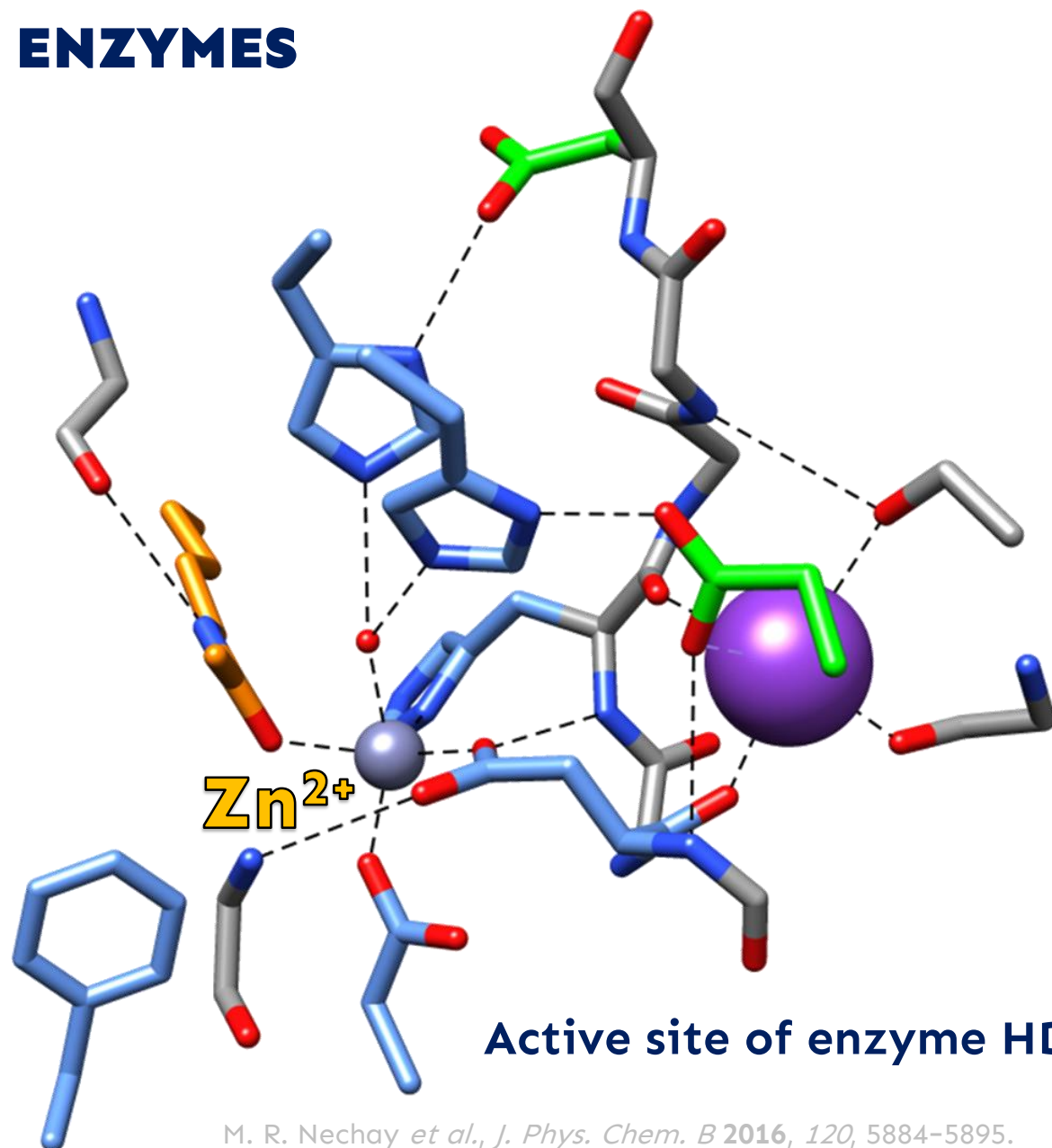


## ENZYMES

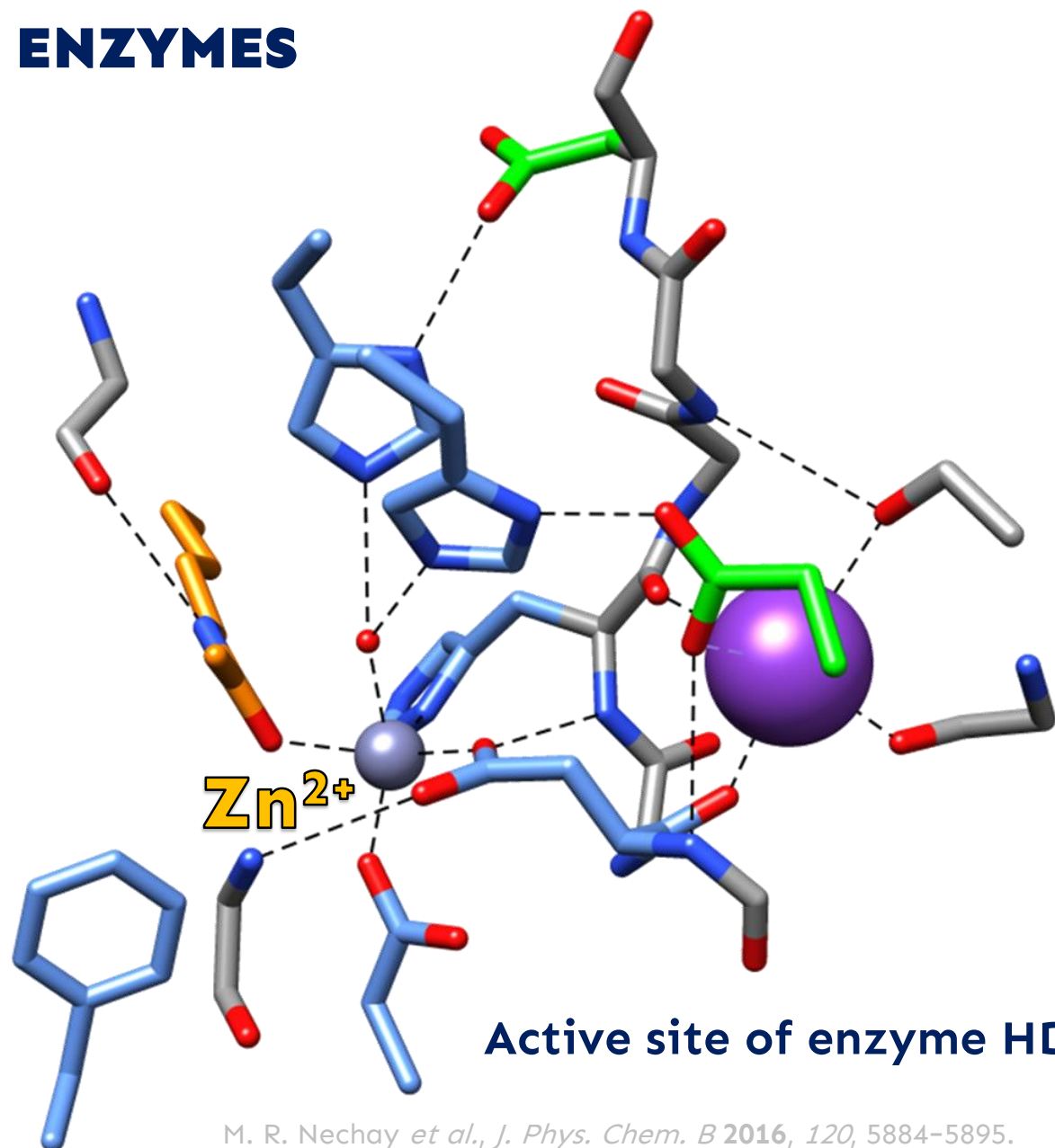


Active site of enzyme HDAC8

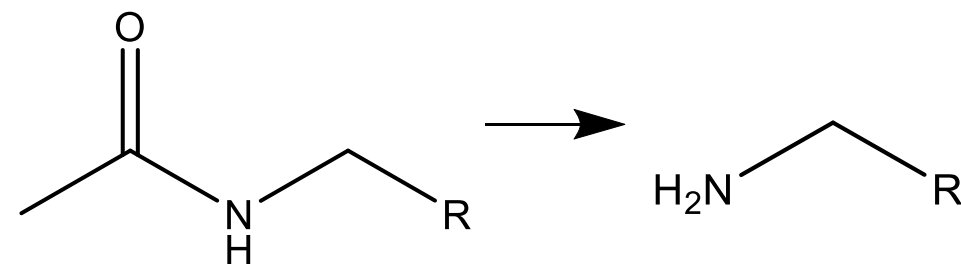
## ENZYMES



## ENZYMES

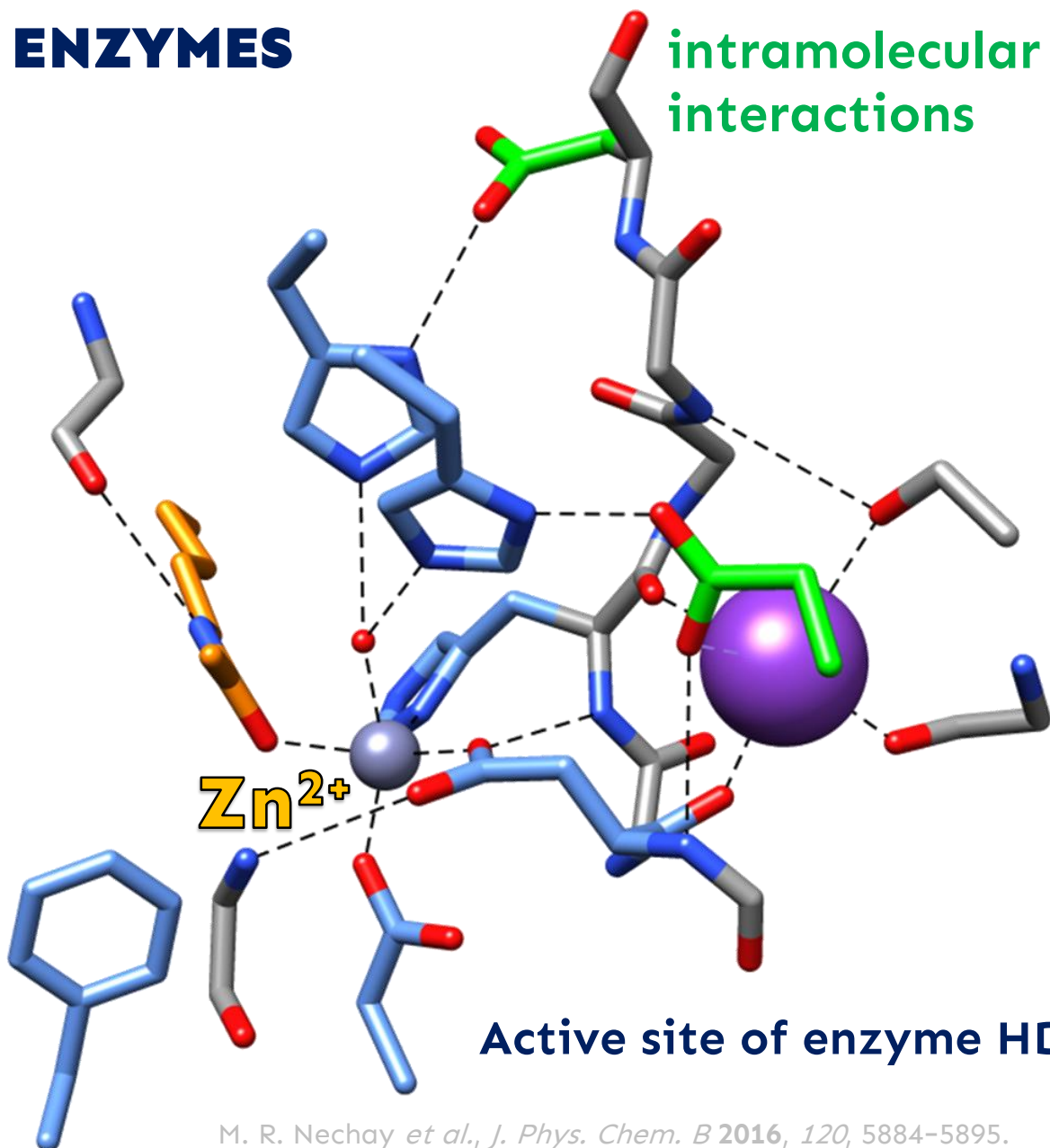


Deacetylation reaction during biosynthesis of proteins

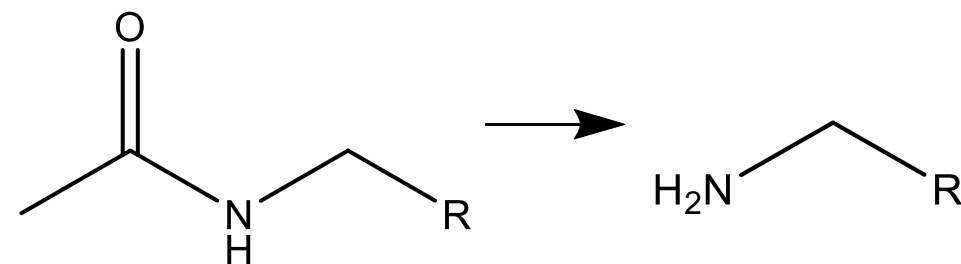


## ENZYMES

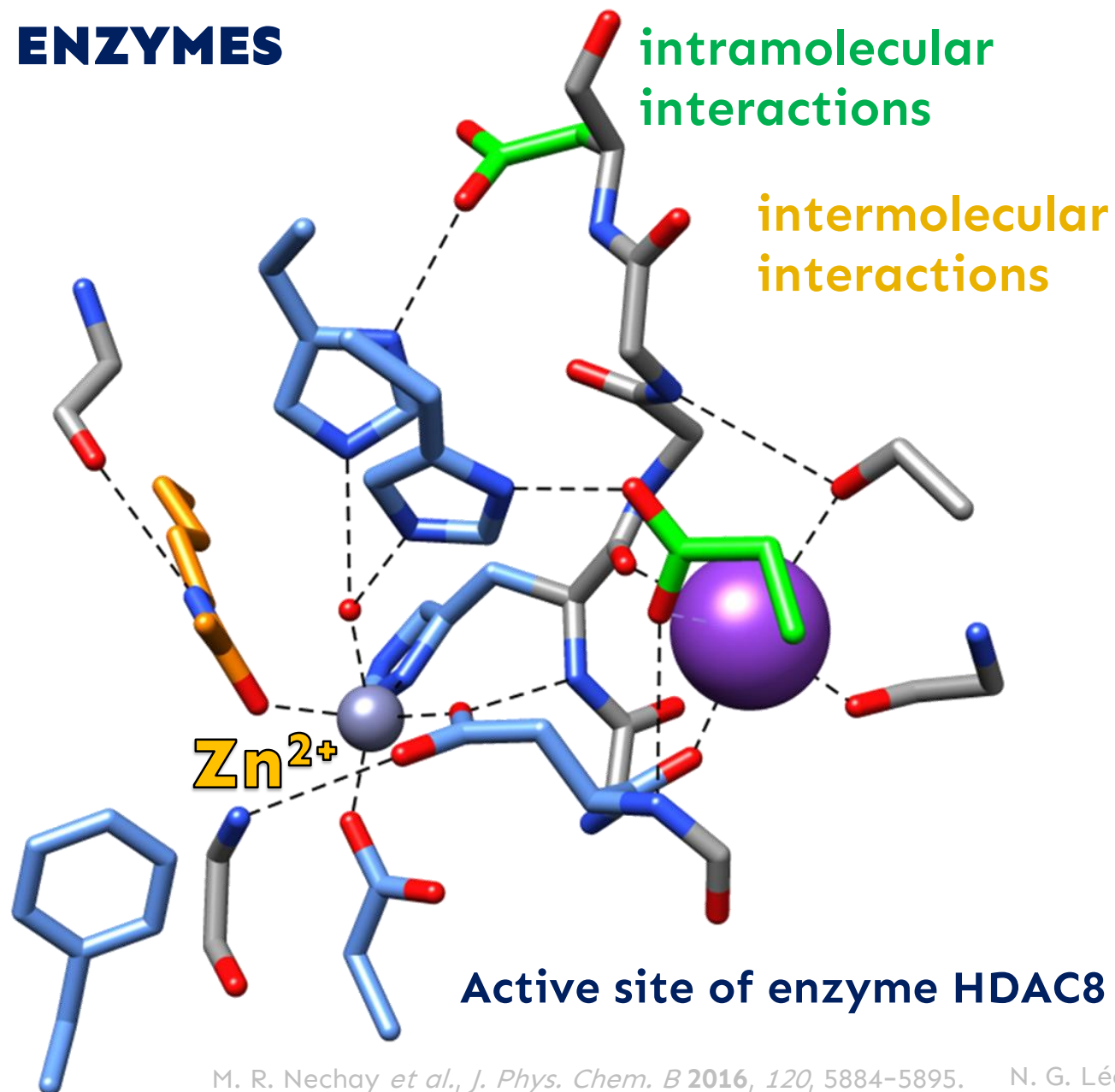
intramolecular  
interactions



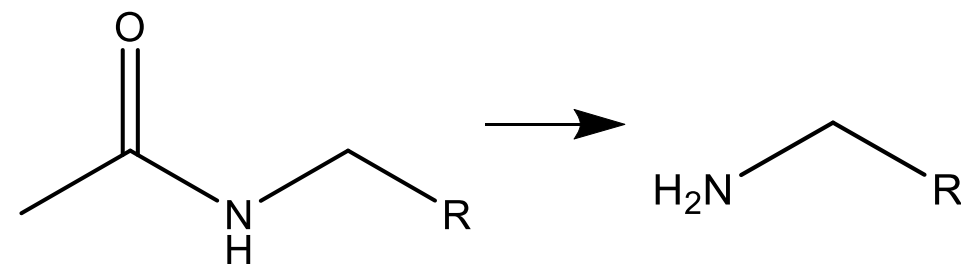
Deacetylation reaction during  
biosynthesis of proteins



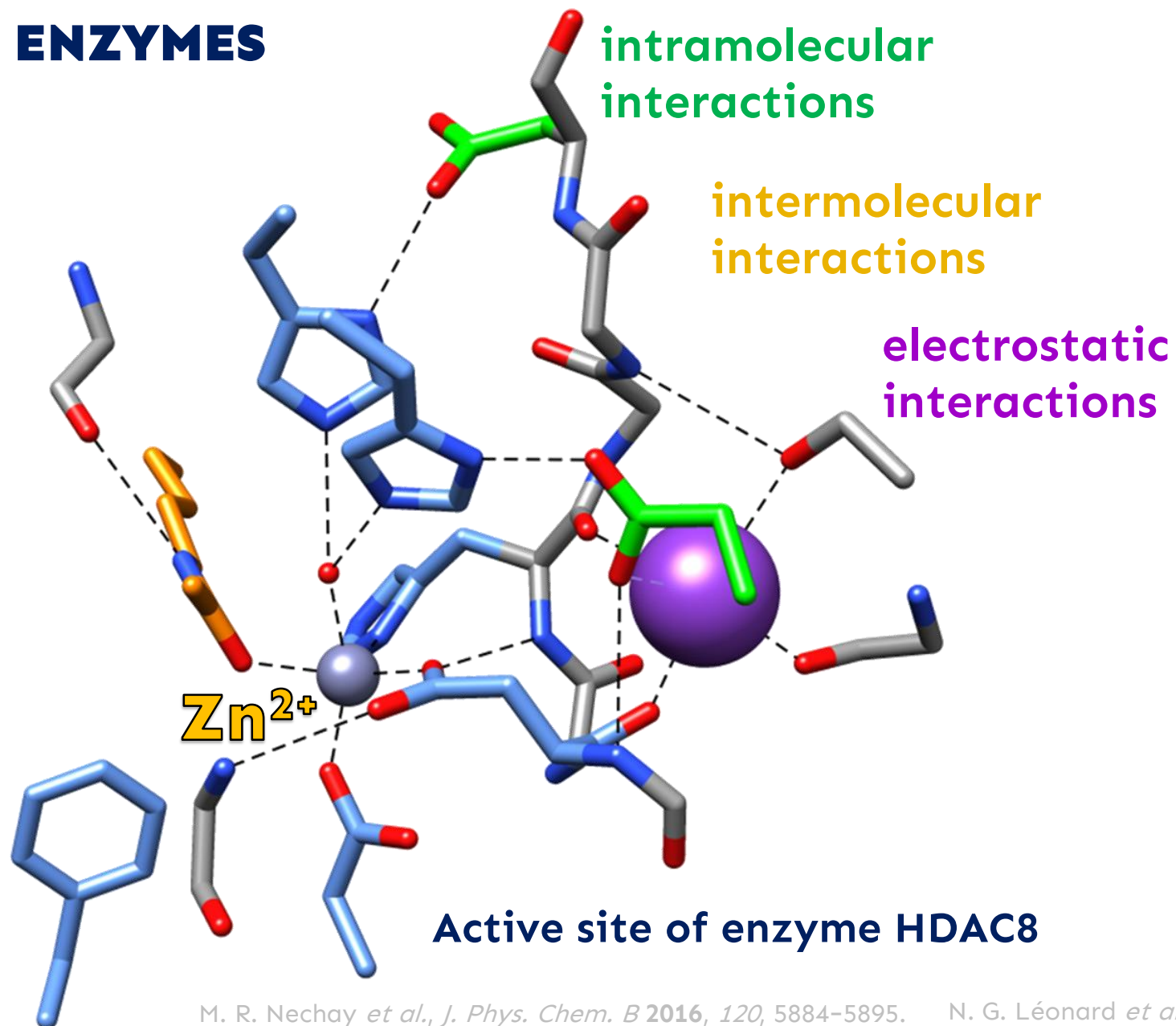
## ENZYMES



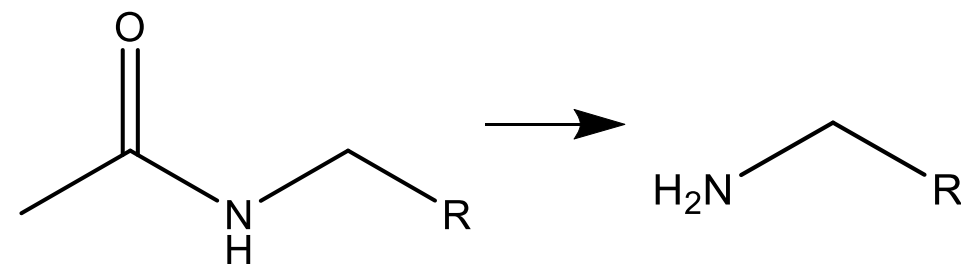
## Deacetylation reaction during biosynthesis of proteins



## ENZYMES

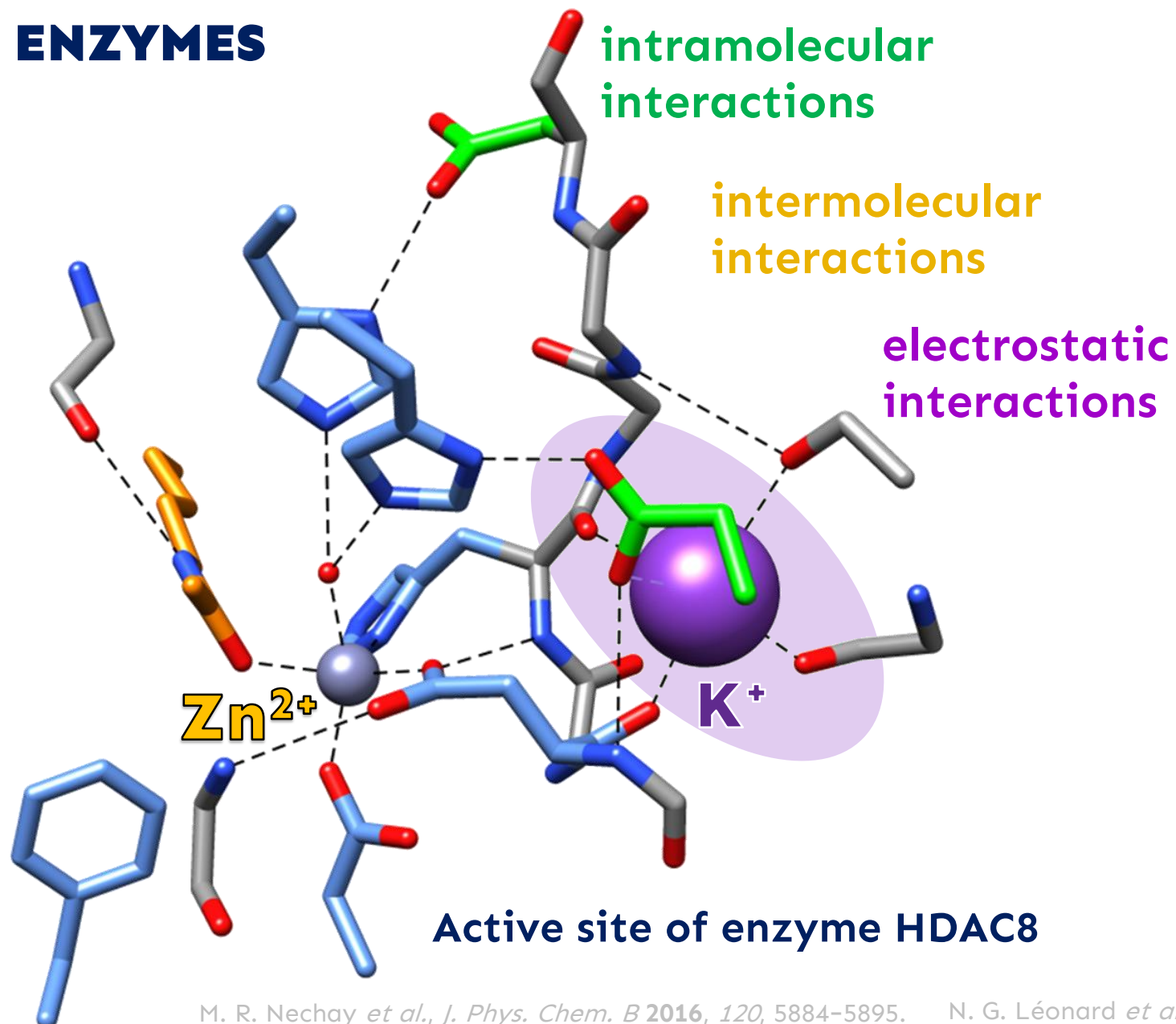


## Deacetylation reaction during biosynthesis of proteins

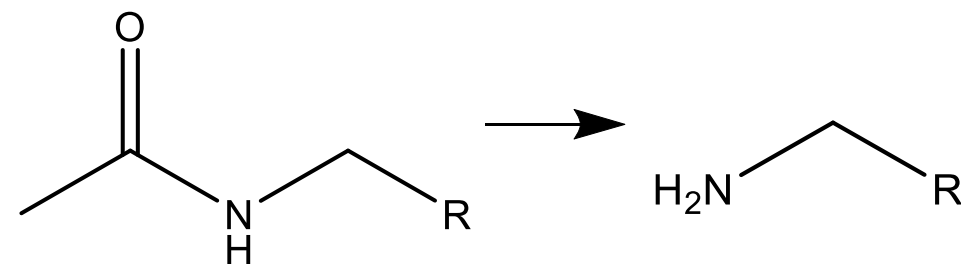




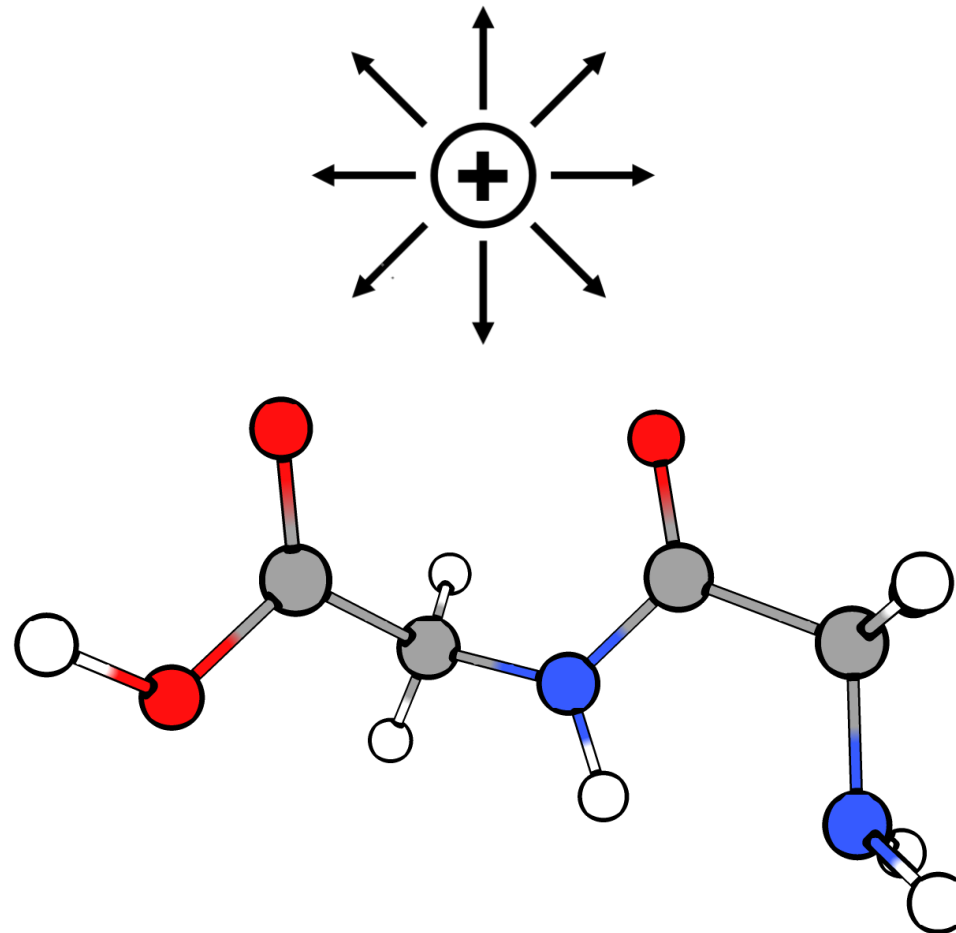
## ENZYMES



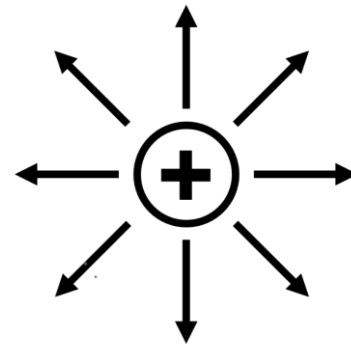
## Deacetylation reaction during biosynthesis of proteins



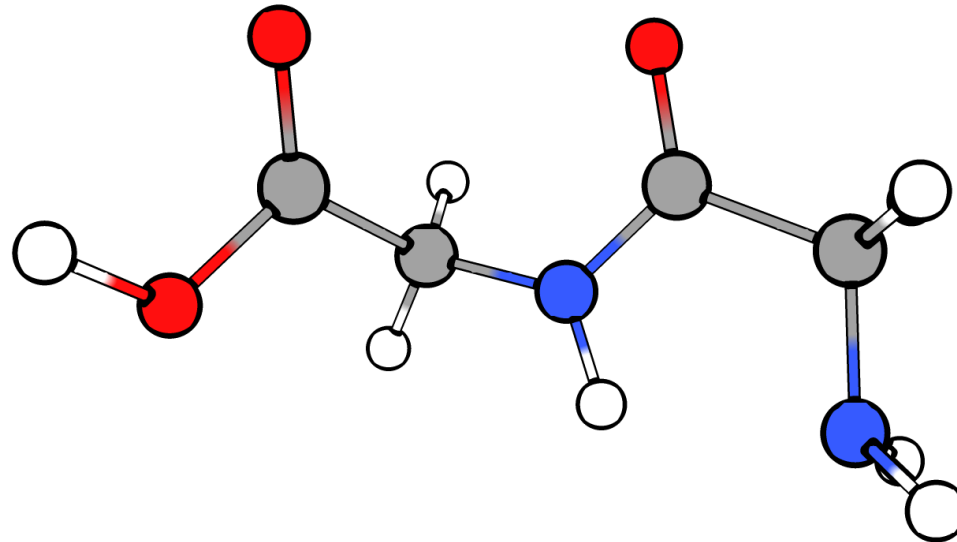
# THE INTERPLAY OF NON-COVALENT INTERACTIONS

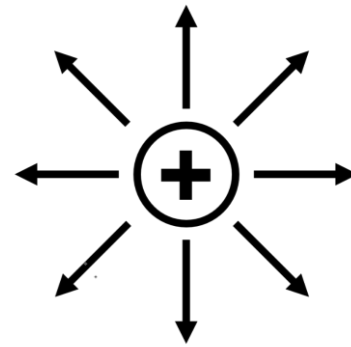


# THE INTERPLAY OF NON-COVALENT INTERACTIONS

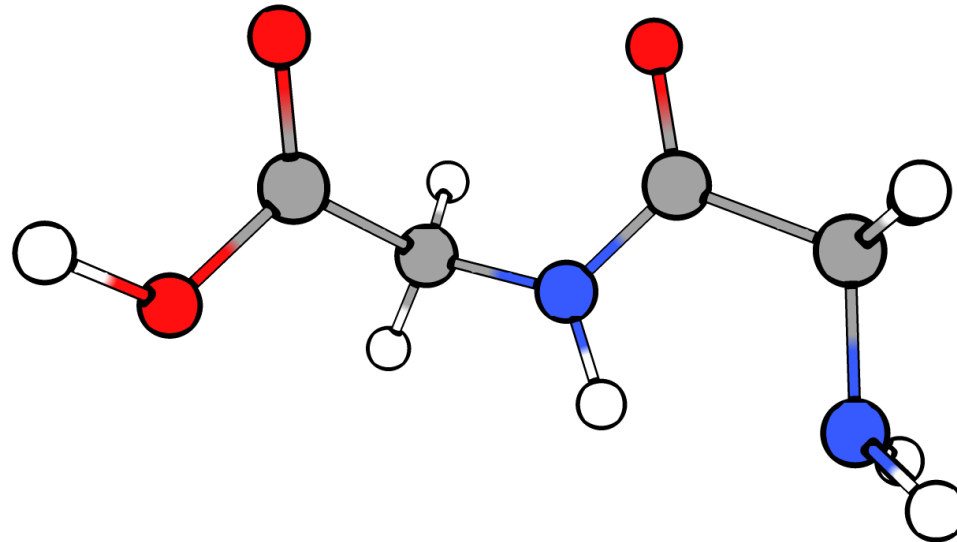


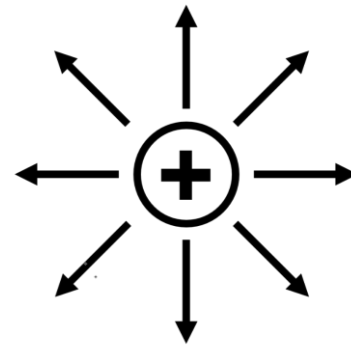
$M^+ : Li^+$



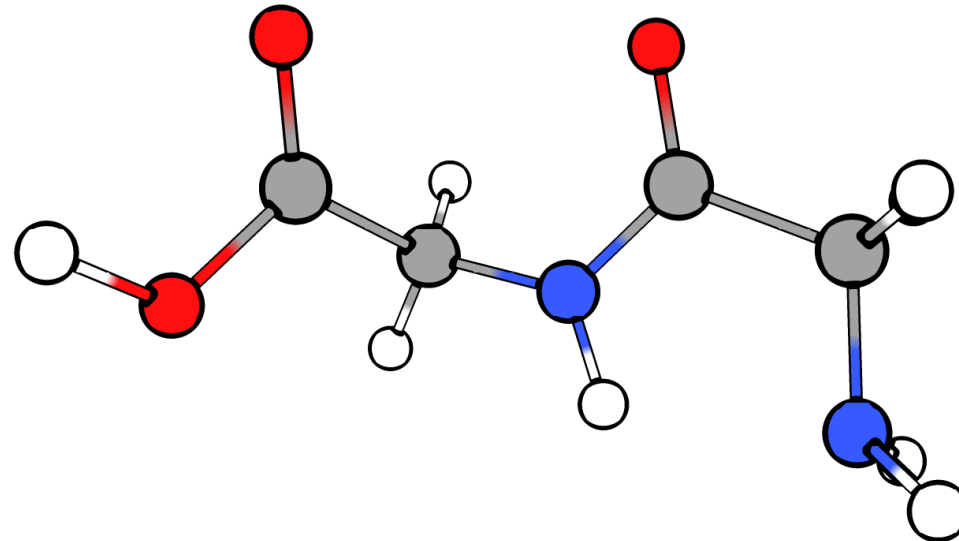


$M^+ : \text{Li}^+, \text{Na}^+, \text{K}^+$

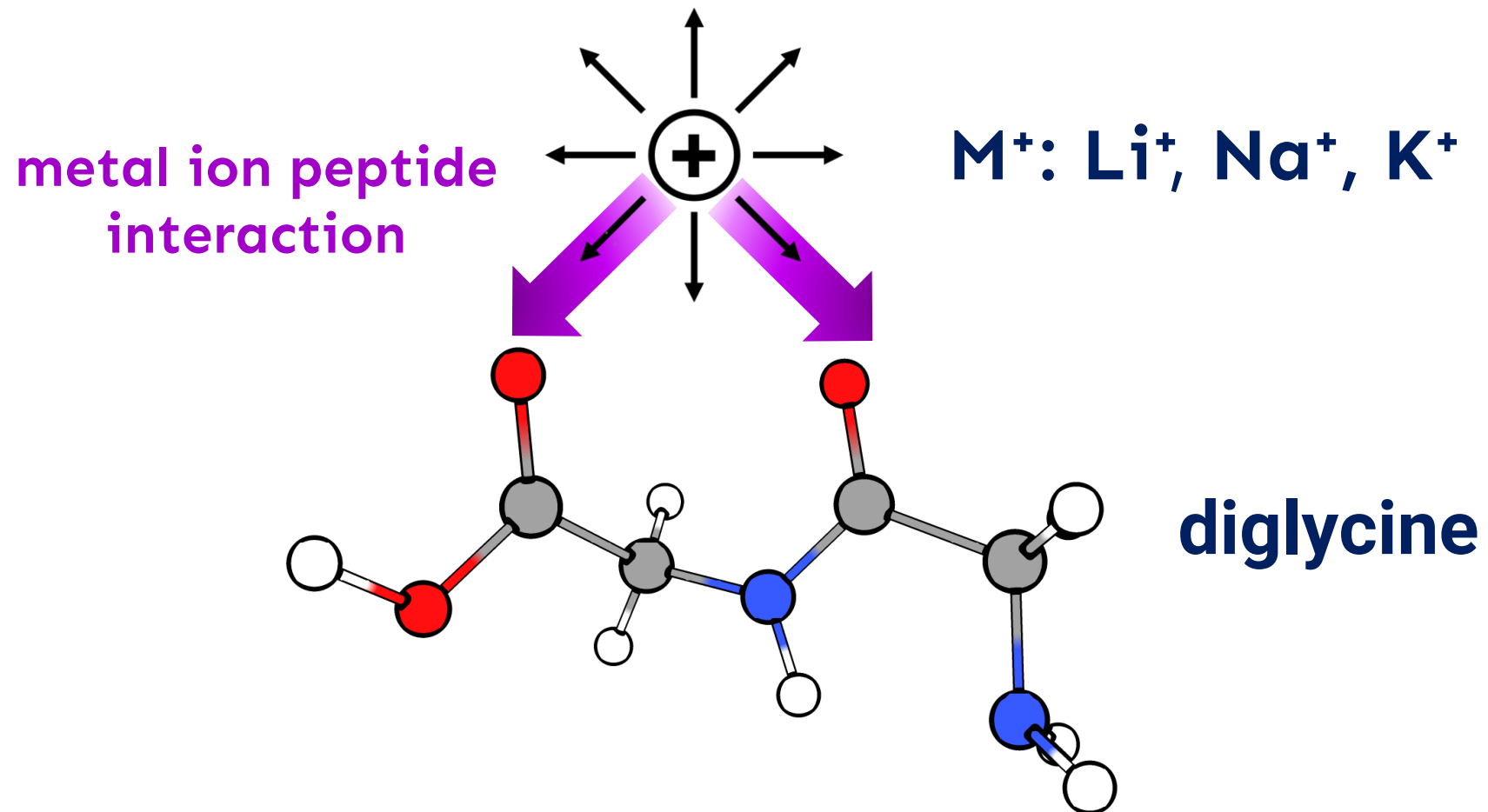


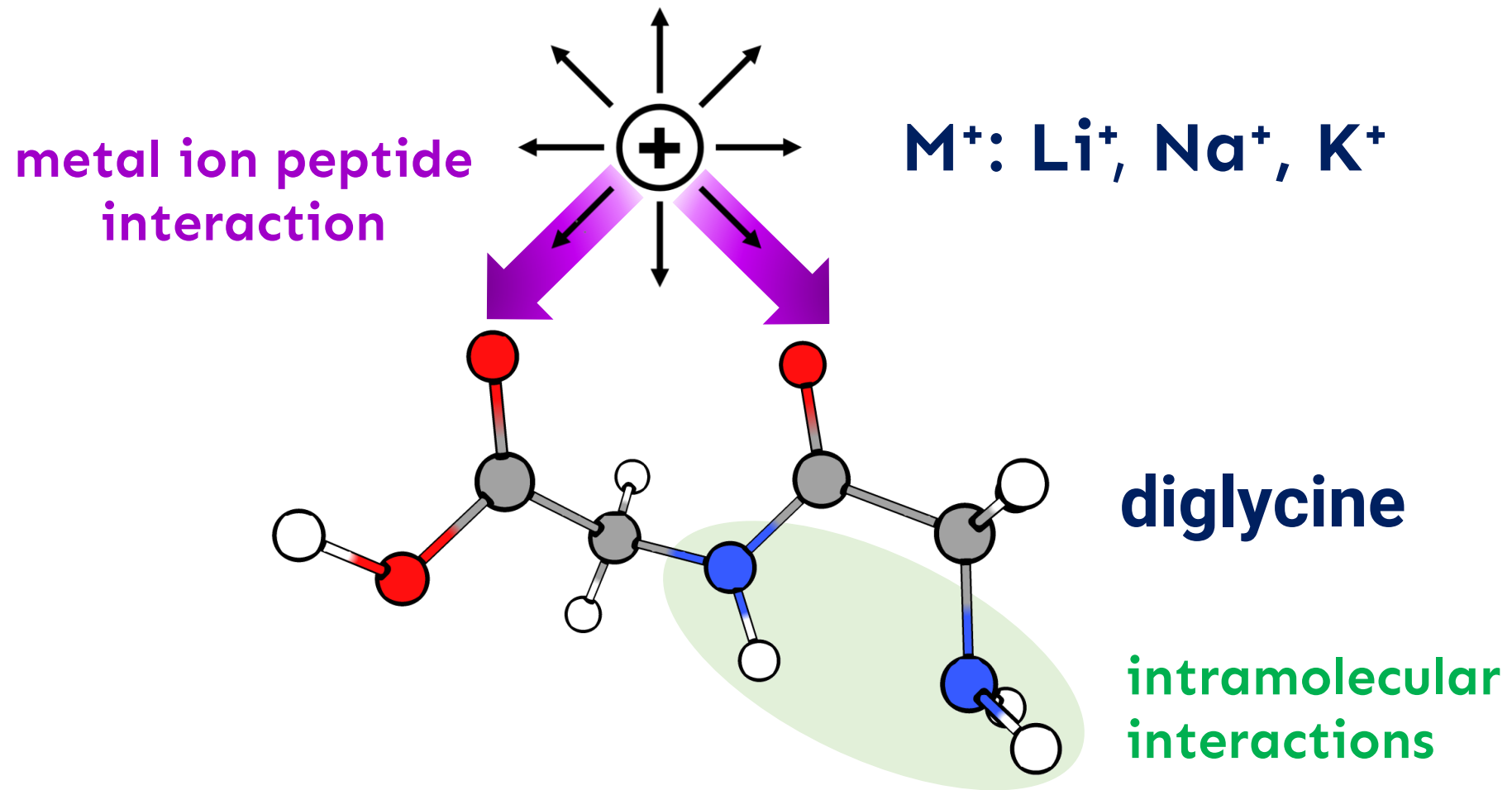


$M^+$ :  $Li^+$ ,  $Na^+$ ,  $K^+$

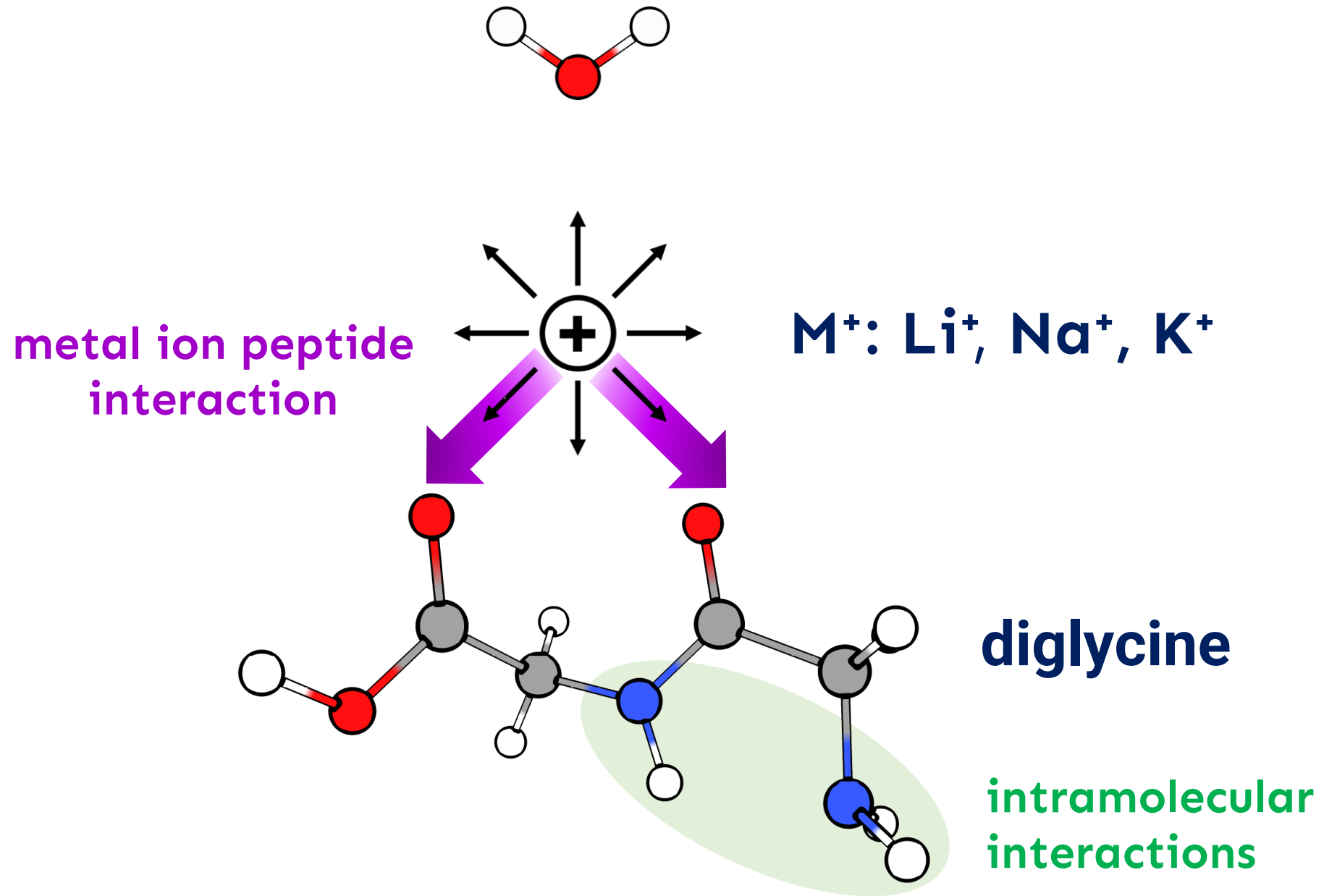


diglycine



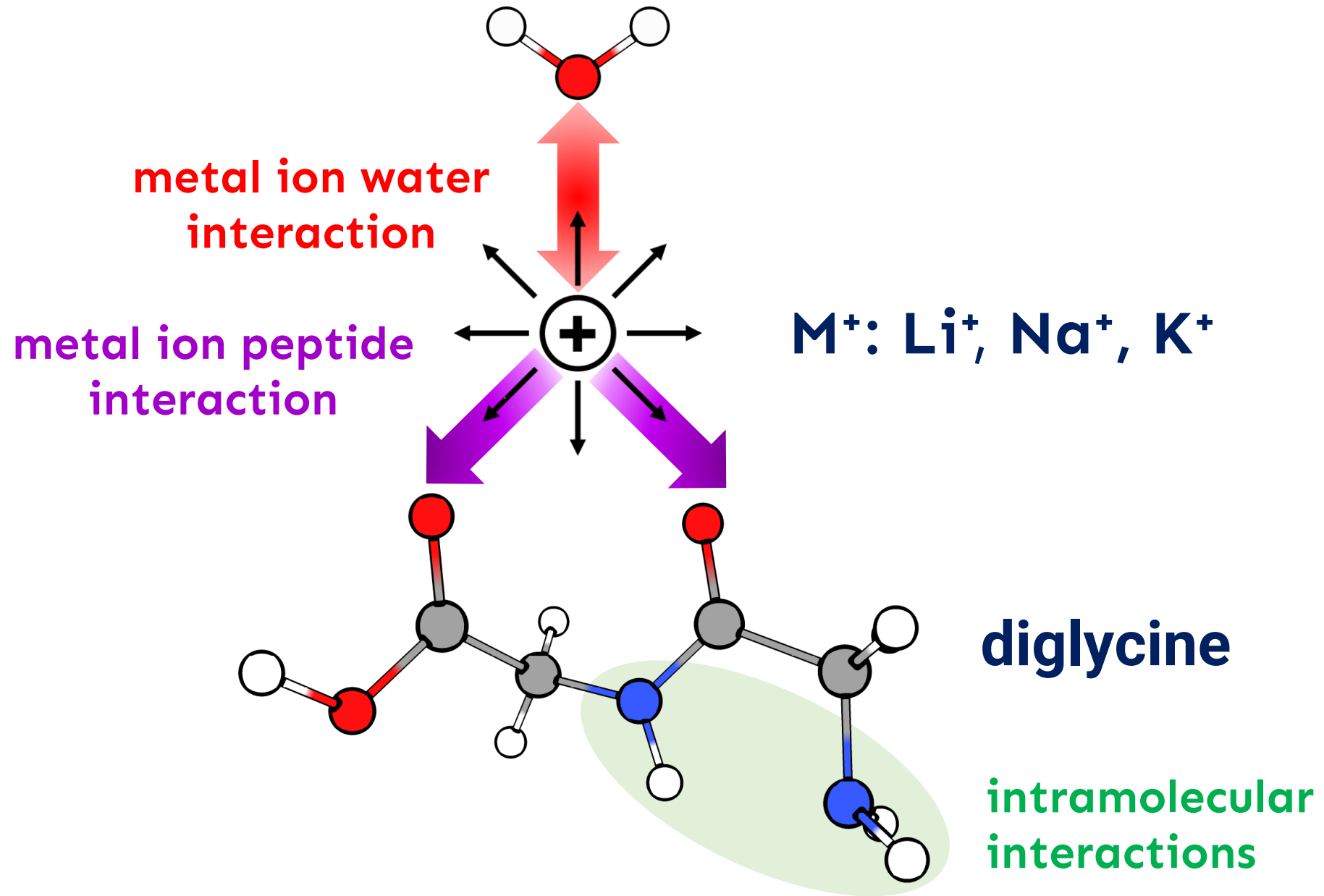


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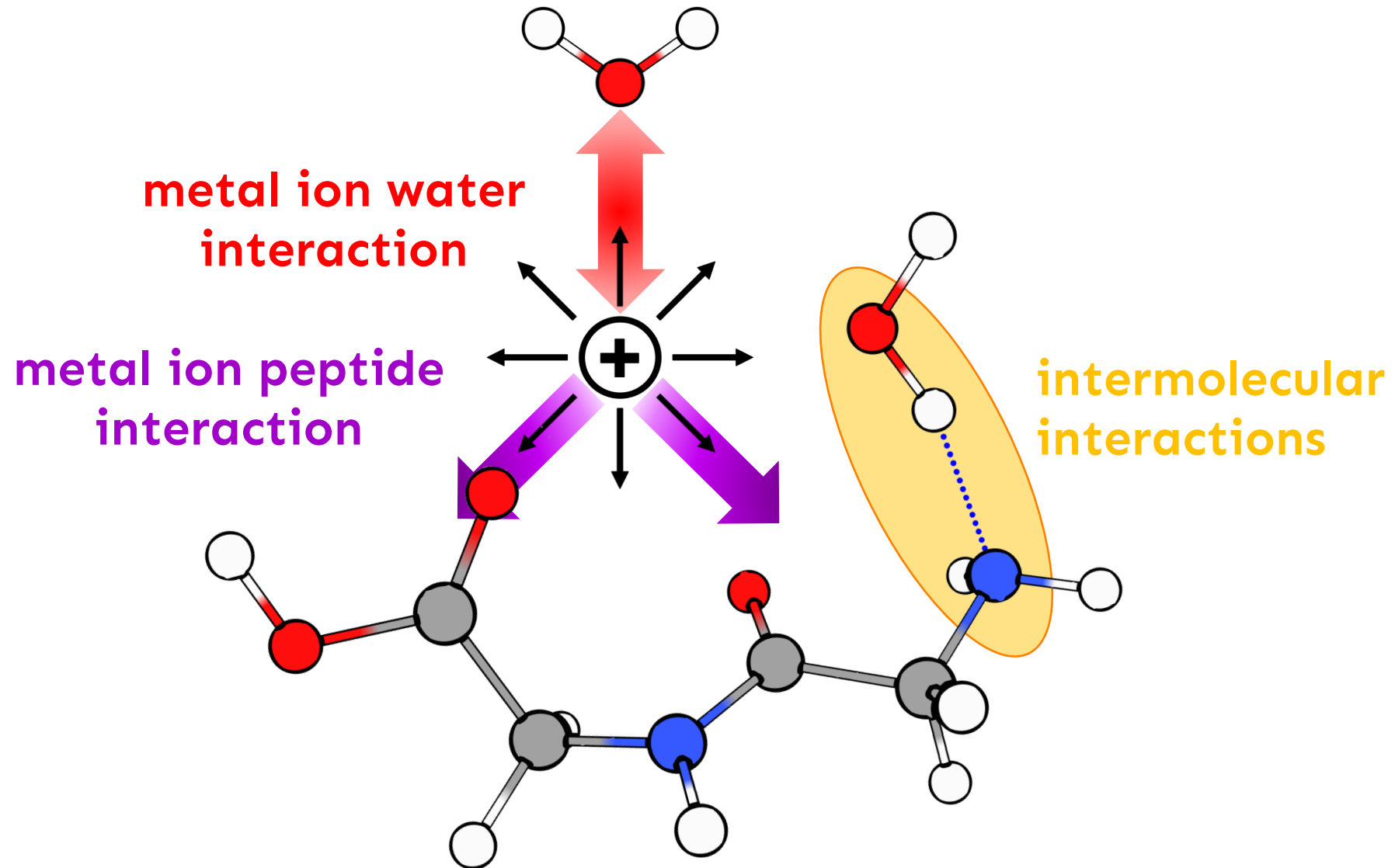


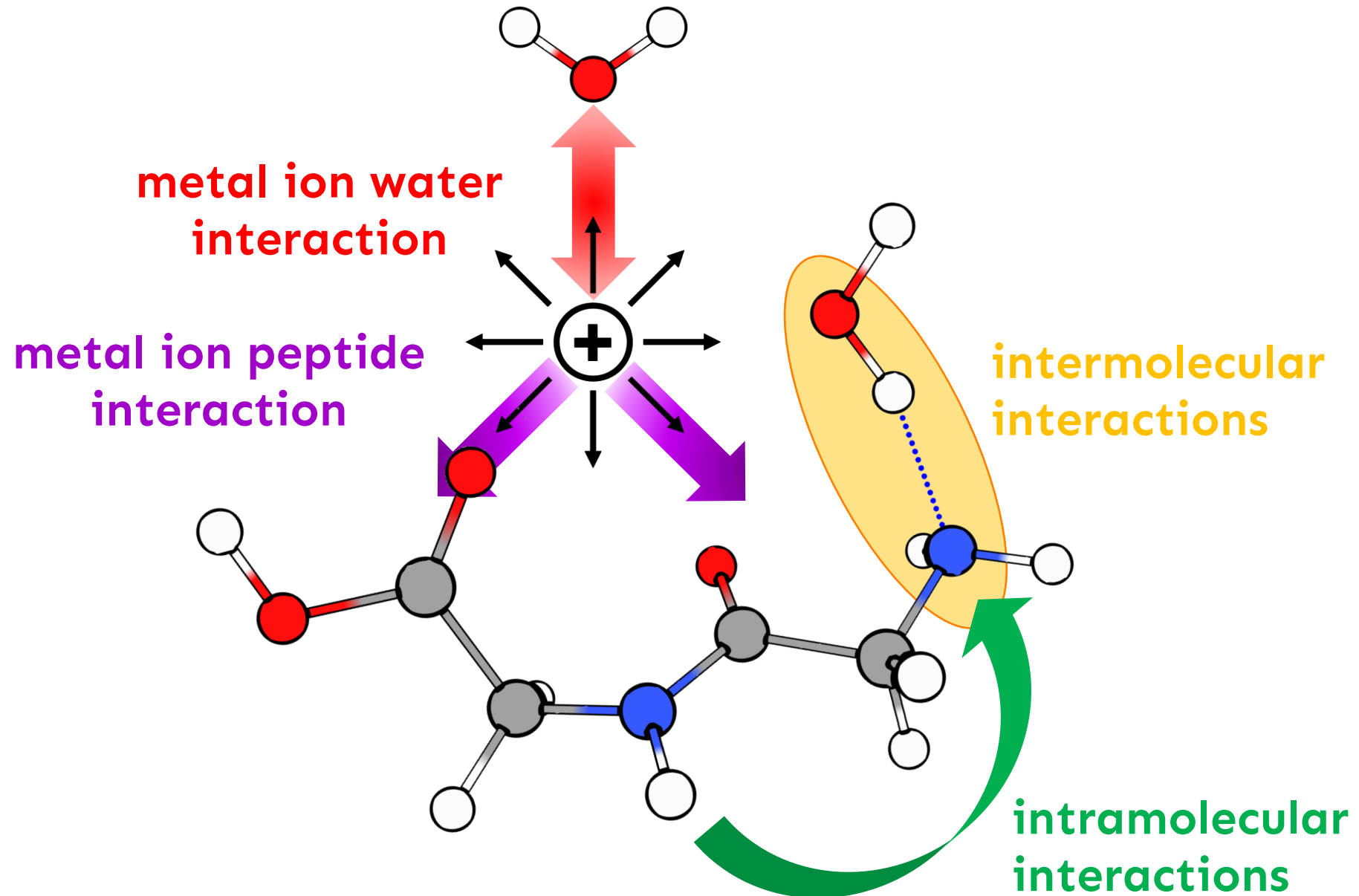


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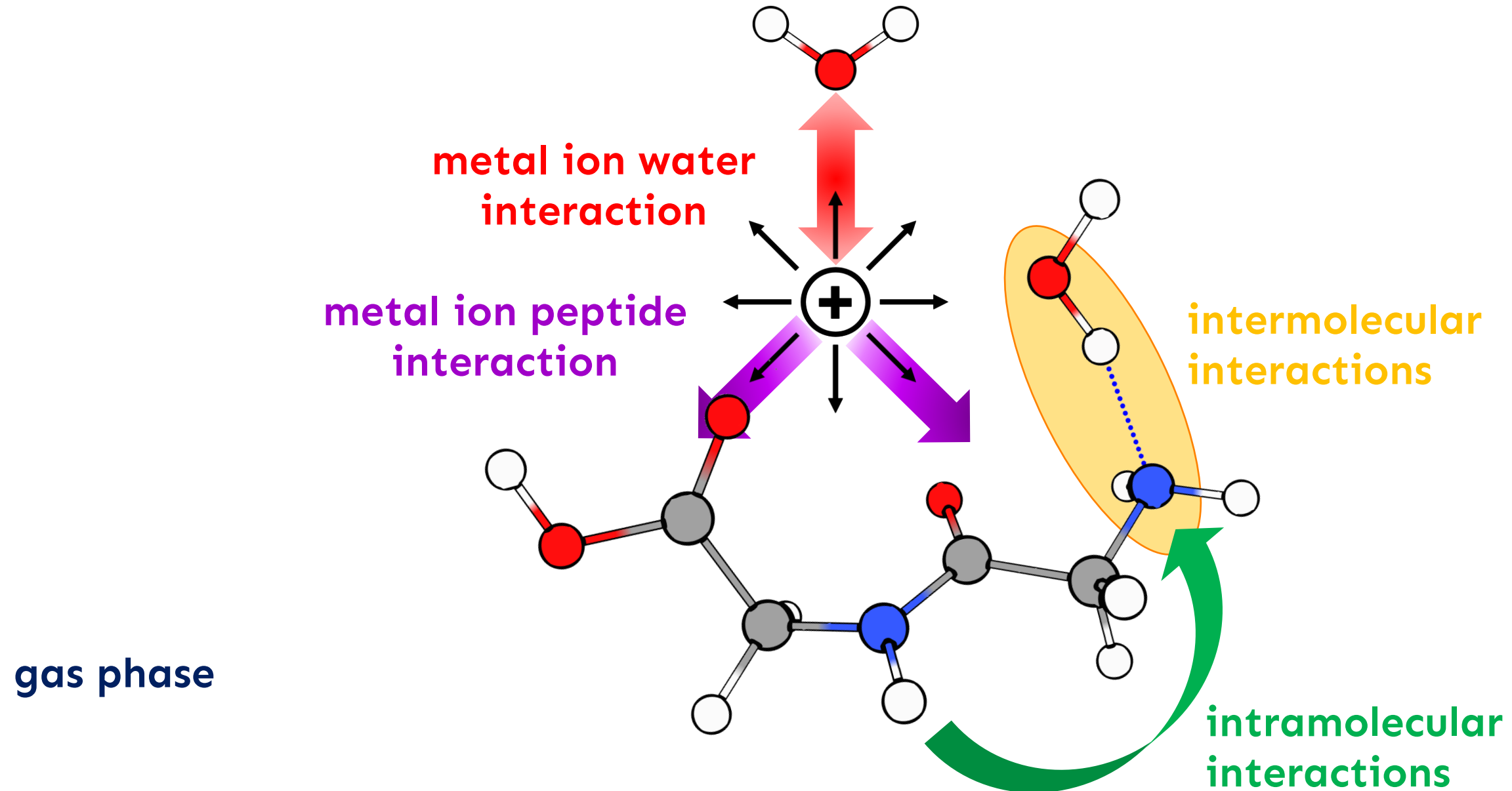


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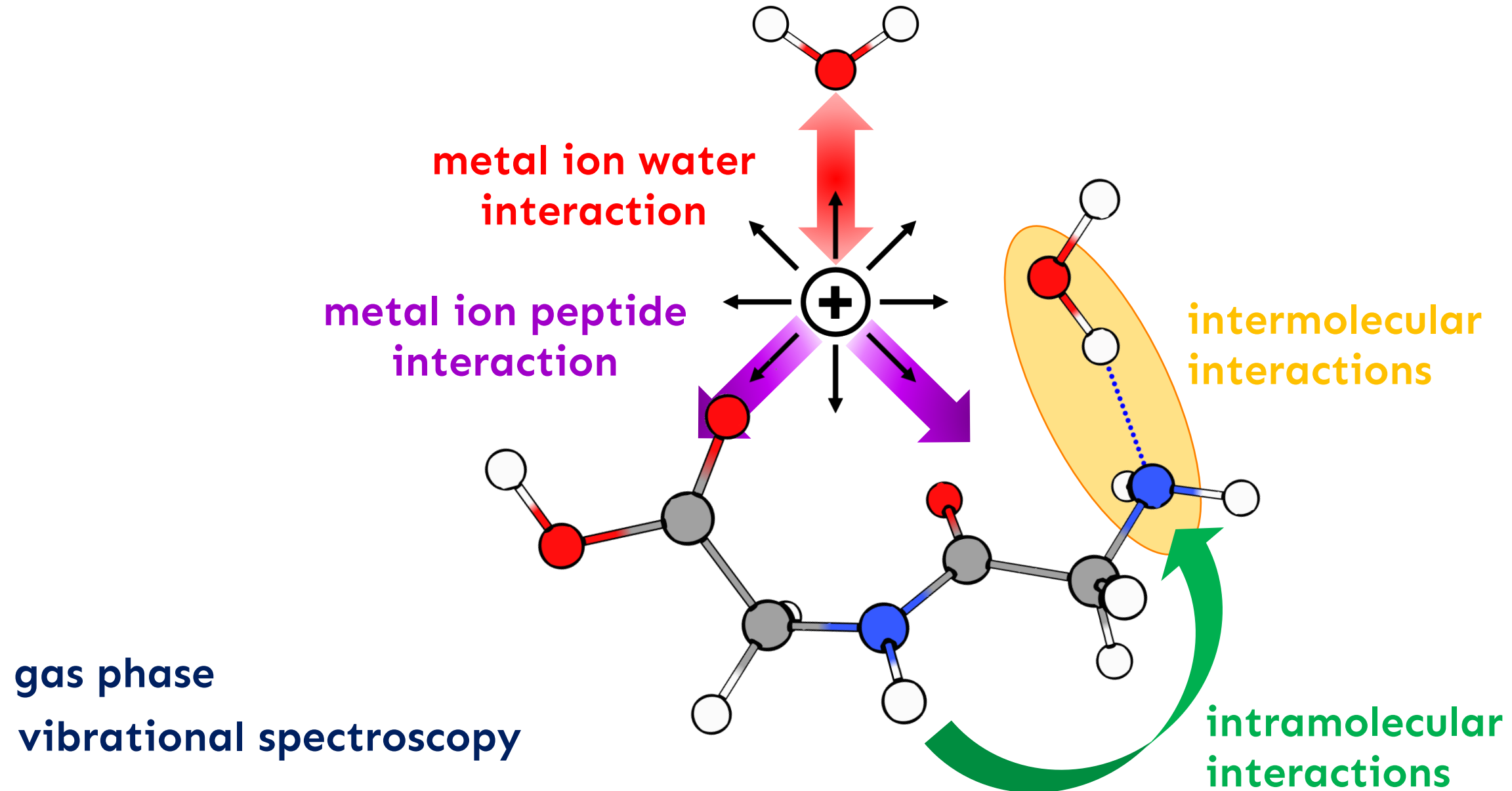


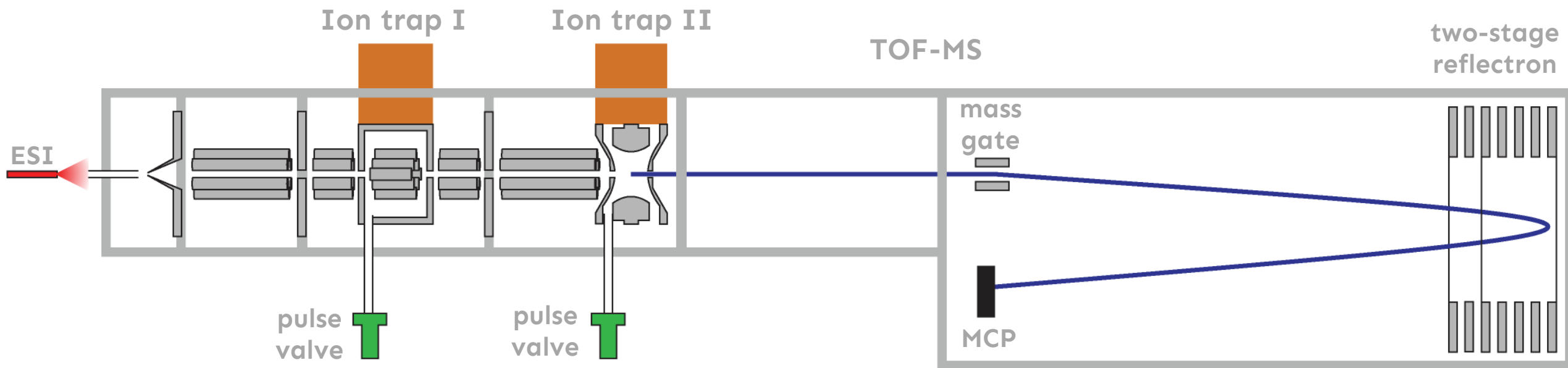


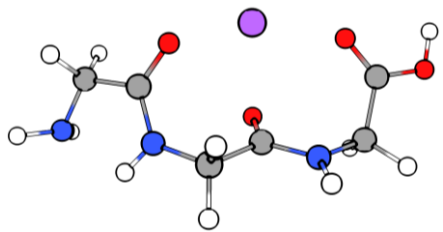
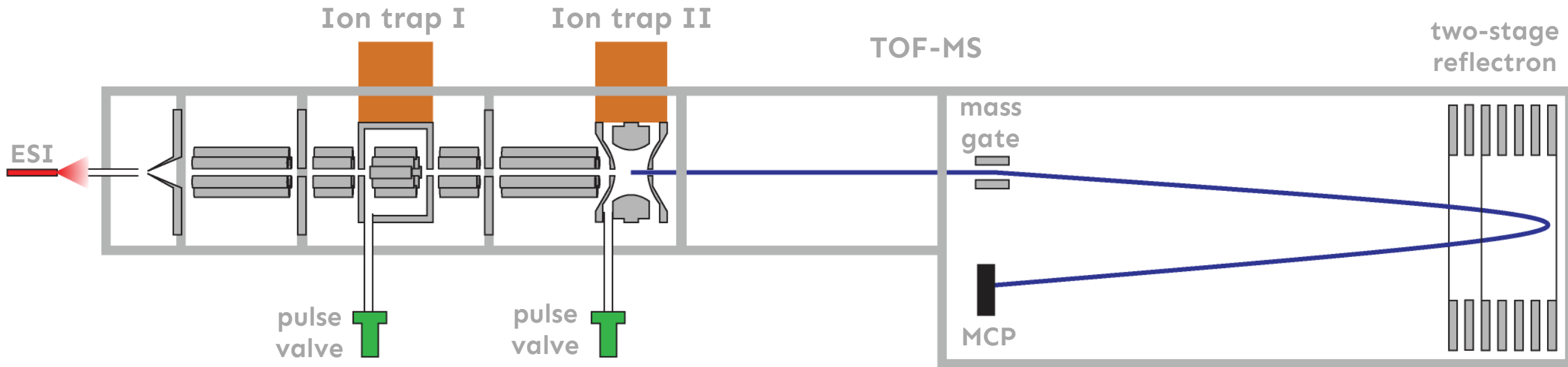
# THE INTERPLAY OF NON-COVALENT INTERACTIONS



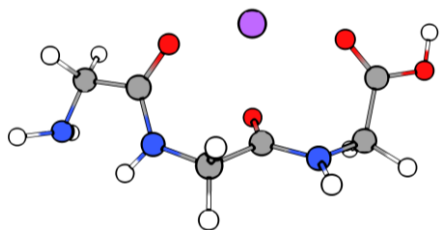
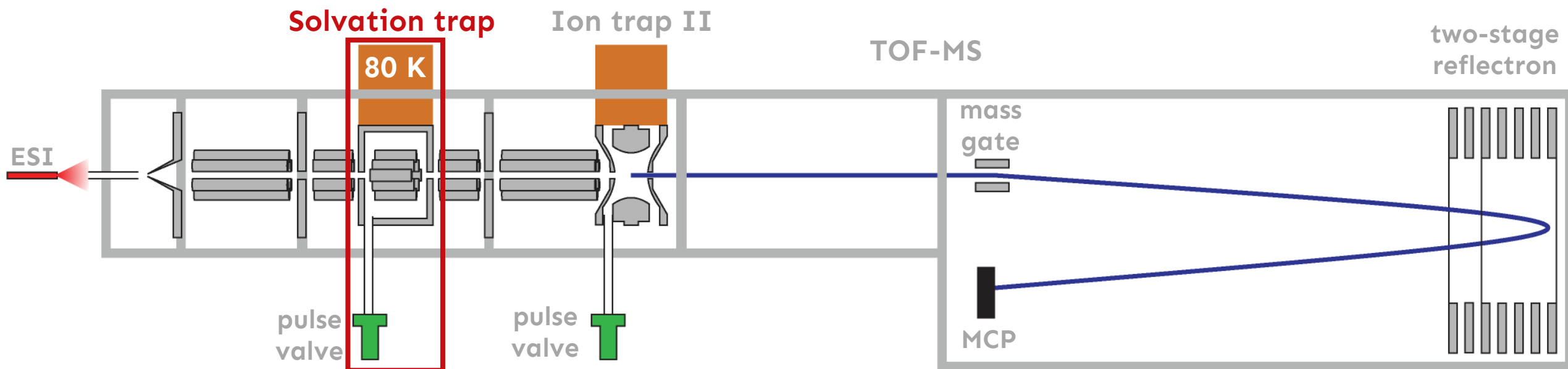
# THE INTERPLAY OF NON-COVALENT INTERACTIONS



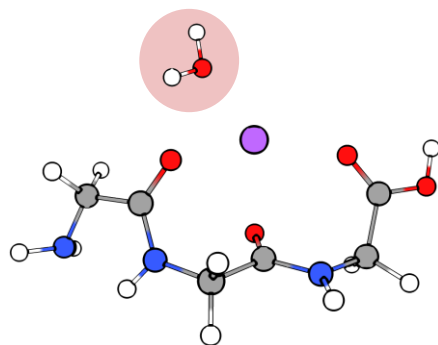




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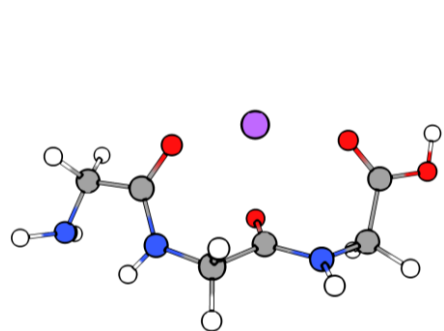
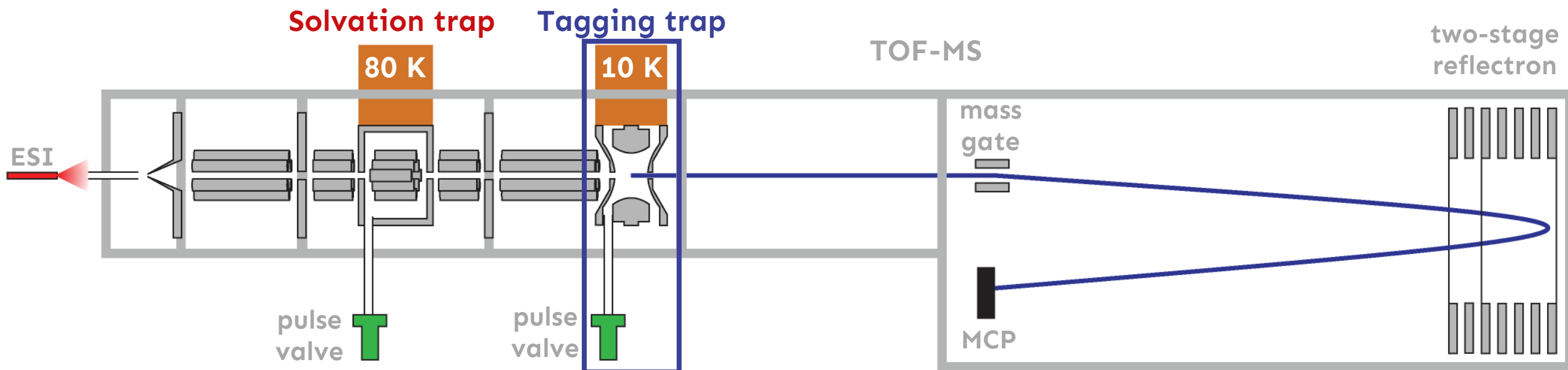


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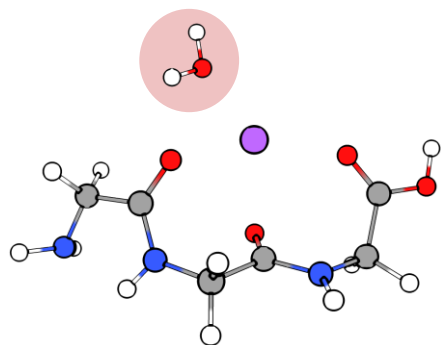


re-condensation of  
water

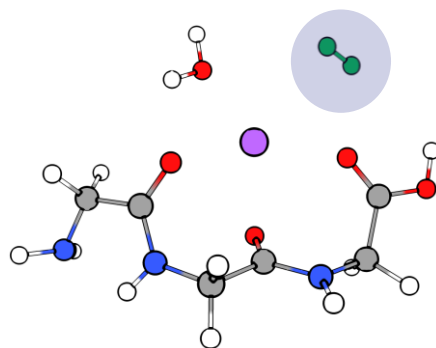




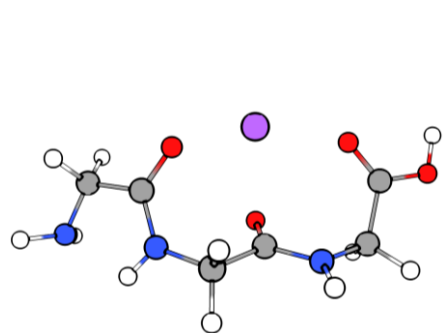
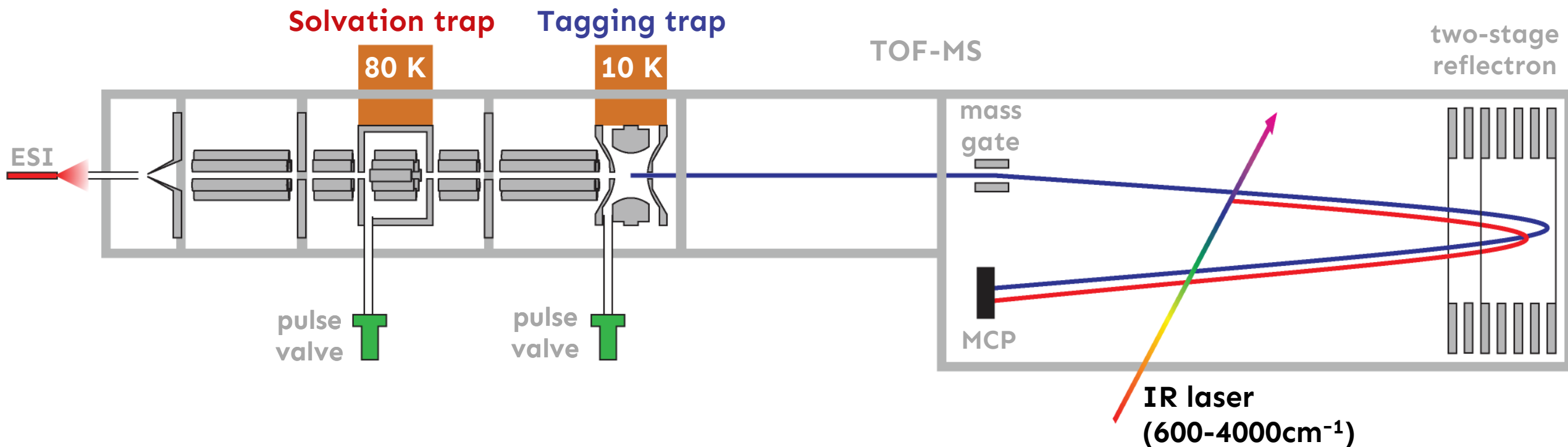
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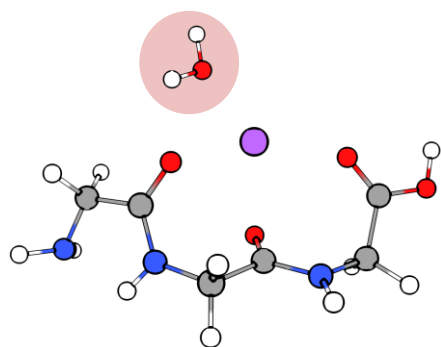
re-condensation of  
water



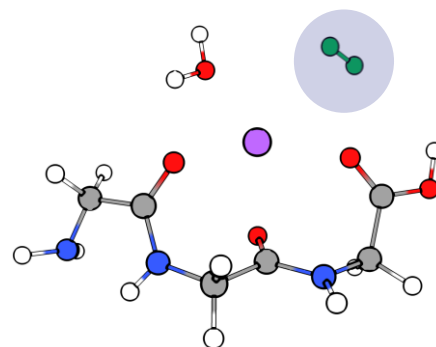
tagging



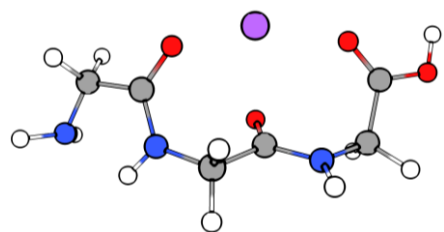
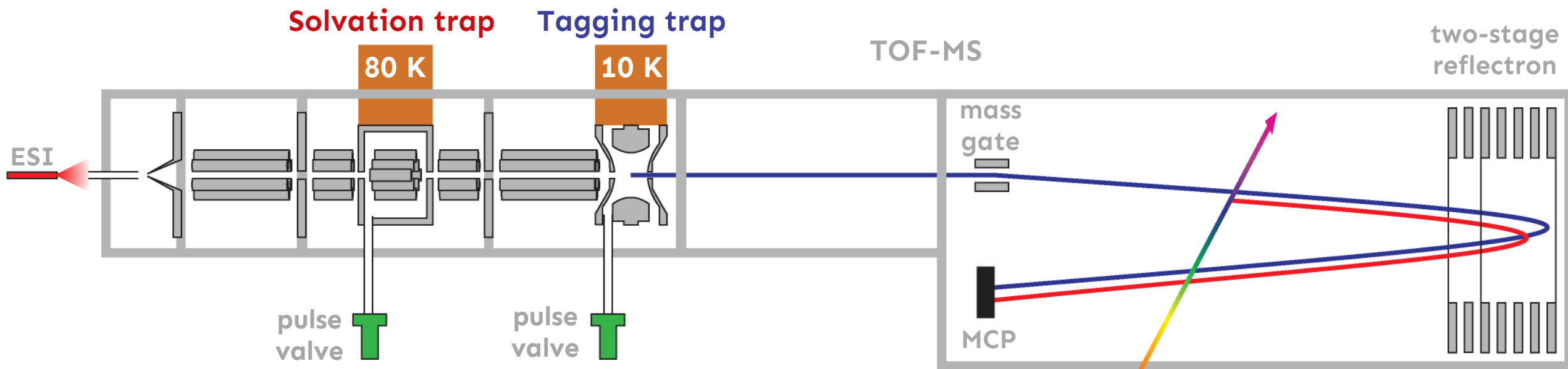
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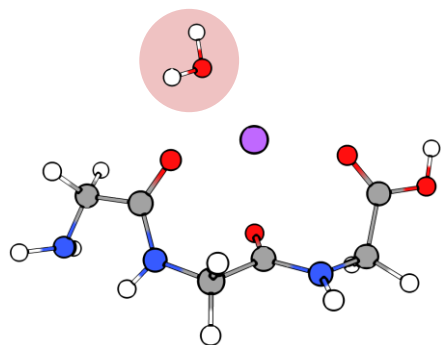
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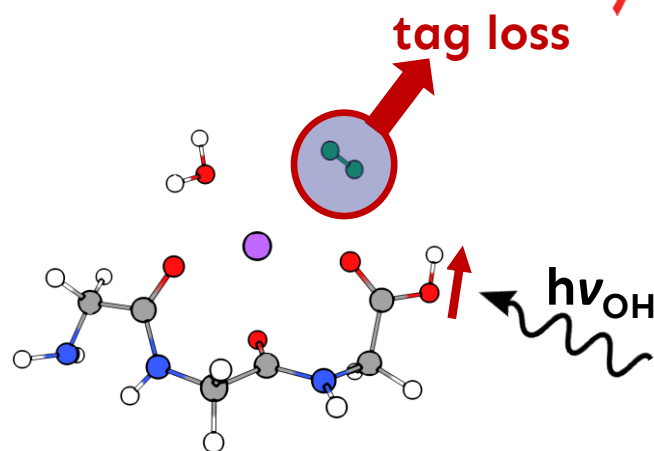
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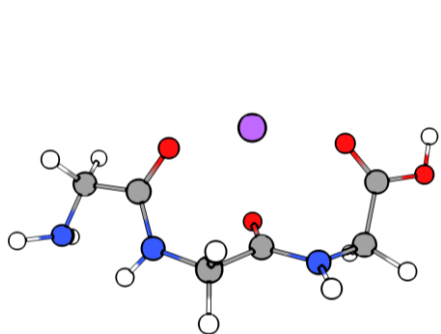
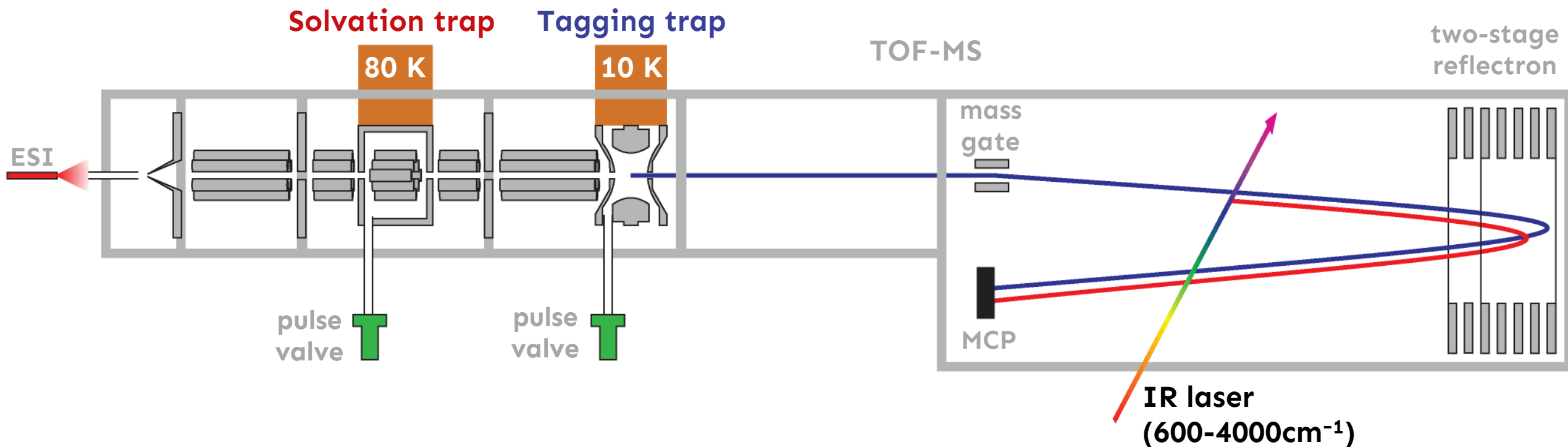
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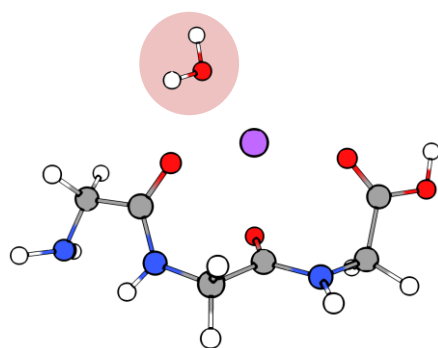
re-condensation of  
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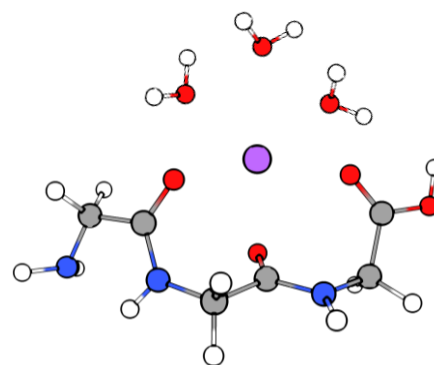
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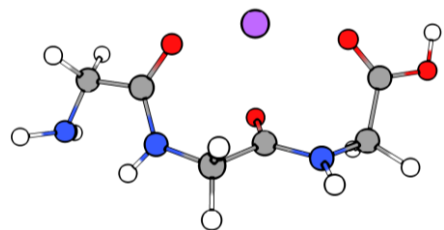
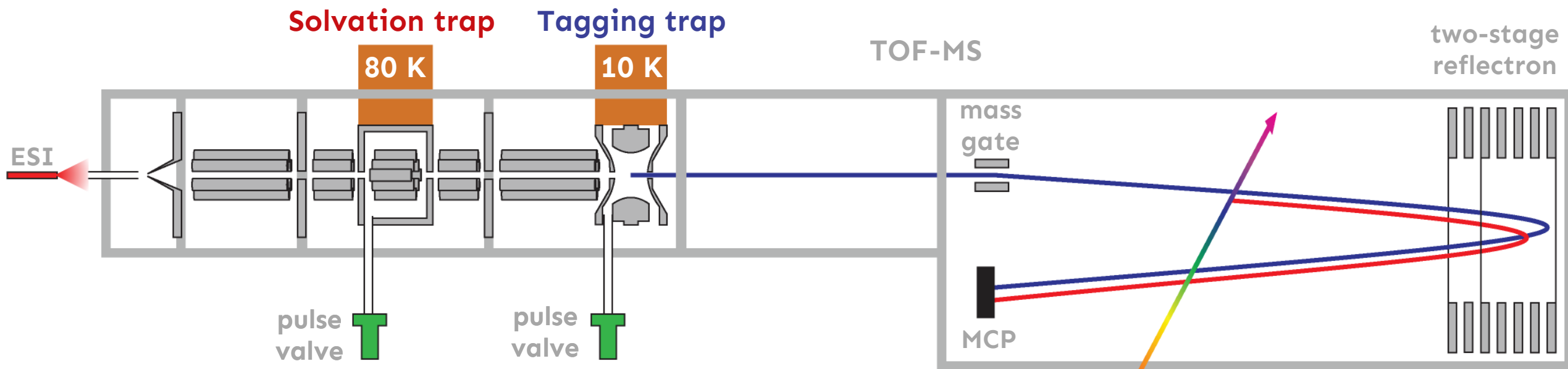
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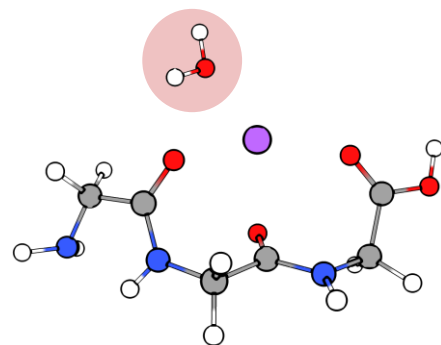
re-condensation of  
water



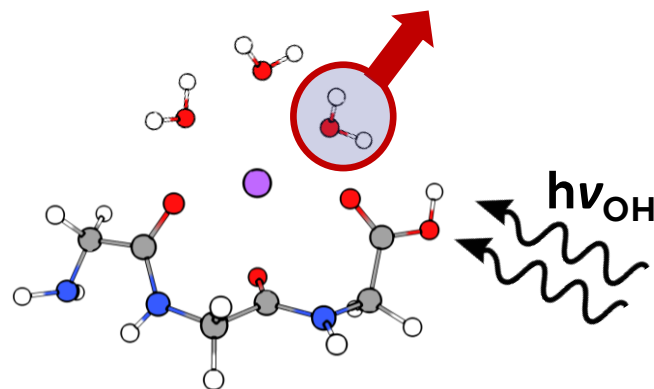
larger water clusters



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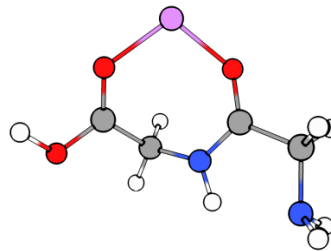
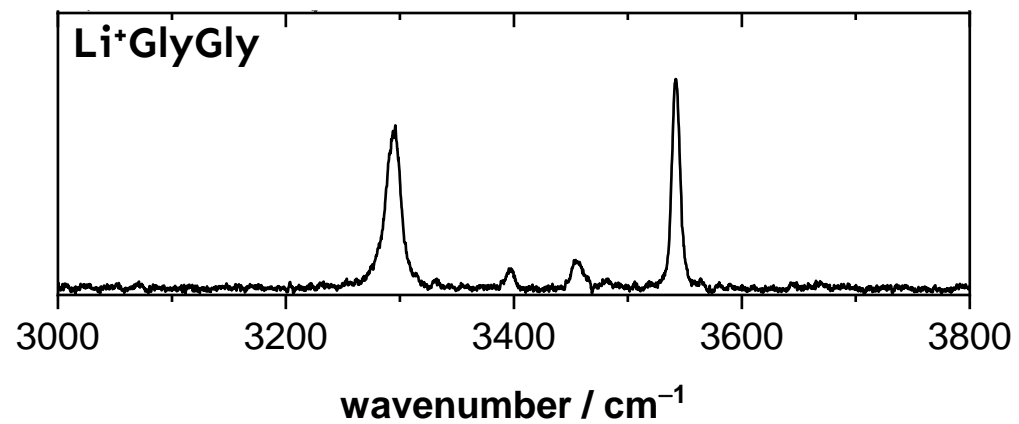


re-condensation of water

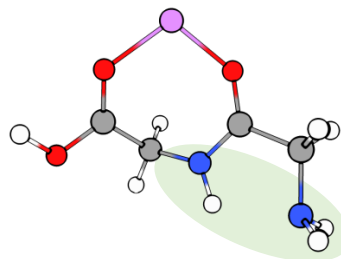
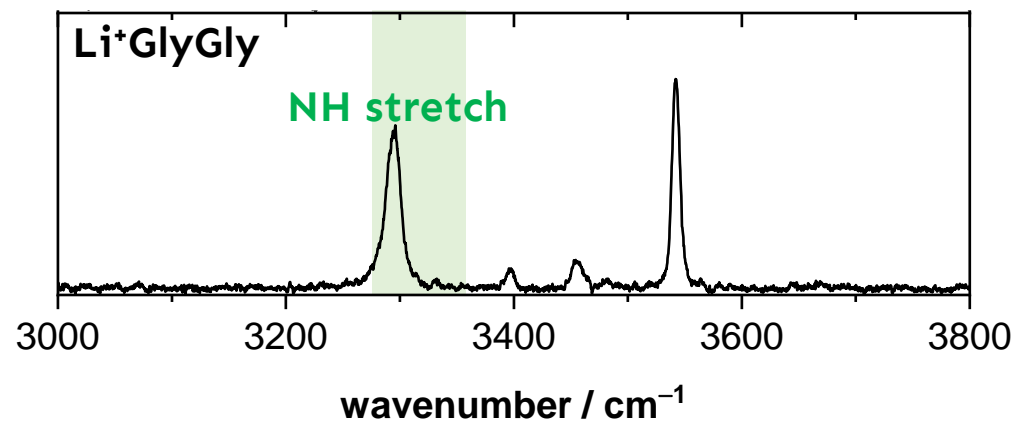


larger water clusters

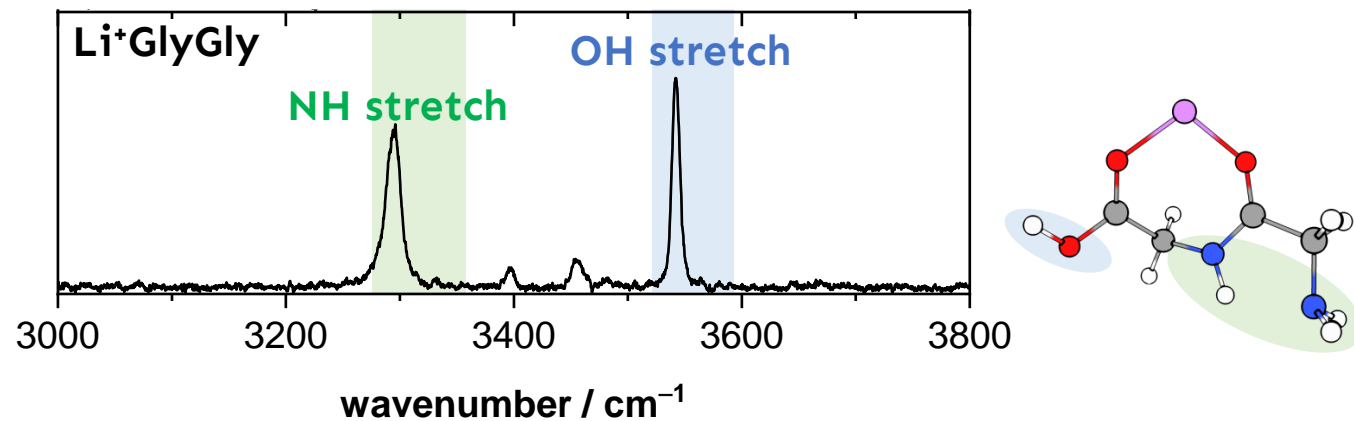
# CHANGES IN STRUCTURE OF Li<sup>+</sup>GlyGly UPON SOLVATION



# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION

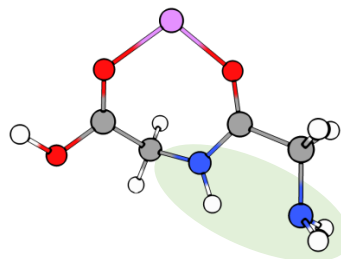
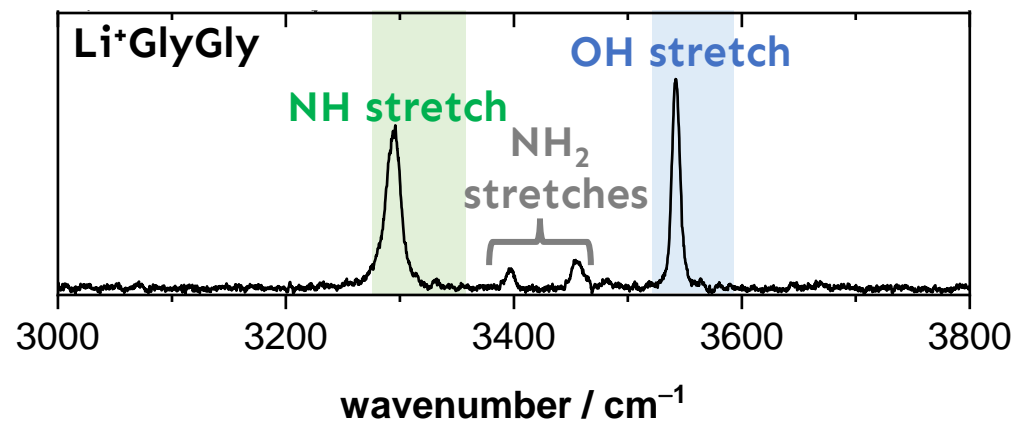


# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION

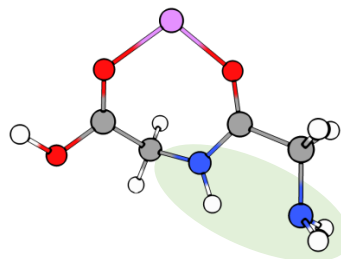
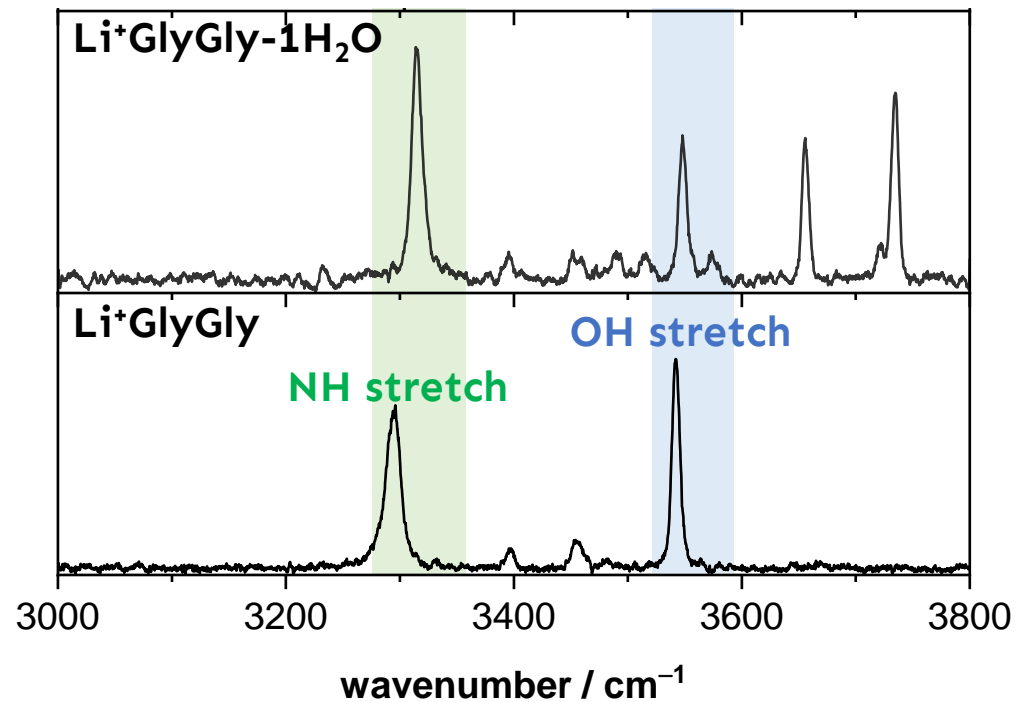




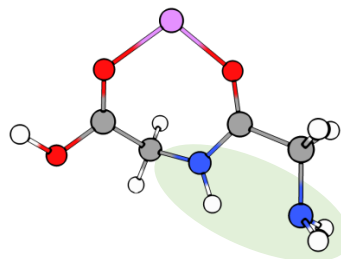
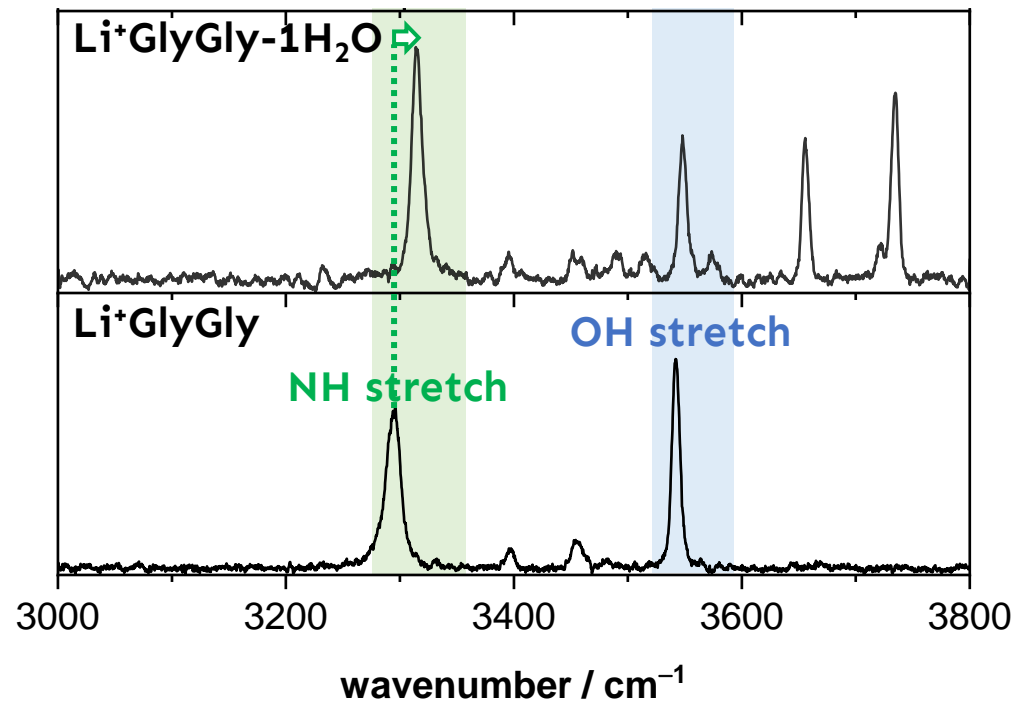
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



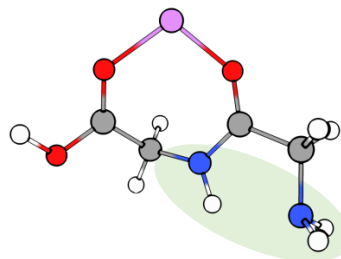
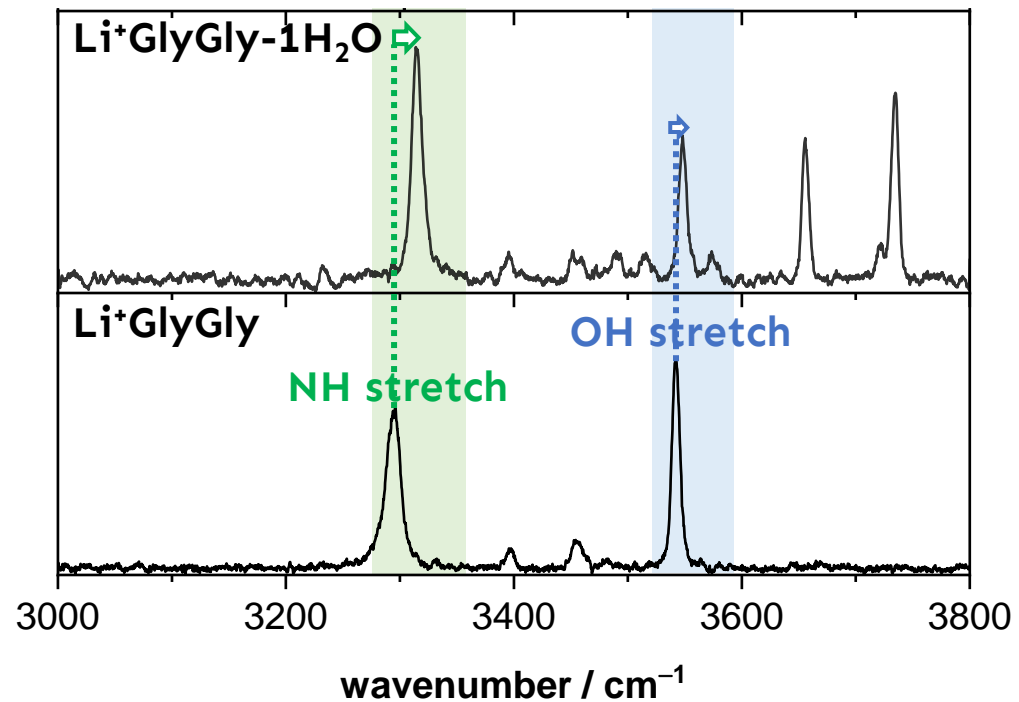
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



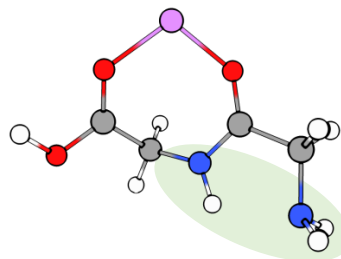
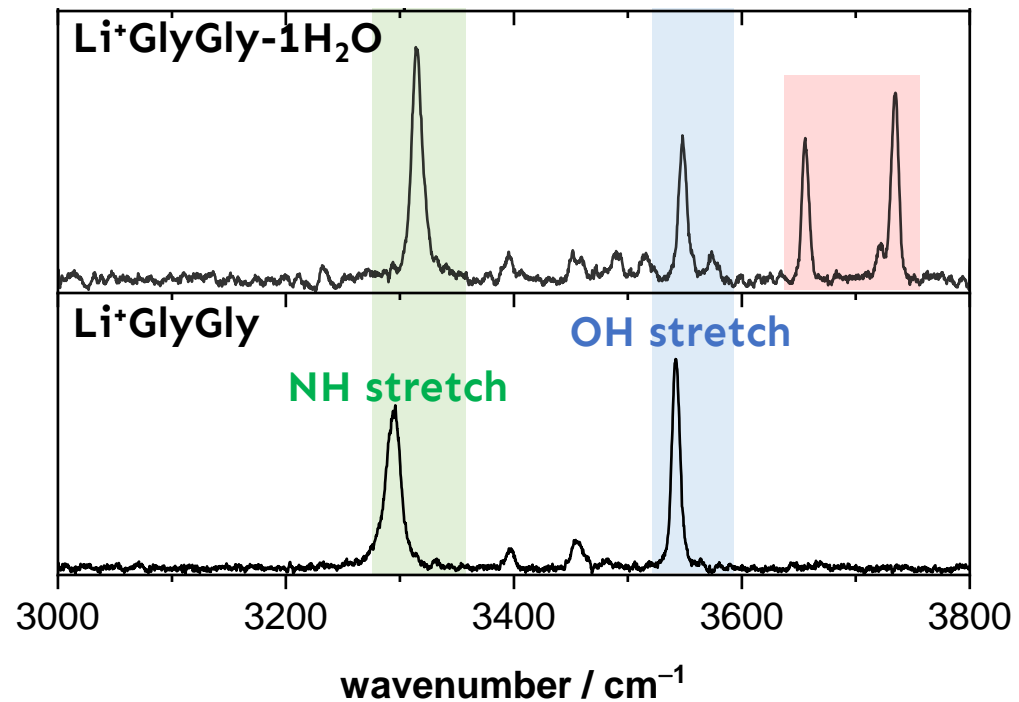
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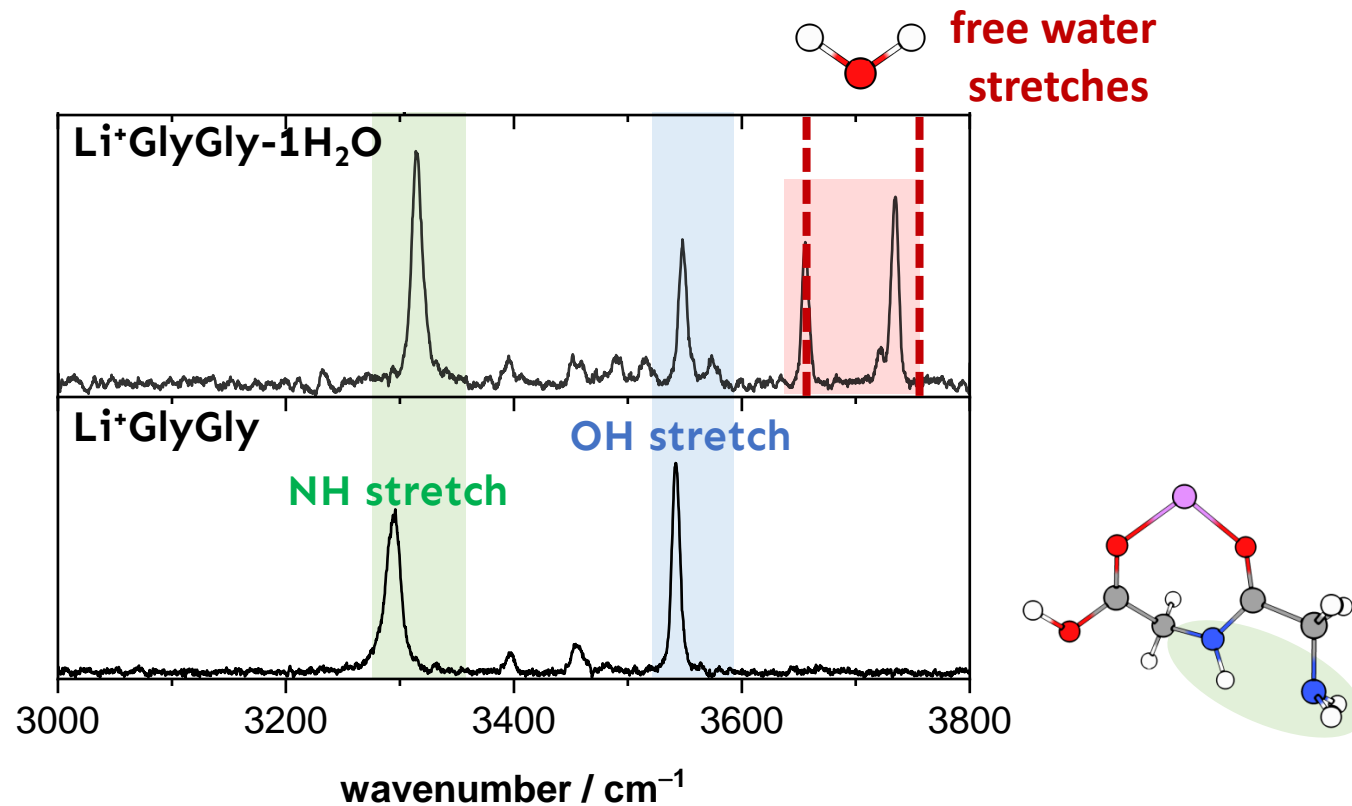
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



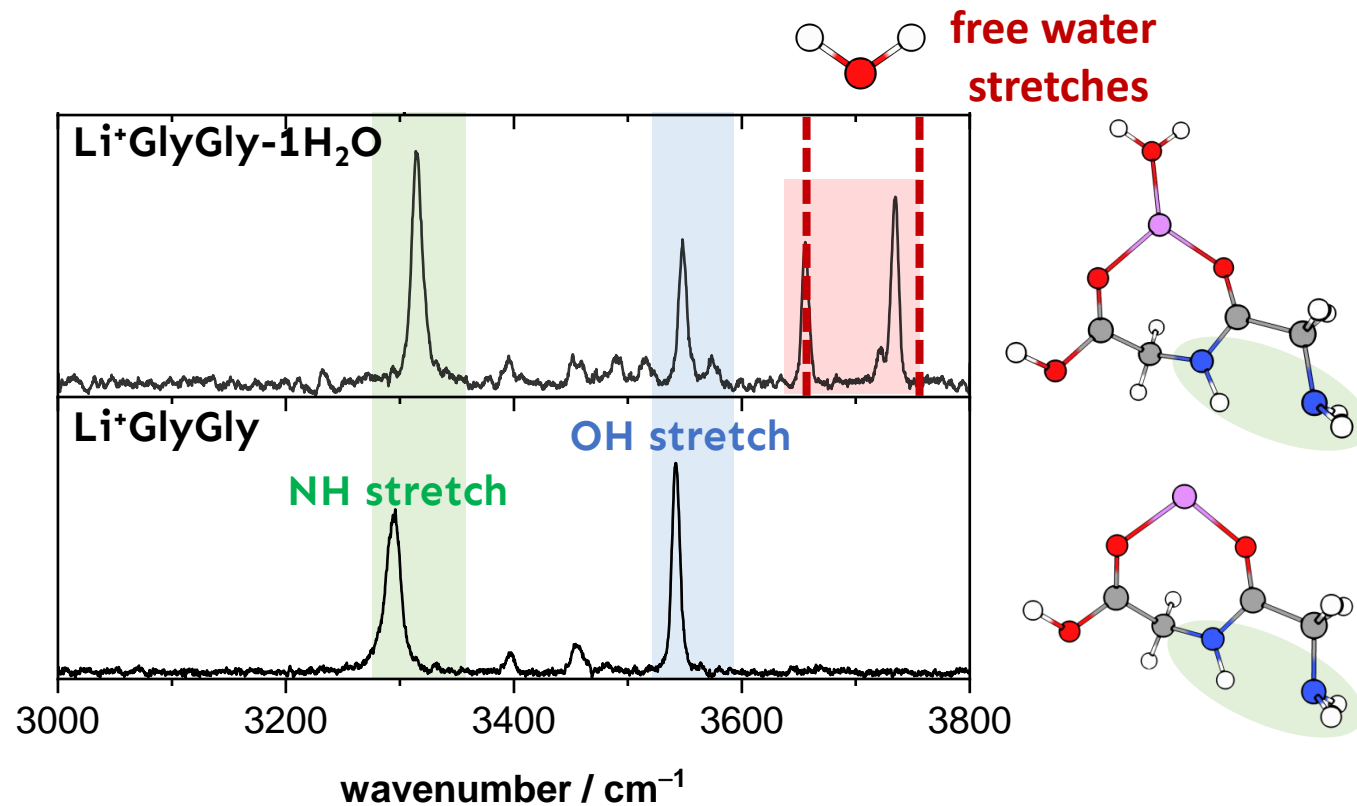
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



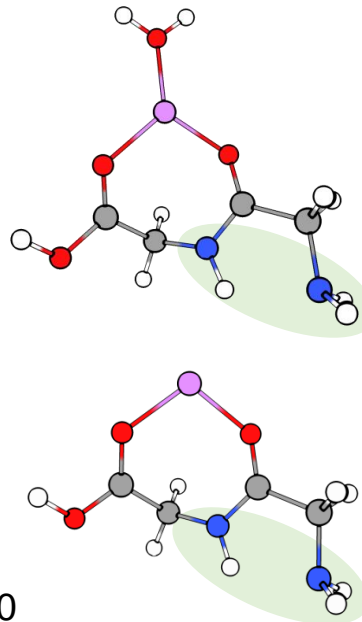
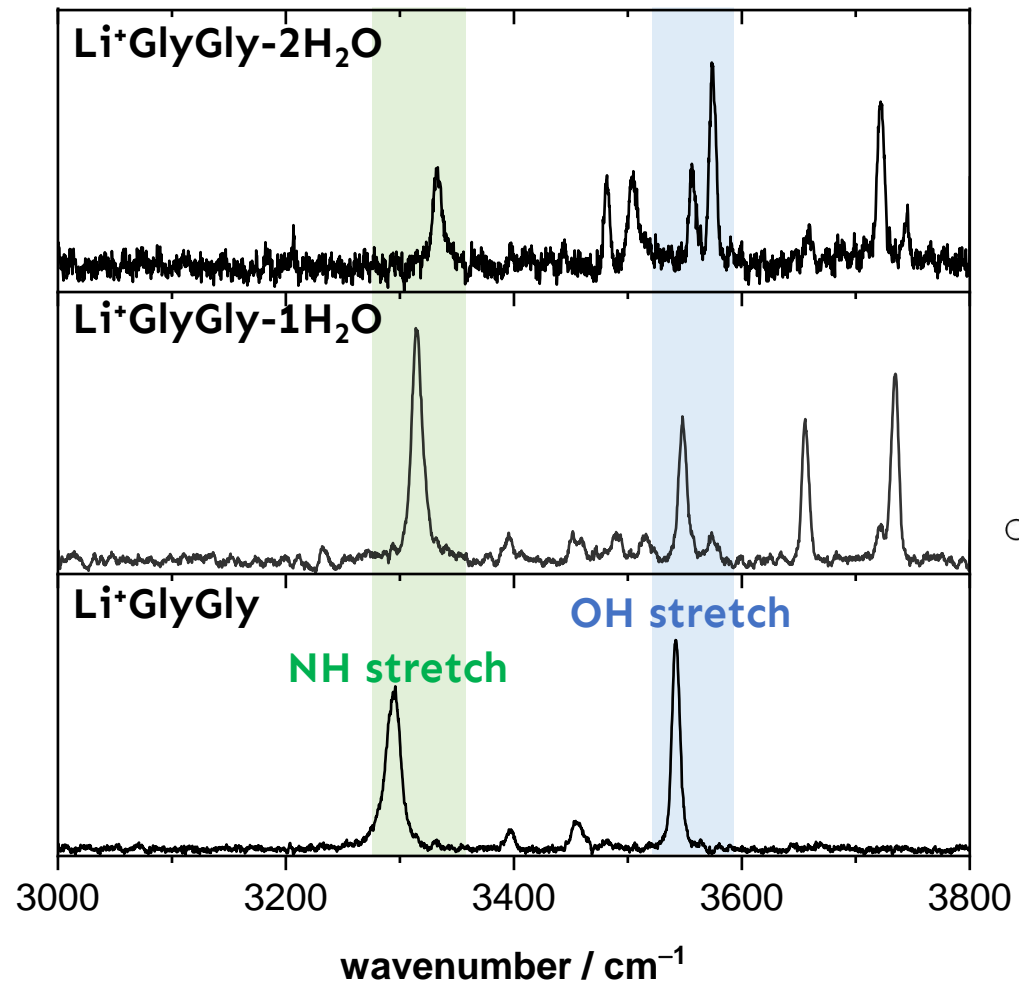
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION

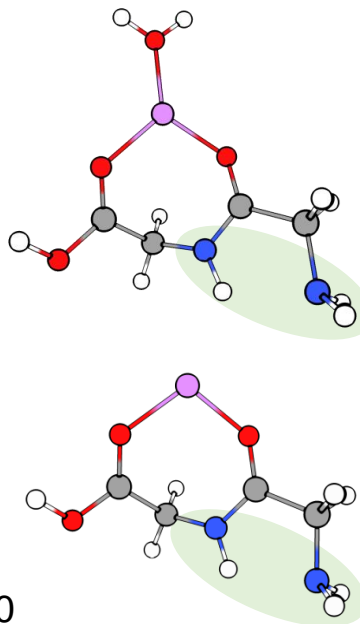
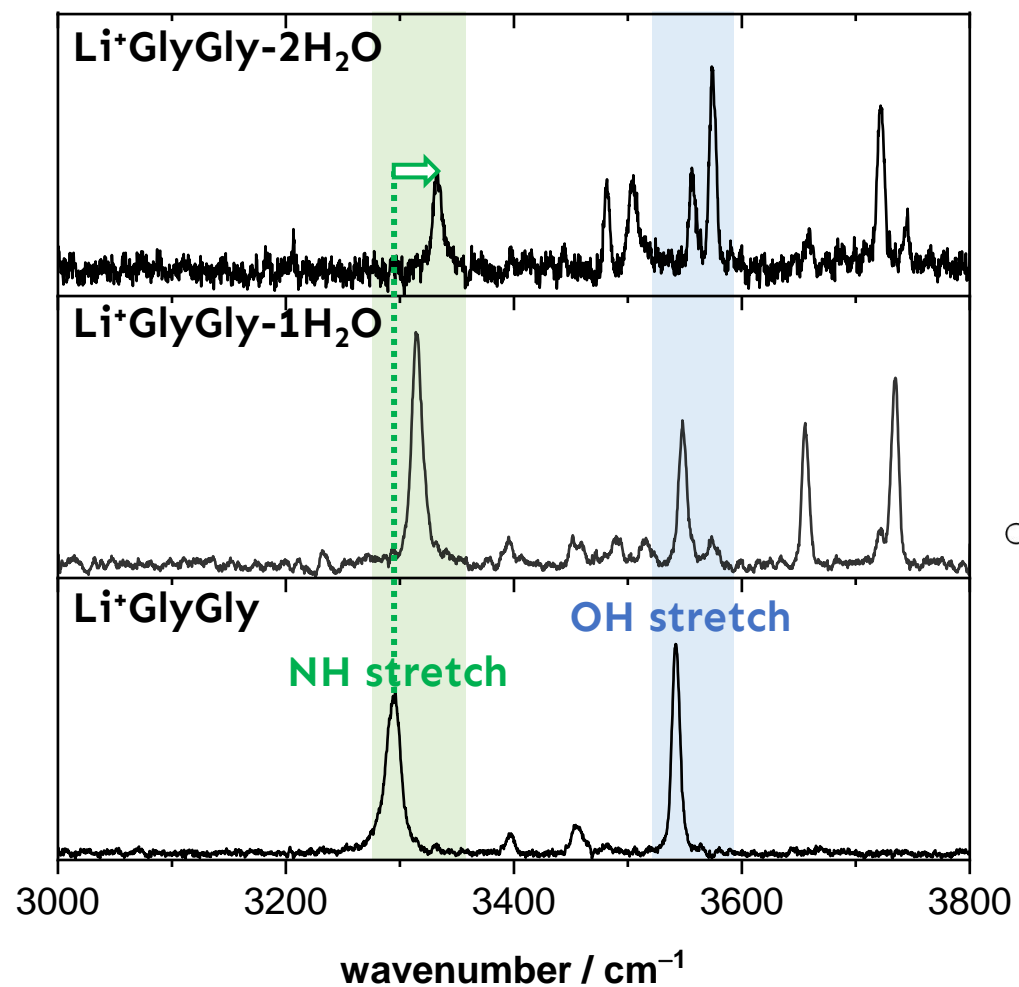


# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION

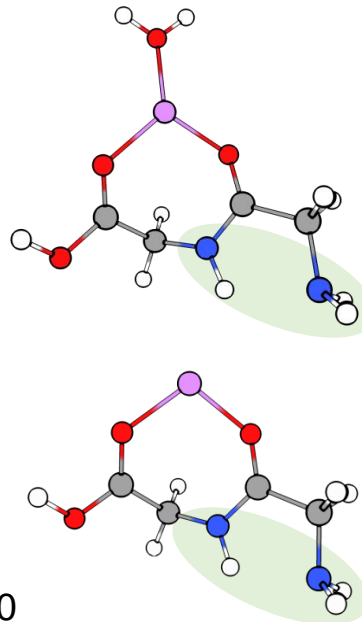
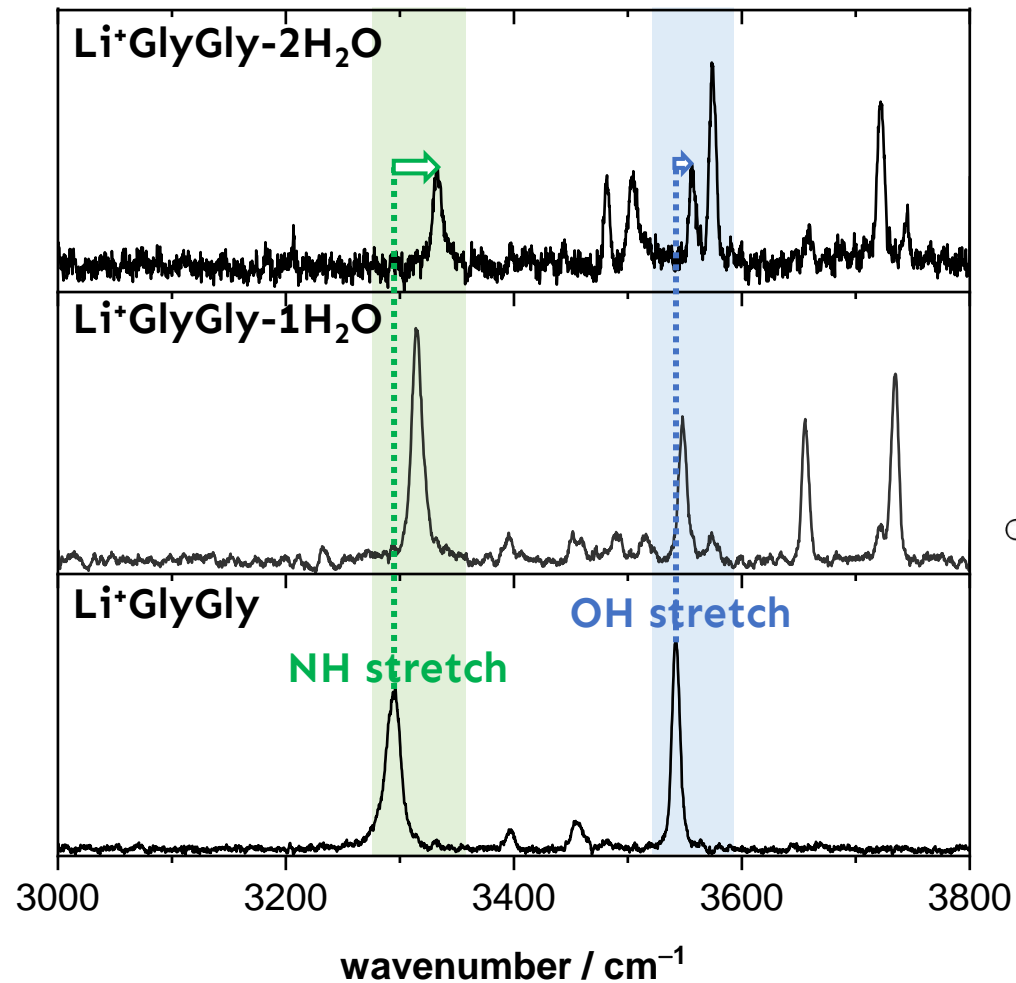




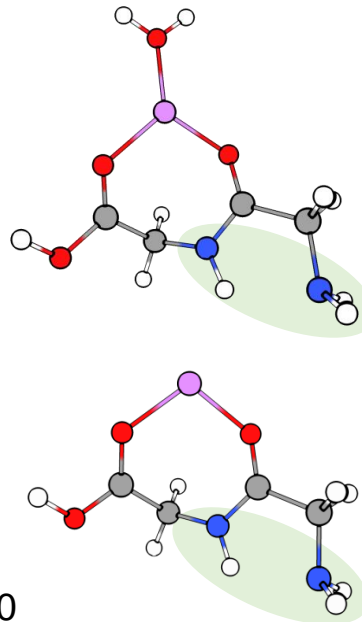
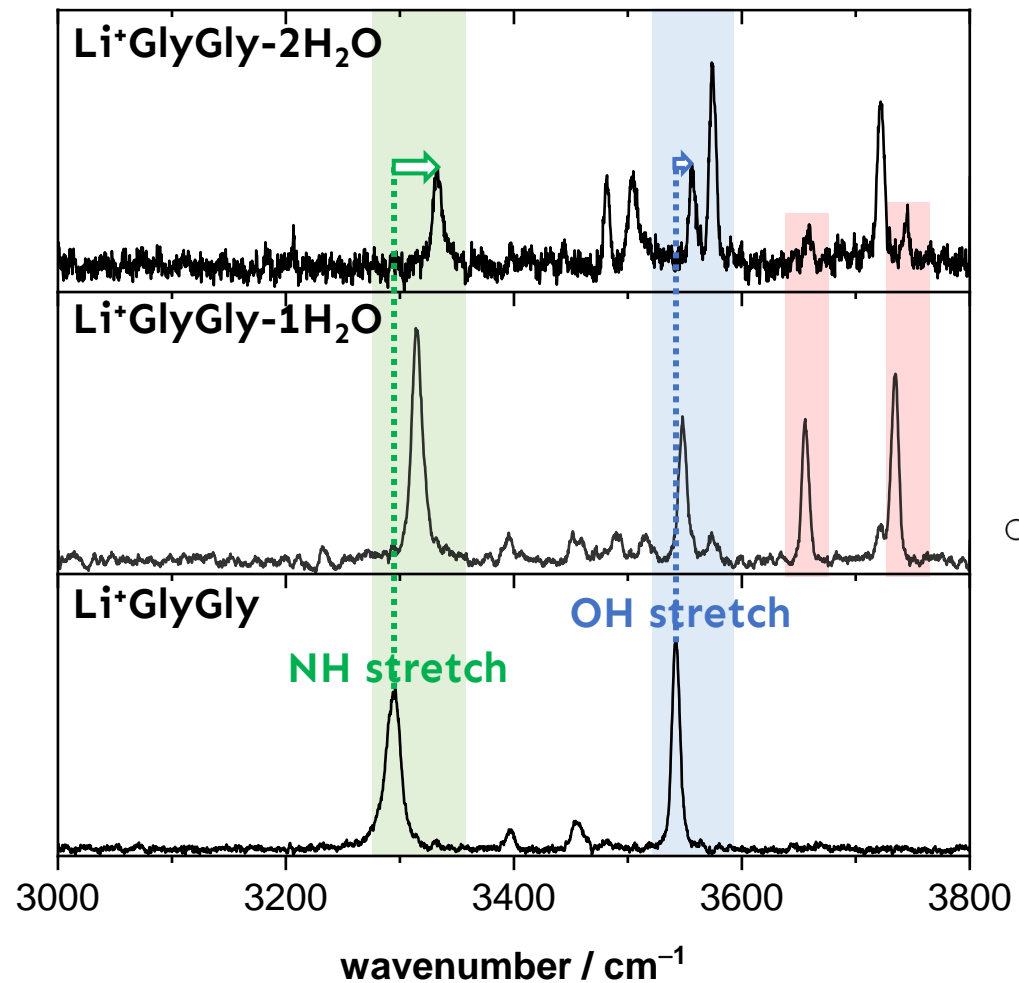
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



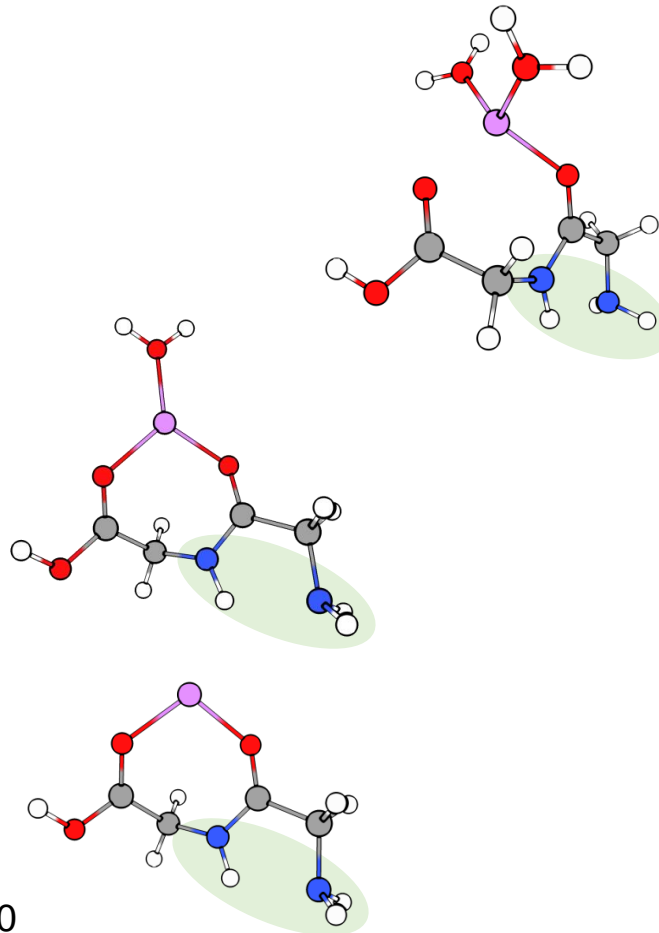
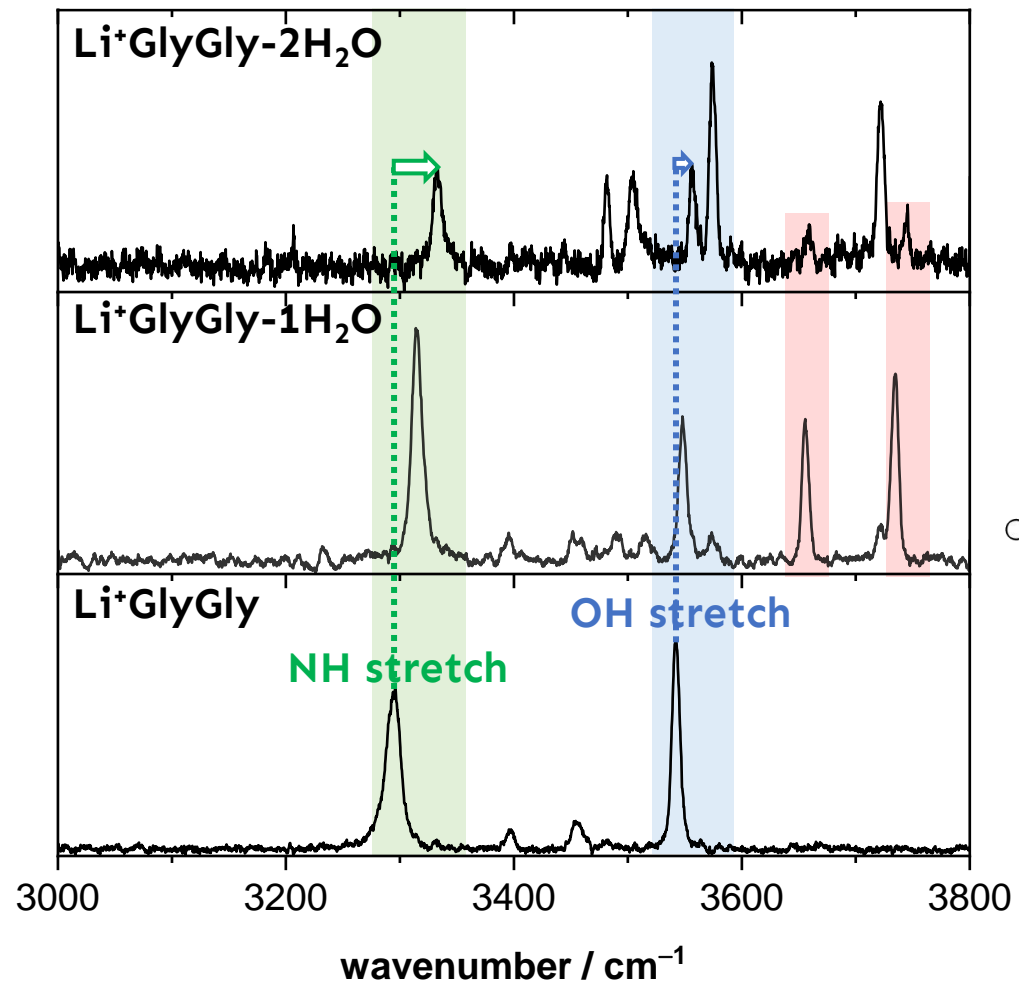
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



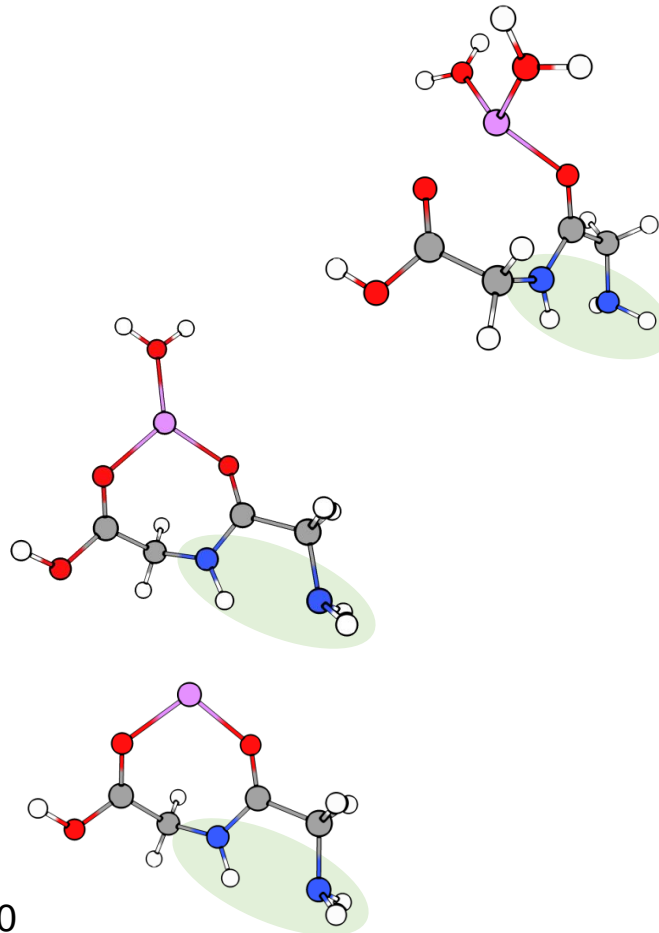
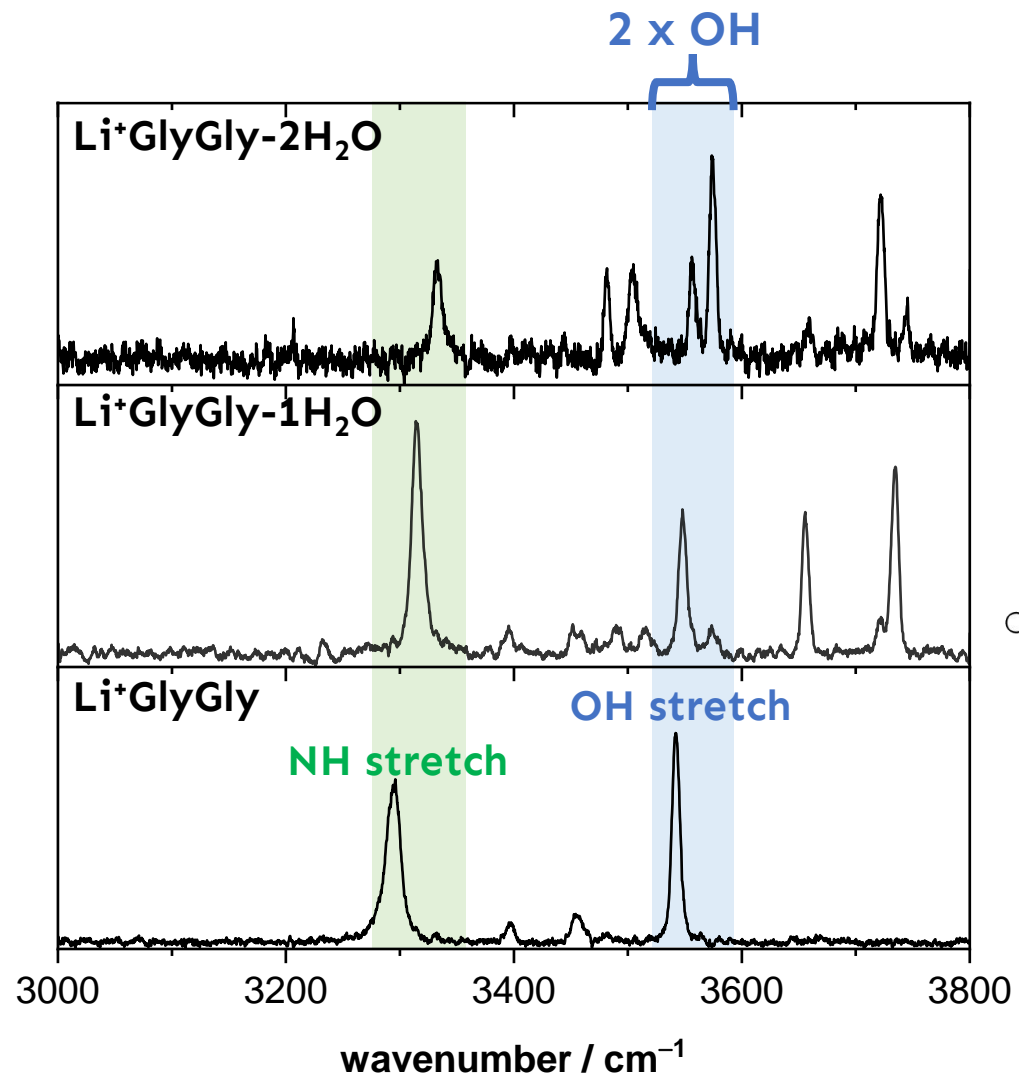
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



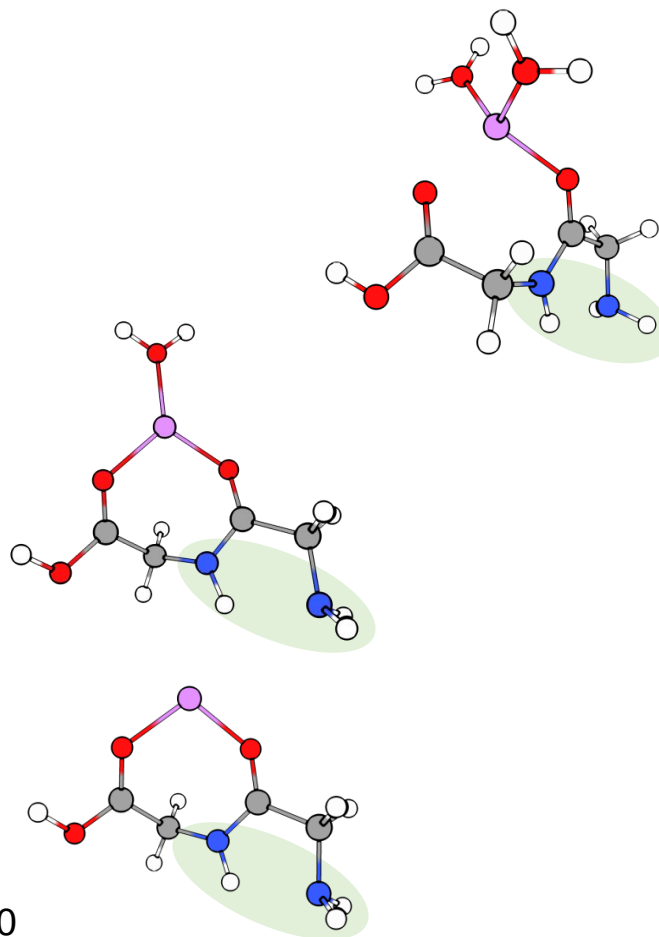
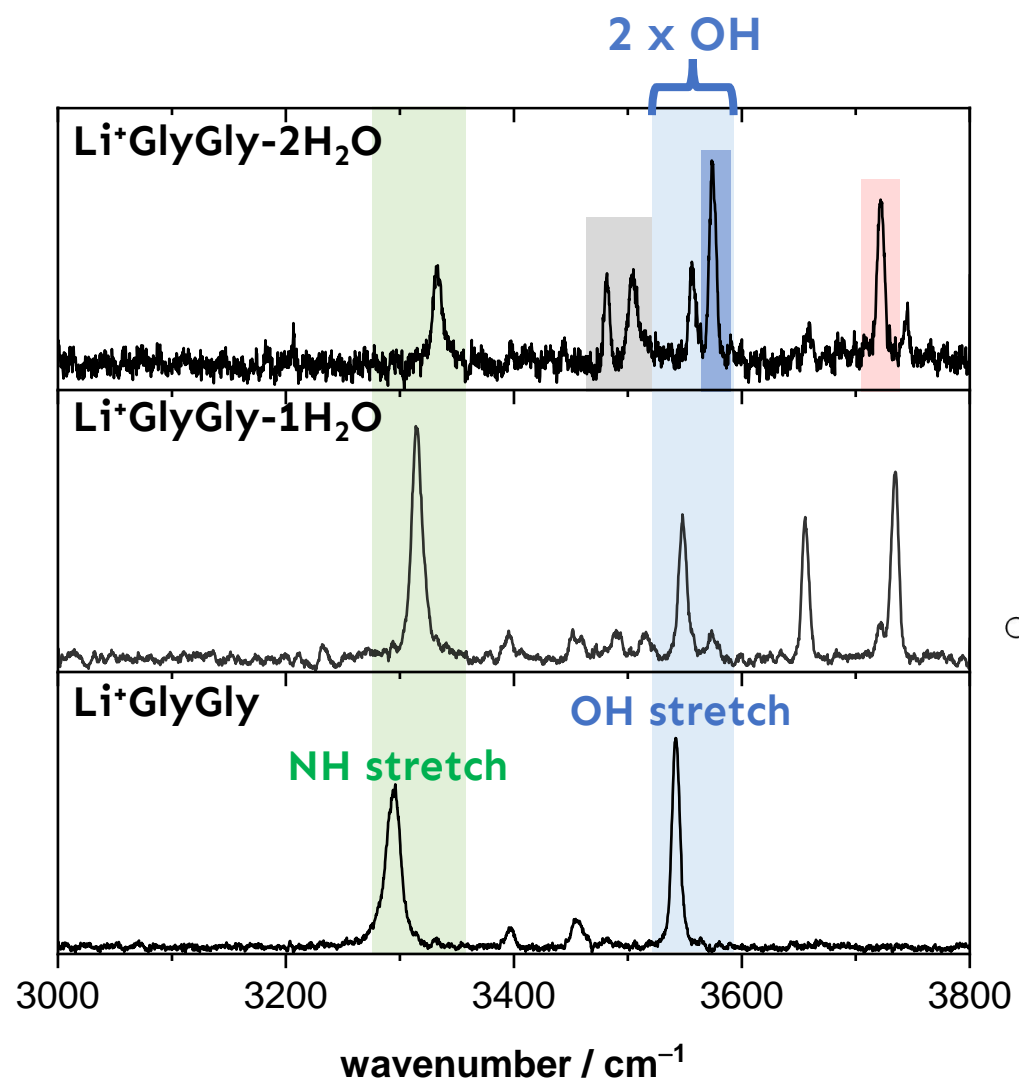
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



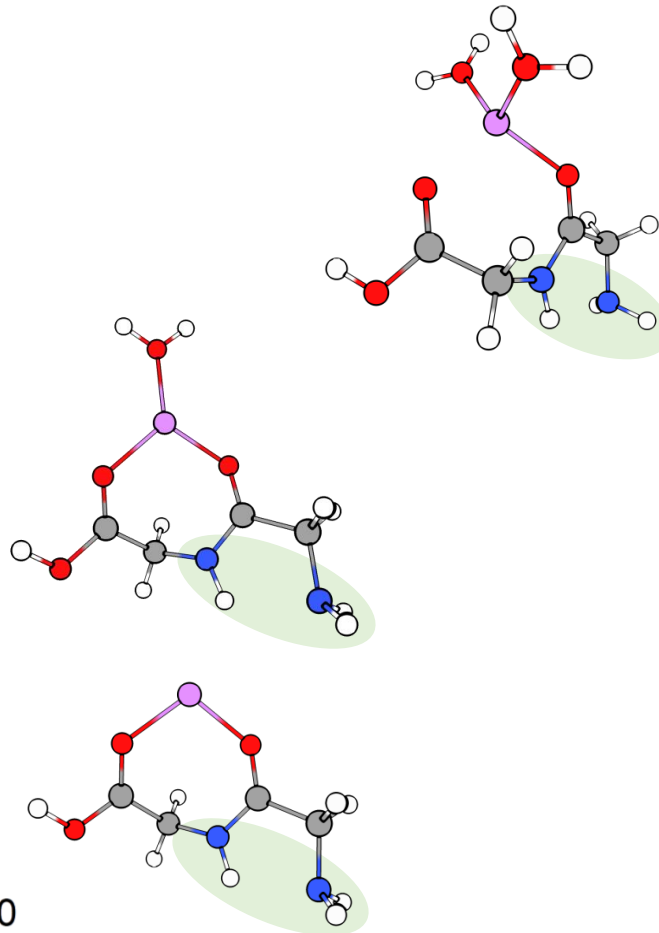
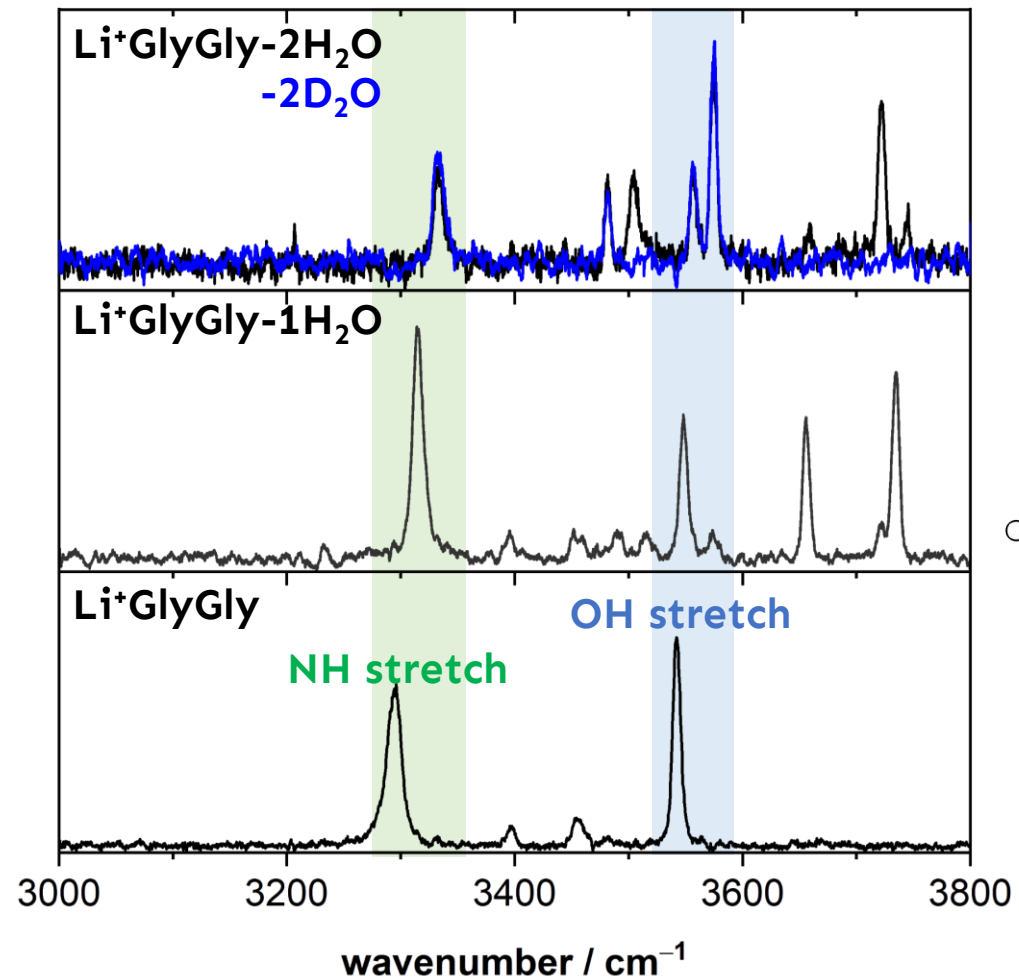
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



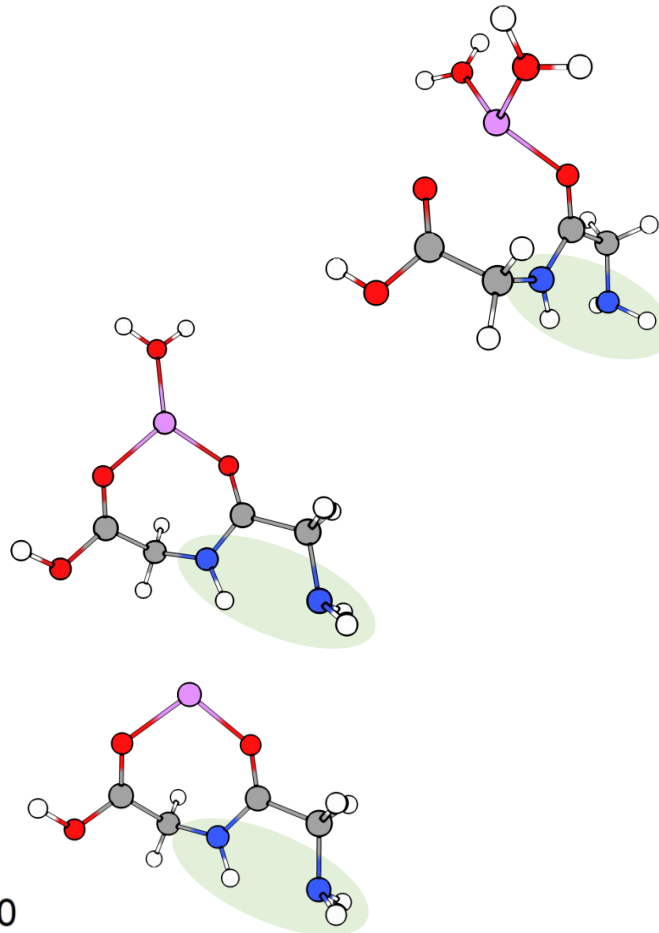
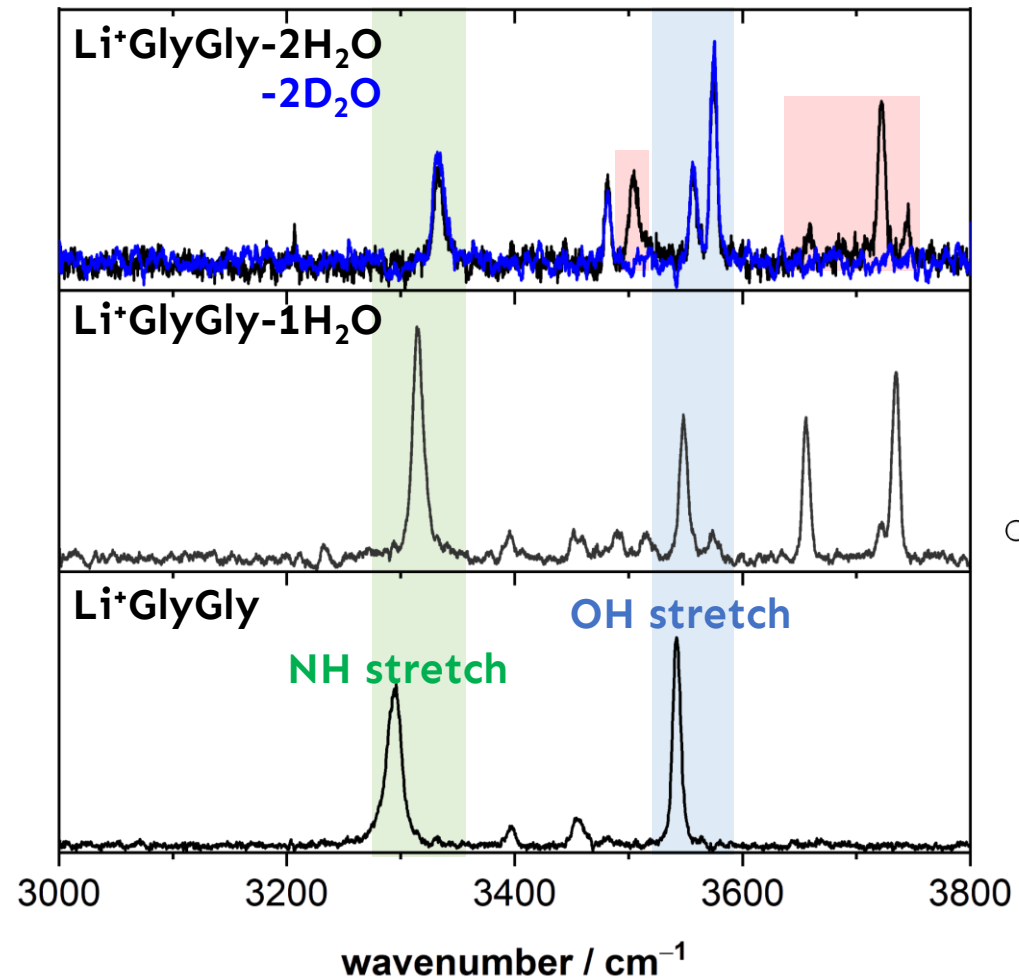
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION

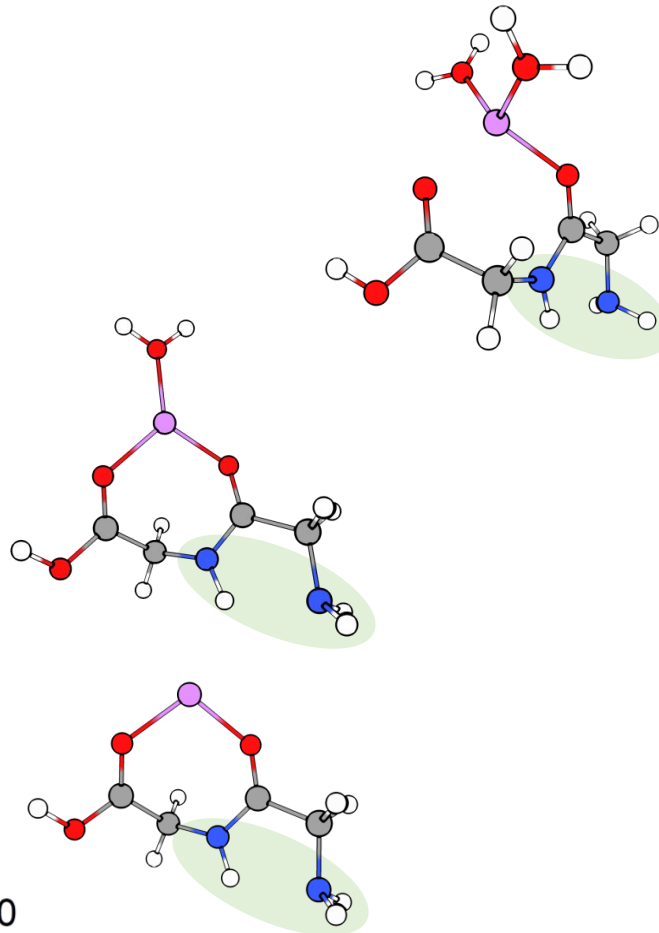
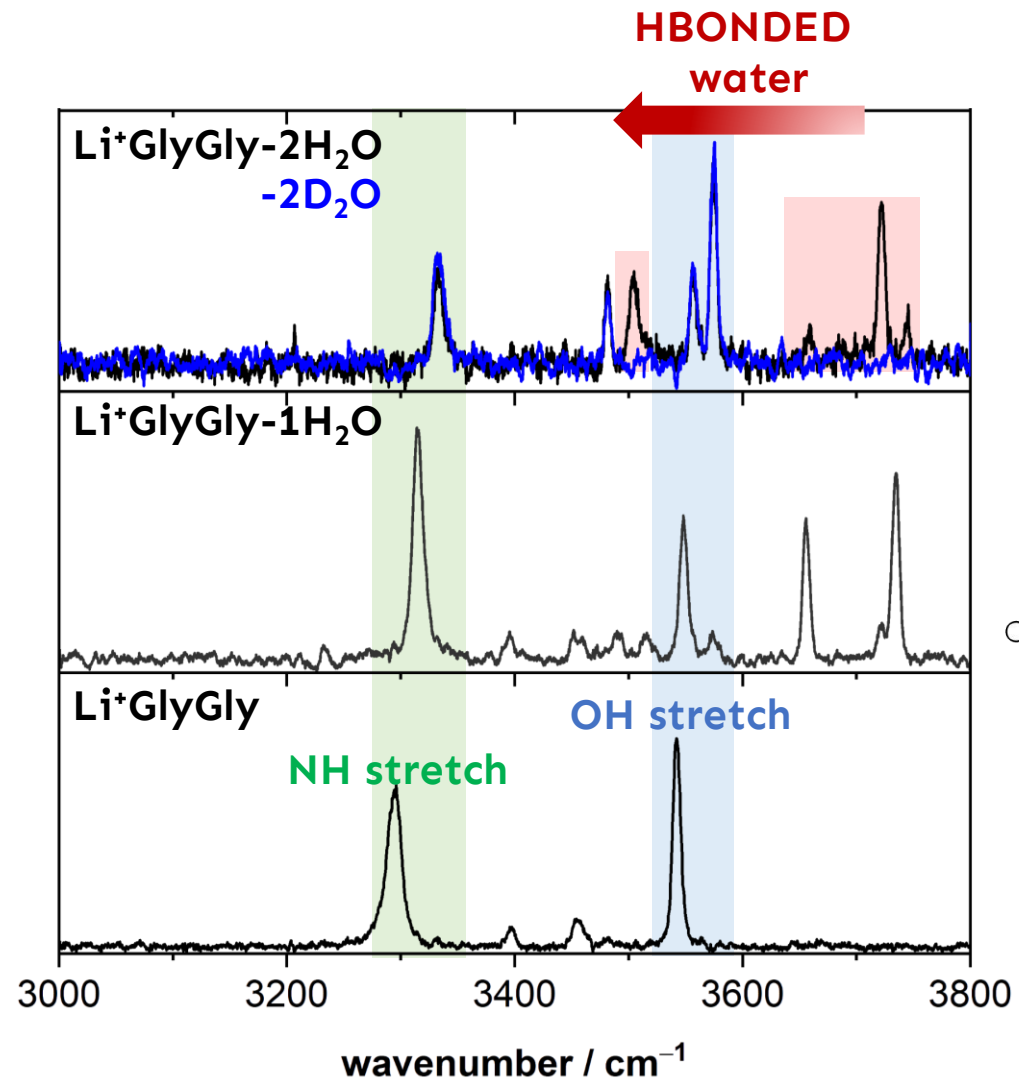


# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION

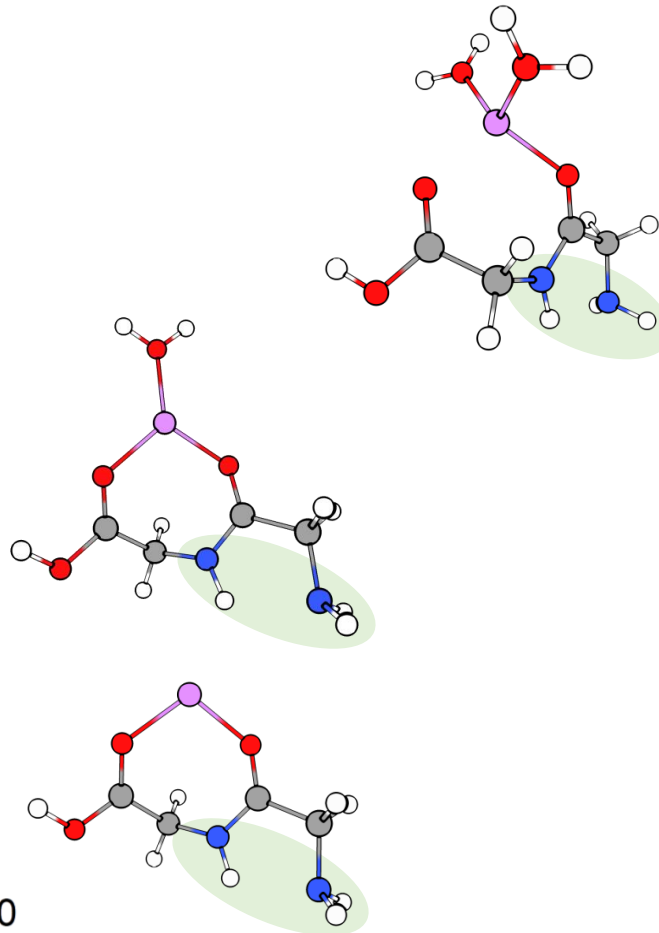
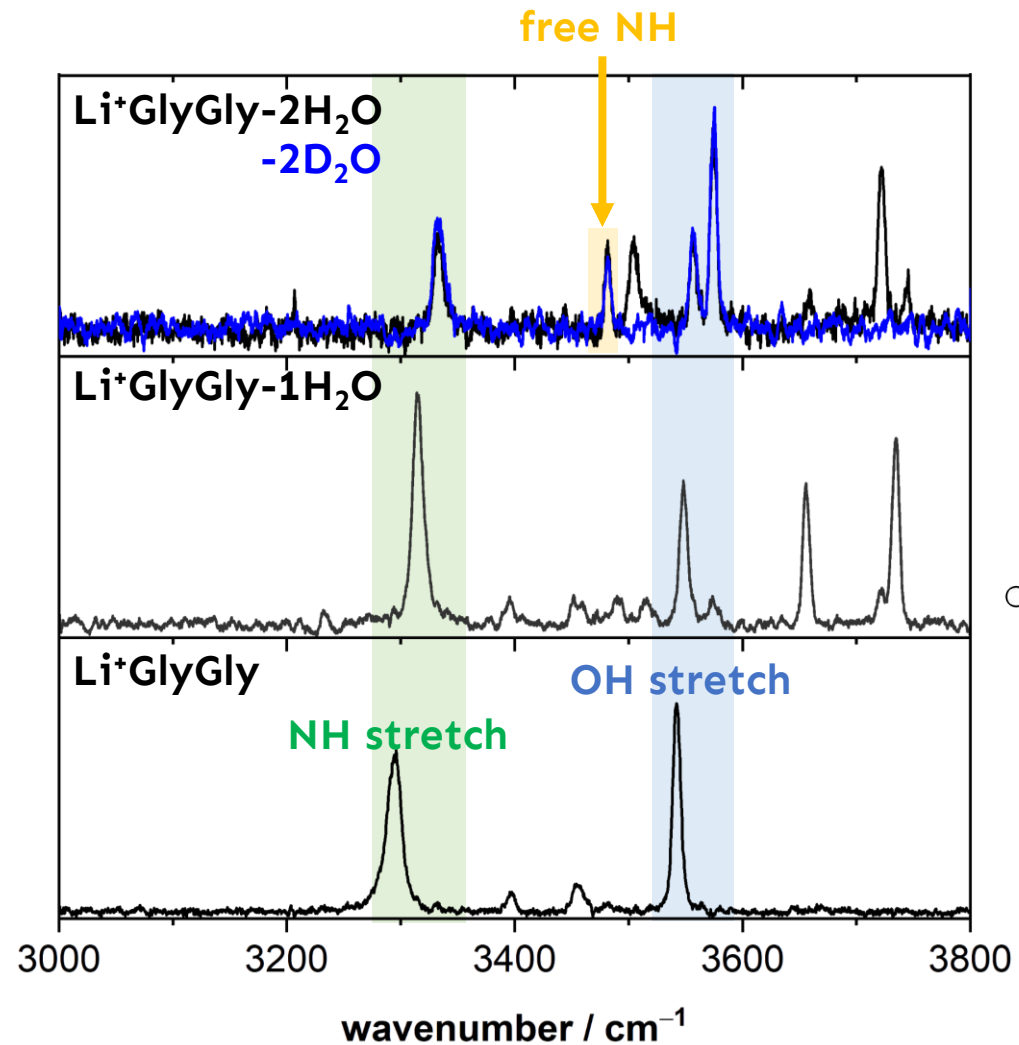




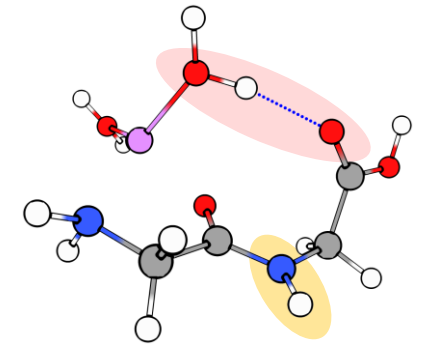
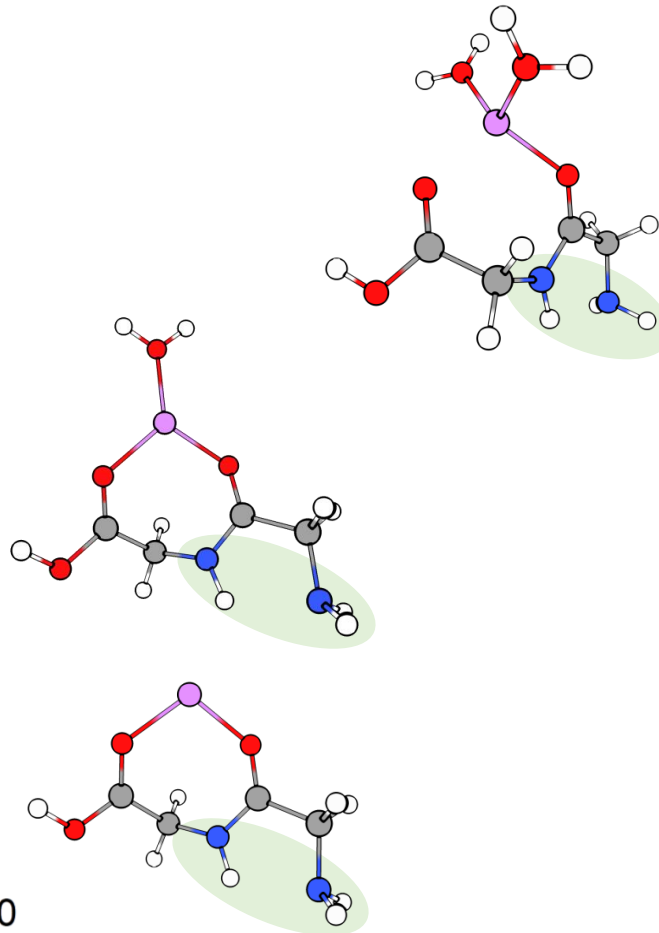
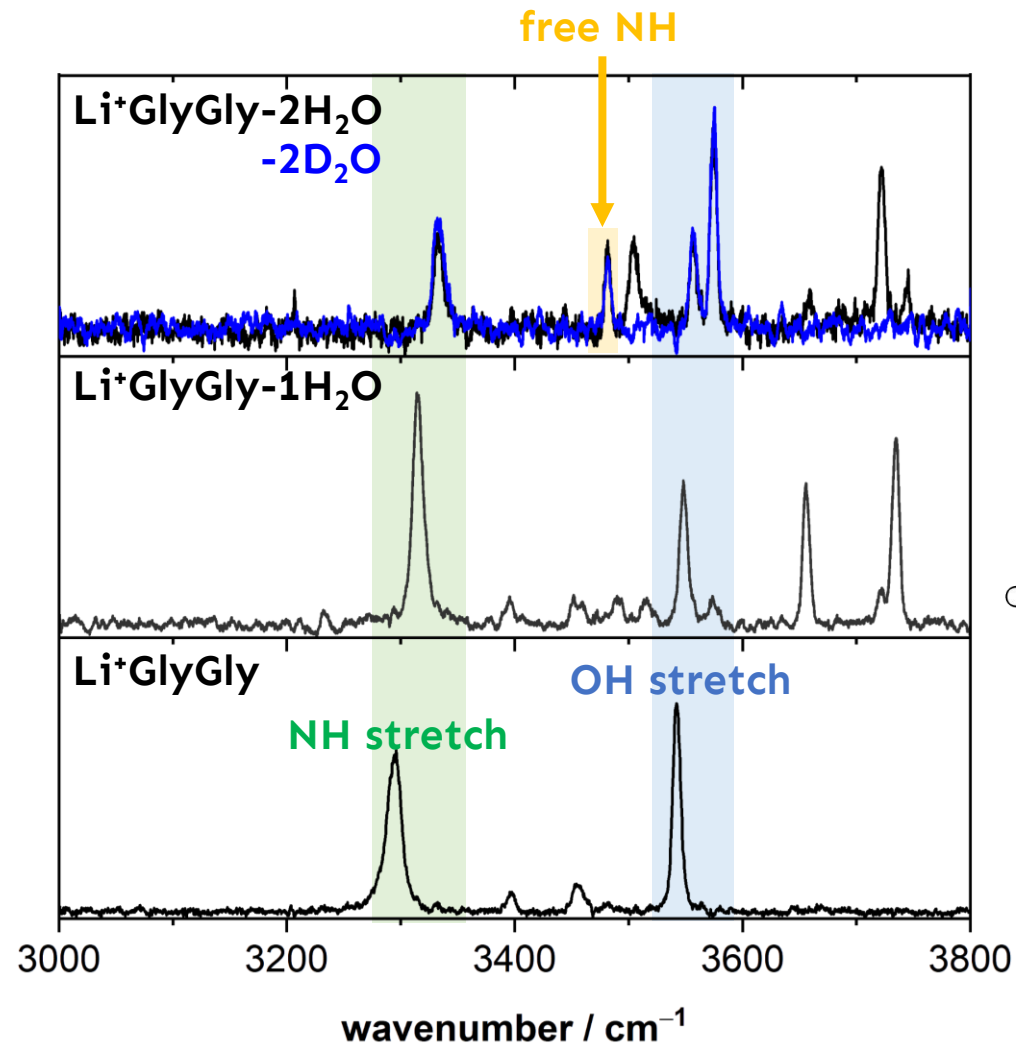
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION

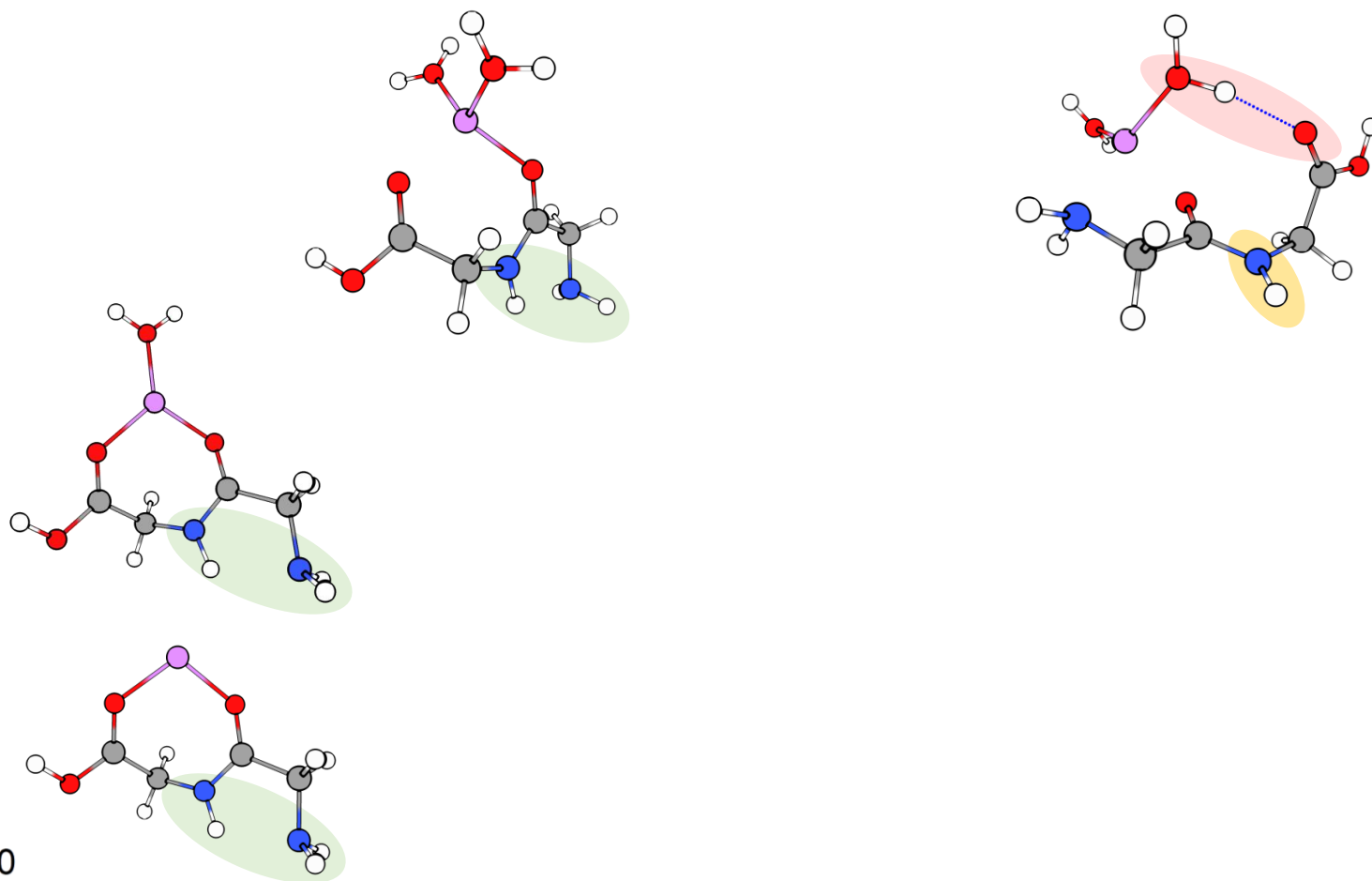
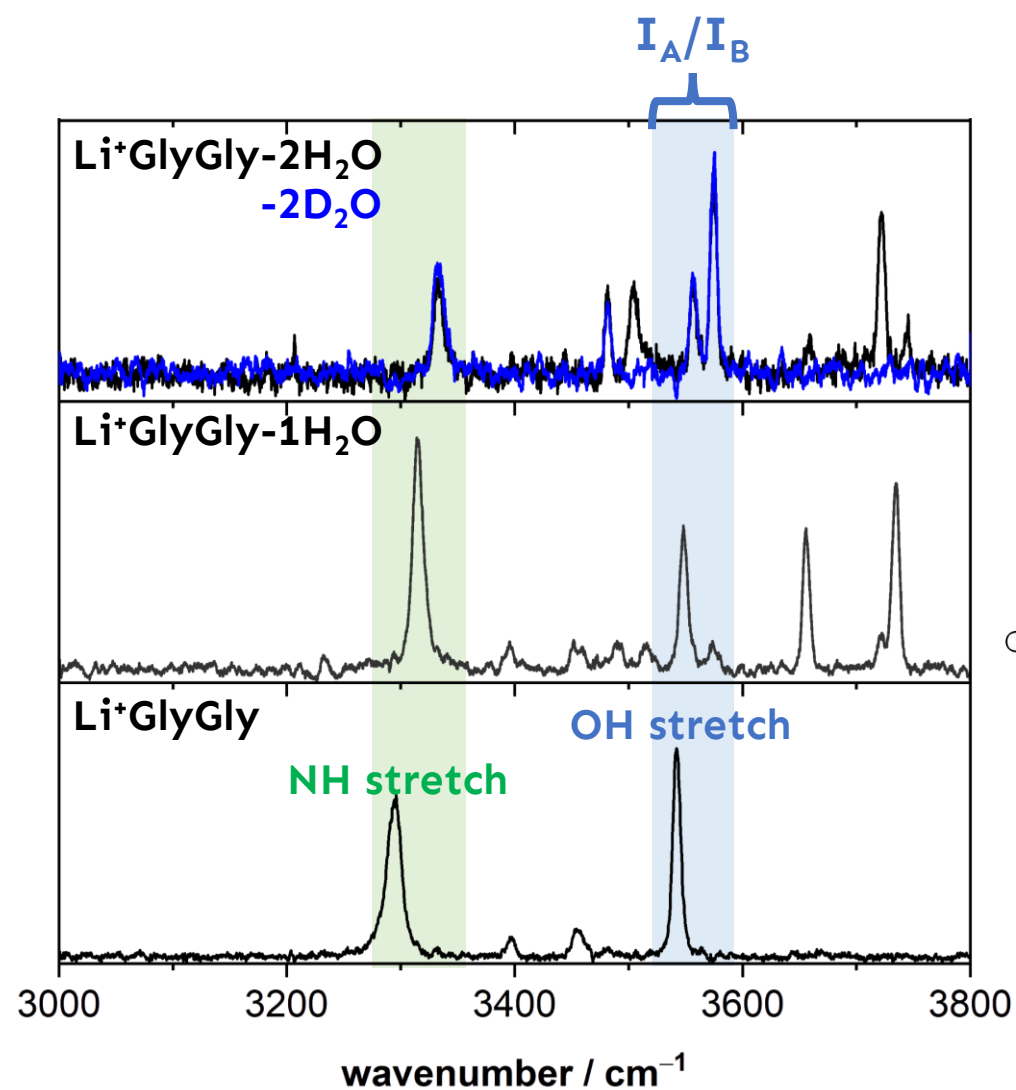


# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION

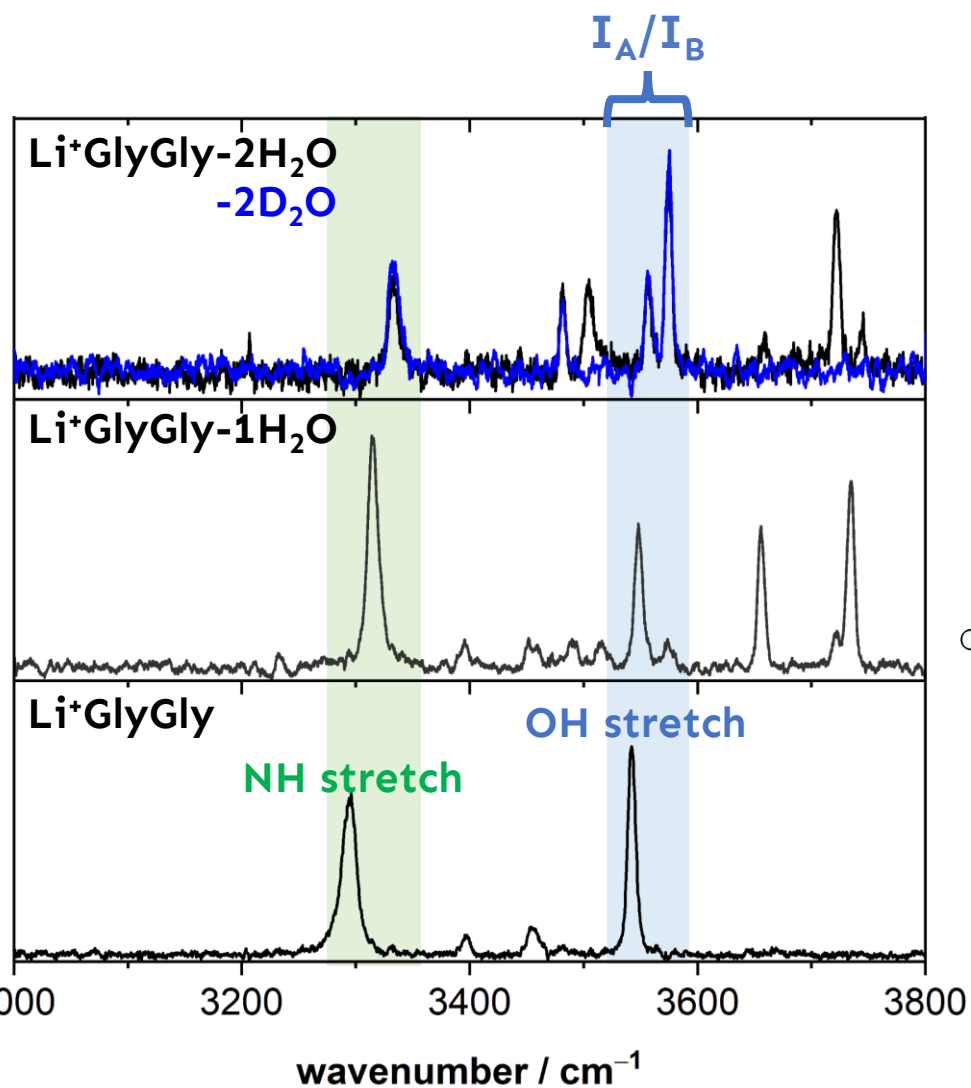


# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION

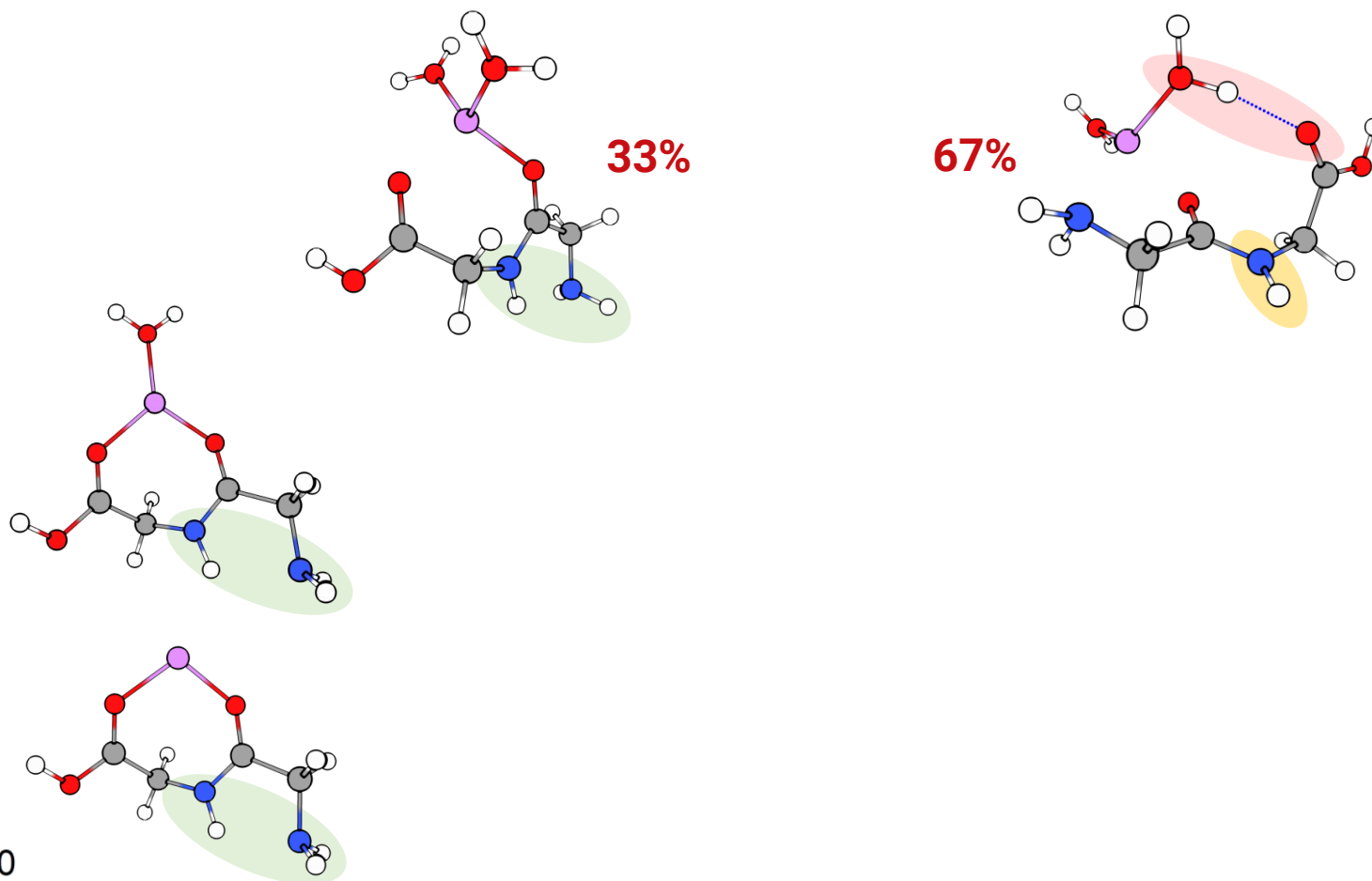
Conformer ratio:  
Comparison of relative OH band intensities



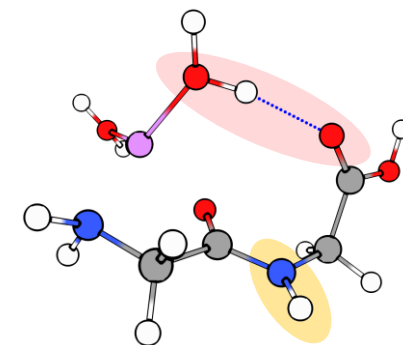
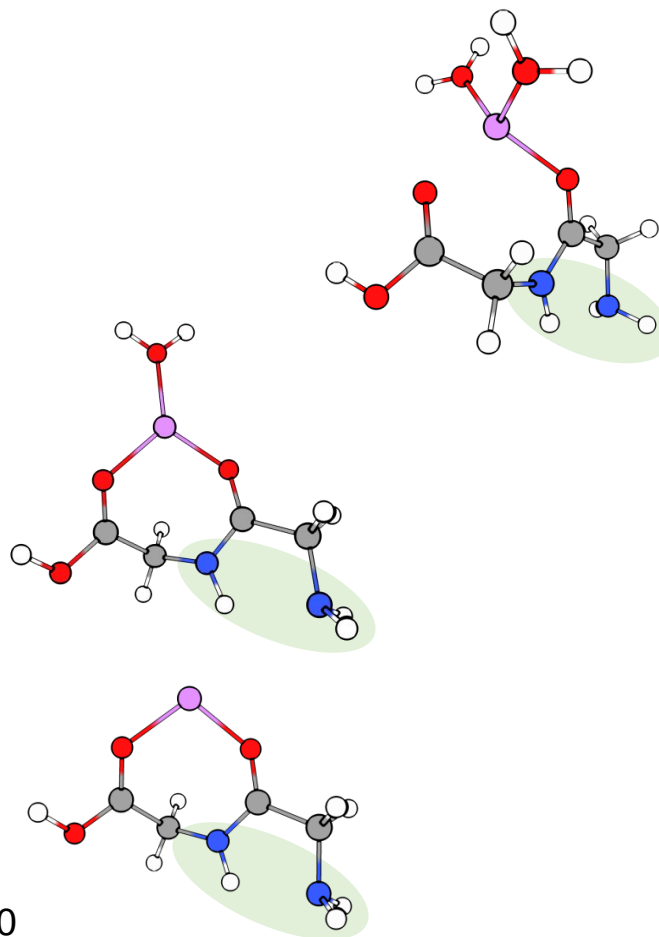
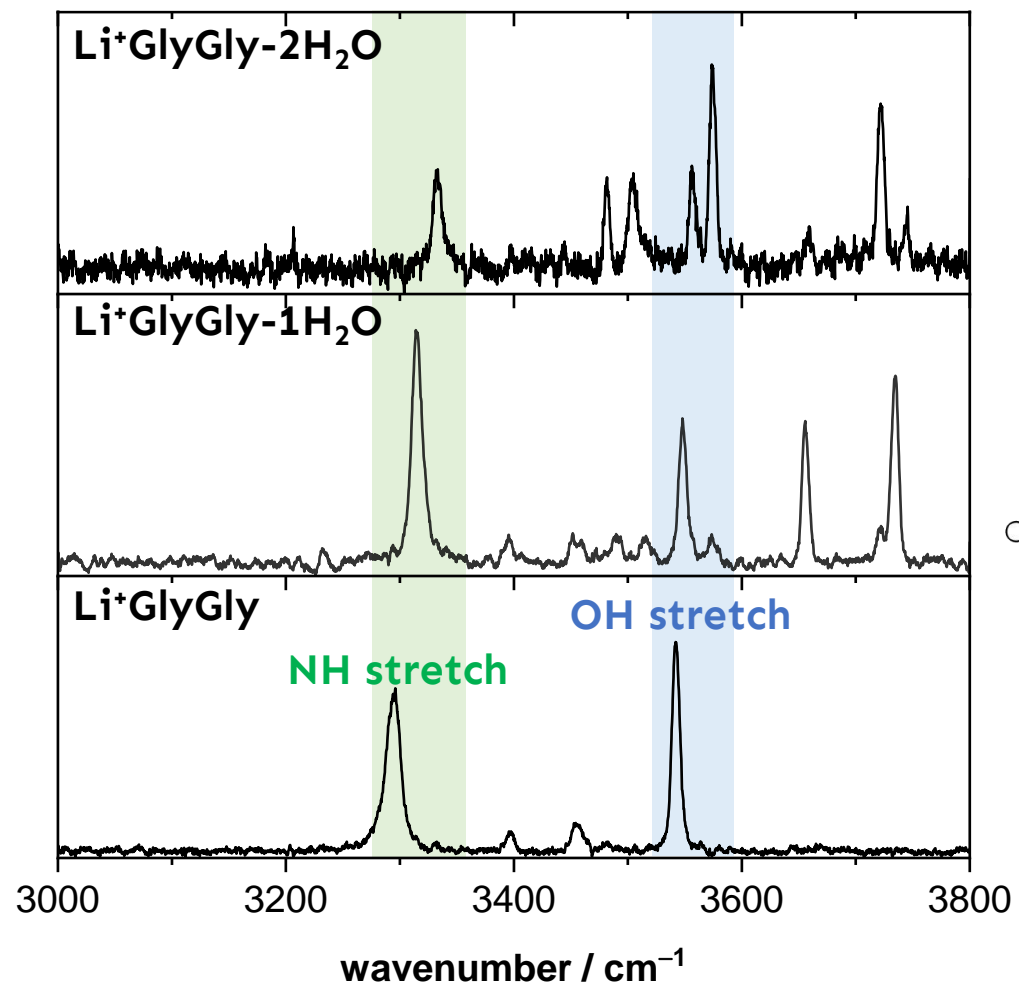
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



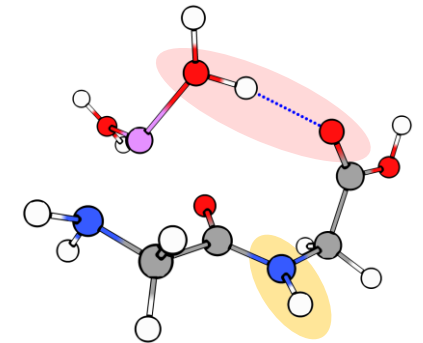
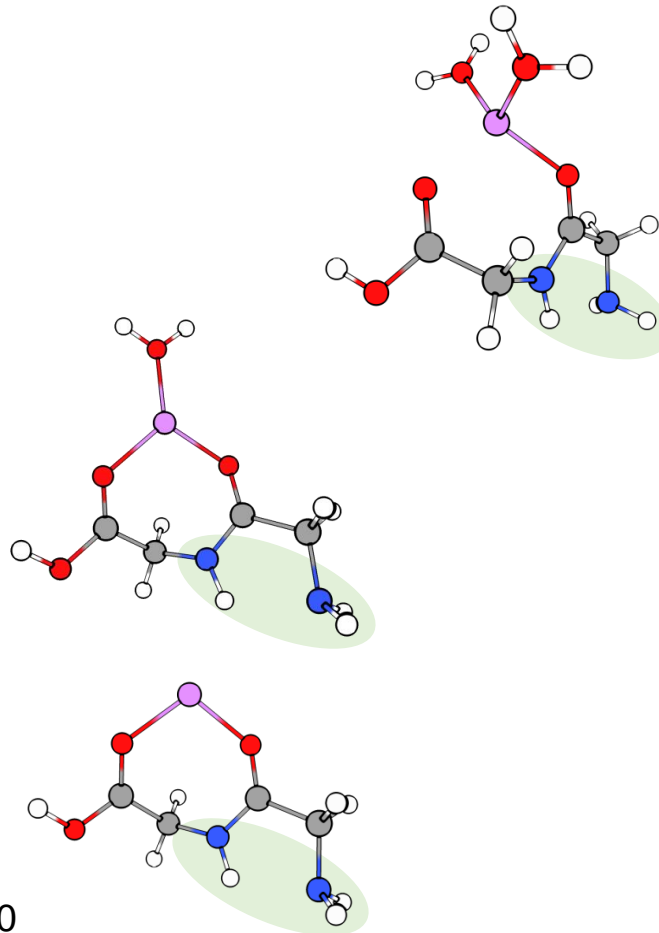
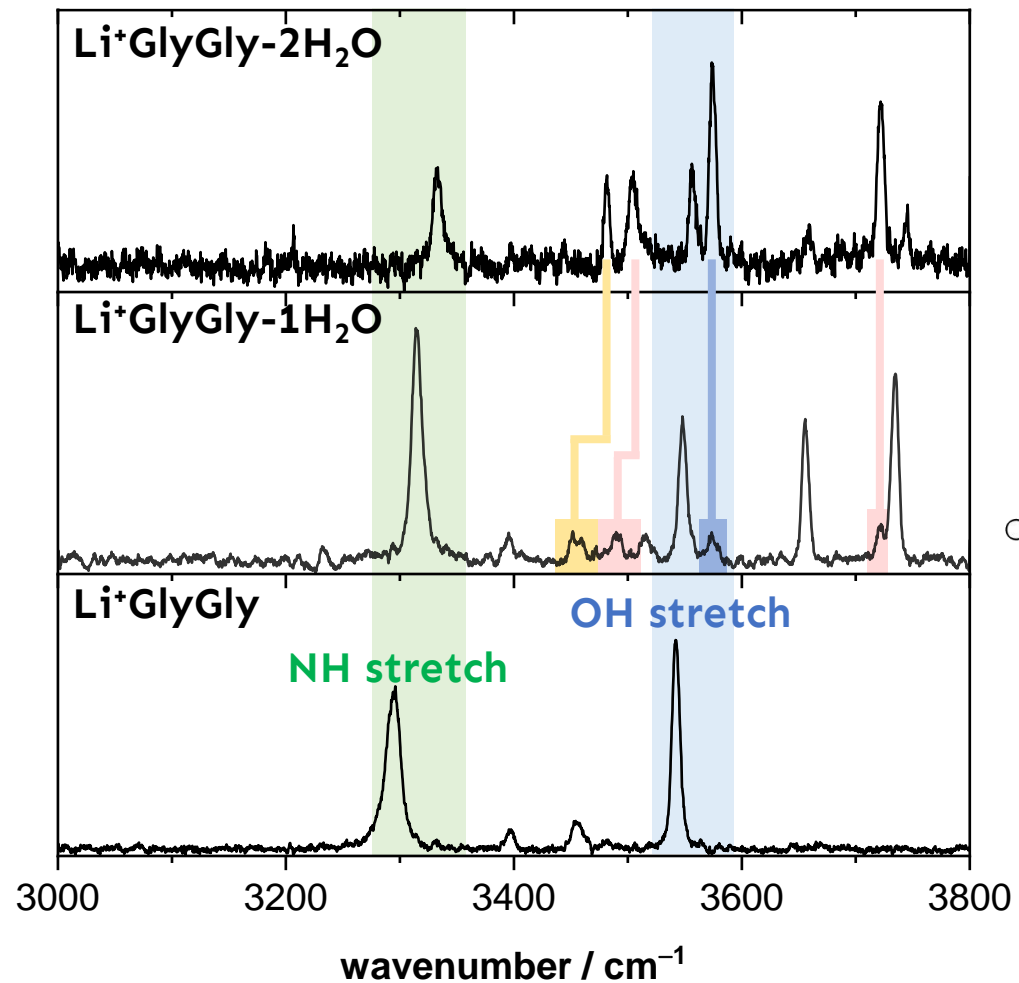
Conformer ratio:  
Comparison of relative OH band intensities



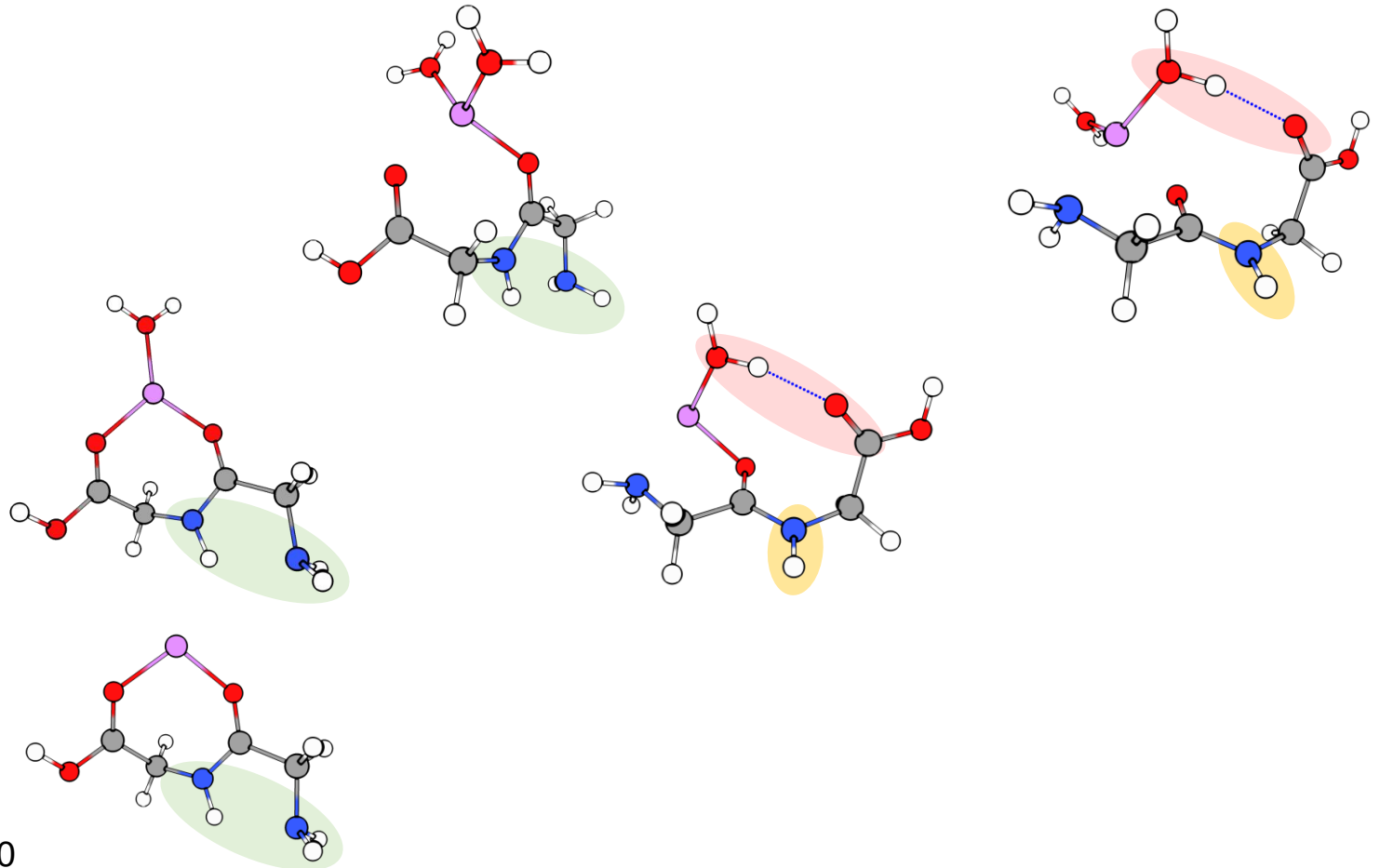
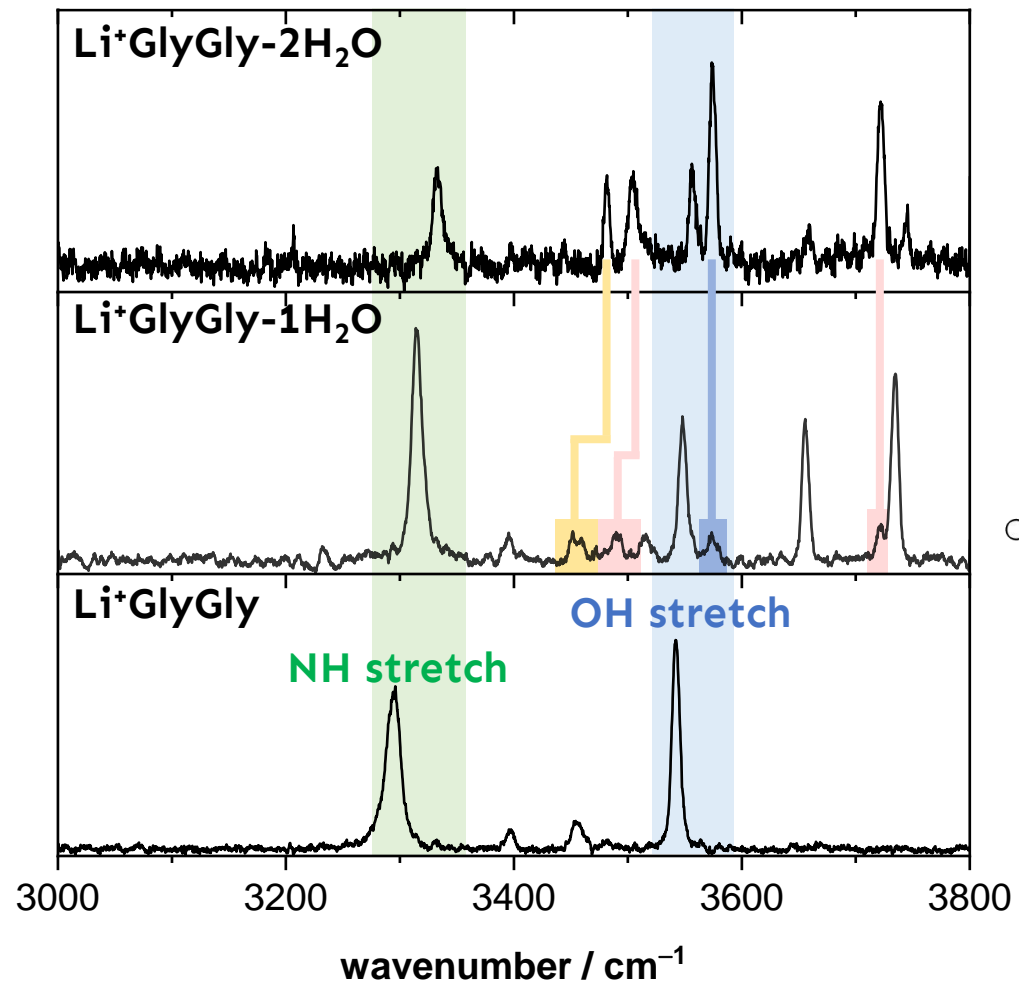
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION

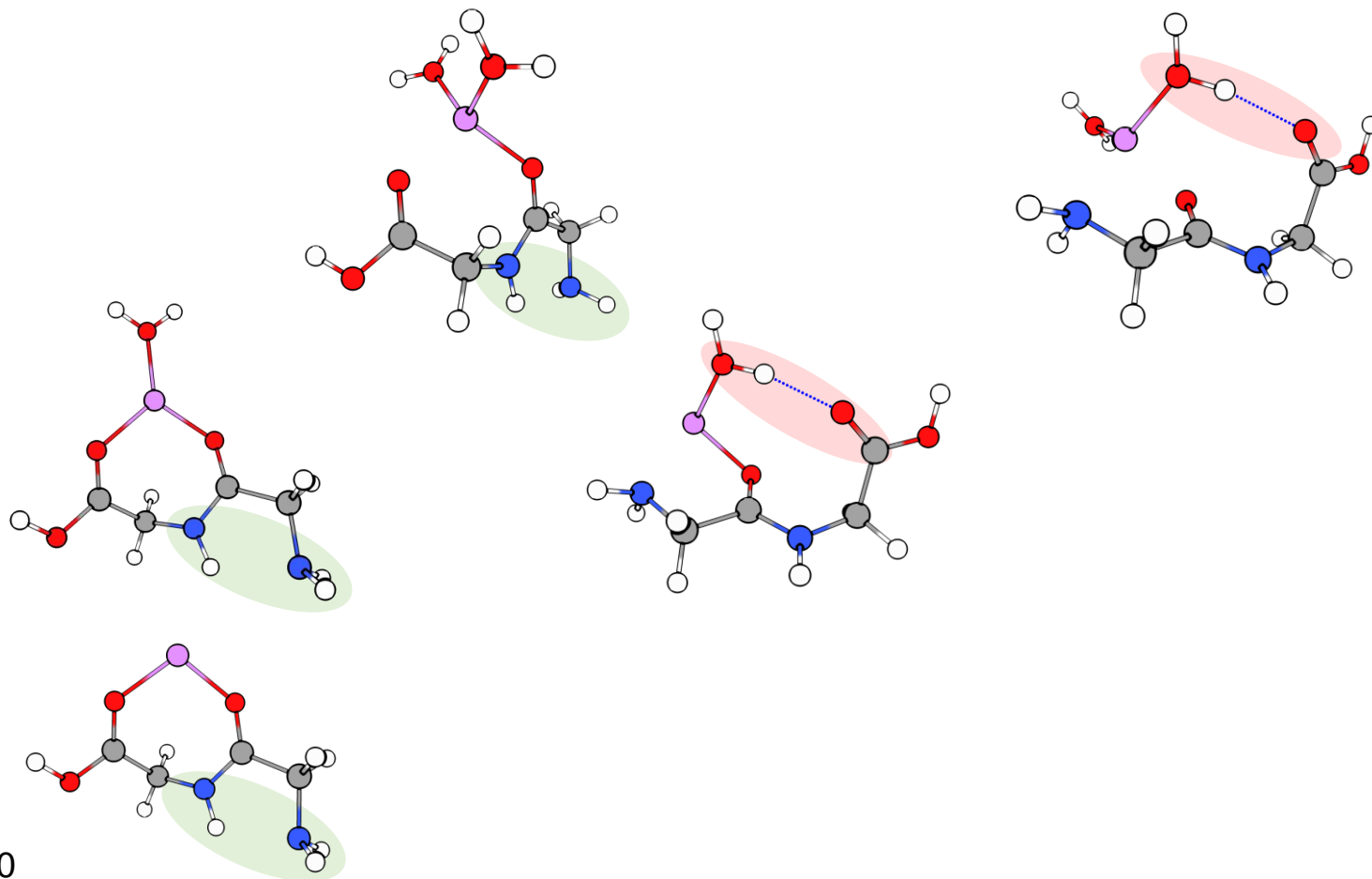
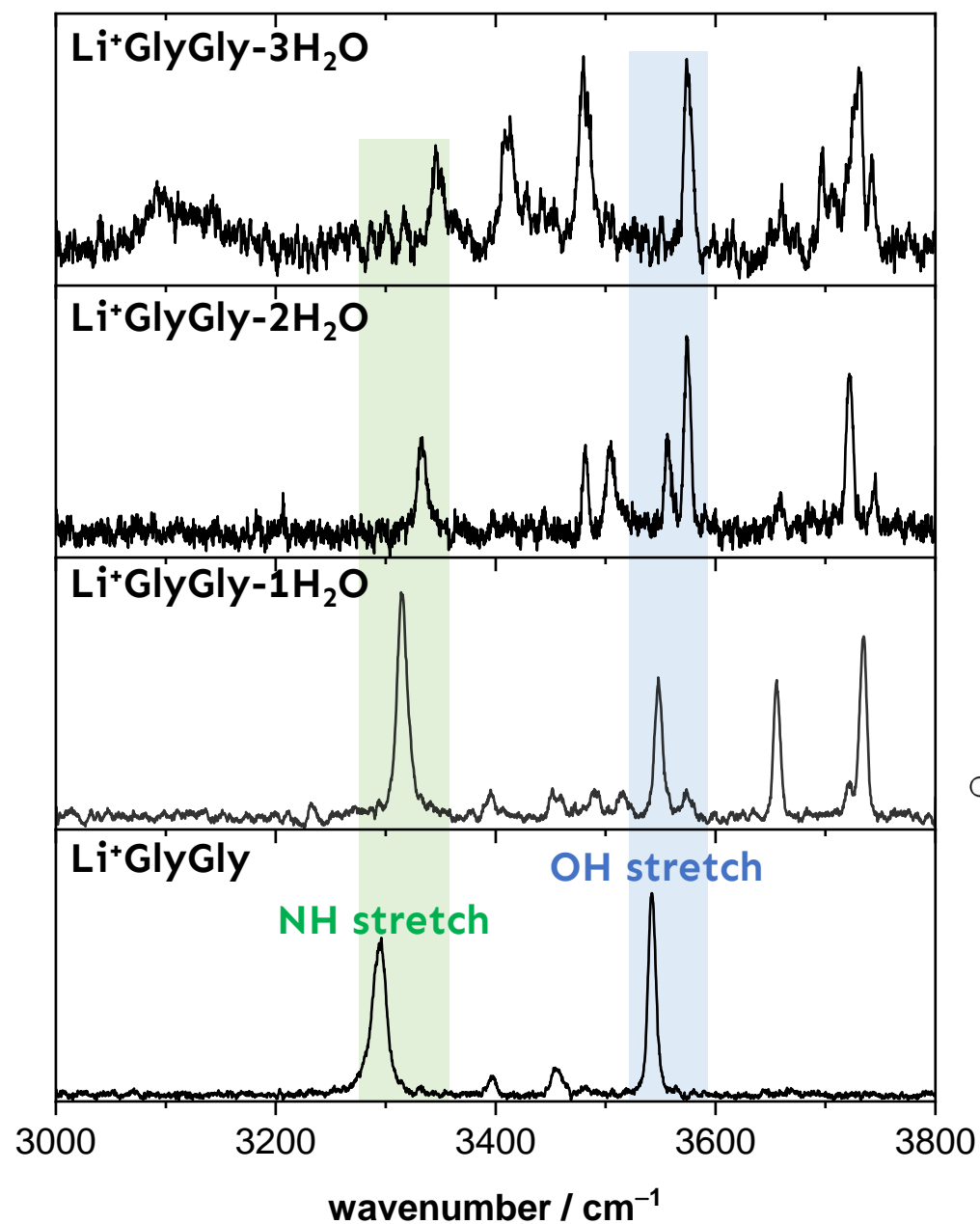


# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION

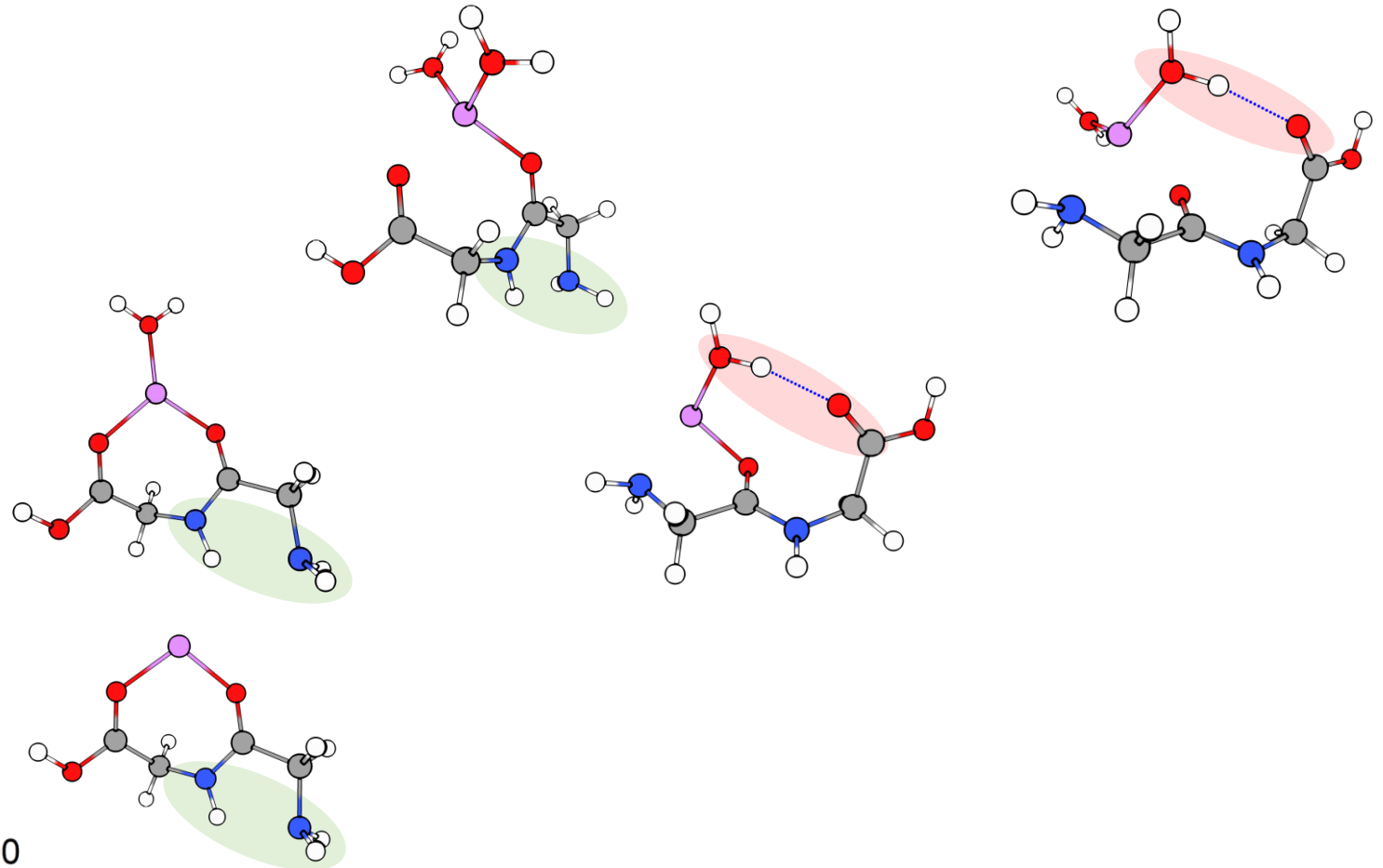
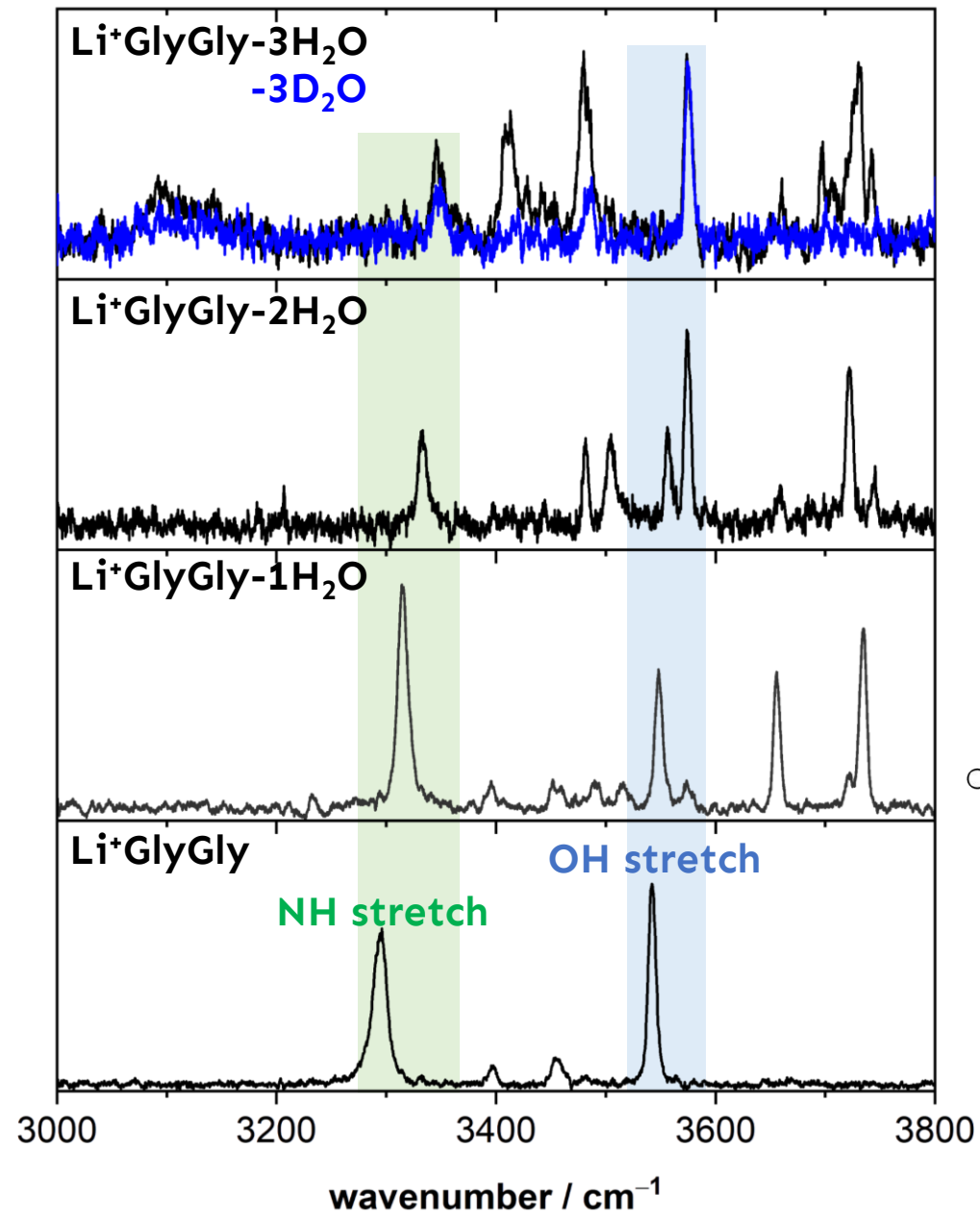




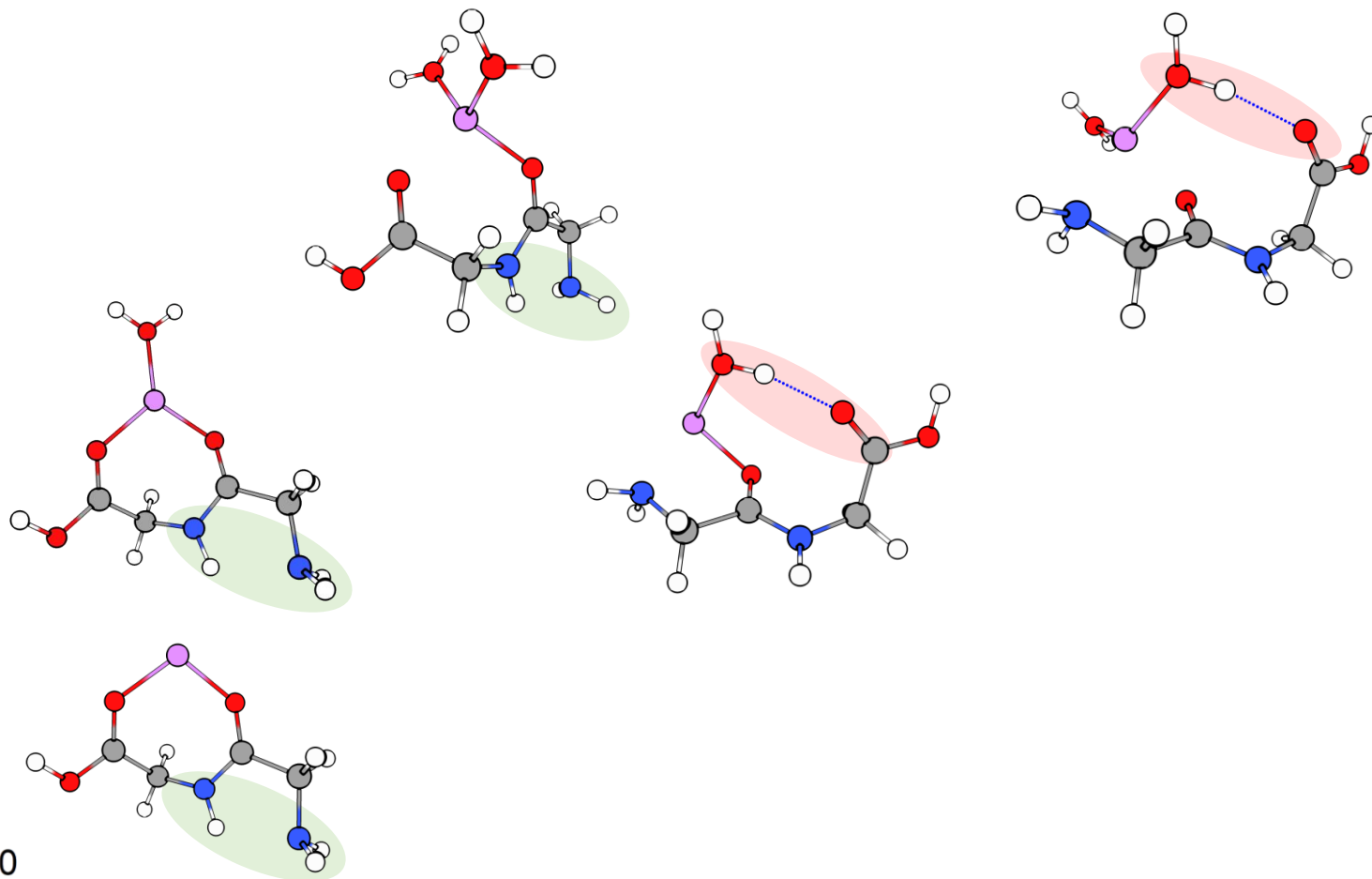
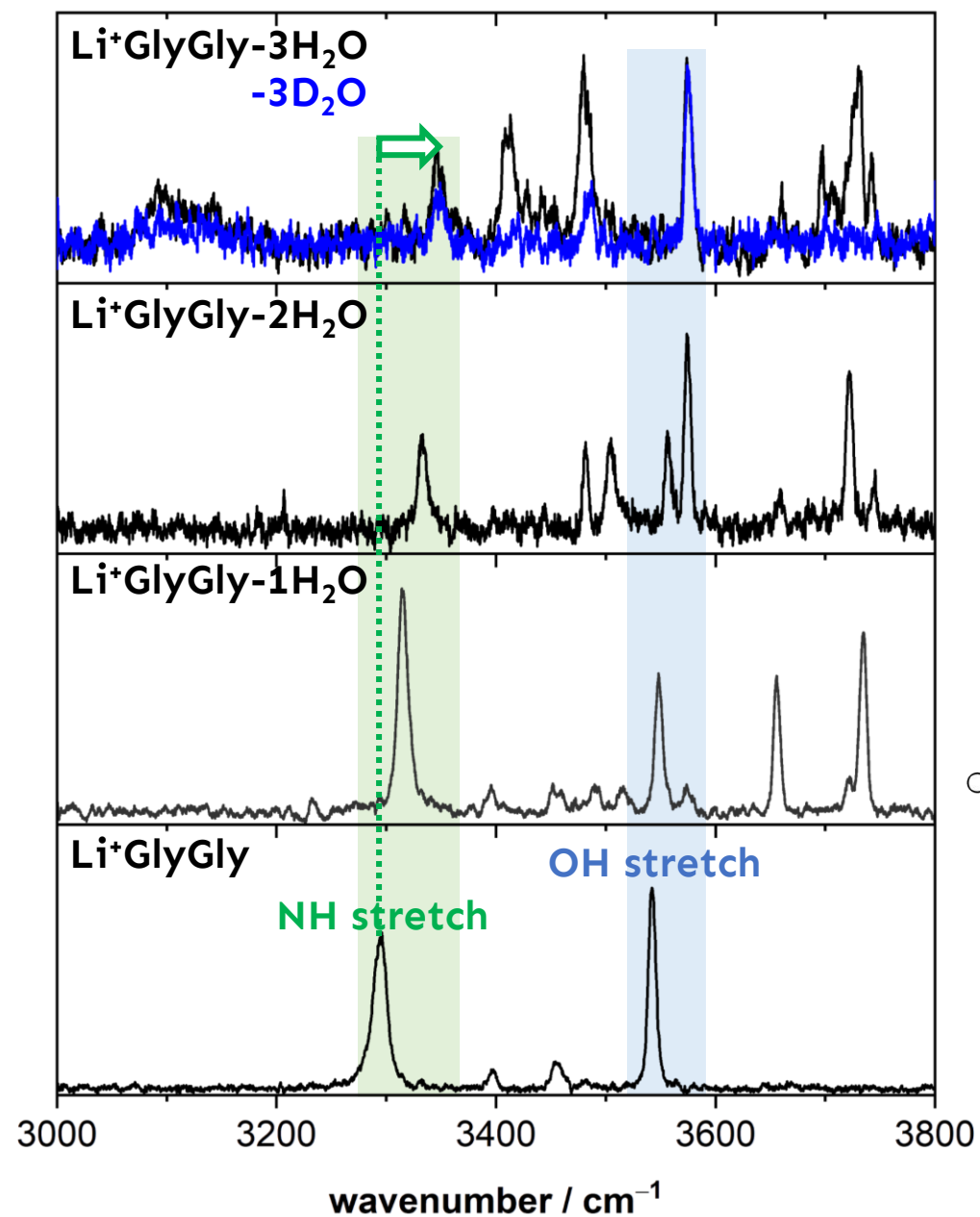
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



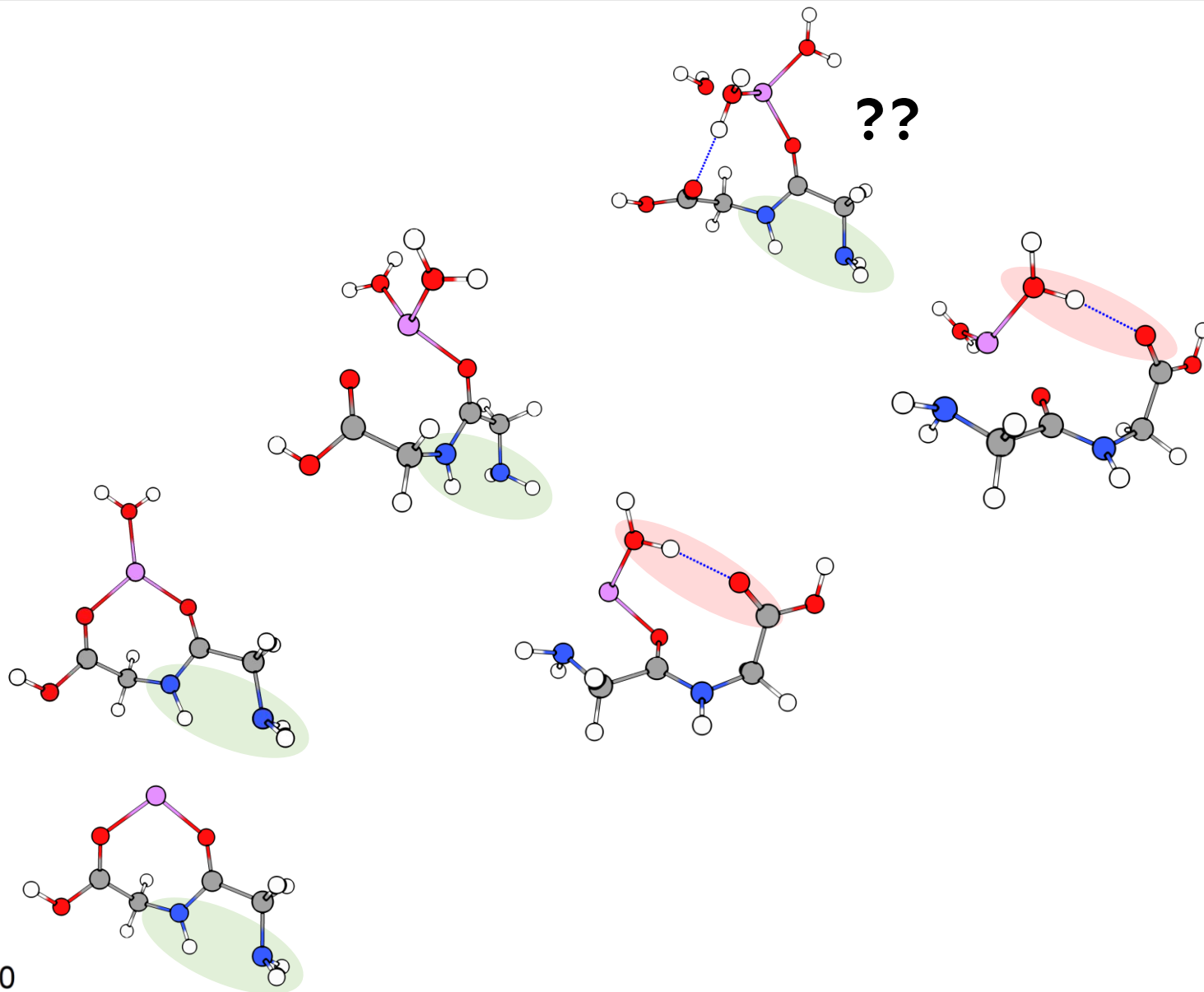
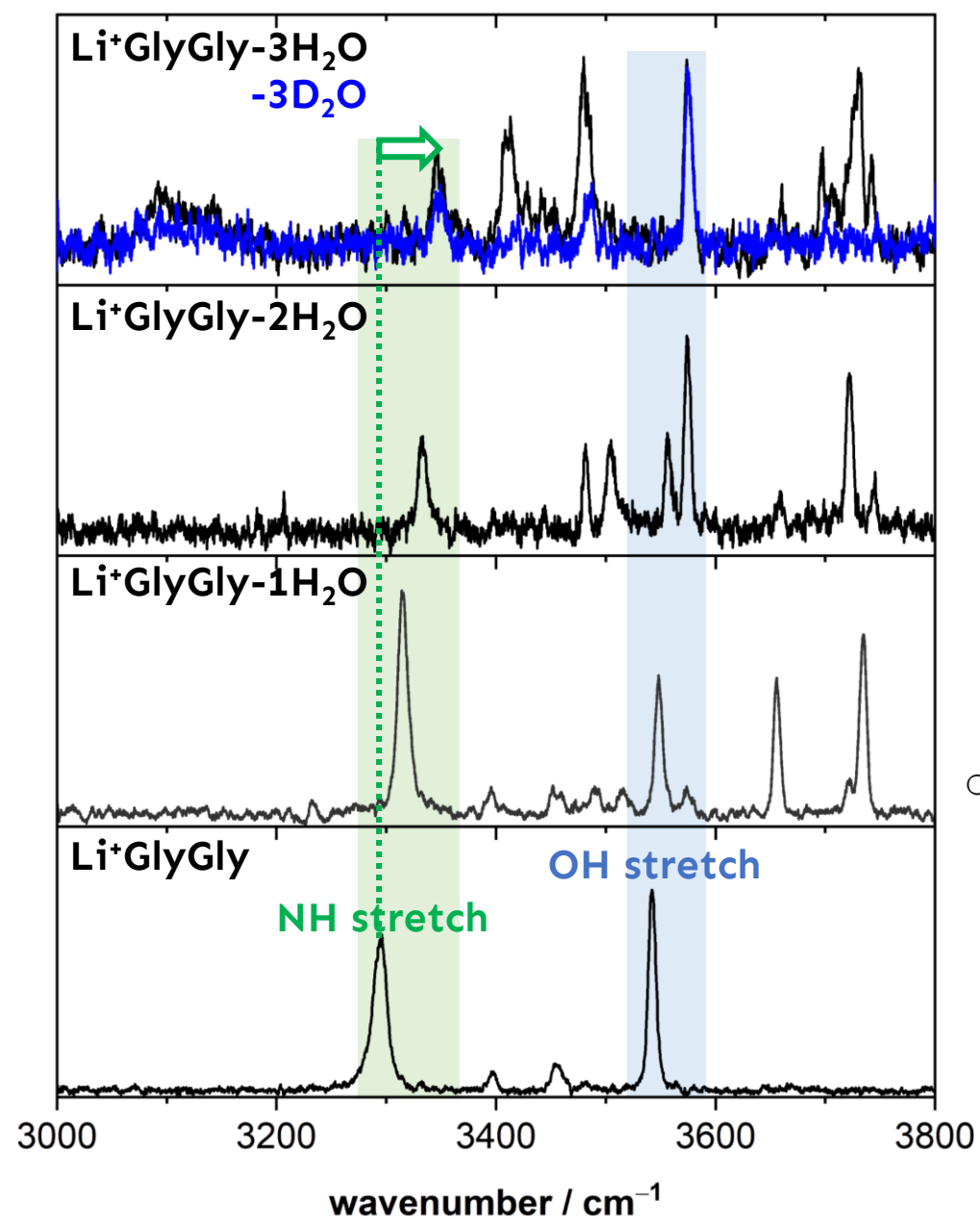
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



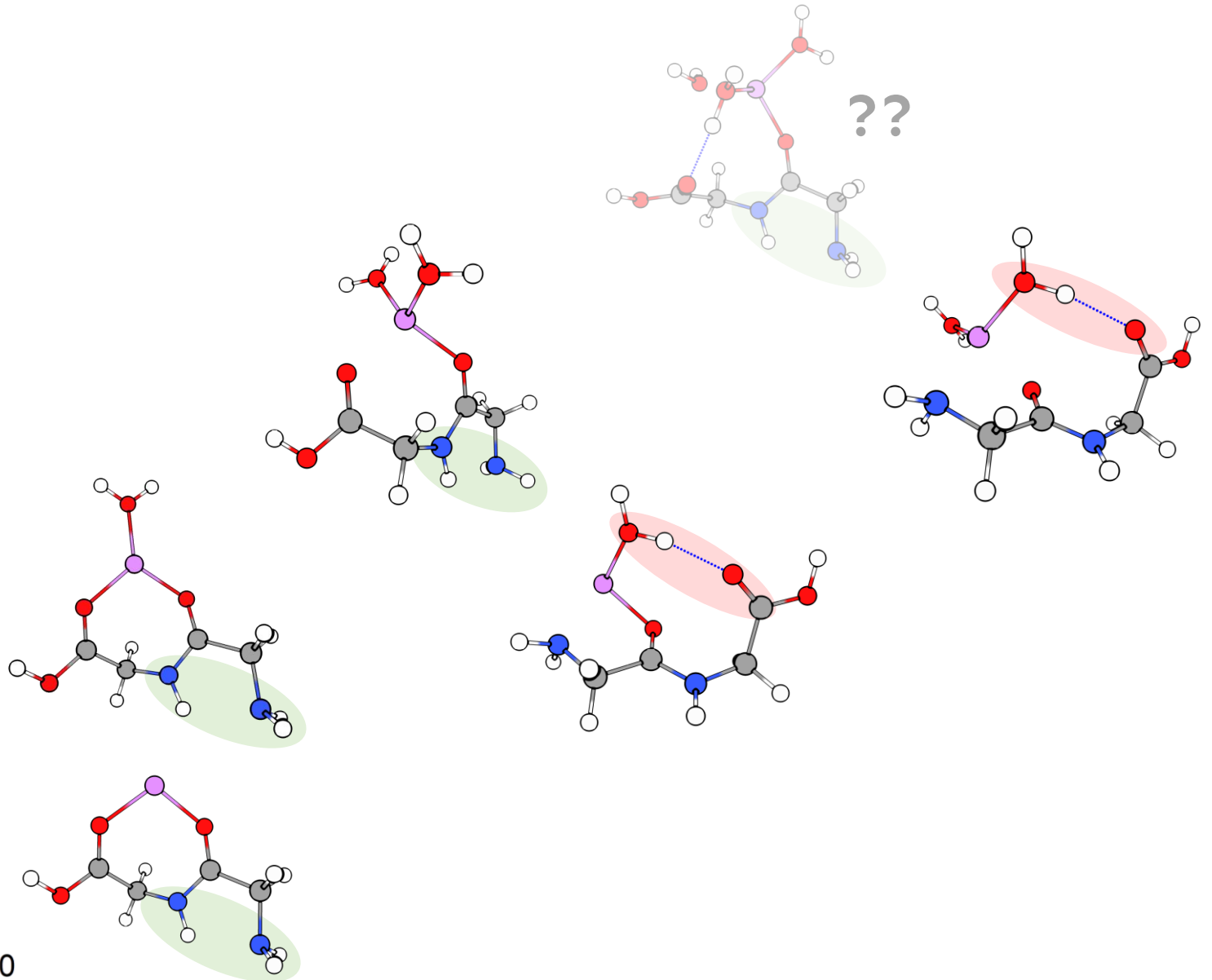
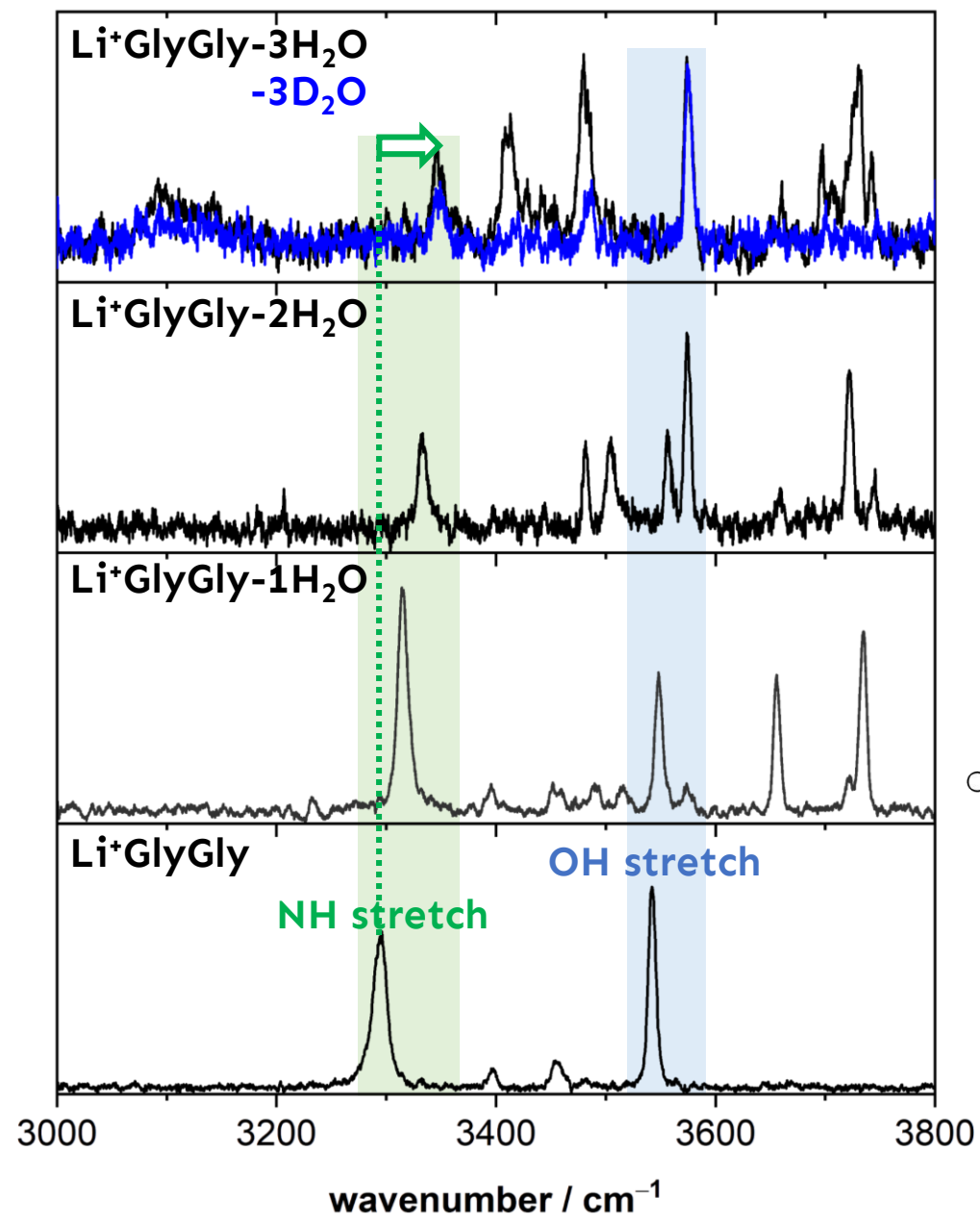
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



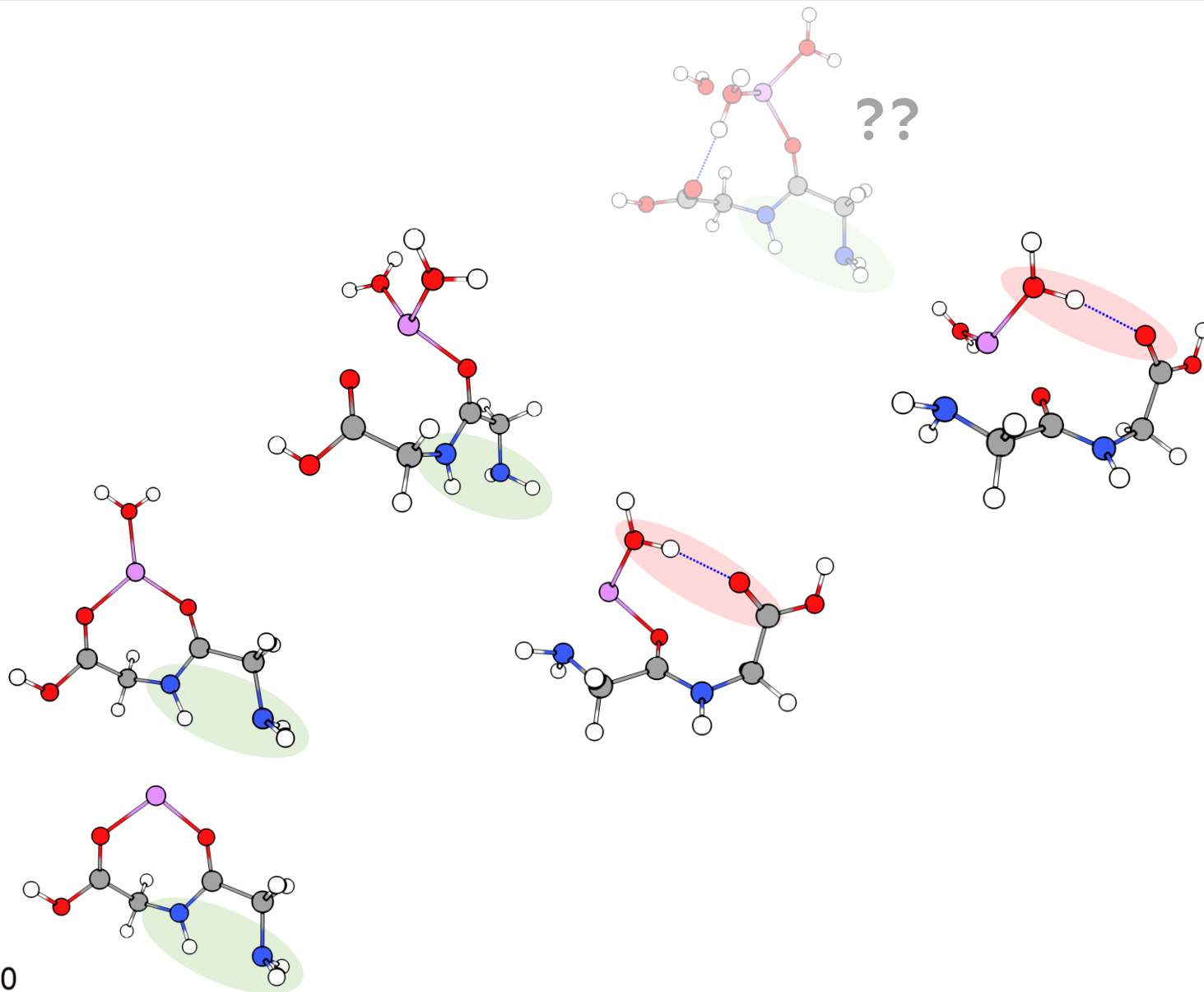
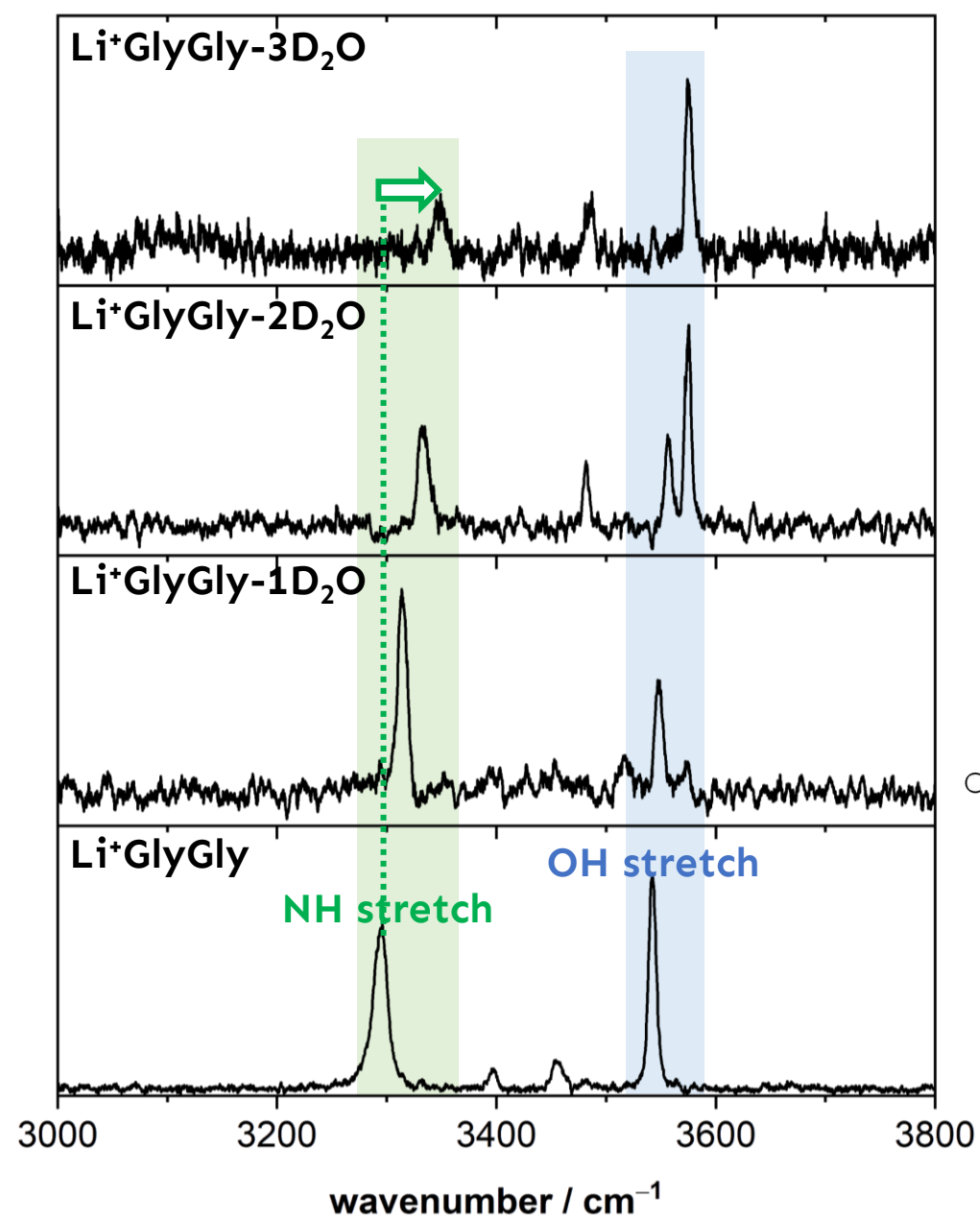
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



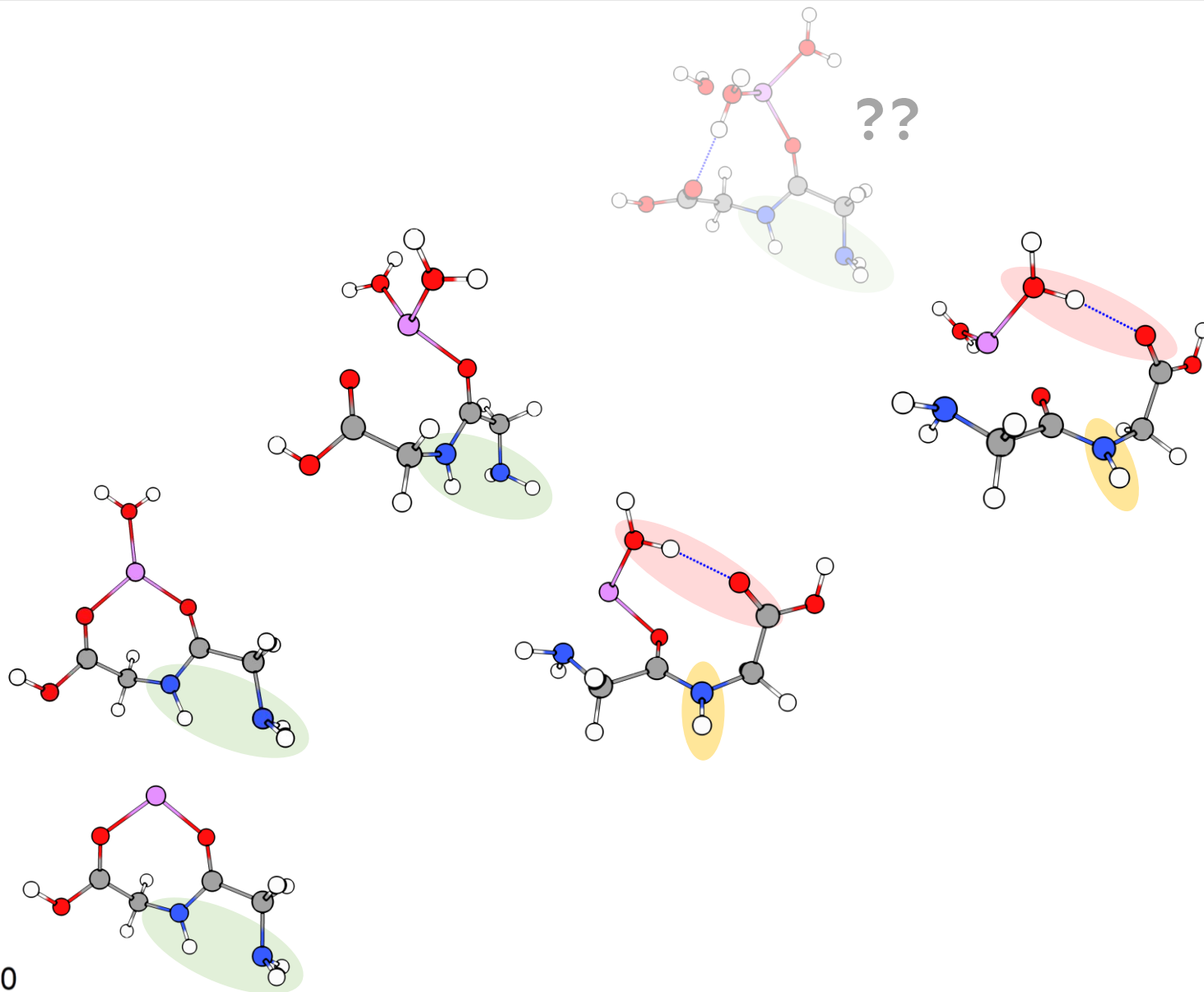
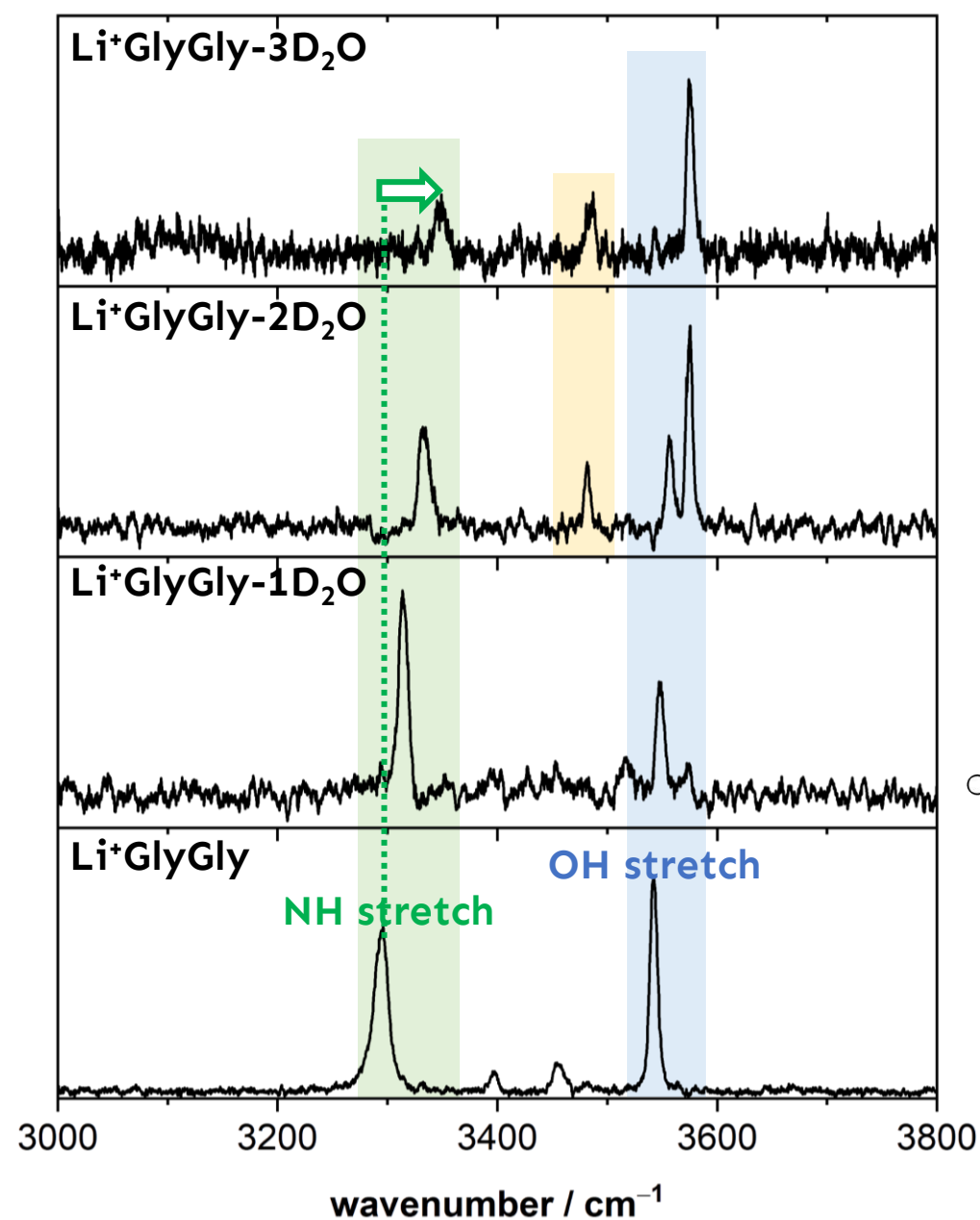
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION



# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION

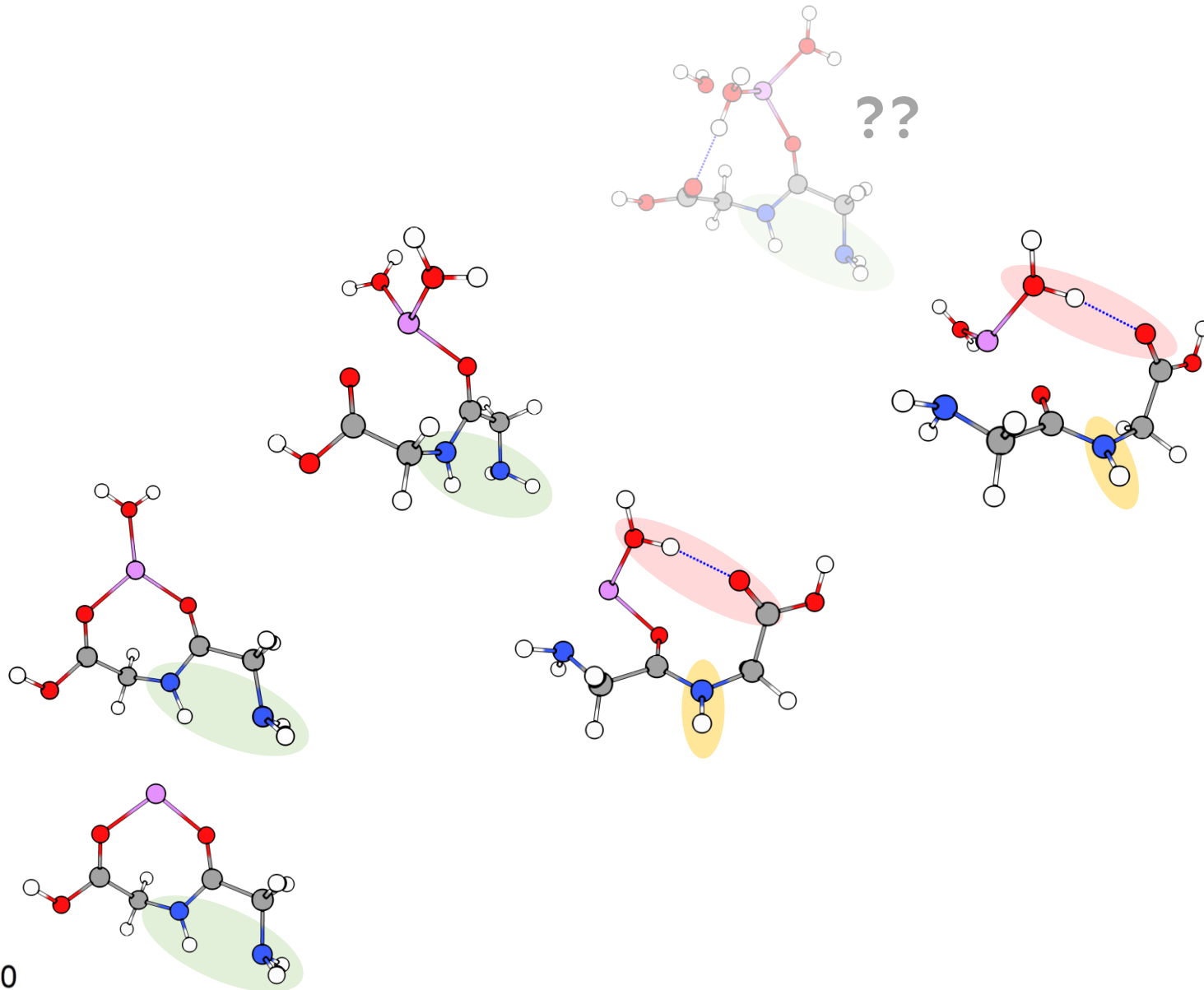
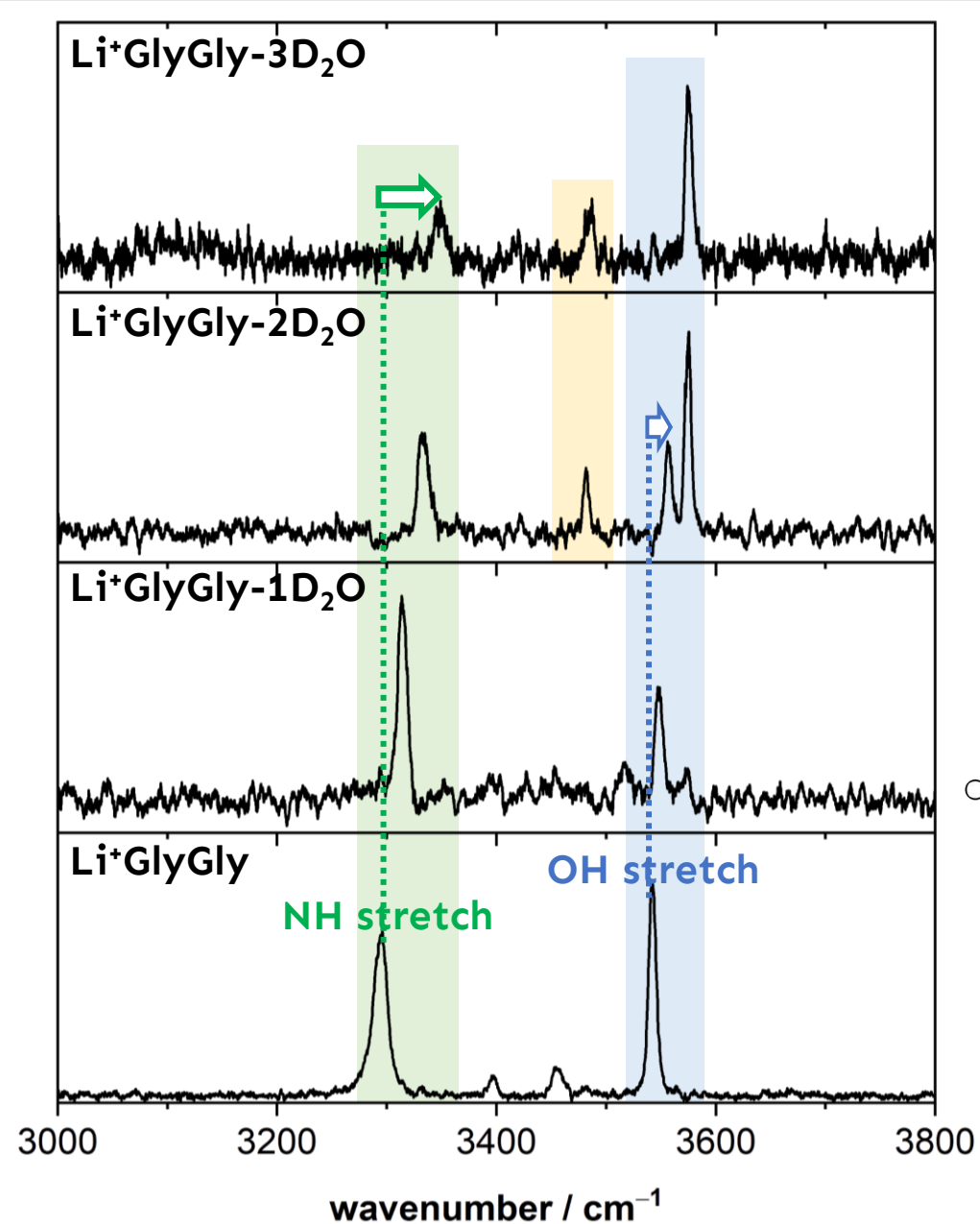


# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION

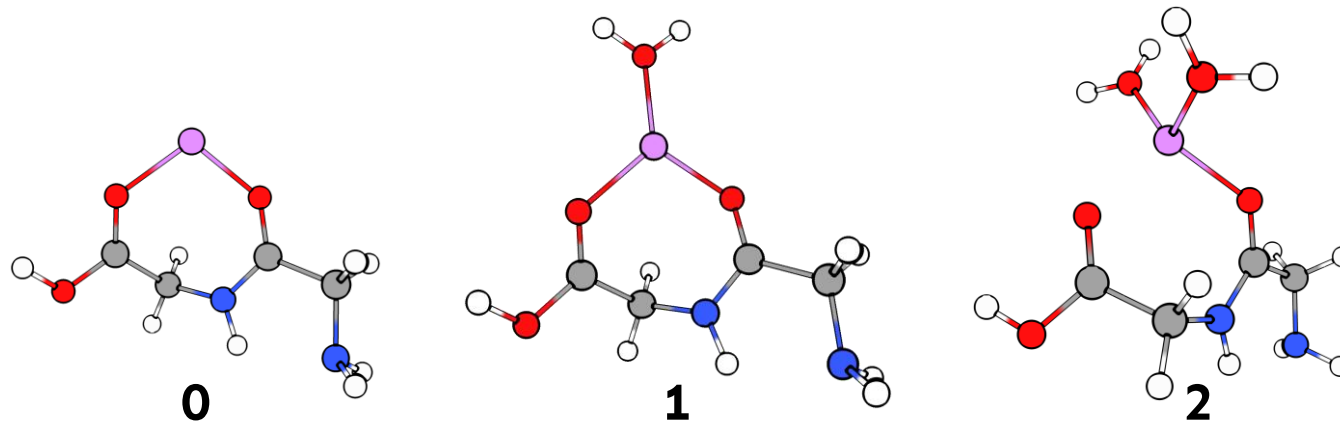
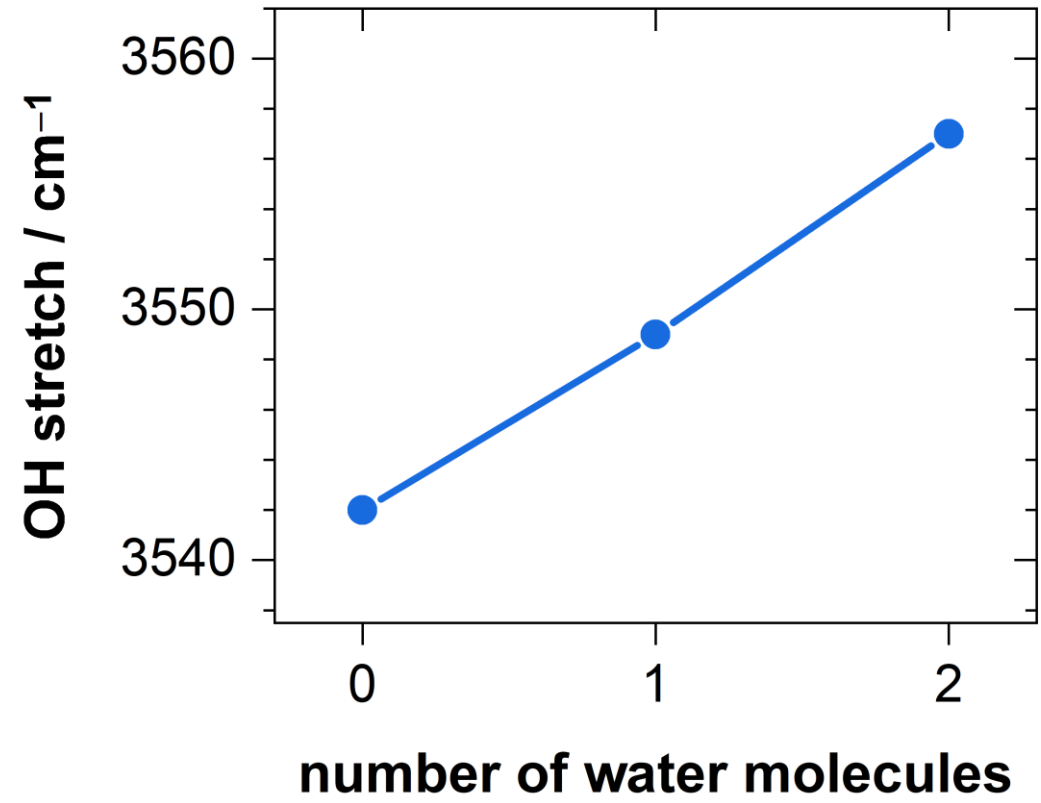


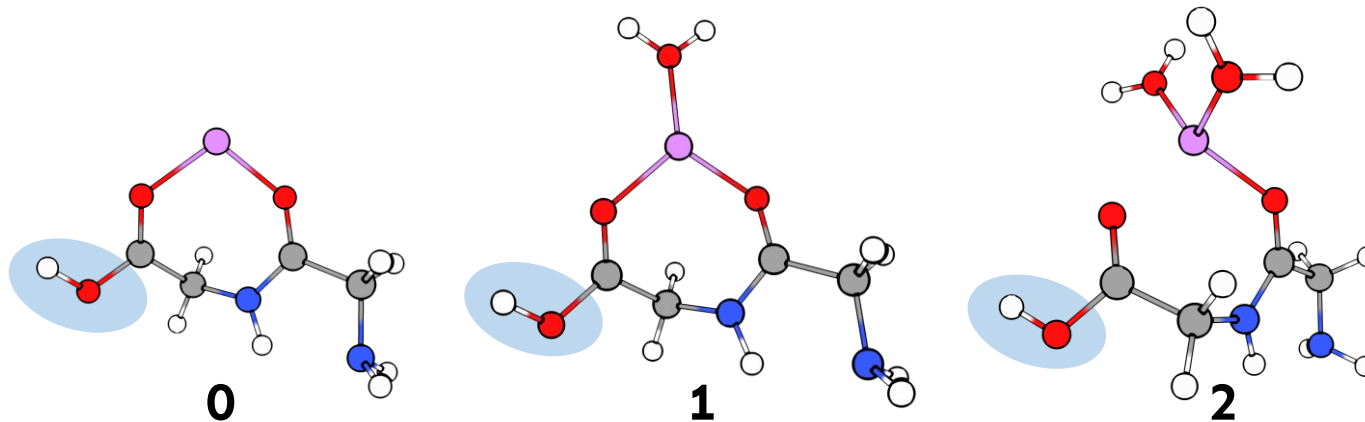
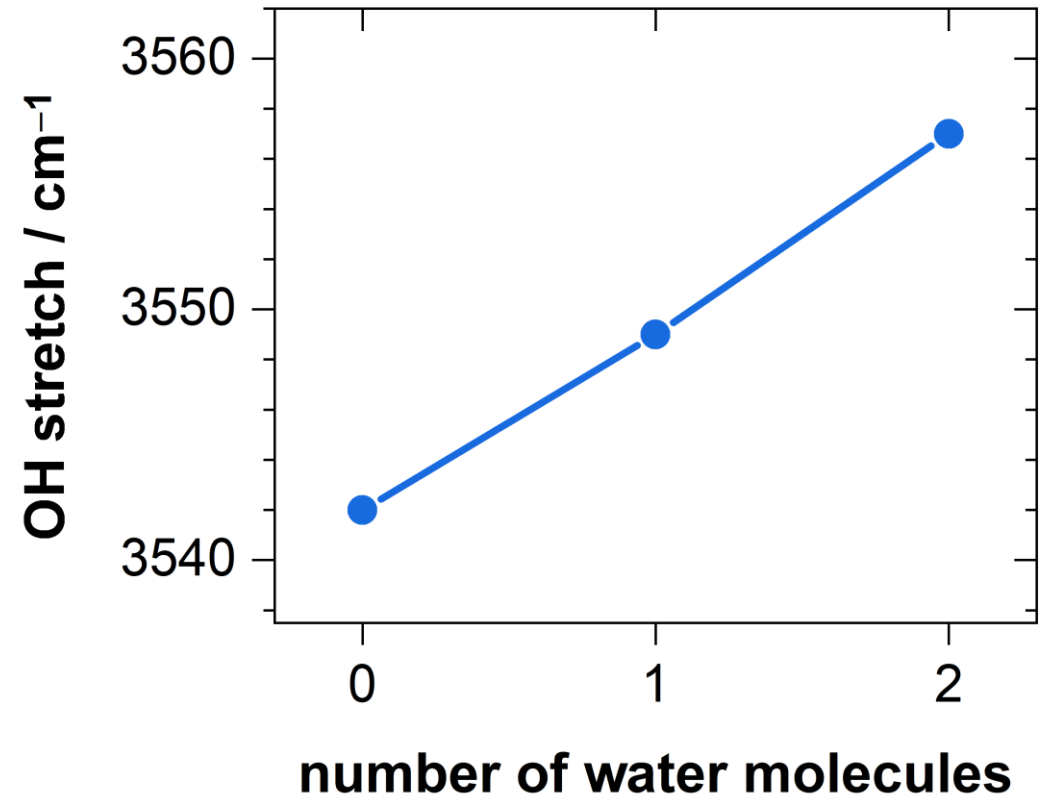


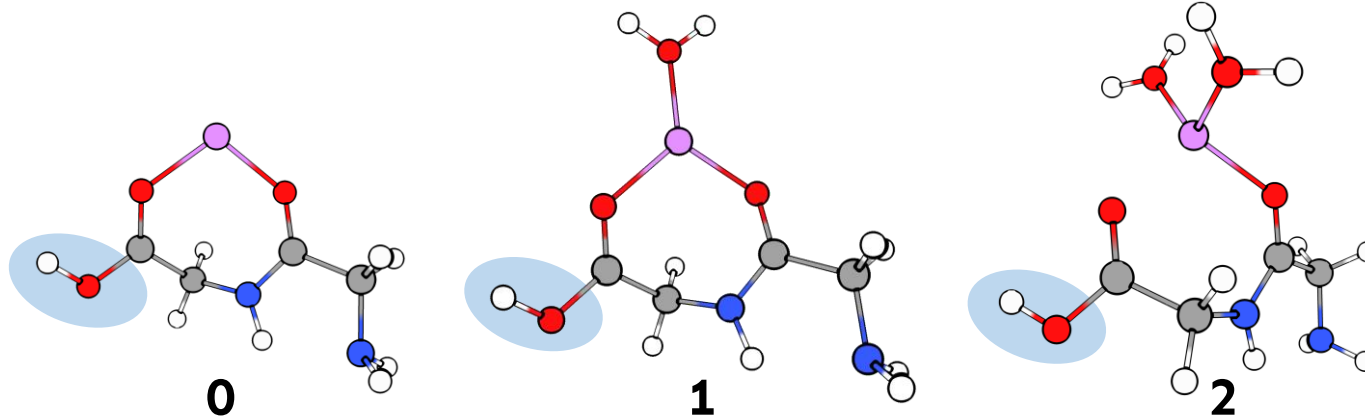
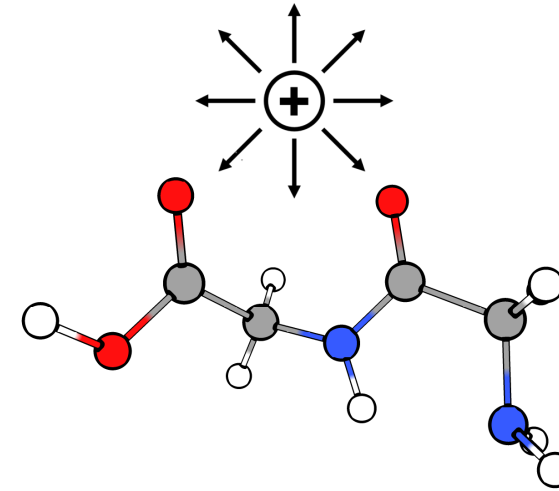
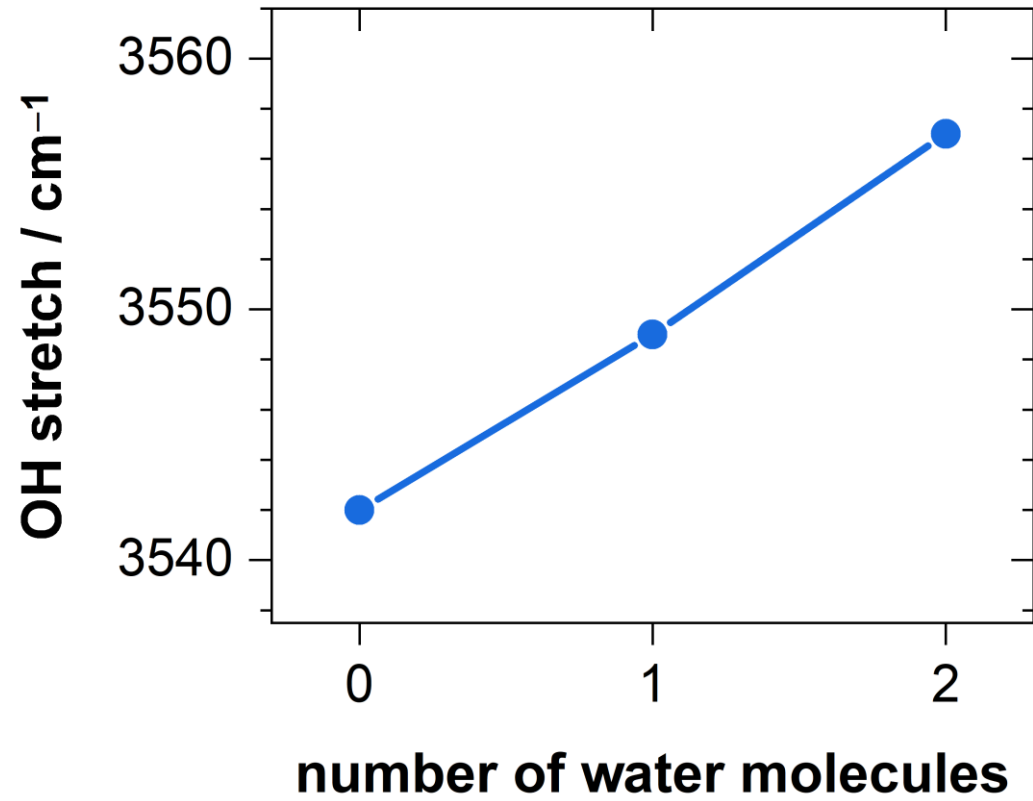
# CHANGES IN STRUCTURE OF $\text{Li}^+\text{GlyGly}$ UPON SOLVATION

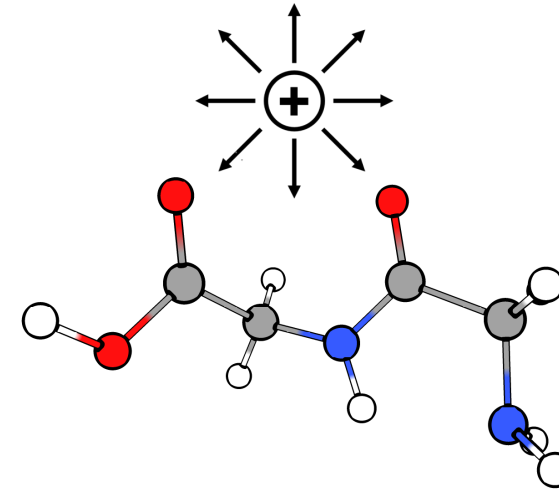
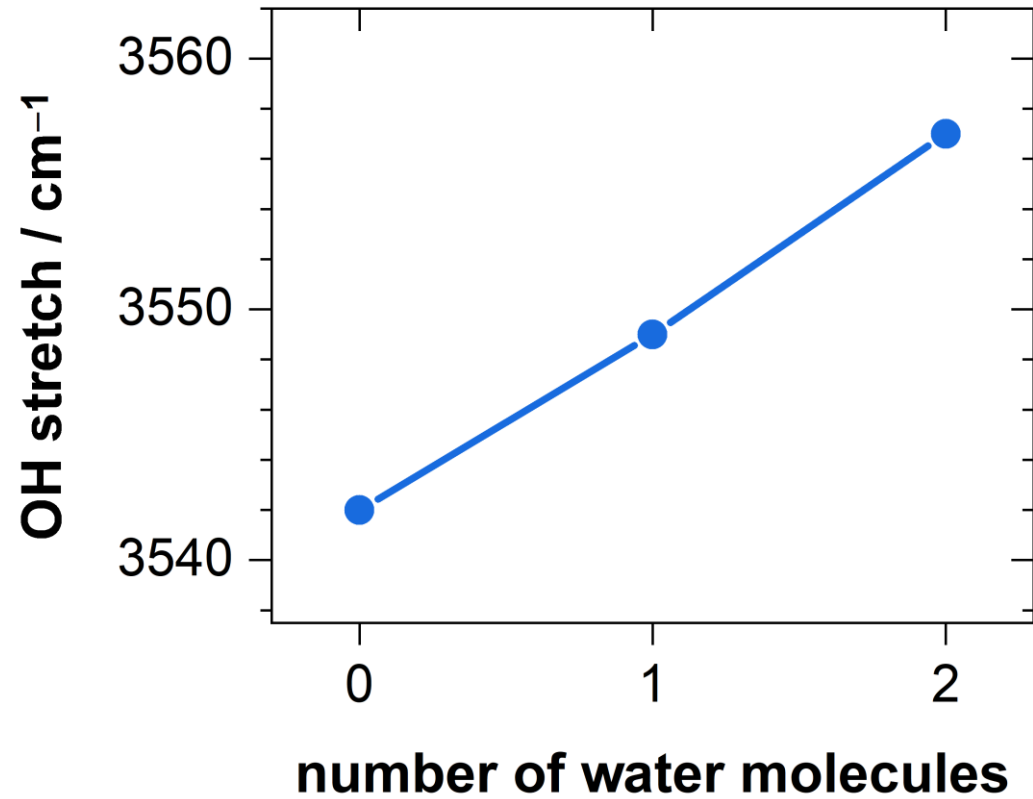






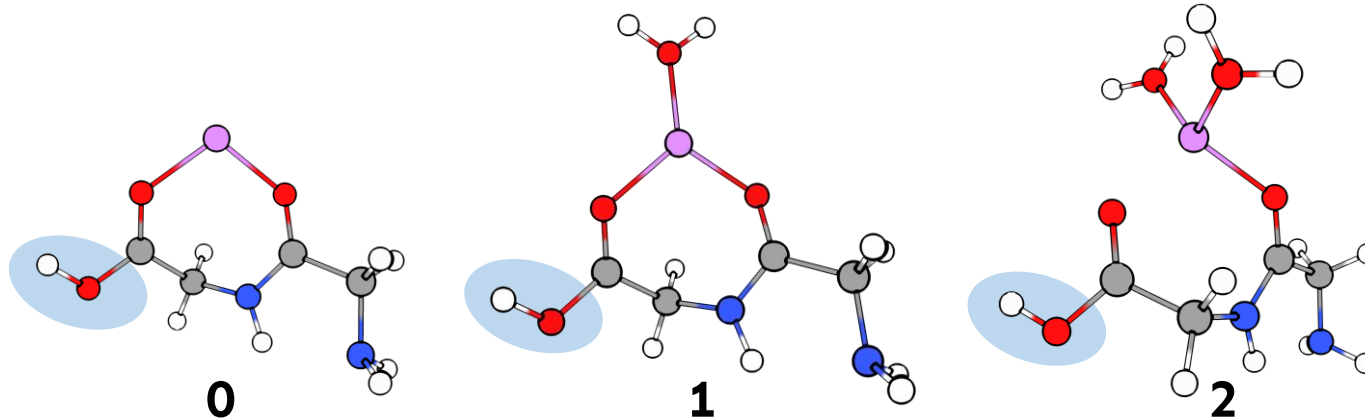


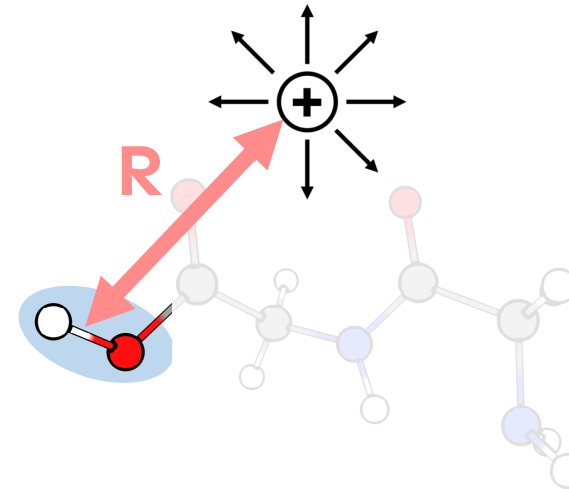
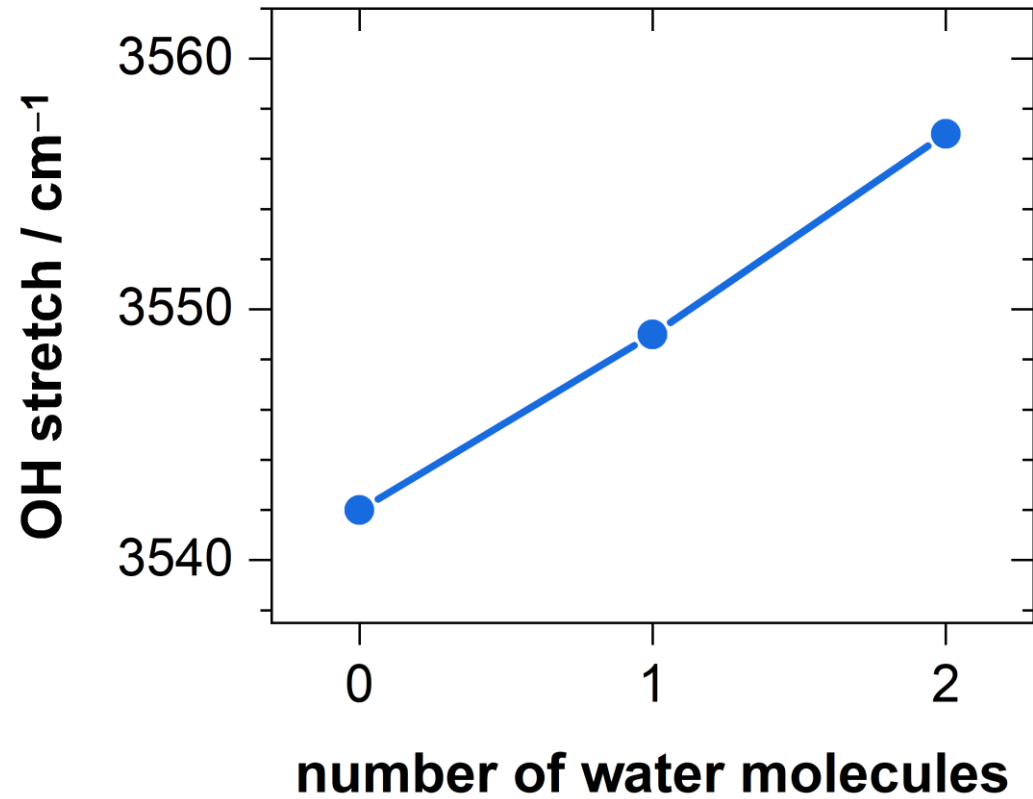




Electric field  
point charge

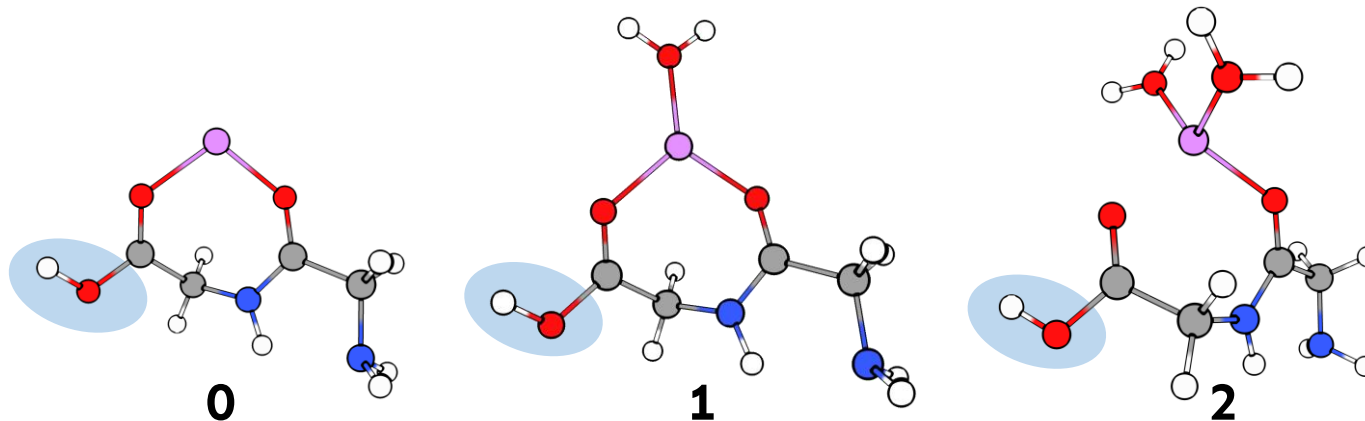
$$\sim \left( \frac{1}{R} \right)^2$$

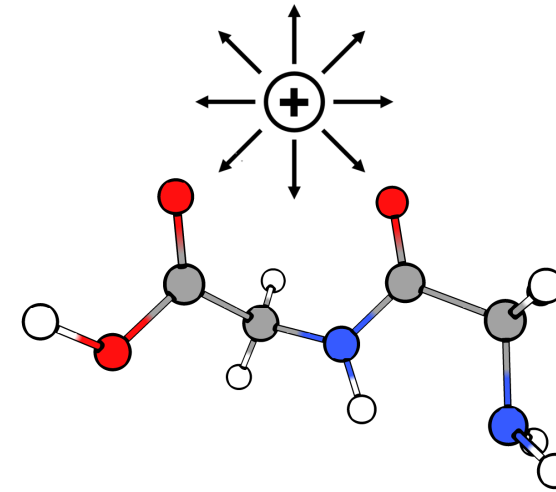
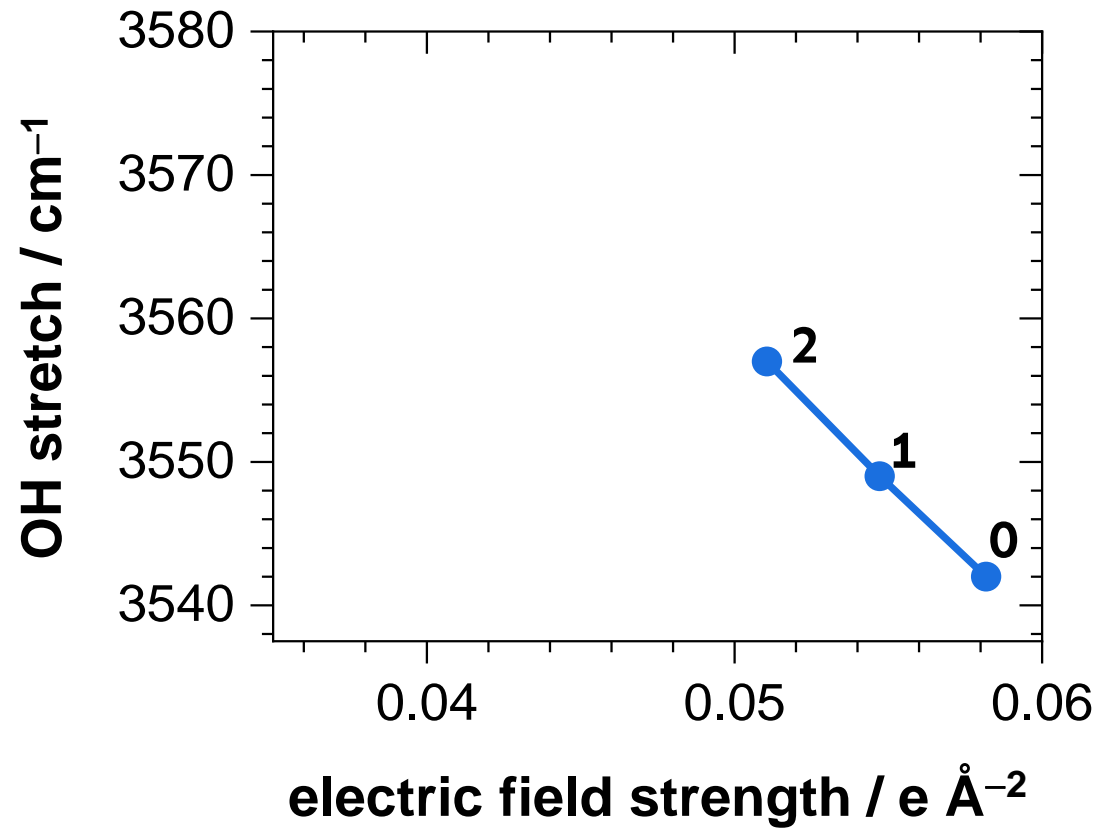




Electric field  
point charge

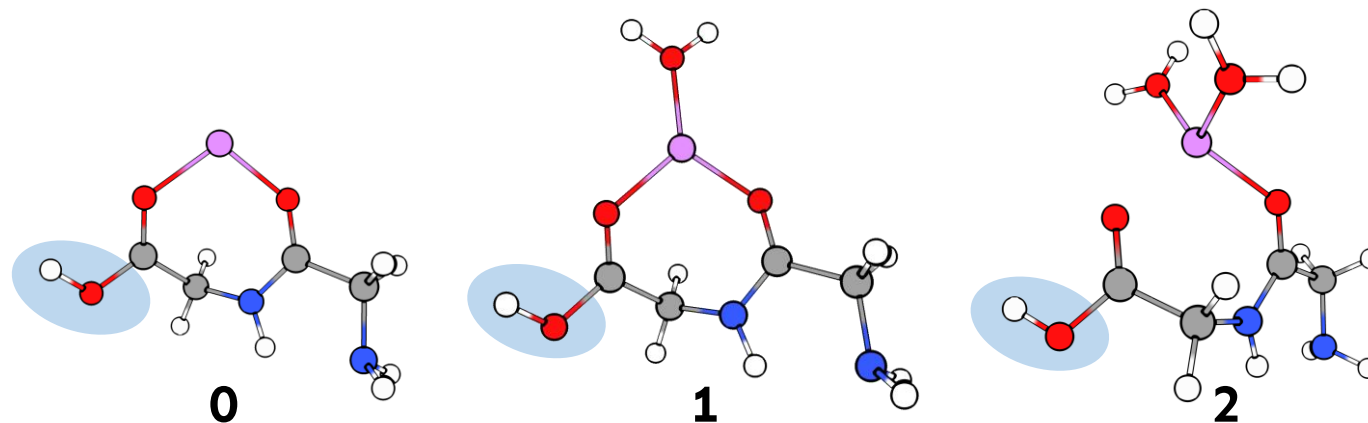
$$\sim \left( \frac{1}{R} \right)^2$$

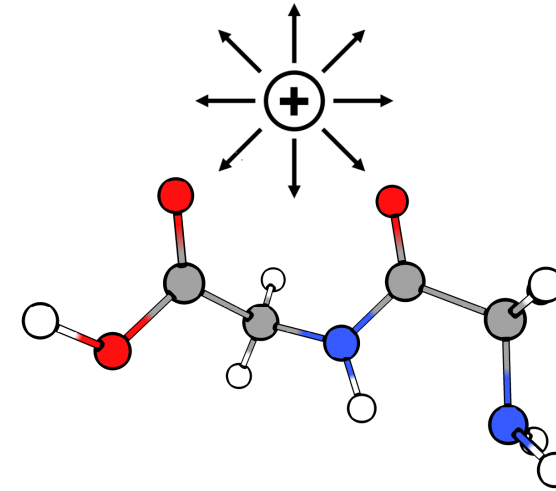
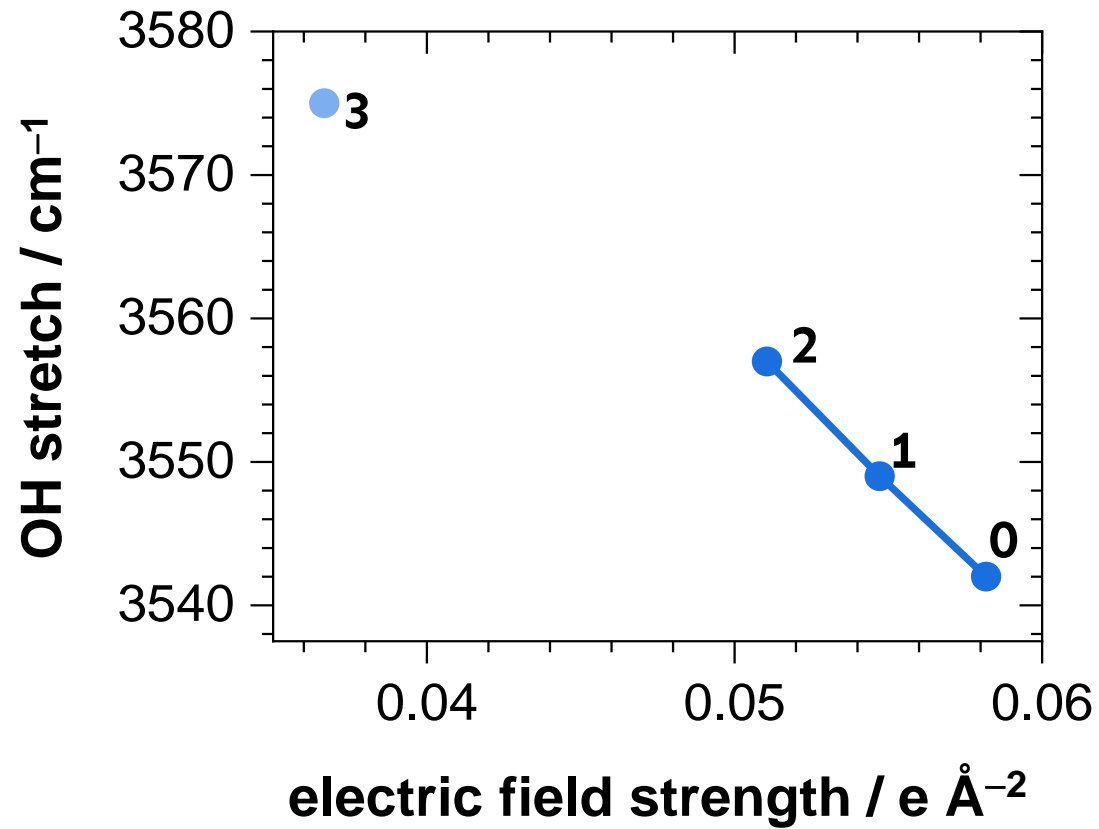




Electric field  
point charge

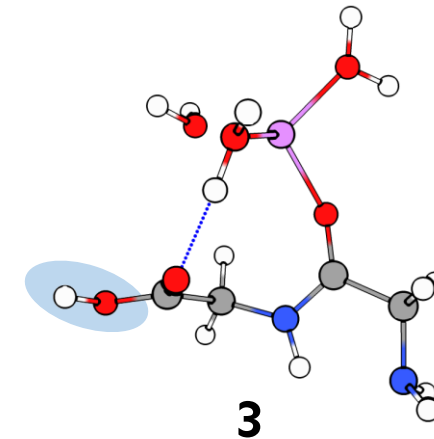
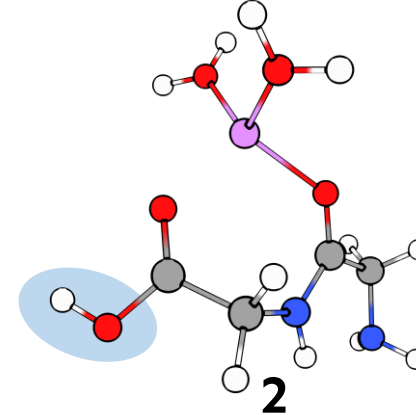
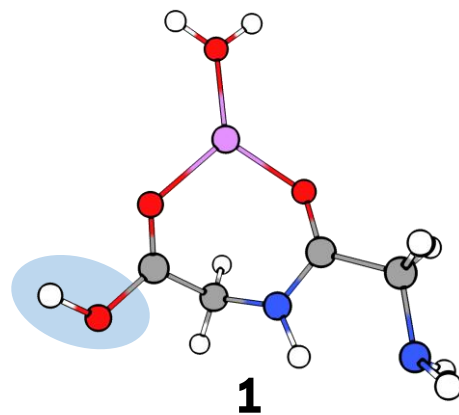
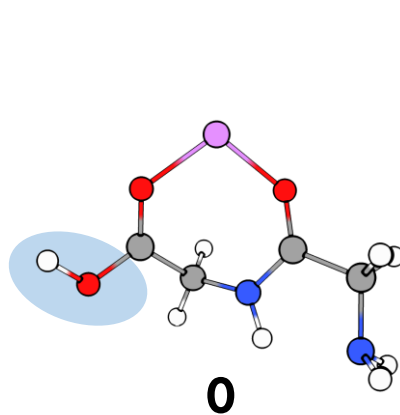
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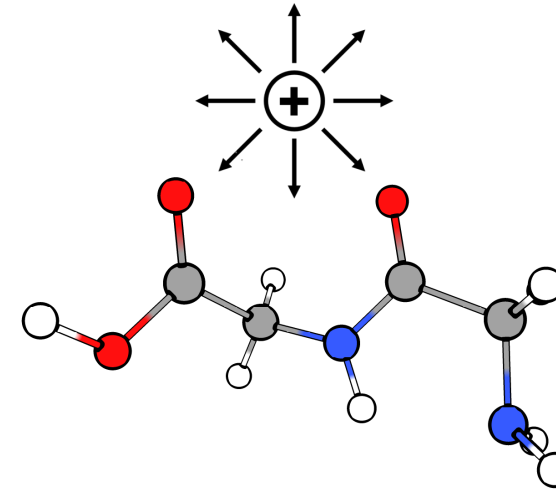
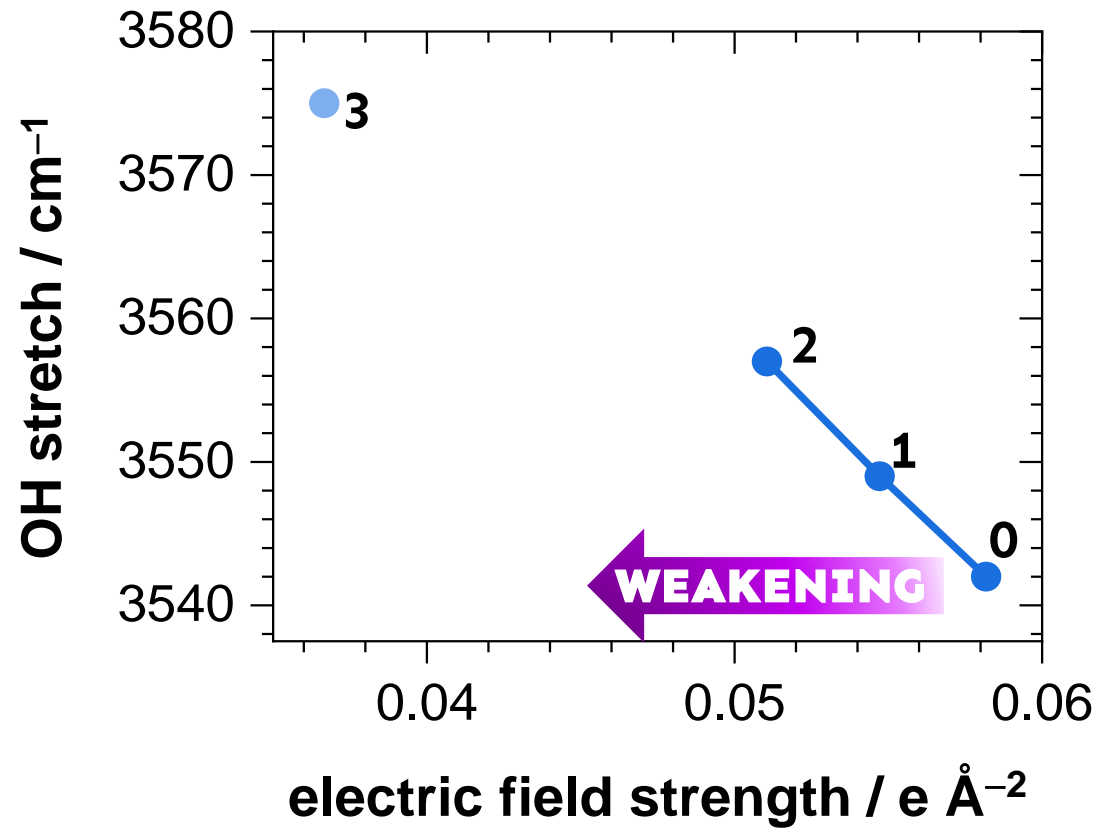




Electric field  
point charge

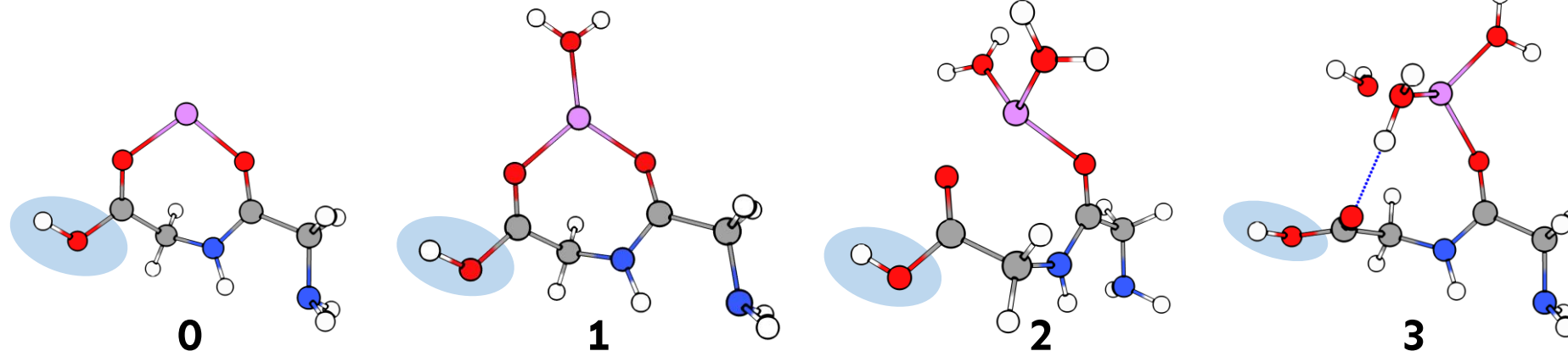
$$\sim \left( \frac{1}{R} \right)^2$$





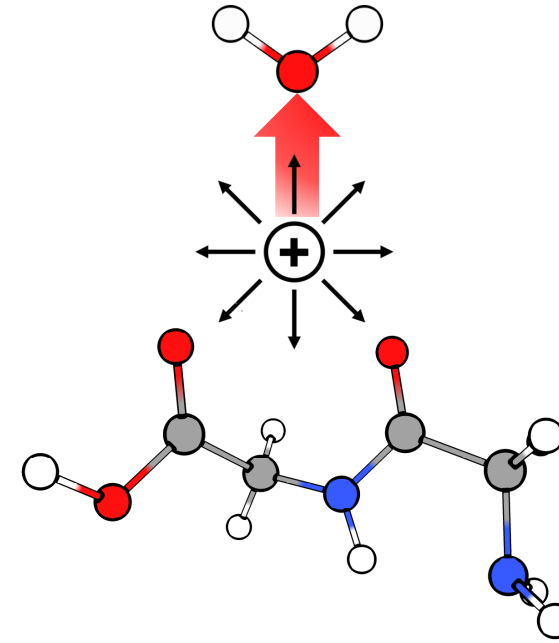
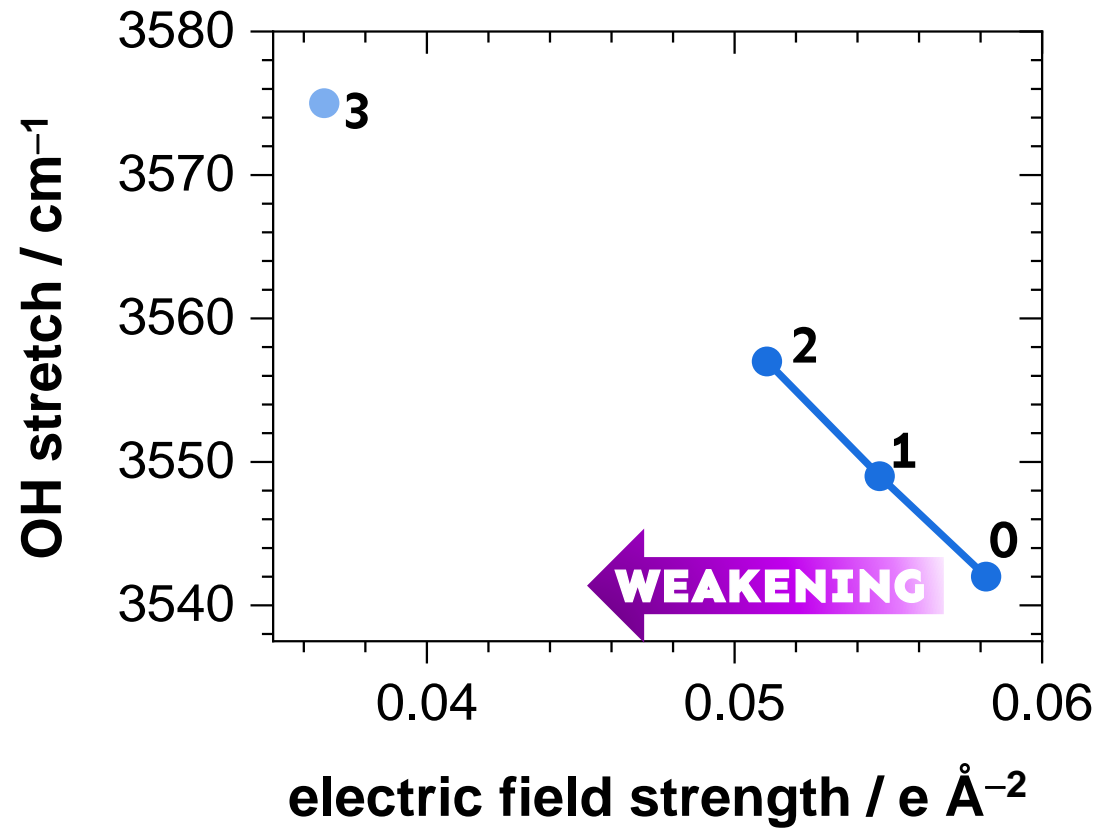
Electric field point charge

$$\sim \left( \frac{1}{R} \right)^2$$



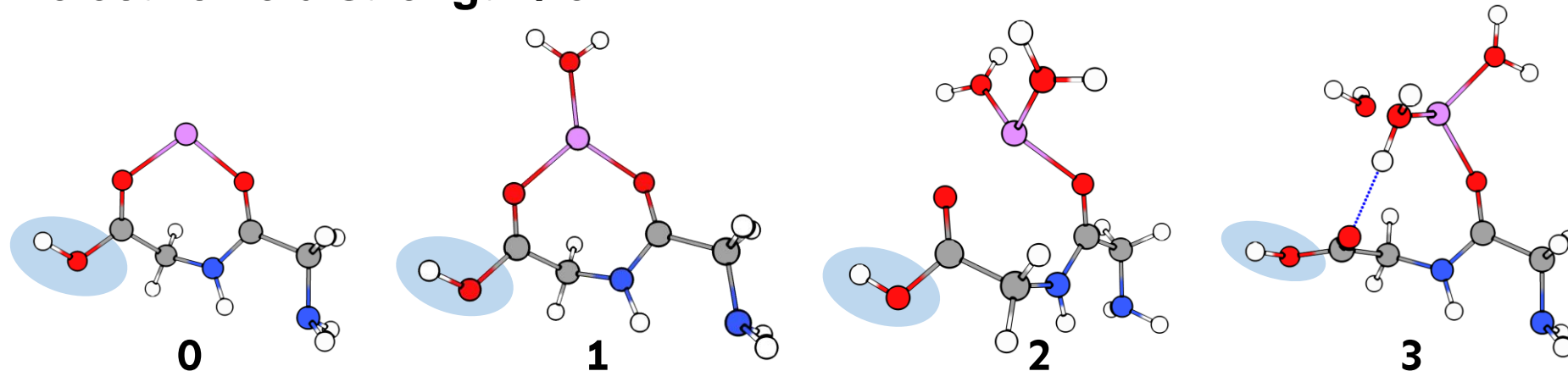


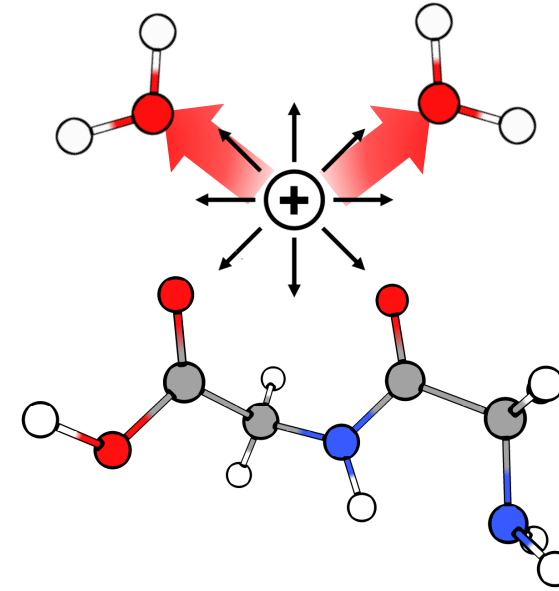
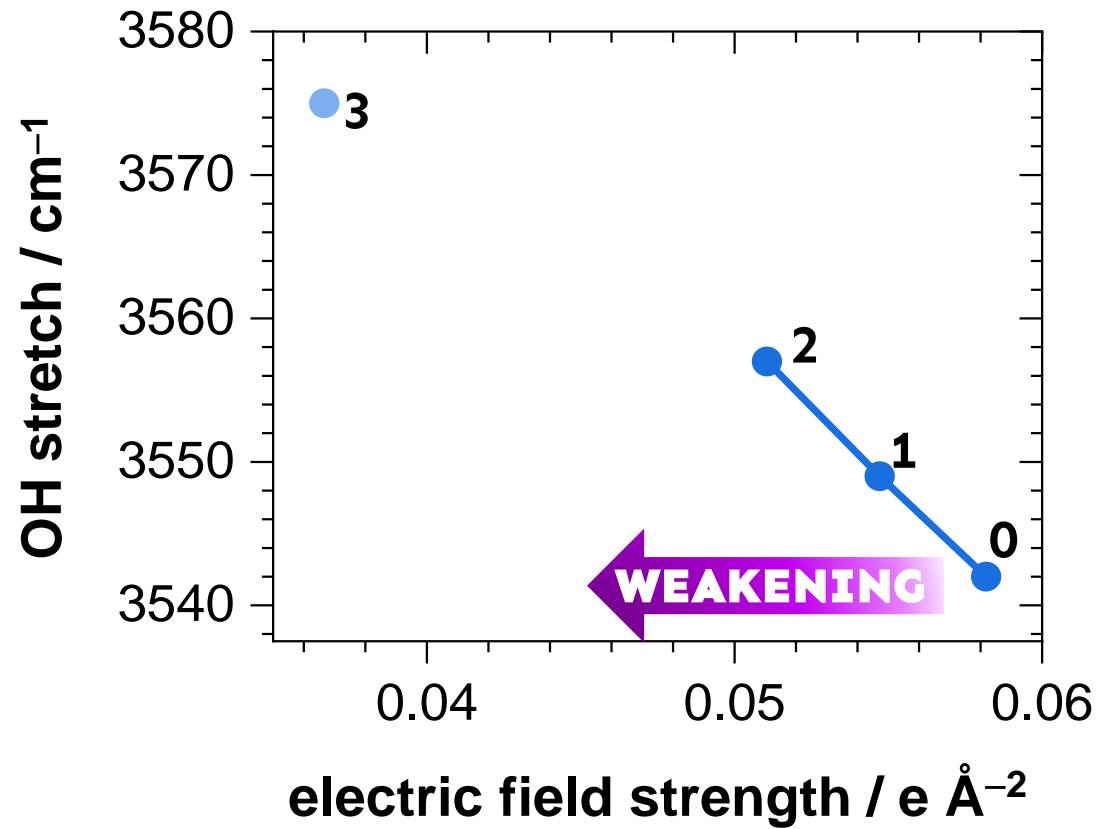
# E-FIELD IMPACT ON VIBRATIONS AND STRUCTURE



Electric field  
point charge

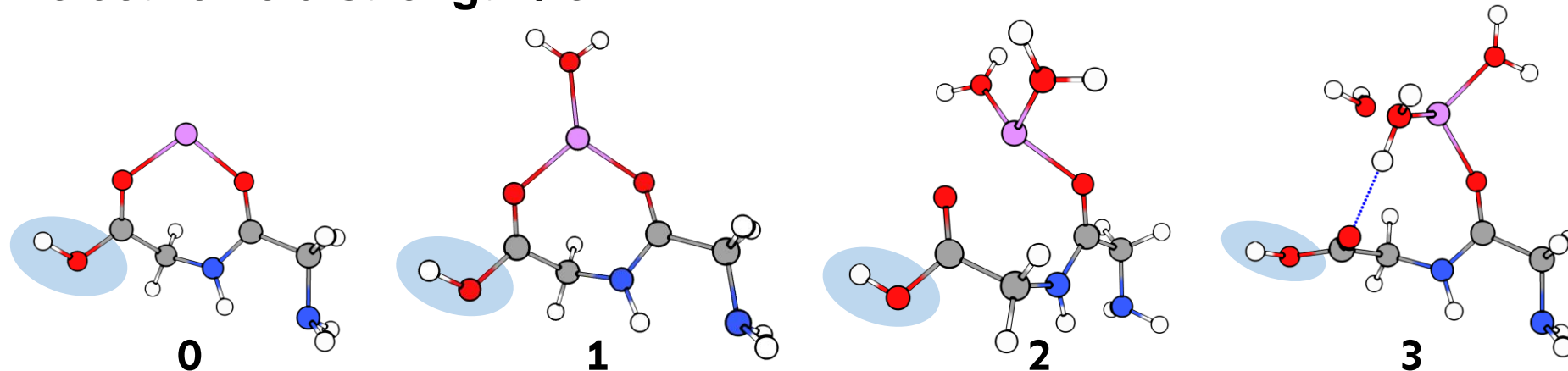
$$\sim \left(\frac{1}{R}\right)^2$$

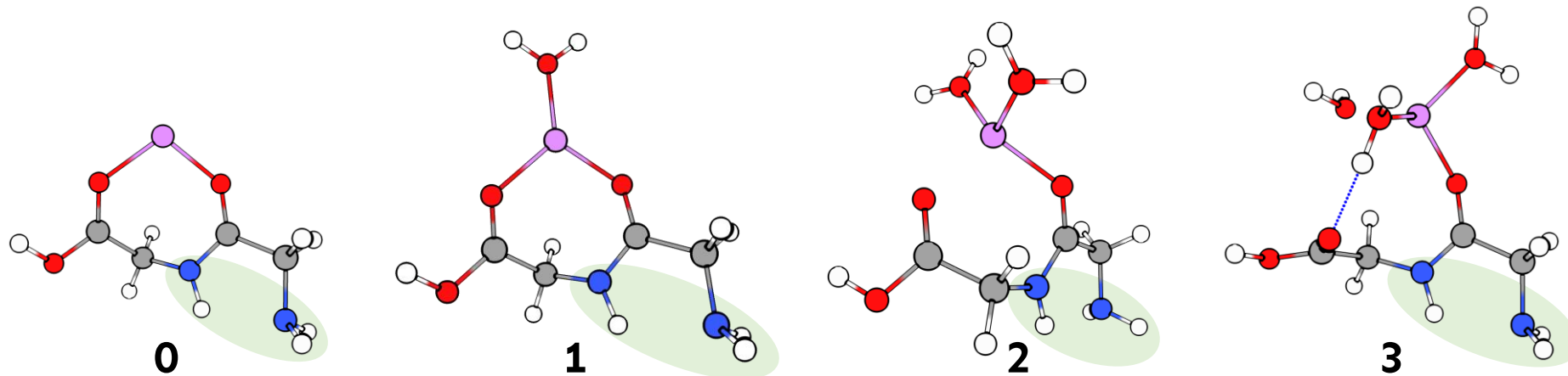




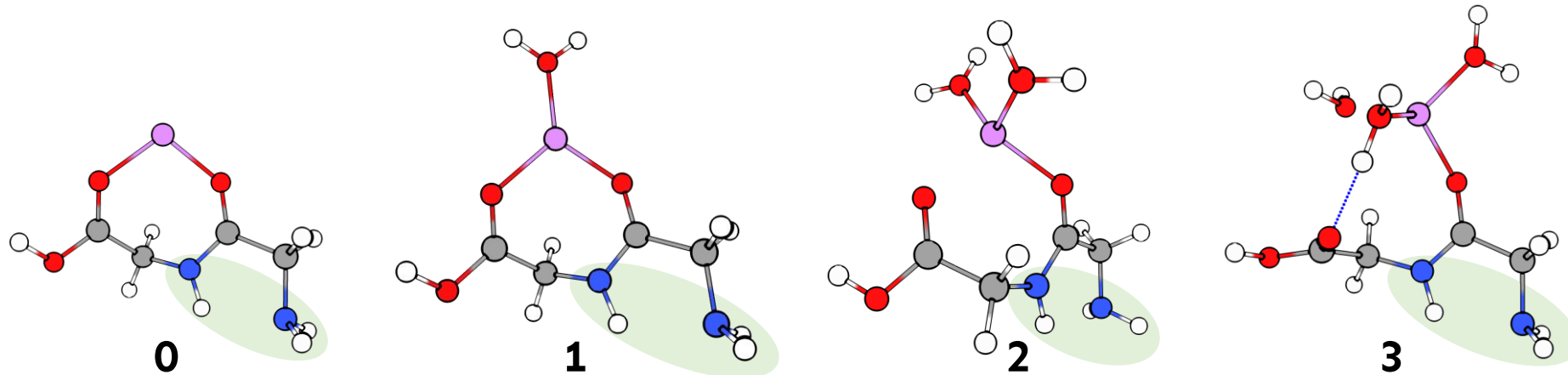
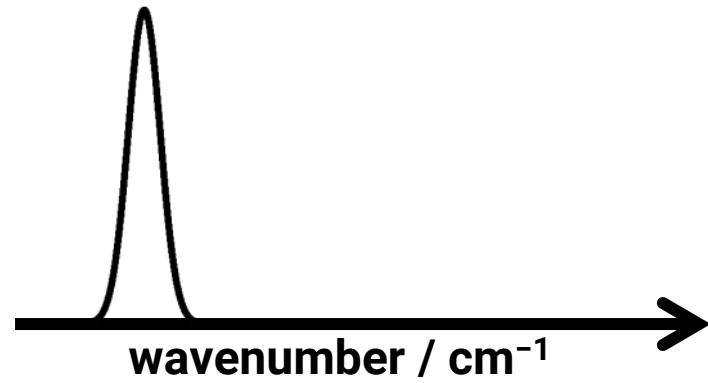
Electric field  
point charge

$$\sim \left( \frac{1}{R} \right)^2$$



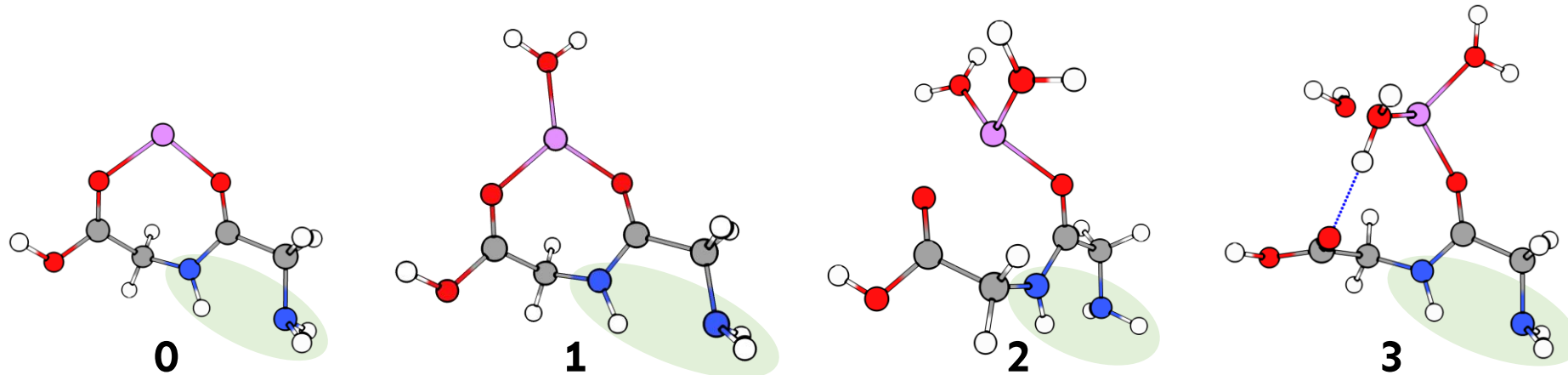
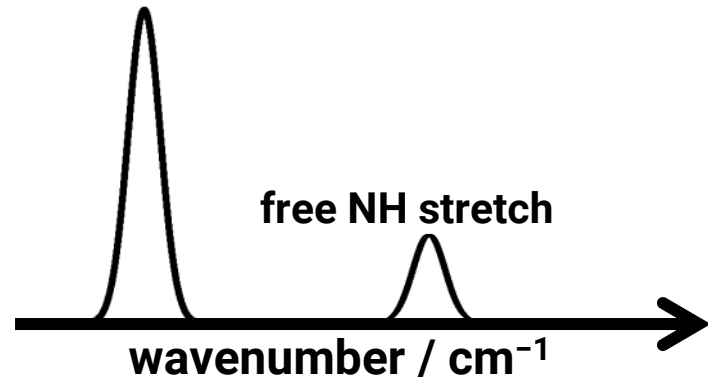


hydrogen bonded  
NH stretch



hydrogen bonded  
NH stretch

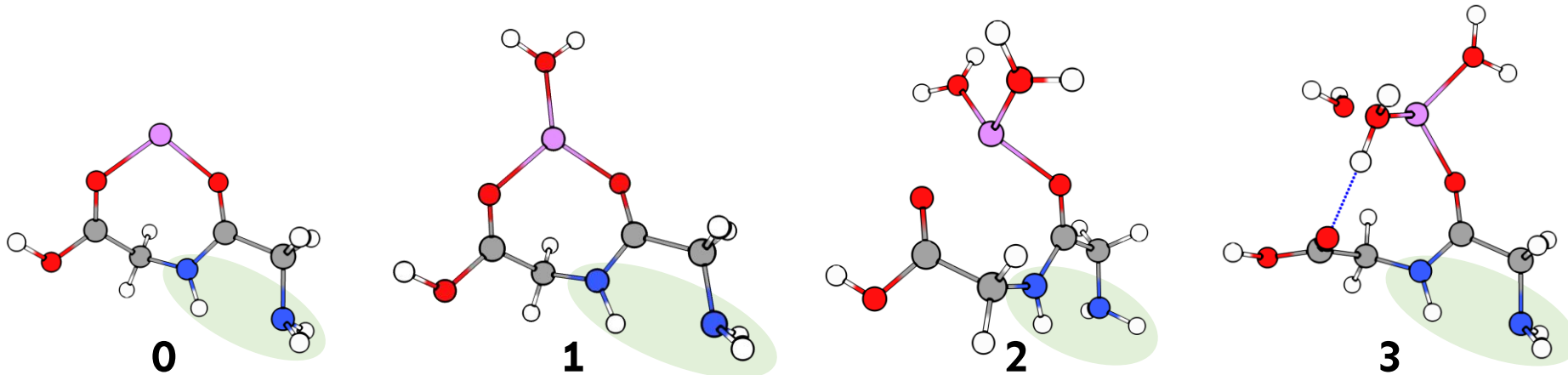
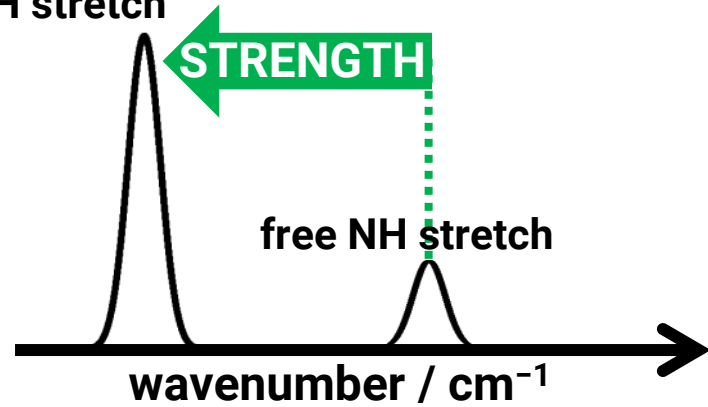
free NH stretch

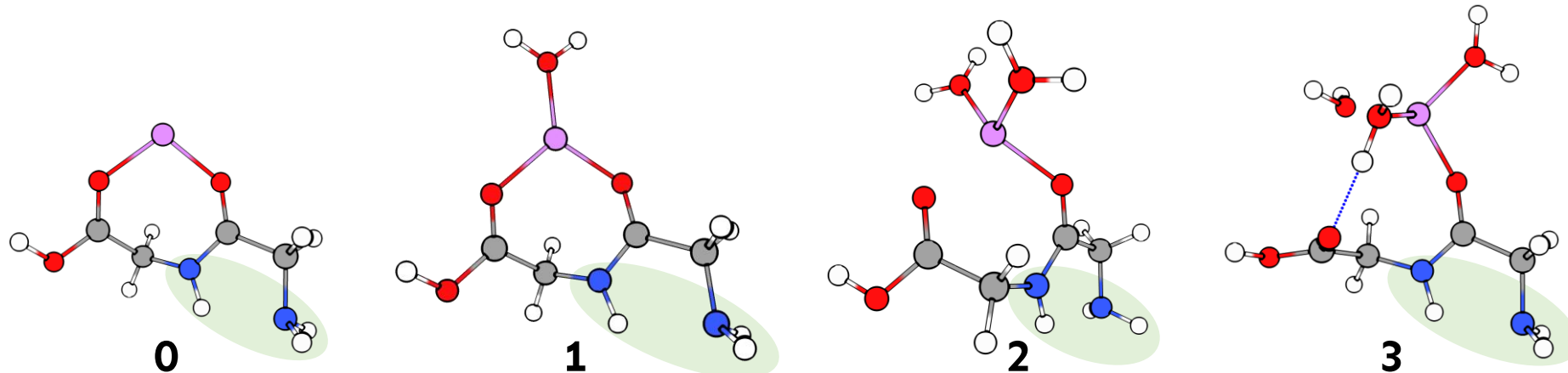
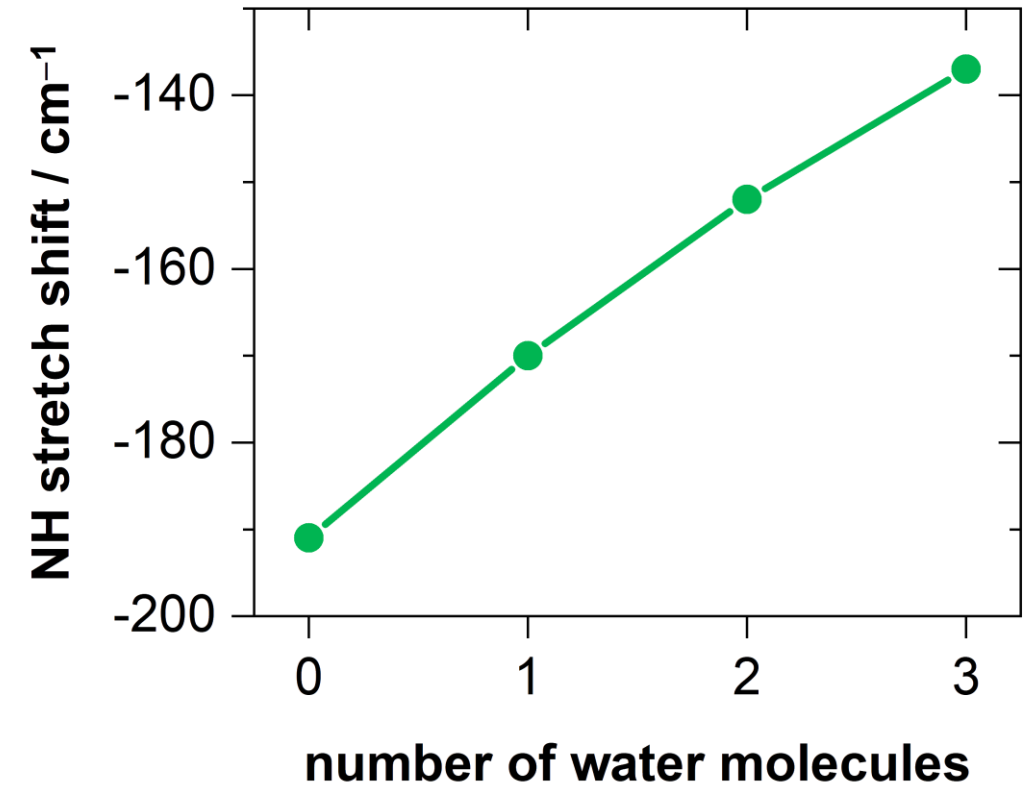
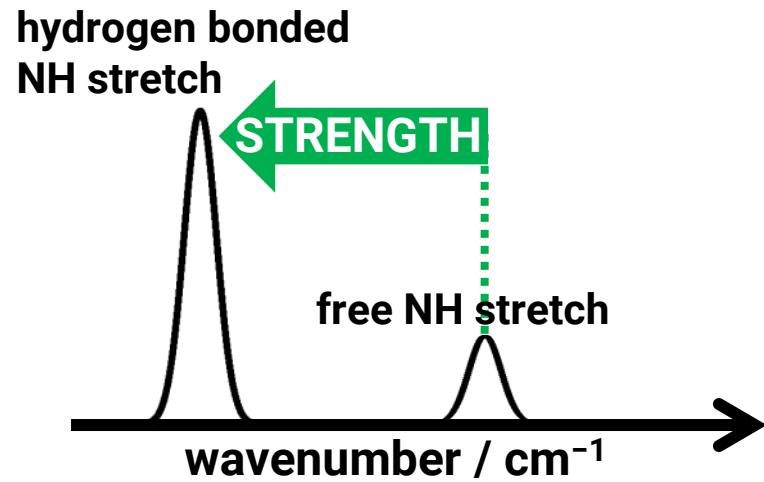


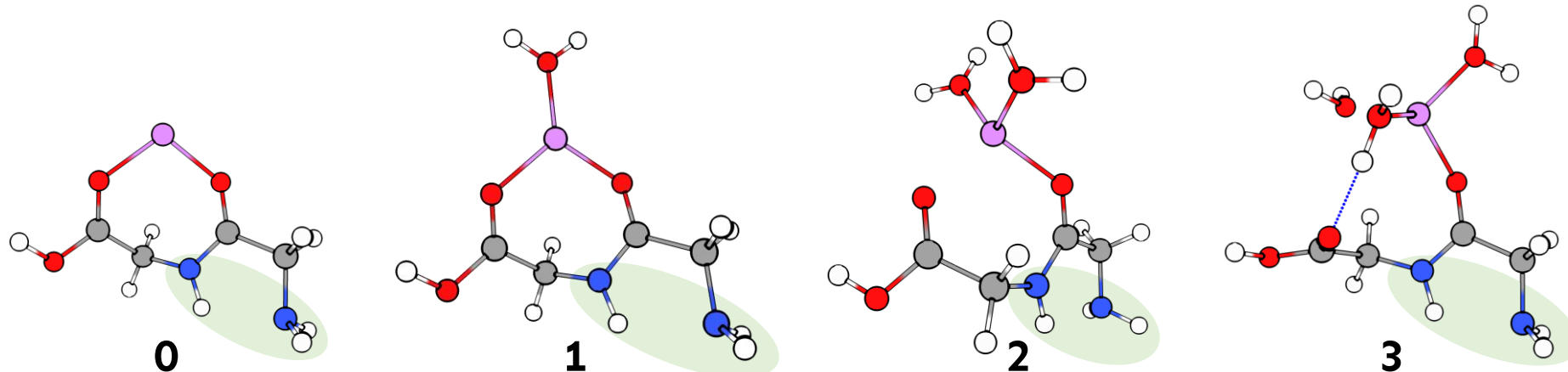
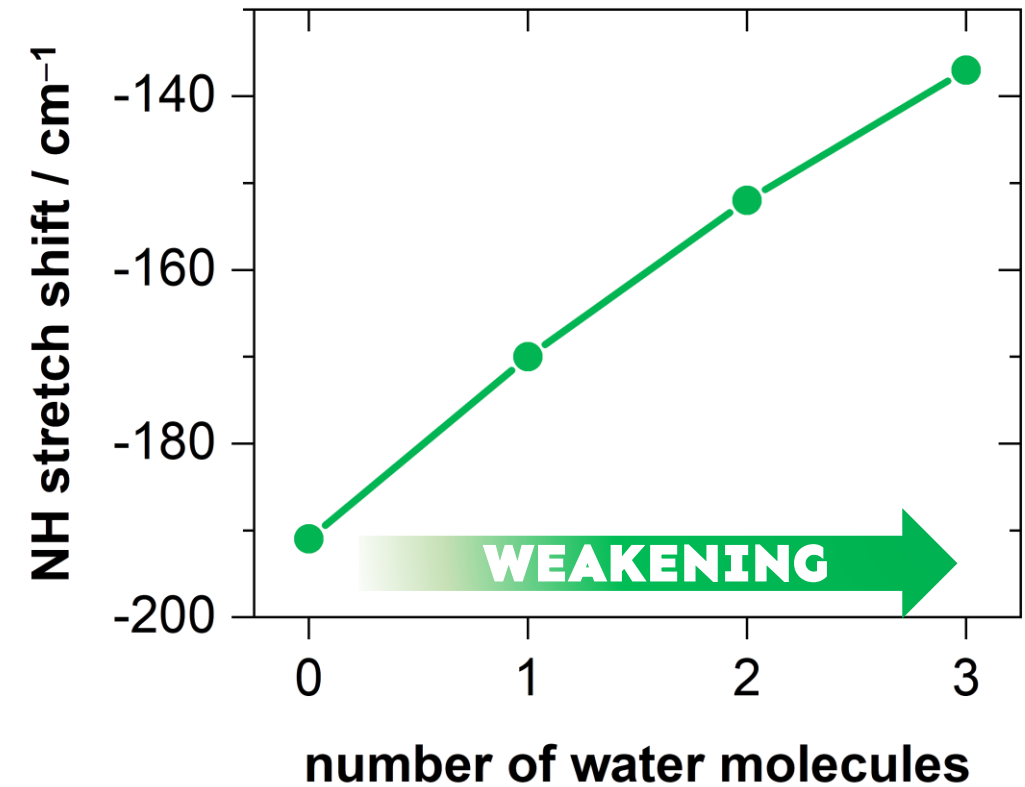
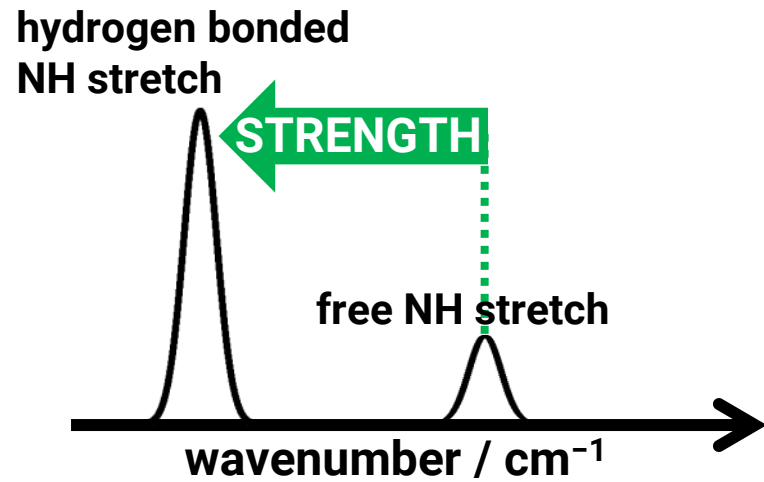
hydrogen bonded  
NH stretch

← STRENGTH

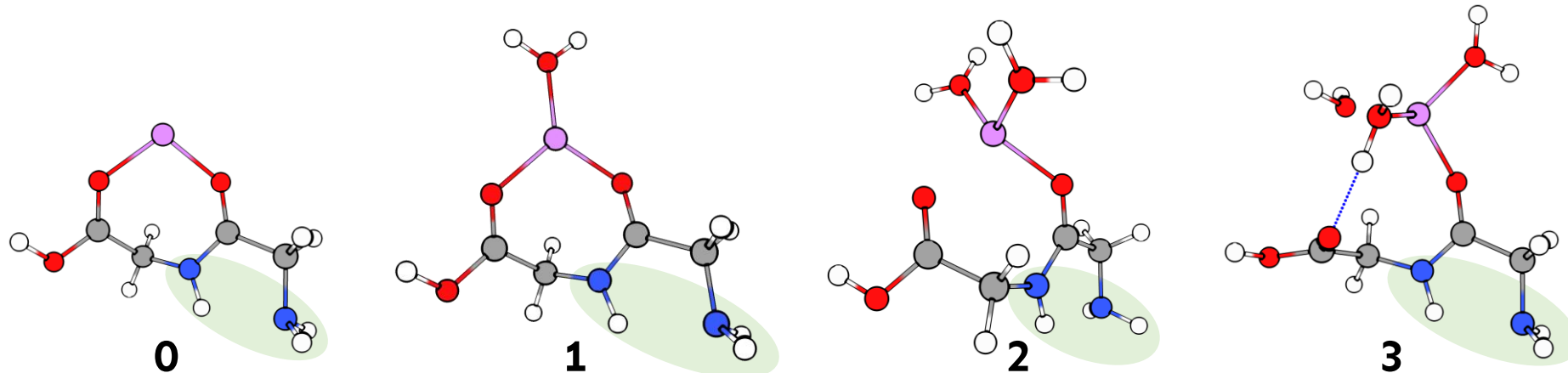
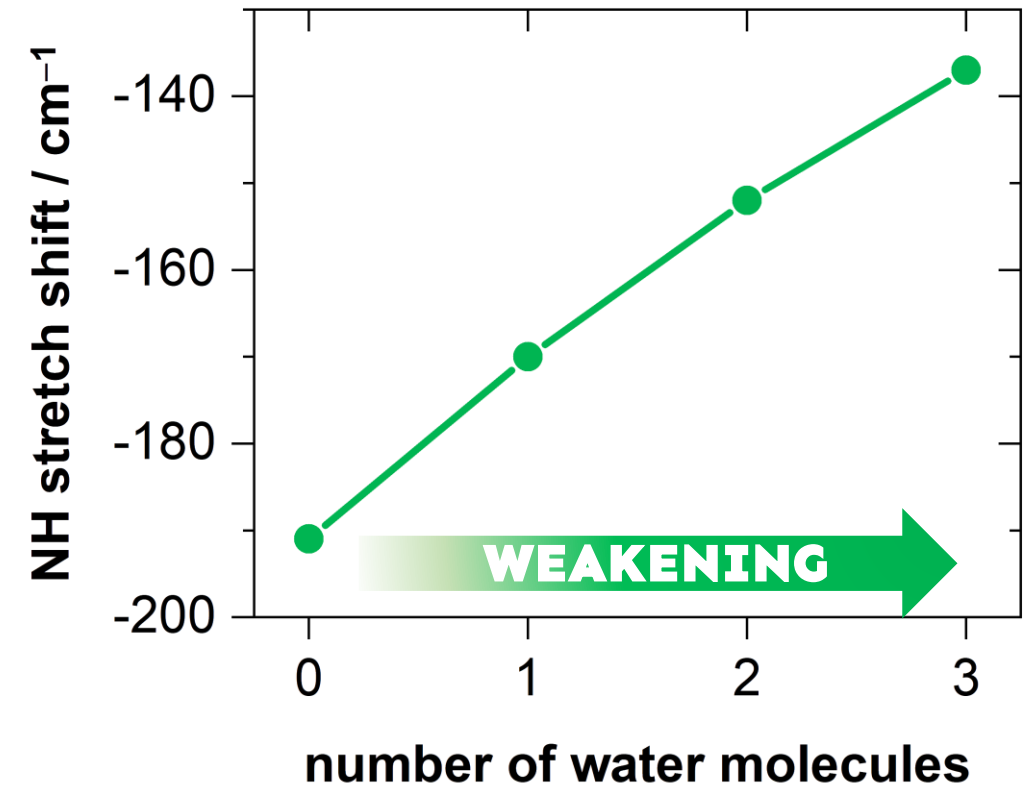
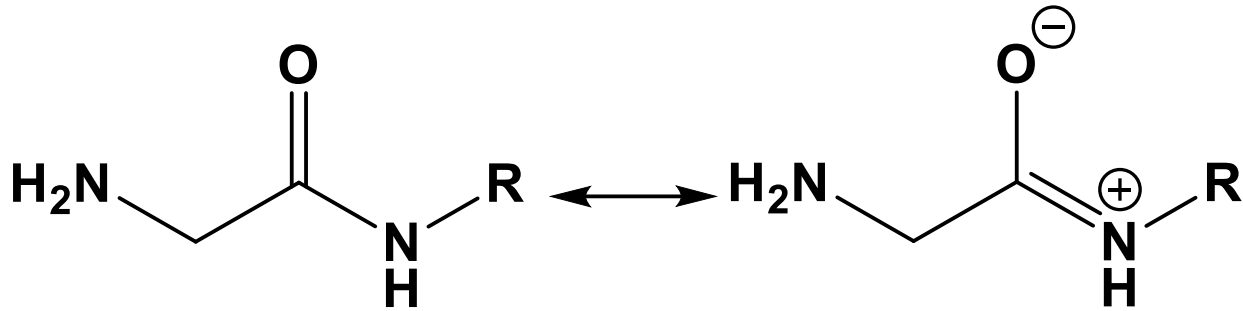
free NH stretch



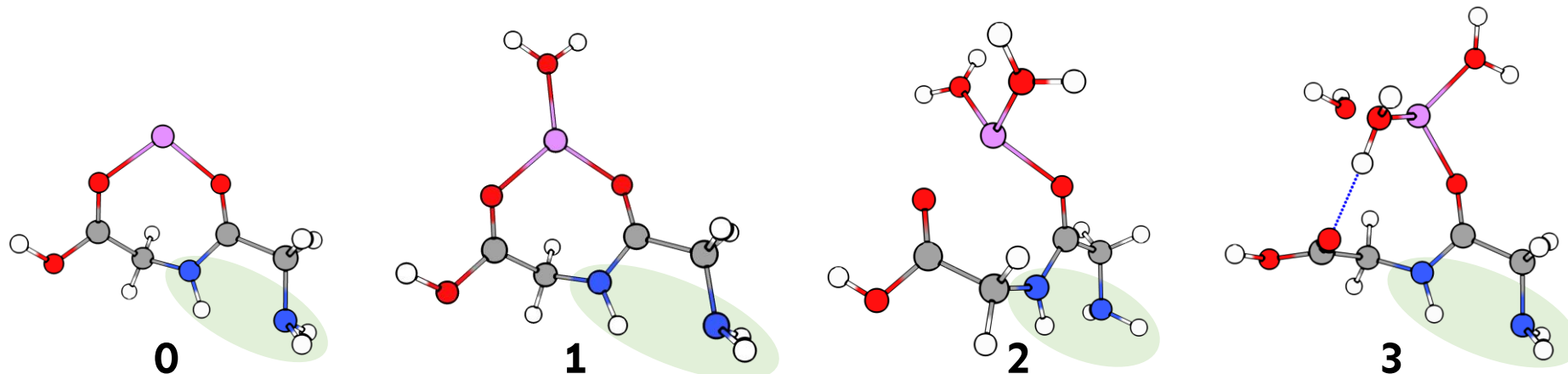
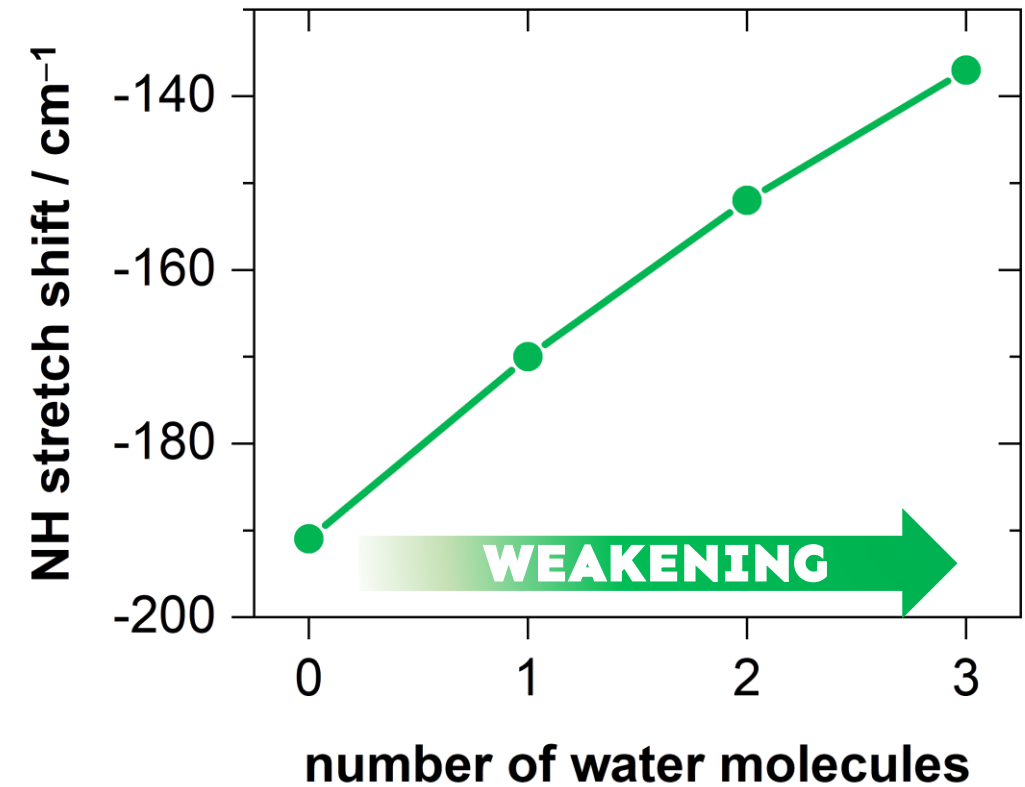
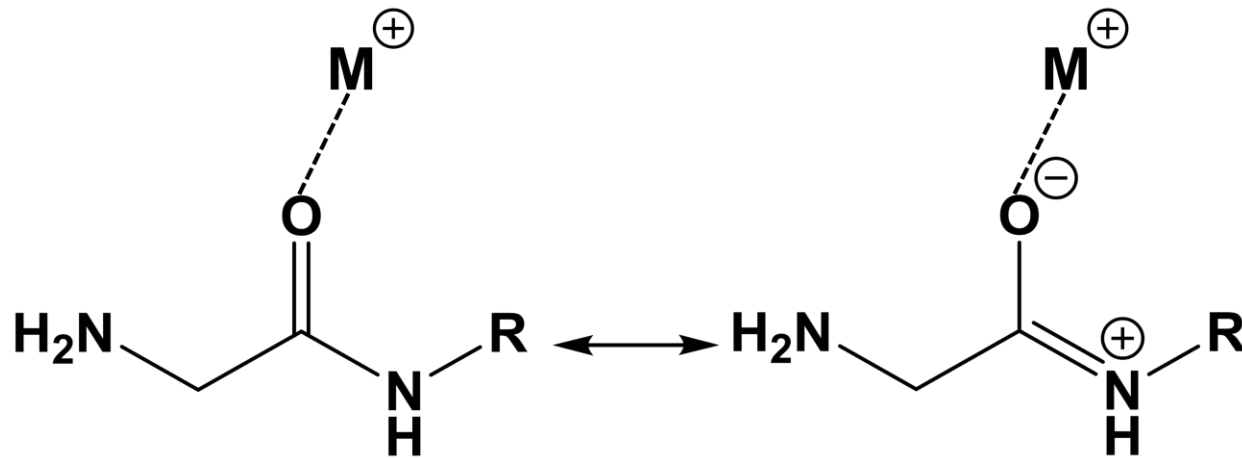


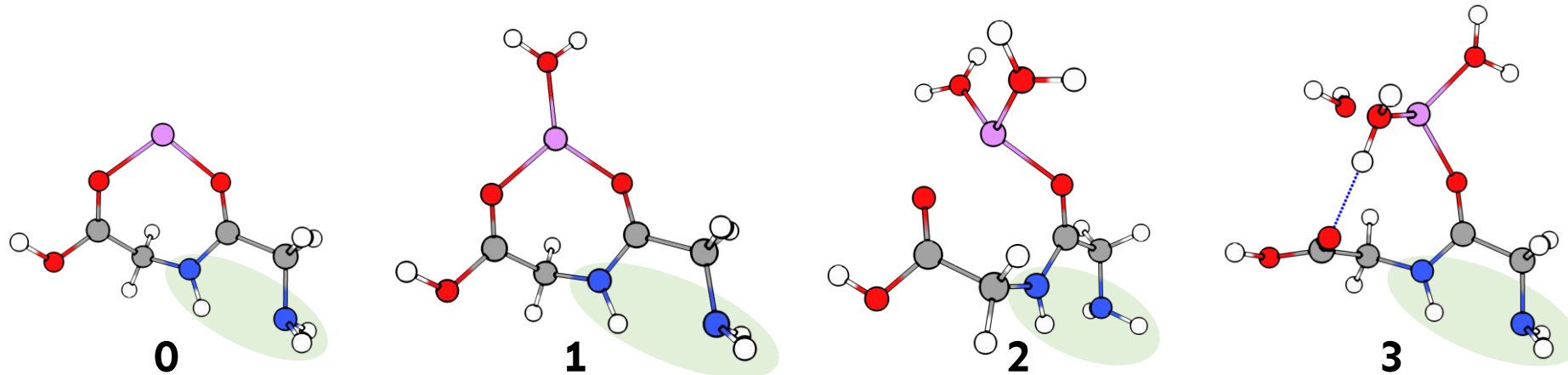
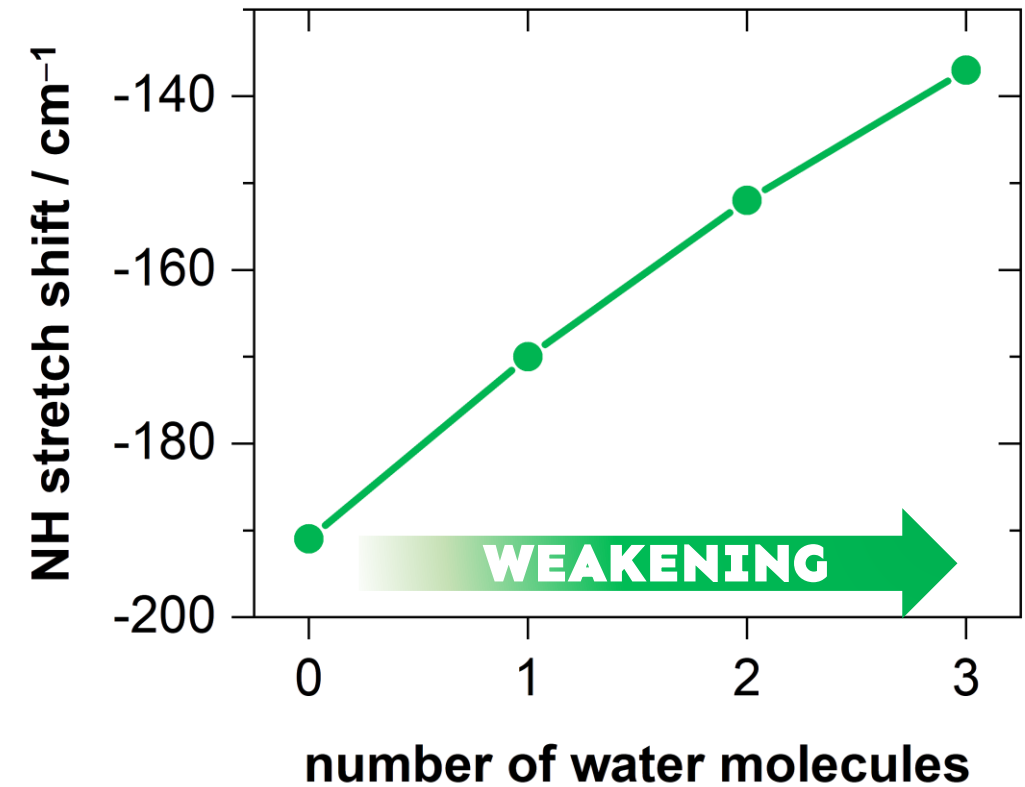
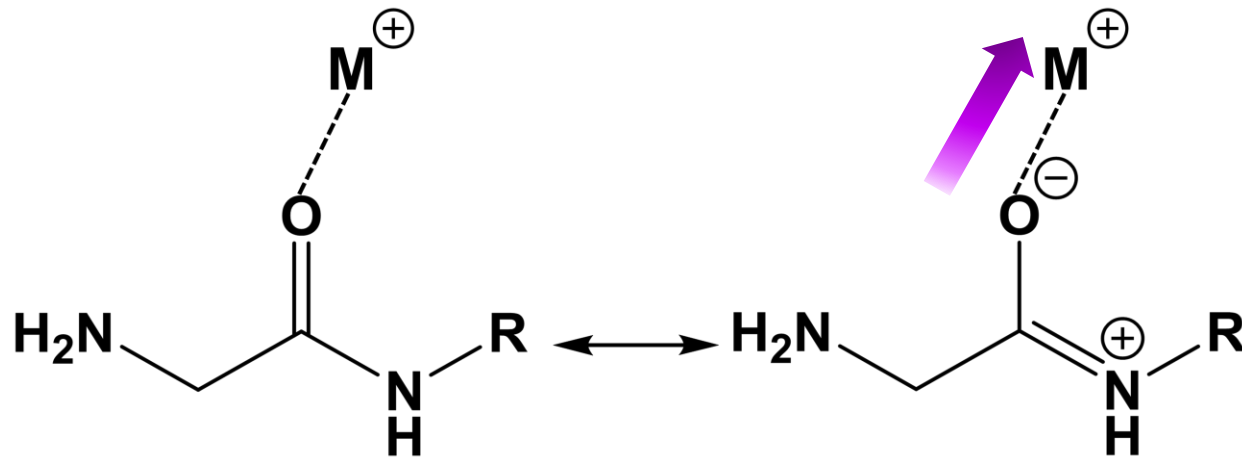




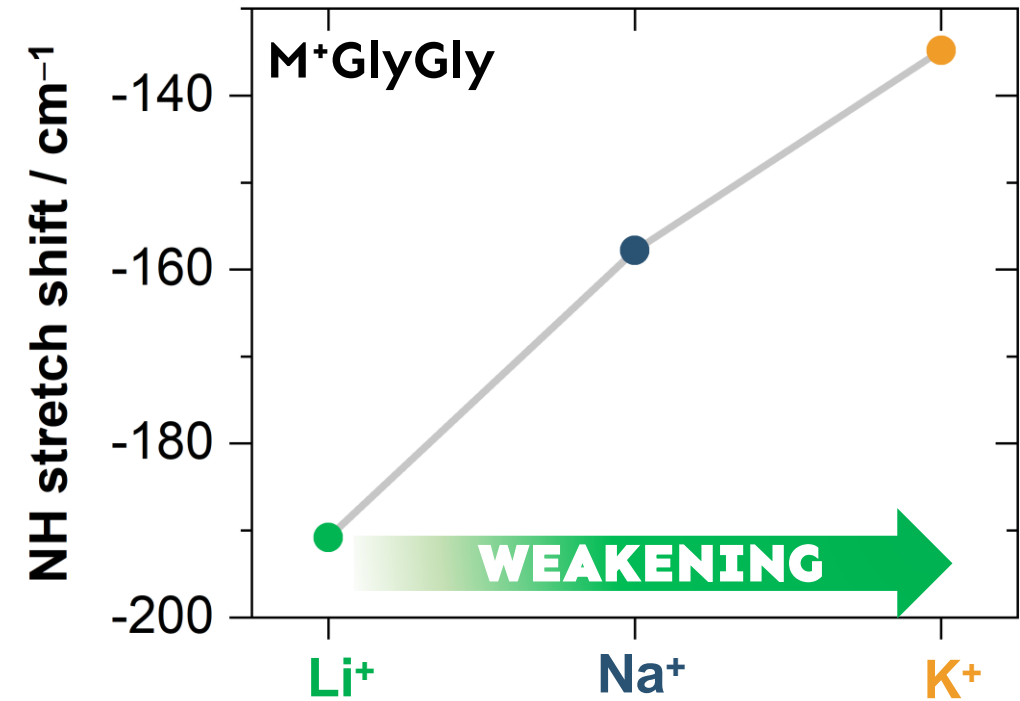
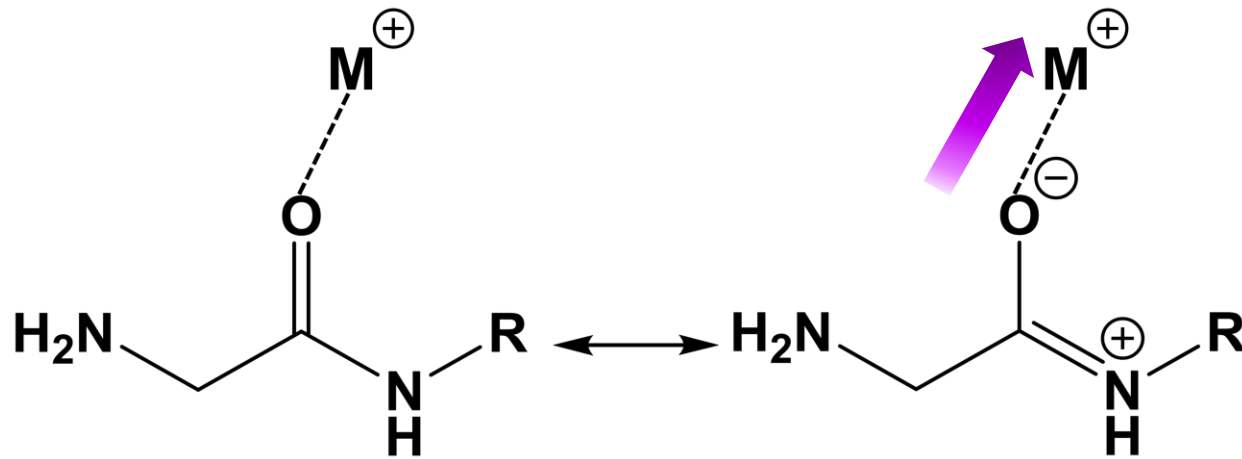


# E-FIELD IMPACT ON VIBRATIONS AND STRUCTURE

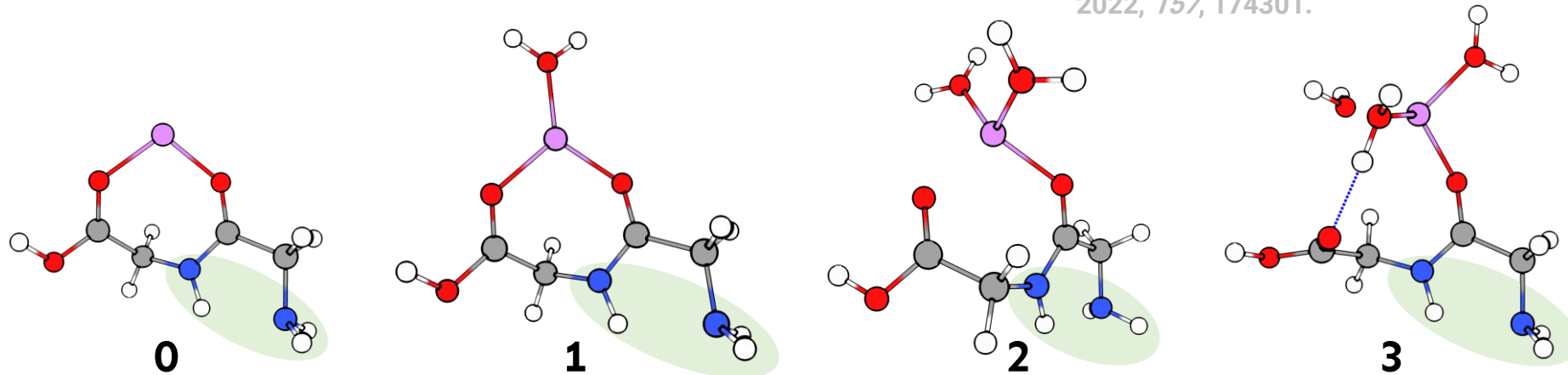


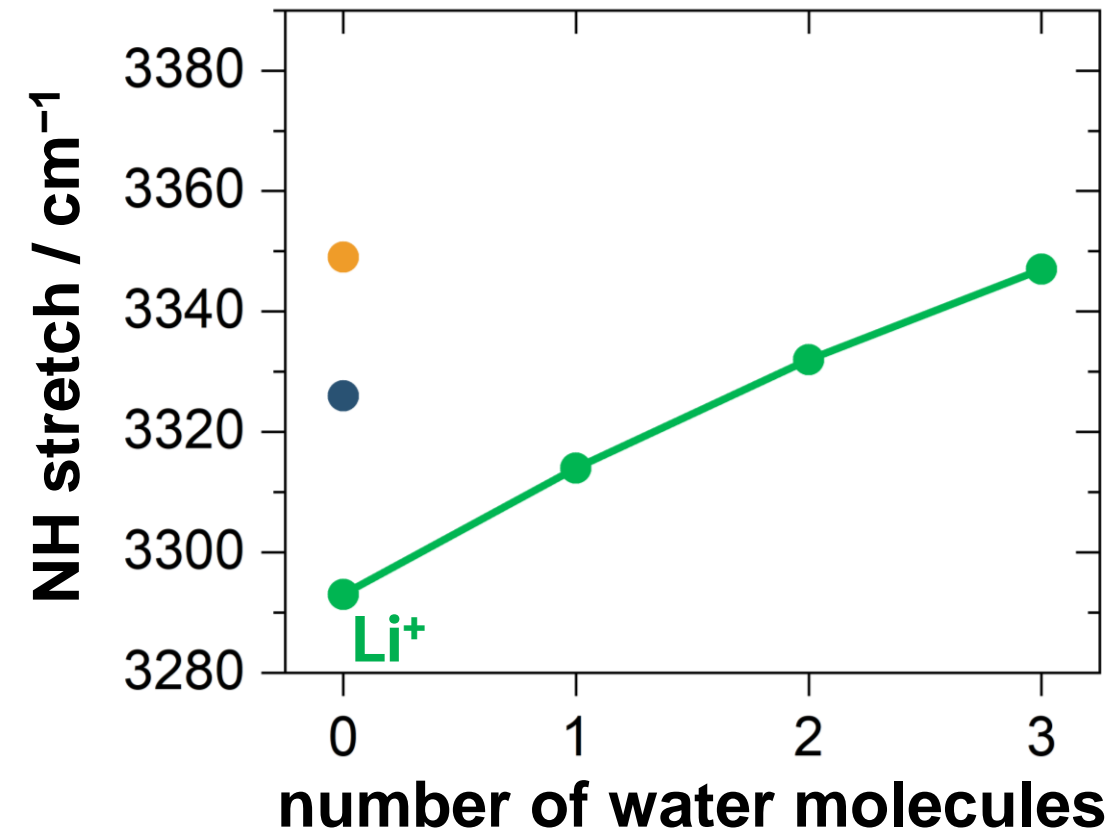


# E-FIELD IMPACT ON VIBRATIONS AND STRUCTURE

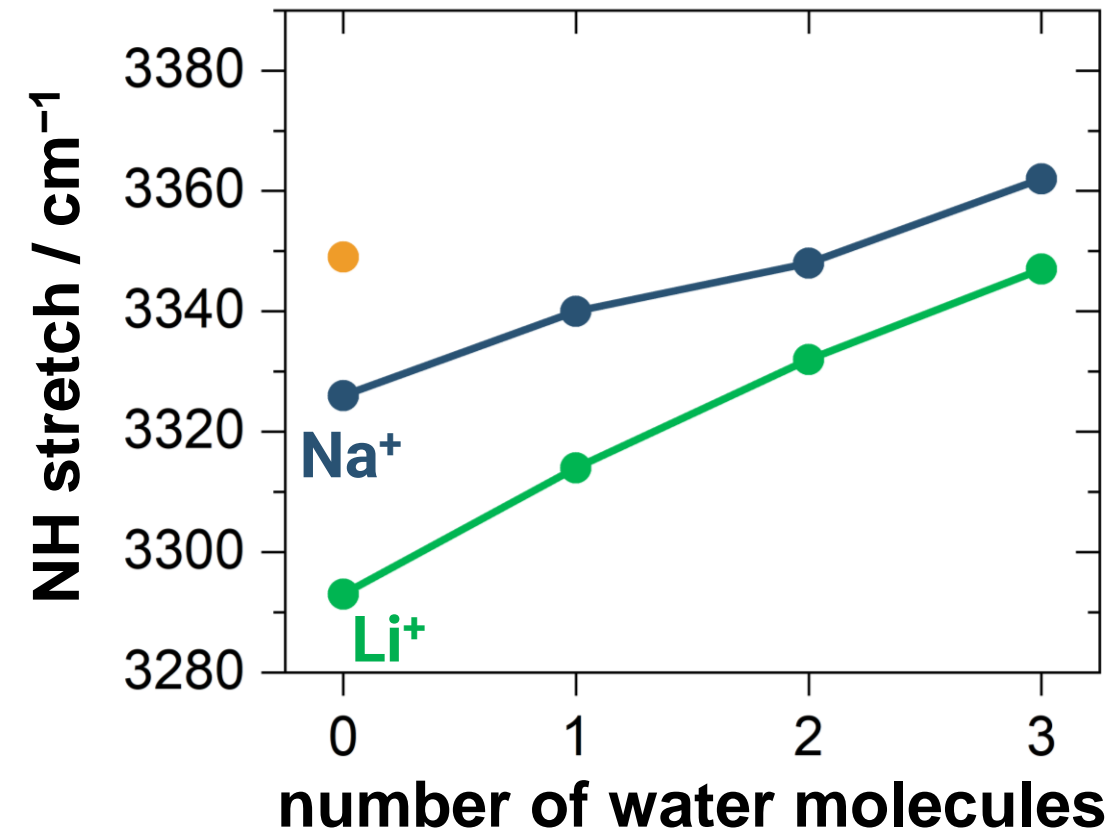


K. A. E. Meyer, K. A. Nickson, E. Garand, *J. Chem. Phys.* 2022, 157, 174301.

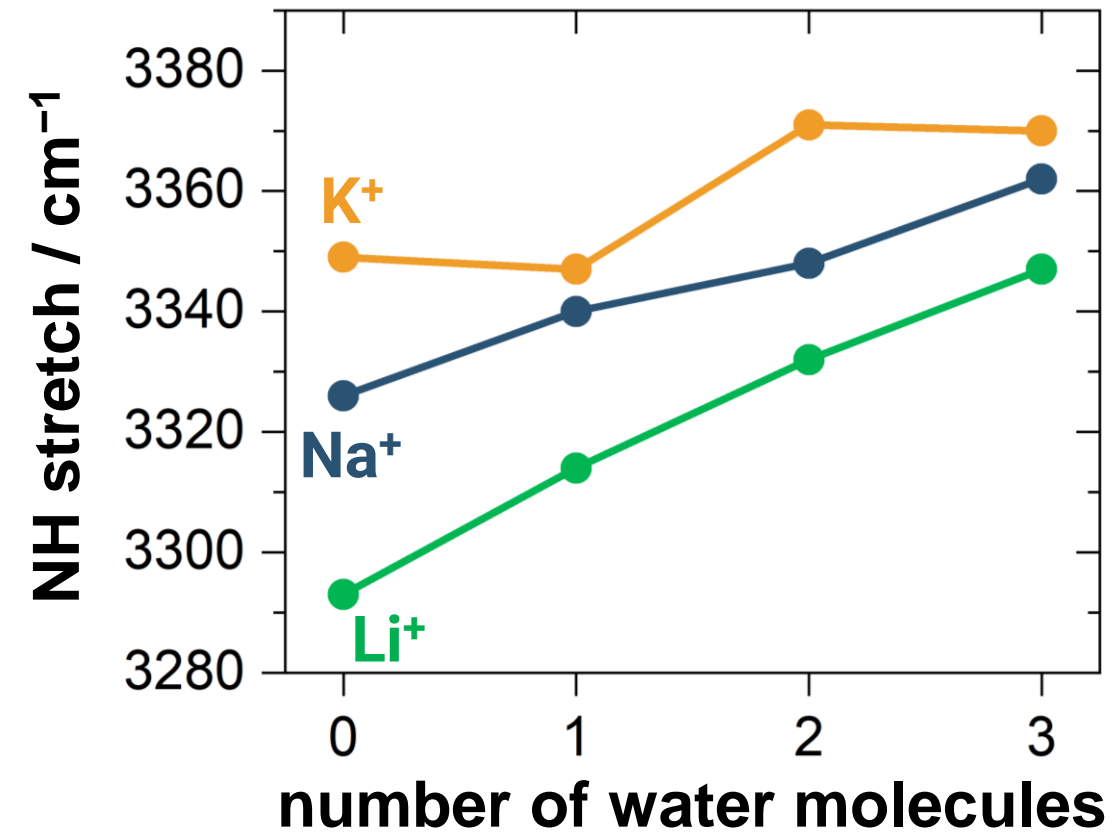




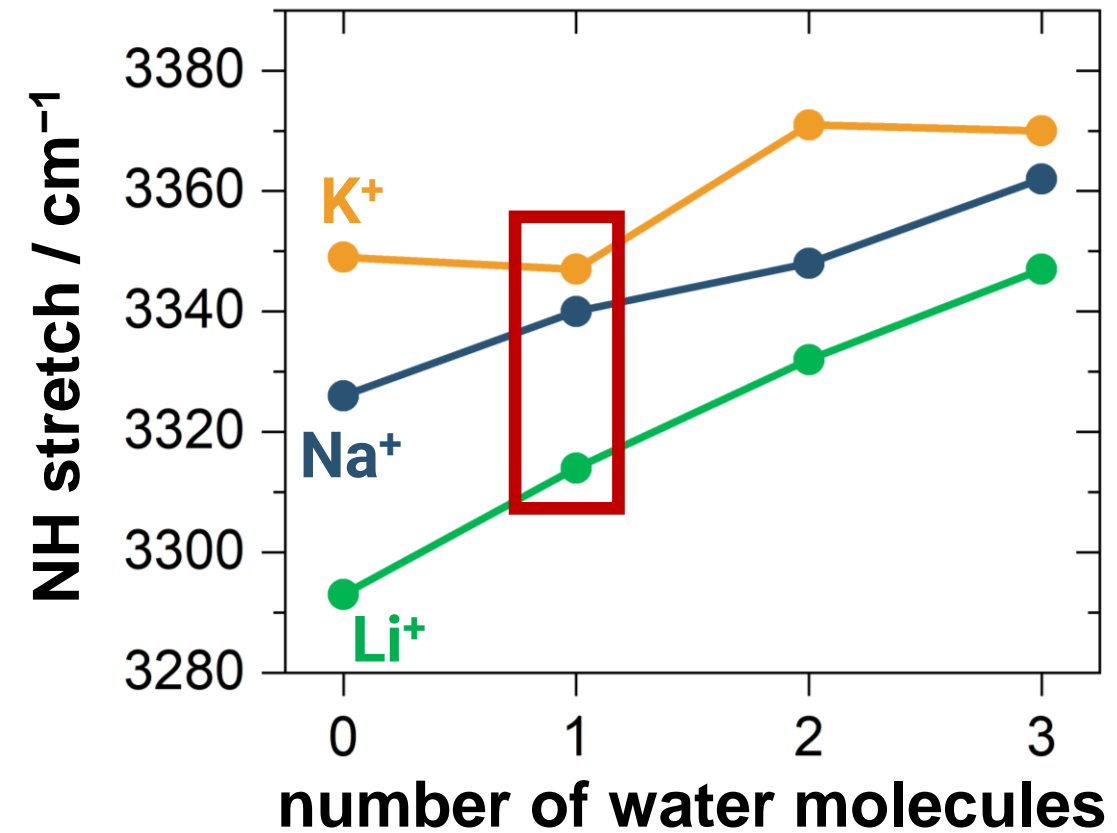
# SOLVATION: IMPACT OF THE METAL ION



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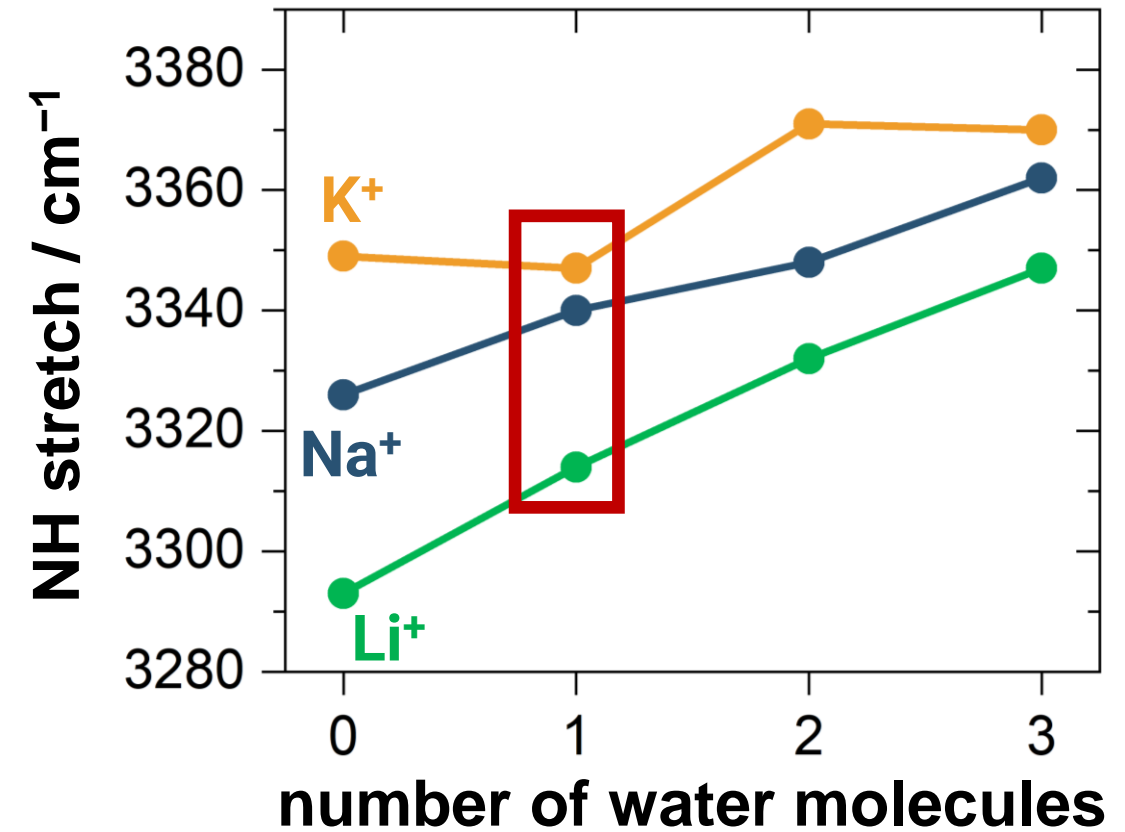
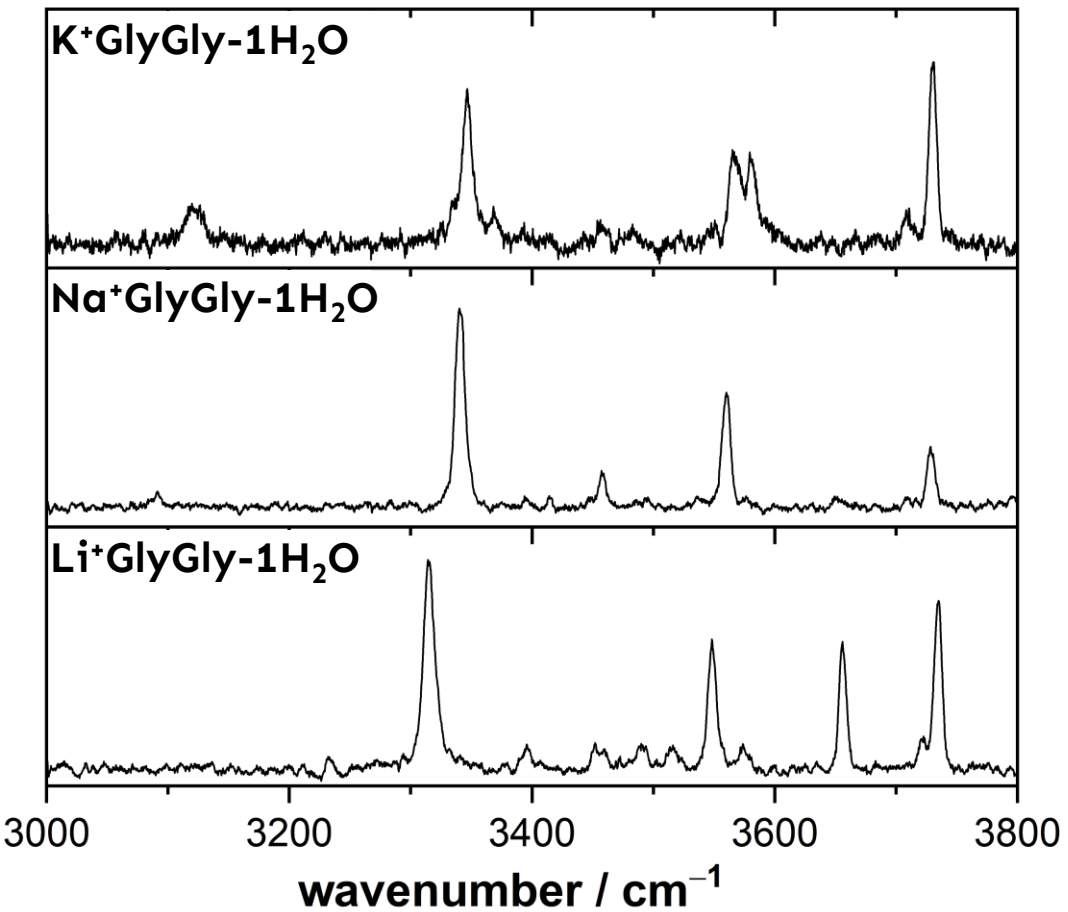


# SOLVATION: IMPACT OF THE METAL ION

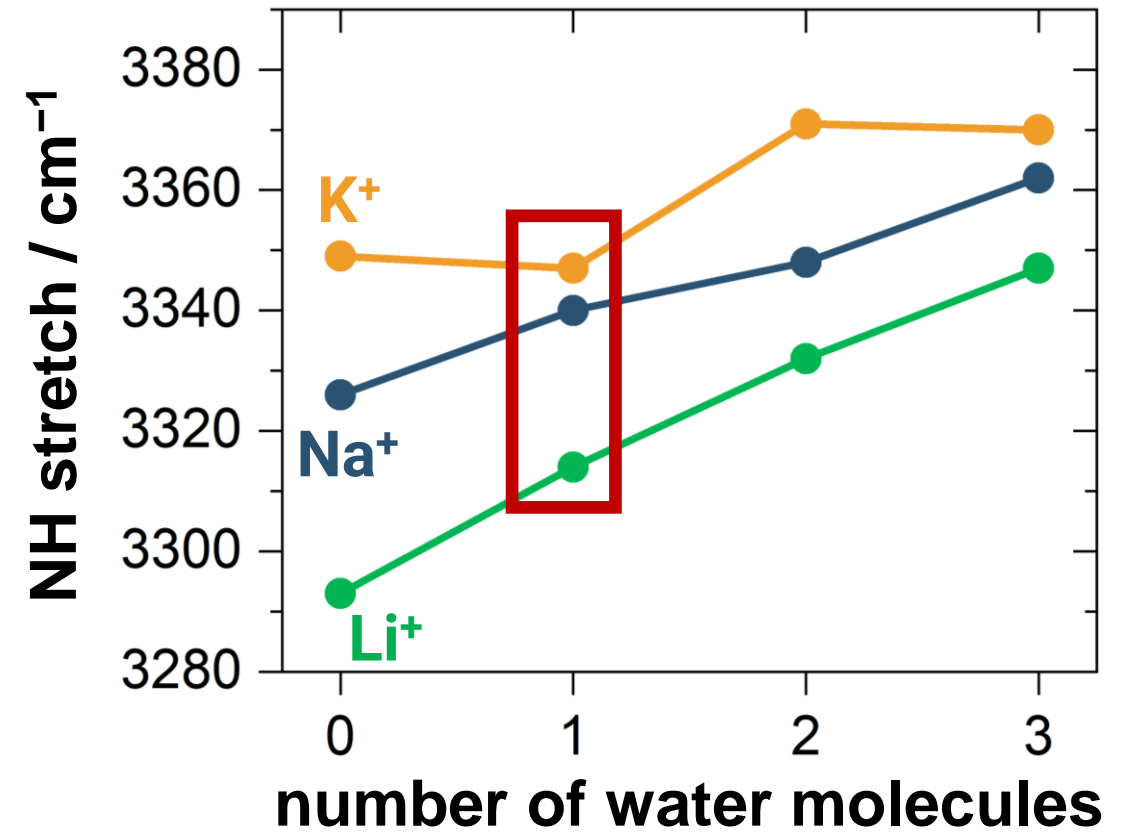
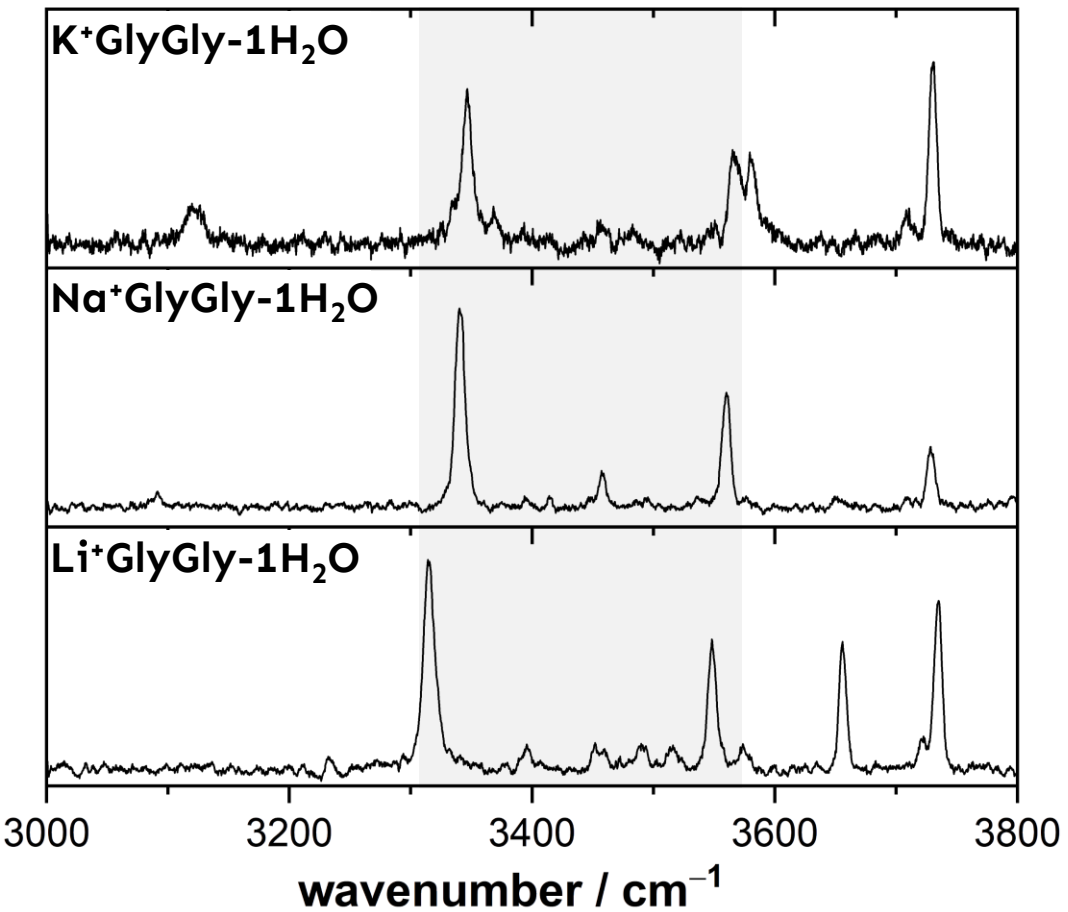




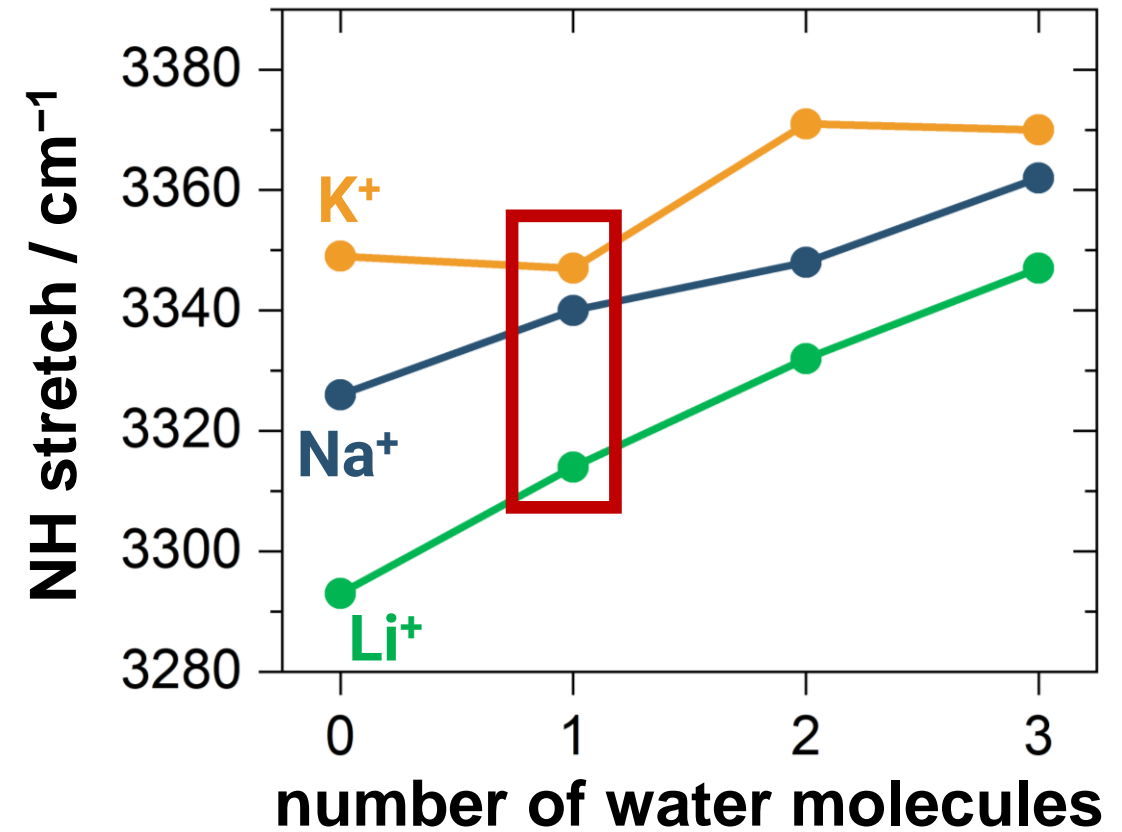
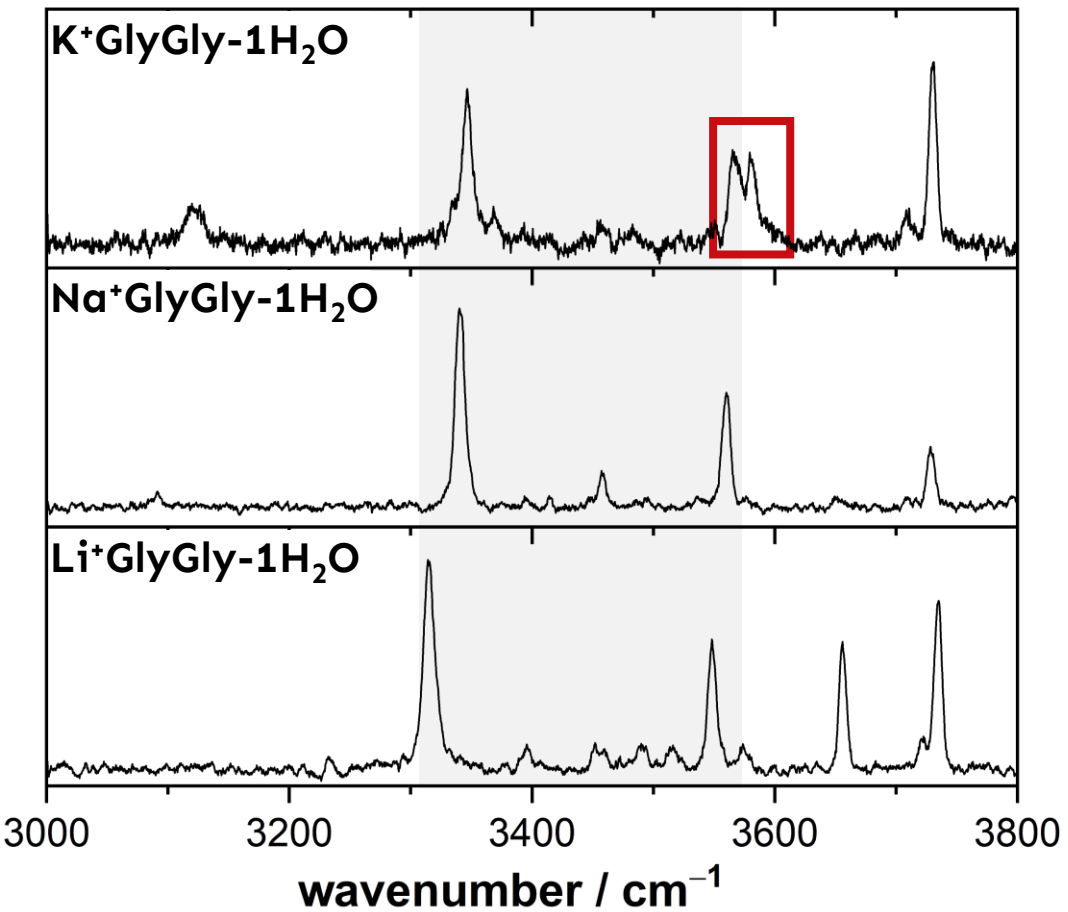
# SOLVATION: IMPACT OF THE METAL ION



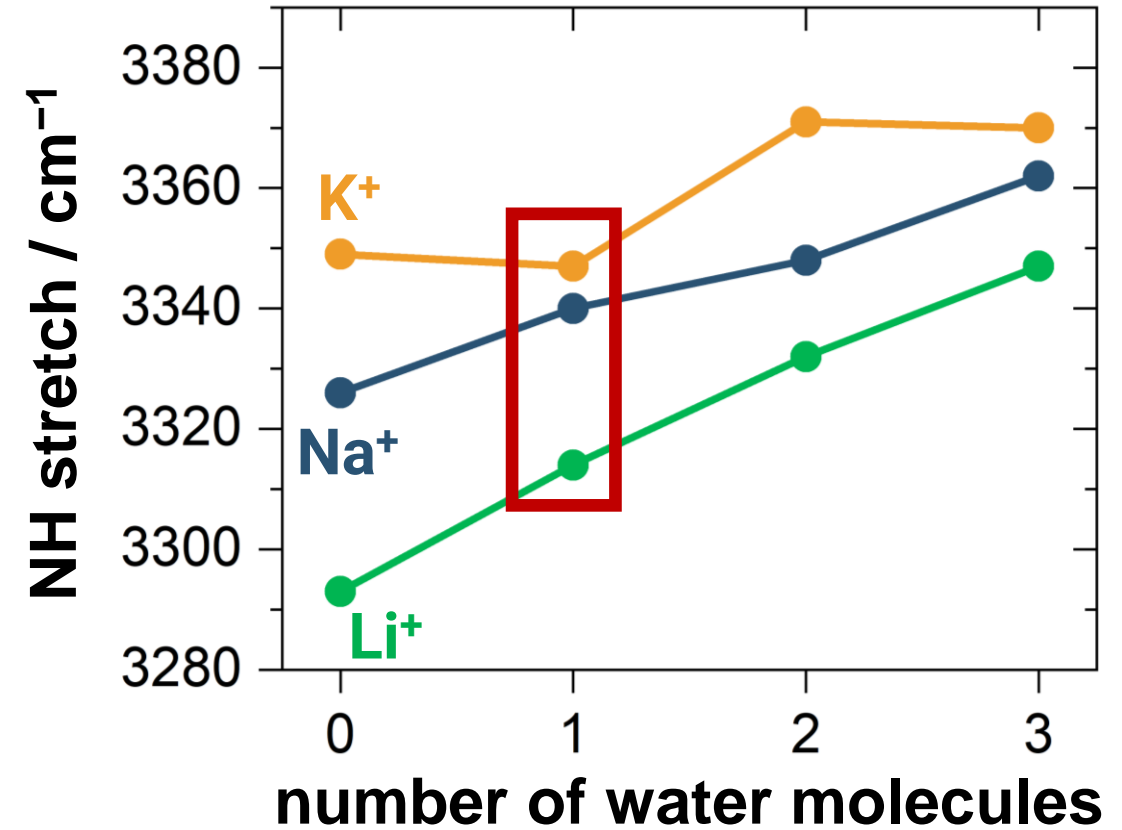
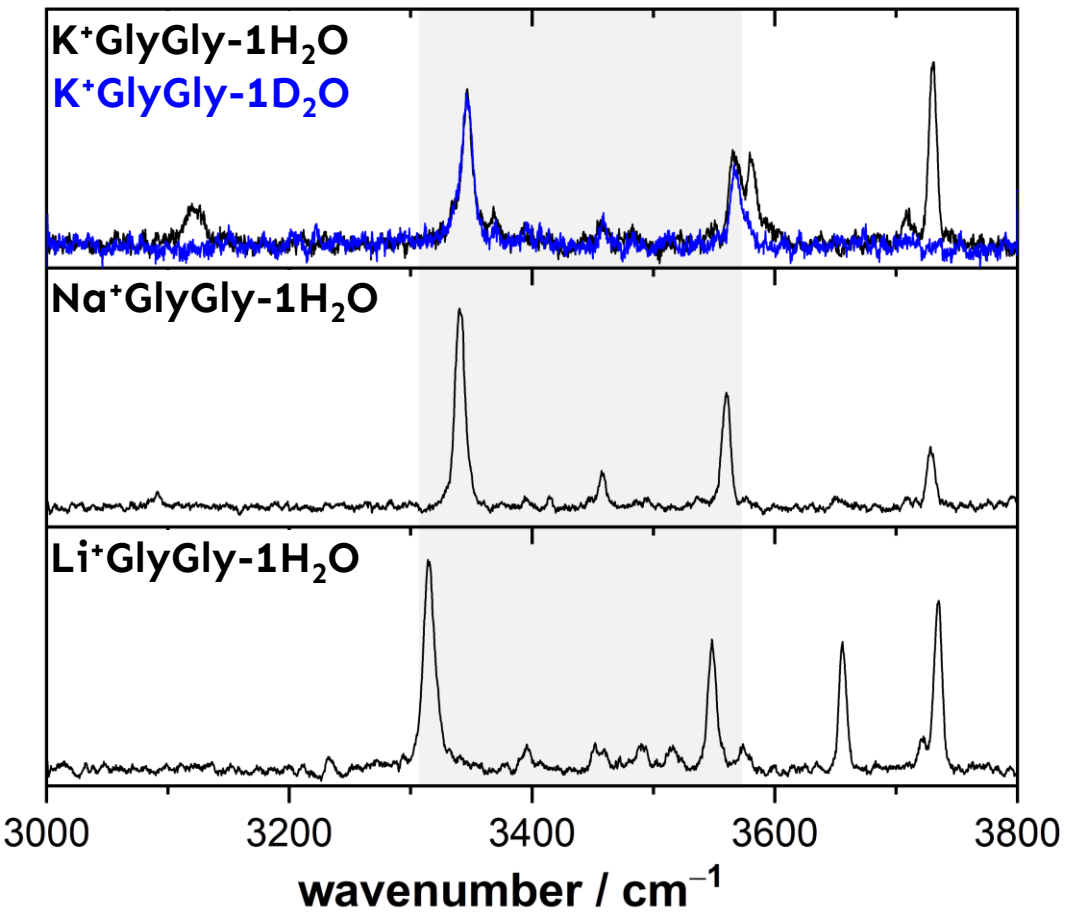
# SOLVATION: IMPACT OF THE METAL ION



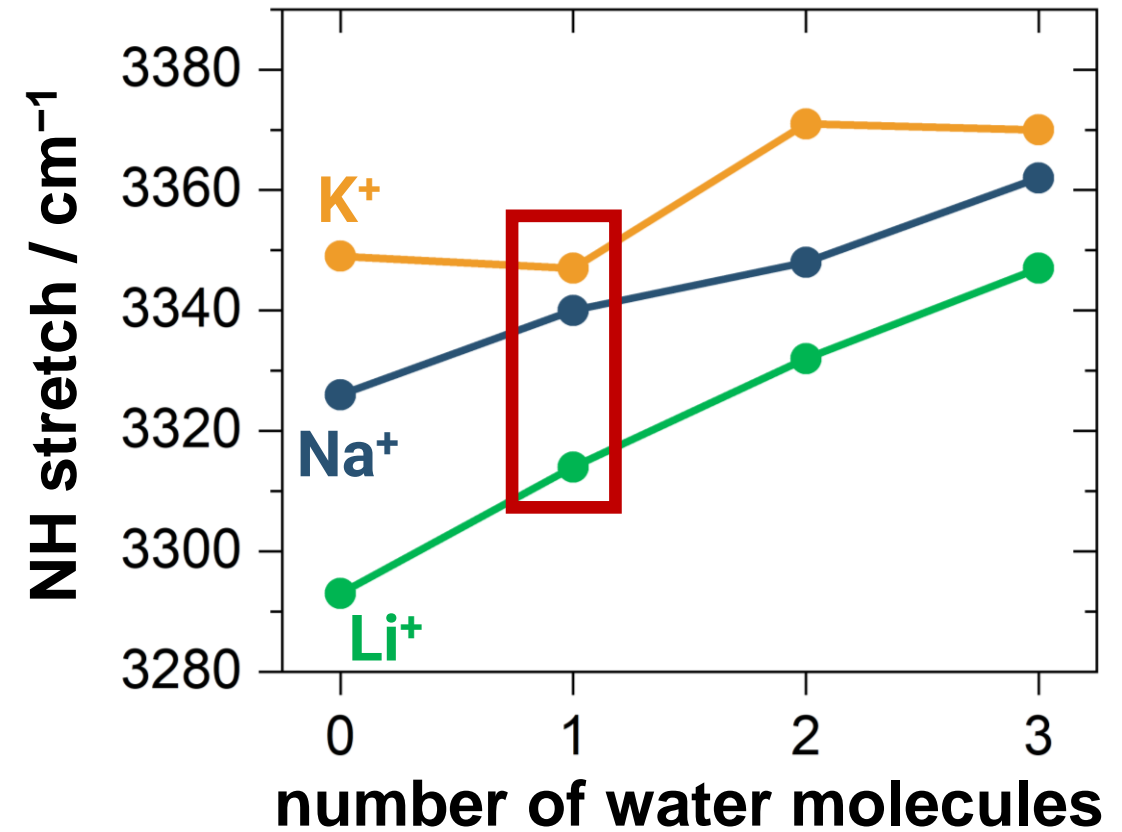
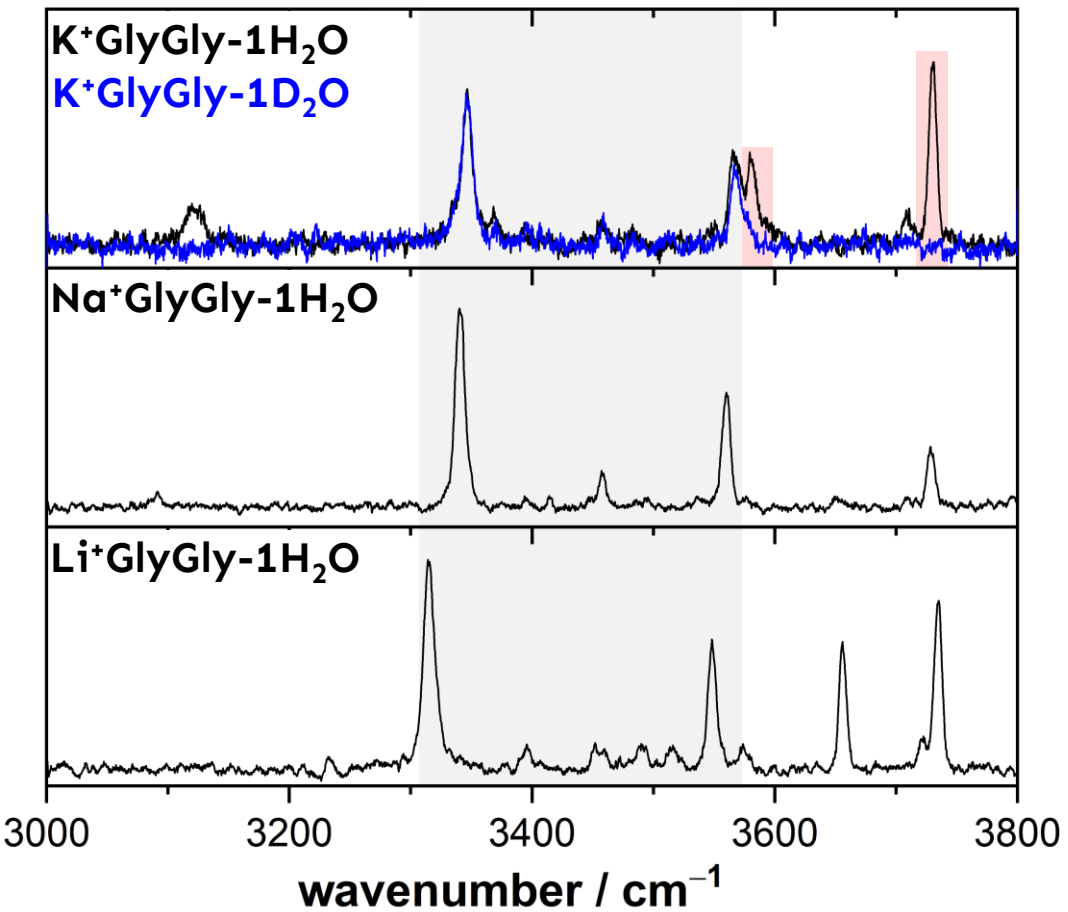
# SOLVATION: IMPACT OF THE METAL ION



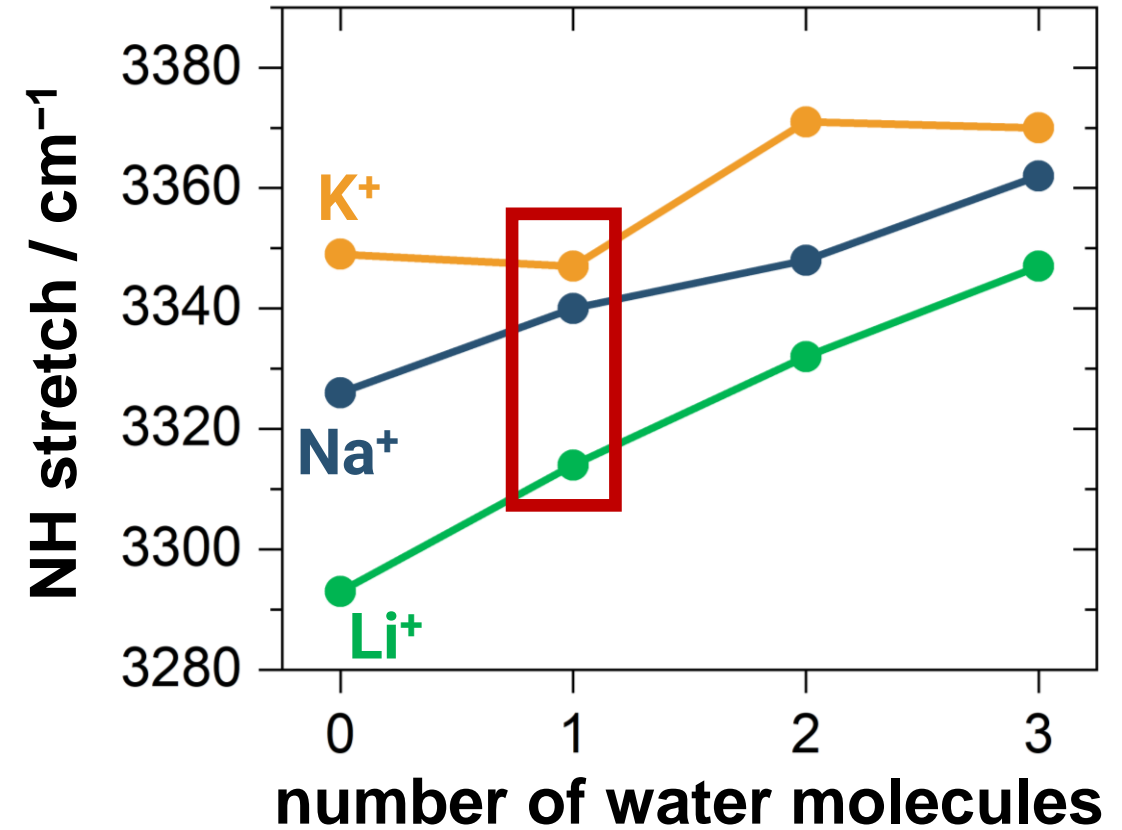
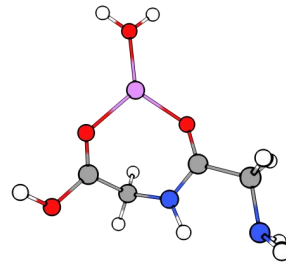
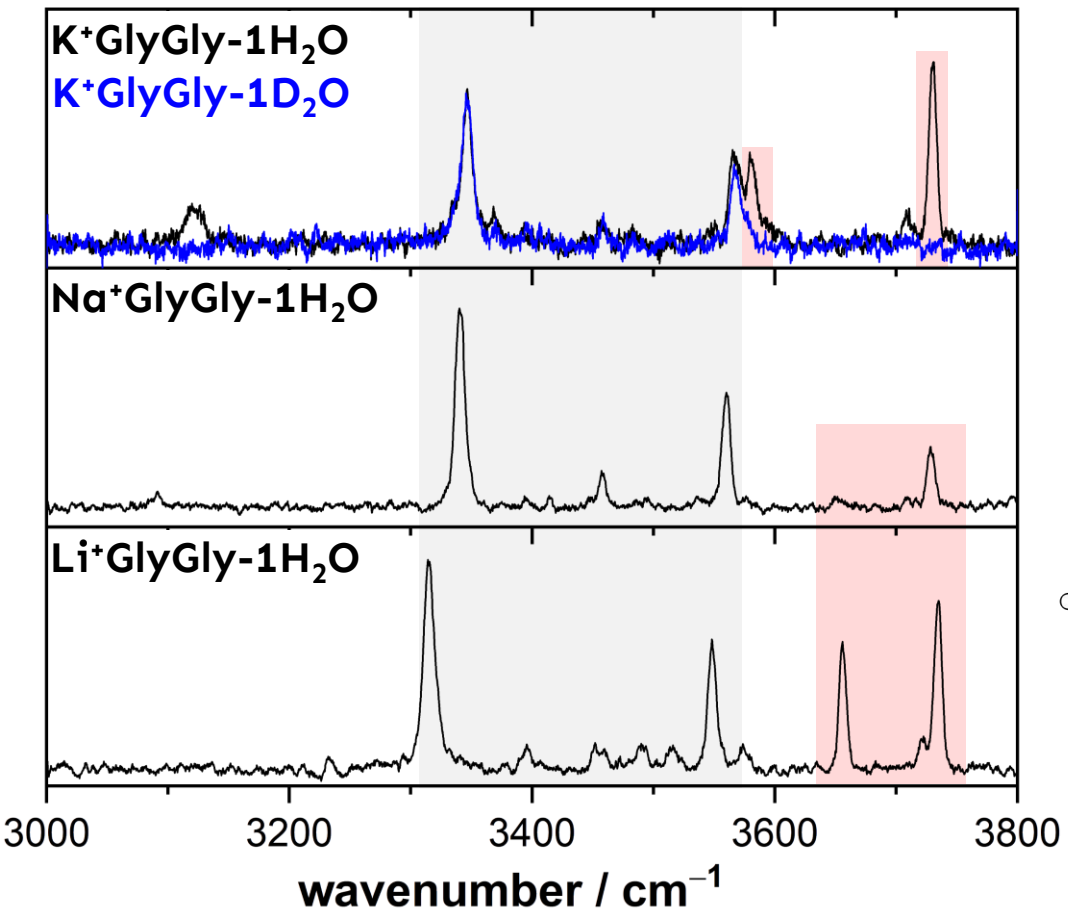
# SOLVATION: IMPACT OF THE METAL ION



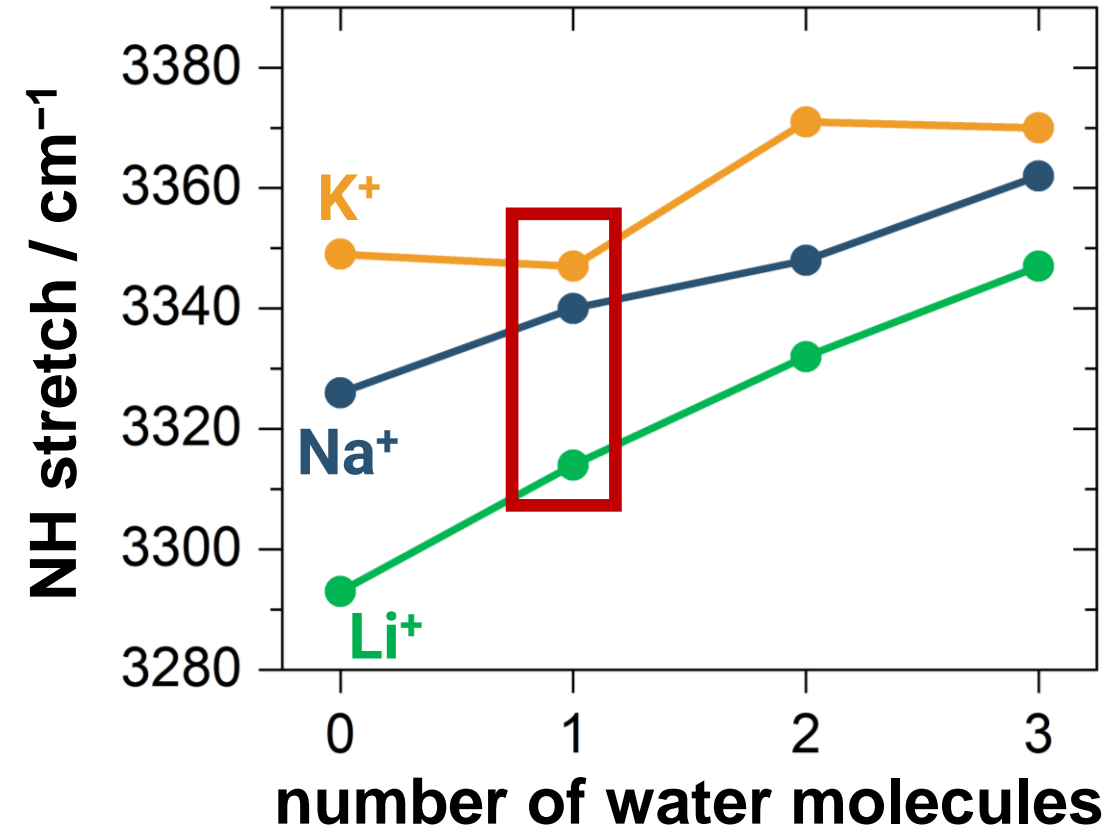
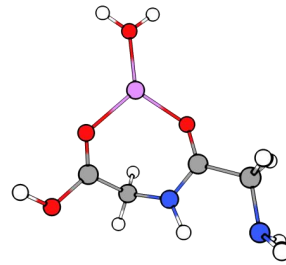
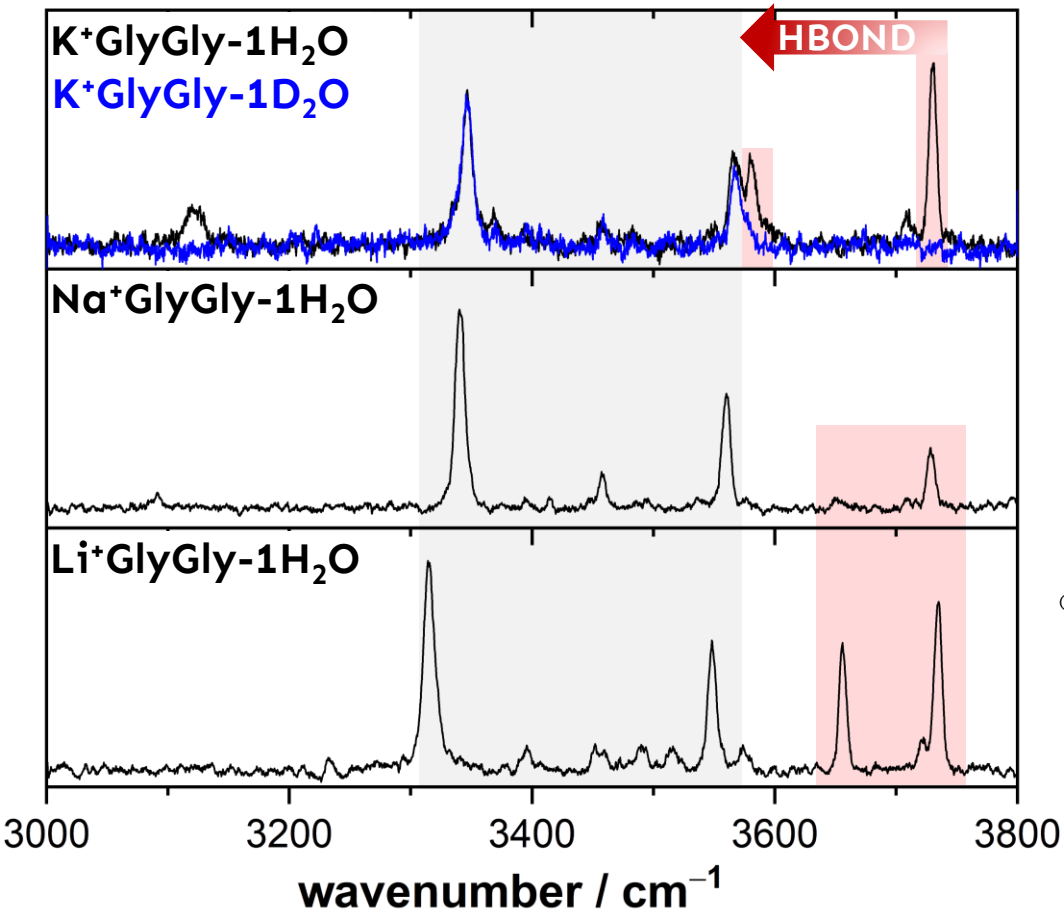
# SOLVATION: IMPACT OF THE METAL ION



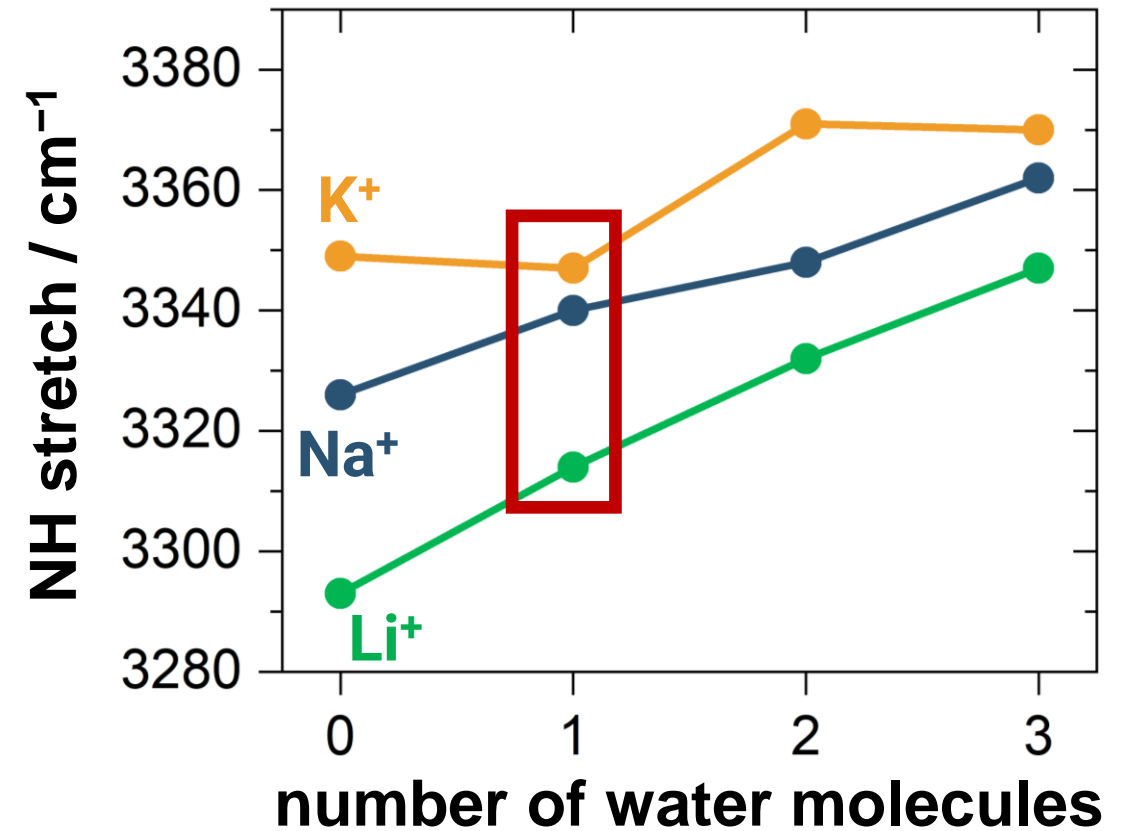
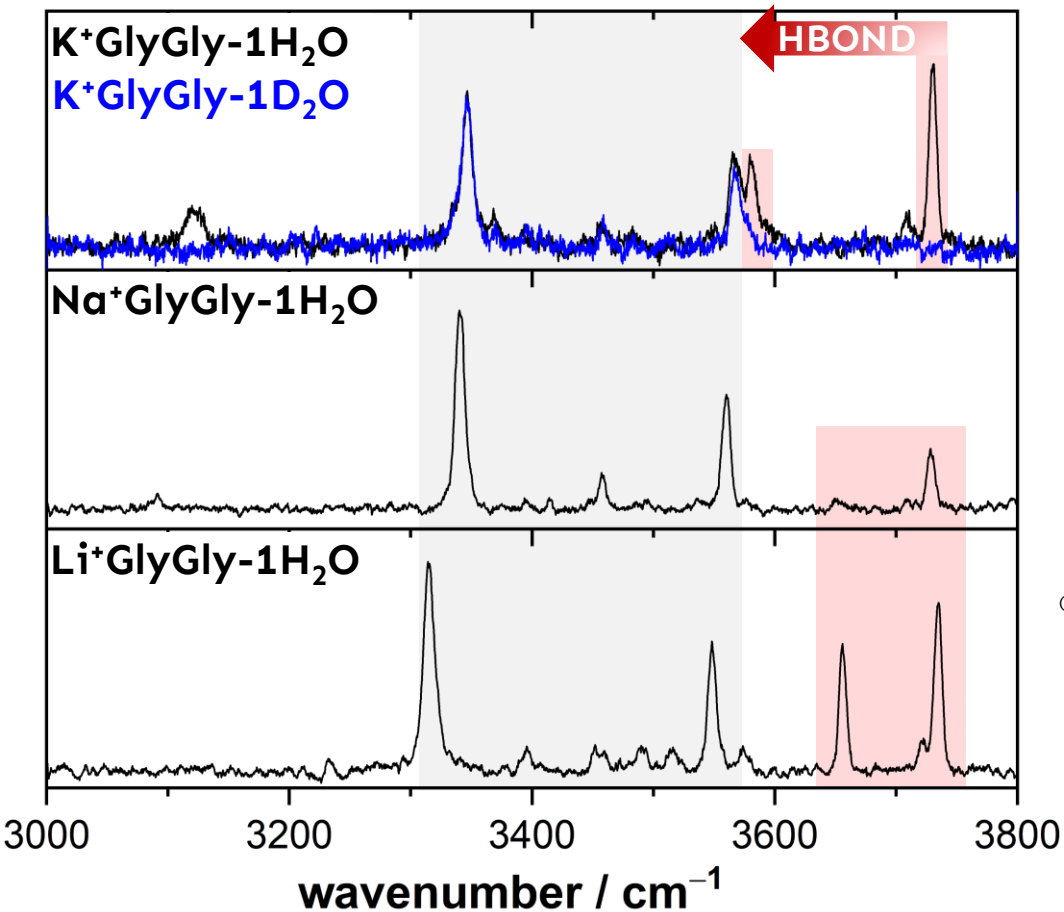
# SOLVATION: IMPACT OF THE METAL ION



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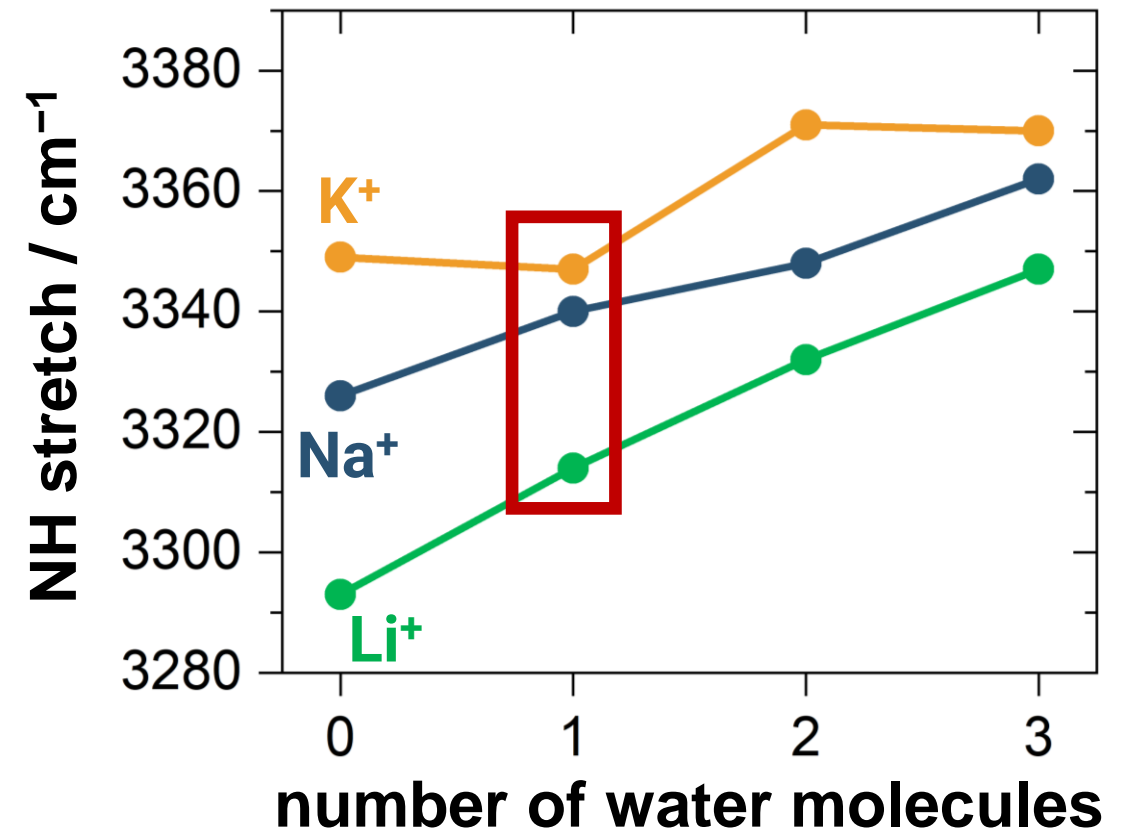
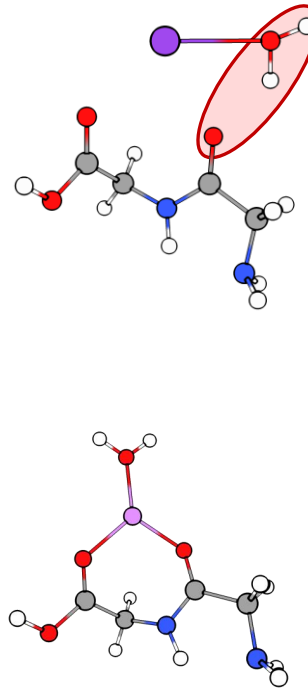
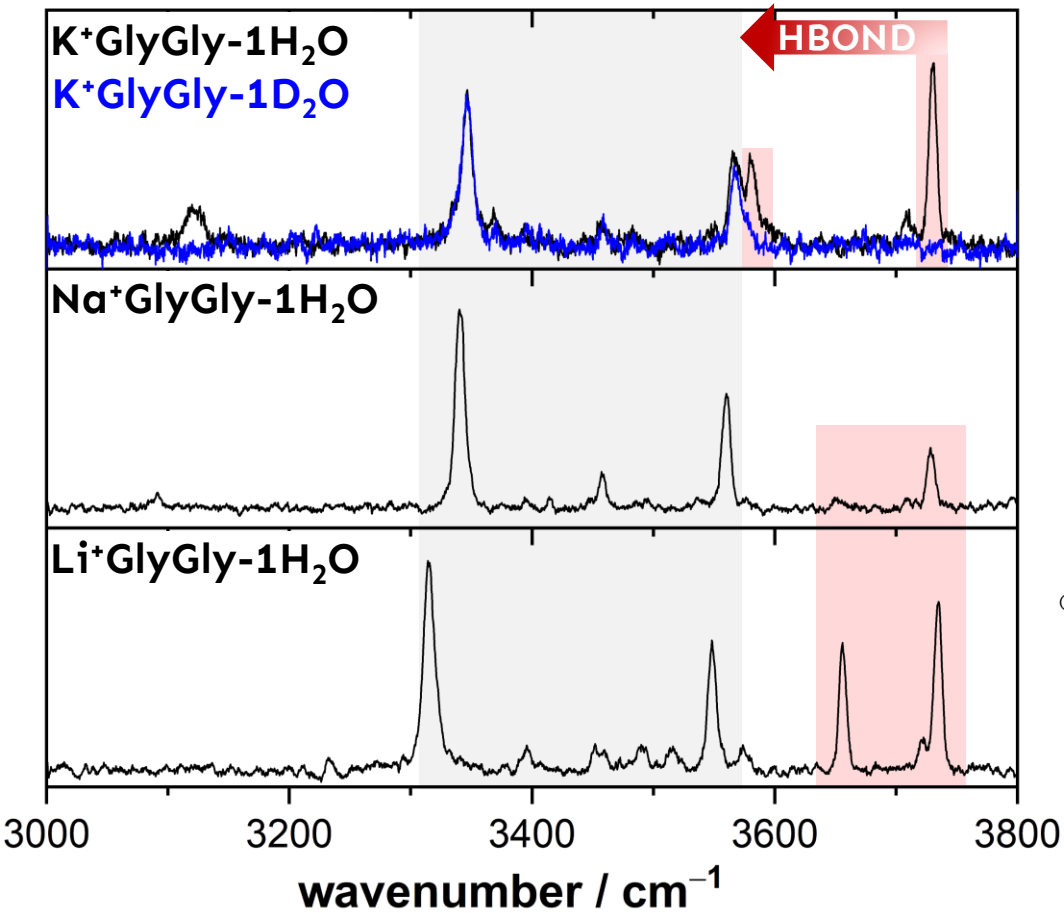


# SOLVATION: IMPACT OF THE METAL ION

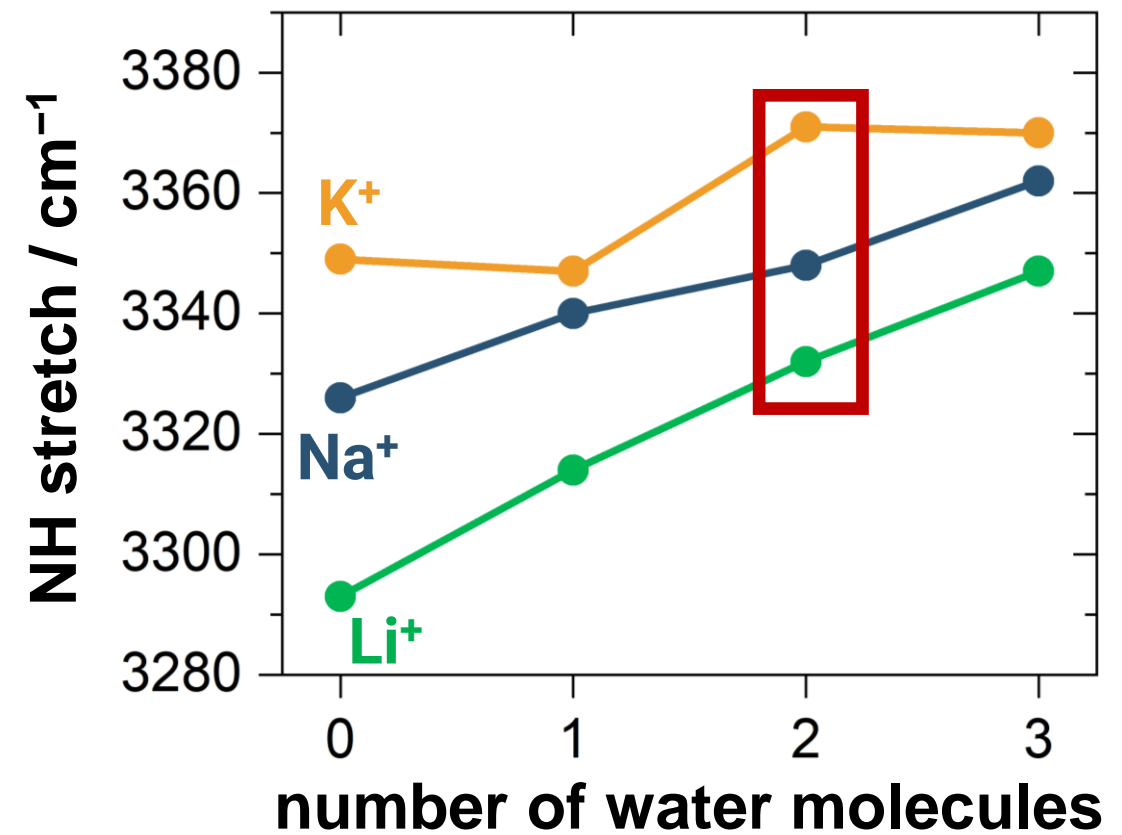
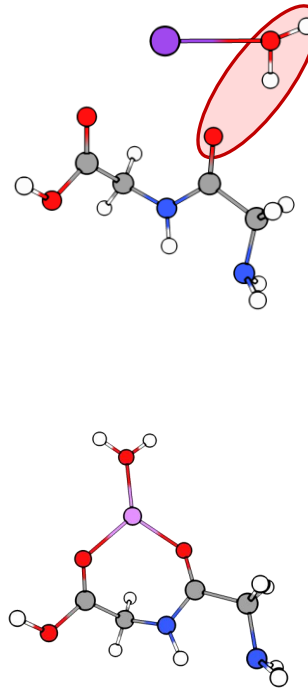
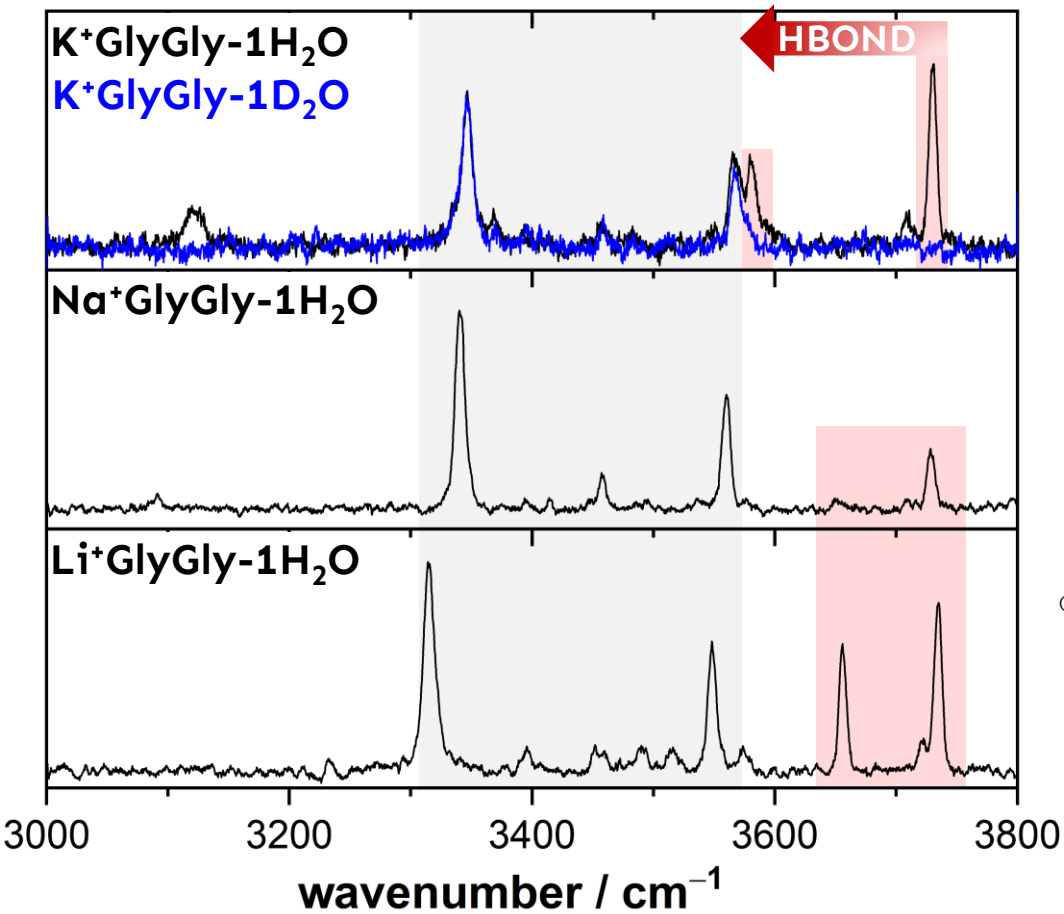




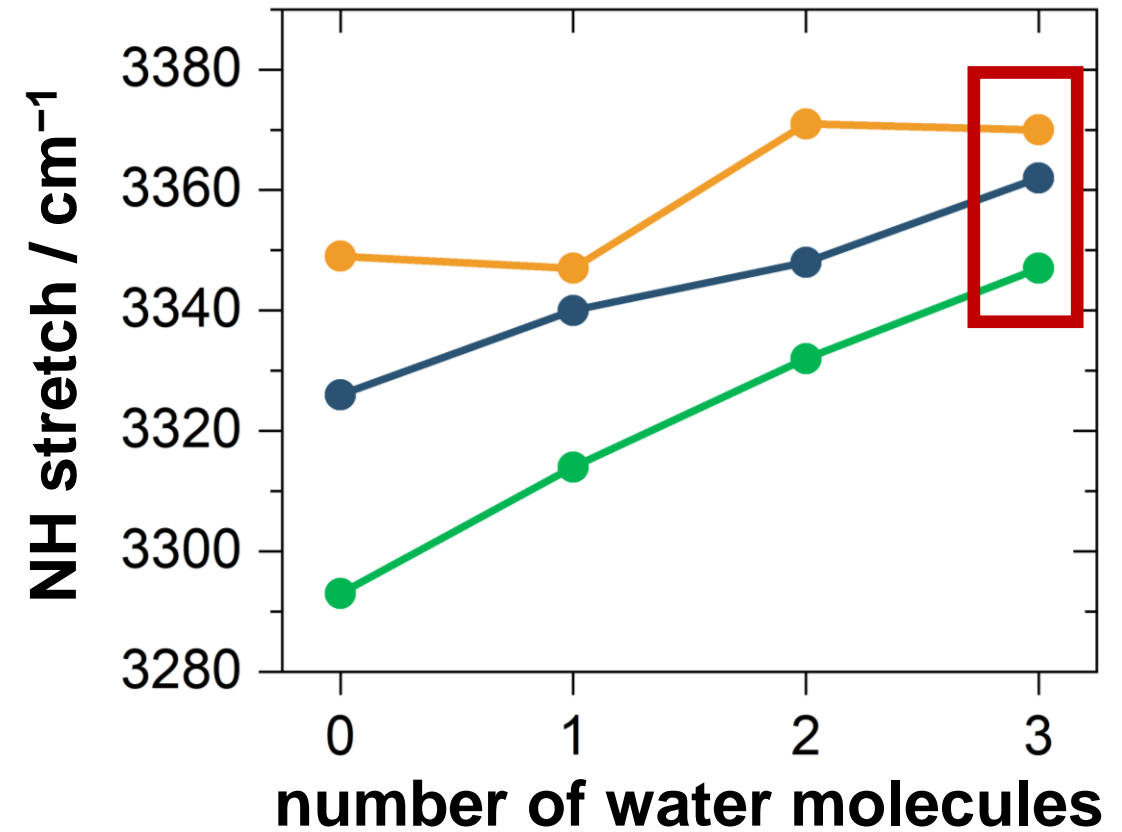
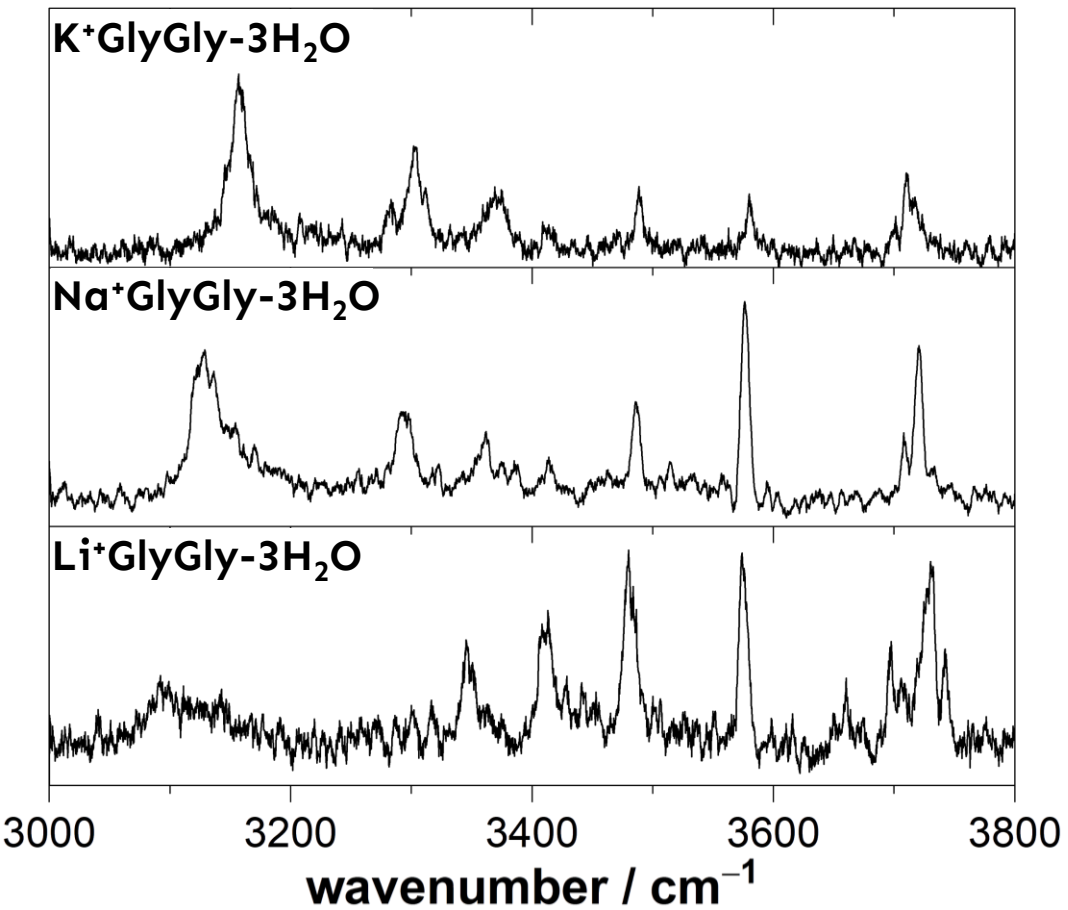
# SOLVATION: IMPACT OF THE METAL ION



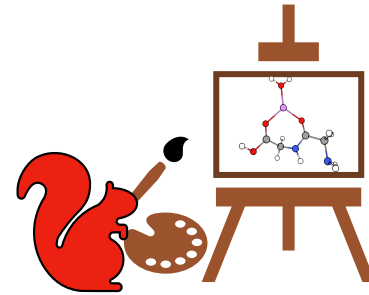
# SOLVATION: IMPACT OF THE METAL ION



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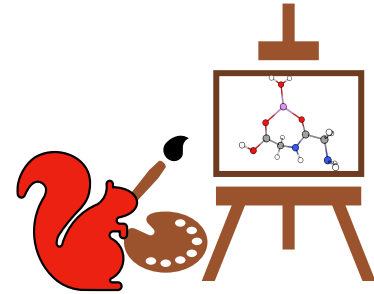


# BENCHMARKING: WHICH METHOD IS THE BEST?



# BENCHMARKING: WHICH METHOD IS THE BEST?

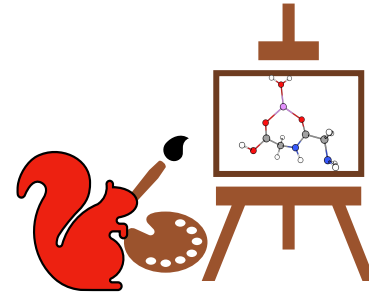
Scaled harmonic vibrational  
frequency calculations



# BENCHMARKING: WHICH METHOD IS THE BEST?

Scaled harmonic vibrational  
frequency calculations

B3YLP-D3

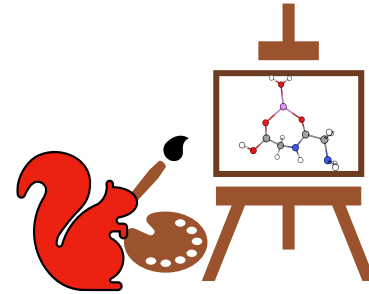


# BENCHMARKING: WHICH METHOD IS THE BEST?

Scaled harmonic vibrational  
frequency calculations

B3YLP-D3

B3LYP



# BENCHMARKING: WHICH METHOD IS THE BEST?

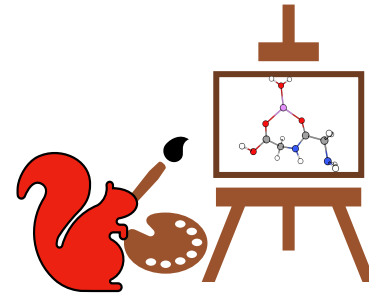
Scaled harmonic vibrational  
frequency calculations

B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X





# BENCHMARKING: WHICH METHOD IS THE BEST?

Scaled harmonic vibrational  
frequency calculations

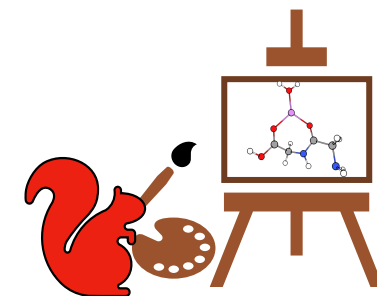
B3YLP-D3

B2PLYP-D3

B3LYP

$\omega$ B97XD

M06-2X



# BENCHMARKING: WHICH METHOD IS THE BEST?

Scaled harmonic vibrational  
frequency calculations

B3YLP-D3

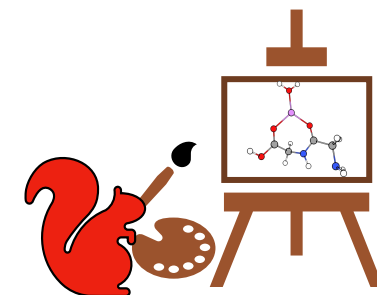
B3LYP

$\omega$ B97XD

M06-2X

B2PLYP-D3

MP2



# BENCHMARKING: WHICH METHOD IS THE BEST?

Scaled harmonic vibrational  
frequency calculations

B3YLP-D3

B3LYP

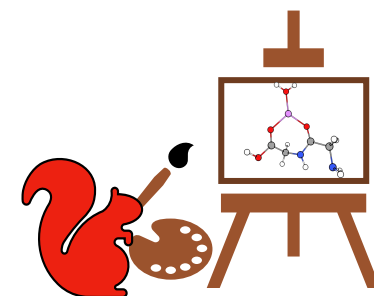
$\omega$ B97XD

M06-2X

B2PLYP-D3

MP2

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?

Scaled harmonic vibrational  
frequency calculations

B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

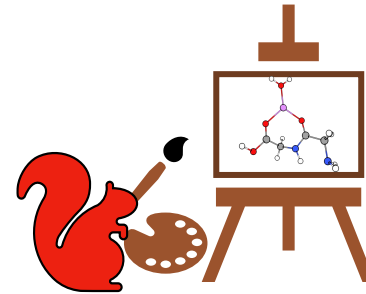
def2TZVP

B2PLYP-D3

MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?

Scaled harmonic vibrational  
frequency calculations

B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

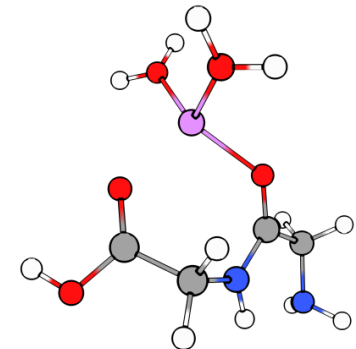
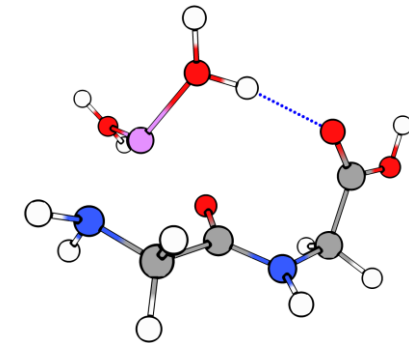
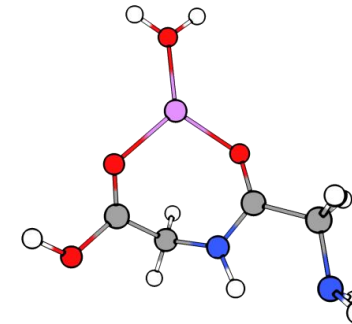
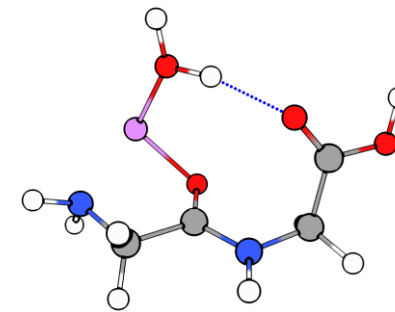
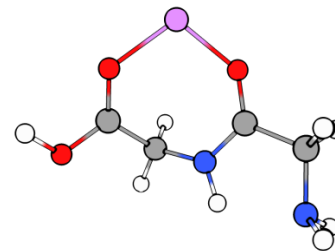
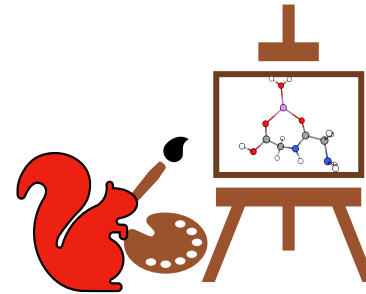
def2TZVP

B2PLYP-D3

MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?

B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

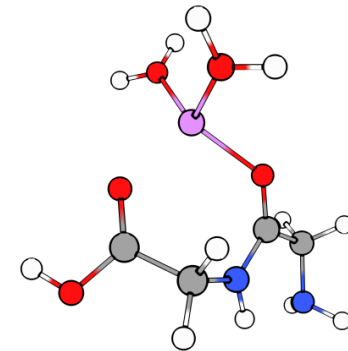
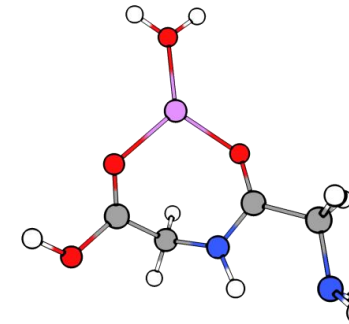
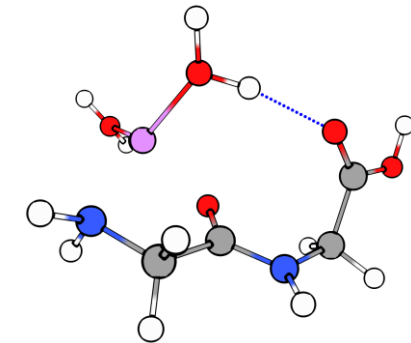
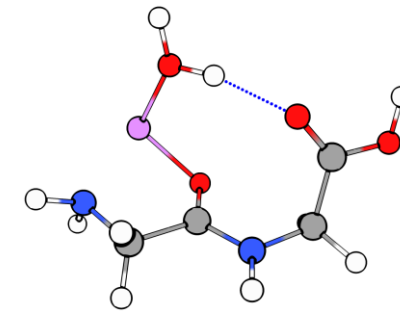
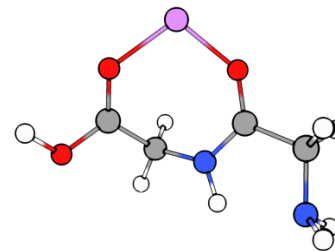
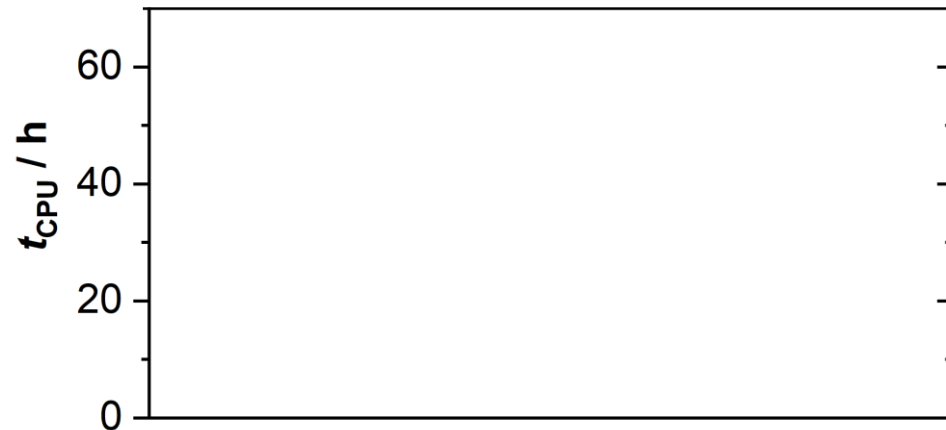
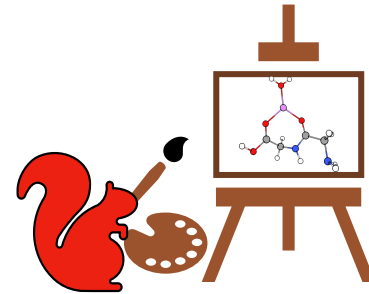
def2TZVP

B2PLYP-D3

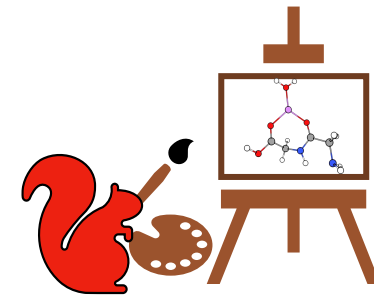
MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

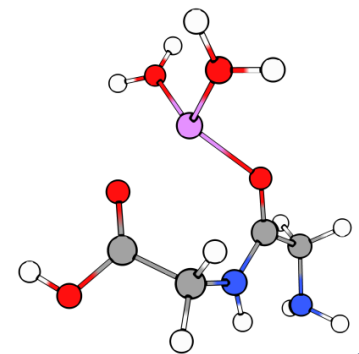
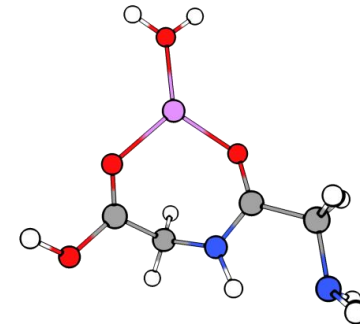
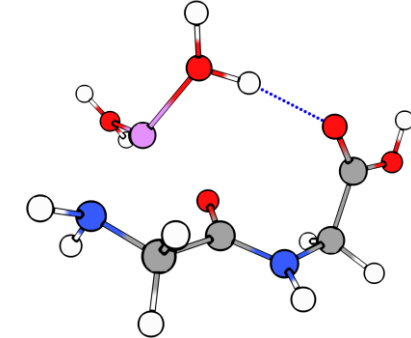
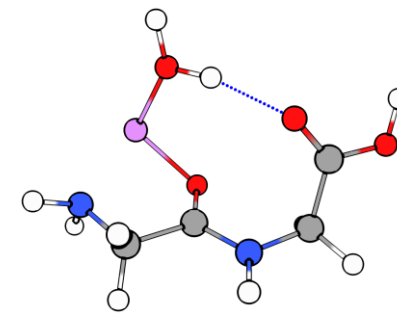
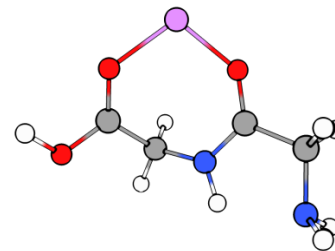
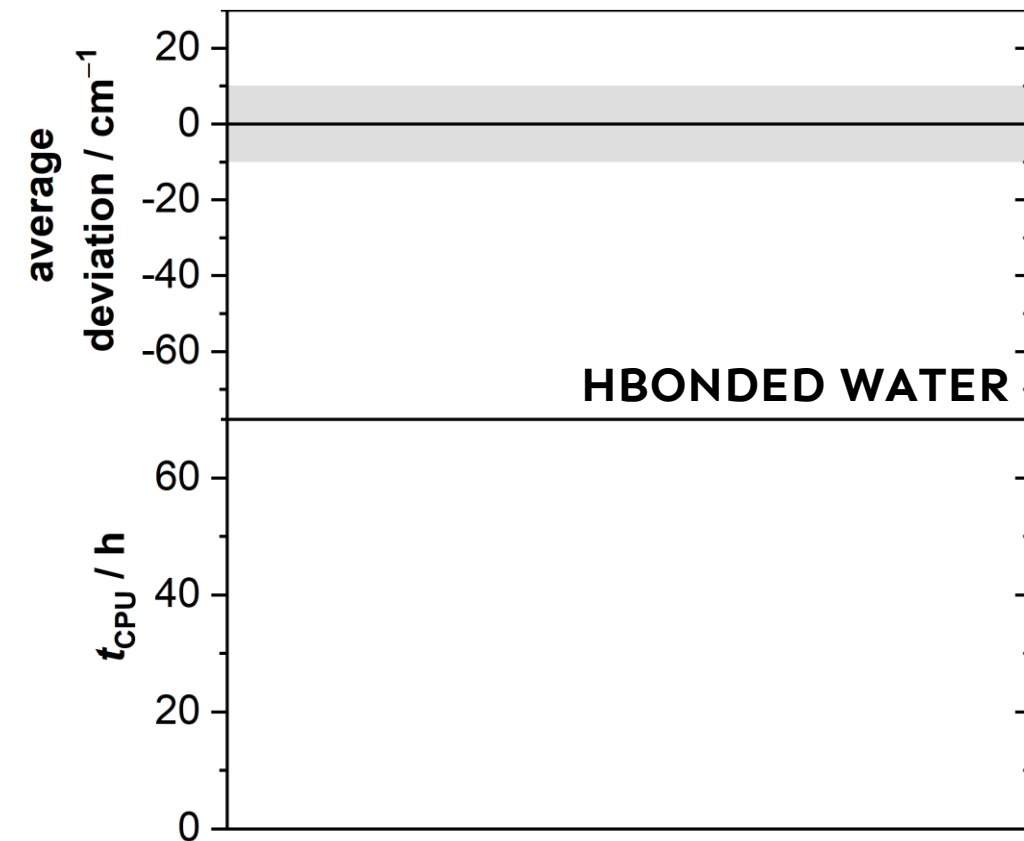
def2TZVP

B2PLYP-D3

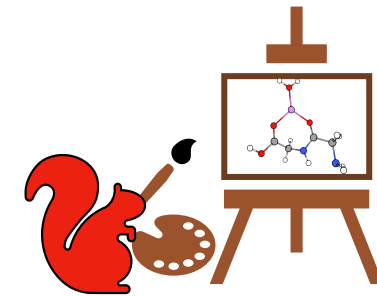
MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

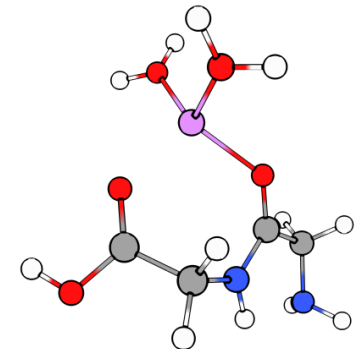
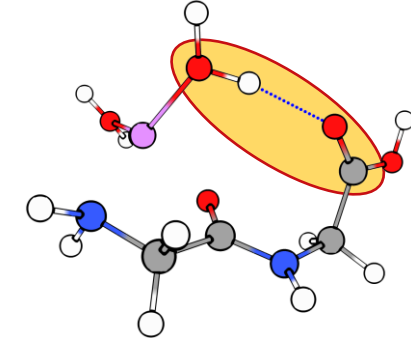
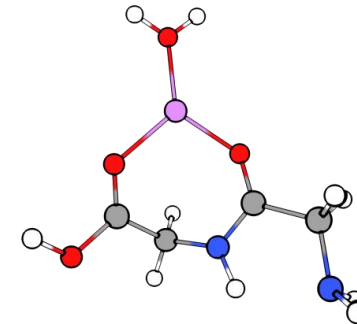
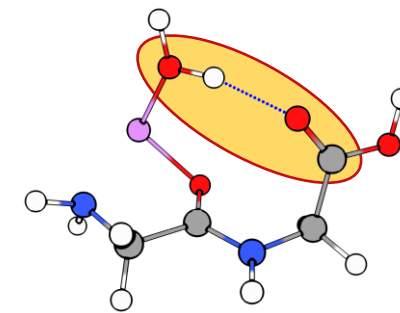
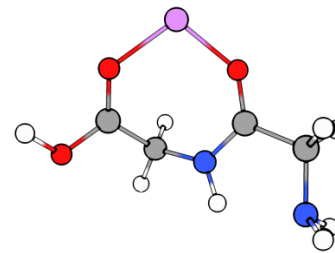
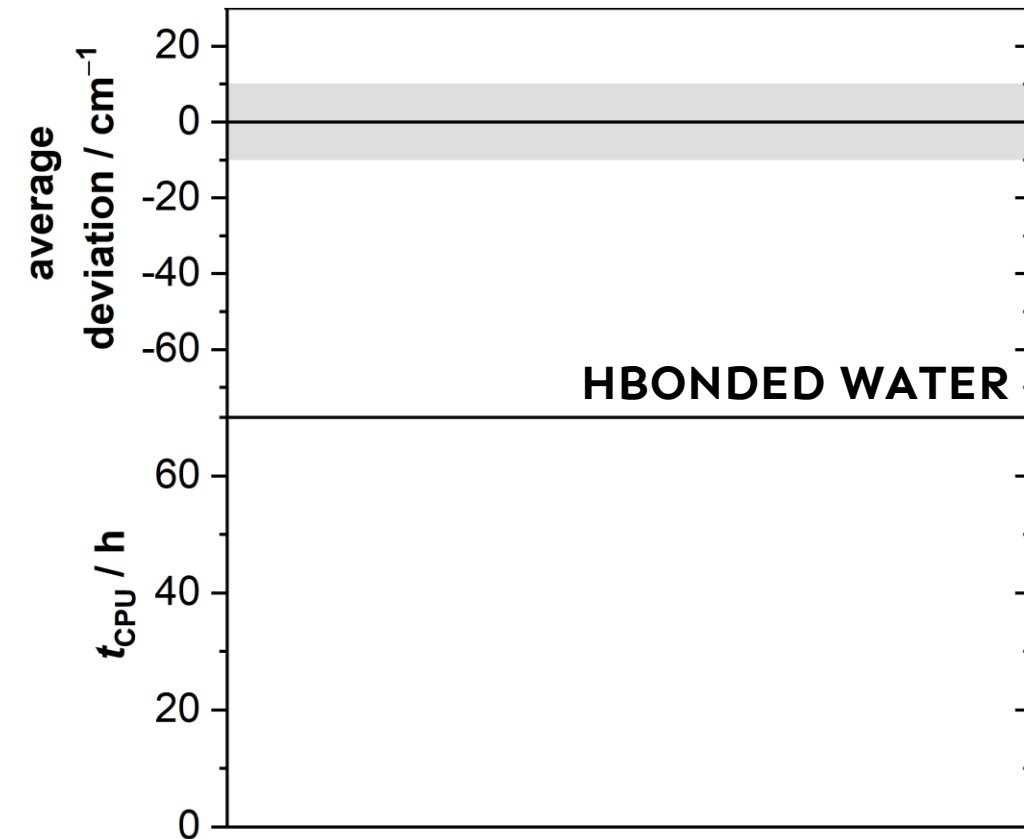
def2TZVP

B2PLYP-D3

MP2

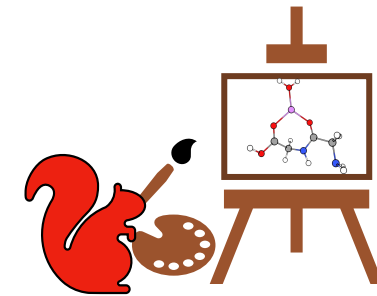
aVTZ

PM3





# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

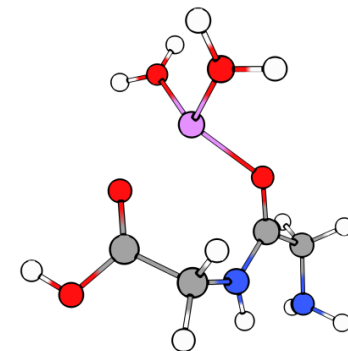
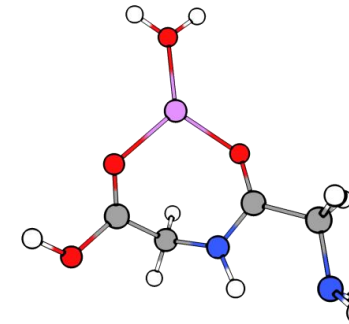
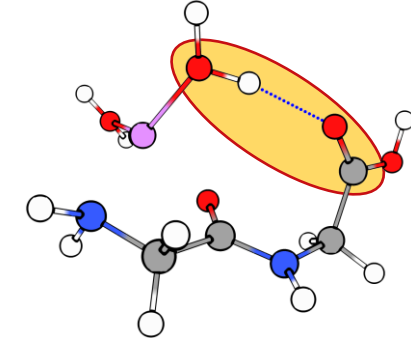
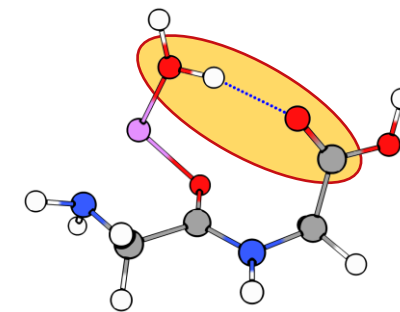
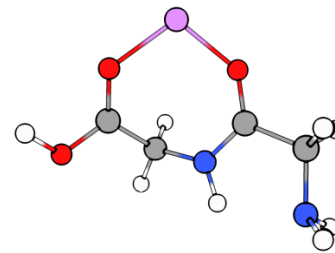
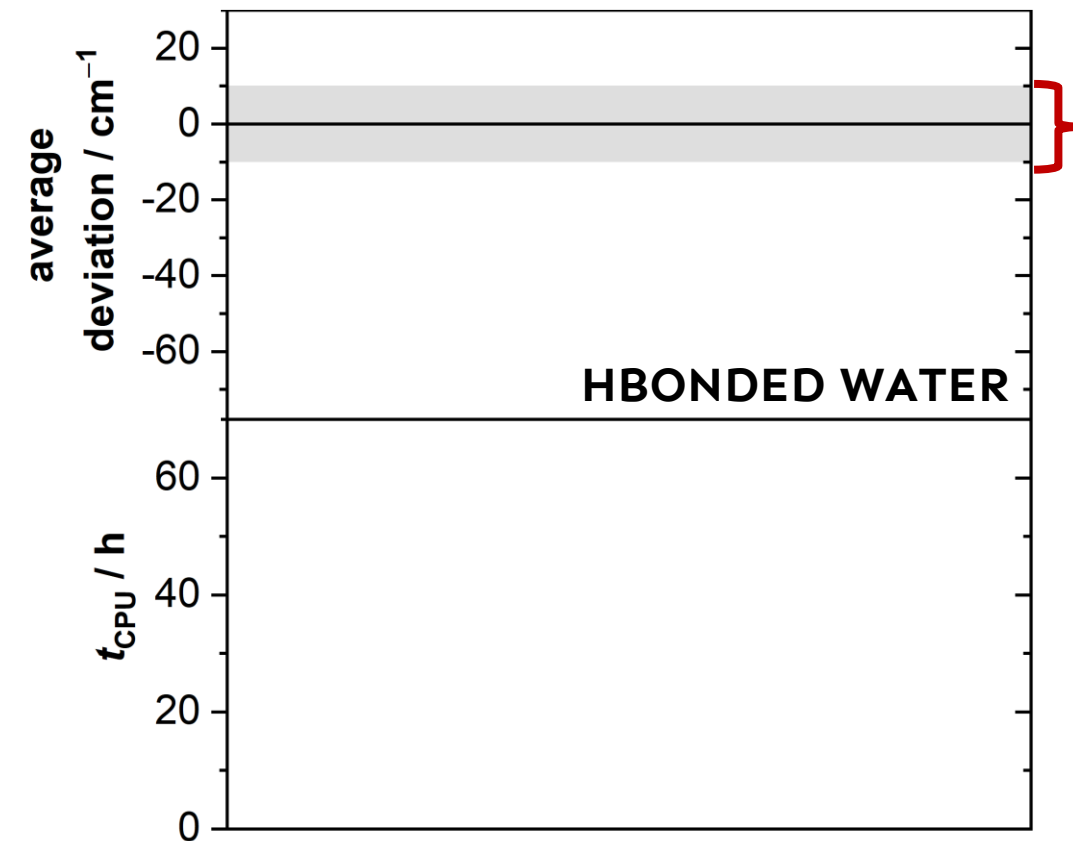
B2PLYP-D3

MP2

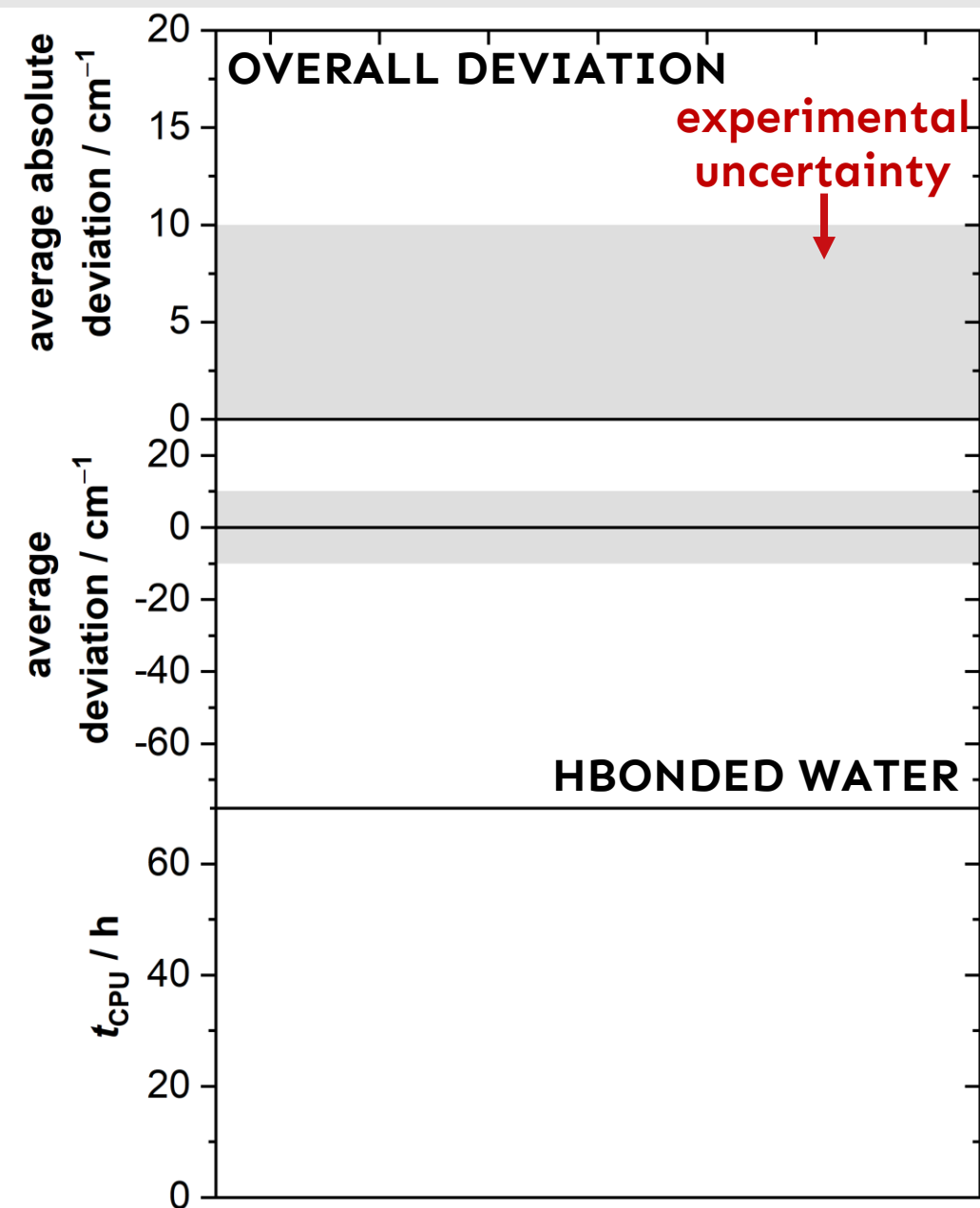
PM3

aVTZ

experimental  
uncertainty



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

ωB97XD

M06-2X

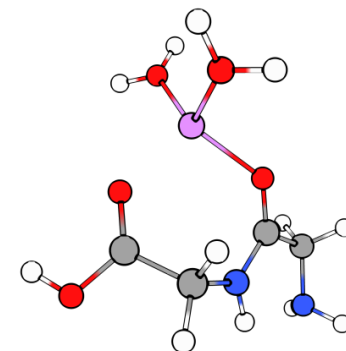
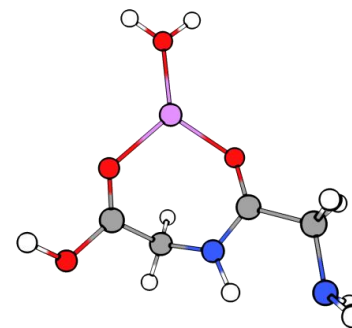
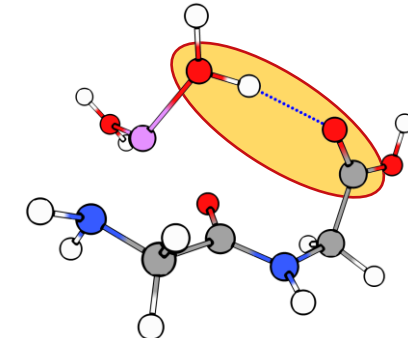
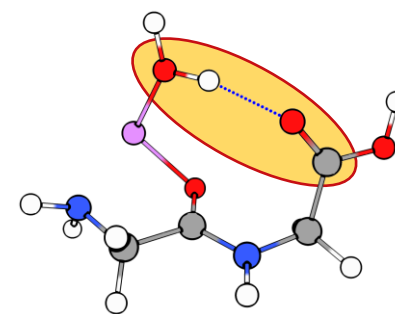
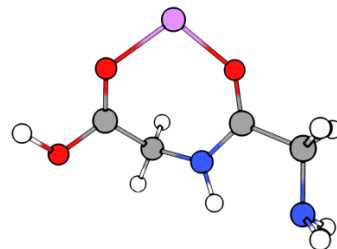
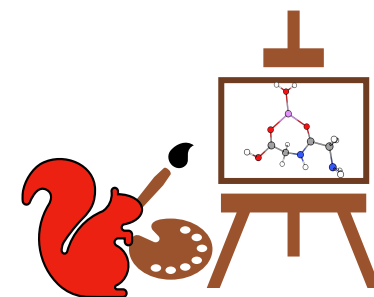
def2TZVP

B2PLYP-D3

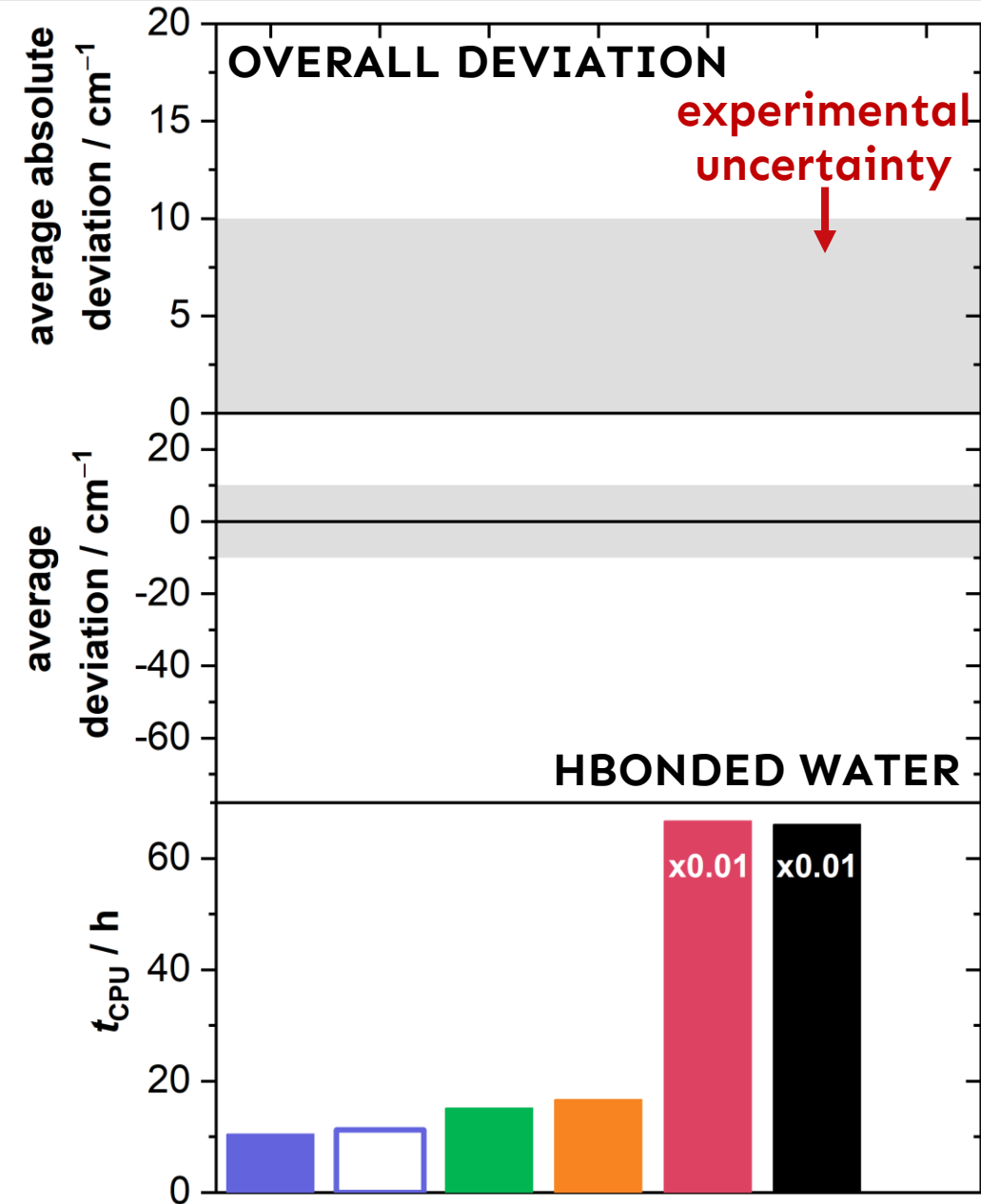
MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

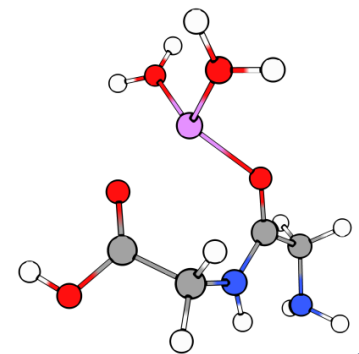
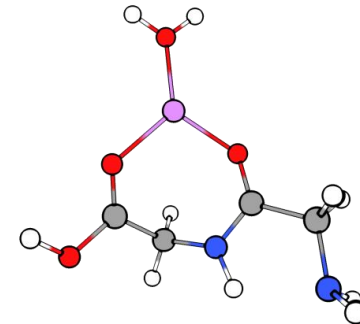
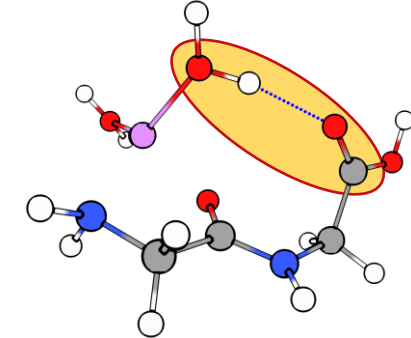
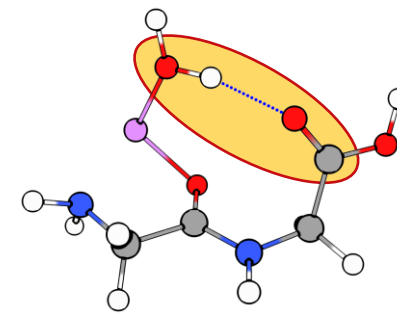
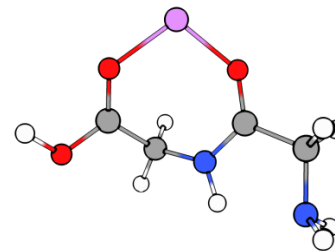
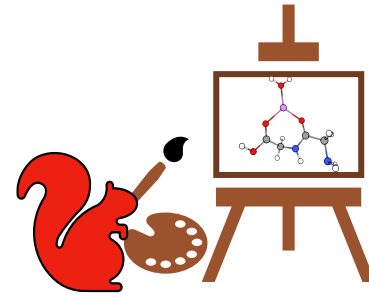
def2TZVP

B2PLYP-D3

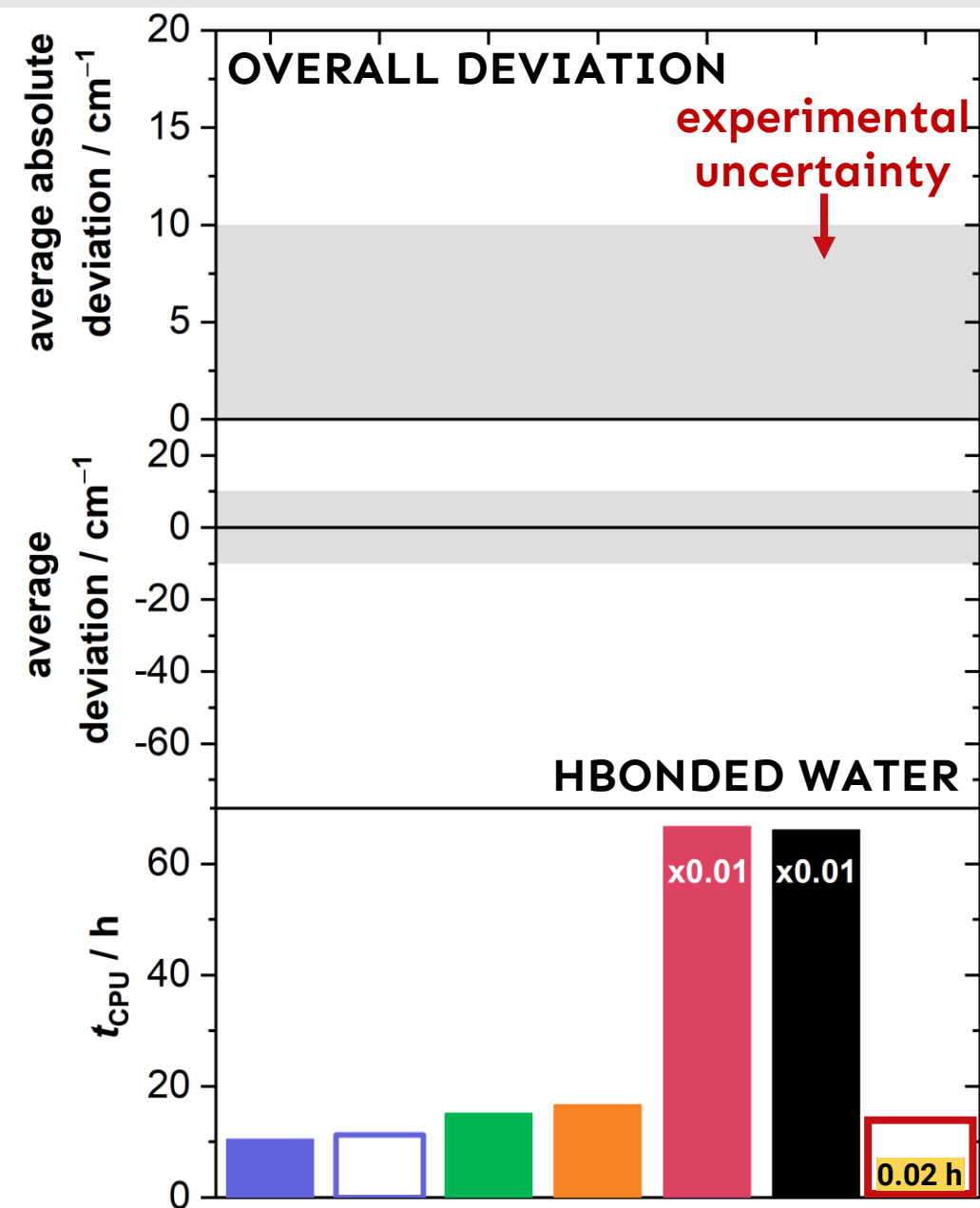
MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

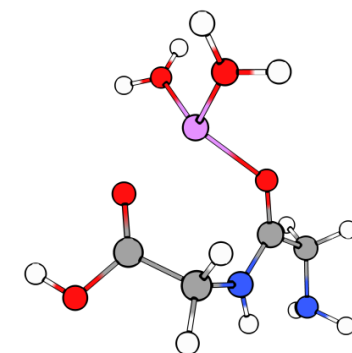
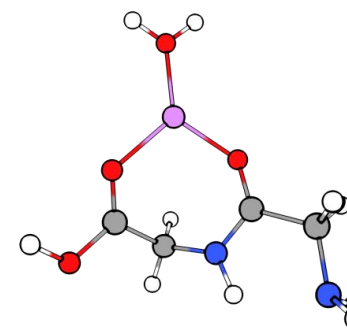
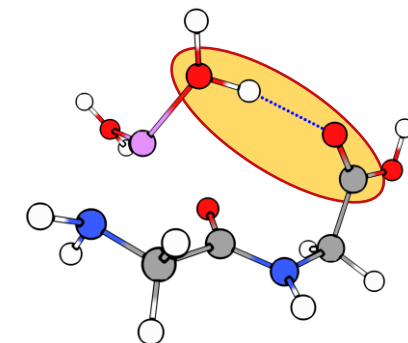
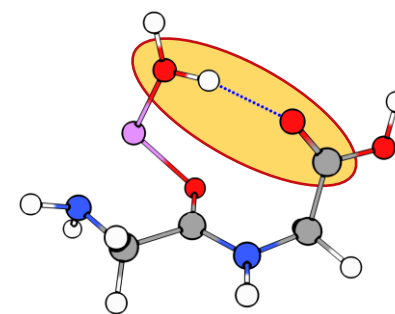
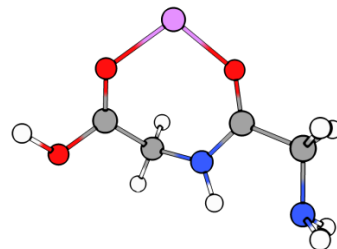
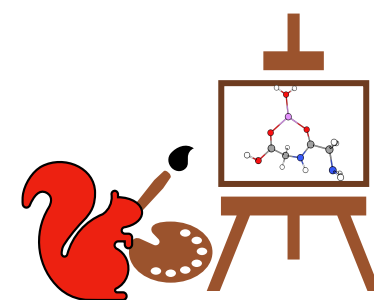
def2TZVP

B2PLYP-D3

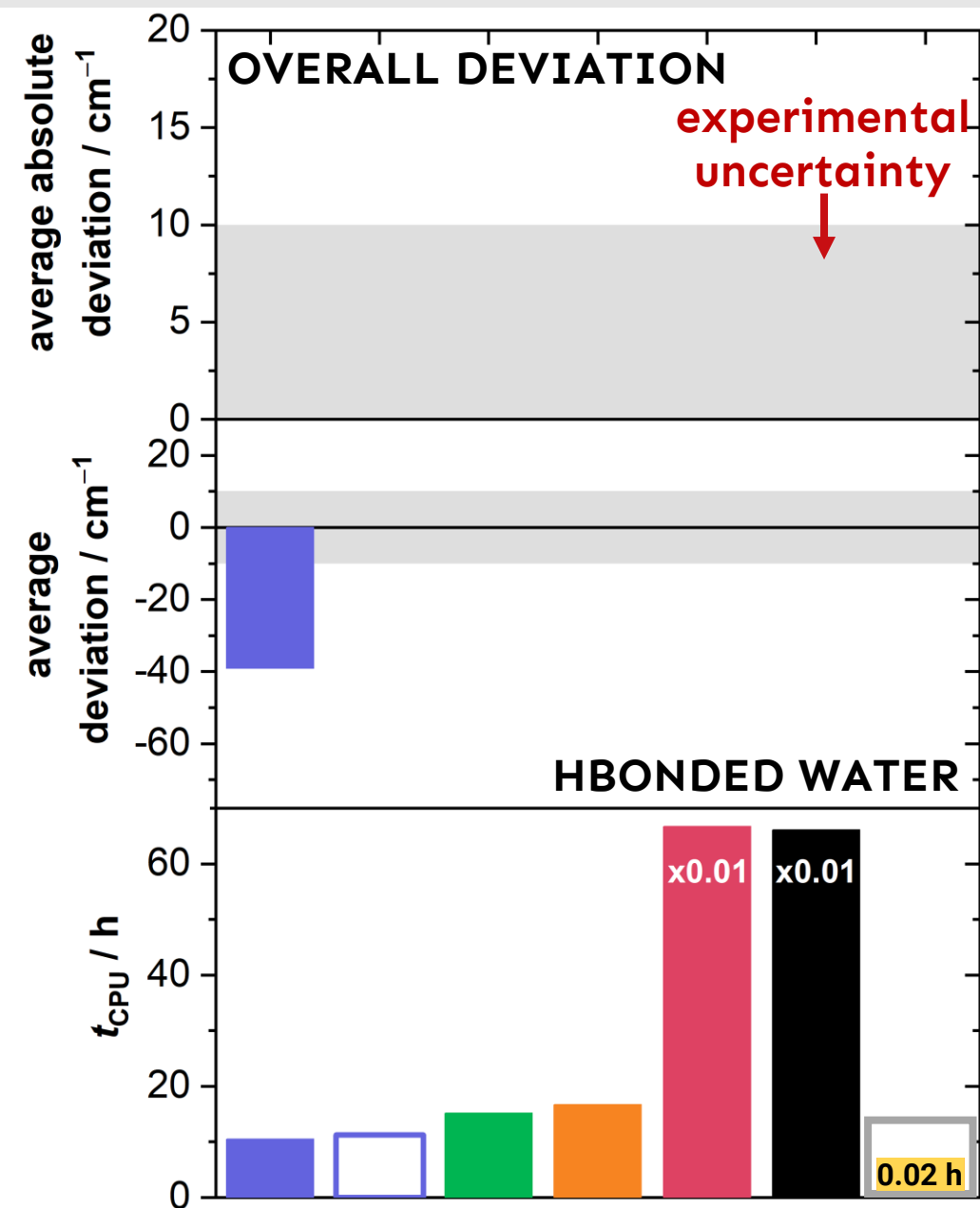
MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

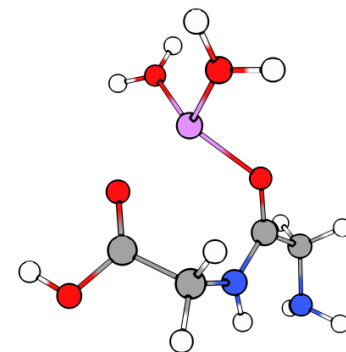
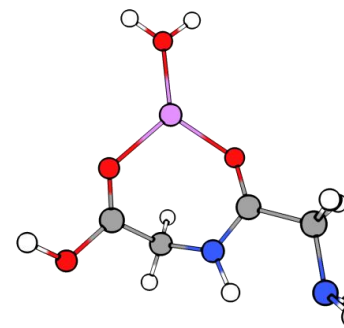
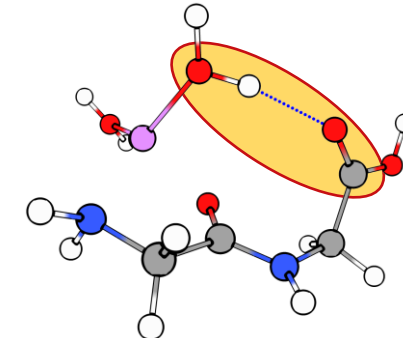
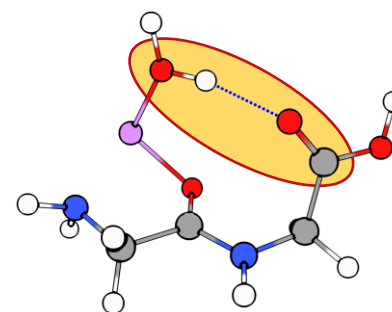
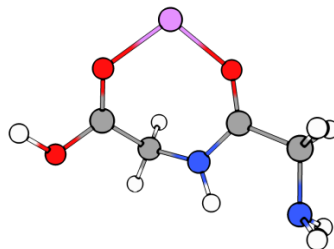
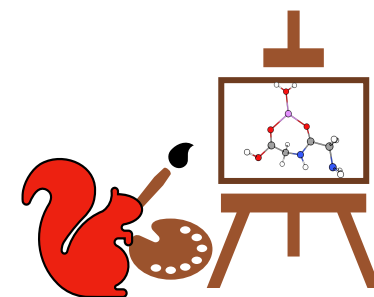
def2TZVP

B2PLYP-D3

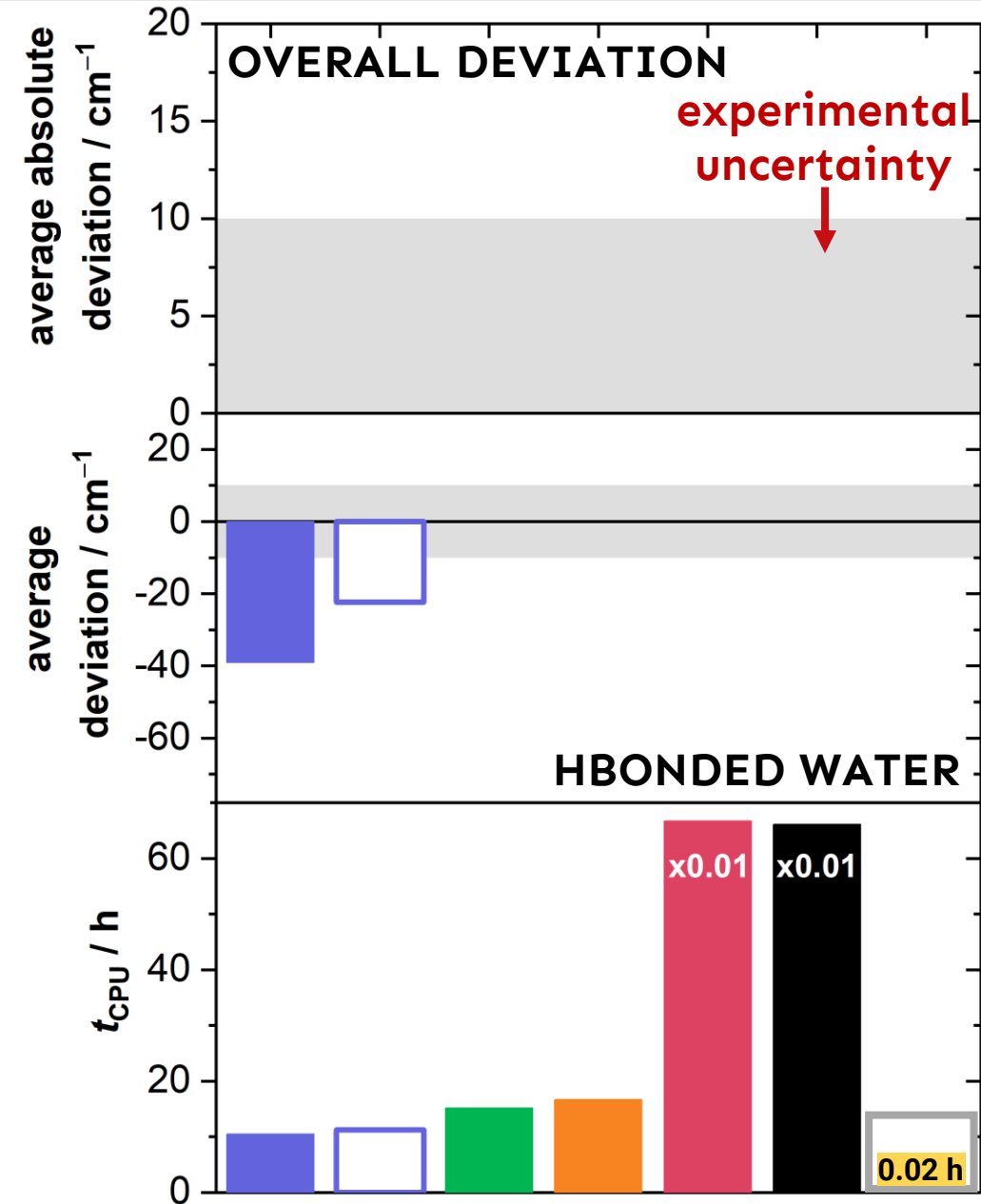
MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

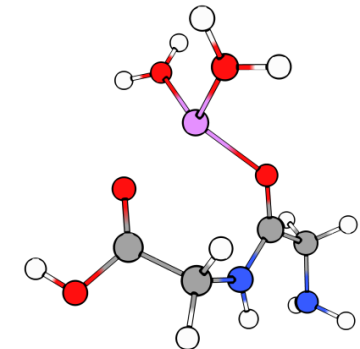
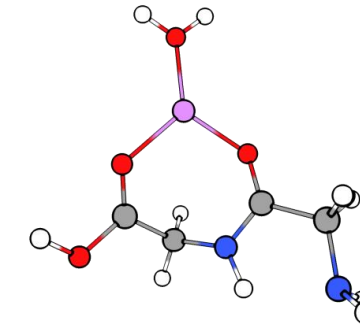
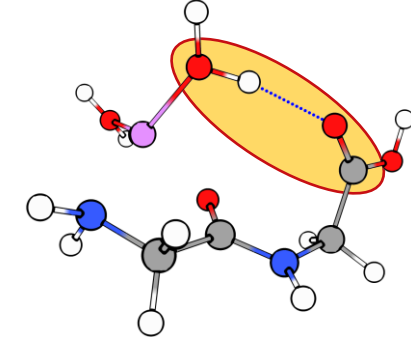
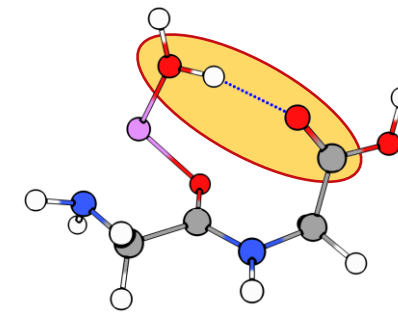
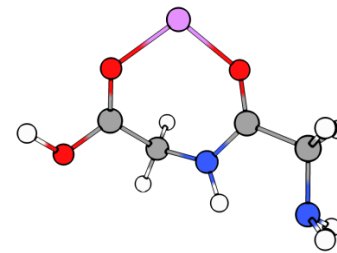
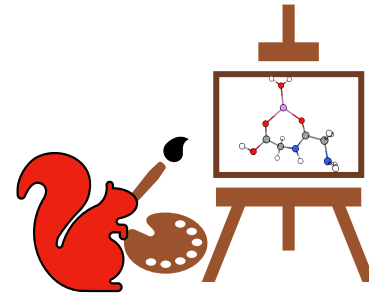
def2TZVP

B2PLYP-D3

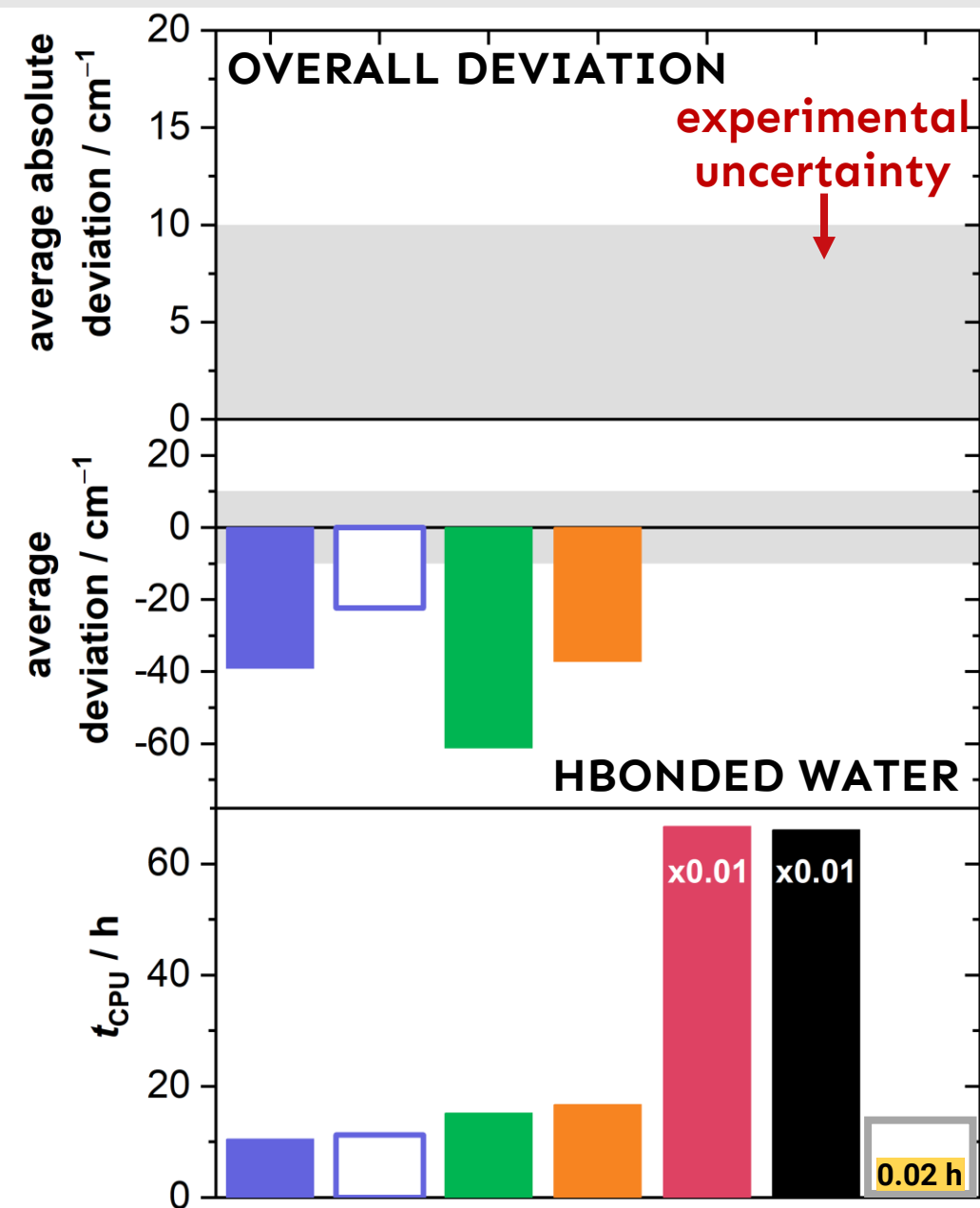
MP2

PM3

aVTZ



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

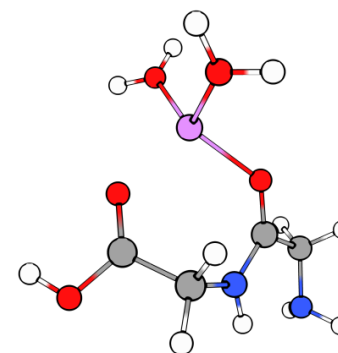
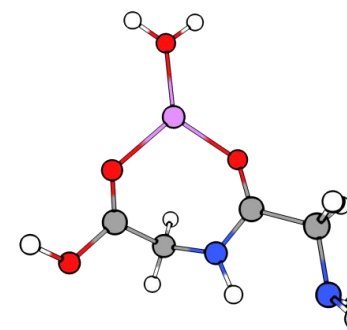
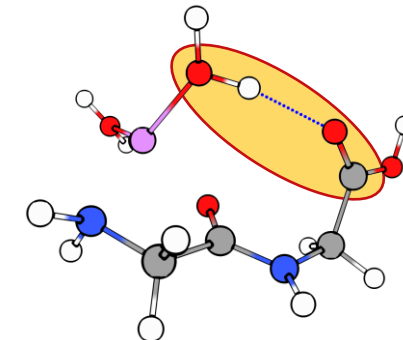
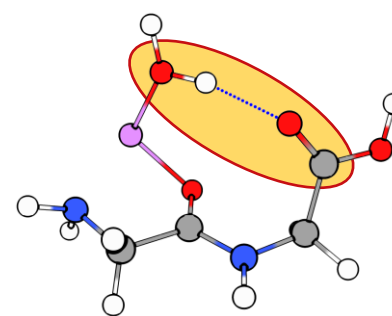
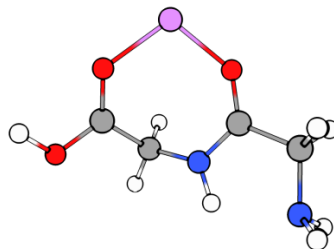
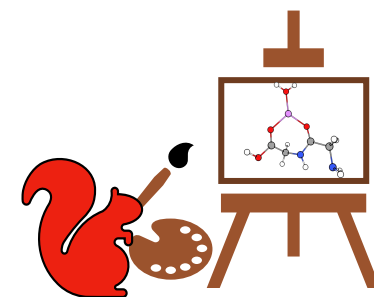
def2TZVP

B2PLYP-D3

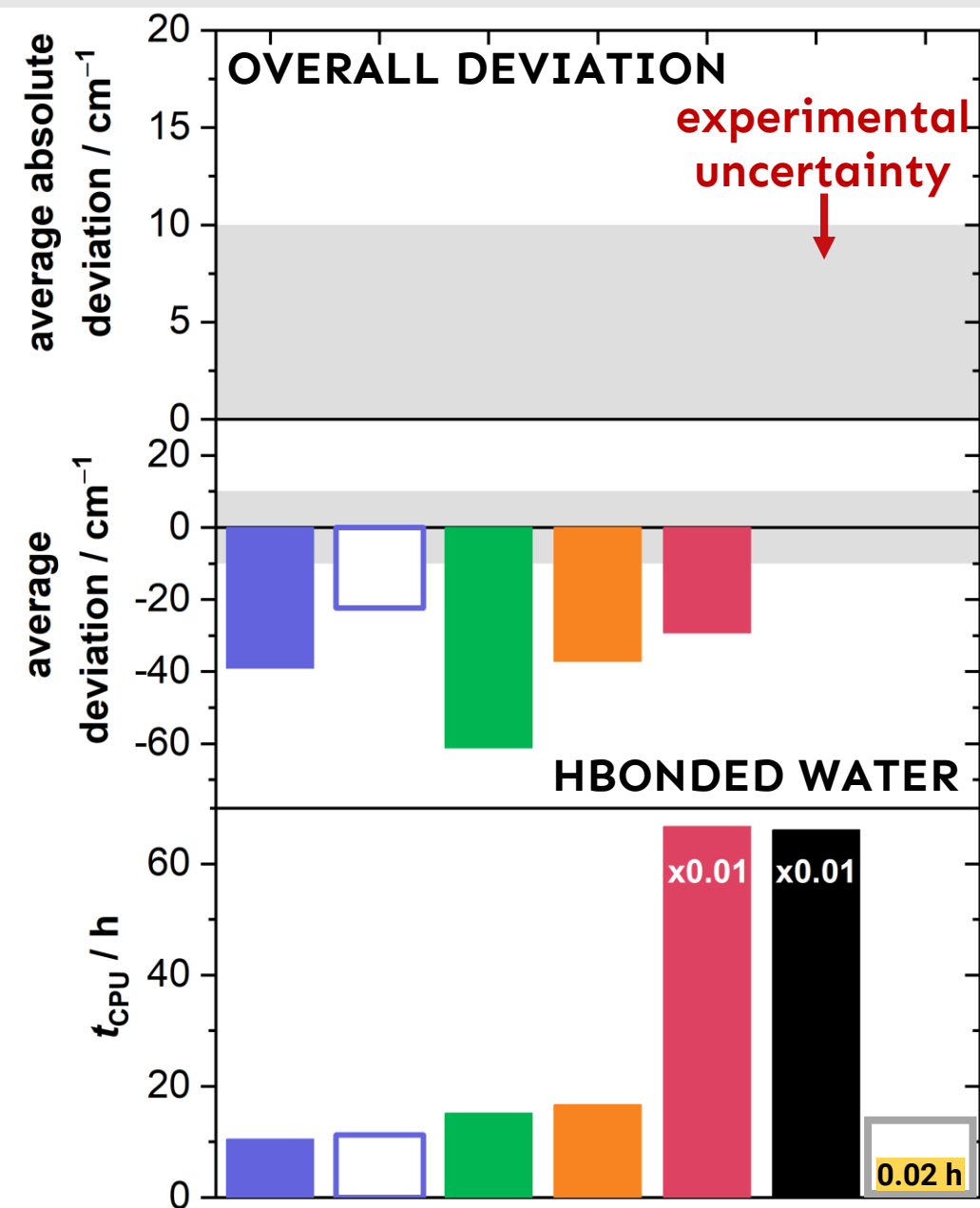
MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

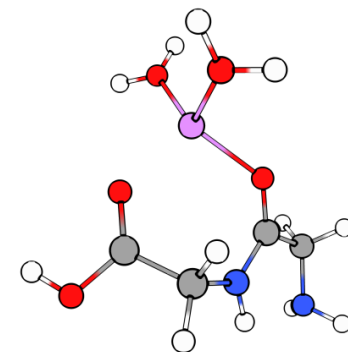
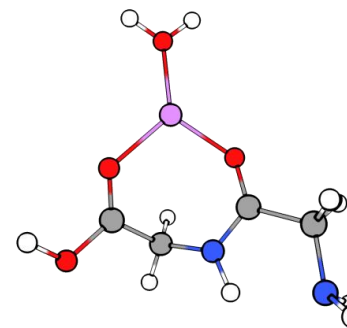
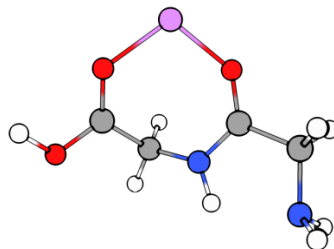
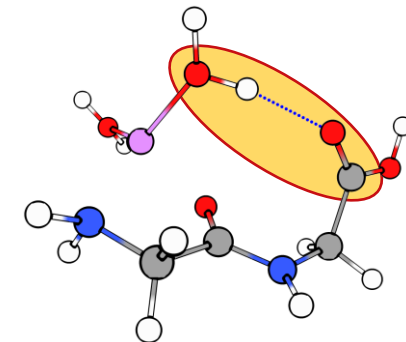
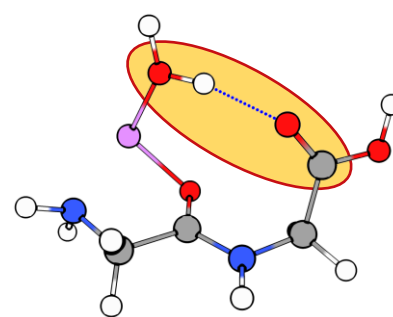
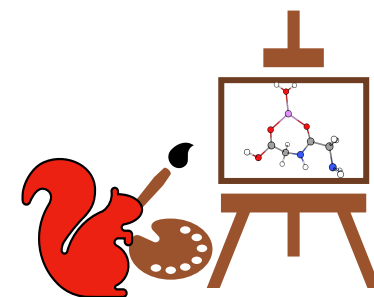
def2TZVP

B2PLYP-D3

MP2

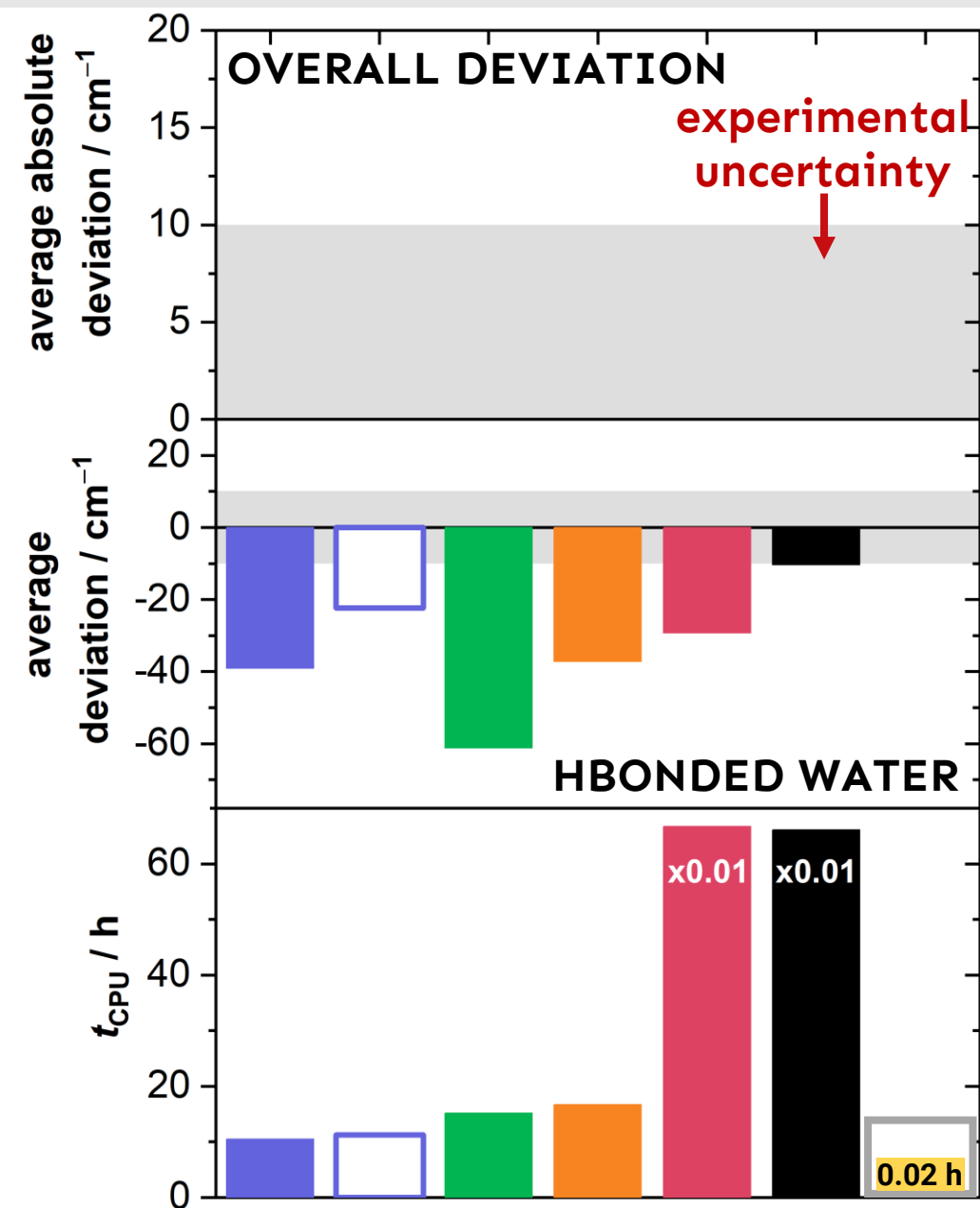
aVTZ

PM3





# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

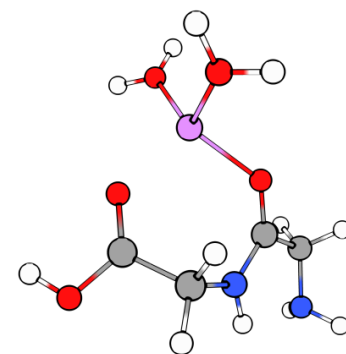
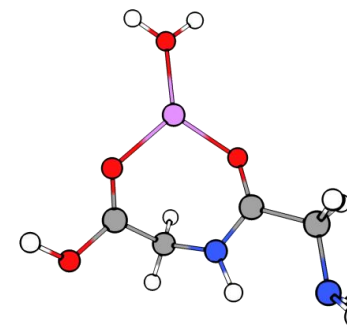
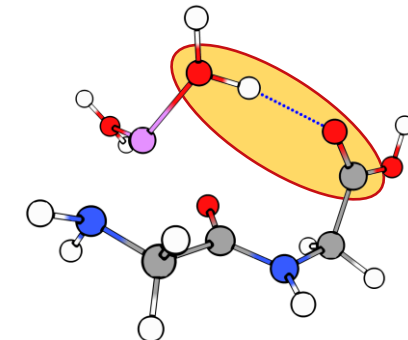
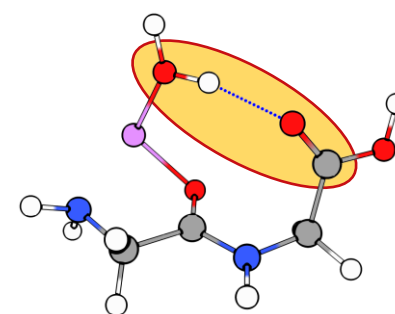
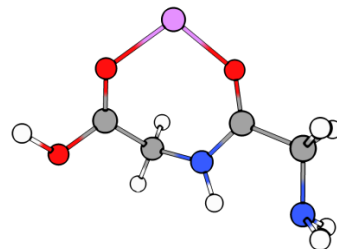
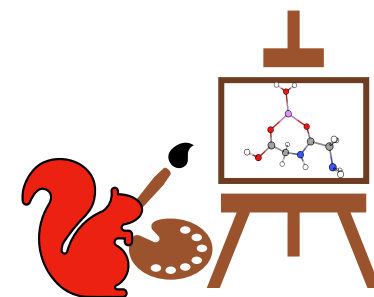
def2TZVP

B2PLYP-D3

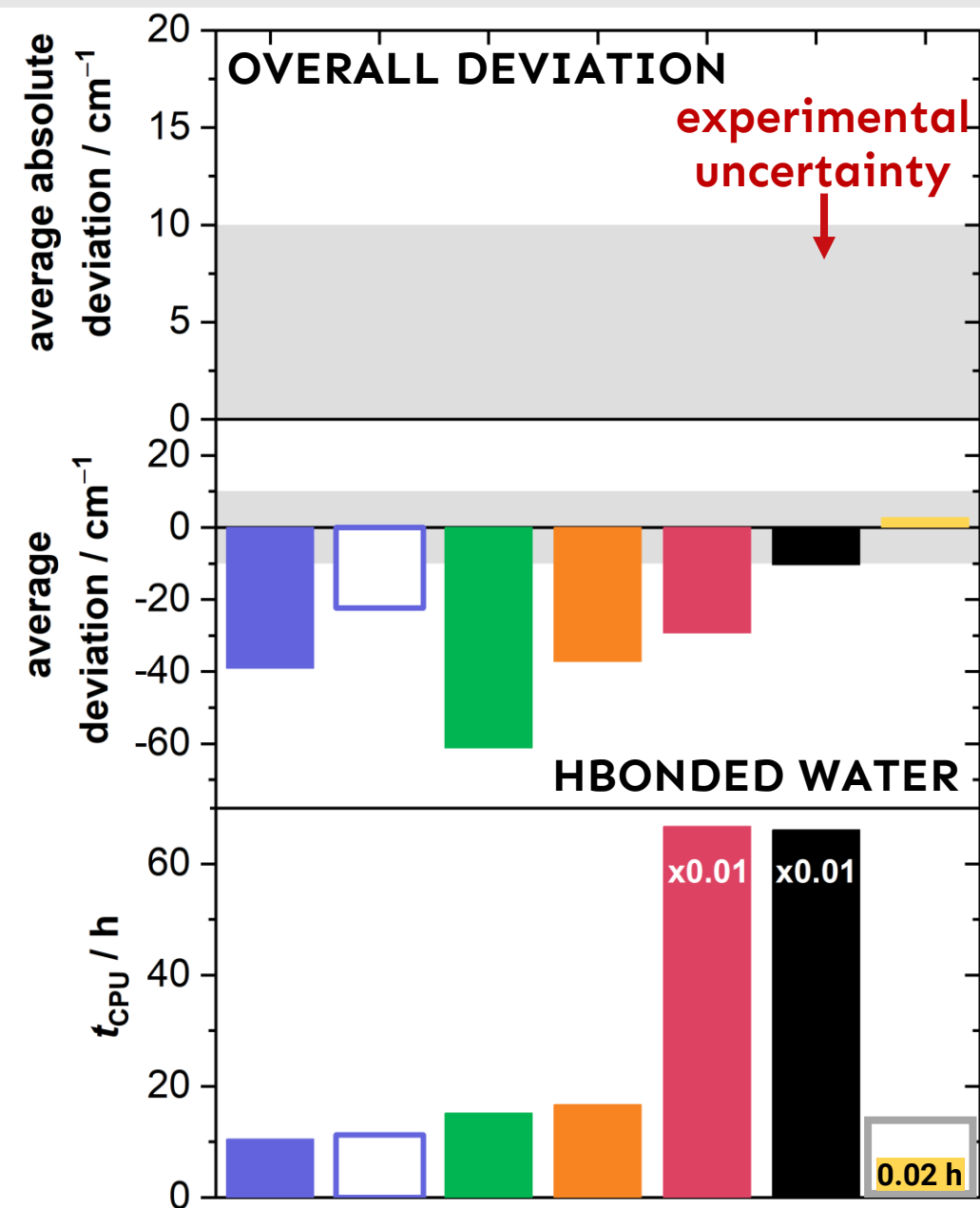
MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

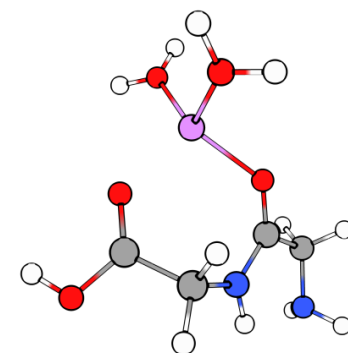
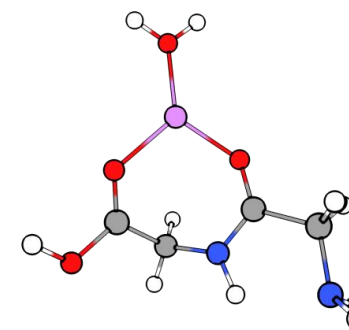
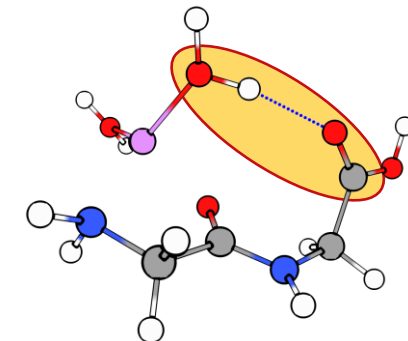
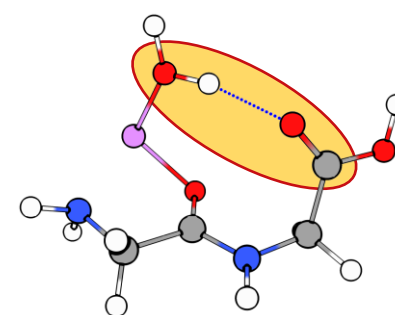
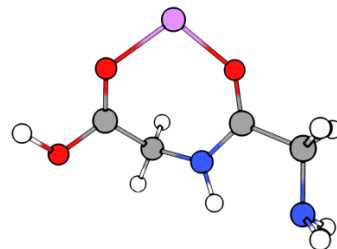
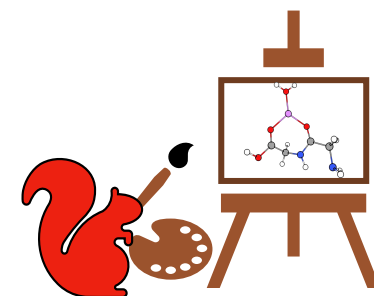
def2TZVP

B2PLYP-D3

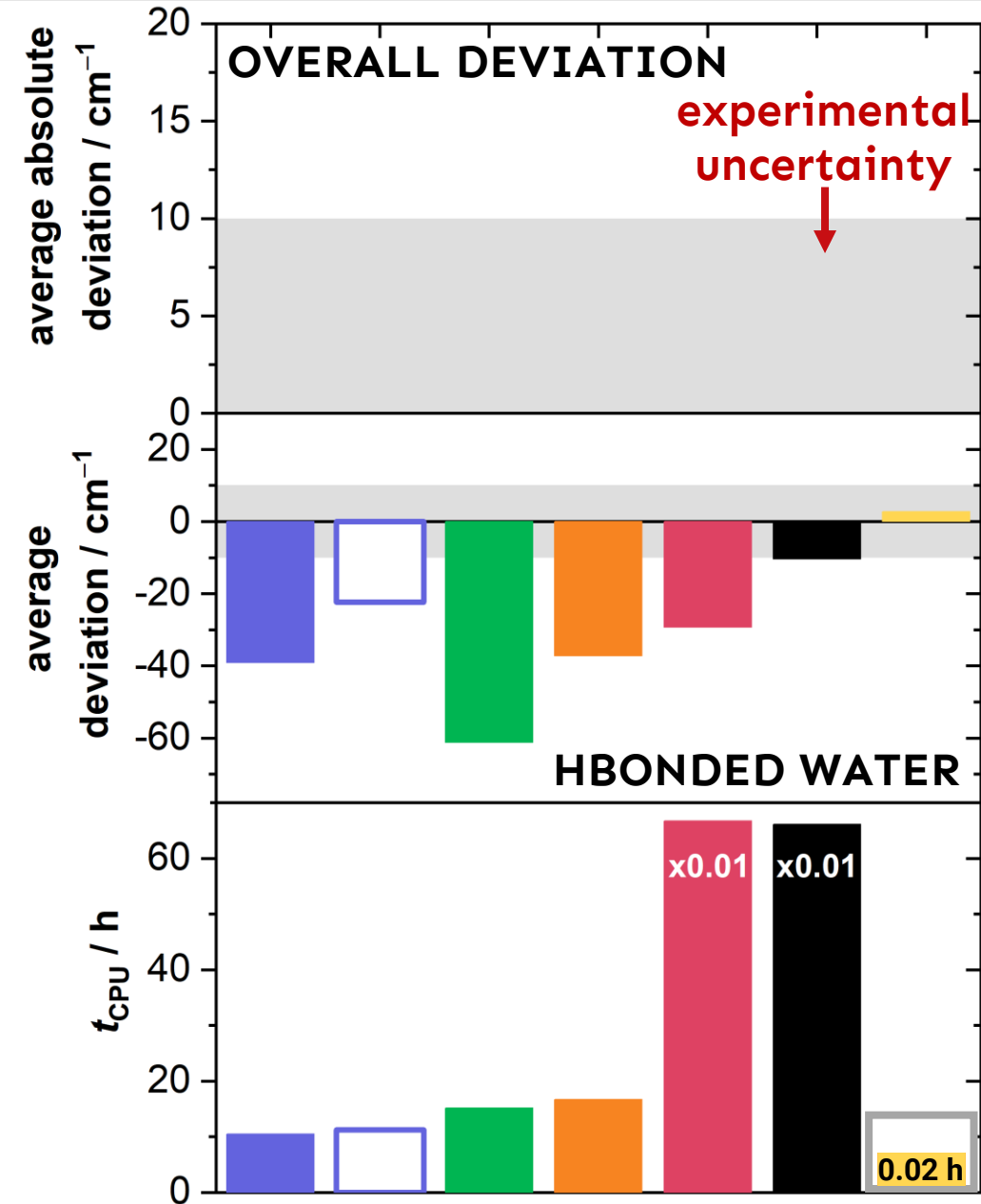
MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

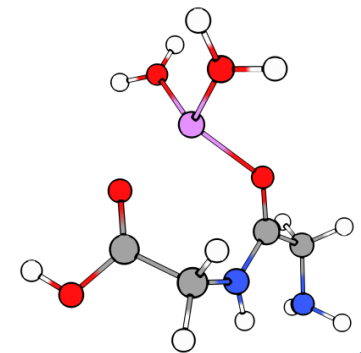
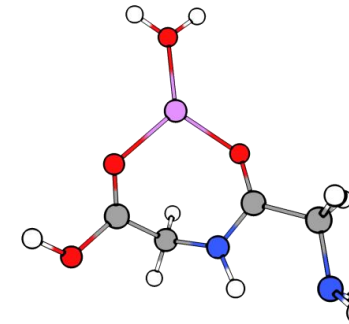
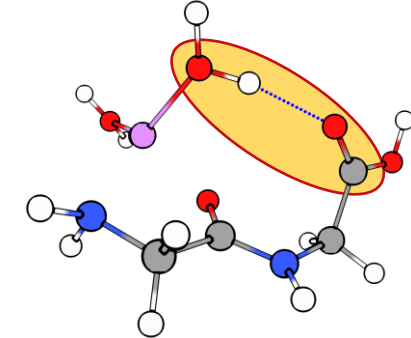
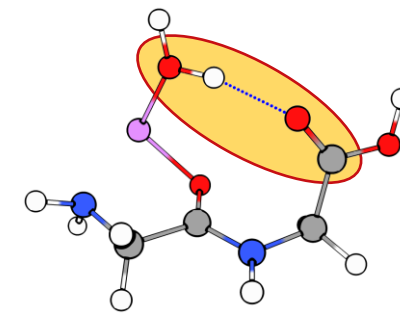
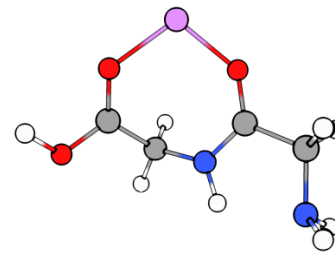
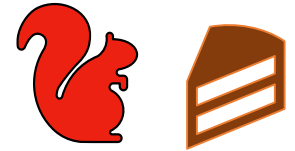
def2TZVP

B2PLYP-D3

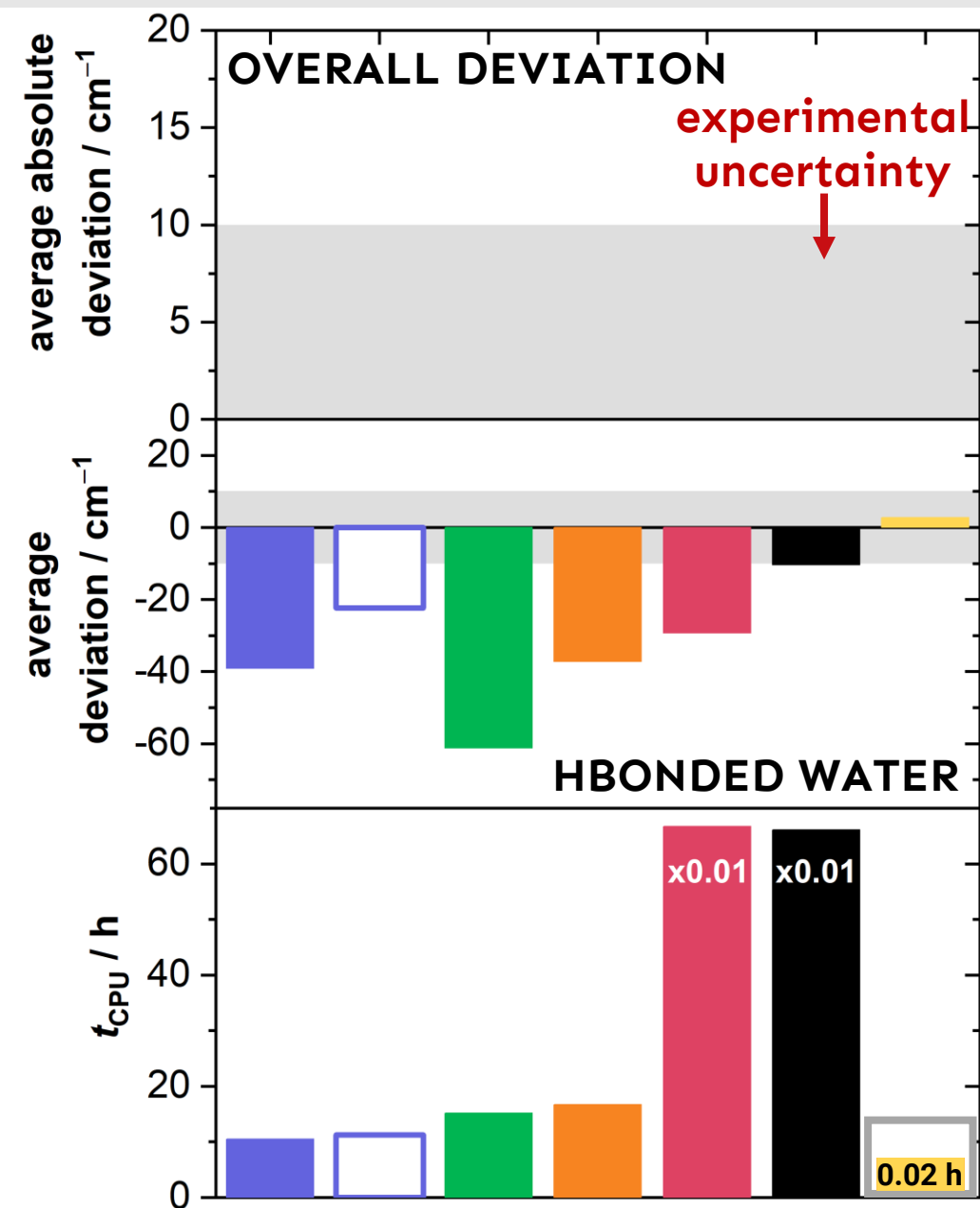
MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

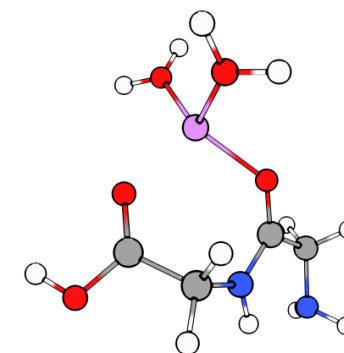
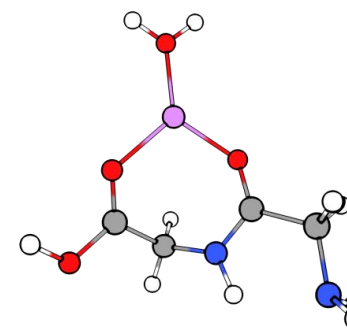
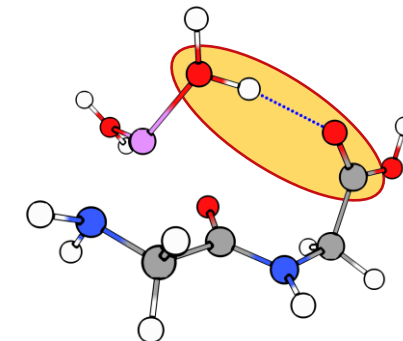
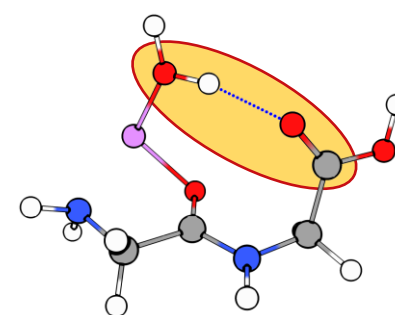
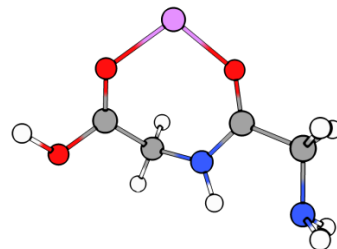
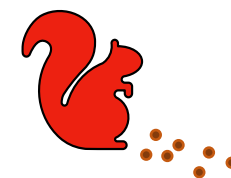
def2TZVP

B2PLYP-D3

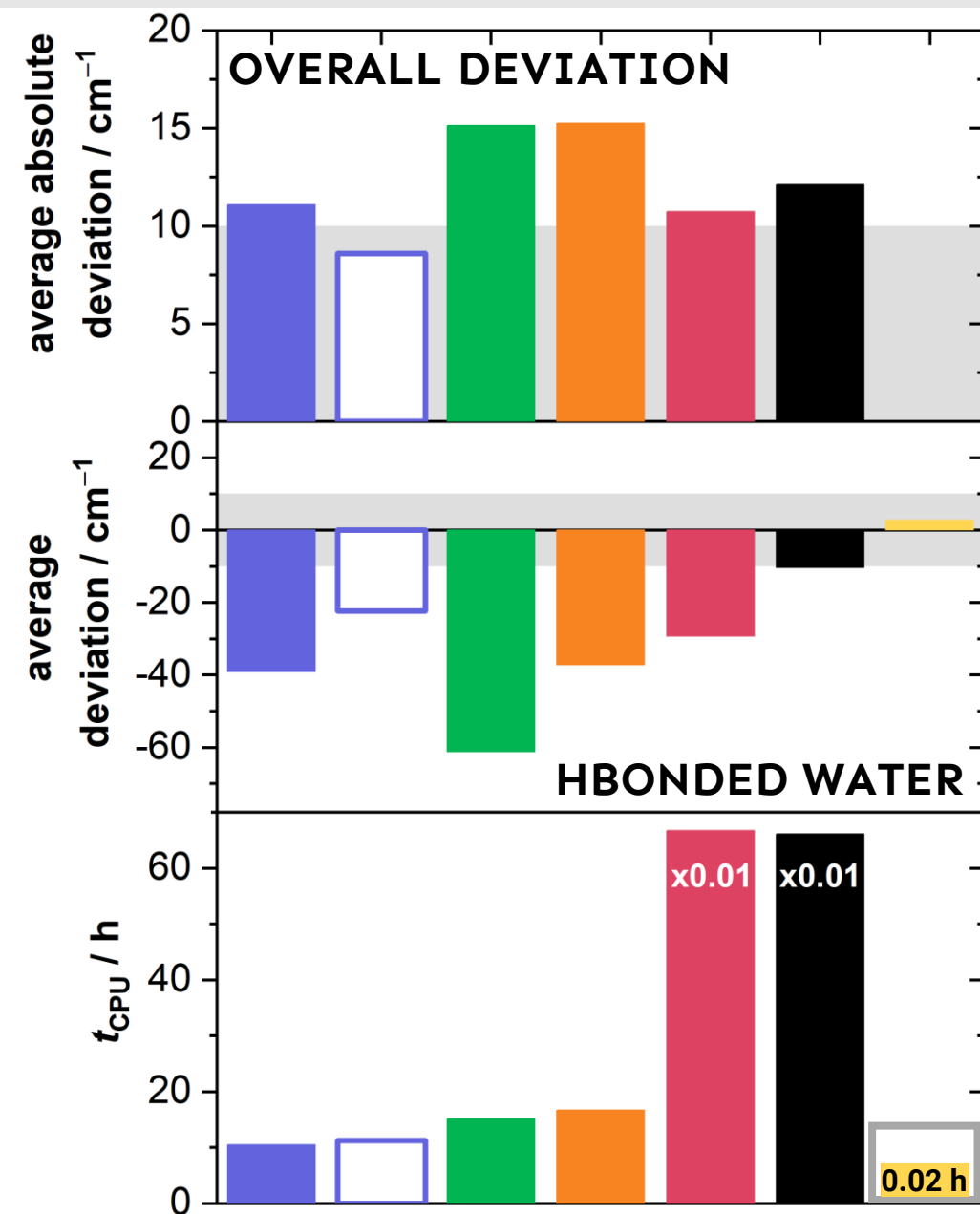
MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

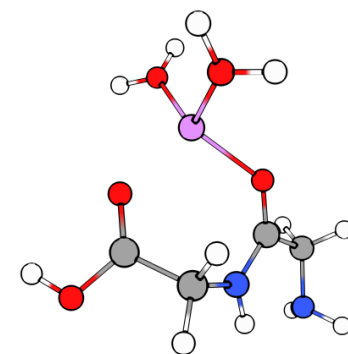
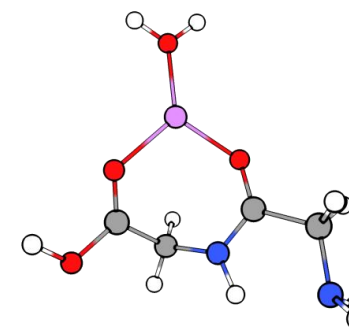
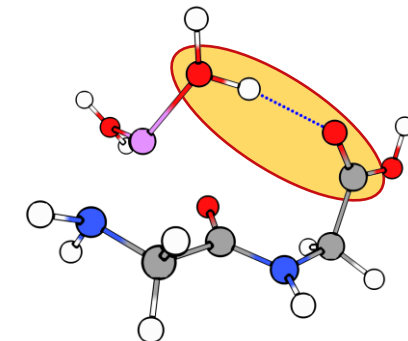
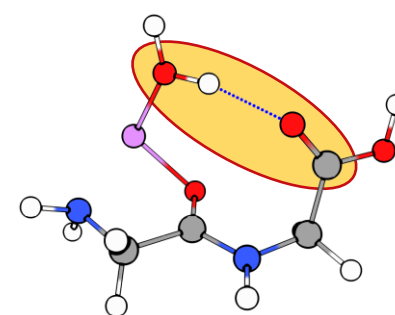
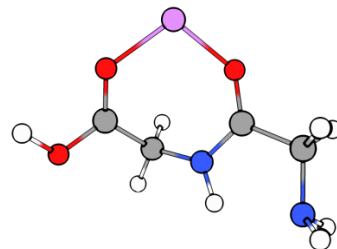
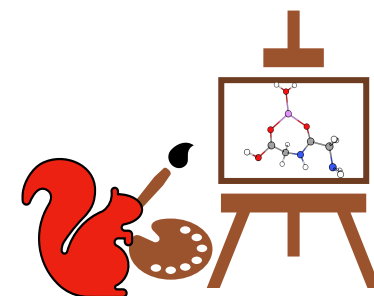
def2TZVP

B2PLYP-D3

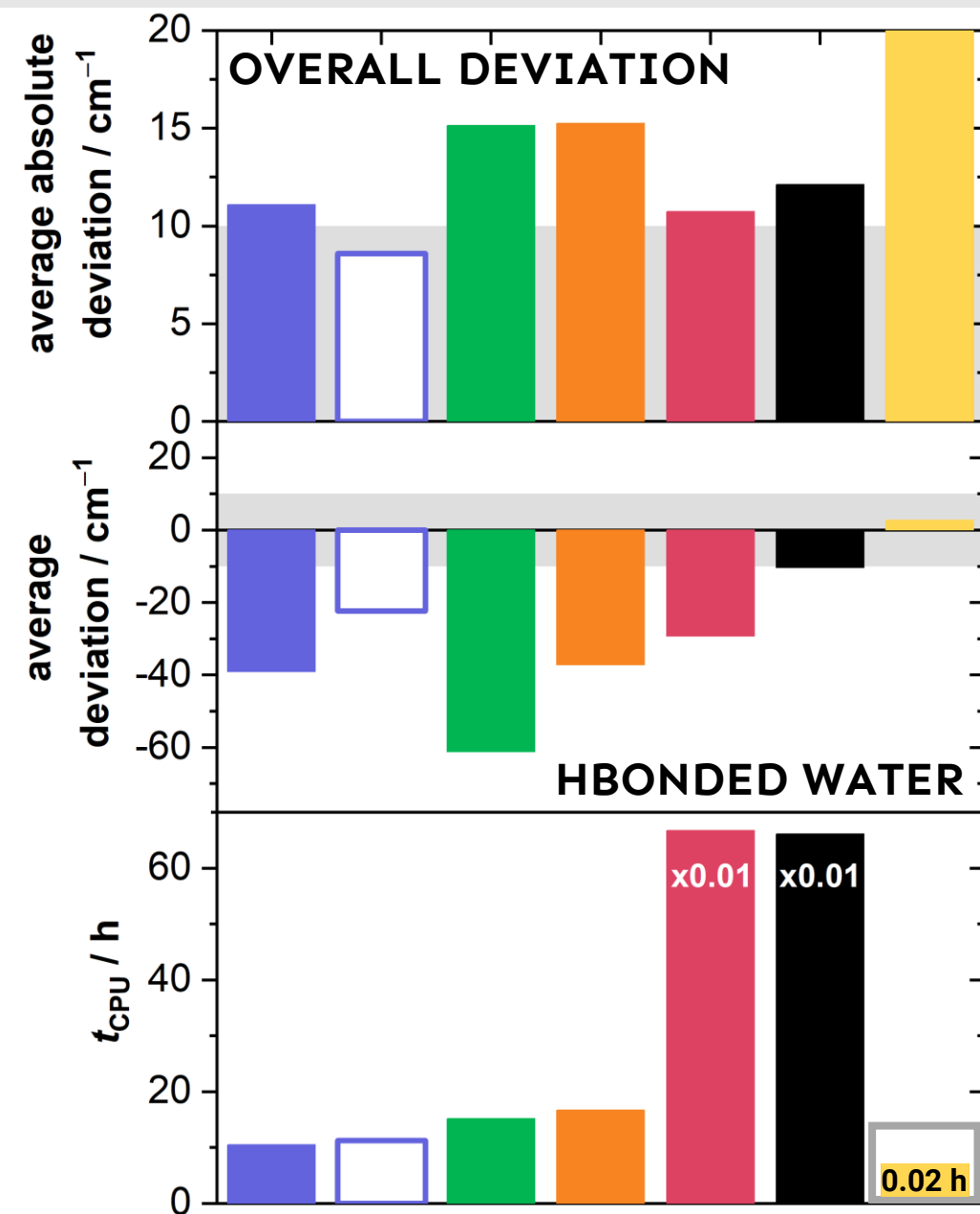
MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

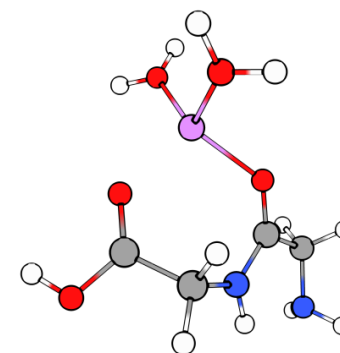
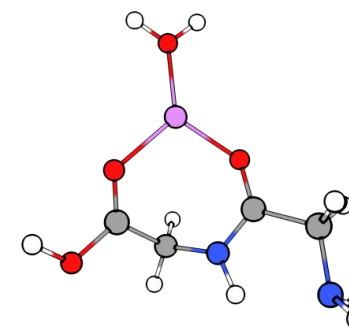
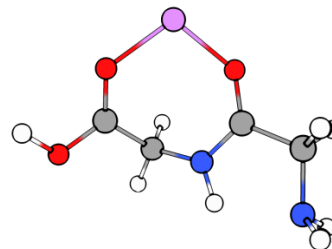
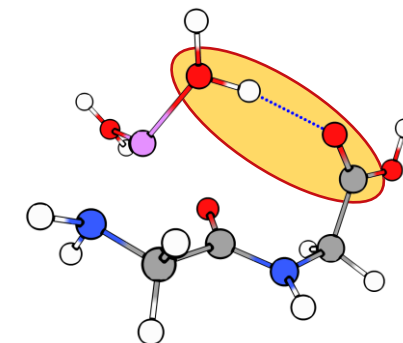
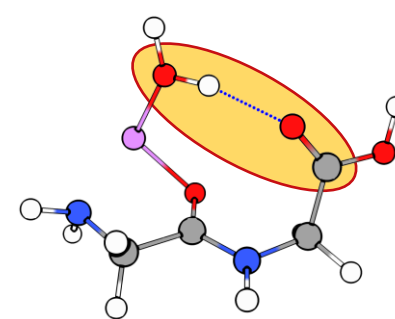
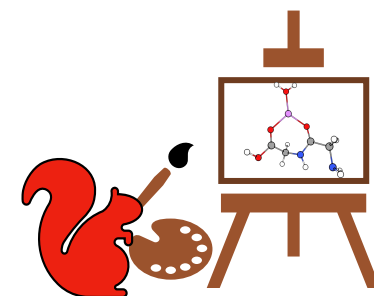
def2TZVP

B2PLYP-D3

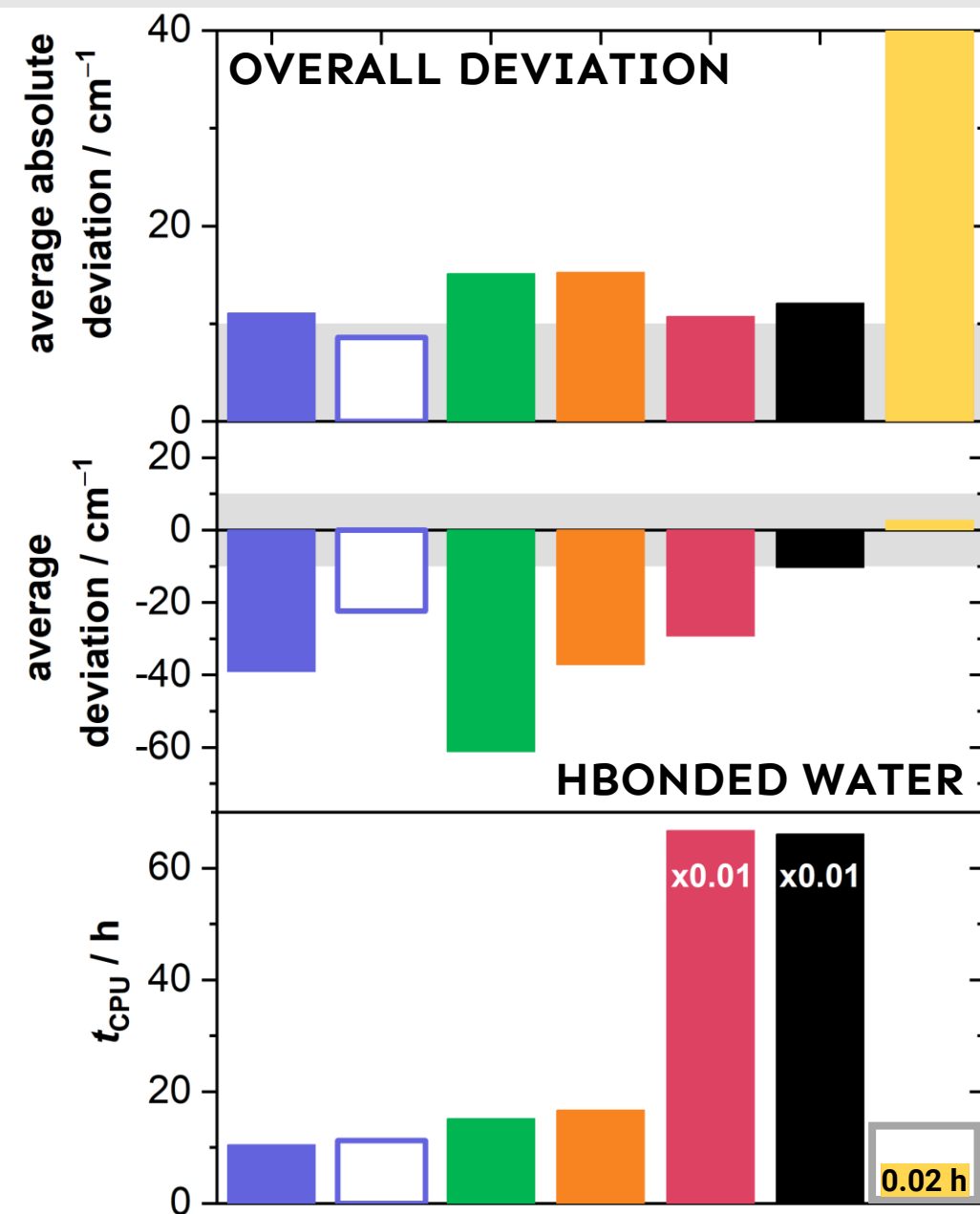
MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

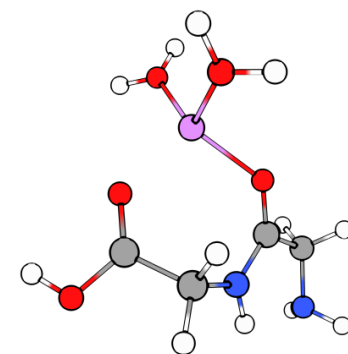
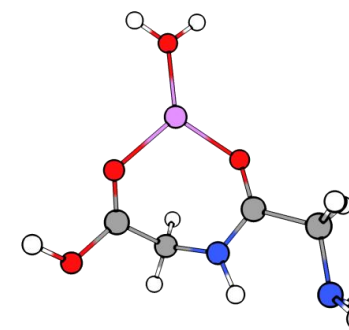
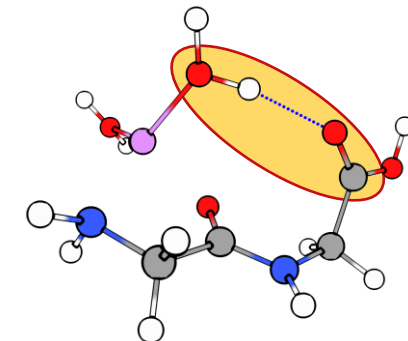
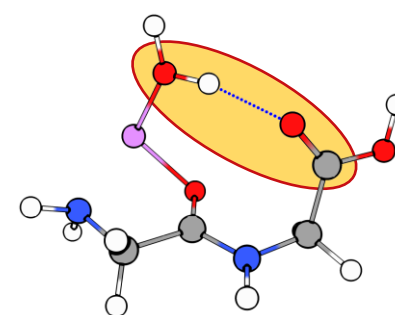
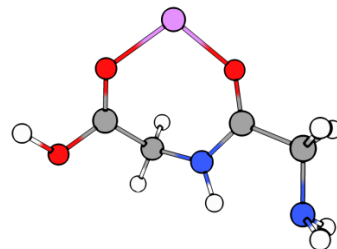
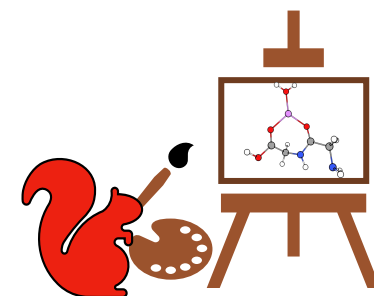
def2TZVP

B2PLYP-D3

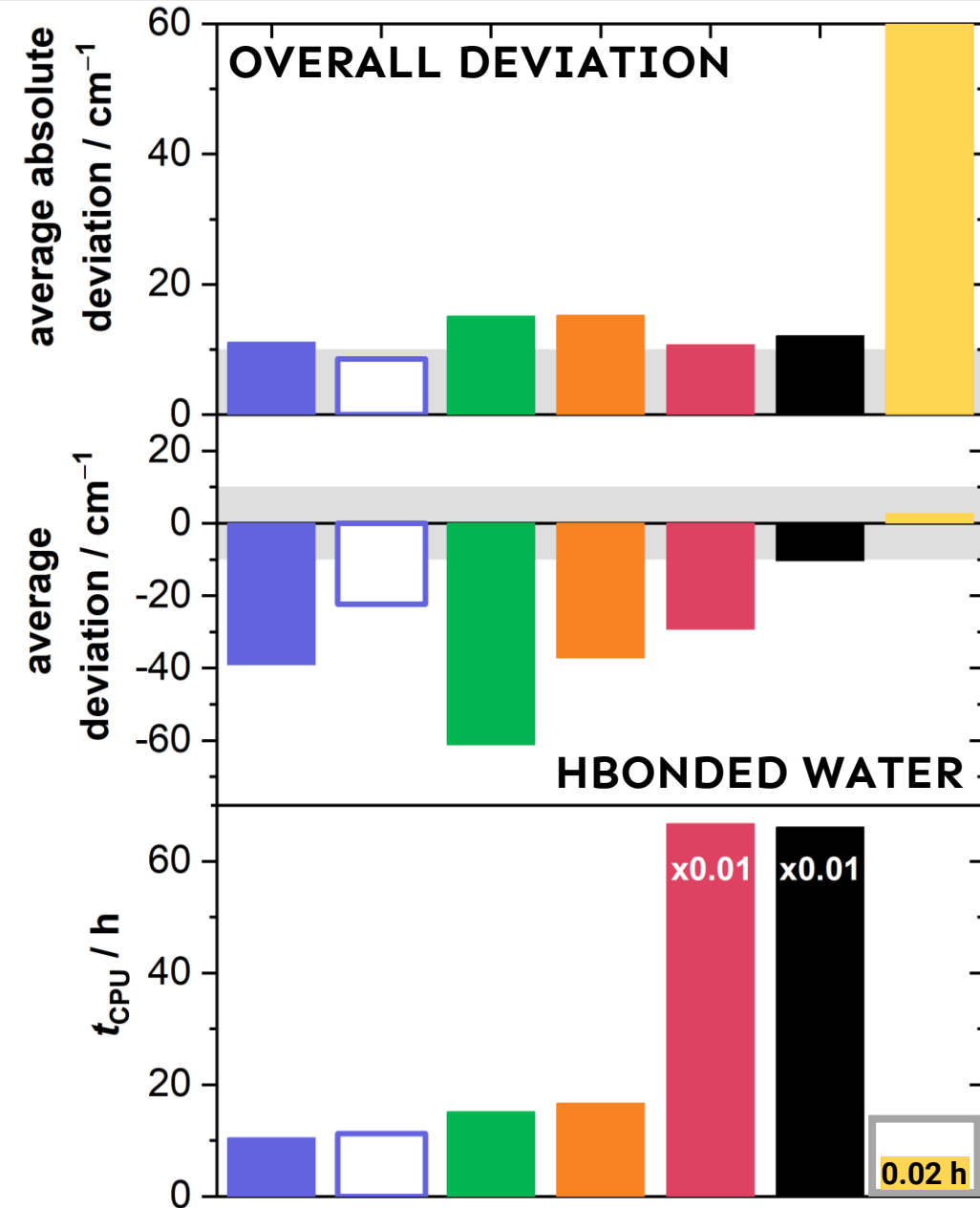
MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

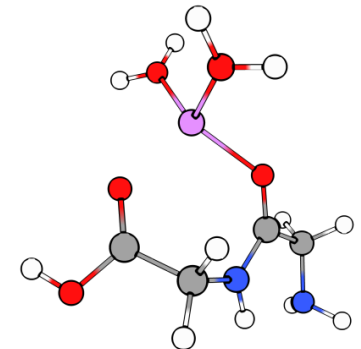
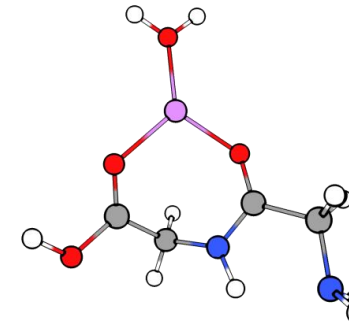
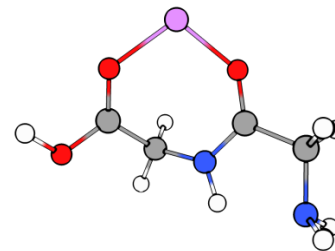
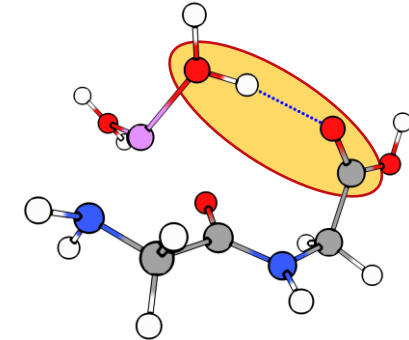
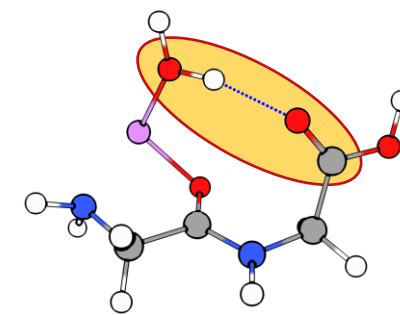
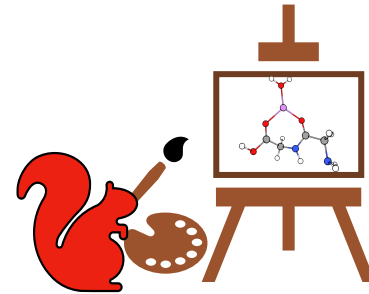
def2TZVP

B2PLYP-D3

MP2

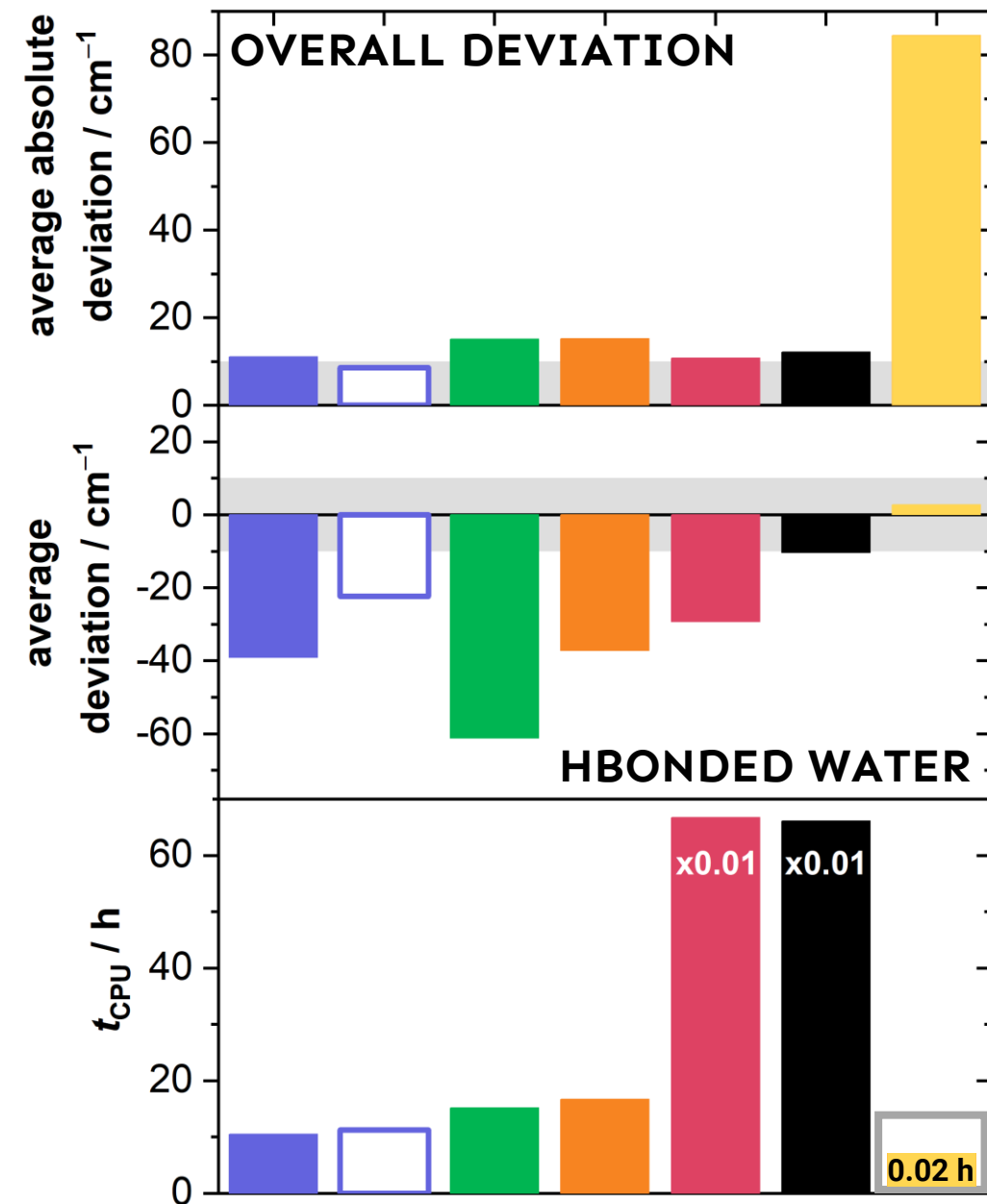
aVTZ

PM3





# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

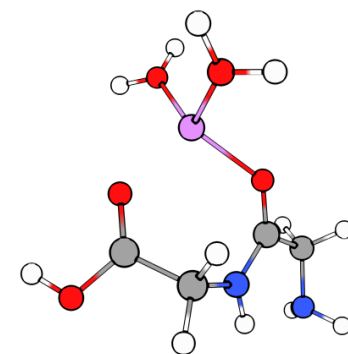
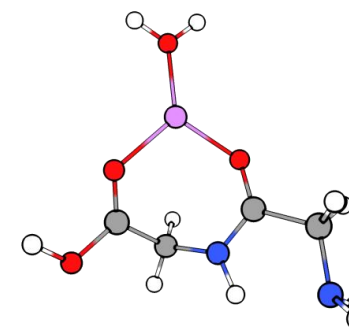
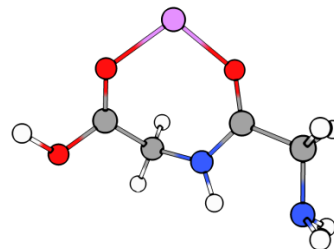
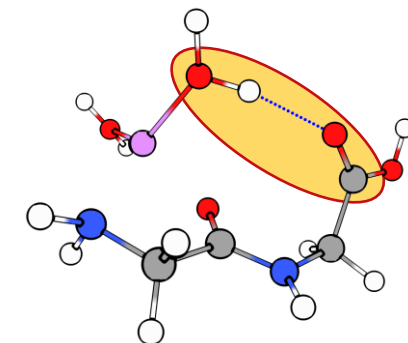
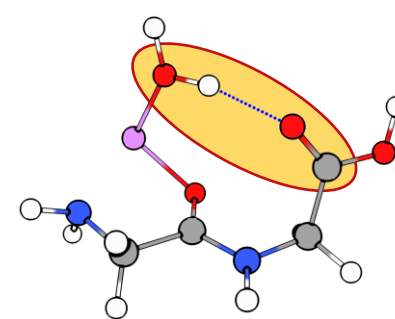
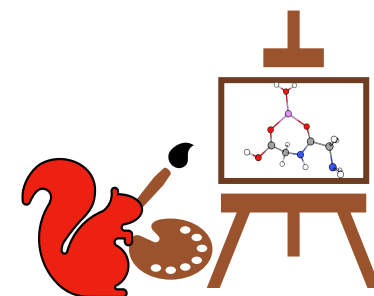
def2TZVP

B2PLYP-D3

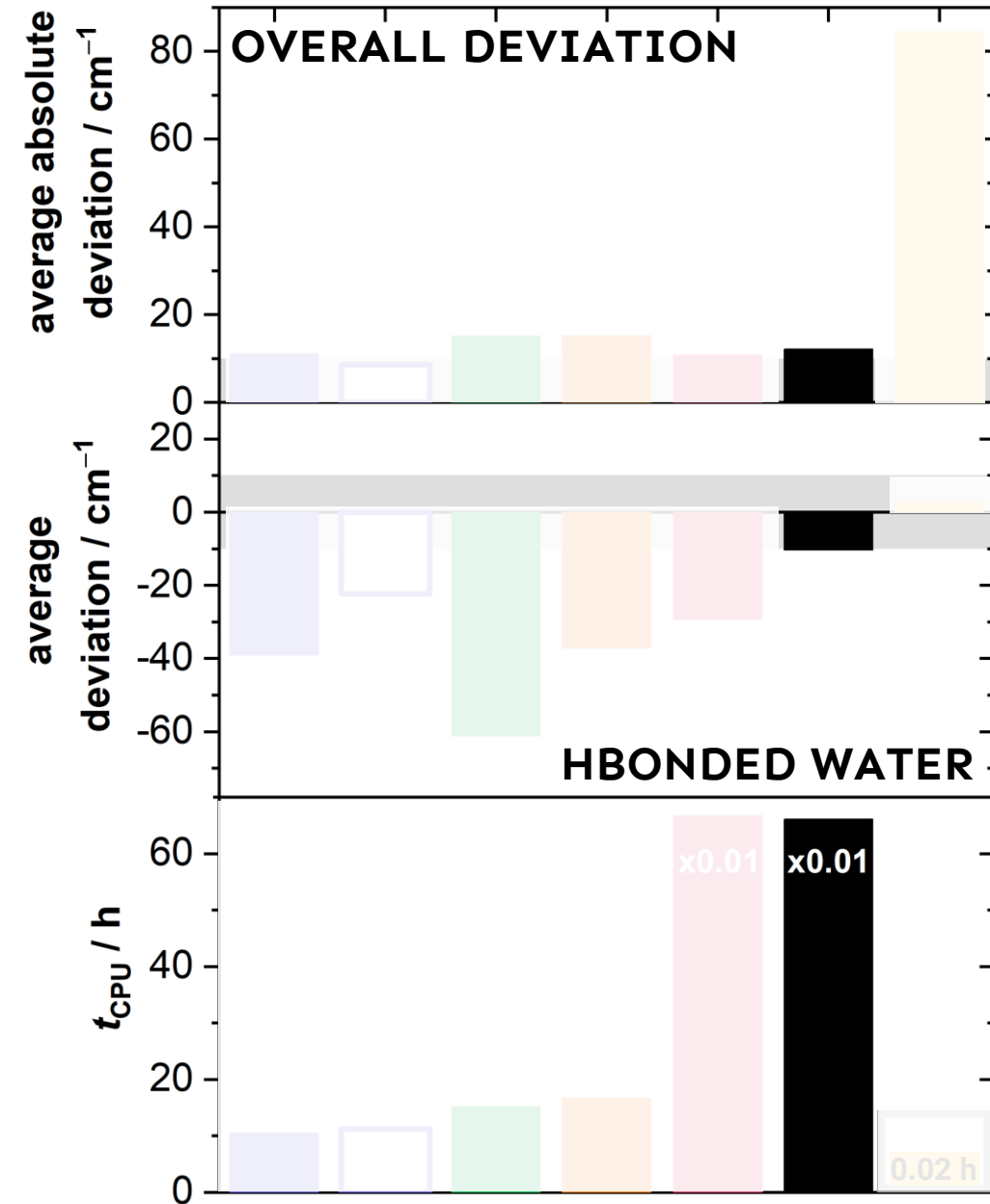
MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

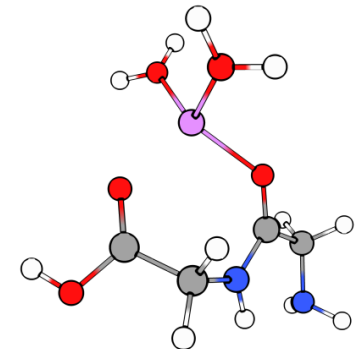
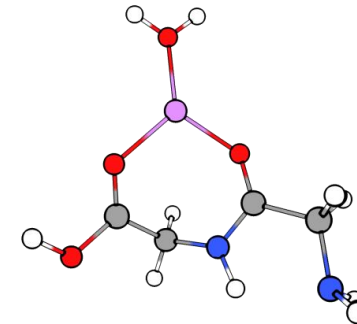
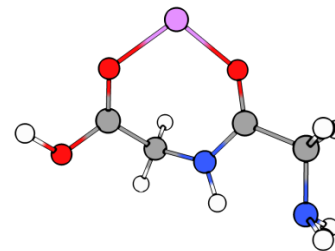
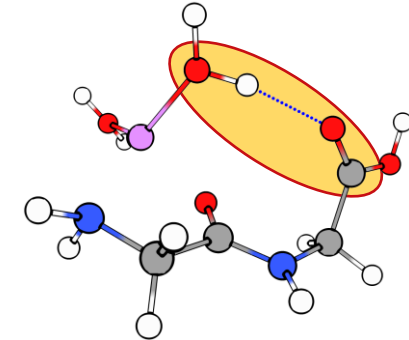
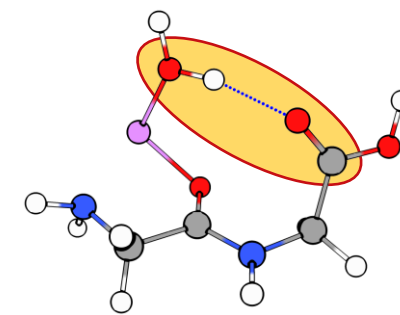
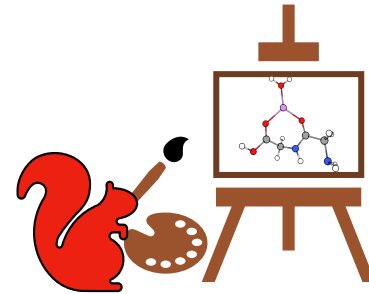
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B2PLYP-D3

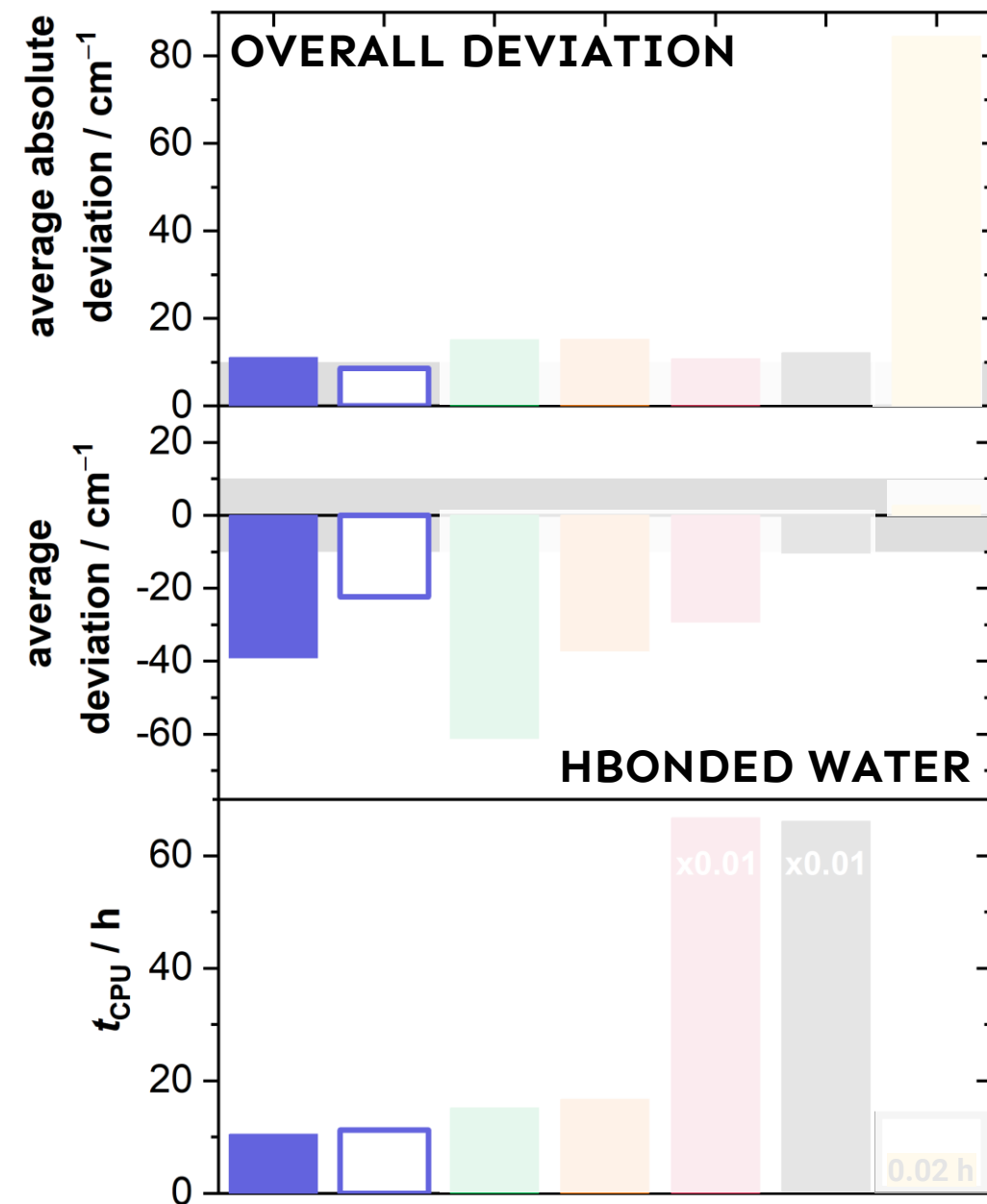
MP2

aVTZ

PM3



# BENCHMARKING: WHICH METHOD IS THE BEST?



B3YLP-D3

B3LYP

$\omega$ B97XD

M06-2X

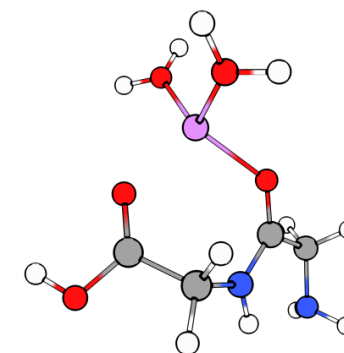
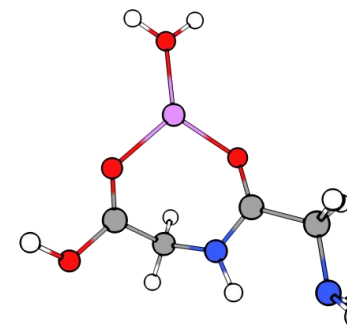
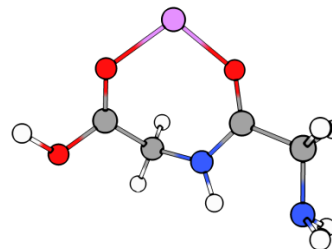
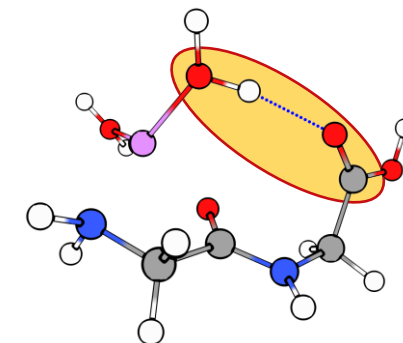
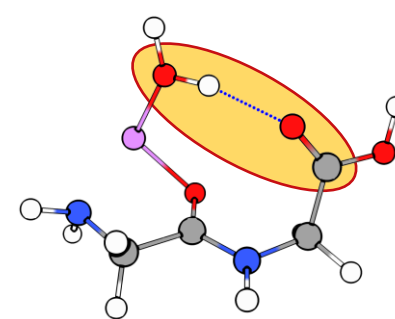
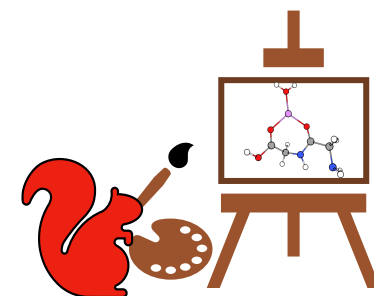
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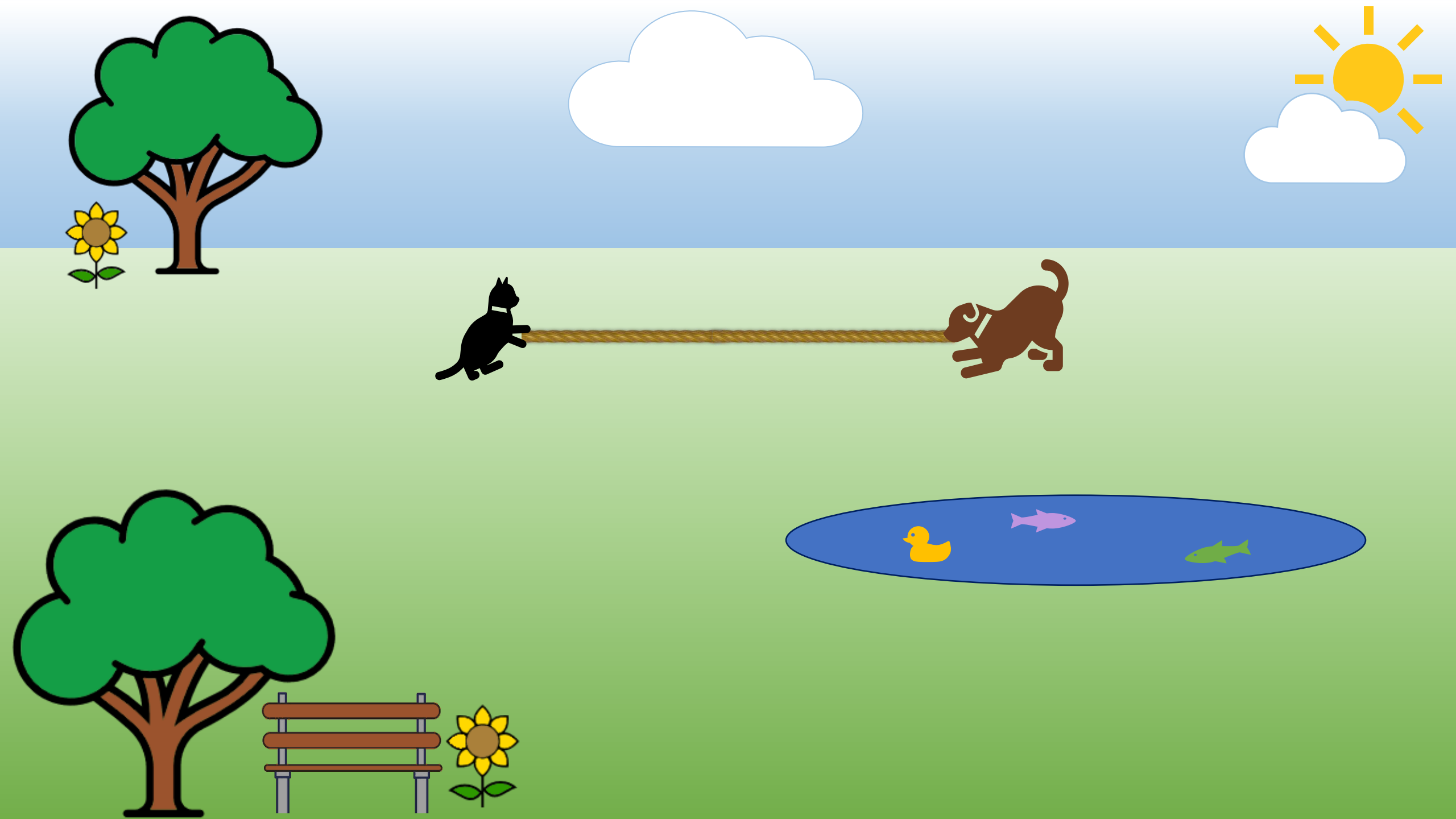
B2PLYP-D3

MP2

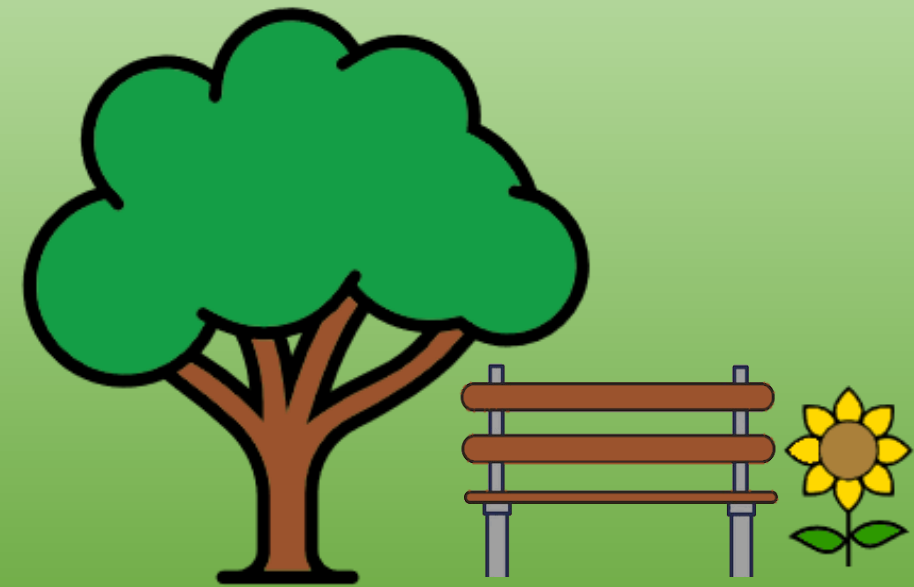
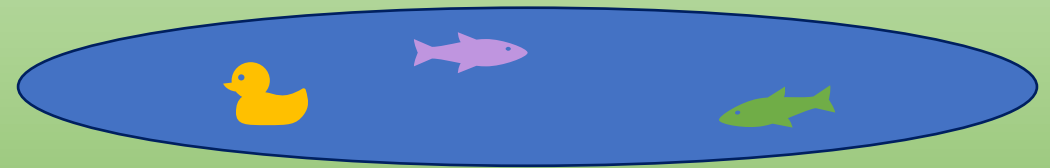
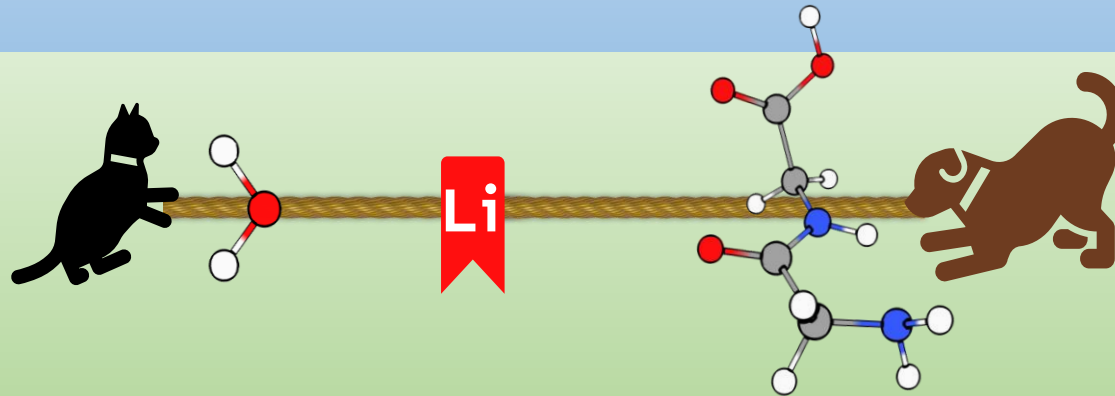
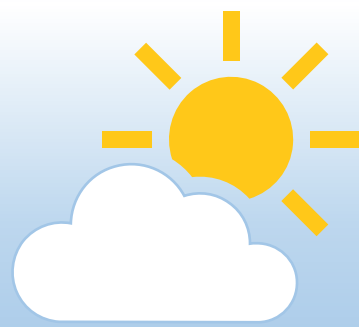
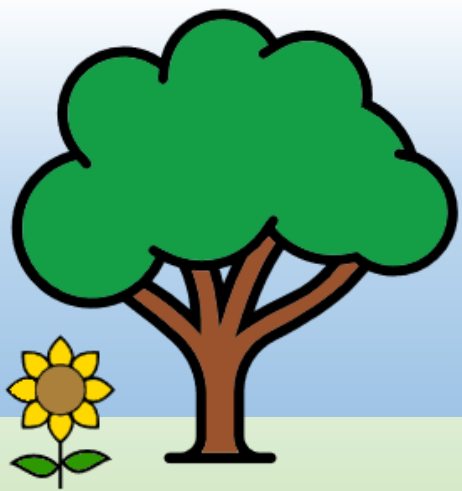
aVTZ

PM3

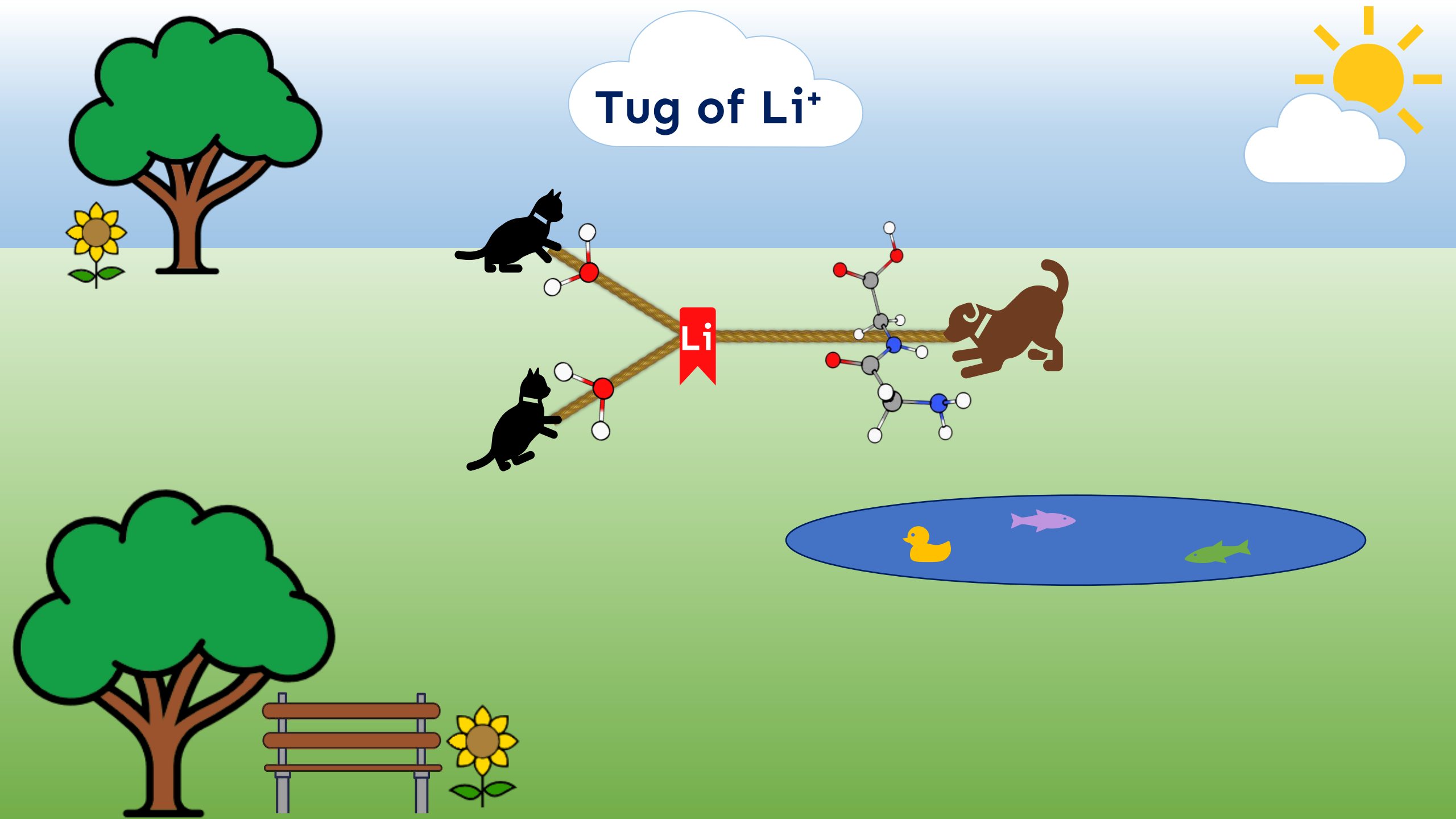




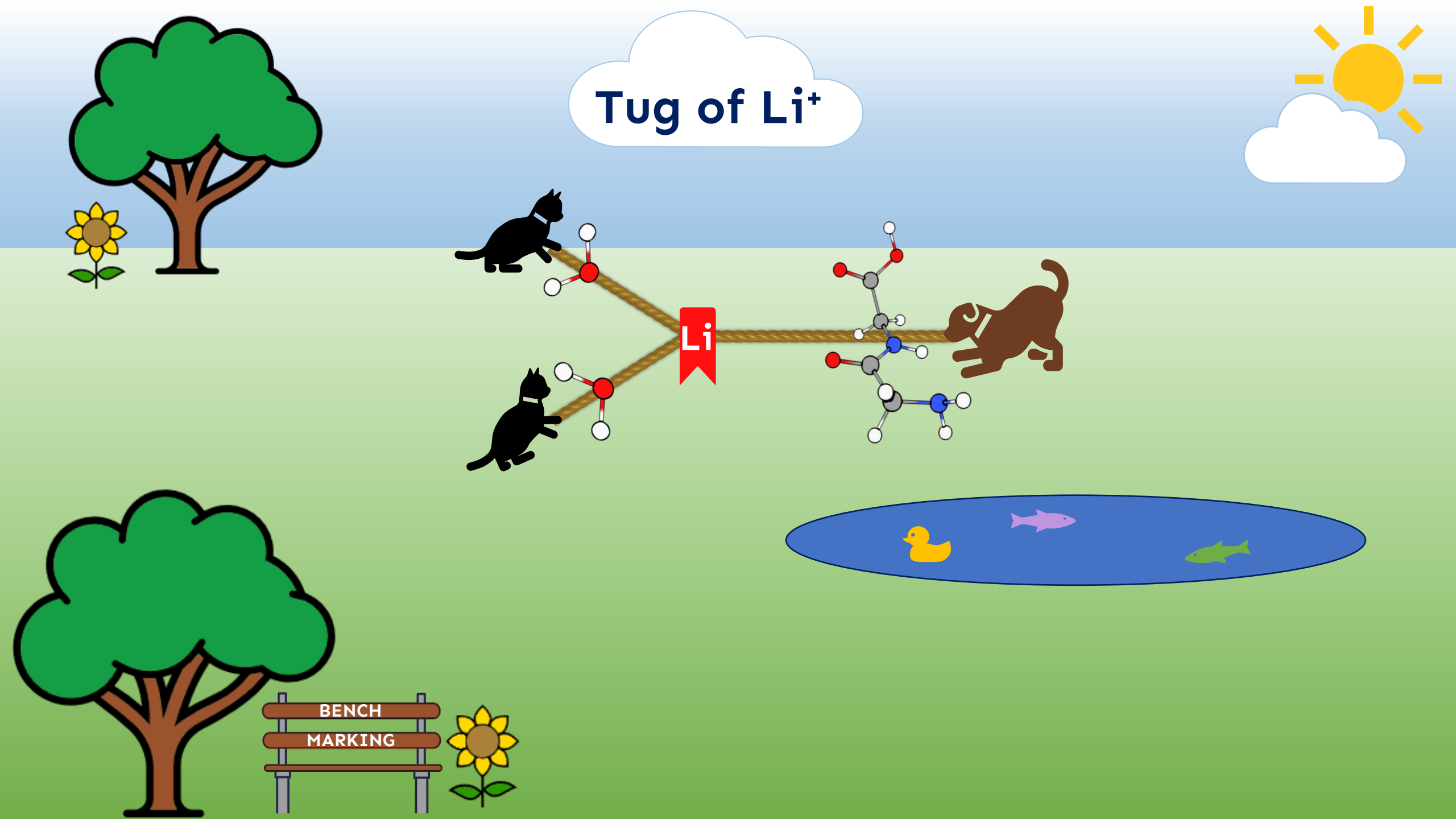
# Tug of Li<sup>+</sup>



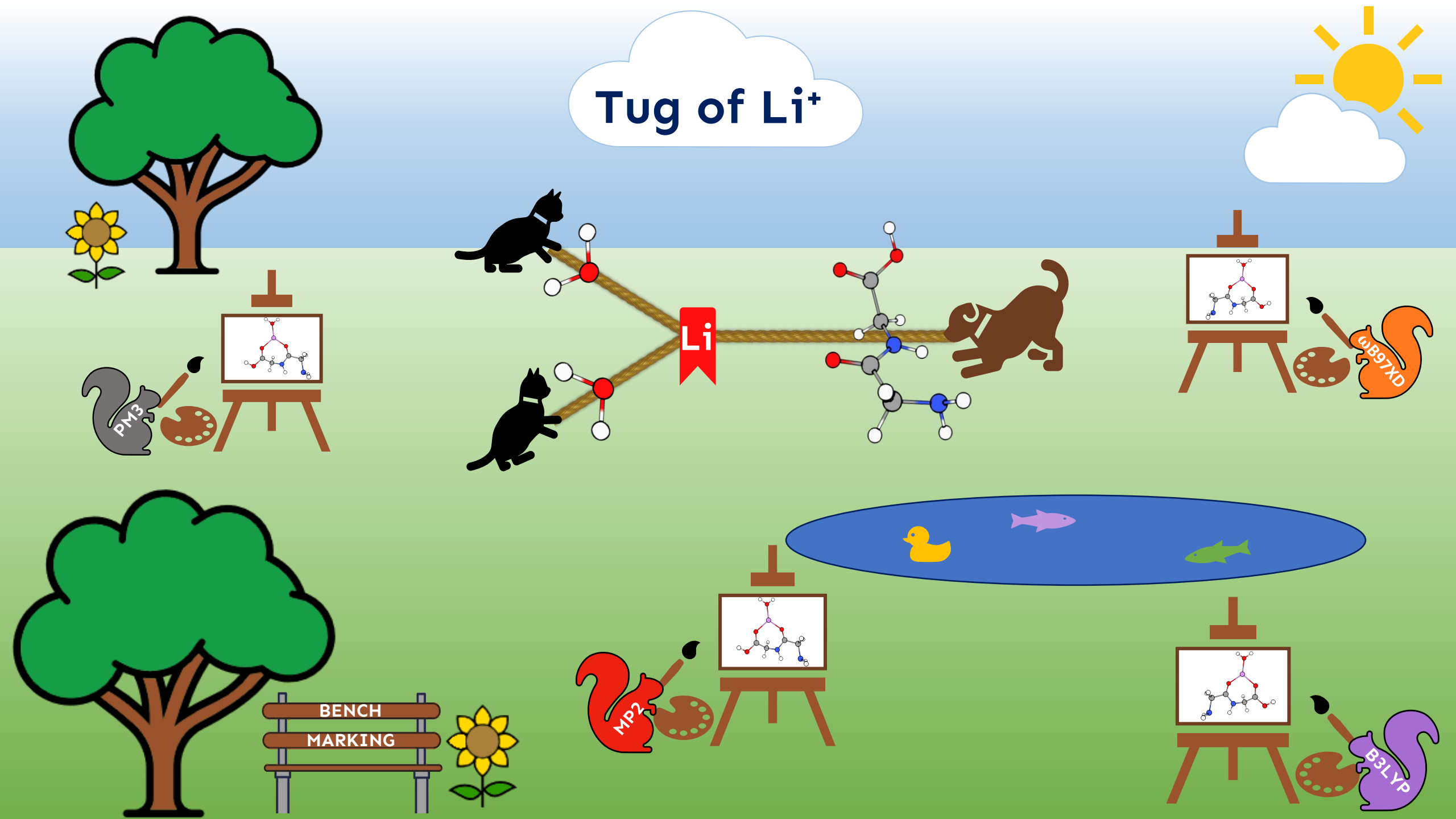
# Tug of Li<sup>+</sup>



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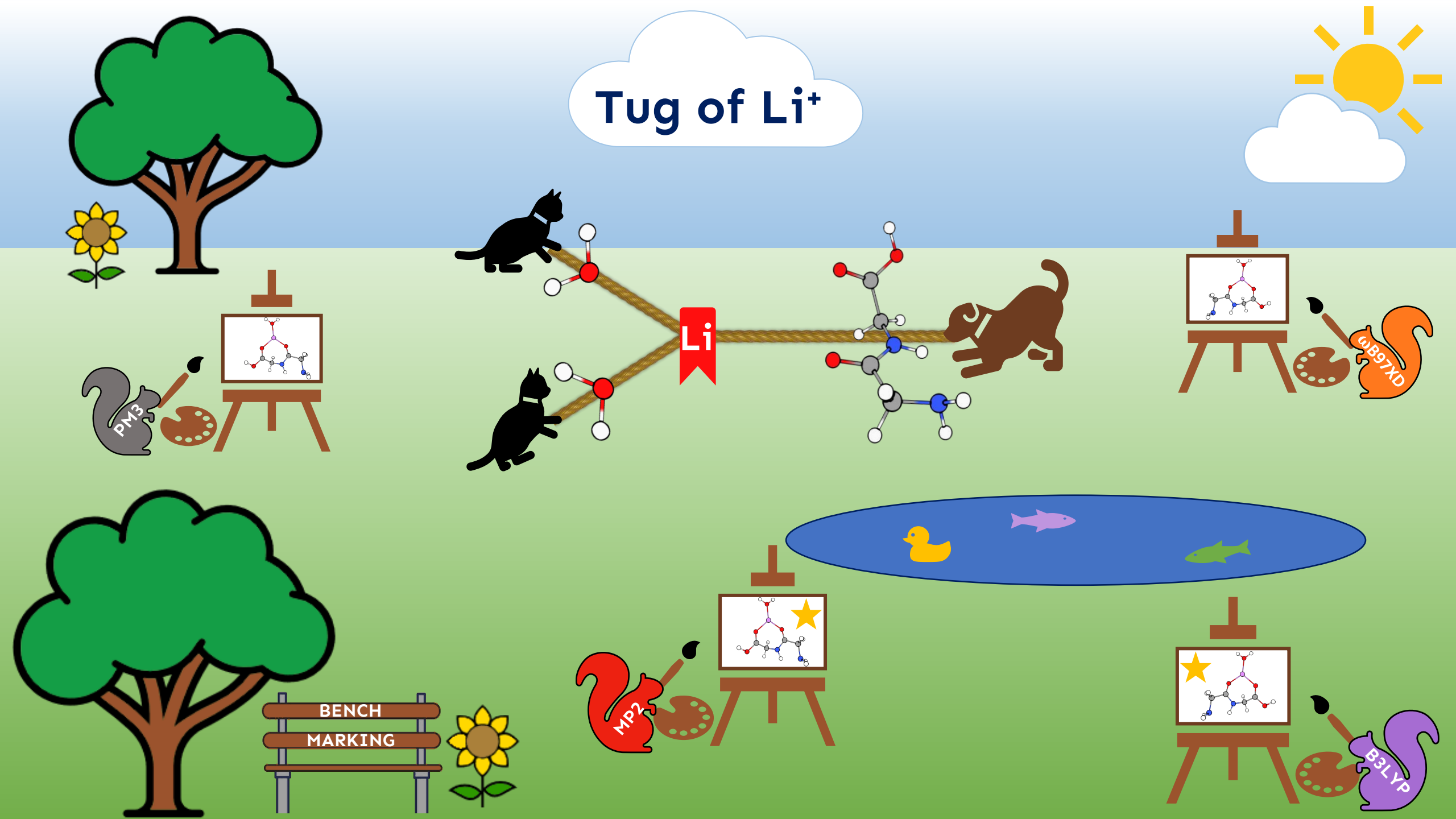


# Tug of Li<sup>+</sup>

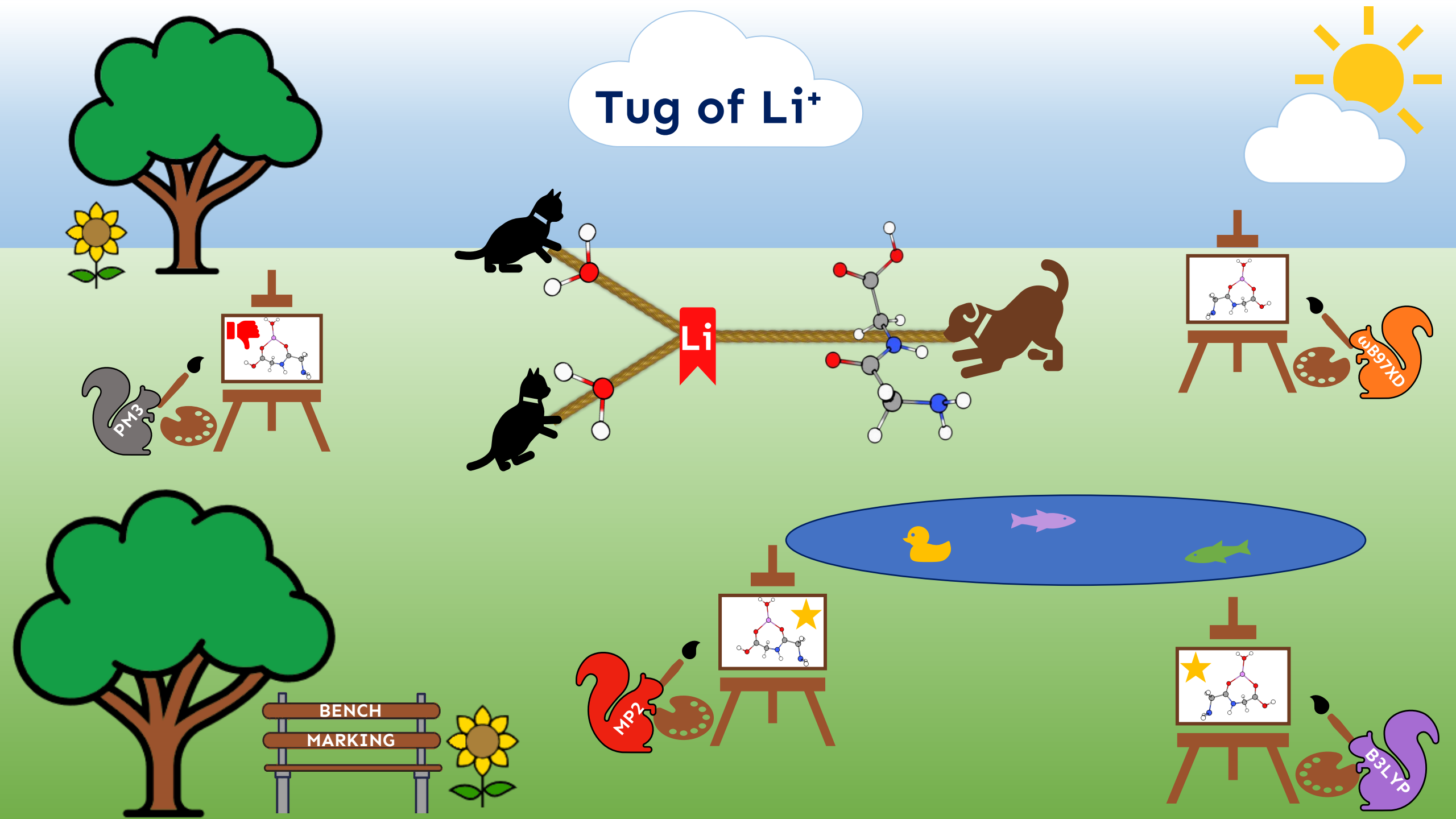




# Tug of Li<sup>+</sup>

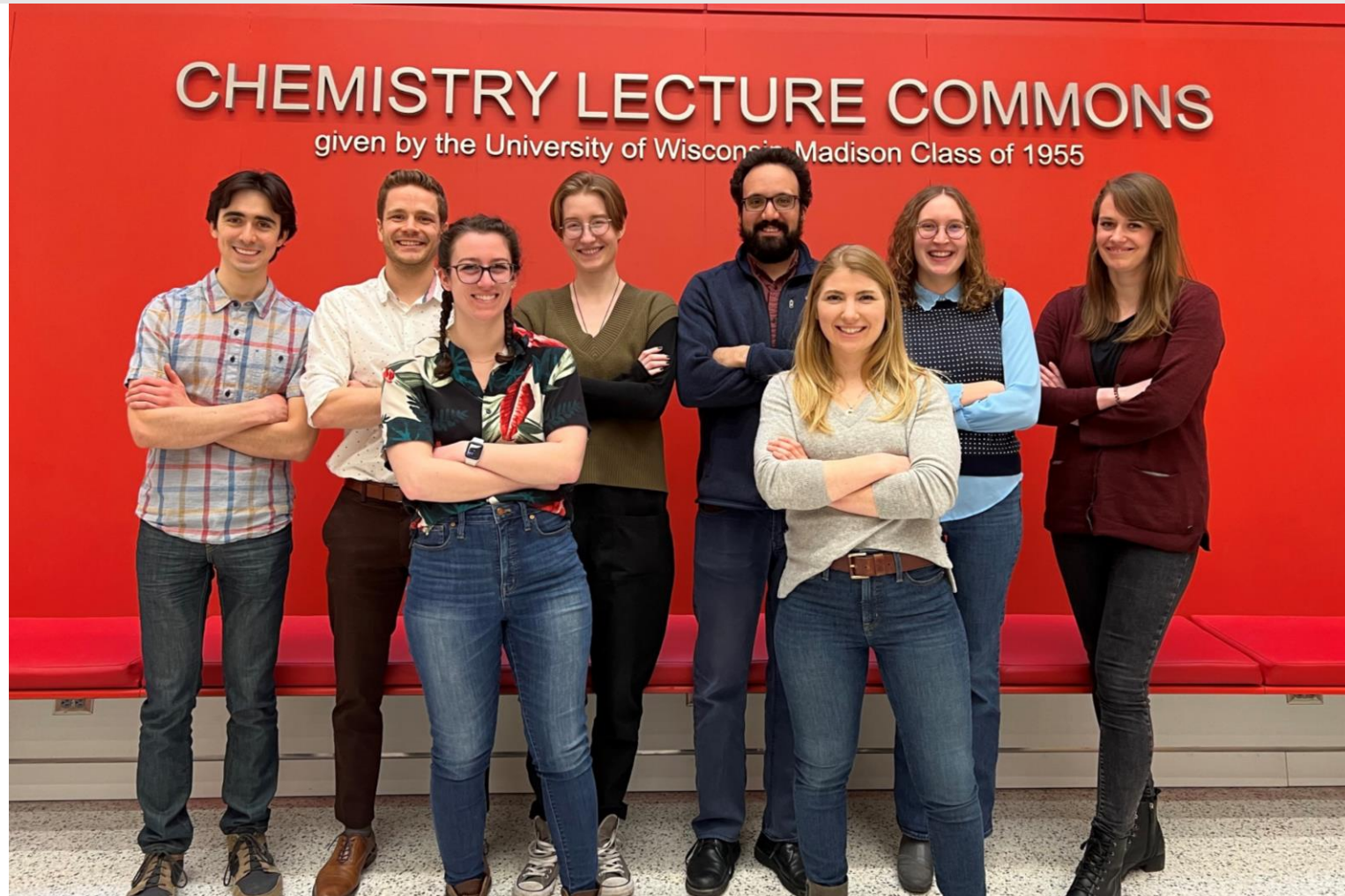


# Tug of Li<sup>+</sup>



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Bri Hopper



# Assignments: $\text{Li}^+\text{GlyGly-1H}_2\text{O}$ and $-2\text{H}_2\text{O}$

