Effect of the Order of the Amino Acids in a Small Peptide

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Introduction

- Protein folding is not yet understood
- Misfolding of proteins leads to various illnesses that could be avoided if the proteins folded correctly.
- The goal was to determine whether hydrogen bonding or the dispersion interactions dominate, and if the order of the amino acids makes a difference.
- Because the dipeptides are composed of the same amino acids, it was predicted that the two lowest energy structures would be similar.
- F = Phenylalanine; Y = Tyrosine

Methods For Each Dipeptide

- 7 Starting structures
- 150 ns simulation using Amber ff99SB
- Selected low energy structures
- DiLabio's method, B3LYP-DCP
  - Dispersion correction potentials are appended to the Gaussian09 input
- Analysis of structures was done with Jmol and ChemBio3D

References

1. Torres, E. and DiLlabio, G. A. *J. Phys. Chem. Lett.*, **2012**, 3, 1738 – 1744.
2. http://www.ualberta.ca/~gdilabio/group.html

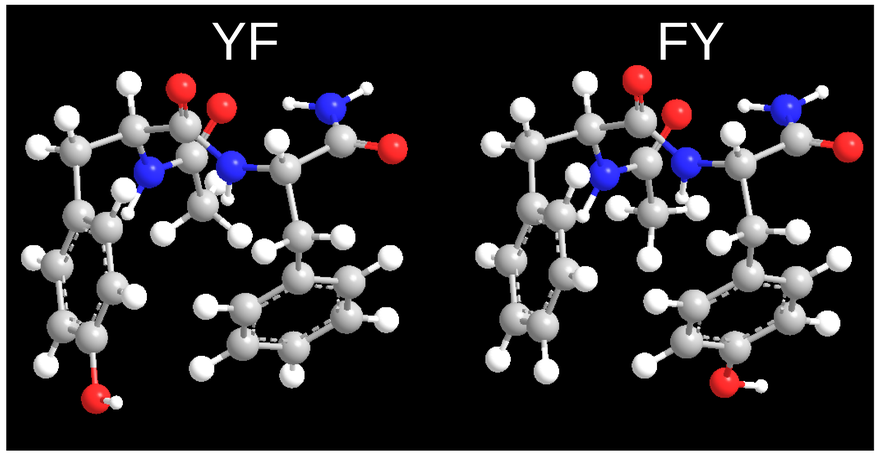

Figure 1. The two lowest energy structures from different peptide arrangements. These structures were found independently of one another.

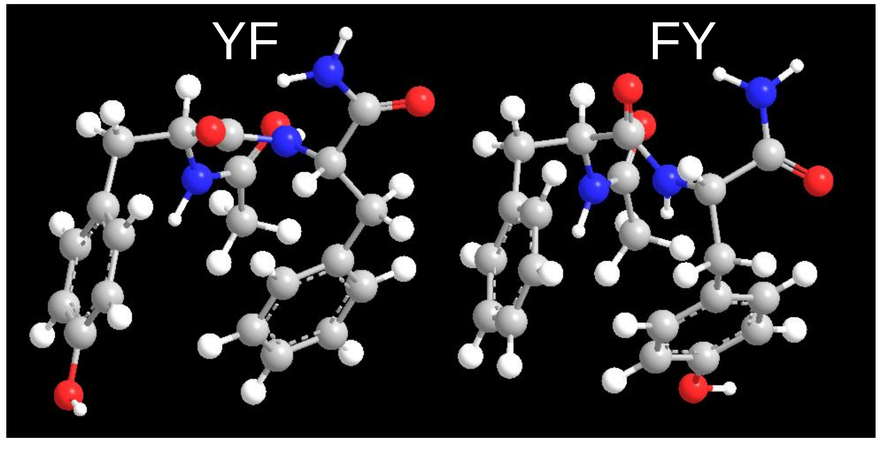

Figure 2. Another pair of low energy structures that are similar
YF relative energy = + 12 kJ/mole
FY relative energy = + 8 kJ/mole

Results

- Lowest energy structures for FY and YF were very similar.
  - Attractions inside the dipeptide created a C10 ring.
- Two other structures were also alike with relatively low energy.
  - Created a C7 ring.
- Two structures in YF were found with relatively low energies; these did not have corresponding FY structures.

Conclusion

- Two pairs of corresponding structures were identified for FY and YF
  - The lowest energy structure for each
  - A structure approx. +10 kJ/mol higher
- Although there are pairs of similar structures, YF can form additional stable structures.
- The interaction of the rings in all of the low energy structures indicates the importance of dispersion interactions.

Acknowledgements

• Purdue North Central
  - Department of Biology and Chemistry
  - College of Science
  - Honors Program
• Rosen Center for Advanced Computing
• LSAMP Indiana