

# Atomic Contact Energies

## Bioinformatics II

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# Structure

## Theoretical Background

What does the energy function model?

## Methods

Implementation of the function.

## Results

Performance Evaluation

## Discussion

# Theoretical Background

# Appetizer



from: <http://thejobmouse.com>

# The Desolation Energy

- ▶ Energy needed for transferring atoms from the solvent (water) into the protein's interior.
- ▶ One possible measure of protein stability
- ▶ The project:
  - ▶ Implement desolation energy by (?)
  - ▶ Evaluate on *CASP11* data

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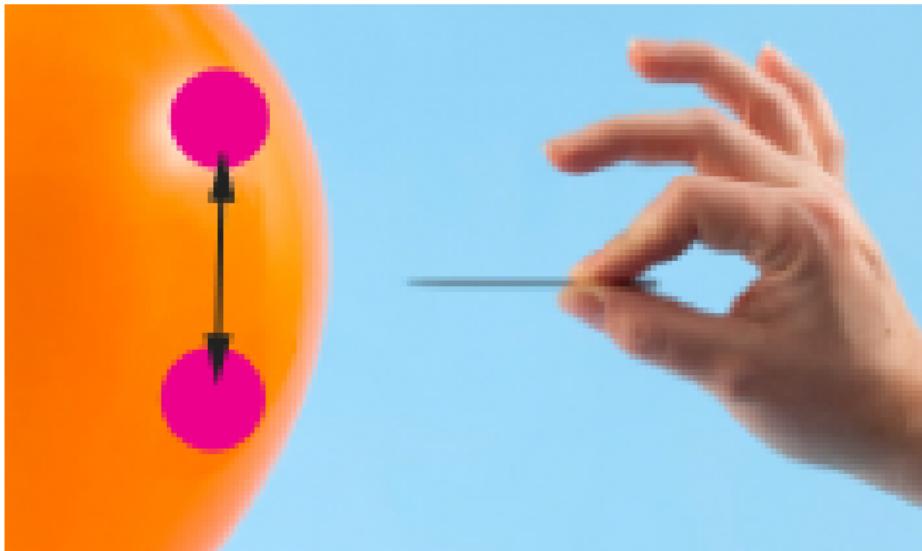
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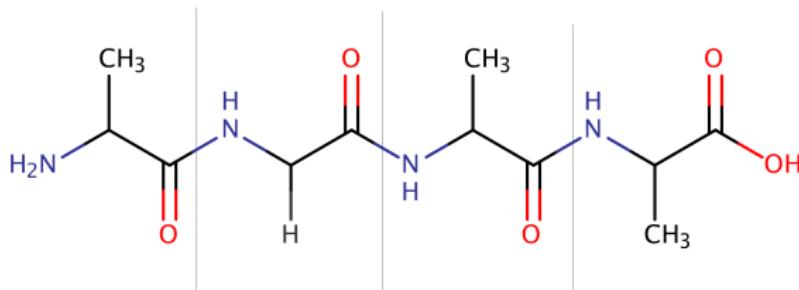
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# Atomic Contacts



Based on a picture from: <http://thejobmouse.com>

# Atomic Contacts Pairs

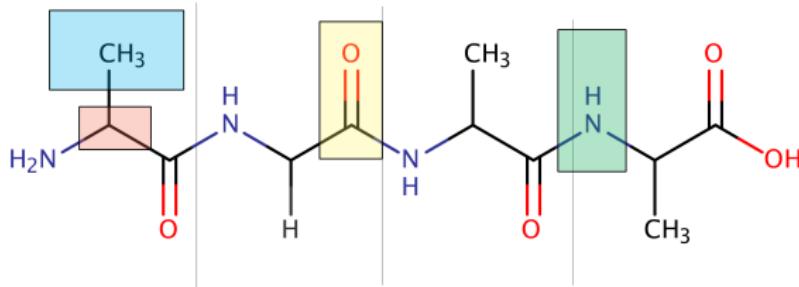


A valid contact pair:

- ▶ Only heavy atoms
- ▶ Distance below 6 Å
- ▶ More than 10 covalent bonds in between

Estimated by connectivity class & residue index differences

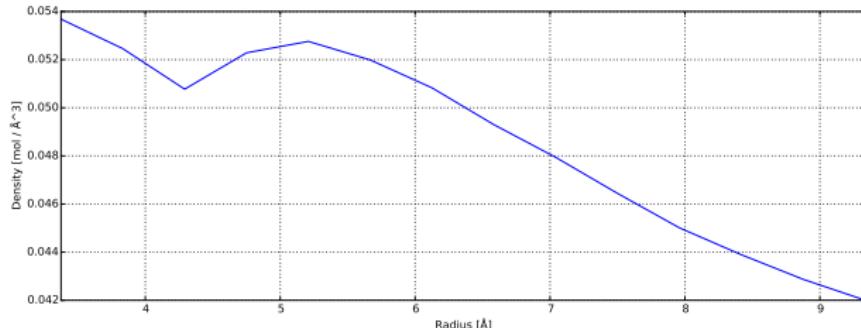
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# Atomic Packaging



- ▶ Number density of interior atoms ( $SAS = 0$ )
- ▶ Relative to a sphere of variable radius
- ▶ Evaluated on non-homologous protein set

# Methods

# Conclusion

Thank you for your attention!

# Bibliography