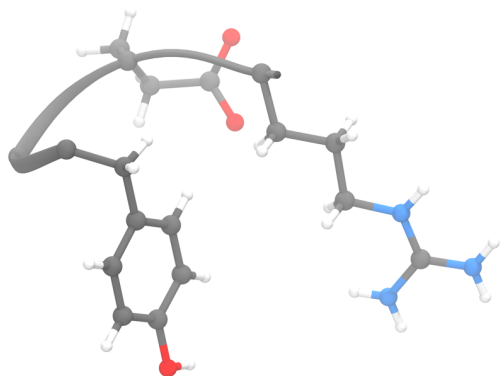


 **Impossible**

2010

QM Calculations

Impossible for proteins.
Limited to small molecules
only

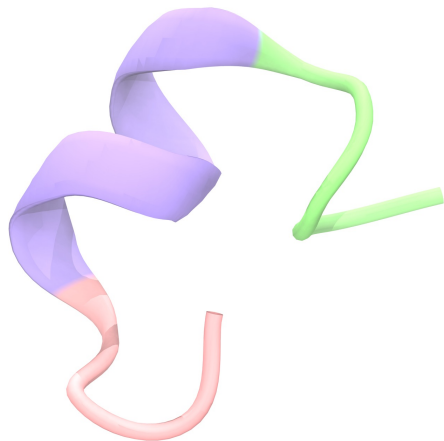


 **Limited**

2012

GPU Accelerated QM

Limited to peptides and very small
proteins (~hundreds of atoms)

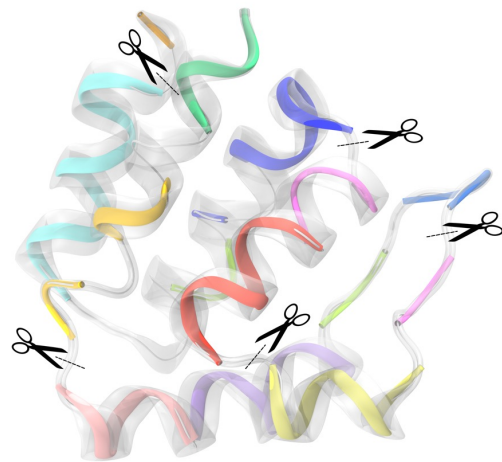


 **Possible**

2017

Q|R with Fragmentation

QM-based protein refinement. Slow,
resource-intensive, no inherent size
limit



 **Practical**

2024

ML Potentials

Fast, rivaling classical force fields,
with QM-level accuracy and no
fragmentation required

