EXPERIMENTING WITH FIASCO FOR PROTEIN STRUCTURE PREDICTION.

WWW.CS.NMSU.EDU/FIASCO/

- Fragment-based Interactive Assembly for protein Structure prediction with COnstraints
- C++ constraint solver
- F. Campeotto (UniUD, NMSU)
- A. Dal Palù (UniPR)
- A. Dovier (UniUD)
- F. Fioretto (UniUD, NMSU)
- E. Pontelli (NMSU)
Experimenting with FIASCO

www.cs.nmsu.edu/fiasco/

Tool: github.com/MatteoDusefante/Java-GUI/

- Interactive GUI
- Multiagent prediction secondary structure
- Constraint solving with fragment assembly
EXPERIMENTING WITH FIASCO

INTERACTIVE GUI

• Demo in a few minutes
• Drives the Design/Prediction workflow
• Interface for constraints handling
• Controls the search tools
• Allows to manually inspect / improve solutions
EXPERIMENTING WITH FIASCO
CoCos (Concurrent Constraint System)

- Secondary structure prediction
- Multiagent based
- Local search
- GPU powered (neighborhood, consistency, energy computation)
- Outputs feasible 3D structure

EXPERIMENTING WITH FIASCO

FIASCO

- Constraint solving for 3D structures
- Fragment assembly
- Propagators for spatial constraints

Special track Constraints in Bioinformatics

Journal Algorithms for Molecular Biology (AMB)

- Edited by: R. Backofen, A. Dal Palu’, A. Dovier, S. Will
- Call in a few weeks
- You can submit at any time
- Open access
- Article cost standard with AMB policies
- IF: 1.86
- www.almob.org/series/constr_and_bioinf
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DEMO!