## AlphaKnot: server to analyze entanglement in structures predicted by AlphaFold methods

- Objective: Detect knots in AlphaFold predicted proteins
- Novelty: considers pLDDT
- Workflow: PDB -> Cα atoms -> HOMFLY-PT (1000 random closings) -> Alexander polynomial for knot map



## HOMFLY-PT

- Invariant
- generalizes Alexander and Jones
- Skein relation

Vs Alexander: computationally less consuming

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- Findings:
  - Case 1: structures with high pLDDT may have unlikely non-trivial topologies
  - Case 2: structures with strictly conserved non-trivial topologies from different organisms
  - Case 3: topology is conserved only between some homological proteins



Fig 4, Niemyska et al.

HOMFLY-PT

- Invariant
- generalizes Alexander and Jones

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Insights:

- Topology is conserved between proteins with the same function but low sequence similarity
- Most knotted proteins are enzymes with an active site in the knot

AlphaKnot Database (entries grouped by knot type): <a href="https://alphaknot.cent.uw.edu.pl/searchdb/?all=False&cats=Knot&organisms=CAEEL.DANRE,DROME,HUMAN,MOUSE,RAT,ECOLI.MYCTU,STAA8,CANAL,SCHPO,YEAST,ARATH,MAIZE,ORYSJ,SOYBN,DICDI,LEIIN,METJA,PLAF7,TRYCC">https://alphaknot.cent.uw.edu.pl/searchdb/?all=False&cats=Knot&organisms=CAEEL.DANRE,DROME,HUMAN,MOUSE,RAT,ECOLI.MYCTU,STAA8,CANAL,SCHPO,YEAST,ARATH,MAIZE,ORYSJ,SOYBN,DICDI,LEIIN,METJA,PLAF7,TRYCC</a>