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Deep learning metrics for protein-protein interfaces in macromolecular assemblies

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Structural models of macromolecular assemblies allow us to determine their function, yet the structural models we rely on are not direct experimental results, but the computational interpretation of many different noisy observations. This risks local errors that can propagate throughout the model. One area where this error can propagate is the interface between different protein chains. Can we use ML as a way to validate protein-protein interfaces and build stronger structures?

Summary

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