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Random Drift Particle Swarm Optimisation Algorithm for Highly Flexible Protein-ligand Docking

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Highlights

- Two algorithms (RDPSO and QPSO) are used to solve molecular docking problems.
- A fast, exact hybrid algorithm (LRDPSO) specialized for docking highly flexible ligands is proposed.
- A thorough experiment result with statistical assessment is presented.
- Specific instances are analyzed in detail to compare algorithms.

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