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Showcasing research from Professor Shuguang Yuan's laboratory, Shenzhen Institutes of Advanced Technology, CAS, China.

Enhancing multifunctional drug screening *via* artificial intelligence

Alpha-Pharm3D is a versatile deep learning method that predicts ligand–protein interactions using 3D PH4 fingerprints by explicitly incorporating geometric constraints. This comprehensive new algorithm enhances substantially not only the prediction interpretability and accuracy of binding affinities of ligands against the target protein. Alpha-Pharm3D outperforms state-of-the-art scoring methods in bioactivity prediction and achieves considerable improvements in both accuracy and success rate, irrespective of data scarcity.

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As featured in:

See Junlin Dong, Chenyang Wu, Tianle Lu, Shiyu Wang *et al.*, *Digital Discovery*, 2025, **4**, 2012.

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