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EDITORIAL

This issue: Drug Design Data Resource Grand Challenge 4, first of two issues

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The Drug Design Data Resource (D3R) enables rigorous assessment of techniques for computer-aided drug design by holding community-wide blinded pose- and affinity-prediction challenges. This is the first of two special issues presenting detailed reports from D3R's Grand Challenge 4 (GC4). The GC4 challenge focused on proteins β-Secretase 1 (BACE1) and Cathepsin S and was run in an analogous manner to the prior three challenges. In Stage 1, participants' ability to predict the poses and affinities of BACE1 ligands was assessed. Then all available BACE1 co-crystal structures were released, and Stage 2 re-tested affinity rankings, this time with the co-crystal structures available to participants. The Cathepsin S component involved only affinity predictions. The reports in this first GC4 special issue discuss a wide range of computational methods and provide insights into factors that may contribute to successful predictions.

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