



## Drug Design Data Resource, Grand Challenge 4, *second of two issues*

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We are delighted to present here the second of two special issues of this journal containing detailed reports from D3R's Grand Challenge 4 (GC4). The first issue can be found at Journal of Computer-Aided Molecular Design, Volume 33, Issue 12, December 2019, Special Issue: Drug Design Data Resource: Grand Challenge 4—Part 1.

The first article of this issue, Part 2, provides our customary overview of the entire challenge, in which we check whether old patterns are again seen and highlight new observations and methodological approaches. This particular challenge focused on proteins  $\beta$ -Secretase 1 (BACE1) and

Cathepsin S and afforded opportunities to test pose-prediction and affinity-ranking and -prediction tools.

We also wish to inform readers that the D3R Grand Challenges are in suspension for now, as the NIH program that funded it has been closed. We hope this project has been useful to you and hope to see it resume in a future iteration.

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