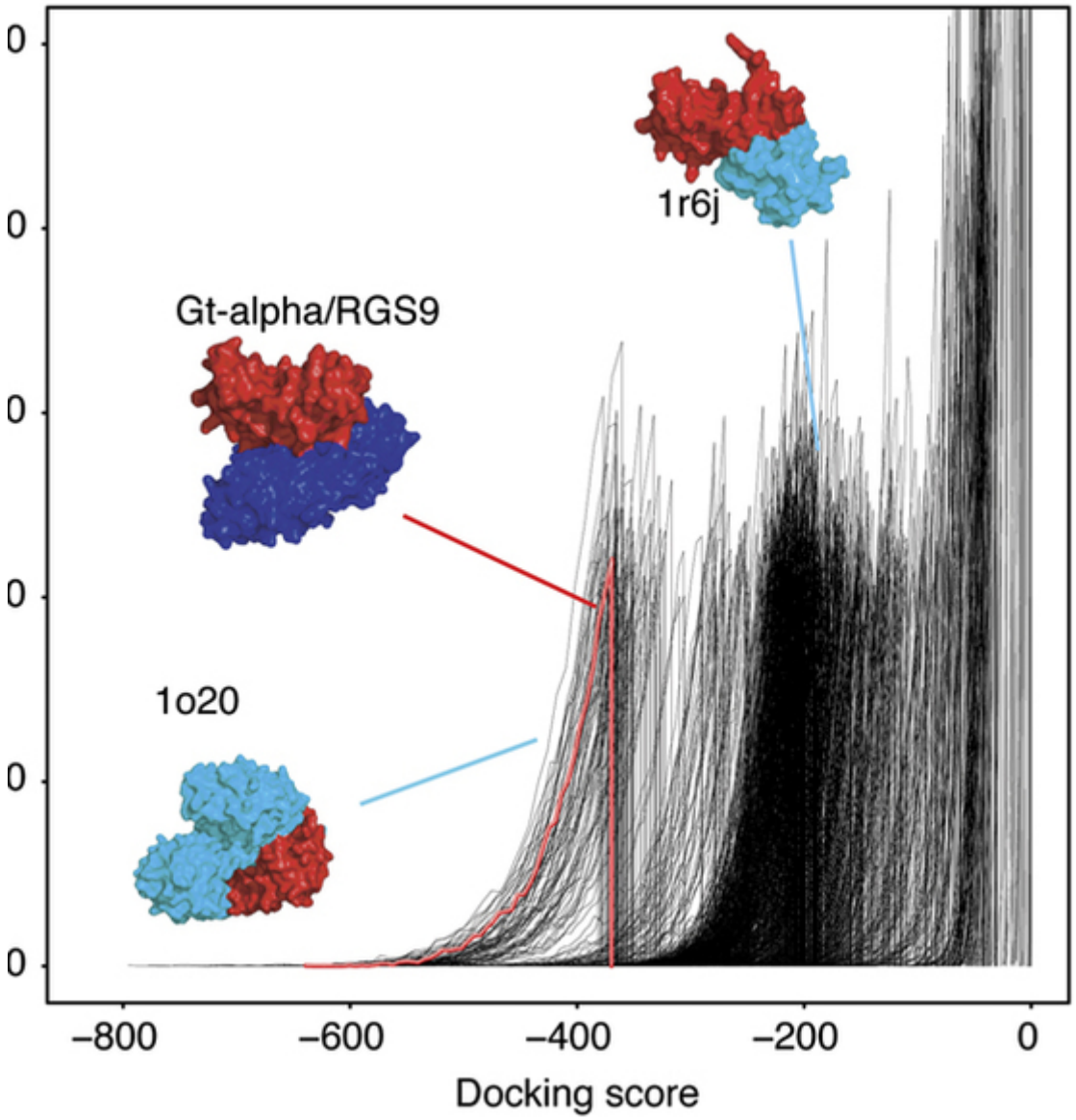
Computational programs used to predict the composition of protein complexes

The prestigious journal Molecular Systems Biology published the first extensive study demonstrating the ability to use computational docking programs to predict protein-protein interactions. These calculations are extremely demanding and were possible thanks to the intensive use of the facilities of the Barcelona Supercomputing Center. The results presented in this paper open new possibilities for the modeling of protein complexes as a step towards the interpretation of cancer related mutations.


1r6j
Gt-alpha/RGS9
1o20
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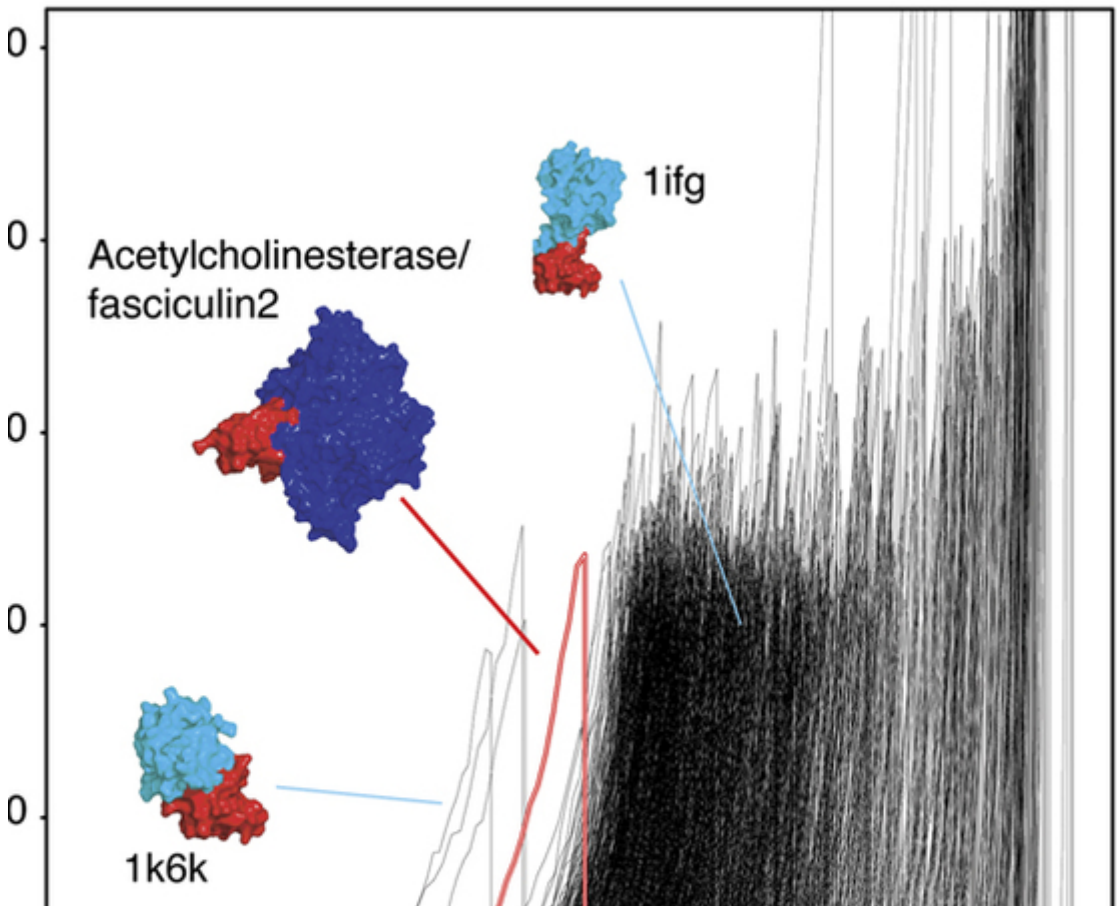
0
0
0
0
−800
−600
−400
−200
0
Docking score


1ifg
Acetylcholinesterase/
fasciculin2
1k6k
0
0
0
0
0