

phage display has a lower stability compared to the mother system. This important result raises the central question of selectivity vs stability. In order to address both aspects, theoretical investigations were conducted using molecular dynamics within the Gomacs suite. Pulling apart the two helices up to 3.00 nm from each other, potentials of mean force were calculated by umbrella sampling with a view to compare the energy barriers of the mother dimer to the phage display variant.

Authors' details

¹Department of Biology, Chemistry and Pharmacy, Freie Universität Berlin, Takustraße 3, 14195 Berlin, Germany. ²Department of Physics, Freie Universität Berlin, Takustraße 3, 14195 Berlin, Germany. ³Fritz Haber Institute, Faradayweg 4-6, 14195 Berlin, Germany.

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