



Dissecting the Supramolecular Dispersion of Fullerenes by Proteins/Peptides: Amino Acid Ranking and Driving Forces for Binding to C₆₀

Tainah Dorina Marforio^{1,*}, Alessandro Calza¹, Edoardo Jun Mattioli¹, Francesco Zerbetto¹ and Matteo Calvaresi^{1,*}

¹ Dipartimento di Chimica “Giacomo Ciamician”, Alma Mater Studiorum - Università di Bologna, Bologna 40126, Italy

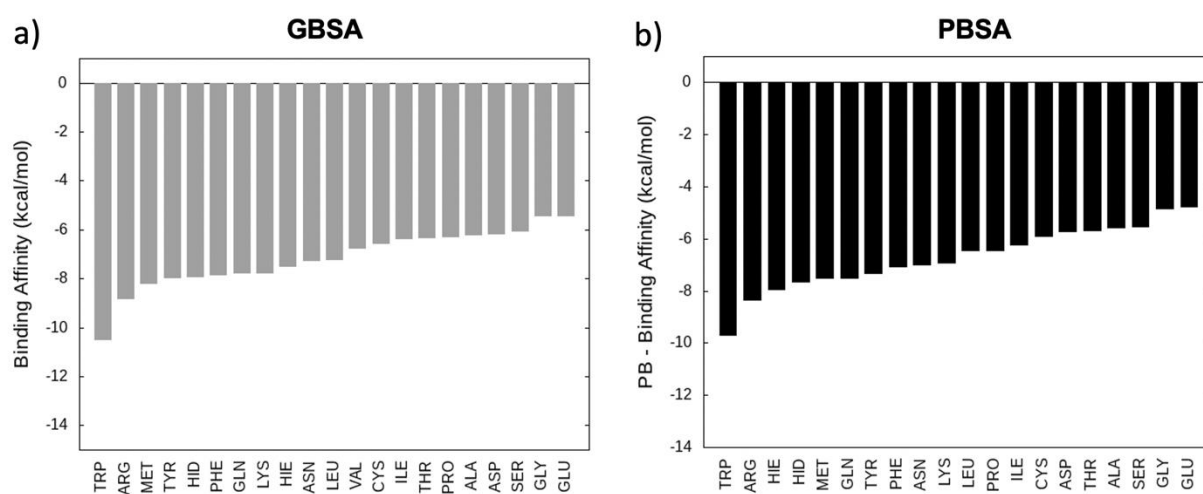
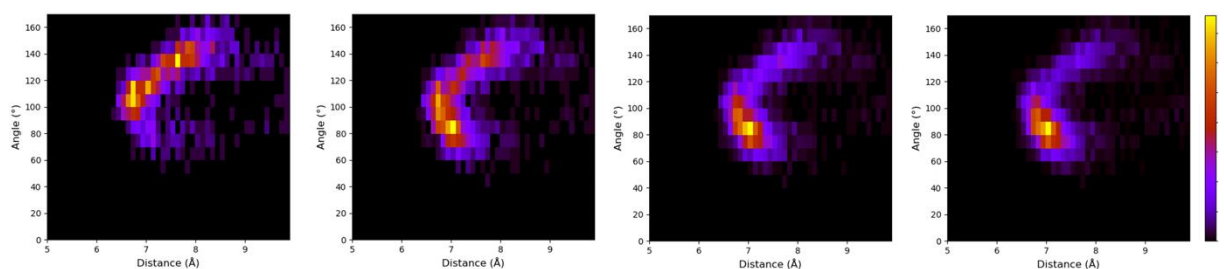


Figure S1. Binding energy between amino acid and C₆₀ calculated by a) MM/GBSA and b) MM/PBSA for the twenty proteinogenic amino acids.

TRP@C₆₀



ARG@C₆₀

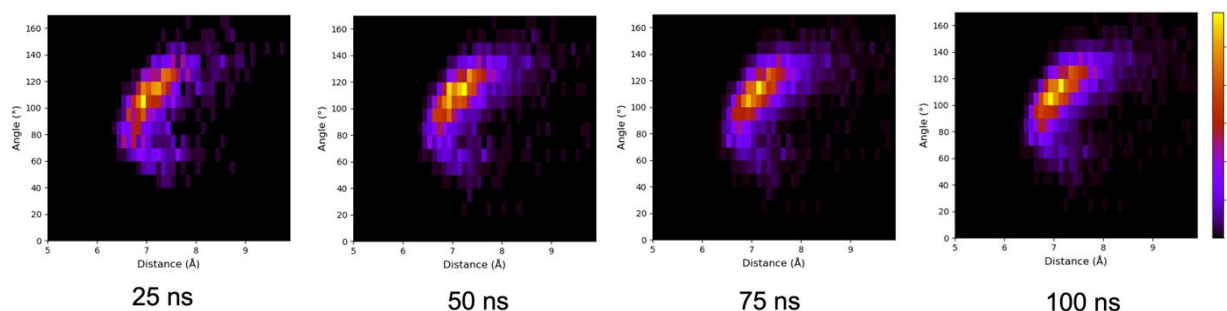


Figure S2. Convergence of the Trp@C₆₀ (top) and Arg@C₆₀ (bottom) FES as a function of the sampling time.