

Supplementary Information

Metallofullerenol Gd@C₈₂(OH)₂₂ Distracts Proline-Rich-Motif from Putative Binding on SH3 domain

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Figure S1. Contribution of hydrogen bonding and hydrophobic packing (denoted by contact surface area) of $\text{Gd@C}_{82}(\text{OH})_{22}$ in its binding to SH3 domain. The number of hydrogen bonds between $\text{Gd@C}_{82}(\text{OH})_{22}$ and SH3 domain is found to be roughly proportional to their contact surface area during this binding process. Our analysis also shows that $\text{Gd@C}_{82}(\text{OH})_{22}$ can form up to 10 hydrogen bonds with SH3 domain, along with $\sim 260 \text{ \AA}^2$ contact surface area. This indicates both the specific hydrogen bonding and non-specific hydrophobic packing contribute to the $\text{Gd@C}_{82}(\text{OH})_{22}$'s binding with SH3 domain.

Figure S2. Time evolution of native contacts (ratios against X-ray structure) between PRM and SH3 domain. While native contacts are frequently observed between SH3 and PRM with no $\text{Gd@C}_{82}(\text{OH})_{22}$ in presence (panel **a**), the addition of $\text{Gd@C}_{82}(\text{OH})_{22}$ nanoparticles is shown to seriously interfere PRM's interaction with SH3 with no obvious native contacts seen (panel **b**). In the absence of $\text{Gd@C}_{82}(\text{OH})_{22}$, we found 2 trajectories out of total 7 showing that PRM is bound almost perfectly at the native binding site of SH3 domain.