Electronic Supplementary Material (ESI) for Nanoscale Advances.

Supplementary Information: Computational Elucidation of Recombinant Fusion Protein Effect on Peptide-Directed Nanoparticles

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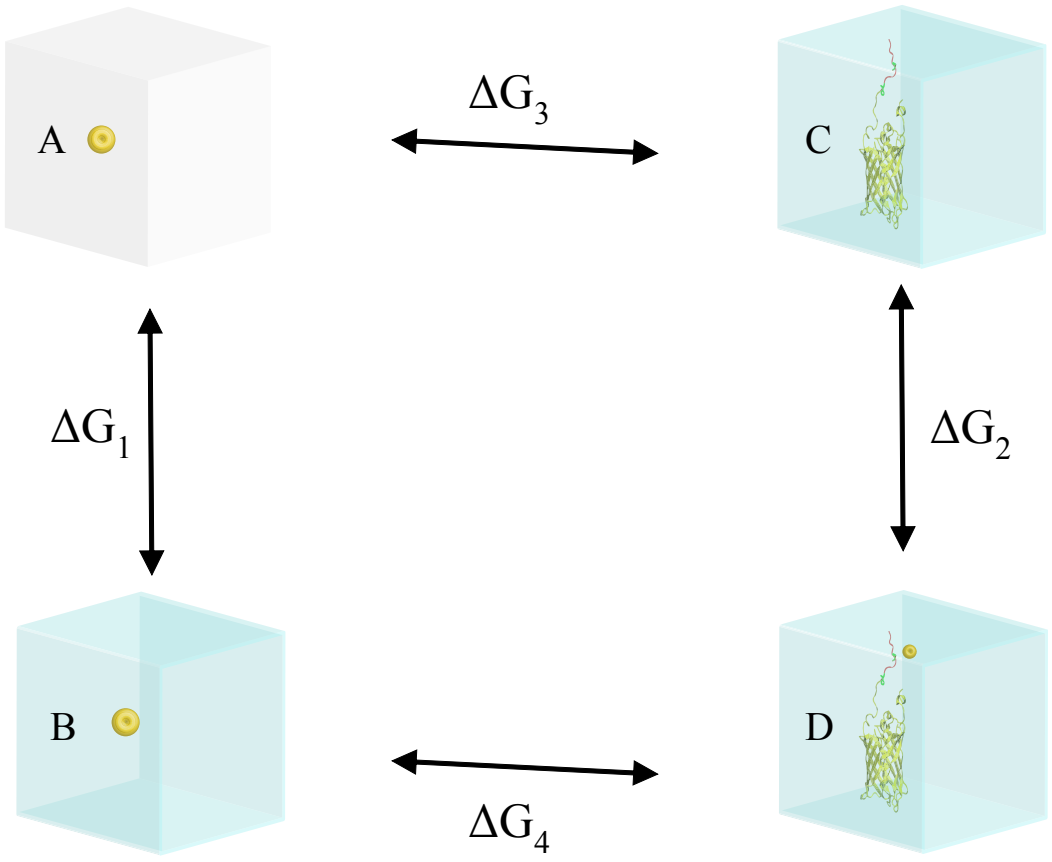
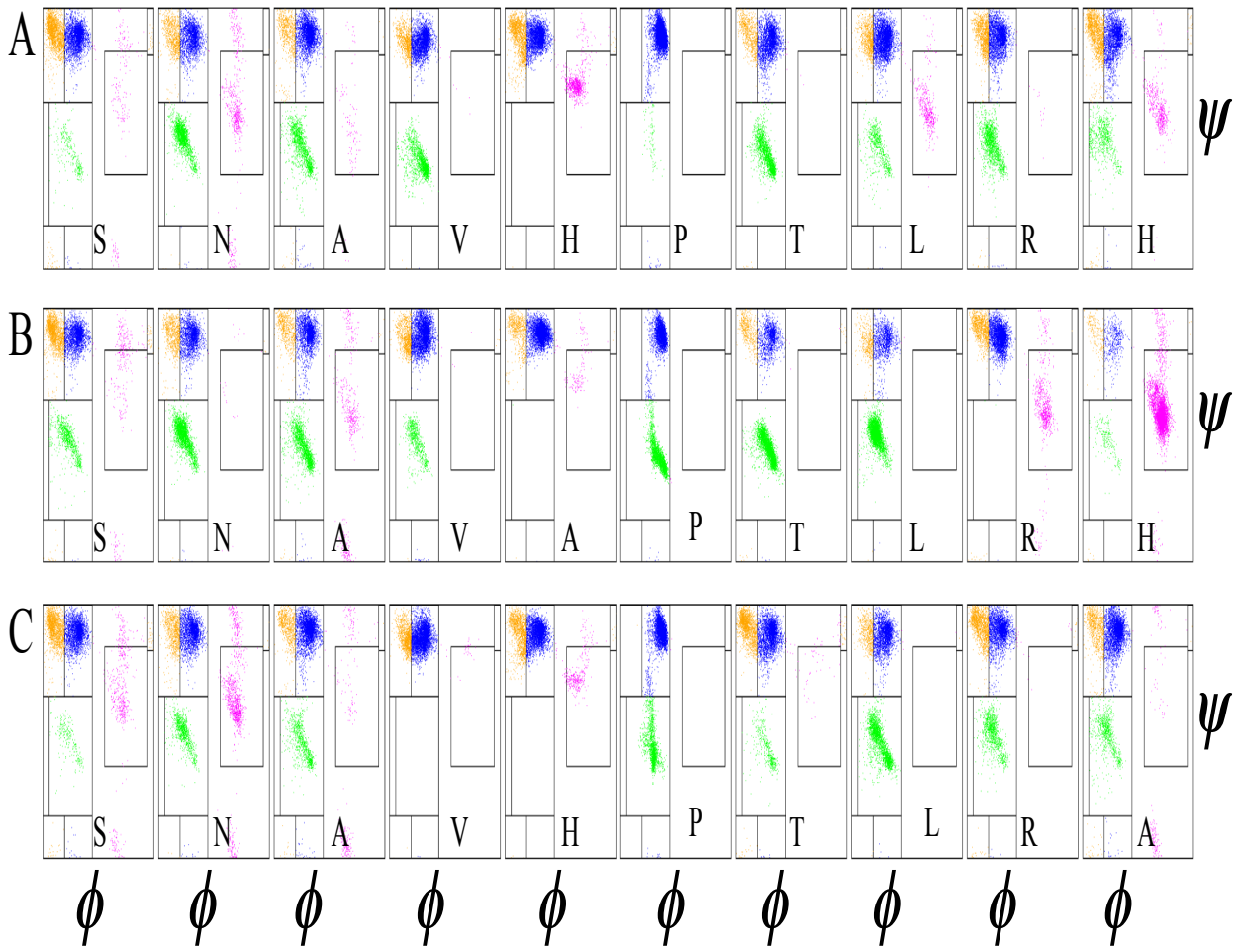
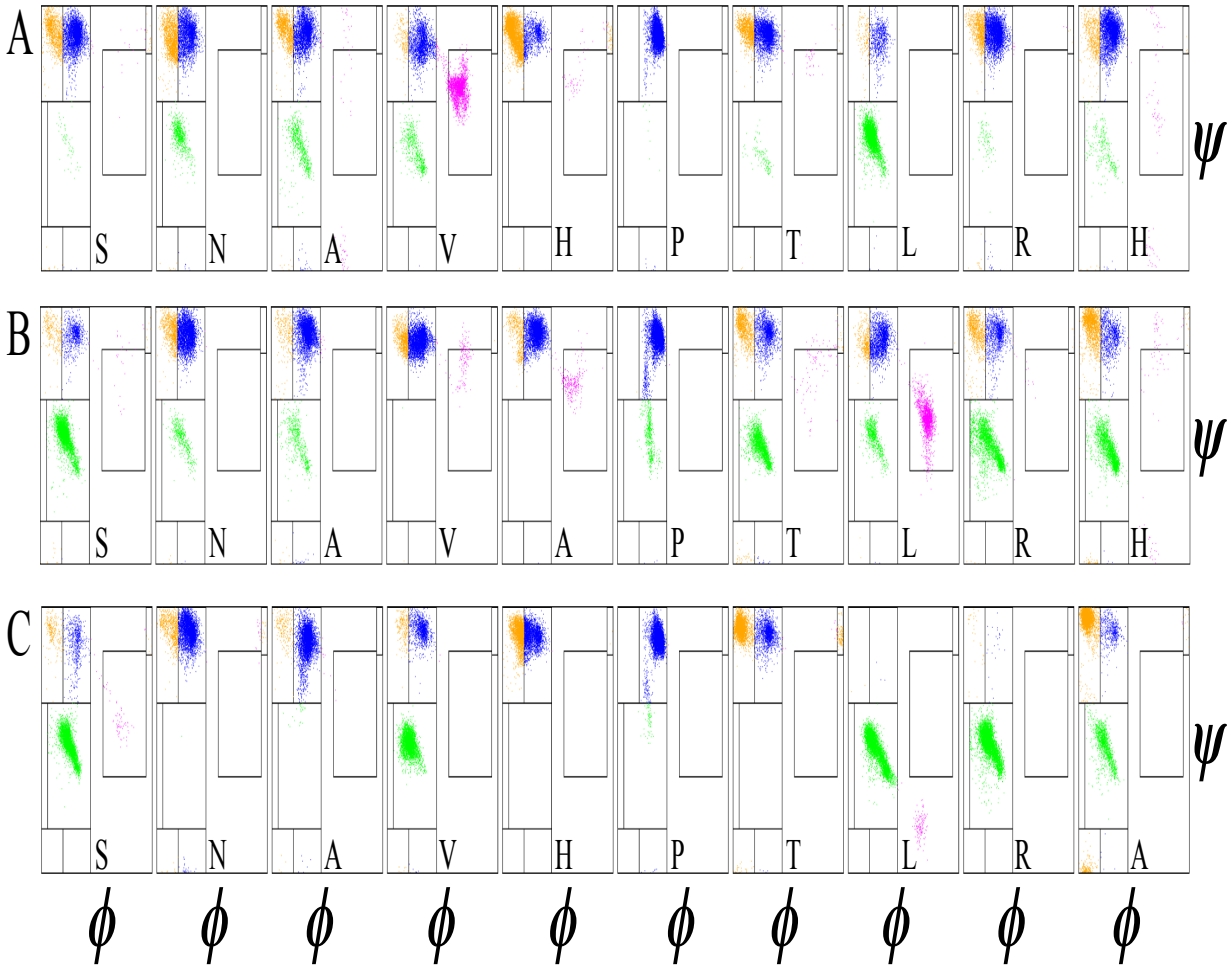


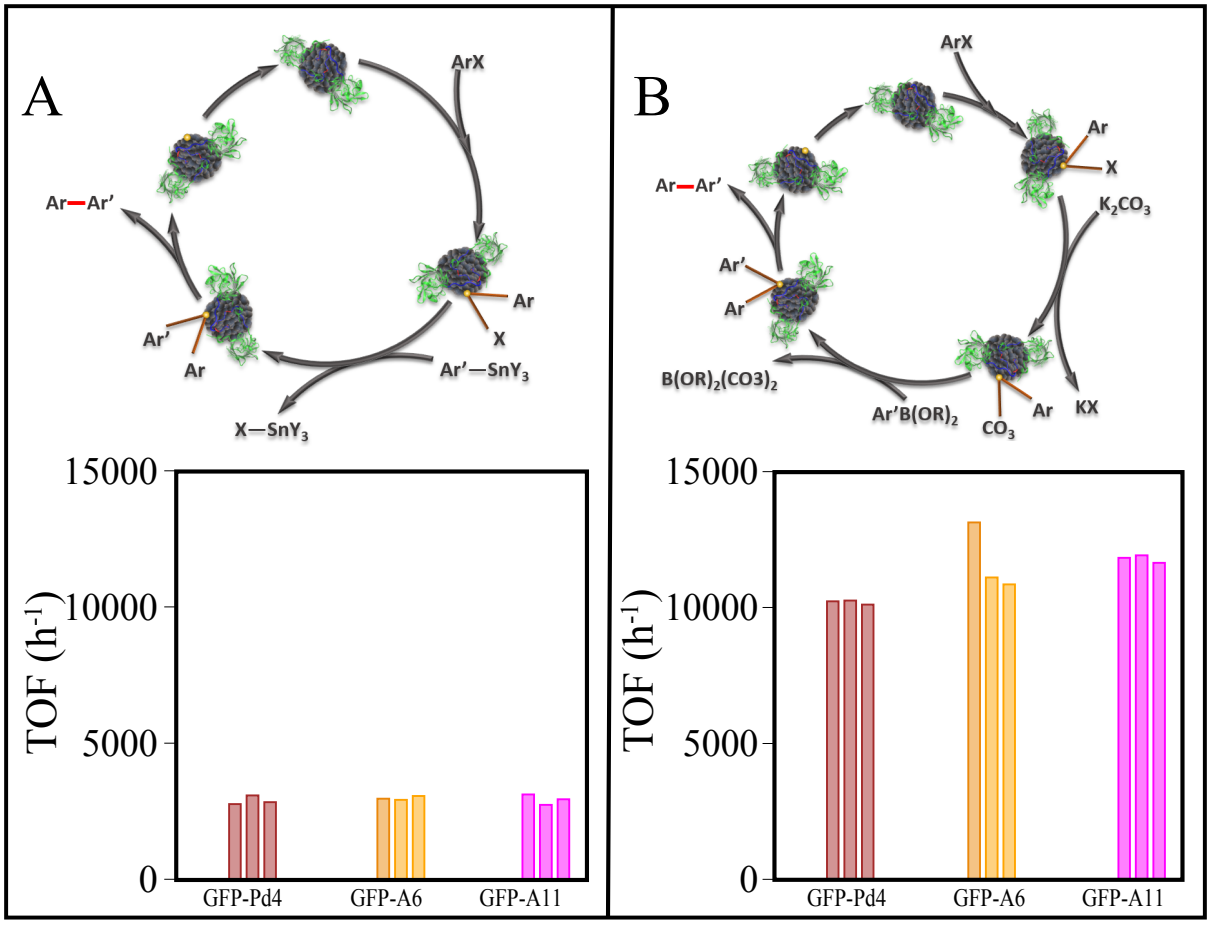
Supplementary Figure 1: Schematic representation of thermodynamics cycle for calculating the relative binding free energy of palladium binding to the histidine of peptides.(A-B) Solvation free energy of palladium ion in the aqueous solution. (C-D) Relative free energy binding of the palladium with the histidines of the peptides. overall binding free energy is derived from $\Delta G_{binding}$ = ΔG_2 - ΔG_1



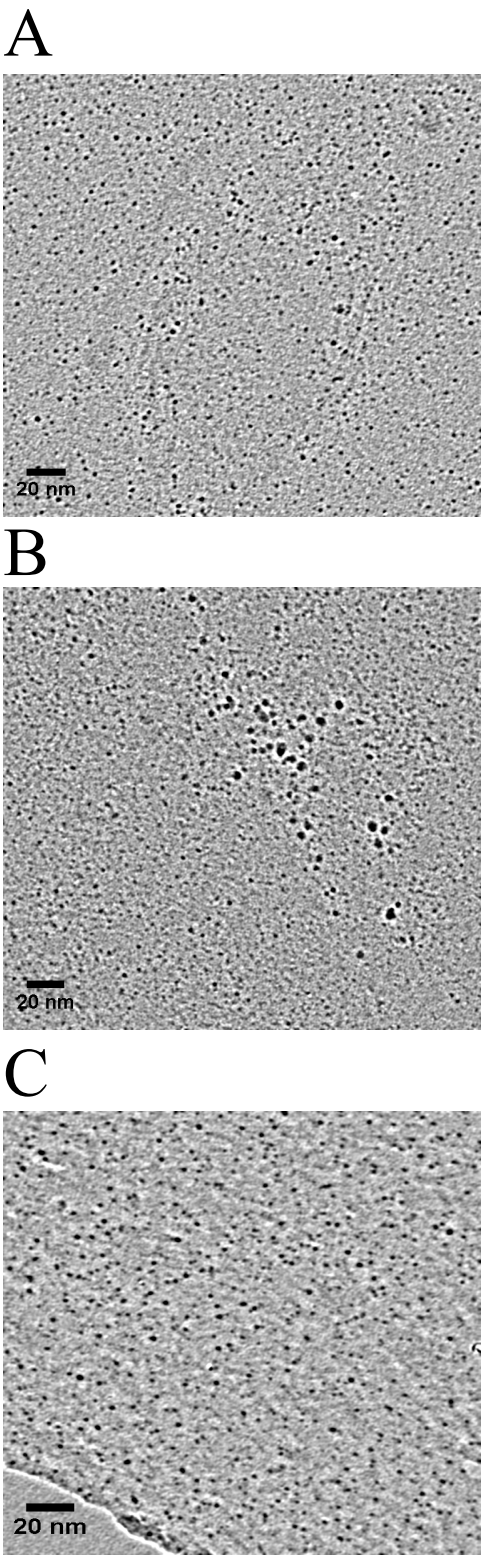
Supplementary Figure 2: Ramachandran plots of residues in free peptides: (A-C) The backbone structure of the residue in peptides Pd4, A6, and A11 respectively. The region definitions are the same as Figure 1A. Orange, blue, pink, green, and gray clusters identify the β, F, α_L, α_R, and N regions, of Ramachandran plot respectively.



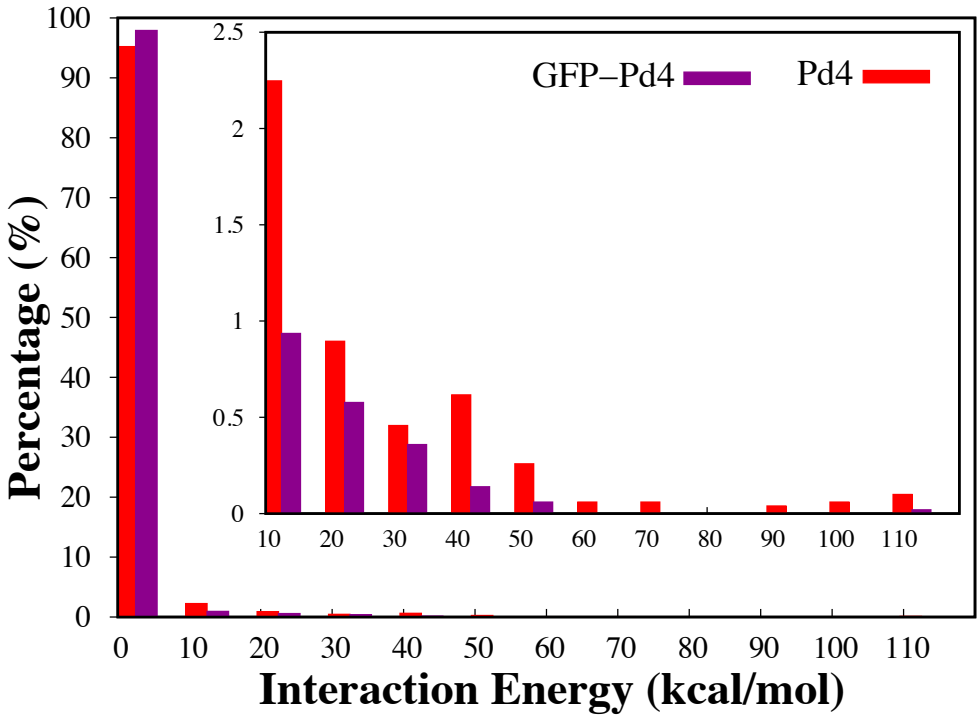
Supplementary Figure 3: Ramachandran plots of residues in GFPuv fusion peptides: (A-C) The backbone structure of the residue in GFP bound peptides Pd4, A6, and A11 respectively. The region definitions are the same as Figure 1A. Orange, blue, pink, green, and gray clusters identify the β, F, α_L, α_R, and N regions, of Ramachandran plot respectively



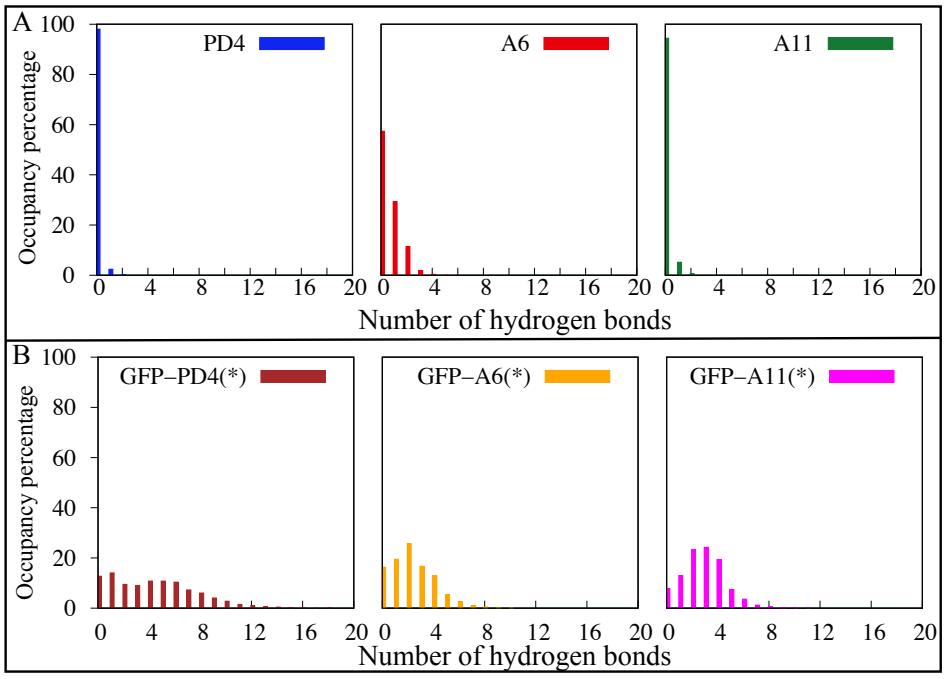
Supplementary Figure 4: Schematic diagram and TOF of (A) Stille coupling and (B) Suzuki-Miyaura coupling reaction for GFP fused peptides Pd4, A6 and A11 respectively.



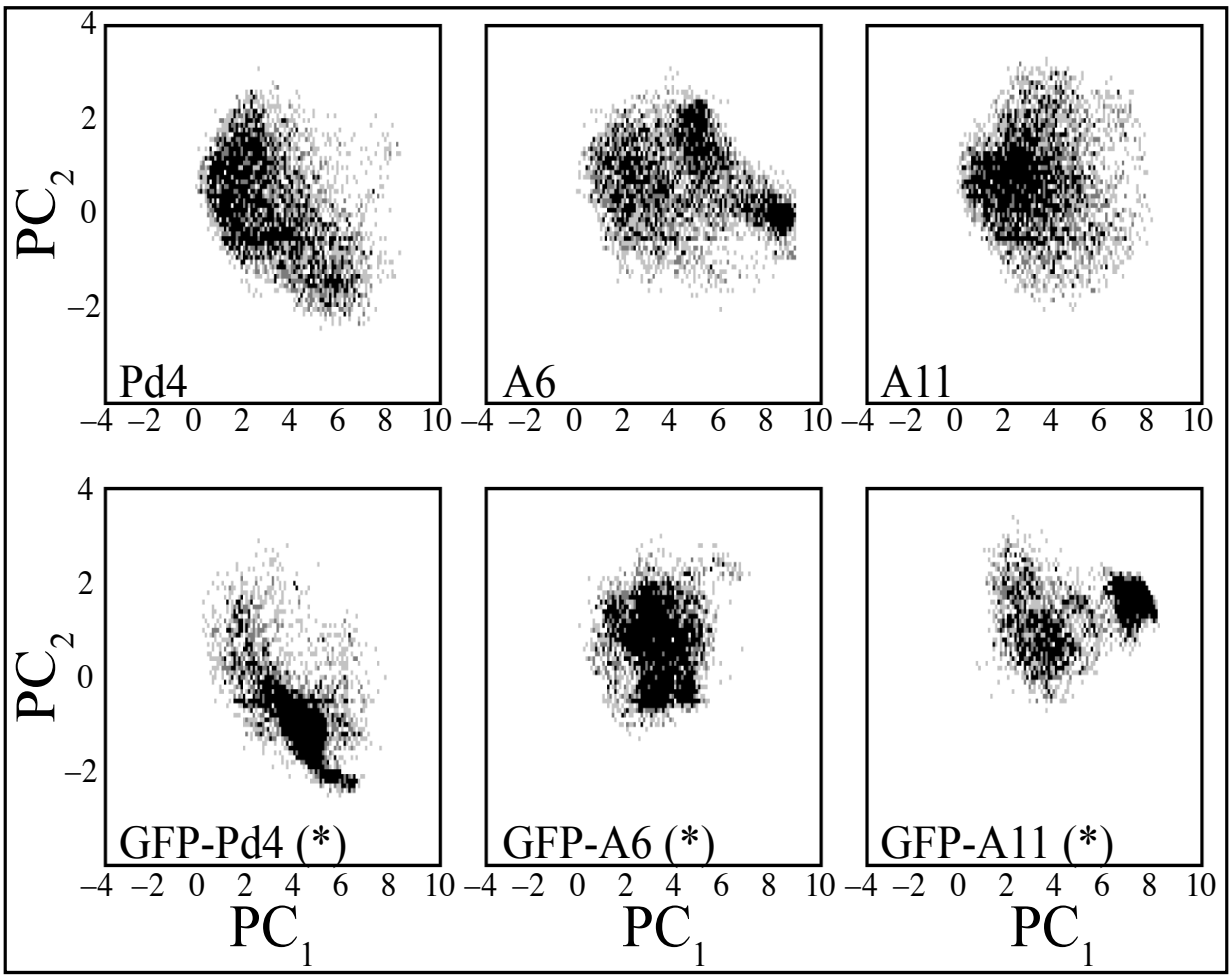
Supplementary Figure 5: (A-C) TEM images of nanoparticles produced from GFPuv-attached peptides Pd4 (A), A6 (B) & A11 (C).



Supplementary Figure 6: His6-His11 interaction energy distribution in the Pd4 and GFP-Pd4 systems. The normalized histograms are built with a bin size of 10 kcal/mol and based on the magnitude of interaction energies. In the inset, the distribution is shown, but the 0–10 bin is left out.



Supplementary Figure 7: The occupancy percentage of hydrogen bonds calculated from the MD simulations for the (A) free peptides and (B) GFPuv fused peptide region. (*) Only the peptide region in the GFPuv fused peptide simulations was used for hydrogen bond analysis. This hydrogen bond analysis was done using a distance cutoff of 3.5 Å and an angle cutoff of 30°.



Supplementary Figure 8: PCA of C-α of peptides in free state and GFP fused simulations. The intensity of the color in the plot represents the relative population of peptide PCA analysis.

Supplementary Table 1: **Optimized condition via coupling reaction of iodobenzene and phenylboronic acid. Solvent, base, and temperature.**

$$\mathrm{Ar{-}X{+}}Ar' \xrightarrow[Solvent,Time,and Temperature]{Catalyst,Base} Ar - Ar' \quad (1)$$

Entry	Solvent	Base (mmol)	Time (h)	Temperature (°C)	Yield[b] (%)
1	EtOH: H_2O (1:1)	KOtBu	3.0	80	47
2	EtOH: H_2O (1:1)	K_2HPO_4	3.0	80	65
3	EtOH: H_2O (1:1)	K_2HPO_4	3.0	80	62
4	EtOH: H_2O (1:1)	K_2CO_3	3.0	80	98
5	EtOH: H_2O (1:1)	K_2CO_3	8.0	80	82
6	EtOH: H_2O (3:1)	K_2CO_3	1.5	80	98
7	EtOH: H_2O (1:1)	K_2CO_3	1.5	80	97
8	EtOH: H_2O (1:3)	K_2CO_3	3.5	80	74

Reaction conditions:iodobenzene (0.1 mmol), phenylboronic acid (0.12 mmol), base (0.3 mmol) and Pd NPs (0.005 μmol) were mixed in solvent and refluxed under N_2. ([b])Yield were determined by HPLC.

Supplementary Table 2: **Optimized condition via coupling reaction of iodobenzene and phenyltin trichloride. Solvent, base, and temperature.**

$$\mathrm{Ar{-}X} + Ar - SnCl_3 \xrightarrow[EtOH:H\_2OandRefulx]{Catalyst,Base} Ar - Ar' \tag{2}$$

Entry	Solvent	Pd (mmol %)	Time (h)	Temperature (°C)	Yield[b] (%)
1	5	KOH	6.0	80	72
2	5	K_2CO_3	6.0	80	34
3	5	K_2HPO_4	6.0	80	36
4	5	CsF	6.0	80	97
5	5	K_3PO_4	48.0	40	58
6	5	K_3PO_4	20.0	60	70
7	10	K_3PO_4	6.0	80	96
8	2	K_3PO_4	16	80	88
9	1	K_3PO_4	16	80	64

Reaction conditions:iodobenzene (0.1 mmol), phenylboronic acid (0.12 mmol), base (0.3 mmol) and Pd NPs (0.005 μmol) were mixed in solvent and refluxed under N_2. ([b])Yield were determined by HPLC.