**Supporting Information**

**Self-Assembly of P22 Protein Cages with Polyamidoamine Dendrimer and Cationic Nanoparticles**

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Sample number ratio calculations for both nanoparticles (NPs): P22 and polyamidoamine G3 (PAMAM): P22 are shown in detail as follows:

1. For PEI-coated iron oxide NPs (Ocean NanoTech),

Number of Fe3O4 NPs, NNPs =

Here, rNPs ~ 5 nm and ρNPs = 5.21 g/cc

NNPs = = 3.67 x 1017 MNPs

Number of P22 particles, NP22 = Moles of P22 particles x Avogadro’s number

Therefore, NP22 = =

NP22 = 3.051 x 1016 MP22

**= 6.5:1**

1. For Au NPs,

Number of Au NPs, NNPs =

Here, rAuNPs ~ 3.5 nm and ρAuNPs = 19.32 g/cc

NAuNPs = = 2.883 x 1017 MNPs

Number of P22 particles, NP22 = Moles of P22 particles x Avogadro’s number

Therefore, NP22 = =

NP22 = 3.051 x 1016 MP22

**= 6.5:1**

1. For PEI-coated CoFe2O4 NPs,

Number of CoFe2O4 NPs, NNPs =

Here, rNPs ~ 6 nm and ρNPs = 5.24 g/cc

NNPs = = 2.11 x 1017 MNPs

Number of P22 particles, NP22 = Moles of P22 particles x Avogadro’s number

Therefore, NP22 = =

NP22 = 3.051 x 1016 MP22

**= 4:1**

1. For PAMAM dendrimers:

Number of PAMAM particles, NPAMAM = Moles of PAMAM x Avogadro’s number

Therefore, NPAMAM = =

NPAMAM = 8.718 x 1019 MPAMAM

Number of P22 particles, NP22 = Moles of P22 particles x Avogadro’s number

Therefore, NP22 = =

NP22 = 3.051 x 1016 MP22

**= 8:1**

The Debye screening length, which determines the electrostatic interaction distance between the particles, is given by:

where, *ε*0 and *ε*r are vacuum permittivity and dielectric constant of the aqueous medium, *k*B is Boltzmann’s constant, *e* is the elementary charge, *T* is the temperature, while *c*i and *z*i are the number density and valencies of the medium electrolyte ions. The following table summarizes the Debye length, pH, and specific mixing conditions of P22 virus-like particles (VLPs) with NPs and PAMAM. Table 1 shows the experimental conditions used for the VLP-NP and VLP-PAMAM interactions.

Table SI. Summary of experiments conducted to investigate the assembly of P22 VLPs through electrostatic interaction with rigid NPs and soft PAMAM dendrimer.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Serial number | Nanoparticle: P22 number ratio or PAMAM: P22 number ratio | NaCl concentration (mM) | pH | | | Debye length (nm) |
| *Nanoparticles: Iron oxide, CoFe2O4, and Au* | | | | | | |
| 1 | 0.9:1 | 0 | 6 | 7 | 7.5 | ∞ |
| 2 | 2.4:1 | 0 | 6 | 7 | 7.5 | ∞ |
| 3 | 4.3:1 | 0 | 6 | 7 | 7.5 | ∞ |
| 4 | 6.5:1 | 0 | 6 | 7 | 7.5 | ∞ |
| 5 | 7:1 | 0 | 6 | 7 | 7.5 | ∞ |
| 6 | 11:1 | 0 | 6 | 7 | 7.5 | ∞ |
| 7 | 0.9:1 | 10 | 6 | 7 | 7.5 | 3.04 |
| 8 | 2.4:1 | 10 | 6 | 7 | 7.5 | 3.04 |
| 9 | 4.3:1 | 10 | 6 | 7 | 7.5 | 3.04 |
| 10 | 6.5:1 | 10 | 6 | 7 | 7.5 | 3.04 |
| 11 | 7:1 | 10 | 6 | 7 | 7.5 | 3.04 |
| 12 | 11:1 | 10 | 6 | 7 | 7.5 | 3.04 |
| 13 | 0.9:1 | 50 | 6 | 7 | 7.5 | 1.36 |
| 14 | 2.4:1 | 50 | 6 | 7 | 7.5 | 1.36 |
| 15 | 4.3:1 | 50 | 6 | 7 | 7.5 | 1.36 |
| 16 | 6.5:1 | 50 | 6 | 7 | 7.5 | 1.36 |
| 17 | 7:1 | 50 | 6 | 7 | 7.5 | 1.36 |
| 18 | 11:1 | 50 | 6 | 7 | 7.5 | 1.36 |
| 19 | 0.9:1 | 100 | 6 | 7 | 7.5 | 0.96 |
| 20 | 2.4:1 | 100 | 6 | 7 | 7.5 | 0.96 |
| 21 | 4.3:1 | 100 | 6 | 7 | 7.5 | 0.96 |
| 22 | 6.5:1 | 100 | 6 | 7 | 7.5 | 0.96 |
| 23 | 7:1 | 100 | 6 | 7 | 7.5 | 0.96 |
| 24 | 11:1 | 100 | 6 | 7 | 7.5 | 0.96 |
| *Polyamidoamine (PAMAM)* | | | | | | |
| 25 | 2:1 | 10 | 7.5 | | | 3.04 |
| 26 | 6:1 | 10 | 7.5 | | | 3.04 |
| 27 | 8:1 | 10 | 7.5 | | | 3.04 |
| 28 | 10:1 | 10 | 7.5 | | | 3.04 |
| 29 | 100:1 | 10 | 7.5 | | | 3.04 |
| 30 | 2.1 | 100 | 7.5 | | | 0.96 |
| 31 | 6:1 | 100 | 7.5 | | | 0.96 |
| 32 | 8:1 | 100 | 7.5 | | | 0.96 |
| 33 | 10:1 | 100 | 7.5 | | | 0.96 |
| 34 | 100:1 | 100 | 7.5 | | | 0.96 |
| 35 | 2:1 | 1000 | 7.5 | | | 0.30 |
| 36 | 6:1 | 1000 | 7.5 | | | 0.30 |
| 37 | 8:1 | 1000 | 7.5 | | | 0.30 |
| 38 | 10:1 | 1000 | 7.5 | | | 0.30 |
| 39 | 100:1 | 1000 | 7.5 | | | 0.30 |

Figure S1 summarizes the hydrodynamic sizes of P22 VLP and the NPs, measured on a dynamic light scattering (DLS) instrument equipped with a Zetasizer (Malvern).



Figure S1. DLS plots showing hydrodynamic sizes of: (a) P22 and (b) PEI-iron oxide NPs, (c) PEI-CoFe2O4 NPs, and (d) Au NPs.

Figure S2 and S3 indicate the influence of pH on the zeta potential of P22 VLPs and PEI-iron oxide NPs, respectively.



Figure S2. Zeta potential of P22 at different pH. (a) pH = 5, (b) pH = 6, and (c) pH = 8.



Figure S3. Zeta potential of PEI-iron oxide NPs at different pH. (a) pH 5.5, (b) pH 6.5, (c) pH 6, and (d) pH 7.

Figure S4a-c are transmission electron microscope (TEM) image showing the assembly of P22 at different NP: P22 number ratio, using PEI-iron oxide NPs as models. Figure S4d is a TEM image of the PEI-CoFe2O4 NPs used in our experiments.



Figure S4. TEM image showing (a) NP packing around P22 at 2.4:1 NP: P22 number ratio, (b) dense monolayer of P22 packed with NPs at 7:1 NP: P22 number ratio, (c) P22 VLP clustering at high NP: P22 number ratio (11: 1), and (b) PEI-CoFe2O4 NPs.

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