

## **Supplementary Material**

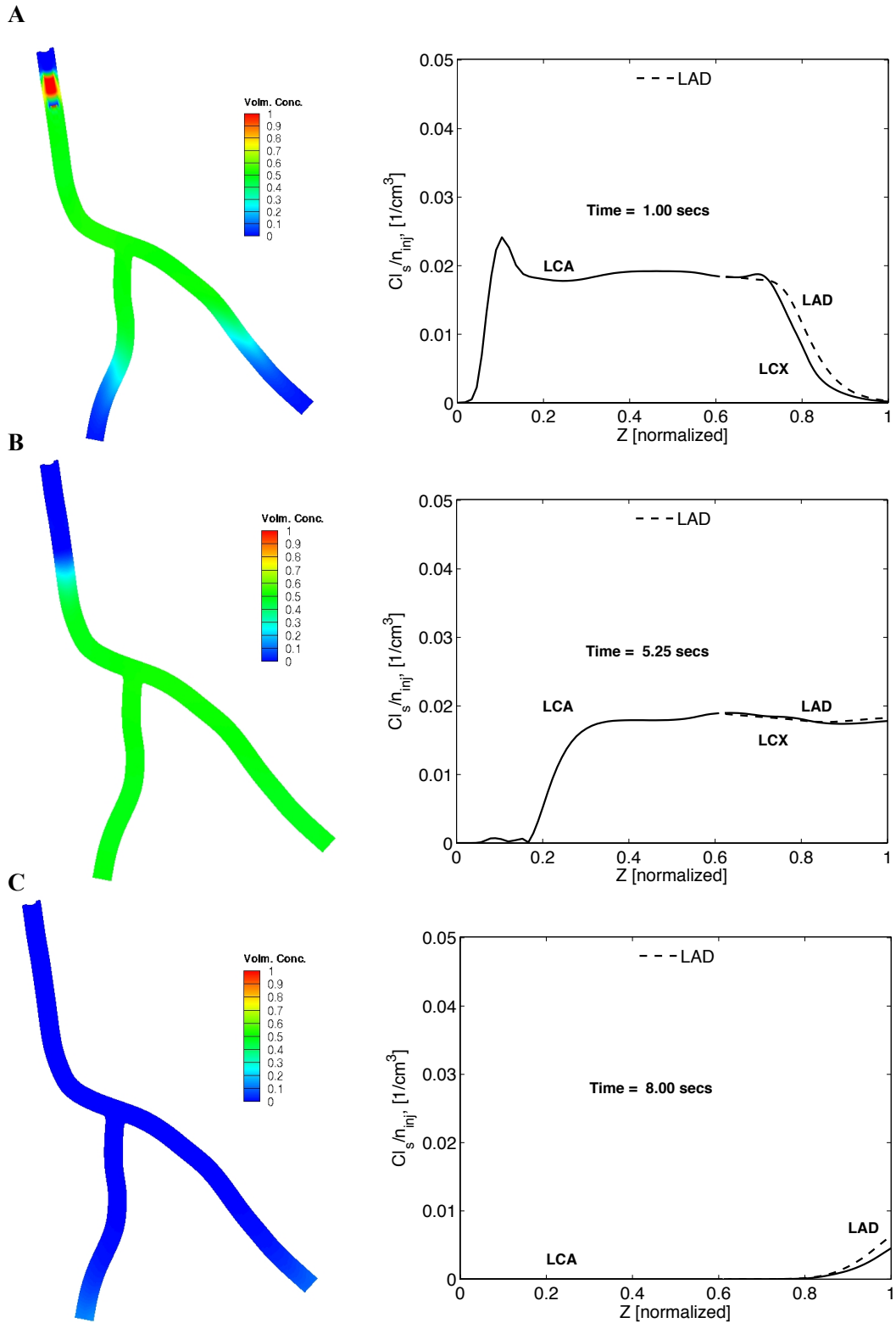
### **Wall Deposition Patterns for Nanoparticles in an Inflamed Patient-Specific Arterial Tree**

Shaolie S. Hossain<sup>a</sup>, Thomas J.R. Hughes<sup>b</sup>, Paolo Decuzzi<sup>a</sup>

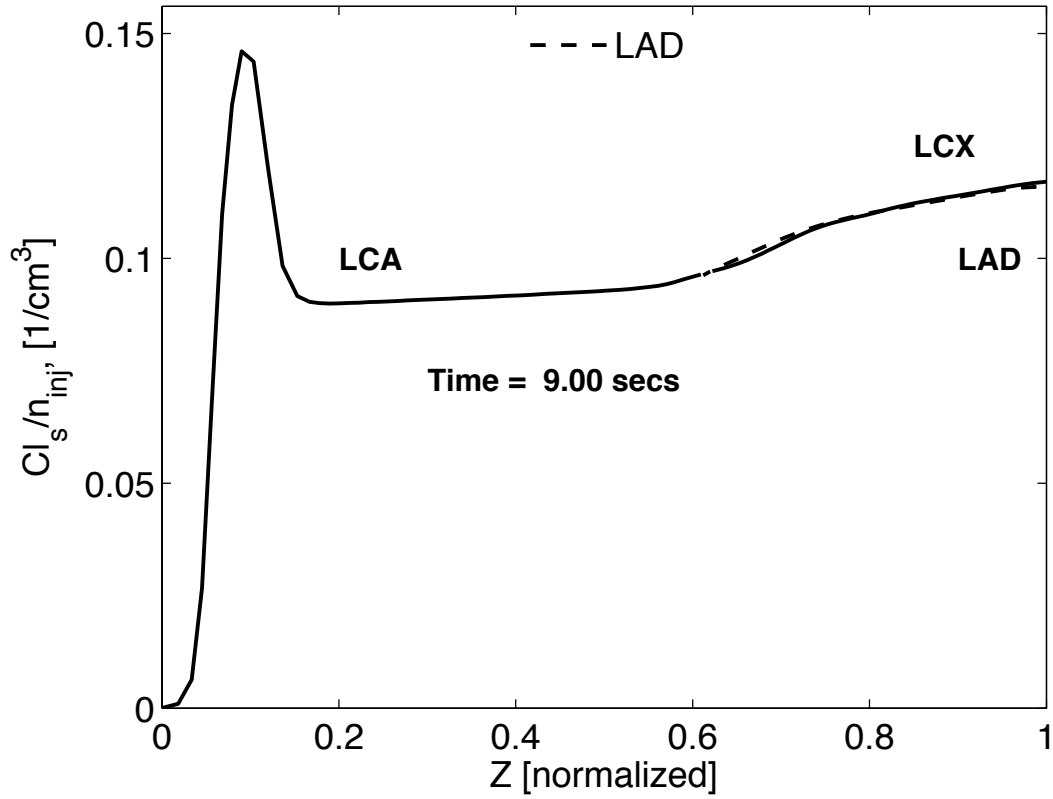
<sup>a</sup>Department of Translational Imaging and Department of Nanomedicine, The Methodist Hospital Research Institute, 6670 Bertner Avenue, Houston, TX 77030, USA

<sup>b</sup>Institute for Computational Engineering and Sciences, The University of Texas at Austin, 201 East 24<sup>th</sup> Street, Stop C0200, Austin, TX 78712, USA

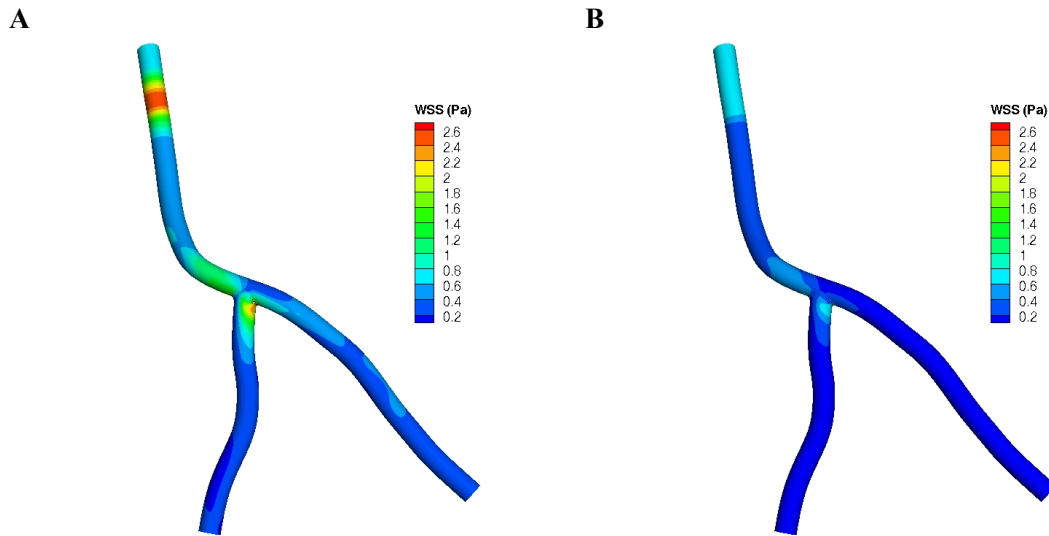
**Supplementary Figure 1:** Time evolution of particle volumetric concentration at A) 1 s, B) 5.25 s, and C) 8 s. Right column plots the area-averaged quantity normalized by the number of particles injected  $n_{inj}$  and averaged over the surface area along the vessel centerline (“Z” direction).



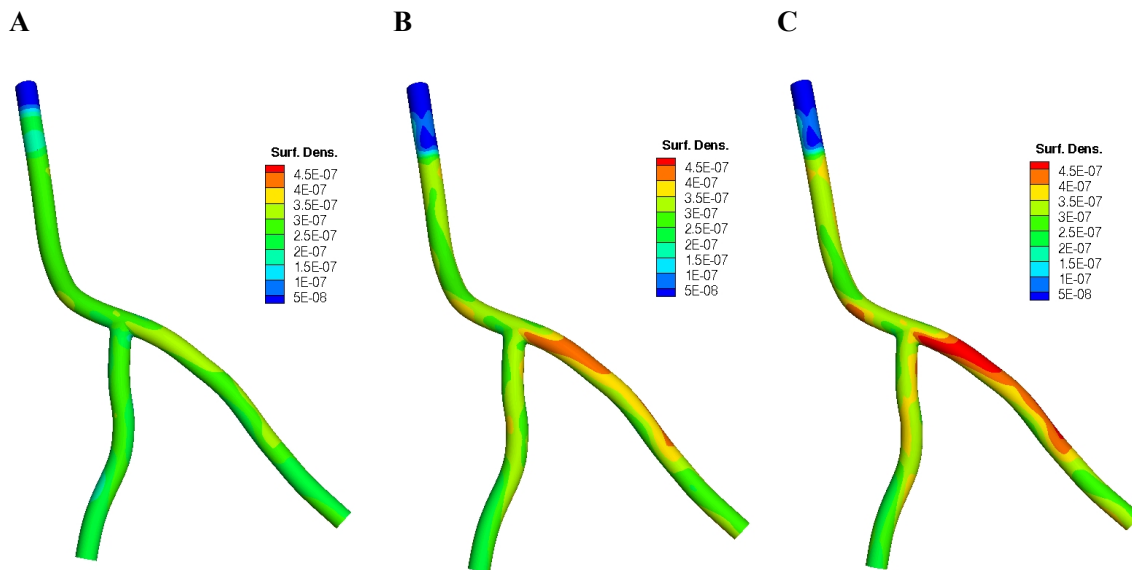
**Supplementary Figure 2:** Time-integrated particle volumetric concentration ( $\text{cm}^{-3}$ )  $C|_s$  at the lumen-wall interface at the end of simulation ( $t = 9$  s) averaged over the circumference of each cross section taken at various “Z”-locations along the vessel centerline.



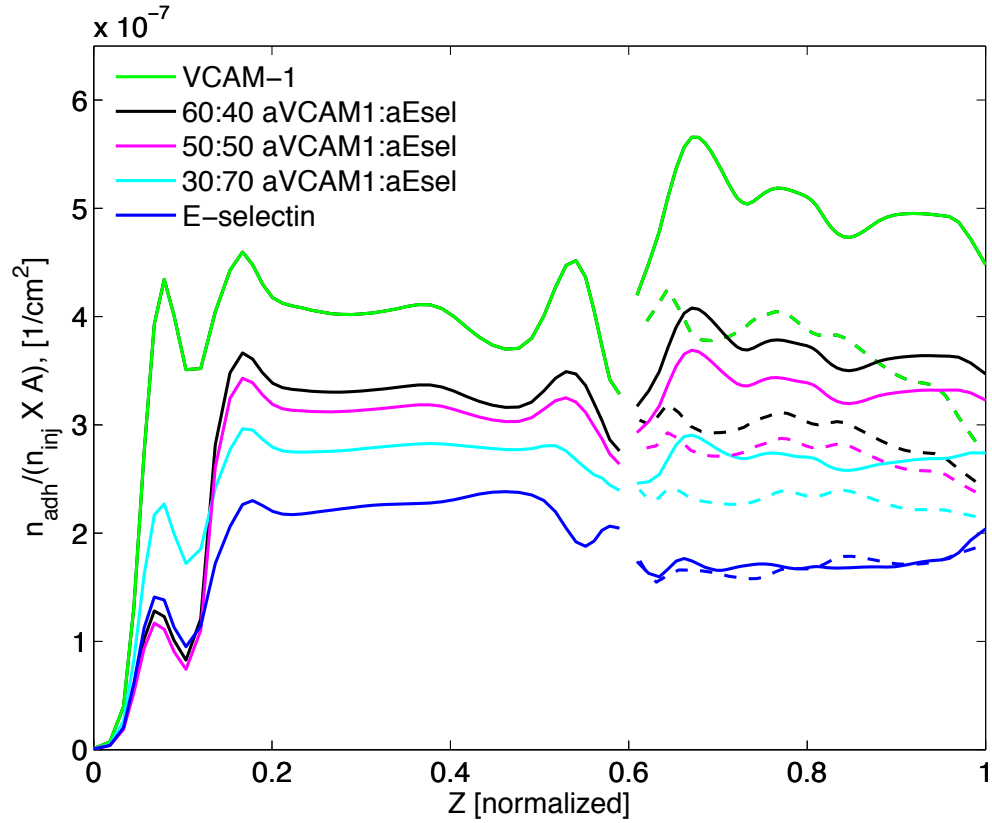
**Supplementary Figure 3:** Time-averaged wall shear stress (WSS) in Pa ( $\text{N}/\text{m}^2$ ) A) during the first 5 s of catheter injection and B) after catheter injection is ceased.



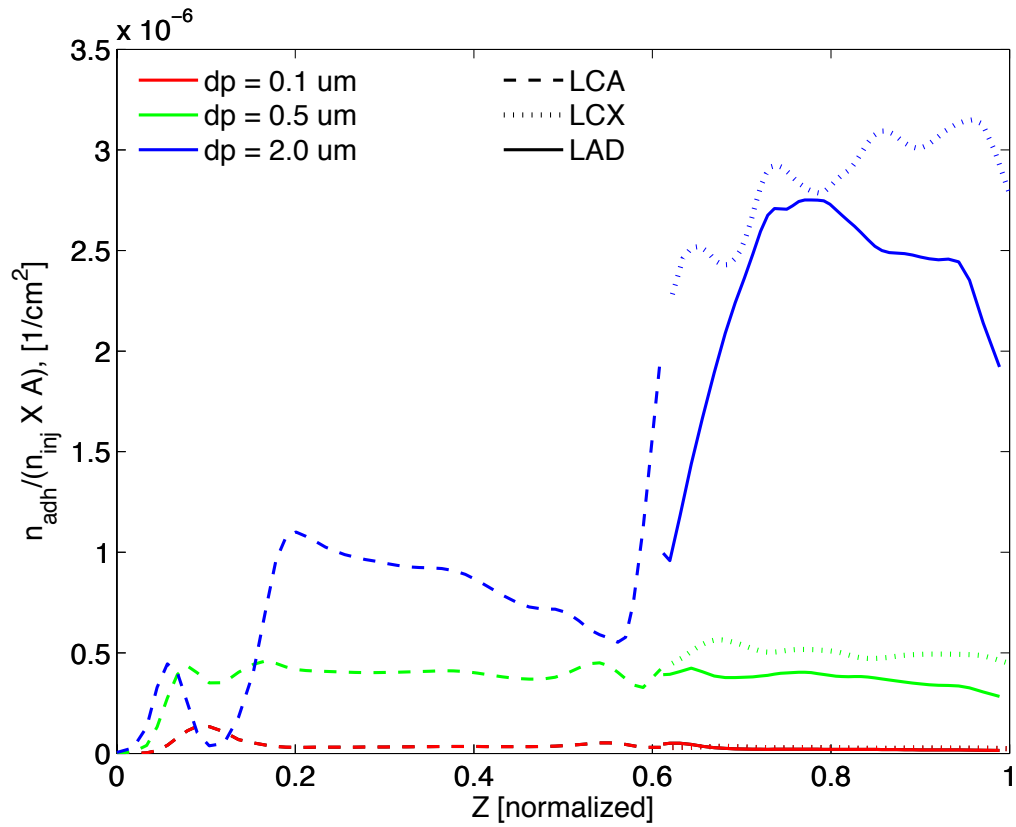
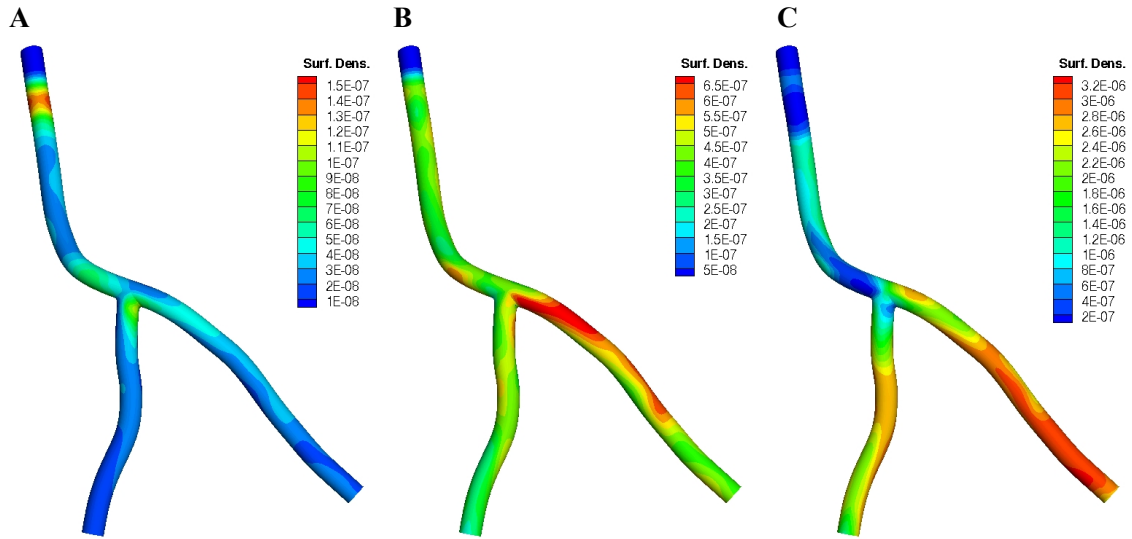
**Supplementary Figure 4:** Comparison between A) 30:70, B) 50:50, and C) 60:40 aVCAM:aEsel targeting in terms of  $(n_{\text{adh}}/n_{\text{inj}} \times A)$ , where  $n_{\text{adh}}$  is the number of adhered particles,  $n_{\text{inj}}$  is the total number of injected particles, and  $A$  is the surface area ( $\text{cm}^2$ ).



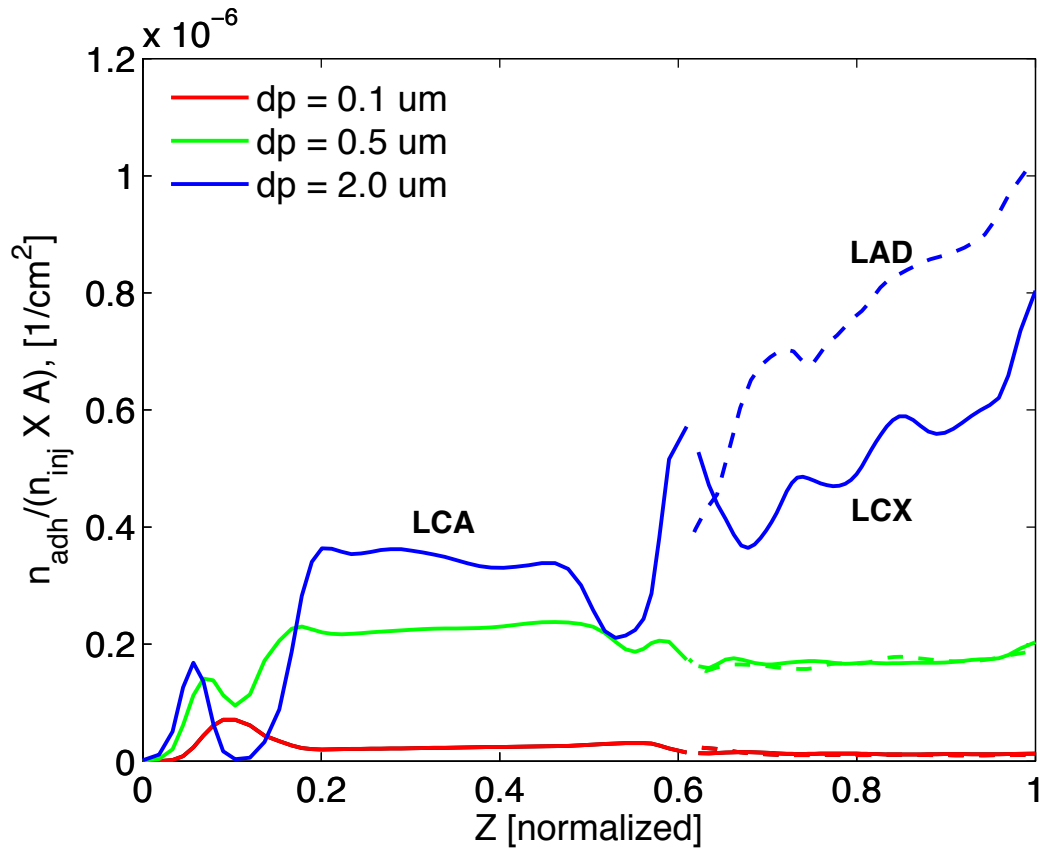
**Supplementary Figure 5: Comparison between different proportions of dual targeting.** The number of adhering  $0.5 \mu\text{m}$  particles averaged over the circumference of each cross section taken at various “ $Z$ ”-locations along the vessel centerline. Here  $n_{\text{adh}}$  is the number of adhered particles,  $n_{\text{inj}}$  is the total number of injected particles, and  $A$  is the surface area ( $\text{cm}^2$ ). Comparison between A) 30:70 aVCAM-aEsel, B) 50:50 aVCAM-aEsel and C) 60:40 aVCAM-aEsel cases. Here dashed line represents the LAD branch.



**Supplementary Figure 6: Comparison of particle size under single receptor (VCAM-1) targeting.** Spatial distribution of different sized particles: A)  $d_p = 0.1 \mu\text{m}$ , B)  $d_p = 0.5 \mu\text{m}$  and C)  $d_p = 2.0 \mu\text{m}$ , in terms of  $n_{\text{adh}}/(n_{\text{inj}} \times A)$ , where  $n_{\text{adh}}$  is the number of adhered particles,  $n_{\text{inj}}$  is the total number of injected particles and  $A$  ( $\text{cm}^2$ ).



**Supplementary Figure 7: Comparison of particle size under single receptor (E-selectin) targeting.** Spatial distribution of different sized particles: A)  $d_p = 0.1 \mu\text{m}$ , B)  $d_p = 0.5 \mu\text{m}$  and C)  $d_p = 2.0 \mu\text{m}$ , averaged over the circumference of each cross section taken at various “Z”-locations along the vessel centerline in terms of  $n_{\text{adh}}/(n_{\text{inj}} \times A)$ . Here,  $n_{\text{adh}}$  is the number of adhered particles,  $n_{\text{inj}}$  is the total number of injected particles and  $A$  ( $\text{cm}^2$ ). The dashed line represents the LAD branch.



**Supplementary Table 1:** Area-averaged NP surface density in the arterial tree segment under the single- and dual-targeting approaches.

Total area-averaged NP surface density, cm <sup>-2</sup>			
NP type	Single - receptor targeting approach		
aICAM-1	7.09 x 10 <sup>-9</sup>	4.51 x 10 <sup>-8</sup>	7.48 x 10 <sup>-8</sup>
aVCAM-1	3.26 x 10 <sup>-8</sup>	4.14 x 10 <sup>-7</sup>	1.87 x 10 <sup>-6</sup>
aEsel	1.82 x 10 <sup>-8</sup>	1.75 x 10 <sup>-7</sup>	4.83 x 10 <sup>-7</sup>
aVCAM-1:aEsel	Dual - receptor targeting approach		
30:70	2.25 x 10 <sup>-8</sup>	2.46 x 10 <sup>-7</sup>	9.03 x 10 <sup>-7</sup>
50:50	2.41 x 10 <sup>-8</sup>	2.86 x 10 <sup>-7</sup>	1.18 x 10 <sup>-6</sup>
60:40	2.55 x 10 <sup>-8</sup>	3.09 x 10 <sup>-7</sup>	1.32 x 10 <sup>-6</sup>

**Supplementary Table 2:** Heterogeneity index, H under the single- and dual-targeting

approaches. Here,  $H = \frac{N_{LCX}}{N_{LAD}}$ , and N is the surface density of particles integrated over the entire surface of the branch and divided by the total surface area of the branch.

Heterogeneity index, H			
NP type	$d_p = 0.1 \mu\text{m}$	$d_p = 0.5 \mu\text{m}$	$d_p = 2.0 \mu\text{m}$
Single-receptor targeting approach			
aICAM-1	1.06	0.88	0.53
aVCAM-1	1.21	1.35	1.22
aEsel	1.04	1.01	0.70
Dual-receptor targeting approach			
30:70	1.11	1.17	0.99
50:50	1.15	1.23	1.08
60:40	1.16	1.26	1.11