SUPPORTING INFORMATION

Dual Peptide Nucleic Acid- and Peptide-functionalized Shell Crosslinked Nanoparticles Designed to Target mRNA toward the Diagnosis and Treatment of Acute Lung Injury

Ritu Shrestha,[†] Yuefei Shen,[‡] Kevin A. Pollack,[†] John-Stephen A. Taylor,^{*,‡} and Karen L. Wooley^{*},[†]

[†]Departments of Chemistry and Chemical Engineering , Texas A&M University, P.O. Box 30012, College Station, Texas 77842-3012, USA

[‡]Department of Chemistry, Washington University in Saint Louis, Saint Louis, Missouri 63130, USA

Supplementary Tables and Figures.

Table S1. MALDI data for PNAs

		Calc. Mass (M+1)	Obsvd. Mass (M+1)
iNOS-240	5'- TGT CCT TTT CCT CTT TCA-K4 -3'	5267.3	5268.6
iNOS-240mm	5'- TGT CCT <u>CC</u> T <u>TT</u> T CTT TCA-K4 -3'	5267.3	5268.5
iNOS-480	5'- TGA AAT CCG ATG TGG CCT-K4-3'	5427.3	5428.3
iNOS-480mm	5'-T <u>AG</u> AAT CC <u>A G</u> TG <u>GT</u> G CCT-K4- 3'	5427.3	5432.5

Table S2. MALDI data for maleimide-PNAs

		Calcd. Mass (M+1) Obsvd. Mass (M+1)	
iNOS-240	5'-Maleimide-TGT CCT TTT CCT CTT TCA-3	4906.7	4909.2
iNOS-240mm	5'-Maleimide- TGT CCT CCT TTT CTT TCA-3	4906.7	4906.9
iNOS-480	5'-Maleimide- TGA AAT CCG ATG TGG CCT-3	5063.8	5064.0
iNOS-480 mm	5'-Maleimide- TAG AAT CCA GTG GTG CCT-3	5063.8	5067.3



Figure S1. TEM images of iNOS PNA-SCK conjugates with and without TAT.



Figure S2. Determination of ODN 240 and 480 binding affinity for iNOS mRNA. Fits of fraction ODN bound to the iNOS mRNA from a Dynabead binding assay to equation 1) as described in the experimental section. The concentration of ODN was 100 pM.



Figure S3. Determination of PNA 240 and 480 binding affinity for iNOS mRNA through a Dynabead competition assay as described in the experimental section. The fraction of mRNA (10 pM) bound to 5'-radiolabeled ODN (1 nM) as a function of PNA concentration (nM) was fit to equation 2) to determine the IC₅₀. The K_d for PNA binding was then determined from the K_d for the ODN and the IC₅₀ for the PNA according to equation 3).



Figure S4. Determination of SCK-PNA 240 and 480 binding affinity for iNOS mRNA through a Dynabead competition assay as described in the experimental section. The fraction of mRNA (10 pM) bound to 5'-radiolabeled ODN (1 nM) as a function of SCK-PNA concentration (nM) was fit to equation 2) to determine the IC₅₀. The K_d for SCK-PNA binding was then determined from the K_d for the ODN and the IC₅₀ for the SCK-PNA according to equation 3).



Figure S5. Determination of TAT-SCK-PNA 240 and 480 binding affinity for iNOS mRNA through a Dynabead competition assay as described in the experimental section. The fraction of mRNA (10 pM) bound to 5'-radiolabeled ODN (1 nM) as a function of TAT-SCK-PNA concentration (nM) was fit to equation 2) to determine the IC50. The K_d for TAT-SCK-PNA binding was then determined from the K_d for the ODN and the IC50 for the TAT-SCK-PNA according to equation 3).