Synthesis, Characterization and Bioimaging of a Fluorescent Rhenium-Containing PNA Bioconjugate

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Table of contents

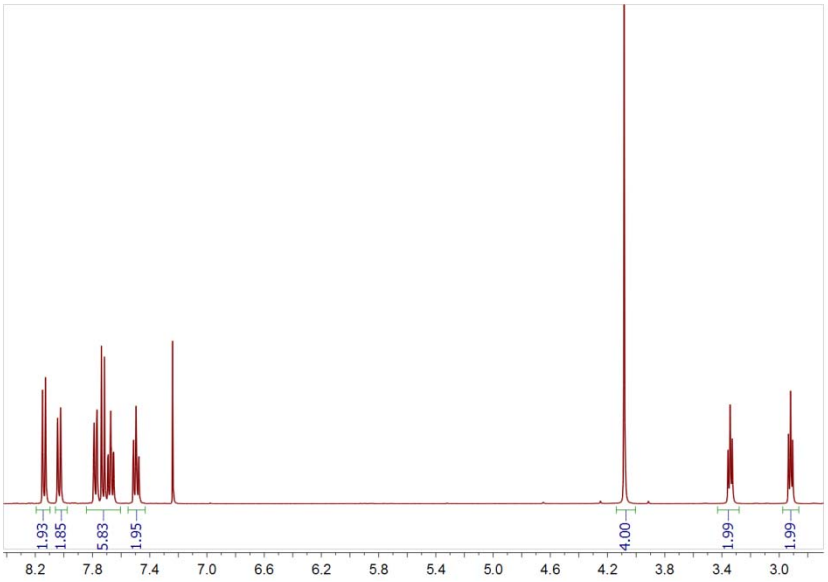

Figure S1. ^{1}H NMR in $CDCl_3$ of ligand **L-N_3.**

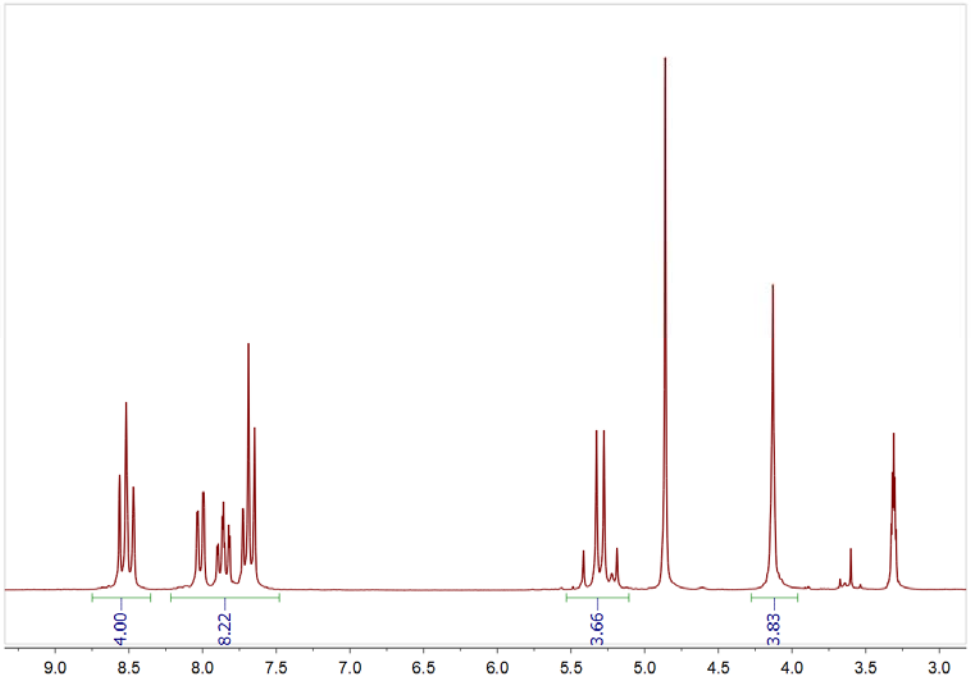

Figure S2. ^{1}H NMR in CD_3OD of **[Re(CO)$_3$(L-N_3)]Br** just after dissolution.

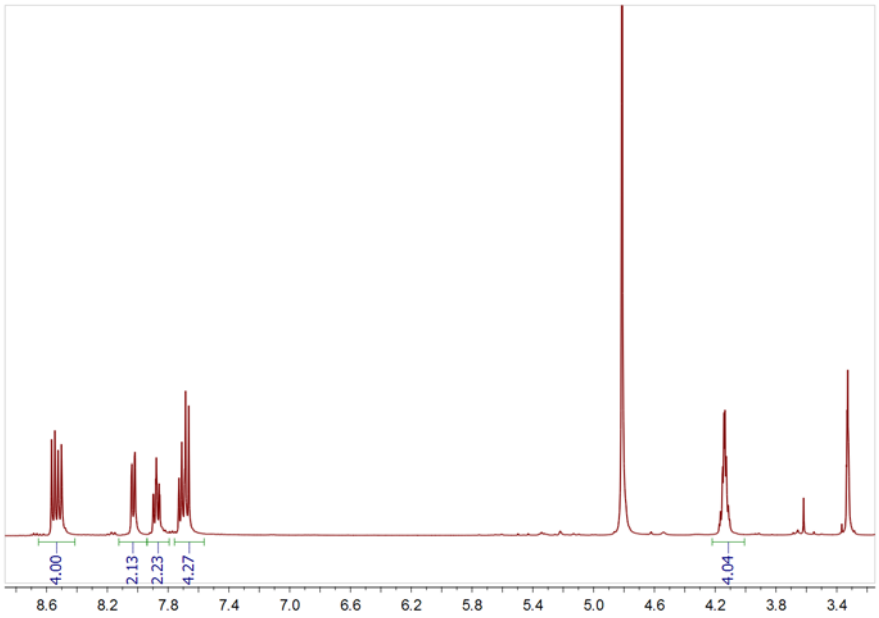

Figure S3. ^{1}H NMR in CD_3OD of **[Re(CO)$_3$(L-N$_3$)]Br** 5 days after dissolution.

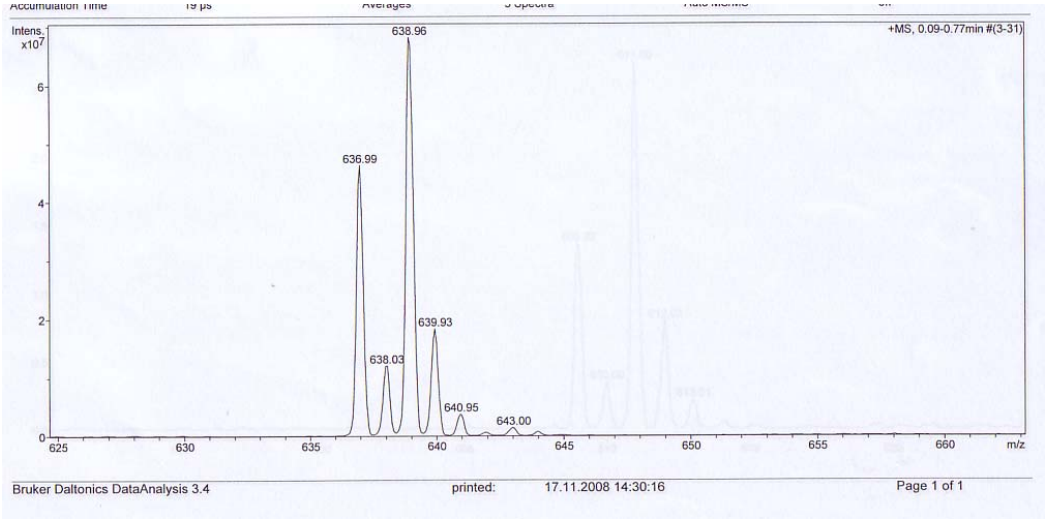

Figure S4. ESI-MS Spectrum of **[Re(CO)$_3$(L-N$_3$)]Br** in MeOH.

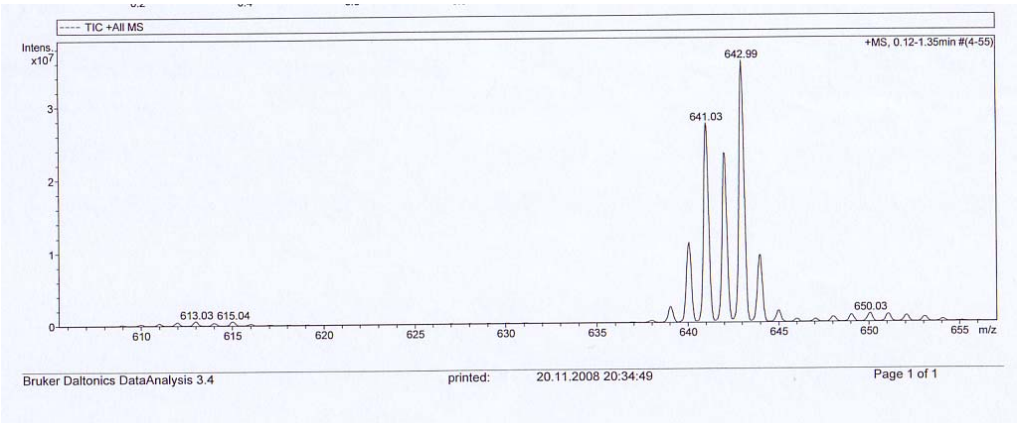

Figure S5. ESI Spectrum of **[Re(CO)$_3$(L-N$_3$)]Br** in CD_3OD 5 days after dissolution.

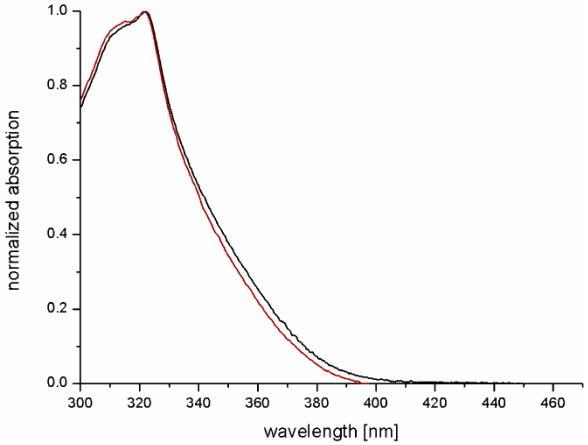

Figure S6. Normalized absorption spectra of **Re(CO)$_3$(L-N$_3$)]Br** in degassed ethylene glycol (black) and in air-saturated water (red) at room temperature.

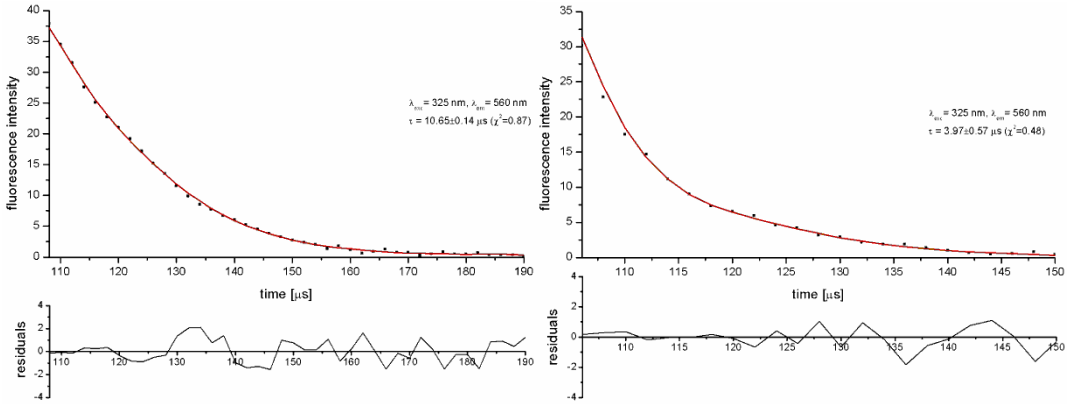

Figure S7. Observed luminescence decay curves (measured at 560 nm) and monoexponential fit (red) of **Re(CO)$_3$(L-N$_3$)]Br** in degassed (left) and air-saturated (right) ethylene glycol at room temperature.

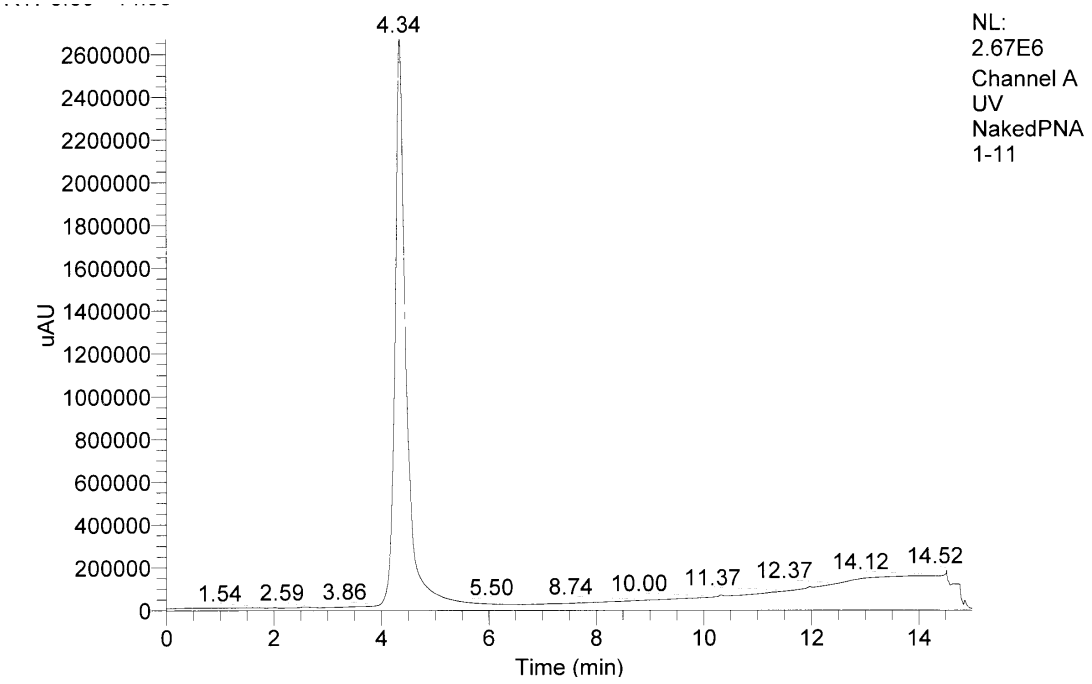

Figure S8. Analytical HPL chromatogram of **Naked-PNA**

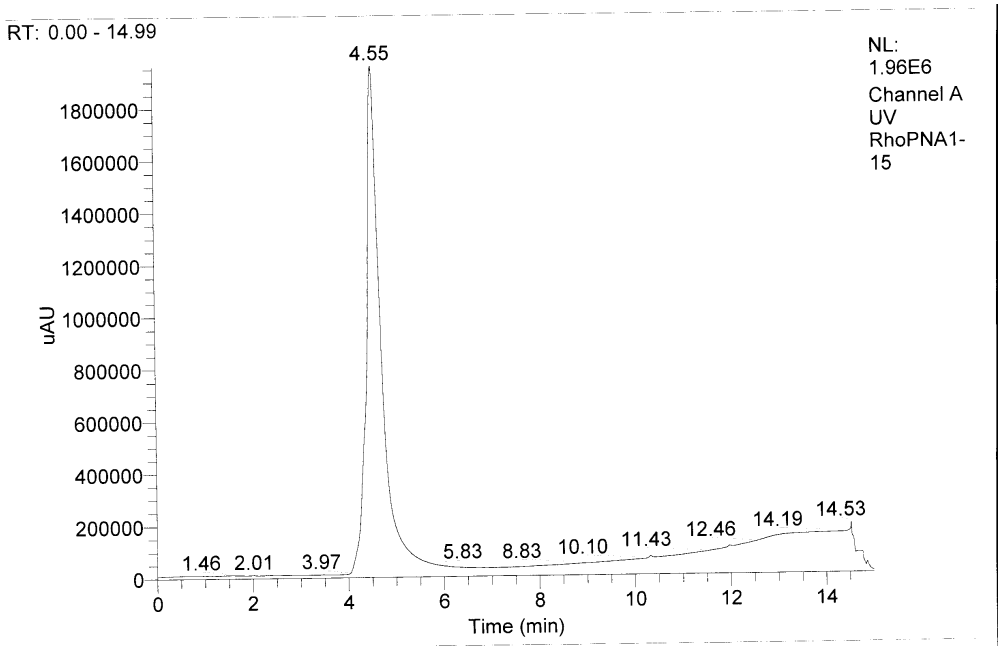

Figure S9. HPL chromatogram of **Rho-PNA**

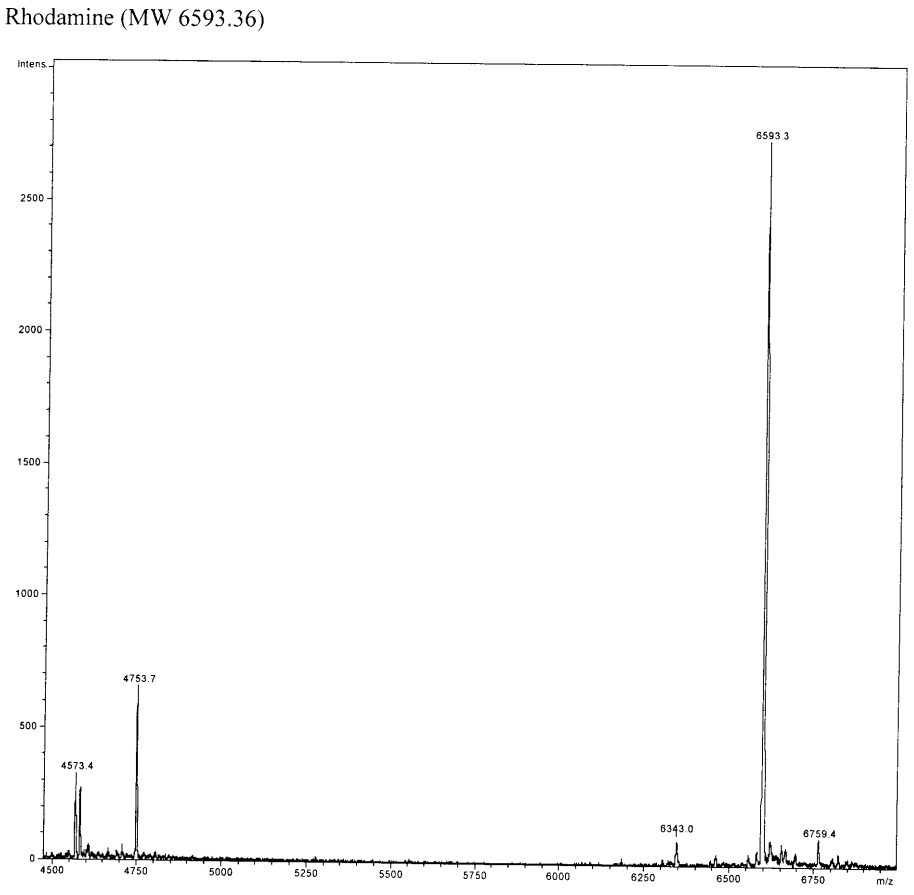

Figure S10. MALDI-TOF mass spectrum of **Rho-PNA**.

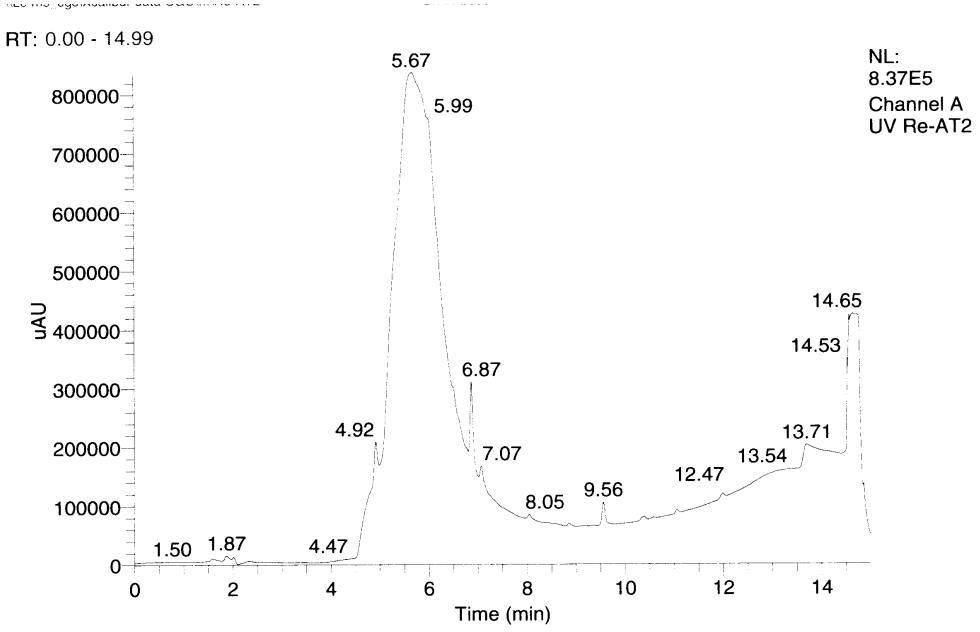

Figure S11. Analytical HPL chromatogram of **Re-PNA**.

Table S1. ESI-MS characterization of **Re-PNA**.

PNA Code	$[M+5H]^{5+}$	$[M+6H]^{6+}$	$[M+7H]^{7+}$	$[M+8H]^{8+}$	$[M+9H]^{8+}$	ν_{CO} / cm^{-1}
Re-PNA	1399.8	1166.8	1000.3	875.4	-	1925, 2031

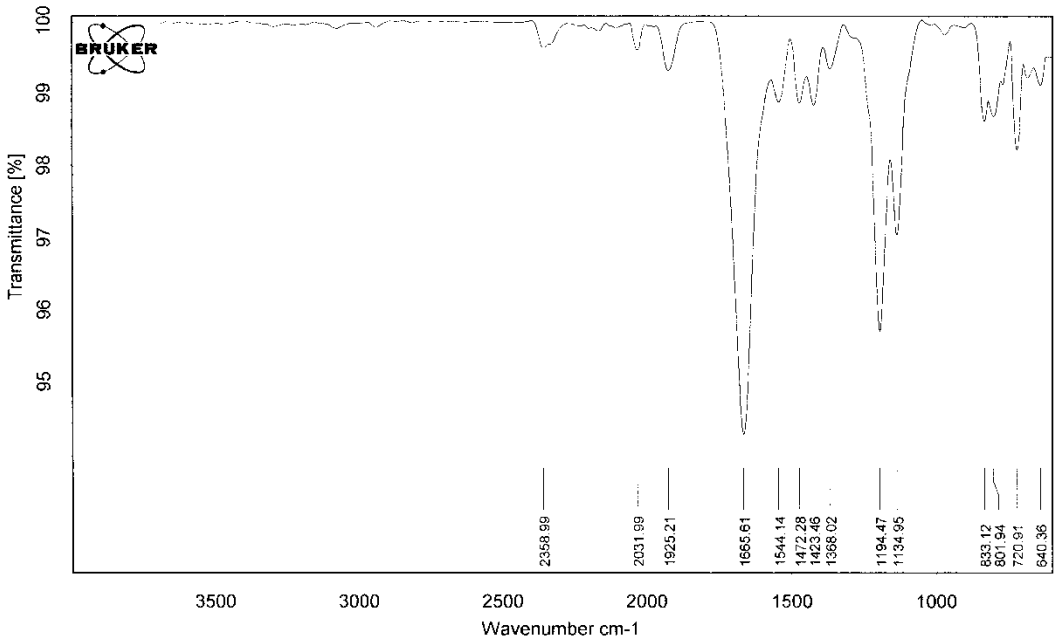

Figure S12. IR Spectrum of **Re-PNA**.

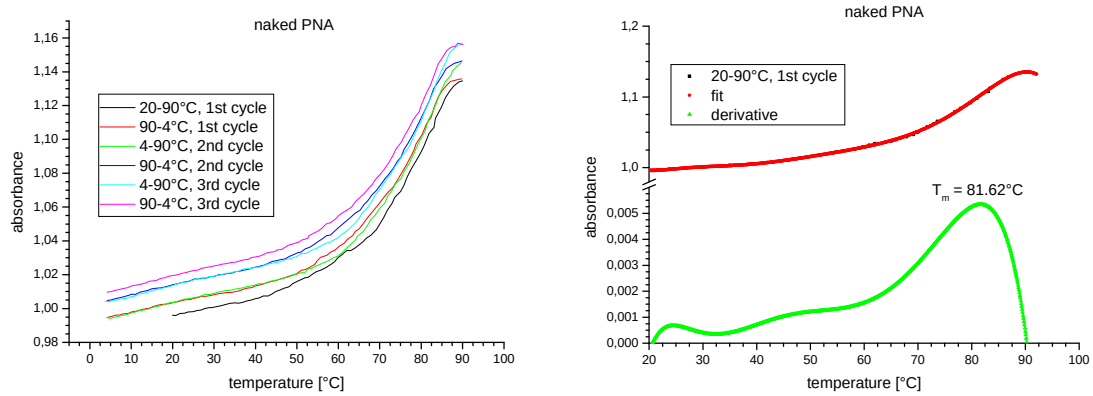

Figure S13. UV-Vis melting spectrum of **Naked-PNA-DNA,** overview (left) and cycle 1 (right).

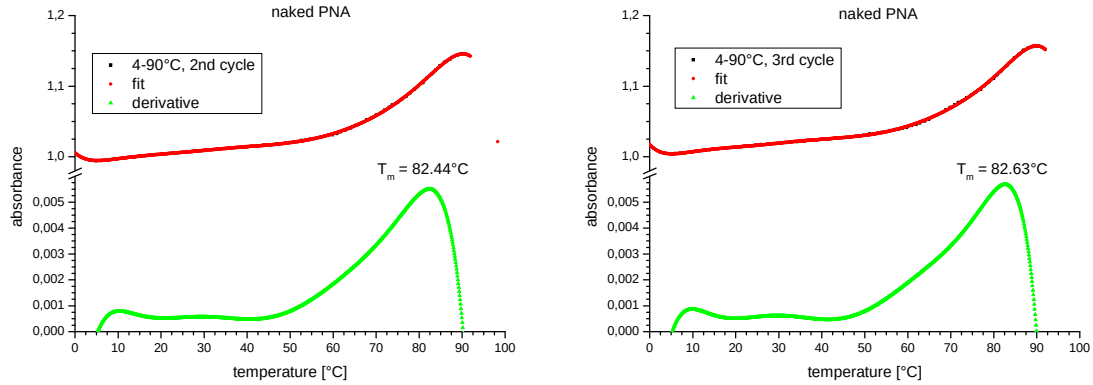

Figure S14. UV-Vis melting spectrum of **Naked-PNA-DNA**, cycle 2 (left) and cycle 3 (right).

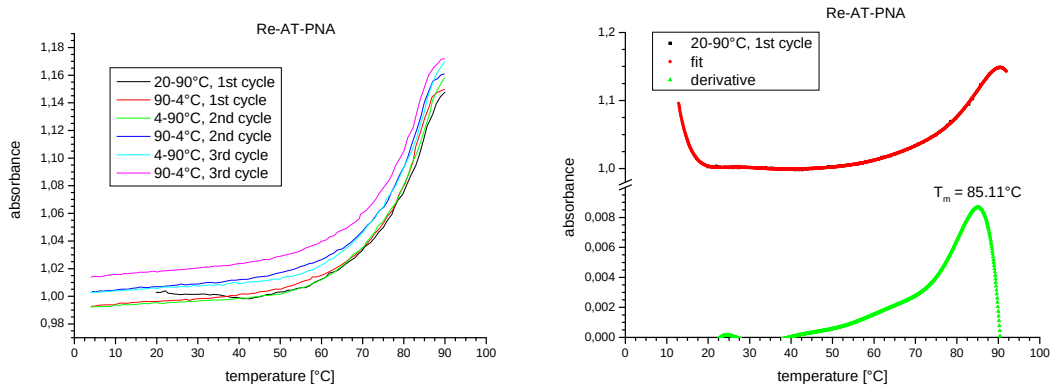

Figure S15. UV-Vis melting spectrum of **Re-PNA-DNA**, overview (left) and cycle 1 (right).

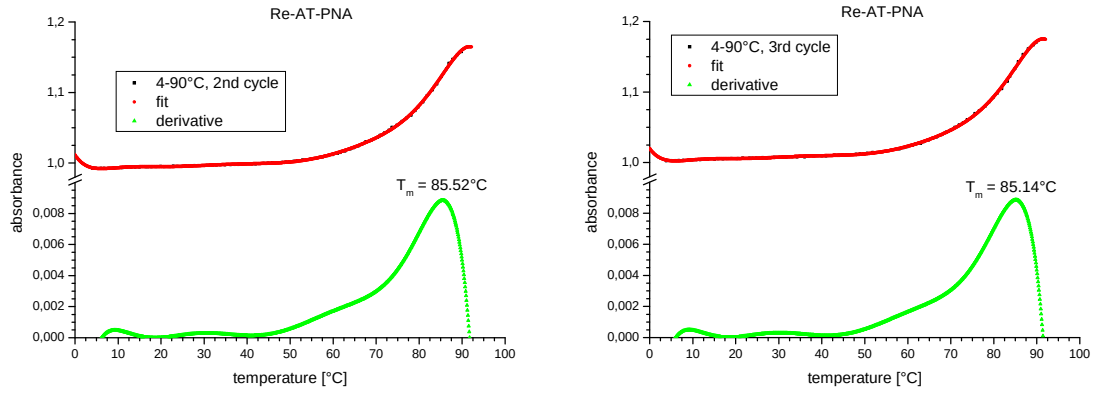

Figure S16. UV-Vis melting spectrum of **Re-PNA-DNA**, cycle2 (left) and cycle 3 (right).

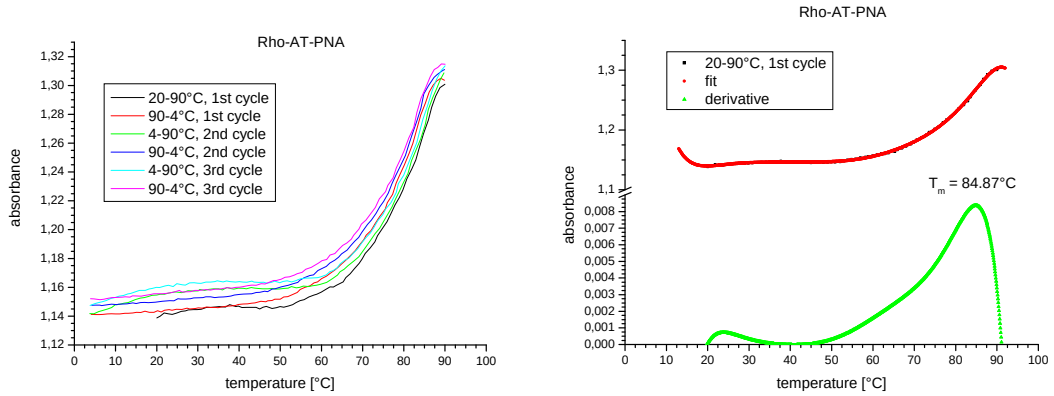

Figure S17. UV-Vis melting spectrum of **Rho-PNA-DNA**, overview (left) and cycle 1 (right).

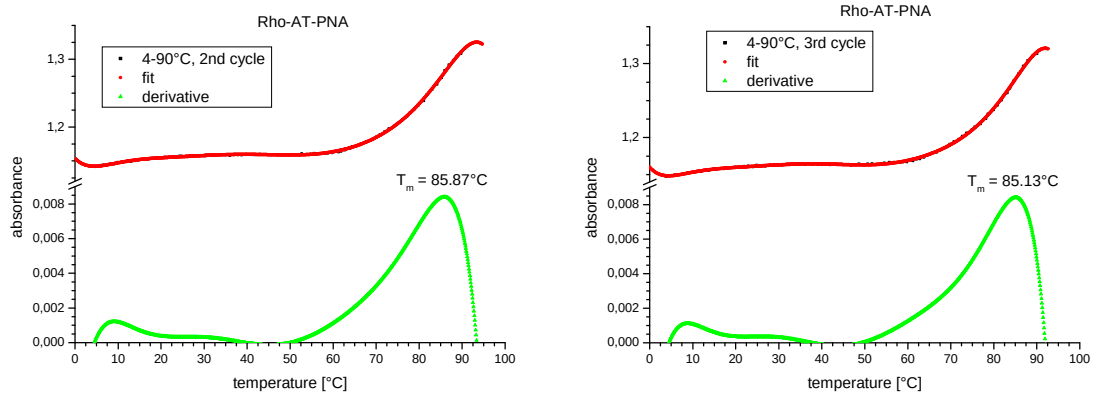

Figure S18. UV-Vis melting spectrum of **Rho-PNA-DNA**, cycle 2 (left) and cycle 3 (right).

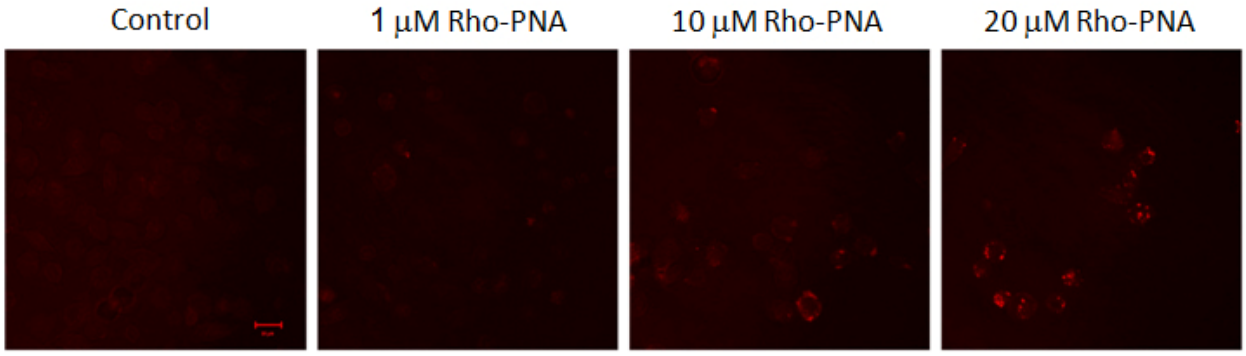

Figure S19. Fluorescence micrographs of HeLa cells one day after delivery of three different concentrations of **Rho-PNA** by electroporation. Scale bar indicates 20 µm in all images.