

Supplementary data

Inhibitory effect of Naphthoquinone-Tryptophan hybrid towards aggregation of PAP f39 semen amyloid

V. Guru KrishnaKumar^{1†}, Satabdee Mohapatra^{1†}, Ashim Paul¹, Elad Arad², Raz Jelinek², Ehud Gazit¹ and Daniel Segal^{1,3*}

¹School of Molecular Microbiology & Biotechnology, Tel Aviv University, Tel Aviv 69978, Israel

²Department of Chemistry and Ilse Katz Institute (IKI) for Nanoscale Science and Technology, Ben Gurion University of the Negev, Beer Sheva 84105, Israel

³Sagol Interdisciplinary School of Neurosciences, Tel Aviv University, Tel Aviv 69978, Israel

† Contributed equally to the work

* Corresponding author; E-mail address: dsegal@post.tau.ac.il (Prof. Daniel Segal)

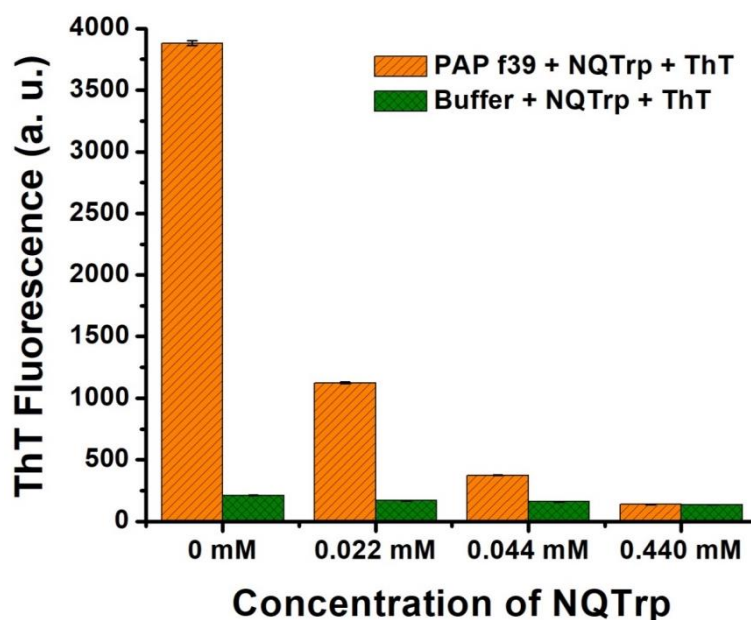


Figure S1. NQTrp shows minimal quenching of ThT fluorescence. ThT (50 μ M) was incubated with various concentrations of NQTrp. ThT fluorescence emission was measured at 480 nm by exciting the dye at 440 nm.

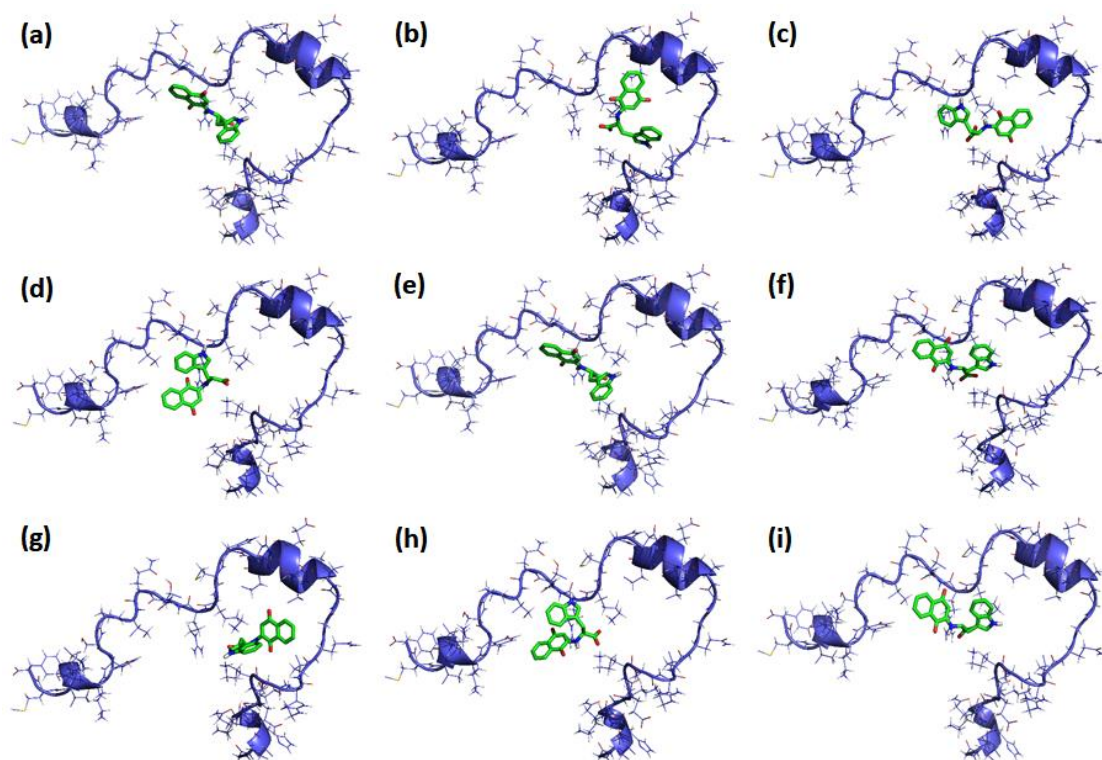


Figure S2. Various docking conformations of PAP f39 monomer and NQTrp.

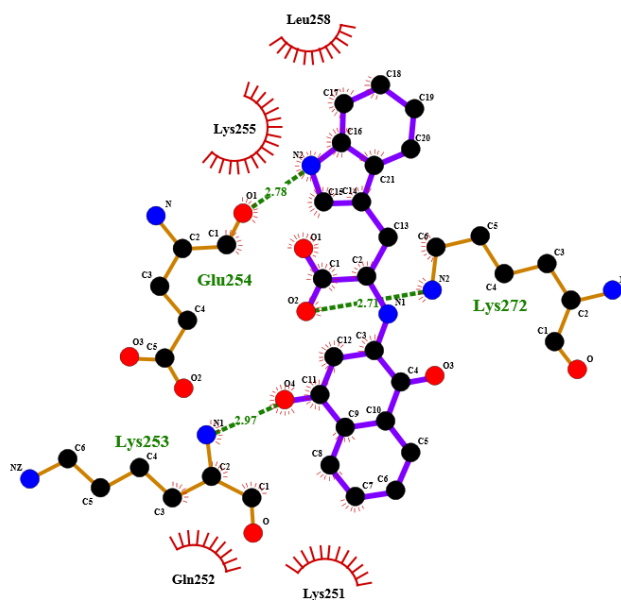


Figure S3. Docking study: Association of NQTrp with PAP f39.

Table S1. Post-docking analysis shows the interaction profile of NQTrp with PAP f39 monomer corresponding to the docked conformers in SI Fig. 2.

Notation	NQTrp association with PAP ₂₄₈₋₂₈₆		Binding Energy (kcal/mol)
	Hydrogen bonds	Hydrophobic Interactions	
a	Lys ₂₇₂	Lys ₂₅₅ , Arg ₂₇₃ , Ala ₂₇₄ , Thr ₂₇₅ , Ile ₂₇₇	-6.99
b	Lys ₂₇₂	Lys ₂₅₅ , Leu ₂₅₈ , Val ₂₆₄ , Asn ₂₆₅ , Leu ₂₆₈ , Asn ₂₆₉	-6.98
c	Lys ₂₅₅ , Lys ₂₇₂	Arg ₂₇₃ , Thr ₂₇₅ , Leu ₂₅₈ , Val ₂₆₄ ,	-6.94
d	Lys ₂₇₂ , Arg ₂₇₃	Lys ₂₅₅ , Ala ₂₇₄ , Thr ₂₇₅ , Ile ₂₇₇ , Tyr ₂₈₀	-6.78
e	Lys ₂₇₂	Lys ₂₅₅ , Arg ₂₇₃ , Ala ₂₇₄ , Thr ₂₇₅ , Ile ₂₇₇ ,	-6.77
f	Lys ₂₇₂	Lys ₂₅₅ , Arg ₂₇₃ , Thr ₂₇₅ , Ile ₂₇₇ ,	-6.69
g	-	Lys ₂₅₅ , Leu ₂₅₈ , Gln ₂₅₉ , Val ₂₆₄ , Leu ₂₆₈ , Lys ₂₆₈	-6.64
h	Lys ₂₅₅ , Lys ₂₇₂	Arg ₂₇₃ , Thr ₂₇₅ , Ile ₂₇₇ , Tyr ₂₈₀	-6.49
i	Lys ₂₇₂	Lys ₂₅₅ , Arg ₂₇₃ , Ala ₂₇₄ , Thr ₂₇₅ , Ile ₂₇₇ ,	-6.40