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Supplementary material

The cytokine IL-1β and piperine complex surveyed by experimental and computational molecular biophysics.

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Received: date; Accepted: date; Published: date

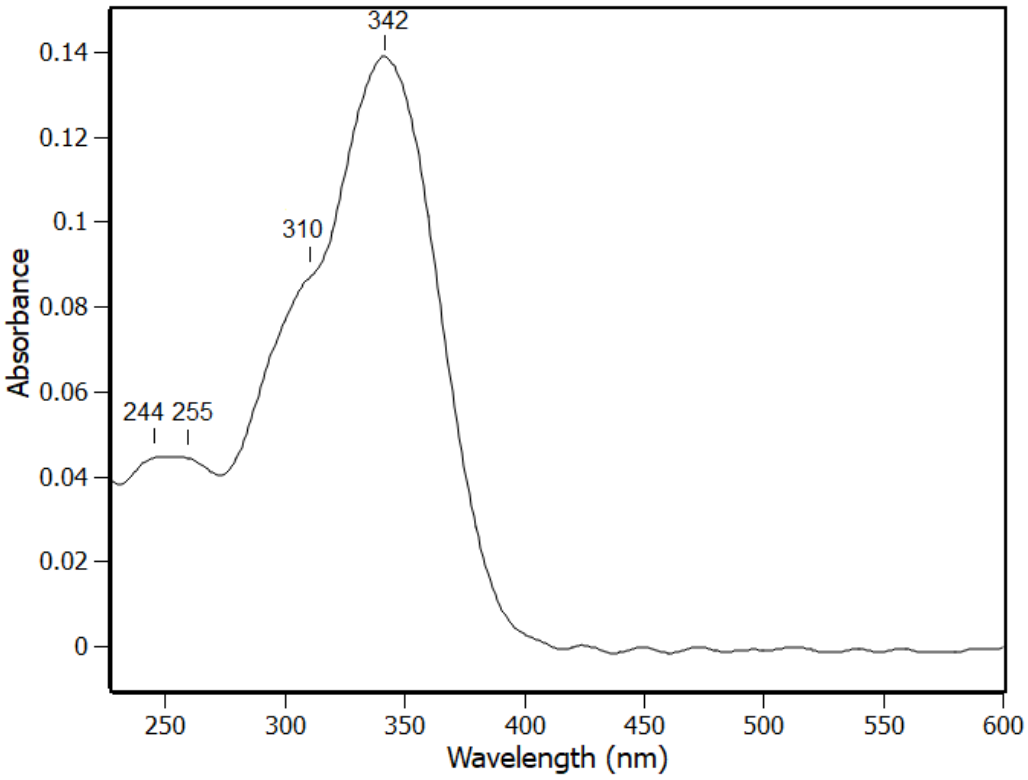


Figure S1: Piperine at 10μM absorption spectrum at dibasic sodium phosphate in pH=7.4 at 298K. Cell length = 1cm

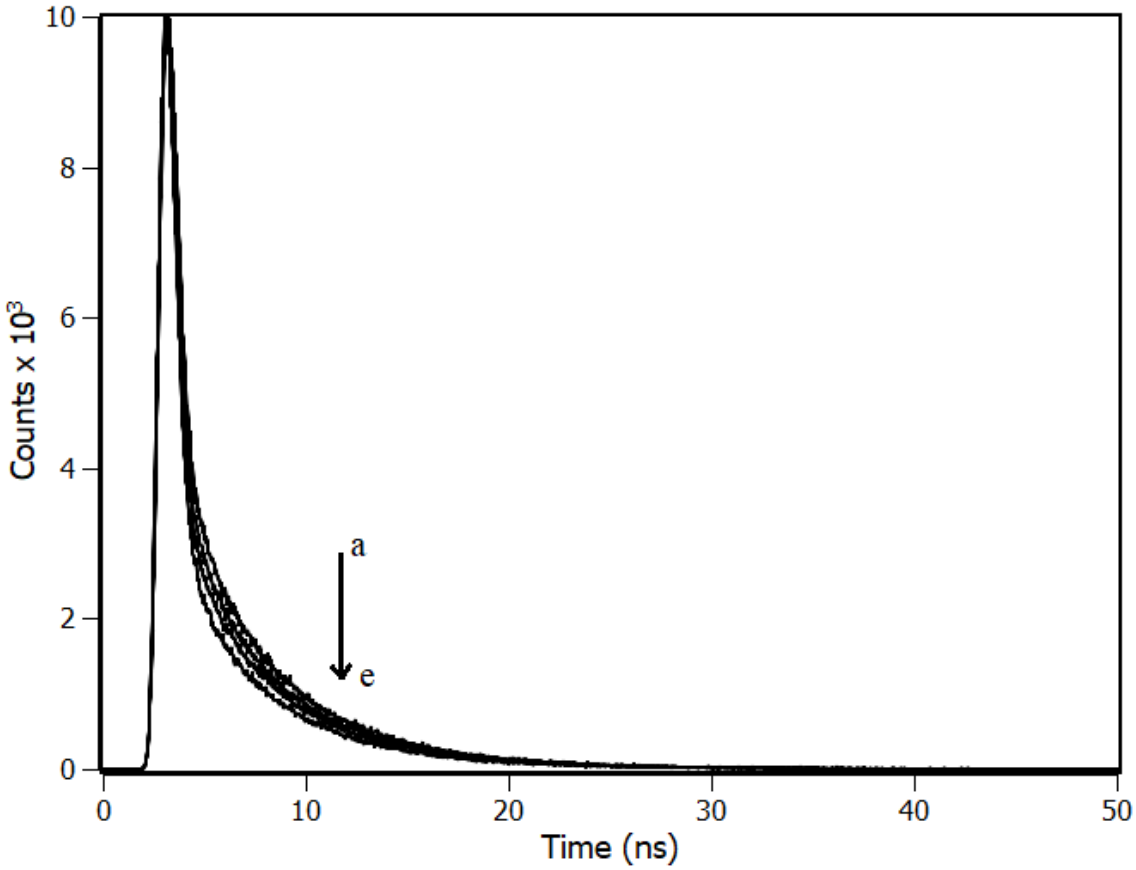
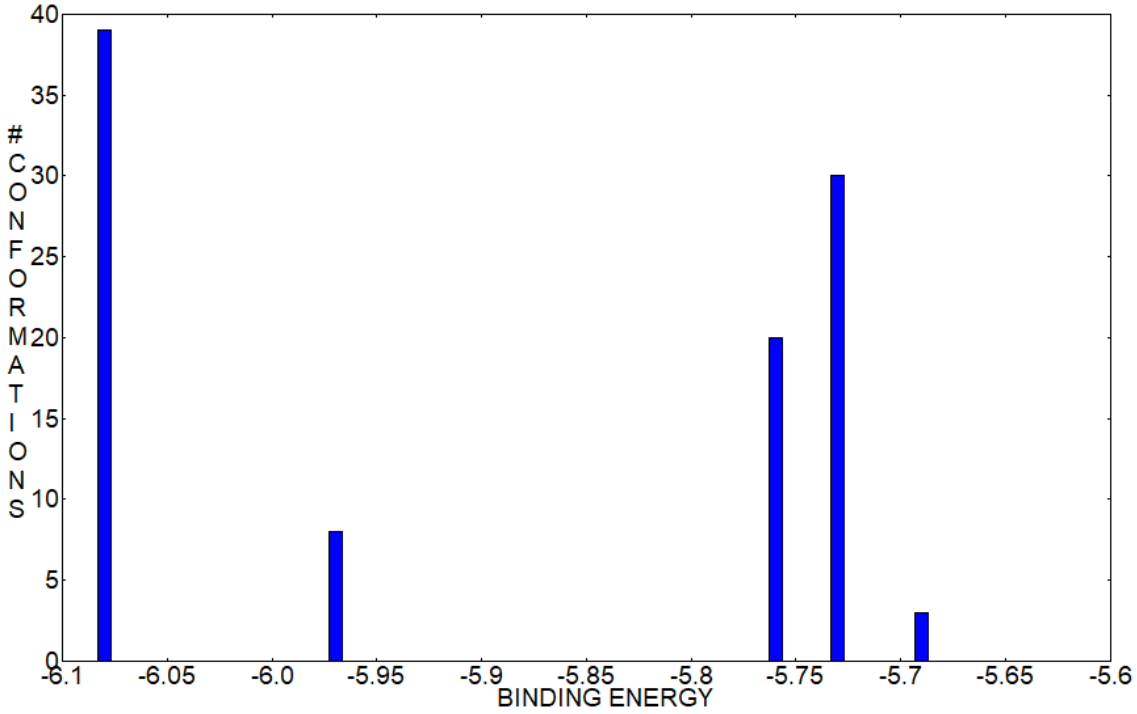


Figure S2: Time-resolved fluorescence decay of (a) IL-1β with Piperine (→e) from 12 to 49μM. [IL-1β] = 10μM, T = 298K and λ_{ex} = 295nm.

Table S1: Tryptophan lifetime in different stoichiometries IL-1β:Piperine.

[piperine](μM)	α_1	τ_1 (ns)	α_2	τ_2 (ns)	τ_{avg} (ns)
0	0.20	0.80	0.66	4.95	4.81
16	0.22	0.79	0.61	4.9	4.76
32	0.26	0.74	0.64	4.92	4.73
49	0.29	0.71	0.62	4.88	4.67



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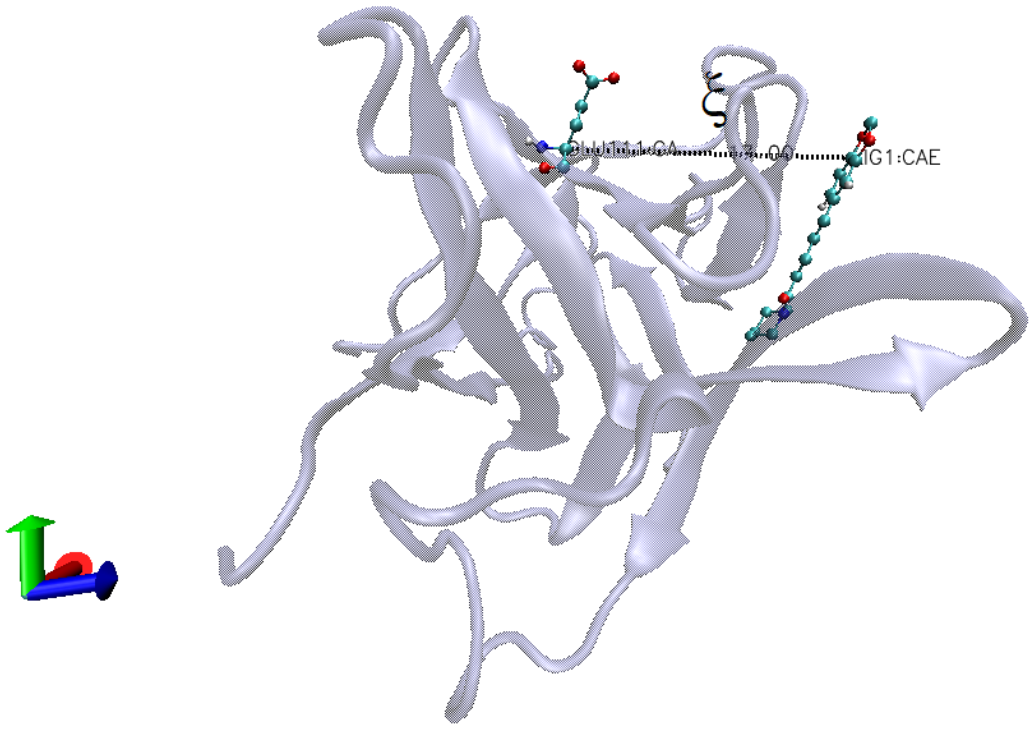
42 Figure S3: Molecular docking clusters with their respectives energy scores



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44 Figure S4: The atoms picked to define the reaction coordinate (ξ). For the protein was chosen the
45 atom CA with index 1129 from the amino acid Glu111. For piperine the atom chosen was CAE with
46 index of 1585.

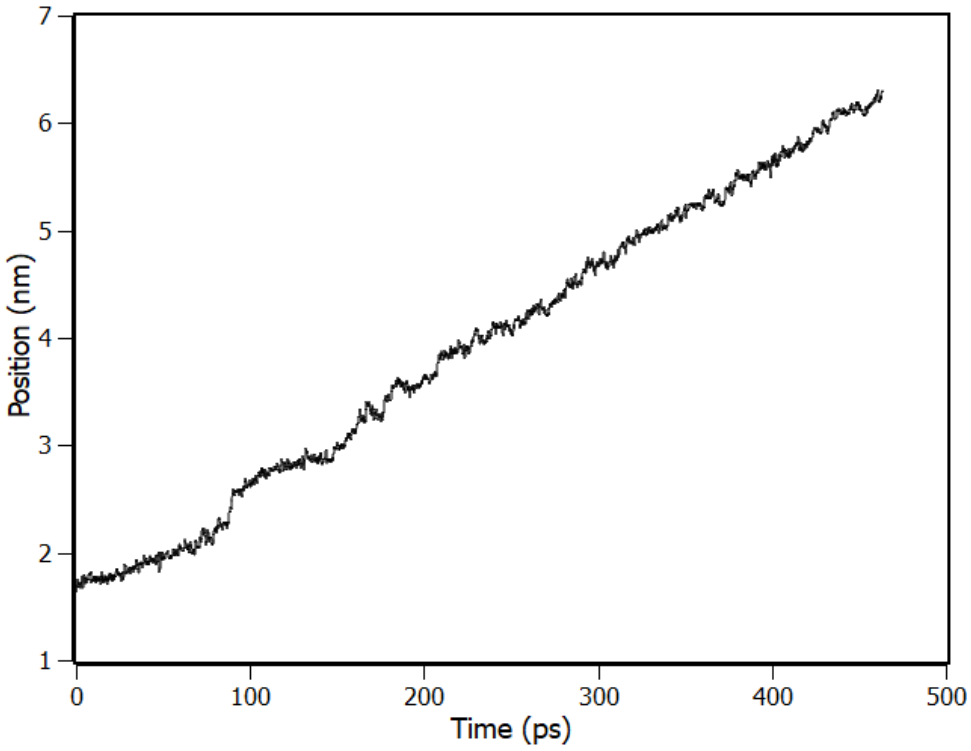

Figure S5: Pulling profile during the pulling simulation. Y-axis is the value of reaction coordinate (ξ) and x-axis is the time of simulation.