

Supporting Information

The inhibitory effects of platinum (II) complexes on amyloid aggregation: a theoretical and experimental approach

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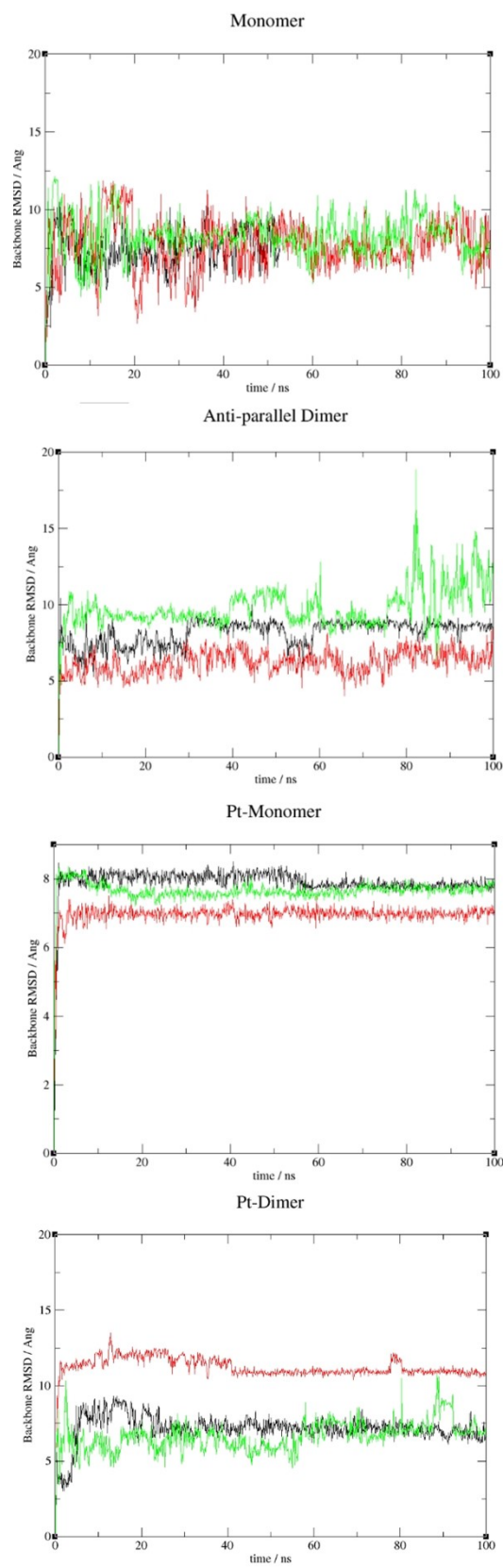


Fig. S1 Time evolution of RMSD relative to initial extended structure.

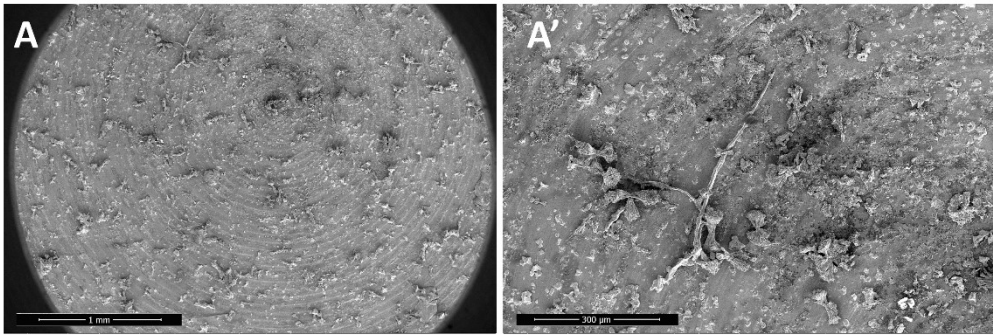


Fig S2. SEM micrographs of (A-A') NPM1₂₆₄₋₂₇₇ + **1**, at 1:5ratio, at 1 mm, and 300 μm.

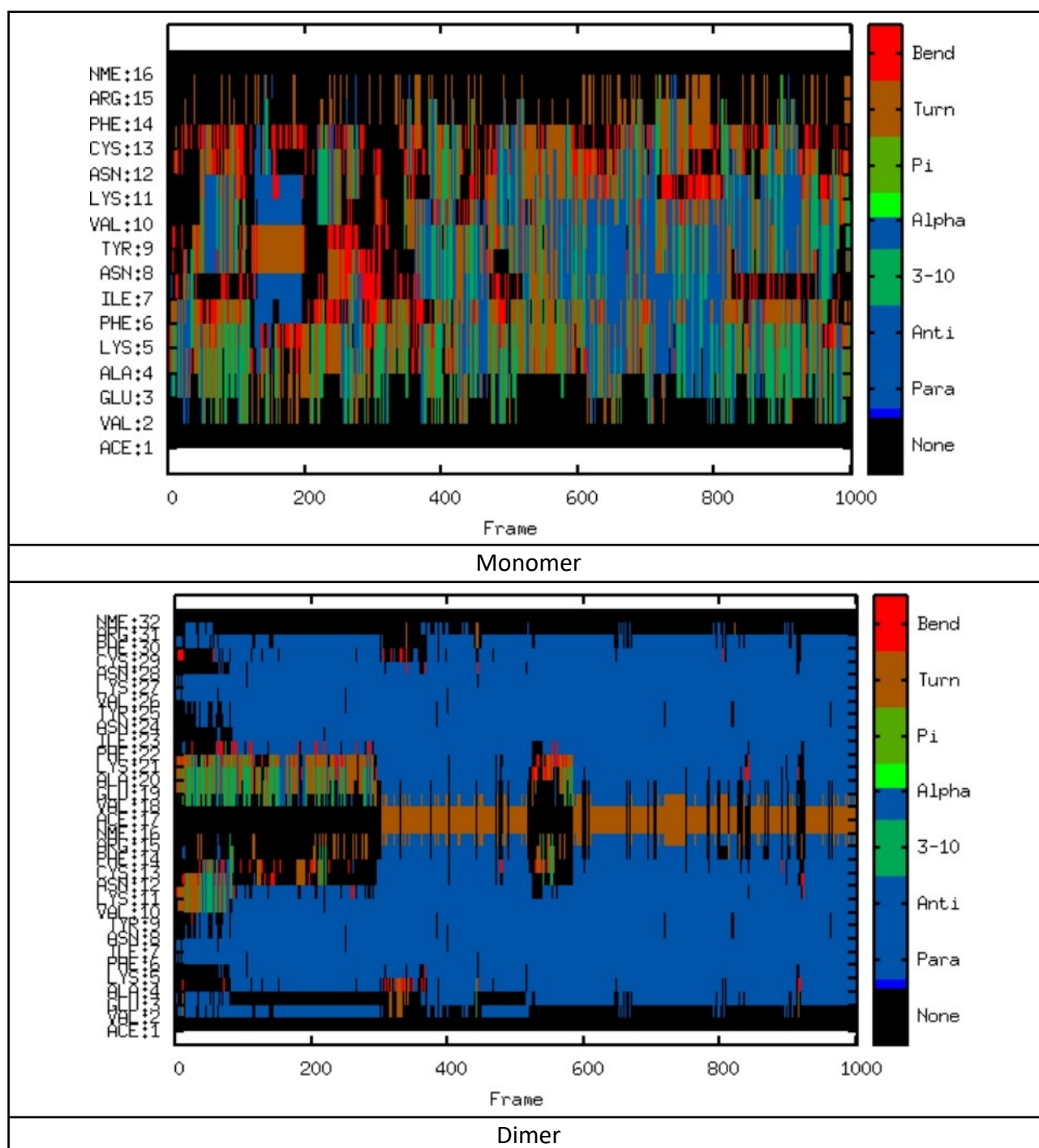


Fig. S3 Time evolution of secondary structure in metal-free monomer and dimer MD simulation.

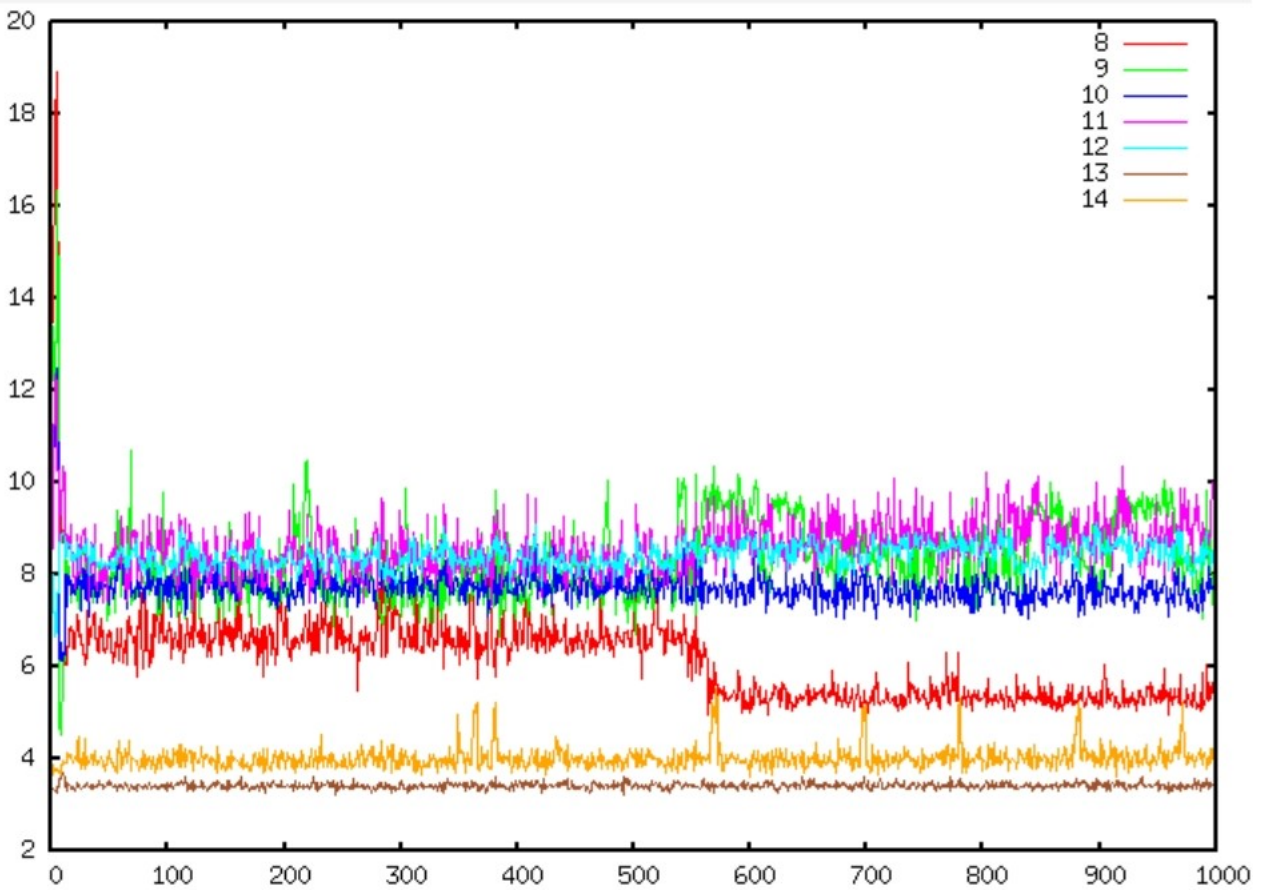
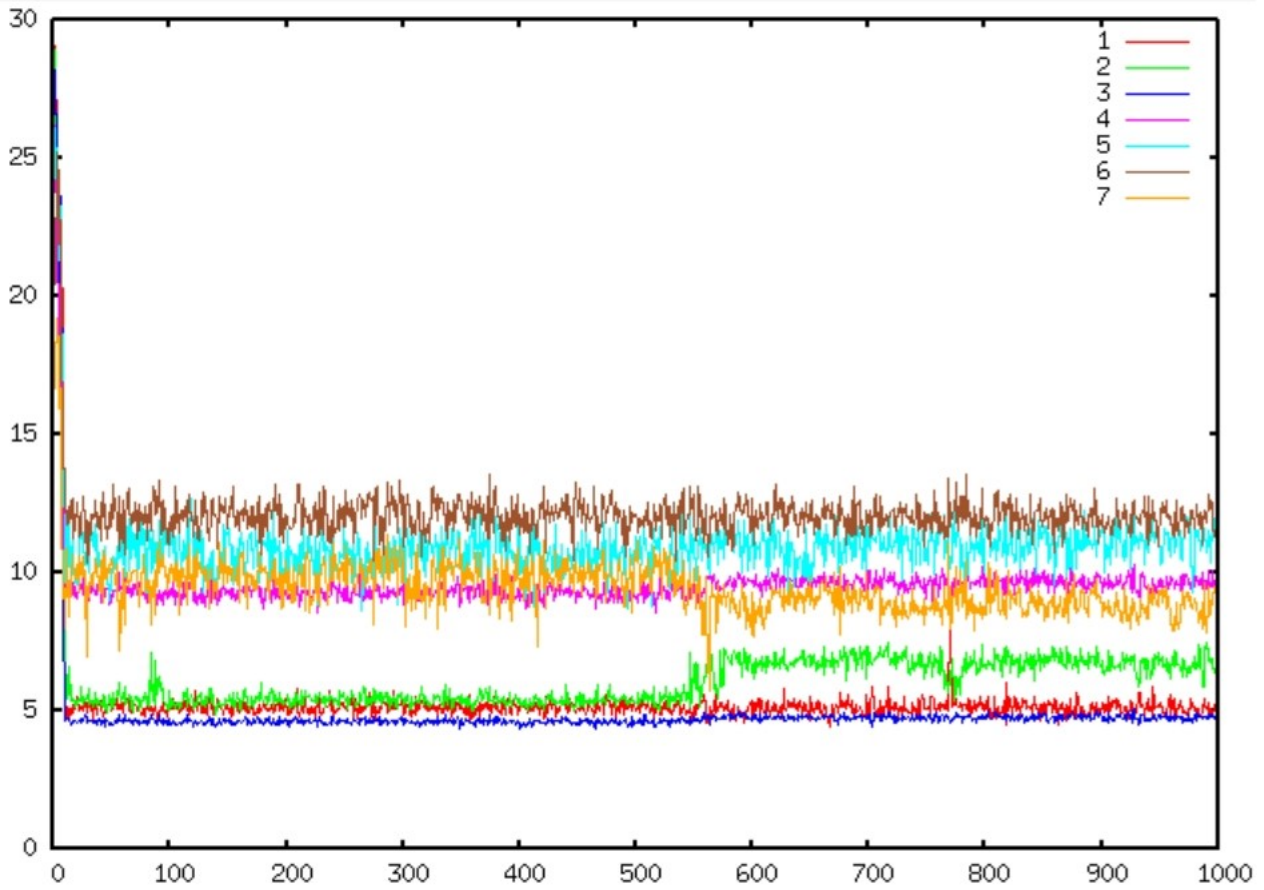


Figure S4: Time evolution of Pt-residue distances (Å) in monomer-2 MD simulation. Numeration refers to the position of single residue into NPM1₂₆₄₋₂₇₇ considering 264 as 1.

Table S1: Deconvolution of CD spectra reported in Figure 5 at indicated times.

	Time(h)	helix	beta	turn	others
NPM1 ₂₆₄₋₂₇₇	0	4.4	33.2	13.9	48.4
	1	3.5	34.8	13.8	47.9
	2	2.0	36.6	13.4	48.0
	3	0.1	37.9	14.3	47.7
	12	0.0	37.1	13.4	49.5
NPM1 ₂₆₄₋₂₇₇ +1	0	4.7	34.9	14.6	45.8
	1	3.1	35.0	14.2	47.7
	2	0.1	36.9	14.5	48.5
	3	0.0	38.7	14.8	46.5
	12	0.0	38.5	13.5	47.9
NPM1 ₂₆₄₋₂₇₇ +2	0	7.9	39.2	14.4	38.5
	1	0.6	39.5	15.2	44.7
	2	0.7	41.6	15.2	42.5
	3	0.0	42.6	14.5	42.9
	12	0.0	41.0	14.5	44.5

Table S2: Bonded parameters from MCPB.py for compound **2** bound to Cys

		Force constant / kcal mol ⁻¹ Å ⁻²	Eqm value / Å or °
BOND	Pt-Nphen	104.1	2.0669
	Pt-NH ₃	109.0	2.0986
	Pt-S	130.0	2.3294
ANGL	S-Pt-Nphen	140.05	91.93
	S-M1-NH ₃	166.04	84.44
	S-M1-NH ₃ b	141.22	176.19
	Nphen-Pt-NH ₃	194.79	176.07
	Nphen-Pt-NH ₃ b	124.71	88.91
	NH ₃ -Pt-NH ₃ b	150.33	94.80