

**Molecular mechanics and quantum chemical calculations
unveil the combating effect of baicalein on human islet amyloid polypeptide
aggregates**

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Supplementary Information:

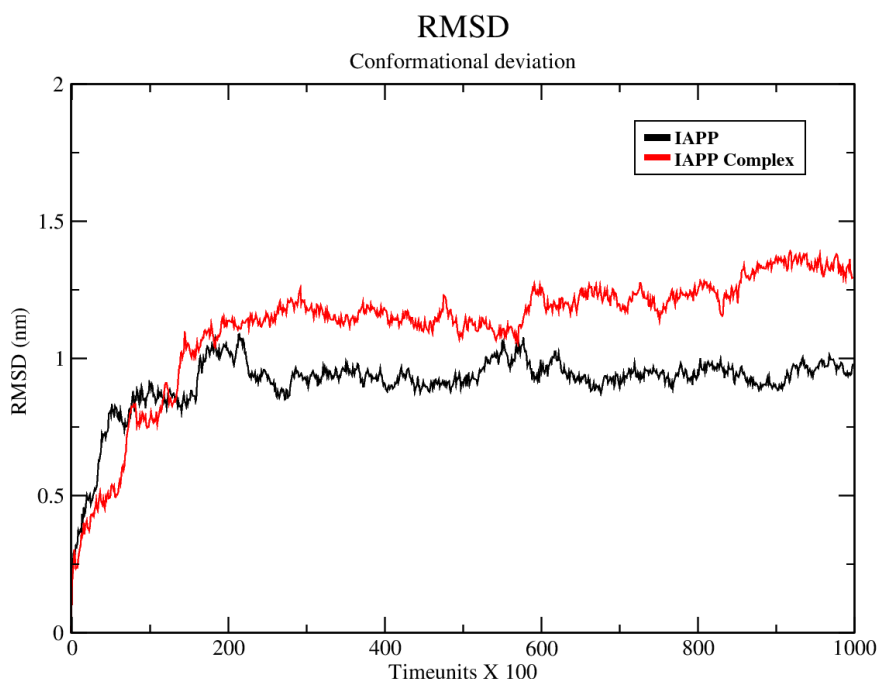


Fig.4 The conformational deviation of the hIAPP and hIAPP complex computed over the period of the simulation time.

Table 1: Statistical reports on mean, standard deviation (SD) and *P*-value of RMSD and RMSF values for the IAPP and IAPP complex.

Conformational statistics	RMSD		RMSF		<i>P</i> -value (<0.05) Significance
	Mean	SD	Mean	SD	
IAPP	0.91	0.11	0.34	0.14	Yes
IAPP Complex	1.11	0.22	0.43	0.15	Yes

Table 2: Statistical studies on the secondary structures of the IAPP and IAPP complex with mean, standard deviation (SD) and *P*-value.

Secondary structure statistics	IAPP		IAPP Complex		<i>P</i> -value (<0.05) Significance
	Mean	SD	Mean	SD	
Helix	0.05	0.40	0.03	0.31	No
Beta-sheets	25.43	4.13	17.31	6.19	Yes
Beta-Bridge	3.85	1.60	5.38	1.97	Yes
Bend	10.69	2.14	11.77	2.91	Yes
Turn	5.97	1.61	4.38	1.46	Yes
Coil	28	5	35.5	7.52	Yes