Computational study of self-assembled hexapeptide inhibitors against amyloid-β (Aβ) aggregation

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Table S1 Interaction energy of hexapeptide-based dimers (kcal/mol) calculated at the M062X/6-311+G(d, p) level of theory in water and DMSO

Hexapeptide	Solvent	KLVFFA	NKGAII	GAIIGL	AIIGLM	MVGGVV	GGVVIA	Self-aggregaion
CTIYWG	Water	-76.9(a) [a]	-78.1(a)	-60.9(p)	-63.7(p)	-63.7(p)	-61.5(p)	-70.8(p)
	DMSO	-80.1(a)	-73.7(a)	-53.0(p)	-56.5(p)	-56.7(p)	-59.0(a)	-63.7(p)
CTLWWG	Water	-84.8(p)	-76.4(a)	-64.0(p)	-65.5(p)	-62.1(a)	-70.8(p)	-68.5(p)
	DMSO	-86.2(p)	-74.2(a)	-58.6(p)	-60.6(p)	-56.0(p)	-69.0(p)	-61.1(p)
GTVWWG	Water	-73.1(p)	-75.0(p)	-58.9(a)	-73.3(p)	-66.0(p)	-59.4(p)	-71.5(p)
	DMSO	-67.8(p)	-72.9(p)	-53.8(a)	-68.5(p)	-59.8(p)	-56.6(p)	-72.5(p)
Self-aggregation	Water	-72.1(a)	-56.7(p)	-63.0(a)	-65.3(p)	-53.1(a)	-59.4(p)	—
	DMSO	-50.1(a)	-53.1(p)	-55.4(a)	-58.5(p)	-46.7(a)	-53.6(p)	

[a] a: antiparallel manner; p: parallel manner.

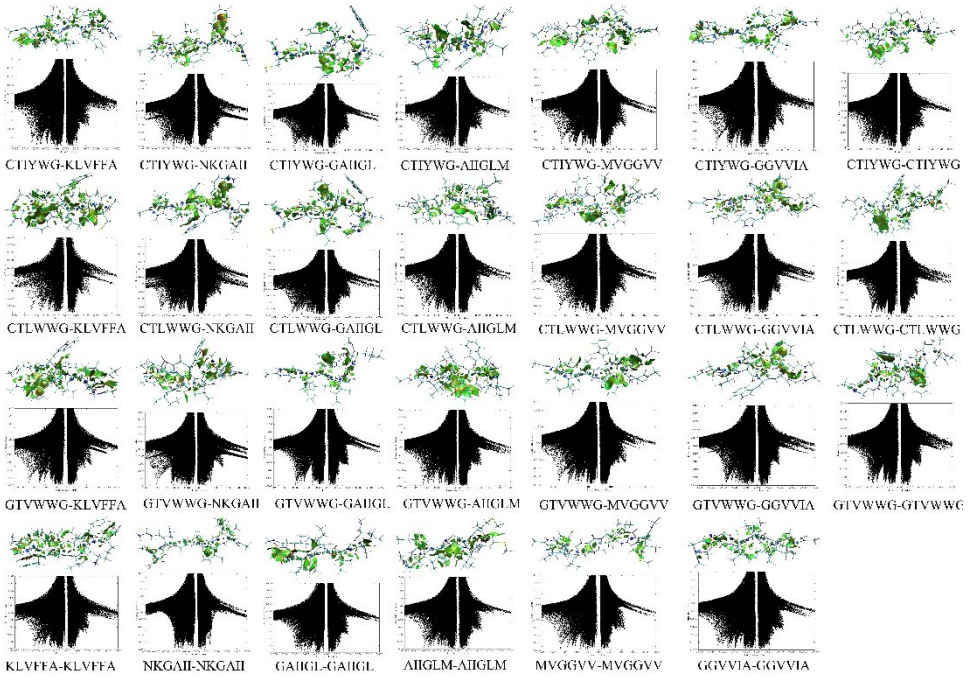

Fig. S1 3D NCI (above) and 2D NCI (below) of dimers. The blue isosurface indicates hydrogen bond effects, and green and yellowish green isosurface indicates van der waal effects.