Inhibiting amyloid β-protein assembly: Size-activity relationships among grape seed-derived polyphenols

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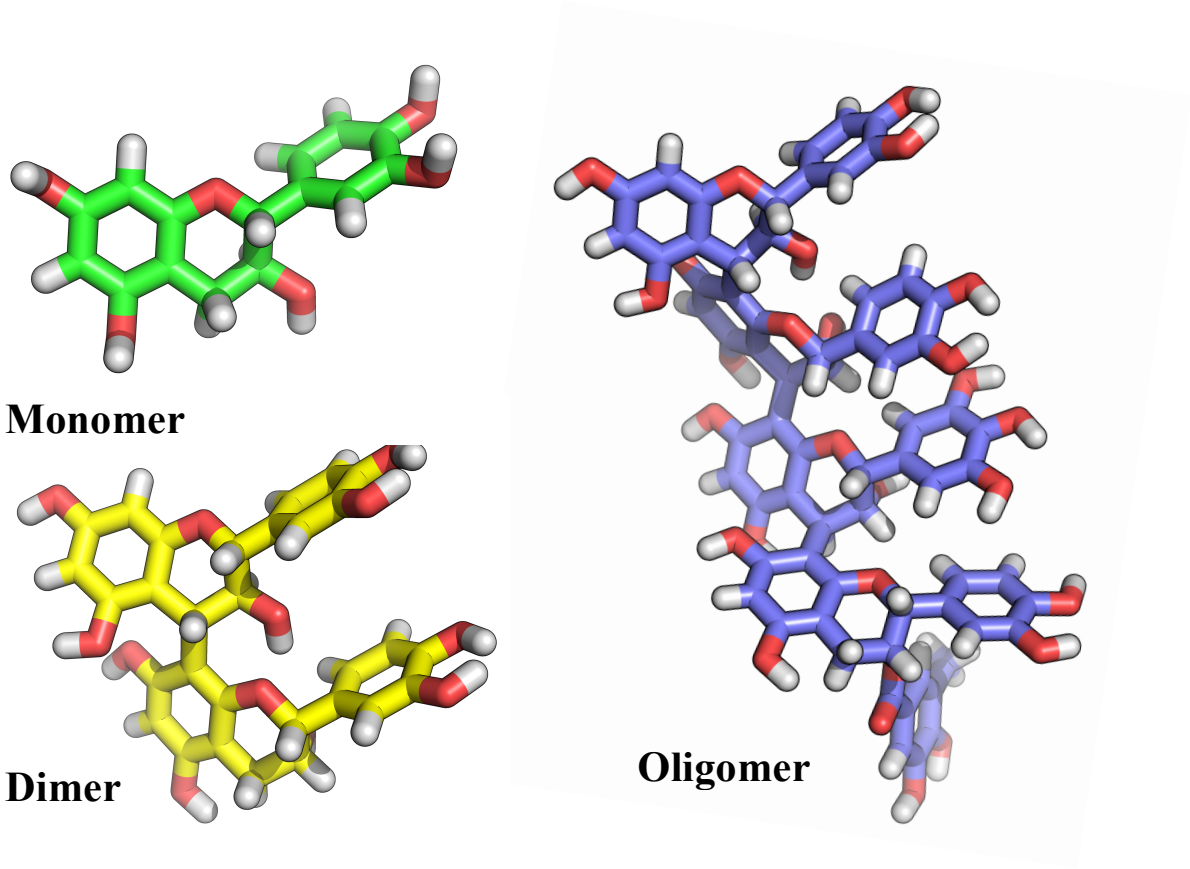

Fig. S1. Three-dimensional structures of the GSPE monomer, dimer, and oligomer, shown in Fig. 1. Monomer (green), dimer (yellow), and oligomer (purple) are shown as stick models with oxygen atoms shown in red and hydrogen atoms shown in white.

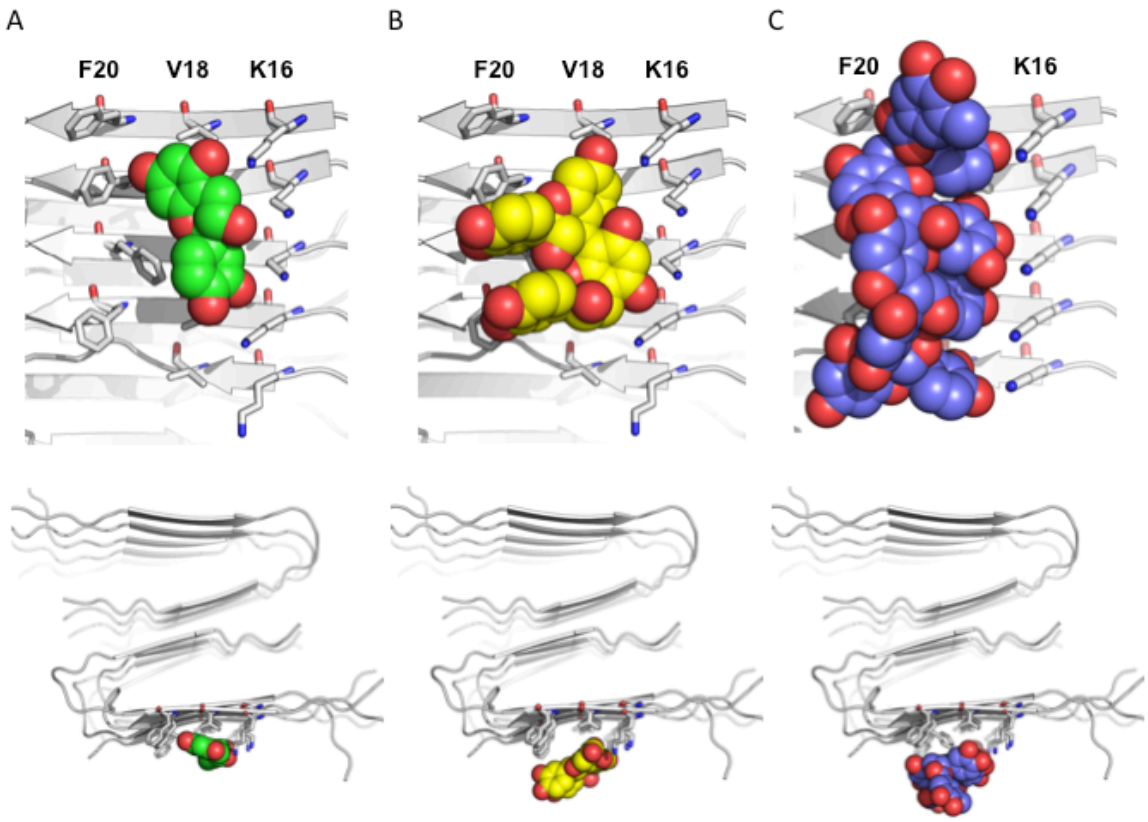

Fig. S2. Structural models of GSPE:fibril interactions. Monomer (A), dimer (B), and oligomer (C) are docked on an Aβ fibril (grey) whose fibril axis extends from the bottom to the top of the figure (top row of figures). These same interactions are viewed looking down the fibril axis in the bottom row of figures. Aβ fibril side-chains are shown in stick representation.

Table S1. Energetics of GSPE:Aβ complexation[a]

GSPE	Binding Energy	Non-bond Potential[b]	Solvation Energy[c]	Electrostatic Potential[d]	H-bond Energy[e]
Monomer	-9	-9	3	-1	-2
Dimer	-10	-13	5	0	-1
Oligomer	-18	-23	10	-1	-4

Table S1. Energetics of GSPE:Aβ complexation. A comparison of the predicted binding energy and physically meaningful energy terms of each model.

[a]- Energies are listed as kcal/mol.

[b]- The attractive portion of the non-bonded Lennard-Jones potential (1).

[c]- LK implicit solvation energy (2).

[d]- Simple Coulombic electrostatics (1).

[e]- Interfacial hydrogen binding energy (3).

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