Supplemental Table 2. Binding energies of the best ligand-hIAPP complexes after docking calculations for PBA, Resveratrol and epigallocatechin gallate (EGCG).

	Cavity	Binding Energy of PBA (kcal/mol) Round0 / Round1	Binding Energy of Resveratrol (kcal/mol) Round0/Round1	Binding Energy of EGCG (kcal/mol) Round0/Round1
Monomer 1	0	-3.6 / -3.4	-4.0 / -3.6	-2.0 / 1.1
Monomer 2	0	-5.3 / -5.2	-6.4 / -6.4	-6.5 / -6.4
Monomer 4	0	-3.7 / -3.7	-4.2 / -4.3	-5.3 / -5.2
	1	-3.8 / -3.8	-3.2 / -3.3	4.1 / 6.9
Dimer 1	0	-4.4 / -4.3	-4.7 / -4.7	-4.5 / -4.5
Dimer 2	0	-4.8 / -4.9	-4.3 / -4.4	-3.0 / -2.9
Dimer 3	0	-4.6 / -4.6	-4.7 / -4.7	-5.6 / -5.6
Oligomer 1	0	-5.6 / -5.6	-7.1 / -7.1	-5.6 / -5.6
	1	-5.9 / -5.9	-6.7 / -6.7	-5.9 / -5.9
	2	-6.5 / -6.5	-7.3 / -7.4	-6.5 / -6.5
	3	-6.0 / -6.0	-5.8 / -5.8	-5.9 / -6.0
	5	-5.7 / -5.7	-6.3 / -6.3	-5.7 / -5.7
Oligomer 2	0	-5.7 / -5.6	-7.0 / -7.0	-5.6 / -5.6
	1	-5.4 / -5.4	-6.1 / -6.1	-5.6 / -5.7
	3	-5.6 / -5.6	-6.9 / -6.9	-5.8 / -5.8
	14	-5.8 / -5.8	-6.4 / -6.4	-5.4 / -5.4