Atomic and dynamic insights into the beneficial effect of the NQTrp inhibitor on Alzheimer's Aβ1-42 Dimer in terms of aggregation and toxicity

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Table S 1. The binding residues to NQTrp from the 11 to 20 Aβ1-42 clusters.

Clusters	Population (%)	Amino acids at binding pockets.		Averaged area of binding interface (Å^2)
		Chain A	Chain B	
11	1.93	E11-V12, Q15-K16, F19, Ser26-N27, I31-I32, M35	D1-H6, Y10, L17-E22, K28-G33, M35-I41	225 ± 6.7
12	1.86	Y10, L17, F20, V24-M35	F4-E11, Q15, V24-G29, I31, G33-G37	263 ± 6.9
13	1.85	Y10, L17-V18, A21, V24-I32, L34-M35	F4-H6, S8-V12, Q15, D23-K28, I31, M35-G37	260 ± 4.9
14	1.79	D1-Y10, V12, Q15, L17-A21, V24, I31, L34	F4, K16-V36, G	288 ± 4.4
15	1.75	A2, F4, Y10-H13, Q15, L17-F19, V24, I31, L34	V12-S25, G29-I41	221 ± 11.8
16	1.65	H6-E22, A30-L34	H14, A21-G37, V39	298 ± 3.0
17	1.61	D1, E3-R5, Y10, F19-F20, G29-G37, V39-I41	H13-A21, D23-G25, K28-I41	247 ± 6.2
18	1.59	D23-V24, S26-L34	R5-S8, E11-F20, E22, V24-G25, G29-A42	288 ± 4.0
19	1.57	V12-Q15, N27-I41	D1, E3-S8, V18-G25, N27-A30, I32, V36-A42	178 ± 1.3
20	1.44	Y10, Q15-E22, S26-I32	H6-Q15, L17-F20, I31-V40	252 ± 10.4

Note: The clusters 12 and 13 have similar binding pocket. The clusters 15 and 17 have similar binding pocket. The cluster 11 has similar binding pocket with cluster 3.

Table S 2. Life-times of exposed side chains to solvent. The residue is defined as exposed when more than 40% of its total side-chain surface area is solvent accessible. Note for Glycine, the lifetime is 0.

Residue	lifetime of exposed to solvent (%)	Residue	lifetime of exposed to solvent (%)
1	94 ± 1	22	87 ± 2
2	63 ± 2	23	78 ± 2
3	77 ± 4	24	41 ± 2
4	57 ± 2	25	0
5	27 ± 4	26	25 ± 2
6	50 ± 3	27	48 ± 4
7	73 ± 3	28	63 ± 3
8	38 ± 2	29	0
9	0	30	34 ± 2
10	41 ± 3	31	41 ± 4
11	76 ± 2	32	44 ± 2
12	40 ± 4	33	0
13	36 ± 4	34	39 ± 3
14	46 ± 4	35	42 ± 3
15	45 ± 2	36	42 ± 2
16	47 ± 3	37	0
17	43 ± 3	38	0
18	41 ± 1	39	49 ± 2
19	50 ± 2	40	47 ± 4
20	57 ± 2	41	64 ± 2
21	35 ± 3	42	73 ± 2

Table S 3. Lifetime of salt bridges. A salt bridge was considered as formed when the distance between the side chain nitrogen atoms of a positively charged residue and the side chain oxygen atoms of negatively charged residues was not more than 3.2 Å.

Salt Bridge Lifetime (%)		Intra-chain	Inter-chain
R5	D1	4.8 ± 2.2	2.3 ± 1.3
	E3	18.6 ± 1.7	2.0 ± 0.9
	D7	31.1 ± 0.2	3.7 ± 1.6
	E11	15.6 ± 2.7	3.2 ± 1.2
	E22	6.1 ± 0.7	4.9 ± 1.3
	D23	0.6 ± 0.1	4.1 ± 1.6
R5 Sum		**76.7 ± 6.2**	**20.2 ± 4.7**
K16	D1	2.6 ±1.7	1.6 ± 1.0
	E3	4.8 ± 2.4	0.7 ± 0.2
	D7	5.8 ± 2.3	0.4 ± 0.3
	E11	7.0 ± 1.9	2.1 ± 0.6
	E22	1.2 ± 0.9	1.7 ± 0.4
	D23	0.6 ± 0.6	1.1 ± 0.5
K16 Sum		**22.1 ± 6.7**	**7.6 ± 0.8**
K28	D1	1.5 ± 0.8	1.3 ± 0.3
	E3	0.6 ± 0.3	0.3 ± 0.1
	D7	0.4 ± 0.4	0.4 ± 0.4
	E11	1.0 ± 0.6	0.5 ± 0.4
	E22	7.0 ± 2.3	0.5 ± 0.5
	D23	9.4 ± 1.2	1.6 ± 0.4
K28 Sum		**19.8 ± 2.0**	**4.6 ± 0.9**