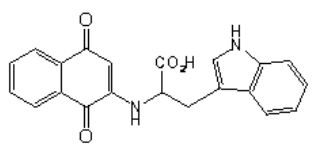
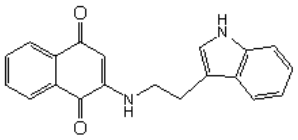
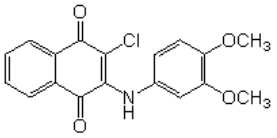


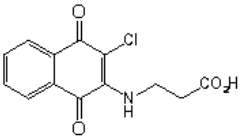
IL, IID



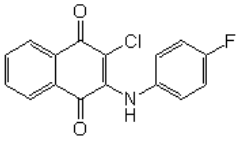
III



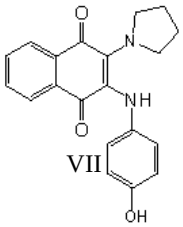
IV



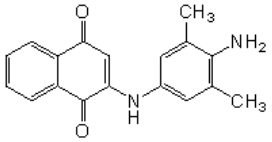
V



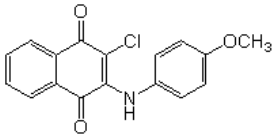
VI



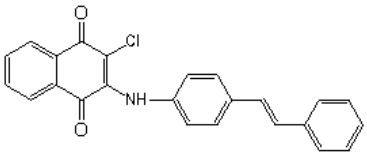
VII



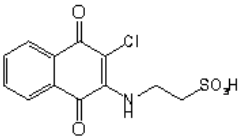
VIII



VIIII



X



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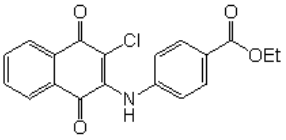

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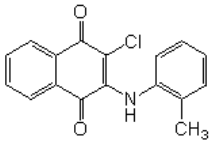

XIII

Figure S1

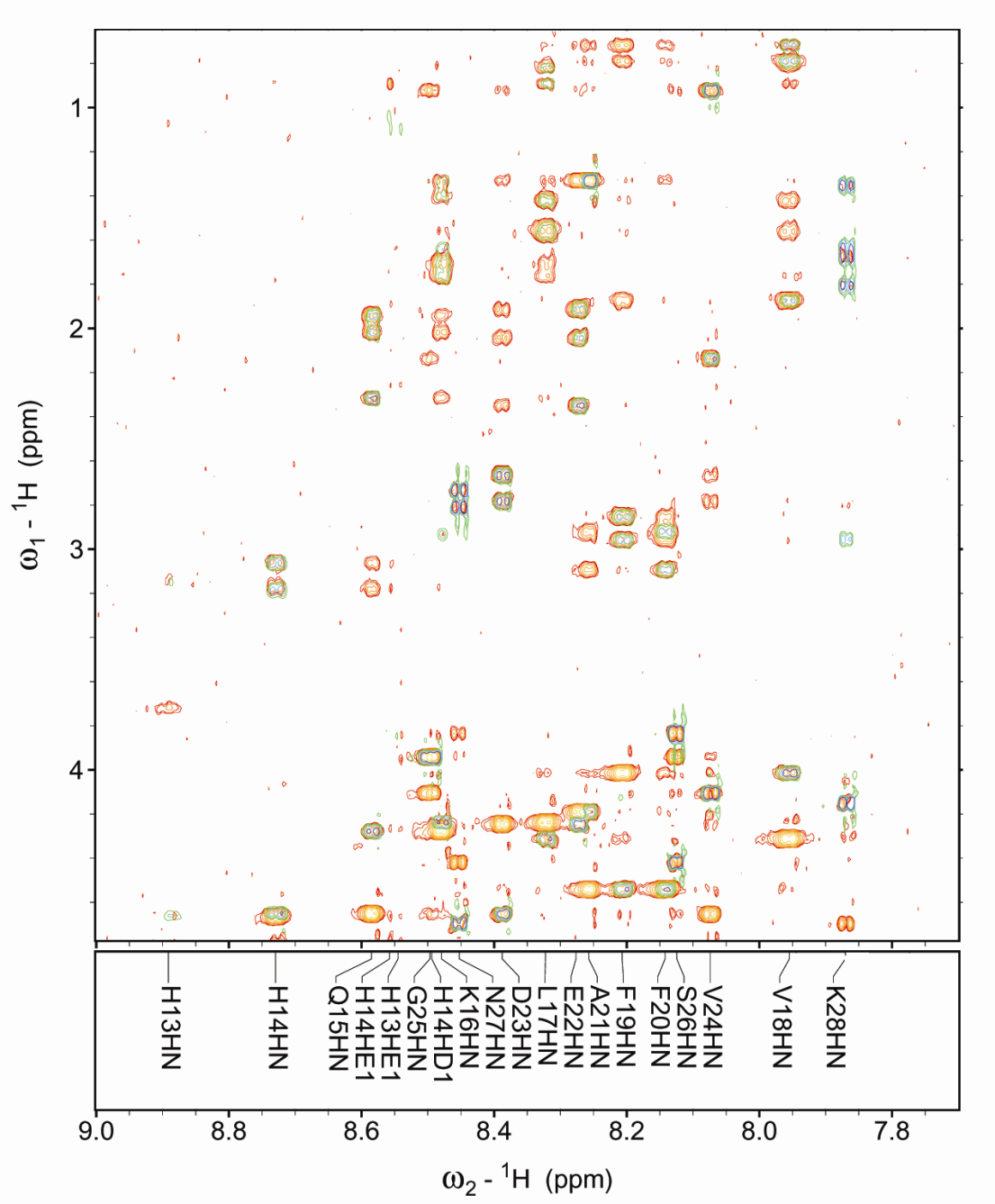
ω1 - 1H (ppm)
1
2
3
4
H13HN
H14HN
Q15HN
H14HE1
H13HE1
G25HN
H14HD1
K16HN
N27HN
D23HN
L17HN
E22HN
A21HN
F19HN
F20HN
S26HN
V24HN
V18HN
K28HN
9.0
8.8
8.6
8.4
8.2
8.0
7.8
ω2 - 1H (ppm)

Figure S2

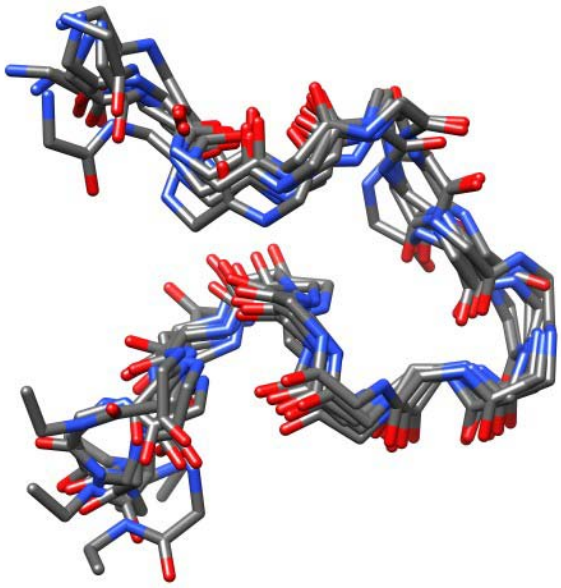

Figure S3

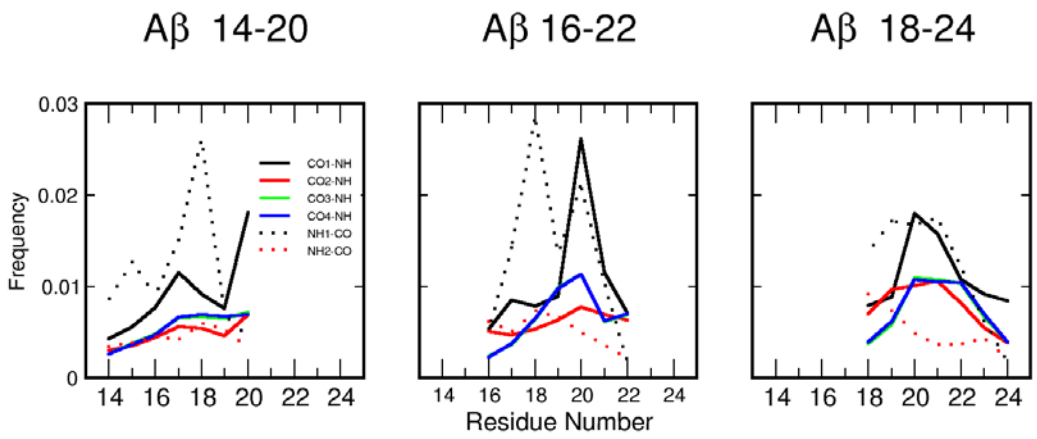
Aβ 14-20
Aβ 16-22
Aβ 18-24
Frequency
0.03
0.02
0.01
0
CO1-NH
CO2-NH
CO3-NH
CO4-NH
NH1-CO
NH2-CO
14 16 18 20 22 24
Residue Number

Figure S4

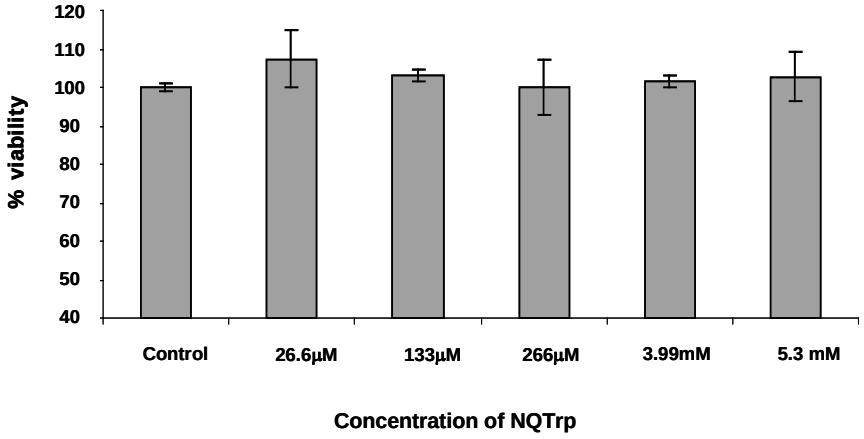
120
110
100
90
80
70
60
50
40
% viability
Control
26.6µM
133µM
266µM
3.99mM
5.3 mM
Concentration of NQTrp

Figure S5

Small molecule	Oligomer Inhibition	Fibril Inhibition
I	+++	+++
II	+++	+++
III	++	+++
IV	-	-
V	-	-
VI	++	-
VII	-	+++
VIII	+	++
VIIII	-	++
X	-	++
XI	-	+
XII	-	++

Table S1

```
!Abeta(12-28) with NQTrp (molar ratio 4:1, respectively)
!i.HN
4:1)
!i.HN
!!Intra-residual restraints.
!i+1.HN
!!Restraints i,i+1.
 assign (resid 16 and name HN) (resid 17 and name HN) 2.3 0.5 0.5
 assign (resid 18 and name HN) (resid 17 and name HN) 3.1 1.3 0.5
 assign (resid 18 and name HN) (resid 19 and name HN) 3.2 1.4 0.5
 assign (resid 24 and name HN) (resid 23 and name HN) 3.2 1.4 0.5
 assign (resid 25 and name HN) (resid 24 and name HN) 2.9 1.1 0.5
 assign (resid 26 and name HN) (resid 25 and name HN) 2.1 0.3 0.5
 assign (resid 26 and name HN) (resid 27 and name HN) 3.2 1.4 0.5
 assign (resid 28 and name HN) (resid 27 and name HN) 2.8 1.0 0.5
!i.FP
!!Intra-residual restraints.
 assign (resid 13 and name HA) (resid 13 and name HN) 5.8 4.0 0.5
 assign (resid 13 and name HB*) (resid 13 and name HN) 2.3 0.5 0.5
 assign (resid 14 and name HA) (resid 14 and name HN) 2.8 1.0 0.5
 assign (resid 14 and name HB2) (resid 14 and name HN) 3.1 1.3 0.5
 assign (resid 14 and name HB1) (resid 14 and name HN) 3.0 1.2 0.5
 assign (resid 14 and name HD2) (resid 14 and name HN) 5.2 3.4 2.3
 assign (resid 14 and name HN) (resid 14 and name HD2) 5.4 3.6 0.5
 assign (resid 15 and name HA) (resid 15 and name HN) 3.1 1.3 0.5
 assign (resid 15 and name HB2) (resid 15 and name HN) 2.3 0.5 0.5
 assign (resid 15 and name HB1) (resid 15 and name HN) 2.6 0.8 0.5
 assign (resid 15 and name HG*) (resid 15 and name HN) 3.4 1.6 0.5
 assign (resid 16 and name HB1) (resid 16 and name HN) 2.4 0.6 0.5
 assign (resid 16 and name HB2) (resid 16 and name HN) 2.7 0.9 0.5
 assign (resid 16 and name HE*) (resid 16 and name HN) 5.8 4.0 0.5
 assign (resid 16 and name HG2) (resid 16 and name HN) 2.1 0.3 0.5
 assign (resid 16 and name HG1) (resid 16 and name HN) 2.5 0.7 0.5
 assign (resid 17 and name HA) (resid 17 and name HN) 3.0 1.2 0.5
 assign (resid 17 and name HB1) (resid 17 and name HN) 3.0 1.2 0.5
 assign (resid 17 and name HD2*) (resid 17 and name HN) 4.0 2.2 0.5
 assign (resid 17 and name HD1*) (resid 17 and name HN) 3.2 1.4 0.5
 assign (resid 18 and name HA) (resid 18 and name HN) 3.1 1.3 0.5
 assign (resid 18 and name HB) (resid 18 and name HN) 3.0 1.2 0.5
 assign (resid 18 and name HG1*) (resid 18 and name HN) 4.0 2.2 0.5
 assign (resid 18 and name HG2*) (resid 18 and name HN) 5.0 3.2 0.5
 assign (resid 19 and name HA) (resid 19 and name HN) 2.0 0.2 0.5
 assign (resid 19 and name HB2) (resid 19 and name HN) 3.0 1.2 0.5
 assign (resid 19 and name HB1) (resid 19 and name HN) 2.9 1.1 0.5
 assign (resid 20 and name HA) (resid 20 and name HN) 2.6 0.8 0.5
 assign (resid 20 and name HB2) (resid 20 and name HN) 3.2 1.4 0.5
 assign (resid 20 and name HB1) (resid 20 and name HN) 3.5 1.7 0.5
 assign (resid 21 and name HA) (resid 21 and name HN) 4.0 2.2 0.5
 assign (resid 21 and name HB*) (resid 21 and name HN) 2.6 0.8 0.5
 assign (resid 22 and name HA) (resid 22 and name HN) 3.5 1.7 0.5
 assign (resid 22 and name HB2) (resid 22 and name HN) 3.0 1.2 0.5
 assign (resid 22 and name HB1) (resid 22 and name HN) 3.2 1.4 0.5
 assign (resid 22 and name HG*) (resid 22 and name HN) 3.2 1.4 0.5
 assign (resid 23 and name HA) (resid 23 and name HN) 3.0 1.2 0.5
 assign (resid 23 and name HB2) (resid 23 and name HN) 3.0 1.2 0.5
```

```
 assign (resid 23 and name HB1) (resid 23 and name HN) 2.9 1.1 0.5
 assign (resid 24 and name HA) (resid 24 and name HN) 3.1 1.3 0.5
 assign (resid 24 and name HB) (resid 24 and name HN) 2.8 1.0 0.5
 assign (resid 24 and name HG*) (resid 24 and name HN) 2.9 1.1 0.8
 assign (resid 25 and name HA*) (resid 25 and name HN) 2.7 0.9 0.5
 assign (resid 26 and name HA) (resid 26 and name HN) 2.2 0.4 0.5
 assign (resid 26 and name HB*) (resid 26 and name HN) 2.8 1.0 0.5
 assign (resid 27 and name HA) (resid 27 and name HN) 2.9 1.1 0.5
 assign (resid 27 and name HB1) (resid 27 and name HN) 3.0 1.2 0.5
 assign (resid 27 and name HB2) (resid 27 and name HN) 4.5 2.7 0.5
 assign (resid 28 and name HA) (resid 28 and name HN) 2.0 0.2 0.5
 assign (resid 28 and name HB2) (resid 28 and name HN) 4.6 2.8 0.5
 assign (resid 28 and name HB1) (resid 28 and name HN) 4.5 2.7 0.5
 assign (resid 28 and name HG*) (resid 28 and name HN) 2.4 0.6 0.5
!i+1.FP
!!Restraints i,i+1.
 assign (resid 12 and name HA) (resid 13 and name HN) 3.1 1.3 0.5
 assign (resid 14 and name HB2) (resid 15 and name HN) 3.5 1.7 0.5
 assign (resid 14 and name HB1) (resid 15 and name HN) 3.2 1.4 0.5
 assign (resid 14 and name HN) (resid 13 and name HD2) 6.4 4.6 2.3
 assign (resid 15 and name HA) (resid 16 and name HN) 2.5 0.7 0.5
 assign (resid 15 and name HB2) (resid 16 and name HN) 2.6 0.8 0.5
 assign (resid 15 and name HB1) (resid 16 and name HN) 2.2 0.4 0.5
 assign (resid 15 and name HG*) (resid 16 and name HN) 3.4 1.6 0.5
 assign (resid 16 and name HB1) (resid 17 and name HN) 4.5 2.7 0.5
 assign (resid 16 and name HB2) (resid 17 and name HN) 5.0 3.2 0.5
 assign (resid 16 and name HG1) (resid 17 and name HN) 4.5 2.7 0.5
 assign (resid 17 and name HA) (resid 18 and name HN) 2.6 0.8 0.5
 assign (resid 17 and name HB1) (resid 18 and name HN) 3.1 1.3 0.5
 assign (resid 17 and name HD1*) (resid 18 and name HN) 4.7 2.9 0.5
 assign (resid 18 and name HA) (resid 19 and name HN) 2.6 0.8 0.5
 assign (resid 18 and name HA) (resid 17 and name HN) 5.0 3.2 0.5
 assign (resid 18 and name HB) (resid 19 and name HN) 4.0 2.2 0.5
 assign (resid 18 and name HG1*) (resid 19 and name HN) 4.0 2.2 0.5
 assign (resid 18 and name HG2*) (resid 19 and name HN) 3.5 1.7 0.5
 assign (resid 19 and name HB2) (resid 20 and name HN) 3.0 1.2 0.5
 assign (resid 19 and name HZ) (resid 20 and name HN) 4.5 2.7 2.3
 assign (resid 20 and name HA) (resid 21 and name HN) 2.7 0.9 0.5
 assign (resid 20 and name HB2) (resid 19 and name HN) 5.5 3.2 0.5
 assign (resid 20 and name HB2) (resid 21 and name HN) 3.3 1.5 0.5
 assign (resid 20 and name HB1) (resid 21 and name HN) 3.3 1.5 0.5
 assign (resid 20 and name HN) (resid 19 and name HZ) 5.0 3.2 2.3
 assign (resid 20 and name HZ) (resid 21 and name HN) 4.5 2.7 2.3
 assign (resid 21 and name HA) (resid 22 and name HN) 3.5 1.7 0.5
 assign (resid 21 and name HB*) (resid 20 and name HN) 4.5 2.7 0.5
 assign (resid 21 and name HN) (resid 20 and name HZ) 5.0 3.2 2.3
 assign (resid 22 and name HA) (resid 23 and name HN) 2.7 0.9 0.5
 assign (resid 22 and name HB2) (resid 23 and name HN) 3.2 1.4 0.5
 assign (resid 22 and name HB2) (resid 23 and name HN) 3.0 1.2 0.5
 assign (resid 22 and name HG*) (resid 23 and name HN) 2.8 1.0 0.5
 assign (resid 23 and name HA) (resid 24 and name HN) 2.8 1.0 0.5
 assign (resid 23 and name HB2) (resid 24 and name HN) 2.6 0.8 0.5
 assign (resid 23 and name HB1) (resid 24 and name HN) 2.6 0.8 0.5
 assign (resid 24 and name HA) (resid 25 and name HN) 3.4 1.6 0.5
 assign (resid 24 and name HB) (resid 25 and name HN) 4.3 2.5 0.5
 assign (resid 24 and name HG*) (resid 23 and name HN) 4.8 3.0 0.8
 assign (resid 24 and name HG*) (resid 25 and name HN) 3.3 1.5 0.8
```

```
 assign (resid 25 and name HA*) (resid 24 and name HN) 5.5 3.7 0.5
 assign (resid 25 and name HA*) (resid 26 and name HN) 2.8 1.0 0.5
 assign (resid 26 and name HA) (resid 27 and name HN) 2.8 1.0 0.5
 assign (resid 26 and name HB*) (resid 27 and name HN) 2.6 0.8 0.5
 assign (resid 27 and name HA) (resid 28 and name HN) 2.5 0.7 0.5
!i+2.FP
!!Restraints i,i+2.
 assign (resid 15 and name HG*) (resid 17 and name HN) 3.9 2.1 0.5
 assign (resid 17 and name HA) (resid 19 and name HN) 5.0 3.2 0.5
 assign (resid 17 and name HB1) (resid 19 and name HN) 4.8 3.0 0.5
 assign (resid 18 and name HA) (resid 20 and name HN) 3.4 1.6 0.5
 assign (resid 18 and name HG1*) (resid 20 and name HN) 5.1 3.3 0.5
 assign (resid 18 and name HG2*) (resid 20 and name HN) 3.2 1.4 0.5
 assign (resid 19 and name HZ) (resid 21 and name HN) 5.1 3.3 2.3
 assign (resid 20 and name HB2) (resid 22 and name HN) 5.5 3.7 0.5
 assign (resid 20 and name HB1) (resid 22 and name HN) 5.0 3.2 0.5
 assign (resid 21 and name HB*) (resid 23 and name HN) 5.0 3.2 0.5
 assign (resid 23 and name HA) (resid 25 and name HN) 5.5 3.7 0.5
 assign (resid 24 and name HA) (resid 26 and name HN) 5.0 3.2 0.5
 assign (resid 24 and name HG*) (resid 22 and name HN) 5.8 4.0 0.8
 assign (resid 24 and name HG*) (resid 26 and name HN) 4.5 2.7 0.8
!i+3.FP
!!Restraints i,i+3.
 assign (resid 18 and name HA) (resid 21 and name HN) 5.5 3.7 0.5
 assign (resid 18 and name HG1*) (resid 21 and name HN) 5.2 3.4 0.5
 assign (resid 18 and name HG2*) (resid 21 and name HN) 2.8 1.0 0.5
 assign (resid 21 and name HA) (resid 24 and name HN) 5.5 3.7 0.5
 assign (resid 23 and name HA) (resid 26 and name HN) 2.8 1.0 0.5
 assign (resid 24 and name HG*) (resid 21 and name HN) 5.5 3.7 0.5
!i-lr.FP
!!Long range (further than i+3.(
 assign (resid 18 and name HA) (resid 24 and name HN) 5.0 3.2 0.5
 assign (resid 18 and name HG1*) (resid 26 and name HN) 6.5 4.7 0.5
 assign (resid 18 and name HG2*) (resid 22 and name HN) 5.3 3.5 0.5
 assign (resid 23 and name HA) (resid 15 and name HN) 2.7 0.9 0.5
!i+1.AL
!!Restraints i,i+1.
 assign (resid 13 and name HA) (resid 12 and name HG*) 4.6 2.8 0.5
 assign (resid 17 and name HA) (resid 18 and name HB) 5.0 3.2 0.5
 assign (resid 17 and name HA) (resid 18 and name HG1*) 4.5 2.2 0.5
 assign (resid 17 and name HA) (resid 18 and name HG2*) 5.5 3.2 0.5
 assign (resid 17 and name HB1) (resid 18 and name HG1*) 5.5 3.7 0.5
 assign (resid 18 and name HA) (resid 17 and name HD1*) 5.5 3.7 0.5
 assign (resid 18 and name HA) (resid 17 and name HD2*) 5.0 3.2 0.5
 assign (resid 18 and name HA) (resid 19 and name HB2) 5.5 3.7 0.8
 assign (resid 18 and name HA) (resid 19 and name HZ) 4.8 3.0 2.3
 assign (resid 18 and name HG2*) (resid 19 and name HE*) 5.5 3.7 2.3
 assign (resid 18 and name HG2*) (resid 19 and name HZ) 4.2 2.4 2.3
 assign (resid 19 and name HB2) (resid 18 and name HG2*) 5.5 3.7 0.5
 assign (resid 19 and name HB2) (resid 20 and name HZ) 5.5 3.7 0.5
 assign (resid 20 and name HB2) (resid 21 and name HB*) 5.0 3.2 0.5
 assign (resid 22 and name HG*) (resid 21 and name HB*) 4.8 3.0 0.5
 assign (resid 23 and name HA) (resid 24 and name HG*) 4.5 3.7 0.8
 assign (resid 23 and name HB1) (resid 24 and name HG*) 5.5 3.7 0.8
 assign (resid 25 and name HA*) (resid 24 and name HG*) 4.5 3.7 0.8
!i+2.AL
!!Restraints i,i+2.
```

```
 assign (resid 15 and name HG*) (resid 17 and name HD2*) 6.0 4.2 0.5
 assign (resid 16 and name HG2) (resid 18 and name HG2*) 5.5 3.7 0.5
 assign (resid 16 and name HG1) (resid 18 and name HG2*) 4.5 3.7 0.8
 assign (resid 17 and name HD1*) (resid 19 and name HE*) 5.5 3.7 2.3
 assign (resid 17 and name HD2*) (resid 19 and name HE*) 5.5 3.7 2.3
 assign (resid 17 and name HD2*) (resid 19 and name HZ) 2.2 0.4 2.3
 assign (resid 18 and name HG2*) (resid 20 and name HE*) 4.7 2.9 2.3
 assign (resid 18 and name HG2*) (resid 20 and name HZ) 4.9 3.1 2.3
 assign (resid 20 and name HB1) (resid 18 and name HG1*) 5.5 3.7 0.5
 assign (resid 20 and name HB1) (resid 18 and name HG2*) 5.5 3.7 2.3
!i+3.AL
!!Restraints i,i+3.
 assign (resid 17 and name HD1*) (resid 14 and name HD2) 5.0 3.2 2.3
 assign (resid 17 and name HD1*) (resid 14 and name HE1) 5.1 3.3 2.3
 assign (resid 17 and name HD2*) (resid 14 and name HD2) 5.5 3.7 2.3
 assign (resid 18 and name HA) (resid 21 and name HB*) 5.0 3.2 0.5
 assign (resid 18 and name HG1*) (resid 21 and name HB*) 5.0 3.2 0.5
 assign (resid 18 and name HG2*) (resid 21 and name HB*) 4.5 2.7 0.5
 assign (resid 21 and name HA) (resid 18 and name HG2*) 5.5 3.7 0.5
 assign (resid 21 and name HA) (resid 24 and name HG**) 5.0 3.2 0.5
 assign (resid 21 and name HB*) (resid 18 and name HG1*) 5.5 3.7 0.5
 assign (resid 24 and name HG1*) (resid 21 and name HB*) 5.3 3.5 0.8
!i-lr.AL
!!Long range (further than i+3.(
 assign (resid 16 and name HG1) (resid 19 and name HE*) 5.5 3.7 0.5
 assign (resid 16 and name HG1) (resid 19 and name HZ) 5.5 3.7 0.5
 assign (resid 16 and name HG1) (resid 20 and name HZ) 5.5 3.7 0.5
 assign (resid 17 and name HD1*) (resid 13 and name HD2) 5.5 3.7 0.5
 assign (resid 18 and name HG2*) (resid 14 and name HD2) 5.6 3.8 0.5
 assign (resid 19 and name HA) (resid 18 and name HG1*) 5.5 3.7 0.5
 assign (resid 19 and name HA) (resid 18 and name HG2*) 5.0 3.2 0.5
 assign (resid 19 and name HA) (resid 21 and name HB*) 4.5 2.7 0.5
 assign (resid 22 and name HG*) (resid 18 and name HG2*) 5.5 3.7 0.5
```

Table S2

Aβ segment	Sequence	Hydrogen bonds[a]				r[b]	
		Inter-peptides		Intra-peptide			
		+	-	+	-	+	-
$A\beta_{14-20}$	Ac-HQKLVFF-NHMe	6.7 ± 0.5	8.5 ± 0.3	0.58 ± 0.04	0.1 ± 0.1	1.88	10.2
$A\beta_{16-22}$	Ac-KLVFFAE-NHMe	5.0 ± 0.3	7.1 ± 0.2	0.97 ± 0.03	0.6 ± 0.1	0.59	1.63
$A\beta_{18-24}$	Ac-VFFAEDV-NHMe	4.0 ± 0.3	6.9 ± 0.3	2.44 ± 0.05	0.8 ± 0.2	0.24	1.01

Table S3

$A\beta_{14-20}$	NH2-CO	CO1-NH	CO2-NH	CO3-NH
NH1-CO	0.021	**0.10**	0.025	**0.099**
NH2-CO	-	0.015	0.011	0.020
CO1-NH	-	-	0.022	**0.064**
CO2-NH	-	-	-	0.031

$A\beta_{16-22}$	NH2-CO	CO1-NH	CO2-NH	CO3-NH
NH1-CO	0.027	**0.12**	0.029	**0.13**
NH2-CO	-	0.020	0.016	0.026
CO1-NH	-	-	0.026	**0.082**
CO2-NH	-	-	-	0.039

$A\beta_{18-24}$	NH2-CO	CO1-NH	CO2-NH	CO3-NH
NH1-CO	0.023	**0.12**	0.037	**0.14**
NH2-CO	-	0.021	0.021	0.032
CO1-NH	-	-	0.036	**0.10**
CO2-NH	-	-	-	0.055

Table S4

Peptide	hydrogen bond pairs	frequency
$A\beta_{14\text{-}20}$	NH1-Val18 CO1-Phe20	0.026
$A\beta_{16\text{-}22}$	NH1-Val18 CO1-Phe20	0.027
	NH1-Phe20 CO1-Phe20	0.024
	NH1-Phe20 CO3-Glu22	0.021
$A\beta_{18\text{-}24}$	NH1-Phe20 CO1-Phe20	0.015
	NH1-Ala21 CO1-Ala21	0.013

Table S5

Inhibitor	**IC_{50} μM**
NQTrp	0.05
ThT	122.19 [1]
Congo Red	10, 1.99 [1,2]
Curcumin	0.8, 0.18 [3,4]
Phenol Red	426.25 [1]
Epiccatechin gallate	3 [5,6]
Epigallocatechin gallate (green tea)	0.18 [6]
THB (2,3,4- Trihydroxybenzophenone)	3.1 [5,6]
4-Hydroxy indole	85 [7]
3-Hydroxyindole	100 [7]
Indole-3-carbinole	200 [7]
several benzofurans	28-85 [8]

Table S6

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