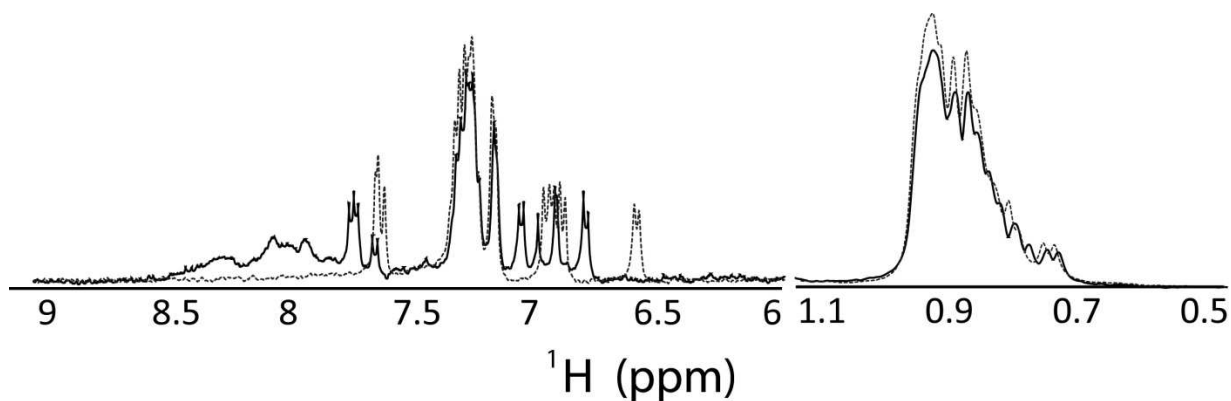


Supporting Information

S1 Spectral changes of A β ₁₋₄₀ from basic to physiological pH

1D ^1H NMR spectra of A β ₁₋₄₀ before (dotted line) and after (full line) adjustment to physiological pH.



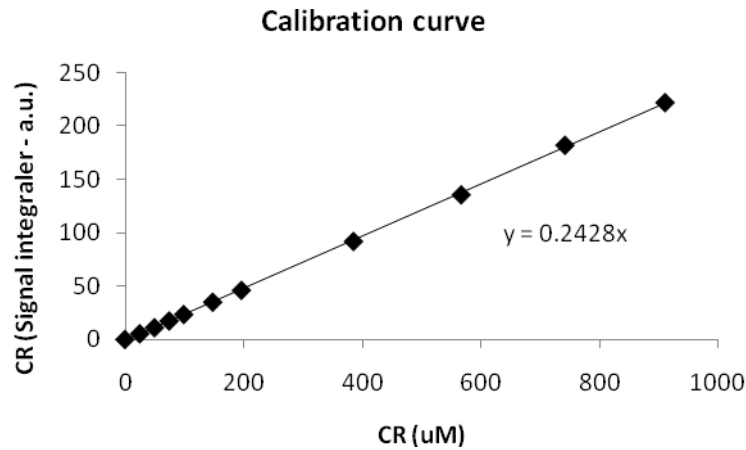
S2 Chemical shift assignments

Assignment of ^1H and ^{15}N chemical shifts for amide groups of A β ₁₋₄₀ recorded at 800 MHz, 25 °C

| Residue | ^{15}N (ppm) | ^1H CS (ppm) | Residue | ^{15}N (ppm) | ^1H CS (ppm) |
|---------|-----------------------|-----------------------|---------|-----------------------|-----------------------|
| E3 | 120.223 | 8.461 | V24 | 120.352 | 8.117 |
| R5 | 123.591 | 8.119 | G25 | 111.591 | 8.529 |
| D7 | 121.568 | 8.257 | S26 | 115.561 | 8.164 |
| S8 | 116.468 | 8.383 | K28 | 121.656 | 8.336 |
| G9 | 110.704 | 8.522 | G29 | 109.445 | 8.413 |
| Y10 | 120.031 | 7.952 | A30 | 123.572 | 8.027 |
| E11 | 122.461 | 8.403 | I31 | 120.37 | 8.123 |
| V12 | 120.809 | 8.051 | I32 | 125.552 | 8.222 |
| Q15 | 121.539 | 8.399 | G33 | 112.68 | 8.431 |
| K16 | 122.583 | 8.354 | L34 | 121.653 | 8.02 |
| L17 | 123.544 | 8.199 | M35 | 121.703 | 8.417 |
| V18 | 121.054 | 7.958 | V36 | 121.857 | 8.183 |
| F19 | 123.966 | 8.211 | G37 | 112.826 | 8.547 |
| F20 | 122.621 | 8.21 | G38 | 108.752 | 8.254 |
| A21 | 126.01 | 8.228 | V39 | 119.829 | 8.054 |
| E22 | 119.859 | 8.352 | V40 | 128.085 | 7.779 |
| D23 | 121.177 | 8.374 | | | |

S3 Congo Red calibration curve.

Signal intensity of CR peaks plotted as a function of CR concentration. The data has been fitted to a linear calibration curve, which subsequently was used to estimate the amount of free CR in solution.



S4 simulations of second binding step using different binding stoichiometries (n_2)

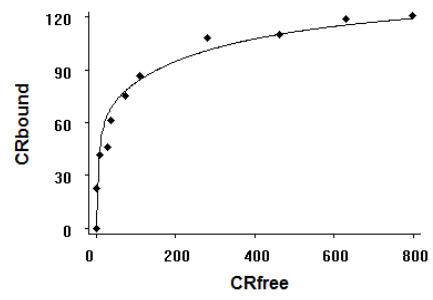
Simulations of the total amount of bound CR have been carried out using the following equation describing a two-state binding:

$$[CR]_{bound} = \frac{n_1 \times [A\beta] \times [CR]_{free}}{K_{d1} + [CR]_{free}} + \frac{n_2 \times [A\beta] \times [CR]_{free}}{K_{d2} + [CR]_{free}}$$

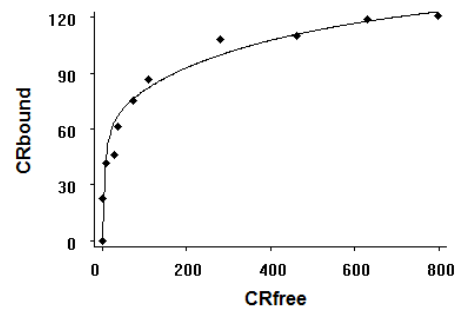
K_{d2} was fitted for different values of n_2 , while n_1 and K_{d1} were fixed at 1 and 5 μ M, respectively.

| n_2 | K_{d2} | Binding curve |
|-------|-------------------|---------------|
| 0.5 | 90.7 ± 127.7 | |
| 0.75 | 180.2 ± 113.1 | |

1.0 319.7 ± 122.3



1.25 498.8 ± 150.4



1.5 698.8 ± 188.0

