Supporting Information for: Copper (I) and copper (II) binding to β-amyloid 16 (Aβ16) studied by electrospray ionization mass spectrometry

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The simulated curves representing the time evolution of the concentrations of Cu(I)- and Cu(II)-Aβ complexes, Cu^{2+} and Aβ were calculated based on empirical chemical kinetics. The static state approximation was applied to this kinetic model i.e. the concentration of Cu^{+} maintained constant during the whole process and the rate equations including all the concentrations of Cu(I)- and Cu(II)-Aβ complexes, Cu^{2+}, Cu^{+}, and Aβ were then given as below:

\[
\frac{d[Cu^I - A\beta]}{dt} = k_1[Cu^I][A\beta] + k_{red}[AA][Cu^II - A\beta]
\]

\[
\frac{d[Cu^II - A\beta]}{dt} = k_2[Cu^II][A\beta] - k_{red}[AA][Cu^II - A\beta]
\]

\[
\frac{d[Cu^II]}{dt} = k_{ox}[Cu^I] - k_2[Cu^II][A\beta]
\]

\[
\frac{d[Cu^I]}{dt} = k - k_{ox}[Cu^I] - k_1[Cu^I][A\beta] = 0
\]

\[
[Cu^I - A\beta] + [Cu^II - A\beta] + [A\beta] = C_0
\]

These equations could be applied to the both presence and absence of reducing agent in the peptide solution just dependent on the assignment of \(k_{red}\) as 0 or not. According to the assumption of the constant concentration of Cu^{+}, the stem of [Cu^I] can be replaced by the expression of the combination of [Aβ], \(k\) and \(k_{ox}\). Then the nonlinear system of ordinary differential equations including Cu(I)- and Cu(II)-Aβ complexes, Cu^{2+} and Aβ could finally be solved by Wolfram Mathematica 7.0.0. Here is the
program written for the resolution of the dynamic equations (\(j = k_1, p = k, l = k_{ox}, k = k_2, m = k_{red}[AA]\)):

```
"Exit[]

system = {
    D[c1[t], t] == j*p/(l + j*c4[t])*c4[t] + m*c2[t],
    D[c2[t], t] == k*c3[t]*c4[t] - m*c2[t],
    D[c3[t], t] == l*p/(l + j*c4[t]) - k*c3[t]*c4[t],
    c1[t] + c2[t] + c4[t] == 10,
    c1[0] == c2[0] == c3[0] == 0
};
param = {
    j -> 85,
    k -> 85,
    m -> 5,
    l -> 400,
    p -> 1.6
};
delta = 10/400; sol = NDSolve[system /. param, {c1[t], c2[t], c3[t], c4[t]}, {t, 0, 10}];
timetable = Table[i*delta, {i, 0, 400}] // N;
Export["CuAB1.xls",
    Transpose[{timetable, sol[[1, 1, 2]] /. {t -> #} & /@ timetable}]]
Export["CuAB2.xls",
    Transpose[{timetable, sol[[1, 2, 2]] /. {t -> #} & /@ timetable}]]
Export["Cu2.xls",
    Transpose[{timetable, sol[[1, 3, 2]] /. {t -> #} & /@ timetable}]]
Export["AB.xls",
    Transpose[{timetable, sol[[1, 4, 2]] /. {t -> #} & /@ timetable}]]
```

Finally, the proper assignments of the rates constants to obtain the solution of the equations are given as follows: \(k = 1.6 \mu M \cdot \text{min}^{-1}\), \(k_1 = k_2 = 85 \mu M^{-1} \cdot \text{min}^{-1}\), \(k_{ox} = 400 \text{ min}^{-1}\), \(k_{red}[AA] = 5 \text{ min}^{-1}\). (\(j=k_1, p=k, l=k_{ox}, k=k_2, m=k_{red}[AA]\))