

Electronic Supplementary Information

Cadmium(II) *N*-Acetylcysteine Complex Formation in Aqueous Solution

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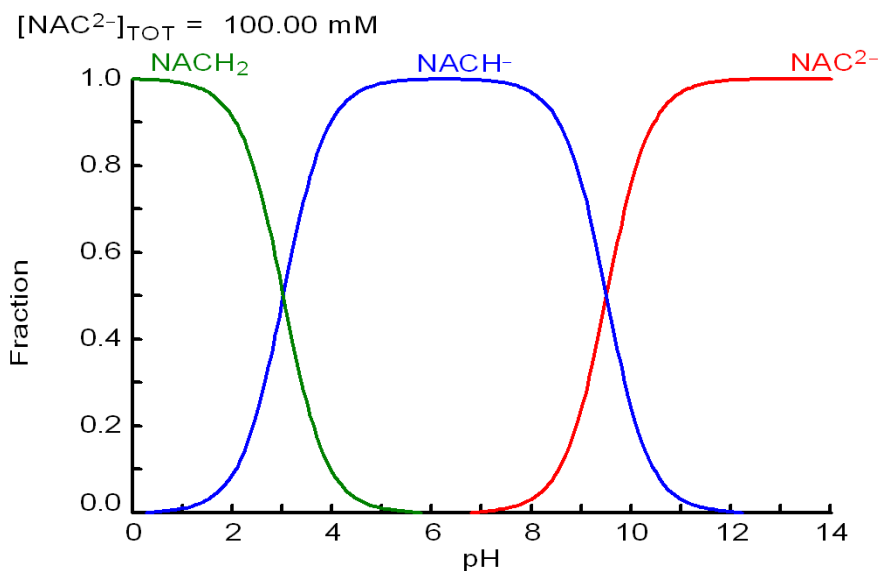


Figure S-1. Fraction diagram calculated with MEDUSA (<http://www.kemi.kth.se/medusa/>) to account for the distribution of the solution species vs. pH in 0.1 M *N*-acetylcysteine solution. The formation constants from *Polyhedron* 9 (1990) 831 -837 were used.

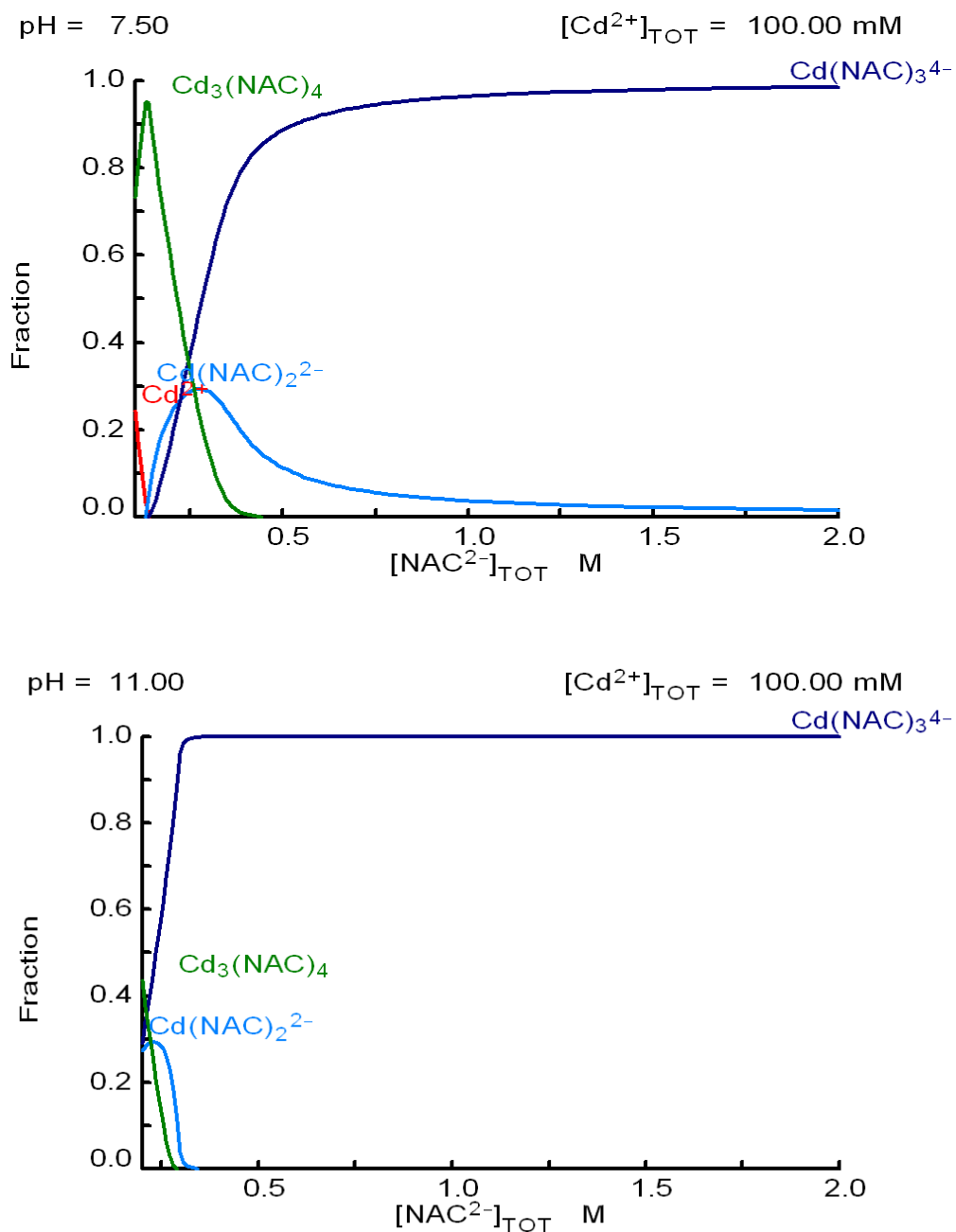


Figure S-2. Fraction diagrams calculated with MEDUSA (<http://www.kemi.kth.se/medusa/>) to account for the calculated distribution of Cd(II) complexes vs. total N-acetylcysteine concentration at pH 7.5 (*top*) and 11.0 (*below*) in aqueous solutions containing [Cd²⁺]_{total} = 0.1 M. For generating these diagrams, the formation constants from *Polyhedron* 9 (1990) 831 -837 were used.

The full input file to the MEDUSA computer program (with $\log\beta$ values for the equilibrium formation constants):

```
3, 13, 0, 0 /MEDUSA, t = 25 C
H+
Cd 2+
NAC 2-
NACH -      , 9.85  1 0 1
NACH2      , 13.16  2 0 1
Cd(NAC)     , 7.05  0 1 1
Cd(NAC)2 2- , 13.49  0 1 2
Cd(NAC)3 4- , 17.41  0 1 3
Cd3(NAC)4   , 35.53  0 3 4
OH-        , -14.0  -1 0 0
Cd(OH)2     , -20.35 -2 1 0
Cd(OH)3-    , -33.3  -3 1 0
Cd(OH)4 2-  , -47.35 -4 1 0
Cd2OH 3+    , -9.39  -1 2 0
Cd4(OH)4 4+ , -32.85 -4 4 0
CdOH+       , -10.08 -1 1 0
Cd 2+, H+,
LAV, -7.0 -12.0
T, 0.1
T, 2.0
T, 0.0
```

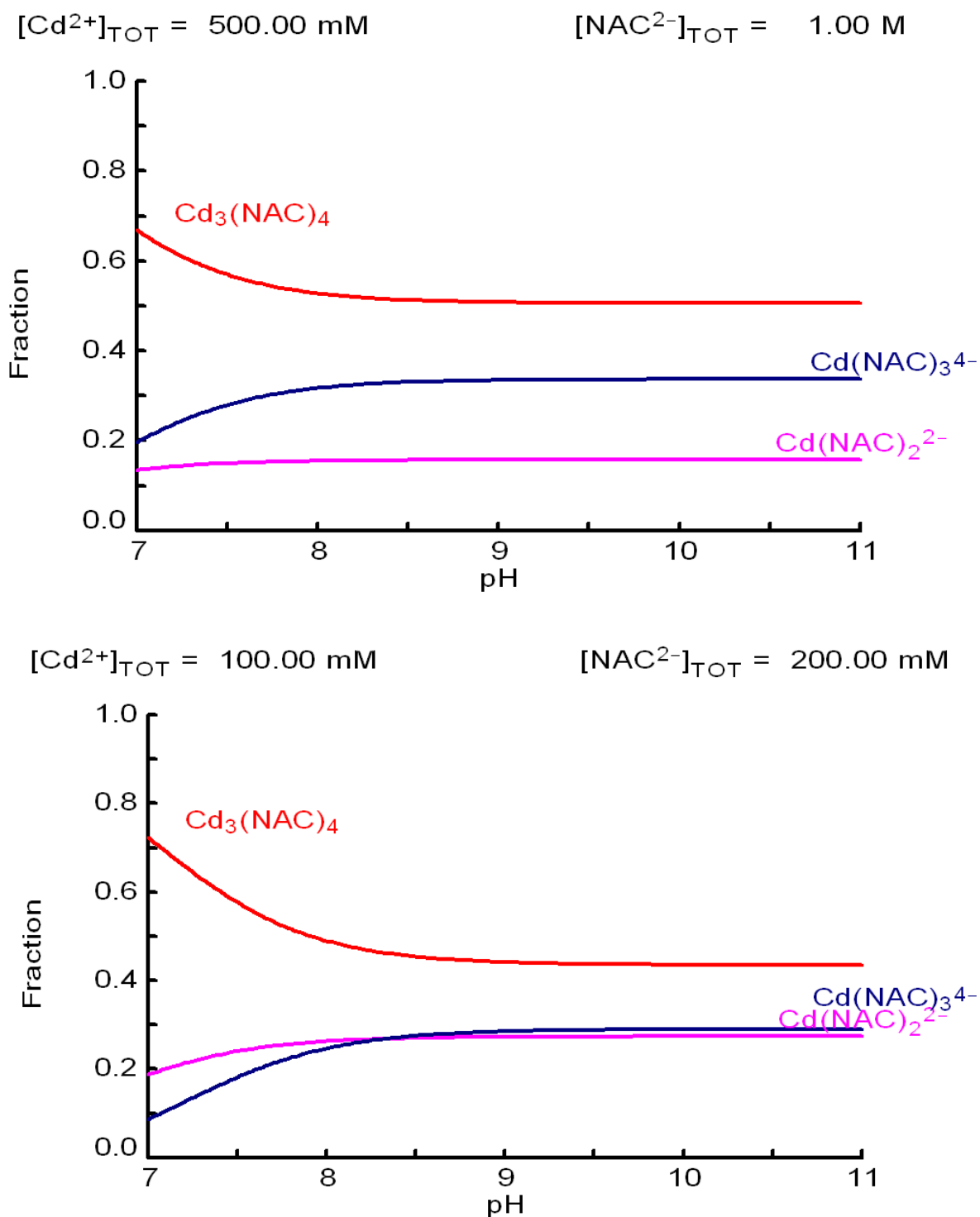


Figure S-3. Fraction diagrams showing the calculated distribution of Cd(II) - NAC complexes vs. pH (according to the formation constants from *Polyhedron* 9 (1990) 831 -837) in aqueous solutions with the H₂NAC/ Cd(II) mole ratio 2.0: (*top*) $c_{Cd(II)} = 0.5 \text{ M}$ (as in solutions **H1** and **H2**); (*below*) $c_{Cd(II)} = 0.1 \text{ M}$ (as in solutions **A1** and **A2**).

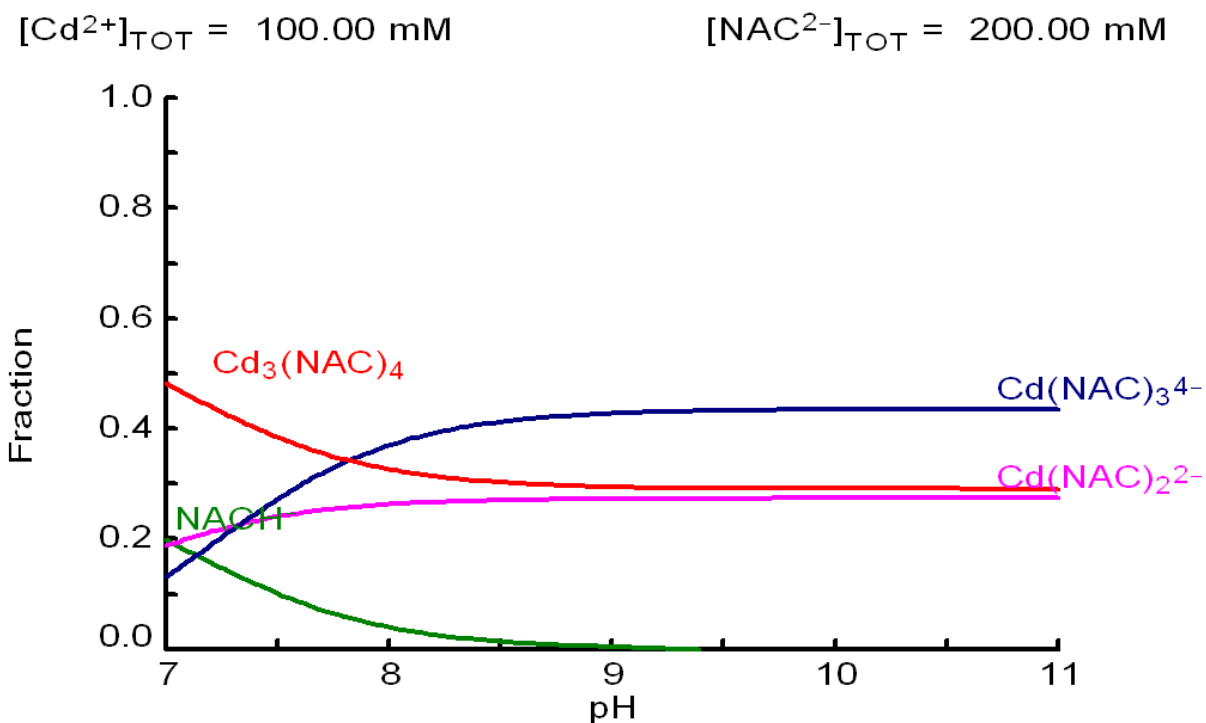


Figure S-4. Fraction diagram showing the calculated distribution of *N*-acetylcysteine in different species (free or as ligand in Cd-complexes) for an aqueous solution with $c_{\text{Cd(II)}} = 0.1 \text{ M}$ and $c_{\text{H}_2\text{NAC}} = 0.2 \text{ M}$. Note that the diagram shows about 10% of the total *N*-acetylcysteine to be present as free HNAC^- ions at $\text{pH} = 7.5$, but at $\text{pH} = 11$ the concentration of free *N*-acetylcysteine in solution is negligible.