

**Table 1.** Calculated pK<sub>a</sub> values for titratable residues in Aβ(1-28) and Aβ(10-42)

Residue	Aβ (1-28)	Aβ (10-42)
NTER	7.1	-
Asp-1	2.9	-
Glu-3	2.4	-
His-6	6.5	-
Asp-7	2.0	-
Glu-11	3.2	3.5
His-13	6.0	6.4
His-14	5.5	6.1
Glu-22	3.4	4.0
Asp-23	2.9	3.8
CTER	2.7	2.9

The standard pK<sub>a</sub> values used are: Asp, 4.0; Glu, 4.4; His, 6.55; α-amino, 7.5; α-carboxyl, 3.8. There is good agreement between the experimentally observed midpoints of the pH profile (3.8 and 6.0) in Aβ (1-40) (1) and the computed highest pK<sub>a</sub> value for carboxyl (4.0) and lowest pK<sub>a</sub> value for histidine (6.1) groups in Aβ (10-42).

1. Kirkitadze MD, Condron MM, Teplow DB (2001) *J Mol Biol* 321: 1103-1119.