

A deeper insight in metal binding to the hCtr1 N-terminus fragment: affinity, speciation and binding mode of binuclear Cu^{2+} and mononuclear Ag^+ complex species

Antonio Magri^{1,#}, Giovanni Tabbi^{1,#}, Irina Naletova^{1,2}, Francesco Attanasio^{1,*}, Giuseppe Arena³ and Enrico Rizzarelli^{1,2,3,*}

¹ Institute of Crystallography, National Council of Research, CNR, S.S. Catania, via P. Gaifami 18, Catania, Italy; antonio.magri@ic.cnr.it, giovanni.tabbi@ic.cnr.it, irina.naletova@ic.cnr.it, francesco.attanasio@ic.cnr.it

² Consorzio Interuniversitario per la Ricerca dei Metalli nei Sistemi Biologici, Via Ulpiani 27, Bari, Italy;

³ Department of Chemical Sciences, University of Catania, Viale A. Doria 6, Catania, Italy; garena@unict.it

AM and GT share the first authorship

* Correspondence: erizzarelli@unict.it; Tel.: +39 095 7385070 (E.R.); francesco.attanasio@ic.cnr.it (F.A.)

Table S1. Log β and pK values for the protonation of the Ctr1₍₁₋₁₄₎.

Species [L _q H _r]	log $\beta^{a,b}$	pK ^b	log β^c	pK ^c
qr				
11	9.64 (3)	9.64	9.84	9.84
12	17.27 (2)	7.63	17.30	7.46
13	24.18 (2)	6.91	24.23	6.93
14	30.47 (1)	6.29	30.46	6.23
15	36.21 (2)	5.74	36.24	5.78
16	40.39 (3)	4.17	40.27	4.03
17	43.21 (1)	2.82	43.20	2.92

^a3 σ in parentheses; ^bThis work; ^cReference 17