
Supplementary Information

Ni(II) Ions May Target the Entire Melatonin Biosynthesis Pathway — a Plausible Mechanism of Nickel Toxicity

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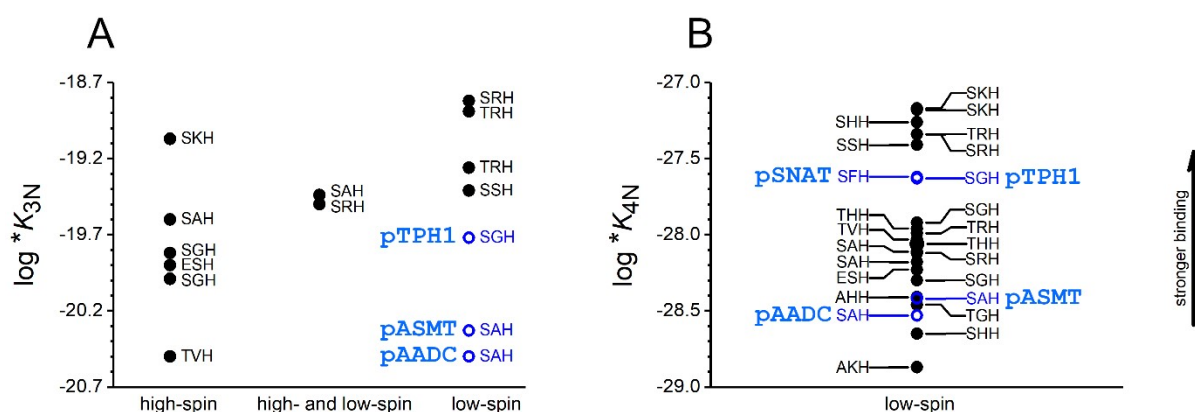


Figure S1. Protonation-corrected logarithmic stability constants of Ni(II) 3N (A, $\log *K_{3N}$), and 4N (B, $\log *K_{4N}$) complexes and spin states of these complexes. The considered peptides are those derived from the melatonin biosynthesis pathway marked by blue open circles, Ac-HALSGHAKV-am (SGH, pTPH1); Ac-TVESAHVQR-am (SAH, pAADC); Ac-ERFSFHAVG-am (SFH, pSNAT); Ac-VRASAHGTE-am (SAH, pASMT); and other, previously studied peptides marked by black dots, Ac-TKYSKHDMN-am (SKH); Ac-GVGTRHKAL-am (TRH); Ac-KMSTVHEIL-am (TVH); Ac-SALSGHLET-am (SGH); Ac-KALTGHLEE-am (TGH); Ac-VKSSSHFNP-am (SSH); Ac-GASGHAKFL-am (SGH); Ac-GASAHWKFL-am (SAH); Ac-GASKHWKFL-am (SKH); Ac-GASRHAKFL-am (SRH); Ac-GASRHWKFL-am (SRH); Ac-GATRHWKFL-am (TRH); Ac-GATHHWKFL-am (THH); Ac-TESHHK-am (SHH); Ac-TASHHK-am (SHH); Ac-TEAHHK-am (AHH); Ac-TESAHK-am (SAH); Ac-TESHAK-am (ESH); Ac-TETHHK-am (THH); Ac-ELAKHA-am (AKH) [1–5].

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