

Phosphatase reactivity by a dicopper(II) complex of a patellamide derivative - possible biological functions of cyclic pseudopeptides.

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Supporting Information

Table S1. Data of the pH profile of the $[\text{Cu}^{II}_2(\text{H}_2\text{pat}^1)(\mu\text{-OH})(\text{H}_2\text{O})_2]^+$ -catalyzed BDNPP hydrolysis (catalyst concentration: 40 μM , BDNPP for the pH dependence: 6.25 mM, pH for the substrate dependence: 7.06, $\mu = 0.45$).

pH	V_0 [M s ⁻¹]	Δ [M s ⁻¹]
6.04	6.64x10 ⁻⁹	2.41x10 ⁻⁹
6.48	1.82x10 ⁻⁸	3.88x10 ⁻⁹
7.06	2.90x10 ⁻⁸	3.34x10 ⁻⁹
7.53	2.37x10 ⁻⁸	3.99x10 ⁻⁹
8.01	1.40x10 ⁻⁸	1.54x10 ⁻⁹
8.51	8.71x10 ⁻⁹	2.08x10 ⁻⁹
9.00	7.14x10 ⁻⁹	1.14x10 ⁻⁹
9.50	4.97x10 ⁻⁹	8.70x10 ⁻¹⁰
10.02	4.42x10 ⁻⁹	2.21x10 ⁻⁹
10.51	4.51x10 ⁻⁹	2.02x10 ⁻⁹
10.99	5.17x10 ⁻⁹	3.73x10 ⁻⁹

Table S2. Data of the BDNPP concentration dependence of the $[\text{Cu}^{II}_2(\text{H}_2\text{pat}^1)(\mu\text{-OH})(\text{H}_2\text{O})_2]^+$ -catalyzed BDNPP hydrolysis (catalyst concentration: 40 μM , pH for the substrate dependence: 7.06, $\mu = 0.45$).

BDNPP [mM]	V_0 [M s ⁻¹]	Δ [M s ⁻¹]
1.00	4.58x10 ⁻⁹	1.37x10 ⁻¹⁰
3.00	1.59x10 ⁻⁸	4.33x10 ⁻⁹
5.00	2.22x10 ⁻⁸	4.03x10 ⁻⁹
6.25	2.90x10 ⁻⁸	3.34x10 ⁻⁹
7.00	3.36x10 ⁻⁸	3.85x10 ⁻⁹
9.00	4.10x10 ⁻⁸	2.35x10 ⁻⁹

Table S3. Kinetic data of the $[\text{Cu}^{II}_2(\text{H}_2\text{pat}^1)(\mu\text{-OH})(\text{H}_2\text{O})_2]^+$ -catalyzed BDNPP hydrolysis.

Catalyst	pH _{max}	V _{0,max}	pK _{a(I)}	pK _{a(II)}	k _{cat} [s ⁻¹] *10 ⁻³	K _M [mM]	k _{cat} /K _M [M ⁻¹ s ⁻¹]
$[\text{Cu}^{II}_2(\text{H}_2\text{pat}^1)(\mu\text{-OH})(\text{H}_2\text{O})_2]^+$	7.21	$1.59 \times 10^{-7} \pm 3.00 \times 10^{-9}$	6.91 ± 0.21	7.31 ± 0.20	3.95 ± 0.07	26.4 ± 2.20	0.15 ± 0.03