

## The impact of two -GlyProGly- motifs on formation of di-copper complexes by His<sub>4</sub>-cyclopeptides

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### Electronic Supplementary Information

Table 1. Backbone structural parameters for considered set of complexes. The data are given in degrees.

		H1	K2	H3	P4	H5	K6	H7	P8
<b>c(HKHP)<sub>2</sub></b> {2N <sub>1m</sub> , 2N <sub>am</sub> <sup>-</sup> }	Φ	-113.5	-150.9	-92.8	77.9	-120.26	-54.0	-115.9	-84.7
	Ψ	-109.4	-17.0	108.5	-172.4	-18.0	-54.7	156.3	72.4
<b>c(HKHP)<sub>2</sub></b> {2N <sub>1m</sub> , 3N <sub>am</sub> <sup>-</sup> }	Φ	-158.3	178.3	-169.3	84.9	-129.4	-61.1	-123.9	-87.2
	Ψ	-5.7	8.0	165.3	-179.3	-71.3	-47.9	74.4	164.1
<b>c(HKHP)<sub>2</sub></b> {2N <sub>1m</sub> , 2N <sub>am</sub> <sup>-</sup> }	Φ	-152.7	-165.1	-106.6	120.5	-151.5	166.3	-164.1	-72.2
	Ψ	-89.3	-3.5	158.3	-113.2	166.7	21.3	117.6	109.7

		H1	K2	H3	G4	P5	G6	H7	K8	H9	G10	P11	G12
<b>c(HKHGPG)</b> {2N <sub>1m</sub> , 2N <sub>am</sub> <sup>-</sup> }	Φ	84.2	132.4	74.0	81.7	-82.7	-99.9	115.4	154.0	115.3	-91.7	-73.1	97.8
	Ψ	-72.5	29.1	150.7	-85.4	158.9	-84.8	-3.3	-47.5	-177.2	-66.3	-47.5	151.7
<b>c(HKHGPG)</b> {2N <sub>1m</sub> , 3N <sub>am</sub> <sup>-</sup> }	Φ	98.7	-170.7	100.4	-153.4	-83.4	-109.8	75.4	52.1	130.0	-90.9	-93.5	-106.7
	Ψ	83.7	-10.9	31.2	177.8	66.1	-87.0	4.8	32.4	-130.8	-64.7	-57.6	-161.5
<b>c(HKHGPG)</b> {2N <sub>1m</sub> , 2N <sub>am</sub> <sup>-</sup> }	Φ	35.2	107.4	87.4	103.7	-58.2	-168.3	177.4	157.5	172.4	-171.8	-148.6	171.4
	Ψ	72.2	17.2	157.2	-135.1	165.5	-156.2	39.9	-0.1	146.5	-59.0	35.2	167.1