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**Figure S1**. Imino region of the NOESY spectra of [Ac-Cys-Gly-Ala-Hse( $p^{3'}$ dGCATGC)-Ala-OH]<sub>2</sub>[S-S] in H<sub>2</sub>O (100mM NaCl, T=5°C, pH=7,  $\tau_m$ = 200 ms).



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**Figure S2**. NMR and UV melting curves of [Ac-Cys-Gly-Ala-Hse( $p^{3'}$ dGCATGC)-Ala-OH]<sub>2</sub>[S-S]. Top: Chemical shift variation versus temperature for H5C2 and H2A3. Middle: Chemical shift variation of the thymine methyl resonance. Nucleopeptide concentrations are 1 mM (solid lines), and 0.1 mM (dashed lines). Bottom: UV melting curve at 2  $\mu$ M nucleopeptide concentration.



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**Table S1**. <sup>1</sup>H-NMR assignments of [Ac-Cys-Gly-Ala-Hse(p<sup>3'</sup>dCGATCG)-Ala]-[p<sup>3'</sup>dCGATGC] (100mM NaCl, T=5°C, pH=7).

Res.	Н4'	н1'	Н6/Н8	н2'	н2"	н3'	Н5'	H2/H5/M	NH <sub>2</sub> (2)	NH <sub>2</sub> (1)	NH
1CYT	4.08	5.76	7.68	2.06	2.46	4.74	3.73	5.945	8.17	7.16	
2gua	4.39	6.00	8.06	2.79	2.79	5.02	4.15				12.93
ЗТНҮ	4.24	5.59	7.38	2.18	2.45	4.92	4.15	1.60			13.65
4ADE	4.47	6.32	8.40	2.80	2.93	5.08	4.14	7.76			
5CYT	4.14	5.71	7.36	1.83	2.31	4.84	4.27	5.47	8.38	6.87	
6GUA	4.38	6.23	7.99	2.74	2.56	4.97					13.17
	HN	HA	HB2/3								
13CYS <sup>+</sup>	8.77	4.90	3.04/3.31								
14GLY	8.96	4.07/3.97									
15ALA	8.34	4.38	1.44								
16HSE	8.63	4.48	2.08/2.29					HG2 4.00			
17ALA	8.09	4.08	1.36								

<sup>+</sup>Acetyl terminal group = 1.82 ppm