Electronic Supplementary Information

Evidences for supramolecular organization of nucleopeptides: synthesis, spectroscopic and biological studies of a novel dithymine L-serine tetrapeptide.

Giovanni N. Roviello*a,b, Domenica Musumeci a,b, Enrico M. Bucci and Carlo Pedone

a Dr. G. N. Roviello, Dr. D. Musumeci, Dr. E. M. Bucci, Prof. C. Pedone
Istituto di Biostrutture e Bioimmagini – CNR, Via Mezzocannone 16, 80134 Napoli, Italy
E-mail: giroviel@unina.it; Fax: +39-(0)81-2534574; Tel: +39-(0)81-2534585

b These authors equally contributed to this work.

This supplementary information provides a comparison between the structures of the dithymine-based nucleopeptide and TpT DNA dinucleoside monophosphate, the LC-ESI MS profiles of oligomer 1, monomers 4 and 5, the CD spectra relative to the DNA-binding studies and the HPLC profiles of the crude mixture relative to the two syntheses of the nucleopeptide 1. The crude material was purified by semipreparative HPLC on a C18 column using a linear gradient of 5 % (for 5 min) to 30 % B’ in A’ over 30 min.

![Figure S 1. Comparison between dithymine tetramerine 1 and TpT DNA dinucleoside monophosphate 2.](image-url)
**Figure S 2.** LC-ESIMS of oligomer 1; $t_R = 9.32$ min; method: 5% (5min) to 40% B in A over 10 min (A=0.05% TFA in H$_2$O, B=0.05% TFA in CH$_3$CN).

**Figure S 3.** LC-ESIMS of Fmoc-L-Ser-OH (4); $t_R = 12.50$ min; method: 15% (5min) to 95% B in A over 15 min (A=0.05% TFA in H$_2$O, B=0.05% TFA in CH$_3$CN).
Figure S 4. LC-ESIMS of Fmoc-L-Ser(T)-OH (5); \( t_R = 12.82 \text{ min} \); method: 15% (5min) to 95% B in A over 15 min (A=0.05% TFA in H$_2$O, B=0.05% TFA in CH$_3$CN).

Figure S 5. CD binding study: 15 μM in nucleobase (T) solution of nucleopeptide 1 + 15 μM in A of DNA (dA$_{12}$) before (green) and after (blue) mixing. Both spectra were recorded at 5 °C in 10 mM phosphate buffer, pH=7.5.
Figure S 6. HPLC profile relative to the crude mixture obtained after the solid phase synthesis of nucleopeptide 1 described in Fig. 2.

Figure S 7. HPLC profile relative to the crude mixture obtained after the solid phase synthesis of nucleopeptide 1 described in Fig. 7.