

Electronic Supplementary Information

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

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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

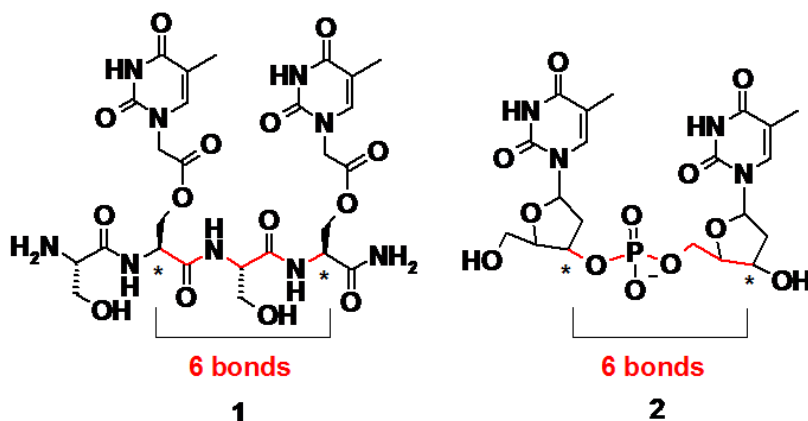


Figure S 1. Comparison between dithymine tetraserine 1 and TpT DNA dinucleoside monophosphate 2.

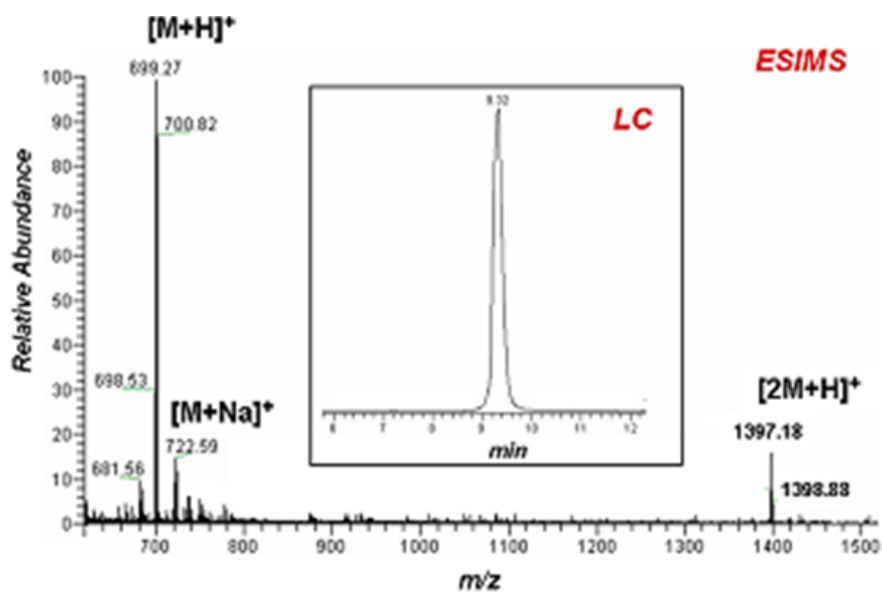


Figure S 2. LC-ESIMS of oligomer 1; t_R = 9.32 min; method: 5% (5min) to 40% B in A over 10 min (A=0.05% TFA in H_2O , B=0.05% TFA in CH_3CN).

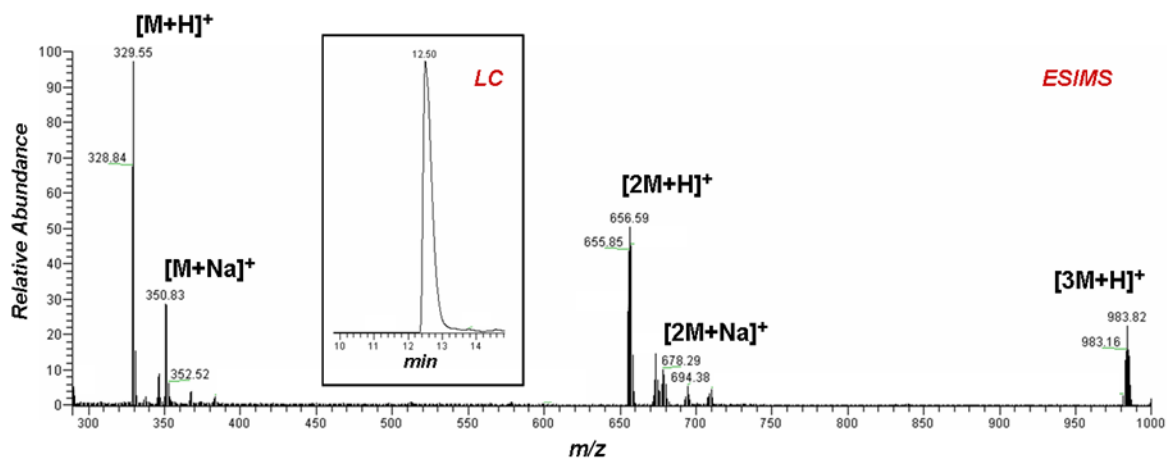


Figure S 3. LC-ESIMS of Fmoc-L-Ser-OH (4); t_R = 12.50 min; method: 15% (5min) to 95% B in A over 15 min (A=0.05% TFA in H_2O , B=0.05% TFA in CH_3CN).

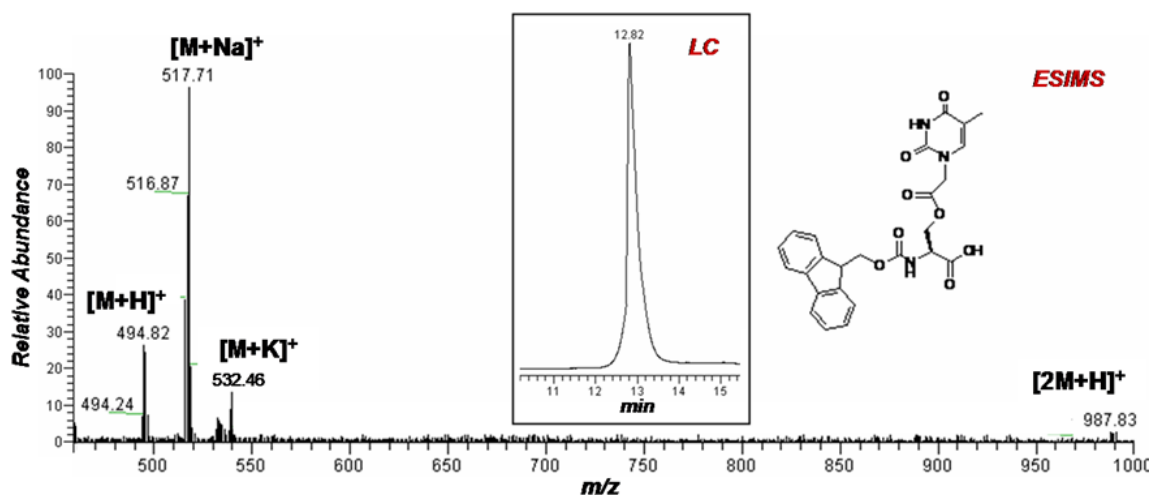


Figure S 4. LC-ESIMS of Fmoc-L-Ser(T)-OH (**5**); t_R = 12.82 min; method: 15% (5min) to 95% B in A over 15 min (A=0.05% TFA in H₂O, B=0.05% TFA in CH₃CN).

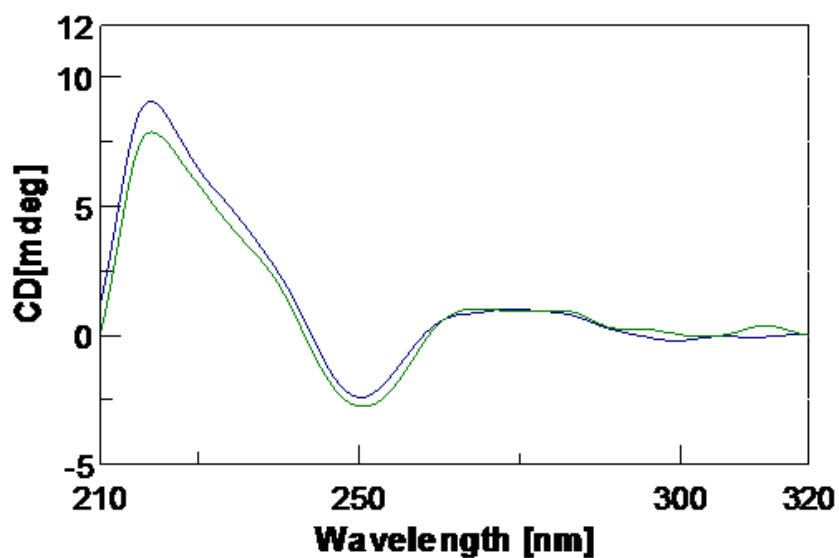


Figure S 5. CD binding study: 15 μ M in nucleobase (T) solution of nucleopeptide **1** + 15 μ M in A of DNA (dA₁₂) before (green) and after (blue) mixing. Both spectra were recorded at 5 °C in 10 mM phosphate buffer, pH=7.5.

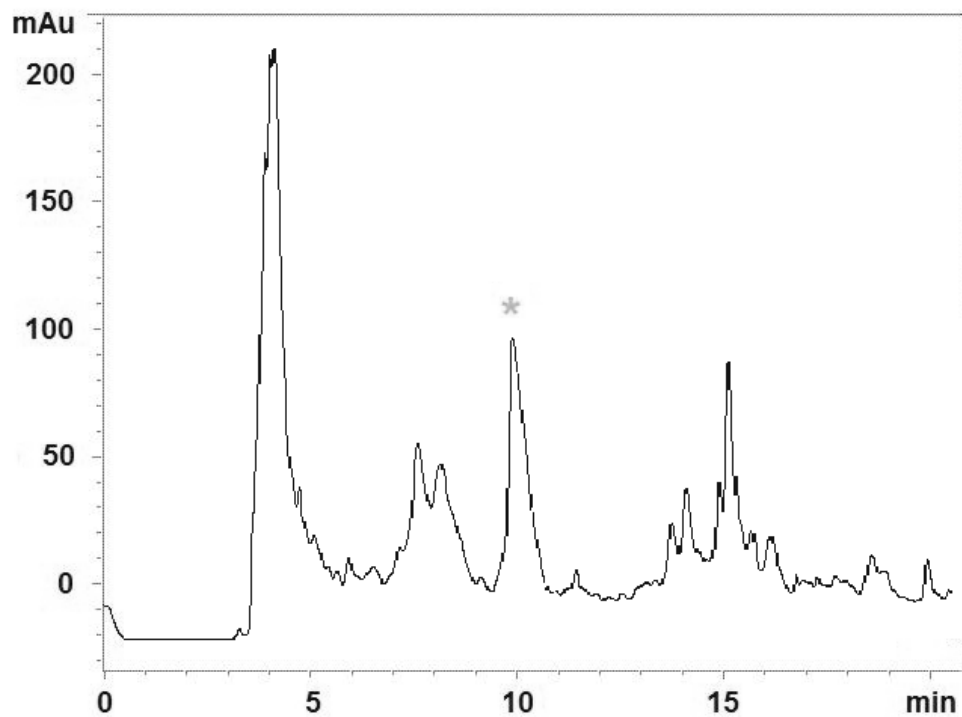


Figure S 6. HPLC profile relative to the crude mixture obtained after the solid phase synthesis of nucleopeptide 1 described in Fig. 2.

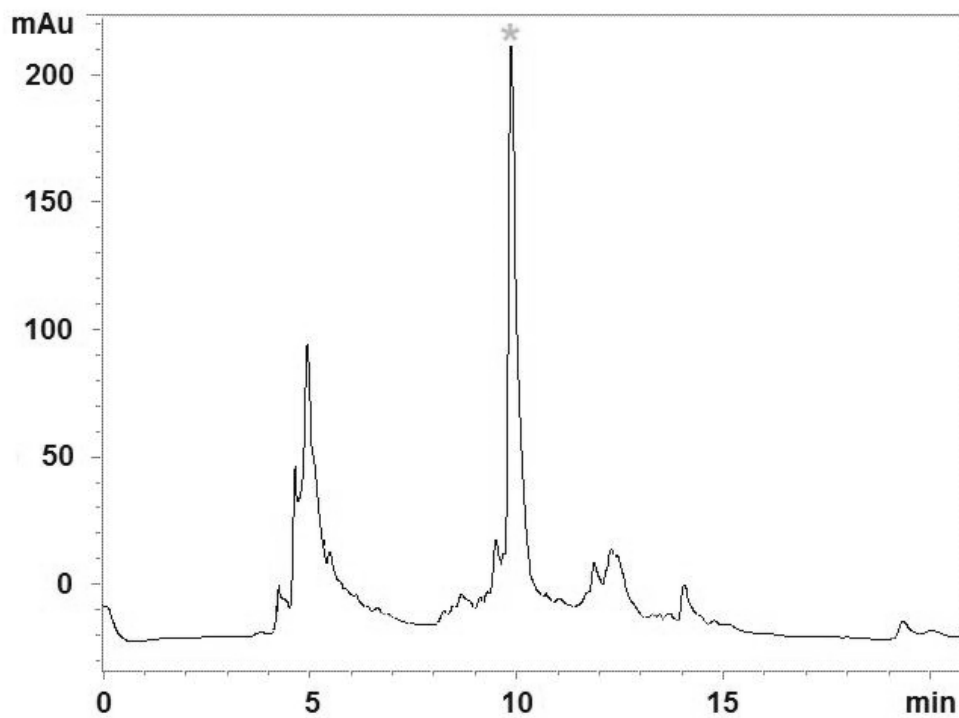


Figure S 7. HPLC profile relative to the crude mixture obtained after the solid phase synthesis of nucleopeptide 1 described in Fig. 7.