

Supplementary Materials

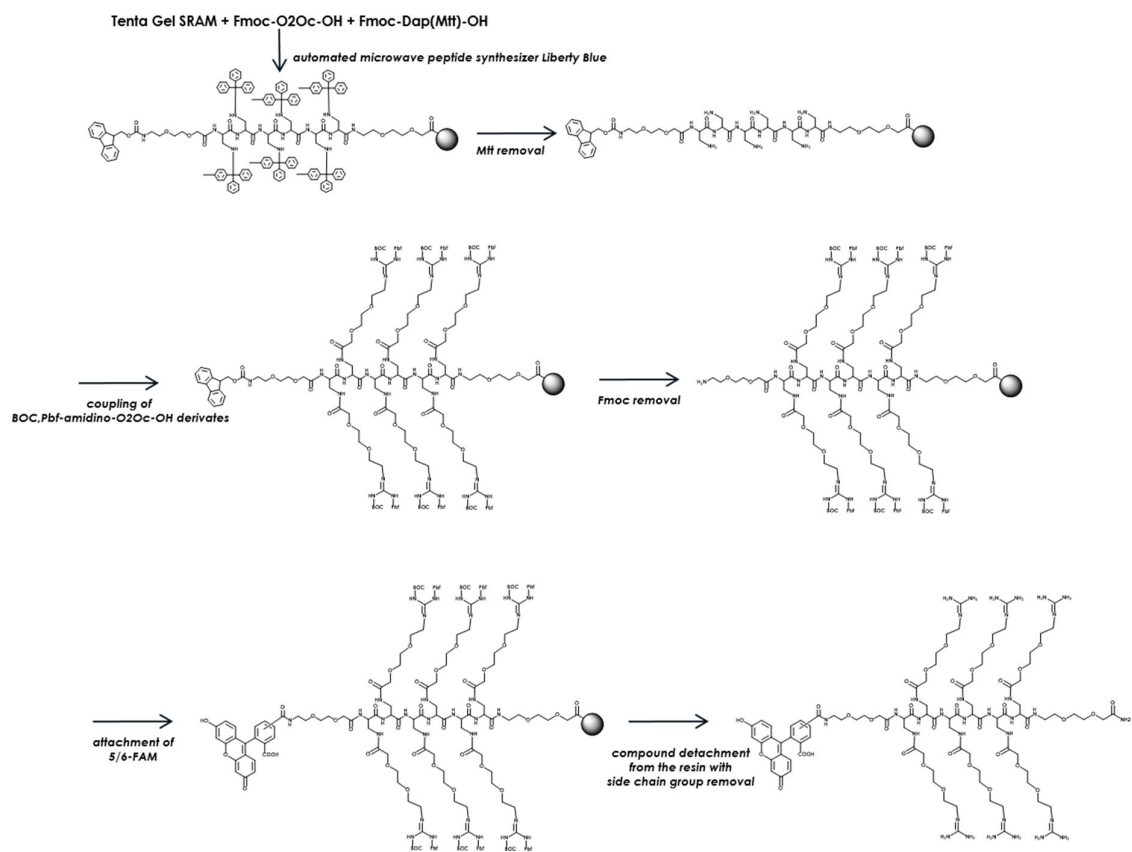


Figure 1S. Scheme of synthesis of compound 5a

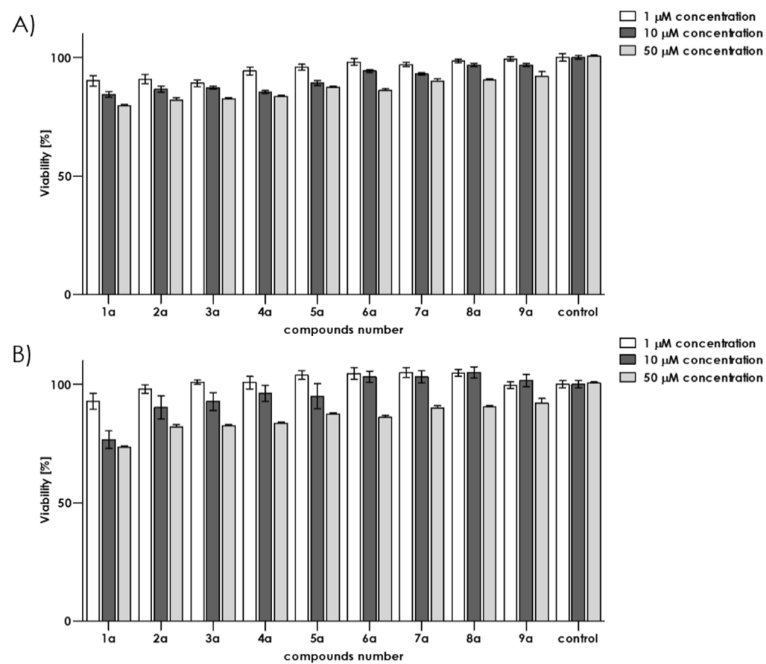


Figure 2S. Cytotoxicity of compounds 1a–9a as assessed by the MTT assay. Two different cell lines were used: A) HB-2 and B) MDA-MB-231.

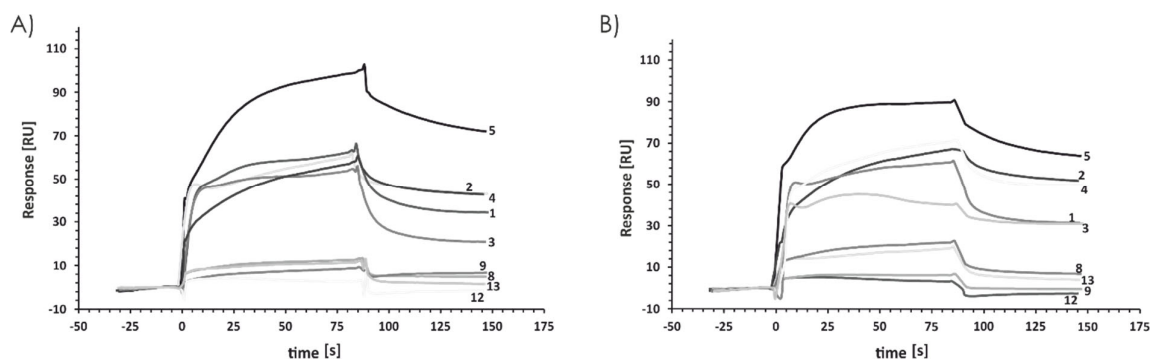
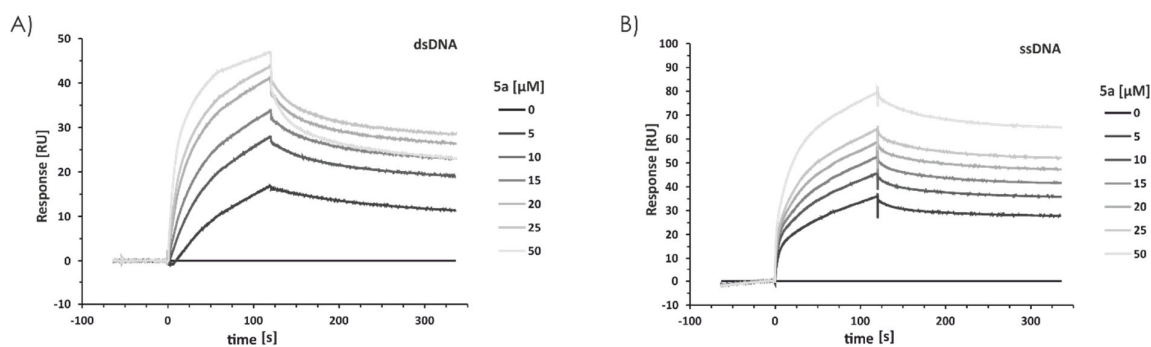


Figure 3S. Surface plasmon resonance SPR analysis of double-stranded DNA (dsDNA) binding by various peptidomimetics. The SPR analysis of dsDNA binding was performed using: A) 50 μM and B) 100 μM of the indicated compounds, flowed over the SA sensor chip surface with immobilized 76 bp biotinylated DNA fragment containing the sequence of beta-actin (*Homo sapiens*). Injections were performed in HBS-EP buffer. HBS-EP was also used as the running buffer.



C)

	k_a	SD	k_d	SD	KD	SD
dsDNA	4.58e02	1.77e02	8.01e-04	2.38e-04	1.81e-06	2.63e-07
ssDNA	6.23e02	2.81e02	1.69e-03	1.42e-03	2.78e-06	2.14e-06

Figure 4S. SPR analysis of DNA binding by compound 5a. The SPR analysis of double-stranded DNA (dsDNA; A) and single-stranded DNA (ssDNA; B) binding by compound 5a was performed using SA sensor chip surface with immobilized 76 bp or 76 nt biotinylated DNA fragment containing the sequence of beta-actin (*Homo sapiens*). An increasing concentration of compound 5a was used, as indicated above. Injections were performed in HBS-EP buffer. HBS-EP was also used as the running buffer. (C) Kinetic constants calculated from at least three experiments using Biacore T200 Evaluation Software

Table 1S. Minimal charge to ratio (N/P) of each compound for efficient complexation with DNA. *minimal N/P ratio resulting in effective complex formation based on EMSA. **ND - no determined

No	Sequence	Minimal N/P ratio*
1	O ₂ Oc(Arg) ₆ -O ₂ Oc-NH ₂	1.5:1
2	O ₂ Oc(D-arg) ₆ -O ₂ Oc-NH ₂	1.5:1
3	O ₂ Oc-(Har) ₆ -O ₂ Oc-NH ₂	1.5:1
4	O ₂ Oc-[Dap(GO1)] ₆ -O ₂ Oc-NH ₂	0.2:1
5	O ₂ Oc-Dap(GO2) ₆ -O ₂ Oc-NH ₂	0.2:1
6	O ₂ Oc-[Dap(O2(GO1))] ₆ -O ₂ Oc-NH ₂	1.5:1
7	O ₂ Oc-[Dap(O2(GO2))] ₆ -O ₂ Oc-NH ₂	1.5:1
8	O ₂ Oc-[Dap(O2)] ₆ -O ₂ Oc-NH ₂	1.5:1
9	O ₂ Oc-[Dap(HO2)] ₆ -O ₂ Oc-NH ₂	No binding
12	O ₂ Oc-[Dap(GO2)] ₂ -O ₂ Oc-NH ₂	ND**
13	O ₂ Oc-[Dap(GO2)] ₄ -O ₂ Oc-NH ₂	1.5:1
14	O ₂ Oc-[Dap(GO2)] ₈ -O ₂ Oc-NH ₂	0.2:1

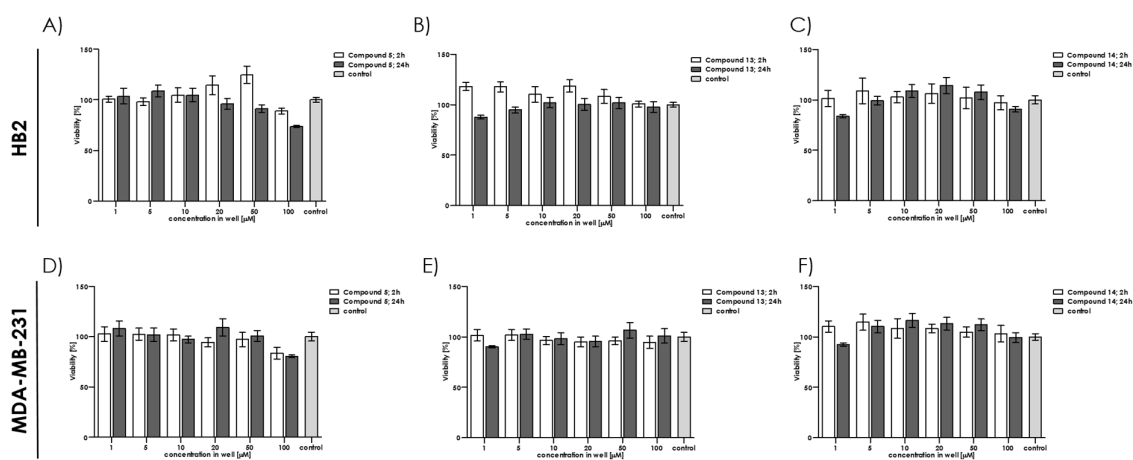


Figure 5S. CCK8 cytotoxicity assay performed for three compounds (5, 13, and 14). Two different cell lines were used: A) HB-2 and B) MDA-MB-231