

Article

Generation and characterization of a DNA-GCN4 oligonucleotide-peptide conjugate: the impact DNA/protein interactions on the sensitization of DNA

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Supplementary materials

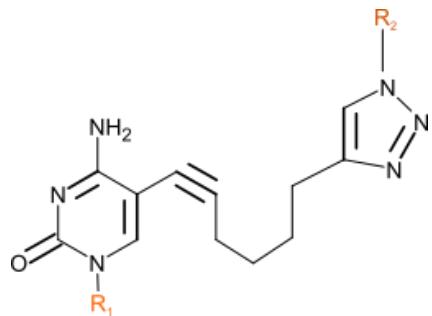


Figure S1. The detailed structure of the linker between oligonucleotide and peptide, R₁ – oligonucleotide residue, R₂ – peptide residue

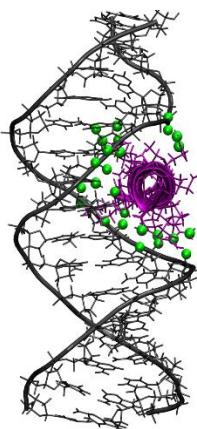


Figure S2. Hydrogen bonding pattern of electrostatic interaction (green) along DNA (gray) and peptide (purple) sequences.

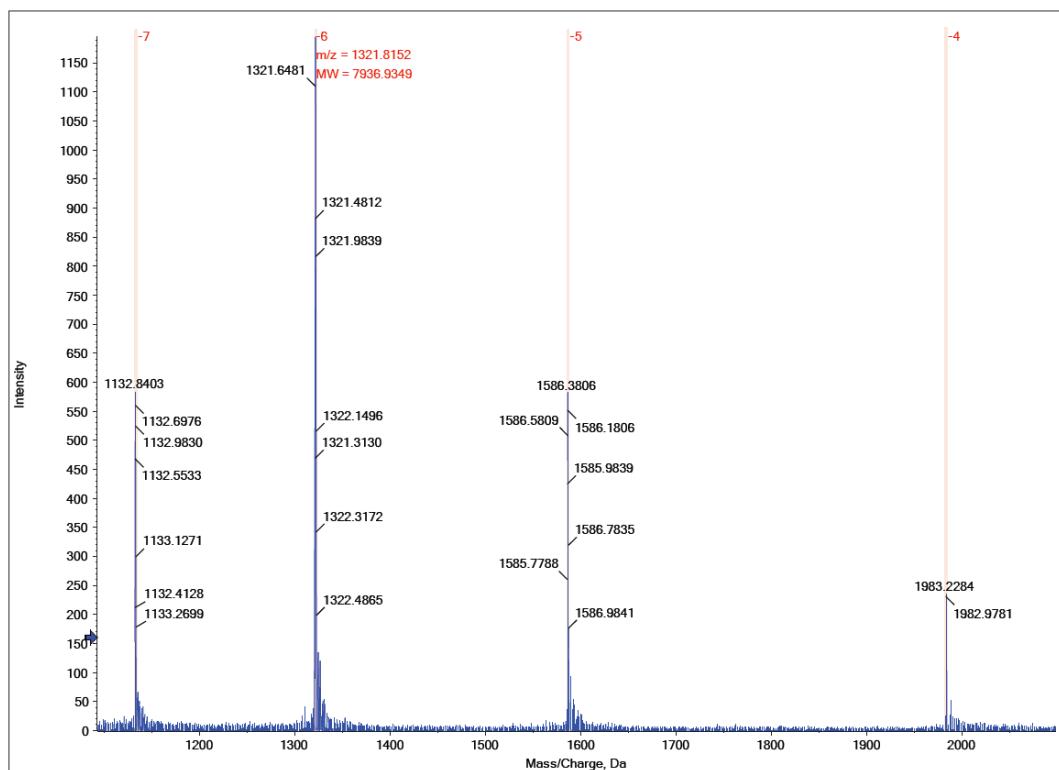


Figure 3. High-resolution mass spectrum of ssDNA*-PEP after purification.

Table S1. Table represent the identified by use of LC-MS fragments after DNase digestion and their representative peak areas. The peak areas where taken and plotted against the charge of the fragment of the oligonucleotide.

	Ret. Time [min]	Strand	Mass [Da]	Fragment	dsDNA	dsDNA-PEP
1	22.667	A	5170.94	whole		
2	23.309	B	5210.94	whole	27100	29380
3	21.687	A	4527.6961	b15		
4	21.412	B	4591.7221	b15	164000	191700
5	21.2	A	3700.3406	w12		
6	21.091	A	4223.5841	b14		
7	20.605	B	4287.6425	b14	6271000	6184000
8	20.169	A	3396.2649	w11		
9	19.988	B	3766.3658	w12	27410	547800
10	19.285	B	3669.4163	b12	6238	12370
11	19.061	A	3606.3835	b12		
12	18.547	A	2754.0029	w11-b15		
13	18.115	A	2794.0151	w9		
14	17.933	B	3356.2966	b11	7919000	11980000
15	17.933	A	3277.2299	b11		
16	16.775	B	2844.0541	w12-b14	6812000	941500
17	16.619	A	2988.1572	b10		

18	16.276	A	2488.9088	w8		
19	15.58	B	2529.9208	w9-b16	347900	74510
20	15.25	B	2505.9057	x8	38100	342100
21	14.909	B	2723.0459	b9	3780000	1778000
22	14.317	A	2136.778	w14-b10/w13-b11		
23	13.247	A/B	2200.808	w7/w14-b10/w9-b15	10420000	5134000
24	11.11	A	2394.9209	b8		
25	11.11	B	2394.9209	w12-b12/w11-b13/w10-b14	25210000	50230
26	10.322	A	1910.6979	w6		
27	10.322	B	1871.6843	w6	620000	5566
28	9.511	B	2079.8061	b7	26490000	3170000
29	8.865	A	1580.5661	w5		
30	8.154	B	1582.5848	w6-b16/w7-b15/w8-b14/w12-b10/w14-b8/	16840000	3184000
31	7.95	B	1750.6962	b6	9316000	1451000
32	7.95	B	1558.5694	w5	1185000	1469000
33	7.613	A	1791.7047	b6		
34	6.861	A	1229.4513	w14-b7/w9-b12/w8-b13		
35	6.498	B	1462.5953	b5	18050000	3575000
36	5.225	A	1488.6024	b5		
37	4.943	A/B	924.3442	w-ACT-b	628700	16150
38	4.547	A/B	949.3552	w-ACG-b		
39	4.162	A/B	964.3576	w-AGT-b		
40	3.88	A/B	940.3425	w-CGT-b	1097000	128100
41	2.957	A/B	964.3624	w-AGT-b		
42	2.787	A/B	940.3425	w-CGT-b		
43	1.715	A/B	682.1904	w-AC-c		
44	1.7-0	A/B	All other fragments			

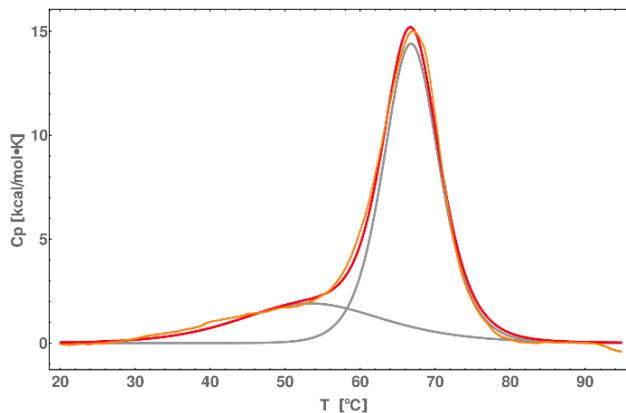


Figure S4. Deconvolution of thermogram (orange line) of dsDNA in 100 mM PBS solution. Gray curves represent the deconvoluted states. The sum of the states is plotted in red.

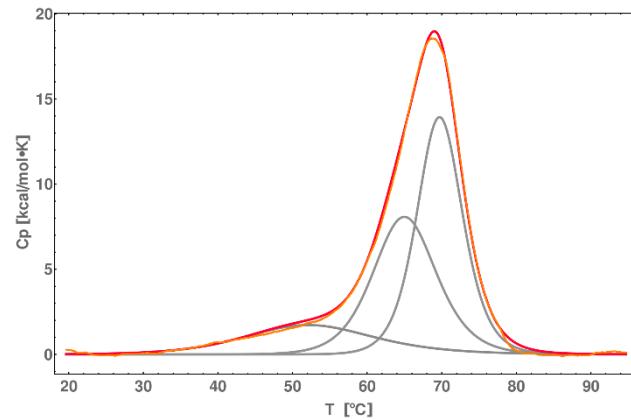


Figure S5. Deconvolution of thermogram (orange line) of dsDNA*-PEP in 100 mM PBS solution. Gray curves represent deconvoluted states. The sum of the states is plotted in red.