Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Electronic Supplementary Information (ESI)

Probing Specific RNA Bulge Conformations by Modified Fluorescent Nucleosides

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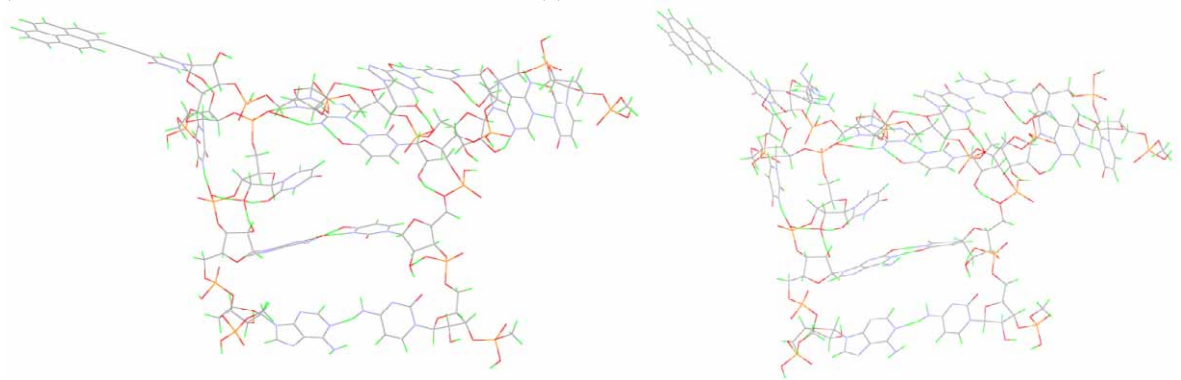
Fig S1.The initial structure of (a) U23^{PY}-RNA, (b) U^{PY}23-RNA-ARG, (c) U25^{PY}-RNA, and (d) U^{PY}25-RNA-ARG

(a) (b)



(c) (d)

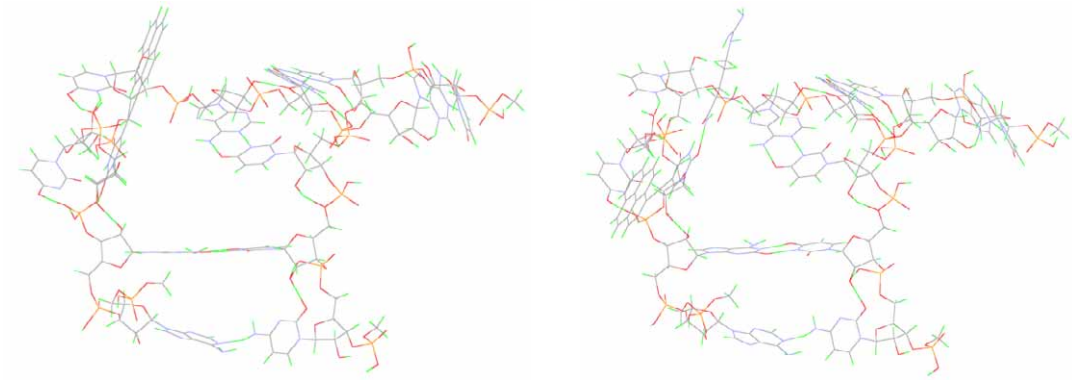
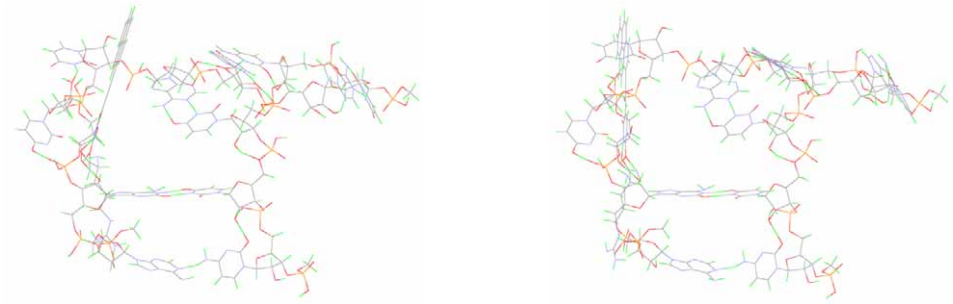
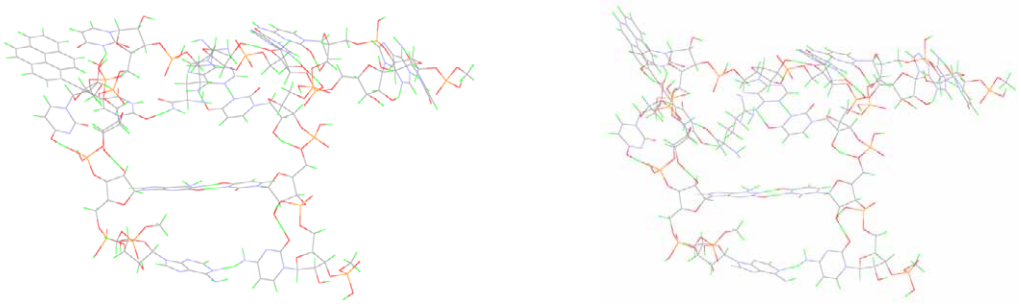


Fig S2. The optimized structures of U^{PY}25-RNA-ARG complexes for various initial structures (a-d). The structures in the left/right column are the initial/optimized structures. In particular for the geometry optimization of U^{PY}25-RNA-ARG, we used four different initial structures.. The four initial structures were generated by rotating the pyrene moiety in different directions. Among them, U^{PY}25-RNA-ARG (d) is the lowest energy conformer, and is denoted as U^{PY}25-RNA-ARG in this manuscript. For U^{PY}25-RNA-ARG (d), the initial structure shows the H-bonding between U^{PY}25 and ARG. After the optimization, the U^{PY}25 and ARG were rotated due to the enhanced interactions between the terminal amino group of ARG and RNA groove as shown.

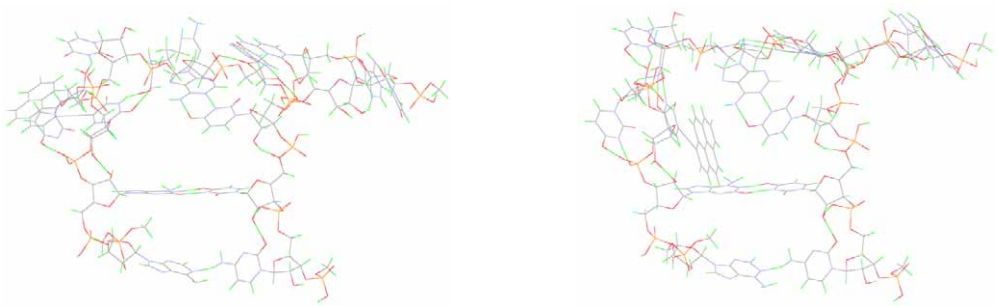
(a)



(b)



(c)



(d)

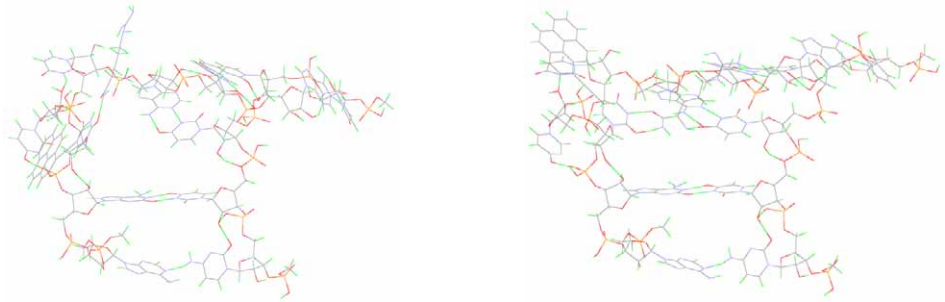
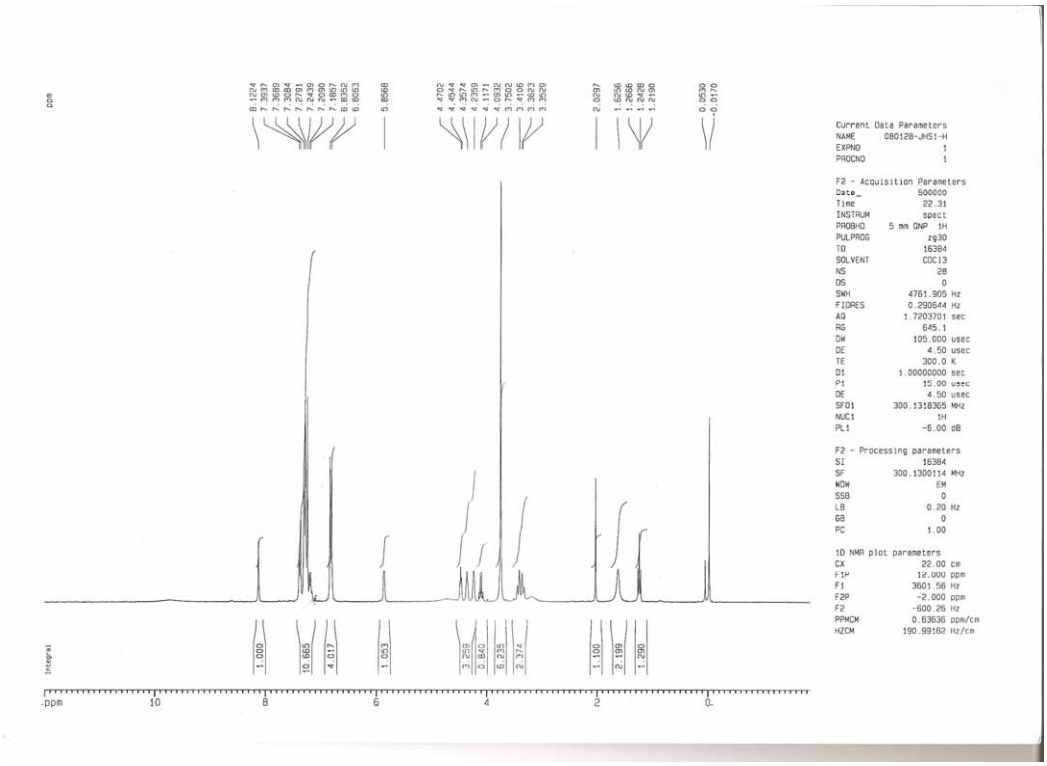


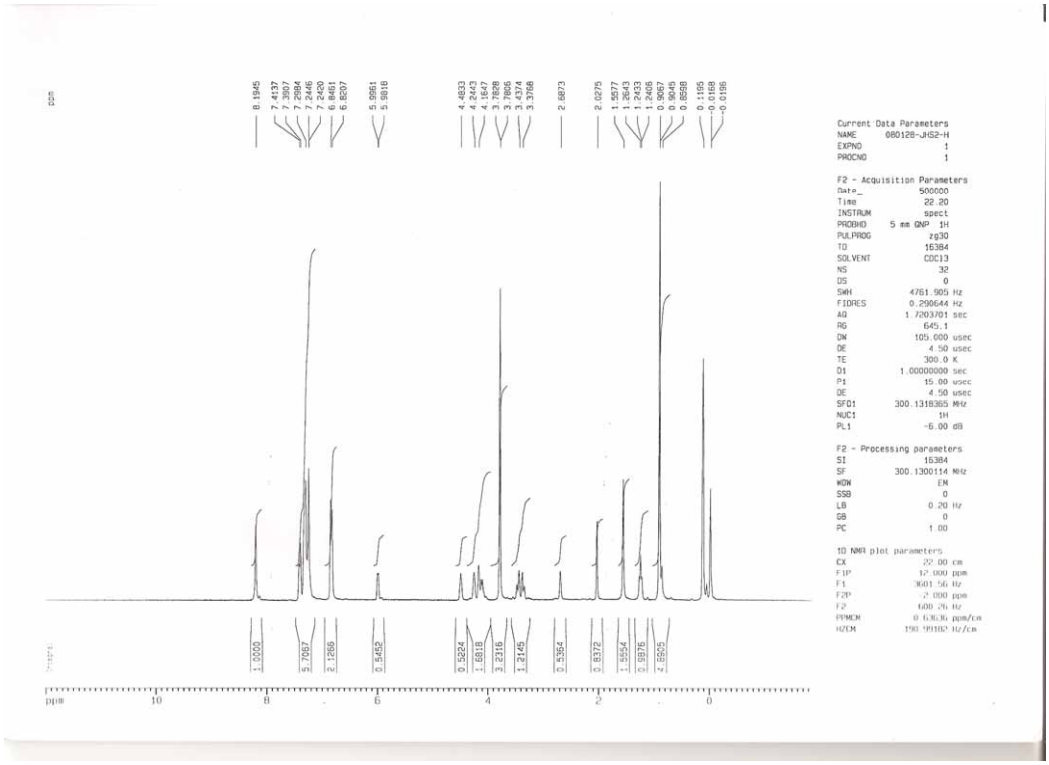
Table S1. Relative energies for the optimized U^{PY}25-RNA-ARG complexes for various initial structures (a-d).

Conformations	Relative energy (kcal/mol)
U^{PY}25-RNA-ARG (a)	18.51
U^{PY}25-RNA-ARG (b)	20.86
U^{PY}25-RNA-ARG (c)	17.84
U^{PY}25-RNA-ARG (d)	0

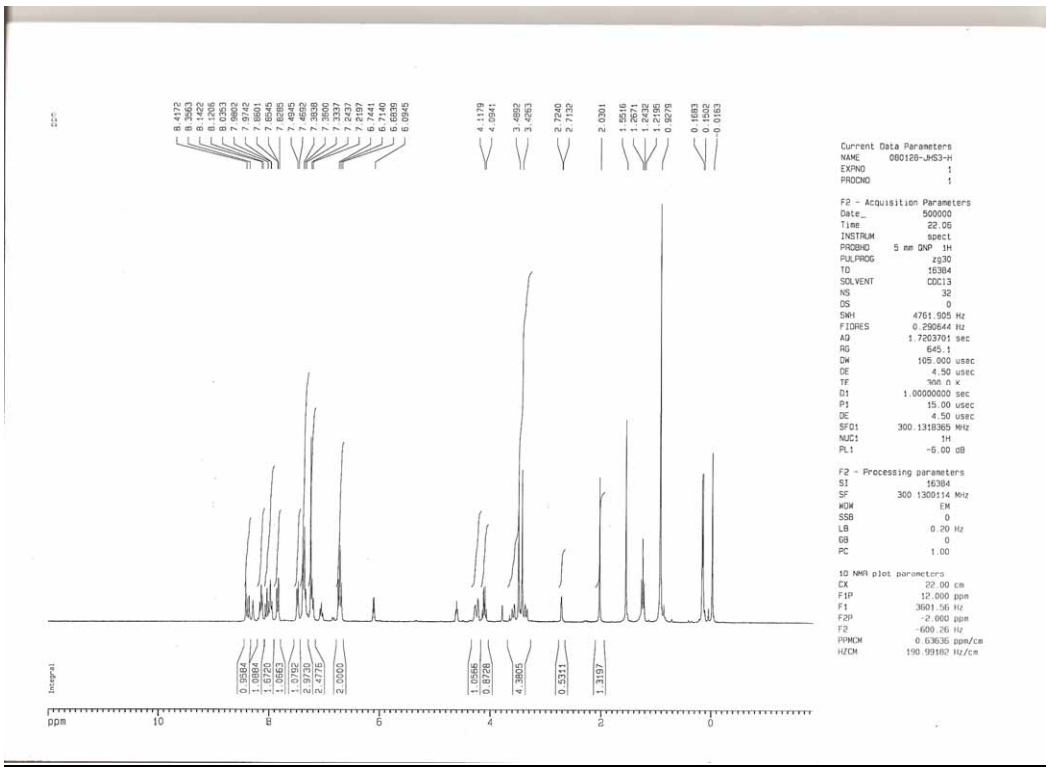
5'-O-[bis(4-methoxyphenyl)phenylmethyl]-5-iodouridine (2)



5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-O-(tert-butyl-dimethylsilyl)-(-)-5-iodouridine (3)



5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-O-(tert-butyl-dimethylsilyl-5-(2-ethynylpyrenyl)uridine (4)



5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-O-(tert-butyl-dimethylsilyl-5-(2-ethynylpyrenyl)uridine 3'-O-[2-cyanoethyl(N,N-diisopropylamino)phosphoramidite (5)

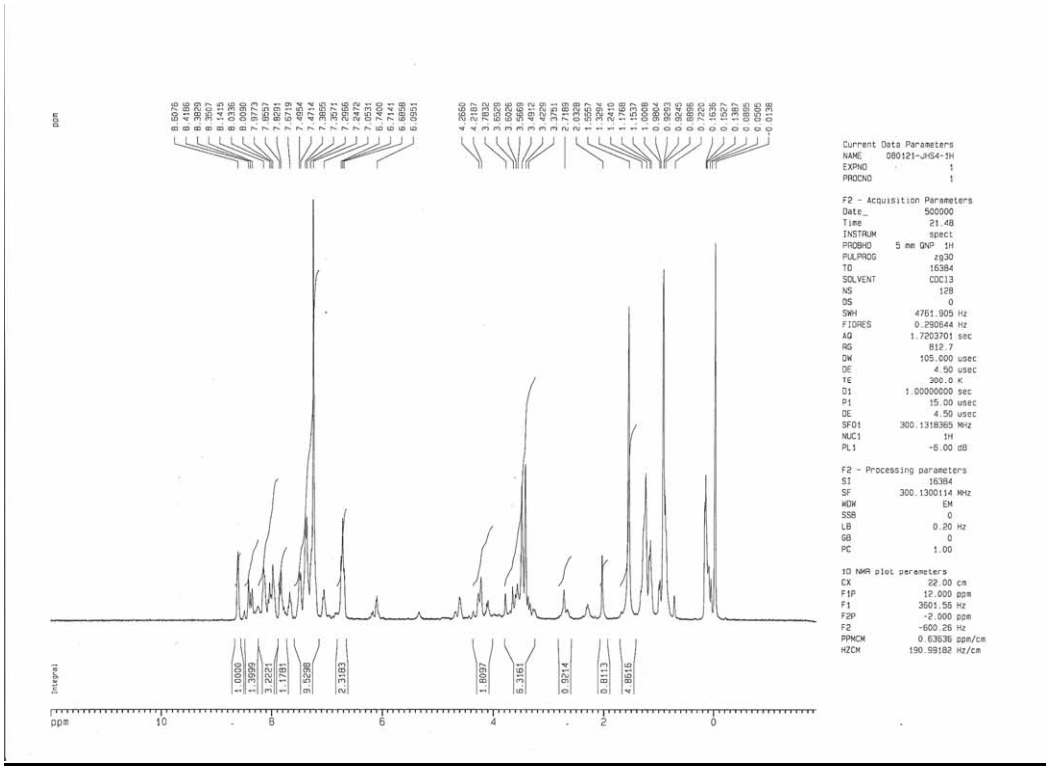
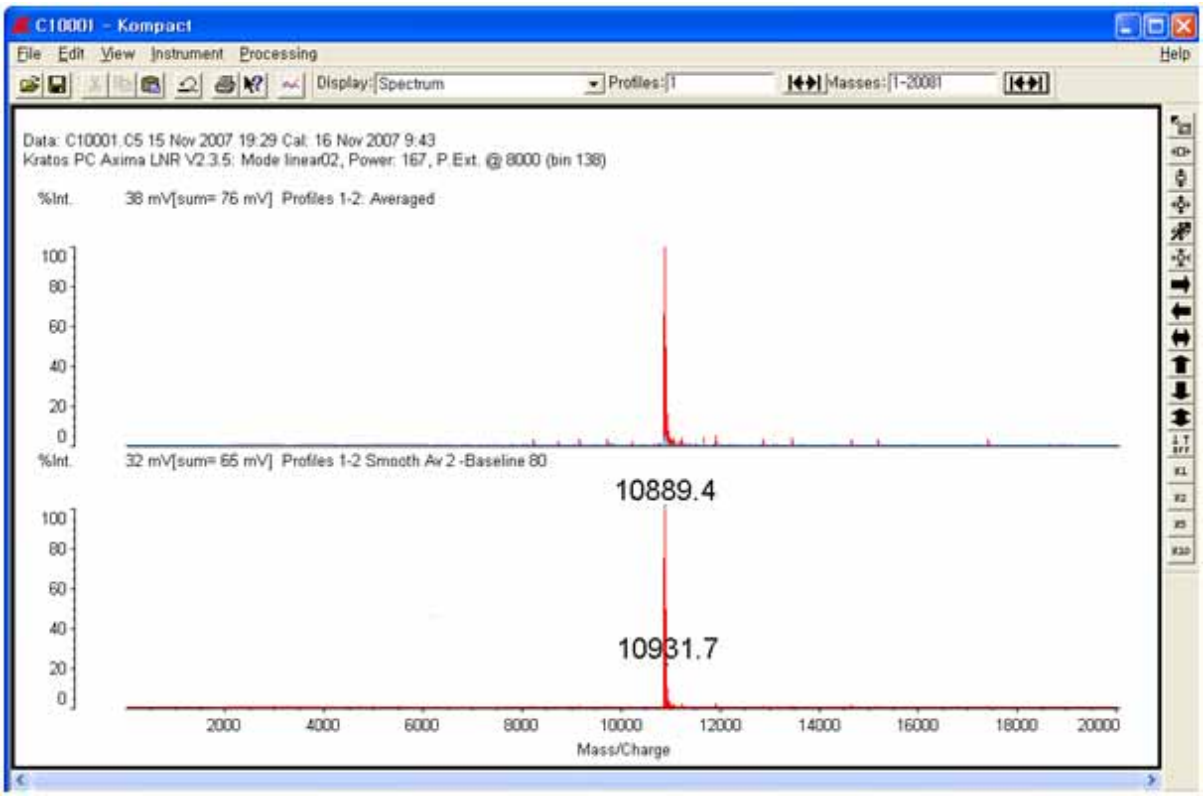


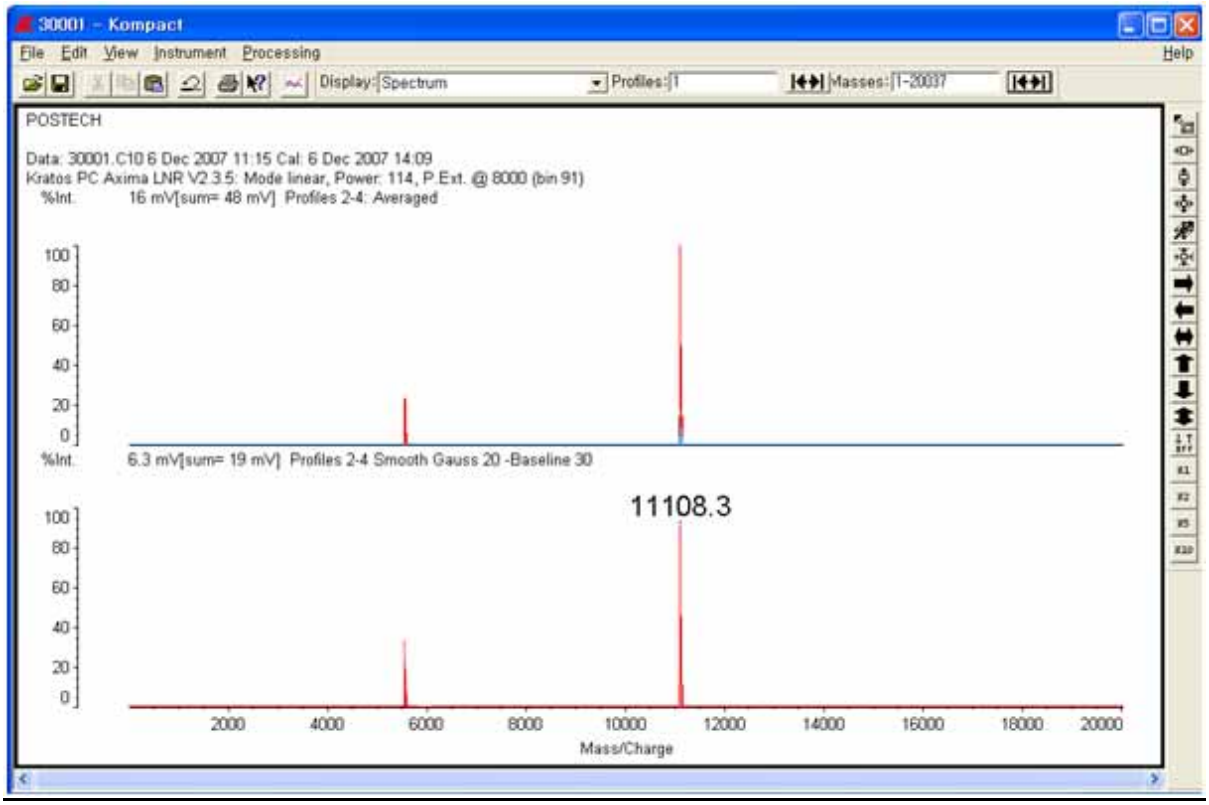
Table S1. MALDI-TOF Mass Spectral Data for the ODNs [M+]

Sequences	Calculated m/z	Found m/z
6 (Control)	10891	10889
7 (U23)	11113	11108
8 (U25)	11113	11117
9 (U31)	11113	11115

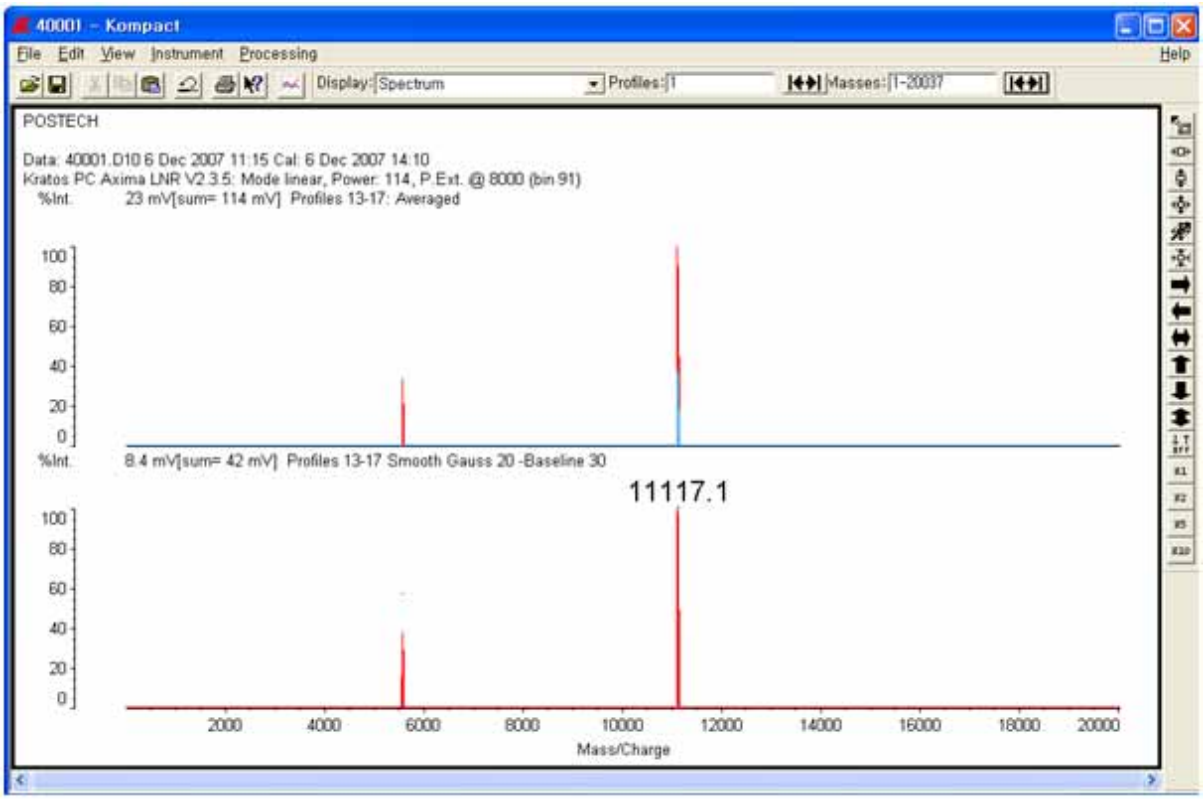
MALDI-TOF data for 6 (Control) RNA



MALDI-TOF data for 7 (U23)



MALDI-TOF data for 7 (U25)



MALDI-TOF data for 7 (U31)