Supplementary material

Conformational Studies of 10-23 DNAzyme in Solution through pyrenyl-labeled 2'-deoxyadenosine Derivatives

Zhiwen Li, Junfei Zhu and Junlin He

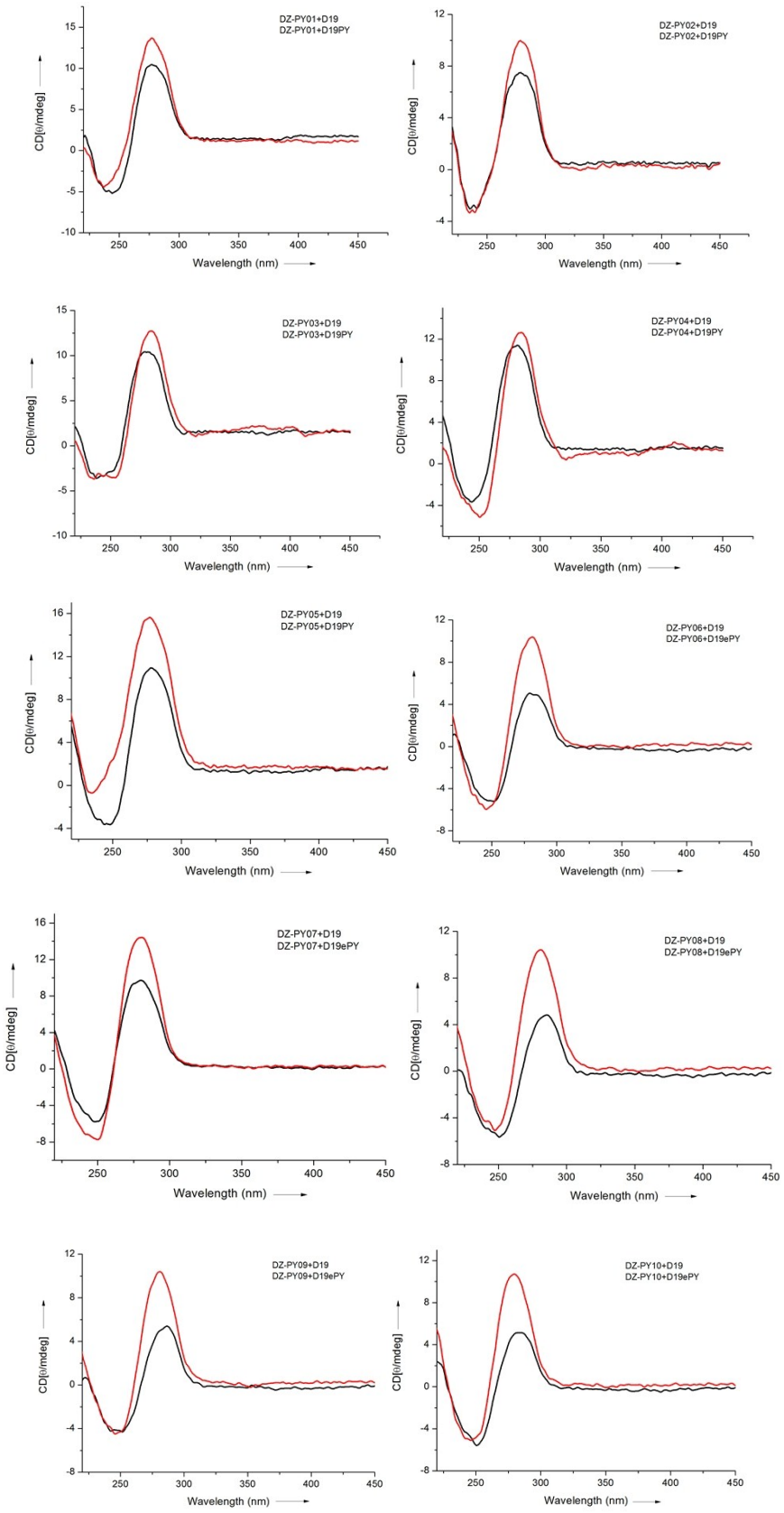


Fig. S1 Comparison of the CD spectra of each DNAzyme with its different substrates **D19** and **D19PY** or **D19ePY**. Each complex (1.1 μM) in the buffer (50 mM Tris-HCl, pH 7.5, 20 mM Mg^{2+}) was used.

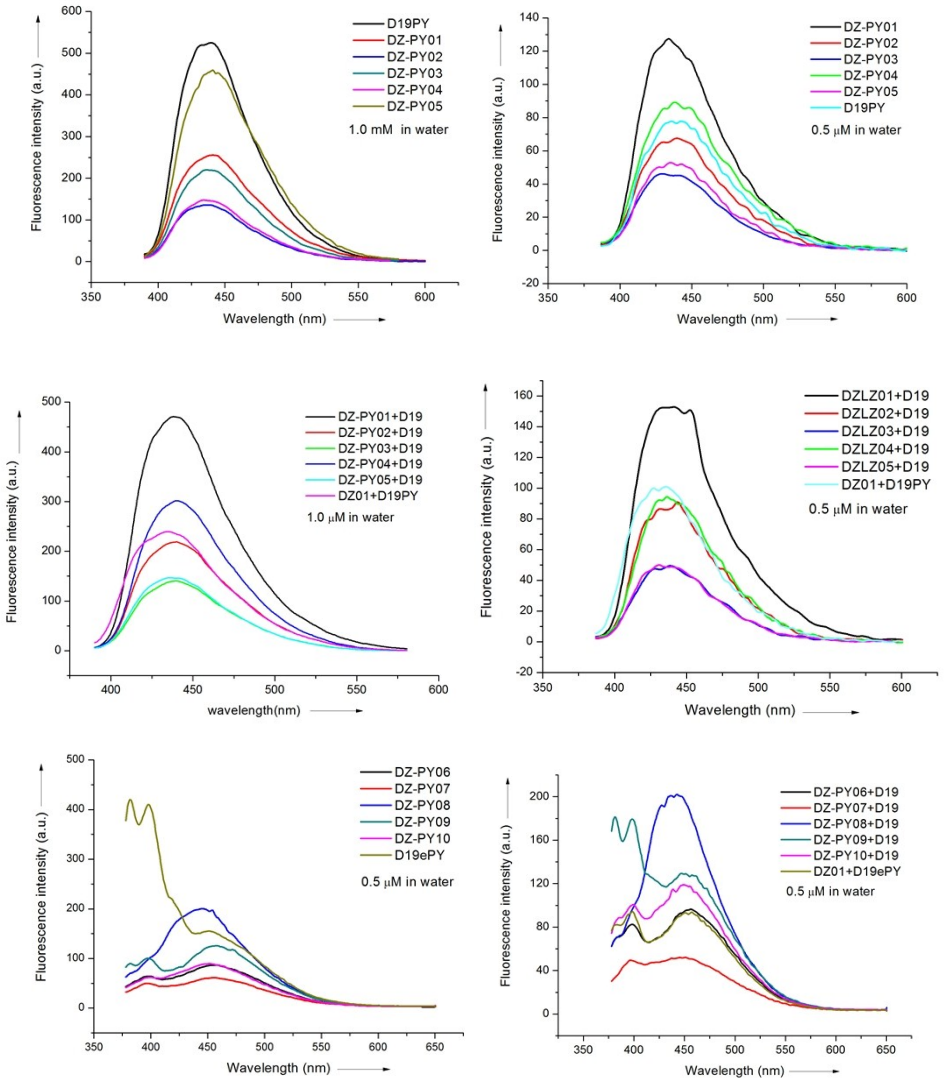


Fig. S2 Comparison of fluorescence spectra of DNAzymes and their complexes at different concentrations. Single oligonucleotides (**DZ-PY01** to **DZ-PY10**, **D19PY**, and **D19ePY**) and the complexes with one pyrenyl group were compared (1.0 μM and 0.5 μM).

Table S1 Fluorescence maxima of the DNAzymes and their complexes

	λ_{max}^{fls} (nm)		λ_{max}^{fls} (nm)
DZ-PY01	439.5	DZ-PY06	455
DZ-PY01+D19	438	DZ-PY06+D19	453.5
DZ-PY01+D19PY	438.5	DZ-PY06+D19ePY	450
DZ-PY02	441	DZ-PY07	458
DZ-PY02+D19	440	DZ-PY07+D19	451.5
DZ-PY02+D19PY	444.5	DZ-PY07+D19ePY	454
DZ-PY03	438	DZ-PY08	446.5
DZ-PY03+D19	440	DZ-PY08+D19	443
DZ-PY03+D19PY	449.5	DZ-PY08+D19ePY	448.5
DZ-PY04	436.5	DZ-PY09	457
DZ-PY04+D19	440	DZ-PY09+D19	453.5
DZ-PY04+D19PY	460-490	DZ-PY09+D19epy	457.5
DZ-PY05	434	DZ-PY10	452.5
DZ-PY05+D19	436	DZ-PY10+D19	447.5
DZ-PY05+D19PY	449	DZ-PY10+D19ePY	451

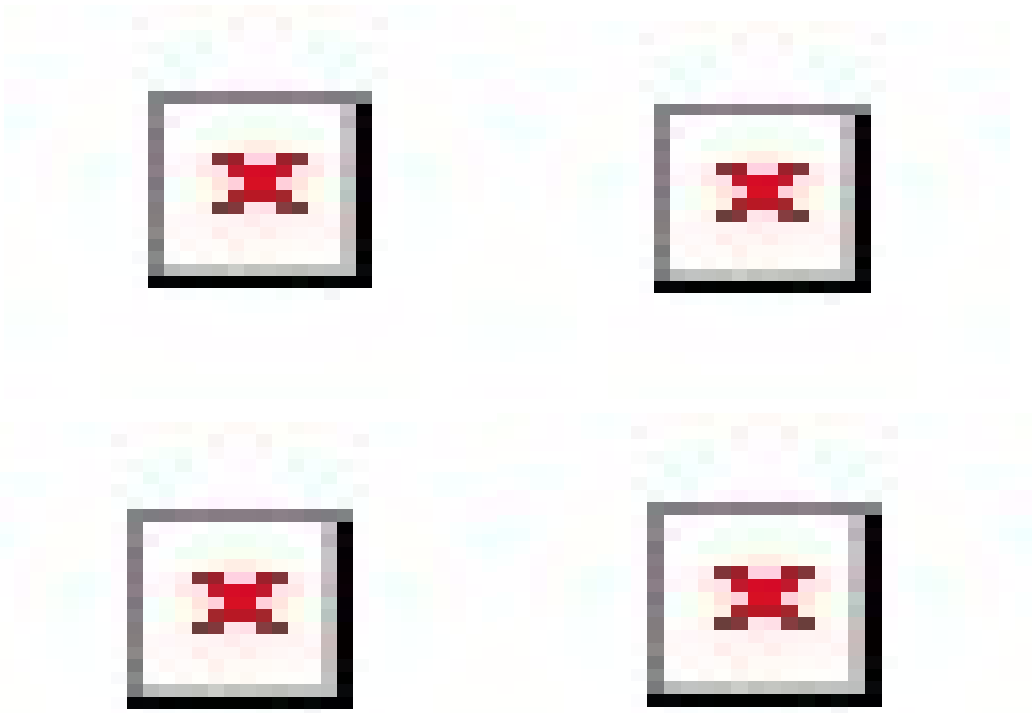


Fig. S3 Comparison of the fluorescence spectra of DNAzymes **DZ-PY06** to **DZ-PY10** in different states. Single oligonucleotides, the complexes with **D19**, and the complexes with **D19ePY** were compared (1.0 μM)

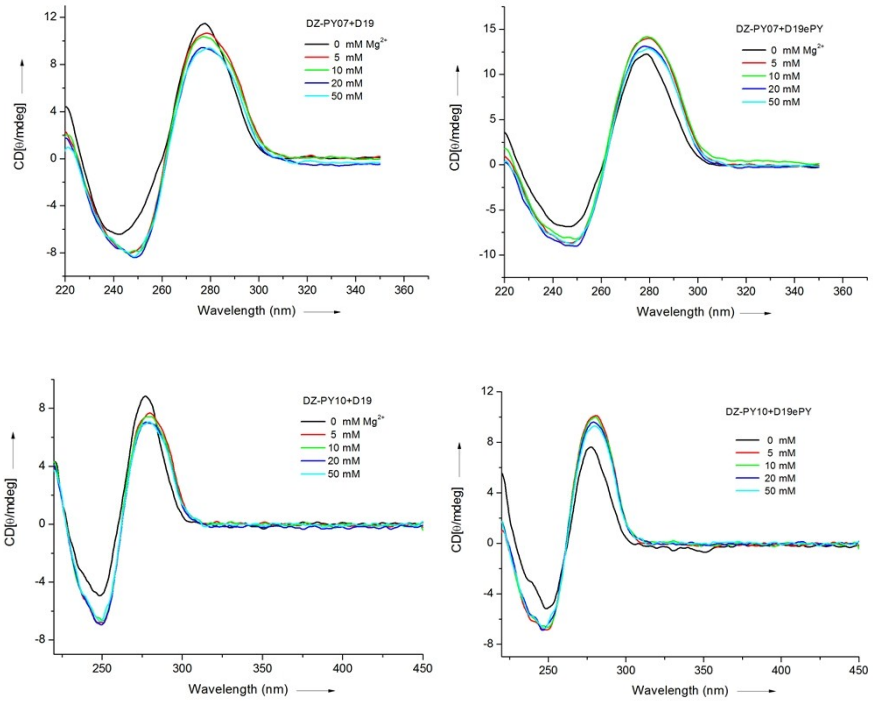
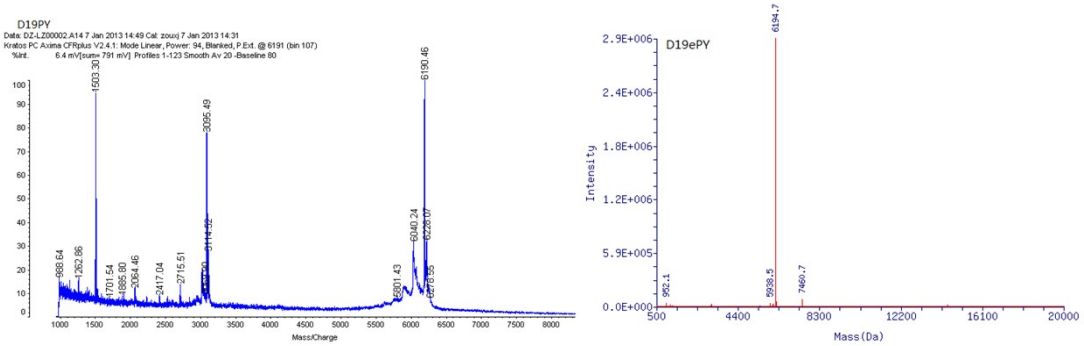
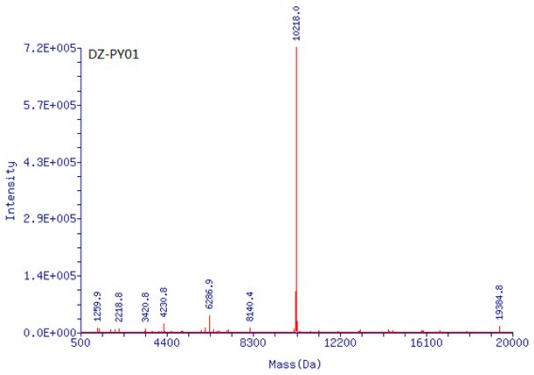
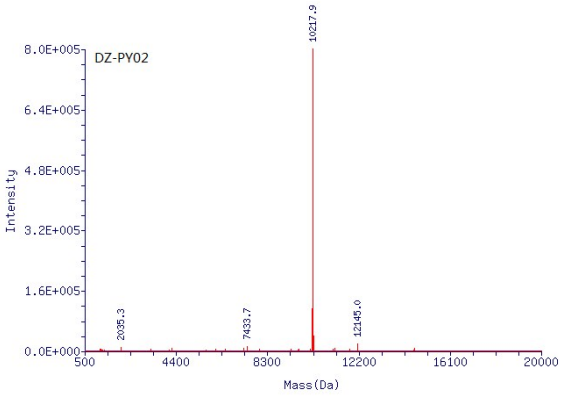
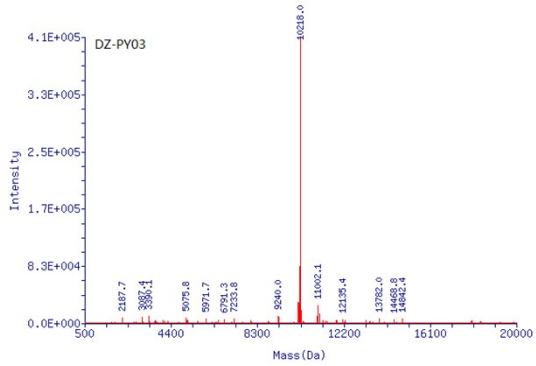


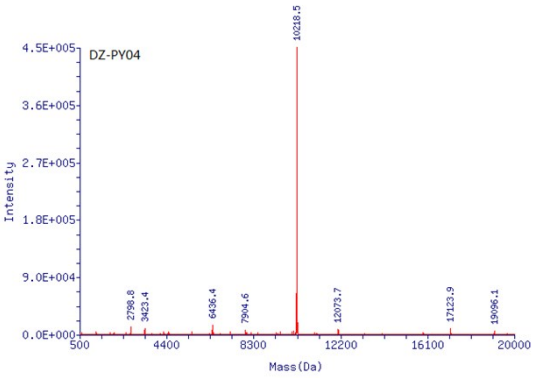
Fig. S4 Comparison of the CD spectra of each DNAzyme-substrate complex in the presence of different concentration of Mg^{2+}. The buffer (50 mM Tris-HCl, pH 7.5) with different concentrations of Mg^{2+} (n = 0, 5, 10, 20, 50 mM) was used for each complex (1.1 μM).

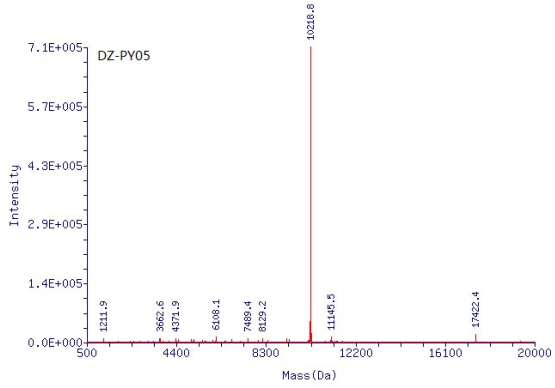


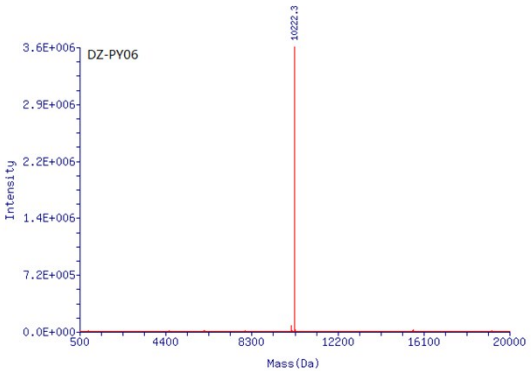

DZ-PY01
Intensity
Mass(Da)
10218.0
1259.9
2218.8
3420.8
4230.8
6286.9
8140.4
19384.8

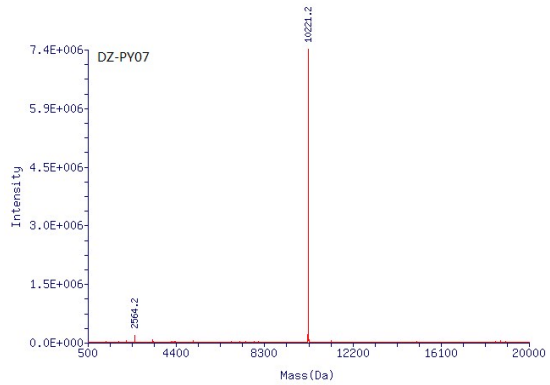

DZ-PY02
Intensity
Mass(Da)
10217.9
2035.3
7433.7
12145.0

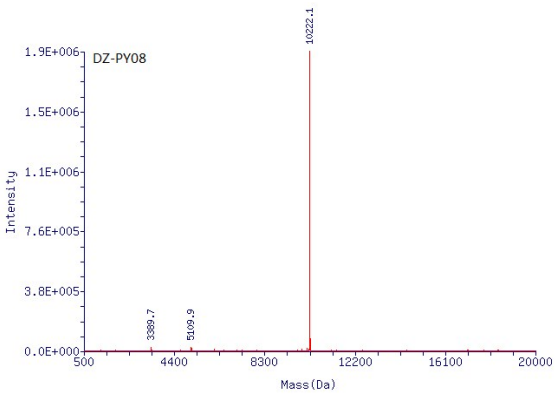

DZ-PY03
Intensity
Mass(Da)
10218.0
2187.7
3980.4
4080.4
5075.8
5971.7
6791.3
7233.8
9240.0
11002.1
12135.4
13782.0
14468.8
14684.4


DZ-PY04
Intensity
Mass(Da)
10218.5
2798.8
3423.4
6436.4
7904.6
12073.7
17123.9
19096.1


DZ-PY05
Intensity
Mass(Da)
10218.8
1211.9
3662.6
4371.9
6108.1
7489.4
8129.2
11145.5
17422.4


DZ-PY06
Intensity
Mass(Da)
10222.3


DZ-PY07
Intensity
Mass(Da)
10221.2
2564.2


DZ-PY08
Intensity
Mass(Da)
10222.1
3389.7
5109.9

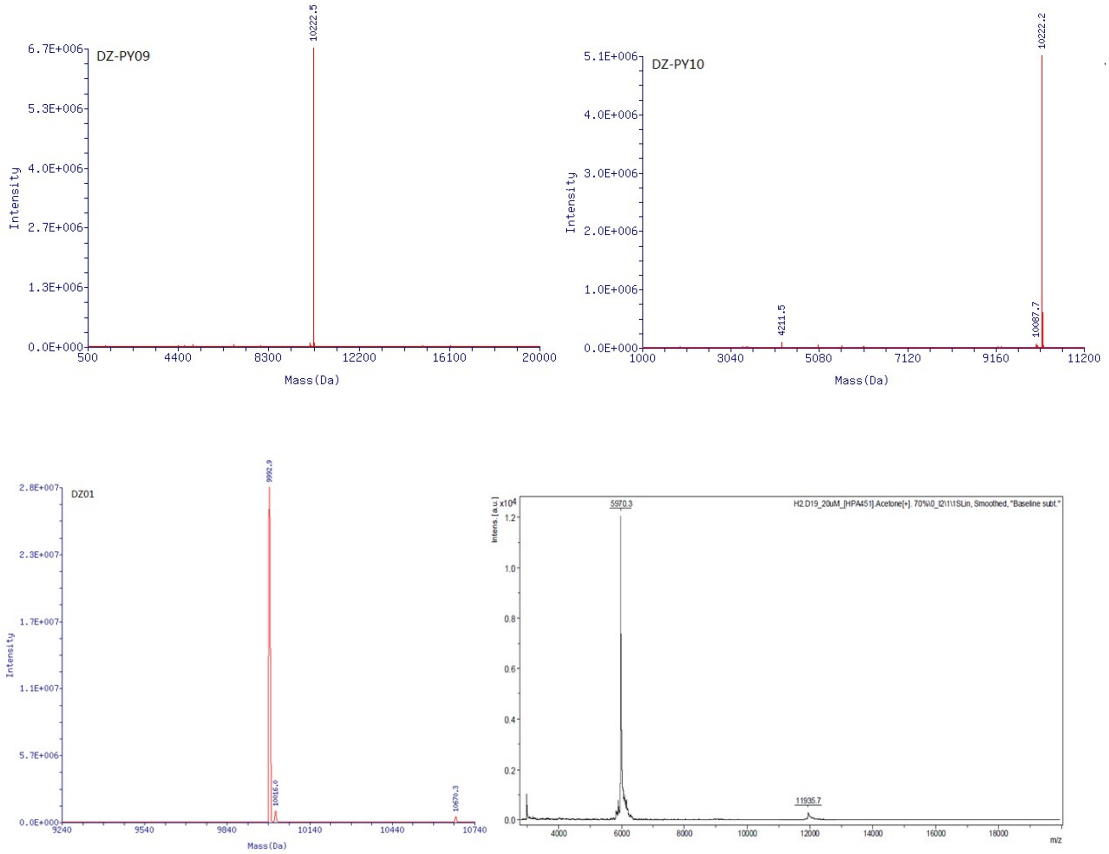
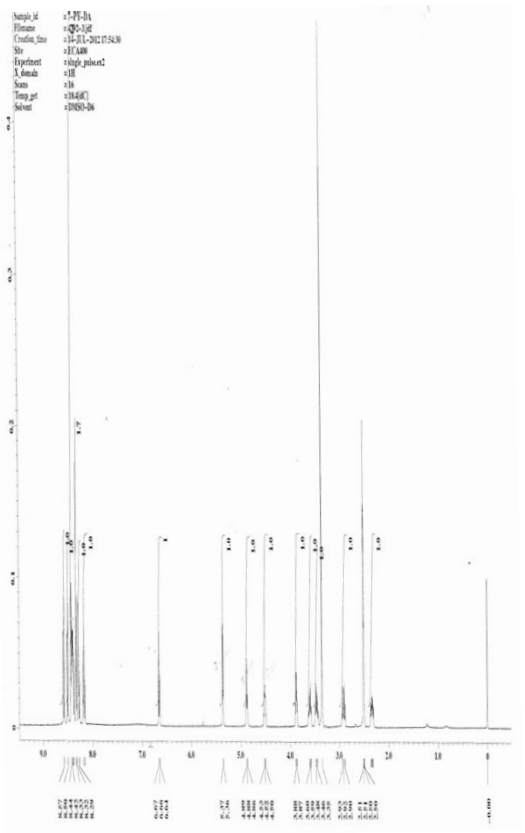
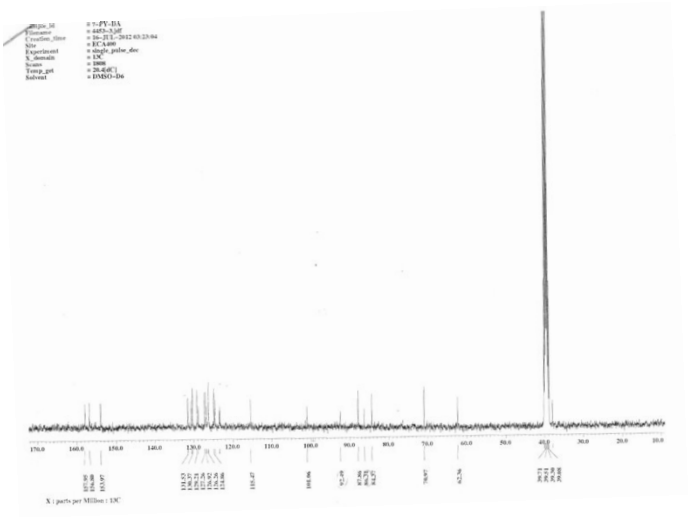


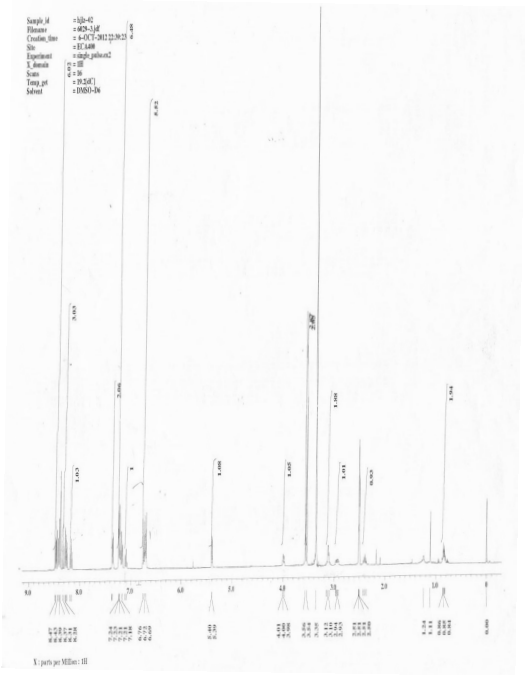
Figure S5 Mass spectra of modified DNAzymes and substrates



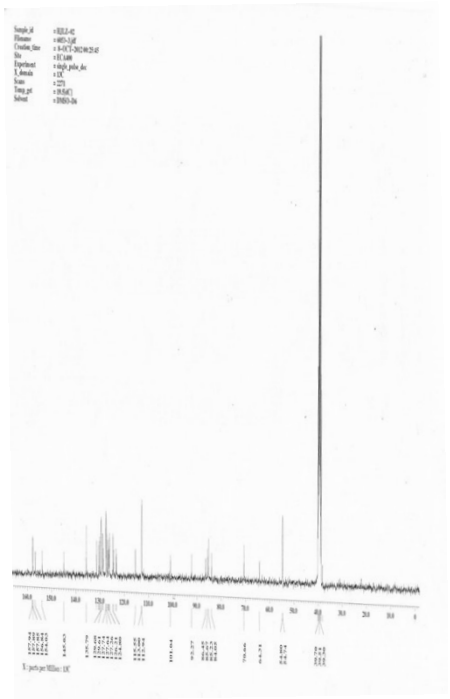
^{1}H NMR of Compound **1**



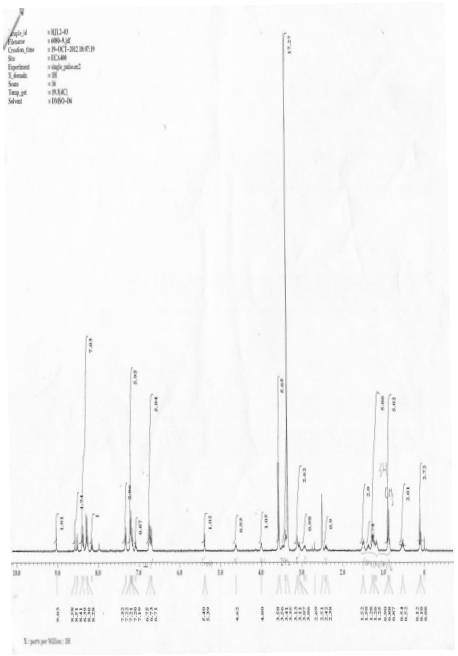
^{13}C NMR of Compound **1**



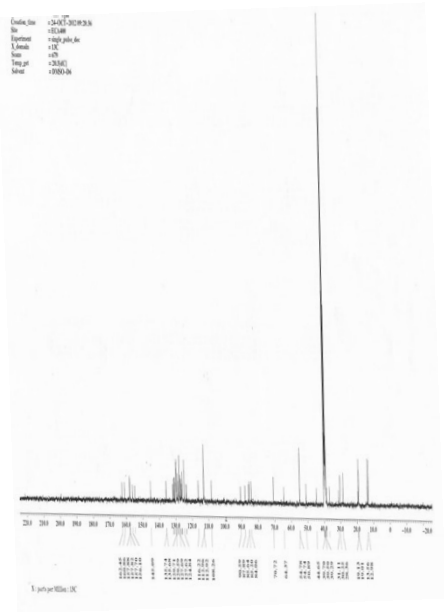
^{1}H NMR of Compound **3**



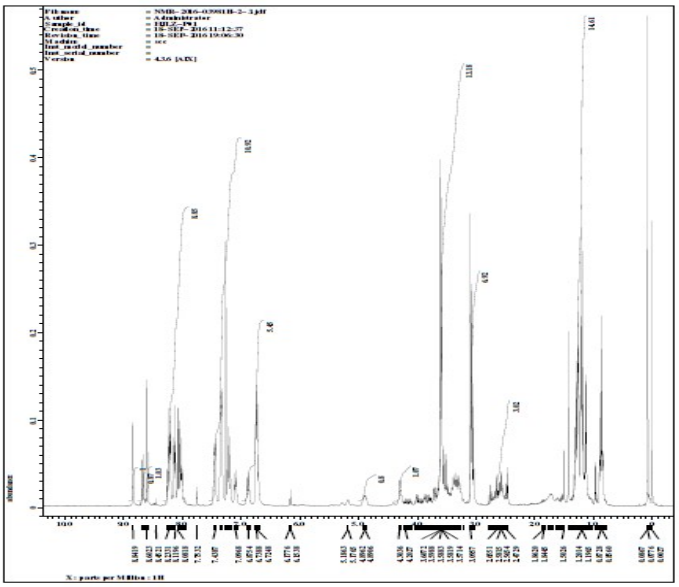
^{13}C NMR of Compound **3**



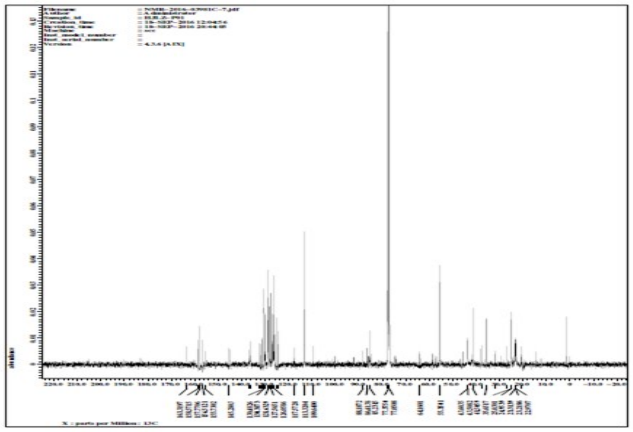
^{1}H NMR of Compound **4**



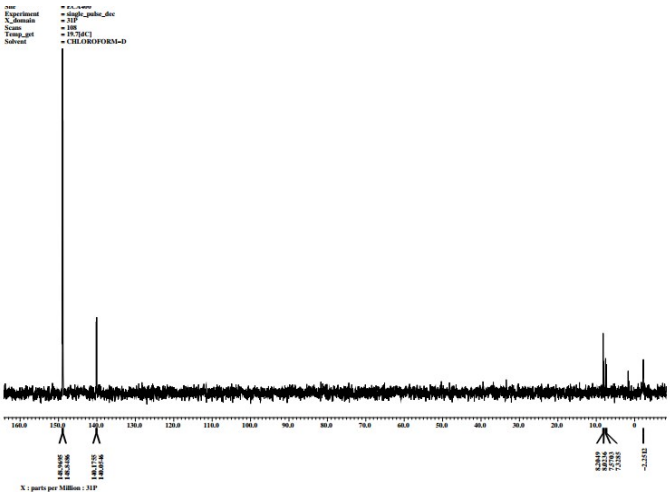
^{13}C NMR of Compound **4**



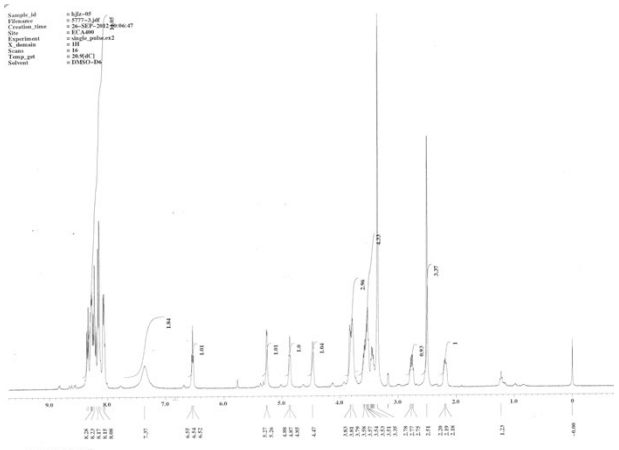
^{1}H NMR of Compound **5**



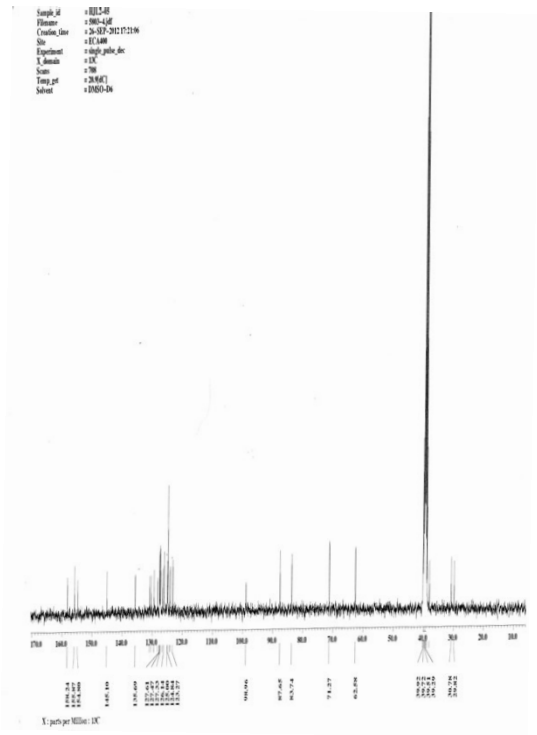
^{13}C NMR of Compound **5**



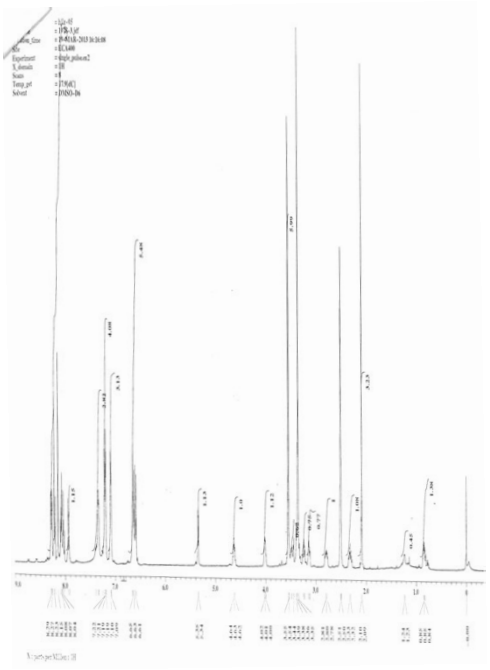
^{31}P NMR of Compound **5**



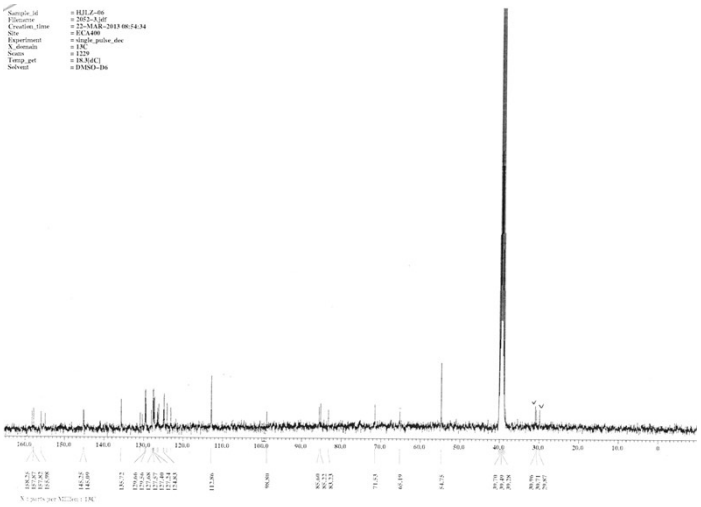
^{1}H NMR of Compound **2**



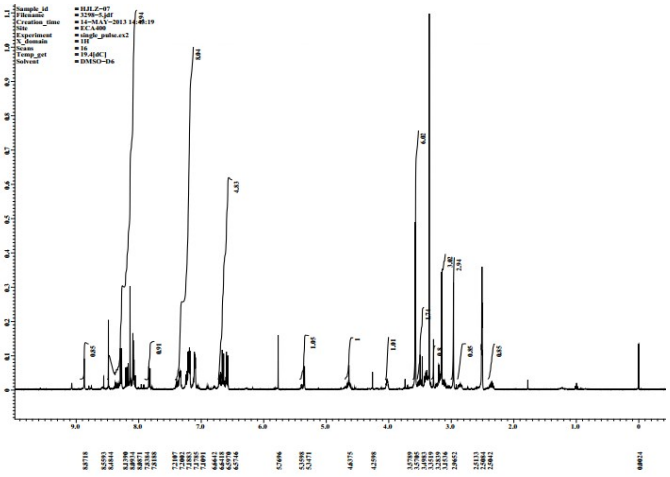
^{13}C NMR of Compound **2**



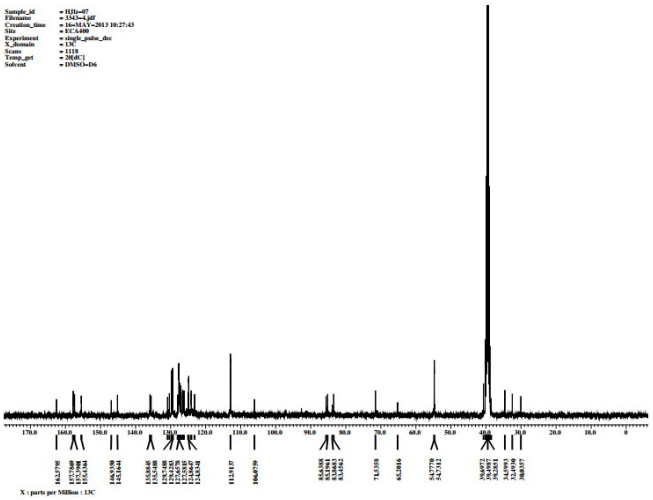
^{1}H NMR of Compound **6**



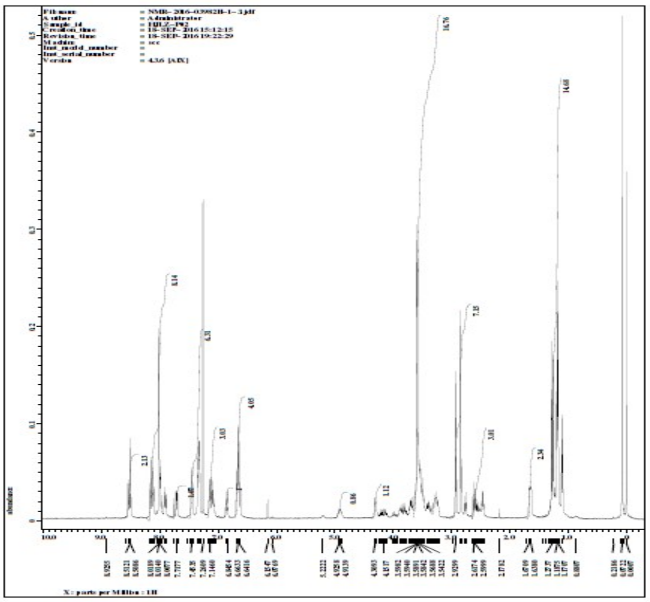
^{13}C NMR of Compound **6**



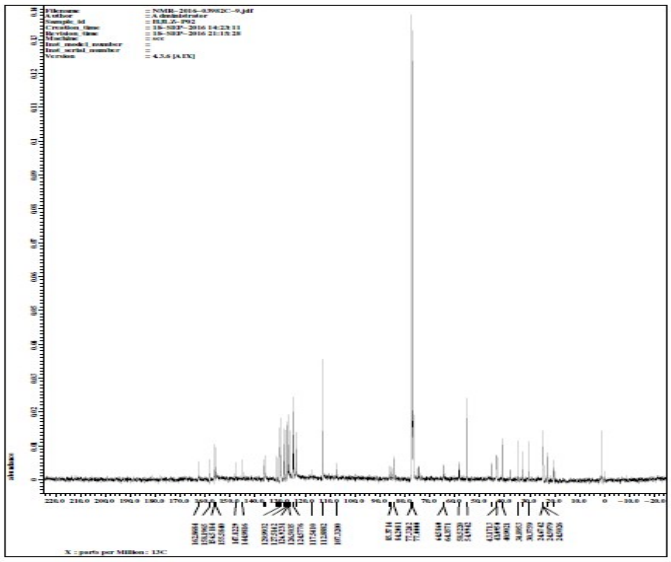
^{1}H NMR of Compound **7**



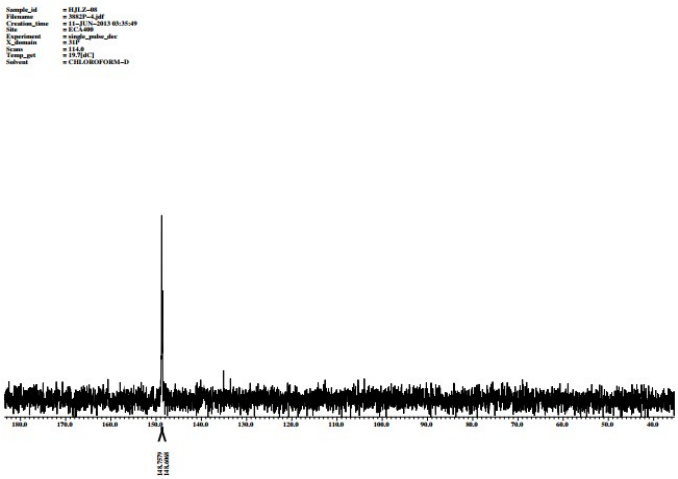
^{13}C NMR of Compound **7**



^{1}H NMR of Compound **8**



^{13}C NMR of Compound **8**



^{31}P NMR of Compound **8**

Fig. S6 NMR spectra of new compounds