Supporting Information for:

a- and β-Stilbenosides as Base-Pair Surrogates in DNA Hairpins

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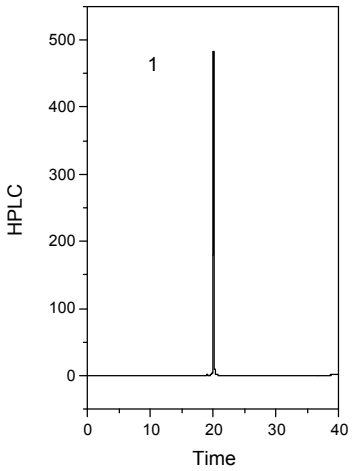
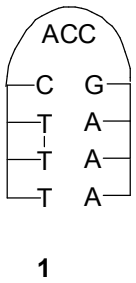
HPLC traces and MALDI-TOF Spectra





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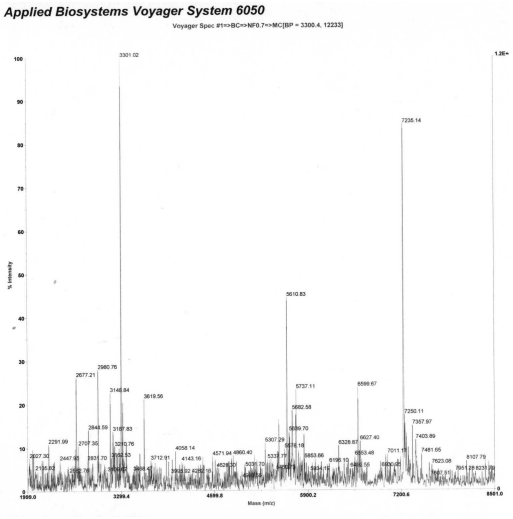
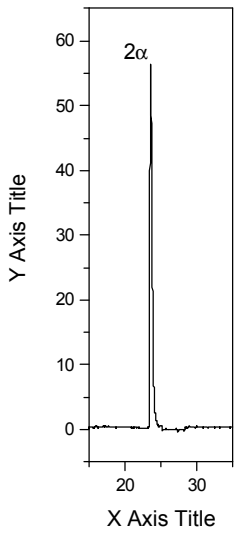
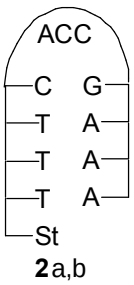
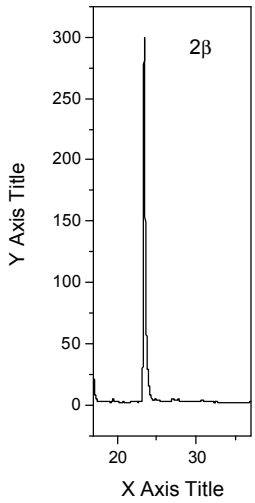
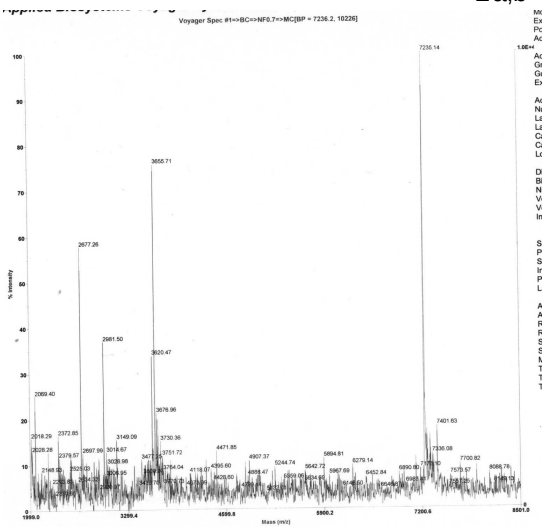


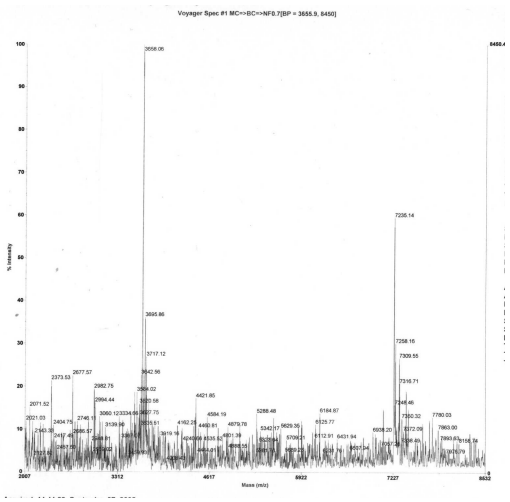


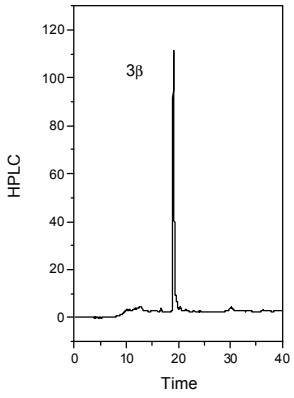


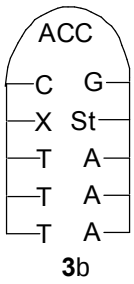
2a,b

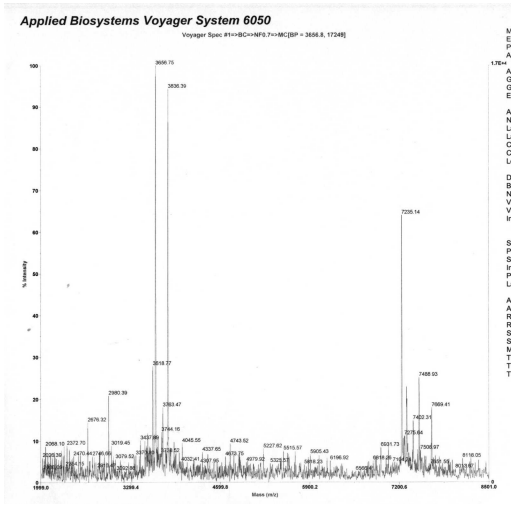


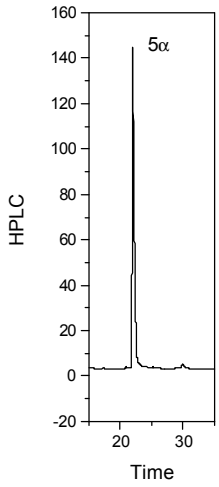


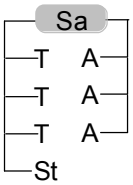




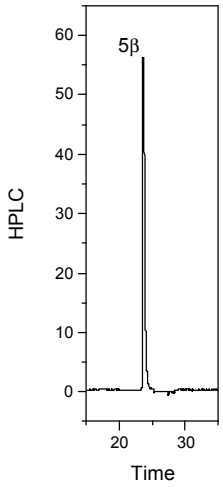


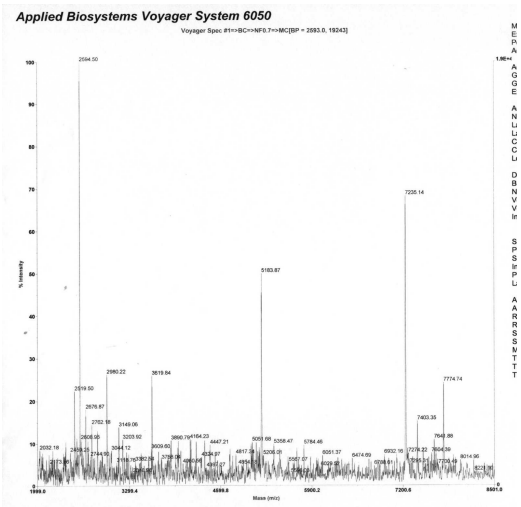



5α
HPLC
Time


Sa
T A
T A
T A
St

5a,b


5β
HPLC
Time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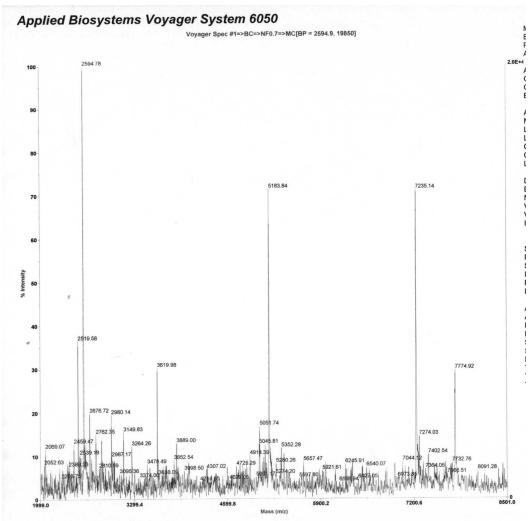
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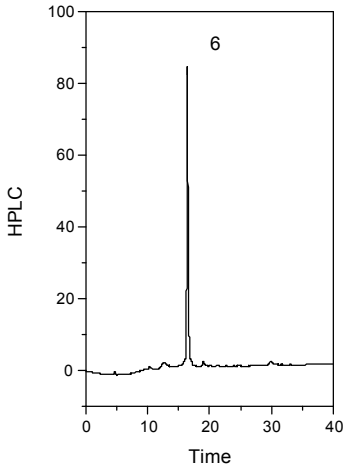
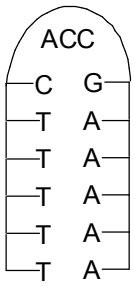
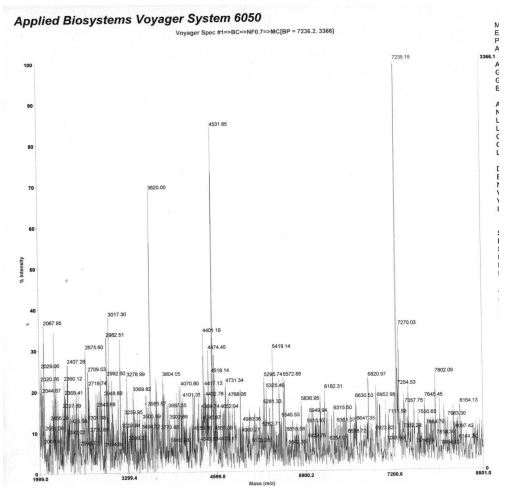

6
HPLC
Time
100
80
60
40
20
0
0
10
20
30
40


ACC
C G
T A
T A
T A
T A
T A

6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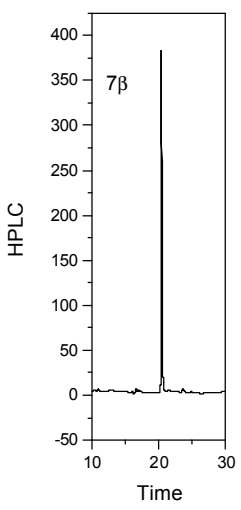
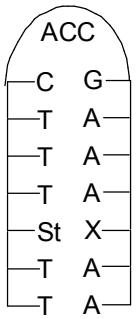
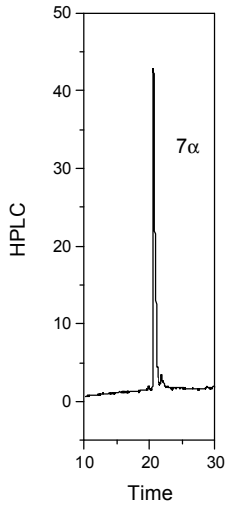
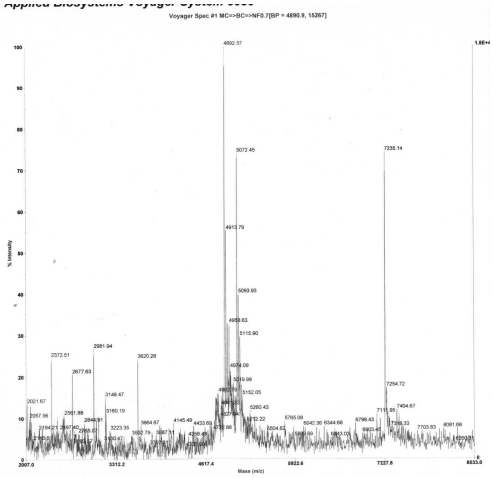
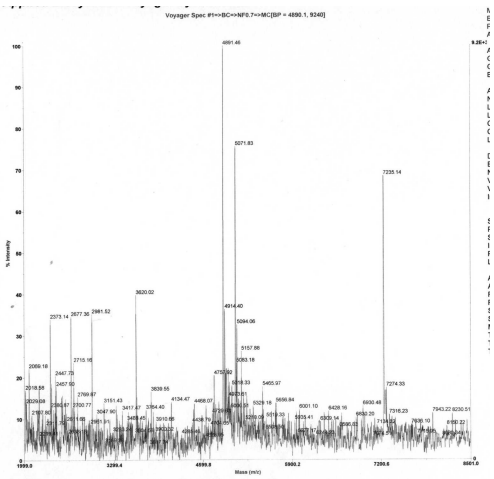


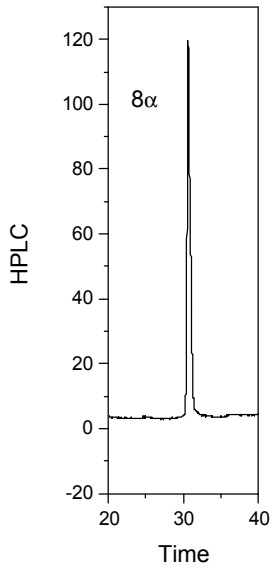


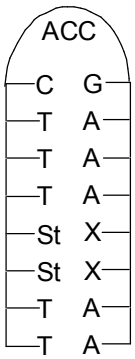
7a,b

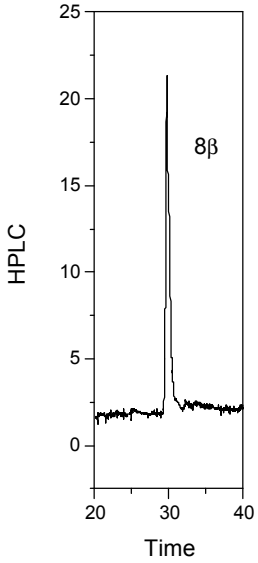




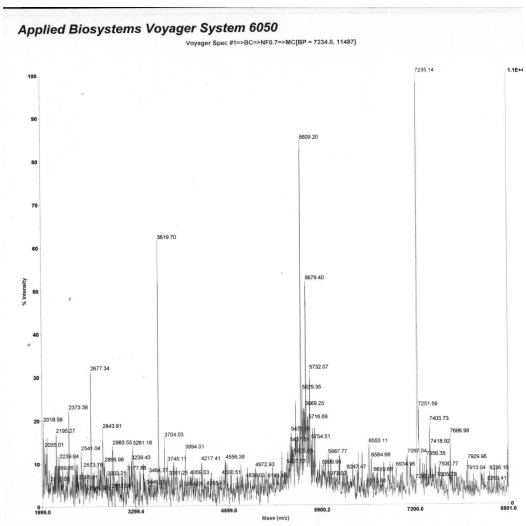



8α
HPLC
Time
120
100
80
60
40
20
0
-20
20
30
40


ACC
C G
T A
T A
T A
St X
St X
T A
T A


8β
HPLC
Time
25
20
15
10
5
0
20
30
40

8a,b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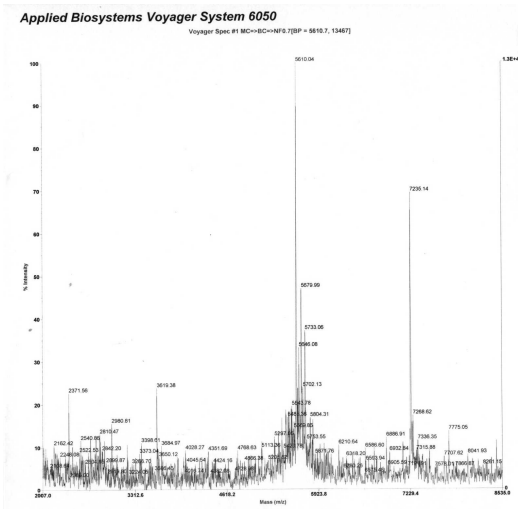
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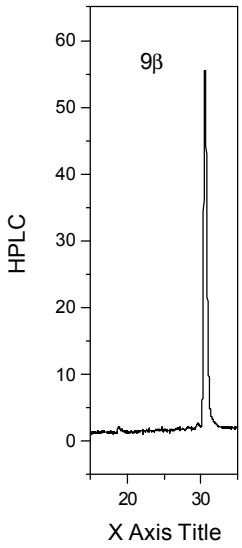
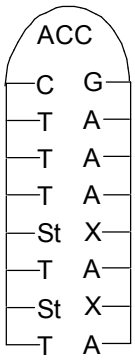
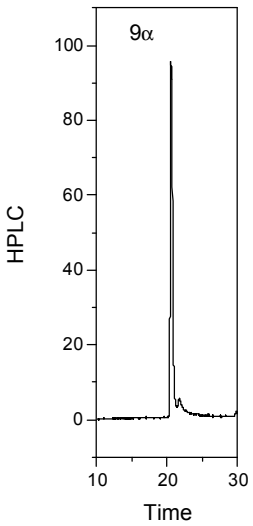
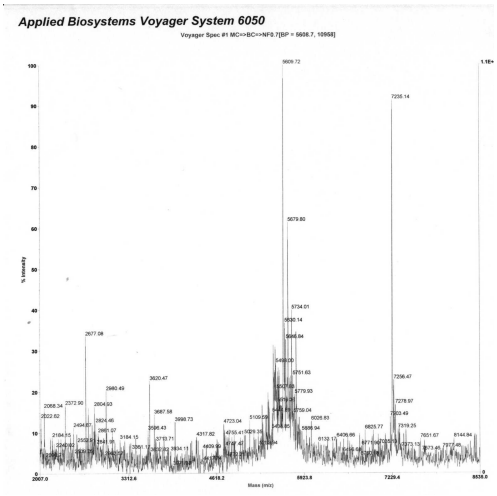
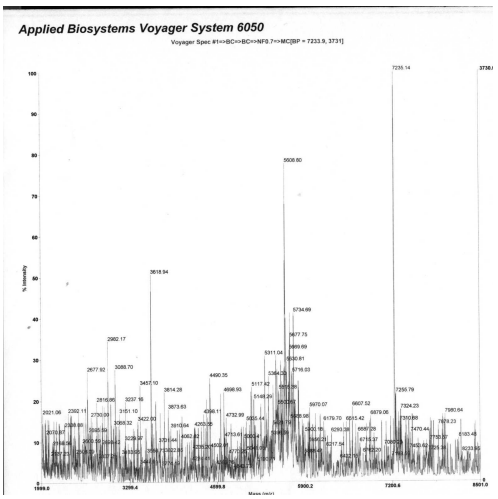




9a,b







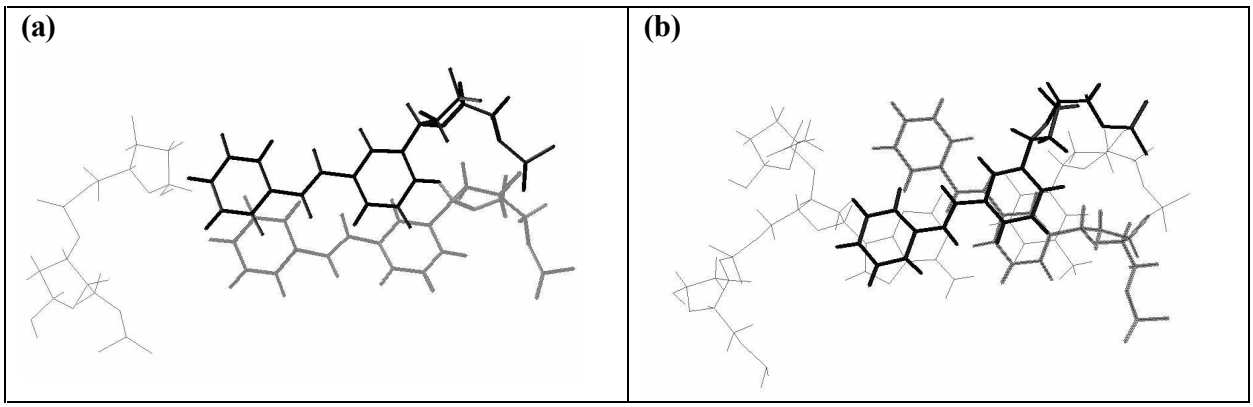
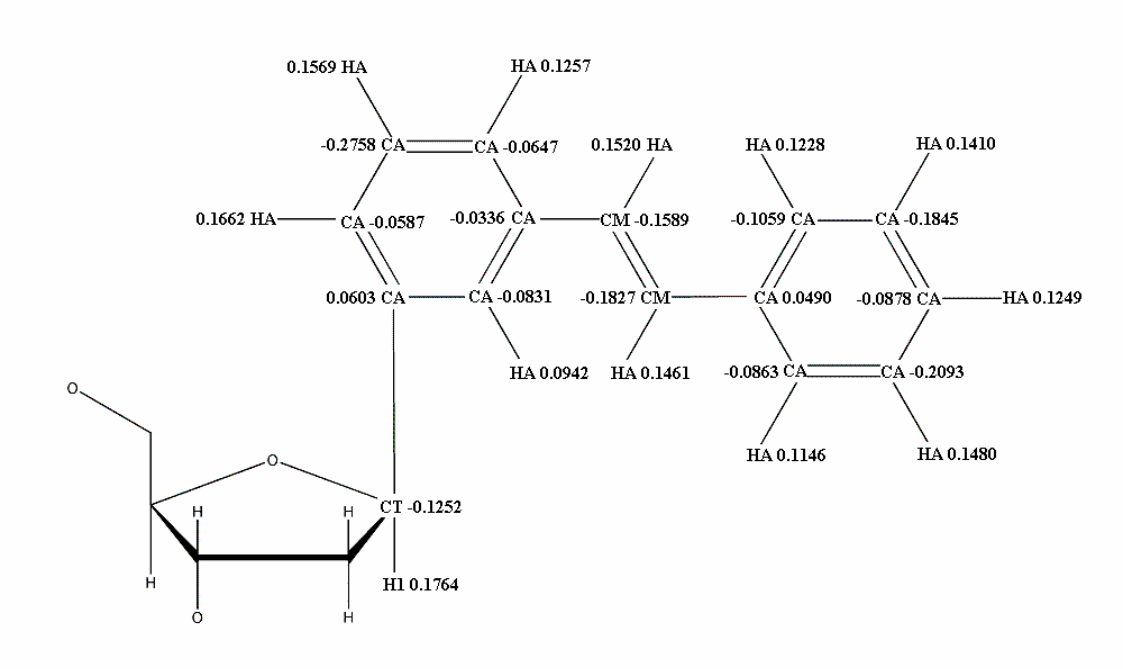


Fig. S1. Averaged truncated structures showing the two stilbenosides for (a) **8β** and (b) **9β** obtained from molecular dynamics simulations. Stilbenosides are bold.

Supporting Information:

Partial atomic charges and atom types of Stilbenosides residues for MD simulation. Partial atomic charges and atom types for other atoms are same as the value provided in ref 1.



References

1 (a) Arnott, S.; Campbell-Smith, P. J.; Chandrasekaran, R. In *Handbook of Biochemistry and Molecular Biology*; 3rd ed.; CRC Press: Cleveland, OH, 1976, pp 411-422. (b) Cornell, W. D.; Cieplak, P.; Bayly, C. I.; Gould, I. R.; Merz, K. M.; Ferguson, D. M.; Spellmeyer, D. C.; Fox, T.; Caldwell, J. W.; Kollman, P. A. *J. Am. Chem. Soc.* **1996**, *118*, 2309-2309.