

Supporting Information for:

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

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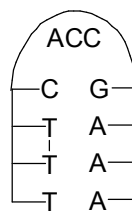
Departments of Chemistry and Immunology and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, 10550 N. Torrey Pines Road, La Jolla, CA 92037

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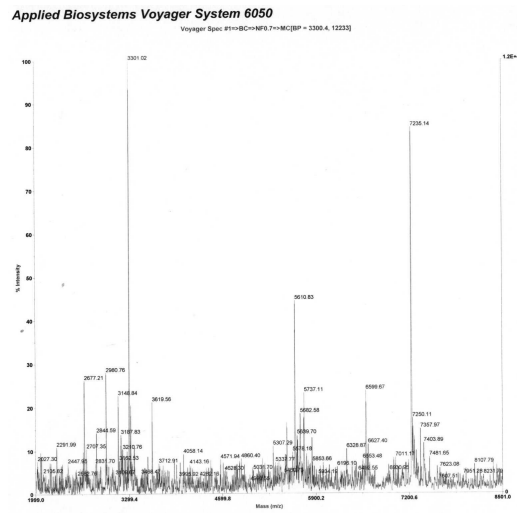
- HPLC and MALDI-TOF Spectra for all new conjugates.
- Averaged truncated structures showing the two stilbenosides for (a) **8 β** and (b) **9 β** obtained from molecular dynamics simulations.
- Partial atomic charges and atom types for the stilbenoside residue.

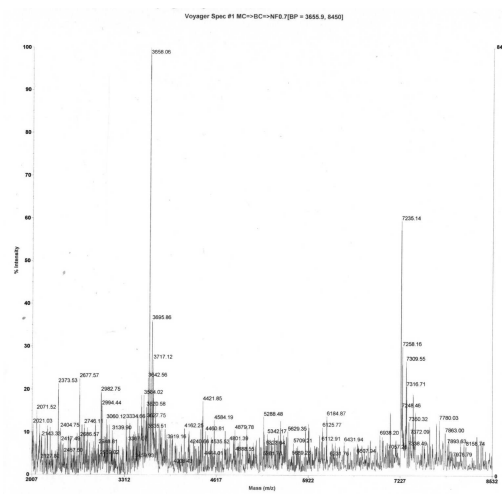
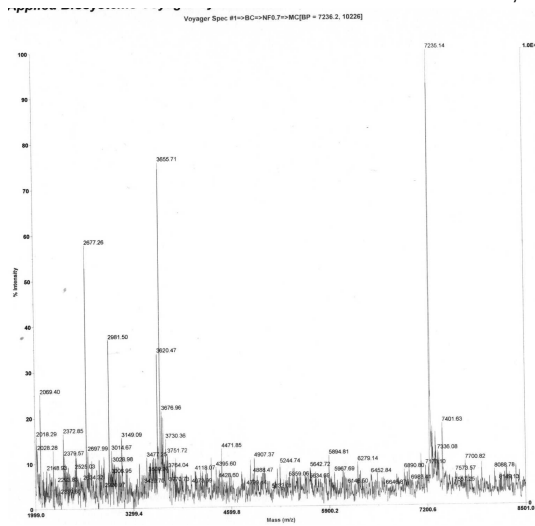
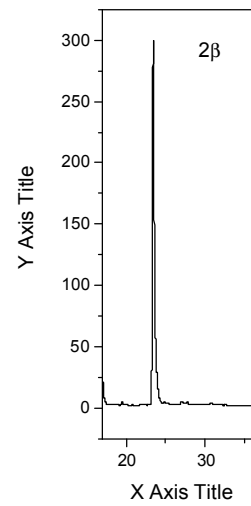
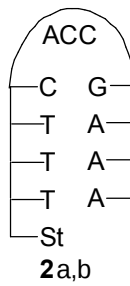
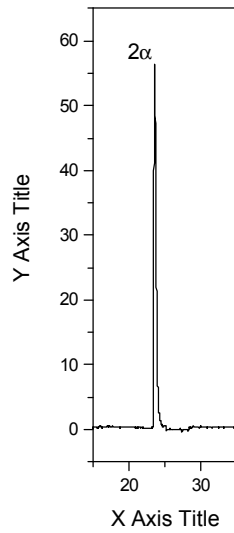
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The chromatogram displays a single, prominent, sharp peak at a retention time of approximately 20 minutes. The peak is labeled with the number '1'. The y-axis, labeled 'HPLC', ranges from 0 to 500. The x-axis, labeled 'Time', ranges from 0 to 40 minutes. The baseline is stable and near zero throughout the run.

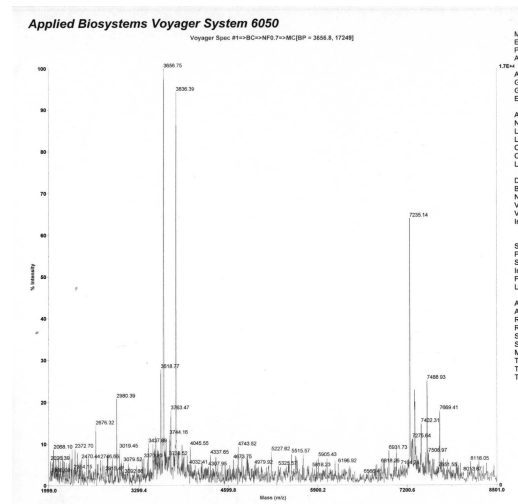
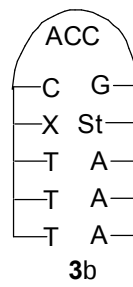
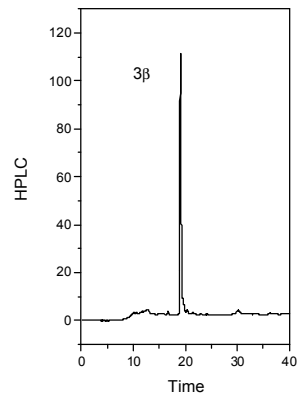


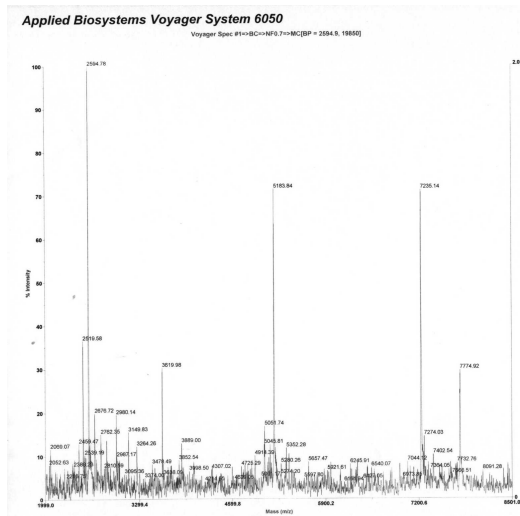
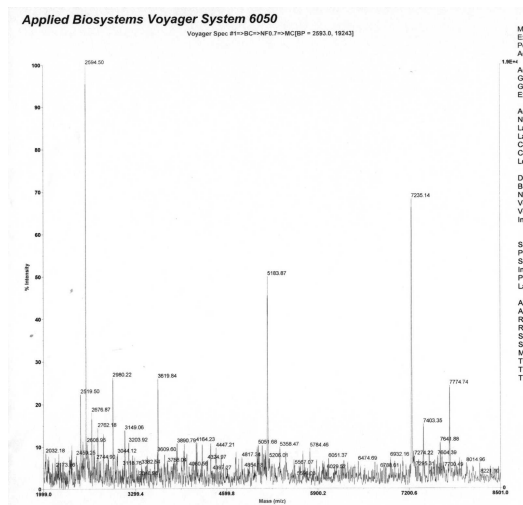
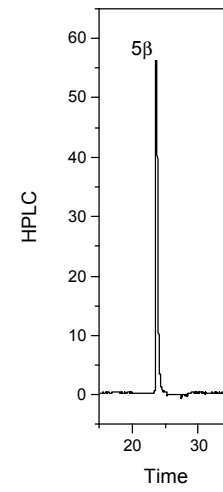
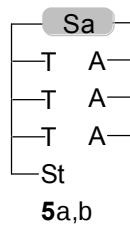
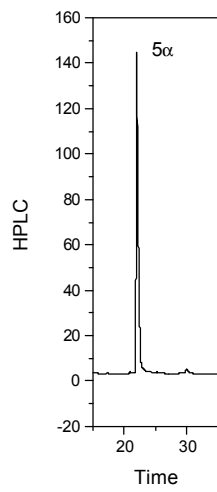
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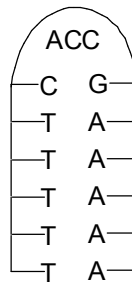


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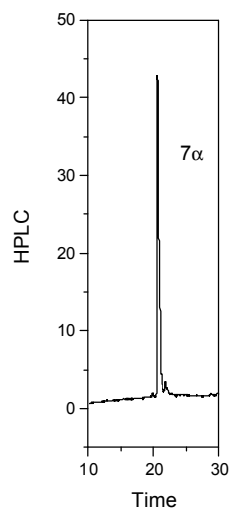
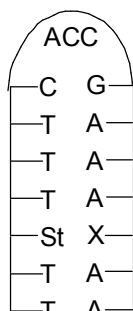
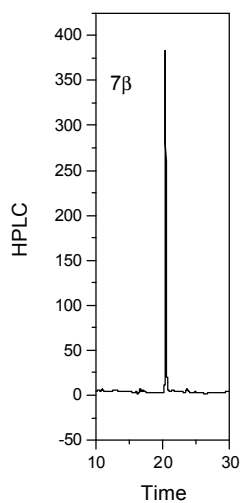


Applied Biosystems Voyager System 6050

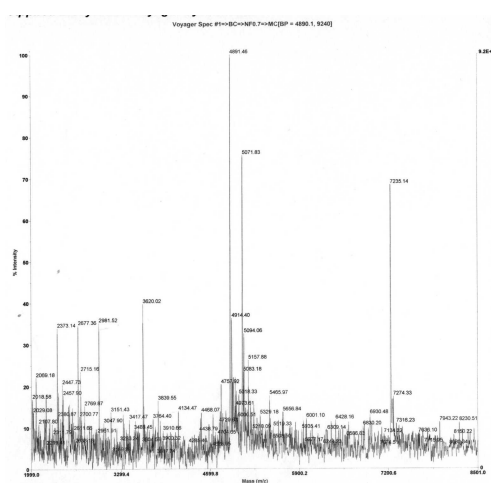
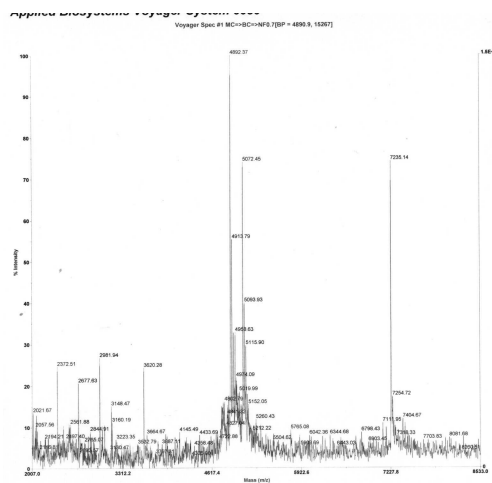
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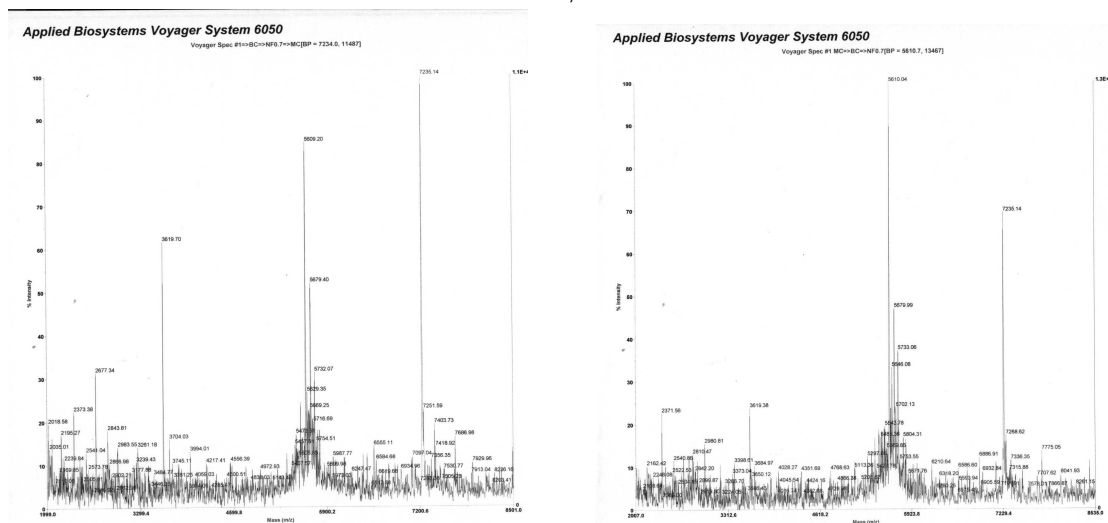
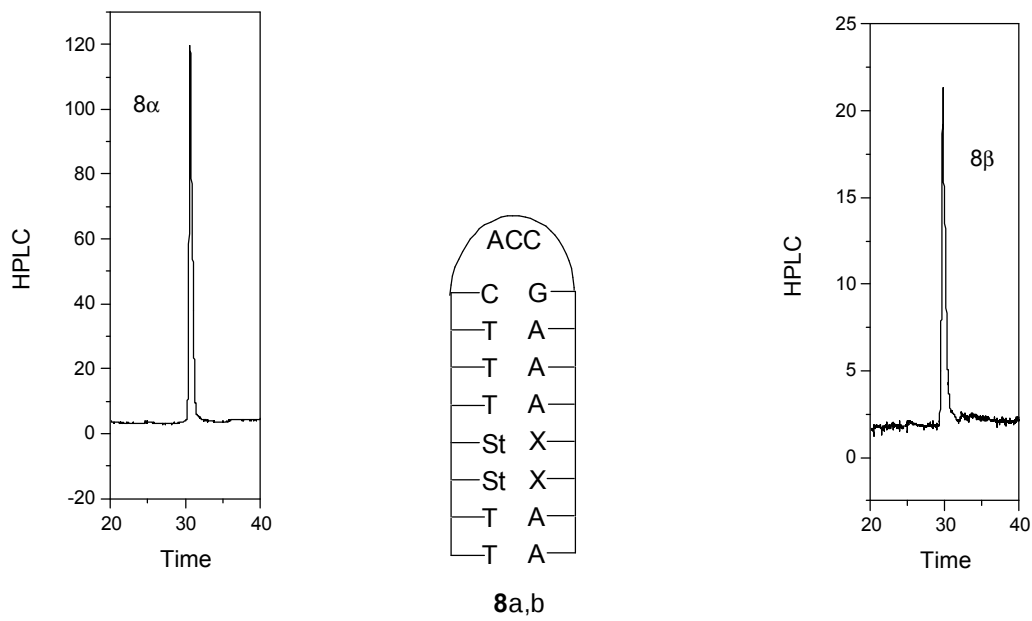
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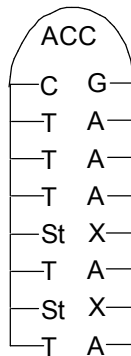
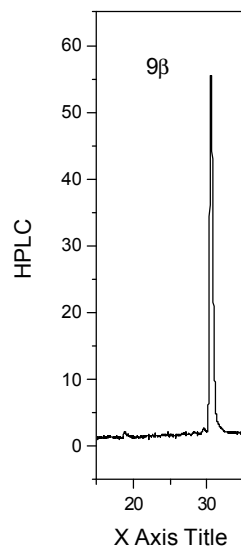
m/z	% Intensity
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2939.06	~20
2950.30	~20
2949.07	~20
2976.60	~25
3017.30	~40
3052.51	~35
3076.42	~25
3176.74	~20
3203.57	~15
3249.30	~15
3262.55	~15
3269.56	~15
3270.57	~15
3271.58	~15
3272.59	~15
3273.60	~15
3274.61	~15
3275.62	~15
3276.63	~15
3277.64	~15
3278.65	~15
3279.66	~15
3280.67	~15
3281.68	~15
3282.69	~15
3283.70	~15
3284.71	~15
3285.72	~15
3286.73	~15
3287.74	~15
3288.75	~15
3289.76	~15
3290.77	~15
3291.78	~15
3292.79	~15
3293.80	~15
3294.81	~15
3295.82	~15
3296.83	~15
3297.84	~15
3298.85	~15
3299.86	~15
3300.87	~15
3301.88	~15
3302.89	~15
3303.90	~15
3304.91	~15
3305.92	~15
3306.93	~15
3307.94	~15
3308.95	~15
3309.96	~15
3310.97	~15
3311.98	~15
3312.99	~15
3313.00	~15
3314.01	~15
3315.02	~15
3316.03	~15
3317.04	~15
3318.05	~15
3319.06	~15
3320.07	~15
3321.08	~15
3322.09	~15
3323.10	~15
3324.11	~15
3325.12	~15
3326.13	~15
3327.14	~15
3328.15	~15
3329.16	~15
3330.17	~15
3331.18	~15
3332.19	~15
3333.20	~15
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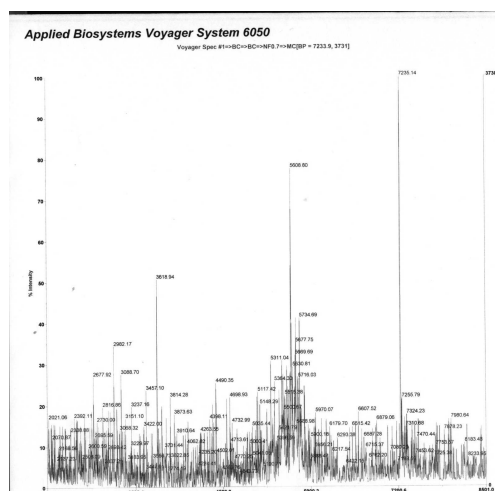
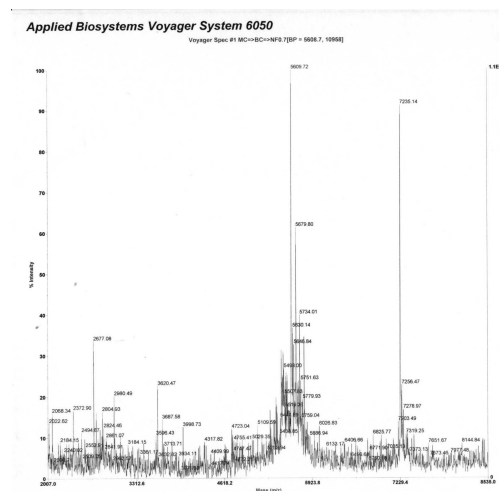
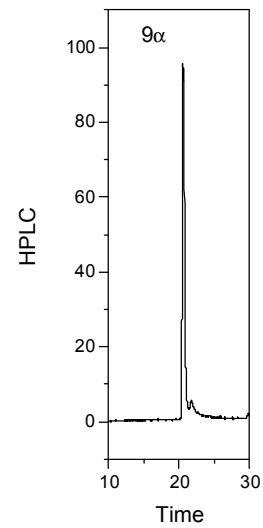
7a,b







9a,b



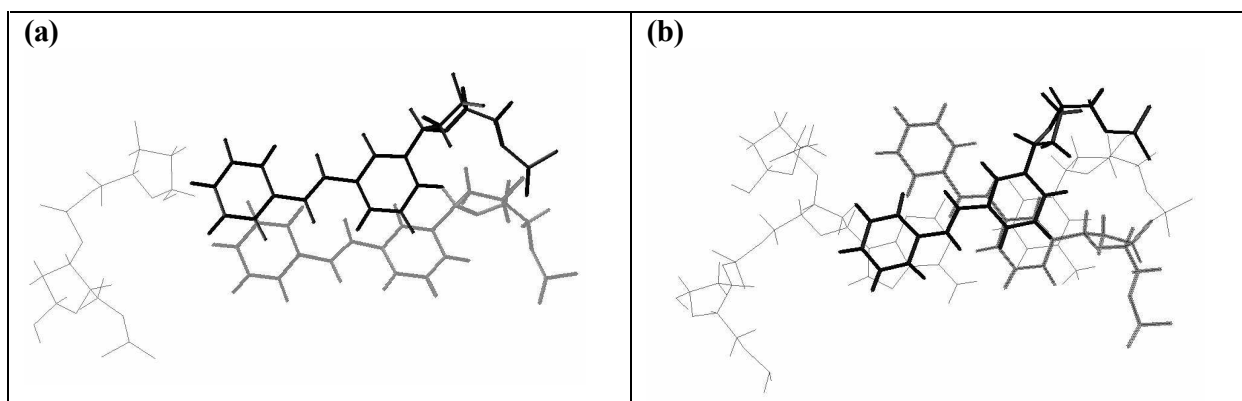
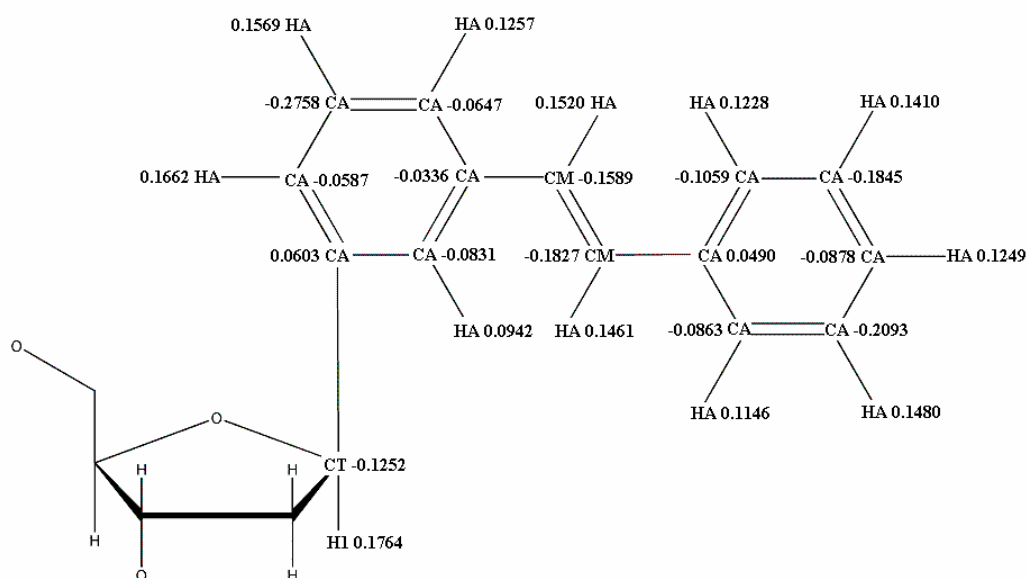


Fig. S1. Averaged truncated structures showing the two stilbenosides for (a) **8β** and (b) **9β** obtained from molecular dynamics simulations. Stilbenosides are bold.

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

- (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.