Electron Supplementary Information

Endonuclease and Exonuclease Activities on Oligodeoxynucleotides Containing Spiroiminodihydantoin Depend on the Sequence Context and the Lesion Stereochemistry

Xin Chen, Aaron M. Fleming, James G. Muller, and Cynthia J. Burrows*

Department of Chemistry, University of Utah, 315 South 1400 East, Salt Lake City, Utah 84112-0850, U.S.A.

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Fig. S1 Anion-exchange HPLC elution for the diastereomers of the dinucleotide 5'-d(Cp[Sp]-3'. The diastereomers elute at 14.1 and 14.6 min, respectively that were products from SVPD digestion of the ODN 5'-d(TTT TTT TAC [Sp]GT)-3' The digestion was done in Tris-HCl (pH 7.8) buffer at 37 °C. (b) Mass spectrum (negative ion) of dCSp dinucleotide from the digestion by snake venom phosphodiesterase (SVPD).



Fig. S2 ESI-MS for the diastereomer mixture of the dinucleotide 5'-d(Cp[Sp])-3'. The calculated mass is $(M-H)^2 = 587.4$; and the experimental mass is $(M-H)^2 = 586.9$.



Fig. S3 Digestion of 5'-d(Ap[Sp])-3' was monitored by RP-HPLC and hypercarb column. (a) HPLC elution of dA, dASp1, dASp2 with a reversed phase column. Retention time: dA(11 min), dASp1 (15 min) and dASp2 (12 min). (b) Sp nucleoside after digestion eluted on hypercarb column.

(a)



(b)



Fig. S4 Digestion efficiency of oligodeoxynucleotides containing Sp with combinations of enzymes.

(a) Digestion of ODNs with enzyme combinations (P1 = nuclease P1).

	GSpC	ASpG	TSpG	CSpG
P1 + SVPD	100%	100%	100%	100%
SVPD + SPD	100 <u>+</u> 1 %	100 <u>+</u> 3 %	70 <u>+</u> 3 %	29 <u>+</u> 8 %

10 GSp2 5 0 _5²∮0 mdegree/OD (240 nm) 260 280 300 320 340 360 380 400 22 240 GSp1 -10 -15 -20 -25 -30 -35 -40-45 wavelength, nm

Fig. S5 ECD spectra for the 5'-d(Gp[Sp])-3' and dSp diastereomers.

8 6 mdegrees/OD (230 nm) dSp1* 4 2 0 -2 -4 dSp2* -6 -8 220 260 320 200 240 280 300 340 Wavelength (nm)

ECD Spectra for the dSp Diastereomers

*The nucleoside numbering scheme is based on the elution order from an anion-exchange HPLC column.

Fig. S6 dSp elution order in and ODN and a free nucleoside. (a) dSp-containing ODN eluted on anion exchange. (b) dSp nucleoside after digestion eluted on hypercarb. The eluting order of these two columns is reversed.



(a)



