Stereospecific Formation of the (*R*)-γ-Hydroxytrimethylene Interstrand N^2-dG:N^2-dG DNA Cross-Links Arising from the γ-OH-1,N^2-Propano-2'-deoxyguanosine Adduct in the 5′-CpG-3′ Sequence

Supporting Information Available

Hai Huang, Hye-Young Kim, Ivan D. Kozekov, Young-Jin Cho, Hao Wang, Albena Kozekova, Thomas H. Harris, Carmelo J. Rizzo, and Michael P. Stone*

Department of Chemistry and Center in Molecular Toxicology, Vanderbilt University, Nashville, Tennessee 37235

*To whom correspondence should be addressed
Telephone 615-322-3589
FAX 615-322-7591
Email: michael.p.stone@vanderbilt.edu

Table S1. NOEs Used in the Molecular Dynamics Simulations and the Corresponding Atom Distances in the Average Structure.

NOE	relative intensity [a]	distance (Å)
$Y^{19} N^2H \rightarrow H^{\alpha 1}$	w	3.8
$Y^{19} N^2H \rightarrow H^{\alpha 2}$	w	4.2
$Y^{19} N^2H \rightarrow H^{\beta 1}$	m	3.6
$Y^{19} N^2H \rightarrow H^{\beta 2}$	s	2.5
$Y^{19} N^2H \rightarrow H^{\gamma}$	m	3.0
$Y^{19} N^2H \rightarrow X^7 N1H$	m	3.5
$X^7 N^2H \rightarrow A^8 H1'$	w	5.5
$X^7 N^2H \rightarrow A^8 H2$	m	3.0
$X^7 N^2H \rightarrow T^{17} N3H$	w	4.6
$X^7 N^2H \rightarrow C^{18} H1'$	w	3.9
$X^7 N^2H \rightarrow C^{18} N^4H1$	w	5.8
$X^7 N^2H \rightarrow Y^{19} H1'$	w	6.0
$X^7 N^2H \rightarrow Y^{19} N1H$	m	3.4
$X^7 N^2H \rightarrow Y^{19} N^2H$	m	3.0
$X^7 N^2H \rightarrow H^{\alpha 1}$	s	2.9
$X^7 N^2H \rightarrow H^{\alpha 2}$	s	2.3
$X^7 N^2H \rightarrow H^{\beta 1}$	w	4.0
$X^7 N^2H \rightarrow H^{\beta 2}$	m	3.5
$X^7 N^2H \rightarrow H^{\gamma}$	m	3.6

[a] Relative intensities: s, strong; m, medium; w, weak.

Complete references 60 and 61.

60. Case, D. A.; Darden, T. A.; Cheatham III, T. E.; Simmerling, C. L.; Wang, J.; Duke, R. E.; Luo, R.; Merz, K. M.; Pearlman, D. A.; Crowley, M.; Walker, R. C.; Zhang, W.; Wang, B.; Hayik, S.; Roitberg, A.; Seabra, G.; Wong, K. F.; Paesani, F.; Wu, X.; Brozell, S.; Tsui, V.; Gohlke, H.; Yang, L.; Tan, C.; Mongan, J.; Hornak, V.; Cui, G.; Berroza, P.; Mathews, D. H.; Schafmeister, C.; Ross, W. S.; Kollman, P. A.; AMBER 9; University of California, San Francisco: San Franciso, 2006.

61. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Pomelli, J.; Ochterski, W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewska, V. G.; Daniels, A. D.; Farkas, O.; Rabuck, A. D.; Raghavachari, K.; Ortiz, J. V. GAUSSIAN 03; Gaussian, Inc., Wallingford, CT, 2004.