

**Differential Base Stacking Interactions Induced by Trimethylene Interstrand DNA  
Cross-links in the 5'-CpG-3' and 5'-GpC-3' Sequence Contexts**

Revised Manuscript

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**Running Title:** Trimethylene Interstrand Cross-Links

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**Table S1.** Backbone Torsion Angles of the Average Structure of the 5'-CpX-3' Cross-Link Compared with the Experimental Data.

nucleotide	experimental (°) <sup>a</sup>		average structure (°)						
	$\delta$	$\epsilon$	$\alpha$	$\beta$	$\gamma$	$\delta$	$\epsilon$	$\zeta$	$\chi$
A <sup>1</sup>	173	-141			63	97	-177	-97	-82
G <sup>2</sup>	160	-140	-80	65	165	148	-166	-79	-140
G <sup>3</sup>	138	-135	-72	-177	43	128	-179	-94	-106
C <sup>4</sup>	88	-144	-62	168	53	97	-160	-72	-130
X <sup>5</sup>	129	-137	-74	169	45	139	-77	134	-85
C <sup>6</sup>	171	-143	-85	145	53	128	-165	-83	-128
C <sup>7</sup>	94	-142	-77	171	50	90	-174	-87	-132
T <sup>8</sup>			-63	173	60	142			-98

<sup>a</sup> Cited from *J. Am. Chem. Soc.* **2001**, *123*, 1730-1739.

**Table S2.** Sugar Torsion Angles of the Average Structure of the 5'-CpX-3' Cross-Link Compared with the Experimental Data.

nucleotide	Experimental <sup>a</sup>		average structure		
	P (°)	Φm (°)	P (°)	Φm (°)	puckering
A <sup>1</sup>	201	49	103	41	O <sub>4</sub> , -endo
G <sup>2</sup>	180	44	183	33	C <sub>3</sub> , -exo
G <sup>3</sup>	149	39	142	36	C <sub>1</sub> , -exo
C <sup>4</sup>	82	44	90	36	O <sub>4</sub> , -endo
X <sup>5</sup>	136	44	142	46	C <sub>1</sub> , -exo
C <sup>6</sup>	237	49	142	33	C <sub>1</sub> , -exo
C <sup>7</sup>	80	34	78	35	O <sub>4</sub> , -endo
T <sup>8</sup>			160	33	C <sub>2</sub> , -endo

<sup>a</sup> Cited from *J. Am. Chem. Soc.* **2001**, *123*, 1730-1739.

**Table S3.** Backbone Torsion Angles of the Average Structure of the 5' -XpC-3' Cross-Link Compared with the Experimental Data.

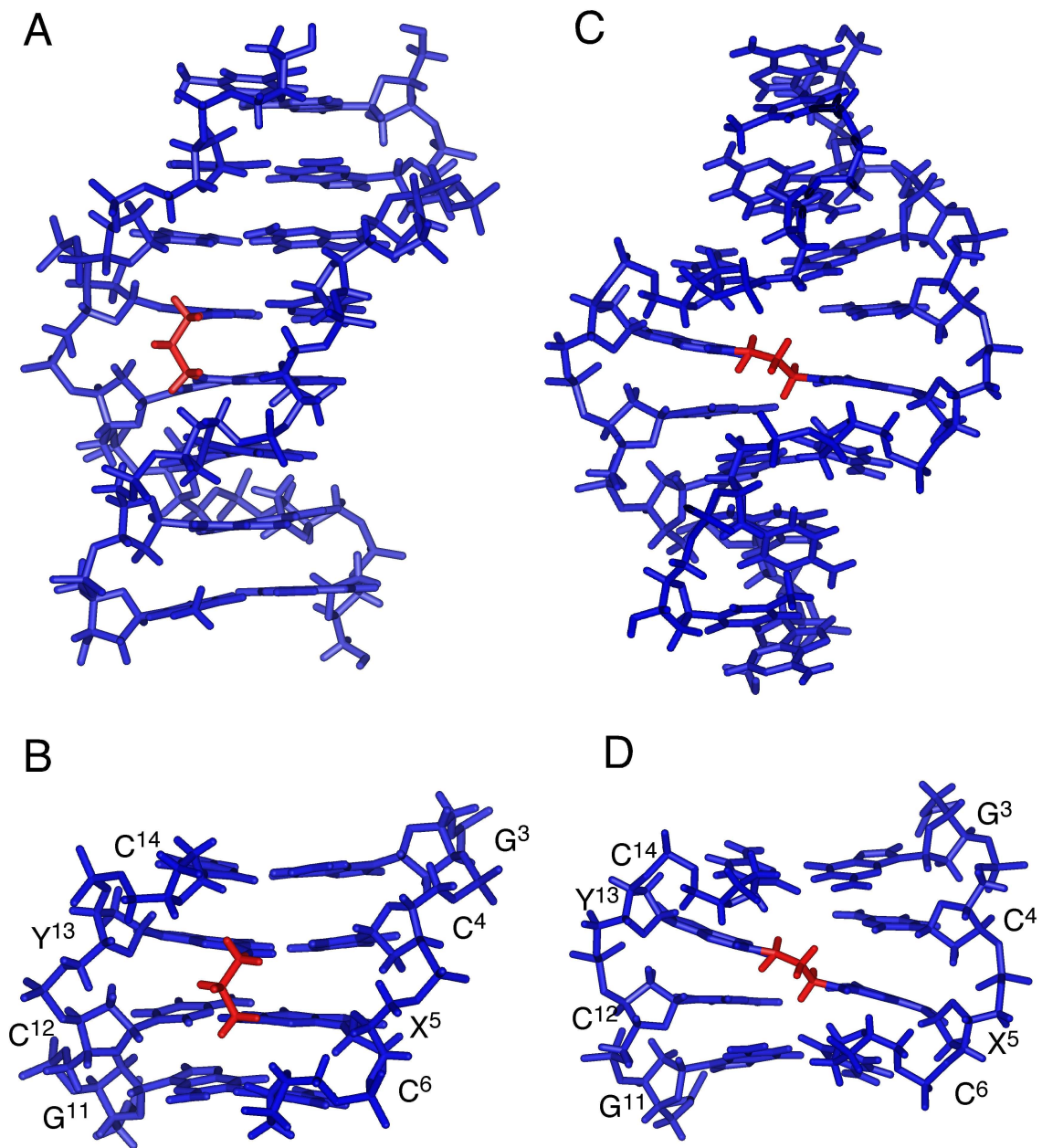
residue	Experimental <sup>a</sup>	average structure						
	$\delta$	$\alpha$	$\beta$	$\gamma$	$\delta$	$\epsilon$	$\zeta$	$\chi$
T <sup>1</sup>	113			-175	126	-180	-91	-116
C <sup>2</sup>	130	-58	162	65	107	-173	-87	-127
C <sup>3</sup>	130	-64	171	56	127	-170	-92	-117
X <sup>4</sup>	138	-80	-168	39	155	-70	164	-86
C <sup>5</sup>	138	-98	139	53	92	-178	-100	-126
G <sup>6</sup>	138	-62	170	63	129	-175	-93	-108
G <sup>7</sup>	130	-64	168	58	122	-174	-93	-116
A <sup>8</sup>	113	-65	174	54	134			-106

<sup>a</sup> Averaged from data in *J. Am. Chem. Soc.* **2003**, *125*, 62-72.

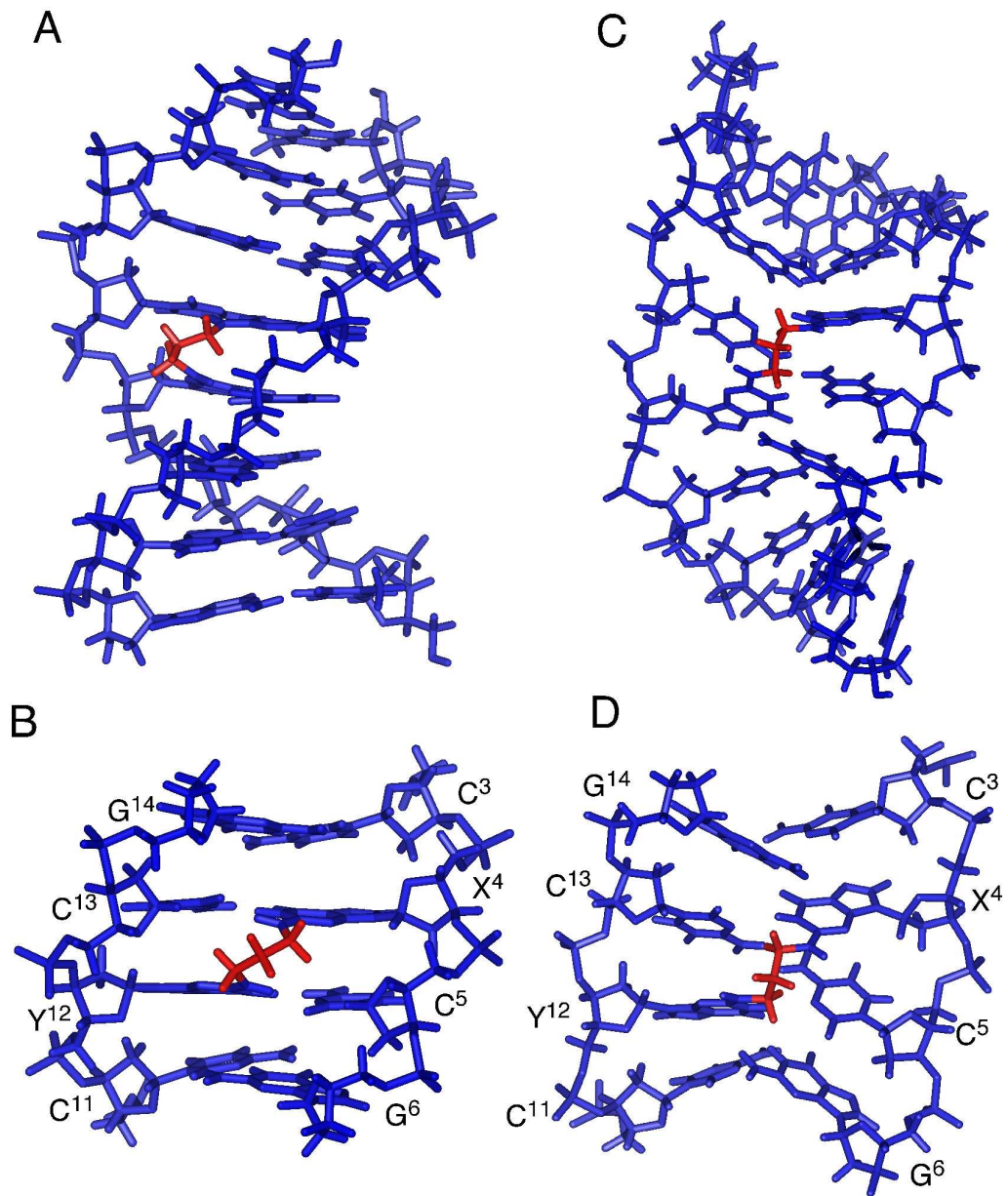
**Table S4.** Sugar Torsion Angles of the Average Structure of the 5'-XpC-3' Cross-Link Compared with the Experimental Data.

nucleotide	Experimental <sup>a</sup>	average structure		
	P (°)	P (°)	Φm (°)	puckering
T <sup>1</sup>	86	145	24	C <sub>2</sub> , -endo
C <sup>2</sup>	131	111	35	C <sub>1</sub> , -exo
C <sup>3</sup>	131	139	36	C <sub>1</sub> , -exo
X <sup>4</sup>	141	162	40	C <sub>2</sub> , -endo
C <sup>5</sup>	141	91	35	O <sub>4</sub> , -endo
G <sup>6</sup>	141	158	25	C <sub>2</sub> , -endo
G <sup>7</sup>	141	132	33	C <sub>1</sub> , -exo
A <sup>8</sup>	86	144	36	C <sub>2</sub> , -endo

<sup>a</sup> Averaged from data in *J. Am. Chem. Soc.* **2003**, 125, 62-72.

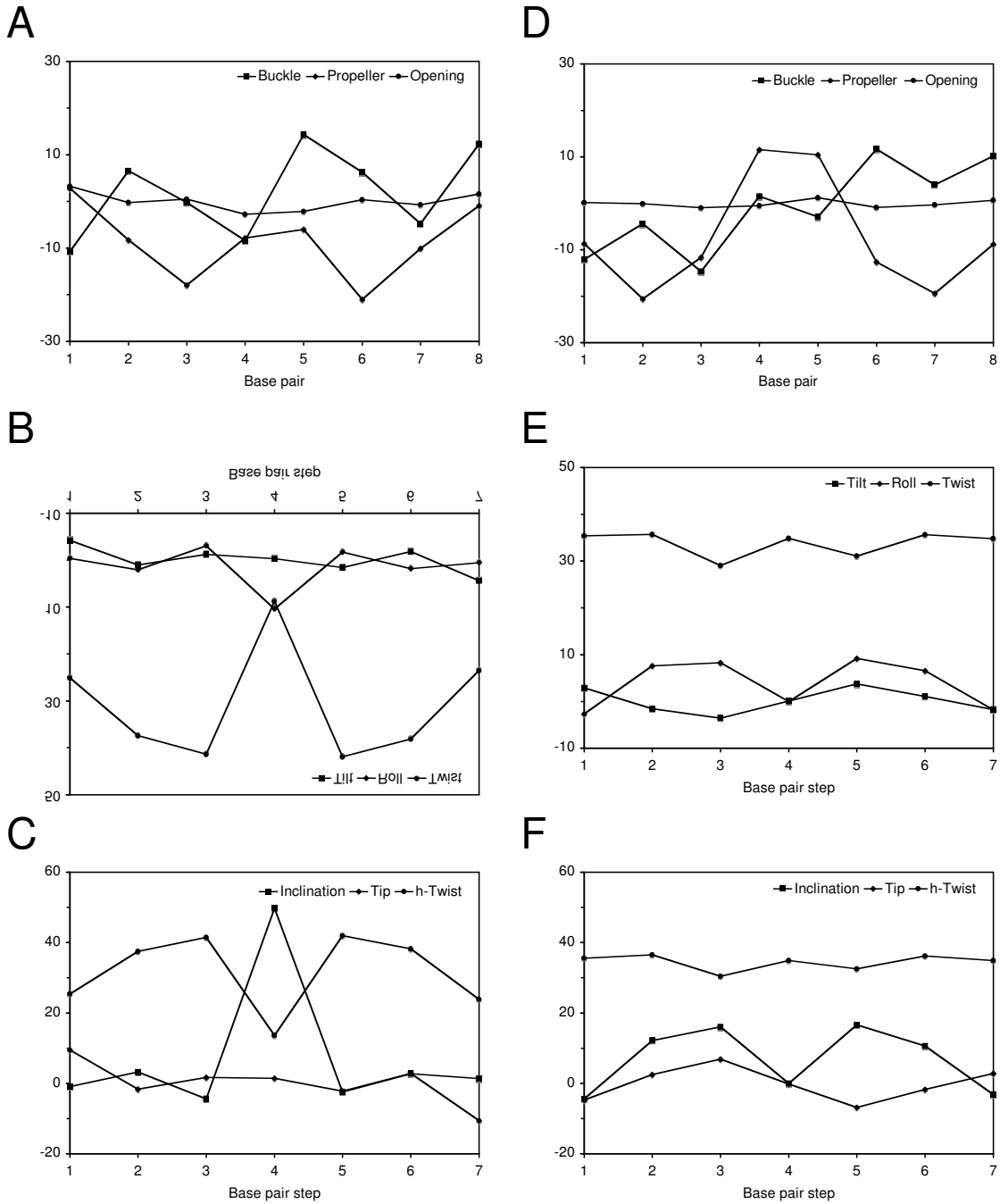


**Figure S1.** Refined structures of the trimethylene interstrand cross-link in the 5'-CpX-3' sequence: (A) new refined structure; (B) expanded view of the new structure from the minor groove; (C) structure refined by Dooley et al. (PDB ID: 1HZ2); (D) expanded view of the structure refined by Dooley et al. from the minor groove. Blue and red sticks represent the nucleotide and the tether, respectively.



**Figure S2.** Refined structures of the trimethylene interstrand cross-link in the 5'-XpC-3' sequence: (A) new refined structure; (B) expanded view of the new structure from the minor groove; (C) structure refined by Dooley et al. (PDB ID: 1LUH); (D) expanded view of the structure refined by Dooley et al. from the minor groove. Blue and red sticks represent the nucleotide and the tether, respectively.





**Figure S3.** Base pairing parameters of the trimethylene cross-links: (A-C) In the 5'-CpX-3' sequence context, significant roll, twist, inclination and h-twist of the cross-linked base pairs are induced; (D-F) In the 5'-XpC-3' sequence context, significant propeller of the cross-linked base pairs is induced.