

**1,*N*<sup>2</sup>-Etheno-2'-Deoxyguanosine Adopts the *syn* Conformation About the Glycosyl Bond When Mismatched with Deoxyadenosine**

**Supporting Information**

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Running Title: 1,*N*<sup>2</sup>-εdG Adduct Opposite Deoxyadenosine

**Table S1.** Non-exchangeable Proton Chemical Shifts of the 1,*N*<sup>2</sup>-εdG•A duplex at pH 5.2, 7 °C.<sup>a,b</sup>

Nucleotide	H8	H6	H1'	H2'	H2''	H3'	H5/H2/CH <sub>3</sub>
C <sup>1</sup>		7.69	5.77	1.99	2.42	4.71	5.92
G <sup>2</sup>	7.99		5.92	2.70	2.75	4.78	
C <sup>3</sup>		7.44	5.57	2.11	2.42	4.87	5.45
A <sup>4</sup>	8.34		6.18	2.67	2.77	5.00	7.62
T <sup>5</sup>		6.62	5.65	1.30	2.44	4.75	1.35
X <sup>6</sup>	7.78		5.83	2.36	nd	nd	
G <sup>7</sup>	7.88		nd	nd	nd	4.98	
A <sup>8</sup>	8.12		6.00	2.71	2.91	5.06	7.15
A <sup>9</sup>	8.12		6.10	2.54	2.87	4.96	7.62
T <sup>10</sup>		7.11	5.86	2.01	2.46	4.82	1.29
C <sup>11</sup>		7.60	6.06	2.23	2.48	4.83	5.63
C <sup>12</sup>		7.74	6.24	2.28	2.28	4.55	5.83
G <sup>13</sup>	7.81		5.61	2.48	2.64	4.81	
G <sup>14</sup>	7.89		5.61	2.72	2.81	5.02	
A <sup>15</sup>	8.27		6.31	2.74	2.97	5.04	7.85
T <sup>16</sup>		7.22	5.96	2.03	2.58	4.85	1.29
T <sup>17</sup>		7.40	6.08	2.13	2.5	4.89	1.50
C <sup>18</sup>		7.66	5.20	2.18	2.40	4.89	5.73
A <sup>19</sup>	8.54		6.14	2.91	3.13	5.14	7.64
A <sup>20</sup>	8.30		6.16	2.62	2.93	5.04	7.61
T <sup>21</sup>		7.01	5.63	1.91	2.32	4.85	1.39
G <sup>22</sup>	7.81		5.77	2.58	2.62	4.95	
C <sup>23</sup>		7.35	5.75	1.93	2.34	4.79	5.38
G <sup>24</sup>	7.93		6.14	2.34	2.62	4.67	

<sup>a</sup> Values in parts per million.

<sup>b</sup> 10 mM phosphate buffer, 100 mM NaCl.

nd- not determined

**Table S2.** Exchangeable Proton Chemical Shifts of 1,*N*<sup>2</sup>- $\epsilon$ dG•A Duplex at pH 5.2, 5 °C.<sup>a,b</sup>

Base Pair	C N <sup>4</sup> H <sub>nbb</sub>	C N <sup>4</sup> H <sub>hb</sub>	G N1H	T N3H
C <sup>1</sup> •G <sup>24</sup>	nd	nd		
G <sup>2</sup> •C <sup>23</sup>	6.6	8.4	13.1	
C <sup>3</sup> •G <sup>22</sup>	6.5	8.3	12.7	
A <sup>4</sup> •T <sup>21</sup>				13.5
T <sup>5</sup> •A <sup>20</sup>				13.3
X <sup>6</sup> •A <sup>19</sup>			nd	
G <sup>7</sup> •C <sup>18</sup>	7.5	7.5	12.5	
A <sup>8</sup> •T <sup>17</sup>				13.6
A <sup>9</sup> •T <sup>16</sup>				13.7
T <sup>10</sup> •A <sup>15</sup>				13.6
C <sup>11</sup> •G <sup>14</sup>	6.9	8.4	12.8	
C <sup>12</sup> •G <sup>13</sup>	nd	nd		

<sup>a</sup> Values in parts per million.

<sup>b</sup> 10 mM phosphate buffer in H<sub>2</sub>O, 100 mM NaCl, pH 5.2.

<sup>c</sup> hb and nbb refer to the hydrogen-bonded and non-hydrogen bonded cytosine amino protons, respectively.

nd, not detected.