

**Stereochemistry of *trans*-4-Hydroxynonenal-Derived Exocyclic 1,*N*<sup>2</sup>-Deoxyguanosine Adducts Modulates Formation of Inter-strand Cross-links in the 5'-CpG-3' Sequence<sup>†</sup>**

Supporting Information

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**Running Title:** Stereospecific Minor Groove Orientations of HNE DNA Adducts

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**Figure S1.** Force field parameters of HNE atoms in cyclic hemiacetal stereoisomers used for rMD calculation

**Table S1.**  $^1\text{H}$  Chemical Shift Assignments of the 5'-CpX-3' Duplex with Stereoisomer **8**.

| Base            | Chemical Shifts (ppm) |          |      |      |      |      |      |      |      |
|-----------------|-----------------------|----------|------|------|------|------|------|------|------|
|                 | H6/H8                 | H2/H5/Me | H1'  | H2'  | H2'' | H3'  | H4'  | H5'  | H5'' |
| G <sup>1</sup>  | 7.99                  |          | 6.03 | 2.68 | 2.80 | 4.86 | 4.27 | 3.75 |      |
| C <sup>2</sup>  | 7.55                  | 5.39     | 6.08 | 2.14 | 2.53 | 4.84 |      |      |      |
| T <sup>3</sup>  | 7.42                  | 1.68     | 5.59 | 2.15 | 2.43 | 4.90 |      |      |      |
| A <sup>4</sup>  | 8.23                  | 7.45     | 6.06 | 2.76 | 2.91 | 5.07 | 4.43 |      |      |
| G <sup>5</sup>  | 7.65                  |          | 5.73 | 2.44 | 2.63 | 4.97 | 4.36 |      |      |
| C <sup>6</sup>  | 7.27                  | 5.32     | 5.57 | 1.96 | 2.25 | 4.80 | 4.11 | 4.20 |      |
| X <sup>7</sup>  | 7.81                  |          | 5.82 | 2.64 | 2.85 | 5.00 | 4.29 | 4.10 | 3.94 |
| A <sup>8</sup>  | 8.04                  | 7.66     | 6.06 | 2.66 | 2.90 | 5.05 | 4.36 | 4.03 | 4.23 |
| G <sup>9</sup>  | 7.55                  |          | 5.80 | 2.44 | 2.69 | 4.90 | 4.34 |      |      |
| T <sup>10</sup> | 7.22                  | 1.26     | 6.04 | 2.13 | 2.52 | 4.84 |      |      |      |
| C <sup>11</sup> | 7.61                  | 5.71     | 6.10 | 2.23 | 2.50 | 4.85 |      |      |      |
| C <sup>12</sup> | 7.69                  | 5.81     | 6.26 | 2.28 | 2.28 | 4.57 | 4.06 |      |      |
| G <sup>13</sup> | 7.84                  |          | 5.65 | 2.48 | 2.67 | 4.82 | 4.17 | 3.66 |      |
| G <sup>14</sup> | 7.85                  |          | 5.59 | 2.70 | 2.80 | 5.03 | 4.38 | 4.07 | 4.14 |
| A <sup>15</sup> | 8.21                  | 7.92     | 6.27 | 2.75 | 2.92 | 5.07 | 4.51 | 4.26 |      |
| C <sup>16</sup> | 7.28                  | 5.23     | 5.81 | 1.94 | 2.46 | 4.67 |      | 4.35 |      |
| T <sup>17</sup> | 7.41                  | 1.54     | 6.03 | 2.18 | 2.51 | 4.87 |      |      |      |

|          |      |      |      |      |      |      |      |      |      |
|----------|------|------|------|------|------|------|------|------|------|
| $C^{18}$ | 7.34 | 5.57 | 6.04 | 1.98 | 2.51 | 4.87 |      | 4.13 | 4.09 |
| $G^{19}$ | 7.77 |      | 5.79 | 2.50 | 2.59 | 4.89 | 4.18 | 4.13 | 4.08 |
| $C^{20}$ | 7.40 | 5.24 | 5.86 | 1.98 | 2.43 | 4.71 | 4.02 |      |      |
| $T^{21}$ | 7.38 | 1.64 | 5.58 | 2.10 | 2.40 | 4.86 |      | 4.10 |      |
| $A^{22}$ | 8.22 | 7.44 | 6.04 | 2.75 | 2.89 | 5.05 | 4.41 |      |      |
| $G^{23}$ | 7.69 |      | 5.82 | 2.48 | 2.65 | 4.95 | 4.36 |      |      |
| $C^{24}$ | 7.41 | 5.37 | 6.14 | 2.12 | 2.20 | 4.47 | 4.05 | 5.24 |      |

**Table S2.**  $^1\text{H}$  Chemical Shift Assignments of the 5'-CpX-3' Duplex with Stereoisomer **10**.

| Base            | Chemical Shifts (ppm) |          |      |      |      |      |      |      |      |
|-----------------|-----------------------|----------|------|------|------|------|------|------|------|
|                 | H6/H8                 | H2/H5/Me | H1'  | H2'  | H2'' | H3'  | H4'  | H5'  | H5'' |
| G <sup>1</sup>  | 8.01                  |          | 6.04 | 2.69 | 2.81 | 4.87 | 4.28 | 3.76 |      |
| C <sup>2</sup>  | 7.56                  | 5.42     | 6.09 | 2.15 | 2.54 | 4.84 | 4.28 | 4.23 | 4.18 |
| T <sup>3</sup>  | 7.43                  | 1.70     | 5.60 | 2.17 | 2.45 | 4.90 | 4.17 |      |      |
| A <sup>4</sup>  | 8.23                  | 7.45     | 6.05 | 2.77 | 2.91 | 5.08 | 4.42 | 4.07 | 4.16 |
| G <sup>5</sup>  | 7.67                  |          | 5.72 | 2.48 | 2.63 | 4.98 | 4.38 | 4.20 |      |
| C <sup>6</sup>  | 7.26                  | 5.27     | 5.50 | 1.93 | 2.25 | 4.80 | 4.10 | 4.20 |      |
| X <sup>7</sup>  | 7.70                  |          | 5.92 | 2.50 | 2.80 | 5.00 | 4.29 | 4.12 | 3.98 |
| A <sup>8</sup>  | 8.02                  | 7.58     | 6.01 | 2.65 | 2.77 | 5.03 | 4.29 |      | 4.14 |
| G <sup>9</sup>  | 7.40                  |          | 5.88 | 2.47 | 2.63 | 4.66 | 4.30 | 4.23 | 4.26 |
| T <sup>10</sup> | 7.38                  | 1.18     | 6.09 | 2.20 | 2.57 | 4.85 |      | 4.21 | 4.19 |
| C <sup>11</sup> | 7.64                  | 5.73     | 6.12 | 2.25 | 2.53 | 4.87 |      | 4.13 |      |
| C <sup>12</sup> | 7.71                  | 5.84     | 6.28 | 2.30 | 2.30 | 4.59 | 4.07 | 4.24 |      |
| G <sup>13</sup> | 7.85                  |          | 5.68 | 2.49 | 2.68 | 4.84 | 4.18 | 3.68 |      |
| G <sup>14</sup> | 7.86                  |          | 5.62 | 2.70 | 2.81 | 5.05 | 4.40 | 4.09 |      |
| A <sup>15</sup> | 8.22                  | 7.95     | 6.31 | 2.76 | 2.95 | 5.08 | 4.52 | 4.22 | 4.27 |
| C <sup>16</sup> | 7.24                  | 5.23     | 5.81 | 1.95 | 2.50 | 4.68 |      | 4.37 |      |
| T <sup>17</sup> | 7.37                  | 1.53     | 6.02 | 2.11 | 2.44 | 4.88 |      |      |      |
| C <sup>18</sup> | 7.38                  | 5.54     | 5.93 | 2.04 | 2.46 | 4.88 | 4.13 | 4.08 | 4.04 |

|          |      |      |      |      |      |      |      |      |      |
|----------|------|------|------|------|------|------|------|------|------|
| $G^{19}$ | 7.89 |      | 5.82 | 2.63 | 2.65 | 4.98 | 4.22 | 4.12 | 4.04 |
| $C^{20}$ | 7.45 | 5.32 | 5.91 | 2.04 | 2.45 | 4.73 |      | 4.18 |      |
| $T^{21}$ | 7.40 | 1.67 | 5.58 | 2.11 | 2.40 | 4.87 | 4.14 |      |      |
| $A^{22}$ | 8.24 | 7.44 | 6.06 | 2.76 | 2.90 | 5.06 | 4.40 | 4.05 | 4.16 |
| $G^{23}$ | 7.70 |      | 5.83 | 2.49 | 2.66 | 4.96 | 4.37 |      |      |
| $C^{24}$ | 7.43 | 5.41 | 6.15 | 2.13 | 2.22 | 4.48 | 4.08 | 4.19 |      |

**Table S3.** NOE restraints utilized in the rMD calculation for the 5'-CpX-3' duplex with stereoisomer **8**.

| Residue 1 |     | Atom 1 | Residue 2 |     | Atom 2 | Lower bond | Upper Bond |
|-----------|-----|--------|-----------|-----|--------|------------|------------|
| 1         | DG5 | H8     | 1         | DG5 | H1'    | 3.33       | 4.51       |
| 1         | DG5 | H3'    | 1         | DG5 | H8     | 2.77       | 4.92       |
| 1         | DG5 | H2'    | 1         | DG5 | H8     | 1.80       | 2.44       |
| 1         | DG5 | H2''   | 1         | DG5 | H8     | 2.99       | 3.93       |
| 1         | DG5 | H2''   | 1         | DG5 | H3'    | 2.14       | 2.82       |
| 2         | DC  | H6     | 1         | DG5 | H8     | 4.67       | 6.31       |
| 2         | DC  | H6     | 1         | DG5 | H2''   | 2.06       | 2.78       |
| 2         | DC  | H5     | 1         | DG5 | H8     | 3.31       | 4.49       |
| 2         | DC  | H5     | 1         | DG5 | H3'    | 4.03       | 5.45       |
| 2         | DC  | H5     | 1         | DG5 | H2''   | 2.60       | 3.46       |
| 2         | DC  | H2'    | 2         | DC  | H6     | 1.91       | 2.59       |
| 3         | DT  | M7     | 2         | DC  | H6     | 2.98       | 4.04       |
| 3         | DT  | M7     | 2         | DC  | H5     | 3.23       | 4.37       |
| 5         | DG  | H3'    | 5         | DG  | H1'    | 3.38       | 4.58       |
| 5         | DG  | H3'    | 5         | DG  | H8     | 3.27       | 4.39       |
| 5         | DG  | H2''   | 5         | DG  | H1'    | 1.93       | 2.61       |
| 6         | DC  | H5'    | 5         | DG  | H1'    | 2.54       | 3.50       |
| 6         | DC  | H6     | 5         | DG  | H8     | 3.60       | 4.92       |

|    |     |      |    |     |     |      |      |
|----|-----|------|----|-----|-----|------|------|
| 6  | DC  | H6   | 5  | DG  | H3' | 3.83 | 5.99 |
| 6  | DC  | H5   | 5  | DG  | H1' | 3.84 | 5.39 |
| 6  | DC  | H5   | 5  | DG  | H8  | 3.15 | 4.27 |
| 6  | DC  | H3'  | 6  | DC  | H6  | 3.14 | 4.24 |
| 6  | DC  | H2'  | 6  | DC  | H3' | 2.24 | 3.02 |
| 6  | DC  | H2'' | 6  | DC  | H5  | 3.12 | 5.54 |
| 6  | DC  | H2'' | 6  | DC  | H3' | 2.42 | 3.28 |
| 9  | DG  | H8   | 8  | DA  | H8  | 3.04 | 4.12 |
| 10 | DT  | H6   | 9  | DG  | H8  | 3.69 | 4.99 |
| 10 | DT  | M7   | 9  | DG  | H8  | 3.01 | 4.07 |
| 10 | DT  | H2'  | 10 | DT  | H6  | 1.91 | 2.59 |
| 11 | DC  | H6   | 10 | DT  | H6  | 3.20 | 5.35 |
| 11 | DC  | H5   | 10 | DT  | H6  | 3.58 | 4.84 |
| 11 | DC  | H5   | 10 | DT  | M7  | 3.61 | 4.89 |
| 11 | DC  | H5   | 10 | DT  | H2' | 2.87 | 3.89 |
| 12 | DC3 | H6   | 12 | DC3 | H1' | 2.85 | 3.85 |
| 12 | DC3 | H5   | 11 | DC  | H6  | 3.52 | 4.76 |
| 12 | DC3 | H3'  | 12 | DC3 | H1' | 3.34 | 4.52 |
| 12 | DC3 | H3'  | 12 | DC3 | H6  | 2.10 | 2.84 |
| 13 | DG5 | H3'  | 13 | DG5 | H1' | 3.06 | 5.01 |
| 13 | DG5 | H2'' | 13 | DG5 | H1' | 1.88 | 2.54 |

|    |    |      |    |     |      |      |      |
|----|----|------|----|-----|------|------|------|
| 14 | DG | H4'  | 13 | DG5 | H1'  | 3.13 | 5.63 |
| 14 | DG | H8   | 14 | DG  | H4'  | 4.42 | 5.61 |
| 14 | DG | H3'  | 14 | DG  | H8   | 3.01 | 4.07 |
| 15 | DA | H8   | 14 | DG  | H8   | 4.02 | 5.37 |
| 15 | DA | H8   | 15 | DA  | H1'  | 2.99 | 4.05 |
| 15 | DA | H2   | 15 | DA  | H1'  | 4.05 | 5.49 |
| 15 | DA | H3'  | 15 | DA  | H1'  | 3.19 | 4.31 |
| 15 | DA | H2'  | 15 | DA  | H1'  | 2.27 | 3.07 |
| 15 | DA | H2'' | 15 | DA  | H1'  | 1.98 | 2.68 |
| 16 | DC | H5'  | 15 | DA  | H1'  | 2.52 | 3.40 |
| 16 | DC | H1'  | 15 | DA  | H1'  | 3.68 | 4.55 |
| 16 | DC | H1'  | 15 | DA  | H2   | 3.50 | 5.50 |
| 16 | DC | H6   | 15 | DA  | H1'  | 2.97 | 4.01 |
| 16 | DC | H6   | 15 | DA  | H8   | 3.43 | 4.65 |
| 16 | DC | H6   | 15 | DA  | H3'  | 4.00 | 5.16 |
| 16 | DC | H6   | 15 | DA  | H2'' | 2.26 | 3.06 |
| 16 | DC | H6   | 16 | DC  | H5'  | 3.48 | 4.55 |
| 16 | DC | H5   | 15 | DA  | H1'  | 4.83 | 6.17 |
| 16 | DC | H5   | 15 | DA  | H8   | 3.22 | 4.36 |
| 16 | DC | H5   | 15 | DA  | H2'  | 2.83 | 3.83 |
| 16 | DC | H5   | 15 | DA  | H2'' | 2.99 | 4.05 |

|    |     |     |    |     |     |      |      |
|----|-----|-----|----|-----|-----|------|------|
| 16 | DC  | H3' | 16 | DC  | H6  | 3.17 | 4.29 |
| 16 | DC  | H2' | 16 | DC  | H5' | 3.78 | 4.70 |
| 17 | DT  | M7  | 16 | DC  | H6  | 2.53 | 3.43 |
| 17 | DT  | M7  | 16 | DC  | H5  | 2.52 | 3.42 |
| 17 | DT  | M7  | 16 | DC  | H3' | 2.95 | 3.99 |
| 17 | DT  | M7  | 16 | DC  | H2' | 2.66 | 3.60 |
| 17 | DT  | H3' | 17 | DT  | M7  | 4.34 | 5.86 |
| 17 | DT  | H2' | 17 | DT  | M7  | 3.02 | 4.08 |
| 18 | DC  | H6  | 17 | DT  | H2' | 2.23 | 3.75 |
| 19 | DG  | H8  | 18 | DC  | H2' | 2.70 | 3.68 |
| 20 | DC  | H6  | 19 | DG  | H8  | 4.20 | 5.38 |
| 20 | DC  | H5  | 19 | DG  | H8  | 3.59 | 4.85 |
| 21 | DT  | M7  | 20 | DC  | H5  | 2.69 | 3.65 |
| 23 | DG  | H3' | 23 | DG  | H8  | 3.39 | 4.51 |
| 24 | DC3 | H6  | 23 | DG  | H8  | 3.76 | 4.65 |
| 24 | DC3 | H5  | 23 | DG  | H8  | 3.84 | 4.74 |
| 24 | DC3 | H5  | 23 | DG  | H3' | 4.92 | 7.00 |
| 24 | DC3 | H3' | 24 | DC3 | H1' | 3.30 | 4.46 |
| 24 | DC3 | H3' | 24 | DC3 | H6  | 3.02 | 3.90 |
| 25 | HNE | M9  | 7  | DGH | H5' | 3.45 | 4.53 |
| 25 | HNE | H1  | 25 | HNE | Q8  | 5.00 | 7.00 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 25 | HNE | H1   | 25 | HNE | H3   | 3.27 | 5.57 |
| 1  | DG5 | Q5'  | 1  | DG5 | H1'  | 4.53 | 5.79 |
| 1  | DG5 | Q5'  | 1  | DG5 | H8   | 3.19 | 4.31 |
| 1  | DG5 | Q5'  | 1  | DG5 | H2'  | 2.97 | 4.03 |
| 1  | DG5 | Q5'  | 1  | DG5 | H2'' | 4.30 | 7.52 |
| 1  | DG5 | H4'  | 1  | DG5 | H8   | 4.06 | 5.48 |
| 2  | DC  | H1'  | 3  | DT  | M7   | 3.72 | 5.04 |
| 2  | DC  | H3'  | 3  | DT  | M7   | 3.27 | 4.43 |
| 2  | DC  | H2'' | 3  | DT  | M7   | 2.78 | 3.76 |
| 3  | DT  | H1'  | 3  | DT  | M7   | 4.00 | 5.40 |
| 5  | DG  | H4'  | 5  | DG  | H1'  | 2.47 | 3.33 |
| 5  | DG  | H4'  | 5  | DG  | H8   | 4.24 | 5.74 |
| 4  | DA  | H3'  | 5  | DG  | H8   | 4.30 | 6.33 |
| 4  | DA  | H2'  | 5  | DG  | H8   | 2.57 | 3.47 |
| 4  | DA  | H2'' | 5  | DG  | H8   | 2.23 | 3.03 |
| 6  | DC  | H1'  | 6  | DC  | H6   | 3.10 | 5.64 |
| 6  | DC  | H1'  | 6  | DC  | H2'  | 2.26 | 3.06 |
| 6  | DC  | H1'  | 7  | DGH | H5'' | 4.13 | 5.27 |
| 6  | DC  | H1'  | 7  | DGH | H8   | 3.23 | 4.37 |
| 6  | DC  | H1'  | 25 | HNE | M9   | 6.38 | 8.64 |
| 6  | DC  | H1'  | 25 | HNE | Q8   | 4.85 | 6.57 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 7  | DGH | H1'  | 7  | DGH | H2'' | 1.80 | 2.44 |
| 8  | DA  | H3'  | 9  | DG  | H8   | 3.37 | 4.55 |
| 8  | DA  | H3'  | 25 | HNE | M9   | 4.86 | 6.58 |
| 8  | DA  | H2'' | 9  | DG  | H8   | 2.23 | 3.01 |
| 9  | DG  | H1'  | 10 | DT  | H6   | 3.43 | 4.63 |
| 10 | DT  | H1'  | 10 | DT  | H6   | 3.26 | 4.42 |
| 10 | DT  | H1'  | 11 | DC  | H5   | 3.44 | 4.66 |
| 9  | DG  | H2'  | 10 | DT  | M7   | 2.77 | 4.03 |
| 9  | DG  | H2'' | 10 | DT  | M7   | 2.56 | 3.46 |
| 10 | DT  | H3'  | 11 | DC  | H5   | 3.82 | 5.06 |
| 12 | DC3 | H4'  | 12 | DC3 | H1'  | 2.37 | 3.21 |
| 11 | DC  | H3'  | 12 | DC3 | H6   | 3.19 | 4.71 |
| 11 | DC  | H2'' | 12 | DC3 | H3'  | 3.52 | 5.18 |
| 13 | DG5 | Q5'  | 13 | DG5 | H1'  | 4.07 | 5.51 |
| 13 | DG5 | Q5'  | 13 | DG5 | H8   | 3.25 | 4.41 |
| 13 | DG5 | Q5'  | 13 | DG5 | H2'  | 3.14 | 4.26 |
| 13 | DG5 | Q5'  | 13 | DG5 | H2'' | 4.79 | 6.47 |
| 14 | DG  | H5'  | 14 | DG  | H8   | 3.40 | 4.60 |
| 15 | DA  | H4'  | 15 | DA  | H1'  | 2.69 | 3.63 |
| 15 | DA  | H4'  | 15 | DA  | H8   | 4.29 | 5.52 |
| 15 | DA  | H4'  | 15 | DA  | H2'' | 3.91 | 4.86 |

|    |     |      |    |     |     |      |      |
|----|-----|------|----|-----|-----|------|------|
| 16 | DC  | H2'' | 17 | DT  | M7  | 3.15 | 4.25 |
| 17 | DT  | H1'  | 18 | DC  | H5  | 3.61 | 4.89 |
| 18 | DC  | H1'  | 18 | DC  | H2' | 2.35 | 3.17 |
| 18 | DC  | H1'  | 19 | DG  | H8  | 4.06 | 5.38 |
| 18 | DC  | H3'  | 18 | DC  | H2' | 1.95 | 2.63 |
| 19 | DG  | H1'  | 19 | DG  | H8  | 3.02 | 4.02 |
| 19 | DG  | H1'  | 20 | DC  | H5  | 3.14 | 4.22 |
| 19 | DG  | H1'  | 25 | HNE | H1  | 4.00 | 5.00 |
| 19 | DG  | H2'' | 20 | DC  | H5  | 2.30 | 3.12 |
| 20 | DC  | H3'  | 21 | DT  | M7  | 3.03 | 4.11 |
| 20 | DC  | H2'  | 21 | DT  | M7  | 2.65 | 3.58 |
| 21 | DT  | H1'  | 21 | DT  | M7  | 5.02 | 6.46 |
| 22 | DA  | H3'  | 23 | DG  | H8  | 4.20 | 5.64 |
| 22 | DA  | H2'' | 23 | DG  | H8  | 2.21 | 2.99 |
| 23 | DG  | H1'  | 24 | DC3 | H1' | 3.48 | 4.70 |
| 23 | DG  | H1'  | 24 | DC3 | H5  | 4.22 | 5.70 |
| 24 | DC3 | H5'  | 24 | DC3 | H1' | 3.56 | 4.32 |
| 24 | DC3 | H4'  | 24 | DC3 | H1' | 2.27 | 3.07 |
| 23 | DG  | H2'' | 24 | DC3 | H3' | 4.45 | 5.93 |
| 7  | DGH | H3'  | 25 | HNE | M9  | 4.15 | 5.61 |
| 7  | DGH | H3'  | 25 | HNE | Q8  | 3.36 | 4.52 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 8  | DA  | H5'  | 25 | HNE | M9   | 2.51 | 3.39 |
| 8  | DA  | H5'  | 25 | HNE | H52  | 3.66 | 8.00 |
| 8  | DA  | H4'  | 25 | HNE | M9   | 4.77 | 6.45 |
| 8  | DA  | H1'  | 25 | HNE | H3   | 2.16 | 2.92 |
| 8  | DA  | H2   | 25 | HNE | H3   | 3.69 | 4.85 |
| 18 | DC  | H2'' | 25 | HNE | H1   | 4.50 | 5.50 |
| 19 | DG  | H4'  | 25 | HNE | H1   | 3.00 | 4.00 |
| 25 | HNE | H4   | 25 | HNE | H1   | 3.04 | 4.14 |
| 5  | DG  | H2'  | 5  | DG  | H8   | 1.95 | 2.63 |
| 6  | DC  | H5   | 5  | DG  | H2'  | 3.14 | 4.26 |
| 6  | DC  | H2'  | 6  | DC  | H5   | 3.52 | 4.41 |
| 9  | DG  | H2'  | 9  | DG  | H8   | 1.96 | 2.66 |
| 10 | DT  | H6   | 9  | DG  | H2'  | 3.04 | 4.12 |
| 10 | DT  | H6   | 9  | DG  | H2'' | 2.30 | 3.10 |
| 10 | DT  | H2'' | 10 | DT  | H6   | 2.86 | 3.68 |
| 10 | DT  | H2'' | 10 | DT  | M7   | 3.90 | 5.08 |
| 11 | DC  | H2'  | 11 | DC  | H6   | 1.96 | 2.42 |
| 13 | DG5 | H2'  | 13 | DG5 | H1'  | 2.23 | 3.01 |
| 14 | DG  | H5'  | 13 | DG5 | H1'  | 2.64 | 3.56 |
| 14 | DG  | H3'  | 14 | DG  | H1'  | 3.65 | 4.78 |
| 14 | DG  | H2'  | 14 | DG  | H1'  | 2.27 | 2.97 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 14 | DG  | H2'' | 14 | DG  | H1'  | 1.92 | 2.60 |
| 15 | DA  | H5'  | 14 | DG  | H1'  | 3.12 | 4.62 |
| 16 | DC  | H2'  | 16 | DC  | H3'  | 1.98 | 2.68 |
| 16 | DC  | H2'' | 16 | DC  | H3'  | 2.35 | 3.19 |
| 18 | DC  | H5   | 17 | DT  | H2'' | 2.19 | 2.95 |
| 20 | DC  | H2'  | 20 | DC  | H1'  | 2.86 | 3.86 |
| 20 | DC  | H2'  | 20 | DC  | H3'  | 1.74 | 2.36 |
| 20 | DC  | H2'' | 20 | DC  | H1'  | 1.78 | 2.40 |
| 20 | DC  | H2'' | 20 | DC  | H3'  | 3.05 | 3.81 |
| 21 | DT  | H5'  | 20 | DC  | H1'  | 2.31 | 2.87 |
| 21 | DT  | M7   | 20 | DC  | H1'  | 4.67 | 6.33 |
| 24 | DC3 | H6   | 23 | DG  | H2'' | 2.08 | 2.82 |
| 24 | DC3 | H2'' | 24 | DC3 | H5   | 3.22 | 5.54 |
| 25 | HNE | M9   | 20 | DC  | H1'  | 5.03 | 6.81 |
| 25 | HNE | H52  | 20 | DC  | H1'  | 3.25 | 4.41 |
| 25 | HNE | H4   | 25 | HNE | H51  | 1.97 | 2.59 |
| 25 | HNE | H4   | 25 | HNE | H52  | 2.32 | 3.04 |
| 1  | DG5 | H1'  | 2  | DC  | H5   | 3.37 | 4.57 |
| 4  | DA  | H8   | 5  | DG  | H8   | 3.37 | 4.57 |
| 5  | DG  | H1'  | 5  | DG  | H2'  | 2.41 | 3.25 |
| 5  | DG  | H1'  | 6  | DC  | H6   | 3.14 | 3.92 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 5  | DG  | H2'' | 6  | DC  | H6   | 2.17 | 3.01 |
| 5  | DG  | H2'' | 6  | DC  | H5   | 2.93 | 4.07 |
| 6  | DC  | H5'  | 6  | DC  | H6   | 3.02 | 4.02 |
| 6  | DC  | H1'  | 6  | DC  | H2'' | 2.02 | 2.72 |
| 7  | DGH | H1'  | 7  | DGH | H8   | 2.97 | 3.91 |
| 7  | DGH | H1'  | 8  | DA  | H8   | 2.55 | 3.45 |
| 7  | DGH | H1'  | 25 | HNE | M9   | 3.79 | 5.13 |
| 7  | DGH | H3'  | 7  | DGH | H2'' | 2.28 | 3.08 |
| 8  | DA  | H5'  | 8  | DA  | H8   | 3.61 | 4.89 |
| 8  | DA  | H5'  | 25 | HNE | Q8   | 2.24 | 3.10 |
| 8  | DA  | H5'  | 25 | HNE | H51  | 3.04 | 4.18 |
| 8  | DA  | H4'  | 8  | DA  | H8   | 4.26 | 5.76 |
| 8  | DA  | H4'  | 25 | HNE | H51  | 2.67 | 3.51 |
| 8  | DA  | H4'  | 25 | HNE | H52  | 4.09 | 5.06 |
| 8  | DA  | H1'  | 8  | DA  | H8   | 2.97 | 4.03 |
| 9  | DG  | H4'  | 9  | DG  | H8   | 3.82 | 5.18 |
| 9  | DG  | H4'  | 9  | DG  | H2'' | 2.93 | 3.83 |
| 9  | DG  | H1'  | 9  | DG  | H8   | 3.74 | 5.06 |
| 9  | DG  | H3'  | 10 | DT  | M7   | 4.00 | 5.39 |
| 10 | DT  | H2'  | 11 | DC  | H6   | 2.75 | 3.41 |
| 11 | DC  | H1'  | 11 | DC  | H2'  | 2.28 | 2.98 |

|    |     |     |    |     |      |      |      |
|----|-----|-----|----|-----|------|------|------|
| 11 | DC  | H1' | 12 | DC3 | H5   | 4.63 | 6.52 |
| 13 | DG5 | H4' | 13 | DG5 | H1'  | 2.48 | 3.36 |
| 13 | DG5 | H3' | 13 | DG5 | H2'' | 2.26 | 2.98 |
| 14 | DG  | H4' | 14 | DG  | H1'  | 2.68 | 3.62 |
| 14 | DG  | H4' | 14 | DG  | H2'' | 2.94 | 3.98 |
| 15 | DA  | H2' | 16 | DC  | H6   | 2.41 | 3.82 |
| 16 | DC  | H1' | 16 | DC  | H6   | 3.51 | 4.75 |
| 16 | DC  | H1' | 16 | DC  | H3'  | 3.87 | 5.31 |
| 16 | DC  | H1' | 16 | DC  | H2'  | 2.34 | 3.06 |
| 15 | DA  | H3' | 16 | DC  | H5   | 4.49 | 6.01 |
| 17 | DT  | M7  | 17 | DT  | H2'' | 3.71 | 4.95 |
| 18 | DC  | H6  | 18 | DC  | H2'  | 1.76 | 2.38 |
| 20 | DC  | H4' | 20 | DC  | H1'  | 2.39 | 3.23 |
| 19 | DG  | H3' | 20 | DC  | H5   | 3.67 | 6.83 |
| 22 | DA  | H8  | 23 | DG  | H8   | 3.45 | 4.59 |
| 22 | DA  | H2' | 23 | DG  | H8   | 2.49 | 4.47 |
| 23 | DG  | H4' | 23 | DG  | H8   | 4.44 | 5.72 |
| 23 | DG  | H1' | 23 | DG  | H3'  | 3.21 | 4.35 |
| 24 | DC3 | H1' | 24 | DC3 | H6   | 2.82 | 4.18 |
| 24 | DC3 | H1' | 24 | DC3 | H2'  | 2.43 | 3.23 |
| 24 | DC3 | H1' | 24 | DC3 | H2'' | 1.84 | 2.50 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 23 | DG  | H2'  | 24 | DC3 | H5   | 3.70 | 5.00 |
| 24 | DC3 | H3'  | 24 | DC3 | H2'  | 1.95 | 2.63 |
| 24 | DC3 | H3'  | 24 | DC3 | H2'' | 2.83 | 3.83 |
| 7  | DGH | H4'  | 25 | HNE | M9   | 2.66 | 3.66 |
| 8  | DA  | H5'' | 25 | HNE | M9   | 3.21 | 4.35 |
| 18 | DC  | H1'  | 25 | HNE | H1   | 4.00 | 5.00 |
| 2  | DC  | H5   | 1  | DG5 | H2'  | 2.46 | 3.32 |
| 2  | DC  | H2'  | 2  | DC  | H5   | 3.39 | 4.31 |
| 2  | DC  | H2'' | 2  | DC  | H5   | 3.72 | 5.51 |
| 3  | DT  | M7   | 2  | DC  | H2'  | 2.70 | 3.66 |
| 4  | DA  | H8   | 3  | DT  | H6   | 3.99 | 5.39 |
| 7  | DGH | H3'  | 7  | DGH | H8   | 3.24 | 4.32 |
| 7  | DGH | H2'  | 7  | DGH | H8   | 2.03 | 2.75 |
| 7  | DGH | H2'  | 7  | DGH | H3'  | 2.04 | 2.76 |
| 7  | DGH | H2'' | 7  | DGH | H8   | 2.81 | 3.69 |
| 8  | DA  | H3'  | 8  | DA  | H8   | 3.14 | 4.04 |
| 8  | DA  | H2'  | 8  | DA  | H1'  | 2.29 | 3.09 |
| 8  | DA  | H2'  | 8  | DA  | H3'  | 2.02 | 2.72 |
| 9  | DG  | H2'' | 9  | DG  | H3'  | 2.19 | 2.97 |
| 12 | DC3 | H5   | 11 | DC  | H2'  | 2.82 | 3.82 |
| 19 | DG  | H3'  | 19 | DG  | H8   | 3.17 | 4.19 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 19 | DG  | H2'' | 19 | DG  | H3'  | 2.44 | 3.30 |
| 20 | DC  | H6   | 19 | DG  | H2'' | 1.72 | 2.88 |
| 21 | DT  | H3'  | 21 | DT  | M7   | 4.74 | 6.42 |
| 21 | DT  | H2'  | 21 | DT  | M7   | 2.98 | 3.86 |
| 21 | DT  | H2'' | 21 | DT  | H3'  | 2.17 | 2.79 |
| 25 | HNE | Q8   | 8  | DA  | H3'  | 4.06 | 5.50 |
| 25 | HNE | H22  | 25 | HNE | H51  | 3.00 | 5.00 |
| 25 | HNE | H21  | 25 | HNE | H51  | 3.00 | 5.00 |
| 25 | HNE | H3   | 8  | DA  | H8   | 3.81 | 5.09 |
| 25 | HNE | H3   | 25 | HNE | H51  | 2.02 | 2.74 |
| 25 | HNE | H1   | 25 | HNE | H51  | 3.50 | 5.50 |
| 1  | DG5 | H1'  | 1  | DG5 | H2'  | 2.25 | 3.05 |
| 1  | DG5 | H1'  | 1  | DG5 | H2'' | 1.91 | 2.59 |
| 1  | DG5 | H3'  | 1  | DG5 | H2'  | 1.71 | 2.31 |
| 2  | DC  | H1'  | 3  | DT  | H6   | 3.32 | 4.50 |
| 4  | DA  | H1'  | 5  | DG  | H8   | 3.27 | 4.43 |
| 5  | DG  | H1'  | 5  | DG  | H8   | 2.96 | 3.94 |
| 5  | DG  | H3'  | 5  | DG  | H2'  | 1.95 | 2.63 |
| 5  | DG  | H3'  | 6  | DC  | H5   | 5.04 | 6.82 |
| 6  | DC  | H3'  | 7  | DGH | H8   | 4.52 | 6.12 |
| 6  | DC  | H2'  | 7  | DGH | H8   | 3.37 | 4.21 |

|    |     |      |    |     |     |      |      |
|----|-----|------|----|-----|-----|------|------|
| 6  | DC  | H2'' | 7  | DGH | H8  | 2.41 | 3.25 |
| 7  | DGH | H5'  | 7  | DGH | H8  | 3.28 | 4.44 |
| 7  | DGH | H5'  | 7  | DGH | H2' | 3.10 | 4.20 |
| 7  | DGH | H5'  | 25 | HNE | Q8  | 3.00 | 4.00 |
| 7  | DGH | H5'' | 7  | DGH | H8  | 3.29 | 5.07 |
| 7  | DGH | H4'  | 7  | DGH | H8  | 4.35 | 5.89 |
| 7  | DGH | H1'  | 7  | DGH | H3' | 3.32 | 4.50 |
| 7  | DGH | H1'  | 25 | HNE | Q8  | 2.29 | 3.09 |
| 8  | DA  | H4'  | 8  | DA  | H1' | 2.11 | 2.85 |
| 8  | DA  | H4'  | 25 | HNE | Q8  | 2.76 | 3.74 |
| 8  | DA  | H4'  | 25 | HNE | Q6  | 4.64 | 5.86 |
| 8  | DA  | H5'' | 8  | DA  | H8  | 4.00 | 5.28 |
| 9  | DG  | H8   | 9  | DG  | H3' | 3.22 | 4.36 |
| 10 | DT  | H6   | 10 | DT  | H3' | 3.74 | 5.06 |
| 10 | DT  | M7   | 10 | DT  | H2' | 3.00 | 3.98 |
| 10 | DT  | H1'  | 11 | DC  | H6  | 3.71 | 5.01 |
| 11 | DC  | H1'  | 11 | DC  | H6  | 2.87 | 3.77 |
| 11 | DC  | H1'  | 12 | DC3 | H6  | 3.31 | 4.89 |
| 11 | DC  | H3'  | 11 | DC  | H2' | 1.88 | 2.54 |
| 13 | DG5 | H3'  | 13 | DG5 | H2' | 1.84 | 2.50 |
| 14 | DG  | H1'  | 14 | DG  | H8  | 2.94 | 3.98 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 14 | DG  | H3'  | 14 | DG  | H2'  | 1.90 | 2.58 |
| 14 | DG  | H3'  | 14 | DG  | H2'' | 2.66 | 3.60 |
| 16 | DC  | H3'  | 17 | DT  | H6   | 3.70 | 4.54 |
| 17 | DT  | H1'  | 17 | DT  | H6   | 2.76 | 3.74 |
| 16 | DC  | H1'  | 17 | DT  | M7   | 3.47 | 4.69 |
| 19 | DG  | H5'  | 19 | DG  | H8   | 3.57 | 4.75 |
| 19 | DG  | H5'  | 25 | HNE | H1   | 3.00 | 4.00 |
| 19 | DG  | H5'' | 19 | DG  | H8   | 4.23 | 5.73 |
| 19 | DG  | H4'  | 19 | DG  | H8   | 3.80 | 5.00 |
| 19 | DG  | H1'  | 19 | DG  | H2'' | 1.99 | 2.69 |
| 20 | DC  | H2'' | 21 | DT  | M7   | 2.98 | 4.02 |
| 21 | DT  | H6   | 21 | DT  | H2'  | 1.73 | 2.35 |
| 21 | DT  | H6   | 22 | DA  | H8   | 3.79 | 5.13 |
| 22 | DA  | H1'  | 23 | DG  | H8   | 3.48 | 4.44 |
| 23 | DG  | H3'  | 23 | DG  | H2'  | 1.90 | 2.58 |
| 23 | DG  | H3'  | 24 | DC3 | H6   | 3.89 | 5.27 |
| 23 | DG  | H2'' | 24 | DC3 | H5   | 2.98 | 4.04 |
| 20 | DC  | H1'  | 25 | HNE | Q8   | 3.52 | 4.62 |
| 20 | DC  | H1'  | 25 | HNE | H51  | 3.50 | 5.50 |
| 8  | DA  | H5'  | 25 | HNE | Q6   | 3.35 | 4.45 |
| 25 | HNE | H52  | 25 | HNE | H22  | 3.93 | 4.67 |

|    |     |     |    |     |      |      |      |
|----|-----|-----|----|-----|------|------|------|
| 25 | HNE | H52 | 25 | HNE | H21  | 3.58 | 4.84 |
| 25 | HNE | H52 | 25 | HNE | H3   | 2.56 | 3.38 |
| 25 | HNE | H52 | 25 | HNE | H1   | 4.08 | 5.52 |
| 25 | HNE | M9  | 25 | HNE | H3   | 3.96 | 5.28 |
| 3  | DT  | H6  | 2  | DC  | H3'  | 3.43 | 4.53 |
| 3  | DT  | H2' | 3  | DT  | H3'  | 1.82 | 2.46 |
| 4  | DA  | H8  | 3  | DT  | H3'  | 4.26 | 5.76 |
| 4  | DA  | H8  | 3  | DT  | H2'  | 3.33 | 4.51 |
| 8  | DA  | H8  | 7  | DGH | H2'' | 1.99 | 2.69 |
| 8  | DA  | H2' | 8  | DA  | H8   | 1.94 | 2.62 |
| 12 | DC3 | H5  | 11 | DC  | H3'  | 4.67 | 6.31 |
| 13 | DG5 | H3' | 13 | DG5 | H8   | 3.83 | 5.19 |
| 13 | DG5 | H2' | 13 | DG5 | H8   | 2.12 | 2.76 |
| 17 | DT  | H6  | 16 | DC  | H2'  | 2.45 | 3.31 |
| 22 | DA  | H8  | 21 | DT  | H3'  | 4.09 | 5.53 |
| 22 | DA  | H8  | 21 | DT  | H2'  | 3.03 | 4.11 |
| 25 | HNE | Q7  | 7  | DGH | H1'  | 3.06 | 4.00 |
| 25 | HNE | H4  | 25 | HNE | Q6   | 2.37 | 3.21 |
| 25 | HNE | H3  | 25 | HNE | Q6   | 3.43 | 4.63 |
| 25 | HNE | H3  | 25 | HNE | H21  | 2.05 | 2.67 |
| 25 | HNE | H1  | 25 | HNE | Q6   | 3.75 | 5.07 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 2  | DC  | H6   | 2  | DC  | H3'  | 2.87 | 3.75 |
| 2  | DC  | H1'  | 2  | DC  | H2'' | 1.71 | 2.31 |
| 3  | DT  | H1'  | 3  | DT  | H6   | 2.89 | 3.85 |
| 3  | DT  | H1'  | 3  | DT  | H3'  | 3.00 | 4.06 |
| 3  | DT  | H1'  | 3  | DT  | H2'  | 2.29 | 3.03 |
| 3  | DT  | H1'  | 3  | DT  | H2'' | 1.80 | 2.44 |
| 3  | DT  | M7   | 3  | DT  | H2'' | 3.83 | 5.03 |
| 4  | DA  | H4'  | 4  | DA  | H2'' | 3.17 | 4.29 |
| 5  | DG  | H3'  | 5  | DG  | H2'' | 2.27 | 3.07 |
| 7  | DGH | H4'  | 7  | DGH | H2'  | 2.83 | 3.83 |
| 7  | DGH | H4'  | 7  | DGH | H2'' | 3.91 | 5.29 |
| 7  | DGH | H3'  | 8  | DA  | H8   | 3.83 | 5.11 |
| 9  | DG  | H4'  | 9  | DG  | H2'  | 3.28 | 4.44 |
| 9  | DG  | H3'  | 10 | DT  | H6   | 3.83 | 6.59 |
| 10 | DT  | H2'' | 11 | DC  | H5   | 2.86 | 3.88 |
| 11 | DC  | H6   | 11 | DC  | H3'  | 2.76 | 3.58 |
| 11 | DC  | H1'  | 11 | DC  | H2'' | 1.71 | 2.31 |
| 11 | DC  | H2'  | 12 | DC3 | H6   | 2.65 | 3.39 |
| 13 | DG5 | H4'  | 13 | DG5 | H8   | 4.04 | 5.10 |
| 13 | DG5 | H1'  | 13 | DG5 | H8   | 2.87 | 3.89 |
| 14 | DG  | H5'' | 14 | DG  | H8   | 3.44 | 4.58 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 16 | DC  | H5   | 16 | DC  | H2'  | 3.34 | 4.40 |
| 17 | DT  | H1'  | 17 | DT  | H2'  | 2.30 | 3.10 |
| 17 | DT  | H3'  | 17 | DT  | H2'  | 1.99 | 2.69 |
| 18 | DC  | H6   | 18 | DC  | H3'  | 2.90 | 3.92 |
| 20 | DC  | H6   | 20 | DC  | H3'  | 2.95 | 3.93 |
| 21 | DT  | H1'  | 21 | DT  | H3'  | 3.22 | 4.36 |
| 21 | DT  | H1'  | 21 | DT  | H2'  | 2.27 | 3.07 |
| 21 | DT  | H1'  | 21 | DT  | H2'' | 1.73 | 2.35 |
| 22 | DA  | H4'  | 22 | DA  | H2'' | 2.68 | 3.62 |
| 23 | DG  | H3'  | 23 | DG  | H2'' | 2.15 | 2.91 |
| 7  | DGH | H5'  | 25 | HNE | Q7   | 4.00 | 6.00 |
| 7  | DGH | H5'  | 25 | HNE | Q6   | 3.80 | 4.90 |
| 8  | DA  | H4'  | 25 | HNE | Q7   | 3.04 | 4.12 |
| 8  | DA  | H4'  | 25 | HNE | H21  | 3.66 | 4.78 |
| 8  | DA  | H3'  | 25 | HNE | Q7   | 4.19 | 5.67 |
| 20 | DC  | H1'  | 25 | HNE | Q7   | 5.42 | 6.92 |
| 20 | DC  | H1'  | 25 | HNE | Q6   | 2.48 | 3.28 |
| 25 | HNE | Q8   | 25 | HNE | H3   | 3.26 | 4.26 |
| 19 | DG  | H5'' | 25 | HNE | H1   | 4.00 | 5.00 |
| 25 | HNE | H22  | 25 | HNE | H1   | 2.50 | 3.50 |
| 2  | DC  | H6   | 1  | DG5 | H3'  | 3.74 | 4.66 |

|   |    |      |   |     |      |      |      |
|---|----|------|---|-----|------|------|------|
| 2 | DC | H2'  | 2 | DC  | H3'  | 2.26 | 3.06 |
| 2 | DC | H2'' | 2 | DC  | H3'  | 2.18 | 2.84 |
| 3 | DT | H6   | 2 | DC  | H6   | 3.37 | 4.57 |
| 3 | DT | H6   | 2 | DC  | H2'  | 2.38 | 3.22 |
| 3 | DT | H6   | 2 | DC  | H2'' | 2.01 | 3.49 |
| 3 | DT | H2'  | 3 | DT  | H6   | 1.92 | 2.60 |
| 3 | DT | H2'' | 3 | DT  | H3'  | 2.13 | 2.77 |
| 4 | DA | H3'  | 4 | DA  | H1'  | 2.95 | 3.89 |
| 4 | DA | H2'  | 4 | DA  | H1'  | 3.01 | 4.07 |
| 4 | DA | H2'  | 4 | DA  | H8   | 1.98 | 2.50 |
| 4 | DA | H2'' | 4 | DA  | H1'  | 1.85 | 2.51 |
| 4 | DA | H2'' | 4 | DA  | H8   | 2.80 | 3.78 |
| 4 | DA | H2'' | 4 | DA  | H3'  | 2.17 | 2.93 |
| 6 | DC | H6   | 5 | DG  | H2'  | 2.69 | 3.99 |
| 6 | DC | H2'  | 6 | DC  | H6   | 1.91 | 2.59 |
| 8 | DA | H8   | 7 | DGH | H2'  | 2.81 | 3.65 |
| 8 | DA | H2'' | 8 | DA  | H8   | 3.22 | 4.00 |
| 8 | DA | H2'' | 8 | DA  | H3'  | 2.10 | 2.84 |
| 9 | DG | H8   | 8 | DA  | H2'  | 2.00 | 2.70 |
| 9 | DG | H2'  | 9 | DG  | H1'  | 2.58 | 3.18 |
| 9 | DG | H2'  | 9 | DG  | H3'  | 1.95 | 2.63 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 9  | DG  | H2'' | 9  | DG  | H1'  | 2.04 | 2.76 |
| 10 | DT  | M7   | 9  | DG  | H1'  | 3.43 | 4.65 |
| 10 | DT  | H3'  | 10 | DT  | M7   | 4.13 | 5.53 |
| 10 | DT  | H2'  | 10 | DT  | H3'  | 1.79 | 2.41 |
| 10 | DT  | H2'' | 10 | DT  | H3'  | 2.37 | 3.11 |
| 11 | DC  | H6   | 10 | DT  | H2'' | 1.97 | 3.38 |
| 11 | DC  | H2'' | 11 | DC  | H3'  | 2.36 | 2.82 |
| 12 | DC3 | H6   | 11 | DC  | H2'' | 2.27 | 3.07 |
| 12 | DC3 | H2'  | 12 | DC3 | H6   | 1.93 | 2.61 |
| 14 | DG  | H8   | 13 | DG5 | H2'' | 2.13 | 2.87 |
| 14 | DG  | H2'  | 14 | DG  | H8   | 2.03 | 2.51 |
| 15 | DA  | H8   | 14 | DG  | H2'  | 2.30 | 3.12 |
| 15 | DA  | H2'  | 15 | DA  | H8   | 2.33 | 3.09 |
| 15 | DA  | H2'  | 15 | DA  | H3'  | 1.84 | 3.40 |
| 15 | DA  | H2'' | 15 | DA  | H8   | 2.87 | 3.77 |
| 15 | DA  | H2'' | 15 | DA  | H3'  | 2.39 | 3.23 |
| 16 | DC  | H2'  | 16 | DC  | H6   | 1.80 | 2.44 |
| 16 | DC  | H2'' | 16 | DC  | H6   | 3.05 | 3.91 |
| 17 | DT  | H6   | 16 | DC  | H2'' | 2.06 | 3.86 |
| 17 | DT  | H2'  | 17 | DT  | H6   | 2.07 | 2.75 |
| 17 | DT  | H2'' | 17 | DT  | H6   | 2.76 | 3.60 |

|    |    |      |    |    |      |      |      |
|----|----|------|----|----|------|------|------|
| 17 | DT | H2'' | 17 | DT | H3'  | 2.17 | 2.75 |
| 18 | DC | H6   | 17 | DT | H2'' | 2.05 | 3.88 |
| 18 | DC | H6   | 18 | DC | H1'  | 2.95 | 3.85 |
| 18 | DC | H5   | 17 | DT | H6   | 3.02 | 3.72 |
| 18 | DC | H5   | 17 | DT | H2'  | 2.51 | 3.39 |
| 18 | DC | H2'' | 18 | DC | H1'  | 2.21 | 2.86 |
| 18 | DC | H2'' | 18 | DC | H6   | 3.17 | 3.81 |
| 18 | DC | H2'' | 18 | DC | H3'  | 2.56 | 3.32 |
| 19 | DG | H8   | 18 | DC | H3'  | 3.50 | 4.52 |
| 19 | DG | H8   | 18 | DC | H2'' | 2.17 | 3.72 |
| 19 | DG | H2'  | 19 | DG | H8   | 2.09 | 3.57 |
| 19 | DG | H2'  | 19 | DG | H3'  | 2.23 | 2.87 |
| 20 | DC | H6   | 19 | DG | H2'  | 2.85 | 3.71 |
| 20 | DC | H5   | 19 | DG | H2'  | 2.51 | 3.39 |
| 20 | DC | H2'  | 20 | DC | H6   | 2.03 | 3.99 |
| 20 | DC | H2'' | 20 | DC | H6   | 2.97 | 3.97 |
| 21 | DT | H6   | 20 | DC | H2'  | 2.89 | 3.54 |
| 21 | DT | H6   | 20 | DC | H2'' | 2.35 | 3.11 |
| 21 | DT | M7   | 20 | DC | H6   | 2.70 | 3.26 |
| 21 | DT | H2'' | 21 | DT | M7   | 3.78 | 5.16 |
| 22 | DA | H2'  | 22 | DA | H1'  | 3.01 | 4.17 |

|    |     |      |    |     |     |      |      |
|----|-----|------|----|-----|-----|------|------|
| 22 | DA  | H2'  | 22 | DA  | H8  | 2.15 | 2.91 |
| 22 | DA  | H2'  | 22 | DA  | H3' | 1.99 | 3.53 |
| 22 | DA  | H2'' | 22 | DA  | H1' | 2.25 | 3.05 |
| 22 | DA  | H2'' | 22 | DA  | H8  | 3.25 | 4.41 |
| 22 | DA  | H2'' | 22 | DA  | H3' | 2.59 | 3.51 |
| 23 | DG  | H1'  | 22 | DA  | H2  | 3.77 | 5.09 |
| 23 | DG  | H2'  | 23 | DG  | H1' | 2.56 | 3.11 |
| 23 | DG  | H2'' | 23 | DG  | H1' | 1.96 | 2.46 |
| 24 | DC3 | H6   | 23 | DG  | H1' | 2.93 | 3.97 |
| 24 | DC3 | H6   | 23 | DG  | H2' | 2.87 | 3.71 |
| 24 | DC3 | H2'  | 24 | DC3 | H6  | 1.94 | 2.58 |
| 25 | HNE | Q7   | 25 | HNE | M9  | 1.91 | 2.59 |
| 25 | HNE | Q8   | 25 | HNE | M9  | 2.37 | 3.78 |
| 25 | HNE | Q6   | 25 | HNE | M9  | 4.44 | 6.08 |
| 25 | HNE | H51  | 25 | HNE | M9  | 3.00 | 5.00 |
| 25 | HNE | H4   | 25 | HNE | M9  | 3.53 | 4.77 |
| 25 | HNE | H4   | 25 | HNE | Q7  | 2.48 | 3.50 |
| 25 | HNE | H4   | 25 | HNE | Q8  | 2.99 | 3.97 |
| 25 | HNE | H22  | 25 | HNE | Q6  | 3.51 | 4.75 |
| 25 | HNE | H22  | 25 | HNE | H4  | 1.95 | 2.63 |
| 25 | HNE | H21  | 25 | HNE | H4  | 2.95 | 3.60 |

|    |     |     |    |     |      |      |      |
|----|-----|-----|----|-----|------|------|------|
| 25 | HNE | H3  | 25 | HNE | Q7   | 2.89 | 3.73 |
| 25 | HNE | H3  | 25 | HNE | H4   | 1.99 | 2.69 |
| 25 | HNE | H3  | 25 | HNE | H22  | 2.04 | 2.76 |
| 25 | HNE | H1  | 25 | HNE | H21  | 1.85 | 2.49 |
| 1  | DG5 | H1' | 2  | DC  | H6   | 2.66 | 3.60 |
| 1  | DG5 | H2' | 2  | DC  | H6   | 2.49 | 3.19 |
| 2  | DC  | H1' | 2  | DC  | H6   | 2.88 | 3.76 |
| 2  | DC  | H1' | 2  | DC  | H3'  | 2.98 | 3.90 |
| 3  | DT  | M7  | 3  | DT  | H2'  | 3.18 | 4.11 |
| 4  | DA  | H4' | 4  | DA  | H1'  | 2.34 | 3.16 |
| 4  | DA  | H4' | 4  | DA  | H8   | 4.32 | 5.84 |
| 4  | DA  | H4' | 4  | DA  | H2'  | 3.15 | 4.25 |
| 3  | DT  | H1' | 4  | DA  | H8   | 3.04 | 3.96 |
| 5  | DG  | H4' | 5  | DG  | H2'  | 2.94 | 3.98 |
| 5  | DG  | H4' | 5  | DG  | H2'' | 3.12 | 4.08 |
| 6  | DC  | H4' | 6  | DC  | H6   | 3.47 | 4.51 |
| 6  | DC  | H1' | 6  | DC  | H3'  | 3.68 | 4.70 |
| 7  | DGH | H1' | 7  | DGH | H2'  | 2.39 | 3.05 |
| 7  | DGH | H1' | 25 | HNE | Q6   | 3.34 | 4.38 |
| 7  | DGH | H1' | 25 | HNE | H51  | 2.45 | 3.39 |
| 7  | DGH | H1' | 25 | HNE | H52  | 3.04 | 4.04 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 8  | DA  | H1'  | 8  | DA  | H2'' | 2.35 | 2.92 |
| 8  | DA  | H1'  | 9  | DG  | H8   | 3.09 | 4.19 |
| 8  | DA  | H4'  | 25 | HNE | H22  | 3.25 | 4.39 |
| 9  | DG  | H4'  | 9  | DG  | H1'  | 2.15 | 2.91 |
| 10 | DT  | H1'  | 10 | DT  | H2'' | 1.91 | 2.59 |
| 11 | DC  | H1'  | 11 | DC  | H3'  | 3.04 | 3.96 |
| 12 | DC3 | H1'  | 12 | DC3 | H2'  | 2.29 | 3.03 |
| 12 | DC3 | H1'  | 12 | DC3 | H2'' | 1.86 | 2.52 |
| 12 | DC3 | H5   | 12 | DC3 | H2'  | 3.24 | 4.38 |
| 12 | DC3 | H3'  | 12 | DC3 | H2'  | 2.21 | 3.07 |
| 12 | DC3 | H3'  | 12 | DC3 | H2'' | 2.59 | 3.51 |
| 13 | DG5 | H1'  | 14 | DG  | H8   | 3.14 | 4.24 |
| 13 | DG5 | H3'  | 14 | DG  | H8   | 3.95 | 5.35 |
| 13 | DG5 | H2'  | 14 | DG  | H8   | 2.27 | 2.99 |
| 14 | DG  | H1'  | 15 | DA  | H8   | 2.96 | 3.86 |
| 14 | DG  | H3'  | 15 | DA  | H8   | 3.67 | 4.97 |
| 14 | DG  | H2'' | 15 | DA  | H8   | 2.04 | 2.76 |
| 16 | DC  | H1'  | 16 | DC  | H2'' | 1.84 | 2.48 |
| 17 | DT  | H1'  | 17 | DT  | H2'' | 2.17 | 2.87 |
| 17 | DT  | H1'  | 18 | DC  | H6   | 2.64 | 3.56 |
| 8  | DA  | H2   | 25 | HNE | H22  | 3.50 | 5.50 |

|    |     |      |    |     |     |      |      |
|----|-----|------|----|-----|-----|------|------|
| 8  | DA  | H2   | 25 | HNE | H21 | 2.88 | 3.82 |
| 18 | DC  | H5'  | 18 | DC  | H6  | 3.08 | 4.02 |
| 18 | DC  | H5'' | 18 | DC  | H6  | 3.26 | 4.43 |
| 19 | DG  | H1'  | 19 | DG  | H2' | 2.38 | 3.22 |
| 19 | DG  | H1'  | 20 | DC  | H6  | 2.26 | 3.06 |
| 19 | DG  | H1'  | 25 | HNE | H51 | 3.50 | 5.50 |
| 19 | DG  | H1'  | 25 | HNE | H52 | 3.02 | 4.02 |
| 20 | DC  | H1'  | 20 | DC  | H6  | 2.95 | 3.99 |
| 20 | DC  | H1'  | 21 | DT  | H6  | 3.23 | 4.23 |
| 20 | DC  | H3'  | 21 | DT  | H6  | 3.52 | 4.66 |
| 21 | DT  | H1'  | 21 | DT  | H6  | 2.91 | 3.67 |
| 21 | DT  | H1'  | 22 | DA  | H8  | 2.97 | 3.95 |
| 21 | DT  | H3'  | 21 | DT  | H2' | 1.75 | 2.37 |
| 22 | DA  | H4'  | 22 | DA  | H1' | 2.50 | 3.38 |
| 22 | DA  | H4'  | 22 | DA  | H8  | 4.05 | 5.03 |
| 22 | DA  | H4'  | 22 | DA  | H2' | 2.93 | 3.97 |
| 23 | DG  | H4'  | 23 | DG  | H1' | 2.22 | 3.00 |
| 23 | DG  | H4'  | 23 | DG  | H2' | 2.86 | 3.82 |
| 23 | DG  | H8   | 23 | DG  | H2' | 1.98 | 2.68 |
| 24 | DC3 | H5   | 24 | DC3 | H2' | 3.66 | 4.66 |
| 7  | DGH | H5'' | 25 | HNE | M9  | 3.68 | 4.98 |

|   |     |      |    |     |     |      |      |
|---|-----|------|----|-----|-----|------|------|
| 7 | DGH | H4'  | 25 | HNE | Q7  | 3.33 | 4.33 |
| 7 | DGH | H4'  | 25 | HNE | Q8  | 2.40 | 3.34 |
| 8 | DA  | H5'  | 25 | HNE | Q7  | 2.25 | 2.97 |
| 8 | DA  | H5'' | 25 | HNE | Q8  | 2.65 | 3.47 |
| 7 | DGH | H5'  | 25 | HNE | H51 | 3.50 | 5.50 |
| 7 | DGH | H5'  | 25 | HNE | H52 | 4.52 | 5.60 |

DGH represents residue X<sup>7</sup> without HNE moiety; HNE with a residue No. 25 represents HNE moiety; M7 represents the methyl protons of thymine; HNE protons were named as: HNE H1 (X<sup>7</sup> H8); HNE H21 (X<sup>7</sup> H7<sup>α</sup>); HNE H22 (X<sup>7</sup> H7<sup>β</sup>); HNE H3 (X<sup>7</sup> H6); HNE H4 (X<sup>7</sup> H11); HNE H51 (X<sup>7</sup> H12<sup>α</sup>); HNE H52 (X<sup>7</sup> H12<sup>β</sup>); HNE Q6 (X<sup>7</sup> H13); HNE Q7 (X<sup>7</sup> H14); HNE Q8 (X<sup>7</sup> H15); HNE M9 (X<sup>7</sup> H16).

**Table S4.** NOE Restraints Utilized in the rMD Calculation for the 5'-CpX-3' Duplex with Stereoisomer **10**.

| Residue 1 |     | Atom 1 | Residue 2 |     | Atom 2 | Lower bond | Upper bond |
|-----------|-----|--------|-----------|-----|--------|------------|------------|
| 1         | DG5 | H3'    | 1         | DG5 | H8     | 3.30       | 4.46       |
| 1         | DG5 | H2''   | 1         | DG5 | H3'    | 2.07       | 2.81       |
| 2         | DC  | H6     | 1         | DG5 | H8     | 3.88       | 5.24       |
| 2         | DC  | H6     | 1         | DG5 | H2'    | 3.04       | 3.76       |
| 2         | DC  | H6     | 1         | DG5 | H2''   | 2.16       | 2.92       |
| 2         | DC  | H5     | 1         | DG5 | H1'    | 3.83       | 5.17       |
| 2         | DC  | H5     | 1         | DG5 | H8     | 3.43       | 4.65       |
| 2         | DC  | H5     | 1         | DG5 | H2''   | 2.44       | 3.30       |
| 2         | DC  | H2'    | 2         | DC  | H6     | 1.91       | 2.59       |
| 2         | DC  | H2''   | 2         | DC  | H6     | 3.01       | 3.69       |
| 3         | DT  | M7     | 2         | DC  | H6     | 3.37       | 4.55       |
| 3         | DT  | M7     | 2         | DC  | H5     | 3.53       | 4.77       |
| 3         | DT  | M7     | 2         | DC  | H2''   | 3.22       | 3.98       |
| 5         | DG  | H3'    | 5         | DG  | H1'    | 2.62       | 4.42       |
| 6         | DC  | H6     | 5         | DG  | H1'    | 3.65       | 4.95       |
| 6         | DC  | H6     | 5         | DG  | H8     | 4.11       | 5.55       |
| 6         | DC  | H6     | 5         | DG  | H3'    | 3.89       | 5.19       |
| 6         | DC  | H5     | 5         | DG  | H1'    | 3.76       | 5.08       |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 6  | DC  | H5   | 5  | DG  | H8   | 3.30 | 4.46 |
| 6  | DC  | H3'  | 6  | DC  | H6   | 3.31 | 4.47 |
| 6  | DC  | H2'  | 6  | DC  | H5   | 3.18 | 4.30 |
| 6  | DC  | H2'  | 6  | DC  | H3'  | 2.09 | 2.83 |
| 6  | DC  | H2'' | 6  | DC  | H5   | 3.62 | 5.62 |
| 6  | DC  | H2'' | 6  | DC  | H3'  | 2.30 | 3.12 |
| 7  | DGH | H8   | 6  | DC  | H6   | 3.69 | 4.99 |
| 7  | DGH | H8   | 6  | DC  | H2'  | 2.69 | 3.65 |
| 8  | DA  | H8   | 7  | DGH | H8   | 3.57 | 4.69 |
| 9  | DG  | H8   | 8  | DA  | H8   | 3.60 | 4.70 |
| 9  | DG  | H8   | 8  | DA  | H3'  | 3.60 | 5.95 |
| 9  | DG  | H3'  | 9  | DG  | H1'  | 2.89 | 3.91 |
| 9  | DG  | H2'' | 9  | DG  | H3'  | 2.21 | 2.81 |
| 10 | DT  | M7   | 9  | DG  | H1'  | 3.92 | 5.30 |
| 10 | DT  | M7   | 9  | DG  | H2'' | 2.78 | 3.76 |
| 10 | DT  | H3'  | 10 | DT  | M7   | 4.05 | 5.47 |
| 10 | DT  | H2'  | 10 | DT  | M7   | 3.06 | 4.14 |
| 11 | DC  | H6   | 10 | DT  | H6   | 4.15 | 5.03 |
| 11 | DC  | H5   | 10 | DT  | H6   | 3.59 | 4.93 |
| 11 | DC  | H5   | 10 | DT  | M7   | 3.79 | 5.13 |
| 12 | DC3 | H5   | 11 | DC  | H6   | 3.61 | 4.77 |

|    |     |      |    |     |     |      |      |
|----|-----|------|----|-----|-----|------|------|
| 12 | DC3 | H3'  | 12 | DC3 | H6  | 2.33 | 3.15 |
| 13 | DG5 | H3'  | 13 | DG5 | H1' | 2.75 | 5.37 |
| 14 | DG  | H5'  | 13 | DG5 | H1' | 2.76 | 3.74 |
| 14 | DG  | H8   | 14 | DG  | H5' | 3.86 | 5.22 |
| 14 | DG  | H3'  | 14 | DG  | H1' | 3.00 | 4.06 |
| 14 | DG  | H3'  | 14 | DG  | H8  | 3.55 | 4.39 |
| 15 | DA  | H8   | 14 | DG  | H8  | 4.18 | 5.38 |
| 15 | DA  | H8   | 15 | DA  | H1' | 3.20 | 4.32 |
| 15 | DA  | H2   | 15 | DA  | H1' | 4.62 | 6.40 |
| 15 | DA  | H3'  | 15 | DA  | H1' | 3.56 | 4.47 |
| 15 | DA  | H2'  | 15 | DA  | H1' | 2.48 | 3.36 |
| 15 | DA  | H2'' | 15 | DA  | H1' | 2.01 | 2.73 |
| 16 | DC  | H5'  | 15 | DA  | H1' | 2.61 | 3.53 |
| 16 | DC  | H1'  | 15 | DA  | H1' | 3.93 | 5.31 |
| 16 | DC  | H1'  | 15 | DA  | H2  | 2.92 | 3.96 |
| 16 | DC  | H6   | 15 | DA  | H1' | 3.10 | 4.66 |
| 16 | DC  | H6   | 15 | DA  | H8  | 3.60 | 4.72 |
| 16 | DC  | H6   | 15 | DA  | H3' | 4.12 | 8.75 |
| 16 | DC  | H6   | 16 | DC  | H5' | 3.94 | 4.89 |
| 16 | DC  | H6   | 16 | DC  | H1' | 3.47 | 4.69 |
| 16 | DC  | H5   | 15 | DA  | H1' | 4.12 | 5.92 |

|    |    |      |    |    |      |      |      |
|----|----|------|----|----|------|------|------|
| 16 | DC | H5   | 15 | DA | H8   | 3.03 | 4.09 |
| 16 | DC | H5   | 15 | DA | H2'  | 3.25 | 4.41 |
| 16 | DC | H5   | 15 | DA | H2'' | 3.54 | 4.72 |
| 16 | DC | H3'  | 16 | DC | H1'  | 3.18 | 4.46 |
| 16 | DC | H3'  | 16 | DC | H6   | 2.73 | 4.46 |
| 16 | DC | H2'  | 16 | DC | H1'  | 2.30 | 3.12 |
| 16 | DC | H2'  | 16 | DC | H5   | 3.47 | 4.37 |
| 16 | DC | H2'' | 16 | DC | H5   | 4.59 | 6.21 |
| 17 | DT | H6   | 16 | DC | H1'  | 3.61 | 4.89 |
| 17 | DT | M7   | 16 | DC | H1'  | 4.00 | 5.42 |
| 17 | DT | M7   | 16 | DC | H6   | 2.64 | 3.58 |
| 17 | DT | M7   | 16 | DC | H5   | 2.75 | 3.73 |
| 17 | DT | M7   | 16 | DC | H2'  | 2.78 | 3.76 |
| 17 | DT | M7   | 16 | DC | H2'' | 3.05 | 4.71 |
| 17 | DT | H2'  | 17 | DT | M7   | 3.43 | 4.65 |
| 18 | DC | H5   | 17 | DT | M7   | 3.97 | 5.37 |
| 19 | DG | H8   | 18 | DC | H3'  | 3.69 | 4.81 |
| 19 | DG | H3'  | 19 | DG | H8   | 3.15 | 4.38 |
| 20 | DC | H6   | 19 | DG | H8   | 3.96 | 5.36 |
| 20 | DC | H5   | 19 | DG | H8   | 3.33 | 4.51 |
| 20 | DC | H5   | 19 | DG | H3'  | 4.09 | 5.53 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 20 | DC  | H3'  | 20 | DC  | H6   | 3.62 | 4.96 |
| 20 | DC  | H2'  | 20 | DC  | H5   | 3.61 | 4.89 |
| 20 | DC  | H2'' | 20 | DC  | H5   | 3.93 | 5.70 |
| 21 | DT  | M7   | 20 | DC  | H5   | 2.87 | 3.87 |
| 21 | DT  | M7   | 20 | DC  | H2'  | 2.81 | 3.81 |
| 24 | DC3 | H6   | 24 | DC3 | H1'  | 3.61 | 5.00 |
| 24 | DC3 | H5   | 23 | DG  | H8   | 3.95 | 5.15 |
| 24 | DC3 | H3'  | 24 | DC3 | H1'  | 3.42 | 5.64 |
| 24 | DC3 | H3'  | 24 | DC3 | H6   | 2.98 | 4.02 |
| 24 | DC3 | H3'  | 24 | DC3 | H5   | 4.68 | 6.20 |
| 1  | DG5 | Q5'  | 1  | DG5 | H1'  | 4.55 | 6.27 |
| 1  | DG5 | Q5'  | 1  | DG5 | H8   | 3.20 | 4.34 |
| 1  | DG5 | Q5'  | 1  | DG5 | H2'  | 3.46 | 4.30 |
| 1  | DG5 | Q5'  | 1  | DG5 | H2'' | 4.19 | 5.67 |
| 2  | DC  | H1'  | 3  | DT  | M7   | 4.37 | 5.45 |
| 5  | DG  | H4'  | 5  | DG  | H1'  | 2.46 | 3.34 |
| 5  | DG  | H4'  | 5  | DG  | H8   | 4.71 | 6.37 |
| 4  | DA  | H3'  | 5  | DG  | H8   | 3.56 | 6.64 |
| 6  | DC  | H4'  | 6  | DC  | H6   | 3.49 | 4.55 |
| 6  | DC  | H1'  | 6  | DC  | H6   | 3.31 | 4.47 |
| 6  | DC  | H1'  | 6  | DC  | H3'  | 3.80 | 4.96 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 6  | DC  | H1'  | 6  | DC  | H2'  | 2.40 | 3.26 |
| 5  | DG  | H2'  | 6  | DC  | H5   | 3.48 | 4.70 |
| 5  | DG  | H2'' | 6  | DC  | H5   | 2.83 | 3.83 |
| 7  | DGH | H5'' | 7  | DGH | H8   | 5.17 | 6.99 |
| 7  | DGH | H1'  | 7  | DGH | H8   | 3.47 | 4.69 |
| 7  | DGH | H1'  | 7  | DGH | H3'  | 3.25 | 4.41 |
| 7  | DGH | H1'  | 7  | DGH | H2'' | 1.83 | 2.47 |
| 7  | DGH | H1'  | 8  | DA  | H8   | 3.56 | 4.51 |
| 7  | DGH | H2'  | 8  | DA  | H8   | 2.41 | 3.19 |
| 8  | DA  | H5'' | 8  | DA  | H8   | 4.37 | 6.10 |
| 8  | DA  | H1'  | 8  | DA  | H3'  | 2.96 | 3.94 |
| 8  | DA  | H2   | 9  | DG  | H1'  | 3.13 | 4.09 |
| 10 | DT  | H1'  | 10 | DT  | H6   | 3.17 | 4.29 |
| 9  | DG  | H2'  | 10 | DT  | M7   | 2.88 | 3.58 |
| 11 | DC  | H5'  | 11 | DC  | H6   | 3.14 | 4.26 |
| 11 | DC  | H1'  | 12 | DC3 | H6   | 3.50 | 4.74 |
| 11 | DC  | H1'  | 12 | DC3 | H5   | 4.46 | 6.04 |
| 11 | DC  | H3'  | 12 | DC3 | H6   | 3.85 | 5.45 |
| 11 | DC  | H3'  | 12 | DC3 | H5   | 4.20 | 5.56 |
| 12 | DC3 | H1'  | 12 | DC3 | H6   | 3.17 | 4.29 |
| 12 | DC3 | H1'  | 12 | DC3 | H3'  | 3.03 | 4.19 |

|    |     |     |    |     |      |      |      |
|----|-----|-----|----|-----|------|------|------|
| 13 | DG5 | Q5' | 13 | DG5 | H1'  | 4.70 | 6.36 |
| 13 | DG5 | Q5' | 13 | DG5 | H8   | 3.30 | 4.46 |
| 13 | DG5 | Q5' | 13 | DG5 | H2'  | 3.40 | 4.60 |
| 13 | DG5 | Q5' | 13 | DG5 | H2'' | 4.18 | 5.52 |
| 13 | DG5 | H4' | 13 | DG5 | H8   | 3.48 | 4.70 |
| 14 | DG  | H4' | 14 | DG  | H1'  | 2.63 | 3.55 |
| 14 | DG  | H4' | 14 | DG  | H8   | 5.05 | 6.41 |
| 15 | DA  | H4' | 15 | DA  | H1'  | 2.73 | 3.69 |
| 15 | DA  | H4' | 15 | DA  | H2'  | 2.84 | 3.84 |
| 15 | DA  | H4' | 15 | DA  | H2'' | 3.66 | 4.96 |
| 17 | DT  | H1' | 18 | DC  | H5   | 2.81 | 5.65 |
| 18 | DC  | H1' | 18 | DC  | H3'  | 3.04 | 3.96 |
| 18 | DC  | H1' | 19 | DG  | H8   | 2.72 | 4.24 |
| 18 | DC  | H6  | 19 | DG  | H8   | 3.39 | 4.51 |
| 18 | DC  | H2' | 19 | DG  | H8   | 2.44 | 3.16 |
| 19 | DG  | H4' | 19 | DG  | H8   | 3.24 | 6.13 |
| 19 | DG  | H1' | 19 | DG  | H8   | 2.95 | 3.93 |
| 19 | DG  | H1' | 20 | DC  | H5   | 2.95 | 3.99 |
| 20 | DC  | H1' | 20 | DC  | H3'  | 2.33 | 5.63 |
| 20 | DC  | H1' | 21 | DT  | M7   | 3.59 | 4.85 |
| 23 | DG  | H4' | 23 | DG  | H8   | 4.82 | 6.31 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 23 | DG  | H1'  | 24 | DC3 | H1'  | 3.66 | 4.96 |
| 24 | DC3 | H4'  | 24 | DC3 | H1'  | 2.52 | 3.40 |
| 23 | DG  | H3'  | 24 | DC3 | H5   | 4.66 | 6.36 |
| 5  | DG  | H3'  | 5  | DG  | H8   | 3.73 | 5.36 |
| 6  | DC  | H6   | 5  | DG  | H2'' | 2.37 | 3.35 |
| 6  | DC  | H2'' | 6  | DC  | H6   | 2.77 | 4.66 |
| 9  | DG  | H3'  | 9  | DG  | H8   | 3.68 | 4.98 |
| 10 | DT  | M7   | 9  | DG  | H3'  | 3.15 | 4.27 |
| 13 | DG5 | H2'  | 13 | DG5 | H1'  | 2.87 | 3.75 |
| 13 | DG5 | H2'' | 13 | DG5 | H1'  | 1.89 | 2.55 |
| 23 | DG  | H2'' | 23 | DG  | H8   | 2.75 | 3.55 |
| 2  | DC  | H3'  | 3  | DT  | M7   | 3.26 | 4.42 |
| 4  | DA  | H1'  | 5  | DG  | H8   | 2.88 | 3.90 |
| 4  | DA  | H2'' | 5  | DG  | H8   | 2.25 | 3.05 |
| 5  | DG  | H5'  | 5  | DG  | H8   | 3.15 | 4.27 |
| 5  | DG  | H1'  | 5  | DG  | H2'' | 1.96 | 2.64 |
| 5  | DG  | H1'  | 6  | DC  | H4'  | 3.24 | 4.24 |
| 6  | DC  | H1'  | 6  | DC  | H2'' | 1.95 | 2.63 |
| 6  | DC  | H1'  | 7  | DGH | H8   | 4.16 | 5.76 |
| 6  | DC  | H3'  | 7  | DGH | H8   | 3.79 | 5.13 |
| 8  | DA  | H2'' | 9  | DG  | H8   | 2.35 | 3.17 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 9  | DG  | H1'  | 9  | DG  | H2'' | 1.80 | 2.44 |
| 12 | DC3 | H4'  | 12 | DC3 | H1'  | 2.45 | 3.31 |
| 13 | DG5 | H4'  | 13 | DG5 | H1'  | 2.48 | 3.36 |
| 14 | DG  | H1'  | 14 | DG  | H2'  | 2.67 | 3.61 |
| 14 | DG  | H1'  | 14 | DG  | H2'' | 1.96 | 2.66 |
| 14 | DG  | H4'  | 14 | DG  | H2'' | 3.01 | 4.07 |
| 15 | DA  | H5'' | 15 | DA  | H8   | 4.18 | 5.66 |
| 15 | DA  | H2'  | 16 | DC  | H6   | 3.06 | 3.92 |
| 15 | DA  | H2'' | 16 | DC  | H6   | 2.16 | 2.92 |
| 17 | DT  | H1'  | 17 | DT  | H2'  | 2.48 | 3.36 |
| 17 | DT  | H1'  | 17 | DT  | H2'' | 1.73 | 2.33 |
| 18 | DC  | H5   | 18 | DC  | H2'  | 3.17 | 4.21 |
| 18 | DC  | H2'' | 19 | DG  | H8   | 2.18 | 2.94 |
| 19 | DG  | H5'  | 19 | DG  | H8   | 3.81 | 5.15 |
| 19 | DG  | H5'' | 19 | DG  | H8   | 4.12 | 6.22 |
| 20 | DC  | H1'  | 20 | DC  | H6   | 3.29 | 4.45 |
| 20 | DC  | H2'' | 21 | DT  | M7   | 2.94 | 3.98 |
| 22 | DA  | H1'  | 23 | DG  | H8   | 3.10 | 4.20 |
| 22 | DA  | H2'' | 23 | DG  | H8   | 2.23 | 3.01 |
| 23 | DG  | H2'  | 24 | DC3 | H5   | 3.43 | 4.55 |
| 24 | DC3 | H1'  | 24 | DC3 | H2'  | 2.38 | 3.69 |

|    |     |     |    |     |      |      |      |
|----|-----|-----|----|-----|------|------|------|
| 24 | DC3 | H1' | 24 | DC3 | H2'' | 1.78 | 2.40 |
| 24 | DC3 | H3' | 24 | DC3 | H2'  | 1.96 | 2.66 |
| 24 | DC3 | H3' | 24 | DC3 | H2'' | 2.76 | 3.79 |
| 11 | DC  | H2' | 11 | DC  | H3'  | 1.98 | 2.68 |
| 17 | DT  | H6  | 16 | DC  | H2'  | 2.81 | 3.65 |
| 1  | DG5 | H4' | 1  | DG5 | H8   | 3.96 | 4.96 |
| 1  | DG5 | H1' | 1  | DG5 | H8   | 3.32 | 4.48 |
| 1  | DG5 | H3' | 1  | DG5 | H2'  | 1.88 | 2.54 |
| 2  | DC  | H1' | 3  | DT  | H6   | 3.48 | 4.35 |
| 3  | DT  | H1' | 3  | DT  | H6   | 2.89 | 3.91 |
| 2  | DC  | H2' | 3  | DT  | M7   | 2.74 | 3.72 |
| 3  | DT  | H3' | 3  | DT  | H2'  | 2.00 | 2.70 |
| 4  | DA  | H2' | 5  | DG  | H8   | 2.99 | 4.41 |
| 5  | DG  | H1' | 5  | DG  | H2'  | 2.50 | 3.38 |
| 5  | DG  | H1' | 6  | DC  | H5'  | 2.68 | 3.62 |
| 7  | DGH | H3' | 7  | DGH | H2'  | 2.21 | 2.99 |
| 8  | DA  | H1' | 8  | DA  | H8   | 3.41 | 4.59 |
| 8  | DA  | H1' | 8  | DA  | H2'  | 2.33 | 3.05 |
| 8  | DA  | H1' | 9  | DG  | H8   | 2.63 | 3.57 |
| 8  | DA  | H3' | 8  | DA  | H2'  | 2.08 | 2.82 |
| 10 | DT  | H6  | 10 | DT  | H2'  | 1.89 | 2.55 |

|    |     |     |    |     |      |      |      |
|----|-----|-----|----|-----|------|------|------|
| 11 | DC  | H1' | 11 | DC  | H3'  | 3.72 | 4.80 |
| 11 | DC  | H1' | 11 | DC  | H2'  | 2.81 | 3.69 |
| 11 | DC  | H1' | 11 | DC  | H2'' | 1.73 | 2.35 |
| 12 | DC3 | H5' | 12 | DC3 | H1'  | 3.51 | 4.57 |
| 12 | DC3 | H5  | 12 | DC3 | H3'  | 4.07 | 5.51 |
| 13 | DG5 | H3' | 13 | DG5 | H2'' | 2.17 | 2.93 |
| 14 | DG  | H1' | 14 | DG  | H8   | 3.03 | 4.11 |
| 14 | DG  | H1' | 15 | DA  | H5'' | 3.81 | 5.88 |
| 14 | DG  | H4' | 14 | DG  | H2'  | 2.91 | 3.95 |
| 15 | DA  | H5' | 15 | DA  | H8   | 3.50 | 4.74 |
| 15 | DA  | H5' | 15 | DA  | H2'  | 3.19 | 4.31 |
| 15 | DA  | H5' | 15 | DA  | H2'' | 4.01 | 5.25 |
| 16 | DC  | H3' | 16 | DC  | H2'  | 2.04 | 2.76 |
| 16 | DC  | H3' | 17 | DT  | M7   | 3.68 | 4.98 |
| 18 | DC  | H3' | 18 | DC  | H2'  | 2.07 | 2.81 |
| 23 | DG  | H4' | 23 | DG  | H1'  | 2.45 | 3.31 |
| 22 | DA  | H3' | 23 | DG  | H8   | 3.75 | 6.05 |
| 2  | DC  | H5  | 1  | DG5 | H2'  | 2.72 | 3.68 |
| 4  | DA  | H8  | 3  | DT  | H2'  | 2.85 | 4.42 |
| 6  | DC  | H6  | 5  | DG  | H2'  | 3.23 | 4.51 |
| 7  | DGH | H3' | 7  | DGH | H8   | 3.43 | 4.65 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 7  | DGH | H2'' | 7  | DGH | H3'  | 2.17 | 2.93 |
| 11 | DC  | H5   | 10 | DT  | H2'  | 2.94 | 3.98 |
| 11 | DC  | H2'  | 11 | DC  | H5   | 3.41 | 4.47 |
| 12 | DC3 | H5   | 11 | DC  | H2'  | 3.02 | 4.11 |
| 12 | DC3 | H2'  | 12 | DC3 | H5   | 3.28 | 4.36 |
| 16 | DC  | H2'' | 16 | DC  | H6   | 2.90 | 3.84 |
| 20 | DC  | H2'  | 20 | DC  | H6   | 1.90 | 2.64 |
| 22 | DA  | H8   | 21 | DT  | H2'  | 2.76 | 3.92 |
| 24 | DC3 | H6   | 23 | DG  | H3'  | 3.92 | 5.76 |
| 1  | DG5 | H1'  | 1  | DG5 | H3'  | 3.50 | 4.74 |
| 1  | DG5 | H1'  | 1  | DG5 | H2'  | 2.40 | 3.32 |
| 1  | DG5 | H1'  | 1  | DG5 | H2'' | 1.95 | 2.63 |
| 1  | DG5 | H1'  | 2  | DC  | H6   | 3.23 | 4.37 |
| 2  | DC  | H5'' | 2  | DC  | H6   | 3.67 | 4.97 |
| 2  | DC  | H4'  | 2  | DC  | H6   | 3.76 | 5.08 |
| 2  | DC  | H1'  | 2  | DC  | H6   | 3.56 | 4.82 |
| 2  | DC  | H1'  | 2  | DC  | H2'  | 2.28 | 2.98 |
| 3  | DT  | H1'  | 3  | DT  | H3'  | 3.19 | 4.31 |
| 3  | DT  | H1'  | 3  | DT  | H2'  | 2.27 | 3.07 |
| 3  | DT  | H1'  | 3  | DT  | H2'' | 1.78 | 2.40 |
| 3  | DT  | H6   | 3  | DT  | H3'  | 3.04 | 4.12 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 4  | DA  | H4'  | 4  | DA  | H2'' | 3.31 | 4.13 |
| 5  | DG  | H8   | 5  | DG  | H2'  | 1.72 | 2.32 |
| 7  | DGH | H4'  | 7  | DGH | H8   | 4.51 | 6.11 |
| 8  | DA  | H8   | 8  | DA  | H3'  | 3.24 | 4.38 |
| 8  | DA  | H1'  | 8  | DA  | H2'' | 1.90 | 2.56 |
| 9  | DG  | H4'  | 9  | DG  | H8   | 3.76 | 4.90 |
| 9  | DG  | H3'  | 9  | DG  | H2'  | 2.10 | 2.92 |
| 10 | DT  | H1'  | 10 | DT  | H2'  | 2.48 | 3.18 |
| 10 | DT  | H2'' | 11 | DC  | H5   | 3.18 | 4.10 |
| 11 | DC  | H6   | 11 | DC  | H3'  | 2.96 | 4.00 |
| 11 | DC  | H6   | 11 | DC  | H2'  | 1.84 | 2.50 |
| 13 | DG5 | H3'  | 13 | DG5 | H2'  | 2.07 | 2.81 |
| 14 | DG  | H1'  | 15 | DA  | H5'  | 2.75 | 3.73 |
| 16 | DC  | H1'  | 16 | DC  | H2'' | 1.80 | 2.44 |
| 17 | DT  | H1'  | 17 | DT  | H3'  | 2.87 | 3.89 |
| 17 | DT  | H2'  | 18 | DC  | H5   | 2.54 | 3.44 |
| 17 | DT  | H2'' | 18 | DC  | H5   | 2.95 | 4.19 |
| 18 | DC  | H1'  | 18 | DC  | H2'  | 2.39 | 3.09 |
| 19 | DG  | H3'  | 20 | DC  | H6   | 4.05 | 5.51 |
| 20 | DC  | H1'  | 20 | DC  | H2'  | 2.30 | 3.04 |
| 21 | DT  | H1'  | 21 | DT  | H3'  | 3.33 | 4.51 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 21 | DT  | H1'  | 21 | DT  | H2'  | 2.37 | 3.13 |
| 21 | DT  | H1'  | 21 | DT  | H2'' | 1.80 | 2.44 |
| 22 | DA  | H4'  | 22 | DA  | H2'' | 2.96 | 3.94 |
| 23 | DG  | H8   | 23 | DG  | H3'  | 3.27 | 4.43 |
| 23 | DG  | H1'  | 23 | DG  | H2'  | 2.32 | 3.04 |
| 24 | DC3 | H5'  | 24 | DC3 | H1'  | 3.43 | 4.63 |
| 23 | DG  | H2'' | 24 | DC3 | H5   | 2.62 | 3.54 |
| 2  | DC  | H3'  | 2  | DC  | H6   | 2.67 | 3.61 |
| 2  | DC  | H3'  | 2  | DC  | H5   | 4.56 | 6.00 |
| 2  | DC  | H2'  | 2  | DC  | H3'  | 1.84 | 2.50 |
| 2  | DC  | H2'' | 2  | DC  | H3'  | 2.53 | 3.29 |
| 3  | DT  | H6   | 2  | DC  | H2'  | 2.60 | 3.52 |
| 3  | DT  | H2'  | 3  | DT  | H6   | 1.79 | 2.43 |
| 4  | DA  | H5'  | 3  | DT  | H1'  | 2.41 | 3.27 |
| 4  | DA  | H8   | 3  | DT  | H1'  | 2.75 | 3.73 |
| 4  | DA  | H8   | 3  | DT  | H6   | 3.58 | 4.84 |
| 4  | DA  | H8   | 4  | DA  | H5'  | 4.05 | 5.47 |
| 4  | DA  | H8   | 4  | DA  | H1'  | 3.06 | 3.96 |
| 4  | DA  | H3'  | 4  | DA  | H1'  | 2.96 | 3.94 |
| 4  | DA  | H2'  | 4  | DA  | H1'  | 2.86 | 3.86 |
| 4  | DA  | H2'  | 4  | DA  | H8   | 2.10 | 2.60 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 4  | DA  | H2'  | 4  | DA  | H3'  | 2.23 | 3.01 |
| 4  | DA  | H2'' | 4  | DA  | H1'  | 1.94 | 2.51 |
| 4  | DA  | H2'' | 4  | DA  | H8   | 2.70 | 3.64 |
| 4  | DA  | H2'' | 4  | DA  | H3'  | 2.61 | 3.31 |
| 5  | DG  | H8   | 4  | DA  | H8   | 3.58 | 4.84 |
| 6  | DC  | H2'  | 6  | DC  | H6   | 1.88 | 2.54 |
| 7  | DGH | H5'  | 6  | DC  | H1'  | 2.49 | 3.37 |
| 7  | DGH | H8   | 7  | DGH | H5'  | 3.42 | 4.62 |
| 7  | DGH | H2'  | 7  | DGH | H8   | 2.01 | 2.73 |
| 7  | DGH | H2'' | 7  | DGH | H8   | 3.27 | 3.93 |
| 8  | DA  | H8   | 7  | DGH | H2'' | 2.03 | 2.81 |
| 8  | DA  | H2'  | 8  | DA  | H8   | 2.26 | 3.06 |
| 9  | DG  | H8   | 8  | DA  | H2'  | 2.81 | 3.79 |
| 10 | DT  | H6   | 9  | DG  | H2'  | 3.02 | 3.86 |
| 10 | DT  | H6   | 9  | DG  | H2'' | 2.03 | 2.81 |
| 10 | DT  | M7   | 9  | DG  | H8   | 3.03 | 4.11 |
| 10 | DT  | H3'  | 10 | DT  | H6   | 3.05 | 4.01 |
| 10 | DT  | H2'  | 10 | DT  | H3'  | 1.85 | 2.49 |
| 10 | DT  | H2'' | 10 | DT  | H6   | 3.21 | 4.25 |
| 10 | DT  | H2'' | 10 | DT  | H3'  | 2.50 | 3.38 |
| 11 | DC  | H6   | 10 | DT  | H2'  | 2.57 | 3.47 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 11 | DC  | H5   | 10 | DT  | H3'  | 4.08 | 5.46 |
| 11 | DC  | H2'' | 11 | DC  | H3'  | 2.18 | 2.88 |
| 12 | DC3 | H6   | 11 | DC  | H2'' | 2.18 | 3.10 |
| 12 | DC3 | H2'  | 12 | DC3 | H6   | 2.18 | 2.98 |
| 12 | DC3 | H2'' | 12 | DC3 | H6   | 2.91 | 3.87 |
| 13 | DG5 | H3'  | 13 | DG5 | H8   | 3.32 | 4.48 |
| 13 | DG5 | H2'  | 13 | DG5 | H8   | 1.98 | 2.68 |
| 14 | DG  | H8   | 13 | DG5 | H3'  | 4.75 | 5.97 |
| 14 | DG  | H8   | 13 | DG5 | H2'  | 2.39 | 3.23 |
| 14 | DG  | H8   | 13 | DG5 | H2'' | 2.21 | 2.86 |
| 14 | DG  | H2'  | 14 | DG  | H8   | 2.11 | 2.61 |
| 15 | DA  | H8   | 14 | DG  | H2'  | 2.84 | 3.84 |
| 15 | DA  | H8   | 14 | DG  | H2'' | 2.38 | 3.22 |
| 15 | DA  | H2'  | 15 | DA  | H8   | 1.89 | 2.57 |
| 15 | DA  | H2'  | 15 | DA  | H3'  | 2.18 | 2.94 |
| 15 | DA  | H2'' | 15 | DA  | H8   | 2.81 | 3.63 |
| 15 | DA  | H2'' | 15 | DA  | H3'  | 2.08 | 2.82 |
| 17 | DT  | H2'  | 17 | DT  | H6   | 2.20 | 3.04 |
| 17 | DT  | H2'  | 17 | DT  | H3'  | 2.25 | 3.11 |
| 17 | DT  | H2'' | 17 | DT  | H6   | 2.98 | 3.79 |
| 17 | DT  | H2'' | 17 | DT  | H3'  | 2.69 | 3.65 |

|    |    |      |    |    |      |      |      |
|----|----|------|----|----|------|------|------|
| 18 | DC | H6   | 17 | DT | H2'  | 2.76 | 3.74 |
| 18 | DC | H5   | 17 | DT | H3'  | 4.20 | 5.68 |
| 18 | DC | H3'  | 18 | DC | H6   | 2.81 | 3.59 |
| 18 | DC | H3'  | 18 | DC | H5   | 4.51 | 6.09 |
| 18 | DC | H2'  | 18 | DC | H6   | 1.95 | 2.43 |
| 18 | DC | H2'' | 18 | DC | H6   | 2.87 | 3.75 |
| 18 | DC | H2'' | 18 | DC | H3'  | 2.13 | 2.89 |
| 19 | DG | H2'  | 19 | DG | H3'  | 2.33 | 3.29 |
| 19 | DG | H2'' | 19 | DG | H3'  | 2.11 | 2.85 |
| 20 | DC | H6   | 19 | DG | H2'  | 3.21 | 4.21 |
| 20 | DC | H6   | 19 | DG | H2'' | 2.38 | 3.04 |
| 20 | DC | H5   | 19 | DG | H2'  | 2.69 | 3.65 |
| 20 | DC | H5   | 19 | DG | H2'' | 2.80 | 3.78 |
| 21 | DT | H6   | 21 | DT | H1'  | 2.83 | 3.75 |
| 21 | DT | M7   | 20 | DC | H6   | 2.47 | 3.35 |
| 21 | DT | H3'  | 21 | DT | M7   | 3.93 | 5.33 |
| 21 | DT | H2'  | 21 | DT | H6   | 2.38 | 3.30 |
| 21 | DT | H2'  | 21 | DT | H3'  | 2.12 | 2.81 |
| 21 | DT | H2'' | 21 | DT | H6   | 2.83 | 3.83 |
| 21 | DT | H2'' | 21 | DT | H3'  | 2.28 | 3.08 |
| 22 | DA | H5'  | 21 | DT | H1'  | 2.42 | 3.28 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 22 | DA  | H8   | 21 | DT  | H1'  | 2.84 | 3.84 |
| 22 | DA  | H8   | 21 | DT  | H6   | 3.68 | 4.98 |
| 22 | DA  | H8   | 21 | DT  | H3'  | 3.45 | 4.67 |
| 22 | DA  | H8   | 22 | DA  | H5'  | 4.02 | 5.22 |
| 22 | DA  | H8   | 22 | DA  | H1'  | 2.85 | 3.85 |
| 22 | DA  | H2'  | 22 | DA  | H1'  | 2.90 | 3.92 |
| 22 | DA  | H2'  | 22 | DA  | H8   | 2.26 | 2.88 |
| 22 | DA  | H2'  | 22 | DA  | H3'  | 2.31 | 2.93 |
| 22 | DA  | H2'' | 22 | DA  | H1'  | 1.83 | 2.47 |
| 22 | DA  | H2'' | 22 | DA  | H8   | 2.75 | 3.73 |
| 22 | DA  | H2'' | 22 | DA  | H3'  | 2.67 | 3.61 |
| 23 | DG  | H8   | 22 | DA  | H2'  | 3.12 | 4.22 |
| 23 | DG  | H2'  | 23 | DG  | H8   | 1.77 | 2.39 |
| 23 | DG  | H2'  | 23 | DG  | H3'  | 1.99 | 2.69 |
| 23 | DG  | H2'' | 23 | DG  | H3'  | 2.07 | 2.79 |
| 24 | DC3 | H6   | 23 | DG  | H2'  | 3.30 | 3.99 |
| 24 | DC3 | H6   | 23 | DG  | H2'' | 2.31 | 3.29 |
| 24 | DC3 | H2'  | 24 | DC3 | H6   | 1.77 | 2.39 |
| 1  | DG5 | H8   | 1  | DG5 | H2'  | 1.93 | 2.61 |
| 1  | DG5 | H8   | 1  | DG5 | H2'' | 3.04 | 3.73 |
| 1  | DG5 | H3'  | 2  | DC  | H6   | 4.00 | 5.42 |

|   |     |      |   |     |      |      |      |
|---|-----|------|---|-----|------|------|------|
| 1 | DG5 | H3'  | 2 | DC  | H5   | 3.87 | 5.23 |
| 2 | DC  | H5'  | 2 | DC  | H6   | 3.50 | 4.74 |
| 2 | DC  | H1'  | 2 | DC  | H3'  | 2.98 | 3.88 |
| 2 | DC  | H1'  | 2 | DC  | H2'' | 1.80 | 2.44 |
| 3 | DT  | H4'  | 3 | DT  | H1'  | 2.54 | 3.36 |
| 3 | DT  | H3'  | 3 | DT  | H2'' | 2.14 | 2.78 |
| 3 | DT  | H3'  | 4 | DA  | H8   | 3.47 | 5.35 |
| 4 | DA  | H5'' | 4 | DA  | H8   | 3.80 | 5.14 |
| 4 | DA  | H4'  | 4 | DA  | H8   | 4.27 | 5.77 |
| 4 | DA  | H4'  | 4 | DA  | H2'  | 3.12 | 4.22 |
| 5 | DG  | H4'  | 5 | DG  | H2'  | 3.35 | 4.53 |
| 5 | DG  | H4'  | 5 | DG  | H2'' | 3.30 | 4.46 |
| 5 | DG  | H3'  | 5 | DG  | H2'  | 2.14 | 2.90 |
| 5 | DG  | H3'  | 5 | DG  | H2'' | 2.18 | 2.88 |
| 6 | DC  | H4'  | 6 | DC  | H1'  | 2.70 | 3.66 |
| 6 | DC  | H5'  | 6 | DC  | H6   | 3.26 | 4.28 |
| 6 | DC  | H2'' | 7 | DGH | H8   | 2.33 | 3.15 |
| 7 | DGH | H3'  | 8 | DA  | H8   | 4.06 | 5.50 |
| 8 | DA  | H4'  | 8 | DA  | H8   | 4.00 | 5.40 |
| 8 | DA  | H1'  | 8 | DA  | H2   | 3.44 | 4.66 |
| 8 | DA  | H3'  | 8 | DA  | H2'' | 2.11 | 2.79 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 9  | DG  | H1'  | 9  | DG  | H8   | 3.13 | 4.03 |
| 9  | DG  | H1'  | 9  | DG  | H2'  | 2.43 | 3.05 |
| 9  | DG  | H3'  | 10 | DT  | H6   | 3.75 | 4.93 |
| 10 | DT  | H1'  | 10 | DT  | H2'' | 1.96 | 2.66 |
| 10 | DT  | H1'  | 11 | DC  | H6   | 2.69 | 3.51 |
| 11 | DC  | H1'  | 11 | DC  | H6   | 2.86 | 3.80 |
| 12 | DC3 | H1'  | 12 | DC3 | H2'  | 2.17 | 2.93 |
| 12 | DC3 | H1'  | 12 | DC3 | H2'' | 2.06 | 2.78 |
| 12 | DC3 | H3'  | 12 | DC3 | H2'' | 2.41 | 3.27 |
| 13 | DG5 | H1'  | 13 | DG5 | H8   | 3.22 | 4.36 |
| 13 | DG5 | H1'  | 14 | DG  | H8   | 3.23 | 4.37 |
| 14 | DG  | H3'  | 14 | DG  | H2'  | 2.04 | 2.76 |
| 14 | DG  | H3'  | 14 | DG  | H2'' | 2.10 | 2.78 |
| 14 | DG  | H3'  | 15 | DA  | H8   | 3.83 | 5.07 |
| 14 | DG  | H1'  | 15 | DA  | H8   | 2.96 | 4.00 |
| 16 | DC  | H6   | 16 | DC  | H2'  | 1.84 | 2.48 |
| 16 | DC  | H3'  | 17 | DT  | H6   | 3.69 | 4.99 |
| 16 | DC  | H2'' | 17 | DT  | H6   | 2.24 | 2.84 |
| 17 | DT  | H1'  | 17 | DT  | H6   | 2.74 | 3.72 |
| 17 | DT  | H1'  | 18 | DC  | H6   | 2.87 | 3.89 |
| 18 | DC  | H1'  | 18 | DC  | H2'' | 2.27 | 2.95 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 19 | DG  | H1'  | 19 | DG  | H3'  | 3.01 | 3.99 |
| 19 | DG  | H1'  | 19 | DG  | H2'  | 2.43 | 3.15 |
| 19 | DG  | H1'  | 19 | DG  | H2'' | 2.20 | 3.08 |
| 19 | DG  | H1'  | 20 | DC  | H6   | 2.66 | 3.60 |
| 19 | DG  | H8   | 19 | DG  | H2'  | 2.12 | 2.98 |
| 20 | DC  | H1'  | 20 | DC  | H2'' | 1.99 | 2.69 |
| 20 | DC  | H1'  | 21 | DT  | H6   | 2.71 | 3.60 |
| 21 | DT  | H4'  | 21 | DT  | H1'  | 2.35 | 3.17 |
| 22 | DA  | H4'  | 22 | DA  | H1'  | 2.49 | 3.37 |
| 22 | DA  | H4'  | 22 | DA  | H8   | 4.57 | 6.19 |
| 22 | DA  | H4'  | 22 | DA  | H2'  | 3.35 | 4.53 |
| 22 | DA  | H5'' | 22 | DA  | H8   | 3.75 | 5.01 |
| 23 | DG  | H1'  | 23 | DG  | H3'  | 3.33 | 4.51 |
| 23 | DG  | H1'  | 23 | DG  | H2'' | 1.78 | 2.42 |
| 23 | DG  | H1'  | 24 | DC3 | H6   | 3.22 | 4.36 |
| 23 | DG  | H1'  | 24 | DC3 | H5   | 4.18 | 5.66 |
| 23 | DG  | H4'  | 23 | DG  | H2'  | 2.92 | 3.94 |
| 23 | DG  | H4'  | 23 | DG  | H2'' | 3.62 | 4.90 |
| 25 | HNE | H1   | 25 | HNE | Q2   | 2.15 | 2.91 |
| 25 | HNE | H1   | 25 | HNE | H3   | 3.50 | 4.50 |
| 25 | HNE | H1   | 25 | HNE | H4   | 3.11 | 4.13 |

|    |     |    |    |     |     |      |      |
|----|-----|----|----|-----|-----|------|------|
| 25 | HNE | H1 | 25 | HNE | H51 | 3.71 | 5.01 |
| 25 | HNE | H1 | 25 | HNE | H52 | 4.00 | 5.00 |
| 25 | HNE | H1 | 25 | HNE | Q6  | 3.00 | 4.00 |
| 25 | HNE | Q2 | 25 | HNE | H51 | 3.50 | 4.50 |
| 25 | HNE | Q2 | 25 | HNE | H52 | 3.00 | 4.00 |
| 25 | HNE | Q2 | 25 | HNE | Q6  | 2.50 | 3.50 |
| 25 | HNE | H3 | 25 | HNE | Q2  | 2.01 | 2.71 |
| 25 | HNE | H3 | 25 | HNE | H4  | 1.79 | 2.43 |
| 25 | HNE | H3 | 25 | HNE | H51 | 3.24 | 4.38 |
| 25 | HNE | H3 | 25 | HNE | H52 | 3.00 | 4.00 |
| 25 | HNE | H3 | 25 | HNE | Q6  | 3.42 | 4.62 |
| 25 | HNE | H4 | 25 | HNE | Q2  | 3.00 | 4.00 |
| 25 | HNE | H4 | 25 | HNE | H51 | 2.00 | 3.00 |
| 25 | HNE | H4 | 25 | HNE | H52 | 1.87 | 2.53 |
| 25 | HNE | H4 | 25 | HNE | Q6  | 2.50 | 3.50 |
| 25 | HNE | Q6 | 25 | HNE | M9  | 2.87 | 3.99 |
| 25 | HNE | Q7 | 25 | HNE | M9  | 2.50 | 3.50 |
| 25 | HNE | Q8 | 25 | HNE | M9  | 2.00 | 3.00 |
| 8  | DA  | H2 | 25 | HNE | H4  | 4.00 | 5.00 |
| 8  | DA  | H2 | 25 | HNE | H51 | 3.50 | 4.50 |
| 8  | DA  | H2 | 25 | HNE | H52 | 2.53 | 3.49 |

|    |     |     |    |     |     |      |      |
|----|-----|-----|----|-----|-----|------|------|
| 8  | DA  | H2  | 25 | HNE | Q6  | 3.00 | 4.00 |
| 8  | DA  | H2  | 25 | HNE | Q7  | 3.00 | 4.00 |
| 8  | DA  | H2  | 25 | HNE | Q8  | 4.50 | 5.50 |
| 7  | DGH | H1' | 25 | HNE | Q2  | 4.50 | 5.50 |
| 7  | DGH | H1' | 25 | HNE | H3  | 3.21 | 4.35 |
| 8  | DA  | H1' | 25 | HNE | H3  | 3.47 | 4.69 |
| 8  | DA  | H1' | 25 | HNE | H51 | 3.20 | 4.50 |
| 8  | DA  | H1' | 25 | HNE | H52 | 2.50 | 3.50 |
| 8  | DA  | H1' | 25 | HNE | Q6  | 3.90 | 5.16 |
| 9  | DG  | H1' | 25 | HNE | Q6  | 4.00 | 5.00 |
| 9  | DG  | H1' | 25 | HNE | Q7  | 2.50 | 3.50 |
| 9  | DG  | H1' | 25 | HNE | Q8  | 3.99 | 5.01 |
| 9  | DG  | H1' | 25 | HNE | M9  | 4.50 | 5.50 |
| 17 | DT  | H1' | 25 | HNE | Q6  | 4.37 | 5.91 |
| 17 | DT  | H1' | 25 | HNE | Q7  | 4.00 | 5.00 |
| 17 | DT  | H1' | 25 | HNE | Q8  | 4.00 | 5.00 |
| 18 | DC  | H1' | 25 | HNE | H1  | 4.16 | 5.48 |
| 18 | DC  | H1' | 25 | HNE | Q2  | 4.00 | 5.48 |
| 18 | DC  | H1' | 25 | HNE | Q6  | 2.89 | 3.97 |
| 18 | DC  | H1' | 25 | HNE | Q7  | 3.67 | 4.97 |
| 18 | DC  | H1' | 25 | HNE | Q8  | 3.69 | 5.13 |

|    |     |      |    |     |      |      |      |
|----|-----|------|----|-----|------|------|------|
| 18 | DC  | H1'  | 25 | HNE | M9   | 4.58 | 6.20 |
| 19 | DG  | H1'  | 25 | HNE | H1   | 3.50 | 4.50 |
| 19 | DG  | H1'  | 25 | HNE | Q2   | 2.45 | 3.31 |
| 19 | DG  | H1'  | 25 | HNE | H3   | 3.71 | 5.95 |
| 25 | HNE | H51  | 9  | DG  | H2'' | 5.00 | 6.00 |
| 25 | HNE | Q7   | 9  | DG  | H2'' | 3.25 | 4.41 |
| 25 | HNE | Q8   | 9  | DG  | H2'' | 4.50 | 5.50 |
| 25 | HNE | H51  | 9  | DG  | H2'  | 5.00 | 6.00 |
| 25 | HNE | Q7   | 9  | DG  | H2'  | 4.12 | 5.58 |
| 8  | DA  | H4'  | 25 | HNE | H51  | 3.50 | 4.50 |
| 8  | DA  | H4'  | 25 | HNE | H52  | 4.00 | 5.00 |
| 8  | DA  | H4'  | 25 | HNE | Q6   | 5.00 | 6.00 |
| 8  | DA  | H4'  | 25 | HNE | Q7   | 5.50 | 6.50 |
| 9  | DG  | H4'  | 25 | HNE | Q6   | 4.00 | 5.00 |
| 9  | DG  | H4'  | 25 | HNE | Q7   | 2.50 | 3.50 |
| 9  | DG  | H4'  | 25 | HNE | Q8   | 4.50 | 5.50 |
| 9  | DG  | H4'  | 25 | HNE | M9   | 3.44 | 4.72 |
| 9  | DG  | H5'  | 25 | HNE | M9   | 4.50 | 5.50 |
| 9  | DG  | H5'' | 25 | HNE | M9   | 4.51 | 6.11 |
| 10 | DT  | H5'  | 25 | HNE | M9   | 4.31 | 5.93 |
| 10 | DT  | H5'' | 25 | HNE | M9   | 4.86 | 6.58 |

|    |    |      |    |     |    |      |      |
|----|----|------|----|-----|----|------|------|
| 18 | DC | H4'  | 25 | HNE | M9 | 2.98 | 4.04 |
| 18 | DC | H5'  | 25 | HNE | M9 | 4.19 | 6.01 |
| 18 | DC | H5'' | 25 | HNE | M9 | 4.21 | 5.63 |
| 19 | DG | H4'  | 25 | HNE | H1 | 2.50 | 3.50 |
| 19 | DG | H5'  | 25 | HNE | H1 | 3.36 | 4.48 |
| 19 | DG | H5'' | 25 | HNE | H1 | 3.67 | 4.89 |
| 20 | DC | H5'  | 25 | HNE | H1 | 4.00 | 5.00 |

DGH represents residue X<sup>7</sup> without HNE moiety; HNE with a residue No. 25 represents HNE moiety; M7 represents the methyl protons of thymine; HNE protons were named as: HNE H1 (X<sup>7</sup> H8); HNE Q2 (X<sup>7</sup> H7); HNE H3 (X<sup>7</sup> H6); HNE H4 (X<sup>7</sup> H11); HNE H51 (X<sup>7</sup> H12<sup>α</sup>); HNE H52 (X<sup>7</sup> H12<sup>β</sup>); HNE Q6 (X<sup>7</sup> H13); HNE Q7 (X<sup>7</sup> H14); HNE Q8 (X<sup>7</sup> H15); HNE M9 (X<sup>7</sup> H16).

**Table S5.** Torsion Angles Derived from rMD Structure of Stereoisomer **8** by 3DNA.

| Base            | alpha | beta   | gamma  | delta | epsilon | zeta   | chi    |
|-----------------|-------|--------|--------|-------|---------|--------|--------|
| G <sup>1</sup>  |       |        | 59.5   | 138.9 | -175.1  | -92.4  | -113.9 |
| C <sup>2</sup>  | -68.7 | 174.0  | 55.4   | 115.6 | -172.7  | -89.0  | -121.3 |
| T <sup>3</sup>  | -65.2 | 169.1  | 55.0   | 121.6 | -172.1  | -92.1  | -116.7 |
| A <sup>4</sup>  | -72.3 | 176.8  | 49.5   | 116.0 | -175.4  | -96.1  | -120.3 |
| G <sup>5</sup>  | -67.5 | 173.7  | 54.0   | 124.8 | 178.2   | -97.9  | -120.3 |
| C <sup>6</sup>  | -63.0 | -178.9 | 55.4   | 126.6 | -172.4  | -102.8 | -125.3 |
| X <sup>7</sup>  | -68.3 | -165.1 | 43.4   | 138.1 | 175.7   | -94.2  | -97.9  |
| A <sup>8</sup>  | -61.7 | 173.2  | 57.3   | 116.5 | -173.6  | -90.4  | -117.2 |
| G <sup>9</sup>  | -65.7 | 169.7  | 52.1   | 116.8 | -177.8  | -95.7  | -122.5 |
| T <sup>10</sup> | -63.5 | 177.5  | 54.2   | 117.5 | -172.1  | -94.3  | -126.0 |
| C <sup>11</sup> | -68.4 | 174.2  | 56.2   | 116.4 | -169.0  | -87.2  | -118.2 |
| C <sup>12</sup> | -72.3 | 165.2  | 51.7   | 88.2  |         |        | -129.5 |
| G <sup>13</sup> |       |        | -178.1 | 96.5  | -174.7  | -92.3  | -142.3 |
| G <sup>14</sup> | -62.4 | -177.9 | 54.7   | 137.2 | -174.9  | -94.4  | -108.6 |
| A <sup>15</sup> | -68.1 | 176.8  | 53.2   | 129.6 | -177.9  | -92.9  | -105.1 |
| C <sup>16</sup> | -65.7 | 169.2  | 57.6   | 104.2 | -171.1  | -89.5  | -130.8 |
| T <sup>17</sup> | -67.9 | 176.0  | 53.5   | 131.6 | -169.3  | -110.6 | -108.1 |
| C <sup>18</sup> | -74.5 | 170.8  | 61.8   | 137.6 | -148.1  | -118.0 | -113.7 |
| G <sup>19</sup> | -53.8 | 139.8  | 55.7   | 108.2 | -178.4  | -107.0 | -127.3 |

|                 |       |       |      |       |        |       |        |
|-----------------|-------|-------|------|-------|--------|-------|--------|
| C <sup>20</sup> | -61.3 | 179.7 | 52.6 | 127.9 | -171.2 | -89.7 | -127.8 |
| T <sup>21</sup> | -66.4 | 175.0 | 52.2 | 124.3 | -173.5 | -90.3 | -116.9 |
| A <sup>22</sup> | -69.3 | 174.6 | 51.1 | 110.1 | -173.1 | -93.6 | -125.3 |
| G <sup>23</sup> | -68.6 | 177.7 | 49.6 | 124.8 | -175.7 | -93.5 | -114.1 |
| C <sup>24</sup> | -66.0 | 170.3 | 56.3 | 118.2 |        |       | -125.8 |

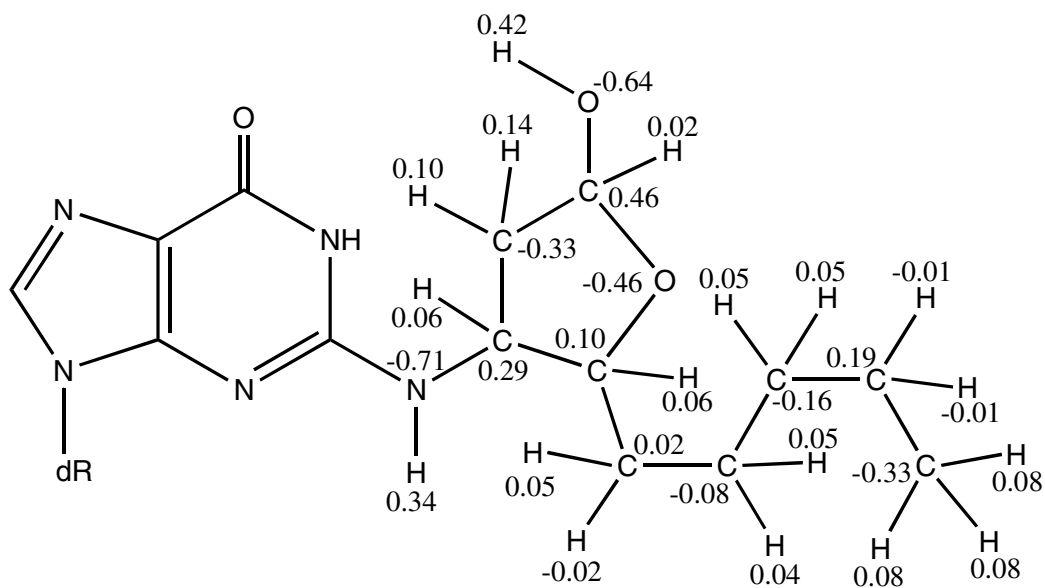
alpha: O3'(i-1)-P-O5'-C5'; beta: P-O5'-C5'-C4'; gamma: O5'-C5'-C4'-C3'; delta: C5'-C4'-C3'-O3';  
epsilon: C4'-C3'-O3'-P(i+1); zeta: C3'-O3'-P(i+1)-O5'(i+1); chi for pyrimidines (Y): O4'-C1'-N1-C2;  
chi for purines (R): O4'-C1'-N9-C4

**Table S6.** Torsion Angles Derived from rMD Structure of Stereoisomer **10** by 3DNA.

| base            | alpha | beta   | gamma  | delta | epsilon | zeta   | chi    |
|-----------------|-------|--------|--------|-------|---------|--------|--------|
| G <sup>1</sup>  |       |        | 53.8   | 141.1 | -177.4  | -99.0  | -113.0 |
| C <sup>2</sup>  | -70.2 | 176.9  | 57.6   | 120.6 | -176.2  | -93.4  | -123.2 |
| T <sup>3</sup>  | -63.3 | 173.0  | 57.0   | 126.6 | -175.5  | -94.7  | -116.8 |
| A <sup>4</sup>  | -68.4 | 177.9  | 51.3   | 128.6 | -178.6  | -101.8 | -115.1 |
| G <sup>5</sup>  | -66.6 | -177.9 | 51.1   | 131.6 | -179.5  | -95.6  | -116.1 |
| C <sup>6</sup>  | -64.0 | 177.1  | 56.8   | 117.5 | -173.8  | -94.3  | -125.1 |
| X <sup>7</sup>  | -67.7 | -178.3 | 49.0   | 124.5 | -171.1  | -89.5  | -111.0 |
| A <sup>8</sup>  | -65.3 | 165.8  | 56.3   | 117.1 | 174.5   | -102.0 | -110.9 |
| G <sup>9</sup>  | -61.9 | 171.1  | 61.6   | 126.7 | -177.7  | -97.5  | -131.8 |
| T <sup>10</sup> | -64.6 | -170.7 | 49.5   | 131.8 | -176.0  | -93.8  | -115.1 |
| C <sup>11</sup> | -65.7 | 171.6  | 56.7   | 116.6 | -169.3  | -90.0  | -122.1 |
| C <sup>12</sup> | -74.4 | 171.0  | 51.2   | 96.1  |         |        | -130.9 |
| G <sup>13</sup> |       |        | -174.0 | 132.4 | -170.2  | -93.7  | -127.1 |
| G <sup>14</sup> | -69.2 | 178.5  | 50.6   | 128.4 | -177.9  | -102.4 | -114.7 |
| A <sup>15</sup> | -66.1 | -179.9 | 54.1   | 133.4 | 177.2   | -96.0  | -110.5 |
| C <sup>16</sup> | -63.3 | 174.1  | 59.8   | 123.1 | -176.2  | -96.9  | -130.1 |
| T <sup>17</sup> | -67.0 | -172.5 | 49.1   | 126.0 | -168.6  | -105.0 | -119.0 |
| C <sup>18</sup> | -70.8 | 175.4  | 57.1   | 125.1 | -179.6  | -93.3  | -107.5 |
| G <sup>19</sup> | -62.4 | 169.7  | 54.1   | 129.5 | -178.5  | -109.1 | -114.2 |

|                 |       |        |      |       |        |        |        |
|-----------------|-------|--------|------|-------|--------|--------|--------|
| C <sup>20</sup> | -65.5 | -179.1 | 55.2 | 136.3 | -175.6 | -93.0  | -117.7 |
| T <sup>21</sup> | -69.1 | 173.4  | 56.6 | 115.3 | -176.8 | -93.4  | -126.6 |
| A <sup>22</sup> | -64.6 | 177.6  | 52.1 | 126.4 | -174.5 | -96.1  | -119.1 |
| G <sup>23</sup> | -68.7 | 179.0  | 50.4 | 124.7 | -178.1 | -101.2 | -113.1 |
| C <sup>24</sup> | -64.6 | 172.4  | 58.4 | 126.8 |        |        | -122.6 |

alpha: O3'(i-1)-P-O5'-C5'; beta: P-O5'-C5'-C4'; gamma: O5'-C5'-C4'-C3'; delta: C5'-C4'-C3'-O3';  
epsilon: C4'-C3'-O3'-P(i+1); zeta: C3'-O3'-P(i+1)-O5'(i+1); chi for pyrimidines (Y): O4'-C1'-N1-C2;  
chi for purines (R): O4'-C1'-N9-C4



**Figure S1.** Force field parameters of HNE atoms in cyclic hemiacetal stereoisomers used for rMD calculation obtained from DFT simulation at B3LYP/6-31G\* level.