Supporting Information

Excited-State Properties and Relaxation Pathways of Selenium-Substituted Guanine Nucleobase in Aqueous Solution and DNA Duplex

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I. Active Spaces

Figure S1. Orbitals included in the active space of 6SeG used in the QM1/MM calculations in the DNA environment. Orbitals in the red frame are excluded in the geometry optimizations. Note that these two orbitals do not correspond to the $\sigma$ and $\sigma^*$ orbitals located on the C-Se bond (as in Fig. 2 of the main text) but to $\pi,\pi^*$ orbitals, which were more favourable for the optimization in DNA.

Figure S2. Orbitals included in the active space of the 6SeG-C base pair used for the QM2/MM calculations in the DNA environment. Orbitals in the red frame are excluded in the geometry optimizations.
II. Superposition of the selected snapshots in water

![Superposition of selected snapshots](image)

Figure S3. Superposition of the ten selected snapshot in water considering the closest solvent molecules in three viewing angles.

III. Electronic Absorption Spectrum of 6SeG in Water

The electronic absorption spectrum of 6SeG in water solution is based on an ensemble of 500 snapshots taken from a previous classical molecular dynamics simulation, where a Gaussian function (FWHM=0.3 eV) centered on the calculated vertical excitation is superposed, see Figure S3.

![Electronic absorption spectrum](image)

Figure S4. Electronic absorption spectrum of 6SeG in water based on an ensemble of 500 snapshots. At each a vertical QM(MS-CASPT2(14,12))/MM excitation energy calculation is done including 13 singlet states state-averaged.

The spectrum exhibits two well-defined absorption bands with maxima at 3.25 eV (381 nm) and 5.58 eV (222 nm), respectively, in good agreement with the experiment
(357 and 209 nm, respectively). Although the predicted intensity of the bands is at variance with experiment, since the simulated first absorption band is more intense than that reported experimentally, the experimental spectrum is fairly reproduced by our simulations.

Regarding the individual contributions of the electronic states to the absorption spectrum: the first absorption band is best represented by the adiabatic $S_2$ state, while the adiabatic $S_3$ state appears with a broad contribution in the range of 250–400 nm. Therefore, we conclude that the $S_3$ is responsible for the shoulder around 300 nm.

IV. Excited State Minima of 6SeG and 6SeG-C in DNA

![Figure S5](image5.png)

Figure S5. QM(CASSCF)/MM optimized excited-state structures of 6SeG in DNA of “D type”, i.e. with the selenium atom in a down position compared to the molecular plane (see also Figure S8).

![Figure S6](image6.png)

Figure S6. QM(CASSCF)/MM optimized excited-state structures of 6SeG in DNA of “C type”, i.e. with the selenium atom lying in the molecular plane, (see also Figure S8).
Figure S7. QM(CASSCF)/MM optimized excited-state structures of 6SeG-C in DNA of “D type”, i.e. with the selenium atom in a down position compared to the molecular plane.

Figure S8. QM(CASSCF)/MM optimized excited-state structures of 6SeG-C in DNA of “C type”, i.e. with the selenium atom lying in the molecular plane.
Figure S9. Definition of “C” (left panel), “U” (middle panel) and “D” (right panel) conformations of 6SeG (yellow) in DNA, in between Guanine and Thymine, above and below, respectively.

V. State Intersection Structures

Figure S10. QM(CASSCF)/MM optimized state intersection structures of 6SeG in DNA of “D type”, i.e. with the selenium atom in a down position below the molecular plane, (see also Figure S8).

Figure S11. QM(CASSCF)/MM optimized state intersection structures of 6SeG-C in DNA of “D type”, i.e. with the selenium atom in a down position below the molecular plane.
VI. Minimum Energy Path in Water

Figure S12. Minimum energy path (MEP) of 6SeG in water along the $S_2$ ($1\pi_{Se\pi^*}$) state (open circle), from the ground-state optimized geometry, computed at QM(CASSCF(12,9))/MM level. Each point generated was followed by a vertical excitation energy calculation at the QM(MS-CASPT2(14,12))/level of theory.

VII. Excited State Relaxation Paths

Figure S13. QM(MS-CASPT2)//MM calculated linearly interpolated internal coordinate (LIIC) paths connecting “D type” critical points (minima and intersection structures) of 6SeG. Favorable relaxation pathway is marked with semi-solid cycles.
Figure S14. QM(MS-CASPT2)//MM calculated linearly interpolated internal coordinate (LIIC) paths connecting “C type” critical points (minima and intersection structures) of 6SeG. Favorable relaxation pathway is marked with semi-solid cycles.

Figure S15. QM(MS-CASPT2)//MM calculated linearly interpolated internal coordinate (LIIC) paths connecting “D type” critical points (minima and intersection structures) of 6SeG-C. Favorable relaxation pathway is marked with semi-solid cycles.
VIII. Tables

Table S1. QM(MS-CASPT2//CASSCF)/MM calculated vertical excitation energies (in eV) of 6SeG in water to the two lowest singlet excited states. Ten snapshots that are randomly sampled from the 1 ns MD simulation are chosen as the starting QM/MM calculations. The calculated root mean square deviations (RMSD) are also given.

| Snapshot | S1 ("nπ") | S2 ("ππ") |
|----------|------------|------------|
| 1        | 2.60       | 3.54       |
| 2        | 2.71       | 3.53       |
| 3        | 2.77       | 3.53       |
| 4        | 2.71       | 3.50       |
| 5        | 2.72       | 3.55       |
| 6        | 2.79       | 3.41       |
| 7        | 2.72       | 3.51       |
| 8        | 2.62       | 3.56       |
| 9        | 2.67       | 3.40       |
| 10       | 2.66       | 3.56       |
| RMSD     | 0.06       | 0.06       |

Table S2. QM(MS-CASPT2//CASSCF)/MM calculated vertical excitation energies (in eV) of 6SeG in DNA to the two lowest singlet excited states. Ten snapshots that are randomly sampled from the 1 ns MD simulation are chosen as the starting QM/MM calculations. The calculated root mean square deviations (RMSD) are also given.

| Snapshot | S1 ("nπ") | S2 ("ππ") |
|----------|------------|------------|
| 1        | 2.68       | 3.39       |
| 2        | 2.70       | 3.43       |
| 3        | 2.67       | 3.41       |
| 4        | 2.86       | 3.35       |
| 5        | 2.79       | 3.42       |
| 6        | 2.70       | 3.38       |
| 7        | 2.64       | 3.45       |
| 8        | 2.62       | 3.34       |
| 9        | 2.72       | 3.37       |
| 10       | 2.65       | 3.40       |
| RMSD     | 0.07       | 0.03       |
Table S3. QM(MS-CASPT2//CASSCF)/MM calculated vertical excitation energies (in eV) of 6SeG-C in DNA to the two lowest singlet excited states. Ten snapshots that are randomly sampled from the 1 ns MD simulation are chosen as the starting QM/MM calculations. The calculated root mean square deviations (RMSD) are also given.

| Snapshot | S1 (1ππ*) | S2 (1ππ*) |
|----------|------------|------------|
| 1        | 2.90       | 3.38       |
| 2        | 2.79       | 3.39       |
| 3        | 2.81       | 3.39       |
| 4        | 2.90       | 3.36       |
| 5        | 2.87       | 3.38       |
| 6        | 2.81       | 3.39       |
| 7        | 2.84       | 3.40       |
| 8        | 2.84       | 3.38       |
| 9        | 2.80       | 3.40       |
| 10       | 2.74       | 3.37       |
| RMSD     | 0.05       | 0.01       |

Table S4. QM(MS-CASPT2(14,12))/MM calculated energies (in eV) of minima and intersection structures of 6SeG in DNA (labelled as U, D, and C) relative to the S0 minimum.

|       | S1 | S2 | T1   | T2   |
|-------|----|----|------|------|
| U     | 2.46 | 3.08 | 2.32 | 2.35 |
| D     | 2.61 | 3.10 | 2.36 | 2.48 |
| C     | 2.48 | 3.22 | 2.39 | 2.43 |

|       | S1/S0 | S2/S1/T2 | T2/T1/S0 |
|-------|-------|----------|----------|
| U     | 2.62/2.58 | -       | 3.04/3.03/2.97 |
| D     | 2.62/2.59 | 3.28/3.19 | -       | 3.03/3.01/2.92 |
| C     | -     | 3.27/3.26/3.26 | - |

Table S5. QM(MS-CASPT2(14,12))/MM calculated energies (in eV) of minima and intersection structures of 6SeG-C in DNA (labelled as U, D, and C) relative to the S0 minimum.

|       | S1 | S2 | T1   | T2   |
|-------|----|----|------|------|
| U     | 2.63 | 2.88 | 2.29 | 2.53 |
| D     | 2.48 | 3.01 | 2.40 | 2.45 |
| C     | 2.81 | 3.04 | 2.36 | 2.67 |

|       | S1/S0 | S2/S1/T2 | T2/T1/S0 |
|-------|-------|----------|----------|
| U     | 2.43/2.40 | 2.90/2.86 | -       | 3.06/2.96/3.03 |
| D     | -     | 3.07/3.04 | -       | 2.97/2.89/2.95 |
| C     | -     | -       | 4.11/4.07/4.10 | - |

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Table S6. QM(MS-CASPT2(14,12))/MM calculated five lowest-lying excited states vertical excitation energies (in eV) of 6SeG-C in DNA, along with excited states characters, where LE and CT represent the local excited state and charge transfer state, respectively.

| Character          | Energy (eV) |
|--------------------|-------------|
| $S_1$ $^1\pi\pi^*$ (LE on 6SeG) | 2.79        |
| $S_2$ $^1\pi\pi^*$ (LE on 6SeG) | 3.29        |
| $S_3$ $^1\pi\pi^*$ (LE on Cyt)   | 4.64        |
| $S_4$ $^1\pi\sigma^*$ (CT)        | 4.77        |
| $S_5$ $^1\pi\pi^*$ (CT)           | 4.83        |

IX. Cartesian Coordinates

MS-CASPT2/PCM and QM(CASSCF)/MM optimized minima and intersection structures of 6SeG and 6SeG-C base pair.

16 (S0)min QM(CASSCF)/MM in water

| Se   | -1.65623547 | 0.83565008 | 1.76789592 |
| C    | -0.97597209 | 0.01721288 | 0.32815484 |
| N    | -1.67284235 | -0.98018992 | -0.35585541 |
| H    | -2.66204180 | -1.00516026 | -0.19283237 |
| C    | -1.21620628 | -1.65501339 | -1.45660295 |
| N    | -2.12638105 | -2.53569491 | -1.99862335 |
| H    | -1.72750743 | -3.07562820 | -2.74124943 |
| H    | -2.59266142 | -3.11459543 | -1.32651161 |
| N    | -0.04788970 | -1.51589173 | -1.97124334 |
| C    | 0.66257699  | -0.49688907 | -1.38025265 |
| N    | 1.89990332  | -0.07234098 | -1.72771411 |
| H    | 2.41071296  | -0.32026755 | -2.55006506 |
| H    | 2.21423065  | 0.94678347  | -0.86127853 |
| N    | 3.14290062  | 1.48570386  | -0.93509235 |
| N    | 1.28001521  | 1.16529119  | 0.01792216  |
| C    | 0.30144785  | 0.24847091  | -0.28050256 |

16 (S1)min QM(CASSCF)/MM in water

| Se   | -1.70124173 | 0.68894911 | 1.97133063 |
| C    | -1.17438345 | 0.08075143 | 0.23890364 |
| N    | -1.85415161 | -1.05031422 | -0.28814920 |
| H    | -2.85552579 | -0.96314013 | -0.31892342 |
| C    | -1.31906462 | -1.78200558 | -1.34420640 |
| N    | -2.21737954 | -2.71222606 | -1.85349036 |
| H    | -1.78510487 | -3.26699362 | -2.56862707 |
| H    | -2.59670515 | -3.30796975 | -1.13791949 |
| N    | -0.13974116 | -1.65784277 | -1.82917696 |
16

(S2) min QM(CASSCF)/MM in water
Se -1.64160682 0.80023964 1.73465732
C -0.87708105 0.01305029 0.17404151
N -1.62283057 -0.96562896 -0.42686224
H -2.59696298 -1.02082660 -0.19905166
C -1.27754718 -1.51037247 -1.66933077
N -2.06751605 -2.62441797 -2.01026058
H -2.07102686 -2.73917444 -3.00882760
H -1.68876054 -3.47014151 -1.61283330
N 0.07832443 -1.46122571 -2.08564335
C 0.77000613 -0.57320321 -1.47830704
N 1.12422729 1.13815118 0.06308121
C 0.14244766 0.22890622 -0.26255811

16

(T1) min QM(CASSCF)/MM in water
Se -1.64219400 0.70420616 1.94775923
C -1.25001680 0.19866567 0.12065176
N -1.91120465 -0.93808558 -0.40894914
H -2.91385020 -0.91270366 -0.36338281
C -1.36731163 -1.73487191 -1.40045145
N -2.26142062 -2.67060428 -1.89749242
H -1.80261807 -3.18329707 -2.51016610
H -2.74922989 -3.16301249 -1.17143995
N -0.17241792 -1.65577180 -1.84965852
C 0.53422334 -0.59204025 -1.30651394
N 1.82068300 -0.22238208 -1.59337101
H 2.37306744 -0.53548561 -2.36347032
C 2.08508471 0.86737092 -0.81319837
H 3.03271123 1.37653570 -0.85391326
N 1.08466732 1.20381444 -0.04722359
C 0.09687041 0.29203806 -0.34858393

16

(T2) min QM(CASSCF)/MM in water
Se -1.77877555 0.55291718 2.00138841
C -1.16041653 0.12259338 0.21267945
N -1.74634178 -1.04692621 -0.33840769
H -2.75010039 -1.05523306 -0.32824318
C -1.16036511 -1.75494433 -1.37261448
N -1.99181153 -2.71866736 -1.91805155
H -1.50207452 -3.28812769 -2.58206505
H -2.43957966 -3.29029893 -1.22355496
|   |   |   |   |   |
|---|---|---|---|---|
| N | 0.02574483 | -1.57388187 | -1.82063294 |   |
| C | 0.66609259 | -0.49549196 | -1.23672236 |   |
| N | 1.92675106 | -0.03806076 | -1.50902336 |   |
| H | 2.49162969 | -0.27989871 | -2.29601530 |   |
| C | 2.11875545 | 1.03996365 | -0.69127477 |   |
| H | 3.03431518 | 1.60603453 | -0.70895193 |   |
| N | 1.10229089 | 1.28571047 | 0.08636315 |   |
| C | 0.17328711 | 0.32201772 | -0.23973648 |   |

16
(S1/S2/T2) CI QM(CASSCF)/MM in water

|   |   |   |   |   |
|---|---|---|---|---|
| Se | -1.69135331 | 0.71396780 | 1.74490095 |   |
| C | -0.90966468 | -0.01693289 | 0.16810308 |   |
| N | -1.63458720 | -0.99314143 | -0.45275750 |   |
| H | -2.60197527 | -1.09184782 | -0.20796719 |   |
| C | -1.28798011 | -1.50658288 | -1.69925658 |   |
| N | -2.06215332 | -2.62375906 | -2.06185449 |   |
| H | -2.06386085 | -2.72533947 | -3.06195761 |   |
| H | -1.67432489 | -3.47367070 | -1.67341601 |   |
| N | 0.07413927 | 1.43244099 | -2.12017582 |   |
| C | 0.74628137 | -0.53991457 | 1.50070568 |   |
| N | 0.26622409 | -0.14115319 | -1.69185665 |   |
| H | 2.56001815 | -0.28379280 | -2.53758572 |   |
| C | 2.27748397 | 0.91949893 | -0.80916339 |   |
| H | 3.21788921 | 1.44542175 | -0.82225494 |   |
| N | 1.29883658 | 1.18845729 | -0.01890356 |   |
| C | 0.29830622 | 0.28439141 | -0.37589451 |   |

16
(S0/T1) ISC QM(CASSCF)/MM in water

|   |   |   |   |   |
|---|---|---|---|---|
| Se | -1.70499000 | 0.43224970 | 2.02880006 |   |
| N | -1.31379238 | 0.36754263 | 0.01958306 |   |
| C | -1.91074454 | -0.85168534 | -0.45748208 |   |
| N | -2.91348138 | -0.85200510 | -0.40759454 |   |
| C | -1.34684953 | -1.67061892 | -1.40795611 |   |
| N | -2.22387064 | -2.61808602 | -1.90288750 |   |
| C | -1.74530386 | -3.32275609 | -2.43166817 |   |
| N | -2.80275906 | -3.03068475 | -1.19470421 |   |
| N | -0.14335313 | -1.63229709 | -1.81228238 |   |
| C | 0.56540426 | -0.56510481 | -1.24386408 |   |
| C | 1.84343714 | -0.19747048 | -1.52039351 |   |
| H | 2.42126107 | -0.54999623 | -2.25966034 |   |
| H | 2.09607375 | 0.91541302 | -0.77387433 |   |
| H | 3.04660794 | 1.41409781 | -0.80303576 |   |
| H | 1.07351428 | 1.28328999 | -0.04240478 |   |
| H | 0.09514789 | 0.35674038 | -0.33316121 |   |

16
(S0)min MS-CASPT2 PCM in water

|   |   |   |   |   |
|---|---|---|---|---|
| Se | 2.41183838 | -0.09566420 | 0.00699822 |   |
| N | -2.49990843 | -1.58905520 | -0.00097685 |   |
| C | -1.59050630 | -2.62536874 | 0.00037770 |   |
| N | -0.32502682 | -2.23193438 | 0.00144987 |   |
| C | -1.76889763 | -0.42324567 | -0.00031184 |   |
| N | -2.26379786 | 0.83446966 | -0.00411308 |   |
| C | -1.29417583 | 1.74912199 | 0.00493140 |   |
| N | -1.60989826 | 3.07539737 | 0.08111611 |   |
|   | S1|min MSCASPT2 PCM in water |   | S2|min MSCASPT2 PCM in water |   | T1|min MSCASPT2 PCM in water |
|---|---|--------------------------|---|--------------------------|---|--------------------------|
| Se | -2.31753320 | -2.23868634 | -2.24406272 |
| N  | 2.50856707  | 2.50219763  | 2.50528862  |
| C  | 1.62675553  | 1.63369563  | 1.63042599  |
| N  | 0.35223086  | 0.37169648  | 0.36282514  |
| C  | 1.77425513  | 1.58641553  | 1.75855132  |
| N  | 2.26136017  | 1.58641553  | 2.23821053  |
| C  | 1.72795797  | 1.72795797  | 1.63013987  |
| N  | -0.06355227 | -0.06355227 | -0.05081154 |
| C  | -0.57917643 | -0.57917643 | -0.58482074 |
| C  | 0.43934374  | 0.43934374  | 0.44214693  |
| H  | 3.52986275  | 3.52986275  | 3.52182529  |
| H  | 2.53182529  | 2.53182529  | 2.50319477  |
| H  | 1.96804321  | 1.96804321  | 1.98352360  |
| N  | -2.0768906  | -0.92692670 | -0.02754597 |
| N  | 0.15901636  | 0.08106456  | 0.14056621  |
| C  | -0.83965547 | -0.83965547 | 0.28588640  |
| N  | -0.01227227 | -0.01227227 | -0.25213020 |
| C  | 0.04472038  | 0.04472038  | 0.04472038  |
| H  | -3.5269876  | -3.5269876  | -3.5269876  |
| H  | -2.57690820 | -2.57690820 | -2.57690820 |
| H  | -0.92680831 | -0.92680831 | -0.92680831 |
| H  | 0.71660648  | 0.71660648  | 0.71660648  |
| H  | -1.92644629 | -1.92644629 | -1.92644629 |

16

S14
16
(T2)min MSCASPT2 PCM in water
Se -2.27194698 -0.16161588 0.73496930
N 2.50788385 -1.56562420 0.07176403
C 1.62399502 -2.61868769 -0.04691686
N 0.36343451 -2.21544884 -0.21806146
C 1.76813457 -0.40928522 0.01137688
N 2.24094735 0.85328652 0.08909173
C 1.25369161 1.76597600 -0.02323201
N 1.58550070 3.09608414 -0.05185199
N -0.06023812 1.44878619 -0.19507242
C -0.58773456 0.15605078 -0.3324045
C 0.45437332 -0.3850837 -0.20679703
H 3.52415611 -1.63331101 0.21791710
H 2.51747235 3.28474798 0.33364129
H 0.86675627 3.72529980 0.32533778
H -0.70477783 2.24465023 -0.32229180
H 1.96310544 -3.65422425 -0.00567374

16
S0-MIN-C (6SeGua in DNA)
N 29.88195123 29.49685739 27.85211766
C 30.83514336 28.49217539 27.89635674
N 30.35309603 27.34658971 28.24296027
C 29.01322211 27.58330471 28.44559882
C 27.97258753 26.69042893 28.80701699
Se 28.07553350 24.89618840 29.13693900
N 26.75361532 27.36810067 28.89157707
C 26.56566729 28.69162330 28.64311795
N 25.29804532 29.15869197 28.83771330
N 27.49508886 29.50965598 28.28886966
C 28.71283726 28.91235760 28.21029786
H 31.86812679 28.68419375 27.67098066
H 25.97616671 28.62393488 29.20491991
H 24.55076857 28.53035627 28.61887259
H 25.16723115 30.07689421 28.46155253
H 30.01405605 30.45834384 27.62435408

16
S1-MIN-C (6SeGua in DNA)
N 29.85804342 29.50057885 27.84510034
C 30.78870343 28.50362152 27.97507734
N 30.29591925 27.38472196 28.41451654
C 28.95754499 27.65057704 28.59351462
C 27.91779597 26.83408368 29.08642454
Se 28.00040951 24.90791538 29.43192286
N 26.62951679 27.43078545 28.97921558

S15
| Element | S16 (9a-Min-C (6SeGua in DNA)) | N  | 29.86942503 | 29.49239368 | 27.84579449 |
|---------|--------------------------------|----|--------------|--------------|--------------|
|         | C                              |    | 30.83708625 | 28.50989216 | 28.03438001 |
|         | N                              |    | 30.37819232 | 27.41885928 | 25.5439784 |
|         | C                              |    | 29.02749406 | 28.0604060 | 28.35164107 |
|         | Se                             |    | 28.00765293 | 24.74952027 | 29.21912330 |
|         | N                              |    | 26.76911395 | 27.47435248 | 29.19433964 |
|         | C                              |    | 26.55080241 | 28.72143951 | 29.7308299 |
|         | N                              |    | 25.27103537 | 29.18133731 | 28.78788092 |
|         | C                              |    | 27.47611705 | 29.50220909 | 28.25098159 |
|         | Se                             |    | 28.04254755 | 26.90604060 | 29.35164107 |
|         | N                              |    | 29.85015114 | 29.49239368 | 27.84579449 |
|         | C                              |    | 30.7766816 | 28.49916325 | 28.03072850 |
|         | N                              |    | 30.26914342 | 27.4029354 | 28.5035304 |
|         | C                              |    | 28.93142178 | 27.6796080 | 28.65483119 |
|         | C                              |    | 27.89685716 | 26.91514521 | 29.22530801 |
|         | Se                             |    | 28.7037224 | 28.93910692 | 28.26541189 |
|         | N                              |    | 31.86539732 | 28.67887196 | 27.76894675 |
|         | C                              |    | 26.0231260 | 27.01219405 | 29.67298224 |
|         | Se                             |    | 27.435248 | 28.72143951 | 29.7308299 |
|         | N                              |    | 30.1163692 | 30.0118412 | 28.25181807 |
|         | C                              |    | 30.0132736 | 30.44353219 | 27.58237269 |

| Element | 16 (9b-Min-C (6SeGua in DNA)) | N  | 29.85015114 | 29.49239368 | 27.84579449 |
|---------|--------------------------------|----|--------------|--------------|--------------|
|         | C                              |    | 30.7766816 | 28.49916325 | 28.03072850 |
|         | N                              |    | 30.26914342 | 27.4029354 | 28.5035304 |
|         | C                              |    | 28.93142178 | 27.6796080 | 28.65483119 |
|         | Se                             |    | 28.04254755 | 26.90604060 | 29.35164107 |
|         | N                              |    | 29.8515114 | 29.49879319 | 27.84685364 |
|         | C                              |    | 30.7766816 | 28.49916325 | 28.03072850 |
|         | N                              |    | 30.26914342 | 27.4029354 | 28.5035304 |
|         | C                              |    | 28.93142178 | 27.6796080 | 28.65483119 |
|         | Se                             |    | 28.01250116 | 24.9759567 | 29.60364292 |
|         | N                              |    | 26.62271306 | 27.47761227 | 29.03304684 |
|  |  |  |  |
|---|---|---|---|
| C | 26.48580298 | 28.79631859 | 28.68909480 |
| N | 25.21464296 | 29.29845393 | 28.84289274 |
| N | 27.42153919 | 29.56232809 | 28.27262103 |
| C | 28.65348542 | 28.95126065 | 28.28643130 |
| H | 31.81631565 | 28.64654918 | 27.76813284 |
| H | 30.19947403 | 27.96509856 | 29.60687790 |
| H | 24.48531898 | 28.67687045 | 28.54813913 |
| H | 25.13007643 | 30.20102190 | 28.41636911 |
| H | 30.01621046 | 30.43893496 | 27.59540601 |
| S1UT2 (6SeGua in DNA) | | | |
| N | 29.83298957 | 29.51139276 | 27.85941445 |
| C | 30.74329164 | 28.46310481 | 27.93255604 |
| N | 30.25278065 | 27.33237828 | 28.24858411 |
| C | 28.87228223 | 27.59987468 | 28.42078971 |
| C | 27.85903023 | 26.83445237 | 28.84960312 |
| Se | 28.07630820 | 24.93615421 | 29.23952042 |
| N | 26.64636128 | 27.42758500 | 28.96186272 |
| C | 28.38689262 | 28.71643302 | 28.46635945 |
| N | 25.17247424 | 24.90359666 | 28.97094194 |
| N | 27.45529727 | 29.57633722 | 28.24241717 |
| C | 28.59911785 | 28.98366055 | 28.17184836 |
| H | 31.78837196 | 28.63063310 | 27.72674312 |
| H | 25.83885443 | 26.90390036 | 28.27948257 |
| H | 24.75396825 | 29.83732961 | 28.27948257 |
| H | 25.35282336 | 29.28539499 | 29.77491486 |
| H | 30.02458943 | 30.45823078 | 27.61887332 |
| S1-MIN-U (6SeGua in DNA) | | | |
| N | 29.84064080 | 29.51235070 | 27.84777609 |
| C | 30.73969478 | 28.47833899 | 27.90109555 |
| N | 30.20724207 | 27.35617902 | 28.28045251 |
| C | 28.88302119 | 27.66105757 | 28.49382518 |
| C | 27.80300112 | 26.83106456 | 28.90938961 |
| Se | 27.69119519 | 24.95597948 | 28.27828515 |
| N | 26.58065539 | 27.54798226 | 28.96534455 |
| C | 26.47001902 | 28.87596059 | 28.64564662 |
| N | 25.20646555 | 29.38856656 | 28.82626053 |
| N | 27.42109734 | 26.2926145 | 28.25120785 |
| C | 28.63895924 | 28.98363216 | 28.22795976 |
| H | 31.77920962 | 28.61550703 | 27.66278854 |
| H | 25.85448439 | 27.18368316 | 29.54657249 |
| H | 24.47303101 | 28.80557617 | 28.46831785 |
| H | 25.14077900 | 30.32459792 | 28.47495577 |
| H | 30.01193982 | 30.45823078 | 27.61887332 |

|  |  |  |  |
|---|---|---|---|
| S2-MIN-U (6SeGua in DNA) | | | |
| N | 29.83815943 | 29.50511185 | 27.85599359 |
| C | 30.76681110 | 28.48531330 | 28.02856180 |
| N | 30.26156400 | 27.39360818 | 28.49025092 |
| C | 28.91220871 | 27.67107424 | 28.64303507 |
| C | 27.86835374 | 26.88798245 | 29.15652420 |
| Se | 27.68999782 | 24.91874113 | 28.30740842 |
| N | 26.64371983 | 27.56040970 | 29.07621998 |
|   |   |   |   |
|---|---|---|---|
| C | 26.48131060 | 28.83539016 | 28.66611971 |
| N | 25.22162851 | 29.35101357 | 28.74593634 |
| N | 27.44854726 | 29.59928396 | 28.24727358 |
| C | 28.64554772 | 28.98229164 | 28.28902846 |
| H | 31.80516168 | 28.62587223 | 27.76412534 |
| H | 25.84721860 | 27.07239146 | 29.43254629 |
| H | 24.46545887 | 27.68524013 | 28.59281351 |
| H | 25.12354531 | 30.21251329 | 28.24606423 |
| C | 30.01387204 | 30.44189387 | 27.56830923 |

**16**

**T1-MIN-U (6SeGua in DNA)**

|   |   |   |   |
|---|---|---|---|
| N | 29.82506165 | 29.51641611 | 27.84484262 |
| C | 30.71051599 | 28.46575552 | 27.88961137 |
| N | 30.17682450 | 27.34710360 | 28.25012842 |
| C | 28.84442303 | 27.65478754 | 28.47050624 |
| C | 27.77504559 | 26.83578450 | 28.91494448 |
| Se | 27.69948331 | 24.97354829 | 28.27418978 |
| N | 26.56293922 | 27.56405872 | 28.99168205 |
| C | 26.44274026 | 28.88769034 | 28.64557286 |
| N | 25.17266171 | 29.39322878 | 28.83395223 |
| N | 27.38625848 | 29.63609996 | 28.23741673 |
| C | 28.60821869 | 28.99291826 | 28.21672464 |
| H | 31.75275541 | 28.96273741 | 27.65517944 |
| H | 25.82562553 | 27.93605622 | 29.55288718 |
| H | 24.44924796 | 28.81237200 | 28.45250822 |
| H | 25.10681794 | 30.32860542 | 28.47942972 |
| H | 30.01214026 | 30.45268887 | 27.57096576 |

|   |   |   |   |
|---|---|---|---|
| N | 29.84989810 | 29.50684638 | 27.84694862 |
| C | 30.75813725 | 28.47828100 | 27.91114058 |
| N | 30.24495584 | 27.35312809 | 28.28961055 |
| C | 28.90881204 | 27.63502044 | 28.49759784 |
| C | 27.85020343 | 26.80947137 | 28.94102247 |
| Se | 27.69198756 | 24.95002322 | 28.28142732 |
| N | 26.61858829 | 27.52022596 | 28.96415984 |
| C | 26.48637625 | 28.84092174 | 28.64931406 |
| N | 25.21783975 | 29.34609385 | 28.81263466 |
| N | 27.43511472 | 29.60489727 | 28.26110158 |
| C | 28.65269450 | 28.97002527 | 28.23329489 |
| H | 31.79656897 | 28.62600109 | 27.67212154 |
| H | 25.86115012 | 27.08580630 | 29.44793193 |
| H | 24.48470183 | 28.74215131 | 28.49277235 |
| H | 25.13924885 | 30.26552023 | 28.42301242 |
| H | 30.01212117 | 30.44901808 | 27.56899433 |

**16**

**T2-MIN-U (6SeGua in DNA)**

|   |   |   |   |
|---|---|---|---|
| N | 29.84989810 | 29.50684638 | 27.84694862 |
| C | 30.75813725 | 28.47828100 | 27.91114058 |
| N | 30.24495584 | 27.35312809 | 28.28961055 |
| C | 28.90881204 | 27.63502044 | 28.49759784 |
| C | 27.85020343 | 26.80947137 | 28.94102247 |
| Se | 27.69198756 | 24.95002322 | 28.28142732 |
| N | 26.61858829 | 27.52022596 | 28.96415984 |
| C | 26.48637625 | 28.84092174 | 28.64931406 |
| N | 25.21783975 | 29.34609385 | 28.81263466 |
| N | 27.43511472 | 29.60489727 | 28.26110158 |
| C | 28.65269450 | 28.97002527 | 28.23329489 |
| H | 31.79656897 | 28.62600109 | 27.67212154 |
| H | 25.86115012 | 27.08580630 | 29.44793193 |
| H | 24.48470183 | 28.74215131 | 28.49277235 |
| H | 25.13924885 | 30.26552023 | 28.42301242 |
| H | 30.01212117 | 30.44901808 | 27.56899433 |

**16**

**S2S1-U (6SeGua in DNA)**

|   |   |   |   |
|---|---|---|---|
| N | 29.83754714 | 29.50962012 | 27.85311800 |
| C | 30.76042021 | 28.46028805 | 27.92344201 |
| N | 30.23763017 | 27.33435096 | 28.25120803 |
| C | 28.88919007 | 27.60372198 | 28.41203604 |
| C | 27.84077400 | 26.79615792 | 28.83646507 |
| Se | 27.40190297 | 25.30423882 | 27.19570496 |
| N | 26.63590191 | 27.51316197 | 28.84237707 |
|   |   |   |   |
|---|---|---|---|
| N | 29.82097729 | 29.51401310 | 27.85572992 |
| C | 30.72252108 | 28.46075446 | 27.95659809 |
| N | 30.17915679 | 27.35508912 | 28.3308679 |
| C | 28.83769981 | 27.66306610 | 28.50203725 |
| C | 27.77319385 | 26.84914978 | 28.8991472 |
| Se | 27.30570326 | 24.50964724 | 27.7877528 |
| N | 26.61033224 | 27.57894237 | 28.9391071 |
| C | 26.46900054 | 28.89296090 | 28.6293743 |
| N | 25.21491568 | 24.9162866 | 27.7803730 |
| C | 27.43729577 | 29.65070785 | 28.2466371 |
| C | 28.61989332 | 29.00373480 | 28.20544378 |
| H | 31.76604846 | 28.59817998 | 27.73324850 |
| H | 25.79119214 | 27.0676054 | 29.2345462 |
| H | 24.44367798 | 28.20883503 | 28.59543303 |
| H | 25.11591234 | 30.32281147 | 28.35830637 |
| H | 30.01092174 | 30.45431060 | 27.58306104 |

**T2T1S0-U (6SeGua in DNA)**

|   |   |   |   |
|---|---|---|---|
| N | 29.82090561 | 29.51179695 | 27.85296411 |
| C | 30.72397985 | 28.48293207 | 27.99056308 |
| N | 30.18036993 | 27.37869648 | 28.33294982 |
| C | 28.83462421 | 27.66468790 | 28.43916224 |
| C | 27.70627163 | 26.79377218 | 28.8920904 |
| Se | 27.66226790 | 25.63153993 | 27.24731602 |
| N | 26.54177973 | 27.64202394 | 28.97028972 |
| C | 26.45022482 | 28.94264988 | 28.6120499 |
| N | 25.2273093 | 29.52129673 | 28.80344741 |
| H | 27.42538582 | 26.69090425 | 28.18259554 |
| C | 28.60164434 | 28.98414022 | 28.74560636 |
| H | 31.77506894 | 28.62445473 | 27.80497967 |
| H | 25.74153647 | 27.23857200 | 29.40763736 |
| H | 24.42832452 | 28.94240931 | 28.64024119 |
| H | 25.16084965 | 30.4279342 | 28.38449691 |
| H | 30.00646940 | 30.40615600 | 27.61142222 |

**T1S0-U (6SeGua in DNA)**

|   |   |   |   |
|---|---|---|---|
| N | 29.82090561 | 29.51179695 | 27.85296411 |
| C | 30.72397985 | 28.48293207 | 27.99056308 |
| N | 30.18036993 | 27.37869648 | 28.33294982 |
| C | 28.83462421 | 27.66468790 | 28.43916224 |
| C | 27.70627163 | 26.79377218 | 28.8920904 |
| Se | 27.66226790 | 25.63153993 | 27.24731602 |
| N | 26.54177973 | 27.64202394 | 28.97028972 |
| C | 26.45022482 | 28.94264988 | 28.6120499 |
| N | 25.2273093 | 29.52129673 | 28.80344741 |
| H | 27.42538582 | 26.69090425 | 28.18259554 |
| C | 28.60164434 | 28.98414022 | 28.74560636 |
| H | 31.77506894 | 28.62445473 | 27.80497967 |
| H | 25.74153647 | 27.23857200 | 29.40763736 |
| H | 24.42832452 | 28.94240931 | 28.64024119 |
| H | 25.16084965 | 30.4279342 | 28.38449691 |
| H | 30.00646940 | 30.40615600 | 27.61142222 |

**S1-MIN-D (6SeGua in DNA)**

|   |   |   |   |
|---|---|---|---|
| N | 29.82402524 | 29.50804934 | 27.82581813 |
| C | 30.73759797 | 28.50288034 | 28.03163536 |
| N | 30.2141803 | 27.4363873 | 28.55415964 |
| C | 28.87790055 | 27.73689720 | 28.67457407 |
| C | 27.80863035 | 26.96611039 | 29.23802265 |
| Se | 28.14608768 | 26.20014136 | 31.05907958 |
| N | 26.56858860 | 27.62532348 | 29.05434855 |
|   |   |   |   |
|---|---|---|---|
| 16 | S2-MIN-D (6SeGua in DNA) |   |   |
| N | 29.81571465 | 29.51062899 | 27.83161044 |
| C | 30.72797174 | 28.46856073 | 27.95315147 |
| N | 30.20547079 | 27.38098101 | 28.40658178 |
| C | 28.86815441 | 27.68123537 | 28.57734235 |
| C | 27.81003982 | 26.89763760 | 29.04676239 |
| Se | 28.14749354 | 26.18976983 | 31.06565171 |
| N | 26.60003106 | 27.60555804 | 29.01879316 |
| C | 26.45768554 | 28.88896210 | 28.62193184 |
| N | 25.22041987 | 24.3562692 | 28.75309401 |
| C | 27.43071963 | 29.63375513 | 28.19485558 |
| C | 28.62117481 | 29.00614130 | 28.20737585 |
| C | 31.76711097 | 28.60344394 | 27.7106950 |
| H | 25.82484445 | 27.15924407 | 29.46193524 |
| H | 24.43036749 | 28.8294006 | 28.66831683 |
| H | 25.12209982 | 30.31343320 | 28.28407204 |
| H | 29.96261226 | 30.40956137 | 27.42573266 |

|   |   |   |   |
|---|---|---|---|
| 16 | T1-MIN-D (6SeGua in DNA) |   |   |
| N | 29.81716462 | 29.50908994 | 27.84883279 |
| C | 30.72735022 | 28.49420317 | 28.05519777 |
| N | 30.21075868 | 27.43611352 | 28.59123543 |
| C | 28.86826388 | 27.73956343 | 28.73093575 |
| C | 27.79025201 | 26.95440641 | 29.23329444 |
| Se | 28.15087264 | 26.20751254 | 31.05534165 |
| N | 26.55333161 | 27.62505195 | 29.03851903 |
| C | 26.44083622 | 28.92883913 | 28.64822497 |
| N | 25.17820910 | 29.45222616 | 28.74000018 |
| N | 27.40631034 | 29.6600348 | 28.23891682 |
| C | 28.61612638 | 29.01758378 | 28.27135444 |
| H | 31.76555086 | 28.60475933 | 27.79436247 |
| H | 25.74878374 | 27.2285249 | 29.46911398 |
| H | 24.42786222 | 28.81786035 | 28.54848450 |
| H | 25.08981747 | 30.31648246 | 28.24255635 |
| H | 29.97220619 | 30.39567883 | 27.42162915 |

|   |   |   |   |
|---|---|---|---|
| 16 | T2-MIN-D (6SeGua in DNA) |   |   |
| N | 29.82791758 | 29.50757124 | 27.82495303 |
| C | 30.74658519 | 28.50095387 | 28.00518586 |
| N | 30.24006972 | 27.42253678 | 28.50856702 |
| C | 28.89741224 | 27.70975690 | 28.64492554 |
| C | 27.85260888 | 26.92682051 | 29.21005187 |
| Se | 28.14654754 | 26.19681428 | 31.06170268 |
| N | 26.60983129 | 27.59563830 | 29.09669839 |
|    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
|    | C  | 26.46176181 | 28.88996309 | 28.67836230 |
|    | N  | 25.19077132 | 29.39574258 | 28.80437749 |
|    | N  | 27.40382285 | 29.62578395 | 28.22608092 |
|    | C  | 28.62433578 | 28.98651441 | 28.21759100 |
|    | H  | 31.78439880 | 28.63571111 | 27.75329843 |
|    | H  | 25.82351392 | 27.13575742 | 29.50475112 |
|    | H  | 24.45048240 | 28.75030955 | 28.60786882 |
|    | H  | 25.08435737 | 30.25808549 | 28.30657877 |
|    | H  | 29.97559174 | 30.40371008 | 27.41744728 |
|    | N  | 25.26047582 | 29.43164812 | 28.81445007 |
|    | N  | 27.46293197 | 29.63329613 | 28.22634037 |
|    | C  | 28.63185406 | 29.00694508 | 28.21171203 |
|    | H  | 25.86326486 | 27.09141795 | 29.37192311 |
|    | H  | 24.44325975 | 28.85960107 | 28.80628207 |
|    | H  | 25.16077681 | 30.37189418 | 28.49430305 |
|    | H  | 30.01196816 | 30.46654619 | 27.62790699 |

16

S2S1-D (6SeGua in DNA)

|    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
|    | N  | 29.82329614 | 29.51425612 | 27.86011100 |
|    | C  | 30.73645821 | 28.45470605 | 27.93949601 |
|    | N  | 30.20651317 | 27.34301696 | 28.30045203 |
|    | C  | 28.86661017 | 27.63415898 | 28.49895705 |
|    | C  | 27.78330500 | 26.81082292 | 28.77372606 |
|    | Se | 27.99530201 | 26.04621987 | 30.88710222 |
|    | N  | 26.60812291 | 27.56849698 | 28.90264308 |
|    | C  | 26.47185390 | 28.86998807 | 28.62247106 |
|    | N  | 25.26047582 | 29.43164812 | 28.81445007 |
|    | N  | 27.46293197 | 29.63329613 | 28.22634037 |
|    | C  | 28.63185406 | 29.00694508 | 28.21171203 |
|    | H  | 31.77912928 | 28.60831905 | 27.72414199 |
|    | H  | 25.86326486 | 27.09141795 | 29.37192311 |
|    | H  | 24.44325975 | 28.85960107 | 28.80628207 |
|    | H  | 25.16077681 | 30.37189418 | 28.49430305 |
|    | H  | 30.01196816 | 30.46654619 | 27.62790699 |

16

T2T1S0-D (6SeGua in DNA)

|    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
|    | N  | 29.82195180 | 29.51521538 | 27.85110627 |
|    | C  | 30.72068329 | 28.46548102 | 27.95464167 |
|    | N  | 30.17385843 | 27.35884307 | 28.33038158 |
|    | C  | 28.83423583 | 27.66986458 | 28.49440505 |
|    | C  | 27.76261008 | 26.83753229 | 28.88055198 |
|    | Se | 28.24360646 | 25.42124842 | 30.96917432 |
|    | N  | 26.60067500 | 27.58363005 | 28.92557147 |
|    | C  | 26.46261385 | 28.90519843 | 28.62110386 |
|    | N  | 25.21420324 | 29.43407834 | 28.78279978 |
|    | N  | 27.43413477 | 29.66034455 | 28.24241109 |
|    | C  | 28.61872835 | 29.00539179 | 28.20476563 |
|    | H  | 31.76587539 | 28.60088483 | 27.73802097 |
|    | H  | 25.77666377 | 27.10194831 | 29.22085966 |
|    | H  | 24.44056572 | 28.82861856 | 28.59378268 |
|    | H  | 25.11938356 | 30.34098371 | 28.37046880 |
|    | H  | 30.01212023 | 30.45442460 | 27.57582190 |

16

T1S0-D (6SeGua in DNA)

|    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
|    | N  | 29.84368634 | 29.50810638 | 27.85463774 |
|    | C  | 30.75028049 | 28.47389645 | 27.86867387 |
|    | N  | 30.23033243 | 27.35465865 | 28.19835619 |
|    | C  | 28.90151607 | 27.63781517 | 28.43547656 |
|    | C  | 27.77329415 | 26.70057026 | 28.73871751 |
|    | Se | 28.35478473 | 26.26472115 | 30.62407476 |
|    | N  | 26.57361171 | 27.50871138 | 28.74689174 |
|     |     |     |                     |                     |
|-----|-----|-----|---------------------|---------------------|
|     |     |     | 29                 | S0-MIN-C (6SeG-Cyt in DNA) |
|     |     |     |                    | N                   |
| 29  |     |     |                    | 29.96042089 | 29.06936119 |
|     |     |     |                    | 30.78976812 | 27.96942208 |
|     |     |     |                    | 30.16427193 | 26.88164829 |
|     |     |     |                    | 28.83640647 | 27.24619507 |
|     |     |     |                    | 27.67786542 | 26.46353458 |
|     |     |     |                    | 27.61799125 | 24.63229816 |
|     |     |     |                    | 26.52196159 | 27.23937785 |
|     |     |     |                    | 26.49186172 | 28.58523236 |
|     |     |     |                    | 25.29608229 | 29.17468820 |
|     |     |     |                    | 27.56461160 | 29.31840459 |
|     |     |     |                    | 28.69557143 | 28.60745717 |
|     |     |     |                    | 31.85801217 | 28.06378842 |
|     |     |     |                    | 25.63857017 | 26.76644723 |
|     |     |     |                    | 24.42691239 | 26.94866655 |
|     |     |     |                    | 25.28810303 | 30.16386462 |
|     |     |     |                    | 21.10621649 | 26.38079551 |
|     |     |     |                    | 22.39224499 | 26.88281219 |
|     |     |     |                    | 22.61224462 | 28.06377329 |
|     |     |     |                    | 23.42990503 | 26.01723329 |
|     |     |     |                    | 23.20685748 | 24.74610130 |
|     |     |     |                    | 24.22300748 | 23.92273928 |
|     |     |     |                    | 21.87219539 | 24.17599006 |
|     |     |     |                    | 20.86647745 | 25.03012496 |
|     |     |     |                    | 25.17257861 | 24.24763001 |
|     |     |     |                    | 24.07061728 | 22.94206513 |
|     |     |     |                    | 21.70143674 | 23.11794962 |
|     |     |     |                    | 19.84649753 | 24.69771661 |
|     |     |     |                    | 30.23813733 | 30.00628412 |
|     |     |     |                    | 20.36263966 | 27.02061316 |
|     |     |     |                    | 29.00863860 | 30.23857900 |
|     |     |     |                    | 25.62459812 | 28.66904302 |
|     |     |     |                    | 25.32314016 | 29.25756612 |
|     |     |     |                    | 27.59422144 | 29.37514021 |
|     |     |     |                    | 28.74035886 | 28.64504896 |
|     |     |     |                    | 31.90540760 | 28.09640380 |
|     |     |     |                    | 25.62276396 | 26.92738138 |
|     |     |     |                    | 24.46243764 | 28.79697176 |
|     |     |     |                    | 25.32220783 | 30.23857900 |
|     |     |     |                    | 21.15948899 | 26.31175392 |
|     |     |     |                    | 22.45074389 | 26.79664994 |
|     |     |     |                    | 22.69067922 | 27.96686925 |
|     |     |     |                    | 23.47024877 | 25.91526788 |

29

|     |     |     |                     | S1-MIN-C (6SeG-Cyt in DNA) |
|-----|-----|-----|---------------------|---------------------|
|     |     |     |                    | N                   |
| 29  |     |     |                    | 30.00863860 | 29.09345770 |
|     |     |     |                    | 30.83856828 | 28.02306596 |
|     |     |     |                    | 30.19831625 | 26.95825987 |
|     |     |     |                    | 28.87789178 | 23.3246398 |
|     |     |     |                    | 27.69264943 | 26.61819397 |
|     |     |     |                    | 27.62559749 | 24.64762129 |
|     |     |     |                    | 26.51453001 | 27.33102588 |
|     |     |     |                    | 26.52459812 | 28.66904302 |
|     |     |     |                    | 25.32314016 | 29.25756612 |
|     |     |     |                    | 27.59422144 | 29.37514021 |
|     |     |     |                    | 28.74035886 | 28.64504896 |
|     |     |     |                    | 31.90540760 | 28.09640380 |
|     |     |     |                    | 25.62276396 | 26.92738138 |
|     |     |     |                    | 24.46243764 | 28.79697176 |
|     |     |     |                    | 25.32220783 | 30.23857900 |
|     |     |     |                    | 21.15948899 | 26.31175392 |
|     |     |     |                    | 22.45074389 | 26.79664994 |
|     |     |     |                    | 22.69067922 | 27.96686925 |
|     |     |     |                    | 23.47024877 | 25.91526788 |
|   | 23.22107432 | 24.65522069 | 28.39884049 |
|---|-------------|-------------|-------------|
| C | 24.21879511 | 23.82765108 | 28.04786661 |
| N | 21.89138059 | 24.09133722 | 28.55573484 |
| C | 20.90105363 | 24.96173734 | 28.80009818 |
| H | 25.13405391 | 24.19186678 | 27.88811933 |
| H | 24.07712214 | 22.84482227 | 27.98852734 |
| H | 21.70607428 | 23.03391300 | 28.47281713 |
| H | 19.87955962 | 24.64564656 | 28.93100886 |
| H | 30.25841550 | 30.03795461 | 28.16433626 |
| H | 20.43509548 | 26.96947867 | 29.10207351 |

**S2-MIN-C (6Se-Cyt in DNA)**

|   | 29.99932319 | 29.14550499 | 28.44128016 |
|---|-------------|-------------|-------------|
| N | 30.84745620 | 28.14385857 | 28.86945910 |
| N | 30.23075168 | 27.10479952 | 29.28781759 |
| C | 28.89573143 | 27.40048470 | 29.13689812 |
| C | 27.73265430 | 26.71264650 | 29.56190523 |
| Se | 27.64078513 | 24.59407513 | 29.17923200 |
| N | 26.56197957 | 27.36106979 | 29.14652605 |
| C | 25.62511564 | 28.61165766 | 28.61900525 |
| N | 25.32054277 | 29.12437333 | 28.35826478 |
| N | 27.59444750 | 29.32252247 | 28.36259943 |
| C | 28.73853046 | 28.66968703 | 28.61378912 |
| H | 31.91799290 | 28.24967714 | 28.81634272 |
| H | 25.68405350 | 26.90187068 | 29.30634080 |
| H | 24.46417783 | 28.70612238 | 28.67522961 |
| H | 25.30247105 | 30.06099449 | 28.01939422 |
| N | 21.19592265 | 26.34600388 | 28.93630964 |
| C | 22.48471105 | 26.83628903 | 28.93054175 |
| O | 22.70906427 | 28.01947190 | 29.10766822 |
| N | 23.51784852 | 25.95597050 | 28.71675377 |
| C | 23.27994140 | 26.48976530 | 28.53916040 |
| N | 24.29222292 | 23.85824208 | 28.27523562 |
| C | 21.94057894 | 24.13071213 | 28.60482902 |
| C | 20.94076625 | 24.99712119 | 28.81474415 |
| H | 25.23503484 | 24.18148949 | 28.39036594 |
| H | 24.14190758 | 22.87398859 | 28.29429372 |
| H | 21.76217573 | 23.0721854 | 28.51332578 |
| H | 19.91603879 | 24.67787134 | 28.90784506 |
| H | 30.23803448 | 30.06849712 | 28.14931983 |
| H | 20.46280479 | 27.00138801 | 29.10557900 |

**11-MIN-C (6Se-Cyt in DNA)**

|   | 29.99876297 | 29.08809368 | 28.39618886 |
|---|-------------|-------------|-------------|
| N | 30.82137470 | 28.01997376 | 28.65951331 |
| N | 30.17715315 | 26.96311907 | 28.99540604 |
| C | 28.85260282 | 27.32713548 | 28.95690765 |
| C | 27.66578272 | 26.63609794 | 29.34802738 |
| Se | 27.65461830 | 24.66428339 | 29.16844847 |
| N | 26.50316871 | 27.34397589 | 28.92993302 |
| C | 26.51080835 | 28.66582829 | 28.63172570 |
| N | 25.31956641 | 29.26522305 | 28.49317269 |
| N | 27.59422958 | 29.37260401 | 28.45157066 |
| C | 28.72571814 | 28.64522487 | 28.58326919 |
| H | 31.89167099 | 28.09386135 | 28.56214258 |
| H | 25.61042011 | 26.90780642 | 29.06155704 |
| H | 24.45802883 | 28.83047114 | 28.76184102 |
| H | 25.33946273 | 30.24997258 | 28.33859549 |
| N | 21.14960914 | 26.32326395 | 28.90859772 |
| C | 22.43750405 | 26.81326193 | 28.89772320 |
| O | 22.67247059 | 27.98762272 | 29.10005770 |
| N | 23.46940252 | 25.92959321 | 28.64689527 |
|   |   |   |   |
|---|---|---|---|
| C | 23.2330124 | 24.6669163 | 28.4721670 |
| N | 24.24200264 | 23.8397142 | 28.16074976 |
| C | 21.89708378 | 24.10281028 | 28.57309563 |
| C | 20.89642414 | 24.97037250 | 28.79371403 |
| H | 25.18462665 | 24.16909667 | 28.22207167 |
| H | 24.10671023 | 22.85131011 | 28.25427332 |
| H | 21.71637052 | 23.04575683 | 28.4773429 |
| H | 19.87324651 | 24.64989585 | 28.89607633 |
| H | 30.26444651 | 30.01900577 | 28.16971567 |
| H | 20.41209171 | 26.97013949 | 29.10027397 |

29
T2-MIN-C (6SeG-Cyt in DNA)

|   |   |   |   |
|---|---|---|---|
| N | 30.03823661 | 29.11654168 | 28.3990653 |
| C | 30.87165500 | 28.05769018 | 28.65129523 |
| N | 30.23376992 | 26.98946636 | 28.97372830 |
| C | 28.91140983 | 27.34644417 | 28.93468551 |
| C | 27.72696680 | 26.63024193 | 29.31088502 |
| Se | 27.65204857 | 24.65218474 | 29.18932225 |
| N | 26.55678906 | 27.31104239 | 28.88957122 |
| C | 26.5522371 | 28.64529890 | 28.57838399 |
| C | 25.34487289 | 29.21229263 | 28.42741307 |
| N | 27.61721848 | 29.36705380 | 28.43163028 |
| C | 28.76906396 | 28.65553182 | 28.57954265 |
| H | 29.03 | 28.01 | 28.03 |
| C | 31.31773822 | 28.1471964 | 28.23508481 |
| C | 31.3174896 | 27.0272678 | 28.62488563 |
| C | 29.50743986 | 27.25528551 | 28.84487736 |
| C | 29.72643941 | 26.4367824 | 29.12417646 |
| C | 28.63632953 | 24.53680317 | 29.39881719 |
| N | 27.22328235 | 26.97668703 | 29.1485669 |
| C | 27.06590176 | 28.3934611 | 29.2360030 |
| N | 25.72029180 | 28.76092279 | 29.22845995 |
| N | 28.04195062 | 29.19651326 | 28.60486220 |
| C | 29.17388767 | 28.64105957 | 28.53676138 |
| H | 32.35141463 | 28.33483912 | 27.99071047 |
| C | 26.49991579 | 26.49998059 | 29.60906289 |
| H | 25.61888548 | 29.74887102 | 29.36521448 |
| H | 25.21734166 | 28.49433355 | 28.39792737 |
| N | 21.39784655 | 24.65242912 | 28.84637232 |
| C | 22.59729218 | 27.1259393 | 28.69452533 |
| O | 22.66797041 | 28.32646194 | 28.80868358 |
| N | 23.71530000 | 26.36763256 | 28.38245996 |

S24
|  |  |  |  |
|---|---|---|---|
| C | 23.38413939 | 24.73541776 | 28.46732979 |
| N | 24.41628986 | 23.92124727 | 28.22430576 |
| C | 22.06452971 | 24.14628770 | 28.62302287 |
| C | 21.05270946 | 24.99485364 | 27.96436818 |
| H | 25.30479369 | 24.31860972 | 27.97040076 |
| H | 24.24671919 | 22.97479638 | 27.96436818 |
| H | 21.90867439 | 23.08208737 | 28.56793420 |
| H | 20.03965240 | 24.65929225 | 28.99726367 |
| H | 30.23698376 | 30.20390652 | 28.17116179 |
| H | 20.54229218 | 26.99772408 | 29.12527124 |

**T1-MIN-U (6SeGua-Cyt in DNA)**

|  |  |  |  |
|---|---|---|---|
| N | 29.95634358 | 29.23752057 | 28.49419015 |
| C | 30.75767794 | 28.13558476 | 28.68590274 |
| N | 30.10079011 | 27.05399518 | 28.87779417 |
| C | 28.77812578 | 27.42690933 | 28.87779417 |
| C | 27.58067047 | 26.65594247 | 28.91008240 |
| Se | 27.56200844 | 25.04977290 | 27.70579294 |
| N | 26.43069247 | 27.47964097 | 28.78032223 |
| C | 26.45656868 | 28.80873677 | 28.56676994 |
| N | 25.27008507 | 24.4991359 | 28.45937944 |
| N | 27.55474328 | 29.51647820 | 28.44031542 |
| C | 28.67219712 | 28.78432648 | 28.56314950 |
| H | 31.83198202 | 28.21027155 | 28.66214113 |
| H | 25.52943197 | 27.03129766 | 28.82533263 |
| H | 24.41637880 | 29.96687701 | 28.71426804 |
| H | 25.29743597 | 30.42596512 | 28.47784594 |
| N | 21.22858275 | 26.29612963 | 28.93804271 |
| C | 22.52204727 | 27.77369116 | 28.88454467 |
| O | 22.76198115 | 27.95864704 | 29.01397767 |
| N | 23.5409301 | 25.87185821 | 28.6860530 |
| C | 23.2860142 | 24.6041729 | 28.58665684 |
| N | 24.29361535 | 23.73811329 | 28.39789946 |
| C | 21.94345139 | 24.06171134 | 28.67352394 |
| C | 20.95603180 | 24.94826059 | 28.85577779 |
| H | 25.23344369 | 24.07981841 | 28.34060617 |
| H | 24.13415989 | 22.75719687 | 28.44036161 |
| H | 21.74691842 | 23.00441001 | 28.60974494 |
| H | 19.92647102 | 24.64671815 | 28.95286948 |
| H | 30.25432068 | 30.1450326 | 28.20287220 |
| H | 20.50505278 | 26.96196180 | 29.10678964 |

|  |  |  |  |
|---|---|---|---|
| C | 22.55591158 | 26.7176557 | 28.83742527 |
| O | 22.82106120 | 27.88903269 | 28.96488331 |
| N | 23.55783677 | 25.78802227 | 28.61821165 |
|   |      |      |      |
|---|------|------|------|
| C | 23.28068731 | 24.52530577 | 28.51563300 |
| N | 24.26681496 | 23.63755009 | 28.30119854 |
| C | 21.92729890 | 24.01054083 | 28.61861404 |
| C | 20.95964010 | 24.91362528 | 28.82712681 |
| H | 25.21807695 | 23.93522118 | 28.34493614 |
| H | 24.08529000 | 22.66178756 | 28.37446470 |
| H | 21.71106101 | 22.95820495 | 28.54815736 |
| H | 19.92735921 | 24.62851094 | 28.94182019 |
| H | 30.25843082 | 30.16384286 | 28.22330241 |
| H | 20.54313161 | 26.93151154 | 29.10272549 |

29

S251-U (6SeGua-Cyt in DNA)

|   |      |      |      |
|---|------|------|------|
| N | 30.08300056 | 29.32637312 | 28.45469105 |
| C | 30.96736880 | 28.27760465 | 28.65158907 |
| N | 30.38712406 | 27.15462117 | 28.82824107 |
| C | 29.03580420 | 27.43723665 | 28.75088050 |
| C | 27.89477913 | 26.62112936 | 28.91904067 |
| Se | 28.00729928 | 24.88429709 | 27.55377396 |
| N | 26.70806015 | 27.33758678 | 28.76155056 |
| C | 26.63671381 | 28.67844951 | 28.53542924 |
| N | 25.42496168 | 29.22448973 | 28.44769810 |
| N | 27.68877824 | 24.48839768 | 28.41307457 |
| C | 28.84501881 | 28.78952524 | 28.52351959 |
| H | 32.03419646 | 24.82842630 | 28.63781931 |
| H | 25.83987792 | 26.82986034 | 28.78204837 |
| H | 24.56886397 | 28.72395490 | 28.61267305 |
| H | 25.39219307 | 30.20580376 | 28.28002356 |
| N | 21.43465023 | 26.24249387 | 28.83231255 |
| C | 22.70095309 | 28.78145697 | 28.75087647 |
| O | 22.88755565 | 27.97065924 | 28.93481027 |
| N | 23.74980446 | 25.94918676 | 28.45429828 |
| C | 23.55727030 | 24.6702960 | 28.29062475 |
| N | 24.58554429 | 23.88943913 | 27.96622407 |
| C | 22.24943808 | 24.05654186 | 28.46425327 |
| C | 21.22892627 | 24.88336541 | 28.73404738 |
| H | 25.49330470 | 24.28375699 | 27.77512951 |
| H | 24.45137170 | 22.91507539 | 27.81501141 |
| H | 22.10911214 | 22.99142317 | 28.38904688 |
| H | 20.22303513 | 24.52830581 | 28.89048811 |
| H | 30.30666913 | 30.28705741 | 28.30467944 |
| H | 20.69315882 | 26.86534092 | 29.07342922 |

29

T2T150-U (6SeGua-Cyt in DNA)

|   |      |      |      |
|---|------|------|------|
| N | 29.79929387 | 29.30677350 | 28.60235950 |
| C | 30.51825109 | 28.12282323 | 28.65773670 |
| N | 29.78913651 | 27.08023732 | 28.67091219 |
| C | 28.48441253 | 27.55638786 | 28.64035546 |
| C | 27.27634698 | 26.86889890 | 28.53172532 |
| Se | 27.42288448 | 25.08906577 | 26.53319534 |
| N | 26.21945786 | 27.74914222 | 28.51831524 |
| C | 26.29899987 | 29.10307849 | 28.53468967 |
| N | 25.14724343 | 29.79103351 | 28.49903292 |
| N | 27.43609646 | 29.75380963 | 28.55561445 |
| C | 28.49263372 | 28.94595655 | 28.60571234 |
| H | 31.59555985 | 28.12877116 | 28.67062160 |
| H | 25.30080246 | 27.33782234 | 28.48672824 |
| H | 24.27494823 | 29.32966580 | 28.68236424 |
| H | 25.21672467 | 30.77017126 | 28.67238942 |
| N | 21.30896253 | 26.33770355 | 28.87629318 |
| C | 22.55419026 | 26.92425203 | 28.83410496 |
| O | 22.69568816 | 28.1279562 | 28.94594797 |
| N | 23.64700857 | 26.11033154 | 28.66011063 |
| C      | 23.52372467 | 24.81824835 | 28.61349239 |
| N      | 24.61994448 | 24.05173606 | 28.55384680 |
| C      | 22.22597533 | 24.16591921 | 28.67723583 |
| C      | 21.15923673 | 24.96743587 | 28.81580100 |
| H      | 25.51045266 | 24.48755226 | 28.40062900 |
| H      | 24.53814138 | 23.10315348 | 28.25898065 |
| H      | 22.12773498 | 23.09327208 | 28.65893935 |
| H      | 20.15795111 | 24.57841069 | 28.90410564 |
| H      | 30.15531424 | 30.23770366 | 28.60281279 |
| H      | 20.52625822 | 26.94036835 | 29.01858879 |

29

T150-U (6SeGua-Cyt in DNA)

| N      | 29.79091471 | 29.26427729 | 28.61643776 |
| C      | 30.46683202 | 28.07649329 | 28.75920643 |
| N      | 29.69333151 | 27.05605465 | 28.76377151 |
| C      | 28.42190987 | 27.57848803 | 28.63309706 |
| C      | 27.09853970 | 26.92976300 | 28.59160793 |
| Se     | 27.21455120 | 26.30112917 | 26.66019039 |
| N      | 26.10709314 | 27.92261473 | 28.80522480 |
| C      | 26.28678198 | 29.26055731 | 28.61974743 |
| N      | 25.16884060 | 30.00378015 | 28.61535004 |
| N      | 27.44132651 | 29.83681262 | 28.47802144 |
| C      | 28.46967780 | 28.94311945 | 28.54644690 |
| H      | 31.54078257 | 28.04139601 | 28.83052678 |
| H      | 25.16760019 | 27.58234906 | 28.83097721 |
| H      | 24.26768614 | 29.59209614 | 28.74542669 |
| H      | 25.27312507 | 30.99189297 | 28.55757387 |
| N      | 21.33865153 | 26.29999909 | 28.86572288 |
| C      | 22.57433167 | 26.90641110 | 28.84423616 |
| O      | 22.70485516 | 28.10733337 | 28.96386312 |
| N      | 23.67935831 | 26.10117656 | 28.69001252 |
| C      | 23.57394322 | 24.81506022 | 28.60944875 |
| N      | 24.69658549 | 24.07920544 | 28.47069871 |
| C      | 22.28734794 | 24.14073894 | 28.64718199 |
| C      | 21.20832173 | 24.92894859 | 28.78401901 |
| H      | 25.57648445 | 24.52696945 | 28.64250040 |
| H      | 24.65792765 | 23.08886923 | 28.57199158 |
| H      | 22.19969327 | 23.06792807 | 28.60098622 |
| H      | 20.21079426 | 24.52638947 | 28.85351028 |
| H      | 30.16649536 | 30.18640440 | 28.63581528 |
| H      | 20.54325521 | 26.89031348 | 28.98966480 |

29

S1-MIN-D (6SeGua-Cyt in DNA)

| N      | 29.95165809 | 29.16717891 | 28.30341339 |
| C      | 30.70307938 | 28.03168337 | 28.46714455 |
| N      | 29.99022224 | 27.00263786 | 28.75560828 |
| C      | 28.70082075 | 27.47205040 | 28.79756642 |
| C      | 27.46990274 | 26.79512406 | 29.08466611 |
| Se     | 27.52486168 | 25.45929699 | 30.59353363 |
| N      | 26.36843003 | 27.67639923 | 29.06861225 |
| C      | 26.46251089 | 28.99920546 | 28.73616550 |
| N      | 25.29860889 | 29.66070775 | 28.67379214 |
| N      | 27.56974076 | 29.62506199 | 28.48480139 |
| C      | 28.65684995 | 28.80661186 | 28.52617649 |
| H      | 31.77243587 | 28.03574835 | 28.33842131 |
| C      | 25.45457523 | 27.26324645 | 29.01793298 |
| H      | 24.42820186 | 29.25224473 | 28.94123612 |
| H      | 23.35309279 | 30.64584468 | 28.50578129 |
| N      | 21.32479045 | 26.36206074 | 28.91366326 |
| C      | 22.57072697 | 26.95100979 | 28.92213557 |
| O      | 22.71597298 | 28.13647838 | 29.13698233 |
| N      | 23.66659119 | 26.14769271 | 28.68041717 |
|    |    |    |    |
|----|----|----|----|
| C  | 23.53769011 | 24.86803505 | 28.52720411 |
| N  | 24.62773908 | 24.12034325 | 28.25316577 |
| C  | 22.24736878 | 24.20428348 | 28.60920153 |
| C  | 21.18022201 | 24.99448079 | 28.80387491 |
| H  | 25.52639216 | 24.54379584 | 28.37729595 |
| H  | 24.58782137 | 23.13899300 | 28.42655900 |
| H  | 22.15087903 | 23.13465630 | 28.53084860 |
| H  | 20.18131620 | 24.59968968 | 28.89627030 |
| H  | 30.27892284 | 30.09046807 | 28.13448649 |
| H  | 20.53768132 | 26.94916399 | 29.07904646 |

29

| S2-MIN-D (6SeGua-Cyt in DNA) |    |    |    |
|------------------------------|----|----|----|
| N  | 30.03070754 | 29.34224634 | 28.32813706 |
| C  | 30.78706396 | 28.20902090 | 28.55258150 |
| N  | 30.10515119 | 27.22092555 | 28.98727786 |
| C  | 28.80991211 | 27.69256432 | 29.06427904 |
| C  | 27.61063208 | 27.06702779 | 29.47069320 |
| Se | 27.72208017 | 26.28127148 | 31.53054721 |
| N  | 26.51627996 | 27.91824828 | 29.32910309 |
| C  | 26.56479735 | 29.19317325 | 28.88017178 |
| N  | 25.40485695 | 28.85944204 | 28.81767927 |
| C  | 27.6340243 | 29.79559838 | 28.5300162 |
| C  | 28.75206168 | 29.01179635 | 28.64236157 |
| H  | 31.84665219 | 28.19811138 | 28.35572237 |
| H  | 25.60833277 | 27.51385201 | 29.47014693 |
| H  | 24.52063347 | 29.40074739 | 28.93998440 |
| H  | 25.43095508 | 30.75953198 | 28.38776990 |
| N  | 21.57827007 | 26.40621822 | 28.97346552 |
| C  | 22.78054240 | 27.07905051 | 28.98972320 |
| O  | 22.83968472 | 28.28378903 | 29.13654692 |
| N  | 23.93315736 | 26.34229112 | 28.8412903 |
| C  | 23.89418296 | 25.05701957 | 28.68665617 |
| N  | 25.05046222 | 24.38191442 | 28.51138738 |
| C  | 22.64944652 | 24.31715739 | 28.66343510 |
| C  | 21.52276551 | 25.03744483 | 28.82265016 |
| H  | 25.89972872 | 24.86920686 | 28.72270360 |
| H  | 25.05934572 | 23.40086324 | 28.6926536 |
| H  | 22.61913164 | 23.24624828 | 28.5532301 |
| C  | 20.54623573 | 24.58149327 | 28.85467287 |
| H  | 30.35269745 | 30.22361314 | 27.98782666 |
| H  | 20.75001235 | 26.94041016 | 29.12290137 |

29

| T1-MIN-D (6SeGua-Cyt in DNA) |    |    |    |
|------------------------------|----|----|----|
| N  | 29.94088609 | 29.14055621 | 28.29621135 |
| C  | 30.69199964 | 27.99715657 | 28.41866852 |
| N  | 29.98008253 | 26.95939379 | 28.67341288 |
| C  | 28.68716962 | 27.42837476 | 28.74036457 |
| C  | 27.45791072 | 26.73201882 | 29.00427057 |
| Se | 27.55648885 | 25.44122273 | 30.60293399 |
| N  | 26.36430531 | 26.12713944 | 28.9384317 |
| C  | 26.45691989 | 28.95619183 | 28.71705044 |
| N  | 25.29497303 | 29.62799306 | 28.69834066 |
| N  | 27.56787960 | 29.59469656 | 28.51008874 |
| C  | 28.6406727 | 28.77298891 | 28.51771726 |
| H  | 31.76066623 | 28.00431144 | 28.28323027 |
| H  | 25.44274271 | 27.21597573 | 28.94878606 |
| H  | 24.41975927 | 29.20098144 | 28.92911623 |
| H  | 25.35177412 | 30.61721493 | 28.60030187 |
| N  | 21.28277250 | 26.39866318 | 28.91680661 |
| C  | 22.5190349 | 26.99780212 | 28.90637681 |
| O  | 22.66258696 | 28.18572243 | 29.11009230 |
| N  | 23.62034223 | 26.20015262 | 28.6353214 |
|  |  |  |
|---|---|---|
| C | 23.50538200 | 24.91905418 |
| N | 24.59782927 | 24.18402045 |
| C | 22.22351824 | 24.24085076 |
| C | 21.15007359 | 25.02486357 |
| H | 25.49700569 | 24.62017647 |
| H | 24.57635952 | 23.19703906 |
| H | 22.13607524 | 23.16914911 |
| H | 20.15659977 | 24.62287298 |
| H | 30.25806785 | 30.07348290 |
| H | 20.49069304 | 26.97970177 |

29

T2-MIN-D (6SeGua-Cyt in DNA)

|  |  |  |
|---|---|---|
| N | 29.96125722 | 29.14464957 |
| C | 30.73719361 | 28.01374327 |
| N | 30.05605584 | 26.96199542 |
| C | 28.75170859 | 27.39666935 |
| C | 28.75170859 | 28.67154487 |
| Se | 27.57293524 | 25.42733767 |
| N | 26.42911970 | 27.54411945 |
| C | 26.48458253 | 28.77239095 |
| N | 25.31859487 | 29.53926285 |
| C | 28.68048313 | 27.31545297 |
| H | 30.18398444 | 29.10499899 |
| H | 25.51625262 | 26.41713728 |
| H | 25.36510182 | 30.52348500 |
| N | 21.27909161 | 26.41713728 |
| C | 22.50927148 | 27.02747324 |
| O | 22.64521841 | 28.21592413 |
| N | 23.61440233 | 26.24153646 |
| C | 23.50927939 | 24.96142343 |
| N | 24.60608005 | 24.23484273 |
| C | 22.23820580 | 24.68253441 |
| C | 21.15923253 | 25.04103830 |
| H | 25.49435000 | 24.68841254 |
| H | 24.60320409 | 23.25601568 |
| H | 22.16290738 | 23.19527979 |
| H | 23.4175407 | 24.63035672 |
| H | 30.25623027 | 30.08610708 |
| H | 20.48334187 | 26.98987672 |

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S2S1-D (6SeGua-Cyt in DNA)

|  |  |  |
|---|---|---|
| N | 30.12008731 | 29.21463852 |
| C | 30.98710069 | 28.13197721 |
| N | 30.39770147 | 27.00356165 |
| C | 29.04849414 | 27.30130938 |
| C | 27.89719850 | 26.49697055 |
| Se | 27.99178044 | 24.8907914 |
| N | 26.72028213 | 27.25697738 |
| C | 26.66946562 | 28.9994676 |
| N | 25.47970896 | 29.18326893 |
| N | 27.74016806 | 29.36974539 |
| C | 28.87583806 | 28.6876459 |
| H | 32.05354670 | 28.27541411 |
| H | 25.84427657 | 26.76289560 |
| H | 24.60288899 | 28.69547817 |
| H | 25.47974660 | 30.17836990 |
| N | 21.44183478 | 26.23834737 |
| C | 22.69984823 | 26.79346615 |
| O | 22.85064342 | 27.99837712 |
| N | 23.78513632 | 25.95122309 |
| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| C       | 23.62792136 | 24.66357510 | 28.59568357 |
| N       | 24.72130369 | 23.87581268 | 28.58878900 |
| C       | 22.31298108 | 24.04550298 | 28.56229665 |
| C       | 21.25878906 | 24.87315252 | 28.62816032 |
| H       | 25.55470104 | 24.28343656 | 28.98769798 |
| H       | 22.18973696 | 22.97616024 | 28.53571207 |
| H       | 20.24347416 | 24.51198503 | 28.65885928 |
| H       | 30.34990278 | 30.18405913 | 28.58401680 |
| H       | 20.66841749 | 26.86749190 | 28.74729209 |
| 29      |            |            |            |
| T2T150-D (6SeGua-Cyt in DNA) |  |  |  |
| N       | 29.79515200 | 29.28330484 | 28.51810551 |
| C       | 30.49694997 | 28.10086422 | 28.69476617 |
| N       | 29.74950374 | 27.08385011 | 28.85978537 |
| C       | 28.45253918 | 27.57809597 | 28.79719193 |
| C       | 27.22636124 | 26.92653045 | 28.92474835 |
| Se      | 27.17931968 | 25.19033492 | 30.97672988 |
| N       | 26.19114491 | 27.81971055 | 28.78569117 |
| C       | 26.29521402 | 29.15567065 | 28.58413069 |
| N       | 25.15265341 | 29.85168236 | 28.46668763 |
| C       | 27.44325920 | 29.77618619 | 28.47810224 |
| C       | 28.48435739 | 28.95236583 | 28.58464510 |
| H       | 31.57417551 | 28.08760553 | 28.67347191 |
| H       | 25.26438653 | 27.42609465 | 28.80914801 |
| H       | 24.27791435 | 29.43825613 | 28.73184219 |
| H       | 25.23878771 | 30.84467652 | 28.48420233 |
| N       | 21.33306285 | 26.38053270 | 28.93576204 |
| C       | 22.55102332 | 27.01706437 | 28.86626167 |
| O       | 22.65777447 | 28.21604906 | 29.05840680 |
| N       | 23.66571069 | 26.25262722 | 28.63886501 |
| C       | 23.59431669 | 24.96218508 | 28.52826511 |
| N       | 24.71538976 | 24.26233679 | 28.27224670 |
| C       | 22.33067221 | 24.25264983 | 28.64532768 |
| C       | 21.23838736 | 25.00595022 | 28.85070368 |
| H       | 25.58901979 | 24.73313040 | 28.42742231 |
| H       | 24.72030301 | 23.29016267 | 28.49510546 |
| H       | 22.27218495 | 23.17866648 | 28.58683218 |
| H       | 20.25680507 | 24.57669521 | 28.97144849 |
| H       | 30.16805243 | 30.19667030 | 28.37587600 |
| H       | 20.53415725 | 26.94300070 | 29.13998900 |

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