Supplementary Materials: How Does Thymine DNA Survive Ultrafast Dimerization Damage?

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1. Computational Details

1.1. Model Setup

In this work, two computational models were built. The first one is comprised of a thymine monomer surrounded by water molecules. And the second one is taken from the RCSB Protein Data Bank (PDB) with code name 1TEZ chain A [1], containing repaired double-helical DNA, amino acid residues, water molecules and FADH. To reduce the computational burden, residues 1 to 237, which are far from the reaction center, were removed from N-terminal. Thirteen Na+ counterions were added using the tleap module of the AMBER10 package [2] to neutralize the system in accordance with experimental conditions. The 285 crystal water molecules in the protein were kept and the AMBER-parm99 force field [3] was employed for the whole system.

1.2. Equilibrium Molecular Dynamics (MD)

The initially constructed systems were equilibrated for 1 ns using classical canonical MD simulations (at 298 K, NVT ensemble). A cutoff radius of 9 Å was used for the real space electrostatic interactions and the van der Waals terms. All MD simulations were performed with the TINKER4.2 package [4]. A cluster analysis of the sampled snapshots generates the appropriate starting structure for the QM/MM calculation.

1.3. QM/MM Computational Protocol

Scheme S1 shows the chosen QM/MM partitioning. To explicitly describe the deactivation paths for the thymine monomer in water box, a small QM1 part containing one thymine molecule was used. To comprehensively account for the decay and dimerization processes for the thymine oligomer, the two adjacent thymine bases were selected as the QM2 part, while the rest of the DNA bases, amino acid residues, crystal water molecules, and counterions were treated with the MM approach. The boundary separating the QM and MM regions was treated by the hydrogen link-atom scheme (see the wavy lines in Scheme S1). To reduce the strong electrostatic interactions between a link atom and its nearest MM atoms, the weight-consistent reparameterization scheme introduced by Olivucci et al. was adopted to adjust the MM point charges near the QM/MM boundaries [5–8]. Specifically, the nearest point charge was set to zero and the other neighboring MM point charges were re-parameterized (see Table S1). For the remaining MM atoms, standard force-field point charges were used.
The chosen QM/MM partitioning: (a) the QM1 subsystem includes the thymine monomer; (b) the QM2 subsystem includes two adjacent thymine bases, while the MM subsystem includes the rest of the DNA bases, amino acid residues, crystal water molecules, and counterions. See the text for details.

Table S1. Re-parameterized point charges (a.u.) for the MM atoms near the QM/MM boundary.

|       | C15  | 0.0000 | C15' | 0.0000 |
|-------|------|--------|------|--------|
| C16   | -0.0754 | -0.0754 |
| C17   | 0.0753  | 0.0753  |
| C18   | 0.1649  | 0.1649  |
| O19   | -0.3431 | -0.3431 |
| O20   | -0.5192 | -0.5192 |
| H21   | 0.1824  | 0.1824  |
| H22   | 0.0818  | 0.0818  |
| H23   | 0.0818  | 0.0818  |

1.3.1. QM Method

The calculations of the QM parts were conducted at the complete active space self-consistent field (CASSCF) level of theory [9,10] with the cc-PVDZ basis set. For the thymine monomer, the ab initio calculations were primarily performed at the CASSCF level of theory with a total of 14 electrons in 10 orbitals (14e/10o). The active orbitals include the O4 lone-pair orbital, all π orbitals and their corresponding π* orbitals (see Figure S2). For the thymine oligomer, 14 electrons in 11 orbitals were chosen as the active space, which includes C5–C6 (C5'–C6') π/π* orbitals, C4–O8 (C4'–O8') π/π* orbitals, O8 lone-pair n orbital and the delocalized π orbitals on the 5'-thymine. All of these orbitals in the active space are shown schematically in Figures S3. Geometry optimizations were performed using a 2-root state-averaged CASSCF approach (S₀ and Sₜₐₜ, equal weights) for the Sₜₐₜ state and a state-specific approach for the S₀ and T₁ state. To consider dynamic electron correlation effects, the single-point energy of the optimized geometries in the above computations was recalculated at the multi-configuration second-order perturbation (CASPT2) level of theory [11,12] based on the zeroth-order six roots state-averaged CASSCF wave functions. These calculations were performed without an ionization potential-electron affinity (IPEA) shift but included an imaginary energy-level shift of 0.2 a.u. to avoid intruder state problems.
1.3.2. Vertical Excitation Energies

Vertical excitation energies, oscillator strengths and transition dipole moments to the lowest five excited singlet states of the QM part at the Franck-Condon (FC) point were computed using the CASPT2//CASSCF and CASSI//CASSCF methods at the CASSCF-optimized S0 minimum.

1.3.3. Optimizations of Minima, Conical Intersections and Paths

Local minima on the excited and ground states were obtained by CASSCF optimizations. The location of conical intersections and singlet/triplet crossings was assessed on the basis of the computed energy gaps for the optimized structures. At the same computational levels, the minimum energy profiles (MEPs) were mapped by intrinsic reaction coordinate (IRC) computations [13,14] to connect above critical points in several possible excited and ground states. The single point energy calculations were carried out at the CASPT2 level of theory, based on optimized geometries using the CASSCF method. Therefore, the MEPs were eventually computed at the CASPT2//IRC/CASSCF level of theory along the unbiased reaction coordinates to gain insight into how the deactivation for the thymine monomer and thymine oligomer takes place.

1.3.4. Packages

The CASSCF calculations were performed using GAUSSIAN03 [15]. The CASPT2 and CASSI calculations were performed using MOLCAS7.6 [16], whereas the MM calculations were conducted under the AMBER99 [3] force field using TINKER4.2 package [4]. The interface between the QM and MM parts was coded by Ferré et al. and included in the Molcas program [17].

2. Charge Translocation Calculations

To further explore the properties of thymine monomer and thymine oligomer in the excited state, a charge translocation calculation was performed based on Mulliken charge population and an appropriate fragment partitioning strategy. As shown in Figure S1, for the thymine monomer, the link nitrogen group and its adjacent –CH group are defined as part I, while the rest part in the ring are defined as part II. For the thymine oligomer, the unexcited thymine base are included as part II. The charge distributions were obtained using a full Mulliken population analysis at the CASPT2//CASSCF level of theory. Table S1 presents the Mulliken charge distributions of part I and II in the ground (S0) and SCT(1ππ*) state upon the photo-excitation of thymine monomer and thymine oligomer.

![Thymine monomer and Thymine oligomer](image)

**Figure S1.** The scheme of fragment partition for charge translocation is shown, for the thymine monomer, the link nitrogen group and its adjacent –CH group are defined as part I, while the rest part in the ring are defined as part II. For the thymine oligomer, the unexcited thymine base are included as part II.
Table S2. Mulliken charge distribution of thymine monomer and thymine oligomer in part I and II in the ground (S₀) and the SCT(1ππ*) state upon the photo-excitation. (unit: e).

|                      | S₀      | SCT(1ππ*) | Charge Translocation |
|----------------------|---------|-----------|---------------------|
| Thymine monomer      |         |           |                     |
| Part I               | 0.1274  | 0.3193    | 0.1919              |
| Part II              | -0.1274 | -0.3193   |                     |
| Thymine oligomer     |         |           |                     |
| Part I               | 0.0830  | 0.2616    | 0.1786              |
| Part II              | -0.0830 | -0.2616   |                     |

3. Selected Orbitals in the Active Space

Diagram of selected orbitals in the active space for the thymine monomer and thymine oligomer.

Figure S2. Molecular orbitals of thymine monomer used in defining the active space for the CASPT2//CASSCF (14e/10o) calculations.
Figure S3. Molecular orbitals of thymine oligomer used in defining the active space for the CASPT2//CASSCF (14e/11o) calculations.

4. Optimized Structures
Figure S4. The structures optimized for the ground and excited states are schematically shown below: (a) the thymine monomer obtained at the CASSCF level of theory; (b) the thymine oligomer obtained at the CASSCF level of theory. Selected key bond lengths (Å) are given (see Section 7 for full Cartesian coordinates obtained at the CASSCF level of theory).

5. Tables

Table S3. Vertical excitation energies (E\textsubscript{\perp}, nm), oscillator strengths (f), transition dipole moments (ΔD.M., Debye), and singly occupied orbitals involved in the different transitions of the thymine monomer. The values were computed with the 6-roots state-averaged CASPT2//CASSCF(14e,10o)/AMBER method.

| Transitions | E\textsubscript{\perp} | f     | ΔD.M. | Singly Occupied Orbitals |
|-------------|----------------|-------|-------|--------------------------|
| S\textsubscript{0}→S\textsubscript{NP} | 255.2 | 7.78 \times 10^{-4} | 4.11→2.80 |
| S\textsubscript{0}→S\textsubscript{CT} | 253.8 | 0.30 | 4.11→5.31 |
Table S4. Vertical excitation energies ($E_{\perp}$, nm), oscillator strengths ($f$), transition dipole moments ($\Delta$D.M., Debye), and singly occupied orbitals involved in the different transitions of the thymine oligomer. The values were computed with the 6-roots state-averaged CASPT2//CASSCF(14e,11o)/AMBER method.

| Transitions | $E_{\perp}$ | $f$   | $\Delta$D.M. | Singly Occupied Orbitals |
|-------------|-------------|-------|--------------|--------------------------|
| $S_0 \rightarrow S_{CT}$ | 257.3 | 0.30 | 7.94→10.39   | -                        |
| $S_0 \rightarrow S_{NP}$ | 256.1 | $5.83 \times 10^{-4}$ | 7.94→5.19    | -                        |
| $S_0 \rightarrow S_{4}$ | 200.3 | $3.84 \times 10^{-2}$ | 7.94→5.17    | -                        |
| $S_0 \rightarrow S_{5}$ | 174.7 | $1.70 \times 10^{-4}$ | 7.94→5.16    | -                        |
Table S5. Absolute energies (A.E., hartree), relative energies (R.E., eV/mol) and MM energies (hartree) for the optimized structures of thymine monomer along the relaxation pathway in the singlet excited state. The corresponding energy profiles are plotted in Figure 1a of the main article.

| Thymine Monomer | RASSCF | MM | CASPT2 |
|-----------------|--------|----|--------|
|                 | A.E.   | A.E. | A.E.   | R.E.   |
| S₀              | -451.60690 | -9.66486 | -452.87549 | 0.00   |
| Root2           | -451.42363 | -9.66486 | -452.87549 | 4.85   |
| Root3(Sₙp(′nπ*)| -451.36081 | -9.66486 | -452.87549 | 4.88   |
| Root4(Sₙπ(′nπ*)| -451.34050 | -9.66486 | -452.87549 | 5.97   |
| Root5           | -451.32206 | -9.66486 | -452.87549 | 6.89   |
| Root6           | -451.28446 | -9.66486 | -452.87549 | 6.39   |
| Path1→(S₄-1)   | -451.60399 | -9.66021 | -452.87142 | 0.23   |
| Root1           | -451.43650 | -9.66021 | -452.87142 | 4.79   |
| Root2(Sₙπ(′nπ*)| -451.37030 | -9.66021 | -452.87142 | 4.83   |
| Root3(Sₙπ(′nπ*)| -451.35999 | -9.66021 | -452.87142 | 4.88   |
| Root4           | -451.32786 | -9.66021 | -452.87142 | 6.89   |
| Root5           | -451.28219 | -9.66021 | -452.87142 | 6.39   |
| Path1→(S₄-2)   | -451.59929 | -9.66097 | -452.86769 | 0.31   |
| Root1           | -451.43944 | -9.66097 | -452.86769 | 4.72   |
| Root2(Sₙp(′nπ*)| -451.37590 | -9.66097 | -452.86769 | 4.82   |
| Root3(Sₙπ(′nπ*)| -451.36482 | -9.66097 | -452.86769 | 5.57   |
| Root4           | -451.32846 | -9.66097 | -452.86769 | 5.57   |
| Root5           | -451.28521 | -9.66097 | -452.86769 | 5.57   |
| Path1→(S₄-3)   | -451.59016 | -9.66500 | -452.86383 | 0.31   |
| Root1           | -451.43902 | -9.66500 | -452.86383 | 4.61   |
| Root2(Sₙp(′nπ*)| -451.38579 | -9.66500 | -452.86383 | 4.74   |
| Root3(Sₙπ(′nπ*)| -451.36479 | -9.66500 | -452.86383 | 5.37   |
| Root4           | -451.32579 | -9.66500 | -452.86383 | 5.37   |
| Root5           | -451.28281 | -9.66500 | -452.86383 | 5.37   |
| Path1→(S₄-4)   | -451.58314 | -9.66588 | -452.85486 | 0.53   |
| Root1           | -451.43635 | -9.66588 | -452.85486 | 4.69   |
| Root2(Sₙp(′nπ*)| -451.38579 | -9.66588 | -452.85486 | 4.68   |
| Root3(Sₙπ(′nπ*)| -451.36290 | -9.66588 | -452.85486 | 5.40   |
| Root4           | -451.32260 | -9.66588 | -452.85486 | 5.40   |
| Root5           | -451.27847 | -9.66588 | -452.85486 | 5.40   |
| Path1→(S₄-5)   | -451.57946 | -9.66610 | -452.85207 | 0.60   |
| Root1           | -451.43443 | -9.66610 | -452.85207 | 4.72   |
| Root2(Sₙp(′nπ*)| -451.38611 | -9.66610 | -452.85207 | 4.65   |
| Root3(Sₙπ(′nπ*)| -451.38611 | -9.66610 | -452.85207 | 4.65   |
| Path1−(SCT(1ππ*))−6 | Root1 | -451.57673 | -9.66665 | -452.84980 | 0.65 |
| Root2(SNP(1nπ*)) | -451.43304 | -452.69947 | 4.74 |
| Root3(SCT(1ππ*)) | -451.38609 | -452.70379 | 4.62 |
| Root4 | -451.36230 | -452.67453 | 5.41 |
| Root5 | -451.31922 | |
| Root6 | -451.27733 | |

| Path1−(SCT(1ππ*))−7 | Root1 | -451.57337 | -9.66666 | -452.84665 | 0.73 |
| Root2(SNP(1nπ*)) | -451.43204 | -452.69849 | 4.76 |
| Root3(SCT(1ππ*)) | -451.38612 | -452.70392 | 4.61 |
| Root4 | -451.36226 | -452.67394 | 5.43 |
| Root5 | -451.31715 | |
| Root6 | -451.27592 | |

| Path1−(SCT(1ππ*))−8 | Root1 | -451.56730 | -9.66635 | -452.84050 | 0.91 |
| Root2 | -451.43134 | -452.69776 | 4.79 |
| Root3(SCT(1ππ*)) | -451.38593 | -452.70363 | 4.63 |
| Root4 | -451.36292 | -452.67374 | 5.44 |
| Root5 | -451.31753 | |
| Root6 | -451.27592 | |

| Path1−(SCT(1ππ*))−9 | Root1 | -451.57363 | -9.66100 | -452.84769 | 0.86 |
| Root2 | -451.43276 | -452.69894 | 4.90 |
| Root3(SCT(1ππ*)) | -451.38775 | -452.70551 | 4.73 |
| Root4 | -451.36165 | -452.67239 | 5.63 |
| Root5 | -451.31582 | |
| Root6 | -451.27599 | |

| Path1−(SCT(1ππ*))−10 | Root1 | -451.57378 | -9.66063 | -452.84487 | 0.94 |
| Root2 | -451.43308 | -452.69762 | 4.95 |
| Root3(SCT(1ππ*)) | -451.38778 | -452.70592 | 4.72 |
| Root4 | -451.36175 | -452.67145 | 5.66 |
| Root5 | -451.31628 | |
| Root6 | -451.27599 | |

| Path1−(SCT(1ππ*))−11 | Root1 | -451.53565 | -9.66181 | -452.81144 | 1.82 |
| Root2 | -451.41074 | -452.67901 | 5.42 |
| Root3(SCT(1ππ*)) | -451.38886 | -452.70848 | 4.62 |
| Root4 | -451.34834 | -452.64667 | 6.30 |
| Root5 | -451.29216 | |
| Root6 | -451.26245 | |

| Path1−(SCT(1ππ*))−12 | Root1 | -451.48831 | -9.66580 | -452.76056 | 3.10 |
| Root2 | -451.39185 | -452.66142 | 5.79 |
| Root3(SCT(1ππ*)) | -451.38555 | -452.71189 | 4.42 |
| Root4 | -451.33319 | -452.61631 | 7.02 |
| Root5 | -451.25707 | |
Table S6. Absolute energies (A.E., hartree), relative energies (R.E., eV/mol) and MM energies (hartree) for the optimized structures of thymine monomer along the relaxation pathway in the triplet excited state. The corresponding energy profiles are plotted in Figure 1b of the main article.

| Thymine Monomer | Path2\(-\text{Sn}(\pi\pi^*)\)-1 | Path2\(-\text{Sn}(\pi\pi^*)\)-2 | Path2\(-\text{Sn}(\pi\pi^*)\)-3 |
|-----------------|-------------------------------|-------------------------------|-------------------------------|
|                 | A.E. | A.E. | A.E. | R.E. | A.E. | A.E. | A.E. | R.E. |
| Root1           | -451.57043 | -9.66756 | -452.84481 | 0.76 |
| Root2(Sn(\pi\pi^*)) | -451.46102 | -452.72115 | 4.12 |
| Root3           | -451.38826 | -452.68130 | 5.21 |
| Root4           | -451.34460 | -452.68494 | 5.11 |
| Root5           | -451.33734 |                           |                           |
| Root6           | -451.27273 |                           |                           |
| Root1           | -451.56125 | -9.66712 | -452.83789 | 0.96 |
| Root2(Sn(\pi\pi^*)) | -451.46244 | -452.72307 | 4.08 |
| Root3           | -451.39159 | -452.68583 | 5.09 |
| Root4           | -451.34142 | -452.68507 | 5.11 |
| Root5           | -451.33653 |                           |                           |
| Root6           | -451.27100 |                           |                           |
| Root1           | -451.56028 | -9.66714 | -452.83688 | 0.98 |
|       | Root2(SNP(1nπ*)) | Root3 | Root4 | Root5 | Root6 |
|-------|-----------------|-------|-------|-------|-------|
|       | −451.46240      | −451.39196 | −451.34103 | −451.33613 | −451.27034 |

Path2–SNP(1nπ*)–4

Snp–Min

|       | Root1 | Root2(SNP(1nπ*)) | Root3 | Root4 | Root5 | Root6 |
|-------|-------|-----------------|-------|-------|-------|-------|
|       | −451.55907 | −9.66850        | −452.83465 | 1.01 |

Path2–Tct(πππ*)–1

|       | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-------|-------|-------|-------|-------|-------|-------|
|       | −451.56531 | −9.66481 | −452.84085 | 0.94 |

Path2–Tct(πππ*)–2

|       | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-------|-------|-------|-------|-------|-------|-------|
|       | −451.57495 | −9.66441 | −452.84897 | 0.73 |

Path2–Tct(πππ*)–3

|       | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-------|-------|-------|-------|-------|-------|-------|
|       | −451.58846 | −9.66467 | −452.85914 | 0.45 |

Path2–Tct(πππ*)–4

|       | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-------|-------|-------|-------|-------|-------|-------|
|       | −451.48893 | −452.76065 | 3.13 |

Path2–Tct(πππ*)–5

|       | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-------|-------|-------|-------|-------|-------|-------|
|       | −451.47932 | −452.74414 | 3.57 |

Path2–Tct(πππ*)–6

|       | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-------|-------|-------|-------|-------|-------|-------|
|       | −451.48297 | −452.75073 | 3.40 |

Path2–Tct(πππ*)–7

|       | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-------|-------|-------|-------|-------|-------|-------|
|       | −451.46635 | −452.72685 | 4.05 |

Path2–Tct(πππ*)–8

|       | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-------|-------|-------|-------|-------|-------|-------|
|       | −451.58884 | −452.85914 | 0.45 |

Path2–Tct(πππ*)–9

|       | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-------|-------|-------|-------|-------|-------|-------|
|       | −451.48893 | −452.76065 | 3.13 |

Path2–Tct(πππ*)–10

|       | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-------|-------|-------|-------|-------|-------|-------|
|       | −451.45025 | −452.71398 | 4.40 |

Path2–Tct(πππ*)–11

|       | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-------|-------|-------|-------|-------|-------|-------|
|       | −451.45469 | −452.71893 | 4.26 |

Path2–Tct(πππ*)–12

|       | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-------|-------|-------|-------|-------|-------|-------|
|       | −451.40894 | −452.69500 | 4.91 |

Path2–Tct(πππ*)–13

|       | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-------|-------|-------|-------|-------|-------|-------|
|       | −451.34377 | −452.62701 | 6.76 |

Path2–Tct(πππ*)–14

|       | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-------|-------|-------|-------|-------|-------|-------|
|       | −451.33898 | −452.62701 | 6.76 |

Path2–Tct(πππ*)–15

|       | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-------|-------|-------|-------|-------|-------|-------|
|       | −451.31844 | −452.62701 | 6.76 |
| Path2−TCT(ππ*)−4 |  |  |  |
|---|---|---|---|
| Root1 | -451.58917 | -9.66559 | -452.85770 | 0.46 |
| Root2 | -451.43316 |  | -452.69994 | 4.75 |
| Root3 | -451.37730 |  | -452.69433 | 4.90 |
| Root4 | -451.36083 |  | -452.67777 | 5.36 |
| Root5 | -451.32234 |  |  |  |
| Root6 | -451.27737 |  |  |  |
| Root1(TCT(ππ*)) | -451.49118 |  | -452.76272 | 3.04 |
| Root2 | -451.43717 |  | -452.70565 | 4.60 |
| Root3 | -451.39582 |  | -452.68381 | 4.90 |
| Root4 | -451.33881 |  | -452.63887 | 5.36 |
| Root5 | -451.32211 |  |  |  |
| Root6 | -451.31310 |  |  |  |

| Path2−TCT(ππ*)−5 |  |  |  |
|---|---|---|---|
| Root1 | -451.58641 | -9.66549 | -452.85541 | 0.52 |
| Root2 | -451.43024 |  | -452.69778 | 4.81 |
| Root3 | -451.37586 |  | -452.69481 | 4.89 |
| Root4 | -451.36039 |  | -452.67648 | 5.39 |
| Root5 | -451.32027 |  |  |  |
| Root6 | -451.27643 |  |  |  |
| Root1(TCT(ππ*)) | -451.49174 |  | -452.76363 | 3.02 |
| Root2 | -451.43418 |  | -452.70347 | 4.66 |
| Root3 | -451.39395 |  | -452.68228 | 5.24 |
| Root4 | -451.33721 |  | -452.63842 | 6.43 |
| Root5 | -451.33031 |  |  |  |
| Root6 | -451.31116 |  |  |  |

| Path2−TCT(ππ*)−6 |  |  |  |
|---|---|---|---|
| Root1 | -451.58305 | -9.66553 | -452.85201 | 0.62 |
| Root2 | -451.42953 |  | -452.69713 | 4.83 |
| Root3 | -451.37539 |  | -452.69358 | 4.93 |
| Root4 | -451.36117 |  | -452.67804 | 5.35 |
| Root5 | -451.31859 |  |  |  |
| Root6 | -451.27678 |  |  |  |
| Root1(TCT(ππ*)) | -451.49332 |  | -452.76452 | 3.00 |
| Root2 | -451.43328 |  | -452.70242 | 4.69 |
| Root3 | -451.39282 |  | -452.68074 | 5.28 |
| Root4 | -451.33444 |  | -452.63584 | 6.50 |
| Root5 | -451.32876 |  |  |  |
| Root6 | -451.30799 |  |  |  |

| Path2−TCT(ππ*)−7 |  |  |  |
|---|---|---|---|
| Root1 | -451.57191 | -9.66443 | -452.84023 | 0.97 |
| Root2 | -451.42834 |  | -452.69620 | 4.89 |
| Root3 | -451.37269 |  | -452.68459 | 5.20 |
| Root4 | -451.36235 |  | -452.68388 | 5.22 |
| Root5 | -451.31154 |  |  |  |
| Root6 | -451.27901 |  |  |  |
| Root1(TCT(ππ*)) | -451.49766 |  | -452.76603 | 2.99 |
| Root2 | -451.43042 |  | -452.69979 | 4.79 |
| Root3 | -451.38897 |  | -452.67677 | 5.41 |
| Root4 | -451.32546 |  | -452.62477 | 6.83 |
| Root5 | -451.32083 |  |  |  |
| Path2–TCT(3ππ*) |  |  |  |  |  |  |  |  |
|---|---|---|---|---|---|---|---|---|
| Root6 |  | −451.29932 |  |  |  |  |  |  |
| Path2–TCT(3ππ*) |  |  |  |  |  |  |  |  |
| Root1 | −451.53031 | −9.67054 | −452.80549 | 1.75 |  |  |  |  |
| Root2 | −451.38635 |  | −452.68507 | 5.02 |  |  |  |  |
| Root3 | −451.35621 |  | −452.67946 | 5.17 |  |  |  |  |
| Root4 | −451.33969 |  | −452.64815 | 6.03 |  |  |  |  |
| Root5 | −451.31312 |  |  |  |  |  |  |  |
| Root6 | −451.28053 |  |  |  |  |  |  |  |
| Root1(TCT(3ππ*)) | −451.49179 |  | −452.75866 | 3.02 |  |  |  |  |
| Root2 | −451.38925 |  | −452.66557 | 5.55 |  |  |  |  |
| Root3 | −451.35393 |  | −452.64149 | 6.21 |  |  |  |  |
| Root4 | −451.31308 |  | −452.61803 | 6.85 |  |  |  |  |
| Root5 | −451.30463 |  |  |  |  |  |  |  |
| Root6 | −451.30009 |  |  |  |  |  |  |  |
| Path2–TCT(3ππ*) |  |  |  |  |  |  |  |  |
| Root1 | −451.51413 | −9.67059 | −452.79137 | 2.13 |  |  |  |  |
| Root2 | −451.35525 |  | −452.68300 | 4.93 |  |  |  |  |
| Root3 | −451.32166 |  | −452.63598 | 6.36 |  |  |  |  |
| Root4 | −451.30857 |  | −452.60834 | 7.11 |  |  |  |  |
| Root5 | −451.28767 |  |  |  |  |  |  |  |
| Root6 | −451.26007 |  |  |  |  |  |  |  |
| Root1(TCT(3ππ*)) | −451.49033 |  | −452.75646 | 3.08 |  |  |  |  |
| Root2 | −451.37292 |  | −452.65188 | 5.92 |  |  |  |  |
| Root3 | −451.33774 |  | −452.62501 | 6.65 |  |  |  |  |
| Root4 | −451.30867 |  | −452.60028 | 7.33 |  |  |  |  |
| Root5 | −451.29680 |  |  |  |  |  |  |  |
| Root6 | −451.29194 |  |  |  |  |  |  |  |
| Path2–TCT(3ππ*) |  |  |  |  |  |  |  |  |
| Root1 | −451.49536 | −9.67442 | −452.76326 | 2.79 |  |  |  |  |
| Root2 | −451.39289 |  |  |  |  |  |  |  |
| Root3 | −451.33982 |  |  |  |  |  |  |  |
| Root4 | −451.32774 |  |  |  |  |  |  |  |
| Root5 | −451.27673 |  |  |  |  |  |  |  |
| Root6 | −451.27461 |  |  |  |  |  |  |  |
| Root1(TCT(3ππ*)) | −451.49052 |  | −452.75202 | 3.09 |  |  |  |  |
| Root2 | −451.38254 |  |  |  |  |  |  |  |
| Root3 | −451.33301 |  |  |  |  |  |  |  |
| Root4 | −451.30623 |  |  |  |  |  |  |  |
| Root5 | −451.29205 |  |  |  |  |  |  |  |
| Root6 | −451.27201 |  |  |  |  |  |  |  |
| Path2–TCT(3ππ*) |  |  |  |  |  |  |  |  |
| Root1 | −451.49091 | −9.67452 | −452.75960 | 2.89 |  |  |  |  |
| Root2 | −451.38593 |  |  |  |  |  |  |  |
| Root3 | −451.33287 |  |  |  |  |  |  |  |
| Root4 | −451.31946 |  |  |  |  |  |  |  |
| Root5 | −451.27905 |  |  |  |  |  |  |  |
| Root6 | −451.27217 |  |  |  |  |  |  |  |
| Root1(TCT(3ππ*)) | −451.48867 |  | −452.75074 | 3.13 |  |  |  |  |
| Root2 | −451.37062 |  |  |  |  |  |  |  |
| Root3 | −451.32352 |  |  |  |  |  |  |  |
| Root4 | −451.30813 |  |  |  |  |  |  |  |
| Root5 | −451.29341 |  |  |  |  |  |  |  |
Table S7. Absolute energies (A.E., hartree), relative energies (R.E., eV/mol) and MM energies (hartree) for the optimized structures of thymine oligomer along the relaxation pathway in the singlet excited state. The corresponding energy profiles are plotted in the right of Figure 2a in the main article.

| Thymine Oligomer | RASSCF | MM | CASPT2 |
|------------------|--------|----|--------|
|                  | A.E.   | A.E.| A.E.   | R.E.  |
| So               | 903.16987 | -29.98257 | -905.75157 | 0.00 |
| Root2(SNP(1nπ*)  | -902.99846 | -905.57357 | 4.84 |
| Root3(SCT(1ππ*)  | -902.91004 | -905.57437 | 4.82 |
| Root4            | -902.89802 | -905.52396 | 6.19 |
| Root5            | -902.87463 | -905.49057 | 7.10 |
| Root6            | -902.87093 | -905.47462 | 7.53 |
| Path3–(SCT(1ππ*))–1 |
| Root1           | -903.16831 | -29.97864 | -905.75118 | 0.11 |
| Root2(SNP(1nπ*)  | -902.99363 | -905.57913 | 4.79 |
| Root3(SCT(1ππ*)  | -902.91749 | -905.58037 | 4.76 |
| Root4            | -902.90783 | -905.53182 | 6.08 |
| Root5            | -902.88193 |
| Root6            | -902.87776 |
| Path3–(SCT(1ππ*))–2 |
| CI(SCT/SNP)      |
| Root1           | -903.16602 | -29.97841 | -905.74987 | 0.15 |
| Root2(SNP(1nπ*)  | -902.99692 | -905.58165 | 4.73 |
| Root3(SCT(1ππ*)  | -902.92147 | -905.58087 | 4.75 |
| Root1 | -903.12917 | -29.97784 | -905.72385 | 0.88  |
|-------|------------|-----------|------------|-------|
| Root2 | -902.99166 | -29.97784 | -905.72385 | 0.88  |
| Root3 | -902.93884 | -29.97784 | -905.72385 | 0.88  |
| Root4 | -902.91592 | -29.97784 | -905.72385 | 0.88  |
| Root5 | -902.89305 | -29.97784 | -905.72385 | 0.88  |
| Root6 | -902.87577 | -29.97784 | -905.72385 | 0.88  |

Path3–(SCT(1ππ*))–4

| Root1 | -903.10404 | -29.98042 | -905.70141 | 1.42  |
|-------|------------|-----------|------------|-------|
| Root2 | -902.97848 | -29.98042 | -905.70141 | 1.42  |
| Root3 | -902.93534 | -29.98042 | -905.70141 | 1.42  |
| Root4 | -902.90938 | -29.98042 | -905.70141 | 1.42  |
| Root5 | -902.89562 | -29.98042 | -905.70141 | 1.42  |
| Root6 | -902.85628 | -29.98042 | -905.70141 | 1.42  |

Path3–(SCT(1ππ*))–5

| Root1 | -903.08919 | -29.97941 | -905.68912 | 1.78  |
|-------|------------|-----------|------------|-------|
| Root2 | -902.96759 | -29.97941 | -905.68912 | 1.78  |
| Root3 | -902.93598 | -29.97941 | -905.68912 | 1.78  |
| Root4 | -902.90253 | -29.97941 | -905.68912 | 1.78  |
| Root5 | -902.89360 | -29.97941 | -905.68912 | 1.78  |
| Root6 | -902.85628 | -29.97941 | -905.68912 | 1.78  |

Path3–(SCT(1ππ*))–6

| Root1 | -903.07060 | -29.97984 | -905.67474 | 2.16  |
|-------|------------|-----------|------------|-------|
| Root2 | -902.96759 | -29.97984 | -905.67474 | 2.16  |
| Root3 | -902.93598 | -29.97984 | -905.67474 | 2.16  |
| Root4 | -902.90253 | -29.97984 | -905.67474 | 2.16  |
| Root5 | -902.89360 | -29.97984 | -905.67474 | 2.16  |
| Root6 | -902.84523 | -29.97984 | -905.67474 | 2.16  |

Path3–(SCT(1ππ*))–7

| Root1 | -903.03505 | -29.97665 | -905.65857 | 2.69  |
|-------|------------|-----------|------------|-------|
| Root2 | -902.94722 | -29.97665 | -905.65857 | 2.69  |
| Root3 | -902.92934 | -29.97665 | -905.65857 | 2.69  |
| Root4 | -902.89054 | -29.97665 | -905.65857 | 2.69  |
| Root5 | -902.87824 | -29.97665 | -905.65857 | 2.69  |
| Root6 | -902.83057 | -29.97665 | -905.65857 | 2.69  |

Path3–(SCT(1ππ*))–8

| Root1 | -903.03353 | -29.97675 | -905.64613 | 3.02  |
|-------|------------|-----------|------------|-------|
| Root2 | -902.95759 | -29.97675 | -905.64613 | 3.02  |
| Root3 | -902.88503 | -29.97675 | -905.64613 | 3.02  |
| Root4 | -902.86467 | -29.97675 | -905.64613 | 3.02  |
| Root5 | -902.80345 | -29.97675 | -905.64613 | 3.02  |
| Root6 | -902.79724 | -29.97675 | -905.64613 | 3.02  |

Path3–(SCT(1ππ*))–9

| Root1 | -903.02520 | -29.97558 | -905.63763 | 3.29  |
|-------|------------|-----------|------------|-------|
| Root2 | -902.95937 | -29.97558 | -905.63763 | 3.29  |
| Root3 | -902.87963 | -29.97558 | -905.63763 | 3.29  |
| Root4 | -902.85448 | -29.97558 | -905.63763 | 3.29  |
| Root5 | -902.79661 | -29.97558 | -905.63763 | 3.29  |
Table S8. Absolute energies (A.E., hartree), relative energies (R.E., eV/mol) and MM energies (hartree) for the optimized structures of thymine oligomer along the relaxation pathway in the singlet excited state. The corresponding energy profiles are plotted in the left of Figure 2a in the main article.

| Thymine oligomer | RASSCF | MM | CASPT2 |
|------------------|--------|----|--------|
|                  | A.E.   | A.E. | A.E.   | R.E.   |
| **Path4–(S\textsubscript{C}\pi\pi\star)–1** | | | |
| Root1            | -903.12917 | -29.97784 | -905.72385 | 0.88 |
| Root2            | -902.99166 | -29.97784 | -905.58784 | 4.83 |
| Root3            | -902.93884 | -29.97784 | -905.58241 | 4.73 |
| Root4            | -902.91592 | -29.97784 | -905.55440 | 5.49 |
| Root5            | -902.89305 | -29.97784 | -905.52842 | 6.25 |
| Root6            | -902.87577 | -29.97784 | -905.51283 | 7.23 |
| **Path4–(S\textsubscript{C}\pi\pi\star)–2** | | | |
| Root1            | -903.09472 | -29.97516 | -905.69336 | 1.76 |
| Root2            | -902.96973 | -29.97516 | -905.56314 | 5.30 |
| Root3            | -902.93575 | -29.97516 | -905.58842 | 4.61 |
| Root4            | -902.90403 | -29.97516 | -905.52842 | 6.25 |
| Root5            | -902.89129 | -29.97516 | -905.51283 | 7.23 |
| Root6            | -902.85252 | -29.97516 | -905.49310 | 8.28 |
| **Path4–(S\textsubscript{C}\pi\pi\star)–3** | | | |
| Root1            | -903.06827 | -29.97601 | -905.68741 | 1.92 |
| Root2            | -902.98199 | -29.97601 | -905.56107 | 5.36 |
| Root3            | -902.93596 | -29.97601 | -905.59017 | 4.57 |
| Root4            | -902.90115 | -29.97601 | -905.52195 | 6.42 |
| Root5            | -902.89067 | -29.97601 | -905.51283 | 7.23 |
| Root6            | -902.84748 | -29.97601 | -905.49310 | 8.28 |
| **Path4–(S\textsubscript{C}\pi\pi\star)–4** | | | |
| Root1            | -903.06827 | -29.97529 | -905.67092 | 2.39 |
| Path 4 | (SCT(1ππ*))−5 | Root 1 | −903.04618 | −29.97364 | −905.65445 | 2.88 |
|--------|----------------|--------|-------------|-------------|-------------|-----|
|        | Root 2(SCT(1ππ*)) | −902.94566 | −905.60097 | 4.34 |
|        | Root 3 | −902.92378 | −905.53844 | 6.04 |
|        | Root 4 | −902.88698 | −905.51268 | 6.74 |
|        | Root 5 | −902.87455 | −905.49499 | 7.19 |
|        | Root 6 | −902.80600 | −905.49499 | 7.19 |

| Path 4 | (SCT(1ππ*))−6 | Root 1 | −903.02460 | −29.97476 | −905.64003 | 3.24 |
|--------|----------------|--------|-------------|-------------|-------------|-----|
|        | Root 2 | −902.95406 | −905.60266 | 4.26 |
|        | Root 3 | −902.88733 | −905.52426 | 6.39 |
|        | Root 4 | −902.84979 | −905.49499 | 7.19 |
|        | Root 5 | −902.80010 | −905.49499 | 7.19 |
|        | Root 6 | −902.79488 | −905.49499 | 7.19 |

| Path 4 | (SCT(1ππ*))−7 | Root 1 | −903.00654 | −29.98014 | −905.63488 | 3.35 |
|--------|----------------|--------|-------------|-------------|-------------|-----|
|        | Root 2 | −902.98266 | −905.62487 | 3.51 |
|        | Root 3 | −902.87222 | −905.55016 | 5.54 |
|        | Root 4 | −902.83084 | −905.49520 | 7.04 |
|        | Root 5 | −902.79157 | −905.49520 | 7.04 |
|        | Root 6 | −902.77666 | −905.49520 | 7.04 |

| Path 4 | (SCT(1ππ*))−8 | CI(SCT/S0)−2 | Root 1 | −902.99919 | −29.981189 | −905.62979 | 3.35 |
|--------|----------------|-------------|--------|-------------|-------------|-------------|-----|
|        | Root 2 | −902.98368 | −905.62824 | 3.39 |
|        | Root 3 | −902.86393 | −905.54427 | 5.67 |
|        | Root 4 | −902.82068 | −905.48924 | 7.17 |
|        | Root 5 | −902.78273 | −905.48924 | 7.17 |
|        | Root 6 | −902.76717 | −905.48924 | 7.17 |

| Path 4 | S0−9 | Root 1 | −903.03472 | −29.97482 | −905.64456 | 3.12 |
|--------|------|--------|-------------|-------------|-------------|-----|
|        | Root 2 | −902.89373 | −905.55186 | 5.64 |
|        | Root 3 | −902.88662 | −905.51989 | 6.51 |
|        | Root 4 | −902.87074 | −905.51989 | 6.51 |
|        | Root 5 | −902.83130 | −905.51989 | 6.51 |
|        | Root 6 | −902.81034 | −905.51989 | 6.51 |

| Path 4 | S0−10 | Root 1 | −903.03949 | −29.97326 | −905.64877 | 3.05 |
|--------|-------|--------|-------------|-------------|-------------|-----|
|        | Root 2 | −902.88427 | −905.53164 | 6.23 |
|        | Root 3 | −902.87787 | −905.53634 | 6.10 |
|        | Root 4 | −902.86589 | −905.53634 | 6.10 |
|        | Root 5 | −902.822766 | −905.53634 | 6.10 |
|        | Root 6 | −902.80912 | −905.53634 | 6.10 |

| Path 4 | S0−11 | Root 1 | −903.05049 | −29.97326 | −905.66130 | 2.70 |
|--------|-------|--------|-------------|-------------|-------------|-----|
|        | Root 2 | −902.88781 | −905.51901 | 6.58 |
|        | Root 3 | −902.86297 | −905.57343 | 5.10 |
| Path4–S0–12 | Root1 | -903.06502 | -29.97230 | -905.67741 | 2.29 |
| | Root2 | -902.89306 | | -905.52466 | 6.45 |
| | Root3 | -902.85173 | | -905.57267 | 5.14 |
| | Root4 | -902.81959 | | | |
| | Root5 | -902.81163 | | | |
| | Root6 | -902.79464 | | | |
| Path4–S0–13 | Root1 | -903.07575 | -29.97199 | -905.69212 | 1.90 |
| | Root2 | -902.89949 | | -905.53499 | 6.18 |
| | Root3 | -902.83938 | | -905.56346 | 5.40 |
| | Root4 | -902.82004 | | | |
| | Root5 | -902.81005 | | | |
| | Root6 | -902.78575 | | | |
| Path4–S0–14 | Root1 | -903.07918 | -29.97167 | -905.69696 | 1.78 |
| | Root2 | -902.90040 | | -905.53714 | 6.13 |
| | Root3 | -902.83596 | | -905.56161 | 5.46 |
| | Root4 | -902.81662 | | | |
| | Root5 | -902.80689 | | | |
| | Root6 | -902.78475 | | | |
| Path4–S0–15 | Root1 | -903.08516 | -29.97155 | -905.70583 | 1.54 |
| | Root2 | -902.90172 | | -905.54110 | 6.02 |
| | Root3 | -902.82583 | | -905.55507 | 5.64 |
| | Root4 | -902.81086 | | | |
| | Root5 | -902.79778 | | | |
| | Root6 | -902.78208 | | | |
| Path4–S0–16 | Root1 | -903.08961 | -29.97138 | -905.71403 | 1.32 |
| | Root2 | -902.90196 | | -905.54949 | 5.92 |
| | Root3 | -902.81628 | | -905.54931 | 5.80 |
| | Root4 | -902.80445 | | | |
| | Root5 | -902.78571 | | | |
| | Root6 | -902.77681 | | | |
| Path4–S0–17 | Root1 | -903.09254 | -29.97136 | -905.72125 | 1.12 |
| | Root2 | -902.90111 | | -905.54839 | 5.83 |
| | Root3 | -902.80772 | | -905.54559 | 5.90 |
| | Root4 | -902.79862 | | | |
| | Root5 | -902.77436 | | | |
| | Root6 | -902.77168 | | | |
| Path4–S0–18 | Root1 | -903.10511 | -29.97175 | -905.73247 | 0.81 |
| | Root2 | -902.90736 | | -905.55083 | 5.75 |
| | Root3 | -902.89787 | | -905.55960 | 5.51 |
| | Root4 | -902.77442 | | | |
| | Root5 | -902.75487 | | | |
| | Root6 | -902.74138 | | | |
Table S9. Absolute energies (A.E., hartree), relative energies (R.E., eV/mol) and MM energies (hartree) for the optimized structures of thymine oligomer along the relaxation pathway in the triplet excited state. The corresponding energy profiles are plotted in Figure 2b in the main article.

| Path4–S0–19 | Path4–S0–20 | Path4–S0–21 |
|--------------|--------------|--------------|
| Root1        | Root1        | Root1        |
| Root2        | Root2        | Root2        |
| Root3        | Root3        | Root3        |
| Root4        | Root4        | Root4        |
| Root5        | Root5        | Root5        |
| Root6        | Root6        | Root6        |
| Path5–(SNP(1nπ*)–1) | Path5–(SNP(1nπ*)–2) | Path5–(SNP(1nπ*)–3) |
| Root1        | Root1        | Root1        |
| Root2        | Root2        | Root2        |
| Root3        | Root3        | Root3        |
| Root4        | Root4        | Root4        |
| Root5        | Root5        | Root5        |
| Root6        | Root6        | Root6        |
| Path5–(SNP(1nπ*)–4) | | |
| Root1        | Root1        | Root1        |
| Root2        | Root2        | Root2        |

| Thymine oligomer | RASSCF A.E. | MM A.E. | CASPT2 A.E. | R.E. |
|------------------|-------------|---------|-------------|------|
| Path5–(SNP(1nπ*)–1) | -903.12883 | -29.98393 | -905.72358 | 0.72 |
| Root1            | -902.99588 | -905.58201 | 4.57       |
| Root2(SNP(1nπ*)) | -902.93988 | -905.57780 | 4.69       |
| Root3            | -902.91776 | -905.56224 | 5.11       |
| Root4            | -902.89325 |           |            |
| Root5            | -902.87890 |           |            |
| Root6            | -903.12495 | -29.98403 | -905.72081 | 0.79 |
| Path5–(SNP(1nπ*)–2) | -903.01792 | -905.59149 | 4.31       |
| Root1            | -902.91645 | -905.57762 | 4.69       |
| Root2(SNP(1nπ*)) | -902.89107 |           |            |
| Root3            | -902.88770 |           |            |
| Path5–(SNP(1nπ*)–3) | -903.11703 | -29.98409 | -905.71395 | 0.98 |
| Root1            | -903.01792 | -905.59919 | 4.10       |
| Root2(SNP(1nππ)) | -902.94912 | -905.56311 | 5.08       |
| Root3            | -902.90510 |           |            |
| Root4            | -902.89458 |           |            |
| Root5            | -902.88566 |           |            |
| Path5–(SNP(1nπ*)–4) | -903.11372 | -29.98427 | -905.71075 | 1.06 |
| Root1            | -903.02088 | -905.60136 | 4.04       |
| Root2(SNP(1nπ*)) | -902.80329 | -905.52179 | 6.54       |
| Root3            | -902.77103 |           |            |
| Root4            | -902.76235 |           |            |
| Root5            | -902.76231 |           |            |
| Root6            | -902.76228 |           |            |
| Root1 | 903.11770 | -29.98437 | -905.71173 | 1.03 |
|---|---|---|---|---|
| Root2 | 903.02403 | -29.98437 | -905.60275 | 4.00 |
| Root3 | 902.93861 | -29.98437 | -905.54904 | 5.46 |
| Root4 | 902.90007 | -29.98437 | -905.55535 | 5.27 |
| Root5 | 902.88234 | -29.98437 | -905.55535 | 5.27 |
| Root6 | 902.87953 | -29.98437 | -905.55535 | 5.27 |

Path5–(SCT(3ππ*)–7

| Root1 | 903.11770 | -29.98430 | -905.71116 | 1.05 |
|---|---|---|---|---|
| Root2 | 903.02488 | -29.98430 | -905.60262 | 4.00 |
| Root3 | 902.93772 | -29.98430 | -905.54745 | 5.50 |
| Root4 | 902.90188 | -29.98430 | -905.54745 | 5.50 |
| Root5 | 902.88640 | -29.98430 | -905.54745 | 5.50 |
| Root6 | 902.87815 | -29.98430 | -905.54745 | 5.50 |
| Path     | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|----------|-------|-------|-------|-------|-------|-------|
| 6        | -902.82225 | -902.98219 | -902.96497 | -902.89293 | -902.88745 | -902.86919 |
| (TCT(3ππ*)−902.82225 | -903.03478 | -902.98219 | -902.994284 | -902.91208 | -902.89909 | -902.89053 |
| 4        | -902.82225 | -902.98219 | -902.994284 | -902.91208 | -902.89909 | -902.89053 |
| (TCT(3ππ*)−902.82225 | -903.04229 | -902.99017 | -902.96833 | -902.94284 | -902.89909 | -902.89053 |
| 2        | -902.82225 | -902.98219 | -902.994284 | -902.91208 | -902.89909 | -902.89053 |
| (TCT(3ππ*)−902.82225 | -903.04958 | -902.99017 | -902.96833 | -902.94284 | -902.89909 | -902.89053 |
| 0        | -902.82225 | -902.98219 | -902.994284 | -902.91208 | -902.89909 | -902.89053 |
| (TCT(3ππ*)−902.82225 | -903.13566 | -902.98396 | -902.92460 | -902.91533 | -902.90158 | -902.87591 |
| 6        | -902.82225 | -902.98219 | -902.994284 | -902.91208 | -902.89909 | -902.89053 |
| (TCT(3ππ*)−902.82225 | -903.05459 | -902.98396 | -902.92460 | -902.91533 | -902.90158 | -902.87591 |
| 4        | -902.82225 | -902.98219 | -902.994284 | -902.91208 | -902.89909 | -902.89053 |
| (TCT(3ππ*)−902.82225 | -903.14364 | -903.01782 | -902.94284 | -902.91533 | -902.90158 | -902.87591 |
| 2        | -902.82225 | -902.98219 | -902.994284 | -902.91208 | -902.89909 | -902.89053 |
| (TCT(3ππ*)−902.82225 | -903.04229 | -903.01782 | -902.94284 | -902.91533 | -902.90158 | -902.87591 |
| 0        | -902.82225 | -902.98219 | -902.994284 | -902.91208 | -902.89909 | -902.89053 |
| (TCT(3ππ*)−902.82225 | -903.14364 | -903.01782 | -902.94284 | -902.91533 | -902.90158 | -902.87591 |
| 6        | -902.82225 | -902.98219 | -902.994284 | -902.91208 | -902.89909 | -902.89053 |
| (TCT(3ππ*)−902.82225 | -903.04229 | -903.01782 | -902.94284 | -902.91533 | -902.90158 | -902.87591 |
| 4        | -902.82225 | -902.98219 | -902.994284 | -902.91208 | -902.89909 | -902.89053 |
| (TCT(3ππ*)−902.82225 | -903.04229 | -903.01782 | -902.94284 | -902.91533 | -902.90158 | -902.87591 |
| 2        | -902.82225 | -902.98219 | -902.994284 | -902.91208 | -902.89909 | -902.89053 |
| (TCT(3ππ*)−902.82225 | -903.04229 | -903.01782 | -902.94284 | -902.91533 | -902.90158 | -902.87591 |
| 0        | -902.82225 | -902.98219 | -902.994284 | -902.91208 | -902.89909 | -902.89053 |
| (TCT(3ππ*)−902.82225 | -903.04229 | -903.01782 | -902.94284 | -902.91533 | -902.90158 | -902.87591 |
| Path6−(TCT\(3\pi\pi^*\))−7 | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-----------------------------|-------|-------|-------|-------|-------|-------|
| Root1(TCT\(3\pi\pi^*\))   | -903.05411 | -902.98252 | -902.93467 | -902.90867 | -902.88852 | -902.85695 |
| Root2                       | -29.98025 | -29.98025 | -29.98025 | -29.98025 | -29.98025 | -29.98025 |
| Root3                       | 1.37    | 4.82   | 5.40   | 6.74   | 6.00   | 6.61   |
| Root4                       | 3.01    | 4.04   | 5.69   | 6.00   | 6.00   | 6.61   |

| Path6−(TCT\(3\pi\pi^*\))−8 | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-----------------------------|-------|-------|-------|-------|-------|-------|
| Root1(TCT\(3\pi\pi^*\))   | -903.04755 | -902.96729 | -902.91388 | -902.90726 | -902.86870 | -902.84287 |
| Root2                       | 1.92   | 4.76   | 5.19   | 6.26   | 6.26   | 6.61   |
| Root3                       | 3.13   | 5.27   | 5.69   | 6.00   | 6.00   | 6.61   |
| Root4                       | 1.86   | 4.04   | 5.69   | 6.00   | 6.00   | 6.61   |

| Path6−(TCT\(3\pi\pi^*\))−9 | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-----------------------------|-------|-------|-------|-------|-------|-------|
| Root1(TCT\(3\pi\pi^*\))   | -903.03927 | -902.95258 | -902.90321 | -902.89242 | -902.84683 | -902.82479 |
| Root2                       | 1.92   | 4.76   | 5.19   | 6.26   | 6.26   | 6.61   |
| Root3                       | 3.13   | 5.27   | 5.69   | 6.00   | 6.00   | 6.61   |
| Root4                       | 1.86   | 4.04   | 5.69   | 6.00   | 6.00   | 6.61   |

| Path6−(TCT\(3\pi\pi^*\))−10 | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|-----------------------------|-------|-------|-------|-------|-------|-------|
| Root1(TCT\(3\pi\pi^*\))   | -903.03461 | -902.94883 | -902.90517 | -902.88337 | -902.81569 | -902.81103 |
| Root2                       | 1.92   | 4.76   | 5.19   | 6.26   | 6.26   | 6.61   |
| Root3                       | 3.13   | 5.27   | 5.69   | 6.00   | 6.00   | 6.61   |
| Root4                       | 1.86   | 4.04   | 5.69   | 6.00   | 6.00   | 6.61   |

| STC(TCT/S0)                     | Root1 | Root2 | Root3 | Root4 | Root5 | Root6 |
|---------------------------------|-------|-------|-------|-------|-------|-------|
| Root1(TCT\(3\pi\pi^*\))       | -903.04387 | -902.94883 | -902.90517 | -902.88337 | -902.81569 | -902.81103 |
| Root2                       | 2.62   | 4.36   | 6.44   | 6.44   | 6.44   | 6.44   |
| Root3                       | 4.36   | 4.36   | 4.36   | 4.36   | 4.36   | 4.36   |
|    | E1 (a.u.) | E2 (a.u.) | DeltaE (a.u.) |
|----|-----------|-----------|---------------|
| Root4 | -902.88308 | -905.53816 | 6.04          |
| Root5 | -902.82477 |           |               |
| Root6 | -902.80177 |           |               |
| Root1(TCT(3ππ*)) | -903.04810 | -905.65828 | 2.78          |
| Root2 | -902.88767 | -905.53421 | 6.15          |
| Root3 | -902.87723 | -905.55138 | 5.69          |
| Root4 | -902.86441 | -905.54919 | 5.74          |
| Root5 | -902.81743 |           |               |
| Root6 | -902.80801 |           |               |
| Path6−S0−1 | -903.05068 | -905.66719 | 2.55          |
| Root2 | -902.93639 | -905.56883 | 5.23          |
| Root3 | -902.88582 | -905.58870 | 4.69          |
| Root4 | -902.88003 | -905.55008 | 5.74          |
| Root5 | -902.85611 |           |               |
| Root6 | -902.84803 |           |               |
| Path6−S0−2 | -903.05897 | -905.67495 | 2.34          |
| Root2 | -902.93121 | -905.55779 | 5.53          |
| Root3 | -902.87982 | -905.52851 | 6.33          |
| Root4 | -902.85145 | -905.57852 | 4.97          |
| Root5 | -902.83640 |           |               |
| Root6 | -902.82041 |           |               |
| Path6−S0−3 | -903.05334 | -905.68683 | 2.00          |
| Root2 | -902.85082 | -905.53151 | 6.23          |
| Root3 | -902.84314 | -905.55263 | 5.66          |
| Root4 | -902.82805 | -905.51568 | 6.66          |
| Root5 | -902.81320 |           |               |
| Root6 | -902.77767 |           |               |
| Path6−S0−4 | -903.05966 | -905.69629 | 1.73          |
| Root2 | -902.83482 | -905.49803 | 7.12          |
| Root3 | -902.82352 | -905.54257 | 5.91          |
| Root4 | -902.81267 | -905.51792 | 6.58          |
| Root5 | -902.78897 |           |               |
| Root6 | -902.78062 |           |               |
| Path6−S0−5 | -903.06598 | -905.70542 | 1.46          |
| Root2 | -902.83750 | -905.49594 | 7.16          |
| Root3 | -902.81059 | -905.53436 | 6.11          |
| Root4 | -902.79778 | -905.51236 | 6.71          |
| Root5 | -902.77768 |           |               |
| Root6 | -902.77076 |           |               |
| Path6−S0−6 | -903.08177 | -905.71738 | 1.13          |
| Root2 | -902.88954 | -905.54427 | 5.84          |
| Root3 | -902.78874 | -905.53828 | 6.00          |
| Root4 | -902.78206 |           |               |
| Root5 | -902.76536 |           |               |
| Root6 | -902.72329 |           |               |
| Path6−S0−7 | -903.06598 | -905.70542 | 1.46          |
|       | Root1     | Root2     | Root3     | Root4     | Root5     | Root6     | Root1     | Root2     | Root3     | Root4     | Root5     | Root6     |
|-------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
|       | -903.09503 | -902.88247 | -902.80581 | -902.79367 | -902.75957 | -902.72490 | -903.10972 | -902.89419 | -902.81788 | -902.80336 | -902.75779 | -902.73738 |
|       | -29.97534  | -29.97532  | -29.97533  | -29.97534  | -29.97532  | -29.97532  | -29.97532  | -29.97532  | -29.97532  | -29.97532  | -29.97532  | -29.97532  |
|       | -905.72688 | -905.54447 | -905.51373 | -905.79367 | -905.52129 | -905.52129 | -905.73885 | -905.55134 | -905.52129 | -905.52105 | -905.52105 | -905.52105 |
|       | 0.86       | 5.83       | 6.66       | 0.54       | 5.64       | 6.66       | 0.54       | 5.37       | 6.46       | 5.44       | 6.44       | 6.44       |

6. Cartesian Coordinates

6.1. Thymine Monomer

|       | So–Min    |         |         |         |         |         | So–Min    |         |         |         |         |         |
|-------|-----------|---------|---------|---------|---------|---------|-----------|---------|---------|---------|---------|---------|
| N     | 0.185476  | -1.653287 | 0.000000 |         |         |         | 1.116523  | -1.240110 | 0.006340 |         |         |         |
| C     | -1.060339 | -1.052397 | 0.000000 |         |         |         | -0.195887 | -1.559472 | -0.005120 |         |         |         |
| H     | -1.897559 | -1.734286 | 0.000000 |         |         |         | -0.505145 | -2.570082 | 0.017820 |         |         |         |
| C     | -1.218752 | 0.286416  | 0.000000 |         |         |         | -1.175638 | -0.426493 | -0.022650 |         |         |         |
| C     | -2.566981 | 0.955575  | 0.000000 |         |         |         | -2.638108 | -0.725675 | 0.005280 |         |         |         |
| H     | -3.146799 | 0.695232  | 0.888980 |         |         |         | -2.441747 | 2.037106  | 0.000000 |         |         |         |
| H     | -3.146799 | 0.695232  | -0.888980 |         |         |         | -3.146799 | 0.695232  | 0.000000 |         |         |         |
| C     | 0.000000  | 1.106790  | 0.000000 |         |         |         | 0.019631  | 2.319392  | 0.000000 |         |         |         |
| O     | 2.034858  | 0.944533  | 0.000000 |         |         |         | 1.352569  | -0.957175 | 0.000000 |         |         |         |
| N     | 1.191679  | 0.406884  | 0.000000 |         |         |         | 0.236428  | -1.476921 | 0.000000 |         |         |         |
| H     | 0.270500  | -2.644337 | 0.000000 |         |         |         | 2.342146  | 1.921237  | 0.007710 |         |         |         |
| \(N\) | \(0.730810\) | \(1.037060\) | \(-0.007110\) |
|-----|------------|------------|-------------|
| \(H\) | \(1.096878\) | \(1.961900\) | \(0.001720\) |
| \(C\) | \(1.644551\) | \(0.045961\) | \(0.007430\) |
| \(O\) | \(2.839591\) | \(0.215813\) | \(-0.000700\) |
| \(H\) | \(1.799114\) | \(-1.976899\) | \(0.009380\) |

\(\text{Sct} - \text{Min}\)

| \(N\) | \(1.119771\) | \(-1.238058\) | \(0.032999\) |
|-----|------------|------------|-------------|
| \(C\) | \(-0.181598\) | \(-1.596741\) | \(-0.058651\) |
| \(H\) | \(-0.456726\) | \(-2.620651\) | \(0.094479\) |
| \(C\) | \(-1.172160\) | \(-0.430422\) | \(-0.046611\) |
| \(H\) | \(-2.917139\) | \(-1.976899\) | \(0.905639\) |

\(\text{Cl(}\text{Sct/So})\)

| \(N\) | \(1.162334\) | \(1.042346\) | \(-0.263248\) |
|-----|------------|------------|-------------|
| \(C\) | \(0.032843\) | \(1.331628\) | \(-0.886719\) |
| \(H\) | \(0.071177\) | \(2.052965\) | \(-1.704964\) |
| \(C\) | \(-1.168235\) | \(0.700011\) | \(-0.381541\) |
| \(C\) | \(-1.406077\) | \(1.232412\) | \(1.064511\) |
| \(H\) | \(-1.516797\) | \(2.315505\) | \(1.051847\) |
| \(H\) | \(-2.359231\) | \(0.817655\) | \(1.396950\) |
| \(H\) | \(-0.646964\) | \(0.980334\) | \(1.816615\) |
| \(C\) | \(-1.030796\) | \(-0.740726\) | \(-0.296916\) |
| \(O\) | \(-1.865129\) | \(-1.605291\) | \(-0.182635\) |
| \(N\) | \(0.327974\) | \(-1.149773\) | \(-0.123341\) |
| \(H\) | \(0.485579\) | \(-2.113117\) | \(0.093964\) |
| \(C\) | \(1.377938\) | \(-0.317455\) | \(0.117311\) |
| \(O\) | \(2.451642\) | \(-0.658032\) | \(0.524231\) |
| \(H\) | \(2.007931\) | \(1.570014\) | \(-0.380930\) |

\(\text{Sn} - \text{Min}\)

| \(N\) | \(1.118267\) | \(-1.237341\) | \(0.044739\) |
|-----|------------|------------|-------------|
| \(C\) | \(-0.253141\) | \(-1.518689\) | \(0.007675\) |
| \(H\) | \(-0.538725\) | \(-2.551897\) | \(0.056292\) |
| \(C\) | \(-1.168598\) | \(-0.446918\) | \(-0.022008\) |
| \(C\) | \(-2.653941\) | \(-0.703861\) | \(-0.021797\) |
| \(H\) | \(-3.013310\) | \(-0.910705\) | \(0.986002\) |
| \(H\) | \(-3.209466\) | \(0.143430\) | \(-0.420720\) |
| \(H\) | \(-2.872031\) | \(-1.575108\) | \(-0.636353\) |
| \(C\) | \(-0.626645\) | \(0.797678\) | \(-0.036345\) |
| \(O\) | \(-1.340757\) | \(1.973560\) | \(0.013733\) |
| \(N\) | \(0.743315\) | \(1.035192\) | \(0.086639\) |
| \(H\) | \(1.104085\) | \(1.939825\) | \(-0.129636\) |
| \(C\) | \(1.656128\) | \(0.009531\) | \(0.011584\) |
| \(O\) | \(2.840365\) | \(0.216224\) | \(-0.059349\) |
|        |          |          |          |          |
|--------|----------|----------|----------|----------|
| H      | 1.778689 | -1.975222 | -0.044953 |
| STC(SNP/TNP/TCT) |          |          |          |          |
| N      | 1.120795 | -1.233804 | 0.048828  |
| C      | -0.250053| -1.516763 | 0.011604  |
| H      | -0.532149| -2.551886 | 0.045354  |
| C      | -1.164688| -0.455414 | -0.035941 |
| C      | -2.652419| -0.702201 | -0.016968 |
| H      | -3.047691| -0.634323 | 0.996749  |
| H      | -3.181849| 0.013410  | -0.644895 |
| H      | -2.864815| -1.702218 | -0.30277 |
| C      | -0.625705| 0.798493  | -0.081720 |
| O      | -1.353355| 1.961125  | 0.051529  |
| N      | 0.742618 | 1.039028  | 0.061322  |
| H      | 1.105331 | 1.936981  | -0.179572 |
| C      | 1.656466 | 0.013888  | 0.012628  |
| O      | 2.842204 | 0.219481  | -0.04265  |
| H      | 1.784882 | -1.971398 | -0.005539 |
|        |          |          |          |          |
| TCT−Min|          |          |          |          |
| N      | 1.136037 | -1.243013 | 0.055026  |
| C      | -0.202653| -1.580820 | -0.112823 |
| H      | -0.487456| -2.597956 | 0.108384  |
| C      | -1.179229| -0.433155 | 0.024707  |
| C      | -2.637720| -0.717310 | 0.012641  |
| H      | -2.914037| -1.303114 | 0.893253  |
| H      | -3.221890| 0.199103  | -0.011243 |
| H      | -2.882069| -1.323233 | -0.862983 |
| C      | -0.660316| 0.910617  | 0.002722  |
| O      | -1.350881| 1.909689  | 0.001241  |
| N      | 0.720175 | 1.040218  | -0.015701 |
| H      | 1.093182 | 1.966793  | -0.017239 |
| C      | 1.644709 | 0.020567  | 0.005134  |
| O      | 2.826107 | 0.245090  | -0.001860 |
| H      | 1.828229 | -1.959657 | 0.025211  |
|        |          |          |          |          |
| STC(TCT/S0) |          |          |          |          |
| N      | 1.162334 | 1.042346  | -0.263248 |
| C      | 0.032843 | 1.331628  | -0.886719 |
| H      | 0.071177 | 2.052965  | -1.704964 |
| C      | -1.168235| 0.700011  | -0.381541 |
| C      | -1.406077| 1.232412  | 1.064511  |
| H      | -1.516797| 2.315505  | 1.051847  |
| H      | -2.359231| 0.817655  | 1.396950  |
| H      | -0.646964| 0.980334  | 1.816615  |
| C      | -1.030796| -0.740726 | -0.296916 |
| O      | -1.865129| -1.605291 | -0.182635 |
| N      | 0.327974 | -1.149773 | -0.123341 |
| H      | 0.485579 | -2.113117 | 0.093964  |
| C      | 1.377938 | -0.317455 | 0.117311  |
| O      | 2.451642 | -0.658032 | 0.524231  |
| H      | 2.007931 | 1.570014  | -0.380930 |
6.2. Thymine Oligomer

|     | So–Min     | Cl(SCT/SNP)  |
|-----|------------|--------------|
| N   | 7.389460   | 7.389460     |
| C   | 6.702690   | 6.702690     |
| H   | 6.542360   | 6.542360     |
| C   | 6.254640   | 6.254640     |
| C   | 5.515260   | 5.515260     |
| H   | 4.496130   | 4.496130     |
| H   | 5.991650   | 5.991650     |
| H   | 5.486430   | 5.486430     |
| C   | 6.538180   | 6.538180     |
| O   | 6.159860   | 6.159860     |
| N   | 7.283710   | 7.283710     |
| H   | 7.643540   | 7.643540     |
| C   | 7.750570   | 7.750570     |
| O   | 8.401140   | 8.401140     |
| N   | 3.784100   | 3.784100     |
| C   | 3.504820   | 3.504820     |
| H   | 3.525040   | 3.525040     |
| C   | 3.196260   | 3.196260     |
| C   | 2.850160   | 2.850160     |
| H   | 1.771080   | 1.771080     |
| H   | 3.252490   | 3.252490     |
| H   | 3.254930   | 3.254930     |
| C   | 3.112730   | 3.112730     |
| O   | 2.718440   | 2.718440     |
| N   | 3.541460   | 3.541460     |
| H   | 3.480570   | 3.480570     |
| C   | 3.898300   | 3.898300     |
| O   | 4.232390   | 4.232390     |
| H   | 7.861800   | 7.861800     |
| H   | 4.266270   | 4.266270     |
| N   | 7.389460   | 7.389460     |
| C   | 6.702690   | 6.702690     |
| H   | 6.542360   | 6.542360     |
| C   | 6.254640   | 6.254640     |
| C   | 5.515260   | 5.515260     |
| H   | 4.496130   | 4.496130     |
| H   | 5.991650   | 5.991650     |
| H   | 5.486430   | 5.486430     |
| C   | 6.538180   | 6.538180     |
| O   | 6.159860   | 6.159860     |
| N   | 7.283710   | 7.283710     |
| H   | 7.643540   | 7.643540     |
| C   | 7.750570   | 7.750570     |
| O   | 8.401140   | 8.401140     |
| N   | 3.784100   | 3.784100     |
| C   | 3.504820   | 3.504820     |
| H   | 3.525040   | 3.525040     |
| C   | 3.196260   | 3.196260     |
| C   | 2.850160   | 2.850160     |
| H   | 1.771080   | 1.771080     |
| H   | 3.252490   | 3.252490     |
| H   | 3.254930   | 3.254930     |
| C   | 3.112730   | 3.112730     |
| O   | 2.718440   | 2.718440     |
| N   | 3.541460   | 3.541460     |
| H   | 3.480570   | 3.480570     |
| C   | 3.898300   | 3.898300     |
| O   | 4.232390   | 4.232390     |
| H   | 7.861800   | 7.861800     |
| H   | 4.266270   | 4.266270     |
|   |   |   |   |
|---|---|---|---|
| H | 1.771080 | 3.580120 | 3.118130 |
| H | 3.252490 | 4.129670 | 3.878740 |
| H | 3.254930 | 3.731830 | 2.170060 |
| C | 3.112730 | 1.530990 | 4.825590 |
| O | 2.718440 | 2.163680 | 5.778470 |
| N | 3.541460 | 0.241170 | 4.996350 |
| H | 3.325050 | -0.143250 | 5.928400 |
| C | 3.898300 | -0.666660 | 4.035240 |
| O | 4.232390 | -1.781710 | 4.356930 |
| H | 7.861800 | 2.030600 | 2.220970 |
| H | 4.266270 | -0.773280 | 2.020570 |

|    |    |    |    |
|---|---|---|---|
| N | 7.413070 | 1.916150 | 3.070240 |
| C | 6.619820 | 2.947210 | 3.411380 |
| H | 6.509630 | 3.763250 | 2.722110 |
| C | 6.159260 | 2.994840 | 4.851390 |
| C | 5.482190 | 4.233430 | 5.335590 |
| H | 4.457380 | 4.018790 | 5.628940 |
| H | 5.980740 | 4.642210 | 6.208600 |
| H | 5.463300 | 4.994720 | 4.557940 |
| C | 6.440900 | 1.933070 | 5.705060 |
| O | 6.084060 | 1.809880 | 6.888890 |
| N | 7.206770 | 0.861770 | 5.168790 |
| H | 7.582470 | 0.184130 | 5.820300 |
| C | 7.733030 | 0.832870 | 3.933820 |
| O | 8.428550 | -0.066080 | 3.511120 |
| N | 3.840340 | -0.226860 | 2.782140 |
| C | 3.585490 | 1.132720 | 2.527640 |
| H | 3.623100 | 1.428320 | 1.491210 |
| C | 3.255300 | 2.028430 | 3.481820 |
| C | 2.898870 | 3.453390 | 3.167730 |
| H | 1.818640 | 3.576220 | 3.138120 |
| H | 3.289150 | 4.134640 | 3.914180 |
| H | 3.310050 | 3.740510 | 2.202730 |
| C | 3.138080 | 1.537130 | 4.858750 |
| O | 2.717010 | 2.169420 | 5.799880 |
| N | 3.541150 | 0.238620 | 5.030200 |
| H | 3.469020 | -0.146640 | 5.960370 |
| C | 3.904350 | -0.667930 | 4.072970 |
| O | 4.229160 | -1.787220 | 4.392300 |
| H | 7.893930 | 2.035310 | 2.182750 |
| H | 4.331690 | -0.767110 | 2.068150 |

|   |   |   |   |
|---|---|---|---|
| N | 7.461908 | 1.872182 | 2.968294 |
| C | 6.332719 | 2.501772 | 3.282239 |
| H | 5.760650 | 2.955940 | 2.482847 |
| C | 6.125641 | 2.802804 | 4.707588 |
| C | 7.232793 | 3.852185 | 4.991311 |
| H | 7.386418 | 4.486333 | 4.122919 |
| H | 6.842934 | 4.481270 | 5.790575 |
| H | 8.204107 | 3.451099 | 5.300025 |
| C | 6.392449 | 1.700391 | 5.620707 |
| Element | X  | Y  | Z  |
|---------|----|----|----|
| O       | 6.110689 | 1.627259 | 6.789222 |
| N       | 7.213685 | 0.702596 | 5.041884 |
| H       | 7.669179 | 0.067136 | 5.693455 |
| C       | 7.880051 | 0.825860 | 3.848761 |
| O       | 8.719365 | 0.048266 | 3.488104 |
| N       | 7.213685 | 0.702596 | 5.041884 |
| C       | 3.612872 | 1.318625 | 2.585392 |
| H       | 3.614374 | 1.628444 | 1.552867 |
| C       | 3.305007 | 2.192778 | 3.569290 |
| H       | 3.011845 | 3.645479 | 3.330565 |
| H       | 1.957946 | 3.867557 | 3.493944 |
| H       | 3.614266 | 4.257680 | 3.999507 |
| C       | 3.263702 | 3.919942 | 2.310036 |
| C       | 3.238476 | 1.678148 | 4.942322 |
| O       | 2.837146 | 2.285331 | 5.904403 |
| N       | 3.661633 | 0.377022 | 5.074098 |
| H       | 3.649744 | -0.021402 | 6.002484 |
| C       | 4.039895 | -0.493502 | 4.090098 |
| O       | 4.404607 | -1.611934 | 4.372987 |
| H       | 7.968134 | 2.130651 | 2.120613 |
| H       | 4.410931 | -0.553438 | 2.080028 |

Cl(Sc/S0)−2

| Element | X  | Y  | Z  |
|---------|----|----|----|
| N       | 7.092819 | 1.862964 | 2.950173 |
| C       | 5.972327 | 2.572264 | 3.268027 |
| H       | 5.714261 | 3.348357 | 2.562011 |
| C       | 5.633029 | 2.775116 | 4.700205 |
| C       | 5.448463 | 4.172356 | 5.241089 |
| H       | 4.478930 | 4.286200 | 5.729809 |
| H       | 6.198135 | 4.384011 | 5.993266 |
| H       | 5.510364 | 4.921654 | 4.456514 |
| C       | 6.191023 | 1.798739 | 5.628049 |
| O       | 5.950604 | 1.774513 | 6.812458 |
| N       | 7.051366 | 0.844927 | 5.075676 |
| H       | 7.548846 | 0.248200 | 5.731607 |
| C       | 7.682728 | 0.981455 | 3.864943 |
| O       | 8.654120 | 0.342002 | 3.569523 |
| N       | 4.239793 | -0.115547 | 2.756919 |
| C       | 4.153365 | 1.314436 | 2.581210 |
| H       | 3.891267 | 1.641389 | 1.590241 |
| C       | 3.679873 | 2.119335 | 3.677872 |
| C       | 3.031697 | 3.435562 | 3.361782 |
| H       | 1.972604 | 3.258297 | 3.172674 |
| H       | 3.125399 | 4.149377 | 4.170456 |
| H       | 3.459896 | 3.874331 | 2.463299 |
| C       | 3.331519 | 1.463112 | 4.947843 |
| O       | 2.769398 | 2.004175 | 5.870631 |
| N       | 3.714135 | 0.152958 | 5.014836 |
| H       | 3.568145 | -0.324440 | 5.892008 |
| C       | 4.193294 | -0.649770 | 3.999507 |
| O       | 4.464991 | -1.800330 | 4.264672 |
| H       | 7.617417 | 2.229002 | 2.157717 |
| H       | 4.749831 | -0.632841 | 2.044065 |
|   | CPD                              |
|---|----------------------------------|
| N | 7.101791 1.609000 2.847776       |
| C | 5.825741 2.230874 3.020127       |
| H | 5.786342 3.090371 2.358397       |
| C | 5.410612 2.632093 4.433457       |
| C | 5.728101 4.092482 5.177419       |
| H | 5.553579 4.783134 4.114382       |
| C | 5.996295 1.689093 5.486422       |
| O | 5.640901 1.716471 6.636235       |
| N | 6.982899 0.822828 5.072048       |
| H | 7.471080 0.307731 5.799977       |
| C | 7.678453 0.889555 3.867885       |
| O | 8.715833 0.301321 3.739653       |
| N | 4.320266 0.006196 2.932808       |
| C | 4.413505 1.466758 2.792149       |
| H | 3.967704 1.757462 1.847310       |
| C | 3.889988 2.300493 3.994569       |
| C | 3.105922 3.524104 3.532119       |
| H | 2.135283 3.221532 3.145122       |
| H | 2.956237 4.231172 4.342294       |
| H | 3.633958 4.047328 2.736174       |
| C | 3.212436 1.551693 5.093935       |
| O | 2.562138 2.073835 5.961660       |
| N | 3.499478 0.221380 5.117981       |
| H | 3.262670 −0.285491 5.958276      |
| C | 4.091837 −0.593960 4.143643      |
| O | 4.278678 −1.727036 4.400987      |
| H | 7.730739 2.114938 2.226094       |
| H | 4.829189 −0.541966 2.244655      |

| SNP−Min |
|---------|
| N −2.130441 −0.227435 −1.462596 |
| C −1.284919 −1.333171 −1.271549 |
| H −1.067406 −1.911489 −2.149799 |
| C −0.906544 −1.706393 0.025454  |
| C −0.123397 −2.969276 0.248725  |
| H 0.864902 −2.777190 0.651068   |
| H −0.639274 −3.614682 0.950078  |
| H −0.019141 −3.500679 −0.693341 |
| C −1.341410 −0.904139 1.037464  |
| O −0.994244 −1.088403 2.356669  |
| N −2.061471 0.267285 0.814445   |
| H −2.553709 0.703085 1.586137   |
| C −2.576355 0.553794 −0.426862  |
| O −3.328865 1.488152 −0.583888  |
| N 1.181810 2.076716 −0.982903   |
| C 1.588692 0.860328 −1.561082   |
| H 1.611320 0.842560 −2.639281   |
| C 1.968897 −0.221425 −0.851242  |
| C 2.460470 −1.488140 −1.490296  |
| H 3.546948 −1.525303 −1.467845  |
|       |       |       |       |
|-------|-------|-------|-------|
| H     | 2.082017 | -2.366385 | -0.980508 |
| H     | 2.128058 | -1.543972 | -2.523811 |
| C     | 1.976208 | -0.097666 | 0.608464 |
| O     | 2.414592 | -0.917169 | 1.386401 |
| N     | 1.421309 | 1.058756  | 1.081482  |
| H     | 1.426809 | 1.195850  | 2.081500  |
| C     | 0.994723 | 2.146114  | 0.356438  |
| O     | 0.549585 | 3.106889  | 0.947370  |
| H     | -2.588778 | -0.218846 | -2.357520 |
| H     | 0.663070 | 2.733883  | -1.569168 |

**STC(Snp/Tnp/Tct)**

|       |       |       |       |
|-------|-------|-------|-------|
| N     | -2.096359 | -0.150056 | -1.480014 |
| C     | -1.332952 | -1.313726 | -1.273419 |
| H     | -1.103355 | -1.891065 | -2.148509 |
| C     | -0.983793 | -1.709662 | 0.017360  |
| C     | -0.205635 | -2.978953 | 0.234887  |
| H     | 0.781158  | -2.784664 | 0.641252  |
| H     | -0.719663 | -3.607122 | 0.931652  |
| H     | -0.090541 | -3.509176 | -0.707511 |
| C     | -1.420003 | -0.907741 | 1.037685  |
| O     | -1.019023 | -1.079945 | 2.344288  |
| N     | -2.060320 | 0.312725  | 0.810398  |
| H     | -2.612227 | 0.716347  | 1.561533  |
| C     | -2.547803 | 0.623205  | -0.438081 |
| O     | -3.286895 | 1.568549  | -0.591908 |
| N     | 1.246600  | 2.063552  | -0.965505 |
| C     | 1.627721  | 0.842147  | -1.549815 |
| H     | 1.653097  | 0.830224  | -2.627968 |
| C     | 1.977938  | -0.253826 | -0.846386 |
| C     | 2.436606  | -1.528376 | -1.494676 |
| H     | 3.521404  | -1.603290 | -1.467519 |
| H     | 2.024044  | -2.398858 | -0.997851 |
| H     | 2.108671  | -1.561411 | -2.530404 |
| C     | 1.975137  | -0.142554 | 0.614441  |
| O     | 2.384819  | -0.980852 | 1.387903  |
| N     | 1.444950  | 1.023445  | 1.092315  |
| H     | 1.454349  | 1.153541  | 2.093206  |
| C     | 1.049119  | 2.126460  | 0.381846  |
| O     | 0.622223  | 3.092618  | 0.967829  |
| H     | -2.576410 | -0.150893 | -2.364980 |
| H     | 0.748368  | 2.737481  | -1.551192 |

**TCT-Min**

|       |       |       |       |
|-------|-------|-------|-------|
| N     | -2.027972 | 0.241743  | -1.595983 |
| C     | -1.256895 | -0.911459 | -1.448986 |
| H     | -1.184390 | -1.538932 | -2.325052 |
| C     | -1.285211 | -1.565958 | -0.089302 |
| C     | -0.657329 | -2.908122 | 0.057017  |
| H     | 0.325400  | -2.827524 | 0.516717  |
| H     | -1.249808 | -3.561312 | 0.686340  |
| H     | -0.535299 | -3.368034 | -0.921158 |
| C     | -1.762475 | -0.800084 | 1.036366  |
| O     | -1.653249 | -1.164434 | 2.189203  |
| Atom | X  | Y  | Z  |
|------|----|----|----|
| N    | -2.339634 | 0.430450 | 0.731157 |
| H    | -2.846735 | 0.913674 | 1.468304 |
| C    | -2.555005 | 0.939115 | -0.530549 |
| O    | -3.147930 | 1.982116 | -0.673783 |
| N    | 1.781503  | 1.947406 | -0.788880 |
| C    | 2.027821  | 0.712291 | -1.416311 |
| H    | 2.175462  | 0.753012 | -2.484043 |
| C    | 2.104498  | -0.462647 | -0.756612 |
| C    | 2.398387  | -1.772004 | -1.432412 |
| H    | 3.446731  | -2.038825 | -1.317020 |
| H    | 1.798053  | -2.573375 | -1.014551 |
| H    | 2.164803  | -1.710994 | -2.492185 |
| C    | 1.971587  | -0.423780 | 0.702639 |
| O    | 2.161065  | -1.355713 | 1.452189 |
| N    | 1.581933  | 0.787784 | 1.205033 |
| H    | 1.507395  | 0.865401 | 2.209484 |
| C    | 1.447736  | 1.974355 | 0.532298 |
| O    | 1.108504  | 2.966470 | 1.131256 |
| H    | -2.375270 | 0.393199 | -2.530623 |
| H    | 1.457043  | 2.724277 | -1.371306 |

| STC(Tc/Sr) |
|------------|
| N          | 7.121285  | 1.611163 | 2.938393 |
| C          | 5.949321  | 2.361571 | 3.277970 |
| H          | 5.900410  | 3.250085 | 2.659563 |
| C          | 5.897490  | 2.702939 | 4.724084 |
| C          | 5.375656  | 4.005024 | 5.244361 |
| H          | 4.353299  | 3.920197 | 5.604904 |
| C          | 5.976232  | 4.325151 | 6.089003 |
| H          | 5.404632  | 4.771684 | 4.473778 |
| C          | 6.417781  | 1.719850 | 5.674316 |
| O          | 6.199819  | 1.774420 | 6.860774 |
| N          | 7.172164  | 0.700533 | 5.113463 |
| H          | 7.695895  | 0.114683 | 5.761203 |
| C          | 7.723322  | 0.764204 | 3.845672 |
| O          | 8.660805  | 0.066843 | 3.554429 |
| N          | 4.267988  | 0.070416 | 2.894243 |
| C          | 4.333315  | 1.520728 | 2.738070 |
| H          | 4.241159  | 1.785117 | 1.692936 |
| C          | 3.318585  | 2.221091 | 3.557615 |
| C          | 2.822930  | 3.577308 | 3.172655 |
| H          | 1.741001  | 3.560527 | 3.062325 |
| H          | 3.072729  | 4.335145 | 3.911333 |
| H          | 3.261014  | 3.883956 | 2.225197 |
| C          | 3.060504  | 1.666854 | 4.878536 |
| O          | 2.464882  | 2.227217 | 5.772846 |
| N          | 3.599553  | 0.421656 | 5.087423 |
| H          | 3.400226  | -0.019495 | 5.973362 |
| C          | 4.117155  | -0.438897 | 4.142226 |
| O          | 4.331147  | -1.586624 | 4.451211 |
| H          | 7.688733  | 2.050390 | 2.224154 |
| H          | 4.778288  | -0.488936 | 2.215524 |
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