**Supporting Information**

# $^{DNS}$C: A Fluorescent, Environmentally Sensitive Cytidine Derivative for the Direct Detection of GGG Triad Sequences

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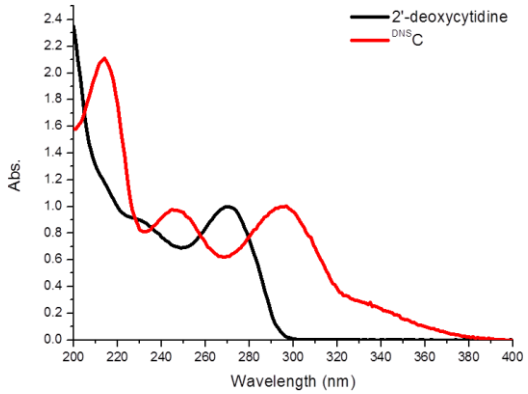
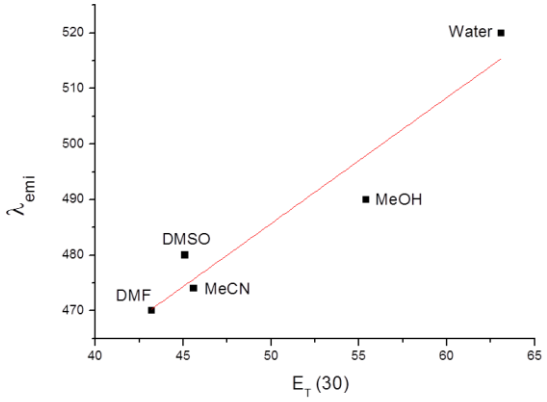



(a)




(b)

**Fig. S1** (a) UV absorption of 2´-deoxycytidine and **$^{DNS}$C** (5 µM; total volume: 1 mL; 20 °C) (b) Plot of fluorescence emission wavelength of $^{DNS}$C versus the ET (30) values.

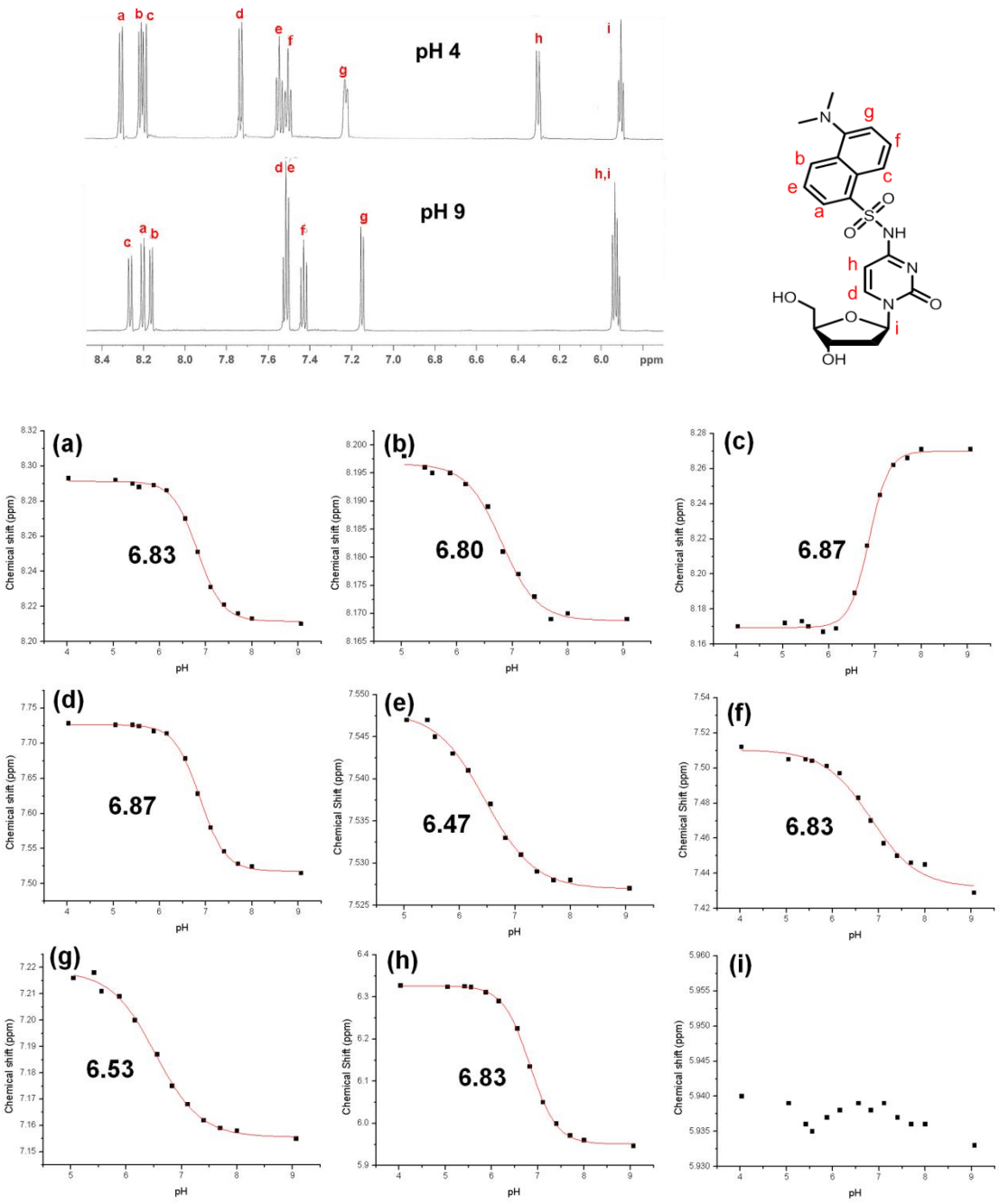



**Fig. S2** NMR spectroscopic titration of $^{DNS}$**C**. The transition pH appeared at pH 6.8, which is the p$K_a$ of the N3 position of $^{DNS}$**C**. Signals were assigned from 2D COSY and HSQC spectra (buffer: 200 mM trizma; 10% DMSO-$d_6$; 3 mM $^{DNS}$**C**, 600 µL).

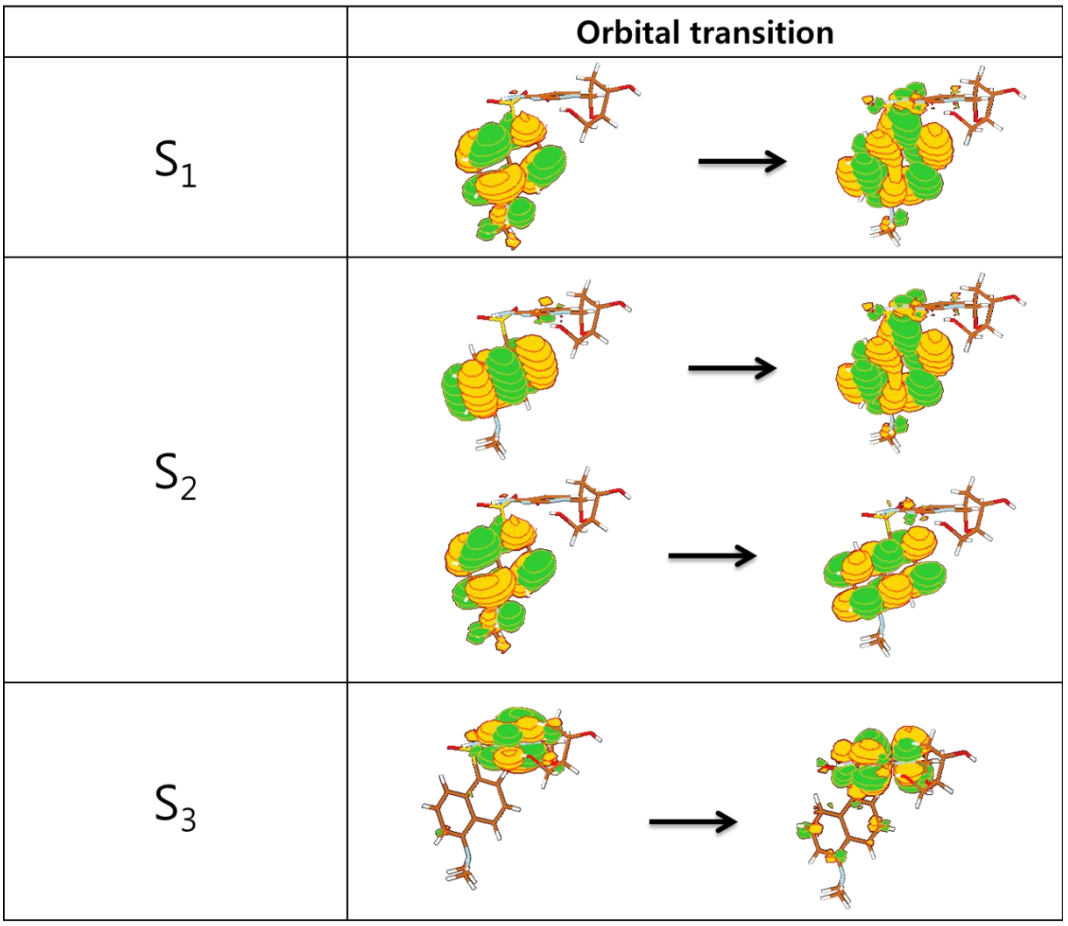



**Fig. S3** Molecular orbital (MO) transitions of $^{DNS}$**C** that contributed significantly to the excited states $S_1$, $S_2$, and $S_3$.

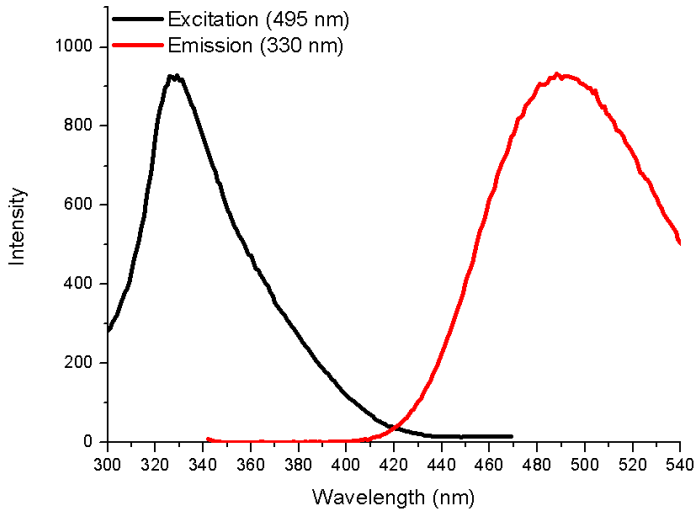



**Fig. S4** Excitation and emission spectra of $^{DNS}$**C** in aqueous solution. $E_{00}$: 420 nm (3.4 mM $^{DNS}$**C**, 100 mM KCl, 50% MeOH).

| ODN name | Sequence (5´ to 3´) | Exact mass | Obs. mass |
|---|---|---|---|
| ODN-A-A | CGA GAA AAA AAG AGC | 4655.1002 | 4655.4605 |
| ODN-A-C | CGA GAA CAC AAG AGC | 4606.3002 | 4606.9386 |
| ODN-A-G | CGA GAA GAG AAG AGC | 4686.3002 | 4686.8933 |
| ODN-A-T | CGA GAA TAT AAG AGC | 4636.3002 | 4637.1941 |
| ODN-C-A | CGA GAA ACA AAG AGC | 4630.7002 | 4630.3345 |
| ODN-C-C | CGA GAA CCC AAG AGC | 4581.9002 | 4580.9557 |
| ODN-C-G | CGA GAA GCG AAG AGC | 4661.9002 | 4661.9299 |
| ODN-C-T | CGA GAA TCT AAG AGC | 4611.9002 | 4612.1425 |
| ODN-G-A | CGA GAA AGA AAG AGC | 4670.7002 | 4670.1179 |
| ODN-G-C | CGA GAA CGC AAG AGC | 4621.9002 | 4621.5972 |
| ODN-G-G | CGA GAA GGG AAG AGC | 4701.9002 | 4701.8273 |
| ODN-G-T | CGA GAA TGT AAG AGC | 4651.9002 | 4651.361 |
| ODN-T-A | CGA GAA ATA AAG AGC | 4645.7002 | 4645.1594 |
| ODN-T-C | CGA GAA CTC AAG AGC | 4596.9002 | 4596.9012 |
| ODN-T-G | CGA GAA GTG AAG AGC | 4676.9002 | 4676.8234 |
| ODN-T-T | CGA GAA TTT AAG AGC | 4626.9002 | 4626.8861 |
| DNS-A | GCT CTT A$^{DNS}$**C**A TTC TCG | 4727.6037 | 4727.8698 |
| DNS-C | GCT CTT C$^{DNS}$**C**C TTC TCG | 4678.8037 | 4679.0445 |
| DNS-G | GCT CTT G$^{DNS}$**C**G TTC TCG | 4758.8037 | 4758.4107 |
| DNS-T | GCT CTT T$^{DNS}$**C**T TTC TCG | 4708.8037 | 4709.1509 |
| Nat-A | GCT CTT ACA TTC TCG | 4494.3002 | 4494.4445 |
| Nat-C | GCT CTT CCC TTC TCG | 4445.5002 | 4445.4753 |
| Nat-G | GCT CTT GCG TTC TCG | 4525.5002 | 4525.4412 |
| Nat-T | GCT CTT TCT TTC TCG | 4475.5002 | 4475.3688 |
| DNS-probe | A CCC TAA C$^{DNS}$**C**C TAA C$^{DNS}$**C**C TAA CCC T | 7286.2216 | 7285.9761 |
| Htelo | A(GGGTTA)$_3$GGGT | 7271.4146 | 7271.0071 |

**Table S1** ODN sequences and their MALDI-TOF MS data.

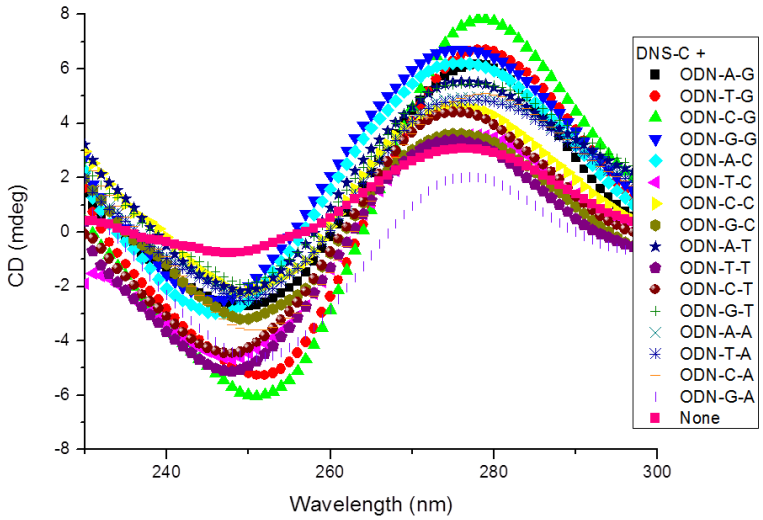



**Fig. S5** CD spectra of single-stranded **DNS-C** and its duplex forms with **ODN-X-Y** sequence incorporating various triads [**ODN-X-Y**: -YXY-; sample concentration, 1.5 μM; buffer, 100 mM tris (pH 9.0); 20 °C; total volume, 1 mL].

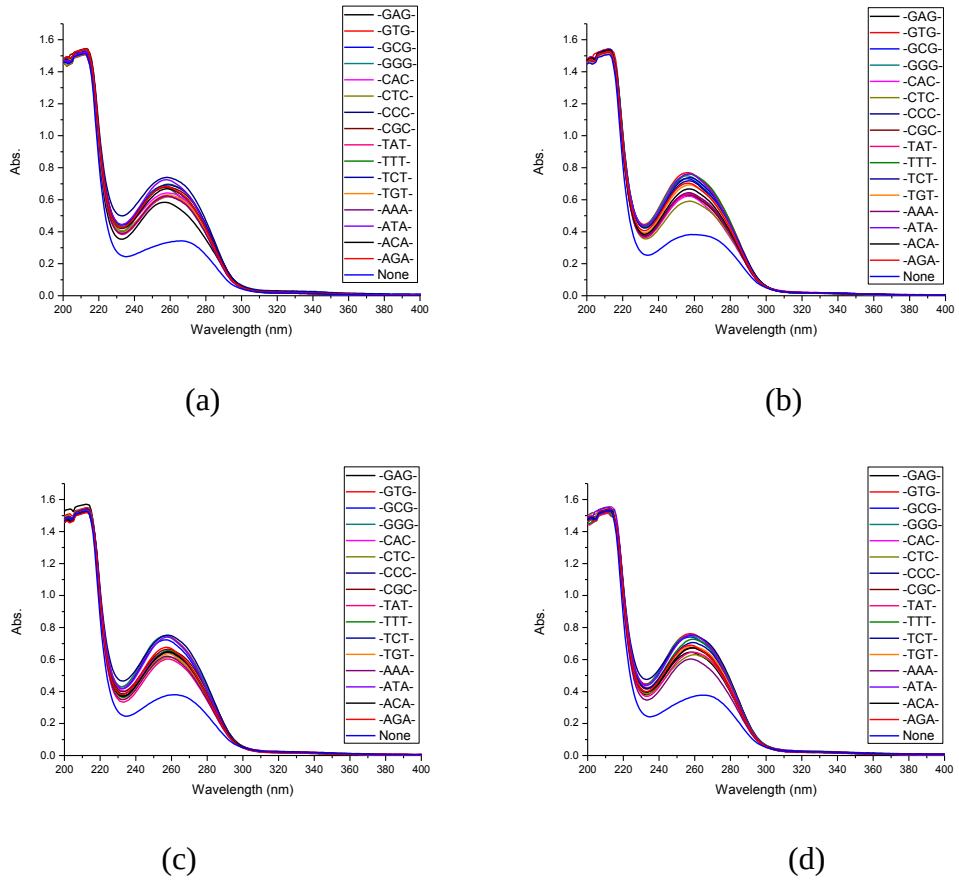



**Fig. S6** UV absorption spectra of single-stranded **DNS-N** strands and of their duplexes with **ODN-X-Y** sequences with various triads: (a) DNS-C, (b) DNS-G, (c) DNS-A, (d) DNS-T (**ODN-X-Y**: -YXY-; sample concentration, 1.5 μM; buffer, 100 mM tris (pH 9.0); excitation: 295 nm; total volume, 1 mL).

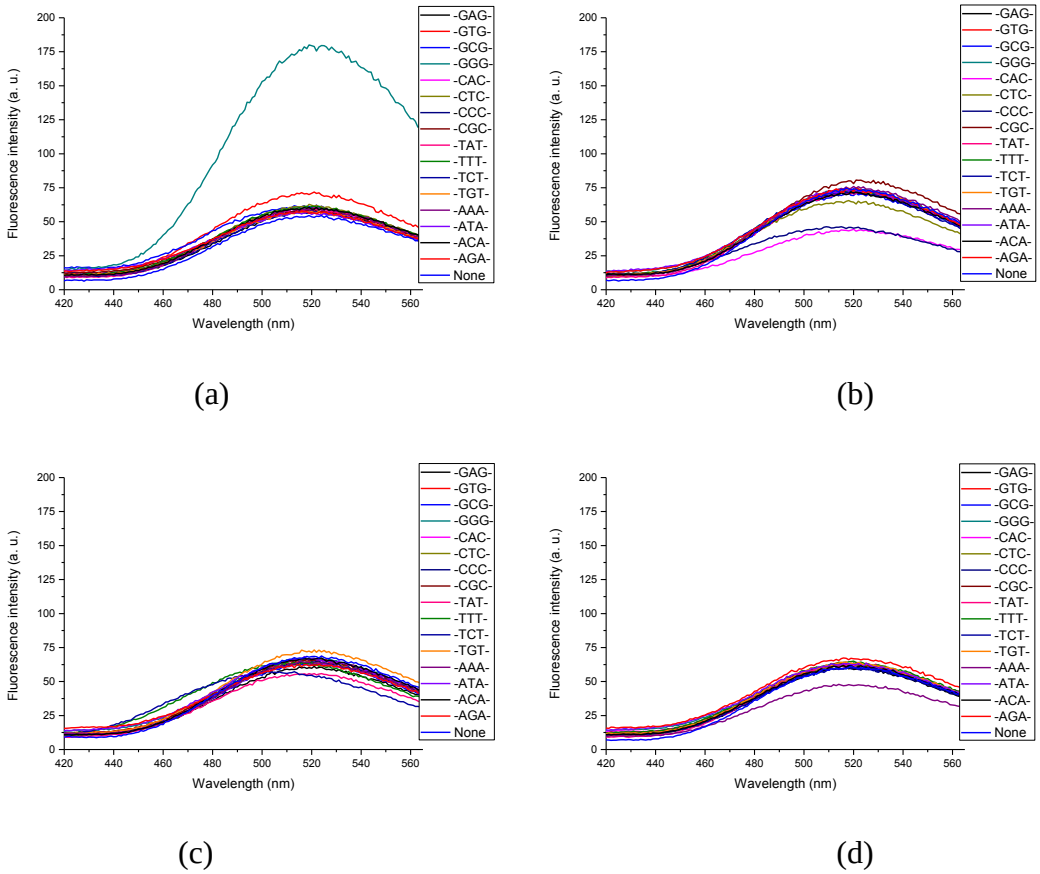



**Fig. S7** Fluorescence spectra of single-stranded **DNS-N** sequences and their duplexes with **ODN-X-Y** sequences with various triads: (a) DNS-C, (b) DNS-G, (c) DNS-A, (d) DNS-T (**ODN-X-Y**: -YXY-; sample concentration, 1.5 μM; buffer, 100 mM tris (pH 9.0); excitation: 295 nm; total volume, 1 mL; excitation and emission slit : 10 nm).

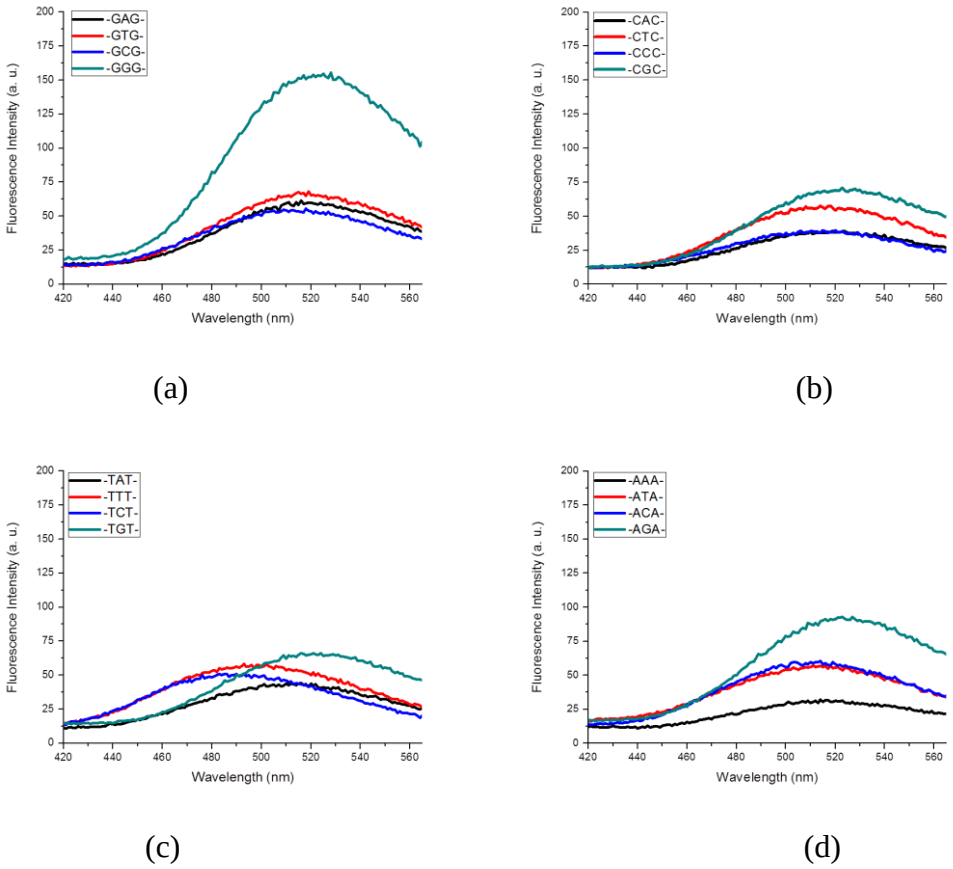



**Fig. S8** Fluorescence spectra of single-stranded **DNS-N** sequences and their duplexes with **ODN-X-Y** sequences with various triads: (a) DNS-C, (b) DNS-G, (c) DNS-A, (d) DNS-T (**ODN-X-Y**: -YXY-; sample concentration, 1.5 μM; buffer, 100 mM tris (pH 9.0), 100 mM NaCl, 20 mM $MgCl_2$; excitation, 295 nm; total volume, 1 mL; excitation and emission slit : 10 nm).

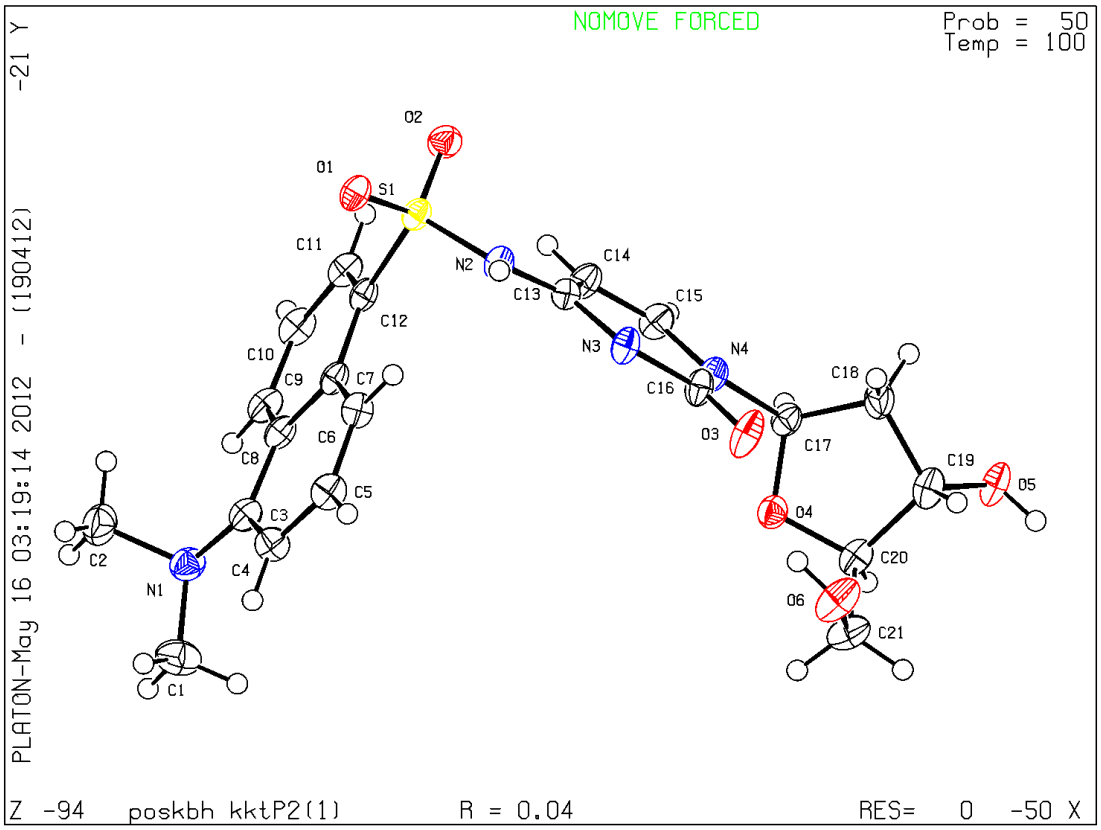
**Table S2**. Crystal data and structure refinement for $^{DNS}$**C**

| | | |
|---|---|---|
| Empirical formula | $C_{21}H_{24}N_4O_6S$ | |
| Formula weight | 460.50 | |
| Temperature | 100(2) K | |
| Wavelength | 0.72999 Å | |
| Crystal system | Monoclinic | |
| Space group | $P2_1$ | |
| Unit cell dimensions | $a$ = 8.2280(16) Å | $\alpha$ = 90° |
| | $b$ = 8.3500(17) Å | $\beta$ = 99.90(3)° |
| | $c$ = 15.938(3) Å | $\gamma$ = 90° |
| Volume | 1078.7(4) Å$^3$ | |
| $Z$ | 2 | |
| Density (calculated) | 1.418 Mg/m$^3$ | |
| Absorption coefficient | 0.167 mm$^{-1}$ | |
| F(000) | 484 | |
| Crystal size | 0.04 × 0.04 × 0.02 mm$^3$ | |
| Theta range for data collection | 2.66–28.00° | |
| Index ranges | $-10 \le h \le 10; -10 \le k \le 10; -19 \le l \le 19$ | |
| Reflections collected | 8814 | |
| Independent reflections | 4600 [$R$(int) = 0.0281] | |
| Completeness to theta = 28.00° | 94.7% | |
| Absorption correction | Empirical | |
| Max. and min. transmissions | 0.9967 and 0.9933 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 4600 / 1 / 294 | |
| Goodness-of-fit on $F^2$ | 1.061 | |
| Final $R$ indices [$I$ > 2sigma($I$)] | $R$1 = 0.0385; $wR$2 = 0.1072 | |
| $R$ indices (all data) | $R$1 = 0.0434; $wR$2 = 0.1091 | |
| Absolute structure parameter | –0.01(6) | |
| Extinction coefficient | 0.078(6) | |
| Largest diff. peak and hole | 0.886 and –0.439 e/Å$^{-3}$ | |

**Table S3**. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$ x $10^3$) for $^{DNS}$**C**. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| S(1) | 6028(1) | 9118(1) | 2223(1) | 21(1) |
| O(1) | 5991(2) | 10848(2) | 2251(1) | 25(1) |
| O(2) | 7627(2) | 8382(2) | 2302(1) | 27(1) |
| O(3) | 2254(2) | 4973(2) | 4323(1) | 33(1) |
| O(4) | 1721(2) | 2095(2) | 3286(1) | 24(1) |
| O(5) | 2731(2) | -1035(2) | 4690(1) | 30(1) |
| O(6) | -501(2) | 2905(2) | 4397(1) | 38(1) |
| N(1) | -5(2) | 8940(2) | -1009(1) | 28(1) |
| N(2) | 5020(2) | 8535(2) | 2955(1) | 23(1) |
| N(3) | 3732(2) | 6646(2) | 3623(1) | 24(1) |
| N(4) | 3930(2) | 3879(2) | 3456(1) | 22(1) |
| C(1) | -1793(3) | 8933(4) | -1201(2) | 39(1) |
| C(2) | 648(3) | 10000(4) | -1601(2) | 39(1) |
| C(3) | 691(2) | 9162(3) | -141(1) | 24(1) |
| C(4) | -194(2) | 9775(3) | 445(1) | 26(1) |
| C(5) | 566(2) | 10006(3) | 1299(1) | 26(1) |
| C(6) | 2190(2) | 9666(2) | 1570(1) | 24(1) |
| C(7) | 3145(2) | 8973(2) | 996(1) | 21(1) |
| C(8) | 2373(2) | 8671(2) | 138(1) | 23(1) |
| C(9) | 3263(3) | 7824(2) | -408(1) | 26(1) |
| C(10) | 4861(3) | 7371(3) | -151(1) | 27(1) |
| C(11) | 5677(2) | 7758(2) | 672(1) | 25(1) |
| C(12) | 4844(2) | 8537(2) | 1233(1) | 21(1) |
| C(13) | 4795(2) | 7000(2) | 3076(1) | 22(1) |
| C(14) | 5488(3) | 5647(2) | 2714(1) | 26(1) |
| C(15) | 5030(2) | 4166(3) | 2915(1) | 27(1) |
| C(16) | 3241(3) | 5143(2) | 3837(1) | 24(1) |
| C(17) | 3435(2) | 2222(2) | 3592(1) | 23(1) |
| C(18) | 3742(3) | 1654(3) | 4514(1) | 31(1) |
| C(19) | 2250(3) | 604(2) | 4593(1) | 28(1) |
| C(20) | 1025(3) | 899(2) | 3759(1) | 25(1) |
| C(21) | -648(3) | 1507(3) | 3878(2) | 33(1) |

**Table S4**. Bond lengths [Å] and angles [°] for $^{DNS}$**C**.




| | |
|---|---|
| S(1)-O(2) | 1.4377(15) |
| S(1)-O(1) | 1.4460(15) |
| S(1)-N(2) | 1.6177(18) |
| S(1)-C(12) | 1.774(2) |
| O(3)-C(16) | 1.222(3) |
| O(4)-C(17) | 1.415(2) |
| O(4)-C(20) | 1.429(2) |
| O(5)-C(19) | 1.426(2) |
| O(5)-H(5) | 0.8400 |
| O(6)-C(21) | 1.424(3) |
| O(6)-H(6) | 0.8400 |
| N(1)-C(3) | 1.415(3) |
| N(1)-C(1) | 1.450(3) |
| N(1)-C(2) | 1.463(3) |
| N(2)-C(13) | 1.313(3) |
| N(2)-H(2) | 0.8800 |
| N(3)-C(13) | 1.370(3) |

| | |
|---|---|
| N(3)-C(16) | 1.379(3) |
| N(4)-C(15) | 1.375(2) |
| N(4)-C(16) | 1.387(2) |
| N(4)-C(17) | 1.469(2) |
| C(1)-H(1A) | 0.9800 |
| C(1)-H(1B) | 0.9800 |
| C(1)-H(1C) | 0.9800 |
| C(2)-H(2A) | 0.9800 |
| C(2)-H(2B) | 0.9800 |
| C(2)-H(2C) | 0.9800 |
| C(3)-C(4) | 1.377(3) |
| C(3)-C(8) | 1.438(3) |
| C(4)-C(5) | 1.409(3) |
| C(4)-H(4) | 0.9500 |
| C(5)-C(6) | 1.361(3) |
| C(5)-H(5A) | 0.9500 |
| C(6)-C(7) | 1.428(3) |
| C(6)-H(6A) | 0.9500 |
| C(7)-C(8) | 1.429(3) |
| C(7)-C(12) | 1.431(3) |
| C(8)-C(9) | 1.419(3) |
| C(9)-C(10) | 1.362(3) |
| C(9)-H(9) | 0.9500 |
| C(10)-C(11) | 1.405(3) |
| C(10)-H(10) | 0.9500 |
| C(11)-C(12) | 1.379(3) |
| C(11)-H(11) | 0.9500 |
| C(13)-C(14) | 1.431(3) |
| C(14)-C(15) | 1.347(3) |
| C(14)-H(14) | 0.9500 |
| C(15)-H(15) | 0.9500 |
| C(17)-C(18) | 1.523(3) |
| C(17)-H(17) | 1.0000 |
| C(18)-C(19) | 1.532(3) |
| C(18)-H(18A) | 0.9900 |
| C(18)-H(18B) | 0.9900 |
| C(19)-C(20) | 1.544(3) |
| C(19)-H(19) | 1.0000 |
| C(20)-C(21) | 1.509(3) |

| | |
|---|---|
| C(20)-H(20) | 1.0000 |
| C(21)-H(21A) | 0.9900 |
| C(21)-H(21B) | 0.9900 |

| | |
|---|---|
| O(2)-S(1)-O(1) | 116.63(9) |
| O(2)-S(1)-N(2) | 112.54(9) |
| O(1)-S(1)-N(2) | 105.24(9) |
| O(2)-S(1)-C(12) | 108.37(9) |
| O(1)-S(1)-C(12) | 106.78(9) |
| N(2)-S(1)-C(12) | 106.72(9) |
| C(17)-O(4)-C(20) | 109.71(15) |
| C(19)-O(5)-H(5) | 109.5 |
| C(21)-O(6)-H(6) | 109.5 |
| C(3)-N(1)-C(1) | 115.65(17) |
| C(3)-N(1)-C(2) | 114.85(17) |
| C(1)-N(1)-C(2) | 109.70(18) |
| C(13)-N(2)-S(1) | 120.13(15) |
| C(13)-N(2)-H(2) | 119.9 |
| S(1)-N(2)-H(2) | 119.9 |
| C(13)-N(3)-C(16) | 126.89(17) |
| C(15)-N(4)-C(16) | 120.34(17) |
| C(15)-N(4)-C(17) | 119.06(16) |
| C(16)-N(4)-C(17) | 120.53(16) |
| N(1)-C(1)-H(1A) | 109.5 |
| N(1)-C(1)-H(1B) | 109.5 |
| H(1A)-C(1)-H(1B) | 109.5 |
| N(1)-C(1)-H(1C) | 109.5 |
| H(1A)-C(1)-H(1C) | 109.5 |
| H(1B)-C(1)-H(1C) | 109.5 |
| N(1)-C(2)-H(2A) | 109.5 |
| N(1)-C(2)-H(2B) | 109.5 |
| H(2A)-C(2)-H(2B) | 109.5 |
| N(1)-C(2)-H(2C) | 109.5 |
| H(2A)-C(2)-H(2C) | 109.5 |
| H(2B)-C(2)-H(2C) | 109.5 |
| C(4)-C(3)-N(1) | 122.63(18) |
| C(4)-C(3)-C(8) | 119.29(18) |
| N(1)-C(3)-C(8) | 118.05(17) |
| C(3)-C(4)-C(5) | 120.45(18) |

| | |
|---|---|
| C(3)-C(4)-H(4) | 119.8 |
| C(5)-C(4)-H(4) | 119.8 |
| C(6)-C(5)-C(4) | 121.79(18) |
| C(6)-C(5)-H(5A) | 119.1 |
| C(4)-C(5)-H(5A) | 119.1 |
| C(5)-C(6)-C(7) | 119.94(18) |
| C(5)-C(6)-H(6A) | 120.0 |
| C(7)-C(6)-H(6A) | 120.0 |
| C(6)-C(7)-C(8) | 118.81(17) |
| C(6)-C(7)-C(12) | 123.69(17) |
| C(8)-C(7)-C(12) | 117.49(16) |
| C(9)-C(8)-C(7) | 118.91(18) |
| C(9)-C(8)-C(3) | 121.59(18) |
| C(7)-C(8)-C(3) | 119.43(17) |
| C(10)-C(9)-C(8) | 121.81(19) |
| C(10)-C(9)-H(9) | 119.1 |
| C(8)-C(9)-H(9) | 119.1 |
| C(9)-C(10)-C(11) | 119.97(18) |
| C(9)-C(10)-H(10) | 120.0 |
| C(11)-C(10)-H(10) | 120.0 |
| C(12)-C(11)-C(10) | 120.17(18) |
| C(12)-C(11)-H(11) | 119.9 |
| C(10)-C(11)-H(11) | 119.9 |
| C(11)-C(12)-C(7) | 121.38(18) |
| C(11)-C(12)-S(1) | 116.57(15) |
| C(7)-C(12)-S(1) | 121.84(14) |
| N(2)-C(13)-N(3) | 115.18(18) |
| N(2)-C(13)-C(14) | 129.44(19) |
| N(3)-C(13)-C(14) | 115.38(17) |
| C(15)-C(14)-C(13) | 118.80(18) |
| C(15)-C(14)-H(14) | 120.6 |
| C(13)-C(14)-H(14) | 120.6 |
| C(14)-C(15)-N(4) | 123.41(19) |
| C(14)-C(15)-H(15) | 118.3 |
| N(4)-C(15)-H(15) | 118.3 |
| O(3)-C(16)-N(3) | 121.14(18) |
| O(3)-C(16)-N(4) | 123.71(18) |
| N(3)-C(16)-N(4) | 115.15(17) |
| O(4)-C(17)-N(4) | 107.76(15) |

| | |
|---|---|
| O(4)-C(17)-C(18) | 107.39(16) |
| N(4)-C(17)-C(18) | 115.56(17) |
| O(4)-C(17)-H(17) | 108.6 |
| N(4)-C(17)-H(17) | 108.6 |
| C(18)-C(17)-H(17) | 108.6 |
| C(17)-C(18)-C(19) | 104.84(17) |
| C(17)-C(18)-H(18A) | 110.8 |
| C(19)-C(18)-H(18A) | 110.8 |
| C(17)-C(18)-H(18B) | 110.8 |
| C(19)-C(18)-H(18B) | 110.8 |
| H(18A)-C(18)-H(18B) | 108.9 |
| O(5)-C(19)-C(18) | 110.31(17) |
| O(5)-C(19)-C(20) | 111.97(17) |
| C(18)-C(19)-C(20) | 104.54(17) |
| O(5)-C(19)-H(19) | 110.0 |
| C(18)-C(19)-H(19) | 110.0 |
| C(20)-C(19)-H(19) | 110.0 |
| O(4)-C(20)-C(21) | 106.76(17) |
| O(4)-C(20)-C(19) | 107.71(16) |
| C(21)-C(20)-C(19) | 114.85(18) |
| O(4)-C(20)-H(20) | 109.1 |
| C(21)-C(20)-H(20) | 109.1 |
| C(19)-C(20)-H(20) | 109.1 |
| O(6)-C(21)-C(20) | 111.11(18) |
| O(6)-C(21)-H(21A) | 109.4 |
| C(20)-C(21)-H(21A) | 109.4 |
| O(6)-C(21)-H(21B) | 109.4 |
| C(20)-C(21)-H(21B) | 109.4 |
| H(21A)-C(21)-H(21B) | 108.0 |

Symmetry transformations used to generate equivalent atoms:

**Table S5**. Anisotropic displacement parameters ($Å^2 \times 10^3$)for $^{DNS}$**C**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[ h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12} ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| S(1) | 24(1) | 17(1) | 25(1) | 1(1) | 8(1) | 0(1) |
| O(1) | 31(1) | 16(1) | 28(1) | 0(1) | 9(1) | -3(1) |
| O(2) | 23(1) | 27(1) | 33(1) | 2(1) | 7(1) | 2(1) |
| O(3) | 54(1) | 20(1) | 34(1) | -2(1) | 27(1) | -4(1) |
| O(4) | 27(1) | 25(1) | 21(1) | 2(1) | 6(1) | -2(1) |
| O(5) | 43(1) | 18(1) | 34(1) | 5(1) | 21(1) | 0(1) |
| O(6) | 42(1) | 25(1) | 54(1) | -7(1) | 29(1) | -2(1) |
| N(1) | 28(1) | 31(1) | 25(1) | -3(1) | 5(1) | -6(1) |
| N(2) | 28(1) | 18(1) | 24(1) | 0(1) | 10(1) | 2(1) |
| N(3) | 32(1) | 17(1) | 24(1) | 1(1) | 12(1) | 0(1) |
| N(4) | 28(1) | 16(1) | 24(1) | 0(1) | 8(1) | 0(1) |
| C(1) | 31(1) | 50(2) | 34(1) | -9(1) | 2(1) | -1(1) |
| C(2) | 46(1) | 43(1) | 27(1) | 5(1) | 5(1) | -11(1) |
| C(3) | 26(1) | 19(1) | 26(1) | -3(1) | 7(1) | -2(1) |
| C(4) | 26(1) | 26(1) | 28(1) | -2(1) | 6(1) | 3(1) |
| C(5) | 28(1) | 26(1) | 27(1) | -5(1) | 12(1) | 3(1) |
| C(6) | 29(1) | 23(1) | 21(1) | -3(1) | 9(1) | 2(1) |
| C(7) | 25(1) | 14(1) | 25(1) | 1(1) | 11(1) | 0(1) |
| C(8) | 27(1) | 18(1) | 26(1) | -2(1) | 10(1) | -3(1) |
| C(9) | 30(1) | 22(1) | 27(1) | -5(1) | 11(1) | -5(1) |
| C(10) | 33(1) | 22(1) | 30(1) | -7(1) | 16(1) | -1(1) |
| C(11) | 25(1) | 18(1) | 35(1) | -1(1) | 13(1) | 2(1) |
| C(12) | 26(1) | 15(1) | 25(1) | 1(1) | 10(1) | 0(1) |
| C(13) | 23(1) | 21(1) | 22(1) | 1(1) | 4(1) | 0(1) |
| C(14) | 28(1) | 23(1) | 33(1) | 0(1) | 15(1) | 1(1) |
| C(15) | 28(1) | 20(1) | 34(1) | -1(1) | 11(1) | 2(1) |
| C(16) | 34(1) | 16(1) | 22(1) | 0(1) | 8(1) | -2(1) |
| C(17) | 27(1) | 15(1) | 29(1) | 0(1) | 7(1) | -1(1) |
| C(18) | 41(1) | 21(1) | 29(1) | 5(1) | -1(1) | -6(1) |
| C(19) | 39(1) | 19(1) | 28(1) | 0(1) | 14(1) | 2(1) |
| C(20) | 32(1) | 19(1) | 26(1) | -5(1) | 12(1) | -3(1) |
| C(21) | 29(1) | 28(1) | 44(1) | -8(1) | 13(1) | -5(1) |

**Table S6** Hydrogen bonds for $^{DNS}$**C** [Å and °].

| D–H···A | *d*(D-H) | *d*(H···A) | *d*(D···A) | <(DHA) |
|---|---|---|---|---|
| O(5)-H(5)···O(6)#1 | 0.84 | 1.86 | 2.681(2) | 165.3 |
| O(6)-H(6)···O(3) | 0.84 | 2.09 | 2.869(2) | 154.4 |

Symmetry transformations used to generate equivalent atoms:

#1 $-x, y - 1/2, -z + 1$

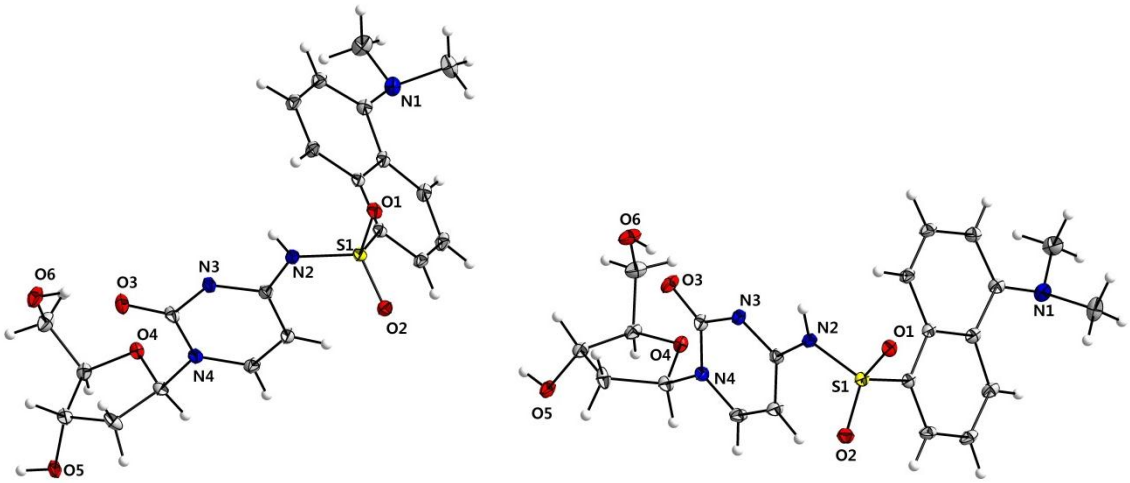



**Fig. S9** Solid state structure of $^{DNS}$**C**, drawn with 30% probability ellipsoids.