Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Electronic Supplementary Information

Characteristics of Excited Triplet States of Thiolated Guanosine Derivatives and Singlet Oxygen Generation

Shoma Miyata,[a] Shunsuke Tanabe,[a] Tasuku Isozaki,[a] Yao–Zhong Xu [b] and Tadashi Suzuki*[a]

[a] *Department of Chemistry and Biological Science, Aoyama Gakuin University, 5–10–1 Fuchinobe, Chuo–ku, Sagamihara, Kanagawa 252–5258, Japan*

[b] *School of Life, Health and Chemical Sciences, The Open University, Milton Keynes MK7 6AA, United Kingdom*

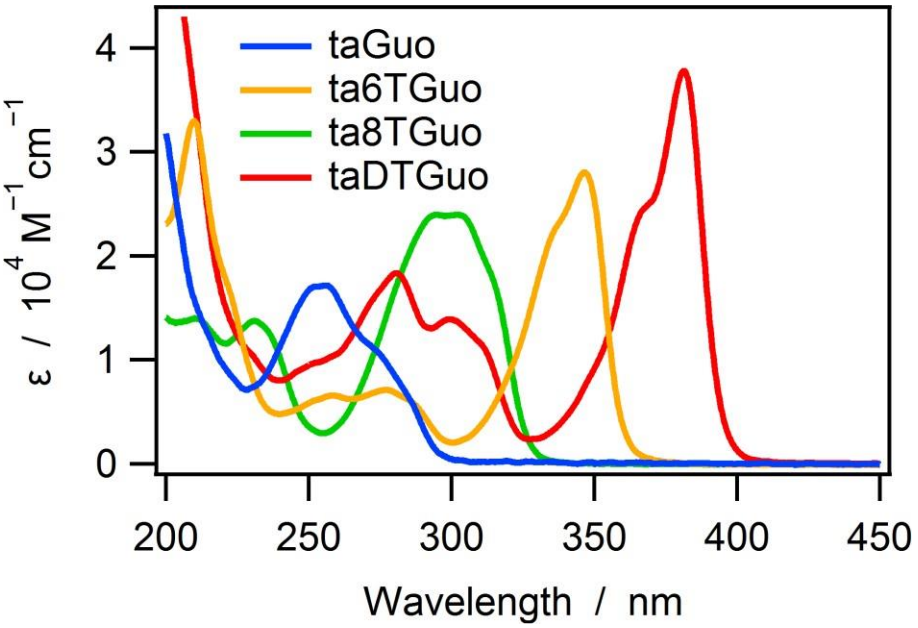

Fig. S1 Absorption spectra of taGuo (blue line), ta6TGuo (yellow line), ta8TGuo (green line) and taDTGuo (red line) in acetonitrile solution. Adopted from reference 1.

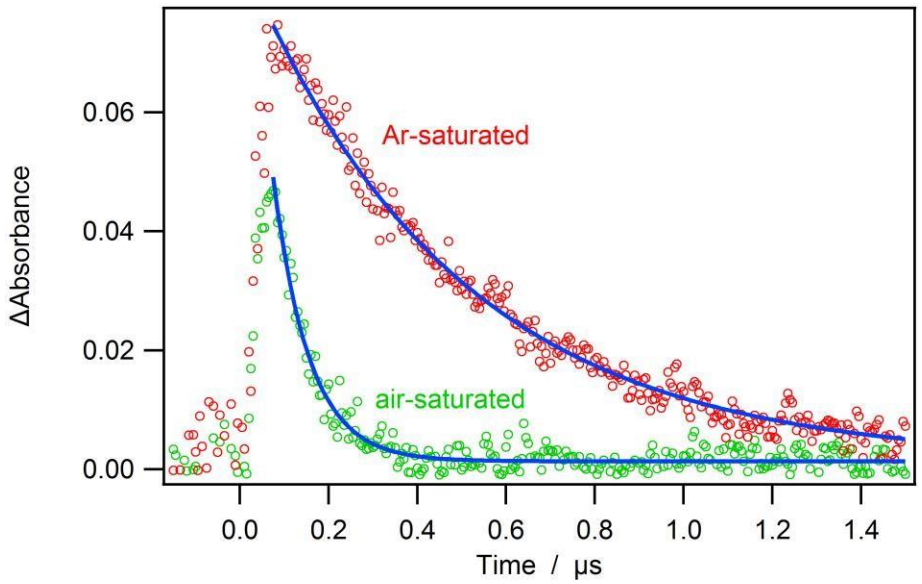

Fig. S2 Transient absorption decays of ta6TGuo (248 μM) at 640 nm in Ar– and air–saturated acetonitrile solution.

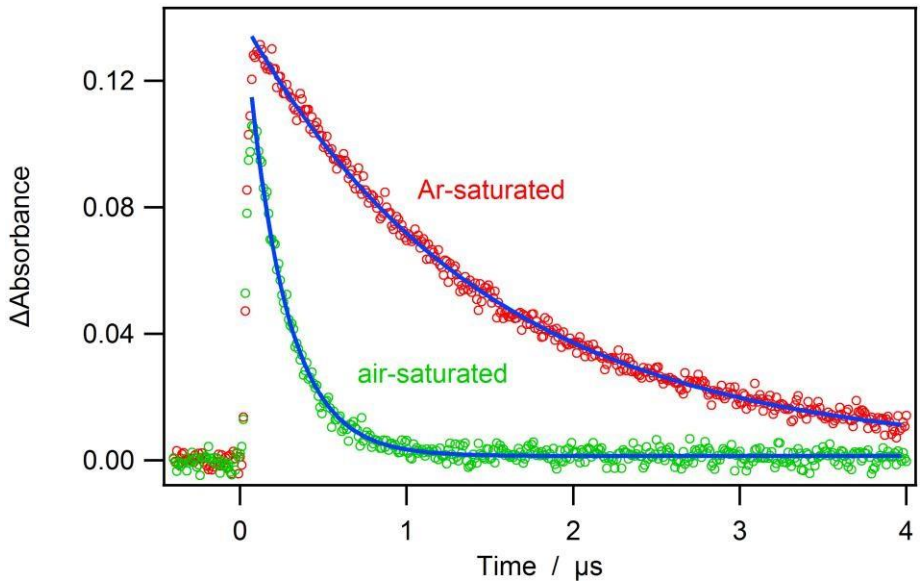

Fig. S3 Transient absorption decays of ta8TGuo (35.8 μM) at 710 nm in Ar– and air–saturated acetonitrile solution.

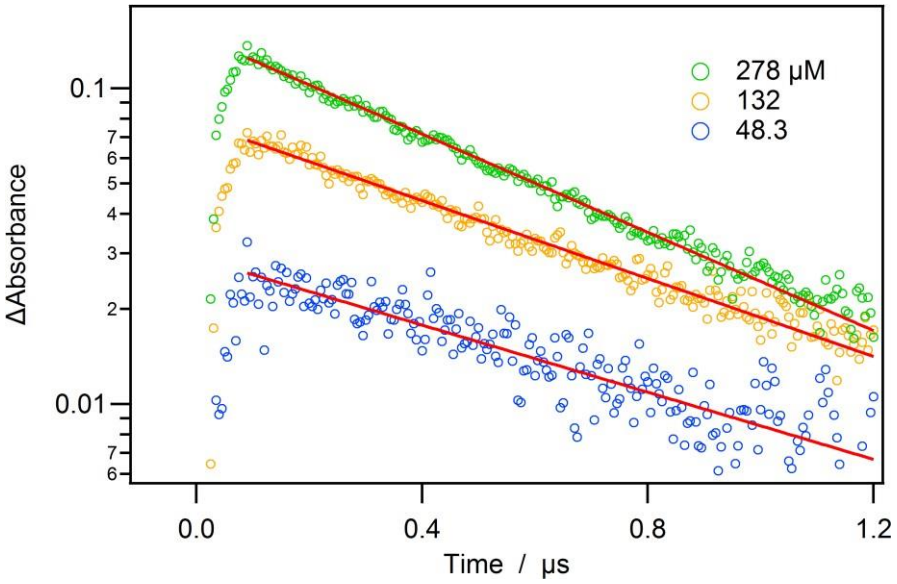

Fig. S4 Transient absorption decays at 640 nm in Ar–saturated acetonitrile solution with several concentrations of ta6TGuo.

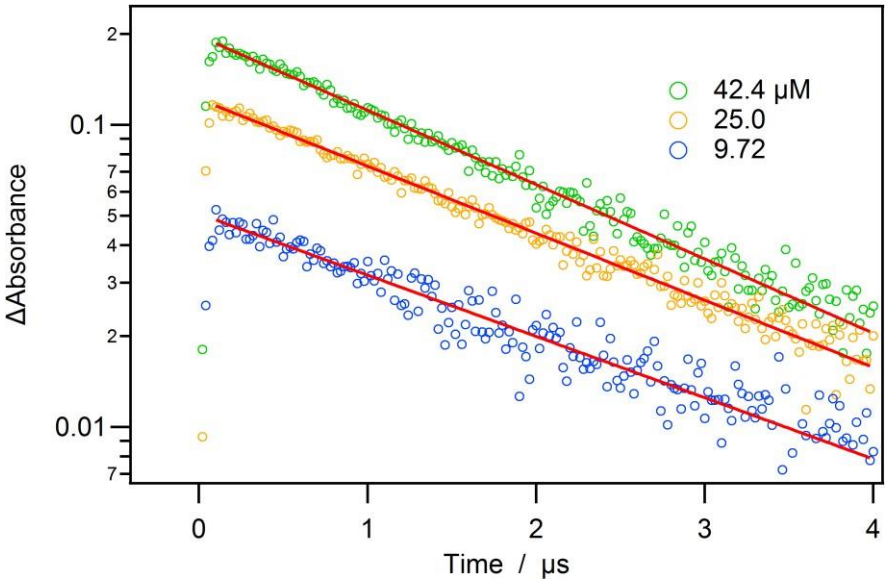

Fig. S5 Transient absorption decays at 710 nm in Ar–saturated acetonitrile solution with several concentrations of ta8TGuo.

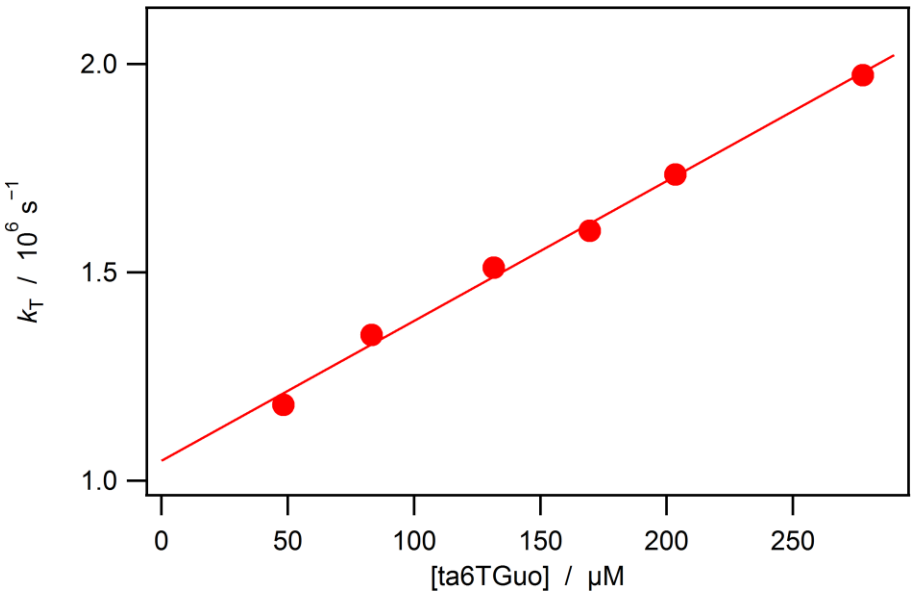

Fig. S6 Plot of the triplet decay rate constant (k_T) of ta6TGuo against the ground–state ta6TGuo concentration.

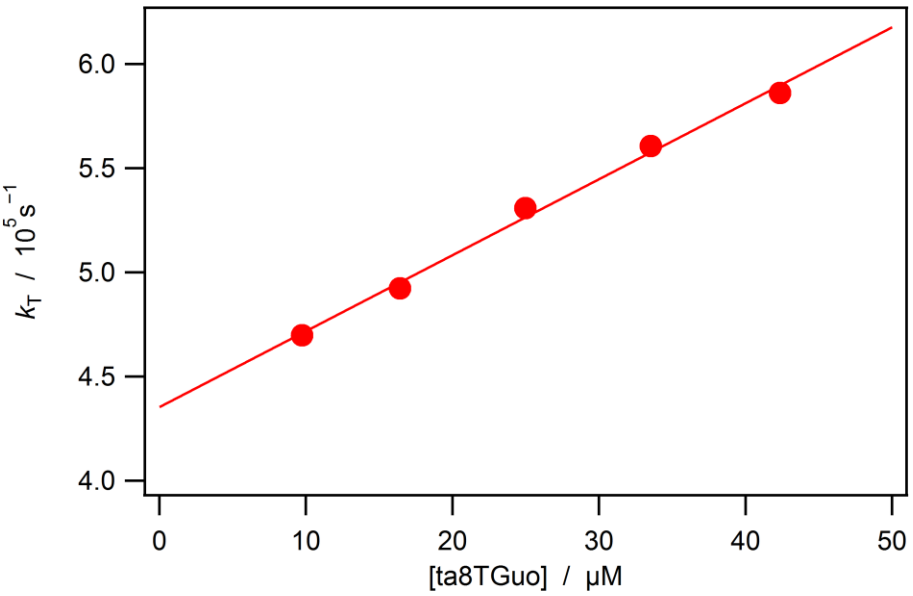

Fig. S7 Plot of the triplet decay rate constant (k_T) of ta8TGuo against the ground–state ta8TGuo concentration.

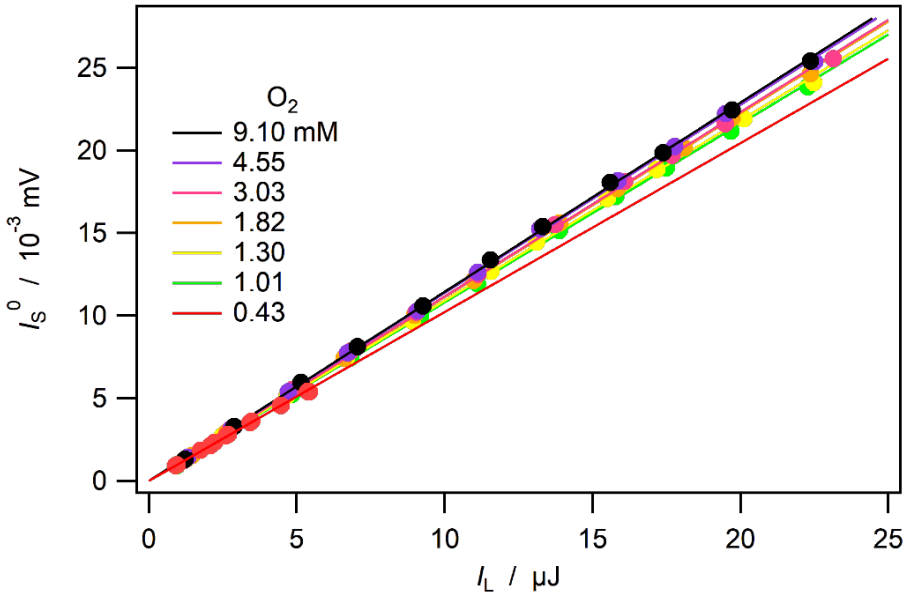

Fig. S8 Plots of the emission intensity maxima (I_S^0) immediately after laser irradiation in taDTGuo solutions (66.7 μM) at several concentration of dissolved oxygen against incident laser power (I_L).

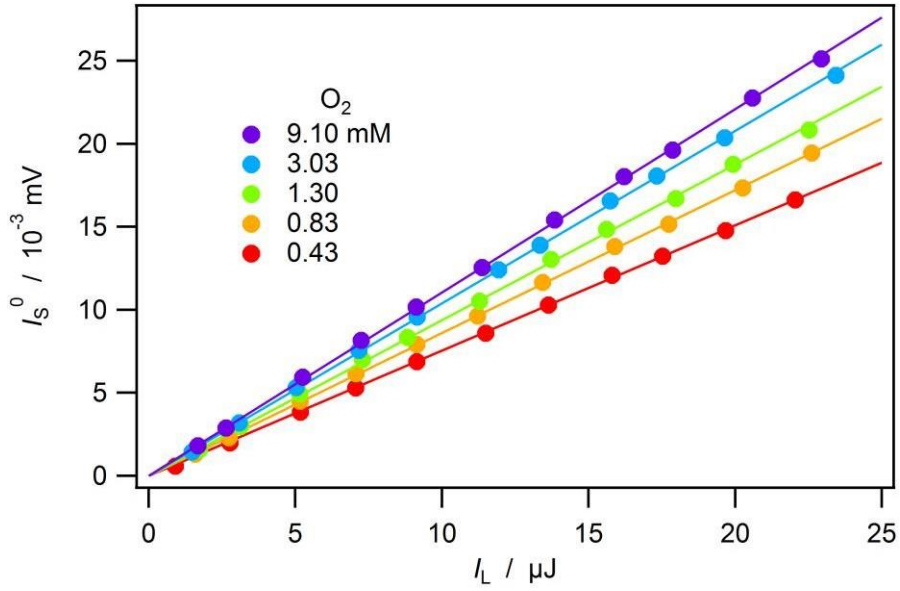

Fig. S9 Plots of the emission intensity maxima (I_S^0) immediately after laser irradiation in ta6TGuo solutions (238 μM) at several concentration of dissolved oxygen against incident laser power (I_L).

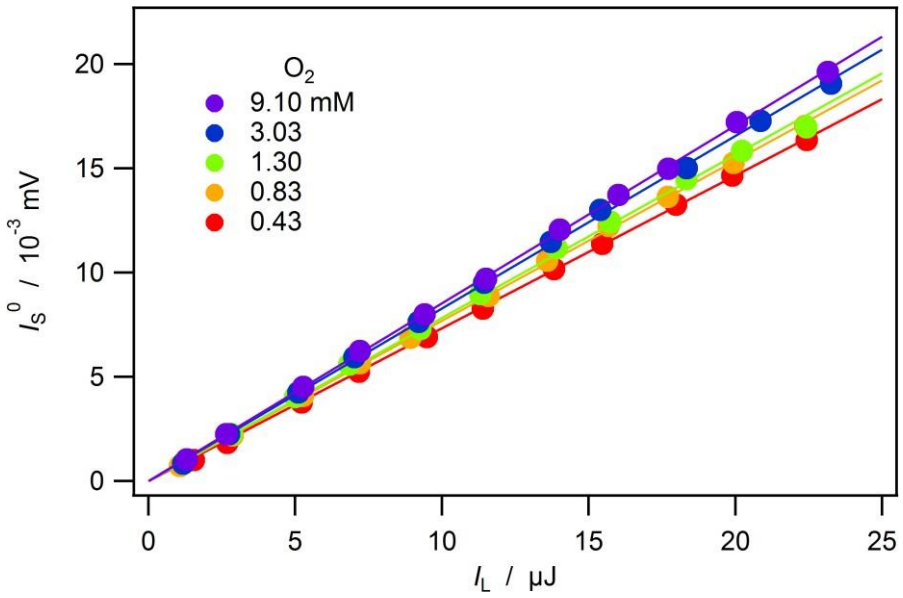

Fig. S10 Plots of the emission intensity maxima (I_S^0) immediately after laser irradiation in ta8TGuo solutions (35.6 µM) at several concentration of dissolved oxygen against incident laser power (I_L).

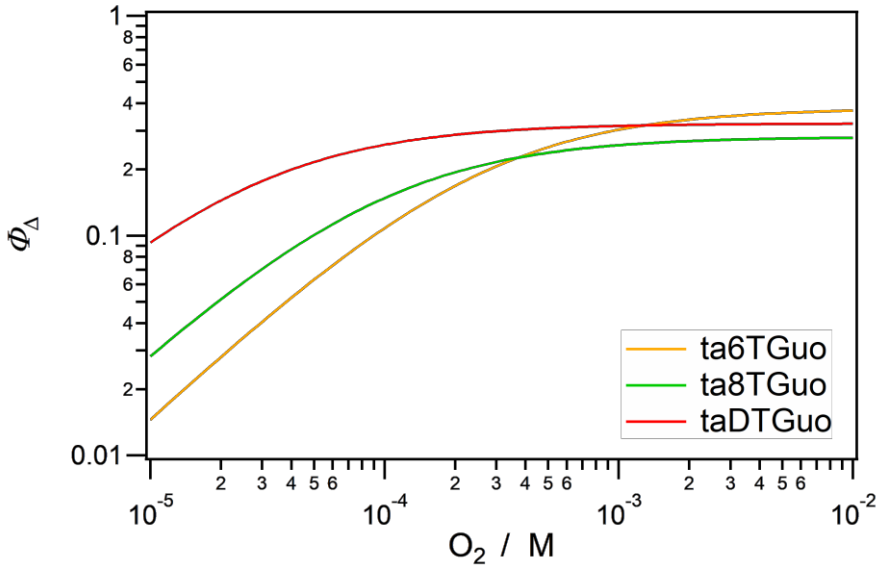

Fig. S11 The simulation curves of the $\emptyset_\Delta$ values under low oxygen concentration such as carcinomatous condition using the kinetics parameters estimated in this study (see Fig. 5a). The concentration of each thioguanosine was 247 µM for ta6TGuo, 35.6 µM for ta8TGuo, and 66.7µM for taDTGuo.

Reference

1. S. Miyata, T. Yamada, T. Isozaki, H. Sugimura, Y.−Z. Xu and T. Suzuki, Absorption Characteristics and Quantum Yields of Singlet Oxygen Generation of Thioguanosine Derivatives, *Photochem. Photobiol*., 2018, **94**, 677–684.