Supporting Information

Rose Bengal-photosensitized oxidation of 4-thiothymidine in aqueous medium: evidence for the reaction of the nucleoside with singlet state oxygen

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**Figure S1.** Transient absorption spectra recorded at different delay times with respect to 532 nm laser excitation of N₂-saturated aqueous solutions of RB at pH 12 (E₅₃₂ ~ 10 mJ/pulse, pulse with ≈ 6 ns). The inset shows the decay trace monitored at 600 nm and the related first-order fitting.

**Figure S2.** Transient absorption spectra recorded at different delay times with respect to 532 nm laser excitation of N₂-saturated aqueous solutions of RB at pH 7 in the presence of S₄TdR 8 × 10⁻⁴ M (E₅₃₂ ~ 10 mJ/pulse, pulse with ≈ 6 ns). The inset shows the decay trace monitored at 600 nm and the related first-order fitting.
Figure S3. Comparison between detailed views (wavenumber range: 550-2000 cm\(^{-1}\)) of the FTIR ATR spectra obtained for: top panels) a 5\times10^{-4} M solution of RB at pH 7 (a) and pH 12 (d), before (black line) and after (dark gray line) irradiation for 1 hour with neon light (emission between 400 and 700 nm); central panels) a 8\times10^{-4} M solution of S\(^4\)TdR in the presence of RB 5\times10^{-4} M at pH 7 (b) and 12 (e), before (black line) and after (dark gray line) irradiation; bottom panels) a 8\times10^{-4} M solution of TdR at pH 7 (c) and 12 (f). See text for details about the assignment of bands emphasized in the figure.
Figure S4. Detailed view (2.14-1.9 ppm) of the $^1$H-NMR spectrum obtained for the reaction mixture containing $2 \times 10^{-4}$ M S$^4$TdR and $5 \times 10^{-4}$ M RB at pH 7 after 1 h of irradiation with neon light (emission between 400 and 700 nm). Signals related to the 7-CH$_3$ protons of 4-thiothymidine (S), thymidine (T) and dimeric 4-thiothymidine (S-Like) are evidenced.
**Figure S5.** Comparison between ESI-MS positive ion spectra obtained for an aqueous solution containing S^4^TdR 2 × 10^{-4} M and RB 5 × 10^{-4} M at pH 7 before (0 h) and after irradiation for 1 h with neon light (emission between 400 and 700 nm). See the text for details about peak assignments. Legend: -ddr = dehydro-deoxyribose neutral loss.