Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

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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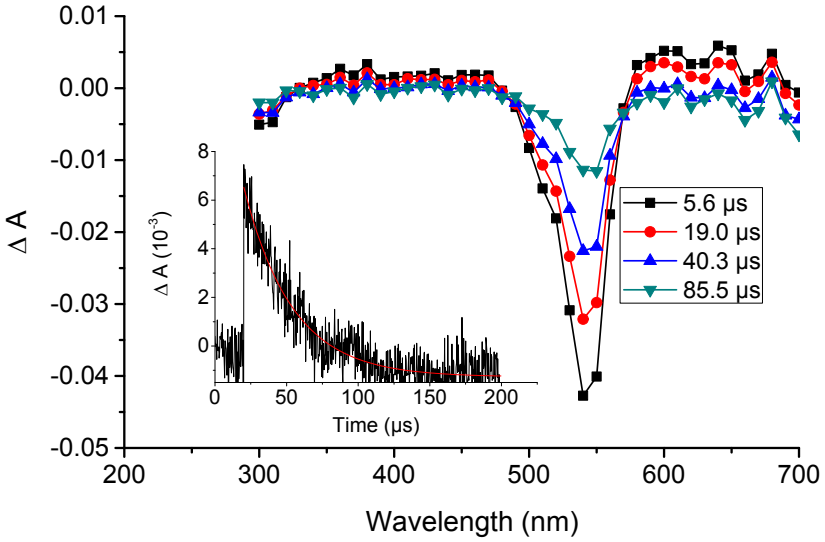

Figure S1. Transient absorption spectra recorded at different delay times with respect to 532 nm laser excitation of N_2-saturated aqueous solutions of RB at pH 12 (E_{532} ~ 10 mJ/ pulse, pulse with ≈ 6 ns). The inset shows the decay trace monitored at 600 nm and the related first-order fitting.

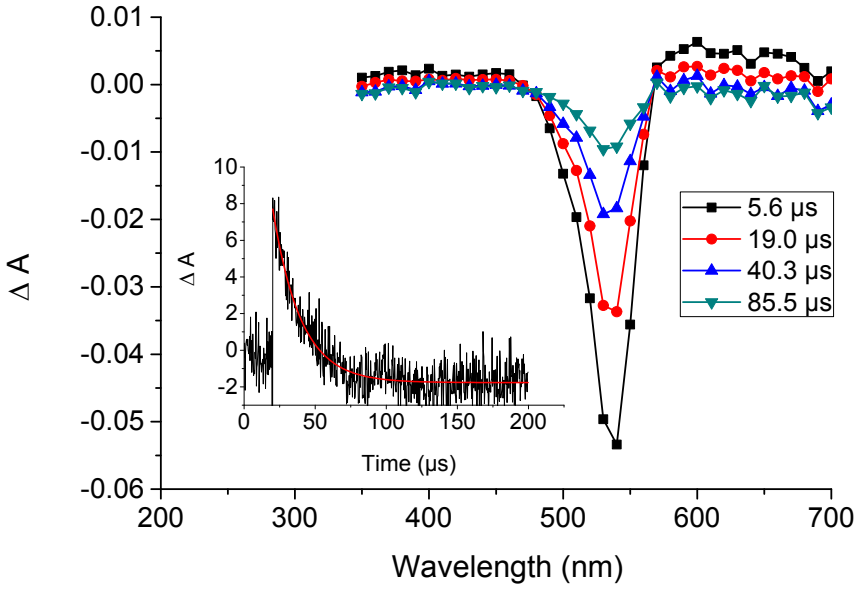

Figure S2. Transient absorption spectra recorded at different delay times with respect to 532 nm laser excitation of N_2-saturated aqueous solutions of RB at pH 7 in the presence of S^4TdR 8×10^{-4} M (E_{532} ~ 10 mJ/ pulse, pulse with ≈ 6 ns). The inset shows the decay trace monitored at 600 nm and the related first-order fitting.

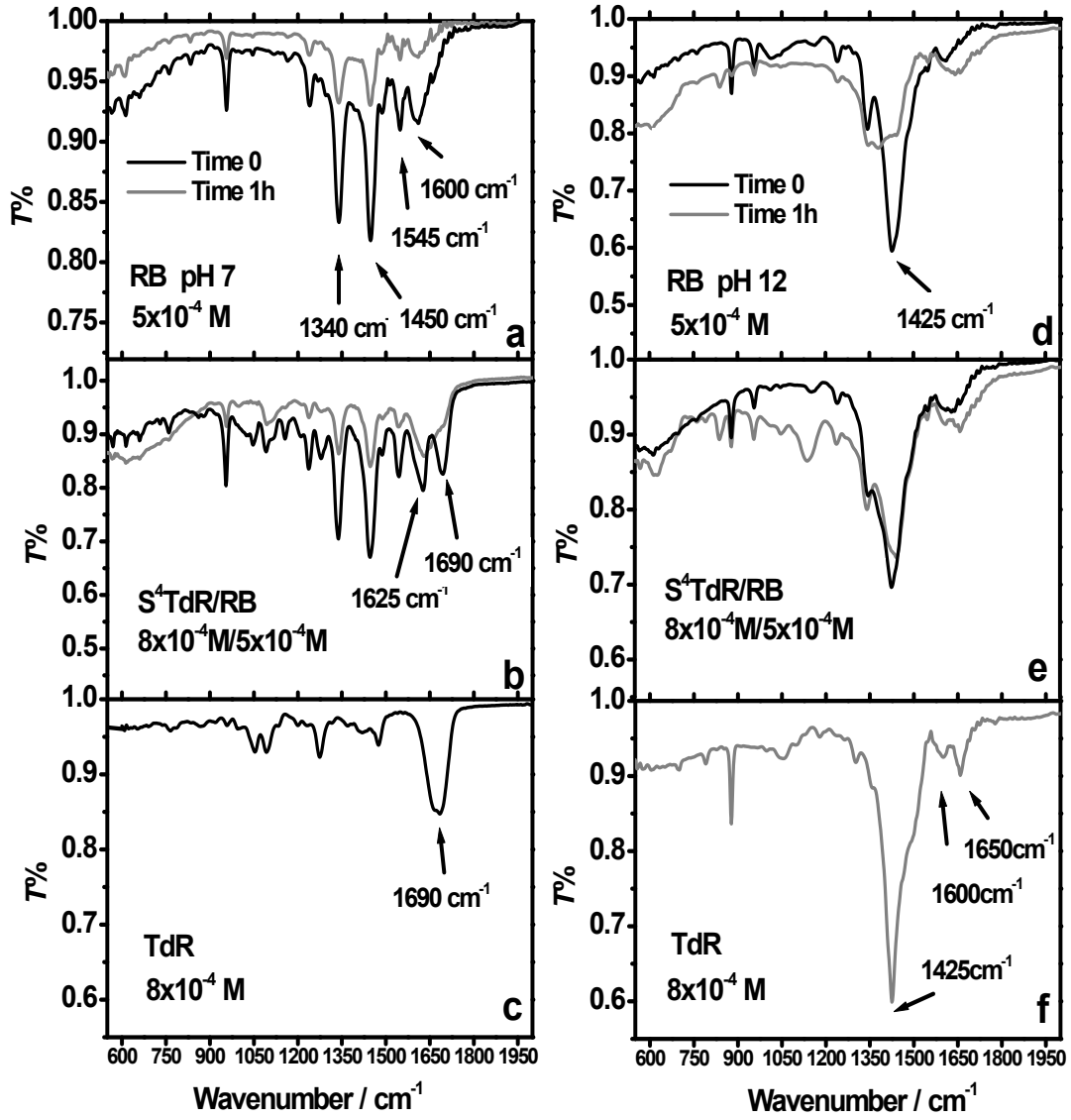

Figure S3. Comparison between detailed views (wavenumber range: 550-2000 cm^{-1}) of the FTIR ATR spectra obtained for: **top panels**) a 5×10^{-4} M solution of RB at pH 7 (a) and pH 12 (d), before (black line) and after (dark gray line) irradiation for 1 hour with neon light (emission between 400 and 700 nm); **central panels**) a 8×10^{-4} M solution of S^4TdR in the presence of RB 5×10^{-4} M at pH 7 (b) and 12 (e), before (black line) and after (dark gray line) irradiation; **bottom panels**) a 8×10^{-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.

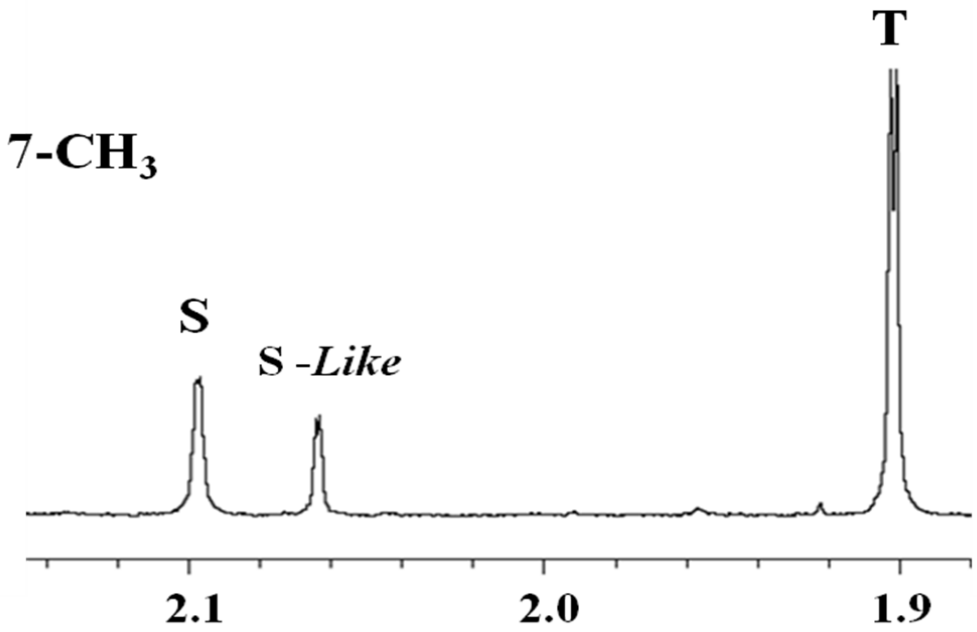

Figure S4. Detailed view (2.14-1.9 ppm) of the ^{1}H-NMR spectrum obtained for the reaction mixture containing 2×10^{-4} M S^{4}TdR and 5×10^{-4} M RB at pH 7 after 1 h of irradiation with neon light (emission between 400 and 700 nm). Signals related to the 7-CH_3 protons of 4-thiothymidine (S), thymidine (T) and dimeric 4-thiothymidine (*S-Like*) are evidenced.

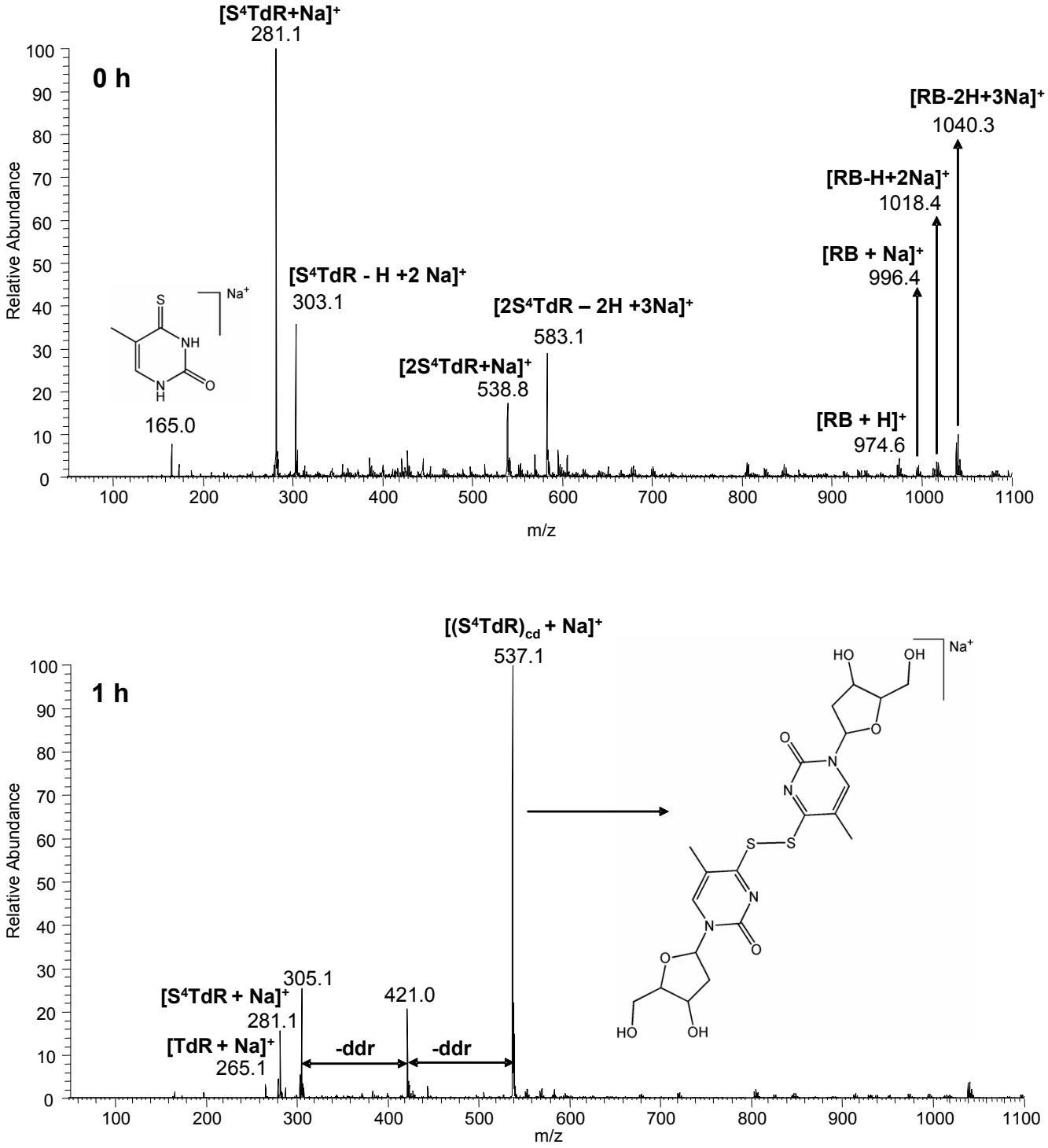

Figure S5. Comparison between ESI-MS positive ion spectra obtained for an aqueous solution containing S^4TdR 2×10^{-4} M and RB 5×10^{-4} M at pH 7 before (0 h) and after irradiation for 1 h with neon light (emission between 400 and 700 nm). See the text for details about peak assignments. Legend: -ddr = dehydro-deoxyribose neutral loss.