Supplementary Material (ESI) for Photochemical & Photobiological Sciences
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Synthetic and photochemical studies of substituted 1-acyl-7-nitroindolines

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Electronic Supplementary Information

Data shown are the progressive photolysis spectra of **8** (Figure S1), UV-visible molar absorbance spectra for **8** and **14** (Figure S2), primary data for the measurement of the hydrolysis rate of **18** (Figure S3), UV-visible molar absorbance spectra for the chromophores of **18** and **32** (Figure S4), a comparison of the UV-visible molar absorbance spectrum for a fully-photolysed solution of **8** with the calculated spectrum of a mixture of its photolysis products **28** and **29** (Figure S5), and the spectrum of the nitrosoindole **31** (Figure S6).

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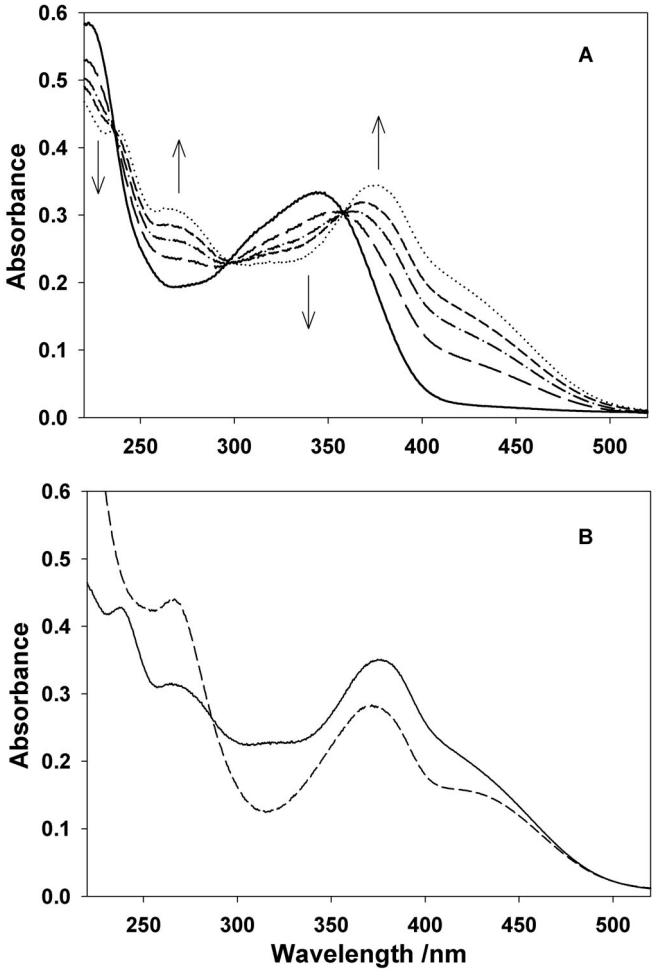

Figure S1. (A) Spectra for progressive photolysis of **8** in 25 mM Na phosphate, pH 7.0–EtOH (9:1), taken before irradiation (—) and after 5 s (– – –), 10 s (– · –), 15 s (---) and 30 s (····) irradiation (350 nm lamps). The vertical arrows indicate the direction of change of absorbance of various bands as the illumination proceeded. (B) Spectra of the solution of **8** after irradiation for 60 s, recorded before (—) and after (---) addition of dithiothreitol. The spectrum at 60 s was identical to that in panel (A) after 30 s irradiation.

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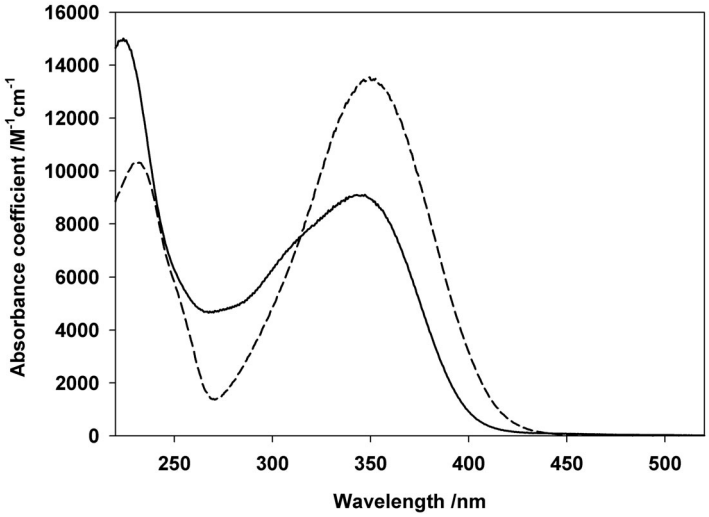

Figure S2. Molar absorbance spectra for 1-acetyl-5,7-dinitroindoline **8** (——) (same chromophore as for the glutamate conjugate **11**) and the 5-nitro compound **14** (------), both determined in 25 mM Na phosphate, pH 7–EtOH (20:1).

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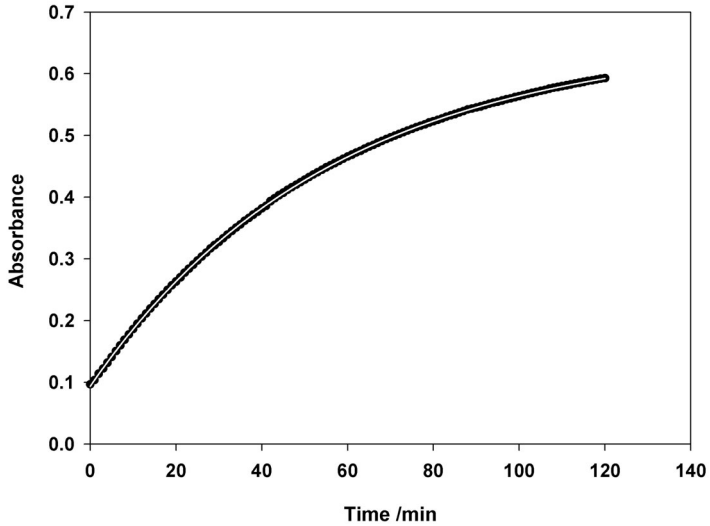

Figure S3. Time recording of the absorbance at 404 nm for a solution of **18** (90 μM) in 62.5 mM 3-cyclohexylamino-1-propanesulfonate (CAPS), pH 11.0, maintained at 30 °C. The symbols (filled circles) are the experimental readings and the superimposed white line is the result of a single exponential fit to these data. Absorbance was monitored for ~3 half lives of the reaction. Figure S4 shows the molar absorbance spectra of the starting compound **18** and the indoline product **32**.

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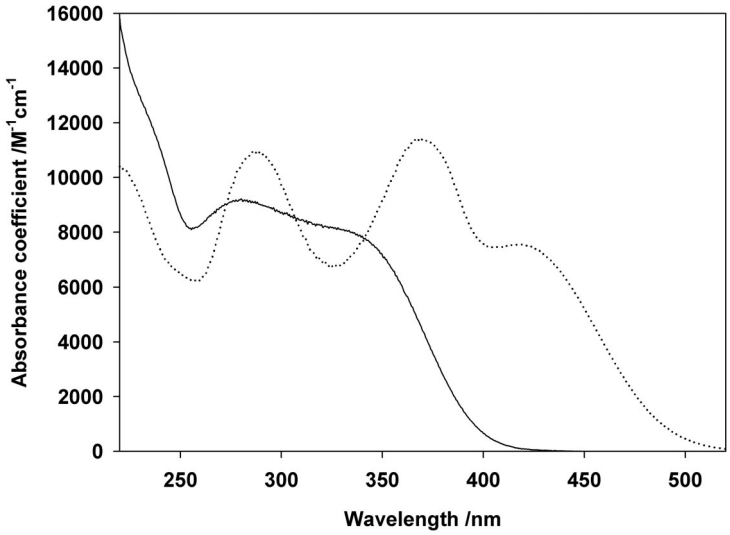

Figure S4. Molar absorbance spectra of 1-acetyl-4-methoxy-5,7-dinitroindoline **9** (——) (same chromophore as for **18**) and its hydrolysis product 4-methoxy-5,7-dinitroindoline **32** (·····), both determined in 25 mM Na phosphate, pH 7–EtOH (9:1). The spectra show the large increase in absorbance at the wavelength (404 nm) used to monitor hydrolysis of **18**.

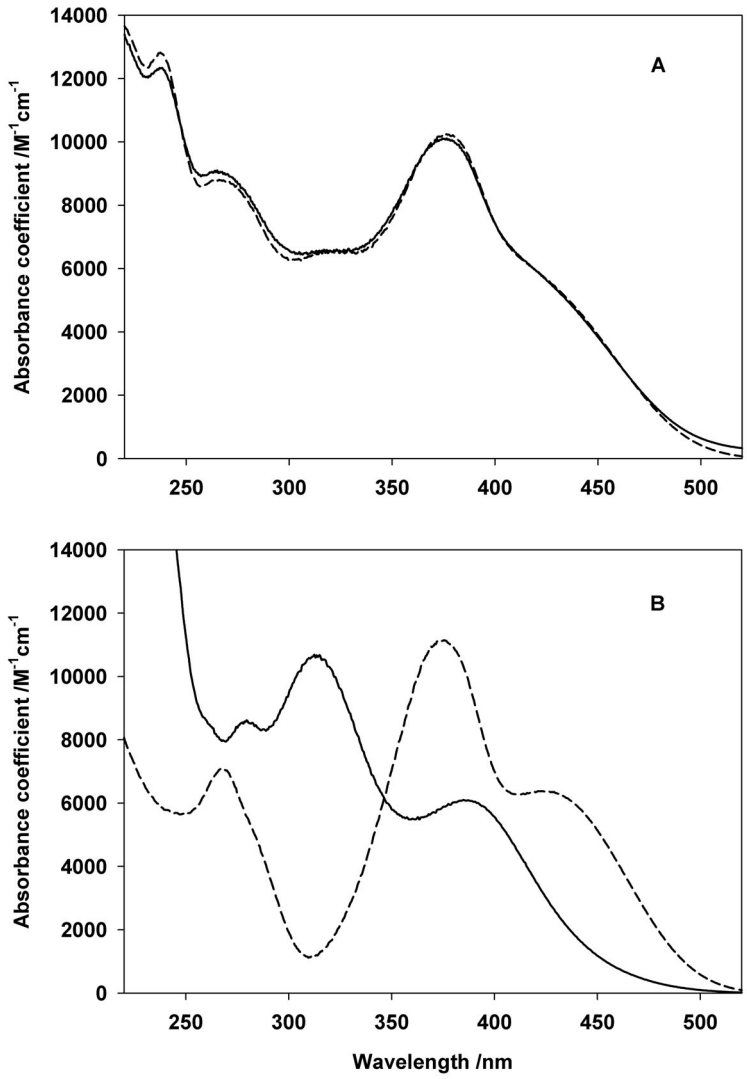

Figure S5. (A) Molar UV-visible absorbance spectrum of an aqueous solution of **8** after irradiation for 60 s (——) and the calculated spectrum (-----) for a mixture of its isolated photolysis products **28** and **29** in a molar ratio of 0.46:0.54 respectively. (B) Individual molar absorption spectra of **28** (——) and **29** (-----).

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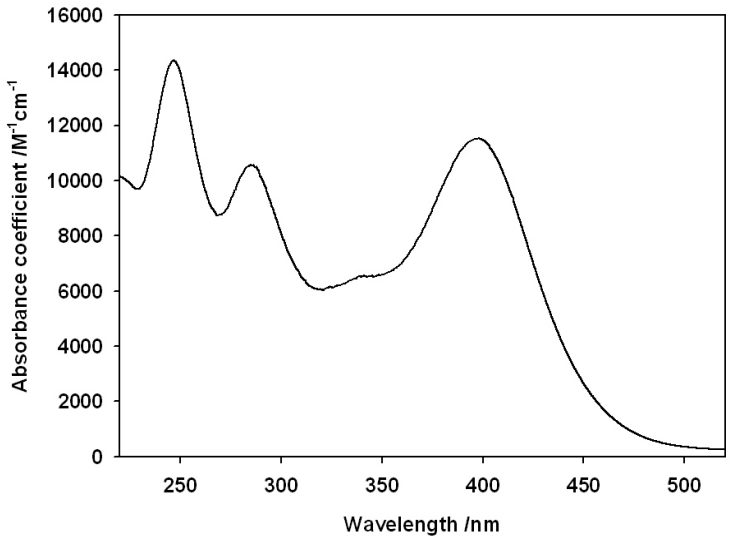

Figure S6. (A) Molar UV-visible absorbance spectrum of an aqueous solution of 4-methoxy-5-nitro-7-nitrosoindole **31** determined in 25 mM Na phosphate, pH 7–EtOH (9:1). Note that the spectrum for 4-methoxy-5,7-dinitroindoline **32** is shown as part of Figure S4.