

Supporting information for:

A new method for the nitrosation of 1,3-diketones applied to 3-ethyl- and 3-methyl pentane-2,4-dione

Emilia Iglesias

Departamento de Química Física e E. Q. I. Facultad de Ciencias. Universidad de La Coruña. 15071-La Coruña, SPAIN. E-mail: emilia.iglesias@udc.es

This supporting information contains:

- i) Spectra of enol tautomerization in water and in aqueous perchloric acid of 3-ethylpentane-2,4-dione, EPD, (Fig. S1 (a) to (c)) and of enol tautomerization of 3-methylpentane-2,4-dione MPD, in aqueous perchloric acid (Fig. S1 (d)).
- ii) Reaction spectra of alkaline hydrolysis for EPD and MPD, Fig. S2.
- iii) The Beer's law behaviour of EPD diluted in aqueous acid medium or in aqueous alkaline medium and immediately made acid, Fig. S3.
- iv) Reaction spectra for the nitrosation of EPD and MPD in acid medium, Fig. S4 (a) and (b).

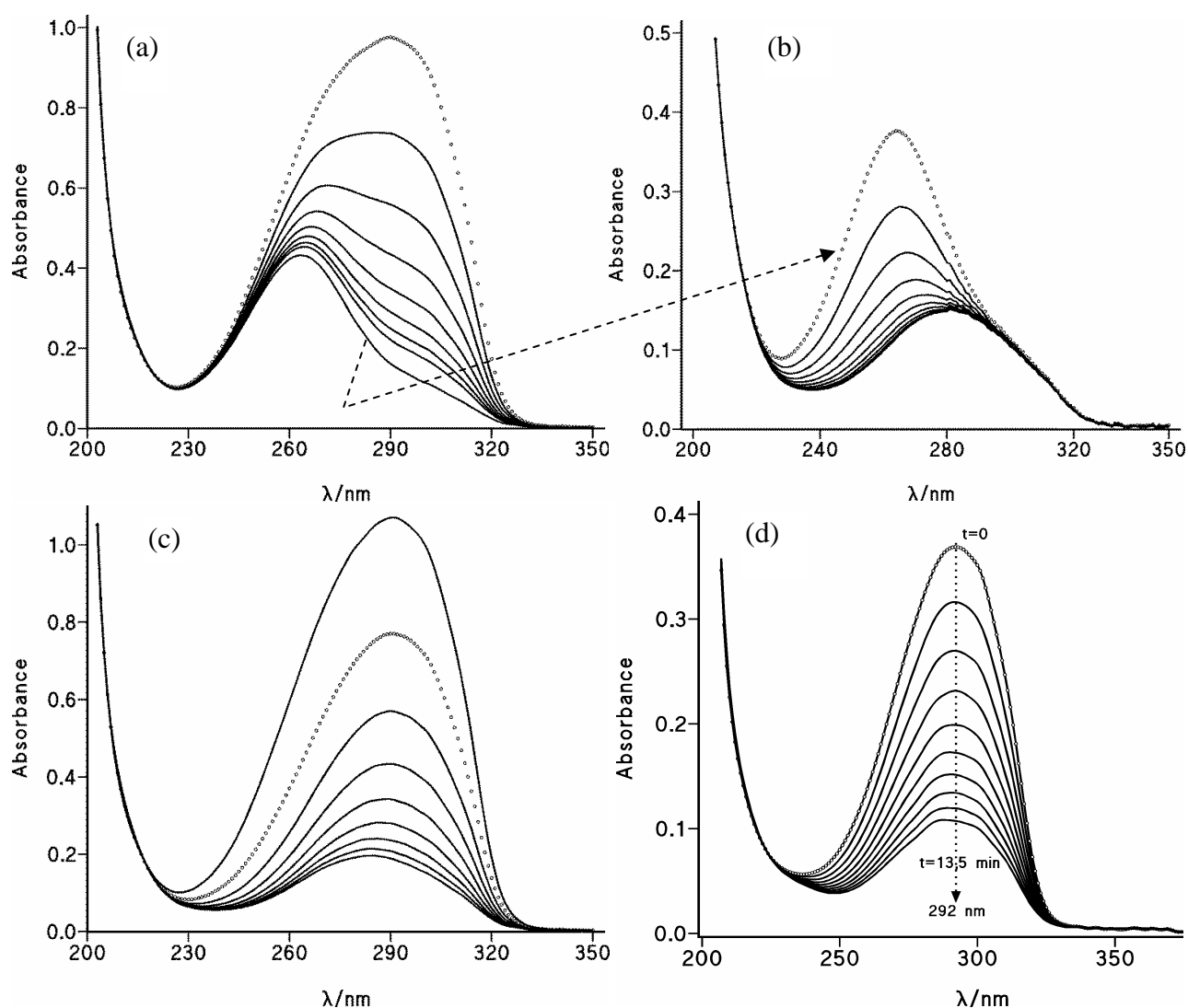


Figure S1. (a)Decreasing absorbance due to enol tautomerization of 3-ethylpentane-2,4-dione (0.41mM) in water; scans at 3 min; (b)the lowest down spectrum of (a) after adding 50 μ L HClO_4 1 M; scans at 3 min interval; (c)decreasing absorbance due tautomerization of 3-ethylpentane-2,4-dione (0.41 mM) in aqueous perchloric acid 0.033 M; scans each 3 min interval. EPD added from the stock dioxane solution. (d)Enol tautomerization of 3-methylpentane-2,4-dione (MPD) 0.113 M at $[\text{H}^+] = 0.034$ M; scans each 1.5 min

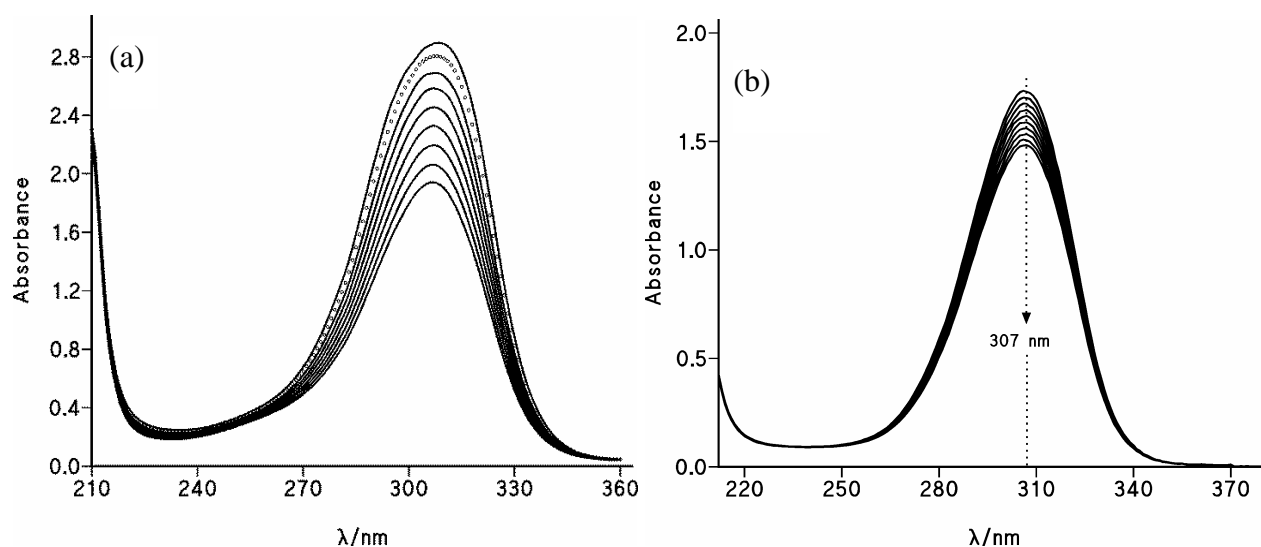


Fig. S2. (a) Reaction spectrum due to alkaline hydrolysis of [EPD] = 0.205 mM in aqueous alkaline medium at $[\text{OH}^-] = 0.033 \text{ M}$; scans at 3 min interval; (b) alkaline hydrolysis of [MPD] = 0.113 mM; $[\text{OH}^-] = 5.0 \text{ mM}$; $I = 0.2 \text{ M}$, scans each 1.2 min

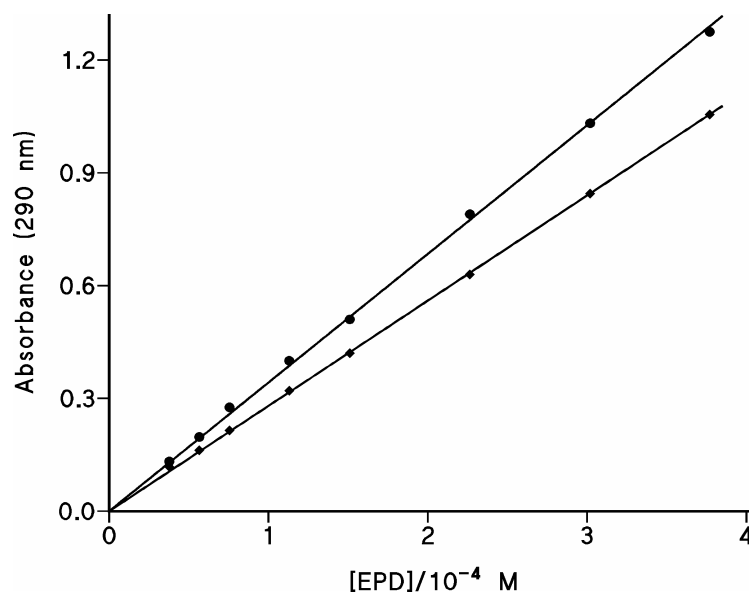


Fig. S3. Absorbance increase as a function of 3-ethylpentane-2,4-dione, EPD, when the ketone dioxane stock solution was diluted (♦) in aqueous acid medium of HClO_4 0.11 M and (●) in aqueous alkaline medium 0.032 M and immediately made acid, $[\text{H}^+] = 0.078 \text{ M}$ (HClO_4).

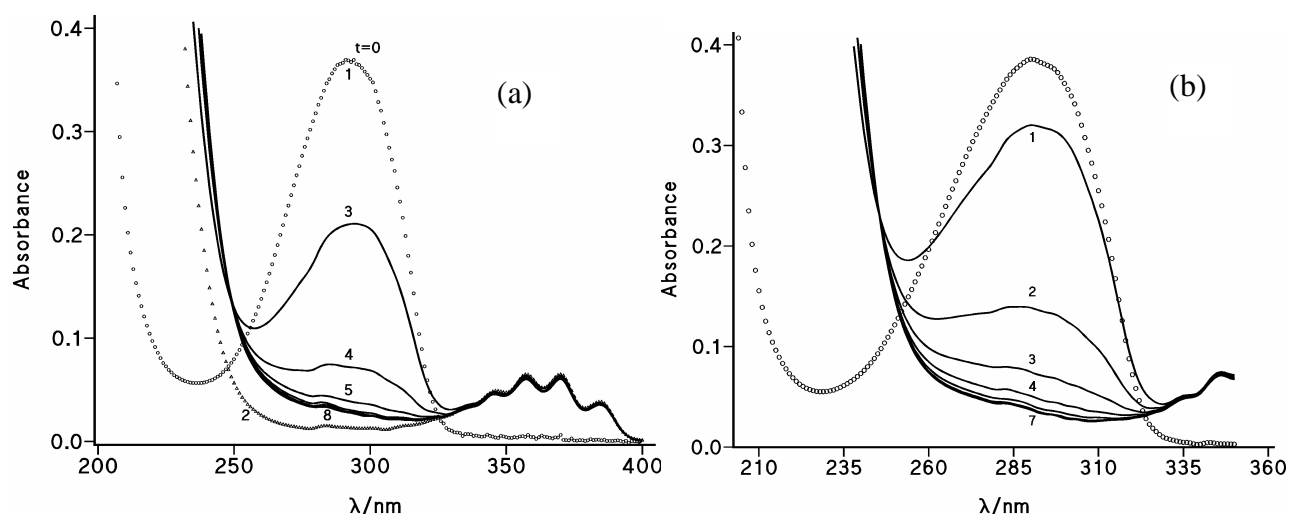


Fig. S4. (a)(o)spectrum of enol of MPD 0.113 mM at [H⁺]=0.034 M; (△)spectrum of HNO₂ 1.13 mM at [H⁺]=0.034 M; scans 3 to 8 correspond to the reaction spectra of [MPD]=0.113 mM; [nit]=1.13 mM and [H⁺]=0.034 M; scans each 1.5 min. (b) (o)spectrum of the enol of EPD 0.103 mM at [H⁺]=0.030 M; scans 1 to 7 correspond to the reaction spectra of [EPD]=0.103 mM; [nit]=1.75 mM and [H⁺]=0.030 M; scans each 2 min.