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

Mathematical description of pH-stat kinetic traces measured during photochemical quinone decomposition

Virág Kiss, Gábor Lehoczki, Katalin Ősz

SUPPORTING INFORMATION

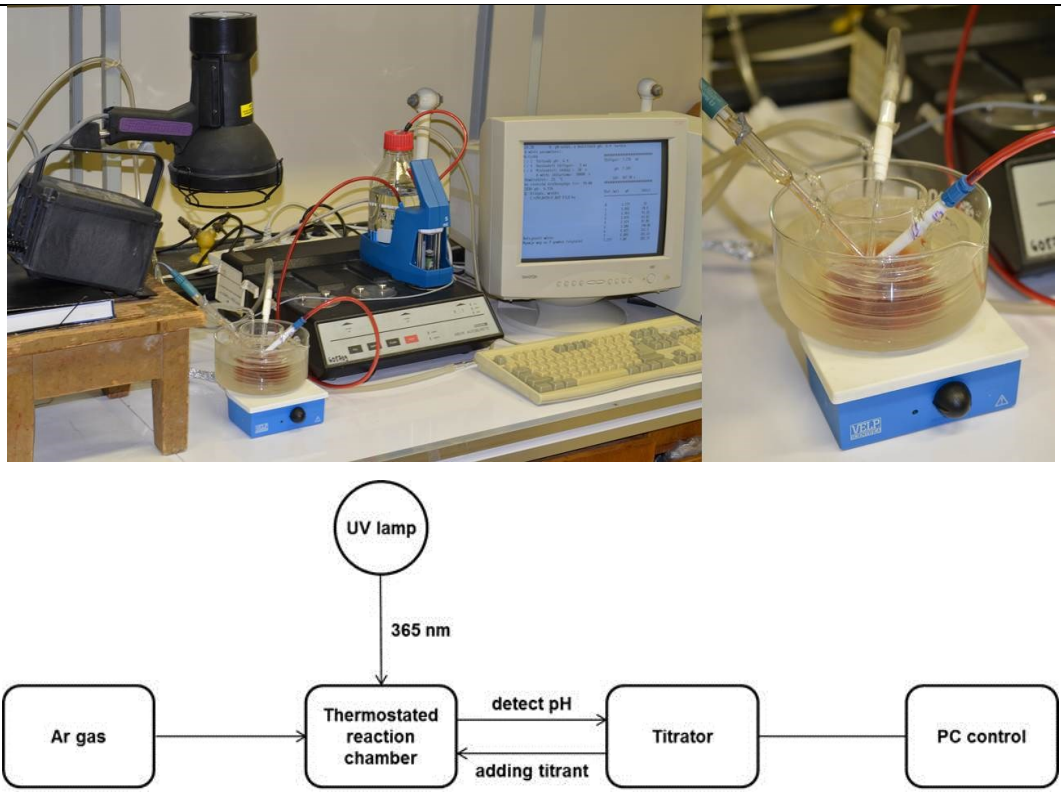

Figure S1 Measurement arrangement for the pH-stat measurements

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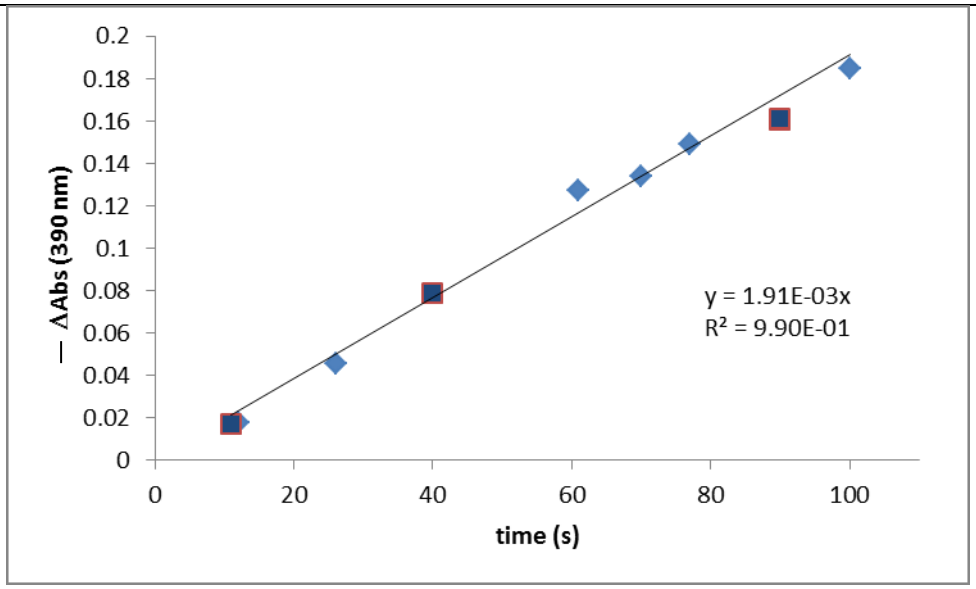

Figure S2 Calibration of the light intensity of the Spectroline FC-100/F UV-A lamp emitting at 365 nm. For these experiments, 30-mg samples of potassium trisoxalatoferrate(III) trihydrate ($K_3[Fe(C_2O_4)_3]\cdot 3H_2O$) were dissolved in 50 cm^3-s of 0.050 mol dm^{-3} aqueous H_2SO_4 solution then illuminated in the photoreactor for 11-100 seconds. The concentration of the Fe(III) reacted was determined from spectrophotometric measurements using the absorbance difference of the original actinometer solution and the solution after illumination.[37] From these measurements, the $-\frac{dA_{390nm}}{dt}$ value in a 1.000 cm cell was $(1.91\pm0.04)\times10^{-3}$ s^{-1}, resulting in a photon flux of 1.46×10^{17} s^{-1} for 50.0 cm^3 sample volumes in the arrangement shown in Figure S1.

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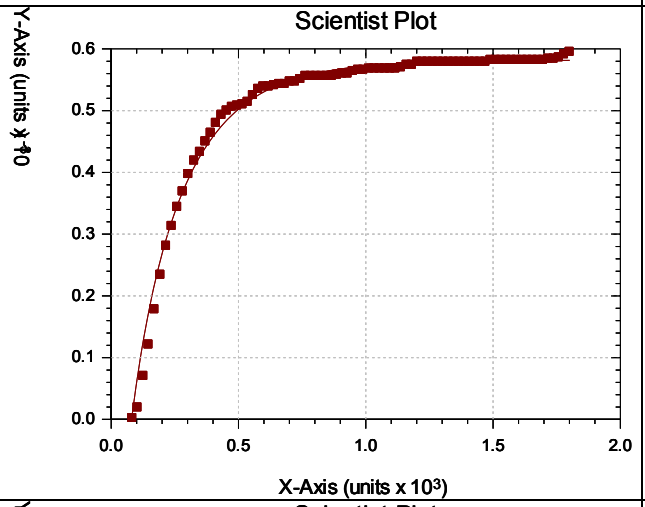
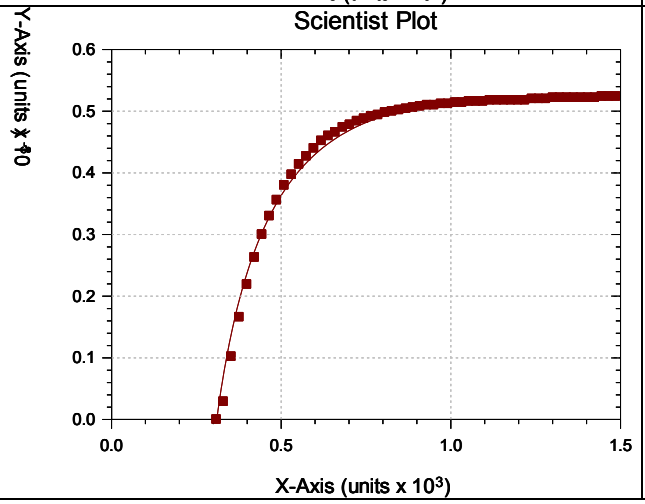
Table S1 Fitted kinetic curves together with the parameters of the quality of the fits

pH	Figure (the dots are the measured data points and the line is the fitted curve)	Sum of squared deviations	R-squared	Paramter correlation	Serial correlation	Skewness	Kurtosis
3.2		1.43094728E-8	0.999377451	-0.659381390 (between α and Φ)	7.95	-0.34	-0.00
3.97		6.42537813E-9	0.999482561	-0.696577428 (between α and Φ)	6.06	-0.66	0.00

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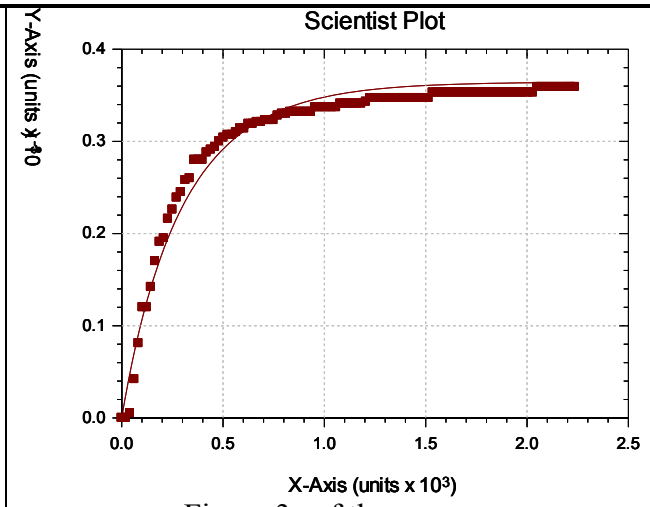
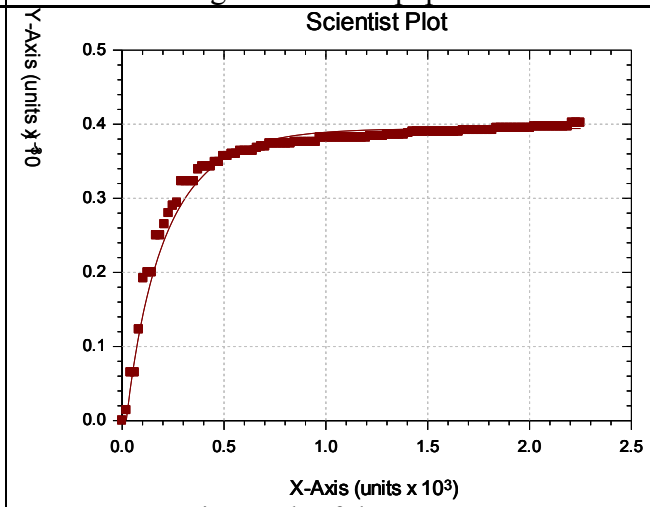
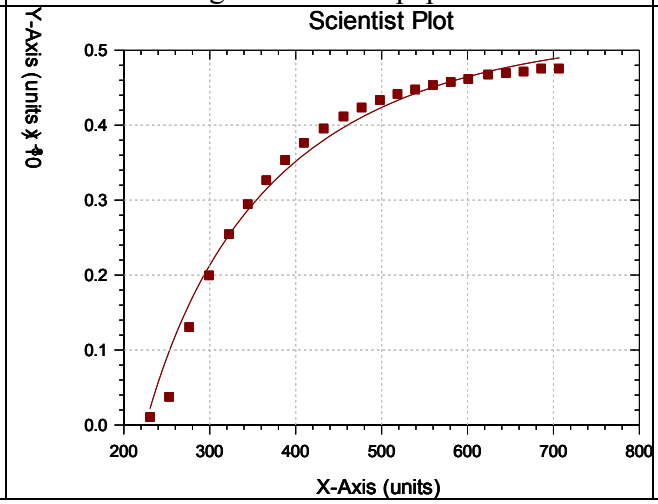
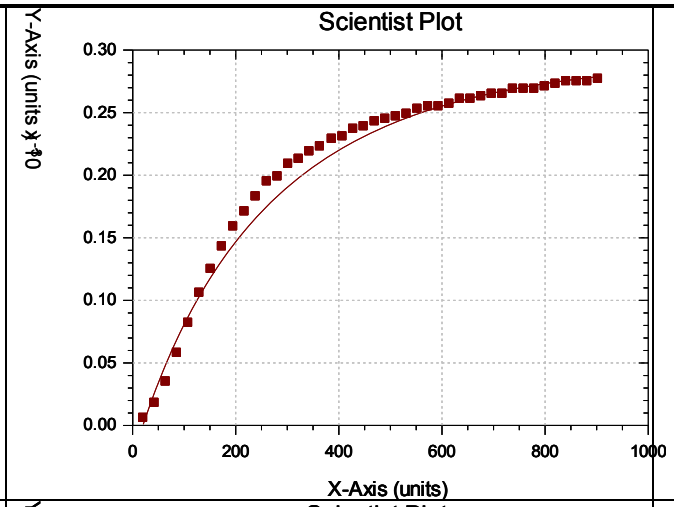
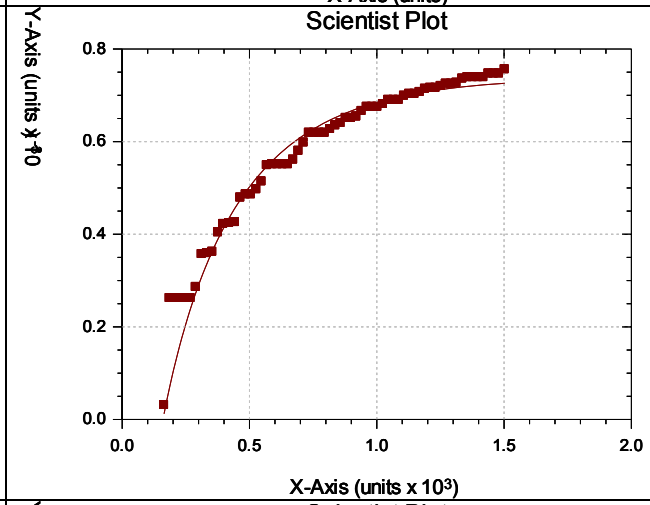
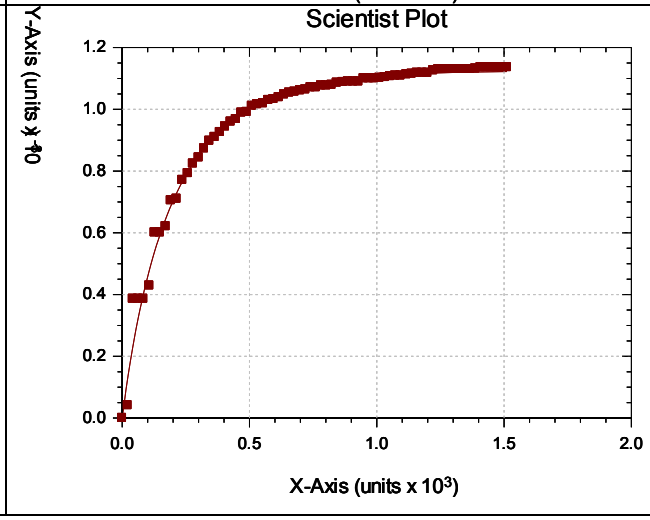
0.00	0.05	9.36	-0.713468793 (between α and ℓ)	0.998485088	1.67844213E-8	 Figure 3a of the paper.	4.3
0.00	-0.44	6.38	-0.560276584 (between α and Φ)	0.999316596	9.87714903E-9	 Figure 3b of the paper.	4.3
-0.49	9.94	3.40	-0.924277574 (between α and Φ)	0.997881474	7.21264142E-9		4.4

Mathematical description of pH-stat kinetic traces measured during photochemical quinone decomposition

Virág Kiss, Gábor Lehoczki, Katalin Ősz

SUPPORTING INFORMATION

4.85		3.52813608E-9	0.998356838	-0.929177106 (between α and Φ)	6.01	-2.10	-0.00
5.6		8.86053768E-8	0.996237847	-0.864785807 (between α and Φ)	5.96	-2.84	-0.00
6.4		4.73715167E-8	0.999343170	-0.706037154 (between α and Φ)	-0.66	-0.55	0.00

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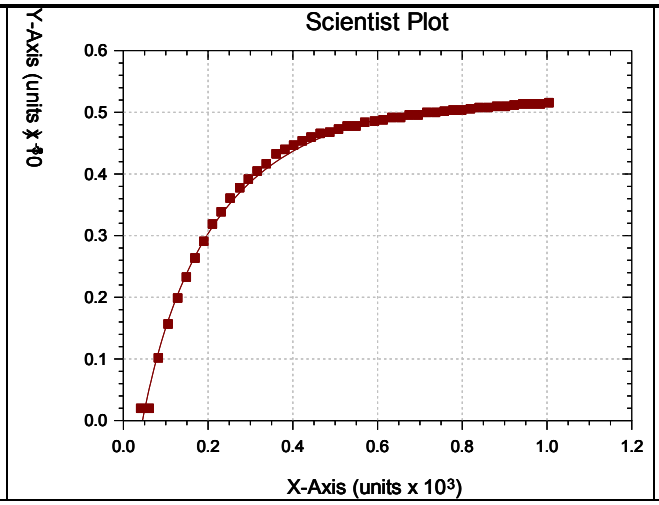
6.75		4.45321607E-9	0.99949648	-0.808158627 (between α and Φ)	2.50	-4.42	0.03

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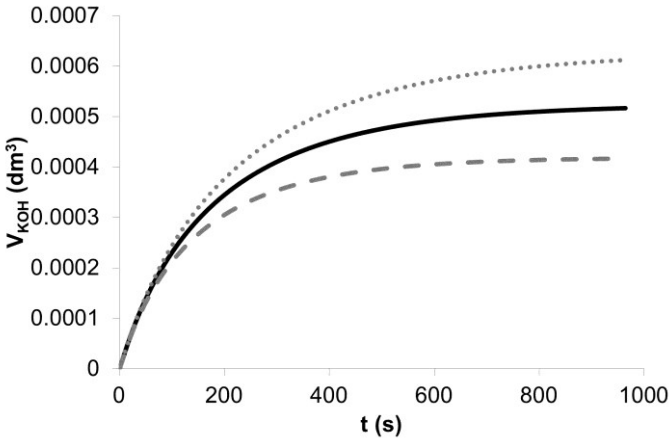
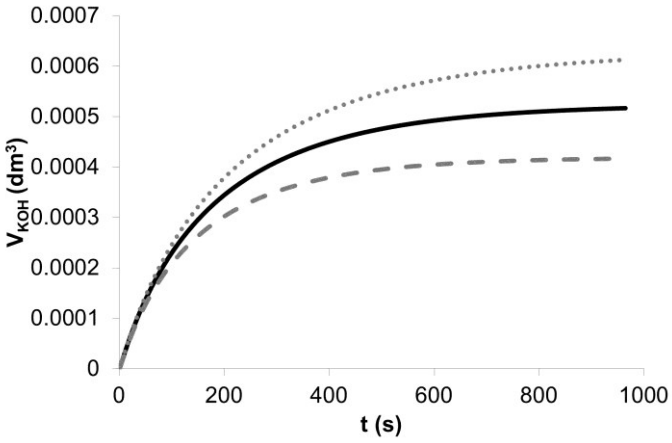
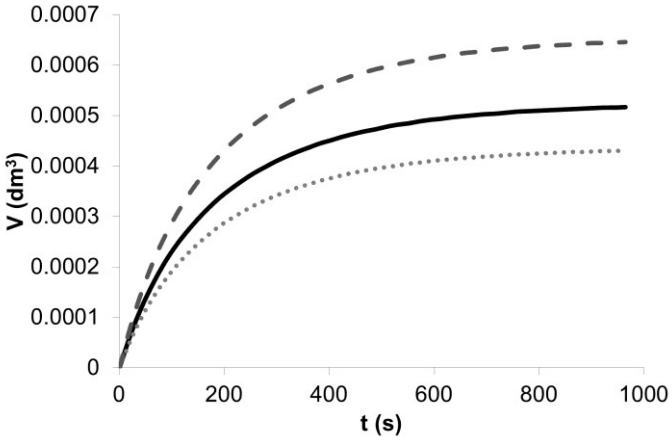
Table S2 Sensitivity analysis of the parameters when decreasing or increasing the parameter values by 20% of the original value. The modified parameters were V_0, c_0, c_{KOH}, α, Φ_P, ε_{Φ}^{ini}, ε_{Φ}^{fin}, Φ and ℓ.

Parameter	Figure
V_0	
c_0	
c_{KOH}	

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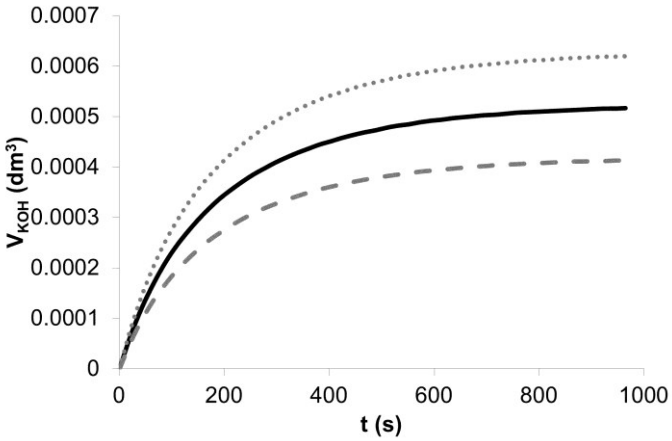
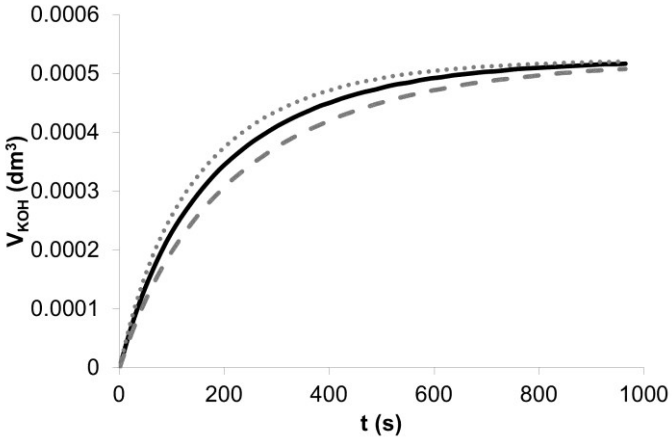
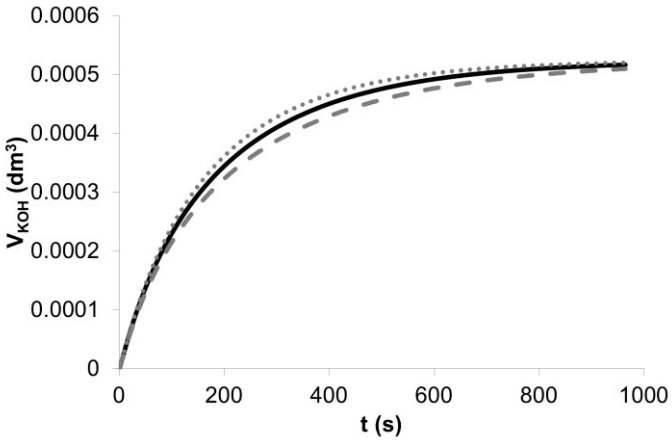
Virág Kiss, Gábor Lehoczki, Katalin Ősz

SUPPORTING INFORMATION

α	 Figure 5b of the paper.
Φ_P	
ε_{Φ}^{ini}	

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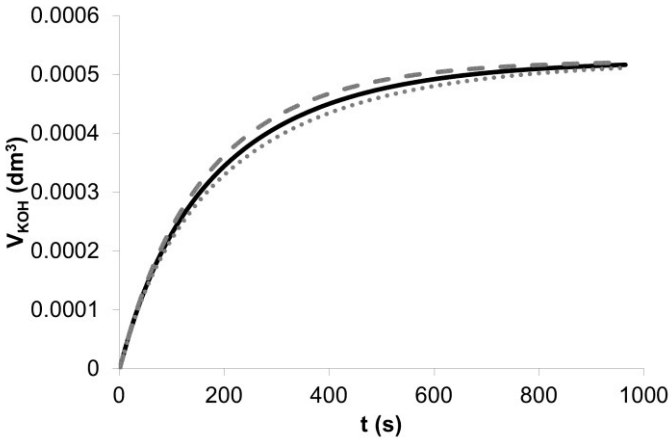
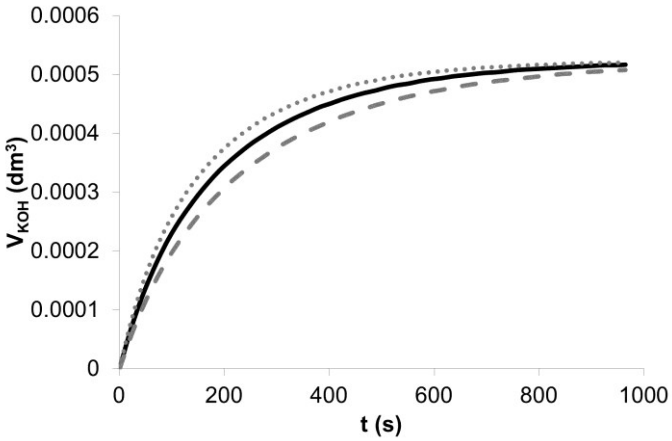
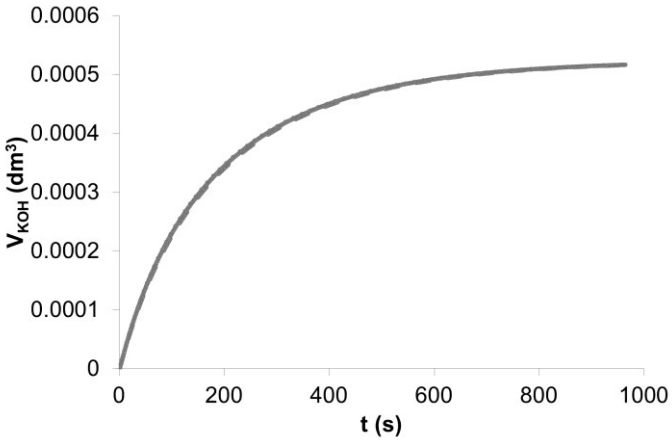
ε_{Φ}^{fin}	
Φ	 Figure 5c of the paper.
ℓ	 Figure 5a of the paper.

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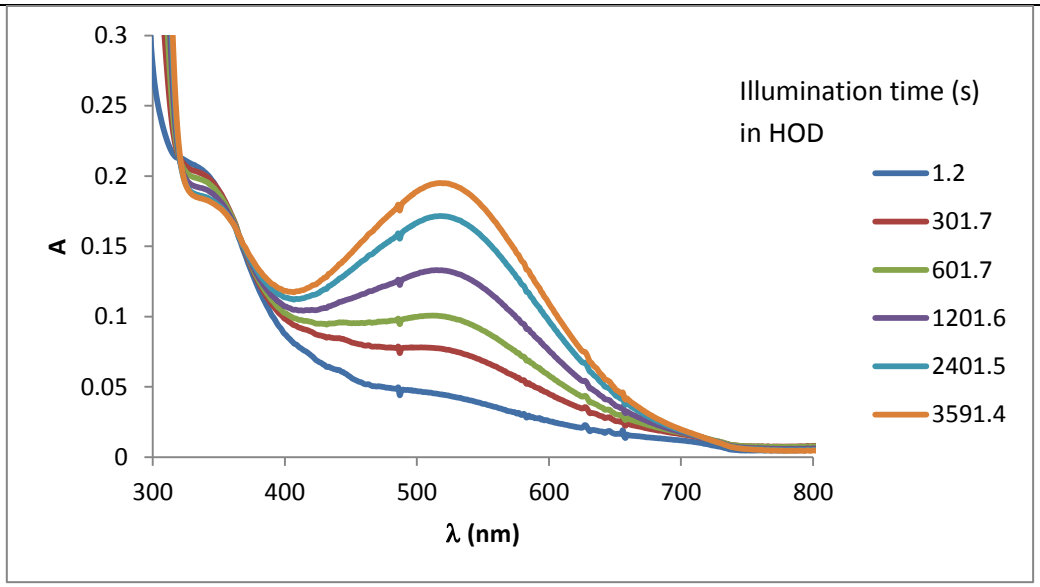

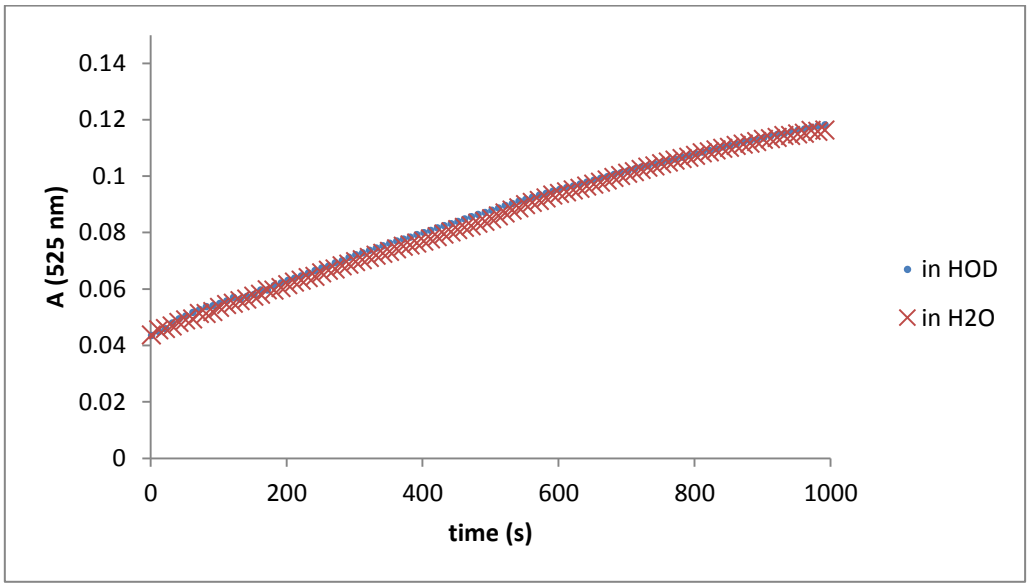

Figure S3 Photochemical decomposition reaction of QR measured in an Agilent 8543 diode array spectrophotometer. The product absorbing at 525 nm is QR-OH.
$c_0 = 5.0\times10^{-4}$ mol dm^{-3}, $V = 2.00$ cm^{-3}

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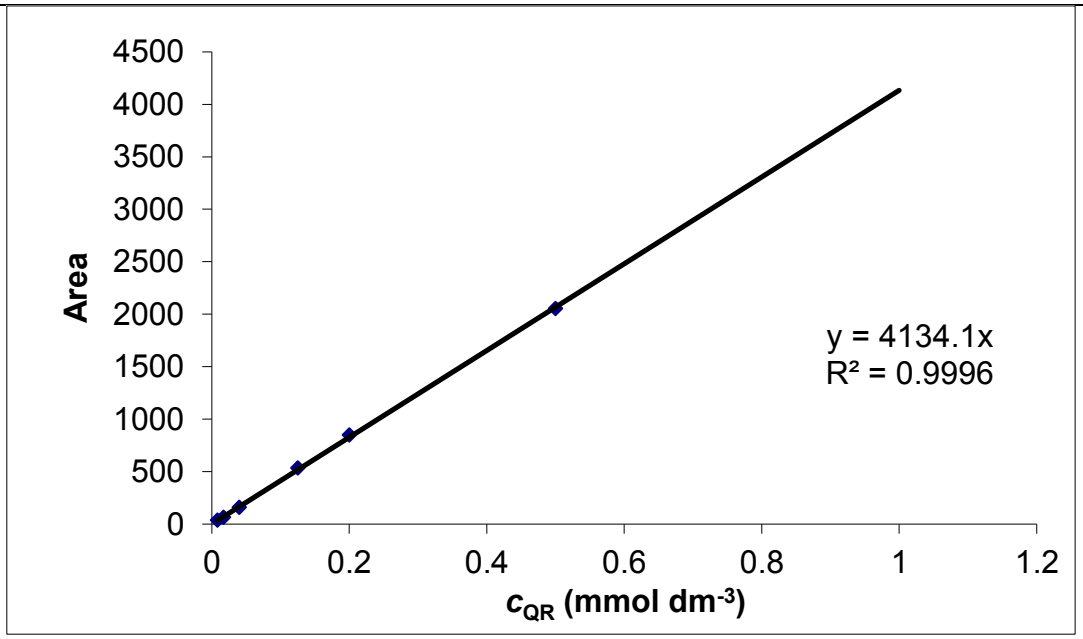

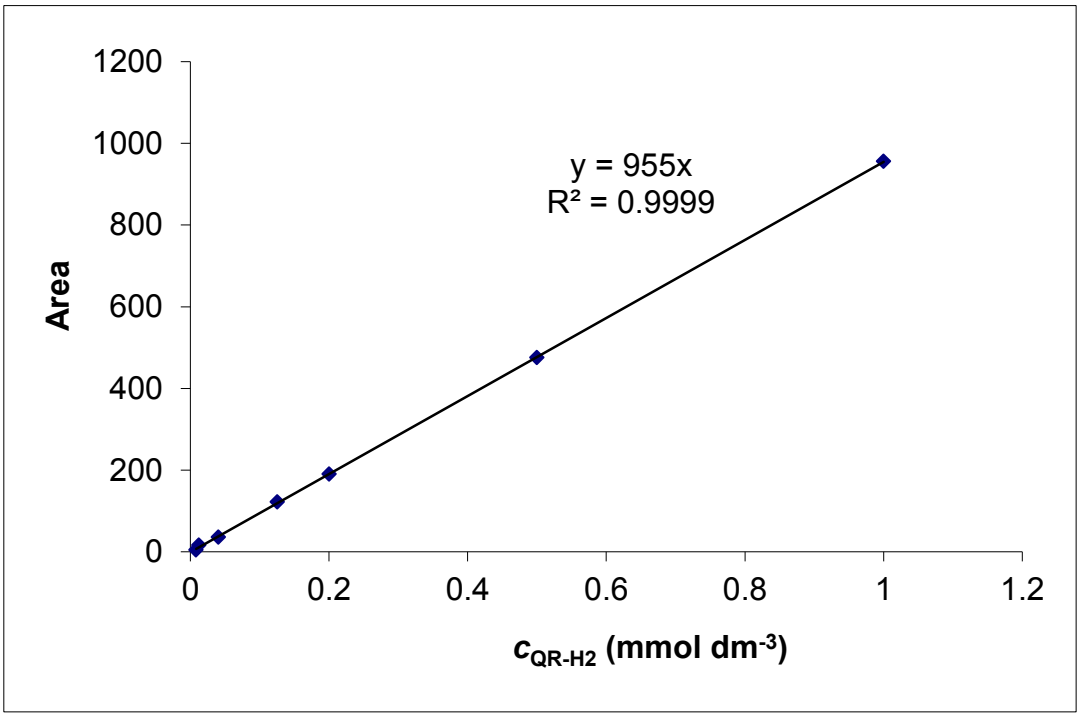

Figure S4 HPLC calibration curves for QR and QR-H_2