Supplementary material for the article:

Dostanić, J.; Lončarević, D.; Zlatar, M.; Vlahović, F.; Jovanović, D. M. Quantitative Structure-Activity Relationship Analysis of Substituted Arylazo Pyridone Dyes in Photocatalytic System: Experimental and Theoretical Study. J. Hazard. Mater. 2016, 316, 26–33. https://doi.org/10.1016/j.jhazmat.2016.05.015

Supplementary Information for:
Quantitative structure-activity relationship analysis of substituted arylazo pyridone dyes in photocatalytic system: Experimental and theoretical study

J. Dostanić[a, 1], D. Lončarević[a], M. Zlatar[b], F. Vlahović[c], D.M. Jovanović[a]

[a] *University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Department of Catalysis and Chemical Engineering, Njegoševa 12, 11000 Belgrade, Serbia*
[b] *University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Department of Chemistry, Njegoševa 12, 11000 Belgrade, Serbia*
[c] *University of Belgrade, Innovation center of the Faculty of Chemistry, 11000 Belgrade, Serbia*

[1] Corresponding author. Tel: +381 11 2630 213; fax: +381 11 2637 977;
E-mail address: jasmina@nanosys.ihtm.bg.ac.rs (J. Dostanić).

Table S1 NPA atomic charges from M062X/6-31+G(d,p) calculations

Substituent, R	C5	N3	N4	C6	O1
OH	-0.0836	-0.2181	-0.2436	0.0837	-0.6397
OCH3	-0.0835	-0.2175	-0.2427	0.0836	-0.6407
H	-0.0814	-0.2115	-0.2514	0.1113	-0.6366
Cl	-0.0792	-0.2118	-0.2585	0.1141	-0.6338
Br	-0.0779	-0.2120	-0.2609	0.1149	-0.6327
CN	-0.0695	-0.2073	-0.2769	0.1465	-0.6251
NO_2	-0.0634	-0.2063	-0.2822	0.1577	-0.6204

Table S2 The first vertical ionization energy (E_i) and electron affinity (E_{ea}) of investigated dyes from M062X/6-31+G(d,p) calculations

Substituent, R	E_i, Hartree	E_{ea}, Hartree
OH	0.143237	0.090062
OCH3	0.141715	0.090811
H	0.146586	0.085983
Cl	0.151357	0.077086
Br	0.151776	0.074779
CN	0.155841	0.059520
NO_2	0.160381	0.057480

Table S3 The condensed Fukui function (f_0) and local softness (s_0) for radical attack of azo nitrogen atoms (N3, N4) and carbon atoms linked to phenyl (C4) and pyridone ring (C5) of the substituted arylazo pyridone dyes calculated by using the M062X/6-31+G(d,p) level of theory and NPA atomic charge; Fukui function for OH radical=0.781; softness for OH radical=1.550. Numbering system used throughout the calculations is shown in Scheme 1. in the main text.

Substituent, R	f_0 [a]				s_0 [b]			
	C5	N3	N4	C6	C5	N3	N4	C6
OH	0.0822	0.0573	**0.1203**	-0.0125	1.5462	1.0780	**2.2623**	-0.2354
OCH3	0.0816	0.0579	**0.1199**	-0.0141	1.6027	1.1392	**2.3558**	-0.2770
H	0.0870	0.0548	**0.1183**	-0.0105	1.4339	0.9054	**1.9530**	-0.1731
Cl	0.0873	0.0531	**0.1142**	-0.0078	1.1757	0.7151	**1.5370**	-0.1059
Br	0.0875	0.0516	**0.1117**	-0.0067	1.1371	0.6703	**1.4510**	-0.0878
COOH	0.0518	0.1017	**0.1075**	0.0128	0.5376	1.0559	**1.1162**	0.1328
CN	0.0927	0.0437	**0.0930**	0.0062	0.9007	0.4254	**0.9041**	0.0611
NO_2	**0.1028**	0.0202	0.0645	0.0252	**0.8108**	0.1597	0.5087	0.1990

[a] condensed radical Fukui function,
[b] local softness.