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

Supporting Information

Photoinduced oxidation of an indole derivative: 2-(1’H-indol-2’-yl)-[1,5]naphthyridine

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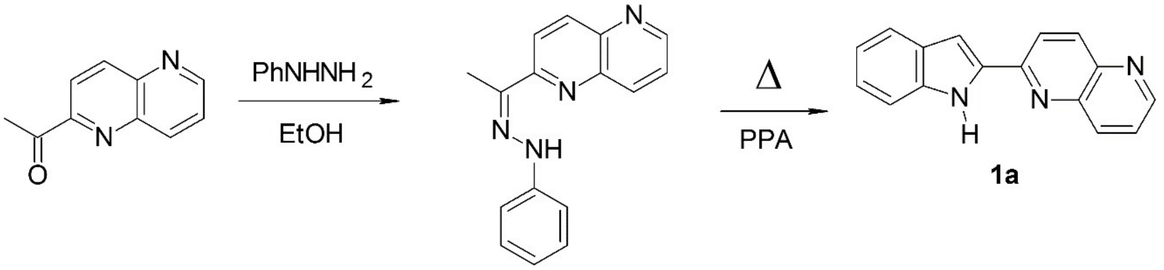


Scheme S1. Preparation of 2-(1’H-indol-2’-yl)-[1,8]naphthyridine (1,5-IN).

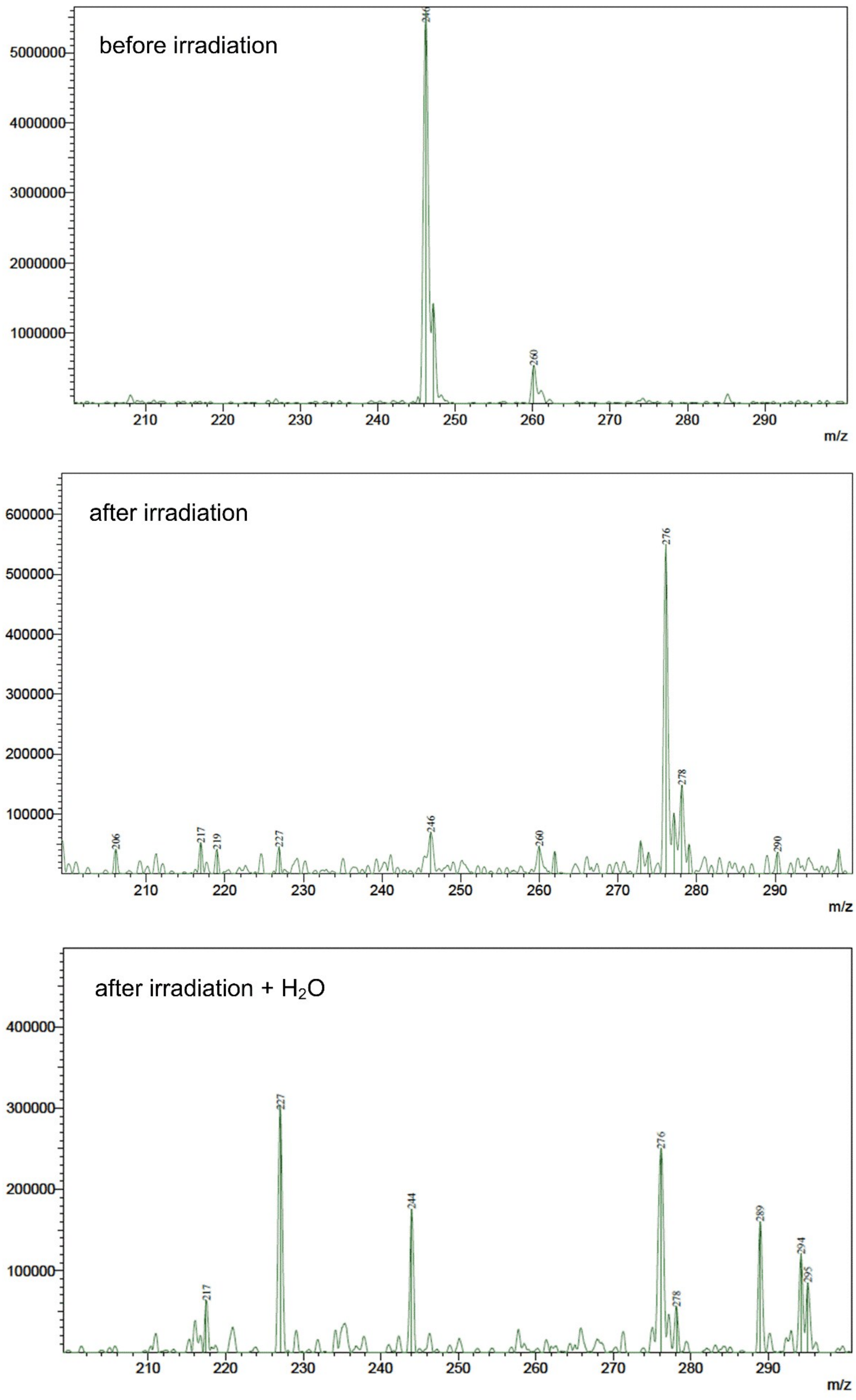


Figure S1(a). The ESI-MS (positive ion mode) spectra of **1** in acetonitrile recorded for the sample before and after 180 min of 365 nm irradiation.

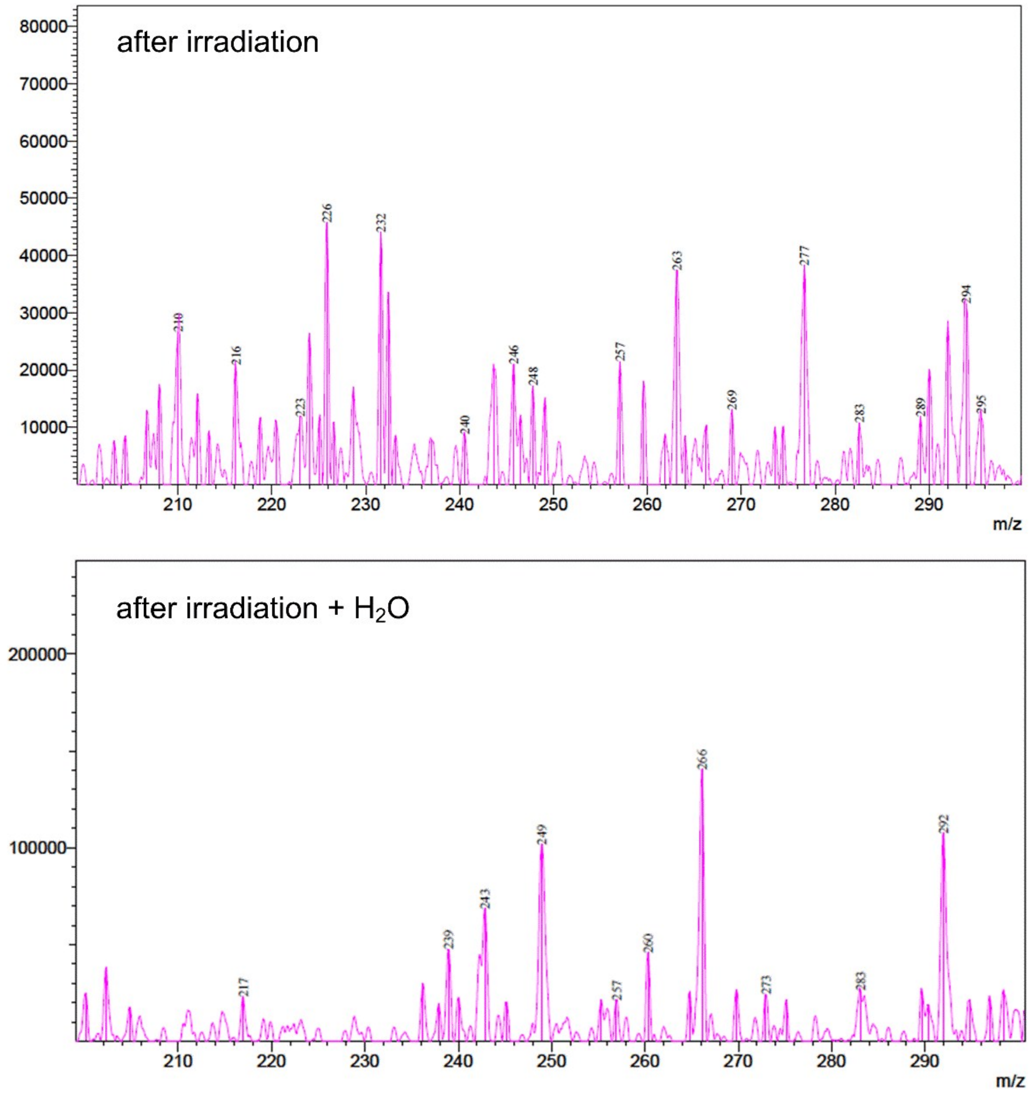


Figure S1(b). The ESI-MS (negative ion mode) spectra of **1** in acetonitrile recorded for the sample before and after 180 min of 365 nm irradiation.

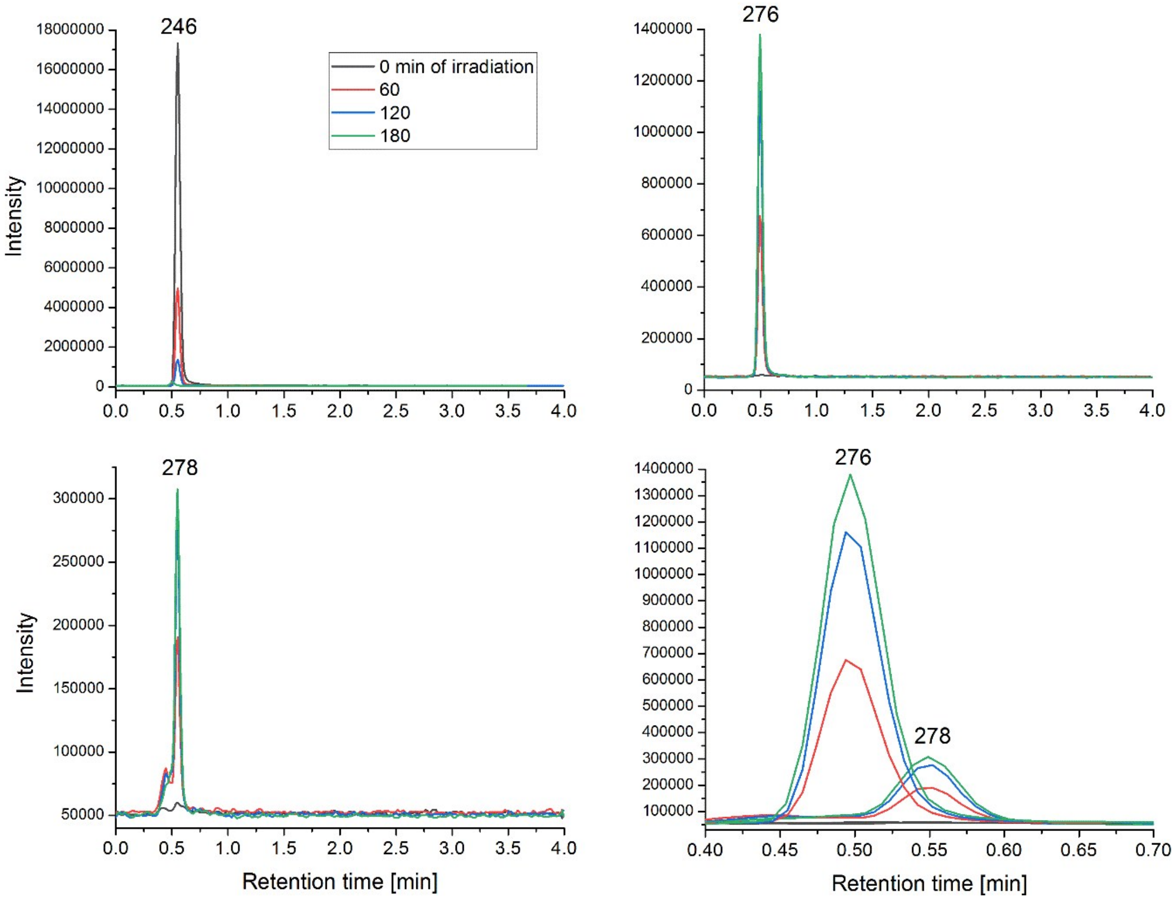
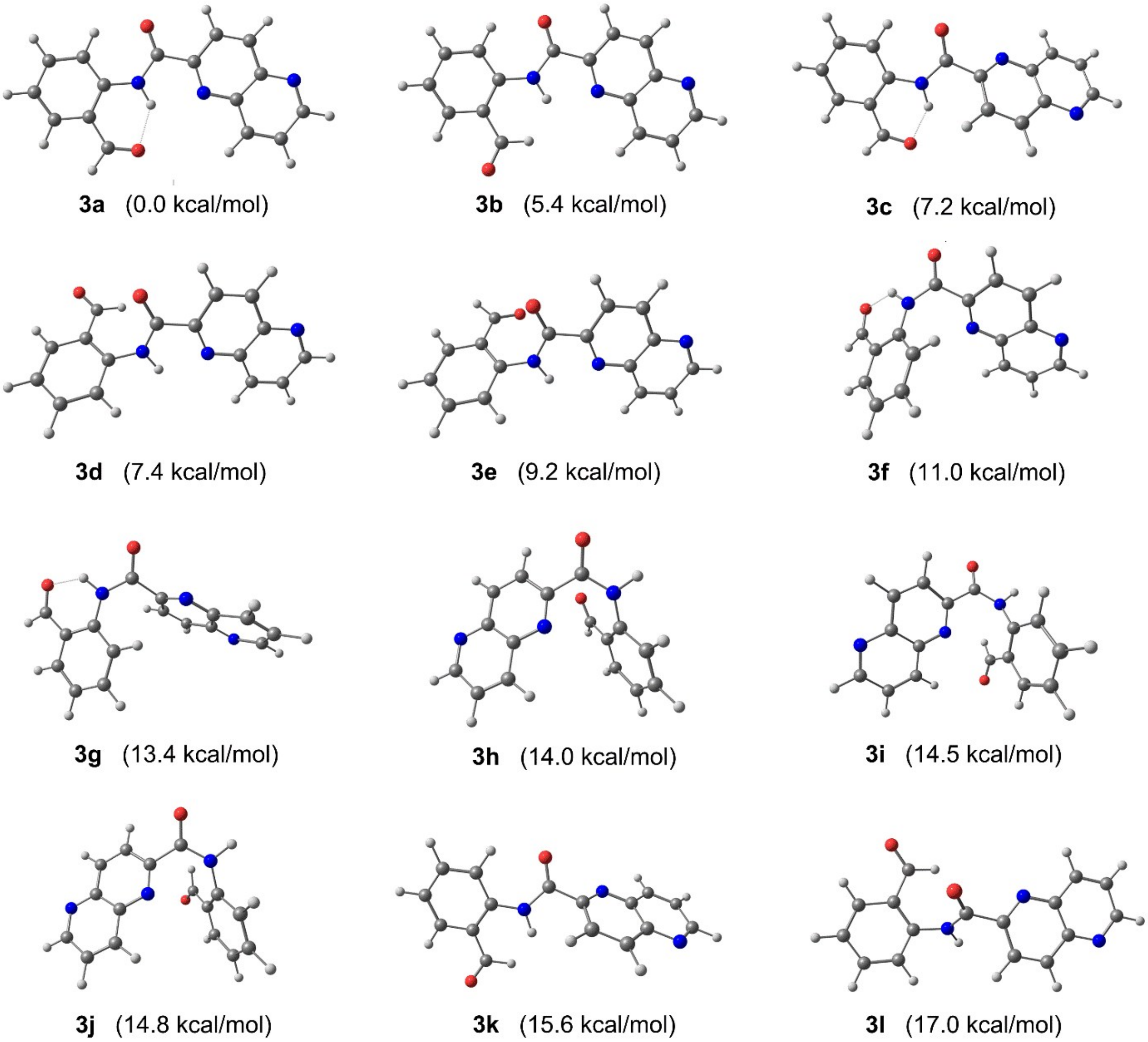


Figure S2. Chromatograms of the positive molecular ions with the m/z equal to 246, 276, and 278 determined for the acetonitrile solution of **1** before and after 0, 120, and 180 min of 365 nm irradiation.



3a (0.0 kcal/mol)

3b (5.4 kcal/mol)

3c (7.2 kcal/mol)

3d (7.4 kcal/mol)

3e (9.2 kcal/mol)

3f (11.0 kcal/mol)

3g (13.4 kcal/mol)

3h (14.0 kcal/mol)

3i (14.5 kcal/mol)

3j (14.8 kcal/mol)

3k (15.6 kcal/mol)

3l (17.0 kcal/mol)

Figure S3. The predicted rotameric structures of **3** with their zero-point corrected relative energies.

Table **S1**. Changes in peak intensity area determined for the positive molecular ions $[M + H]^+$ with m/z equal to 246, 276, and 278 under 180 min of 365 nm irradiation of **1**.

Irradiation time (min)	246 (RT = 0.551)	276 (RT = 0.497)	278 (RT = 0.549)
0	50881811	-	-
	50731629	-	-
60	13781565	1888976	464700
	13226932	1873970	413864
120	3846179	3279823	769163
	3849012	3377147	753515
180	599370	4168758	1027555
	585887	4177554	982295

Table S2. TD-DFT/B3LYP/6-31+G(d,p) calculated energies ($\tilde{\nu}$, cm^{-1}) and oscillator strengths (*f*) corresponding to the vertical transitions to low-lying electronic states (S_1-S_{15}) of **1a**, **1b**, **2a**, **2b**, **3a**, and **3b** structures.

State	**1a**		**1b**		**2a**		**2b**		**3a**		**3b**	
	$\tilde{\nu}$	*f*	$\tilde{\nu}$	*f*	$\tilde{\nu}$	*f*	$\tilde{\nu}$	*f*	$\tilde{\nu}$	*f*	$\tilde{\nu}$	*f*
S_1	25471	0.3055	24522	0.1978	27532	0.0001	27202	0.0000	28071	0.0000	27023	0.1063
S_2	27633	0.1723	28412	0.1314	30053	0.6521	29818	0.5420	28123	0.1695	28547	0.0000
S_3	30140	0.0000	29272	0.0000	33316	0.0465	32994	0.0216	30045	0.0000	29063	0.0001
S_4	31245	0.2637	31444	0.5593	34243	0.0257	33962	0.0193	30951	0.0546	30694	0.0952
S_5	34251	0.1207	34404	0.0191	34524	0.0012	33987	0.0001	32127	0.0006	31986	0.0005
S_6	36526	0.1667	36380	0.0005	36144	0.0011	35185	0.0006	34116	0.0394	33370	0.0001
S_7	37144	0.0004	36434	0.1354	36538	0.0815	36235	0.1337	34421	0.0000	33554	0.0253
S_8	38082	0.0418	37685	0.0000	37049	0.0478	36964	0.0311	36004	0.1115	34431	0.0131
S_9	38485	0.0156	37809	0.0304	37113	0.0001	37111	0.0027	36402	0.0000	35386	0.2502
S_{10}	39632	0.0035	38235	0.0489	37597	0.0747	37852	0.1901	36609	0.1060	36118	0.0000
S_{11}	39981	0.0244	38716	0.0034	38132	0.0008	38010	0.0002	37225	0.1028	36907	0.0755
S_{12}	40952	0.0012	39752	0.0088	38320	0.0000	38724	0.0004	37284	0.0004	38130	0.0004
S_{13}	41220	0.0487	41504	0.0241	39733	0.0000	40053	0.0000	38377	0.0010	39040	0.1772
S_{14}	41722	0.0163	41578	0.0000	40987	0.0000	40627	0.0821	38811	0.0191	39448	0.0008
S_{15}	43048	0.0132	41682	0.0012	42330	0.1566	41495	0.0001	39379	0.0525	40570	0.0014

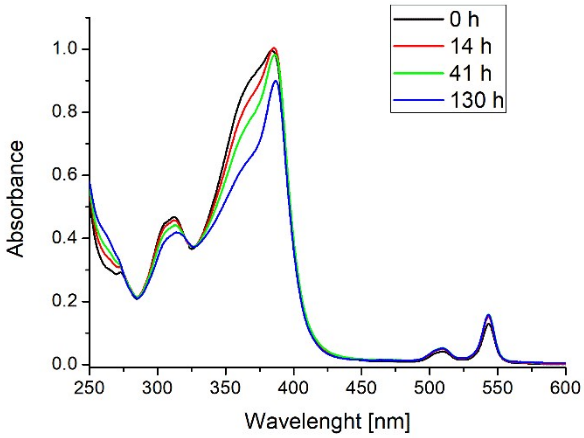


Figure S4. Changes in absorption upon 543 nm irradiation of mixture of **1** and **PdOEP** in acetonitrile.

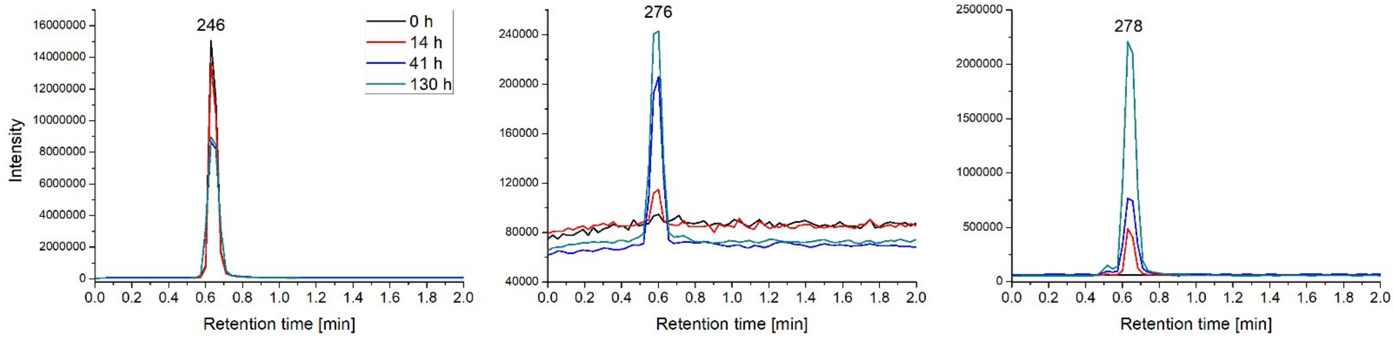


Figure S5. Chromatograms of the positive molecular ions with the m/z equal 246, 276 and 278 determined in the acetonitrile mixture solution of **1** and **PdOEP** before and after 0, 14, 41 and 130 h of 543 nm irradiation.