

Supplementary materials

Synthesis, Characterization and Photodynamic Activity Against Bladder Cancer Cells of Novel Triazole-Porphyrin Derivatives

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1. Photophysical characterization of TZ-POR 7a-f and formulations PVP-TZ-POR 7a-f

Table S1. Photophysical data of TZ-POR 7a-f and formulations PVP-TZ-POR 7a-f.

TZ-POR	λ_{\max} (nm) (log ϵ) ^a	λ_{em} (nm) ^a	Stokes shift (nm) ^a	ϕ_f^b	PVP-TZ-POR	λ_{\max} (nm) (log ϵ) ^a	λ_{em} (nm) ^a	Stokes shift (nm) ^a	ϕ_f^b
	424 (5.31)					424 (5.22)			
	522 (4.23)					521 (4.16)			
7a	561 (3.99)	659, 728	5	0.14	7a	560 (3.90)	659, 726	6	0.10
	599 (3.84)					598 (3.72)			
	654 (3.59)					653 (3.45)			
	424 (5.11)					424 (5.31)			
	521 (4.03)					521 (4.27)			
7b	560 (3.77)	659, 727	5	0.08	7b	560 (4.00)	659, 726	6	0.07
	598 (3.58)					598 (3.82)			
	654 (3.29)					653 (3.54)			
	423 (5.99)					422 (5.65)			
	521 (3.96)					521 (4.59)			
7c	561 (3.72)	660, 727	6	0.09	7c	560 (4.37)	657, 726	5	0.11
	598 (3.53)					598 (4.21)			
	654 (3.26)					652 (4.04)			
	423 (5.64)					423 (5.12)			
	521 (4.54)					521 (4.04)			
7d	560 (4.26)	659, 726	5	0.13	7d	559 (3.78)	659, 727	6	0.09
	598 (4.09)					598 (3.61)			
	654 (3.82)					653 (3.37)			
	423 (5.21)					423 (5.12)			
	521 (4.12)					521 (4.09)			
7e	560 (3.84)	659, 727	6	0.09	7e	559 (3.82)	659, 729	6	0.04
	598 (3.67)					598 (3.65)			
	653 (3.36)					653 (3.41)			
	423 (5.35)					424 (5.36)			
7f	521 (4.31)	659, 727	5	0.11	7f	521 (4.08)	660, 726	8	0.08
	560 (4.03)					560 (3.80)			

598 (3.86)	598 (3.61)
654 (3.58)	652 (3.28)

^a in DMF/H₂O (9:1)

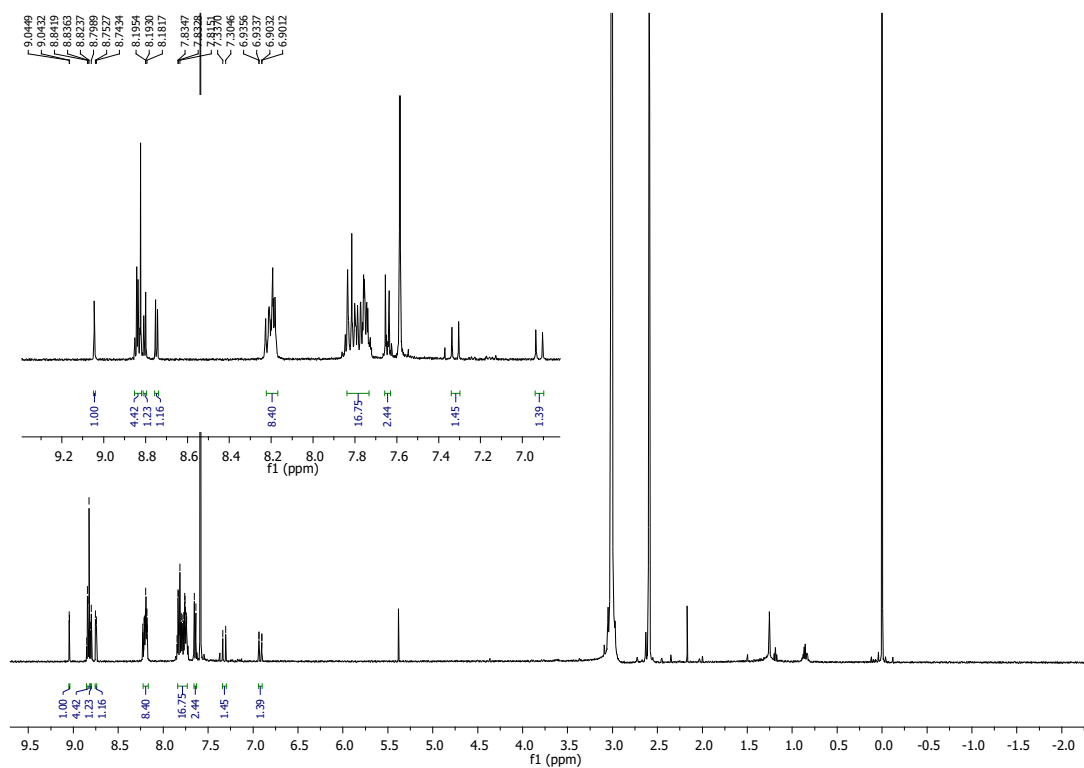
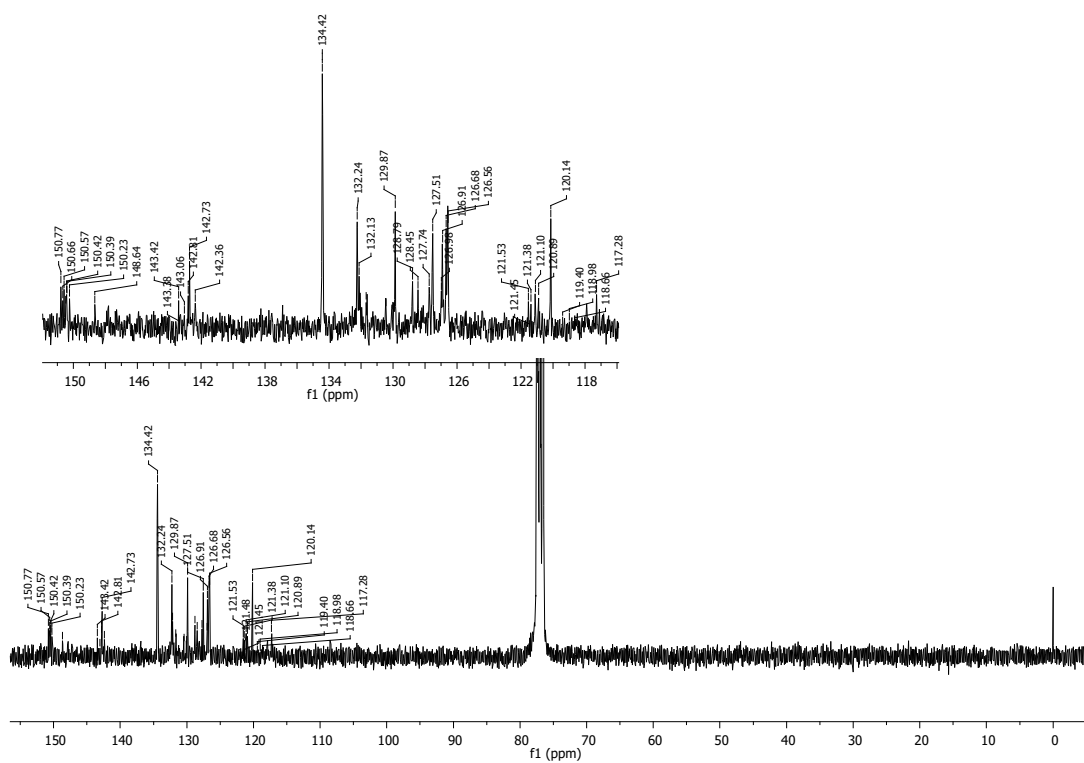
^b TPP in DMF as reference ($\phi_F = 0.12$)

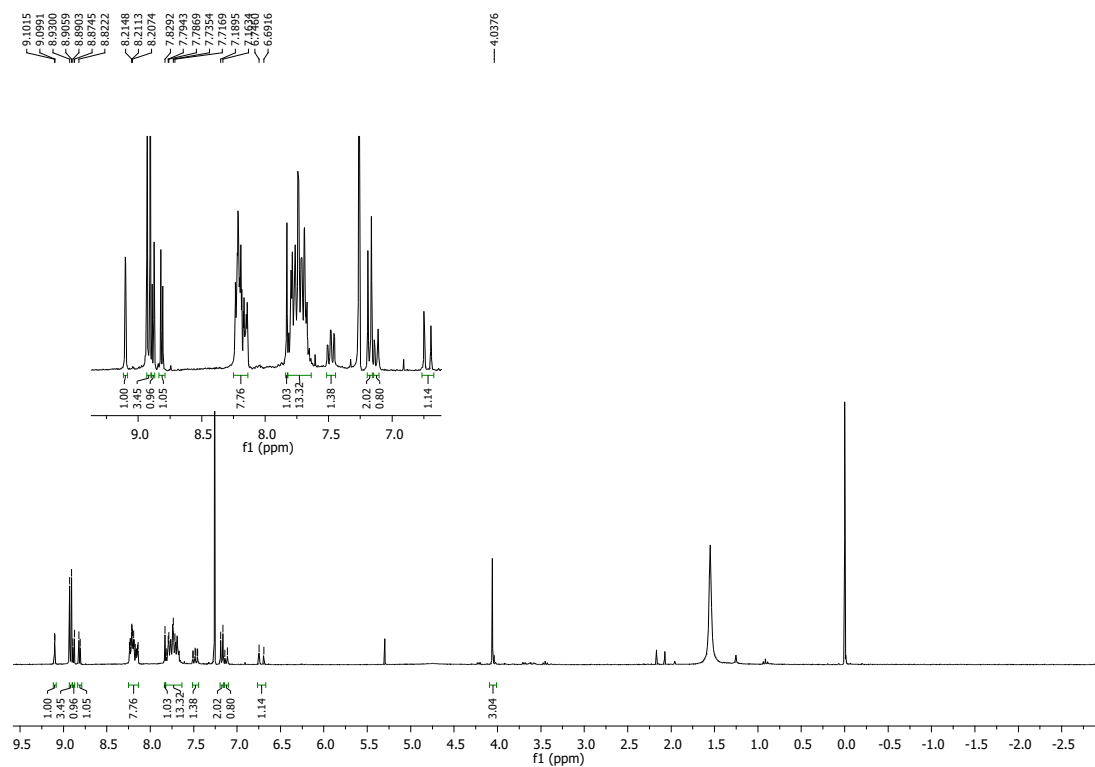
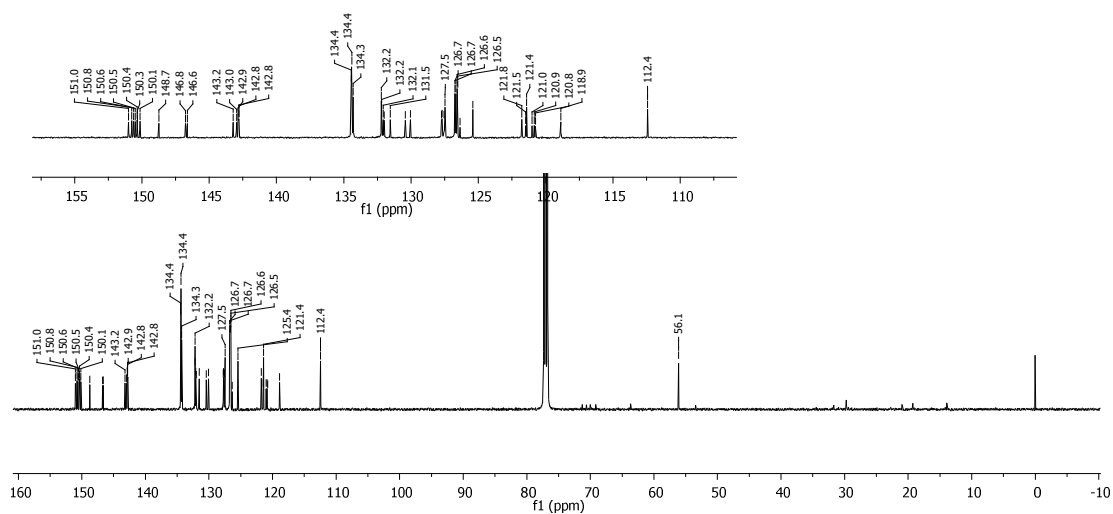
2. Photostability Studies of Formulations PVP-TZ-POR 7a–f

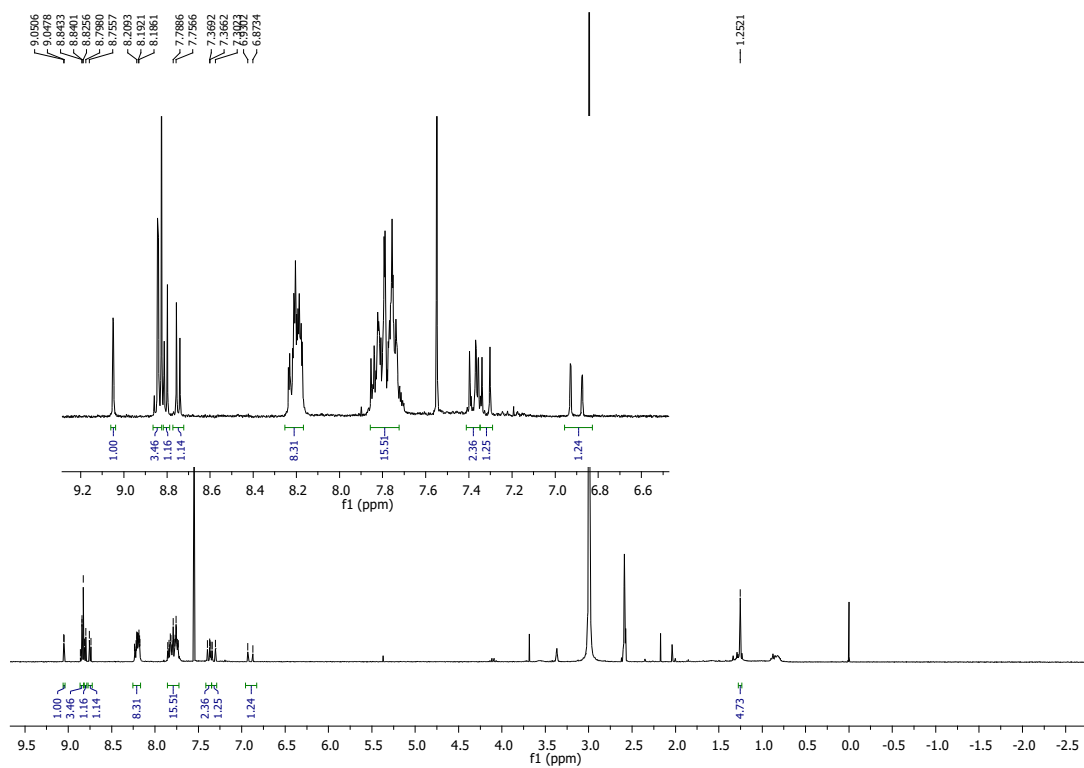
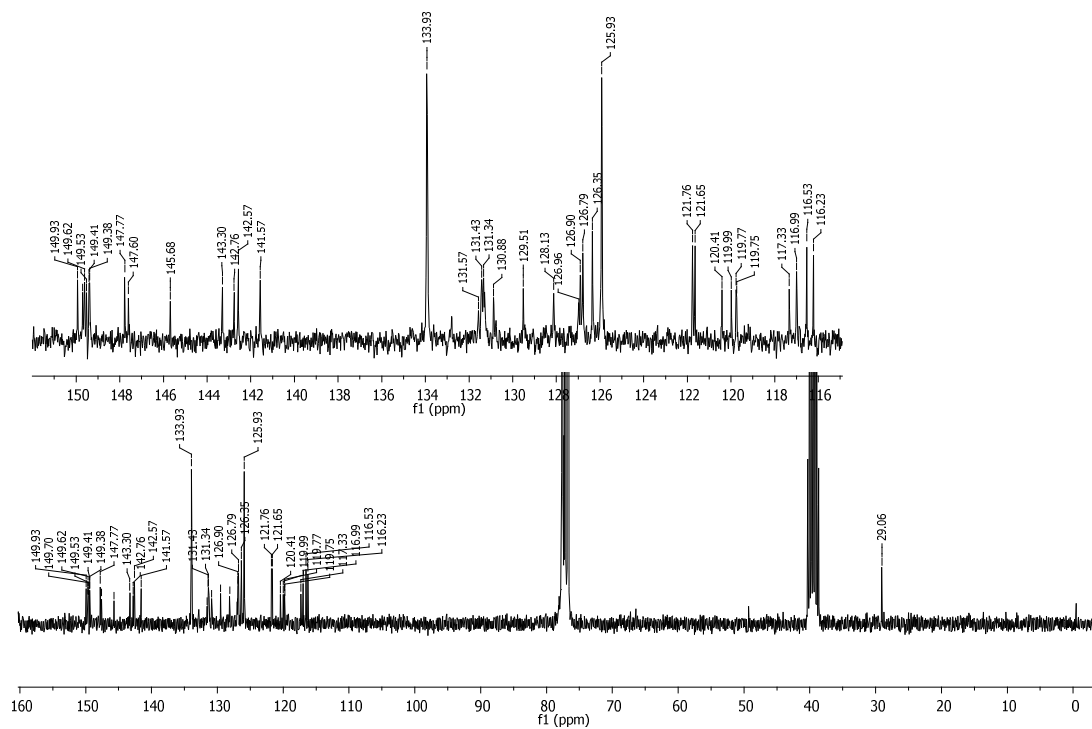
Table S2. Photostability of 10 μ M of PVP-TZ-POR 7a–f, after irradiation with white light at a fluence rate of 20 mW.cm⁻² for different periods of time (0–60 min).*

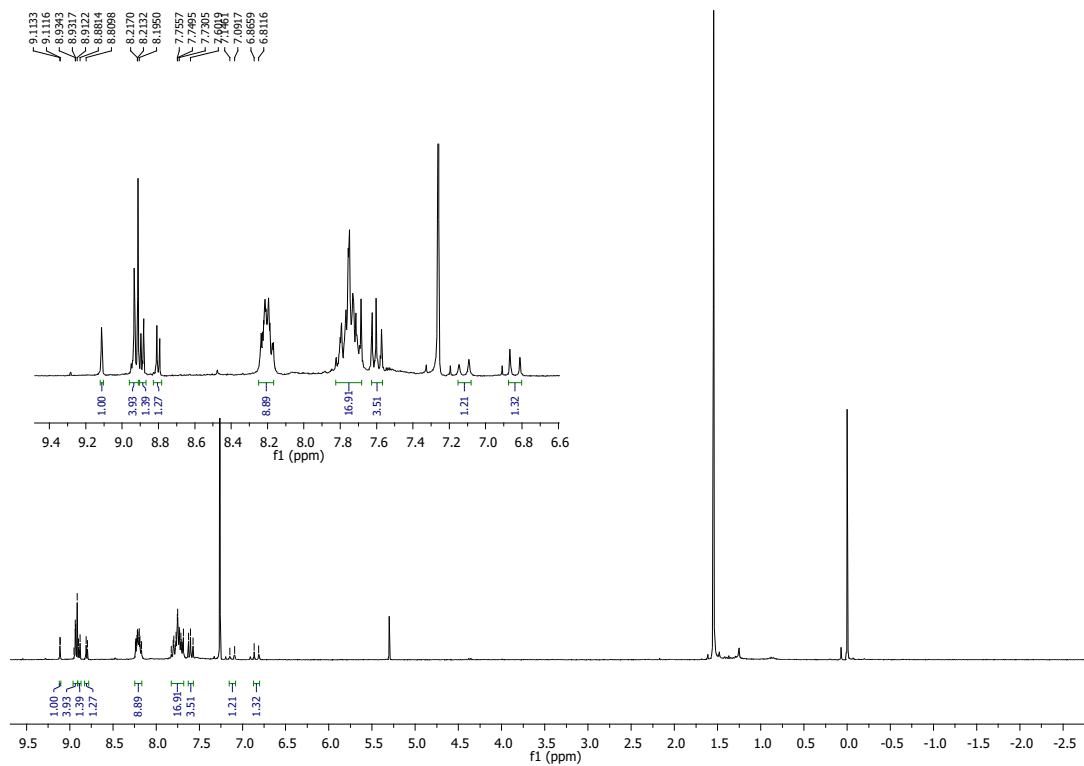
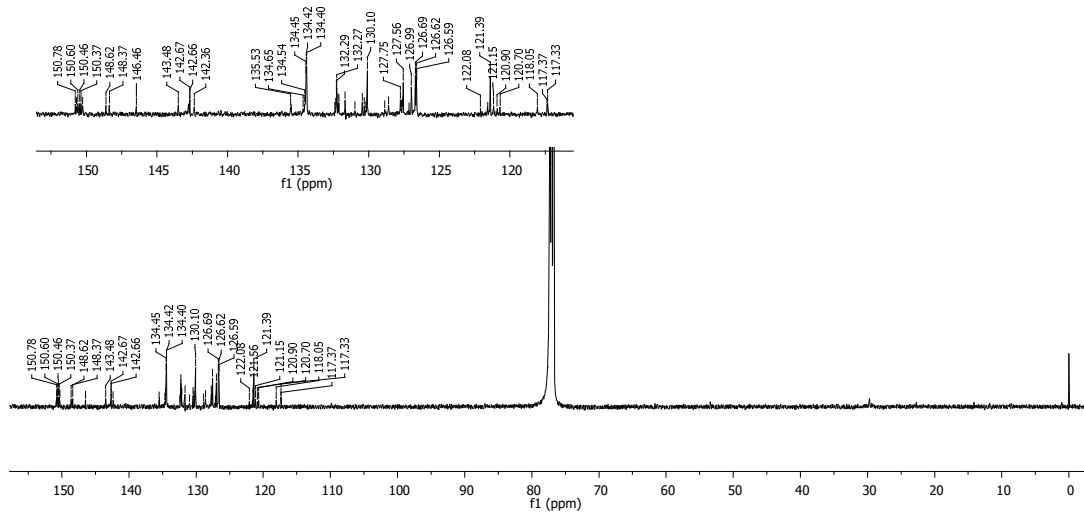
PS	λ (nm)	Irradiation Time (min)							
		0	10	20	30	40	50	60	
PVP-TZ-POR 7a	420	100	96	94	93	92	90	89	
PVP-TZ-POR 7b	420	100	97	95	93	92	90	89	
PVP-TZ-POR 7c	420	100	96	94	92	91	89	88	
PVP-TZ-POR 7d	420	100	96	94	93	91	90	91	
PVP-TZ-POR 7e	420	100	98	96	95	94	94	94	
PVP-TZ-POR 7f	420	100	95	94	93	91	91	91	
PVP-TPP	420	100	98	97	97	96	95	95	

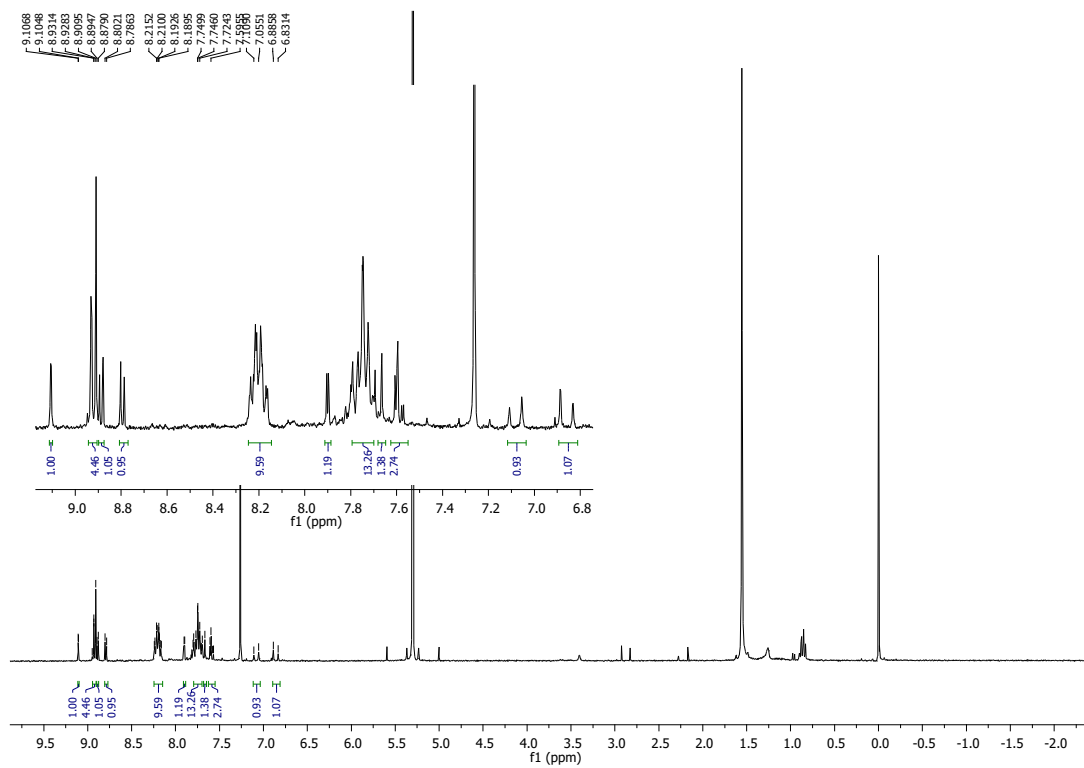
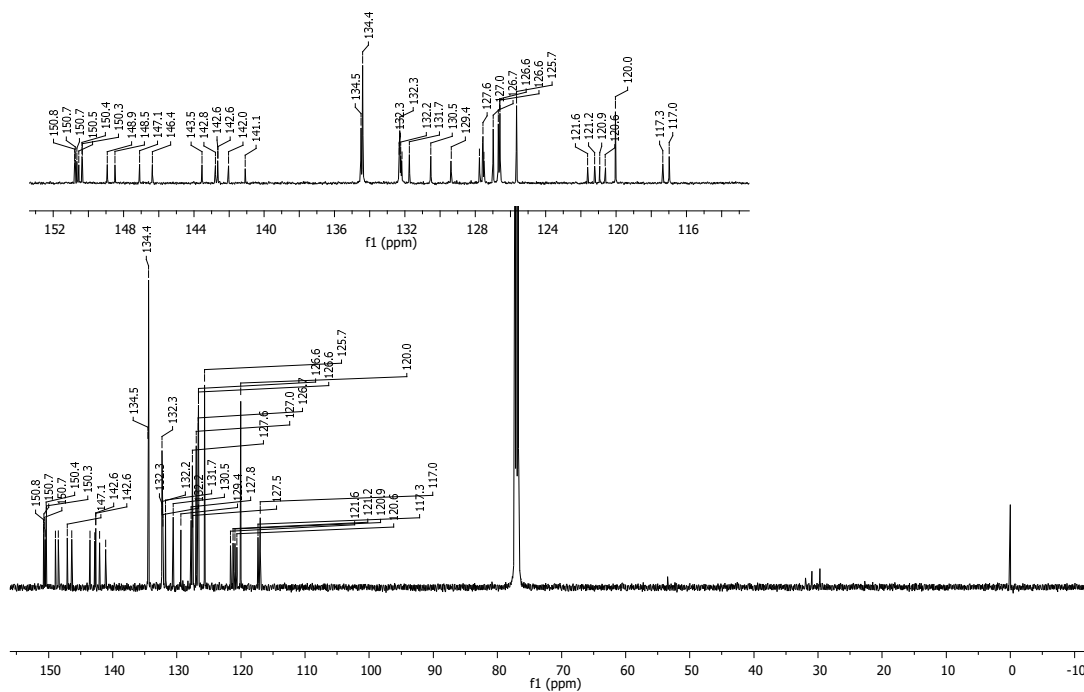
*The results are presented in percentage calculated by the ratio of residual absorbance at 420 nm at different periods of time and absorbance before irradiation.

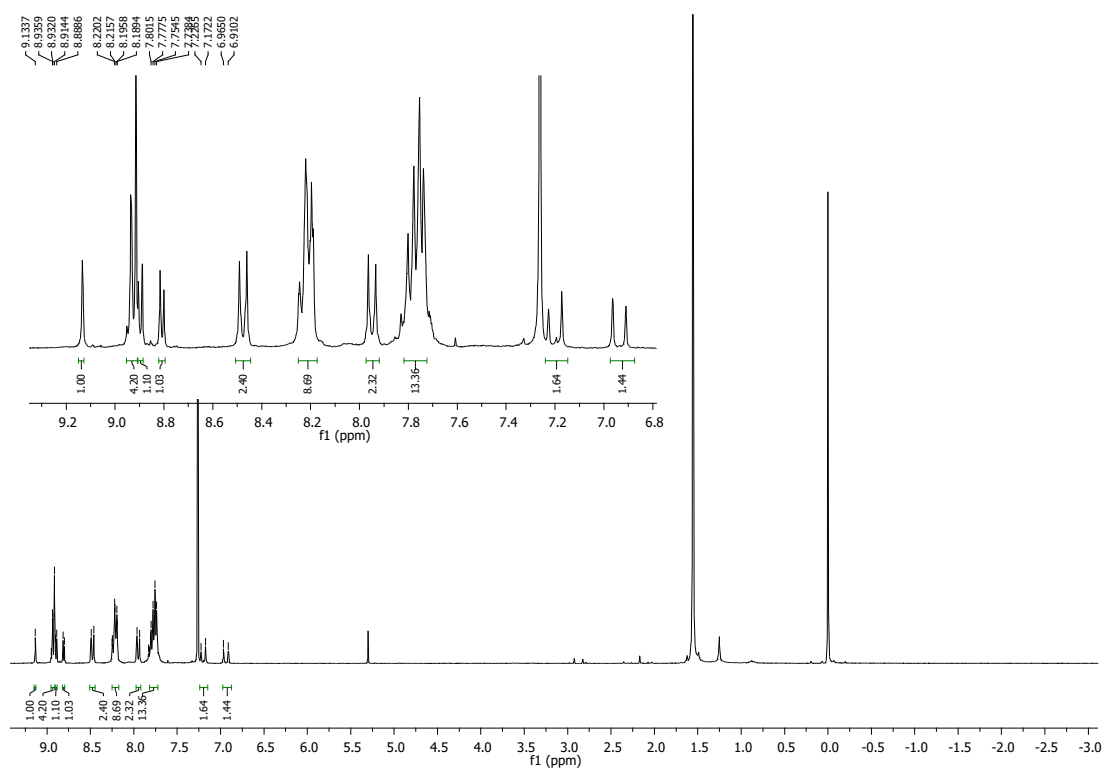
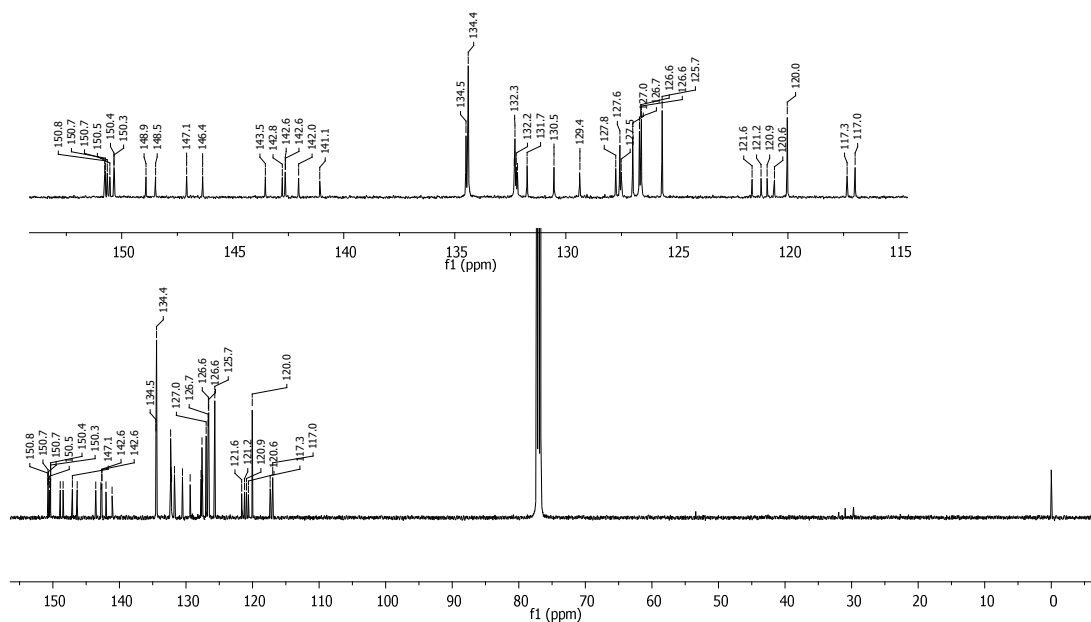
3. ^1H and ^{13}C NMR and HRMS spectra of TZ-POR 6a–f and 7a–fFigure S1. ^1H NMR of TZ-POR 6a in CDCl_3 .Figure S2. ^{13}C NMR of TZ-POR 6a in CDCl_3 .

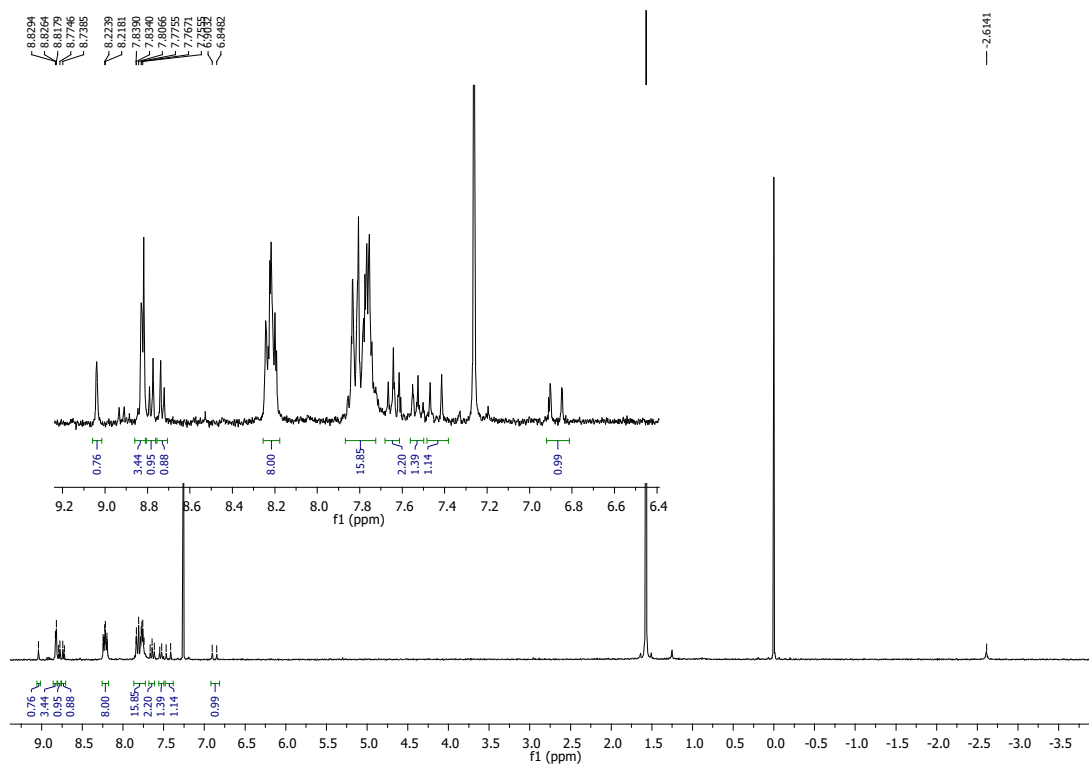
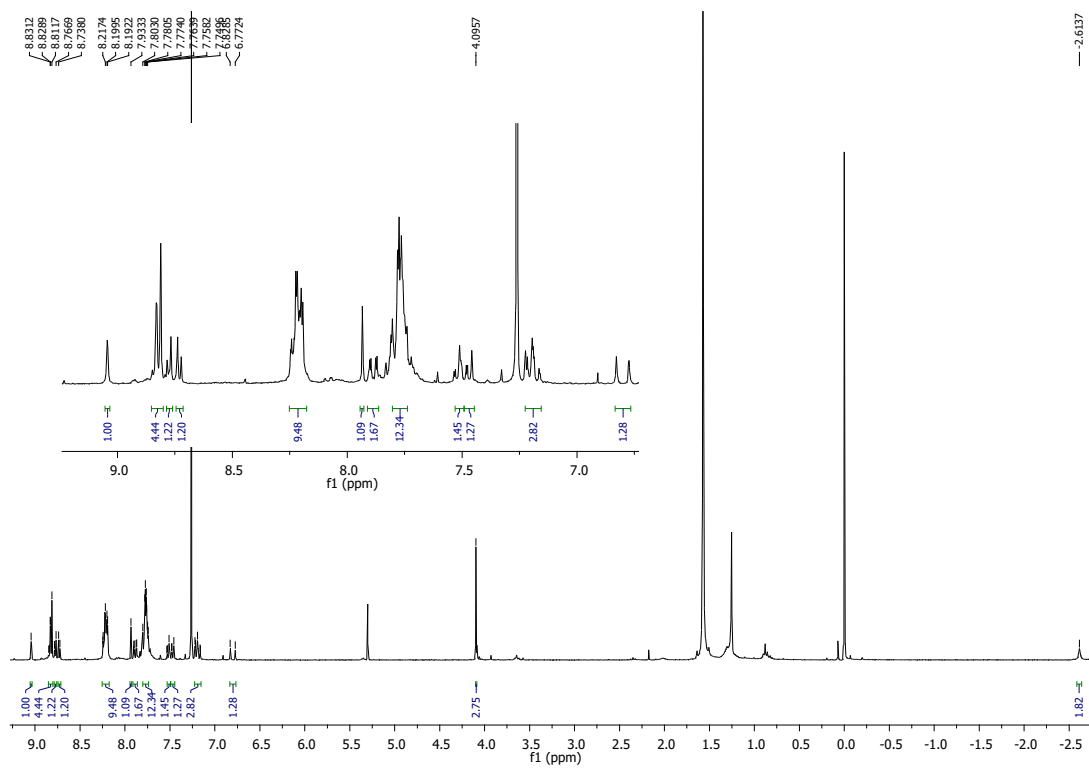
Figure S3. ^1H NMR of TZ-POR **6b** in CDCl_3 .Figure S4. ^{13}C NMR of TZ-POR **6b** in CDCl_3 .

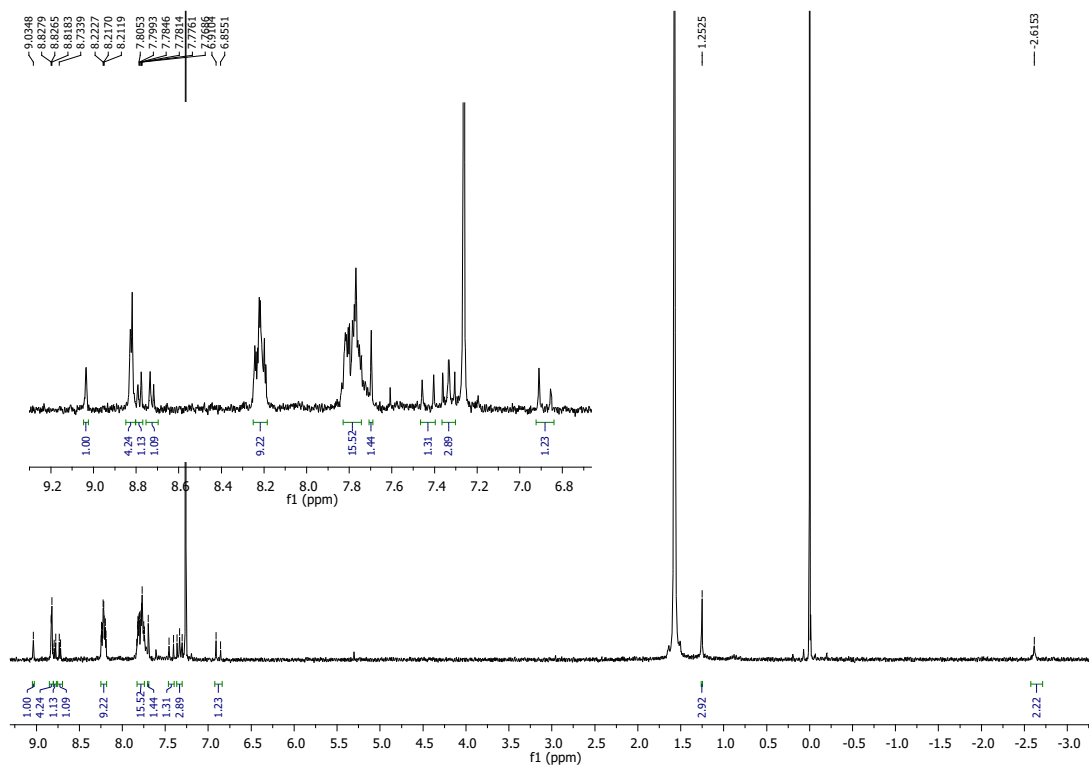
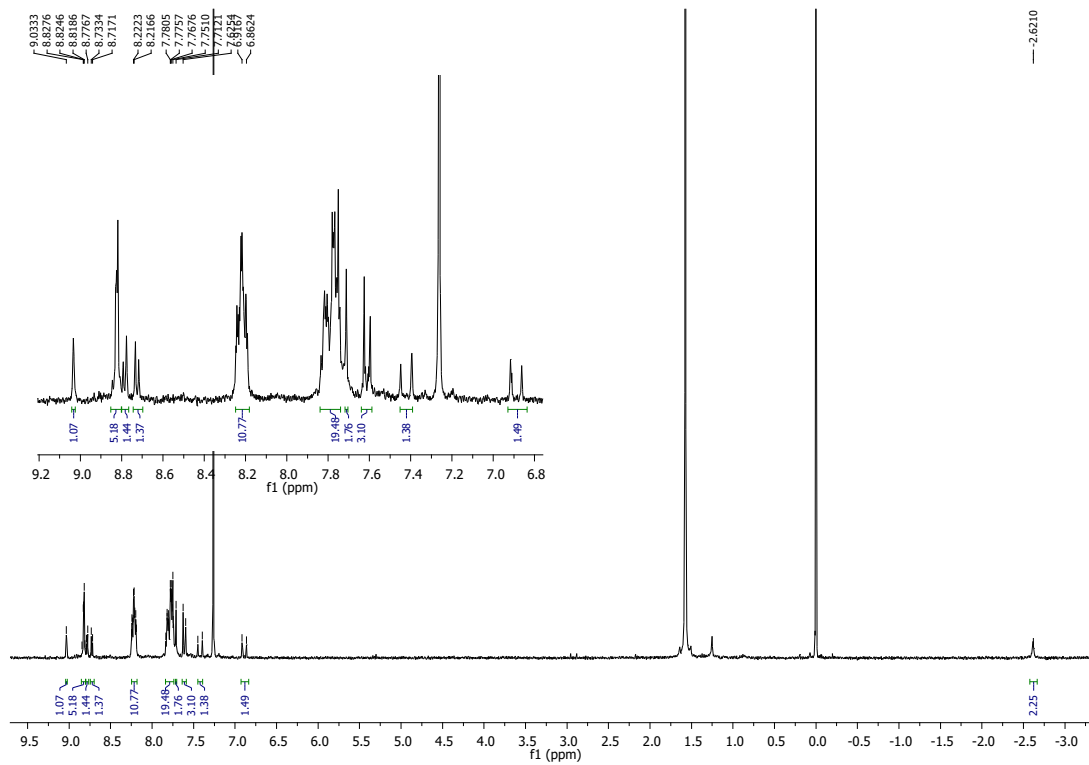
Figure S5. ^1H NMR of TZ-POR 6c in CDCl_3 .Figure S6. ^{13}C NMR of TZ-POR 6c in CDCl_3 and DMSO-d_6 .

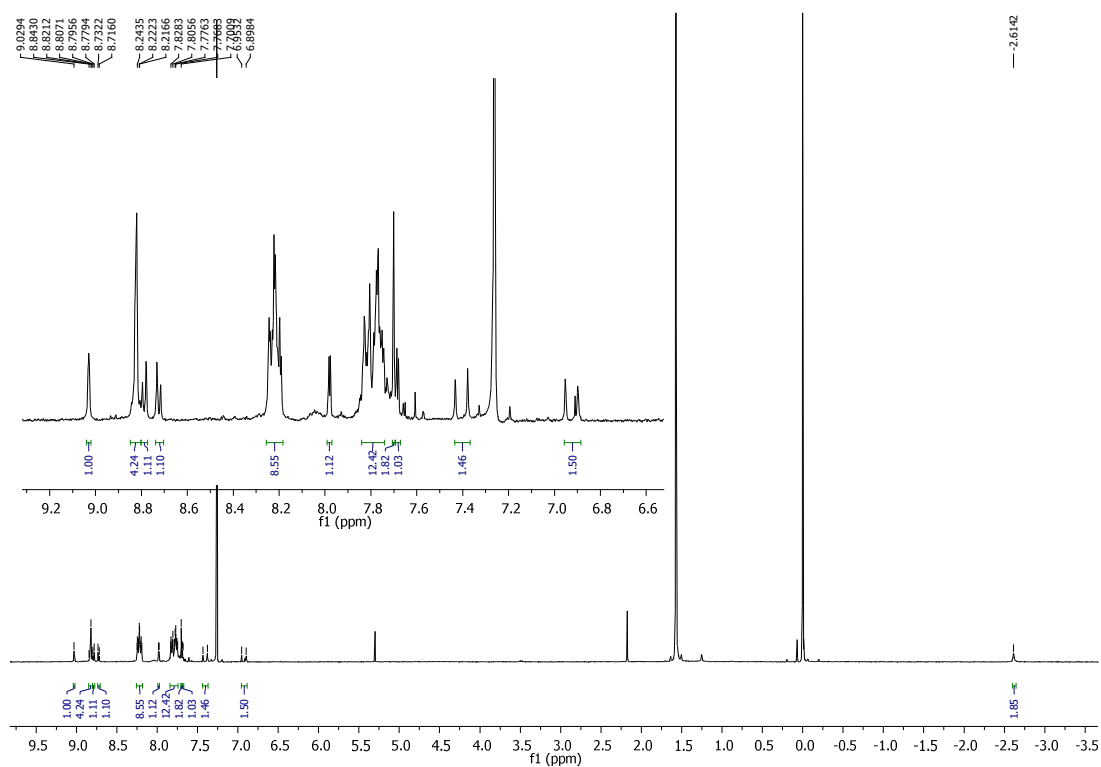
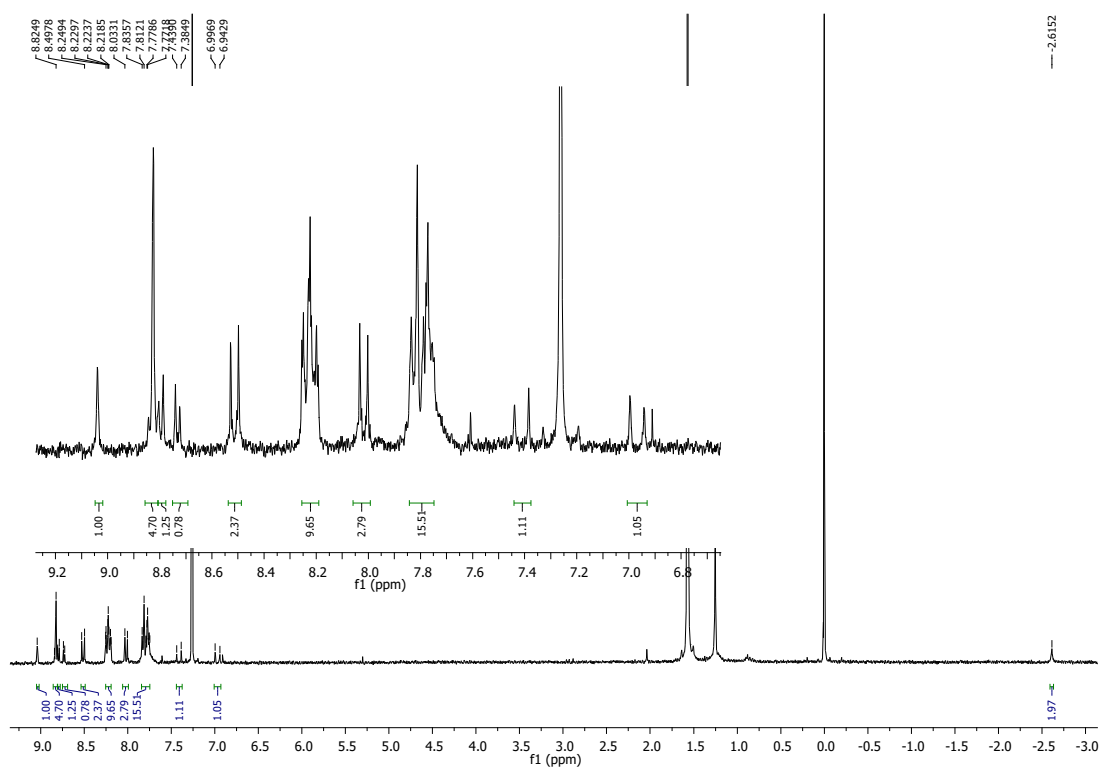
Figure S7. ¹H NMR of TZ-POR 6d in CDCl₃.Figure S8. ¹³C NMR of TZ-POR 6d in CDCl₃.

Figure S9. ¹H NMR of TZ-POR 6e in CDCl₃.Figure S10. ¹³C NMR of TZ-POR 6e in CDCl₃.

Figure S11. ^1H NMR of TZ-POR 6f in CDCl_3 .Figure S12. ^{13}C NMR of TZ-POR 6f in CDCl_3 .

Figure S13. ¹H NMR of TZ-POR 7a in CDCl₃.Figure S14. ¹H NMR of TZ-POR 7b in CDCl₃.

Figure S15. ¹H NMR of TZ-POR 7c in CDCl₃.Figure S16. ¹H NMR of TZ-POR 7d in CDCl₃.

Figure S17. ¹H NMR of TZ-POR 7e in CDCl₃.Figure S18. ¹H NMR of TZ-POR 7f in CDCl₃.

3. Cellular Uptake of PVP-TZ-POR 7a,c,d,f and PVP-TPP

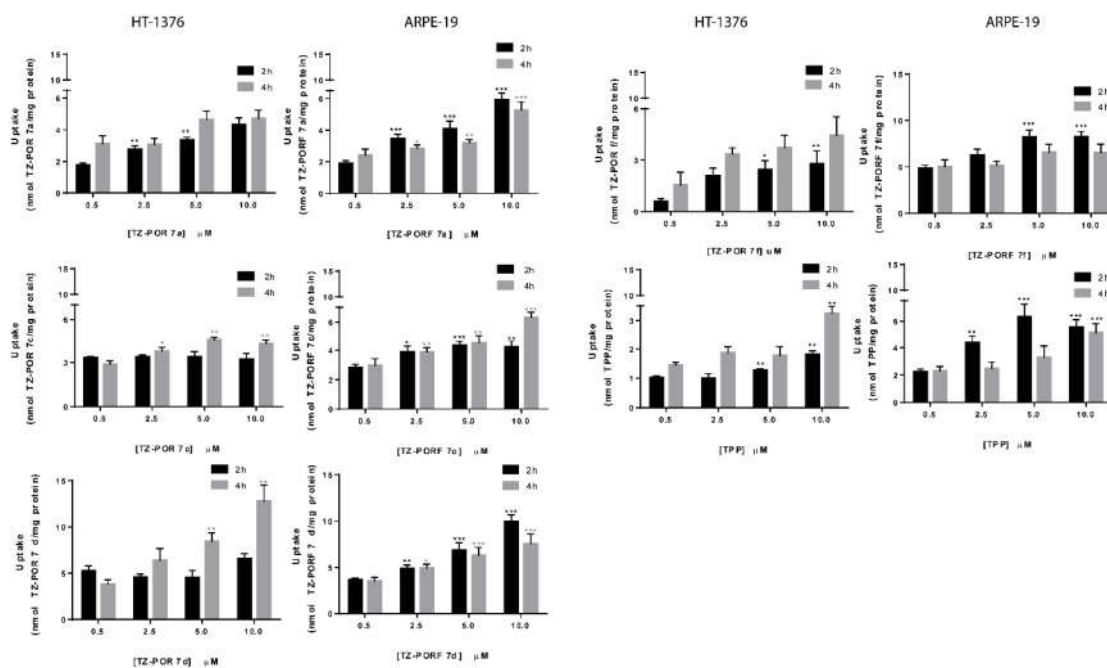


Figure S19. Intracellular uptake of PVP-TZ-POR 7a,c,d,f and PVP-TPP by HT-1376 and ARPE-19 cells. Data are the mean \pm S.D. of at least three independent experiments performed in triplicates. * ($p < 0.05$), ** ($p < 0.01$), *** ($p < 0.001$), significantly different from uptake of PSs.

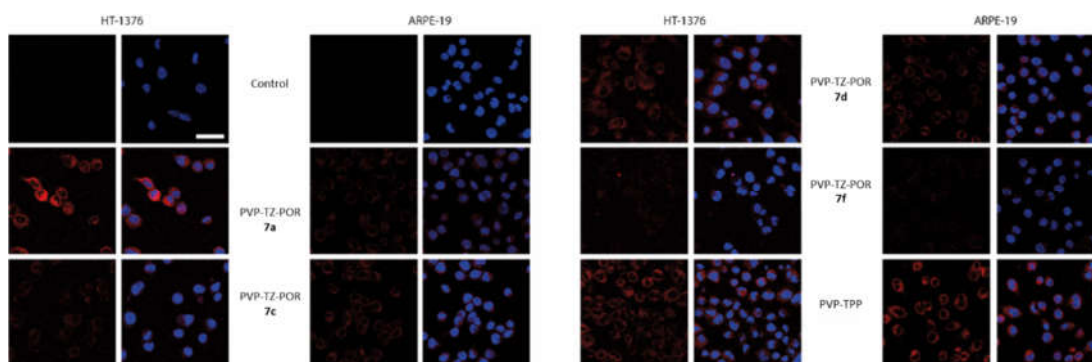


Figure S20. Representative fluorescence images of HT-1376 and ARPE-19 cell lines incubated with 10 μ M of PSs PVP-TZ-POR 7a,c,d,f and PVP-TPP (red) for 4 h in darkness and cell nucleus stained with DAPI (blue). Scale bars 20 μ m.

4. Cell Viability of HT-1376 and ARPE-19 Cells After PDT Treatment with PVP-TZ-POR 7a-d, PVP-TPP and PVP

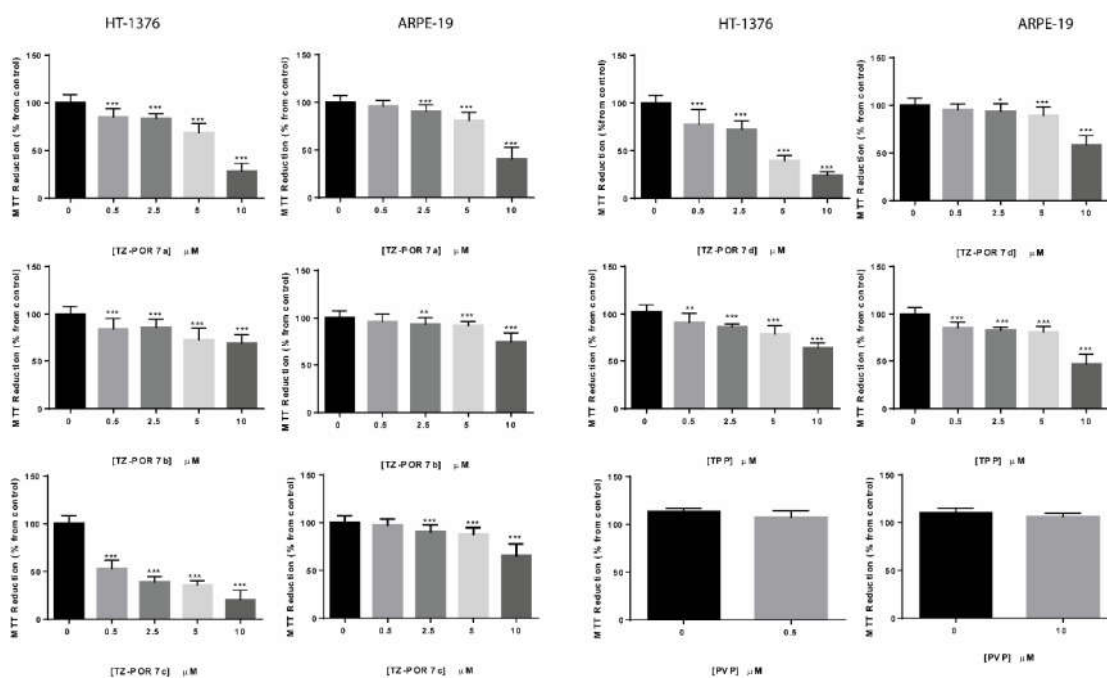


Figure S21. Cell survival of HT-1376 and ARPE-19 cells, incubated in the dark during 4 h with PSs PVP-TZ-POR 7a-d, PVP-TPP and PVP at different concentrations and irradiated with white light for 40 min with an irradiance of 20 mW.cm⁻². Data are the mean value ± S.D. of at least three independent experiments performed in triplicates. *(*p* < 0.05), **(*p* < 0.01), ***(*p* < 0.001), significantly different from MTT reduction (%).

5. Dark toxicity of PVP-TZ-POR 7a-d, PVP-TPP and PVP in HT-1376 and ARPE-19 cells

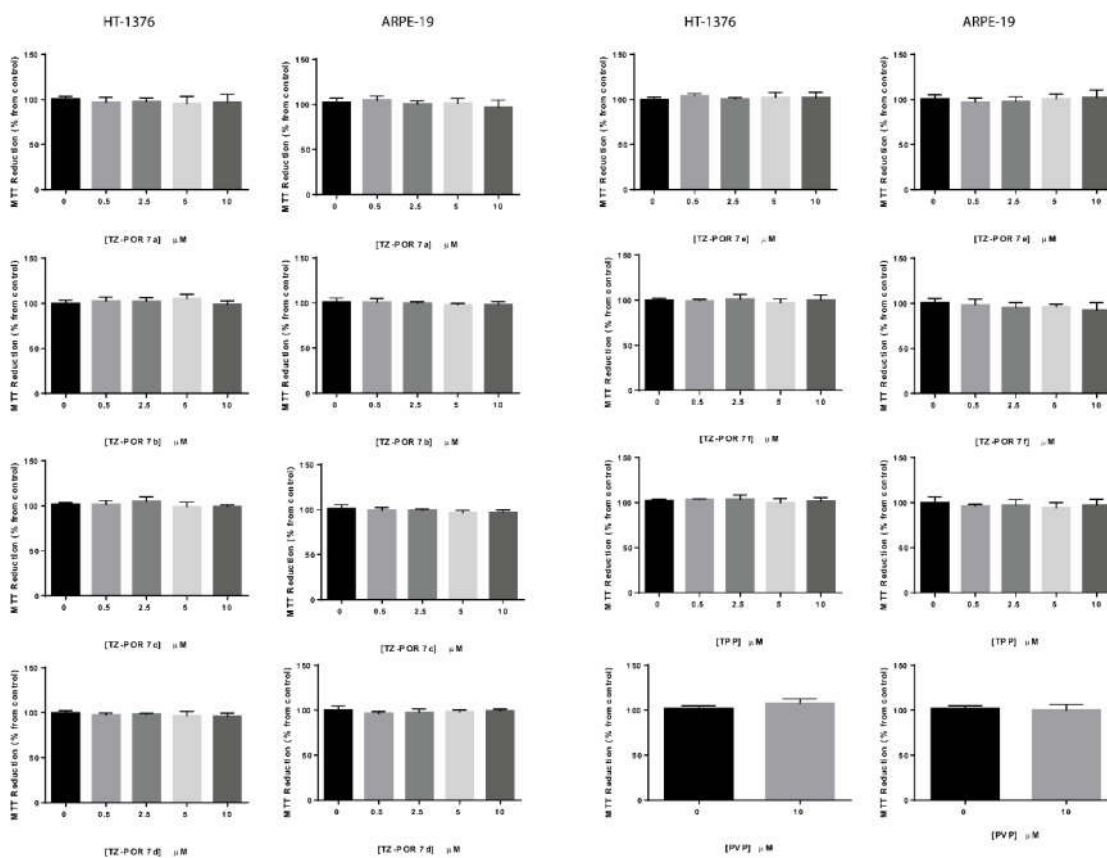


Figure S22. Cell survival of HT-1376 and ARPE-19 cells, incubated in the dark during 4 h with PSs PVP-TZ-POR 7a-f, PVP-TPP and PVP at different concentrations. Data are the mean value \pm S.D. of at least three independent experiments performed in triplicates.