

Supporting Information

For

Two new bulky substituted Zn porphyrins bearing carboxylate anchoring groups as promising dyes for DSSCs

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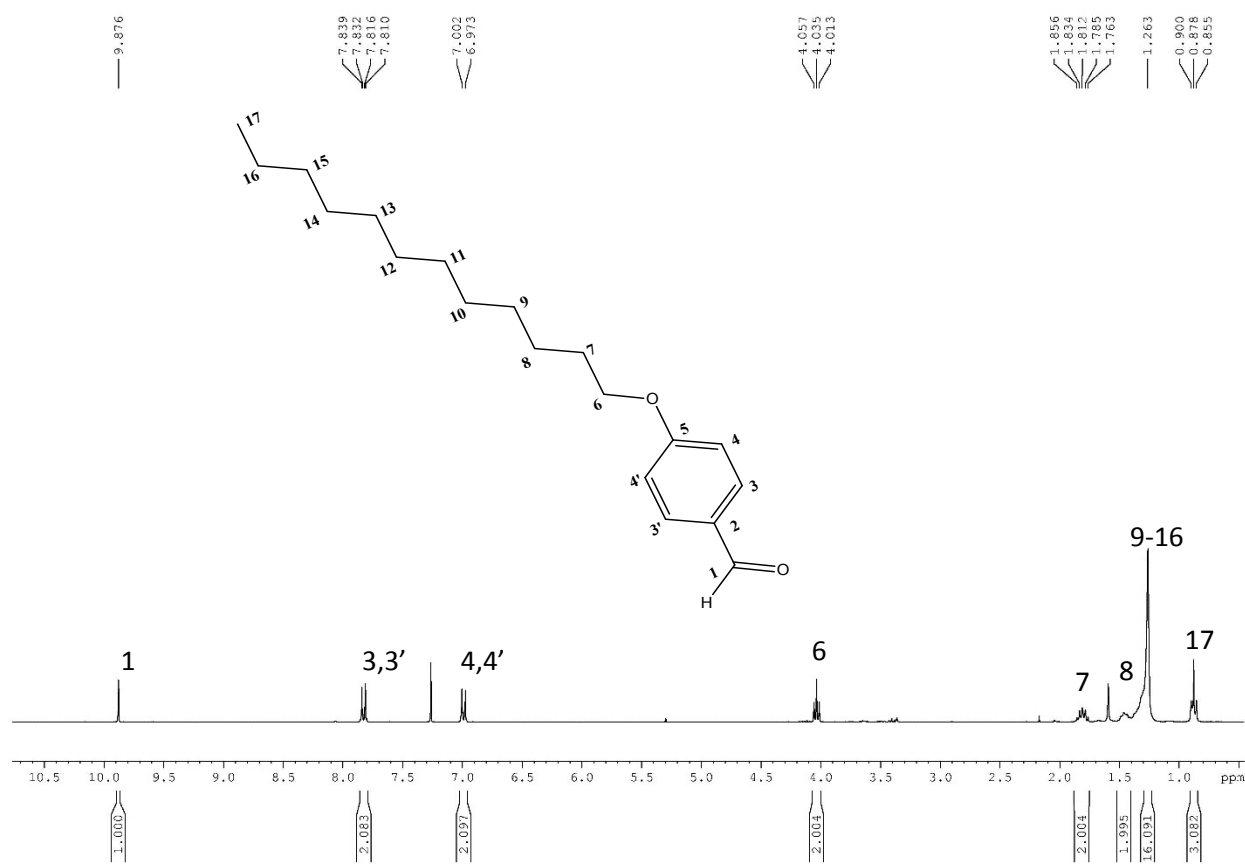


Figure S1. ^1H NMR spectrum of 1 (300MHz, CDCl_3)

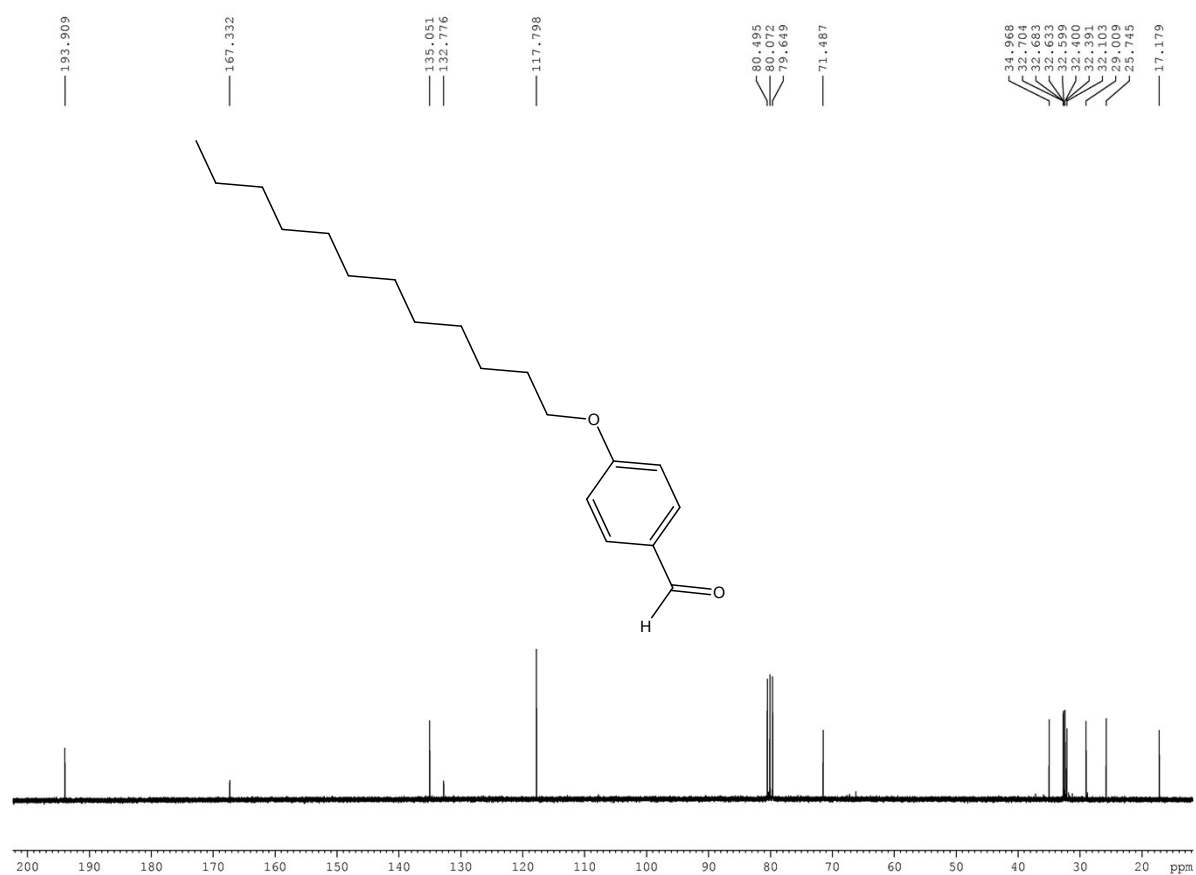
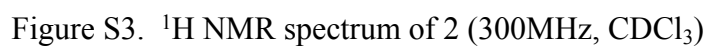


Figure S2. ^{13}C NMR spectrum of 1 (300MHz, CDCl_3)



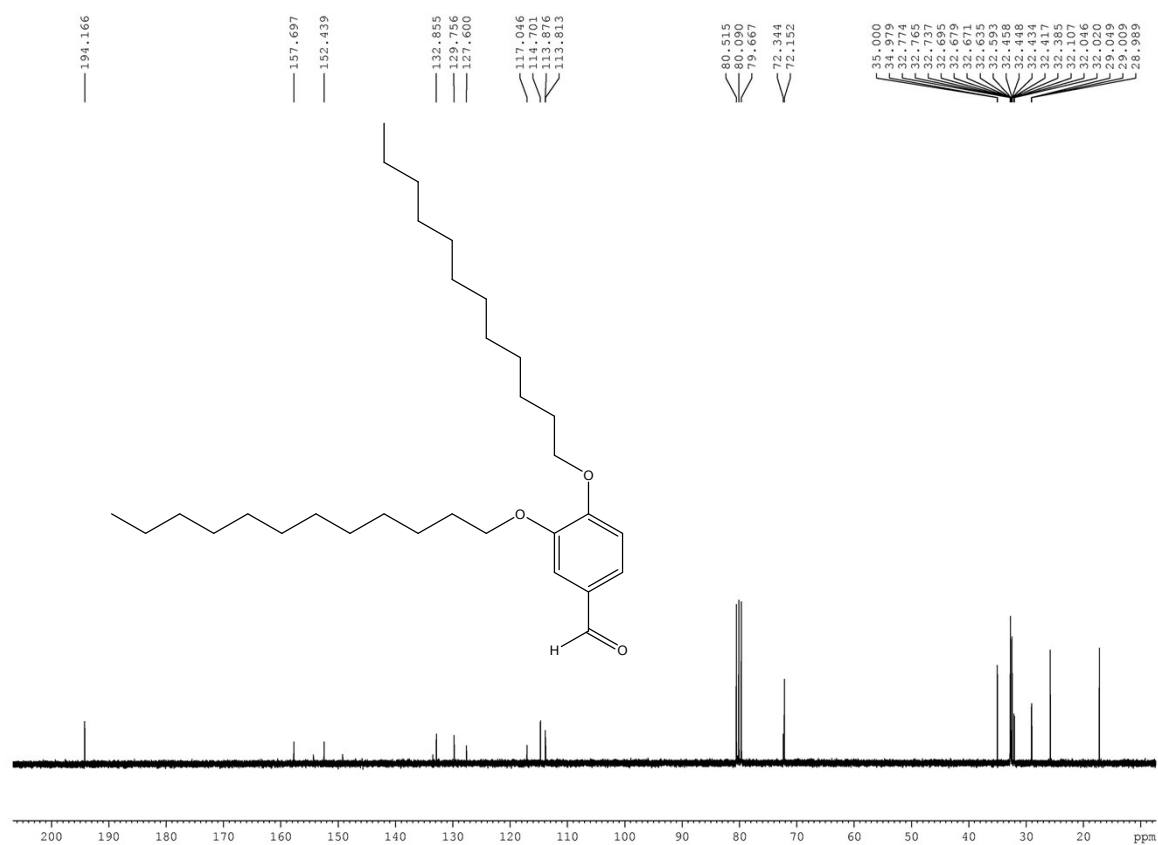


Figure S4. ^{13}C NMR spectrum of 2 (300MHz, CDCl_3)

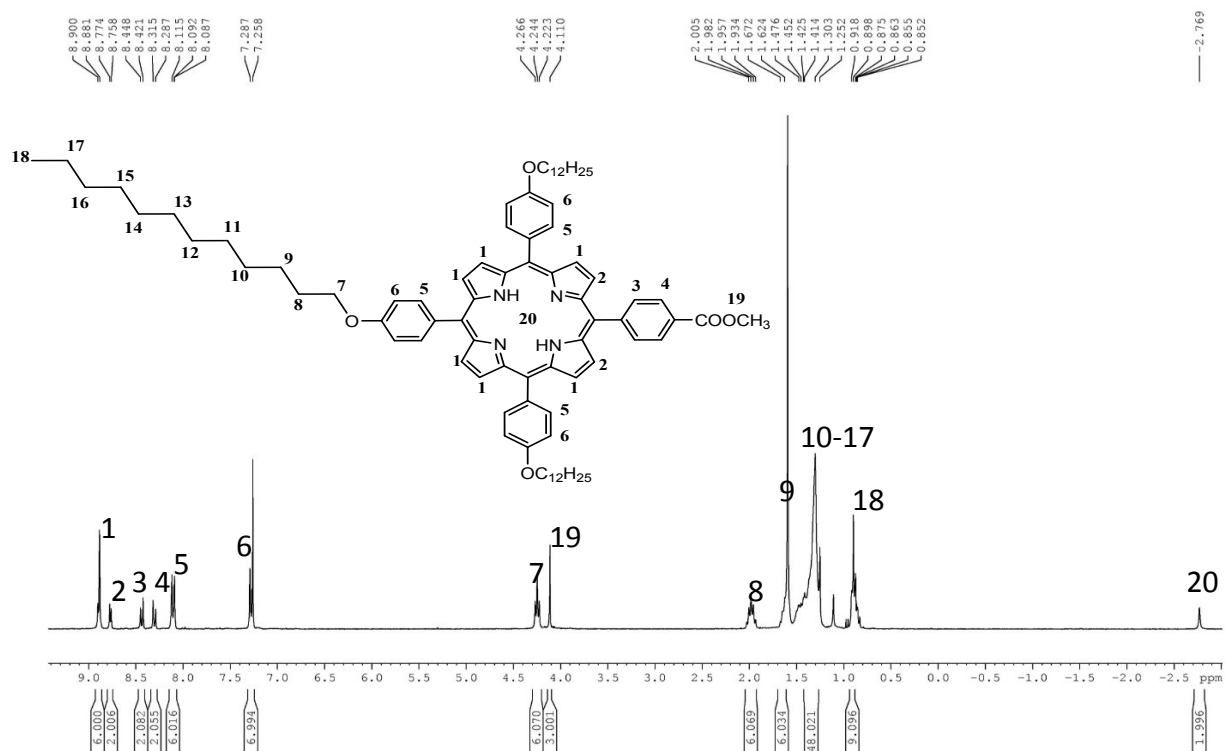


Figure S5. ^1H NMR spectrum of 3 (300MHz, CDCl_3)

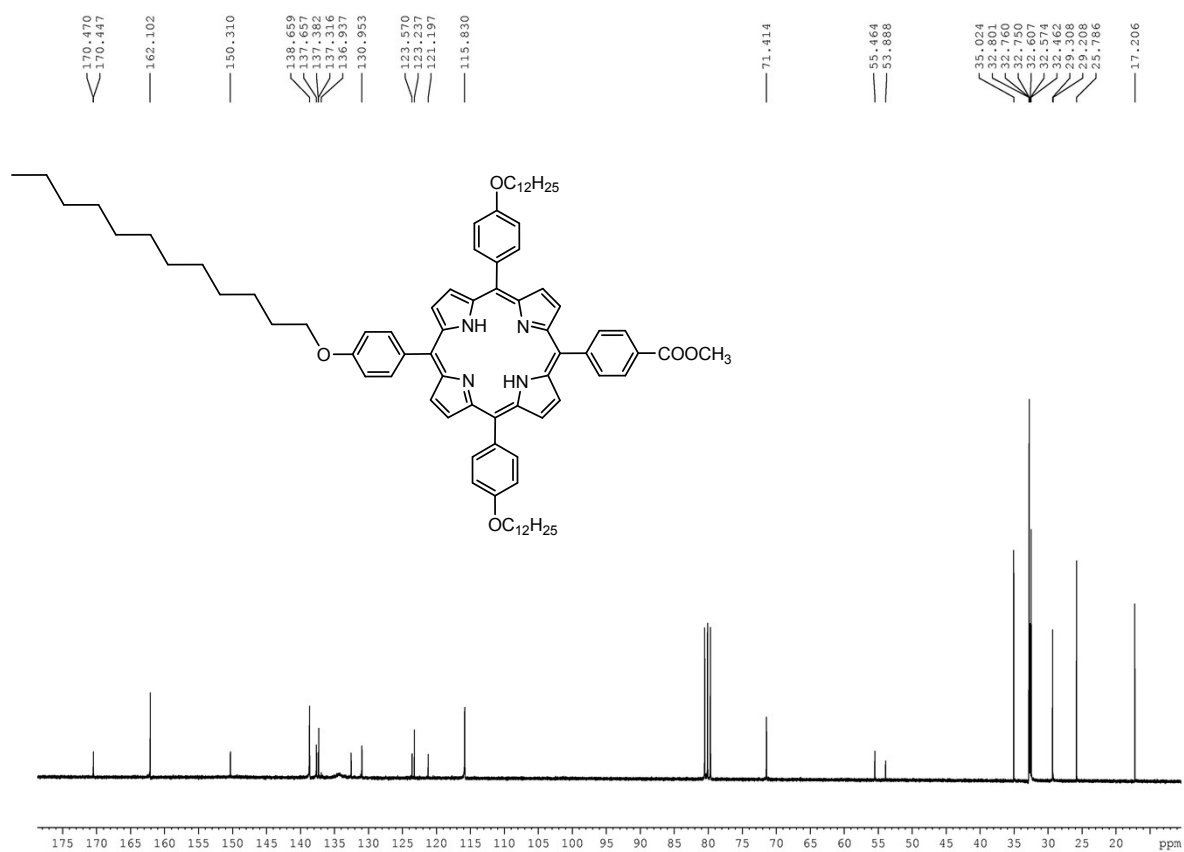


Figure S6. ^{13}C NMR spectrum of 3 (300MHz, CDCl_3)

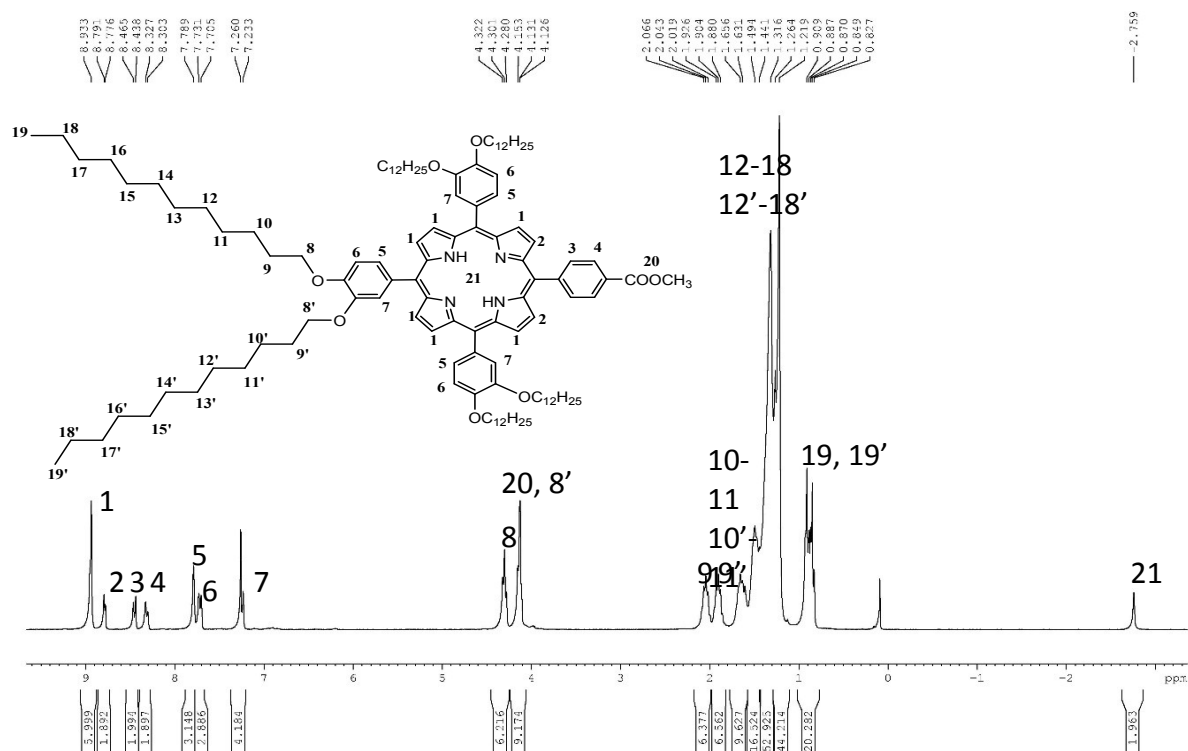


Figure S7. ^1H NMR spectrum of 4 (300MHz, CDCl_3)

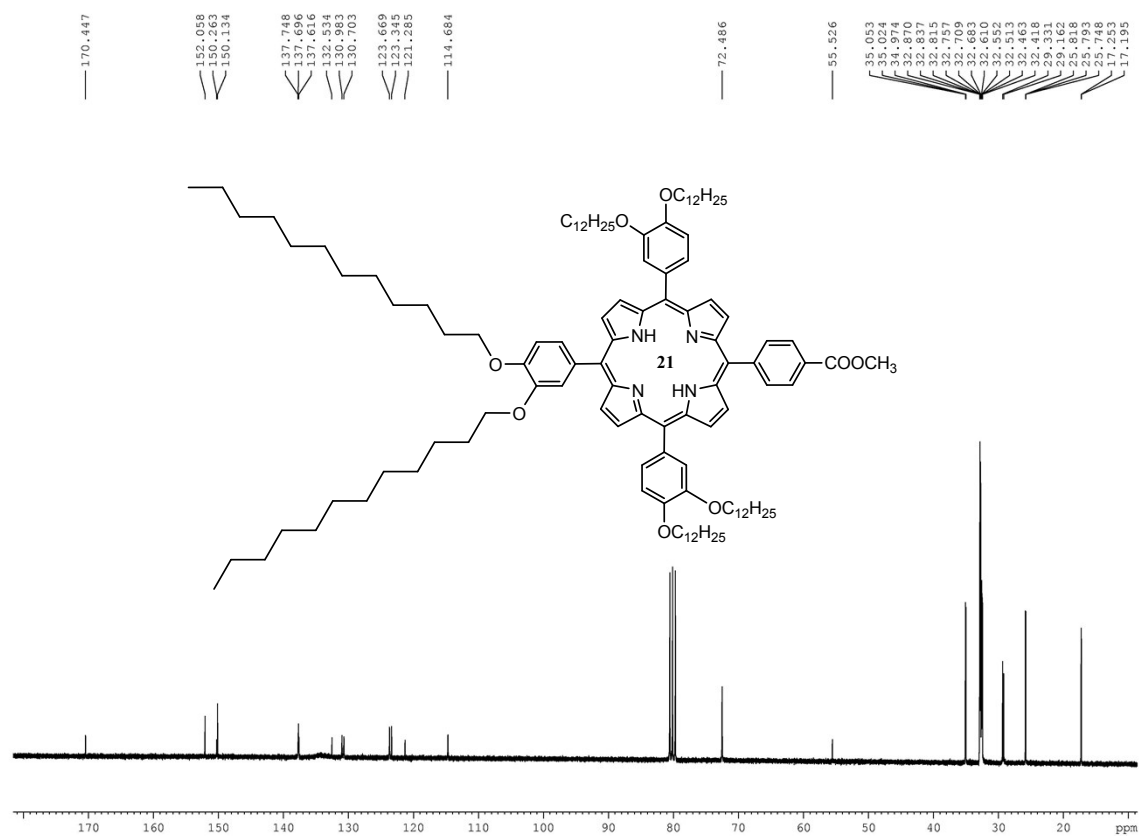


Figure S8. ¹³C NMR spectrum of 4 (300MHz, CDCl₃)

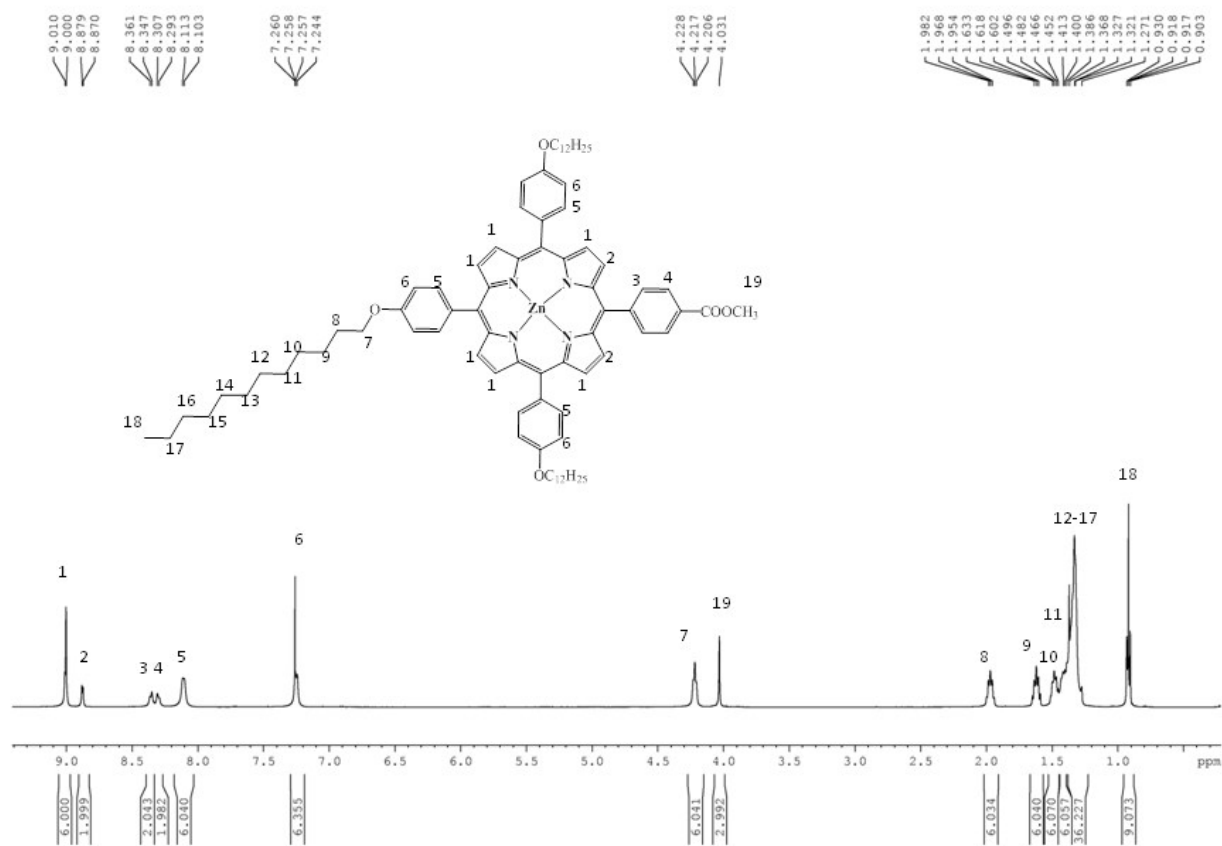


Figure S9. ^1H NMR spectrum of 5 (500MHz, CDCl_3)

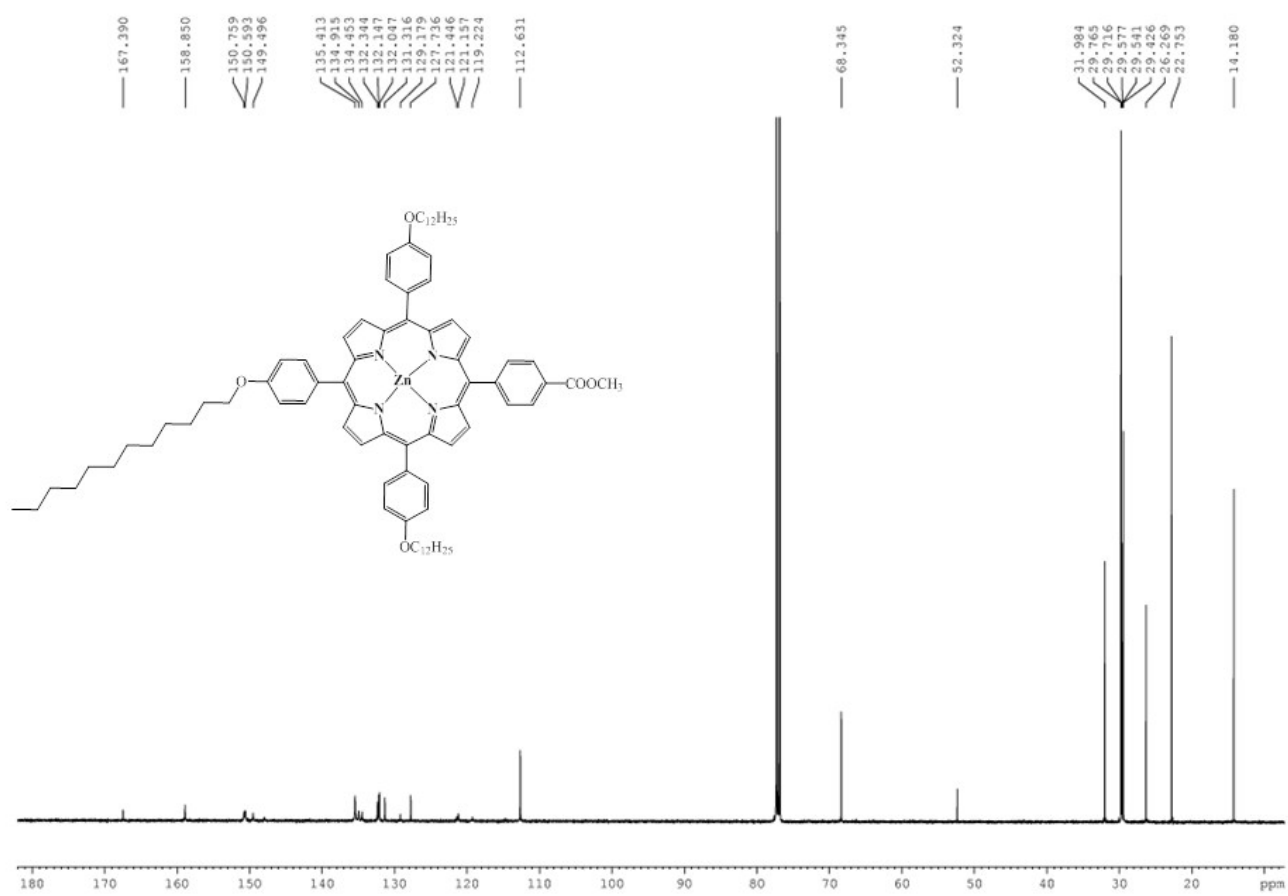


Figure S10. ^{13}C NMR spectrum of 5 (500MHz, CDCl_3)

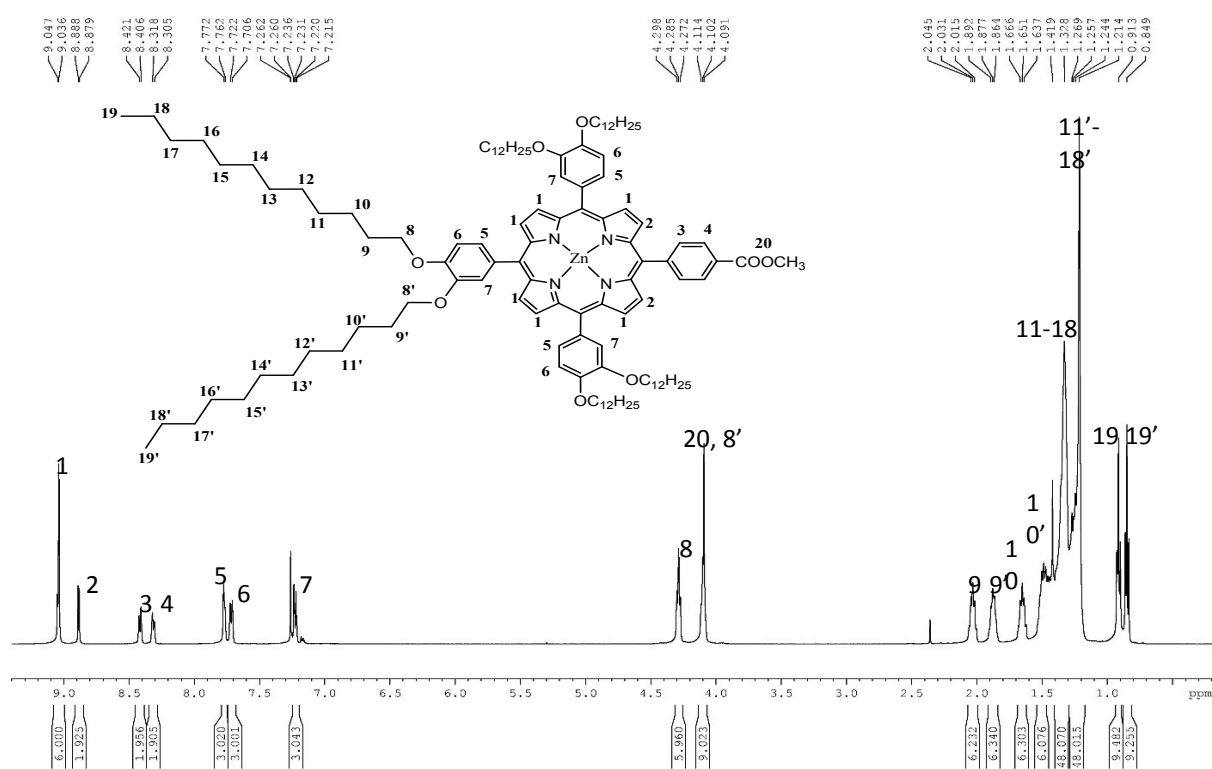


Figure S11. ¹H NMR spectrum of 6 (300MHz, CDCl₃)

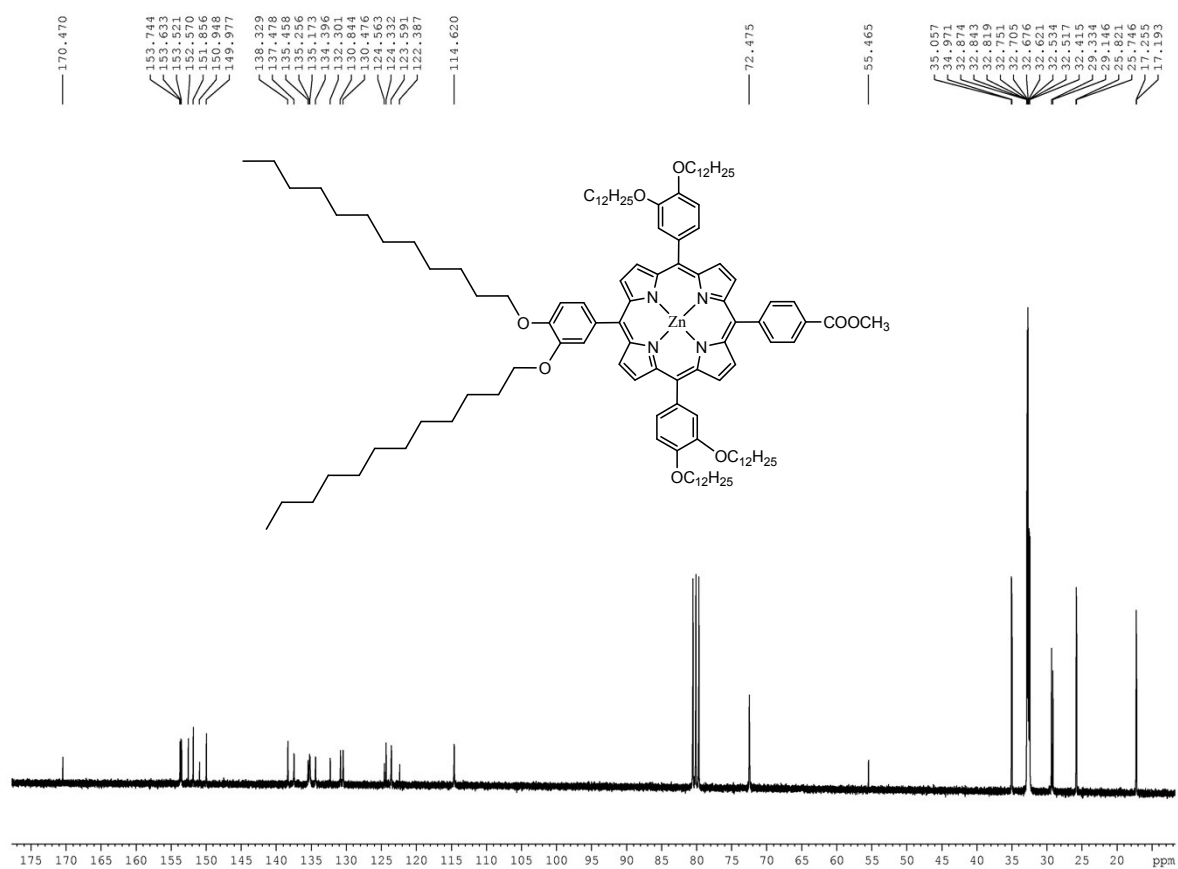


Figure S12. ¹³C NMR spectrum of 5 (300MHz, CDCl₃)

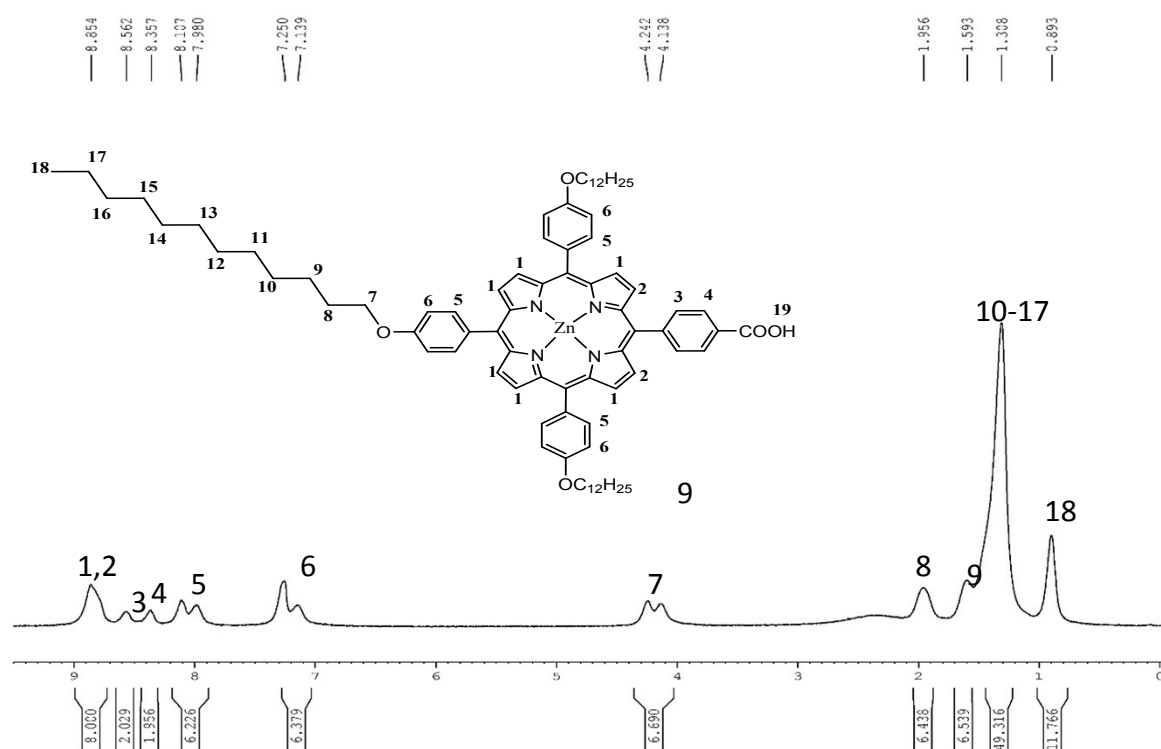


Figure S13. ^1H NMR spectrum of ZnP3C (500MHz, CDCl_3)

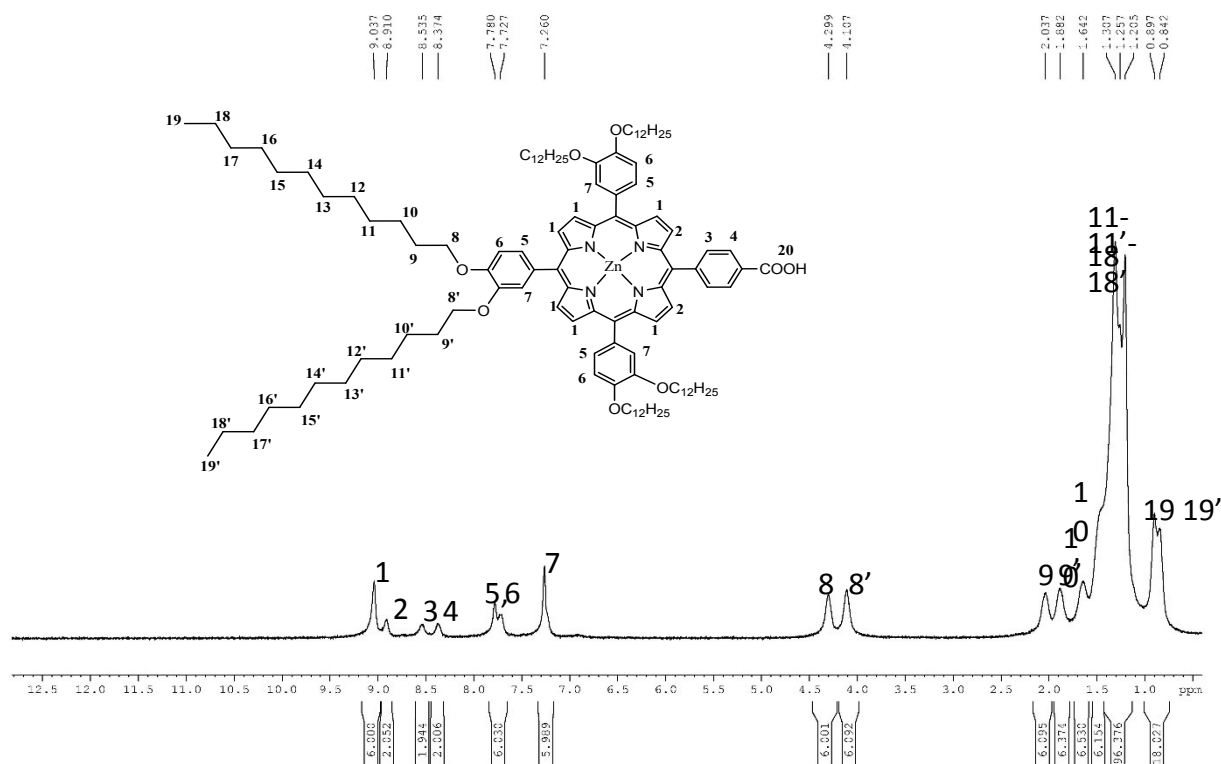


Figure S14. ^1H NMR spectrum of ZnP6C (500MHz, CDCl_3)

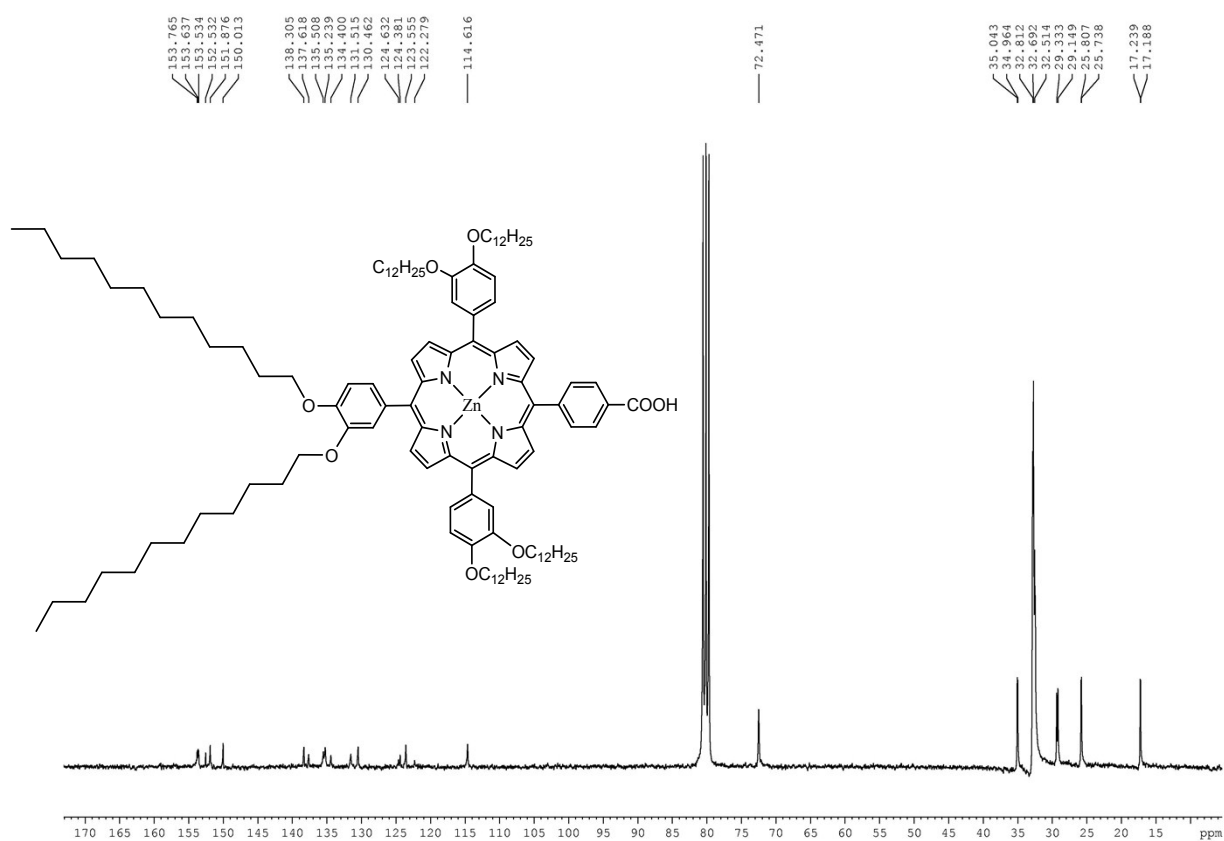


Figure S15. ^{13}C NMR spectrum of ZnP6C (500MHz, CDCl_3)

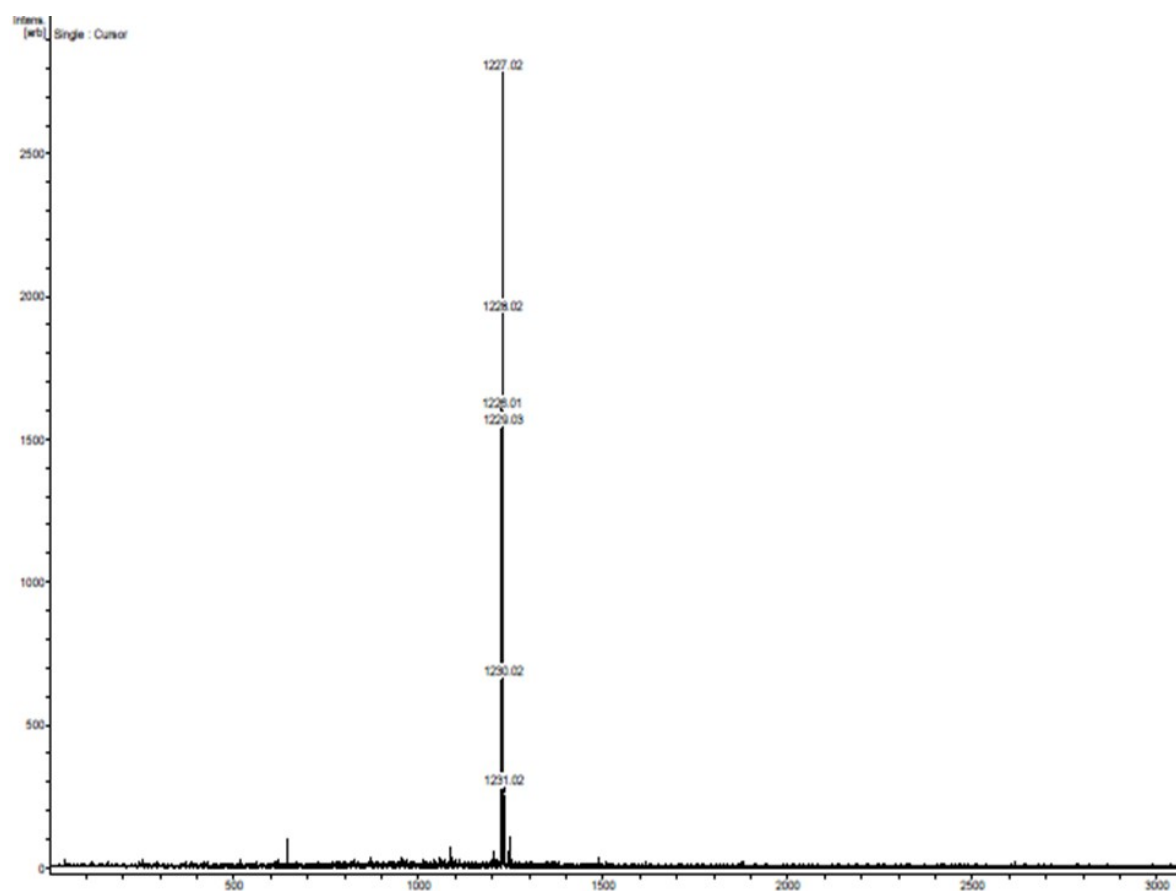


Figure S16. Mass spectrum of compound 3

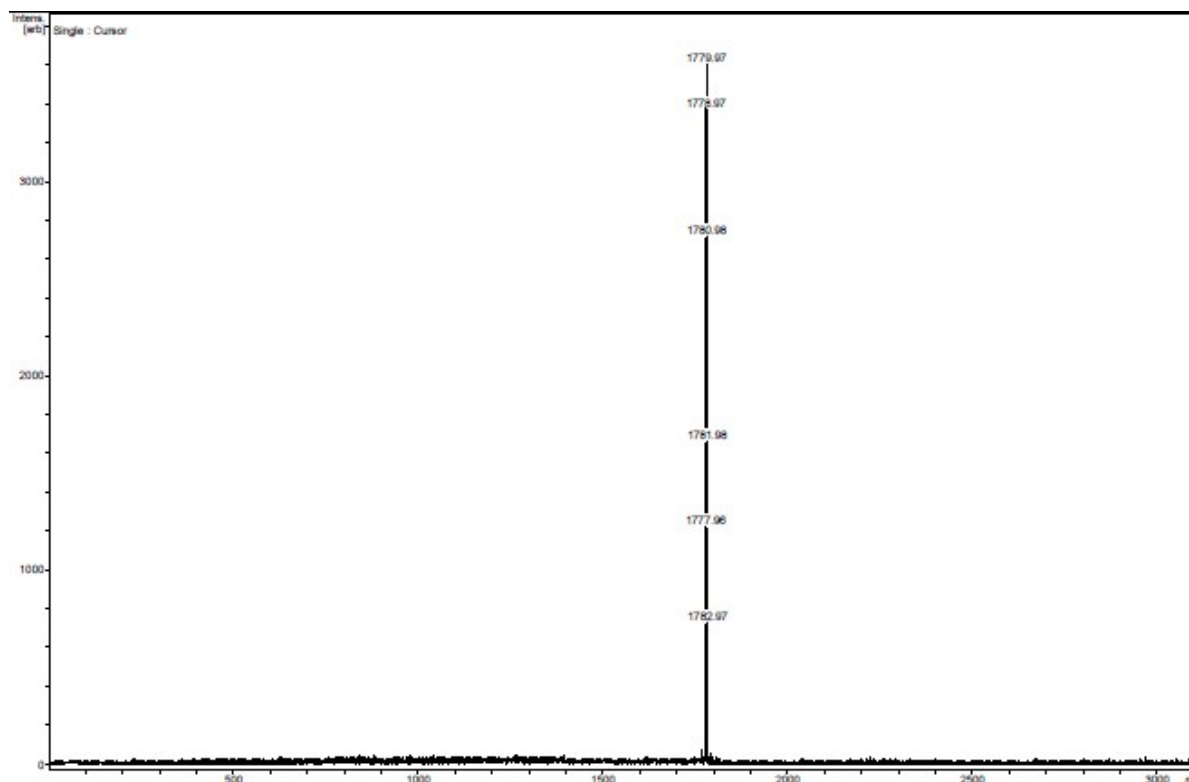


Figure S17. Mass spectrum of compound 4

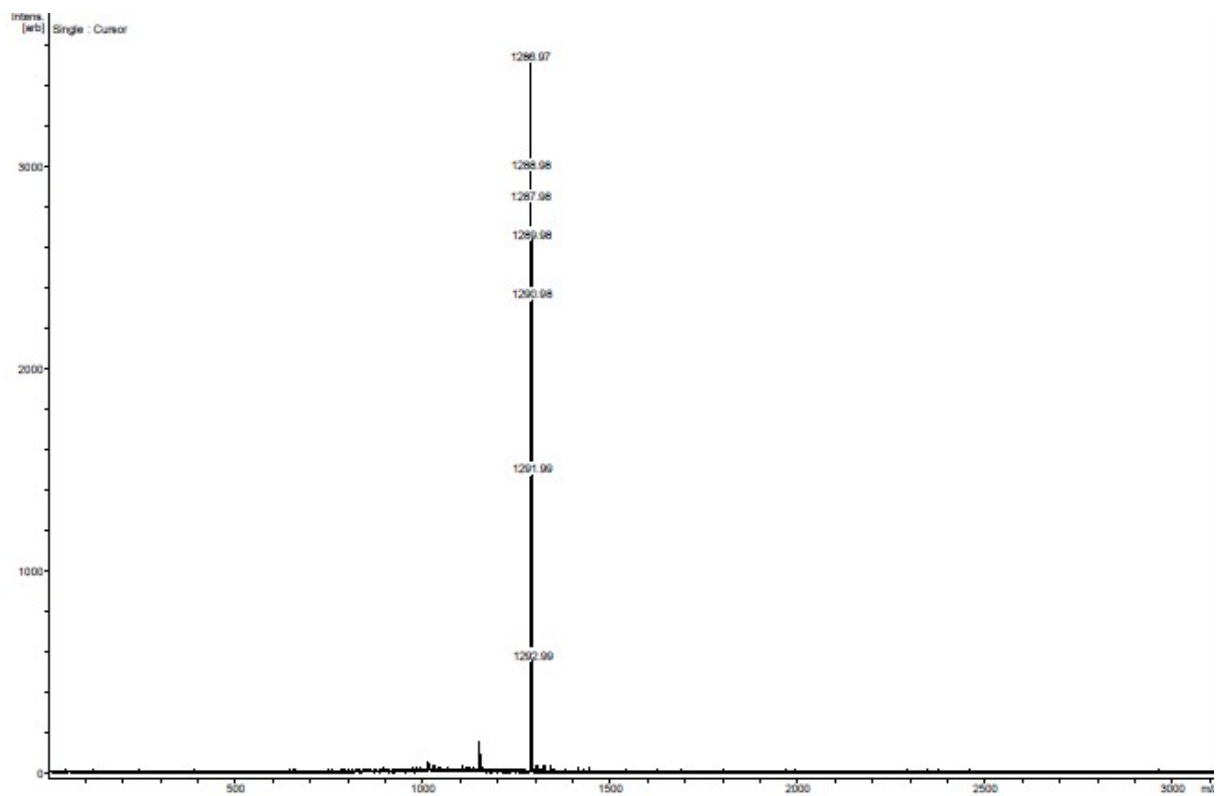


Figure S18. Mass spectrum of compound 5

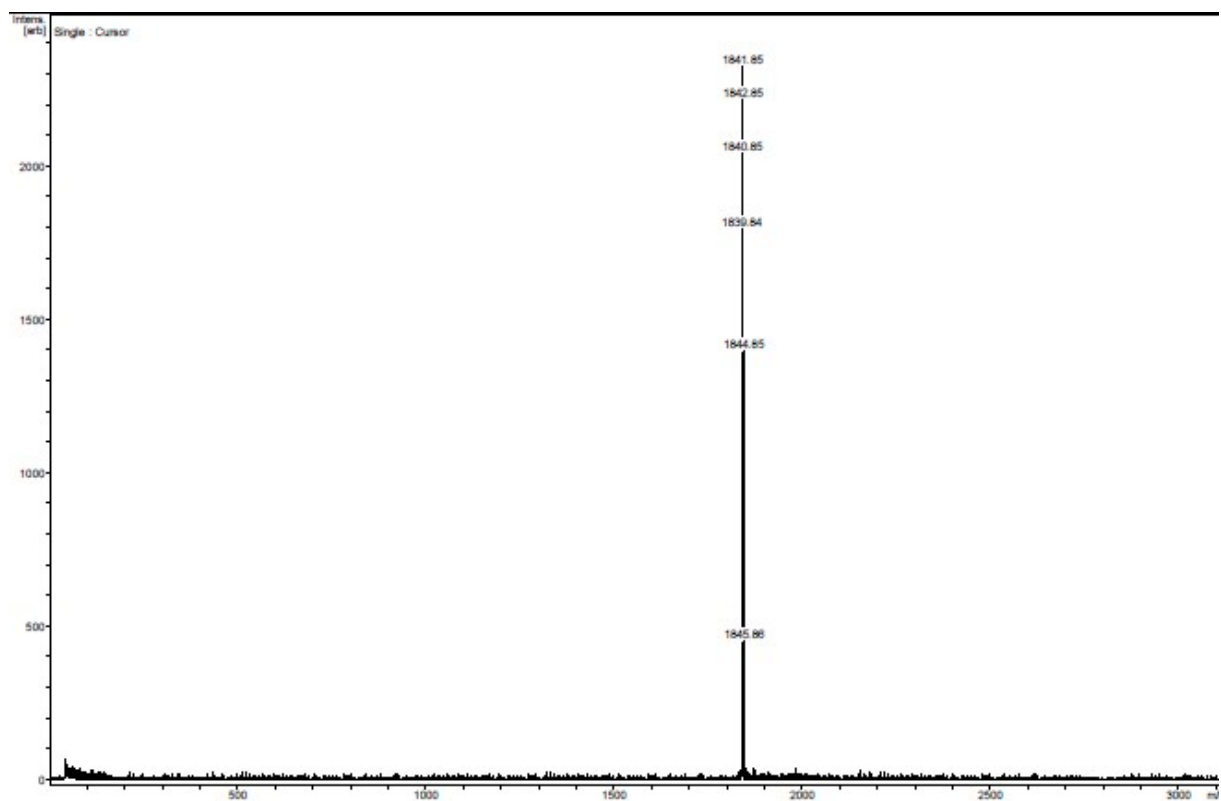


Figure S19. Mass spectrum of compound 6

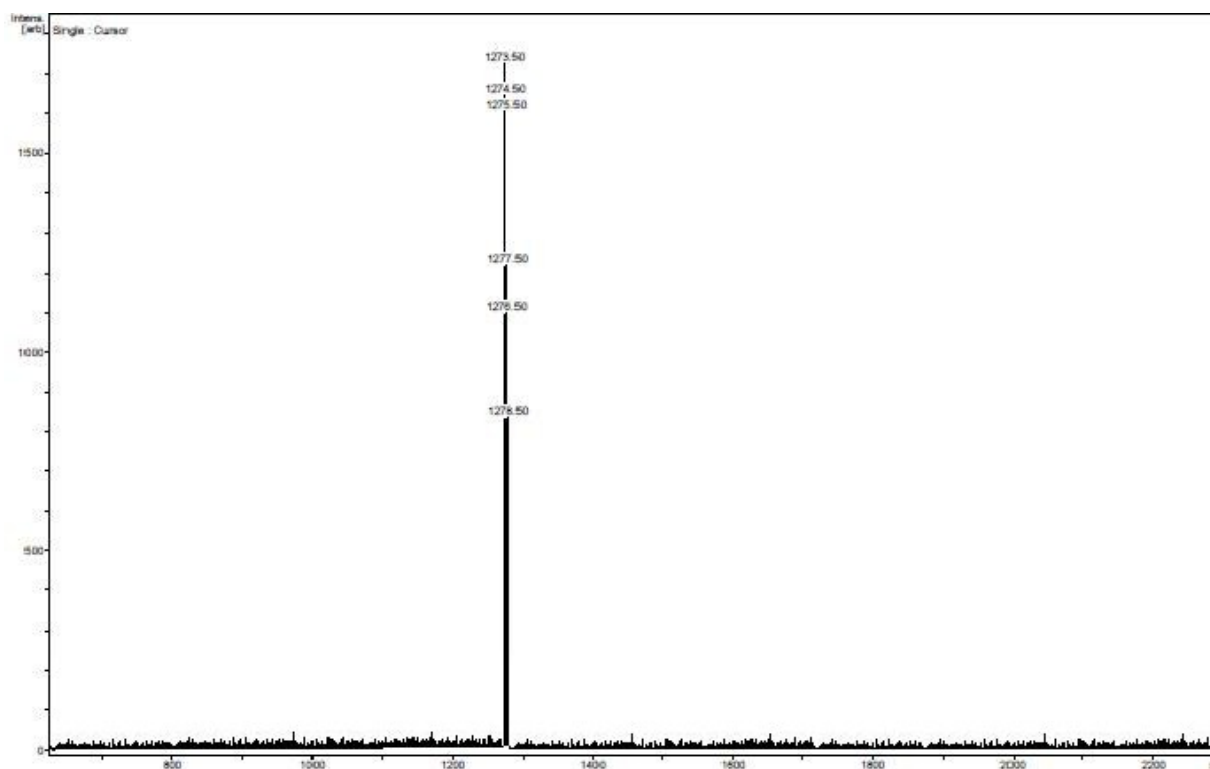


Figure S20. Mass spectrum of compound ZnP3C

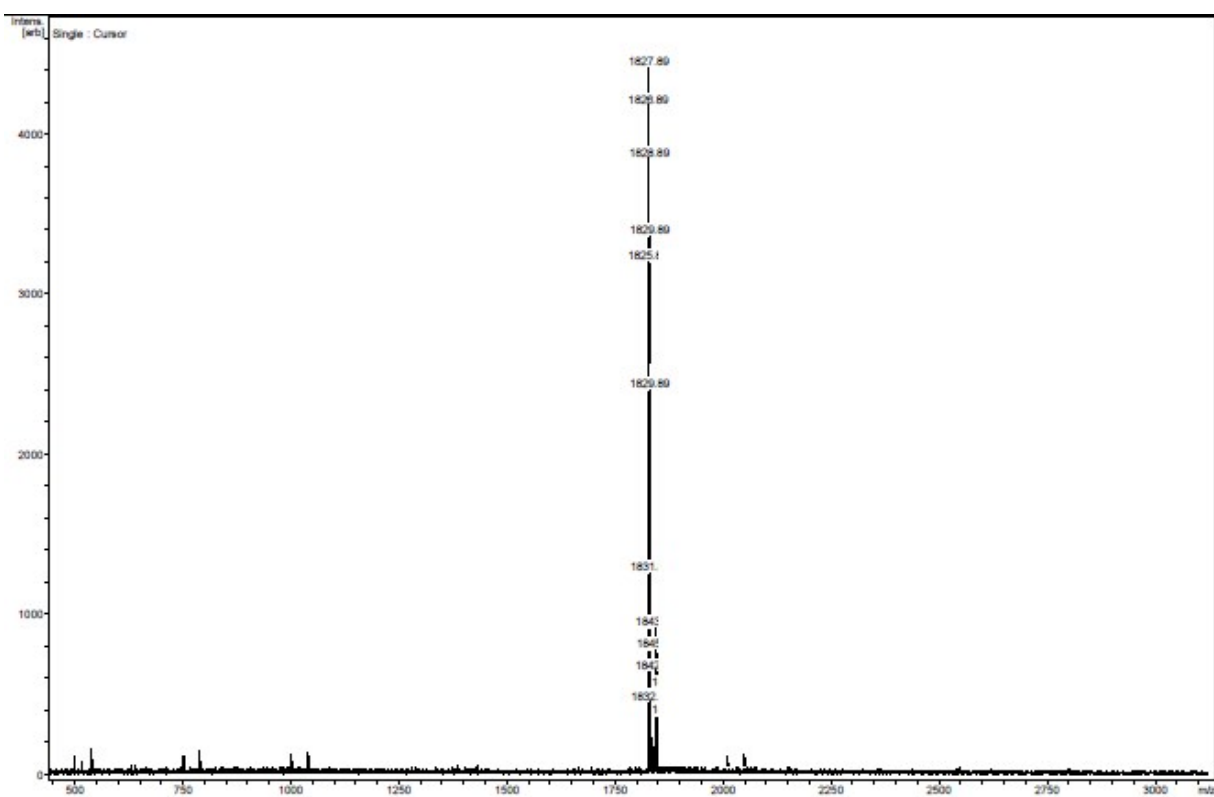


Figure S21. Mass spectrum of compound ZnP6C

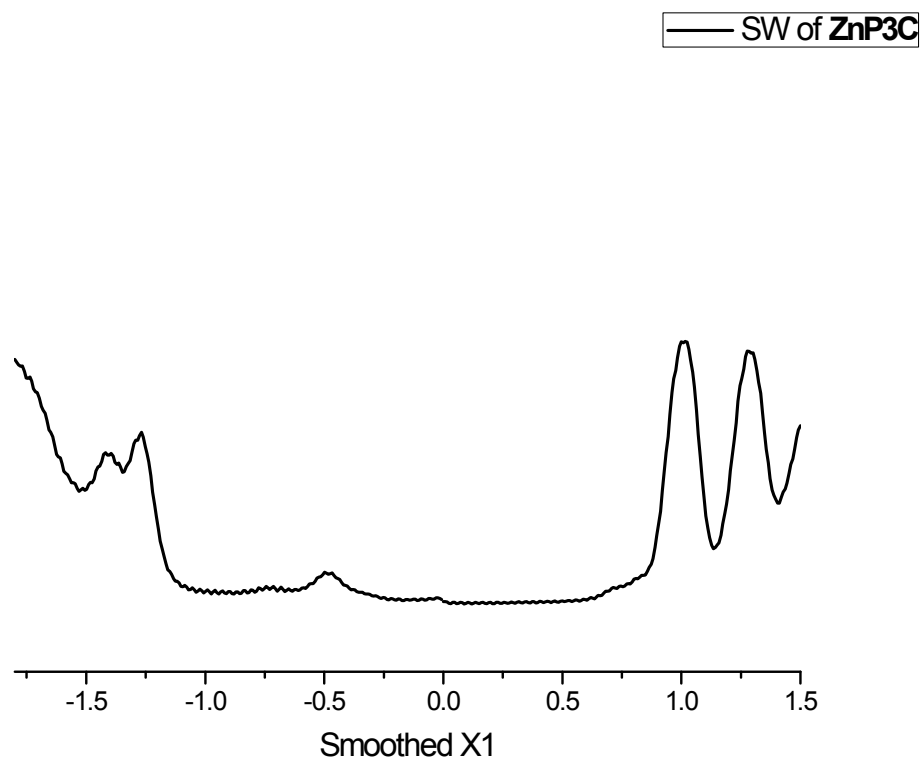


Figure S22. Square wave voltammogram of compound ZnP3C

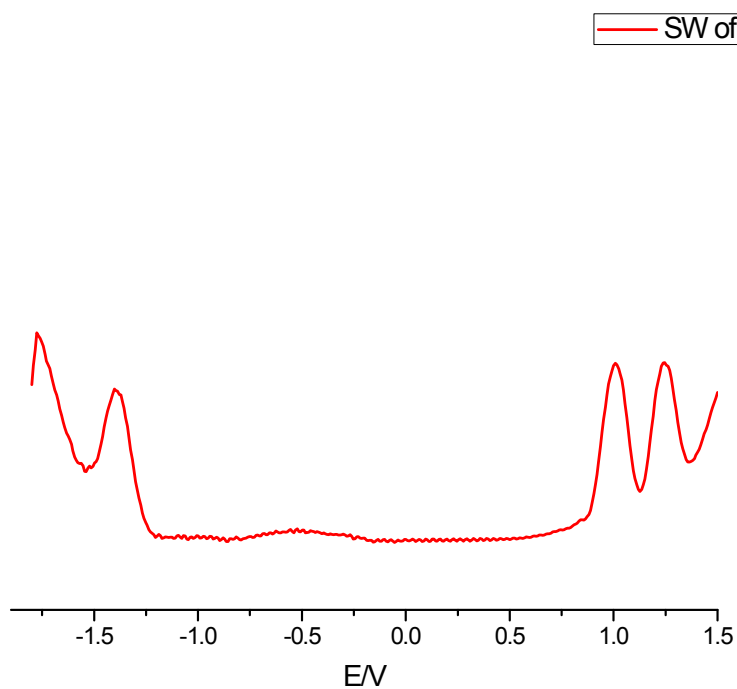


Figure S23. Square wave voltammogram of compound ZnP6C

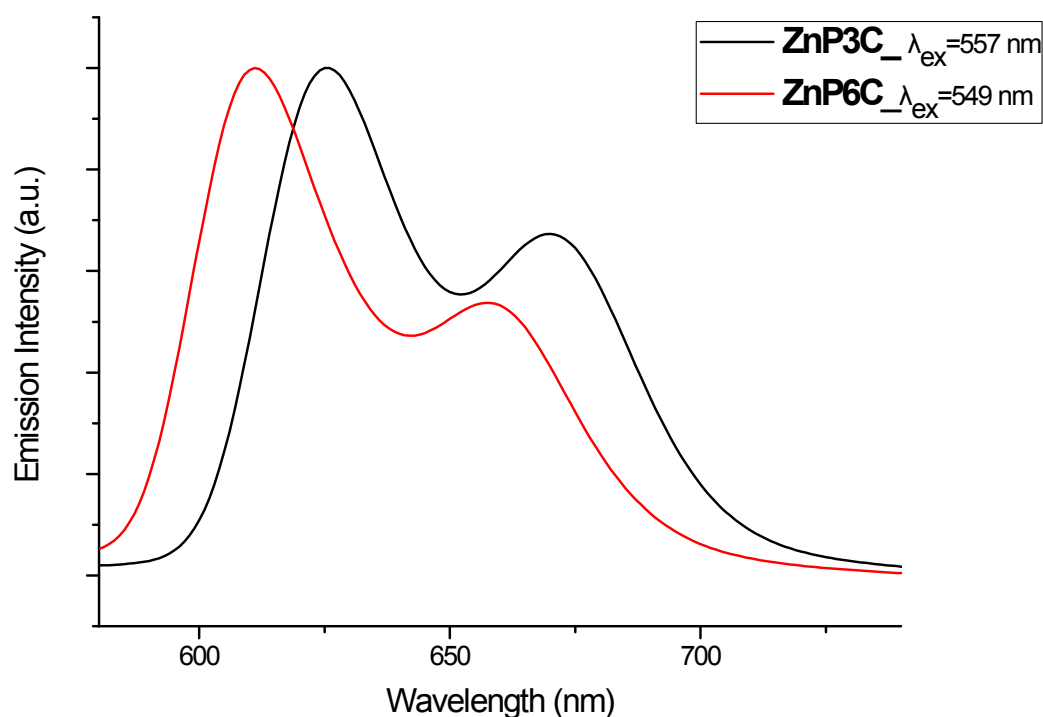


Figure S24. Emission spectra of compounds ZnP3C (black line) and ZnP6C (red line)

Table S1. Cartesian coordinates of gas phase geometry optimized structure of ZnP3C calculated by DFT at the B3LYP / 6-31G(d) level. E = - 3807.6691108 Hartree / particle.

	x	y	z
C	-1.526001000	-0.841751000	-1.309064000
C	-0.480971000	-1.692956000	-1.508124000
C	0.685240000	-0.880879000	-1.780786000
N	0.324216000	0.446024000	-1.767757000
C	-1.020300000	0.502477000	-1.481255000
C	-1.305135000	5.251076000	-1.649266000
C	-2.120922000	4.188101000	-1.402859000

C	-1.314744000	2.993369000	-1.528514000
N	-0.027873000	3.349439000	-1.859659000
C	0.007650000	4.721198000	-1.948449000
C	-1.793170000	1.676842000	-1.355498000
C	4.611347000	4.952247000	-3.132782000
C	3.558223000	5.798739000	-2.959122000
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N	2.811559000	3.675540000	-2.481649000
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C	3.123924000	-0.600795000	-2.299767000
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H	0.840599000	13.607504000	-3.234162000
H	-1.306233000	11.431369000	-3.465310000
H	0.140325000	11.552826000	-4.491070000
H	-5.435734000	2.014075000	1.577690000
H	1.863653000	9.881397000	-0.768677000
H	2.059961000	-5.480669000	0.269050000

Table S2. Cartesian coordinates of gas phase geometry optimized structure of ZnP6C calculated by DFT at the B3LYP / 6-31G(d) level. E = - 5448.5616254 Hartree / particle.

	x	y	z
C	-1.482806000	-0.834417000	-1.269076000
C	-0.434519000	-1.682795000	-1.462726000
C	0.733053000	-0.867769000	-1.720094000
N	0.369351000	0.458554000	-1.705058000
C	-0.978538000	0.511477000	-1.432490000
C	-1.279801000	5.257966000	-1.635066000
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