Supporting Information

Chiral recognition of amino acid esters by a novel oxalic amide-linked bisporphyrin

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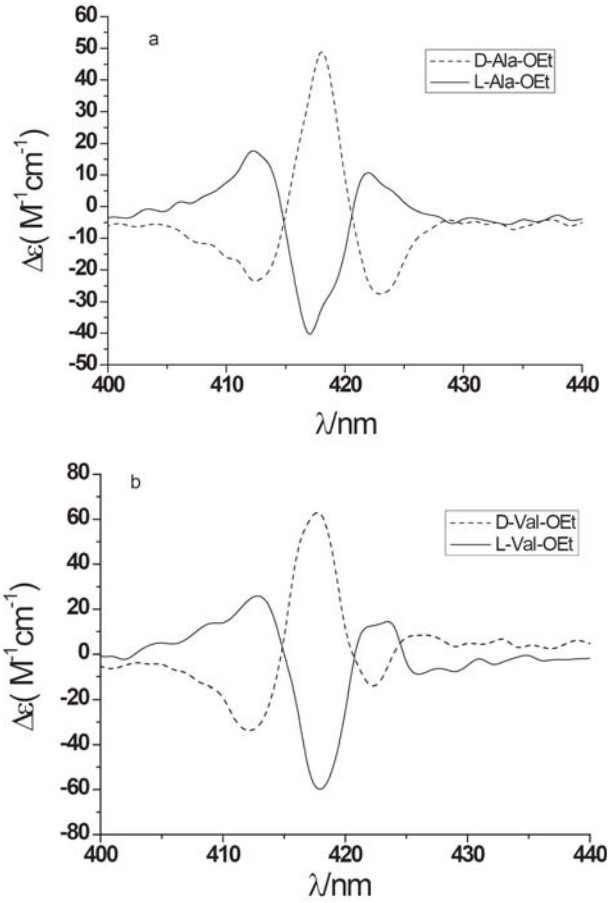

Figure S1. Circular dichroism spectra of a solution of compound **1** (3.4×10^{-6} M) and 400 equivalents of (a) L- (solid line) and D- (dash line) alanine ethyl ester, (b) L-(solid line) and D-(dash line) valine ethyl ester in methylene dichloride at 25 °C.

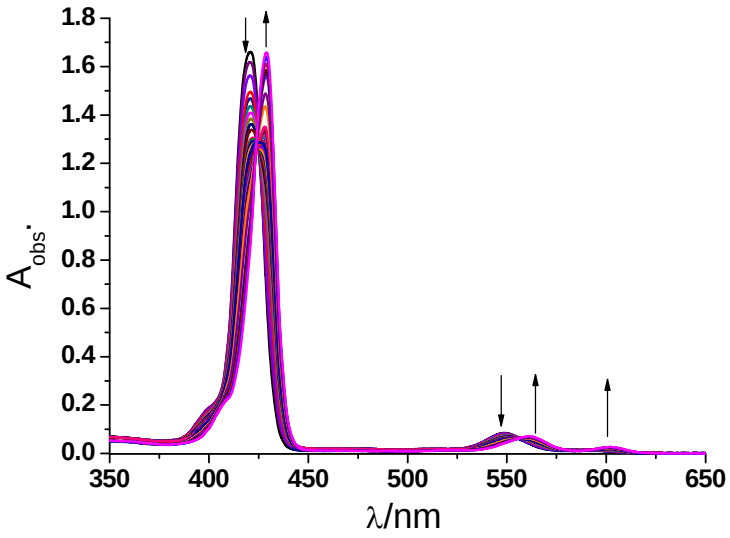

Figure S2. UV-visible spectral changes of compound 1(3.0×10^{-6} M) in methylene dichloride upon addition of D-Phe-OEt as the host: guest molar ratio changes from 1:0 to 1:167.5 at 25℃. Arrows indicate absorbance changes with increasing guest concentrations.

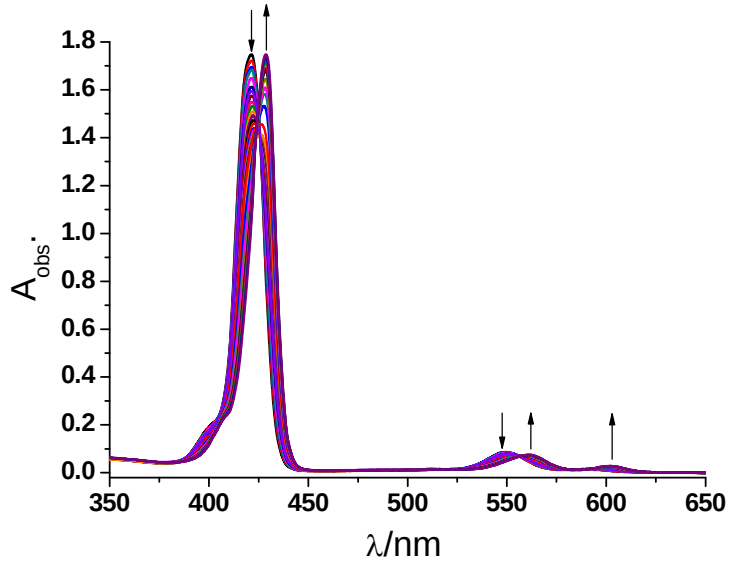

Figure S3. UV-visible spectral changes of compound 1(3.2×10^{-6} M) in methylene dichloride upon addition of D-Ala-OEt as the host: guest molar ratio changes from 1:0 to 1:167.5 at 25℃. Arrows indicate absorbance changes with increasing guest concentrations.

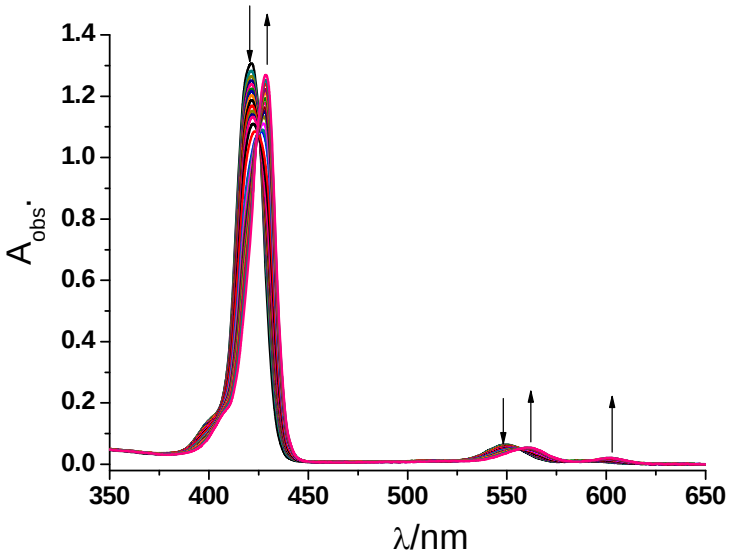

Figure S4. UV-visible spectral changes of compound 1(2.4×10^{-6} M) in methylene dichloride upon addition of L-Ala-OEt as the host: guest molar ratio changes from 1:0 to 1:250 at 25℃. Arrows indicate absorbance changes with increasing guest concentrations.

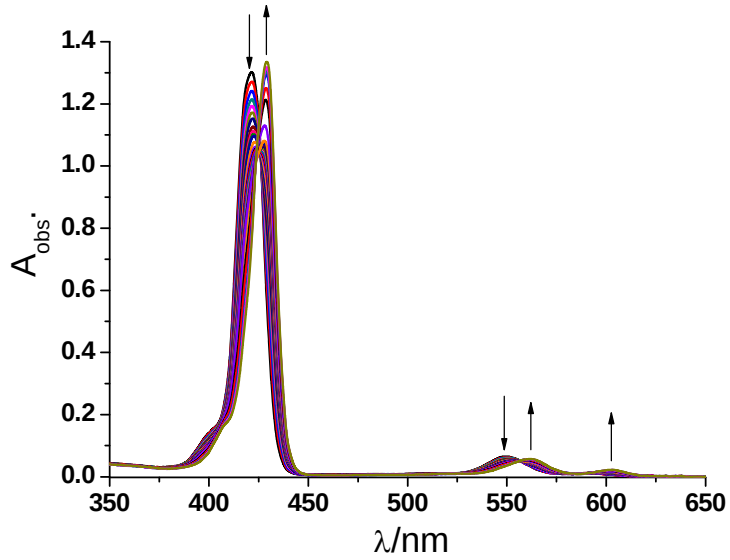

Figure S5. UV-visible spectral changes of compound 1(2.4×10^{-6} M) in methylene dichloride upon addition of D-Leu-OEt as the host: guest molar ratio changes from 1:0 to 1:250 at 25℃. Arrows indicate absorbance changes with increasing guest concentrations.

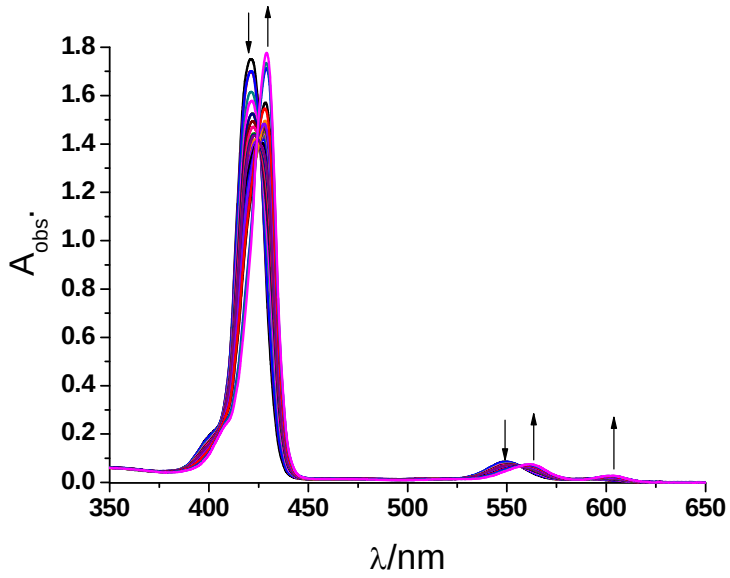

Figure S6. UV-visible spectral changes of compound 1(3.2×10^{-6} M) in methylene dichloride upon addition of L-Leu-OEt as the host: guest molar ratio changes from 1:0 to 1:167.5 at 25℃. Arrows indicate absorbance changes with increasing guest concentrations.

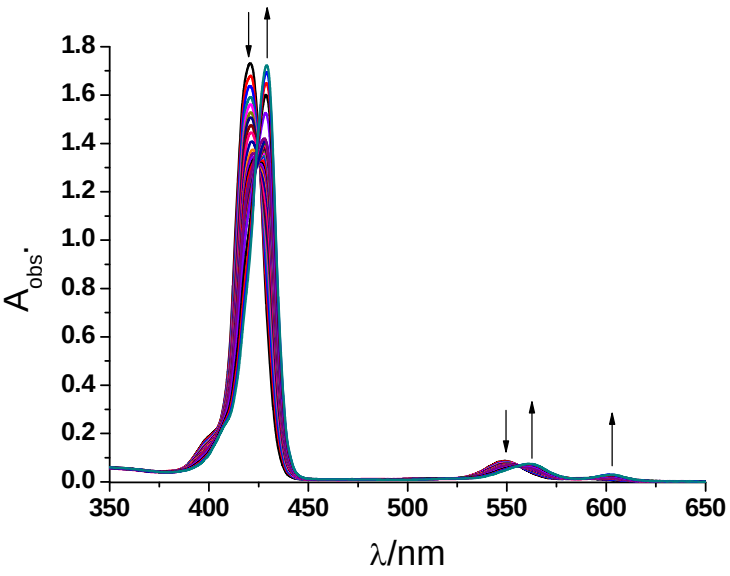

Figure S7. UV-visible spectral changes of compound 1(3.2×10^{-6} M) in methylene dichloride upon addition of D-Phg-OEt as the host: guest molar ratio changes from 1:0 to 1:167.5 at 25℃. Arrows indicate absorbance changes with increasing guest concentrations.

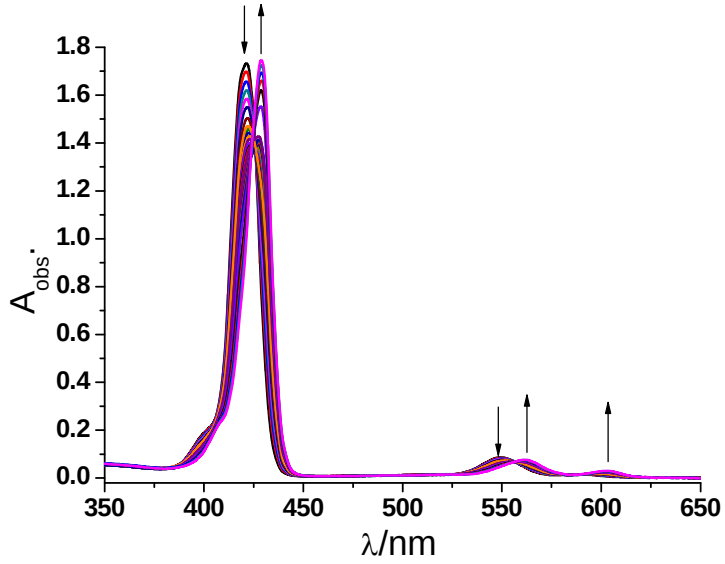

Figure S8. UV-visible spectral changes of compound 1(3.2×10^{-6} M) in methylene dichloride upon addition of L-Phg-OEt as the host: guest molar ratio changes from 1:0 to 1:167.5 at 25℃. Arrows indicate absorbance changes with increasing guest concentrations.

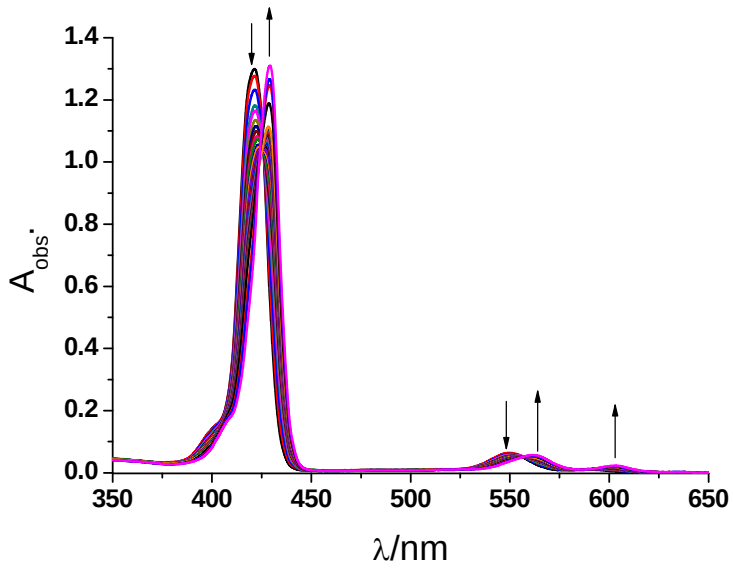

Figure S9. UV-visible spectral changes of compound 1(2.4×10^{-6} M) in methylene dichloride upon addition of D-Val-OEt as the host: guest molar ratio changes from 1:0 to 1:250 at 25℃. Arrows indicate absorbance changes with increasing guest concentrations.

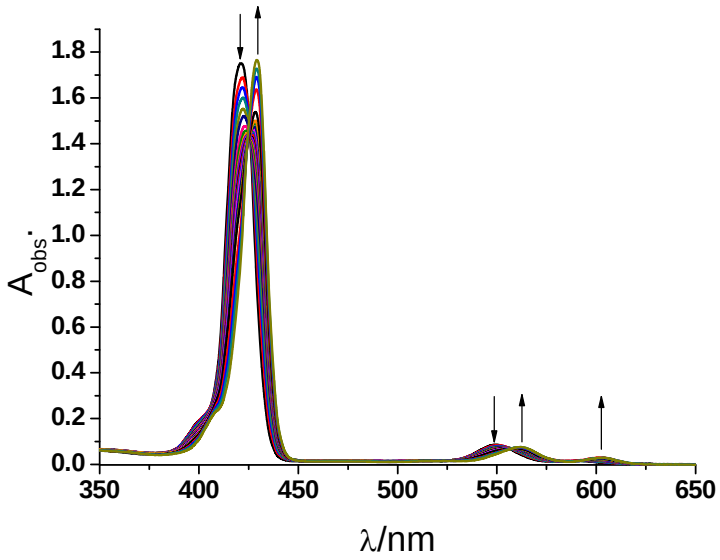

Figure S10. UV-visible spectral changes of compound 1(3.2×10^{-6} M) in methylene dichloride upon addition of L-Val-OEt as the host: guest molar ratio changes from 1:0 to 1:167.5 at 25℃. Arrows indicate absorbance changes with increasing guest concentrations.

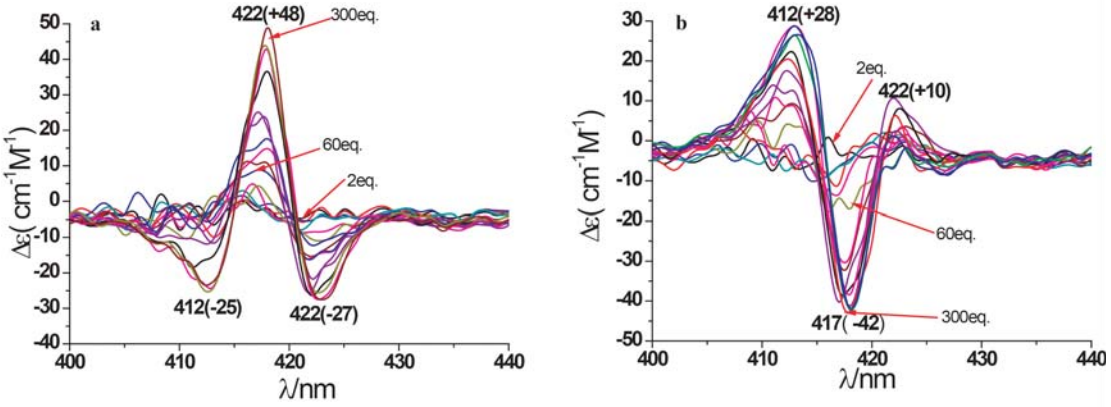

Figure S11. Circular dichroism spectra of a solution of compound **1** (3.4×10^{-6}M) and from 1:2 to 1:300 equivalents of (a) D- alanine ethyl ester, (b) L- alanine ethyl ester in methylene dichloride at 25 °C.

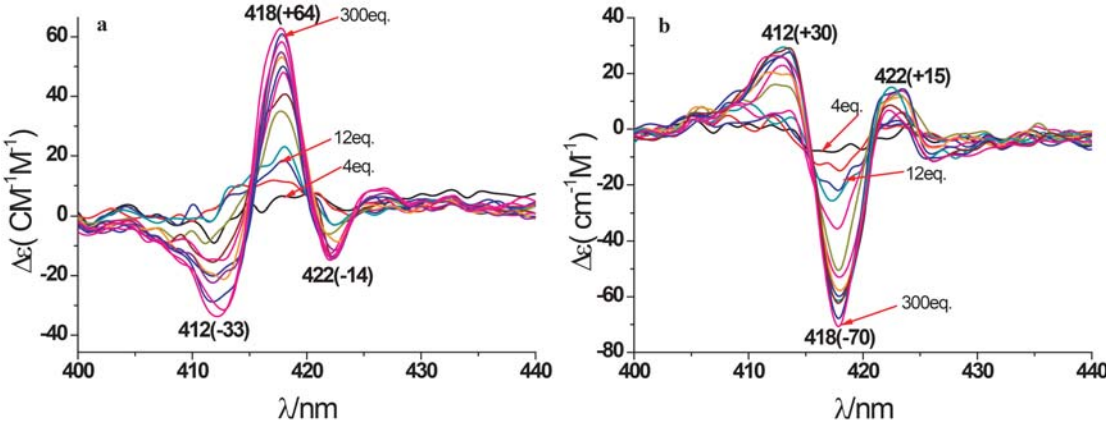

Figure S12. Circular dichroism spectra of a solution of compound **1** (3.4×10^{-6}M) and from 1:4 to 1:300 equivalents of (a) D- valine ethyl ester, (b) L- valine ethyl ester in methylene dichloride at 25 °C.

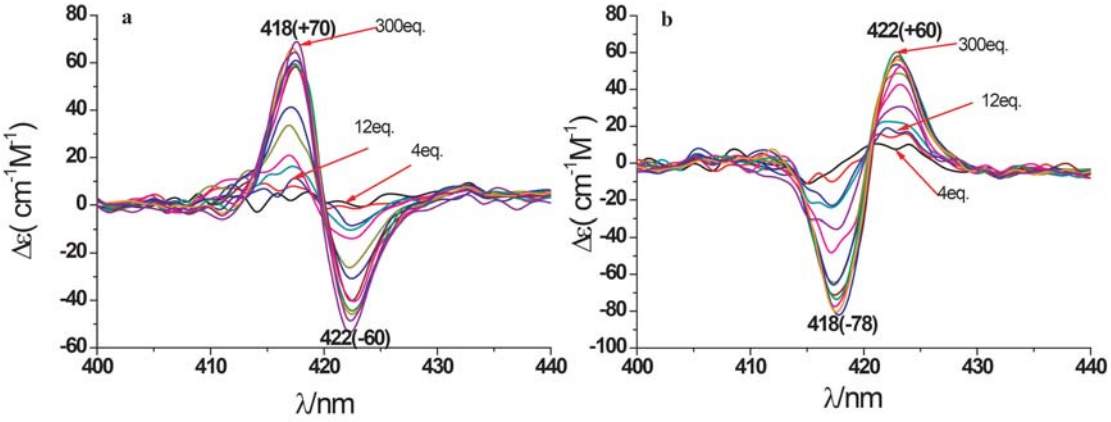

Figure S13. Circular dichroism spectra of a solution of compound **1** (3.4×10^{-6}M) and from 1:4 to 1:300 equivalents of (a) D- leucine ethyl ester, (b) L- leucine ethyl ester in methylene dichloride at 25 °C.

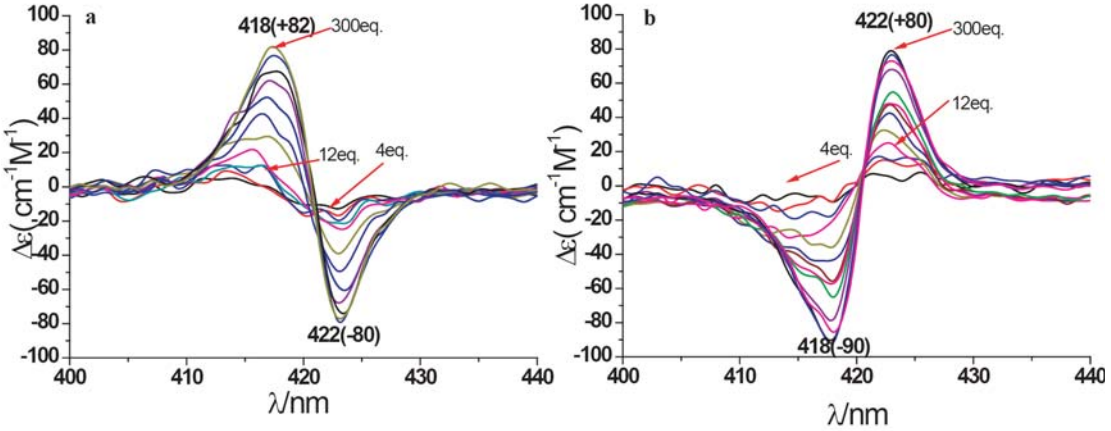

Figure S14. Circular dichroism spectra of a solution of compound **1** (3.4×10^{-6}M) and from 1:4 to 1:300 equivalents of (a) D- phenyl alanine ethyl ester, (b) L- phenyl alanine ethyl ester in methylene dichloride at 25 °C.

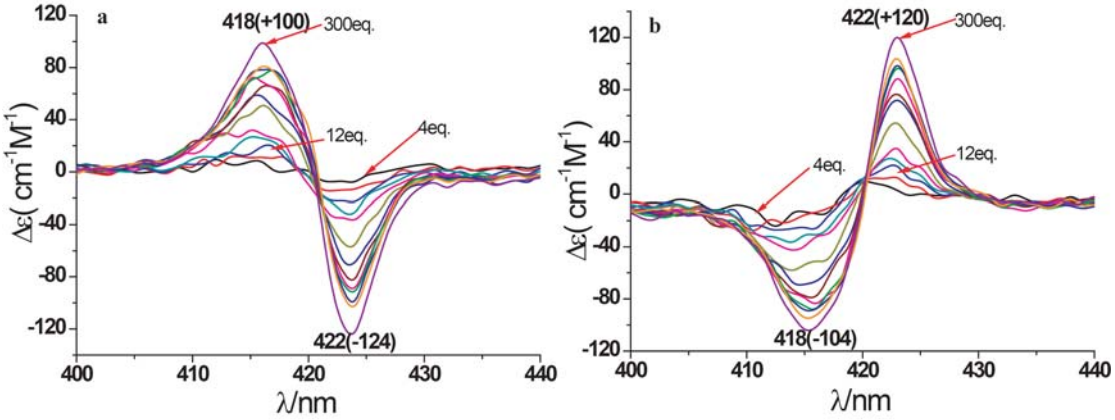

Figure S15. Circular dichroism spectra of a solution of compound **1** (3.4×10^{-6}M) and from 1:4 to 1:300 equivalents of (a) D- phenylglycine ethyl ester, (b) L-phenylglycine ethyl ester in methylene dichloride at 25 °C.

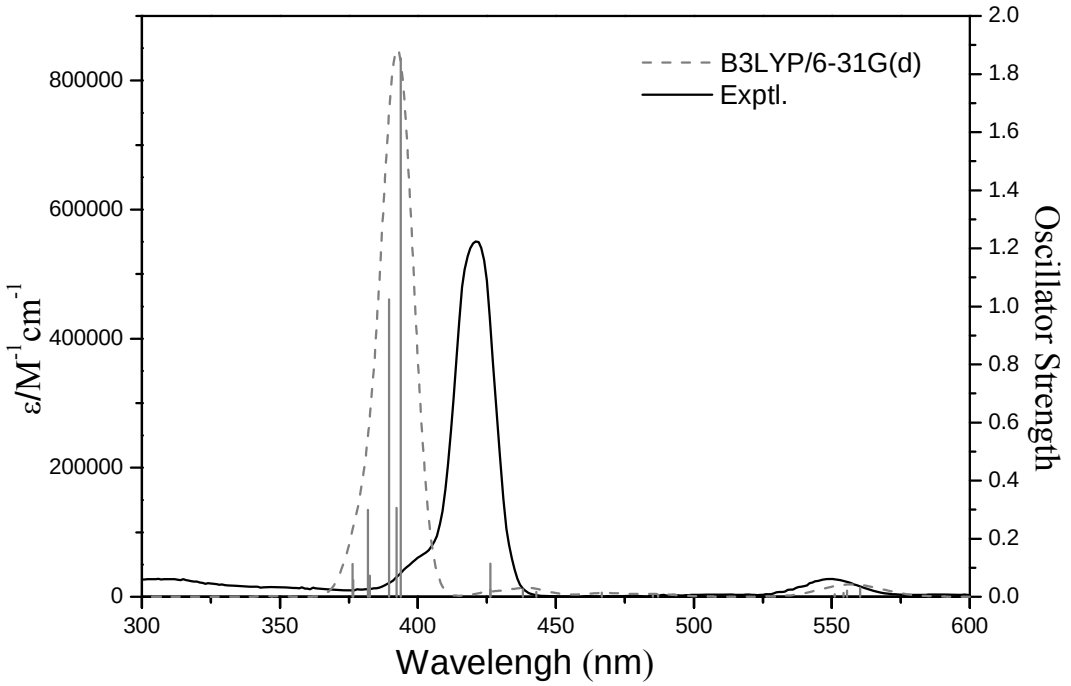

Figure S16. UV-vis spectrum of complex formed between compound **1** and L-Phe-OEt. (black line), calculated UV-vis curve at the B3LYP/6-31G* level (dash line), and oscillator strengths for the different transitions (gray bars).

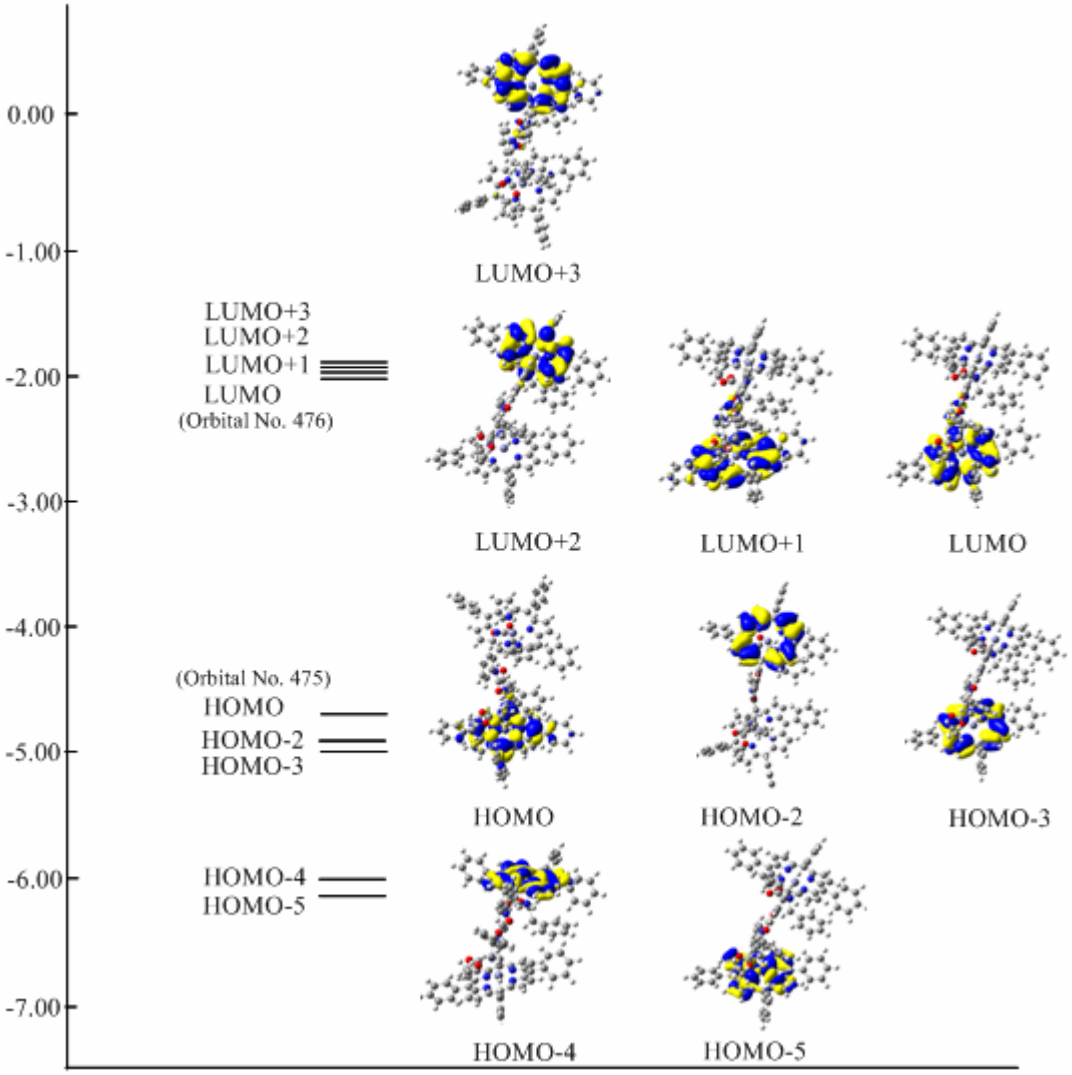

Figure S17. Selected HOMO and LUMO orbital plots at the B3LYP/6-31G* level.

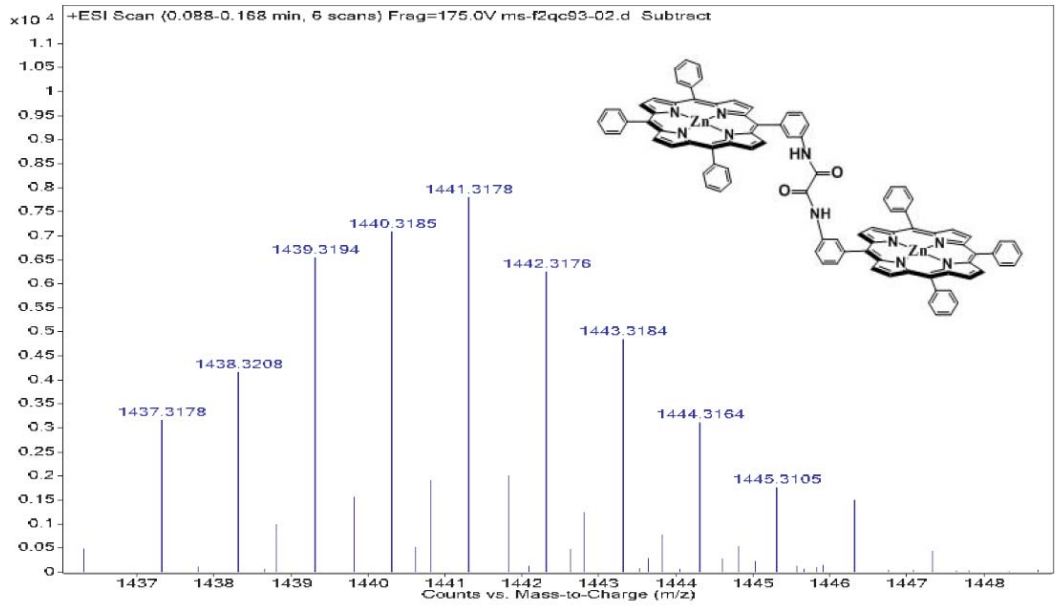

Figure S18. Mass spectrum of the compound **1**.

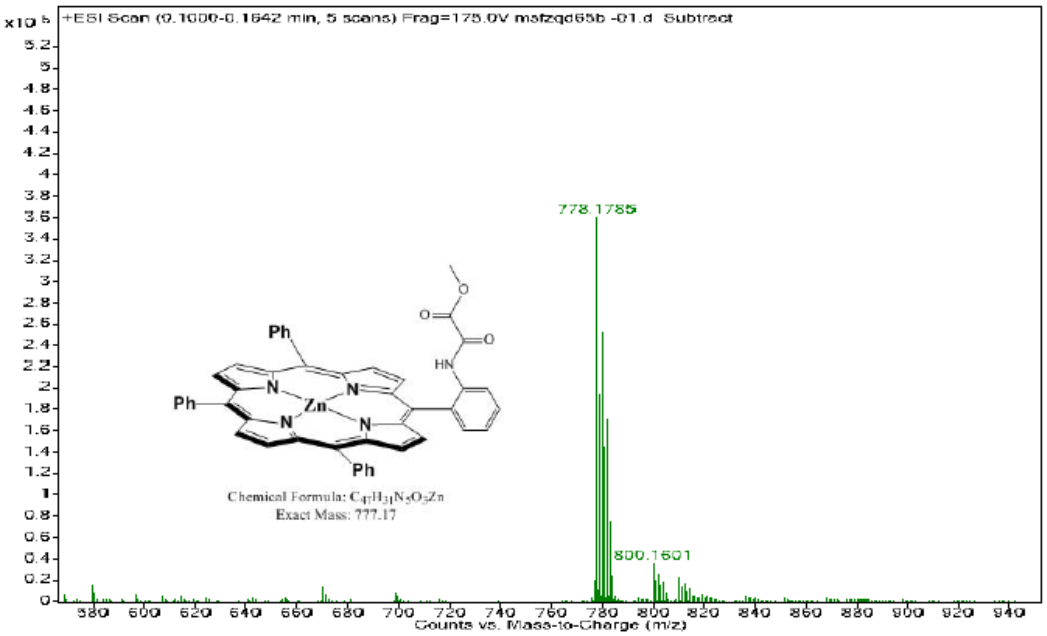

Figure S19. Mass spectrum of the compound **2**.

Table S1. Selected bond distances for the calculated structure of complex **1**·(L-Phe-OEt)$_2$

bond	distance (Å)
Zn(1)-N(55)	2.1754
Zn(1)-N(2)	2.0865
Zn(1)-N(3)	2.0857
Zn(1)-N(4)	2.0906
Zn(1)-N(5)	2.0946
Zn(108)-N(109)	2.0976
Zn(108)-N(110)	2.0833
Zn(108)-N(111)	2.0794
Zn(108)-N(112)	2.0997
Zn(108)-N(162)	2.1717
N(55)---O(165)	3.2065
N(162)---O(58)	3.0654

Table S2 Main Experimental and Calculated Optical Transitions

Orbital Excitations	Character	Calcd/nm	f [a]	Exptl/nm
HOMO-2 →LUMO+3	π→π*	394	1.8540	422
HOMO-3 →LUMO	π→π*			
HOMO-3 →LUMO+1	π→π*	392	0.3055	
HOMO-2 →LUMO+3	π→π*			
HOMO-2 →LUMO+2	π→π*	390	1.0245	
HOMO-4 →LUMO+2	π→π*, MLCT	382	0.2986	416
HOMO-5 →LUMO	π→π*, MLCT			
HOMO-4 →LUMO+3	π→π*, MLCT	377	0.0570	
HOMO-5 →LUMO+1	π→π*, MLCT	376	0.1133	
HOMO-4 →LUMO+3	π→π*, MLCT			

[a] Oscillator strength