Organic &
Biomolecular
Chemistry

Electronic Supplementary Information for

Amino acid derivatives of perylenediimide and their N–H···O peptide bond dipoles-templated solid state assembly into stacks

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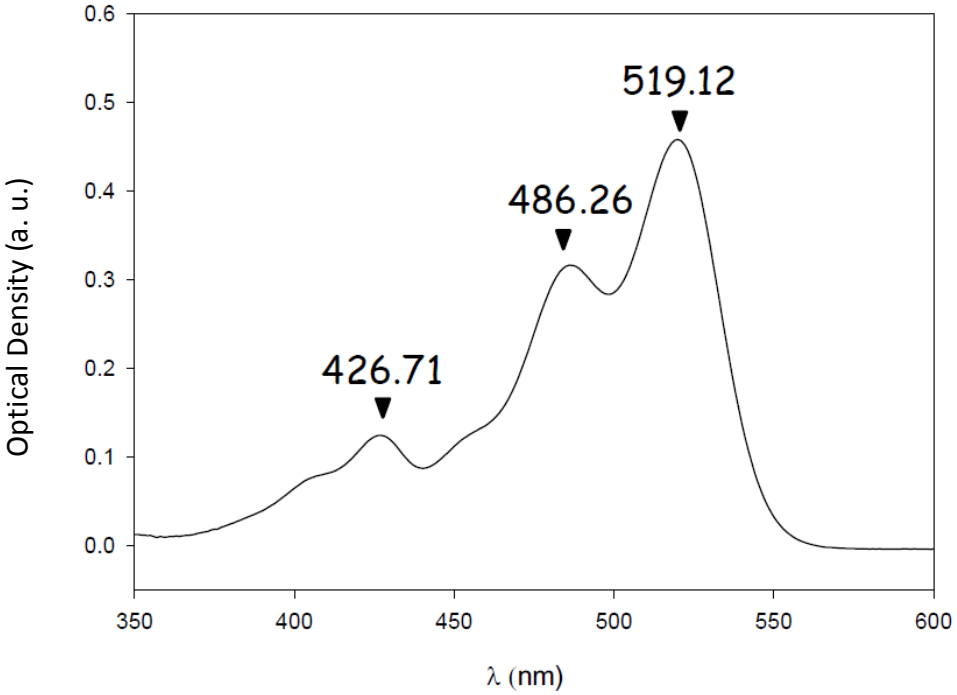
Figure S1. UV-visible absorption spectra for dichloromethane solutions of **2a-b** and tetrahydrofurane solutions of **1**.

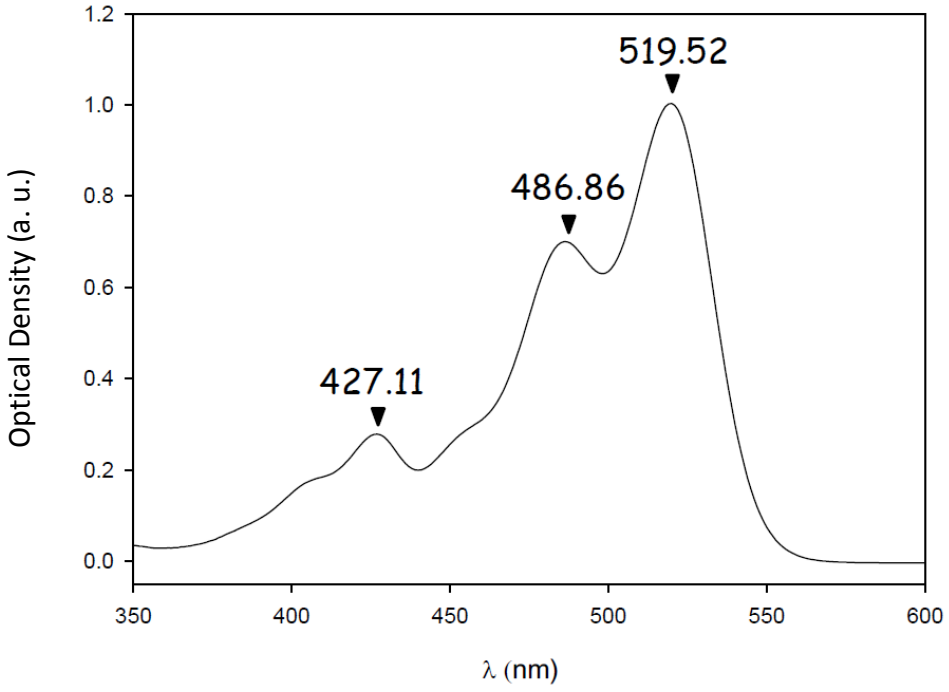
Figure S2. Cyclic voltammograms of compounds **2a** and **2b** and CV of precursor **1**.

Figure S3. Molecular conformations of PDI-(*Cl*$_4$)-[Gly-Ala(OEt)]$_2$, **2a** (Fig. S3a) and PDI-(*Cl*$_4$)-[Gly-Val(OEt)]$_2$, **2b** (Fig. S3b) in solid state.

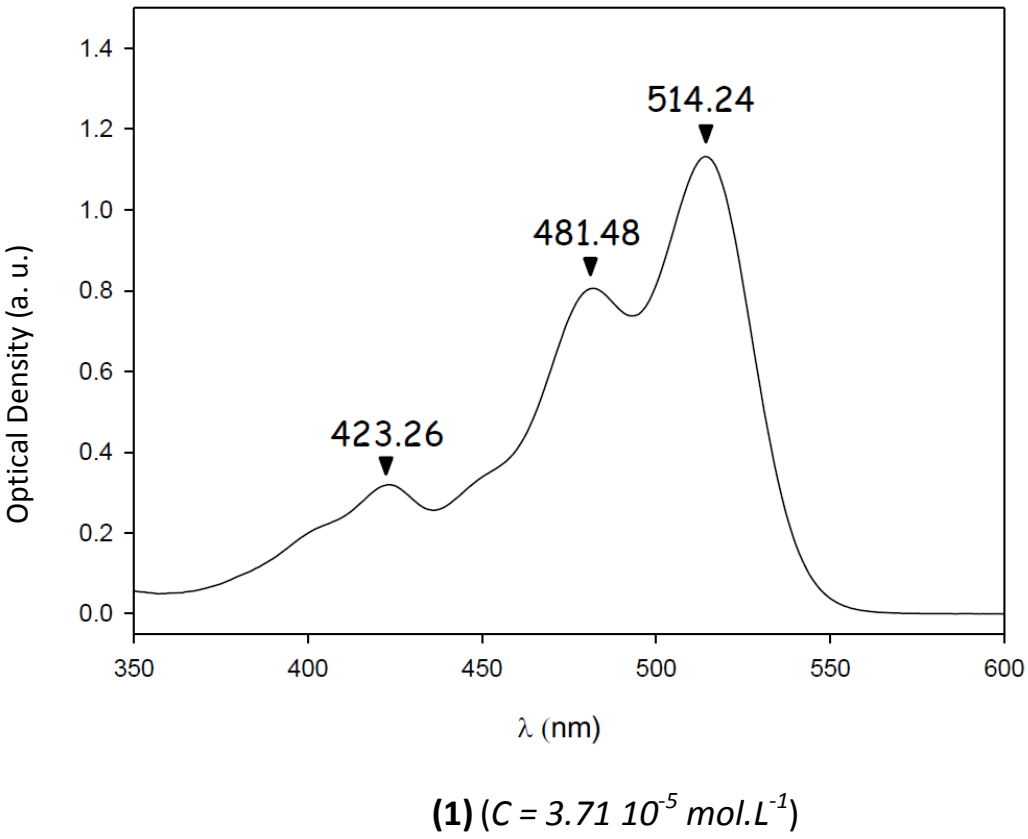
Figure S4. Overlap modes for (a) PDI-(*Cl*$_4$)-[C_2H_4OH][4-(*n*-C_5H_{11})]; (b) PDI-(*Cl*$_4$)-[4-(*n*-$C_{12}H_{25}$)C_6H_4]; (c) PDI-(*Cl*$_4$)-[Gly-Ala(OEt)]$_2$, **2a**; and (d) PDI-(*Cl*$_4$)-[Gly-Val(OEt)]$_2$, **2b**.



(2a) ($C = 1.19\ 10^{-5}\ mol.L^{-1}$)



(2b) ($C = 2.23\ 10^{-5}\ mol.L^{-1}$)



(1) ($C = 3.71\ 10^{-5}\ mol.L^{-1}$)

Figure S1. UV-visible absorption spectra for dichloromethane solutions of **2a-b** and tetrahydrofurane solutions of **1**.

Electrochemical experiments were carried out with a Biologic SP-150 potentiostat at 293 K. Cyclic voltammetry was performed in a three-electrode cell equipped with a platinum-plate counter electrode and a platinum working electrode (0.125 cm^2). Reference electrode was $Ag/AgNO_3$ (0.01 M CH_3CN) and all the potentials are reported *vs*. Fc^+/Fc.

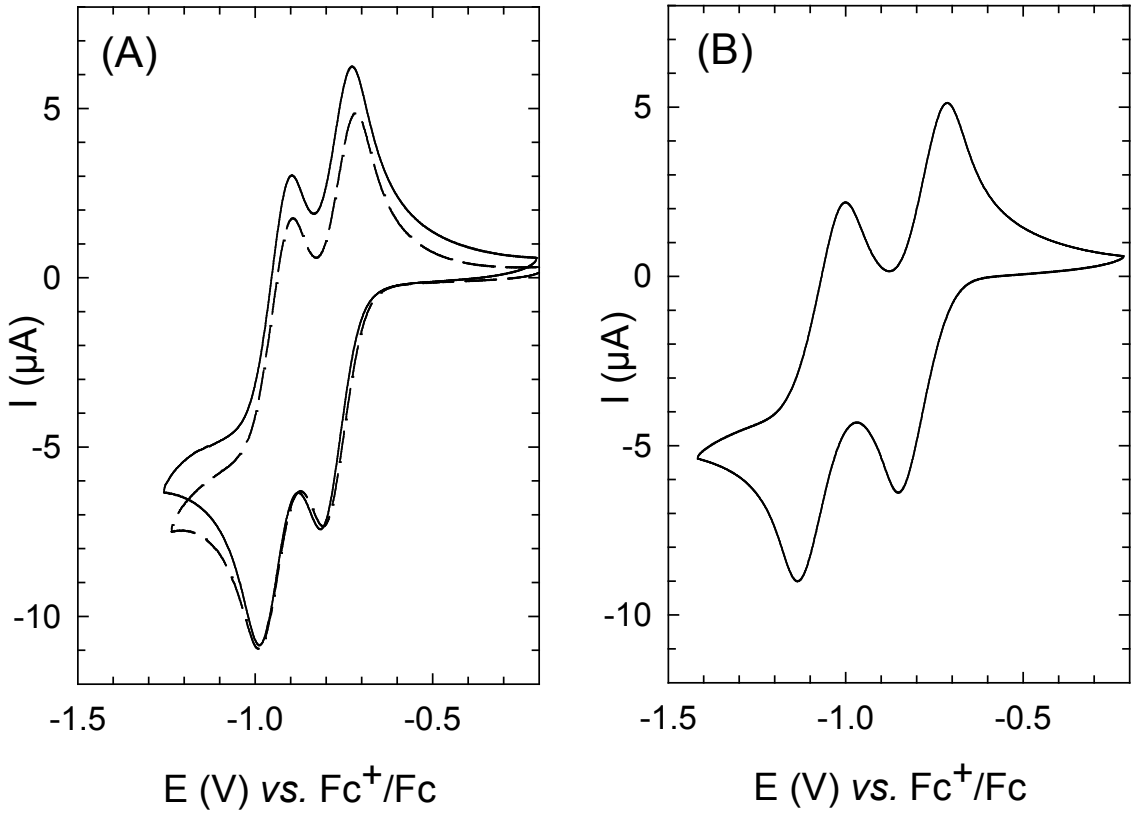
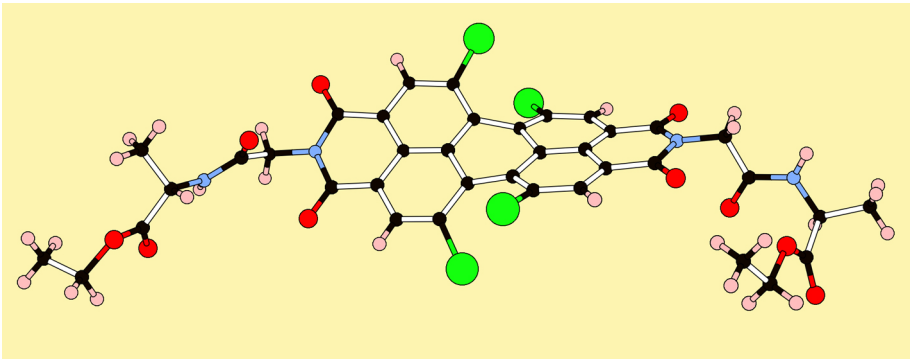
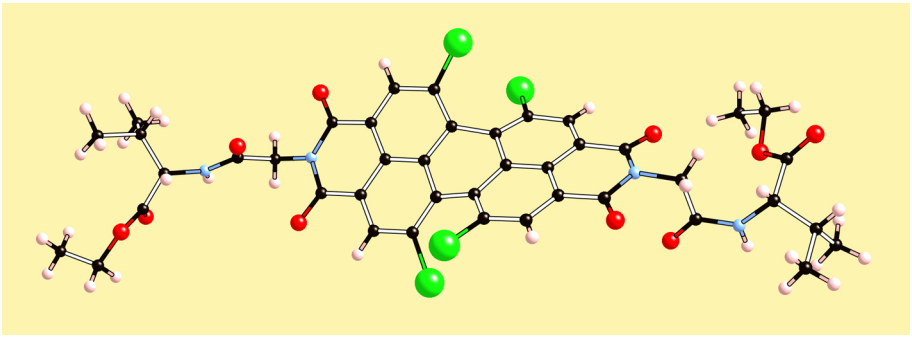


Figure S2. (A) Cyclic voltammograms (CVs) of compounds **2a** (solid line) and **2b** (dash line) in 0.1 M nBu_4NPF_6/CH_2Cl_2, (B) CV of precursor **1** in 0.1 M nBu_4NPF_6/THF. All CVs were performed at 0.1 V s^{-1}.

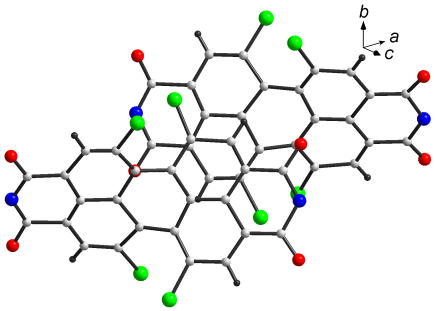


(a)

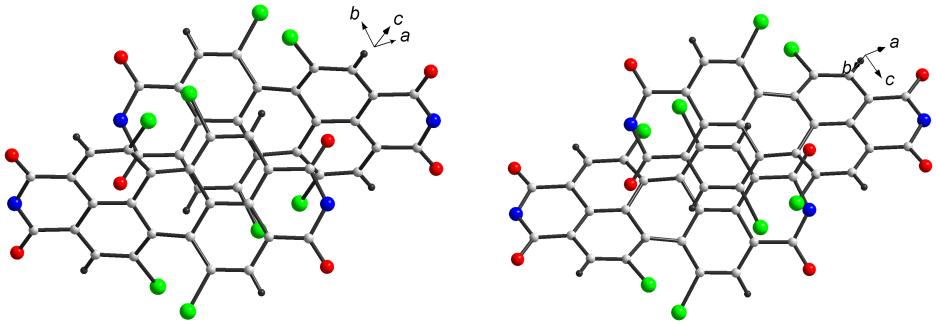


(b)

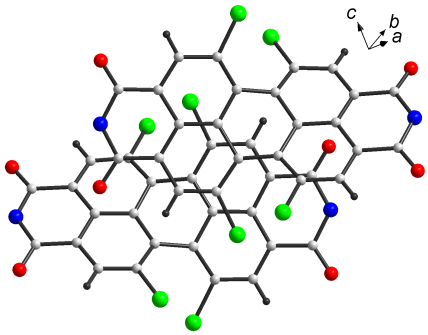
Figure S3. Molecular conformations of PDI-(Cl_4)-[Gly-Ala(OEt)]$_2$, **2a** (Fig. S3a) and PDI-(Cl_4)-[Gly-Val(OEt)]$_2$, **2b** (Fig. S3b) in the solid state.



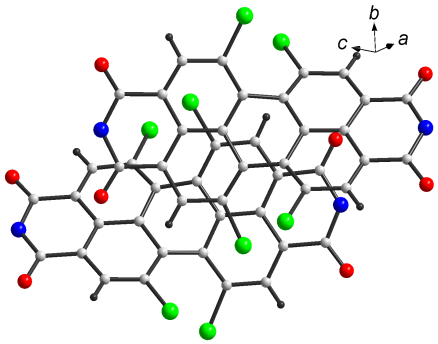
(a)



(b)



(c)



(d)

Figure S3. Overlap modes for (a) PDI-(*Cl*$_4$)-[C_2H_4OH][4-(*n*-C_5H_{11})]; (b) PDI-(*Cl*$_4$)-[4-(*n*-$C_{12}H_{25}$)C_6H_4]; (c) PDI-(*Cl*$_4$)-[Gly-Ala(OEt)]$_2$, **2a**; and (d) PDI-(*Cl*$_4$)-[Gly-Val(OEt)]$_2$, **2b**.