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

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Auteur	Lemouchi, Cyprien [1], Simonov, Sergey [2], Zorina, Leokadiya [3], Gautier, Christelle [4], Hudhomme, Piétrick [5], Batail, Patrick [6]
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Résumé en anglais	A methodology is proposed to provide direct access in good yields to peptide residues-appended perylenediimides PDI-(Cl-4)-[Gly-Ala(OEt)](2), 2a, PDI-(Cl-4)-[Gly-Val(OEt)](2), 2b and PDI-(Cl-4)-[Gly-Gly(OEt)](2), 2c from a generic perylenediimide (PDI) platform symmetrically functionalized with carboxylic acids at the imide sites, PDI-(Cl-4)-[Gly(OH)](2), 1. The latter is obtained in good purity by a non classical two-steps route avoiding the many, notoriously cumbersome successive chromatography steps typical of PDI chemistry, and including a single final purification allowing to crystallize the water soluble pure diacid 1, of great interest in its own right for further developments in a variety of fields. Then, the synthesis, crystallization and analysis of the crystal structures of 2a and 2b reveal a common pattern of self-assembly of the outer peptide residues based on collections of parallel N-H center dot center dot center dot O peptidic hydrogen bonds running alongside stacks where the constraints imposed upon on the inner PDI skeletons by long range interaction of these parallel electric dipoles reduce the dihedral angles around the bay regions by as much as 11% down to 32 degrees.
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