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Biocompatible pillar[5]arene-based ionic liquids containing amino acid fragments as potential water treatment systems

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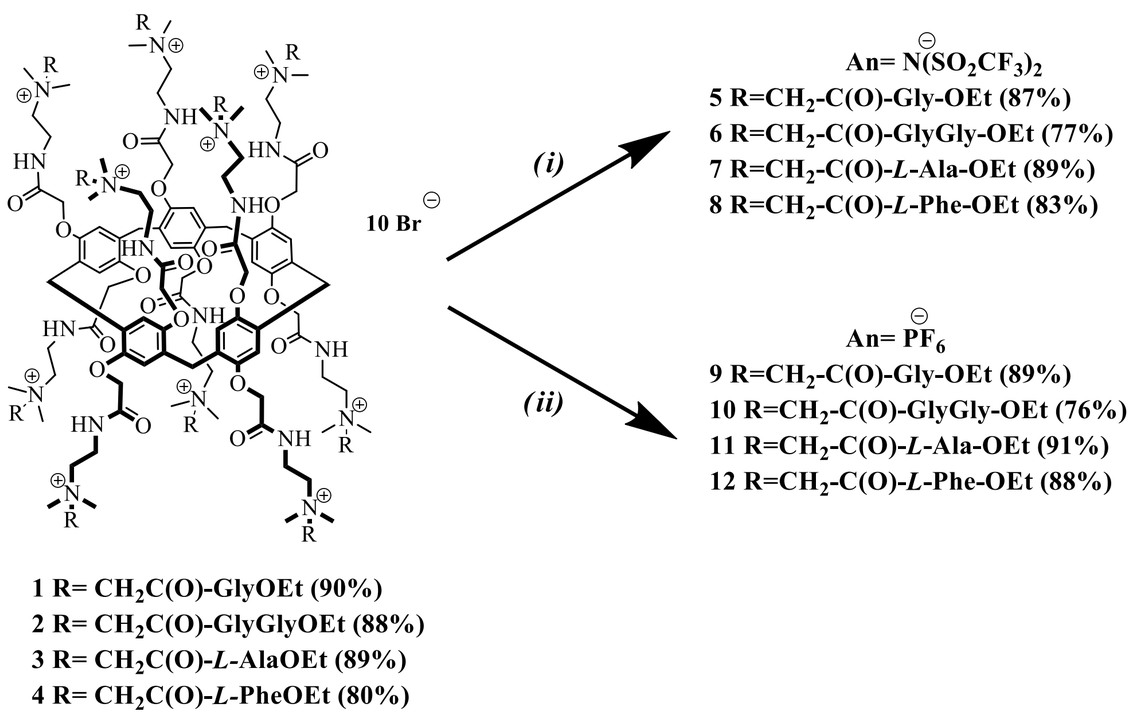
INTRODUCTION & AIM

Ionic liquids (**IL**s) are a rapidly growing area of technology and materials science due to their unique properties such as adsorption, recyclability, polarity, and thermal and electrochemical stability. Pillar[5]arenes are a new class of molecular receptors that have proven to be effective drug delivery systems by forming "host-guest" complexes and agents for the selective recognition of biopolymers. The development of ILs based on a non-toxic biomimetic macrocyclic pillar[5]arene platform will lead to a new generation of materials with programmable properties. The purpose of this work is the synthesis of new **IL**s based on decasubstituted pillar[5]arenes with amino acid fragments (glycine, glycylglycine, *L*-alanine, and *L*-phenylalanine) and the study of their thermal stability and the effect of substituents and counterions, as well as the absorption of water-soluble pollutants.



Scheme 1. (*i*) $LiN(SO_2CF_3)_2$, H_2O; (*ii*) KPF_6, H_2O.

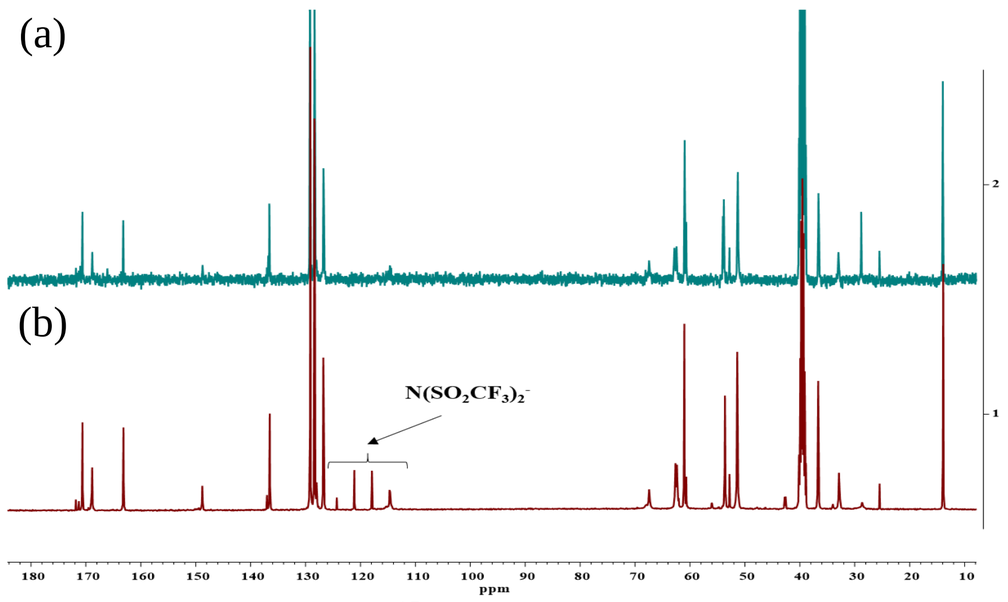


Figure 1. Fragments of ^{13}C NMR spectra of compound **4** (a), **8** (b) (DMSO-d_6, 25ºC, 100 MHz).

Table 1. Melting points (°C) of macrocycles **1-12**.

R-	Counter ion		
	Hal⁻	**$N(SO_2CF_3)_2^-$**	**PF_6^-**
CH_2-C(O)-Gly-OEt	119 (**1**)	57 (**5**)	88 (**9**)
CH_2-C(O)-GlyGly-OEt	121 (**2**)	74 (**6**)	82 (**10**)
CH_2-C(O)-L-Ala-OEt	120 (**3**)	63 (**7**)	81 (**11**)
CH_2-C(O)-L-Phe-OEt	93 (**4**)	61 (**8**)	68 (**12**)

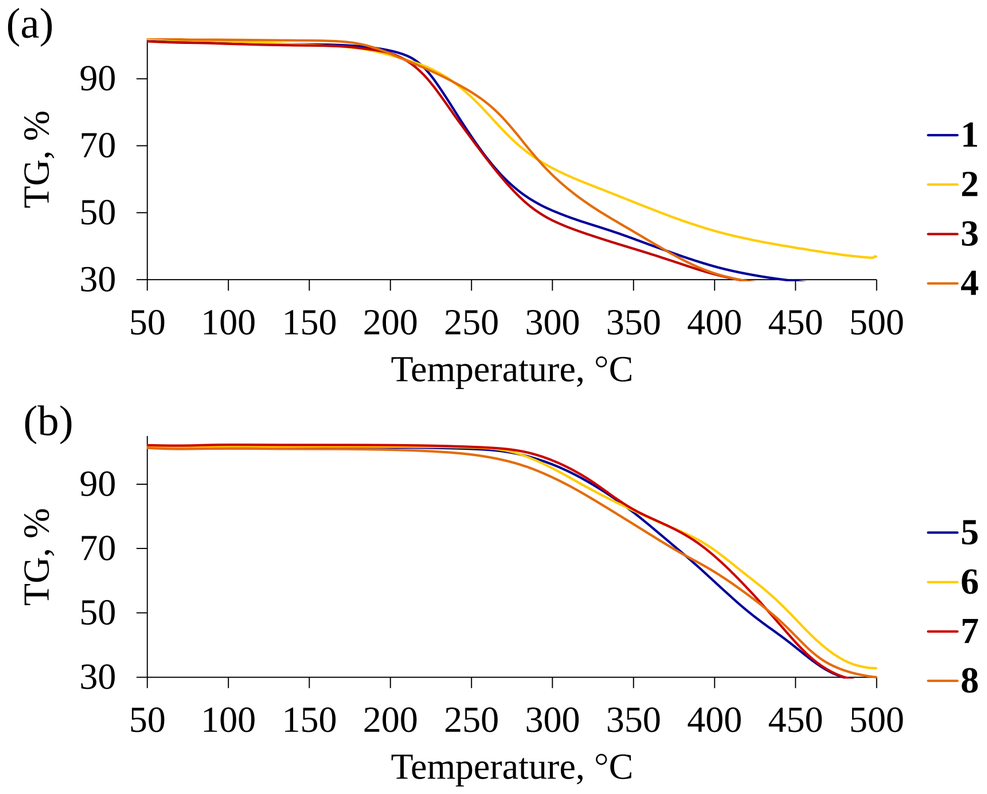


Figure 2. TG curves of the compounds **1-4** (a), and obtained **IL**s **5-8** (b).

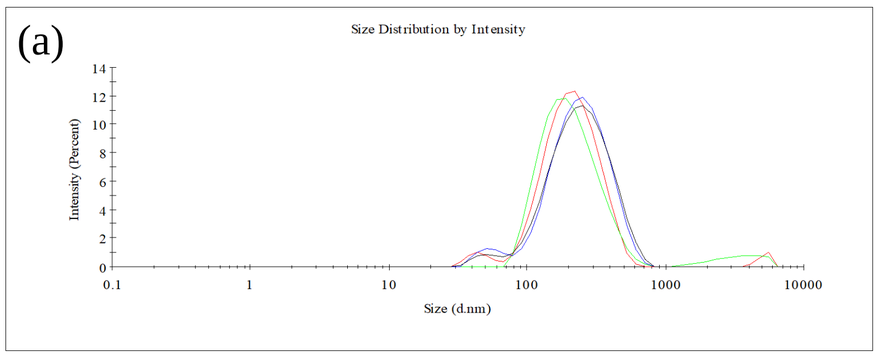


Figure 3. Size distribution of associates formed by macrocycle **1** and **PC** at 1:1 ratio (H_2O, C=1×10^{-4} M) (a), procaine (**PC**) structure (b).

CONCLUSION

In this work, macrocyclic **IL**s based on biomimetic derivatives of pillar[5]arene were synthesized for the first time. The dependence of the melting temperature on the structure of the macrocycle and the nature of the introduced amino acid fragment was revealed. Replacement of halide ions by **$N(SO_2CF_3)_2^-$** leads to a significant decrease in the melting temperature of the studied pillar[5]arenes 57-74 °C, as compared to **PF_6^-** 68-88 °C. An increase in the thermostability of the obtained **IL**s compared to water-soluble derivatives **1-4** was shown. The ability of macrocycles **1-4** to interact with the water-soluble drug procaine was investigated. Pillar[5]arenes **1** and **2** are able to form monodisperse systems with **PC** with an average particle diameter of about 200 nm. Further, the ability of **IL**s **5-12** to absorb **PC** from aqueous solution was investigated and it was shown that **IL**s **9**, **10** exhibit the highest absorption ability, according to UV-visible absorption spectroscopy.

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