Synthesis of new fluorescent amino acids with triazolopyridine core: Diacids sensors

ESI

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S1: Materials and Methods
S2: $^1$H NMR Spectra of starting material
S3: NMR Spectra of new compounds
S1: Materials and Methods

Starting materials, if commercially available, were purchased and used as such. The solvents used were of spectroscopic or equivalent grade. When known compounds had to be prepared by literature procedures, pertinent references are given. Melting points or ranges (m.p.) given were determined on a Büchi B-545 heated stage. $^1$H and ($^1$H decoupled) $^{13}$C nuclear magnetic resonance (NMR) spectra were recorded at 300 and 75 MHz. Chemical shifts are reported in δ units, parts per million (ppm), and were measured relative to the signals for residual deuterated Chlorophrom or deuterated methanol. Coupling constants (J) are given in Hz. Coupling patterns are abbreviated as, for example, s (singlet), d (doublet), t (triplet), q (quartet), td (triplet of doublets), m (multiplet), app. s (apparent singlet) and br. (broad). COSY and DEPT/ed-HSQC experiments were performed for all compounds. IR spectra were recorded using FT-IR ATR. HRMS were recorded using TOF electro-spray ionization (ESI-positive). UV-Visible spectra were measured on an Agilent 8453 spectrometer equipped with a Peltier temperature controller system (±0.1 °C). The emission spectra were recorded with a PTI MO- 5020 spectrofluorimeter in the 300–700 nm range.
S2: $^1$H NMR Spectra of starting material
S3: NMR Spectra of new compounds

(2S)-2-[[6-([1,2,3]triazolo[1,5-a]pyridin-3-yl)pyridin-2-yl-amino] propanoic acid 4a.

(2S)-3-Methyl-2-[[6-([1,2,3]triazolo[1,5-a]pyridin-3-yl)pyridin-2-yl]amino] butanoic acid 4b

(2S)-1-[6-([1,2,3]Triazolo[1,5-a]pyridin-3-yl)pyridin-2-yl] pyrrolidine-2-carboxylic acid. 4c

(2S)-3-(1H-Indol-3-yl)-2-[[6-([1,2,3]triazolo[1,5-a]pyridin-3-yl)pyridin-2-yl]amino} propanoic acid. 4d

(2S)-3-(4-Hydroxyphenyl)-2-[[6-([1,2,3]triazolo[1,5-a]pyridin-3-yl)pyridin-2-yl]amino} propanoic acid 4e

(2S)-3-Phenyl-2-[[6-([1,2,3]triazolo[1,5-a]pyridin-3-yl)pyridin-2-yl]amino] propanoic acid. 4f
4a

MeOD-d₄

*= AcOEt #= EtOH &_= Cl₃CH
MeOD-d₄

4a

*= AcOEt #= EtOH & Cl₃CH
MeOD-d₄


**Chemical Structure**

![Chemical Structure Image]

**Image Description**

The image contains a chemical structure labeled as **4c**. The molecule consists of atoms and bonds that form a specific compound. The structure is shown in a diagram format, with labels indicating different parts of the molecule.

**Solvent**

The solvent used is **CDCl₃**.

**NMR Spectrum**

The image also includes an NMR (Nuclear Magnetic Resonance) spectrum, which is a graphical representation of the chemical shifts and multiplets of the protons in the molecule. The x-axis represents the chemical shift in ppm, while the y-axis represents the resonance intensity.
DEPT-135
CDCl₃

4c
1D-NOE experiences with compound 4c
MeOD-d$_4$

4f