CHEMISTRY
A EUROPEAN JOURNAL

Supporting Information

Tuning the stacking properties of C_3-symmetrical molecules by modifying a dipeptide motif

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Supporting information

Chiral HPLC

Compound **6a** was in first instance obtained via direct coupling of glycyl-L-phenylalanine with 3,4,5-trioctyloxyaniline. The product of this reaction was measured on the Daicel Chiralcel OD column (Figure SI_1 I (left)). The HPLC trace shows two broad peaks of which the area underneath each peak is almost equal. From this it can be deduced that compound **6a** racemized (e.e. = 0%). The synthetic routes towards compounds **6a-e** were then adjusted and the desired amino acids were reacted one-by-one. The HPLC trace of compound **6a** obtained via the second synthetic approach is shown in Figure SI_1 II (right). By applying this new synthetic route racemization is suppressed to less than 1%.

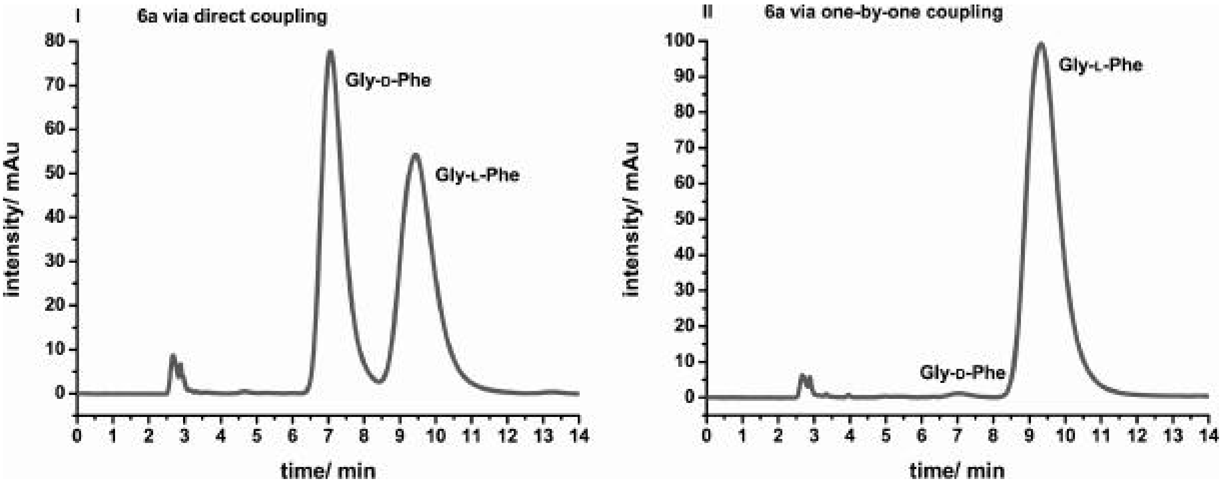

Figure SI_1. Chiral HPLC traces for compounds **6a** measured on a Daicel Chiralcel OD column; I (left) via direct coupling and II (right) via one-by-one coupling; eluent: isopropanol/hexane 1/9 (v/v); λ = 260 nm; c = 0.35 mg.mL^{-1}; injection volume = 5 μL.

Figure SI_2 I (left) shows that compounds **6b**, **6c** and **6e** can be baseline-separated using the Pirkle-type column. Compounds **6b** and **6d** cannot be separated using this column. The Daicel Chiralcel OD column was then used to try to separate compounds **6b** and **6d**. Figure SI_2 II (right) shows that the two compounds can be separated although the peaks are not completely baseline-separated.

Nevertheless, the obtained separation is good enough to determine whether a mixture of these two molecules is present or not. Using both graphs depicted above the optical purity of each of the molecules can be calculated. The enantiomeric excess (e.e.) of all molecules appears to be > 99%.

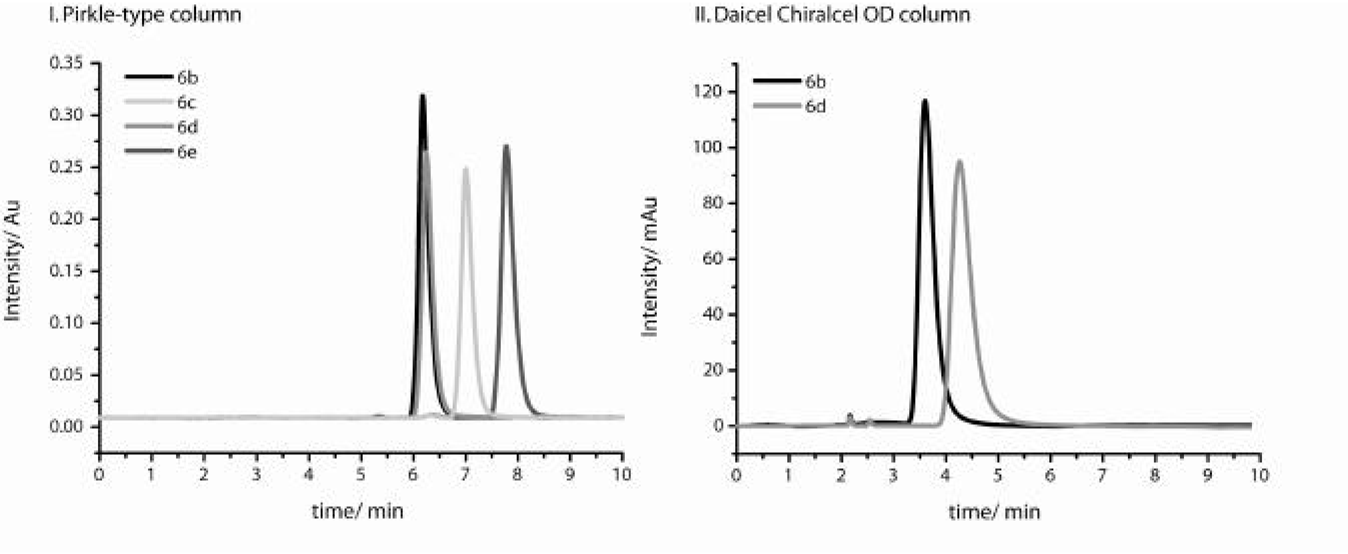

Figure SI_2. Chiral HPLC traces for compounds **6b-e** measured on a Pirkle-type column (I) and on a Daicel Chiralcel OD column; eluent: isopropanol/hexane 1/9 (v/v); λ = 260 nm; c = 0.5 mg/mL; injection volume = 20 μL.

DSC diagrams

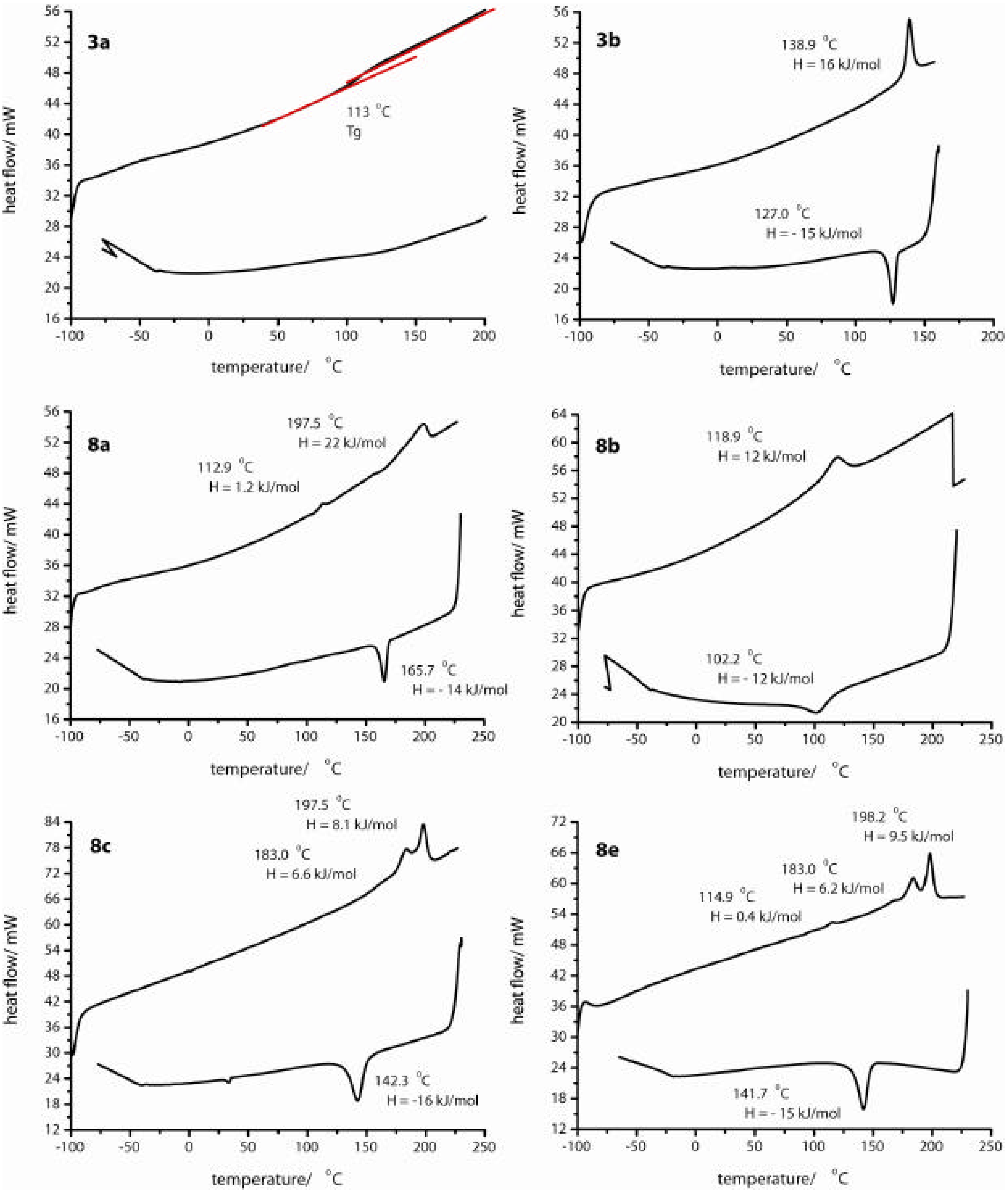

Figure SI_3. The maxima of the transitions T [°C] and the corresponding enthalpies ?H [kJ.mol^{-1}] for compounds **3a-b** and **8a-e** (third heating run; 40 °C.min^{-1}).

Temperature dependent CD

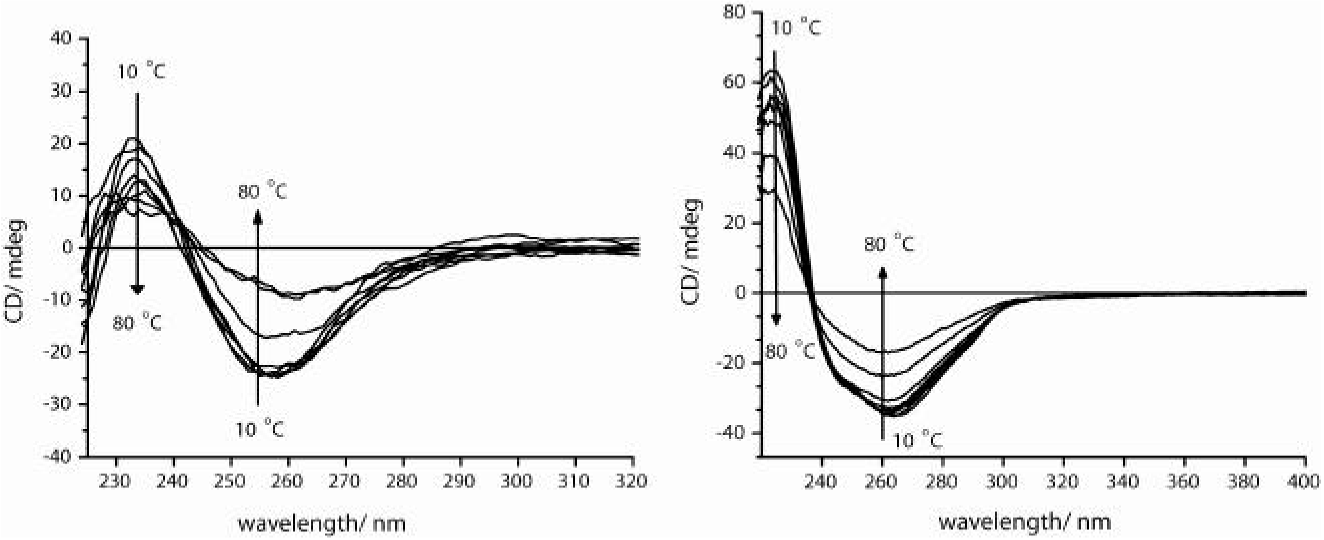

Figure SI_4. Temperature dependent CD measurements for compounds **3a** (left) and **8a** (right) at ? = 255 nm and ? = 263 nm, respectively, in heptane, 2 × 10^{-5} M from 10 °C in steps of 10 °C to 80 °C.

XRD diagrams of compound 3a.

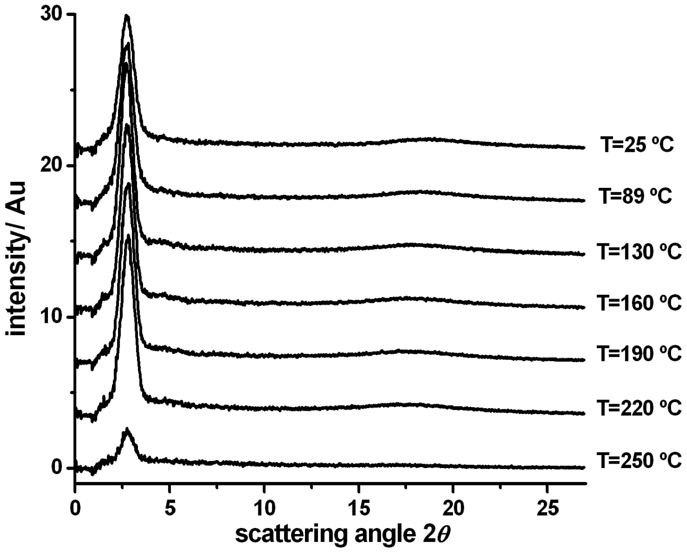

Figure SI_5. XRD diagrams of compound **3a** at different temperatures.