Supporting information

Axially Chiral Trifluoromethylbenzimidazolylbenzoic Acid: A Chiral Derivatizing Agent for α-Chiral Primary Amines and Secondary Alcohols to Determine Absolute Configuration

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Conformational stability of axially chiral acid 2 (TBBA)

A sample of enantiomerically pure acid 2 (5 mg/mL) in ethylene glycol was heated in a heating block Amigochem, which was preheated to the selected temperature. In time intervals, aliquots (200 µL) were taken, diluted with MeOH (800 µL), and analyzed by chiral SFC. The racemization rate constant $k_{\text{rac}}$ was calculated according to Equation 1 (the value shown is the average value of $k_{\text{rac}}$) and, subsequently, this value was used in Equation 2 to calculate the energy barrier for racemization $\Delta G_{\text{rac}}^\ddag$. The half-life of racemization was calculated according to Equation 3. The lower $\Delta G_{\text{rac}}^\ddag$ value was used to calculate the rate constant and half-life of racemization at room temperature (table S1).

$$\ln \left( \frac{R_0}{R_0 - x} \right) = k_{\text{rac}} \cdot t$$

Eq. 1

$$\Delta G_{\text{rac}}^\ddag = -RT \ln \left( \frac{hk_{\text{rac}}}{\kappa T k_B} \right)$$

Eq. 2

$$t_{1/2_{\text{rac}}} = \frac{\ln 2}{k_{\text{rac}}}$$

Eq. 3

$R_0$ = initial concentration of the enantiomer, $x$ = concentration of the racemate at time $t$, $h$ = Planck constant, $k_B$ = Boltzman constant, $\kappa$ = transimission coefficient (equals to 1), $T$ = temperature, $R$ = gas constant, $k_{\text{rac}}$ = racemization rate constant, $\Delta G_{\text{rac}}^\ddag$ = energy barrier for racemization, $t_{1/2_{\text{rac}}}$ = half-life of racemization

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SFC chromatograms of acid 2

Racemic mixture

Enantiopure samples: (M)-TBBA (top), (P)-TBBA (bottom)

Conditions:
90% CO2, 10% MeOH +0,1% DEA + 0,1% TFA + 1% H2O, column CHIRALPAK IA3,
flow: 2,2 ml/min, column temperature: 38˚C, abpr: 2000, make-up pump flow: 0,45 ml/min (MeOH)
Relevant conformers of compounds \((R,P/M)-8\) and \((R,P/M)-20\)

**Compound \((R,P)-8\)**

- **Most stable conformer**
  - Boltzmann weight: 0.414
  - NMR irrelevant: non-selective shielding of both substituents at the same time

- **2nd most stable**
  - \(\Delta G = +1.01 \text{ kJ/mol}\)
  - Boltzmann weight: 0.276
  - NMR relevant: selective shielding on methyl substituent

- **3rd most stable**
  - \(\Delta G = +1.99 \text{ kJ/mol}\)
  - Boltzmann weight: 0.186
  - NMR irrelevant: shielding effect is not produced on any of the substituents

- **4th most stable**
  - \(\Delta G = +3.06 \text{ kJ/mol}\)
  - Boltzmann weight: 0.120
  - NMR irrelevant: shielding effect is not produced on any of the substituents
**Compound (R,M)-8**

Most stable conformer
Boltzman weight: 0.60
NMR irrelevant: shielding effect is not produced on any of the substituents

2nd most stable ΔG= +1.15 kJ/mol
Boltzman weight: 0.378
NMR relevant: shielding effect produced selectively on phenyl substituent

**Compound (R,P)-20**

Most stable conformer
Boltzman weight: 0.579
NMR relevant

2nd most stable ΔG= +1.26 kJ/mol
Boltzman weight: 0.349
NMR irrelevant: shielding effect is not produced on any of the substituents

**Compound (R,M)-20**

Most stable conformer
Boltzman weight: 0.928
NMR irrelevant: shielding effect is not produced on any of the substituents

2nd Most stable conformer ΔG= +7.5 kJ/mol
Boltzman weight: 0.045
NMR relevant
### Compound (R,P)-8

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NMR spectra

Compound 4
Compound 5
Compound (P)-7

residual solvents from chromatography

residual DCM
Compound (M)-7
Compound (P)-8

Method B
Compound (M)-8
Method B

N N
H
C
H
F
F

140.48 140.72 141.0 141.5
f1 (ppm)
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115.68 117.80 119.96 121.99 122.13
124.56 125.81 126.58 127.61 128.80
129.54 130.28 130.97 131.33 131.81
135.36 137.47 140.48 140.72 141.10
141.40 141.89 164.25

140.48 140.72 141.0 141.5
f1 (ppm)
0.00 0.02 0.04 0.06 0.08
115.68 117.80 119.96 121.99 122.13
124.56 125.81 126.58 127.61 128.80
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135.36 137.47 140.48 140.72 141.10
141.40 141.89 164.25
Compound (P)-9
Method B
Compound (M)-9
Method B
Compound (P)-10

Method B

[Chemical structure and spectra diagrams]
Compound (M)-10

Method B
Compound (M)-11

Method B
Compound (P)-12

Method B
Compound (P)-13
Method B
Compound (M)-13
Method B

Chloroform-d

N
N
O
N
H
C
H
3
O
O
C
H
3
F
F
F

S36
Compound (P)-14
Method B
Compound (P)-15
Compound (M)-15

[Chemical Structure Image]
**Compound (M)-16**

[Chemical structure diagram]

**NMR Spectra**

- f1 (ppm) values:
  - 4.60, 4.65, 4.70
  - 2.60, 1.11, 1.13, 1.15
  - 1.02, 1.10, 1.13, 1.10
  - 1.07, 1.10, 1.06

**Chemical Shifts**

- Chloroform-d
  - 7.34, 7.71, 7.76, 7.93, 7.95, 8.24, 8.25, 8.26

**Spectral Data**

- Additional spectral data points are visible in the diagram, indicating the presence of various chemical shifts and peak intensities.
Compound (P)-17

The diagram shows the 1H NMR and 13C NMR spectra of Compound (P)-17. The 1H NMR spectrum displays peaks at various ppm values, indicating the chemical shifts of the protons in the molecule. The 13C NMR spectrum shows the chemical shifts of the carbon atoms, with peaks at specific ppm values, including those for the fluorine atoms and the aromatic carbons. The structures of the compound are also depicted, highlighting the presence of fluorine atoms and oxygen functionalities.
Compound (P)-20

[Chemical structure and NMR spectra]

Chloroform-d
Compound (M)-20

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Compound (P)-22
Compound (M)-22
Compound (P)-23
NMR assignment of compounds \((R,P/M)-8, (R,P/M)-20, (S,P/M)-22, (S,P/M)-23\)

Figure S1: Atom numbering used for Table S2

Compounds \((R,P)-8\) and \((R,M)-8\)

Compounds \((S,P)-20\) and \((S,M)-20\)

Compounds \((S,P)-14\) and \((S,M)-23\)

Compounds \((S,P)-15\) and \((S,M)-22\)
Table S2: $^1$H, $^{13}$C, $^{15}$N and $^{19}$F Chemical Shifts of Compounds (R,P)-8, (R,M)-8, (R,P)-20, (R,M)-20 in CDCl₃.

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$^a$ $\delta$($^{15}$N) $^b$ $J(^{19}$F, $^{13}$C) $^c$ $J(^{15}$N, $^{1}$H) = 89.5 Hz $^d$ $J(^{15}$N, $^{1}$H) = 89.1
In case of compounds (S,P)-22, (S,M)-22, (S,P)-23 and (S,M)-23 not all signals were assigned due to extensive overlaps and being further away from the chiral centre and therefore being less important for the structural assignment. Atom numbering is shown in figure S1.

Table S2 (cont.): $^1$H, $^{13}$C, $^{15}$N and $^{19}$F Chemical Shifts of Compounds (S,P)-22, (S,M)-22, (S,P)-23 and (S,M)-23 in CDCl$_3$.

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$^a$ $\delta$(15N)  $^b$ $\delta$(19F, 13C)  $^c$ $\delta$(15N, 1H) = 89.5 Hz  $^d$ $\delta$(15N, 1H) = 89.1
$^{1}H-^{19}F$-HOESY NMR spectra
In order to obtain more information about conformational model, especially, rotation of amidic moiety, $^{1}H-^{19}F$-HOESY experiment was conducted which showed following interactions (red).

Compound $(R,P)$-8
Compound (R,M)-8
X-ray structure determination of $\text{(R,P)-8}$

**Experimental details and results**

Crystals suitable for crystallographic study were obtained by a slow evaporation of ethyl acetate. Although many attempts to prepare single crystals, utilizing different types of solvents, mixtures of solvents as well as types of crystallizations such as evaporation of solvent(s) and diffusion techniques, were done and complete sets of X-ray data of several crystals were obtained, the experimentally studied crystal were not of good quality (Rint factors were higher that 0.13 in all the cases). This fact influenced the process of refinement of X-ray data as well as the final result. For all that, we believe that the obtained data ambiguously revealed and confirmed the molecular and crystal structures of $\text{(R,P)-8}$.

X-ray data collection of $\text{8R-P}$ was carried out on a D8 QUEST single crystal X-ray diffractometer (Bruker) equipped with a PHOTON 100 CMOS detector, using Mo–Ka radiation ($\lambda = 0.71073$ Å). The data collection and reduction were performed using the APEX3 software package. The structure was solved by a direct method (SHELXS) and refined with the Bruker Software Package [SHELXTL]. The F19a, F20a and F21a atoms were disordered over two positions. H-atoms were positioned theoretically and refined using a riding model. The structural data was deposited in the Cambridge Crystallographic Data Centre under the accession number CCDC 1871600. The graphics were drawn and additional structural calculations were performed by DIAMOND and Mercury software. The molecular structure is depicted in figure S2, crystal data and structure refinement can be found in Table S3.

The structure of $\text{(R,P)-8}$ consists of seven individual and crystallographically independent molecules situated within the unit cell (Figure S3). Moreover, the crystal structure is stabilized by hydrogen bonds of the N–H···O and N–H···N types (Figure S4) as well as some other non-covalent C–H···F, C–H···O and C–H···C contacts.

**Figure S2.** The molecular structure of $\text{(R,P)-8}$ (CCDC 1871600) together with the atom labelling scheme. The thermal ellipsoids are drawn at the 50% probability level. Only one of the seven crystallographically independent molecules is depicted for clarity.
Figure S3. A view of crystal packing of seven crystallographically independent molecules of \((R,P)-8\) within the unit cell.

Figure S4. A part of the crystal structure of \((R,P)-8\) showing the N–H···O and N–H···N hydrogen bonds (green dashed lines).

References
(S1) Wolf, C. Dynamic Stereochemistry of Chiral Compounds; 2007.
(S3) G. M. Sheldrick, Acta Cryst., 2015, C71, 3.
(S4) K. Brandenburg, Diamond Version 4.0.3., Crystal Impact GbR, Bonn, Germany (2015).
Table S3. Crystal data and structure refinement for (R,P)-8.

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