# READ ME File for *Data for the paper 'Minimising conformational bias in fluoroprolines through vicinal difluorination'*

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Raw data for the paper **“Minimising conformational bias in fluoroprolines through vicinal difluorination”**, authored by Gert-Jan Hofman, Emile Ottoy, Mark E. Light, Bruno Kieffer, Ilya Kuprov, José C. Martins, Davy Sinnaeve and Bruno Linclau.

NMR datasets are for Bruker TopSpin 3.

Ac-Pro-OMe

1. 1D 1H, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 1 s.
2. 1D 1H, solvent = D2O, T = 298 K, 500 MHz, D1 = 1 s.
3. 1D 1H, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 15 s. This experiment was used for the determination of the *cis/trans* ratios.
4. 1D 1H, solvent = D2O, T = 298 K, 500 MHz, D1 = 15 s. This experiment was used for the determination of the *cis/trans* ratios.

Ac-(4*R*)-FPro-OMe (**1**)

1. 1D 1H, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 1 s.
2. 1D 1H, solvent = D2O, T = 298 K, 500 MHz, D1 = 1 s.
3. 1D 19F with 1H decoupling, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 1.5 s.
4. 1D 19F with 1H decoupling, solvent = D2O, T = 298 K, 500 MHz, D1 = 1.5 s.
5. 1D 19F with 1H decoupling, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 15 s. This experiment was used for the determination of the *cis/trans* ratios.
6. 1D 19F with 1H decoupling, solvent = D2O, T = 298 K, 500 MHz, D1 = 15 s. This experiment was used for the determination of the *cis/trans* ratios.

Ac-(4*S*)-FPro-OMe (**2**)

1. 1D 1H, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 1 s.
2. 1D 1H, solvent = D2O, T = 298 K, 500 MHz, D1 = 1 s.
3. 1D 19F with 1H decoupling, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 1.5 s.
4. 1D 19F with 1H decoupling, solvent = D2O, T = 298 K, 500 MHz, D1 = 1.5 s.
5. 1D 19F with 1H decoupling, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 15 s. This experiment was used for the determination of the *cis/trans* ratios.
6. 1D 19F with 1H decoupling, solvent = D2O, T = 298 K, 500 MHz, D1 = 15 s. This experiment was used for the determination of the *cis/trans* ratios.

Ac-(3*R*)-FPro-OMe (**3**)

1. 1D 1H, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 1 s.
2. 1D 1H, solvent = D2O, T = 298 K, 500 MHz, D1 = 1 s.
3. 1D 19F with 1H decoupling, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 1.5 s.
4. 1D 19F with 1H decoupling, solvent = D2O, T = 298 K, 500 MHz, D1 = 1.5 s.
5. 1D 19F with 1H decoupling, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 15 s. This experiment was used for the determination of the *cis/trans* ratios.
6. 1D 19F with 1H decoupling, solvent = D2O, T = 298 K, 500 MHz, D1 = 15 s. This experiment was used for the determination of the *cis/trans* ratios.
7. 1D 19F with 1H decoupling, solvent = D2O, T = 308 K, 500 MHz, D1 = 15 s.
8. 2D 19F-19F EXSY with 1H decoupling, solvent = D2O, T = 308 K, 500 MHz, D1 = 15 s, τm = 500 ms.
9. 2D 19F-19F EXSY with 1H decoupling, solvent = D2O, T = 308 K, 500 MHz, D1 = 15 s, τm = 750 ms.
10. 2D 19F-19F EXSY with 1H decoupling, solvent = D2O, T = 308 K, 500 MHz, D1 = 15 s, τm = 1000 ms. These last four experiments were used to determine the *cis/trans* exchange rates.

Ac-4,4-F2Pro-OMe (**5**)

1. 1D 1H, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 1 s.
2. 1D 1H, solvent = D2O, T = 298 K, 500 MHz, D1 = 1 s.
3. 1D 19F with 1H decoupling, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 1.5 s.
4. 1D 19F with 1H decoupling, solvent = D2O, T = 298 K, 500 MHz, D1 = 1.5 s.
5. 1D 1H, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 15 s. This experiment was used for the determination of the *cis/trans* ratios.
6. 1D 1H, solvent = D2O, T = 298 K, 500 MHz, D1 = 15 s. This experiment was used for the determination of the *cis/trans* ratios.
7. 1D 1H, solvent = D2O, T = 308 K, 500 MHz, D1 = 15 s.
8. 2D 1H-1H EXSY, solvent = D2O, T = 308 K, 500 MHz, D1 = 15 s, τm = 500 ms.
9. 2D 1H-1H EXSY, solvent = D2O, T = 308 K, 500 MHz, D1 = 15 s, τm = 750 ms.
10. 2D 1H-1H EXSY, solvent = D2O, T = 308 K, 500 MHz, D1 = 15 s, τm = 1000 ms. These last four experiments were used to determine the *cis/trans* exchange rates.

Ac-(3*S*,4*R*)-F2Pro-OMe (**7**)

1. 1D 1H, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 1 s.
2. 1D 1H, solvent = D2O, T = 298 K, 500 MHz, D1 = 1 s.
3. 1D 19F, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 1.5 s.
4. 1D 19F, solvent = D2O, T = 298 K, 500 MHz, D1 = 1.5 s.
5. 1D 1H, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 15 s. This experiment was used for the determination of the *cis/trans* ratios.
6. 1D 1H, solvent = D2O, T = 298 K, 500 MHz, D1 = 15 s. This experiment was used for the determination of the *cis/trans* ratios.
7. 2D 1H-1H NOESY, solvent = CDCl3, T = 298 K, 500 MHz, D1 = 1 s, τm = 600 ms. This experiment was used for the assignment of the rotamers.
8. 2D 1H-1H NOESY, solvent = D2O, T = 298 K, 500 MHz, D1 = 1 s, τm = 600 ms. This experiment was used for the assignment of the rotamers.
9. 1D 1H, solvent = D2O, T = 308 K, 500 MHz, D1 = 15 s.
10. 2D 1H-1H EXSY, solvent = D2O, T = 308 K, 500 MHz, D1 = 15 s, τm = 500 ms.
11. 2D 1H-1H EXSY, solvent = D2O, T = 308 K, 500 MHz, D1 = 15 s, τm = 750 ms.
12. 2D 1H-1H EXSY, solvent = D2O, T = 308 K, 500 MHz, D1 = 15 s, τm = 1000 ms. These last four experiments were used to determine the *cis/trans* exchange rates.