

SUPPLEMENTARY MATERIALS

Preliminary SAR of a novel series of pyrazole SKF-96365 analogues as potential Store-Operated Calcium Entry (SOCE) inhibitors

Camille D. Dago^{1,2}, Paul Le Maux¹, Thierry Roisnel³, Christophe Brigaudeau^{4,5}, Yves-Alain Bekro², Olivier Mignen^{4,5,*} and Jean-Pierre Bazureau^{1,6,*}

¹ Institut des Sciences Chimiques de Rennes (ISCR), UMR CNRS 6226, groupe CORINT, Université de Rennes 1 (UR1), Campus de Beaulieu, Bât. 10A, 263 Avenue du Général Leclerc, CS 74205, 35042 Rennes Cedex, France

² Laboratoire de Chimie Bio Organique et de Substances Naturelles (LCBOSN), Université Nangui Abrogoua (UNA), BP 802, Abidjan, Côte d'Ivoire

³ Institut des Sciences Chimiques de Rennes (ISCR), UMR CNRS 6226, Centre de Diffractométrie X (cdifx), Université de Rennes 1 (UR1), Campus de Beaulieu, Bât. 10B, 263 Avenue du Général Leclerc, CS 74205, 35042 Rennes Cedex, France

⁴ Laboratoire Canalopathies & Signalisation Calcique, Inserm U1277, Université de Bretagne Occidentale (UBO), 22 Avenue Camille Desmoulins, 29200 Brest Cedex, France

⁵ CalciScreen platform, Université de Bretagne Occidentale (UBO), 22 Avenue Camille Desmoulins, 29200 Brest Cedex, France

⁶ S2Wave platform SFS ScanMAT, Université de Rennes 1 (UR1), Campus de Beaulieu, Bât. 10A, 263 Avenue du Général Leclerc, CS 74205, 35042 Rennes Cedex, France

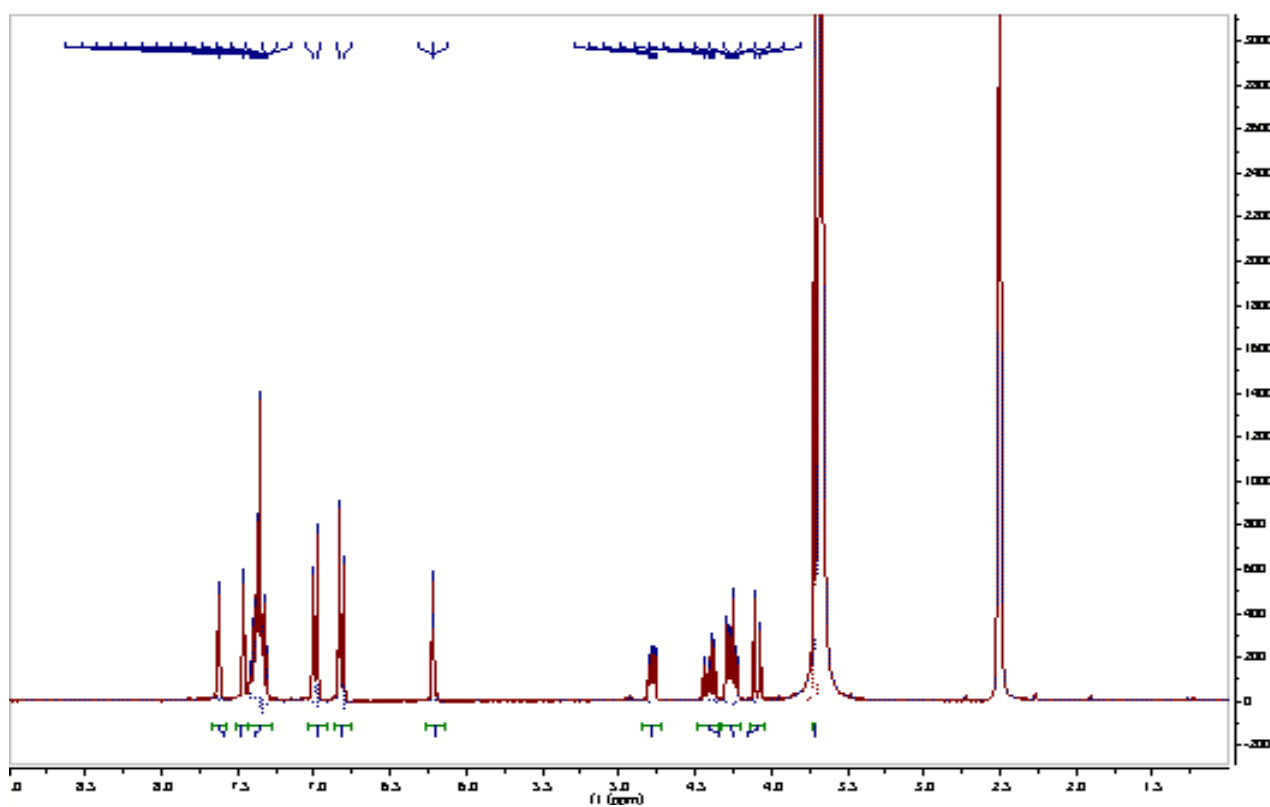
Fax: +33 (0)223 236 374. Phone: +33(0)2 223 236 603.

E-mail: jean-pierre.bazureau@univ-rennes1.fr

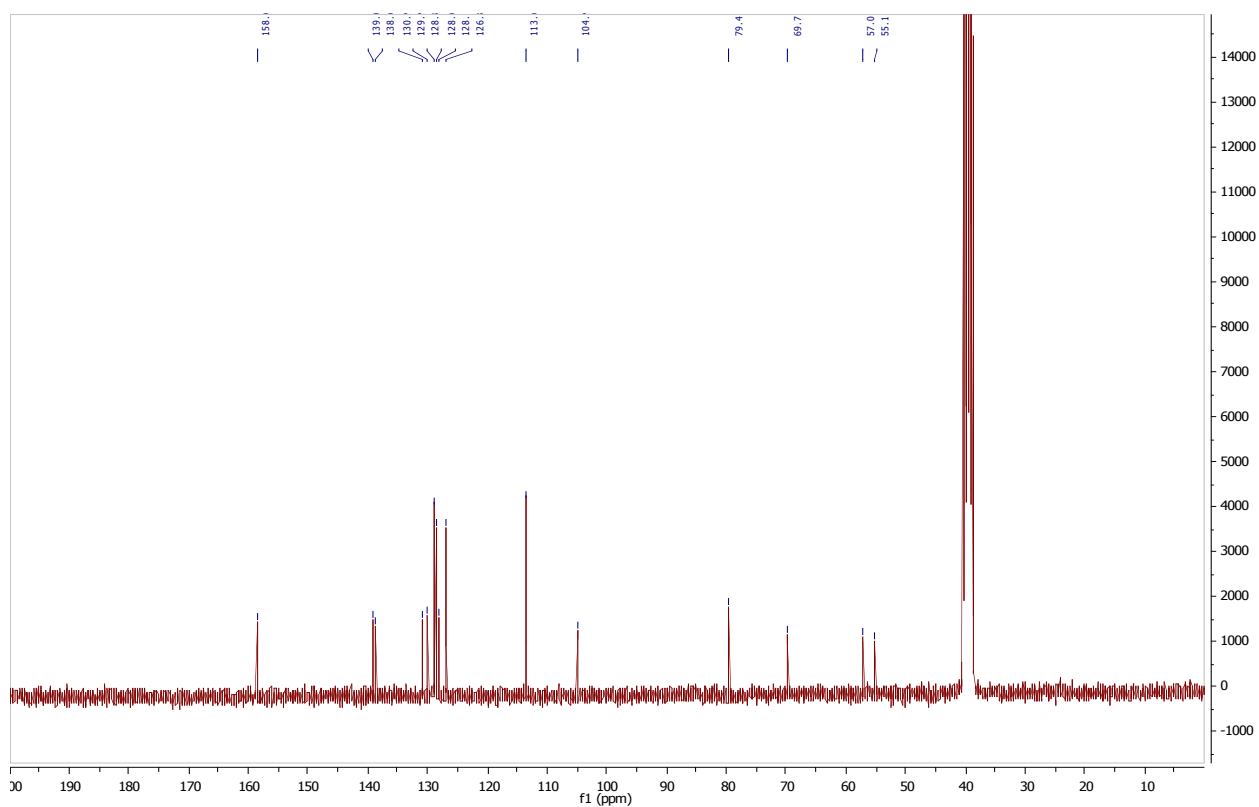
Part 1:

- ¹H NMR in DMSO-*d*₆ solution of isolated (*IR*, *IS*) 1-[β-(phenylalkoxy)-phenethyl]-1*H*-pyrazolium hydrochloride (**7a-e**)
- ¹³C NMR in DMSO-*d*₆ solution of isolated (*IR*, *IS*) 1-[β-(phenylalkoxy)-phenethyl]-1*H*-pyrazolium hydrochloride (**7a-e**)

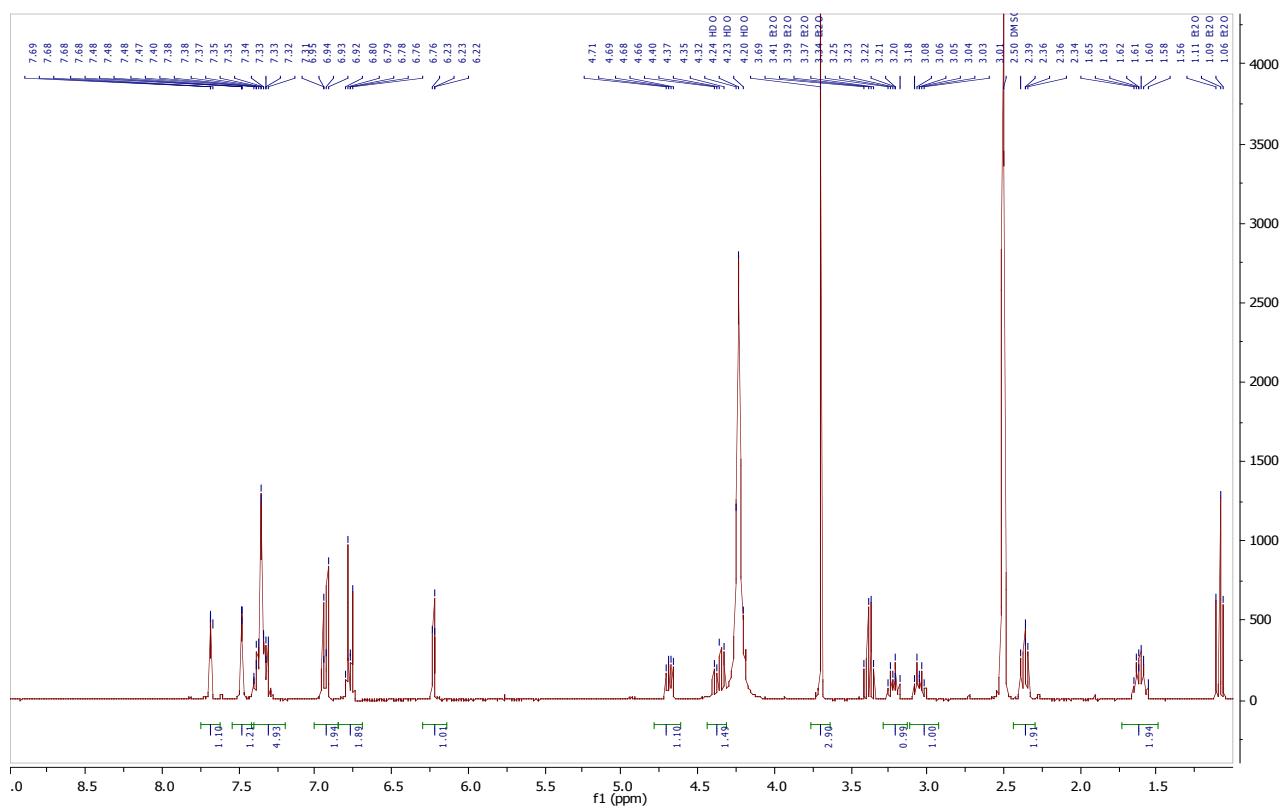
- ^1H NMR in $\text{DMSO-}d_6$ solution of (*1R, 1S*) 1-[β -((4-methoxybenzyl)oxy)-phenethyl]-1*H*-pyrazolium hydrochloride (**7a**)



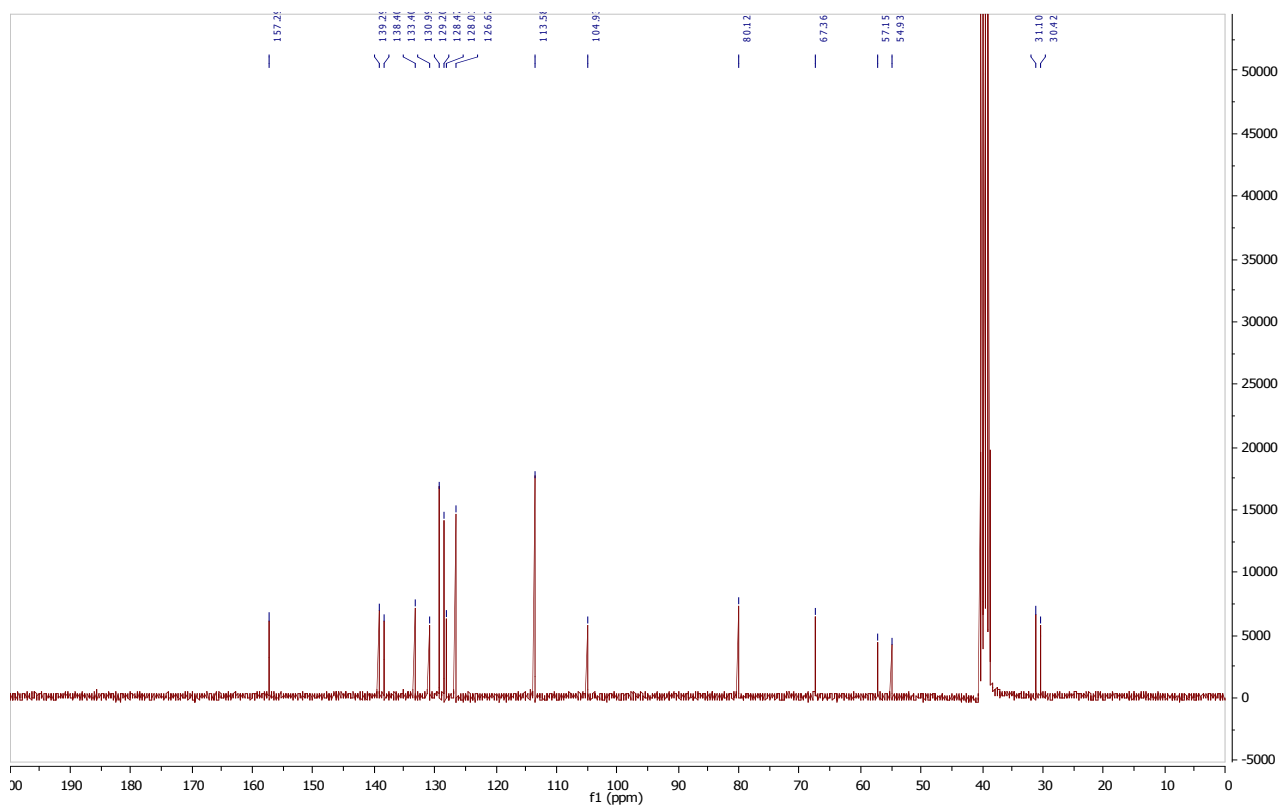
- ^{13}C NMR in $\text{DMSO-}d_6$ solution of (*1R, 1S*) 1-[β -((4-methoxybenzyl)oxy)-phenethyl]-1*H*-pyrazolium hydrochloride (**7a**)



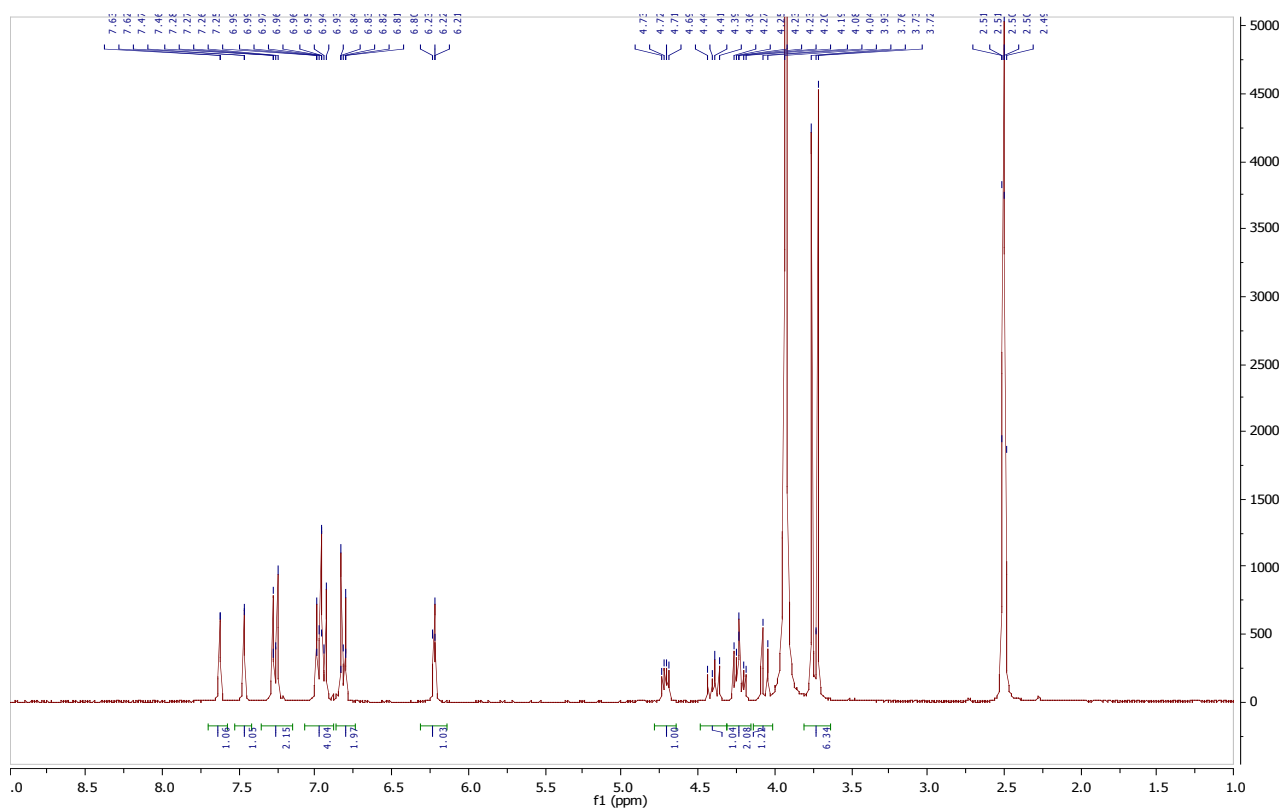
- ^1H NMR in $\text{DMSO-}d_6$ solution of (*1R, 1S*) 1-[β -((3-(4-methoxyphenyl)propyl)oxy)-phenethyl]-1*H*-pyrazolium hydrochloride (**7b**)



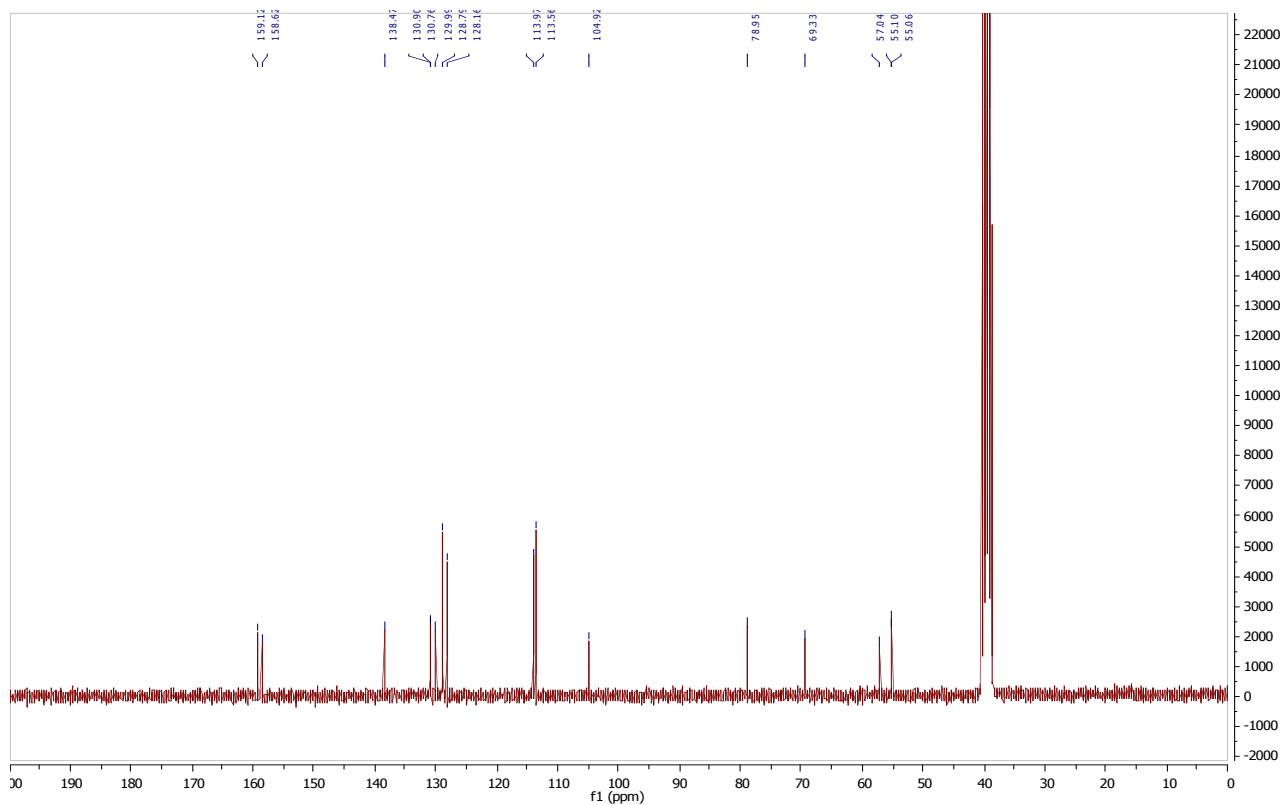
- ^{13}C NMR in $\text{DMSO-}d_6$ solution of (*1R, 1S*) 1-[β -((3-(4-methoxyphenyl)propyl)oxy)-phenethyl]-1*H*-pyrazolium hydrochloride (**7b**)



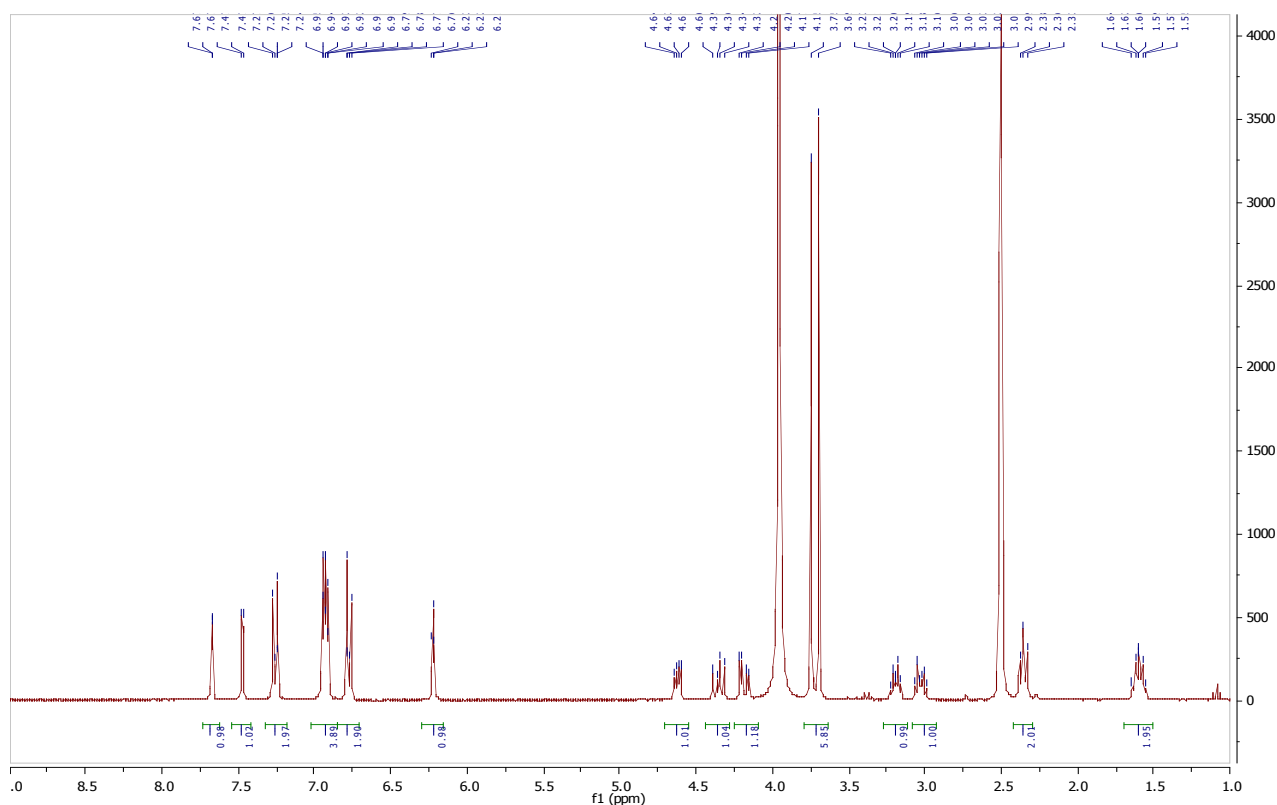
- ^1H NMR in $\text{DMSO-}d_6$ solution of (*IR*, *IS*) 1-[β -((4-methoxybenzyl)oxy)-(4-methoxyphenethyl)]-1*H*-pyrazolium hydrochloride (**7c**)



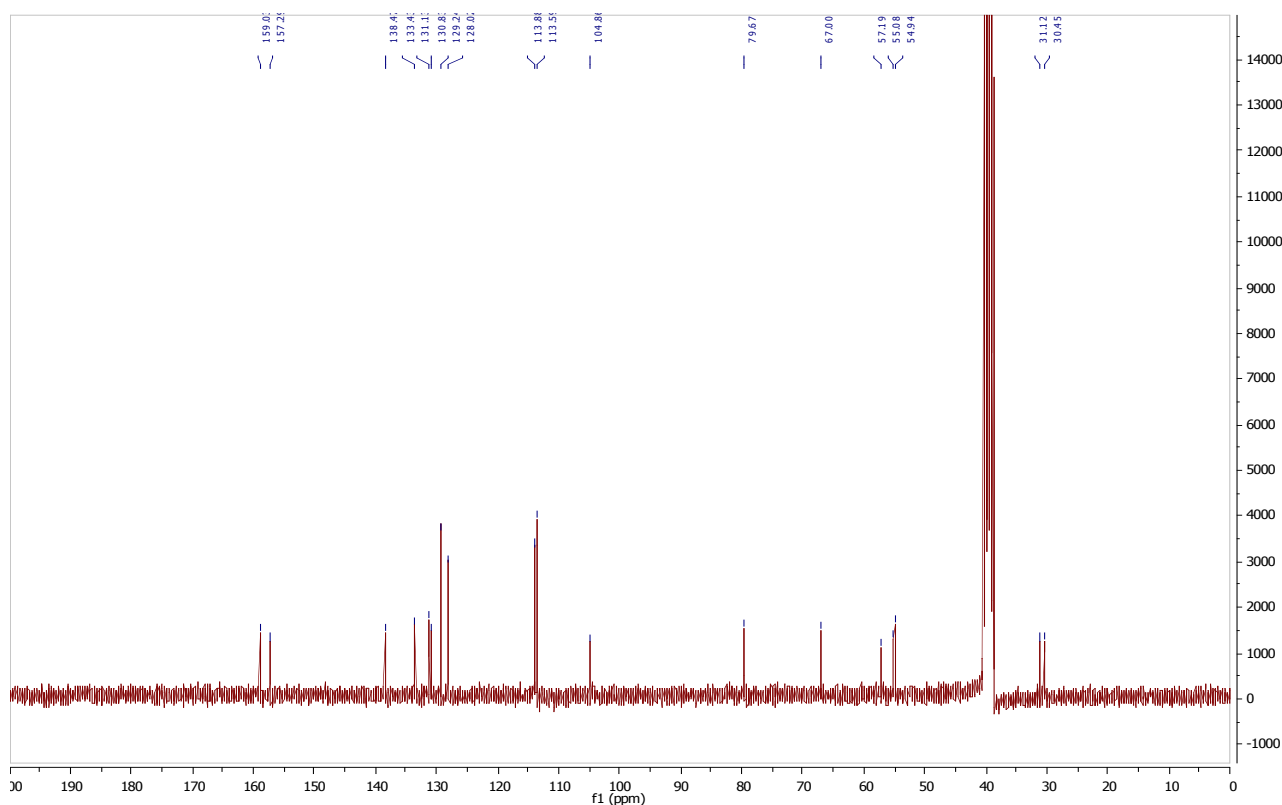
- ^{13}C NMR in $\text{DMSO-}d_6$ solution of (*IR*, *IS*) 1-[β -((4-methoxybenzyl)oxy)-(4-methoxyphenethyl)]-1*H*-pyrazolium hydrochloride (**7c**)



- ^1H NMR in $\text{DMSO-}d_6$ solution of (*IR*, *IS*) 1-[β -((4-methoxyphenyl)-(3-(4-methoxyphenyl)propoxyethyl)]-1*H*-pyrazolium hydrochloride (**7d**)



- ^{13}C NMR in $\text{DMSO-}d_6$ solution of (*IR*, *IS*) 1-[β -((4-methoxyphenyl)-(3-(4-methoxyphenyl)propoxyethyl)]-1*H*-pyrazolium hydrochloride (**7d**)



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Fax: +33 (0)223 236 374. Phone: +33(0)2 223 236 603.

E-mail: jean-pierre.bazureau@univ-rennes1.fr

Part 2:

- Chiral HPLC chromatograms obtained for resolution of (±)-(1*R*, 1*S*) 1-(4-methoxyphenyl)-2-(1*H*-pyrazol-1-yl)ethan-1-ol **4b** with (-)-(1*R*)-CSA and (+)-(1*S*)-CSA using the method of "half-quantities"
- Chiral HPLC chromatogram obtained for racemic (1*R*, 1*S*) 1-[β-((4-methoxyphenyl)-(3-(4-methoxyphenyl)propoxyethyl))-1*H*-pyrazolium hydrochloride (**7d**):

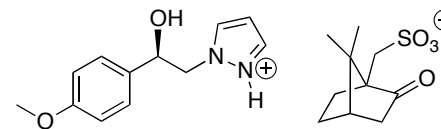
- Chiral HPLC analysis obtained for diastereoisomer (-)-(1S)-**4b**/(-)-(1R)-CSA:

Column: Chiracel OJ-H (250 x 4.60 mm)

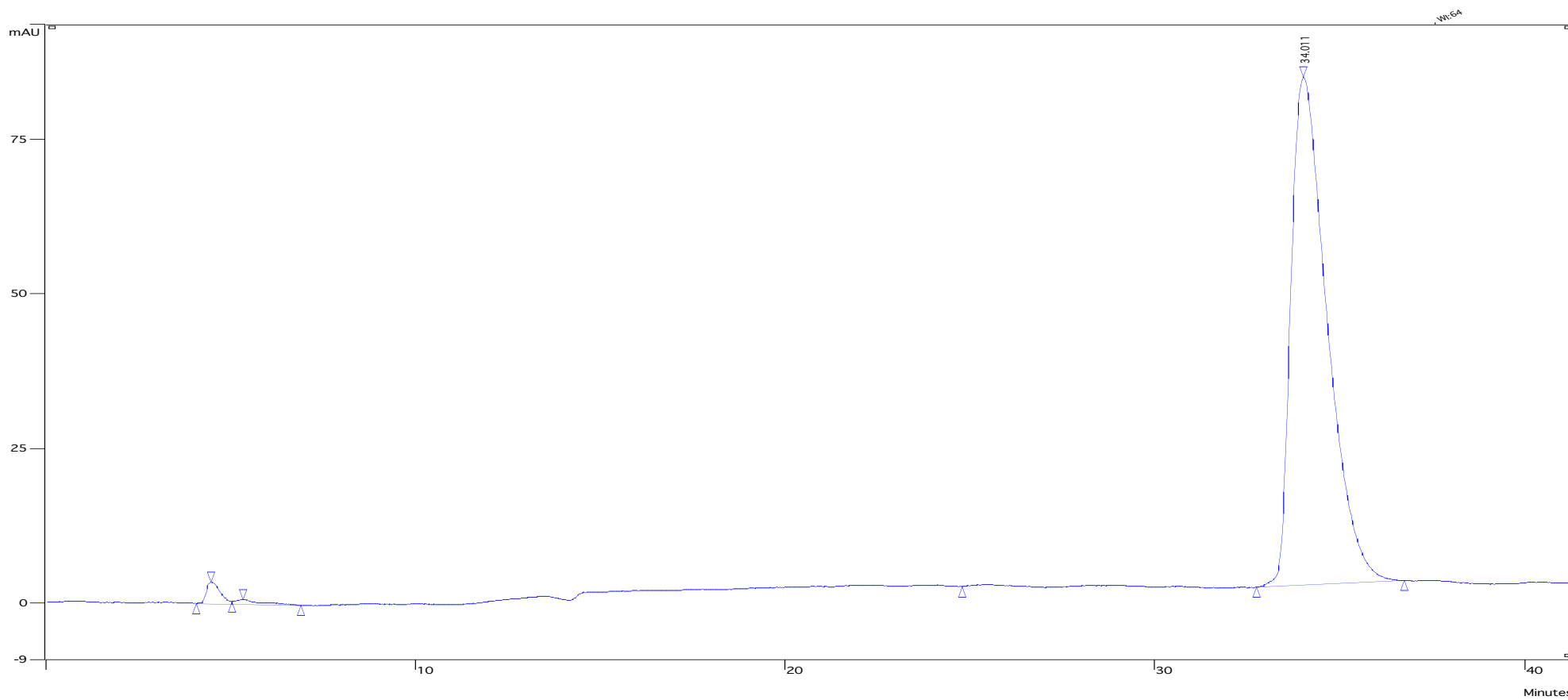
Detector: UV, 220 nm

Eluent: hexane/*i*-PrOH (94:6 v/v)

Flow rate: 0.8 mL/min.



Retention time = 34.0 min.



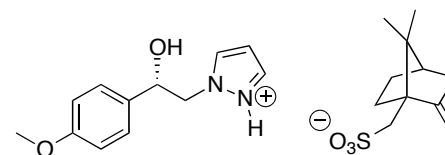
- Chiral HPLC analysis obtained for diastereoisomer (+)-(1*R*)-**4b**/(+)-(1*S*)-CSA:

Column: Chiracel OJ-H (250 x 4.60 mm)

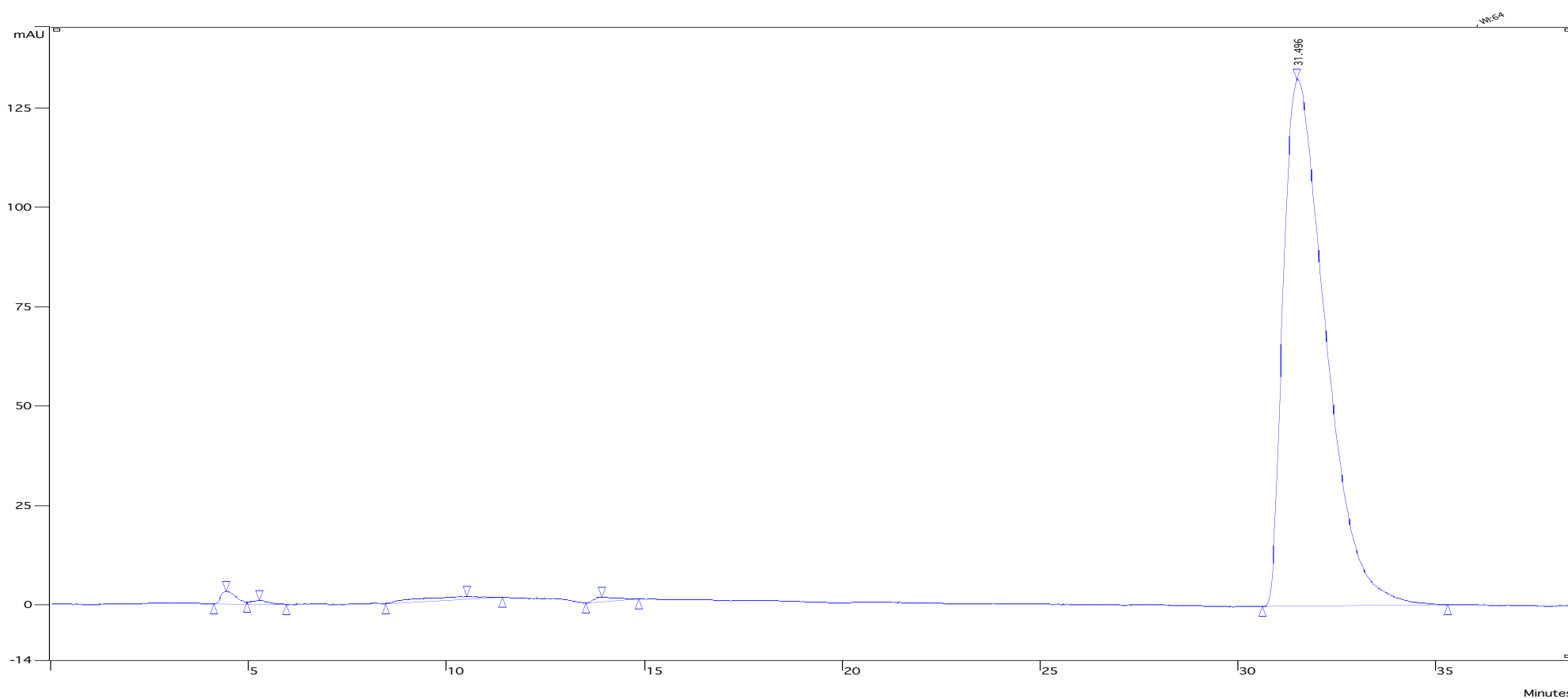
Detector: UV, 220 nm

Eluent: hexane/*i*-PrOH (94:6 v/v)

Flow rate: 0.8 mL/min.



Retention time = 31.5 min.



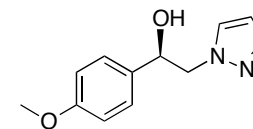
- Chiral HPLC analysis obtained for enantiomer (-)-(1S)-**4b**:

Column: Chiralcel OJ-H (250 x 4.60 mm)

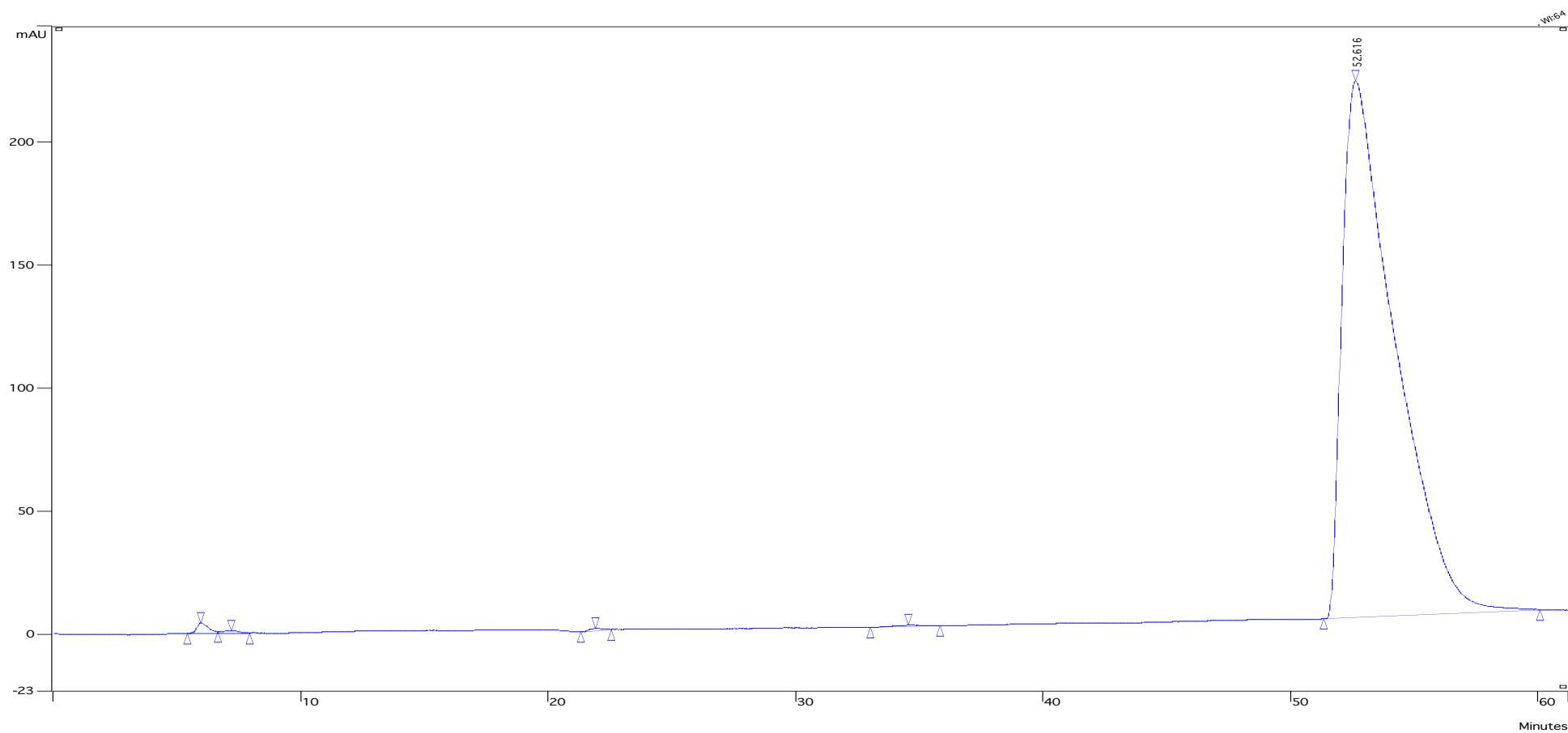
Detector: UV, 220 nm

Eluent: hexane/*i*-PrOH (94:6 v/v)

Flow rate: 0.6 mL/min.



Retention time = 52.6 min.



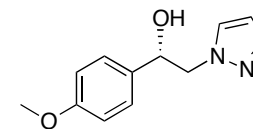
- Chiral HPLC analysis obtained for enantiomer (+)-(1*R*)-**4b**:

Column: Chiracel OJ-H (250 x 4.60 mm)

Detector: UV, 220 nm

Eluent: hexane/*i*-PrOH (94:6 v/v)

Flow rate: 0.6 mL/min.



Retention time = 63.5 min.

