

Supplementary Material

Synthesis of optically active vicinal fluorocyclopentanols and fluorocyclopentanamines by enzymatic deracemization

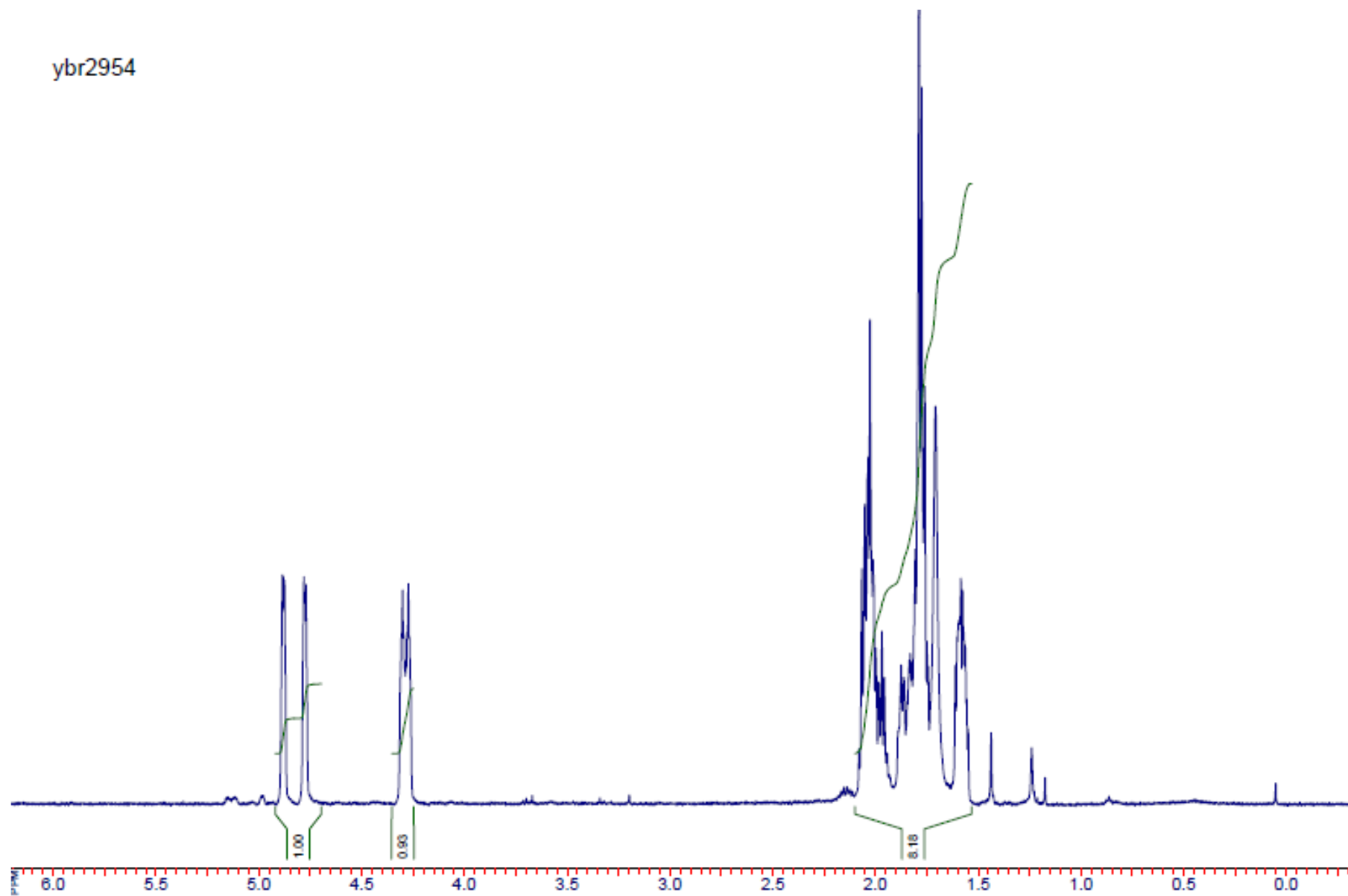
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Murmanska Str., 1, Kiev, Ukraine
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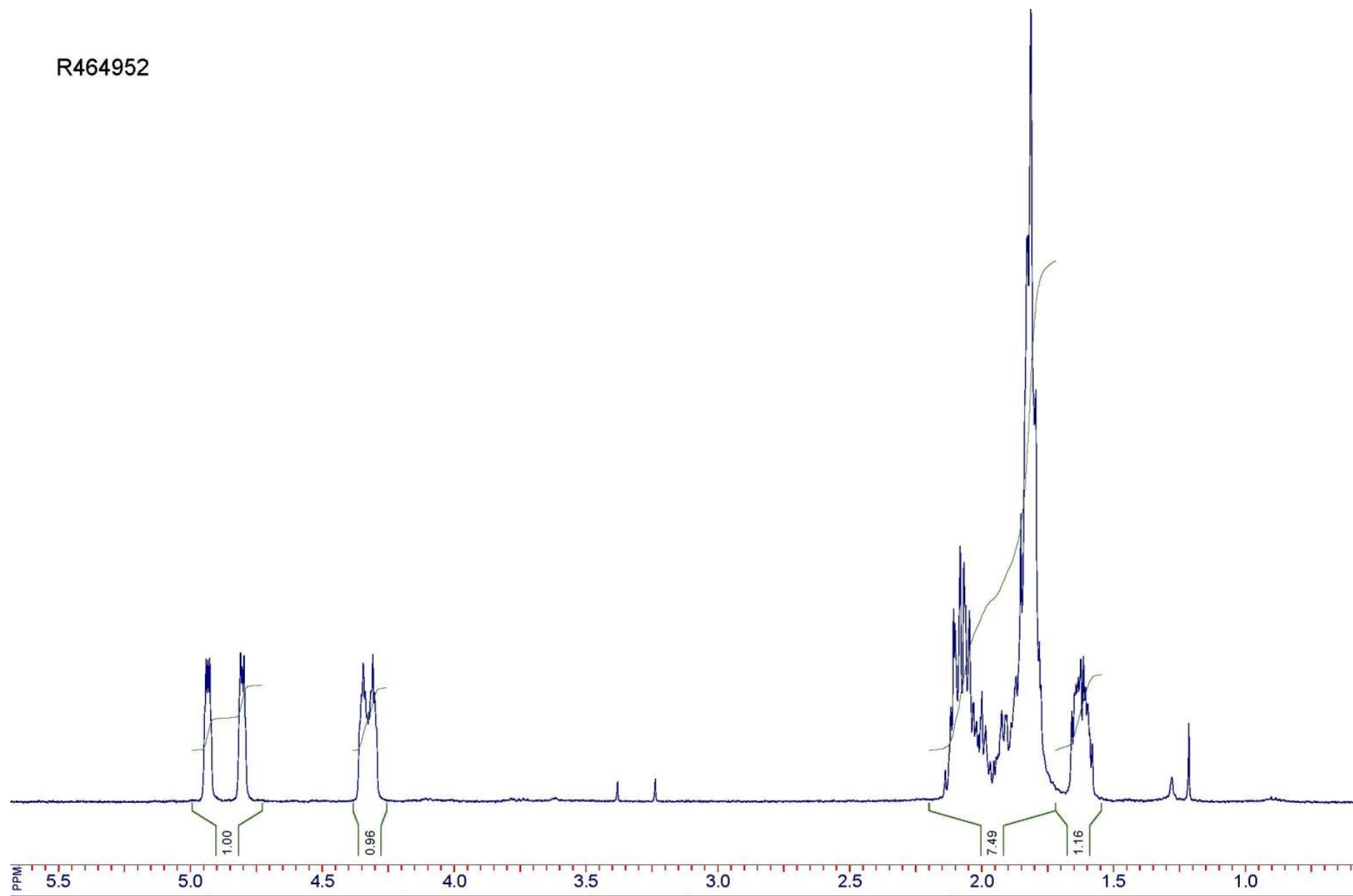
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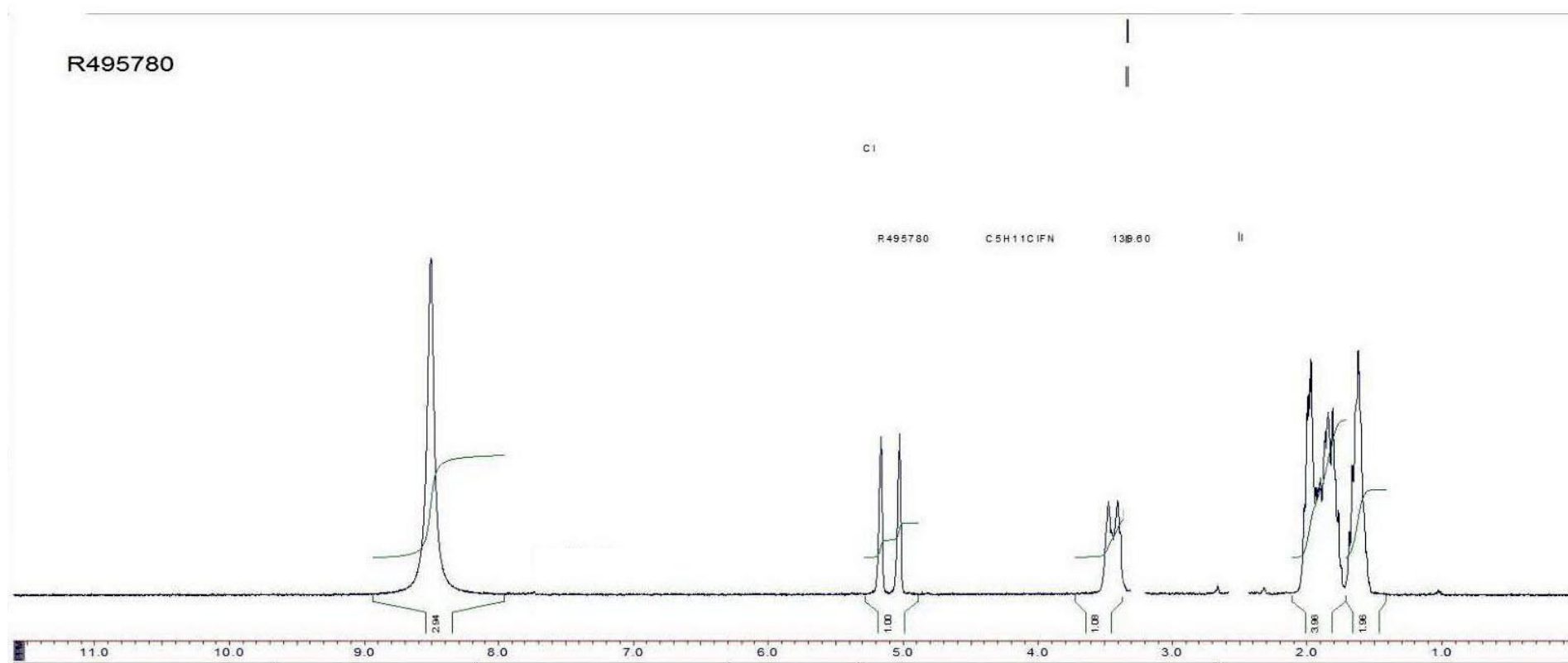
ybr2954

 ^1H NMR spectrum (500MHz, CDCl_3) of (R,R)-2-fluorocyclopentan-1-ol 4

R464952

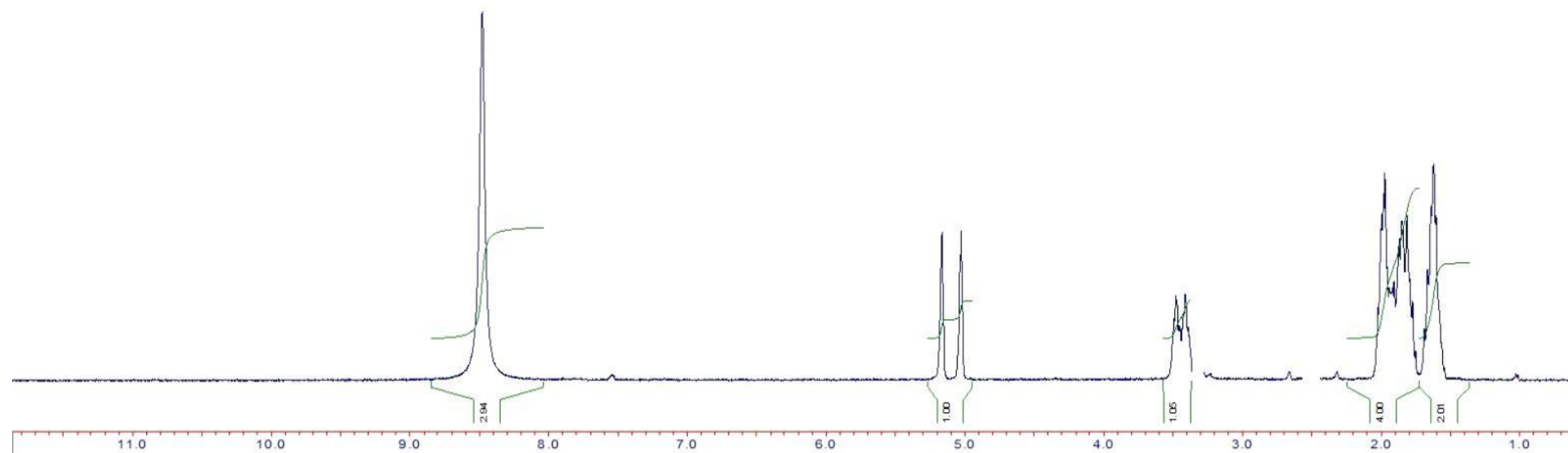
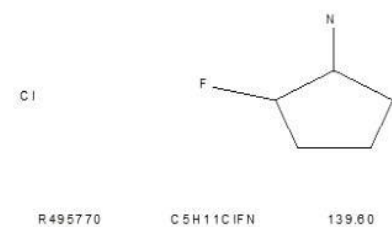


¹H NMR spectrum (500MHz, CDCl₃) of (*S,S*)-2-fluorocyclopentan-1-ol **3**

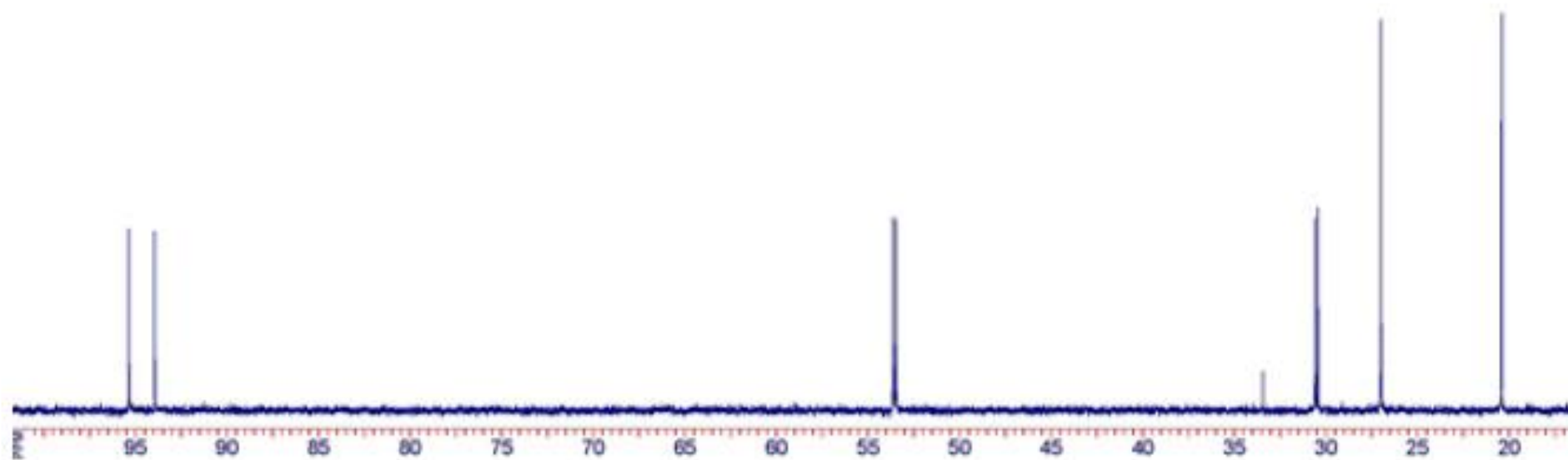


^1H NMR spectrum (500 MHz, DMSO- d_6) of (1S,2R)-fluorocyclopentane-1-amine hydrochloride **14**

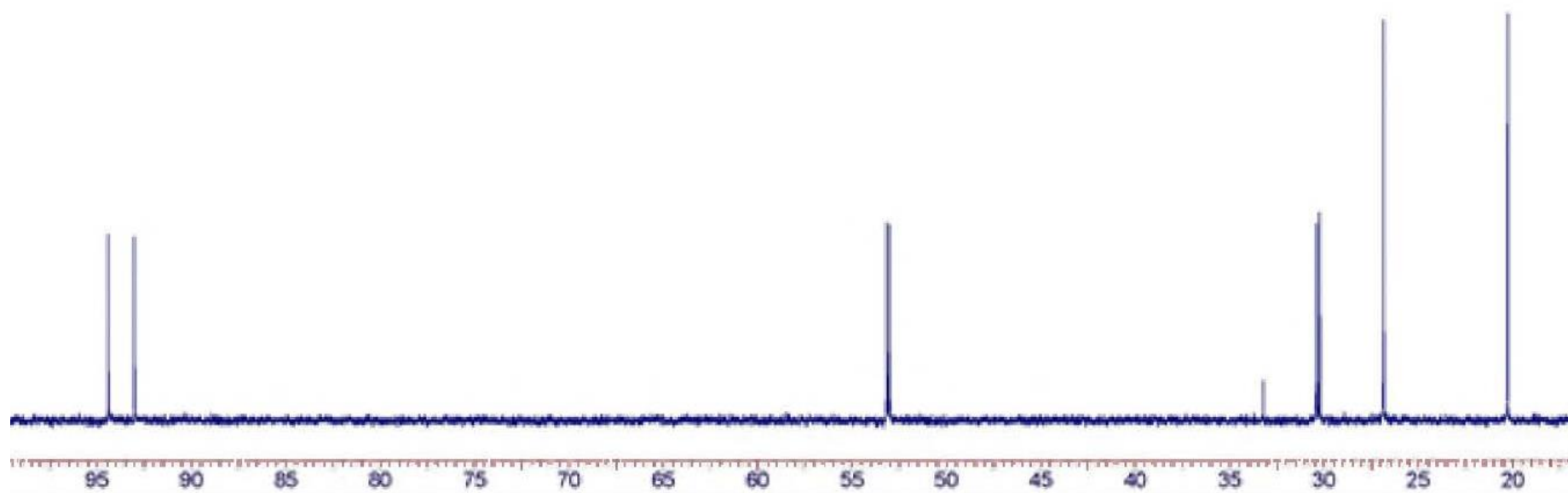
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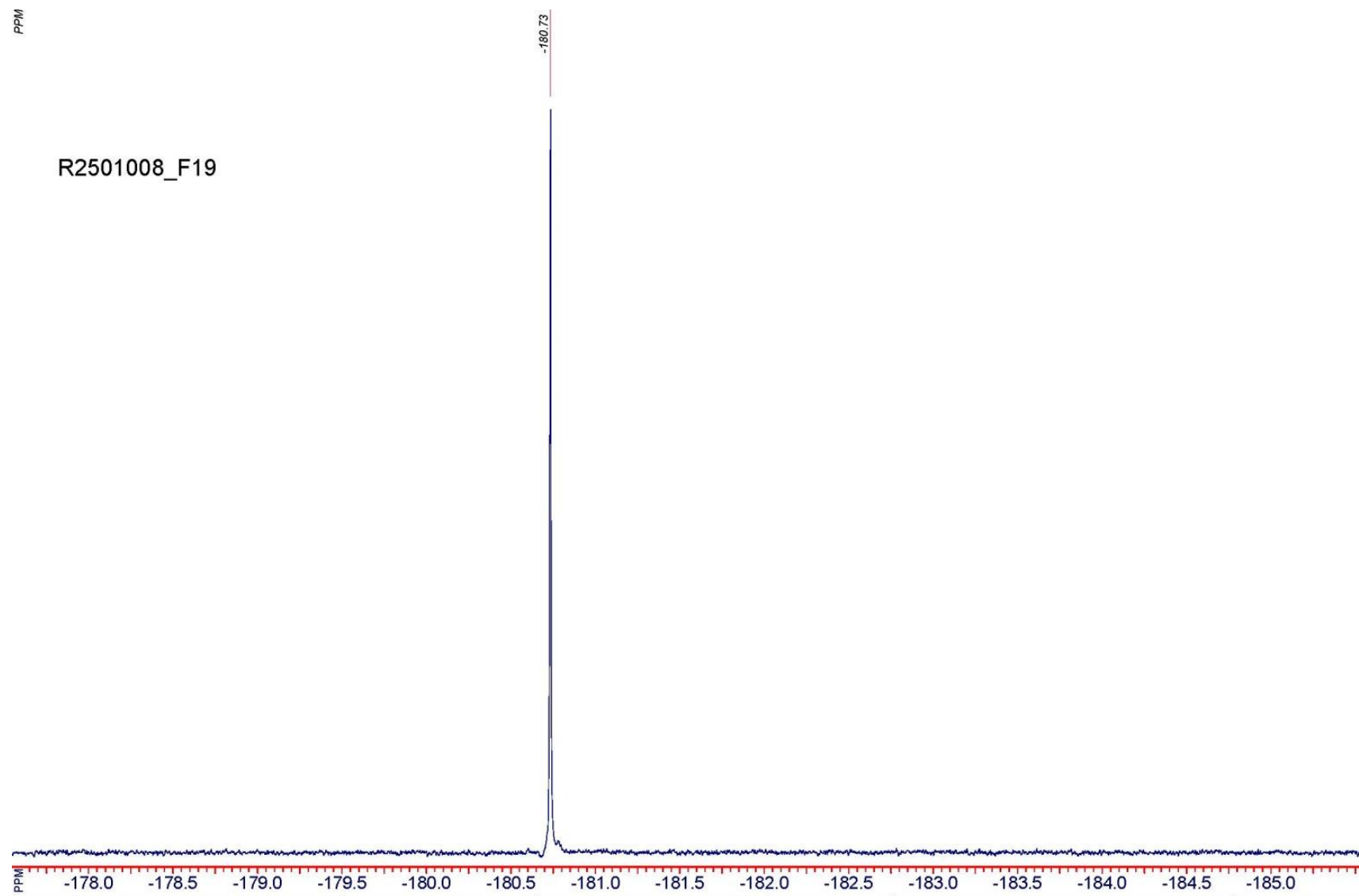
¹H NMR spectrum (500 MHz, DMSO-d₆) of (1*R*,2*S*)-fluorocyclopentane-1-amine hydrochloride **12**



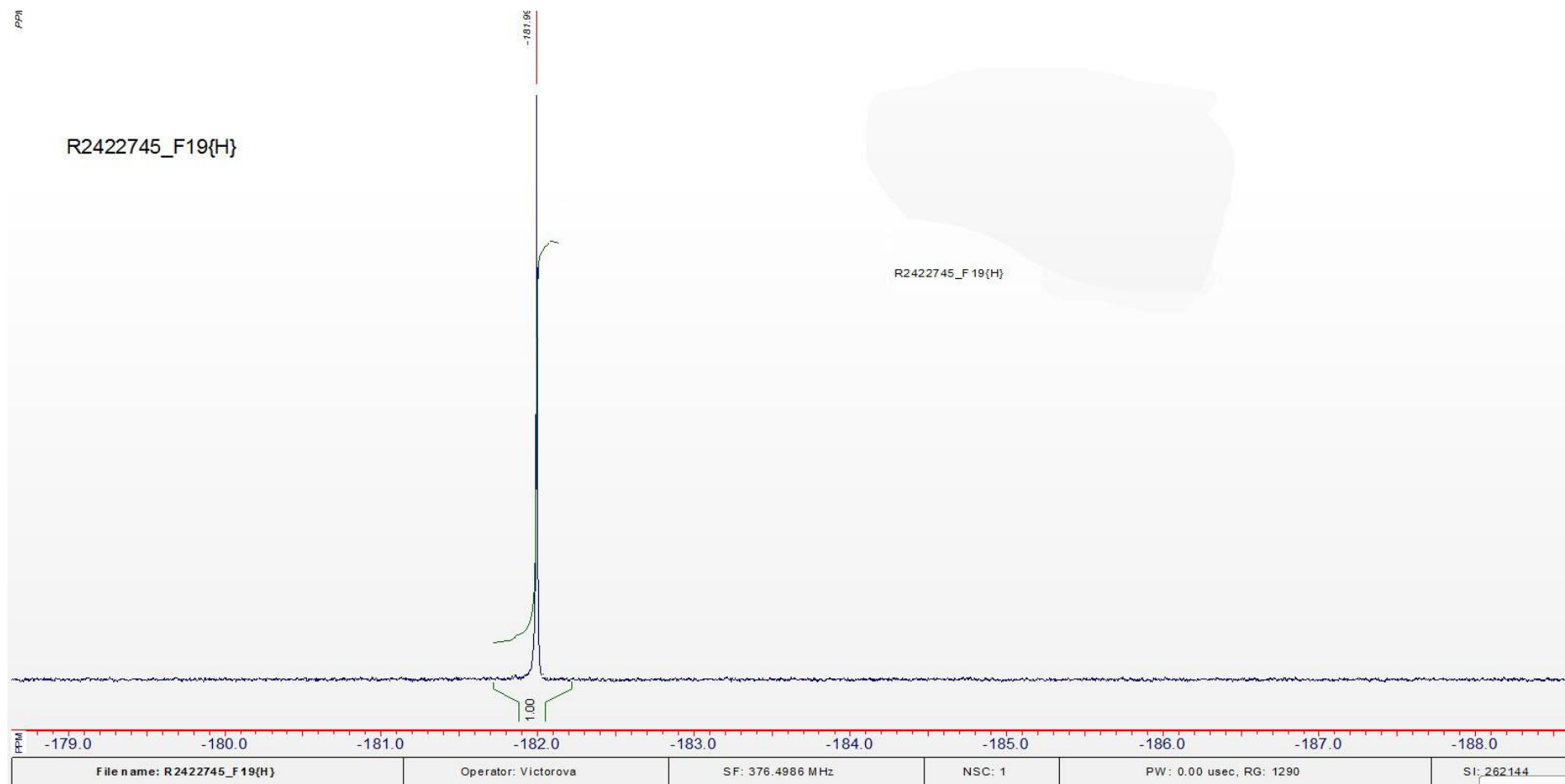
^{13}C NMR spectrum of (*R,S*)-2-fluorocyclopentan-1-ol **2**



^{13}C NMR spectrum of (S,R)-2-fluorocyclopentan-1-ol **1**

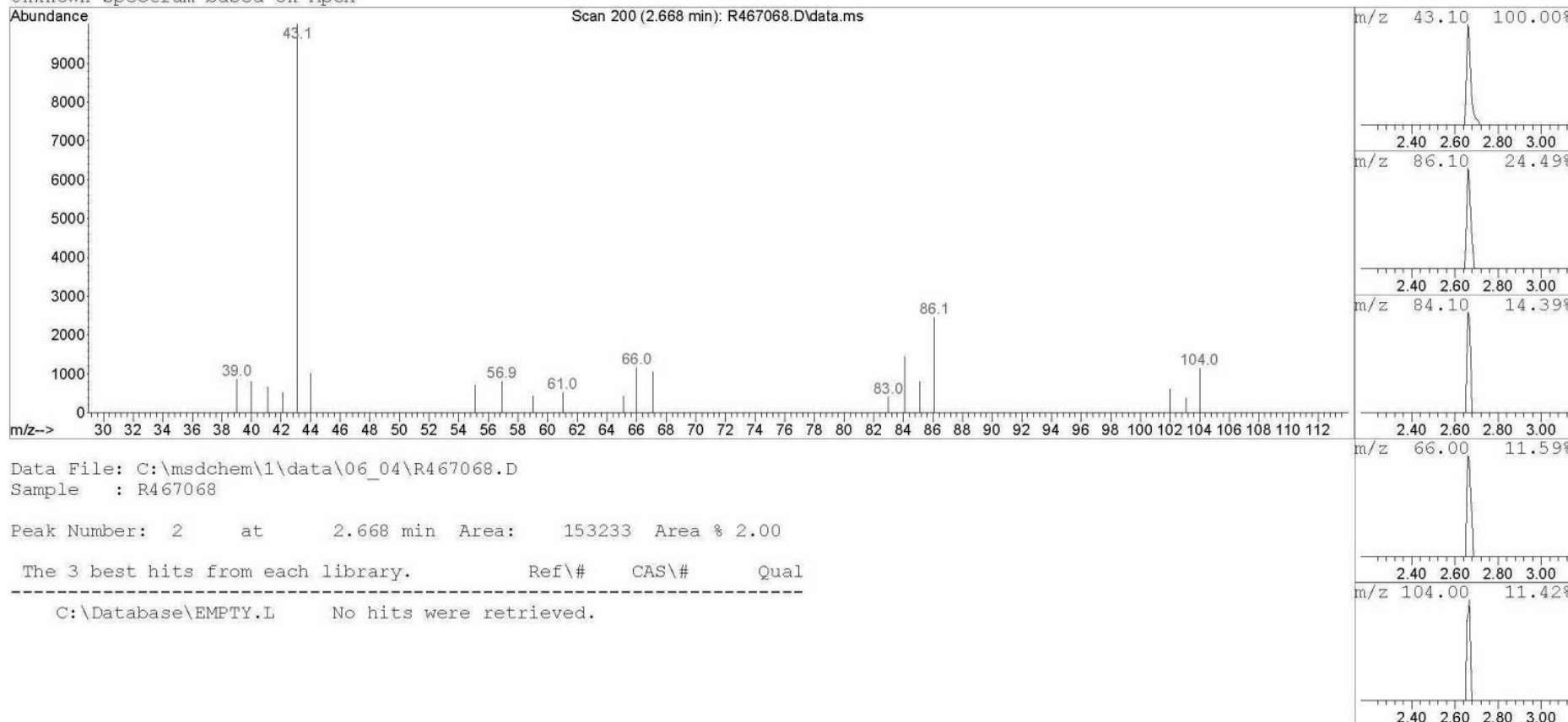


^{19}F NMR spectrum (CDCl_3) of (*S,S*)-2-fluorocyclopentan-1-ol **3**

 ^{19}F NMR spectrum of (*R,S*)-2-fluorocyclopentan-1-ol **2**

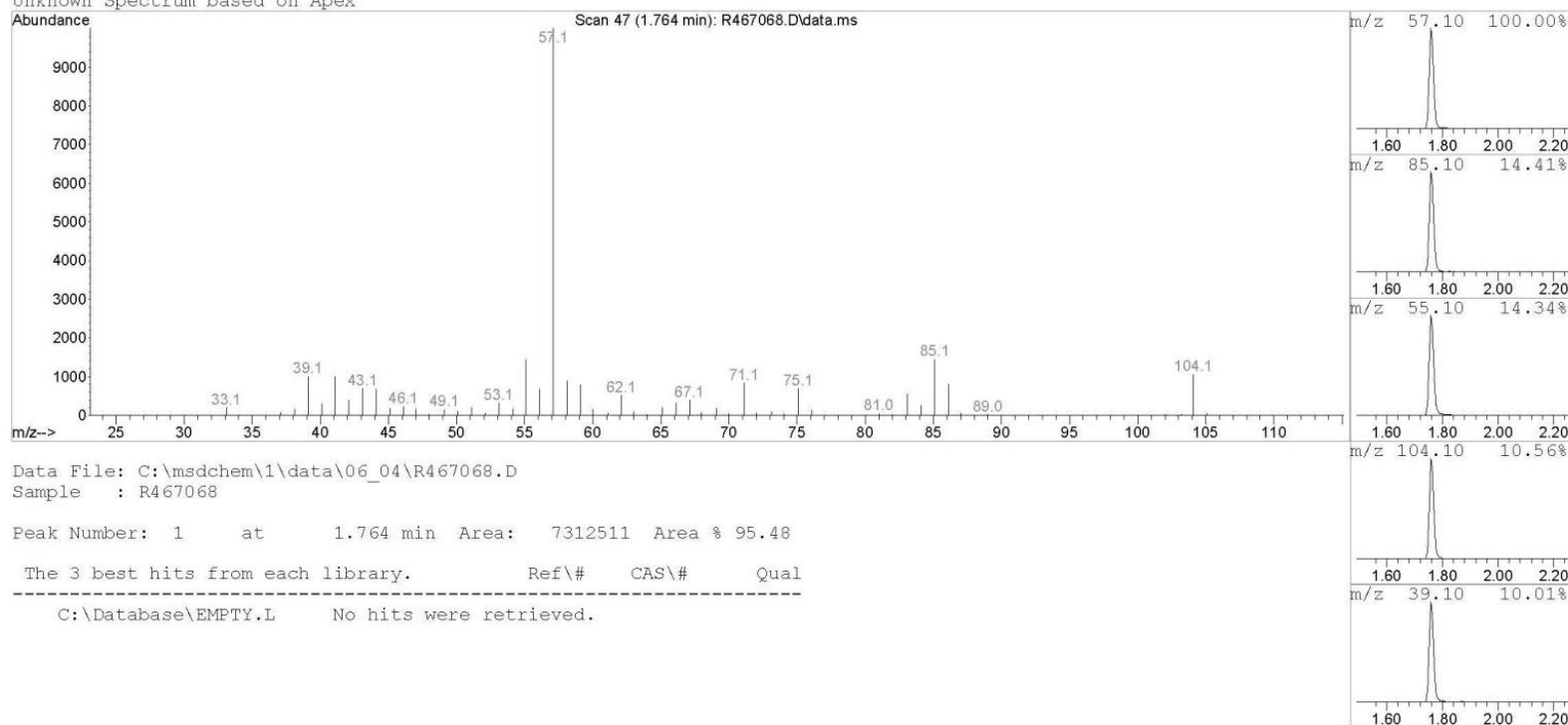
Library Search Report - ChemStation Integrator

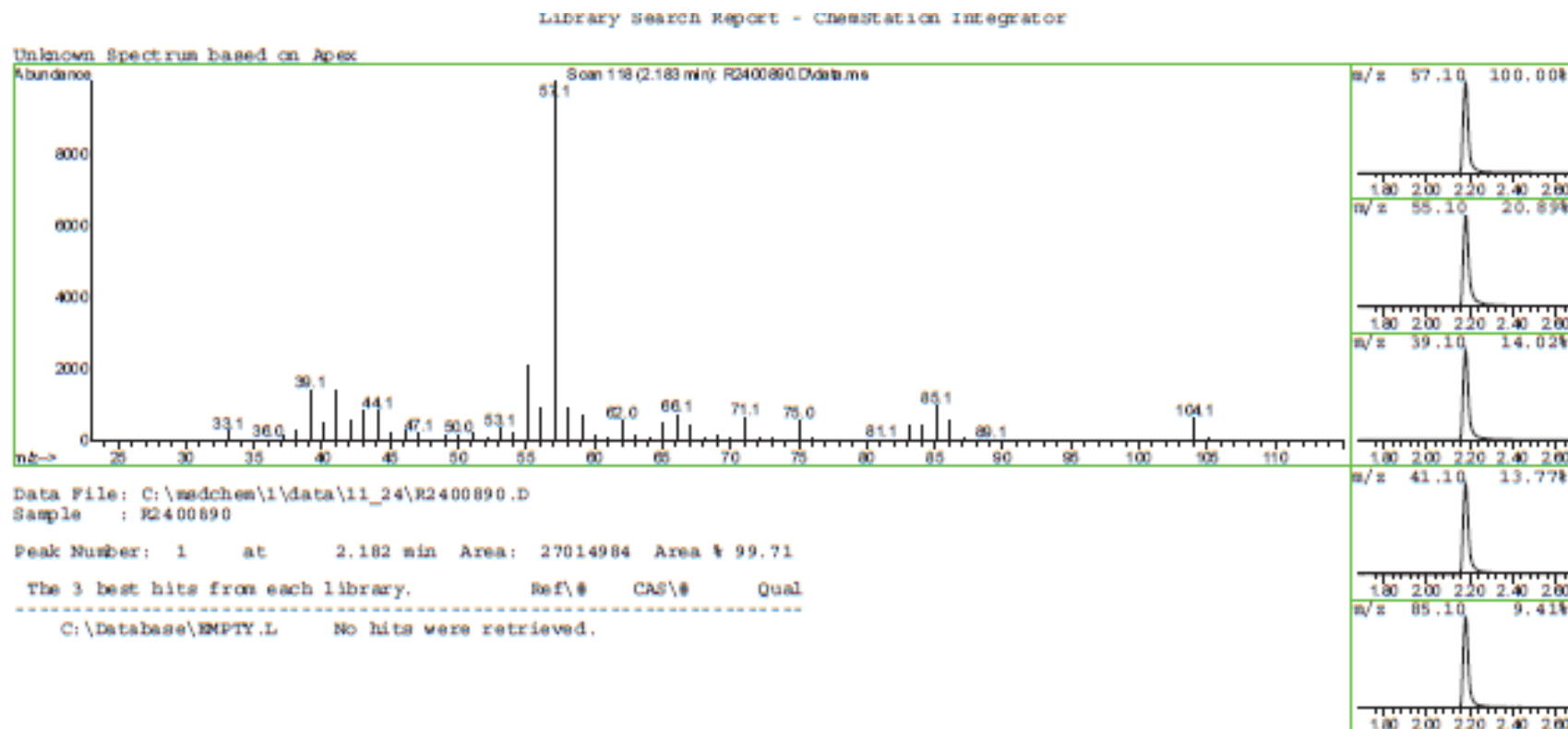
Unknown Spectrum based on Apex

Mass spectrum of (1*R*,2*S*)-2-fluorocyclopentan-1-ol **3**

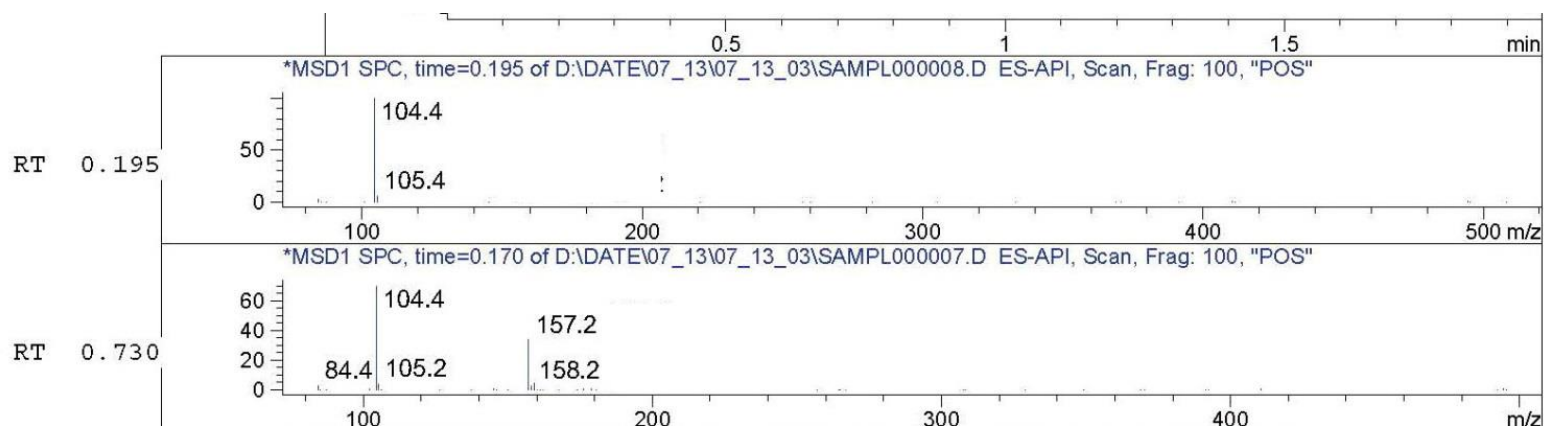
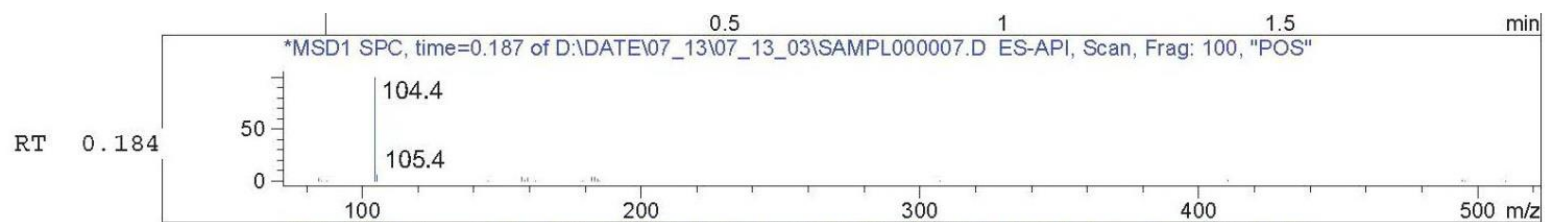
Library Search Report - ChemStation Integrator

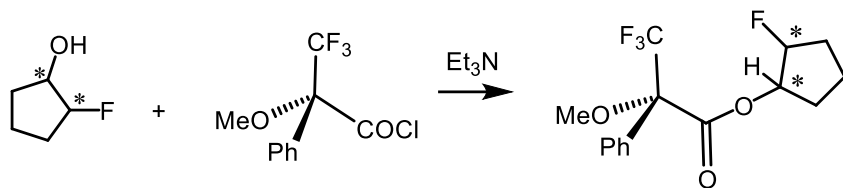
Unknown Spectrum based on Apex

Mass-spectrum of (*R,R*)-2-Fluorocyclopentane-1-ol **4**



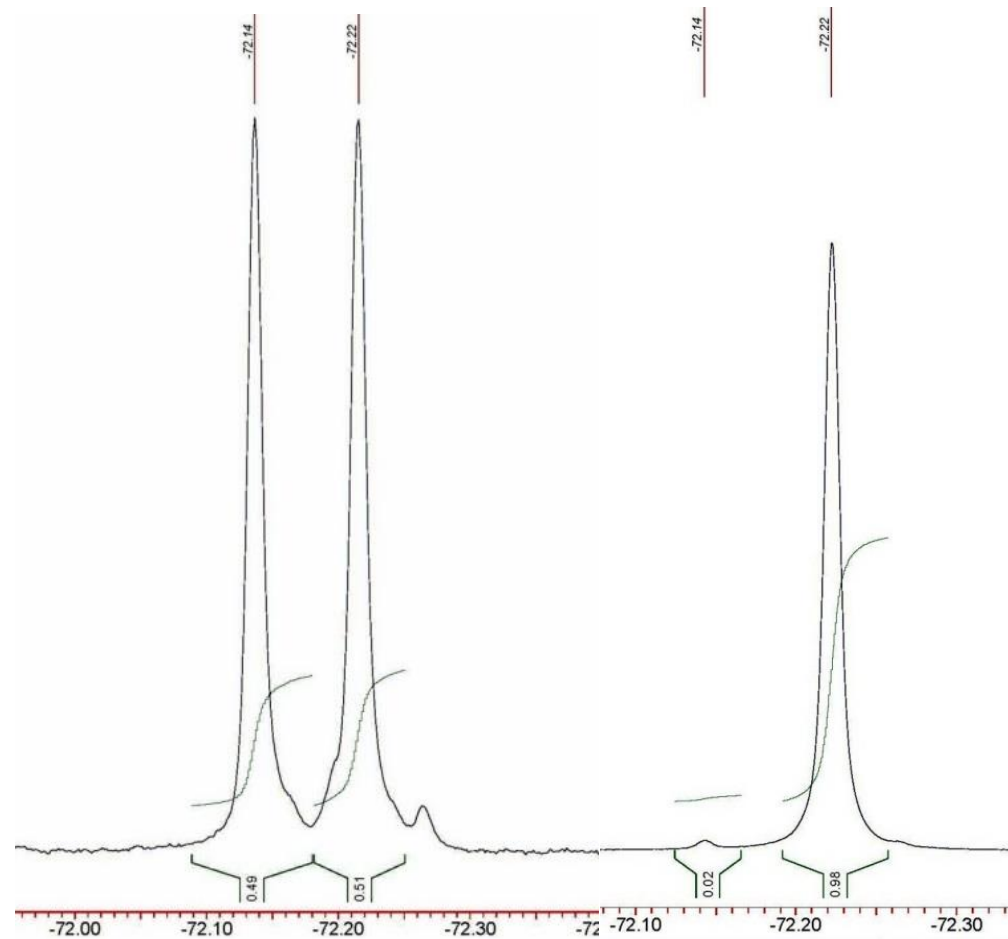
Mass-spectrum of (S,S)-2-fluorocyclopentan-1-ol **3**

Mass-spectrum of (1*S*,2*R*)-2-fluorocyclopentane-1-amine hydrochlorideMass-spectrum of (1*R*,2*S*)-2-fluorocyclopentane-1-amine hydrochloride **13**

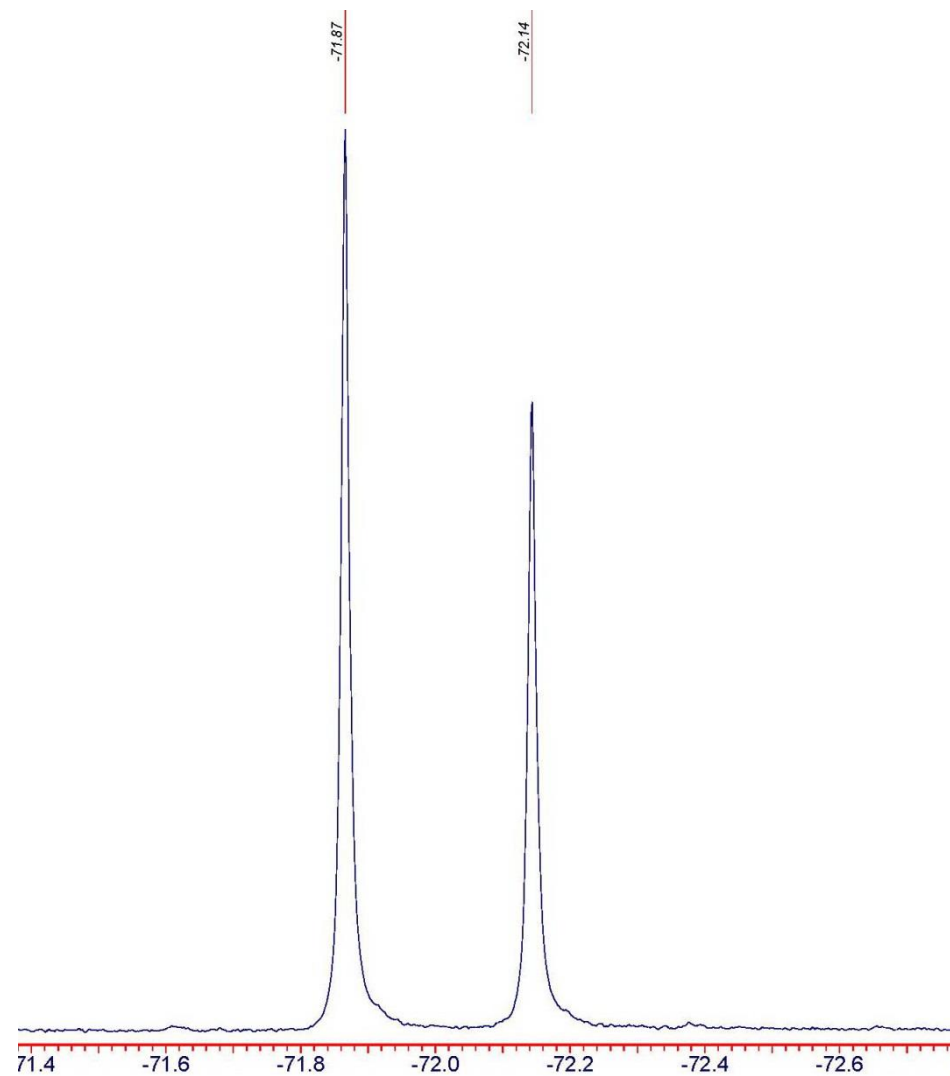
Determination of optical purity of resolved stereoisomers

a) To 10 mg (4.7 mmol) of racemic 2,1-bromoindanol and 0.01 ml of triethylamine in 2 ml of diethyl ether was added 13 mg (5.17 mmol) of Mosher acid chloride in the solution of 1 ml of diethyl ether with stirring and cooling to $-20\text{ }^{\circ}\text{C}$. After 10 min, the reaction mixture was centrifuged; the solvent was evaporated in vacuo, 1 ml of CDCl_3 was added to the residue, the solution was placed to NMR tube, ^1H and ^{19}F NMR spectroscopic analyses were performed (See NMR spectra below);

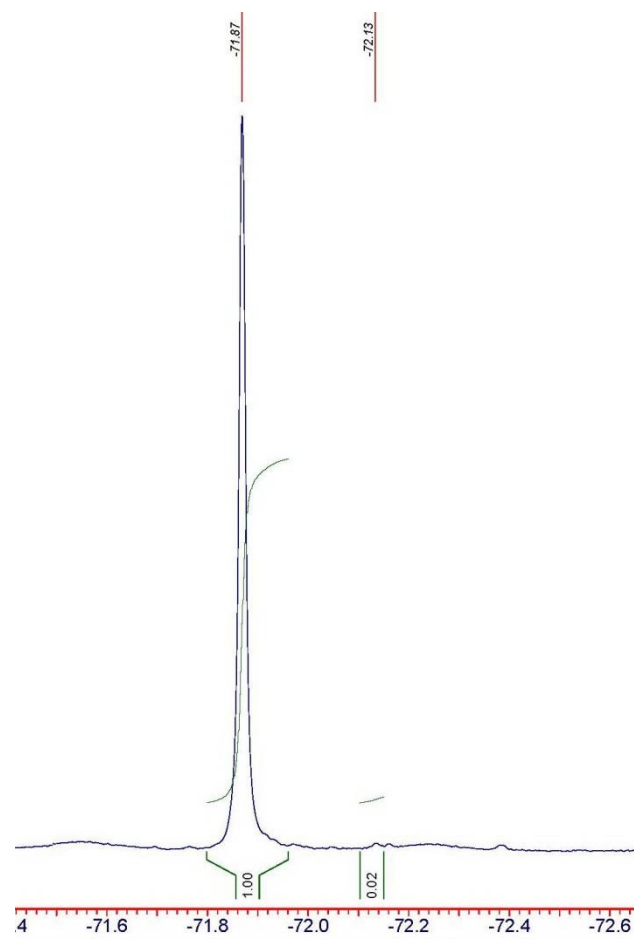
b) The resolved 2-bromo-2,3-dihydro-1H-inden-1-ol stereoisomers were analyzed analogously (See NMR spectra) below.



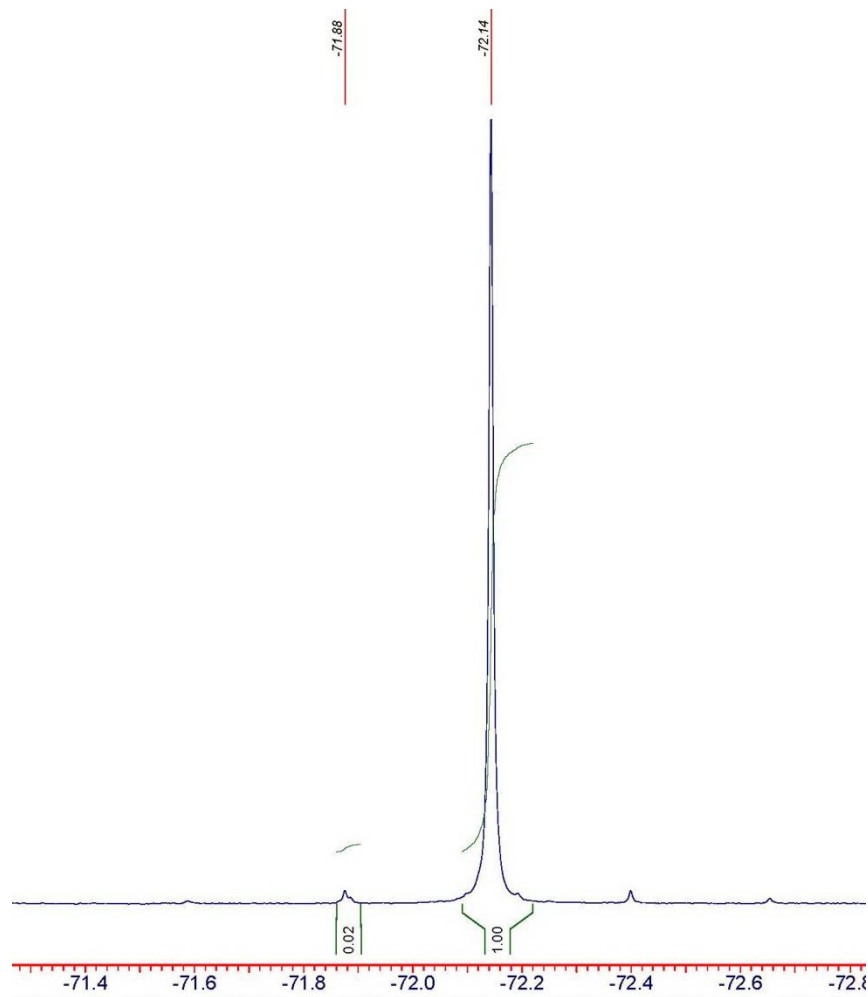
^{19}F Spectra of Mosher derivative of 2-fluorocyclopentan-1-ol: A) racemate; B) (1*S*,2*R*)-Stereoisomer **1**



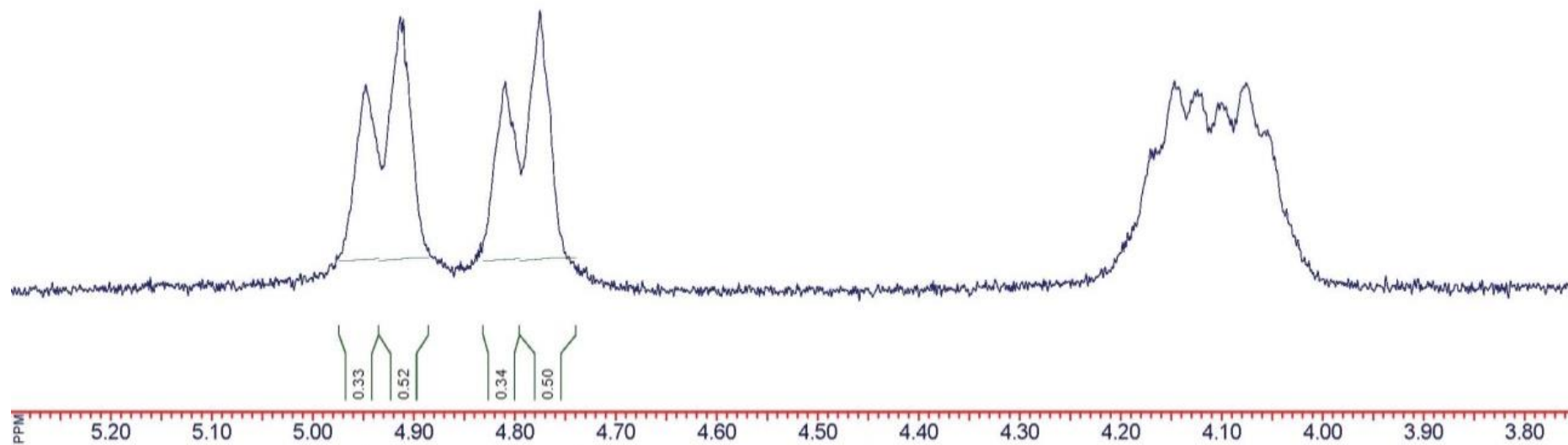
^{19}F Spectra of Mosher derivative of (*rac*)-2-fluorocyclopentan-1-ol



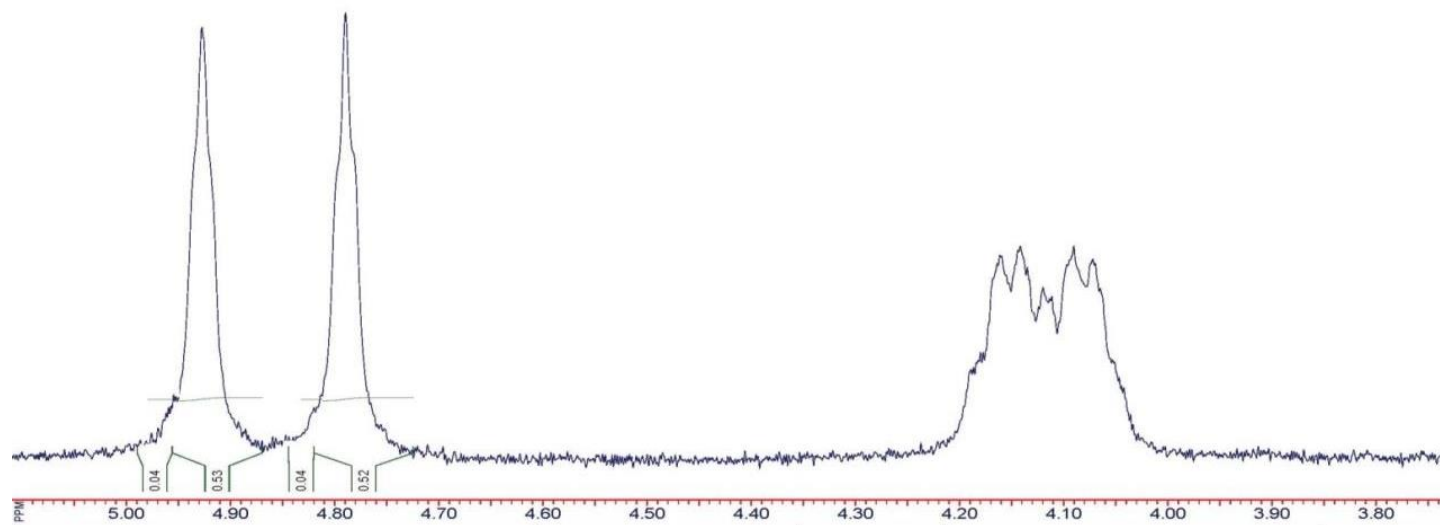
^{19}F Spectra of Mosher derivative of (*R,S*)-2-fluorocyclopentan-1-ol **2**



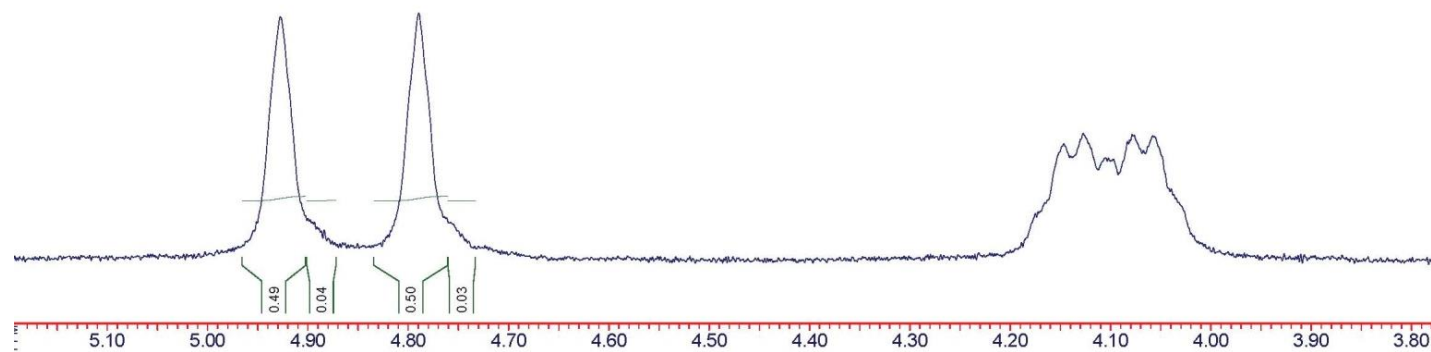
^{19}F Spectra of Mosher derivative of (*S,R*)-2-fluorocyclopentan-1-ol



¹H NMR spectrum of Mosher derivative of racemic fluorocyclopentane-1-amine hydrochloride

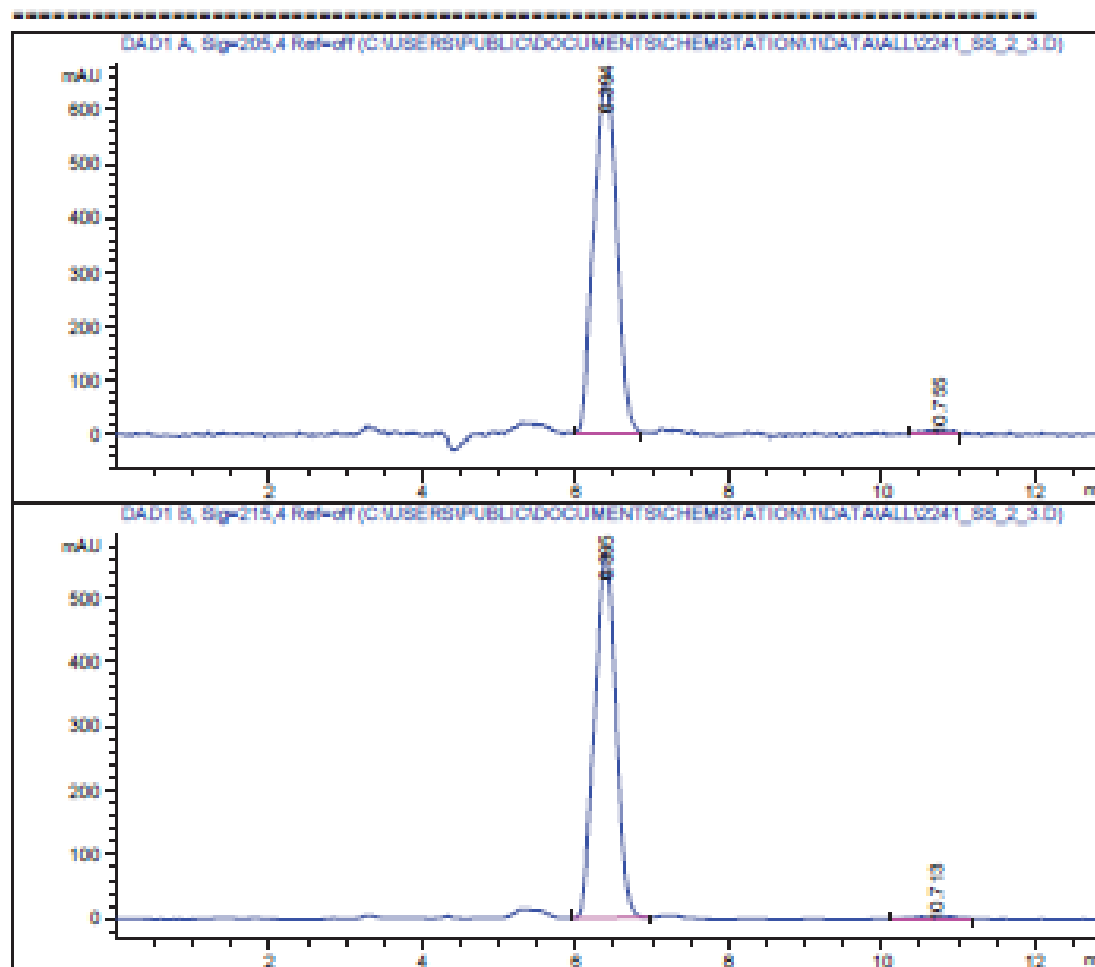


¹H NMR spectrum of Mosher derivative of (1*S*,2*R*)- fluorocyclopentane-1-amine hydrochloride **14**



¹H NMR spectrum of Mosher derivative of (1*R*,2*S*)- fluorocyclopentane-1-amine hydrochloride **12**

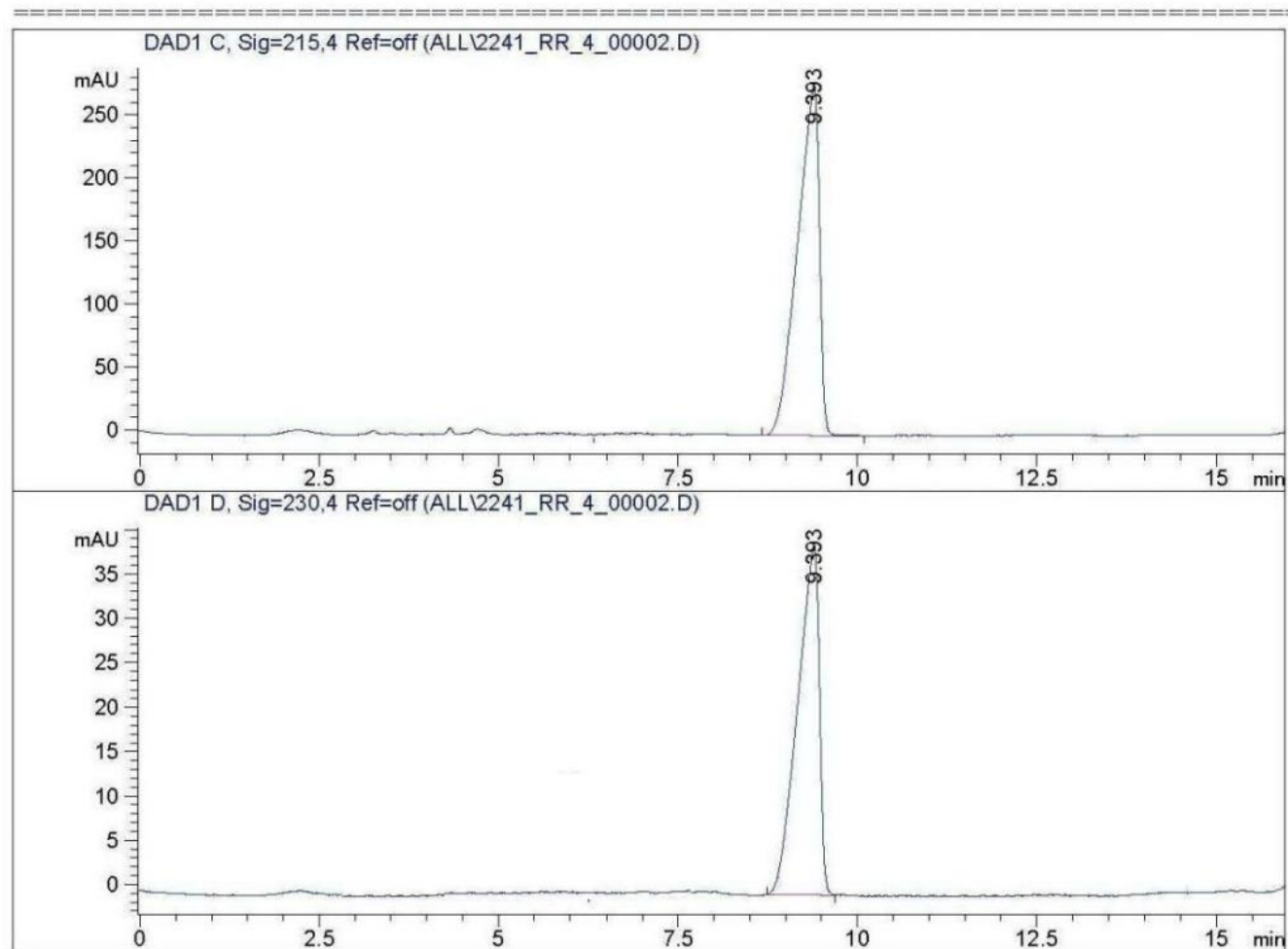
Sample Info: Chiralcel OD-H(258*4.6mm, 5µm), Hexane-IPA, 98-18, 1.8 ml/
min



chiral HPLC analysis on Chiralcel AD-H column of (1*S*,2*R*) 2-fluorocyclopentan-1-ol 1

Injection Volume: 1 mkl

Sample Info: OJ-H, Hexane-IPA, 90-10, 1.0ml/min, with Mosher's acid

chiral HPLC analysis on Chiralcel AD-H column of (1*R*,2*S*) 2-fluorocyclopentan-1-ol 2