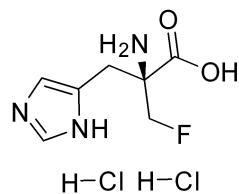


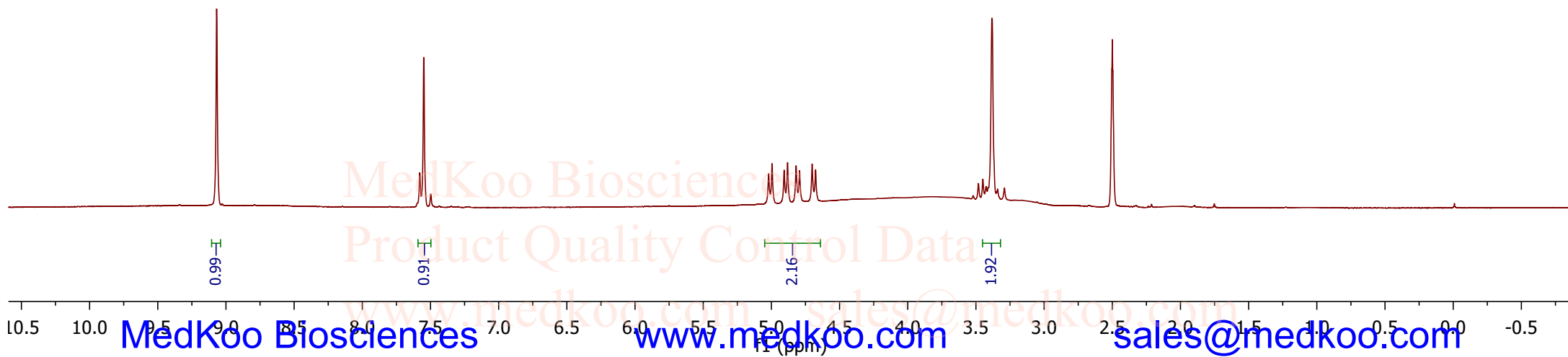
# (S)-alpha-Fluoromethylhistidine HCl HNMR Analysis in DMSO

MedKoo Biosciences  
Product Quality Control Data  
www.medkoo.com sales@medkoo.com



MedKoo Cat#: 525854  
Name: (S)-alpha-Fluoromethylhistidine HCl  
CAS#: 81839-27-2 (HCl)  
Lot#: YXM200504  
Chemical Formula: C7H12Cl2FN3O2  
Molecular Weight: 260.09

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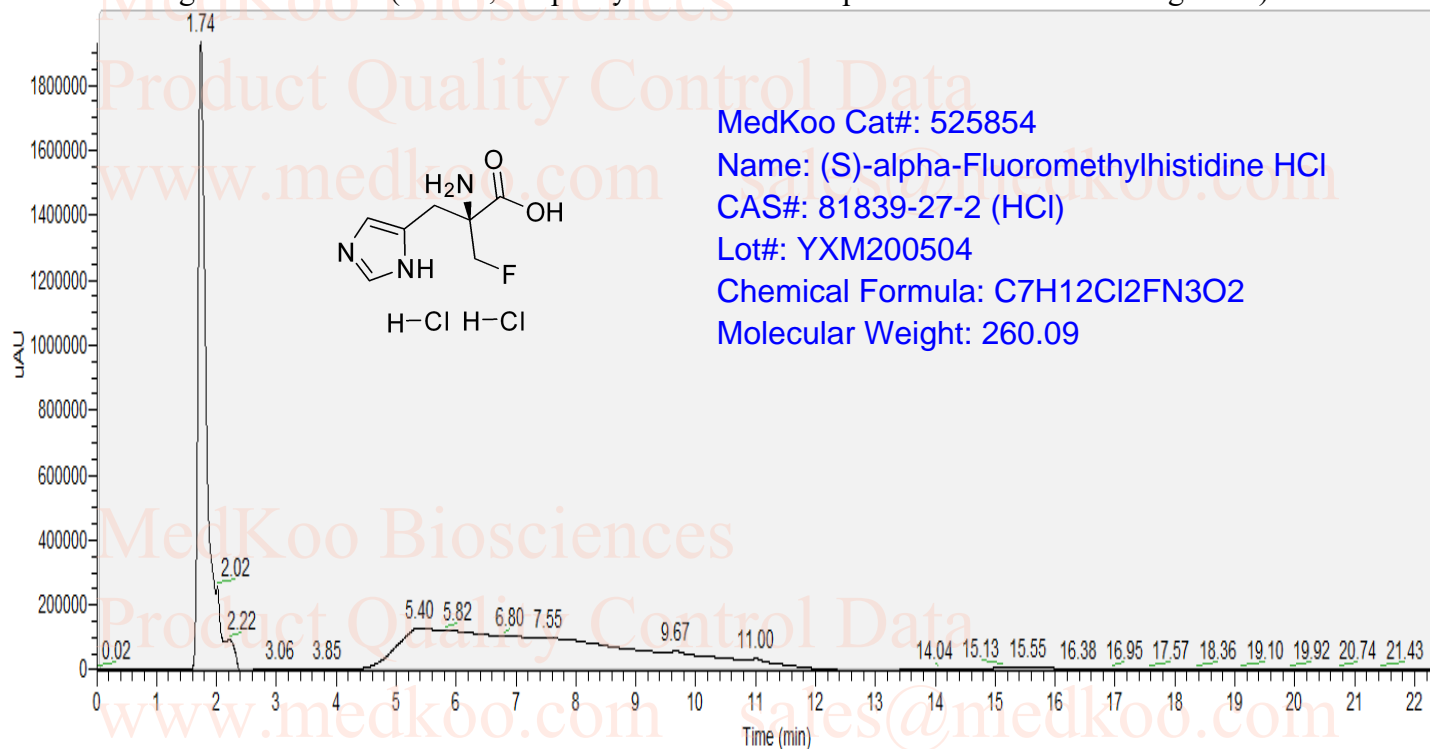


## LC-MS Analytical Report

MedKoo Cat#:	Product Name:	Lot#:
525854	(S)-alpha-Fluoromethylhistidine HCl	YXM200504

- Instrument: Agilent LC/MS system (1100 HPLC and MSD Trap XCT Plus mass spectrometer with UV-Vis detector).
- HPLC condition:
  - Mobile phase A: H<sub>2</sub>O with 0.1% formic acid; Mobile phase B: ACN with 0.1% formic acid.
  - Flow rate: 0.25 ml/min.
  - Column: Phenomenex Gemini 3u C<sub>6</sub>-phenyl 110 A (100 × 2 mm).
  - Gradient: 0-1 min, 50% A; 5-8.5 min, 0% A.
- MS condition: Nebulizer, dry gas and dry temperature are 30 psi, 8L/min, and 350°C, respectively.

UV chromatogram at 210 nm (overall, the purity is 99.1%. Bump in 5-9 min is from background):





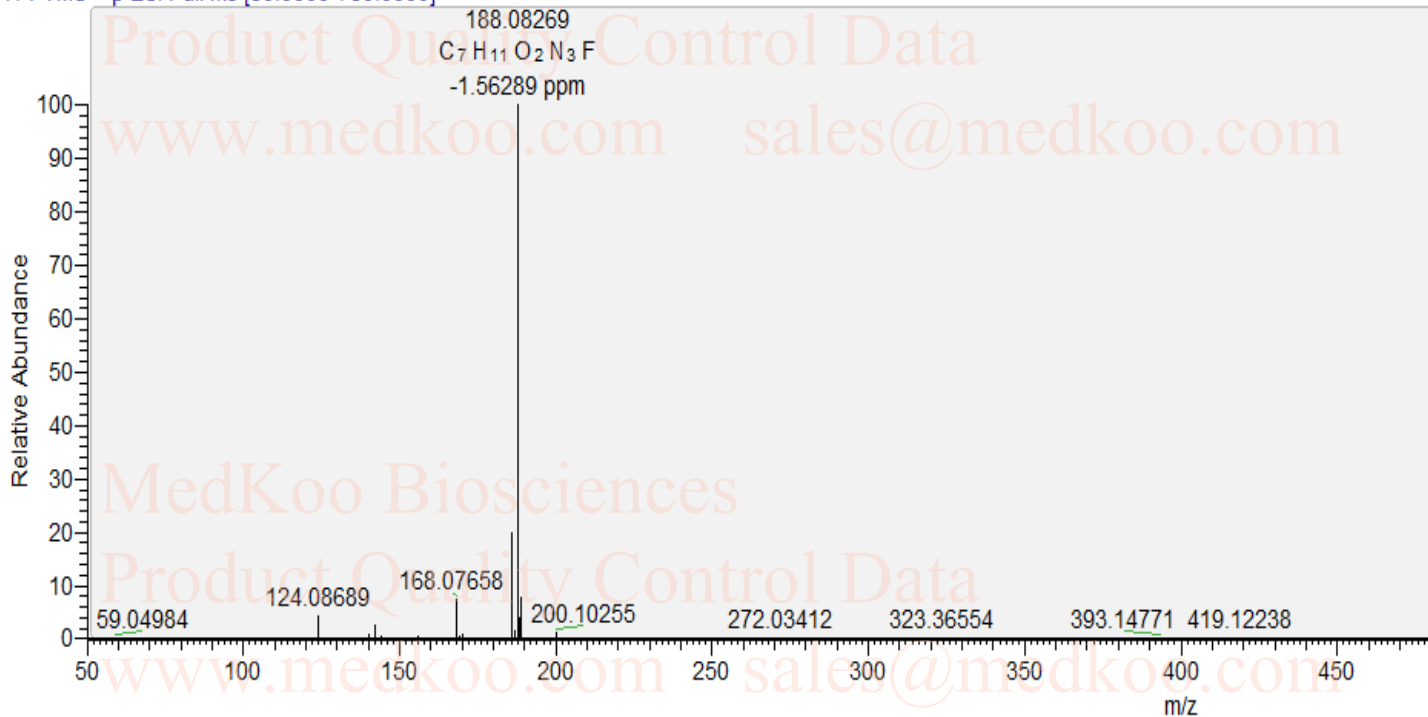
## LC-MS Analytical Report

MedKoo Cat#:	Product Name:	Lot#:
525854	(S)-alpha-Fluoromethylhistidine HCl	YXM200504

Chemical structure	CAS# and Theoretical analysis
<p>Chemical structure of (S)-alpha-Fluoromethylhistidine HCl. The structure shows a histidine ring with a fluoromethyl group at the alpha position. The carboxylic acid group is shown as a zwitterion (H<sub>2</sub>N<sup>+</sup> and COO<sup>-</sup>), and the fluoromethyl group is shown as a zwitterion (CH<sub>2</sub>F<sup>+</sup> and H<sup>-</sup>). The structure is labeled with H-Cl H-Cl.</p>	<p>MedKoo Cat#: 525854 Name: (S)-alpha-Fluoromethylhistidine HCl CAS#: 81839-27-2 (HCl) Lot#: YXM200504 Chemical Formula: C<sub>7</sub>H<sub>12</sub>Cl<sub>2</sub>FN<sub>3</sub>O<sub>2</sub> Molecular Weight: 260.09 Free base: Chemical Formula: C<sub>7</sub>H<sub>10</sub>FN<sub>3</sub>O<sub>2</sub> Exact Mass: 187.0757; Molecular Weight: 187.17</p>

Mass spectrum (positive electrospray ionization) from above peak 1.7 min:

525854 #179 RT: 1.75 AV: 1 NL: 3.74E9  
T: FTMS + p ESI Full ms [50.0000-750.0000]



Note: High-resolution mass spectrum confirms target compound ( $[M + H]^+$ ): If the error between the theoretical m/z and the experimental m/z is less than 5 ppm, it is considered as a match.