Datasheet Mapenterol-D$_{11}$

Reference number : EU/CRL: 44

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MAPENTEROL-D11

Name : 4-amino-3-chloro-α-[(1,1-dimethylpropyl)amino]methyl]-5-(trifluoromethyl)benzenemethanol-D11
Synonym : mapenterol-D11
Molecular formula : C_{14}H_{9}ClD_{11}F_{3}N_{2}O (74.3%)
Cas # : not available
Molecular weight : 335.8 (fumarate: 451.9)
Indication of purity : >95%

Last update : 1998.01.06

Methods used for characterization

I IR spectroscopy
II UV spectroscopy
III Mass spectrometry
IV Mass spectrometry after TMS-derivatisation
I **IR SPECTROSCOPY**

Instrument: Bruker IFS-55 FTIR; detector DTGS  
Sampling technique: KBr-tablet.

![IR Spectroscopy Graph](image)

II **UV SPECTROSCOPY**

Instrument: Cary 3 UV-Visible Spectrophotometer  
Concentration Mapenterol-D₁₁ fumarate=0.111 mM; solvent methanol  
ε₂₄₆.₀ nm=16030  
ε₃₀₈.₅ nm=4250

![UV Spectroscopy Graph](image)
III  MASS SPECTROMETRY

Instrument: Hewlett Packard 5989 A MS
GC-MS spectrum, DIP = direct inlet probe

![Graph showing GC-MS spectrum with m/z values and abundance]

Average of 2.296 to 2.394 min.: 97101699.D (-)

IV  MASS SPECTROMETRY AFTER TMS-DERIVATISATION

Instrument: Hewlett Packard 5970 MSD
MS spectrum, Full Scan (EI)

![Graph showing MS spectrum after TMS-derivatisation with m/z values and abundance]

Average of 7.998 to 8.036 min.: 97042903.D (-,*