

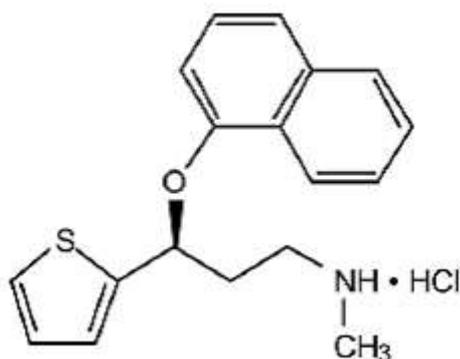
Answer on Question#59432 - Chemistry - Inorganic Chemistry

Question:

1. what are all the possible points of isomerism in duloxetine hydrochloride and assign stereodescriptors to any alkenes, chiral centres?
2. the infrared, mass spectroscopic and ^1H and ^{13}C NMR data for duloxetine hydrochloride

Solution:

Duloxetine hydrochloride is (+)-(*S*)-*N*-methyl- γ -(1-naphthoxy)-2-thiophenepropylamine hydrochloride. The empirical formula is $\text{C}_{18}\text{H}_{19}\text{NOS} \cdot \text{HCl}$, which corresponds to a molecular weight of 333.88. The structural formula is:



Answer:

- 1) Duloxetine hydrochloride should R-isomer - (3*R*)-*N*-Methyl-3-(naphthalen-1-yloxy)-3-(thiophen-2-yl)propan-1-amine HCl:



Stereo descriptors alkenes to chiral centers are R and S.

- 2) **Mass:** $M+297$; **$^1\text{H-NMR}$ (DMSO- d_6):** δ 1.8 (m, 2H), 2.5 (s, 6H), 2.4-2.6 (m, 2H), 5.9-6.0 (m, 1H), 6.9-7.0 (m, 2H), 7.1-7.3 (m, 3 H), 7.4-7.6 (m, 3H), 7.9 (m, 1H), 8.2 (m, 1H) & **IR (cm^{-1}):** 780, 1091(Ether), 1395, 1583(Amine, bend), 2771, 2946, 3056(Amine, str).