

Int= average of normalized integrals values

MW =molecular weight

P = Purity (as percent value)

m = mass

n= number of protons giving rise to a given NMR signal (The total number of protons is set to one because an average of all normalized integrals is carried out)

 $\begin{array}{ll} n_{EC} = 1 & n_3 = 1 \\ Int_{EC} = 1.105 & Int_3 = 1.010 \\ MW_{Ec} = 88.06 & MW_3 = 245.32 \\ M_{EC} = 8.9 \text{ mg} & m_3 = 22.5 \text{ mg} \end{array}$

 $P_{EC} > 99 \%$

$$P(\%) = \left(\frac{n_{EC} \cdot Int_3 \cdot MW_3 \cdot m_{EC}}{n_3 \cdot Int_{EC} \cdot MW_{EC} \cdot m_3}\right) \cdot P_{EC} = 96.4\%$$

