

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)

 $\begin{array}{ll} n_{EC} = 1 & n_1 = 1 \\ Int_{EC} = 1.00 & Int_1 = 0.860 \\ MW_{Ec} = 88.06 & MW_1 = 178.2 \\ m_{EC} = 9.1 \text{ mg} & m_1 = 18.0 \text{ mg} \end{array}$

 $P_{EC} > 99 \%$

$$P(\%) = \left(\frac{n_{EC} \cdot Int_1 \cdot MW_1 \cdot m_{EC}}{n_1 \cdot Int_{EC} \cdot MW_{EC} \cdot m_1}\right) \cdot P_{EC} = 87\%$$

