

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)

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 $\begin{array}{lll} n_{EC} = 1 & & n_1 = 1 \\ Int_{EC} = 1.00 & & Int_1 = 1.01 \\ MW_{Ec} = 88.06 & & MW_1 = 178.2 \\ m_{EC} = 8.8 \text{ mg} & & m_1 = 18.1 \text{ mg} \end{array}$

 $P_{EC} > 99 \%$

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$$P(\%) = \left(\frac{n_{EC} \cdot Int_1 \cdot MW_1 \cdot m_{EC}}{n_1 \cdot Int_{EC} \cdot MW_{EC} \cdot m_1}\right) \cdot P_{EC} = 98\%$$

