

¹H NMR (400 MHz, CDCl₃) of compound 2 + EC as internal standard

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)

 $\begin{array}{lll} n_{EC} = 1 & n_2 = 1 \\ Int_{EC} = 1.00 & Int_2 = 1.043 \\ MW_{Ec} = 88.06 & MW_2 = 392.63 \\ M_{EC} = 4.5 \text{ mg} & m_2 = 20.8 \text{ mg} \\ P_{EC} > 99 \, \% & \end{array}$

$$P(\%) = \left(\frac{n_{EC} \cdot Int_2 \cdot MW_2 \cdot m_{EC}}{n_2 \cdot Int_{EC} \cdot MW_{EC} \cdot m_2}\right) \cdot P_{EC} = 99.5\%$$