OS-QNMR-Step-2

8.33 8.32 8.31 8.12 8.12 8.10
7.68 7.68 7.67 7.66 7.10 7.10 7.08 7.08 7.00 7.00 6.99 6.98 6.98 6.96 6.96
4.44 4.43 4.42 4.41
3.92 3.91 3.89 3.89 3.80 3.79 3.78 3.17 3.16 3.14
2.68
1.25 1.04 1.03
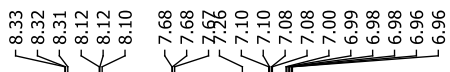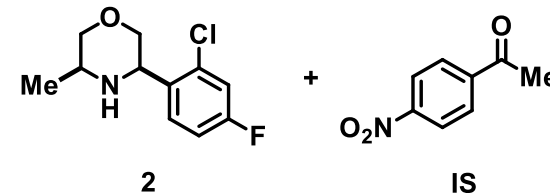
Int = Average of normalized integrals values
MW = Molecular weight
P = Purity (as percent value)
m = mass
n = number of protons giving rise to a given NMR signal (The total number of protons is set to one because an average of all normalized integrals is carried out)

2   **IS**

$n_{IS} = 1$ $n_2 = 1$
$Int_{IS} = 1.01$ $Int_2 = 1.005$
$MW_{IS} = 165.15 \ g/mol$ $MW_2 = 229.68 \ g/mol$
$m_{IS} = 2.47 \ mg$ $m_2 = 3.44 \ mg$
$P_{IS} = 98\%$

$$P \, [\%] = \frac{n_{IS} \cdot Int_2 \cdot MW_2 \cdot m_{IS}}{n_2 \cdot Int_{IS} \cdot MW_{IS} \cdot m_2} \cdot P_{IS} = 97 \ \%$$

2.01 2.00 1.01 0.93 1.02 1.02 1.06 1.08 2.37 3.06 1.96 2.98

f1 (ppm)
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5