



q ^1H NMR (Run 1)

Internal Standard (TMB)	Product
$n_{is} = 3$	$n_{pr} = 2$
$int_{is} = 3.00$	$int_{pr} = 1.85$
$m_{is} = 14.0 \text{ mg}$	$m_{pr} = 35.6 \text{ mg}$
$MW_{is} = 168.19 \text{ g}\cdot\text{mol}^{-1}$	$MW_{is} = 395.96 \text{ g}\cdot\text{mol}^{-1}$
Purity _{is} = 99.8%	Isomer ratios = 1:1.9:18.0 (m:o:p)

$$\text{Molar ratio} = \frac{\left[\frac{Int_{pr}}{n_{pr}}\right]}{\left[\frac{Int_{is}}{n_{is}}\right]} = \frac{1.85/2}{3/3} = 0.925$$

$$wt\%_p = \frac{m_{is} \times MW_{pr} \times \text{molar ratio} \times P_{is}}{m_{pr} \times MW_{is}} = \frac{14.0 \times 395.96 \times 0.925 \times 99.8}{35.6 \times 168.19} = 85.5\%$$

$$wt\%_o = \frac{1.9}{18.0} \times wt\%_p = 9.0\%$$

$$wt\%_m = \frac{1.0}{18.0} \times wt\%_p = 4.7\%$$

$$wt\%_{pr} = wt\%_p + wt\%_o + wt\%_m = 99.2\%$$