

# Supplementary material for the manuscript: Marginalization in nonlinear mixed-effects models – a practical approach

## Vinclozolin study

Table 1: Parameter estimates for the Vinclozolin case study.

Parameter	Coefficient	Random effect s.d.	Correlation structure		
Steepness ( $\beta_1$ )	0.538	0.538	1	-0.893	0.859
Upper asymptote ( $\beta_2$ )	1987.3	758.9	-0.893	1	-0.537
ED50 ( $\beta_4$ )	0.101	0.070	0.859	-0.537	1
Residuals ( $\epsilon_{ij}$ )		100.091			

## Spinach data

Table 2: Parameter estimates for the Spinach case study.

Parameter	Coefficients		Random effect s.d.
	Bentazon	Diuron	
Steepness ( $\beta_1$ )	0.604	1.751	0.000
Lower asymptote ( $\beta_2$ )	0.086	0.036	0.007
Upper asymptote ( $\beta_3$ )	1.303	1.980	0.337
ED50 ( $\beta_4$ )	1.433	0.203	0.000
Residuals ( $\epsilon_{ij}$ )			0.071

## CellTiter - Blue Cell Viability Assay Data

Table 3: Random effect parameter estimates for the Blue Cell Viability Assay case study. Estimates for the fixed effects are:  $\beta_1 = 1.875$ ,  $\beta_2 = 1960.9$ ,  $\beta_4 = 2.877$ , and  $\beta_5 = 0.542$ .

Random effect	Parameter	Random effect s.d.	Random effect correlation			
Day	Steepness ( $\beta_1$ )	0.114	1	0.800	0.878	-0.030
	Upper asymptote ( $\beta_2$ )	792.43	0.800	1	0.989	0.576
	ED50 ( $\beta_4$ )	0.451	0.878	0.989	1	0.452
	Asymmetry ( $\beta_5$ )	0.074	-0.030	0.576	0.452	1
Plate (within Day)	Steepness ( $\beta_1$ )	0.131	1	0.689	-0.707	-0.937
	Upper asymptote ( $\beta_2$ )	192.54	0.689	1	-1.000	-0.898
	ED50 ( $\beta_4$ )	0.280	-0.707	-1.000	1	0.909
	Asymmetry ( $\beta_5$ )	0.078	-0.937	-0.898	0.909	1
Residuals	( $\epsilon_{ij}$ )	187.958				