

Parameter	Calibration				Validation			
	Mean	Min	Max	SD	Mean	Min	Max	SD
C12:0	0.088	0.131	0.049	0.015	0.087	0.049	0.130	0.016
C13:0	0.002	0.010	0.001	0.001	0.002	0.001	0.040	0.004
C14:0	1.492	2.316	1.041	0.212	1.503	1.068	2.316	0.228
C15:0	0.054	0.165	0.023	0.014	0.051	0.025	0.095	0.012
C16:0	25.666	31.167	18.784	2.193	25.846	20.606	30.243	2.236
C17:0	0.345	0.694	0.176	0.092	0.341	0.171	0.625	0.086
C18:0	13.052	20.384	8.644	1.855	13.260	9.088	20.229	2.090
C20:0	0.216	0.387	0.116	0.043	0.217	0.126	0.356	0.045
C22:0	0.013	0.085	0.002	0.013	0.012	0.003	0.052	0.010
Total SFA	40.950	51.733	29.687	3.589	41.337	32.284	51.141	3.781
C14:1	0.015	0.042	0.006	0.006	0.016	0.006	0.034	0.006
C16:1	2.578	4.621	1.566	0.595	2.583	1.566	4.261	0.622
C17:1	0.310	0.815	0.121	0.105	0.305	0.134	0.723	0.099
C18:1	45.303	55.434	36.335	3.698	45.307	37.883	55.055	3.592
C20:1	1.038	1.603	0.837	0.227	1.030	0.684	1.312	0.173
C22:1	0.023	0.088	0.006	0.019	0.026	0.007	0.080	0.021
Total MUFA	49.275	58.949	39.403	3.931	49.287	40.844	58.709	3.819
C18:2 n6	8.335	3.232	17.236	2.920	7.989	3.463	15.182	3.177
C18:3 n3	0.617	0.200	1.549	0.261	0.587	0.211	1.310	0.224
C20:2 n6	0.421	0.148	0.933	0.163	0.409	0.154	0.844	0.163
C20:3 n3	0.127	0.041	0.381	0.055	0.124	0.041	0.379	0.048
C20:3 n6	0.045	0.008	0.093	0.015	0.044	0.009	0.094	0.012
C20:4 n6	0.108	0.028	0.210	0.036	0.106	0.033	0.191	0.035
C20:5 n3	0.004	0.001	0.017	0.003	0.004	0.001	0.012	0.002
C22:4 n6	0.048	0.014	0.106	0.017	0.047	0.019	0.100	0.019
C22:5 n3	0.037	0.008	0.115	0.016	0.036	0.008	0.086	0.012
Total PUFA	9.773	3.765	20.484	3.380	9.376	4.025	17.507	3.690
n3 PUFA	0.787	0.271	1.975	0.320	0.752	0.283	1.708	0.288
n6 PUFA	8.956	3.456	18.483	3.115	8.594	3.715	16.150	3.409

Table S1. Descriptive statistics of fatty acid profile from data set used in calibration and validation (expressed as % of total identified fatty acids).