Supplementary Material

Partial Least Squares Regression Method to Predict Docosahexaenoic and Eicosapentaenoic Acids in Fish Oil Supplements

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Table S2. Spectral interval used in the siPLS models to predict DHA, EPA, and ω-3 PUFA for fish oil supplements.

Compound	**Interval 1**		**Interval 2**	
	Wavelength	**Assignment**	**Wavelength**	**Assignment**
DHA	3092–2866	3009, =C–H *cis* stretching; 2962, asymmetric C–H (CH_3) 2922, CH_2 asymmetric stretching 2871, CH_2 symmetric stretching	1504–1279	1462, CH_2 folding
EPA			1730–1505	1657, C=C stretching (*cis*)
ω-3 PUFA			1957–1731	1743 and 1734, carbonyl stretch TG and EE

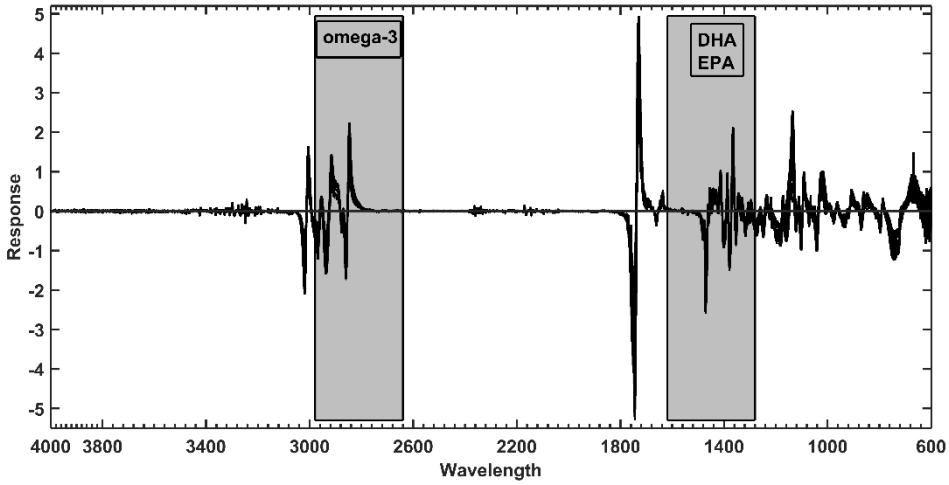

Figure S1. Spectral regions selected to improve prediction of ω-3, DHA and EPA by the si-PLS models.