

Supplementary Materials

Table S1: Percent of models with R^2 and R^2 values that are both higher than 0.9 or 0.5 for different predictive variables and different resolutions using different preprocessing methods.

Dependent variable		Raw spectra	1 st Derivative	2 nd Derivative	Normalization	NOR 1 st Der	NOR 2 nd Der	SNV	SNV 1 st Der	SNV 2 nd Der	WA	WA 1 st Der	WA 2 nd Der	WD	WD 1 st Der	WD 2 nd Der
Palmitic acid	$R^2 \geq 0.9$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	$R^2 \geq 0.5$	53	53	28	69	61	39	72	64	36	56	53	47	47	33	25
Linoleic acid	$R^2 \geq 0.9$	64	53	25	78	64	39	92	64	39	75	50	47	44	39	17
	$R^2 \geq 0.5$	100	78	72	100	83	72	100	83	72	100	89	75	81	75	72
α -linolenic acid	$R^2 \geq 0.9$	92	72	64	100	72	67	100	72	67	89	89	75	75	75	53
	$R^2 \geq 0.5$	100	89	75	100	89	75	100	89	75	100	100	86	94	83	78
Oleic acid	$R^2 \geq 0.9$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	$R^2 \geq 0.5$	39	22	17	42	36	25	53	39	25	42	36	25	28	25	22
Elaidic acid	$R^2 \geq 0.9$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	$R^2 \geq 0.5$	3	6	6	19	6	3	6	6	3	3	3	0	6	0	0
Stearic acid	$R^2 \geq 0.9$	6	0	0	3	8	0	0	6	0	6	0	0	0	0	0
	$R^2 \geq 0.5$	58	36	28	64	39	28	58	31	28	56	39	31	39	25	31
Unsaponifiable matter	$R^2 \geq 0.9$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	$R^2 \geq 0.5$	8	8	0	8	3	3	11	3	3	8	3	3	3	0	0
Acid value	$R^2 \geq 0.9$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	$R^2 \geq 0.5$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Saponification value	$R^2 \geq 0.9$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	$R^2 \geq 0.5$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Ester value	$R^2 \geq 0.9$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	$R^2 \geq 0.5$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Hydroxy value	$R^2 \geq 0.9$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	$R^2 \geq 0.5$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Iodine value	$R^2 \geq 0.9$	28	31	22	53	72	44	53	67	56	28	36	44	28	56	25
	$R^2 \geq 0.5$	100	97	72	100	100	75	100	100	75	100	100	89	94	83	75
Peroxide value	$R^2 \geq 0.9$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	$R^2 \geq 0.5$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Resolution																
2 cm ⁻¹	$R^2 \geq 0.9$	14	12	5	18	13	6	21	12	6	14	12	10	10	10	1
	$R^2 \geq 0.5$	35	20	13	37	23	12	39	23	13	36	27	16	21	12	12
4 cm ⁻¹	$R^2 \geq 0.9$	12	10	8	16	15	10	17	15	12	13	13	13	11	13	8
	$R^2 \geq 0.5$	35	35	22	42	37	25	39	37	25	35	33	31	33	28	21
8 cm ⁻¹	$R^2 \geq 0.9$	17	15	13	20	22	19	19	21	19	18	15	15	13	16	13
	$R^2 \geq 0.5$	37	35	33	37	37	37	37	36	35	37	37	35	37	36	37

R^2 – both determination coefficients; 1st Der – first derivative; 2nd Der – second derivative; NOR – normalized spectra; SNV – spectra normalized with standard normal variate; WA – approximate wavelet coefficients of spectra; WD – detailed wavelet coefficients of spectra.

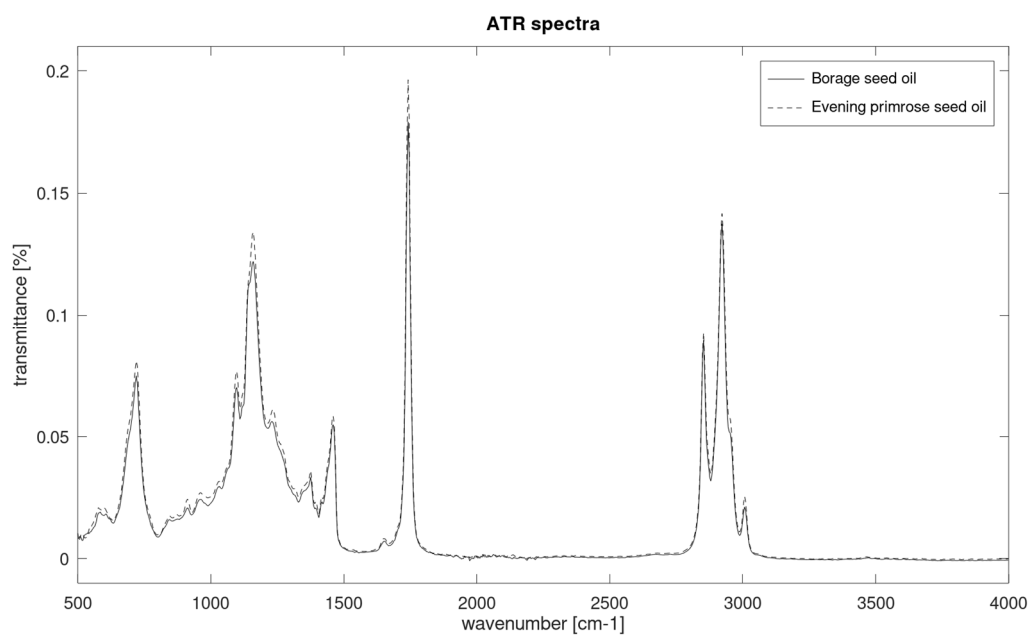


Figure S1: Average ATR spectra of borage seed oil and evening primrose seed oil samples.

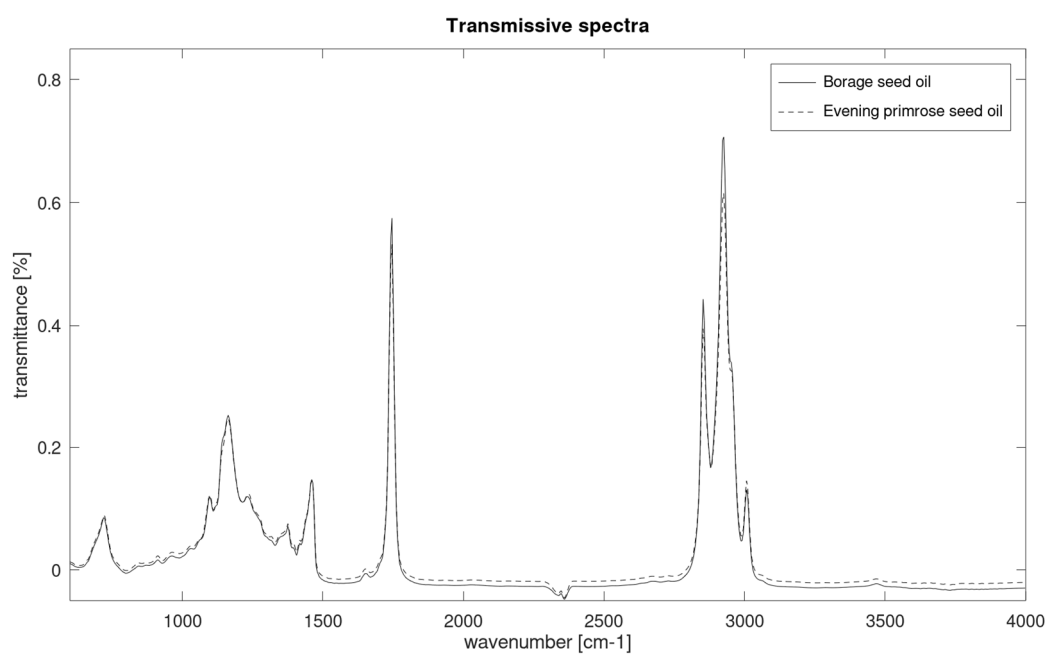


Figure S2: Average transmissive spectra of borage seed oil and evening primrose seed oil samples.