

Table 5. Coefficients (a, b, c, d and e) and Statistics (sample size, n, correlation coefficient, R, root mean squared errors, RMSE and ratio of prediction to deviation, RPD) of the equations obtained by fitting of ABS<sub>390</sub> during the heating treatment and the proportion of monounsaturated (% MUFA), omega-6 (% ω-6) and omega-3 (% ω-3) in the unheated oils.

Eq.	Volatile Compounds	x <sub>1</sub>	x <sub>2</sub>		n	a × 10 <sup>5</sup>	b × 10 <sup>5</sup>	c × 10 <sup>5</sup>	d × 10 <sup>5</sup>	e × 10 <sup>5</sup>	R	R <sup>2</sup>	R <sup>2</sup> <sub>pred</sub>	RMSE	RMSE <sub>pred</sub>	RPD <sub>pred</sub>	
1	Alkanals	MUFA	RM		63	-14.7	-36.3	-0.56	2.1		0.895	0.800		6.00 × 10 <sup>6</sup>			
					42	-13.9	-35.2	-0.56	2.1		0.890	0.793	0.821	6.17 × 10 <sup>6</sup>	5.61 × 10 <sup>6</sup>	2.42	
					21	-16.5	-28.4	-0.55	2.2		0.905	0.818	0.794				
2	Alkenals	MUFA	RM		63	25.5	-59.7	-1.59	3.6		0.758	0.617		1.53 × 10 <sup>7</sup>			
					42	27.3	-59.6	-1.66	3.6		0.765	0.618	0.600	1.57 × 10 <sup>7</sup>	1.51 × 10 <sup>7</sup>	1.62	
					21	20.6	-59.7	-1.41	3.6		0.784	0.615	0.618				
3	Alkadienals	ω-3	RM		63	-29.9	69.5	-2.00	-0.7		0.933	0.871		1.10 × 10 <sup>7</sup>			
					42	-34.7	71.9	-1.83	-0.7		0.933	0.870	0.877	1.10 × 10 <sup>7</sup>	1.02 × 10 <sup>7</sup>	2.92	
					21	-22.5	65.5	-2.15	-0.6		0.937	0.878	0.870				
4	Alkadienals	ω-6	RM		63	80.8	8.59	-4.03	1.2		0.930	0.865		1.10 × 10 <sup>7</sup>			
					42	82.4	7.84	-4.19	1.3		0.929	0.863	0.874	1.12 × 10 <sup>7</sup>	1.04 × 10 <sup>7</sup>	2.88	
					21	79.4	9.68	-3.94	1.1		0.935	0.874	0.863				
5	Total aldehydes	MUFA	ω-3	RM		63	141	-48.5	-4.30	6.3	-8.6	0.879	0.773		2.79 × 10 <sup>7</sup>		
						42	170	-45.9	-4.70	6.2	-9.2	0.878	0.771	0.800	2.85 × 10 <sup>7</sup>	2.52 × 10 <sup>7</sup>	2.29
						21	75.2	-53	-3.40	6.4	-7.4	0.883	0.780	0.785			
6	Total aldehydes	MUFA	ω-6	RM		63	-397	-58	2.00	6.5	7.1	0.877	0.770		2.80 × 10 <sup>7</sup>		
						42	-399	-56	2.00	6.5	7.5	0.875	0.766	0.786	2.89 × 10 <sup>7</sup>	2.61 × 10 <sup>7</sup>	2.22
						21	-397	-61	2.22	6.6	6.4	0.883	0.780	0.771			

RM: Regression model

CV: Cross Validation

DCV: Double-Cross Validation

$$\text{Volatile Compound} = a + b \times \text{ABS}_{390} + c \times x_1 + (d \times \text{ABS}_{390} \times x_1) + e \times x_2$$