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Letter to the Editor

Sir:

The term "selectivity" (SR), when used in reference to a hydrogenated oil or a hydrogenation catalyst, has come to mean the ratio of 2 reaction rates, the rate of hydrogenation of linoleic acid, a diene, divided by the rate of hydrogenation of oleic acid, monoene. The SR may be used as a criterion for catalyst selection and also processing conditions.

To determine the SR, hydrogenation of an oil using a specific set of processing conditions and catalyst is accomplished. The fatty acid composition of the starting and ending samples is determined and from those data and a computer, the reaction rates may be calculated and the SR determined. Because a computer is not always available, Albright (1) published a set of curves he had calculated so that the SR could be found from these graphs. However, the hydrogenation must be continued for some time to enable one to use the graphs. Also, the linolenic selectivity (LnSR) curves published by Allen (2) require a calculation before the graphs can be used.

Unfortunately, the reaction rate equations used to calculate the selectivities do not have closed solutions, so the calculation is accomplished by an iterative process which needs considerable speed and memory in a computer; the small computers and calculators now available are too slow.

Thus, there is a need for a rapid, simple method to calculate SR and LnSR from fatty acid composition data using a calculator.

The graphs published by Albright for the estimation of Selectivity Ratio by the hydrogenation of soybean oil are a family of lines. Such a family may be expressed as shown in Equation I, where S_o, S are the starting and ending stearic content, and L_o, L, the starting and ending linoleic. Albright's data for the SR of soybean oil were used to substitute into the equation and the 4 constants were calculated. Thus, for soybean oil the equation becomes:

$$SR = (100\ S\text{-}S_o)[1/((1.2603(Exp(2.0652(L/L_o))))\text{-}(.07713)(Exp(-2.2988(L/L_o))))]$$

This expression may be evaluated by a good calculator.

Also, the functional form of the Linolenic Selectivity (LnSR) curves calculated by Allen may be expressed as:

$$L/L_o = (Ln/Ln_o)^b,$$

$$SR = \frac{100}{S - S_o}\left[\frac{1.0}{a e^{b\left(\frac{L}{L_o}\right)} - c e^{-d\left(\frac{L}{L_o}\right)}}\right]$$

a = 1.260 c = 0.771

b = 2.065 d = 2.299

Equation I

where b is a function of the LnSR. The LnSR constants are inversely proportional to the estimated (b) and 2 coefficients are necessary to obtain the LnSR constants. The constants were evaluated by linear regression from knowns for soybean oil hydrogenation. Thus, the equation becomes:

$$LnSR = (0.6989\ (1n\ \overline{Ln_o}/1n\ \overline{L_o})) + .3011,$$

where Ln_o, Ln are start and ending linolenic and L_o, L are the linoleic acid in soybean oil.

These equations permit the calculation of the SR and LnSR by a calculator from the fatty acid composition of the starting and ending hydrogenated samples of soybean oil.

Table I shows the results of calculation of the SR and LnSR by a computer evaluation of reaction rate constants and the results obtained from the equations solved by a TI-59 calculator. As shown, the results are comparable. The program for the TI-59 calculator is available from the author.

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TABLE I

	Fatty acid composition					SR		Ln SR	
S_o	S	L_o	L	Ln_o	Ln	Computer	Calculator	Computer	Calculator
4.44	4.67	51.12	32.61	6.74	1.99	94.6	96.0	2.2	2.2
4.44	4.79	51.12	34.46	6.74	0.09	58.0	58.2	8.1	8.0
4.44	9.57	51.12	42.30	6.74	0.01	3.2	3.6	14.2	14.1
4.44	7.00	51.12	45.20	6.74	0.05	7.1	7.3	10.4	10.6
4.44	6.74	51.12	37.40	6.74	0.10	31.1	32.1	9.4	9.7