

The USDA Nutrient Database for Standard Reference Provides
Comprehensive Food Composition Data on Fats and Fatty Acids.
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Abstract

The 1997 report *Food, Nutrition and the Prevention of Cancer: a Global Perspective*, cited fourteen dietary recommendations concerning cancer prevention. One of the recommendations is to limit consumption of fatty foods, particularly those of animal origin and to choose modest amounts of appropriate vegetable oils. Epidemiological research on dietary intake and diseases and subsequent dietary counseling requires the existence of comprehensive food composition tables. The Agricultural Research Service's Nutrient Data Laboratory (NDL) acquires, evaluates and disseminates composition data on foods eaten in the US. As part of that mission, the NDL develops accurate and representative values for fats, oils and lipid components. The data can be disseminated for a variety of nutrients of emerging public health interest including positional and geometric isomers of fatty acids. NDL has developed the National Food and Nutrient Analysis Program, an extensive nationwide sampling and analysis program, to generate accurate and current analytical data. Foods being analyzed include a variety of traditionally high fat foods such as margarines (retail and industrial), and salad dressings. Data will be disseminated in the USDA Nutrient Database for Standard Reference (SR), and related databases developed for use in food consumption surveys. These databases are widely used by epidemiologists in analyzing dietary intakes of individuals. In addition, data from these databases serve as the core data for most commercial food composition databases used in the US and are selectively incorporated into some foreign databases where foods are similar. Margarine/spread data in SR are being updated to reflect current market trends in fat levels from 0% to the traditional 80% fat margarine. This poster will summarize market data, present new fatty acid profiles for 70% fat spread and 80% fat margarine and demonstrate the individual fatty acids and fatty acid totals which can be disseminated in SR.

USDA Compiling Food Composition Data for 100+ Years

- The USDA published its pioneering food composition tables in 1896 with publication of Bulletin No. 28, the Chemical Composition of American of American Food Materials, by W.O. Atwater and C.D. Woods. Percentages of five components (water, protein, fat, carbohydrate and ash) were reported, along with % refuse and calories/pound.
- In 1945, USDA food tables were expanded to 11 nutrients.
- In 1950, Agricultural Handbook No. 8, the Composition of Foods—Raw, Processed, Prepared was first published. Over the years, Handbook No. 8 grew into 22 individual food group sections. By this time, the scope of the nutrient list had been enlarged to include proximates, 9 minerals, 9 vitamins, individual fatty acids, total saturated, monounsaturated and polyunsaturated fatty acids, cholesterol, total phytosterols, and 18 amino acids.
- In 1989, data could be accessed through a dial-up Bulletin Board as well as printed sections.
- In 1992, printed sections were abandoned in favor of all data being made available at no charge on the NDL Web site (www.nal.usda.gov/fnic/foodcomp) or at nominal cost on CD-ROM.

Meeting Expanded Data Needs

- Along with this progress, a need developed to add new nutrients and new functionality to the Nutrient Databank System. A multi-year databank redesign project, called AIM-NDBS (Architecture and Integration Management-Nutrient Databank System), was thus begun. In conjunction with this redesign project, a multi-year analytical project, the National Food and Nutrient Analysis Program (NFNAP), was initiated to provide significantly improved analytical food composition data in the USDA Nutrient Data Laboratory databases.
- These major projects support the **mission of the Nutrient Data Laboratory:**
To develop authoritative food composition databases and state of the art methods to acquire, evaluate, compile and disseminate composition data on foods available in the United States.

The New USDA Nutrient Databank System -- How Do You Benefit?

New Fields of Information, including:

- Derivation codes – give specific information on how the value was determined. e.g.
 - A analytical values with complete documentation
 - S values based on product standard, such as enrichment level
- Added statistical fields
 - Number of acceptable studies
 - Minimum and maximum values
 - Degrees of freedom
 - Error bounds define range in which mean values expected to fall
 - Lower EB lowest mean value expected (95% confidence level)
 - Upper EB highest mean value expected (95% confidence level)
- Confidence Codes indicate data quality based on evaluation of
 - Sample plan
 - Sample handling
 - Analytical methods
 - Analytical quality control
 - Number of samples analyzed
 - References cite sources of nutrient data

More Nutrients:

- Nutrients in upcoming SR releases will include expanded lipid components as well as a large number of additional nutrients including carotenoids, vitamin E isomers, folate expressed as folic acid in mcg, food folate in mcg, and dietary folate equivalents.
- Additions to lipid components are starting to be populated with SR14.
- For some components of emerging public health interest, data will first be released in special interest tables on the NDL Web site. Release 1.2 of the USDA-Iowa State University database on the Isoflavone Content of Foods is presently available under the Food Composition Products heading. Additional datasets of isoflavone and flavonoid values will be provided as data become available through contract analyses.

Many specific fatty acid isomers, including:

- Positional isomers: Differ in the position of the double bond
e.g. omega position
omega-3 (n-3) fatty acids: The 1st double bond is at the 3rd carbon from the methyl end
omega-6 (n-6) fatty acids: The 1st double bond occurs at the 6th carbon
- Geometric isomers: Differ in the configuration of the hydrogen atoms attached to carbons joined by double bonds.
cis isomers have hydrogen atoms on the same side of the double bond
trans isomers have hydrogen atoms on opposite sides of the double bond
See tables 3 and 7 for levels of 18:1c and 18:1t in 80% margarine and 70% spread

More fatty acid totals:

In SR13

Saturated fatty acids

Monounsaturated fatty acids

Polyunsaturated fatty acids

+

Starting in SR14

Also:

Total trans fatty acids

Total trans monoenoic acid

Total trans polyenoic acid

Margarines and Spreads Sampled Through the National Food and Nutrient Analysis Program (NFNAP)

NFNAP was established in 1997 as a coordinated effort between the Nutrient Data Laboratory and NIH/National Heart, Lung, and Blood Institute with 17 other Institutes and Offices. The program has 5 specific aims:

1. Identify Key Foods for sample and analysis

Approximately 667 foods have been identified as Key Foods, collectively contributing 75% of the US population intake of nutrients of public health significance. Additional items prioritized for sampling and analysis include ethnic foods, foods making significant contributions to children's diets, some foods newly introduced to the market and ingredients which are of high usage in commercial food products.

Margarines and spreads are leading contributors of fat, calories, vitamin E, mono- and polyunsaturated fatty acids and are high contributors of vitamin A, saturated fats and sodium. Therefore, these products were among the first identified in 1997 for sampling and analysis.

2. Evaluate existing data for scientific quality

Major changes have occurred in margarine-type product formulations. The variation in fat levels, as well as brand differences in types of oils used, were taken into account in the sampling:

- Fat levels sampled ranged from 0 - 80%.
Existing database fat levels ranged from 20% - 80%.
Based on Nielsen market share data, the mean fat level of margarine-type products consumed by the US population was found to be 56%. 80% fat margarine has declined in both market share and in number of available brands.
Fat level categories sampled for NFNAP analysis were:
 - 80% ([product standard for margarine)
 - 70%
 - 37% - 60%
 - less than 37% but greater than 0%
 - 0% (fat free)
- Tremendous variation in types of oils, level of hydrogenation
- Variations in physical form from soft tub to hard stick

3. Devise and implement a nationally-based sampling survey of foods available in US markets

A population-based sampling plan was developed for margarines to ensure a representative sample of brands, fat levels, oil blends and physical forms purchased from grocery stores across the US. Nielsen market share data were used to determine volume sales of products available in grocery stores. Products were sampled in a variety of package sizes as well as over a variety of brands. Samples were picked up in 12 Generalized Consolidated Metropolitan Statistical Areas (gCMSAs), adapted from Census Areas. Products, including store brands, were statistically selected for pick-up from outlets across 4 regions of the US and 3 strata within each region. For each of the 5 fat ranges selected for sampling, a unique sampling plan was developed. Composite samples consisting of up to 24 sample units were prepared. Each composite usually consisted of sample units of a single brand. For 70% spread, 12 composites were prepared, providing an effective sample size of 288.

4. Analyze sampled foods under USDA-supervised laboratory contracts

Strict quality control procedures were developed based on use of standard reference materials and thorough documentation to maximize reliability and accuracy of analytical data. Beginning with SR15, Expert Confidence Codes, indicators of the reliability of data, will be released.

Fatty acids in margarine-type products were analyzed by a modification of method described by Sampugna et al. J. Chromatogr. 249: 245; 1982.

- Direct transesterification of margarine
- Mini column liquid chromatography
- SP-2380 liquid phase on 25m fused silica capillary column
- Standards used to determine retention times and response factors

Analyses of phytosterols in margarines were based on gas chromatographic procedures described in Method 45.4.06 (AOAC 16th ed. 1995). Data for margarine include stigmasterol, campesterol, and beta-sitosterol.

5. Incorporate the new data into the existing database

New Data will be released in SR14 for:

- Traditional 80% fat stick margarine containing regular regular and hydrogenated corn and soybean oils (data for selected nutrients shown in Tables 1-4) and
- 70% spread containing soybean and hydrogenated soybean oils (Tables 5-8)

Data for remaining margarines and spreads will be released in SR15:

These items will include fat-free, 0-37% fat, and 37-60% fat spreads as well as additional oil blends for 80% margarine and 70% spreads. Selected fat components are reported in this poster to demonstrate the new statistics to be disseminated from the redesigned databank system as well as present some of the new fatty acid isomers and totals which can now be disseminated in the USDA National Nutrient Database for Standard Reference.

Table 1. Proximate data for NDB No. 04628

Margarine, 80% fat, stick, includes regular and hydrogenated corn and soybean oils

Nutr No	Name	Value/ 100g food	Unit	No. Data pts	SE	Lower EB	Upper EB	No. of studies	Min	Max
255	Water	17.17	g	8	0.077	16.99	17.35	1	16.76	17.37
208	Calories	705	Kcal							
203	Protein	0.18	g	4	0.001	0.17	0.18	1	0.17	0.18
204	Total lipid (fat)	78.77	g	8	0.700	77.11	80.42	1	75.68	81.42
207	Ash	1.94	g	8	0.024	1.89	2.00	1	1.83	2.05
205	Carbohydrate by difference	1.94	g							

Table 2. Saturated fatty acid data for NDB No. 04628

Nutr No	Name	Value/ 100 g food	Unit	No. Data pts	SE	Lower EB	Upper EB	No. of studies	Min	Max
606	Fatty acids, total saturated	14.787	g							
611	12:0	0.000	g	8	0.000			1	0.000	0.000
612	14:0	0.069	g	8	0.003	0.062	0.077	1	0.061	0.084
613	15:0	0.000	g	8	0.000			1	0.000	0.000
614	16:0	8.135	g	8	0.107	7.882	8.388	1	7.494	8.533
653	17:0	0.000	g	8	0.000			1	0.000	0.000
614	18:0	6.047	g	8	0.117	5.770	6.325	1	5.742	6.734
615	20:0	0.263	g	8	0.006	0.250	0.277	1	0.232	0.284
624	22:0	0.271	g	8	0.007	0.256	0.287	1	0.238	0.294
654	24:0	0.000	g	8				1	0.000	0.000

Table 3. Monounsaturated fatty acid data for NDB No. 04628

Nutr No	Name	Value/ 100 g food	Unit	No. Data pts	SE	Lower EB	Upper EB	No. of studies	Min	Max
645	Fatty acids, Total monounsaturated	37.201	g							
625	14:1	0.000	g	8	0.000			1	0.000	0.000
626	16:1 undifferentiated	0.000	g							
673	16:1c	0.000	g	8	0.000			1	0.000	0.000
662	16:1t	0.000	g	8	0.000			1	0.000	0.000
617	18:1 undifferentiated	37.201	g							
674	18:1c	17.515	g	8	0.439	16.476	18.554	1	15.266	19.166
663	18:1t	19.686	g	8	0.415	18.706	20.666	1	17.508	21.242
628	20:1	0.000	g	8	0.000			1	0.000	0.000
630	22:1 undifferentiated	0.000	g	8	0.000			1	0.000	0.000
671	24:1c	0.000	g	8	0.000			1	0.000	0.000

Table 4. Polyunsaturated fatty acid, trans total, and sterol data for NDB No 04628

Nutr No	Name	Value/ 100 g food	Unit	No. Data pts	SE	Lower EB	Upper EB	No. of studies	Min	Max
646	Fatty acids, total polyunsaturated	23.097	g							
618	18:2 undifferentiated	20.877	g							
675	18:2 n-6 c,c	20.174	g	8	0.746	18.410	21.938	1	16.629	22.868
666	18:2i	0.703	g	8	0.162	0.320	1.086	1	0.206	1.432
619	18:3 undifferentiated	2.220	g							
851	18:3 n-3 c,c,c	2.220	g	8	0.253	1.622	2.818	1	1.654	3.458
672	20:2 n-6 c,c	0.000	g	8	0.000	0.000	0.000	1	0.000	0.000
689	20:3 undifferentiated	0.000	g	8	0.000	0.000	0.000	1	0.000	0.000
620	20:4 undifferentiated	0.000	g	8	0.000	0.000	0.000	1	0.000	0.000
629	20:5 n-3	0.000	g	8	0.000	0.000	0.000	1	0.000	0.000
631	22:5 n-3	0.000	g	8	0.000	0.000	0.000	1	0.000	0.000
605	Fatty acids, total trans	19.686	g							
693	Fatty acids, total trans-monoenoic	19.686	g							
638	Stigmasterol	28	mg	4	1.105	24.59	31.62	1	26	31
639	Campesterol	41	mg	4	2.622	32.83	49.52	1	34	46
641	Beta-sitosterol	117	mg	4	14.160	72.18	162.30	1	88	143

Table 5. Proximate data for NDB No 04629
Margarine, 70% vegetable oil spread, soybean and soybean (hydrogenated)

Nutr No	Name	Value/ 100g food	Unit	No. Data pts	SE	Lower EB	Upper EB	No. of studies	Min	Max
255	Water	27.41	g	10	0.44	21.78	33.05	1	26.85	27.68
208	Calories	619	Kcal							
203	Protein	0.21	G	10	0.05	- 0.42	0.83	1	0.18	0.27
204	Total lipid (fat)	69.40	g	10	1.24	53.68	85.11	1	68.65	70.98
207	Ash	1.85	g	10	0.06	1.02	2.67	1	1.76	1.89
205	Carbohydrate by difference	1.13	g							

Table 6. Saturated fatty acid data for NDB No 04629

Nutr No	Name	Value/ 100 g food	No. Data pts	Unit	SE	Lower EB	Upper EB	No. of studies	Min	Max
606	Fatty acids, total saturated	12.623		g						
611	12:0	0.000	10	g	0.000	0.000	0.000	1	0.000	0.000
612	14:0	0.041	8	g	0.009	- 0.071	0.152	1	0.029	0.046
613	15:0	0.000	10	g	0.000	0.000	0.000	1	0.000	0.000
614	16:0	7.005	10	g	0.120	5.486	8.524	1	6.933	7.158
653	17:0	0.000	10	g	0.000	0.000	0.000	1	0.000	0.000
614	18:0	5.085	10	g	0.040	4.580	5.590	1	5.034	5.109
615	20:0	0.233	10	g	0.006	0.152	0.315	1	0.229	0.241
624	22:0	0.258	10	g	0.002	0.229	0.287	1	0.257	0.261
654	24:0	0.000	10	g	0.000	0.000	0.000	1	0.000	0.000

Table 7. Monounsaturated fatty acid data for NDB No 04629

Nutr No	Name	Value/ 100 g food	Unit	No. Data pts	SE	Lower EB	Upper EB	No. of studies	Min	Max
645	Fatty acids, Total monounsaturated	36.733	g							
625	14:1	0.000	g	10	0.000				0.000	0.000
626	16:1 undifferentiated	0.000	g							
673	16:1c	0.000	g	10	0.000	0.000	0.000	1	0.000	0.000
662	16:1t	0.000	g	10	0.000	0.000	0.000	1	0.000	0.000
617	18:1 undifferentiated	36.733	g							
674	18:1c	17.506	g	10	0.462	11.630	23.383	1	17.228	18.098
663	18:1t	19.227	g	10	0.039	18.725	19.728	1	19.203	19.277
628	20:1	0.000	g	10	0.000	0.000	0.000	1	0.000	0.000
630	22:1 undifferentiated	0.000	g	10	0.000	0.000	0.000	1	0.000	0.000
671	24:1c	0.000	g	10	0.000	0.000	0.000	1	0.000	0.000

Table 8. Polyunsaturated fatty acid, trans total, and sterol data for NDB No 04629

Nutr No	Name	Value/ 100 g food	Unit	No. Data pts	SE	Lower EB	Upper EB	No. of studies	Min	Max
646	Fatty acids, total polyunsaturated	16.299	g							
618	18:2 undifferentiated	14.723	g							
675	18:2 n-6 c,c	13.656	g	10	0.267	10.263	17.050	1	13.496	13.998
666	18:2i	1.067	g	10	0.618	- 6.787	8.920	1	0.695	1.858
619	18:3 undifferentiated	1.575	g							
851	18:3 n-3 c,c,c	1.575	g	10	0.198	- 0.935	4.086	1	1.322	1.694
672	20:2 n-6 c,c	0.000	g	10	0.000	0.000	0.000	1	0.000	0.000
689	20:3 undifferentiated	0.000	g	10	0.000	0.000	0.000	1	0.000	0.000
620	20:4 undifferentiated	0.000	g	10	0.000	0.000	0.000	1	0.000	0.000
629	20:5 n-3	0.000	g	10	0.000	0.000	0.000	1	0.000	0.000
631	22:5 n-3	0.000	g	10	0.000	0.000	0.000	1	0.000	0.000
605	Fatty acids, total trans	19.227	g							
693	Fatty acids, total trans-monoenoic	19.227	g							
638	Stigmasterol	25	mg	6	0.757	15.290	34.539	1	24	26
639	Campesterol	31	mg	6	0.304	26.859	34.584	1	31	31
641	Beta-sitosterol	81	mg	6	2.067	54.723	107.251	1	80	84

Key components of lipid handling procedures:

- Data in units other than g/100 g food are converted in the databank system using Sheppard factors. These factors were published in a 1992 FDA publication by A.J. Sheppard entitled Lipid Manual, Methodology Suitable for Fatty Acid-Cholesterol Analysis.
- Release of data for some specific geometric and positional isomers in SR
- Consistency for our data users: isomeric values summed to yield estimates of the amount of undifferentiated fatty acid, for example:

18:3 n-3 c,c,c *Newly reported nutrient in SR14*

18:3 n-6 c,c,c *Newly reported nutrient in SR14*

18:3 undifferentiated (existing nutrient number 619)

Conclusion

Multi-year analytical programs coordinated by the Nutrient Data Laboratory have been designed to provide fully documented data on additional components of public health significance for release in the USDA Nutrient Database for Standard Reference (SR). Some of the nutrients which will be appearing in future releases of SR include: positional and geometric isomers of fatty acids, alpha-tocopherol, individual carotenoids, retinol in micrograms, and folate expressed as, food folate, added folic acid and dietary folate equivalents. Specific isomers of fatty acids will not be available for all foods in SR, but will be disseminated when available from contract analyses or from the scientific literature. Nationally-based sampling plans have been developed and full documentation is electronically recorded of all stages of the process from pickup of samples through analysis of composited samples. With a fully redesigned databank system, critical data from many of these fields will be disseminated with each release of the USDA Nutrient Database for Standard Reference (SR).

Numerous changes have been made to lipid handling procedures in the redesigned databank system to allow for dissemination of data on positional and geometric isomers of fatty acids. For the two margarine/spreads analyzed under the NFNAP protocol, the only trans fatty acid found was 18:1t. The level of this fatty acid increased with fat level from 19.227 for the 70% fat spread to 19.686 for 80% fat margarine. Cis and trans isomers for these items were totaled in the AIM system to provide users with a value for the undifferentiated fatty acid, nutrient 617, which has historically been disseminated for many SR items and for all items in the survey nutrient database. Such summations will be provided in SR whenever specific fatty acid isomers have been quantified.