Enhanced Formulation Estimations in USDA National Nutrient Databank.

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Abstract

In redesigning the National Nutrient Databank (NNDB), the Nutrient Data Laboratory (NDL) gave high priority to improved estimation methods. The cereal industry has been an important data provider for the NNDB, with some data provided by industry and released on a brand name basis. Also, considerable data are used for aggregation with similar products producing representative generic profiles. For the database used for food consumption surveys, complete nutrient profiles are needed for more than 3000 foods. Rarely are values available for the more than 50 nutrients required. NDL is now conducting national sampling and analysis of many Key Foods and processed food ingredients. Data for these items will be released in NDL's Standard Reference (SR) product. These analytical values are also used to complete profiles of multi-ingredient foods. Ingredients being analyzed include wheat flours and a variety of oils and shortenings important in many cereal-based foods. For aggregated generic items, missing values are calculated in a variety of ways. One of the most useful is the NNDB formulation program that uses SAS least square fitting techniques to estimate a formulation and proceeds with calculations of all missing nutrient values based on the estimated ingredient proportions. As part of the NNDB Redesign, the formulation program is being validated by comparisons of estimated and analytical values for the same products. Combined with improved processed food ingredient data, this enhanced formulation program will provide better nutrient estimations for cereal products in USDA food composition database products.

Fig. 1

Label Ingredients Entered
in Order of Predominance

Fig. 2

Food Specialist Enters Nutrients on Serving Size Basis
System Algorithms Convert Values to 100 g Basis

Nutrient Data Bank System - REAL

Action Edit Query Record Utility Main Menu Outlier Reports Help Window

Initial Food Item View

| Main Menu | | < | > | | Run Query | Impact Report | Associate | ☐ | Calculator |

Source Category

Identifier `122843` Type `Individual ▼` Created By `NNGAINE` FS Approved ☐ `Label ▼`

Creation Date `08-07-2000` QC Panel Approved ☐

Brand Name ☐

Food Group `18` Sub Group `[ ]` Modification Date `08-08-2000` Proprietary ☐

Sponsoring Org
`[ ]` ... New

Initial Name `Mission Corn Tortillas-Extra Thin, Composite C9813J, Sample Unit NF9907WE`

Database
`[ ]` ... New

Edited Name `[ ]`

Study
`NFNAP C99W3a`

Manufacturer `[ ]` ... New   Help

1 of 1

| SAMP PLAN | HANDLING | LABEL INFO | NAME | WEIGHT | NUTRIENTS | COMPONENTS | PREP METHOD | LANGUAL |

Initial

	Number	Name	Add Nutr	Value	Unit	Number Datapts	Source Code	Deriv Code	Chg Code	Add/Mod Date	Reject Flag	
X	208	Energy	☐	90.0000	kcal ▼	1				07-AUG-2000	☐	...
X	203	Protein	☐	2.0000	g ▼	1				07-AUG-2000	☐	...
X	204	Total lipid (fat)	☐	1.0000	g ▼	1				07-AUG-2000	☐	...
X	205	Carbohydrate, by difference	☐	18.0000	g ▼	1				07-AUG-2000	☐	...
X	291	Fiber, total dietary	☐	1.0000	g ▼	1				07-AUG-2000	☐	...
X	269	Sugars, total	☐	.0000	g ▼	1				07-AUG-2000	☐	...
X	301	Calcium, Ca	☐	2.0000	% DV ▼	1				07-AUG-2000	☐	...
X	303	Iron, Fe	☐	2.0000	% DV ▼	1				07-AUG-2000	☐	...
X	304	Magnesium, Mg	☐		mg ▼					07-AUG-2000	☐	...

Fiber Subtraction Indicator ☐

Help   View Label Ingred

c:\ndbs\fooditem.fmb Multi Nutrient ☐ Multiple   Dry Basis ☐

Moisture % `[ ]` Total Lipid `[ ]`

Moisture Source `[ ]` Lipid Source `[ ]`

Factors   Print

Record: 9/30   List of Values <OSC> <DBG>

Fig. 3
Analytical Data Entry into NNDB System

- Analytical data entered on 100 g food basis

- Derivation Codes automatically generated by System provide valuable information about data sources. e.g.

  A= analytical data with full documentation, including analytical methods and sampling

Fig. 4

Ingredient Listings for 4 Brands of Corn Tortillas
Used in Formulation Estimations

Brand A	**Brand B**	**Brand C**	**Brand D**
Corn	Corn		
Lime	Lime	Corn flour	Corn flour
Water	Water	Water	Water
Cellulose gum	Cellulose gum	Cellulose gum	Fumaric acid
Propionic acid	Propionic acid	Potassium sorbate	Potassium sorbate
Phosphoric acid	Phosphoric acid	Calcium propionate	Calcium propionate
Benzoic acid	Benzoic acid	Lime	Lime
			Propionic acid
			Phosphoric acid
			Sodium propionate
			Dextrose

Fig. 5
NNDB Ingredients Entered

Nutrient Data Bank System - REAL

Action Edit Query Record Utility Main Menu Outlier Reports Help Window

Formulation View

| Main Menu | Save | < ▷ | Tab Copy | Run Query | Formulate | Calculator |

Identifier `131599`   Type `Formulated`   Created By `RCUTRUFELLI`

Food Group `19`   Sub Group `   `   Creation Date `10-03-2001`

Modification Date `10-03-2001`

Initial Name `corn tortilla`   Brand Name ☐

Edited Name `Corn tortilla run 4` LIST   Approved ☐

Ingredient Basis `    ` ...   Component Basis `    ` ...   Target Nutrient Basis `    ` ... Help

Food Supply ☐   Ingredient ☐   PDS ☐   SR ☐   Special ☐   Proprietary ☐

Lipid Conversion Factor `.8600`   Retinol Factor `9.9787`   **4 of 4**

| SOURCE | INGREDIENTS | TARGET | PRODUCT | NUTRIENTS | NAME | WEIGHT | PREP INST |

Ingredient List

	Rank	Food Item Identifier	NDB NO	Edited Name	Ingred Subst	Lower Bound	Exact Amount	Upper Bound	Relax Order	Est. % Wt.	% Fat Loss	Nutr Lost w/ Fat	% Moist Loss	Ret ID	
X	1	68377	20016	Corn flour, whole-grain, yel	☐	0	☐	100	☐	59.194		☐		0301	...
X	2	68900	42062	Added calcium	☑	0	☐	50	☑	.052		☐			...
X	3	66519	14429	Water, municipal	☐	0	☐	50	☑	39.704		☐			...
X	4	69063	42243	Gums, plant exudates (incl	☐	0	☐	.5	☐	.5		☐			...
X	5	69662	47019	Acetic acid	☑	0	☐	.5	☐	.5		☐			...
X	6	69053	42233	Added sodium	☑	0	☐	100	☑	.05		☐			...
X					☐		☐		☐			☐			...

| Select Ingredients | Water Ingredients | Refresh | Formulation Report | Common Substitutions | Help |

Record: 4/4   <OSC> <DBG>

Fig. 6
Food Specialist Adds Constraints
to Guide Formulation Estimation

Fig. 7
**Food Specialist Checks Key Nutrient Field,
Selecting Nutrients for Best-fit Match to Label Nutrients
by Regression Techniques**

Fig. 8

Constraints Applied to Formulation Program
Run With Label Claim Corn Tortilla Data

- Rank order of ingredients is the first determinant of relative ingredient percents

  Corn flour was consistently the first ingredient in corn tortillas and therefore was assigned rank order of 1. Order was relaxed for water to accommodate differences among brands and the possible shifting of water predominance order due to drying of dough ingredients during commercial preparation of tortillas. Relaxed order for added minerals reflected differences in types and order of additives between brands.

- Lipid, energy, calcium, sodium and vitamin A were keyed for best-fit formulation purposes. The formulation program outputs the formulation which produces nutrient values most closely approximating known values for keyed nutrients.

- Upper bounds were applied by the food specialist to further narrow formulation estimations. The most vital upper bound applied was to limit moisture to 50%, since most other nutrient levels are dependent on the moisture level of a product. The upper bound chosen was based on previously released database values for corn tortillas (44.1% in SR14). Organic acid bounds were based on ingredient supplier information as to normal usage levels.

Fig. 9

Considerations in Selecting NNDB Ingredients
for Use in Formulation Program

- NNDB ingredients are selected which most closely approximate the label ingredients.

- Ingredient substitutions are often required for functional food additives. For corn tortillas, acetic acid, added sodium and added calcium served this purpose.

- Additives may be ignored in formulation program listings if they will not contribute to the formulation estimation or provide a needed nutrient value. Potassium was not listed as an ingredient because the label provided no potassium value for matching. The Food Specialist therefore must remember to reject any potassium output from the corn tortilla formulation.

- Occasionally 2 or more NNDB ingredients are required to represent a single label ingredient. Bran, for example, is often added to cereal-based formulations in combination with all-purpose flour to simulate custom milled flours which may be used in commercial products.

Fig. 10

Flour Tortilla Label Claim Data,
Aggregation of 18 Brands

Fig. 11
Flour Tortilla Estimations Using
Label Claim Data

Fig. 11

Flour Tortilla Estimations Using Label Claim Data

target_tab: Previewer

File   View   Help

Formulation Target Tab Report

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Identifier 131608   **Type** Formulated   **Created By** GHOLCOMB   **FS Approved** N
                                                               Creation Date 03-OCT-2001   **Brand Name** N
Food Group 08   **Sub Group**   **Modification Date** 03-OCT-2001   **Proprietary** N

Initial Name   AACC Flour Tortilla Formulation, label claim data

Edited Name   AACC Flour Tortilla Formulation, label claim data

Number	Name	Target Value	Calculated Value	Unit	Key Nutrient	Model Error
203	Protein	7.7047	7.7046	g	Y	.00
204	Total lipid (fat)	6.9286	6.9288	g	Y	.00
205	Carbohydrate, by difference	50.8299	57.0283	g	N	12.19
208	Energy	301.3434	321.2908	kcal	N	8.43
269	Sugars, total	2.0616		g	N	
291	Fiber, total dietary	2.5299	2.0137	g	Y	- 20.41
301	Calcium, Ca	119.4000	119.6460	mg	Y	.21
303	Iron, Fe	2.5394	3.4637	mg	N	36.40
307	Sodium, Na	683.0470	683.3760	mg	Y	.05
404	Thiamin	0.4965	0.4684	mg	N	- 5.67
405	Riboflavin	0.1517	0.3316	mg	N	118.58
406	Niacin	3.3154	3.9629	mg	N	19.53
417	Folate, total	102.6316	80.3975	mcg	N	- 21.66
601	Cholesterol	0.0000	0.0000	mg	N	
606	Fatty acids, total saturated	1.7514	1.7514	g	N	.00

Total Model Error: 20.66

Fig. 12
Flour Tortilla Estimations, Analytical Data Formulation 1
Results in Low Protein and Mg Values

target_tab: Previewer

File View Help

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Formulation Target Tab Report

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Identifier 131606   **Type** Formulated   **Created By** GHOLCOMB   **FS Approved** N
                                                            Creation Date 03-OCT-2001   **Brand Name** N
Food Group 18   **Sub Group**   **Modification Date** 03-OCT-2001   **Proprietary** N

Initial Name AACC Flour Tortilla Formulation, calculated protein, ash, Mg low

Edited Name AACC Flour Tortilla Formulation, analytical data, run 1

Number	Name	Target Value	Calculated Value	Unit	Key Nutrient	Model Error
203	Protein	8.3115	7.1747	g	Y	- 13.68
204	Total lipid (fat)	7.7130	7.7126	g	Y	- .01
207	Ash	2.3920	0.7558	g	N	- 68.40
255	Water	30.4377	30.4377	g	Y	.00
301	Calcium, Ca	128.5000	128.9567	mg	Y	.36
303	Iron, Fe	3.3400	3.2261	mg	N	- 3.41
304	Magnesium, Mg	22.0333	15.5051	mg	Y	- 29.63
306	Potassium, K	154.6667	74.3455	mg	N	- 51.93
307	Sodium, Na	636.3330	636.7368	mg	Y	.06
309	Zinc, Zn	0.5412	0.4932	mg	N	- 8.87
312	Copper, Cu	0.1423	0.1015	mg	N	- 28.70
315	Manganese, Mn	0.4977	0.4743	mg	N	- 4.70
410	Pantothenic acid	0.1640	0.3042	mg	N	85.49

Total Model Error: 43.73

Fig. 13
Flour Tortilla Estimations, Analytical Data
Final Formulation with Wheat Bran Added

- Illustrates the use of more than 1 NNDB ingredient to represent a single label ingredient.
- The first formulation gave undesirably low protein and magnesium values. The commercial flour used in tortillas may contain more bran than the flour used in the formulation.
- Wheat bran therefore was added as a 'relaxed order' ingredient, allowing the System to find the optimal rank order for matching keyed nutrients.

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File View Help

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Formulation Target Tab Report

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Identifier 131607	**Type** Formulated	**Created By** GHOLCOMB		**FS Approved** N
		Creation Date 03-OCT-2001		**Brand Name** N
Food Group 18	**Sub Group**	**Modification Date** 03-OCT-2001		**Proprietary** N

Initial Name AACC Flour Tortilla Formulation, analytical data, final, wheat bran added

Edited Name AACC Flour Tortilla Formulation, final

Number	Name	Target Value	Calculated Value	Unit	Key Nutrient	Model Error
203	Protein	8.3115	7.2343	g	Y	- 12.96
204	Total lipid (fat)	7.7130	7.7130	g	Y	.00
207	Ash	2.3920	0.8148	g	N	- 65.94
255	Water	30.4377	30.4372	g	Y	.00
301	Calcium, Ca	128.5000	128.6024	mg	Y	.08
303	Iron, Fe	3.3400	3.2926	mg	N	- 1.42
304	Magnesium, Mg	22.0333	22.0351	mg	Y	.01
306	Potassium, K	154.6667	86.2746	mg	N	- 44.22
307	Sodium, Na	636.3330	636.7377	mg	Y	.06
309	Zinc, Zn	0.5412	0.5661	mg	N	4.61
312	Copper, Cu	0.1423	0.1110	mg	N	- 22.03
315	Manganese, Mn	0.4977	0.5943	mg	N	19.40

Total Model Error: 13.11

Fig. 14
Flour Tortillas
Ratio of Analytical/Estimated Values

AIM_NDBS

File View Help

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Food Item Nutrient Comparison - Ratio Report

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Identifier 1	131558			**Identifier 2**	131607		
Type	Compiled			**Type**	Formulated		
Edited Name	AACC Flour Tortillas 8/14/2001			**Edited Name**	AACC Flour Tortilla Formulation, final		

Nutrient Number	Nutrient Name	Value 1	Source Code 1	Value 2	Source Code 2	Ratio
255	Water	30.4377	1	30.4372	4	1.0000
208	Energy	307.2463	4	310.3084	4	.9901
268	Energy	1285.5187	4	1311.7407	4	.9800
203	Protein	8.3115	1	7.2343	4	1.1489
204	Total lipid (fat)	7.7130	1	7.7130	4	1.0000
207	Ash	2.3920	1	.8148	4	2.9356
205	Carbohydrate, by difference	51.1458	4	52.9886	4	.9652
301	Calcium, Ca	128.5000	1	128.6024	4	.9992
303	Iron, Fe	3.3400	1	3.2926	4	1.0144
304	Magnesium, Mg	22.0333	1	22.0351	4	.9999
306	Potassium, K	154.6667	1	86.2746	4	1.7927
307	Sodium, Na	636.3333	1	636.7377	4	.9994
309	Zinc, Zn	.5412	1	.5661	4	.9559
312	Copper, Cu	.1423	1	.1110	4	1.2829
315	Manganese, Mn	.4977	1	.5943	4	.8374

Summary of Validation Results

Food Specialists at the Nutrient Data Laboratory are validating the Formulation Program of the National Nutrient Databank System with a variety of food products. This poster presents data comparing nutrient values for corn and flour tortillas calculated through the Formulation Program with values derived from both label claims and through a rigorous analytical protocol, the National Food and Nutrient Analysis Program (NFNAP).

As can be seen from Fig. 7 and Fig.11, the Formulation Program produced good correspondence with label claim data. Due to the limited number of nutrients available from a label, Food Specialists often find that applying constraints such as lower and/or upper bounds provides critical guidance to the program in optimizing a formulation.

Numerous reports and statistical procedures have been built into the NNDB for comparison and quality control purposes. Fig.14 shows a Nutrient Comparison Report used as part of the Formulation validation procedure. Nutrients calculated through the Formulation program were compared with analytical values from flour tortillas sampled nationwide through the NFNAP.   Data are presented as ratios of analytical /calculated. A ratio of 1 indicates an exact correspondence of calculated and analytical values.   Ratios for 13 of the nutrients fell within a narrow range of 0.84 to 1.28, showing excellent correspondence between calculated and analytical values. No attempt was made to match ash and potassium values due to the large number of mineral-containing functional additives.

The Formulation Program, when guided by the expertise of knowledgeable Food Specialists, can be an effective tool in estimating nutrient values. As more analytical data become available, both from industry and from the NFNAP program, validations will be run a variety of food matrices.

Cooking Yields

- Additional constraints to the Formulation Program which will be investigated include addition of cooking yield adjustments for moisture and fat losses and gains (e.g. moisture losses during reheating of tortillas and fat uptake during frying of meats).

- Considerable cooking yields work is being conducted in NDL's food preparation laboratory and will be incorporated into electronic tables with existing published data. Preliminary Cooking Yields are shown below in Fig. 15. Cooking yields and retentions values will be published on the NDL Web site at

    www.usda.gov/fnic/foodcomp

Fig. 15

Preliminary Cooking Yields for Refrigerated
Flour Tortillas, heated for serving

Heating Method	% Yield
Microwave	95
Oven	98
Skillet	96