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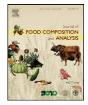
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Improvements to the International Life Sciences Institute Crop Composition Database

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ABSTRACT

In May 2003, the International Life Sciences Institute (ILSI) released Version 1.0 of the Crop Composition Database (http://www.cropcomposition.org), a comprehensive public database that provides information on the natural variability in composition of conventionally bred crops. Currently, the database contains more than 115,000 data points representing 132 compositional components in corn, soybean and cotton. In 2009 the database logged more than 30,000 site visits from 122 countries around the world. ILSI has made a number of improvements to the original database and recently developed Version 4.0, which will be released for public access in 2010. Version 4.0 presents an intuitive graphical-user interface (GUI), significantly increased performance, added security, and additional features such as unit conversion and multiple output options. Another notable improvement in Version 4.0 is the Summary of Search Results tool, which allows users to immediately view data of interest and guides the preparation of output reports. This paper summarizes some of the enhanced features and usage of the database, which continues to be a valuable tool for characterizing the composition of conventional crops.

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1. Introduction: a report from the ILSI International Food Biotechnology Committee Task Force on Crop Composition

Repositories of food composition data have increased in number, size and utility throughout the past century (Atwater and Woods, 1896; Chatfield, 1949; Conrad et al., 1982). Personal computers and the Internet have hastened this trend (Day, 1985), and a variety of composition data sources are available via traditional media and the World Wide Web (Charrondiere et al., 2002; Kitta et al., 2005). Examples include the USDA National Nutrient Database for Standard Reference (http://www.ars.usda. gov/ba/bhnrc/ndl), INFOODS (http://www.fao.org/infoods), and EuroFIR (http://www.eurofir.net).

Like most databases, composition databases are designed to reflect the needs of specific user communities (Pennington, 2008), which may limit utility or functionality for other users. For example, many food composition databases do not provide information for crop tissues grown in different countries over multiple years. In some cases analytical methods are not provided, or their performance parameters are not available. In addition, composition data are often aggregated (rather than consisting of individual analyses) and do not make it possible for the user to assess the natural compositional variation that exists within different crops.

Understanding this natural compositional variation is essential for safety assessments of new germplasm and genetically modified (GM) products. These safety assessments also require knowledge about the composition of conventional crops (i.e. non-GM). When these data are combined with side-by-side experimental

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comparisons of a transgenic crop and its conventional counterpart and the scientific literature, one can determine if food or feed derived from a GM crop is substantially equivalent to its conventional (non-GM) counterpart and, if so, it is very likely that the GM crop is as safe and nutritious as the corresponding conventional crop. This comparative safety assessment process (sometimes called substantial equivalence) is well accepted by regulatory agencies (US FDA, 1992; OECD, 1993; WHO, 1995; FAO, 1996; Codex Alimentarius, 2003).

The International Life Sciences Institute (ILSI; http://www.ilsi.org) is a non-profit worldwide foundation established in 1978 to advance the understanding of scientific issues relating to nutrition, food safety, toxicology, risk assessment and the environment. ILSI also works to provide the scientific basis for global harmonization in these areas. By bringing together scientists from academia, government, industry and the public sector, ILSI seeks a balanced approach to solving problems of common concern for the well being of the general public.

To aid investigations of substantial equivalence, ILSI maintains the Crop Composition Database (ILSI-CCDB; http://www.cropcomposition.org), which is a public database that provides information on the natural compositional variability of conventional crops (Ridley et al., 2004). The ILSI-CCDB is a compilation of crop analyses from a number of companies engaged in agricultural life sciences. Through ILSI, these composition data have been standardized and pooled to make the information available to academia, government agencies, industry and the general public.

The ILSI-CCDB has undergone an extensive redesign (Version 4.0) to add requested functions, increase performance, enhance security, and prepare the database for the addition of new composition data. The purpose of this paper is (a) to summarize how these objectives were achieved in Version 4.0 of the ILSI-CCDB, and (b) to introduce users to the improved graphical-user interface (GUI) and new features of the ILSI-CCDB. In addition, the methods for database validation and beta testing are discussed. ILSI expects to launch Version 4.0 in 2010.

2. The ILSI-CCDB

In 2009 the ILSI-CCDB logged more than 30,000 site visits from 122 countries. The current version of the ILSI-CCDB (Version 3.0) includes more than 115,000 data points for 132 proximates, nutrients, bioactive non-nutrients and secondary metabolites in corn, soybean and cotton. Samples were collected from controlled field trials at multiple worldwide locations, under the guidelines of the U.S. Environmental Protection Agency Good Laboratory Practices (US EPA, 1989), and are traceable back to the source. Each data point in the database is linked to a validated, published method, a field site location and the year of sample harvest. Currently, no samples from GM crops are in the database, and the conventional data serve as a reference point for crop composition prior to the introduction of modern agricultural biotechnology.

In addition to providing central tendency statistics (i.e. mean values), a key feature of the ILSI-CCDB is that it provides a measure of statistical dispersion for individual analytes (i.e. range values). This feature allows users to better understand the natural variation of these analytes in crop tissues of interest. For example, Fig. 1 shows the central tendency and statistical dispersion for total fat (Fig. 1A) and crude protein (Fig. 1B) in more than 1100 corn samples obtained from 1995 to 2004 from 10 field locations around the world. The data indicate that these two analytes in corn grain exhibit natural variation that approximates a Gaussian distribution. Similar observations have been reported for ash, protein, fat and carbohydrate in corn and soybean (Herman et al., 2010). In fact, this observation holds for many analytes in the ILSI-CCDB (data not shown), which has important implications for investigations of

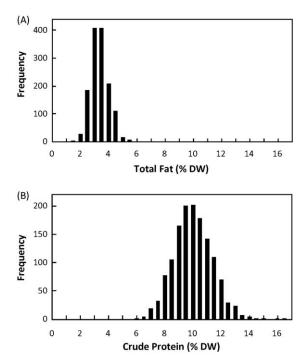


Fig. 1. Total fat and Crude protein in conventional corn grain. The analytes were measured in more than 1100 grain samples and the data were binned prior to plotting the histograms. These results indicate that these analytes (in corn grain) exhibit natural variation that approximates a Gaussian distribution. Minimum, maximum, and mean values for each analyte are also shown.

compositional equivalence. Specifically, the natural variation in crop composition should be carefully considered during comparative safety assessments of conventional and GM crops.

In addition to incorporating recurring user requests, Version 4.0 includes notable changes to the software and hardware for the database. Version 4.0 has been improved by moving from an outdated Perl interface to an intuitive Java-based GUI. To increase performance and security, the Java code for Version 4.0 accesses data files that are organized with the 11g StandardEdition One platform (Oracle Corp., CA) and is maintained on a new PowerEdge R200 server (Dell Inc., TX). Additional data were not added during the upgrade to Version 4.0 so that it could first be tested for performance and stability, and validated for accuracy. It is expected that a large amount of new (existing) data will be added to the ILSI-CCDB after Version 4.0 is released.

3. New features and options in the ILSI-CCDB

The new GUI for Version 4.0 is comprised of four primary screens. Screen 1 (Fig. 2) is the Welcome portal for the ILSI-CCDB. This screen provides users with relevant information about the database, such as *Privacy Policy, Terms of Use, About the ILSI CCDB*, and *How to Cite this Database*. All users should read the disclaimer statement at the bottom of Screen 1. Users access the database search functions via the *Database Search* button on the Welcome page.

Screen 2 (Fig. 3) allows users to select primary search criteria including crop type, tissue type, year(s) of sample harvest and field site location(s). Simple instructions are located at the left of this and subsequent screens. Screen 2 also allows users to activate the *Analyte Filters* option to filter the data by a range of values and/or analysis method, if desired.

Screen 3 is accessed via the *View Summary of Search Results* button. Screen 3 (Fig. 4) has three functions, all of which are useful new features of the ILSI-CCDB. First, using the *Summary of Search Results* tool, users can quickly review data and determine if a search refinement is necessary, prior to generating an output report. The

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About the ILSI-CCDB		•Other Web Sites of	of Interest			
Register For Updates		•Help				
		© 2003-2010 International Life Sci	ences Institute			

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Fig. 2. Welcome portal for Version 4.0 of the ILSI Crop Composition Database. This screen of the new GUI provides users with relevant information about the database, such as *Sources of Data, Database Structure, How to Submit Data,* and other useful links. The homepage for the International Life Sciences Institute can be accessed using the link in the upper left corner. Users access the database search functions via the *Database Search* button on the Welcome page.

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Crop Composition	Database		
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Disclaimer: The database is provided "as is" and without warranty of any kind, whether express or implied. ILSI and its member companies expressly disclaim implied warranties of merchantability, fitness for a particular purpose, and noninfringement. In no event shall ILSI or any of its member companies be liable to database users or any third party in any way, including, without limitation, for direct, indirect, consequential, incidental, reliance, or special damages. Because it is not feasible to provide in this database statistical analyses for search results derived from all combinations of selection oriteria, the responsibility for any statistical analyses and interpretation of results rests with the user.

Fig. 3. Selecting primary search criteria in Version 4.0 of the ILSI Crop Composition Database. The *Primary Search Criteria* tool allows users to select crop type, tissue type, year(s) of sample harvest, and field site location(s). This screen also allows users to activate the *Analyte Filters* option to filter the data by a range of values and/or analysis method. Simple instructions are located at the left of the screen.

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Fig. 4. The Summary of Search Results tool, the Create Report from Search Results tool, and the Select Fields for Report Output tool in Version 4.0 of the ILSI Crop Composition Database. The Summary of Search Results tool allows users to quickly review data and determine if a search refinement is necessary, prior to generating an output report. The Create Report from Search Results tool allows the user to create and organize a specific analyte list for an output report. Meta-data can be added to the output report using the Select Fields for Report Output tool. Simple instructions are located at the left of the screen.

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Fig. 5. Selecting the format of output reports in Version 4.0 of the ILSI Crop Composition Database. The *Select Report Format* tool allows users to select the format for output reports. Three report formats are available in the *Report Type* panel; each of these formats can be generated in the portrait or landscape orientations and output as HTML, PDF or a comma delimited file (CSV). Header text can be added using the *Report Info* panel. Simple instructions are located at the left of the screen.

Summary of Search Results tool allows one to determine quickly the sample number (n), minimum, maximum, and mean values for any analyte in the database. The *Create Report from Search Results* tool allows the user to create and organize a specific analyte list for an output report. Meta-data can be added to the output report using the *Select Fields for Report Output* tool. In essence, the data/information contained in a desired output report and how that data/information is organized are defined using the *Create Report from Search Results* tool and the *Select Fields for Report Output* tool. The options in these two tools allow one to consider the potential effects of different variables (e.g. analysis method, crop yield or location of field site) on datasets of interest.

Screen 4 is accessed via the *Report Options* button. Users of the ILSI-CCDB represent a broad cross-section of researchers in plant, animal and food sciences, and the needs of users are variable. Thus, Version 4.0 allows more flexibility in the format of output reports. The new features on Screen 4 (Fig. 5) allow one to select the format for output reports. Three report formats are available (*Summary Report, Detailed Report*, or *Tabular Report*). Each of these formats can be generated in the portrait or landscape orientations, and output as HTML, PDF or a comma delimited file (CSV). CSV files can be transferred to Excel, SAS, MATLAB, or the R programming language for advanced statistical analyses and graphics. Screen 4 also includes text fields for adding header-type information to output reports (e.g. name of the study director, study title, document number, etc.). Output reports are generated using the *Run Report* button.

4. Units of measure in Version 4.0

A diverse range of needs has led to the adoption of many different units of measure to describe the composition of food and feeds. For example, food composition databases often use fresh

weight (FW) units of measure since foods are usually consumed in a hydrated form, while vitamins are typically expressed as mg/100 g FW to compare the nutritional value of fresh fruits or vegetables. By comparison, investigations of compositional equivalence are typically conducted with units of measure that apply broadly across analyte categories such as % dry weight (DW). Other examples include the formulation of animal diets that use mg of amino acid per g DW of grain (mg/g DW), while the development of nutritionally enhanced crops typically express data as relative percentage (e.g. % of total fatty acids). Therefore, to meet these diverse needs, Version 4.0 of the ILSI-CCDB allows users to view and output composition data in multiple units of measure, including % DW, % FW, mg/100 g FW, mg/g DW and mg/g FW. In addition, amino acids and fatty acids can be expressed as a relative percentage (i.e. % Total AA or % Total FA), and some nutrients (e.g. ferulic acid, p-coumaric acid) can be expressed as parts per million FW (ppm FW). Minerals are expressed as mg/kg DW and ppm FW, and calories are expressed as kcal/100 g DW and kcal/100 g FW. This flexibility with units of measure is a notable enhancement to the ILSI-CCDB.

All analytes in the database have been assigned a primary unit of measure, which is shown in the right column of the new *Summary of Search Results* tool (Fig. 4). To maximize performance and simplify usage of this tool, composition data may be viewed only in the primary unit of measure. If secondary units of measure (or multiple units of measure for a single analyte) are preferred, Version 4.0 of the ILSI-CCDB requires that data with secondary units of measure be generated in an output report.

4.1. Methods of analysis and LOQ in Version 4.0

Precision of measurement varies with the specific nutrient being measured, the method used, and the laboratory conducting the analysis (Phillips et al., 2007). Thus, each data point in the ILSI-CCDB is associated with a specific method of analysis, a method code and a literature citation for the method. All data in the ILSI-CCDB originate from methods that are validated and internationally accepted. Meta-data for methods can be accessed by activating the *Analysis Method* option in the *Select Fields for Report Output* tool on Screen 3 (Fig. 4).

The importance of the Limit of Quantitation (LOQ) for understanding food composition data has been recognized previously (Holden et al., 2005). The LOQ is defined as the lowest point at which the method can quantify the amount of an analyte in the sample. It typically represents some multiple of the Limit of Detection (MacDougall et al., 1980). The LOQ for an individual method can vary among studies and laboratories depending on calibration standards, matrix effects and instrumentation. As shown in Fig. 4, the Summary of Search Results tool reports the number of samples within a search that are below the LOQ. For example, raffinose was measured in 737 corn grain samples and 73 of the observed values for raffinose in this tissue were below the LOQ (denoted as 73 < LOQ). The data that contribute to the minimum, maximum and mean values for raffinose do not include the 73 data points that are below the LOQ. The LOQ meta-data can also be accessed by activating the Samples Below LOQ and Samples Above LOQ options in the Select Fields for Report Output tool on Screen 3 (Fig. 4).

4.2. Using Version 4.0 of the ILSI-CCDB: a step-by-step example

Direct your web browser to http://www.cropcomposition.org. On Screen 1 (Fig. 2), press the *Database Search* button to initiate a database query.

On Screen 2 (Fig. 3) use the pull-down menus to select a *Crop Type* (corn) and a *Tissue Type* (grain). If no selections are made in the pull-down menus for *Crop Year*(s), *Country*(s), and *Region*(s), the primary search criteria will default to All Years, Any Country, and Any Region. For this example, accept these defaults by ignoring these three pull-down menus; ignore *Analyte Filters* (optional) as

well. Press the *View Summary of Search Results* button near the bottom of Screen 2. It will require ~30 s to process this initial query because the server is accessing all data and meta-data for more than 1350 corn grain samples.

On Screen 3 (Fig. 4), in the Summary of Search Results tool, activate the "check-box" buttons adjacent to Bio Actives, Minerals, and Other Metabolites for a quick-view of the composition data for these analytes in corn grain. Note that phytic acid levels were measured in 1163 corn grain samples and that phytic acid was below the LOQ in 6 of these 1163 samples. Thus, all data and meta-data for this analyte derived from 1157 samples (1163 - 6 = 1157) and the minimum, maximum and mean values for phytic acid in this tissue are 0.102% FW, 1.421% FW, and 0.665% FW, respectively. These results indicate that corn grain is relatively rich in phytic acid. The Summary of Search Results tool also reports that sodium and furfural were measured in 1145 and 547 grain samples, respectively, and sodium was below the LOQ in 928 of the 1145 samples while furfural was below the LOQ in 533 of the 547 samples. These results indicate that corn grain contains very little sodium (mean = 29.00 ppm FW, n = 217) and furfural (mean = 3.081 ppm FW, n = 14). Thus, measuring sodium and furfural in corn grain may not be critical for comparative safety assessments of conventional and GM corn products.

Next, use the *Create Report from Search Results* tool to select *Bio Actives* in the pull-down menu under *Analyte Type* (Fig. 4). Select phytic acid in the pull-down menu under *Analyte*. Select % FW in the pull-down menu under *Units*. Press the *Add Analyte*(s) button to add phytic acid (% FW) to the *Analyte List* for the output report. Repeat these steps, but select % DW in the pull-down menu under *Units*. Press the *Add Analyte*(s) button to add phytic acid (% FW) to the *Analyte List* for the output report. Repeat these steps, but select % DW in the pull-down menu under *Units*. Press the *Add Analyte*(s) button to add phytic acid (% DW) to the *Analyte List* for the output report. Use this same approach to create an *Analyte List* that includes phytic acid (% FW and % DW), Vitamin B₃ (mg/100 g FW), iron (ppm FW), sodium (ppm FW), and furfural (ppm FW). If desired, the red " × " button can be used to remove an analyte from the *Analyte List*. For certain *Analyte Types*



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Fig. 6. An example of an HTML output report from Version 4.0 of the ILSI Crop Composition Database. Data for a single analyte (phytic acid in corn grain) is shown with two units of measure (% DW and % FW). This HTML output report also shows meta-data for the analysis methods used to measure this analyte. Output reports in this format can be saved as a PDF using the pull-down menu labeled *Output Format* and the *Go* button.

(e.g. fatty acids) the pull-down menu under *Analyte* includes the selection of *All Fatty Acids*; this option allows users to populate the *Analyte List* with all fatty acids via a single use of the *Add Analyte*(s) button. After creating an *Analyte List* for the output report, use the "check-box" buttons in the *Select Fields for Report Output* tool (Fig. 4) to include meta-data for *Number of Samples, Samples Below LOQ, Samples Above LOQ* and *Analysis Method* in the output report. For this example do not change the default settings for *Minimum Value, Maximum Value, Mean Value, Analyte Type* and *Analyte*. Press the *Report Options* button.

On Screen 4 (Fig. 5), in the *Report Options* tool, select the "checkbox" button for *Summary Report*. Use the pull-down menus under *Report Orientation* and *Output Format* to select the landscape orientation and HTML format, respectively. Enter "Short Title 123" in the text field under *Title* and enter "Short Description 123" in the text field under *Description*. Press the *Run Report* button.

One example of an HTML *Summary Report* is shown in Fig. 6. To print this report use the pull-down menu labeled *Output Format* and the *Go* button to save a PDF to your desktop. Note that this output report shows that the phytic acid values were derived using three methods that are identified by method codes and literature citations. For example, method A0036 (*Journal of Agricultural and Food Chemistry*, 19(3): 551–554, 1994) was used for measuring phytic acid in 927 of the 1163 samples. If statistical analyses or graphical representations of the data are desired, the 1163 phytic acid values (including values that were below the LOQ) can be retrieved using the *Detailed Report* option in the *Report Options* tool (see Fig. 5).

5. Validation and beta testing of Version 4.0

Quality control checks are conducted during sample analysis to monitor method performance, and original or certified copies of the data are archived by the data sources. Analysis for data outliers is the responsibility of each data source prior to database submissions. An exhaustive cross-validation of Version 4.0 has been completed. This validation effort included a complete review of all raw data files and thorough comparisons of output from Version 3.0 and Version 4.0. Extensive cross-validations were completed for the output in the *Summary of Search Results* tool, *Summary Report* output, *Detailed Report* output, and *Tabular Report* output. The cross-validation work was conducted on all crop types, all tissue types, and all analyte types.

Considering the substantial redesign of the ILSI-CCDB, ILSI sought opportunities to beta test Version 4.0. Following a suggestion from the user community, ILSI agreed to provide a hands-on training workshop for Version 4.0 of the ILSI-CCDB. The daylong session was attended by 20 participants from FDA, ILSI member companies and ILSI staff. Participant feedback confirmed that search features and key attributes of Version 4.0 had been well developed. Workshop participants also encouraged ILSI to consider adding non-OECD analytes to the database, additional data on existing crops, and additional crops. Some participants indicated the same level of comprehensive information for GM crops would be extremely useful.

6. Conclusions and future directions

The release of Version 1.0 of the ILSI-CCDB took place in May 2003. Subsequent versions expanded the database and incorporated additional data for forage and grain/seed. Database performance diminished as the size of the database and user community increased. To meet the needs of this international user community, the ILSI Crop Composition Task Force embarked on a complete redesign of the ILSI-CCDB to add user-requested functions, increase performance, enhance security and prepare

the database for a large addition of new (existing) composition data. Following the addition of new data, the ILSI Crop Composition Task Force expects to further improve performance, search and output options in future upgrades to the ILSI-CCDB. It is hoped that future versions of the database will include data submitted from scientists and other researchers, representing a variety of public and private organizations. These future enhancements will provide additional leverage for understanding crop composition and completing safety assessments for new crop varieties.

Citing the ILSI-CCDB

For a general citation of the ILSI-CCDB please cite Ridley et al., 2004 and Alba et al., 2010. In addition, the following citation format is suggested when referring to datasets obtained from the ILSI-CCDB: ILSI, 2010. International Life Sciences Institute Crop Composition Database, Version 4.0, http://www.cropcomposition.org [month, day, year (when the cited data were retrieved)].

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