### **Best Practices for Preparing Ecological Data to Share**

Bob Cook Environmental Sciences Division Oak Ridge National Laboratory

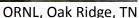


#### Best Practices for Preparing Ecological Data Sets, ESA, August 2010

#### Presenter

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Data







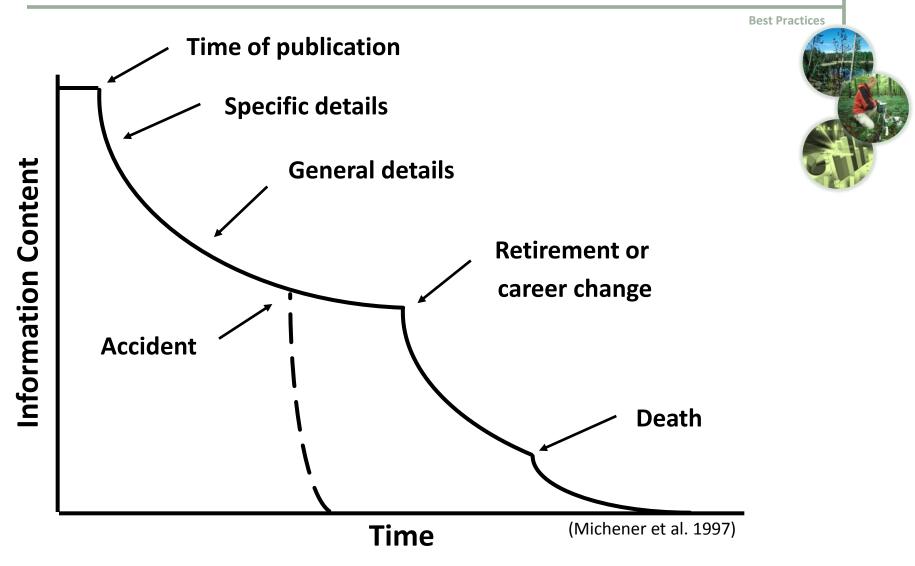




#### Information to let you find, understand, and use the data

- descriptors
- -documentation

# Poor data practice results in loss of information (data entropy)



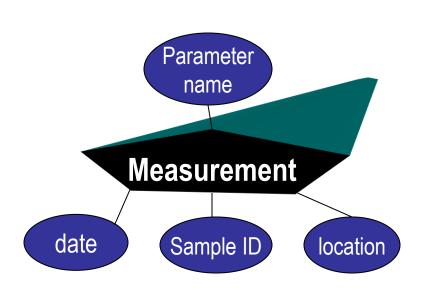
# **The 20-Year Rule**

- The metadata accompanying a data set should be written for a user 20 years into the future--what does that investigator need to know to use the data?
- Prepare the data and documentation for a user who is unfamiliar with your project, methods, and observations



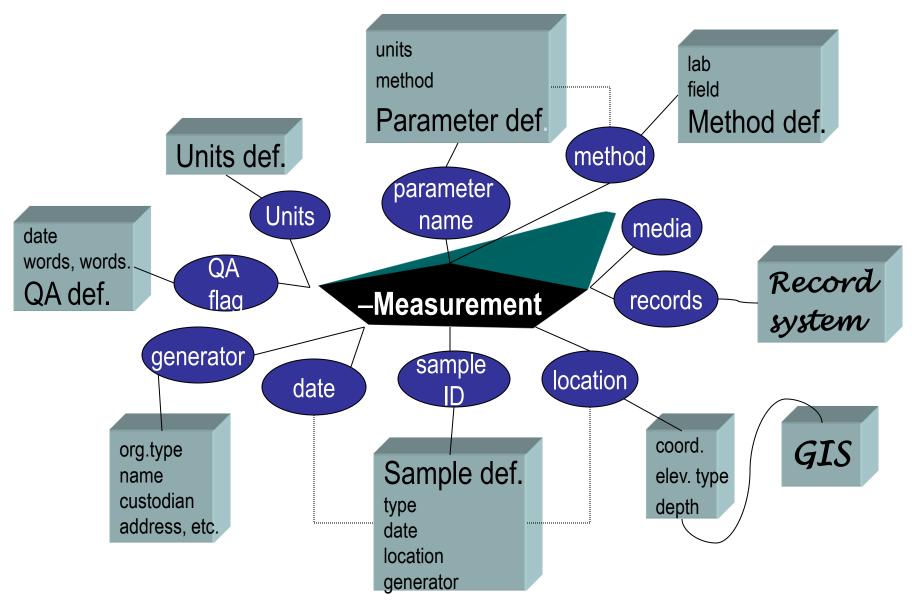
#### **Metadata needed to Understand Data**

-The details of the data ....



**Best Practices** 

### **Metadata Needed to Understand Data**



- 1. Define the contents of your data files
- 2. Use consistent data organization
- 3. Use stable file formats
- 4. Assign descriptive file names
- 5. Preserve information
- 6. Perform basic quality assurance
- 7. Assign descriptive data set titles
- 8. Provide documentation
- 9. Protect your data
- 10. Acknowledge contributions



### **1. Define the contents of your data files**

 Content flows from science plan (hypotheses) and is informed from requirements of final archive

- Best Practices
- Keep a set of similar measurements together in one file (e.g., same investigator, methods, time basis, and instruments)
  - No hard and fast rules about contents of each files

#### **1. Define the Contents of Your Data Files**

### **Define the parameters**

- Use commonly accepted parameter names that describe the contents (e.g., precip for precipitation)
- Use consistent capitalization (e.g., not temp, Temp, and TEMP in same file)
- Explicitly state units of reported parameters in the data file and the metadata
  - SI units are recommended

#### **1. Define the Contents of Your Data Files**

#### **Define the parameters** (cont)

- Choose a format for each parameter, explain the format in the metadata, and use that format throughout the file
  - e.g., use yyymmdd; January 2, 1999 is 19990102
  - Use 24-hour notation (13:30 hrs instead of 1:30 p.m. and 04:30 instead of 4:30 a.m.)
  - Report in both local time and Coordinated Universal Time (UTC)
  - See Hook et al. (2007) for additional examples of parameter formats
    - http://daac.ornl.gov/PI/bestprac.html#prac3



#### 1. Define the Contents of Your Data Files (cont)

Column	Description	Units/Format
SITE	k=Kataba forest, p=Pandamatenga, m=Near Maun, e=HOORC/MPG Maun tower, o=Okwa river crossing, t=Tshane, skukuza=Skukuza Flux Tower	text
SPECIES	Scientific name up to 25 characters	text
DATE	Date of measurement	yyyymmdd
BA	Woody plant basal area	m2/ha
SEBA	Standard error of BA	m2/ha
DENSITY	Woody plant density (number of trees per hectare)	number/ha
SEDEN	Standard error of DENSITY (n=42 for KT, n=49 for Skukuza)	number/ha
STEMS	Number of stems per hectare (/ha)	number/ha
HEIGHT	Basal area-weighted average height	m2/ha
WOOD	Aboveground woody plant wood dry biomass	kg/ha
LEAF	Aboveground woody plant leaf dry biomass	kg/ha
LAI	Leaf Area Index calculated by allometry	m2/m2

**Best Practices** 

Scholes (2005)

#### 1. Define the contents of your data files

#### Site Table

Site Name	Site Code	Latitude (deg)	Longitude (deg)	Elevation (m)	Date
Kataba (Mongu)	k	-15.43892	23.25298	1195	29-Feb-00
Pandamatenga	р	-18.65651	25.49955	1138	7-Mar-00
Skukuza Flux Tower	skukuz a	-31.49688	25.01973	365	15-Jun-00

. . . . . .

Scholes, R. J. 2005. SAFARI 2000 Woody Vegetation Characteristics of Kalahari and Skukuza Sites. Data set. Available on-line [http://daac.ornl.gov/] from Oak Ridge National Laboratory Distributed Active Archive Center, Oak Ridge, Tennessee, U.S.A. doi:10.3334/ORNLDAAC/777

**Best Practices** 

#### 2. Use consistent data organization (one good approach)

Each row in a file represents a complete record, and the columns represent all the parameters that make up the record.

Station	Date	Temp	Precip
Units	YYYYMMDD	С	mm
HOGI	19961001	12	0
HOGI	19961002	14	3
HOGI	19961003	19	-9999

Note: -9999 is a missing value code for the data set

#### 2. Use consistent data organization (a 2<sup>nd</sup> good approach)

Parameter name, value, and units are placed in individual columns.

This approach is used in relational databases.

Station	Date	Parameter	Value	Unit
HOGI	19961001	Temp	12	С
HOGI	19961002	Temp	14	С
HOGI	19961001	Precip	0	mm
HOGI	19961002	Precip	3	mm



#### 2. Use consistent data organization (cont)

**Best Practices** 

- Be consistent in file organization and formatting
  - don't change or re-arrange columns
  - Include header rows (first row should contain file name, data set title, author, date, and companion file names)
  - column headings should describe content of each column, including one row for parameter names and one for parameter units

### 3. Use stable file formats

- Use text (ASCII) file formats for tabular data
  - (e.g., .txt or .csv (<u>c</u>omma-<u>s</u>eparated <u>v</u>alues)
  - within the ASCII file, delimit fields using commas, pipes (|), tabs, or semicolons (in order of preference)
- Use GeoTiffs / shapefiles for spatial data
- Avoid proprietary formats
  - They may not be readable in the future



#### 3. Use consistent and stable file formats (cont)

**Best Practices** 

SAFARI 2000 Plant and Soil C and N Isotopes, Southern Africa, 1995-2000
SITE, COUNTRY, LAT, LONG, DATE, START\_DEPTH, END\_DEPTH, CHARACTERISTICS, C, N, d13C, d15N
units, none, decimal degrees, decimal
degrees, yyyy/mm/dd, cm, cm, none, percent, percent, per mil, per mil
USGS-1, Botswana, -21.62, 27.37, 1999/07/12, 5, 20, Hardveld, 0.67, 0.052, -17, 8.9
USGS-2, Botswana, -21.07, 27.42, 1999/07/12, 5, 20, Hardveld, 0.68, 0.063, -18.3, 8
USGS-3, Botswana, -20.72, 26.83, 1999/07/12, 5, 20, Hardveld, 0.94, 0.087, -17, 6.8
USGS-4, Botswana, -20.52, 26.41, 1999/07/12, 5, 20, Hardveld, 0.53, 0.04, -19.9, 5.5
USGS-5, Botswana, -20.55, 26.15, 1999/07/12, 5, 20, Lacustrine, 2.11, 0.162, -15.2, 5.9
...
USGS-30, Botswana, -19.81, 23.63, 1999/07/18, 5, 20, Alluvium, 0.67, 0.063, -19.2, 11.8
USGS-31, Botswana, -20.62, 22.74, 1999/07/18, 5, 20, Hardveld, 0.23, 0.014, -16.8, 16.2

Aranibar, J. N. and S. A. Macko. 2005. SAFARI 2000 Plant and Soil C and N Isotopes, Southern Africa, 1995-2000. Data set. Available on-line [http://daac.ornl.gov/] from Oak Ridge National Laboratory Distributed Active Archive Center, Oak Ridge, Tennessee, U.S.A. doi:10.3334/ORNLDAAC/783

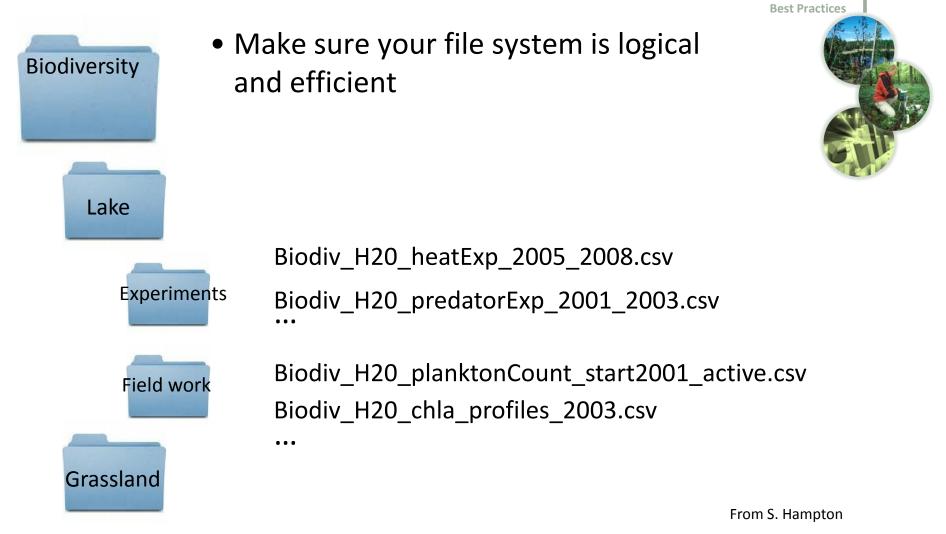
# 4. Assign descriptive file names

**Best Practices** 

- File names should be <u>unique</u> and <u>reflect the file</u> <u>contents</u>
- Bad file names
  - Mydata
  - 2001\_data
- A better file name
  - bigfoot\_agro\_2000\_gpp.tif
    - BigFoot is the project name
    - Agro is the field site name
    - 2000 is the calendar year
    - GPP represents Gross Primary Productivity data
    - tif is the file type GeoTIFF

A STORY TOLD IN FILE NAMES:			
Location: 😂 C:\user\research\data			~
Filename 🔺	Date Modified	Size	Туре
🔀 data_2010.05.28_test.dat	3:37 PM 5/28/2010	420 KB	DAT file
🚦 data_2010.05.28_re-test.dat	4:29 PM 5/28/2010	421 KB	DAT file
👸 data_2010.05.28_re-re-test.dat	5:43 PM 5/28/2010	420 KB	DAT file
👸 data_2010.05.28_calibrate.dat	7:17 PM 5/28/2010	1,256 KB	DAT file
👸 data_2010.05.28_huh??.dat	7:20 PM 5/28/2010	30 KB	DAT file
関 data_2010.05.28_WTF.dat	9:58 PM 5/28/2010	30 KB	DAT file
👸 data_2010.05.29_aaarrrgh.dat	12:37 AM 5/29/2010	30 KB	DAT file
👸 data_2010.05.29_#\$@*&!!.dat	2:40 AM 5/29/2010	0 KB	DAT file
👸 data_2010.05.29_crap.dat	3:22 AM 5/29/2010	437 KB	DAT file
関 data_2010.05.29_notbad.dat	4:16 AM 5/29/2010	670 KB	DAT file
🔀 data_2010.05.29_woohoo!!.dat	4:47 AM 5/29/2010	1,349 KB	DAT file
👸 data_2010.05.29_USETHISONE.dat	5:08 AM 5/29/2010	2,894 KB	DAT file
🕲 analysis_graphs.xls	7:13 AM 5/29/2010	455 KB	XLS file
ThesisOutline!.doc	7:26 AM 5/29/2010	38 KB	DOC file
Notes_Meeting_with_ProfSmith.txt	11:38 AM 5/29/2010	1,673 KB	TXT file
🗀 JUNK	2:45 PM 5/29/2010		Folder
😝 data_2010.05.30_startingover.dat	8:37 AM 5/30/2010	420 KB	DAT file

# 4. Assign descriptive file names **Organize files logically**



#### 5. Preserve information

- Keep your raw data raw
  - No transformations, interpolations, etc, in raw file



Raw Data	File		-### GI	iles_zoop_temp_regress_4jun08.r	
Giles_zoop0	Count_Diel_2	001_2003.csv	—### Lc	oad data	
ТАХ	COUNT	TEMPC	–Giles< read.cs	<- sv("Giles_zoopCount_Diel_2001_2003.csv")	
C	3.97887358	-	-### Lc	ook at the data	
F	0.97261354 0.53051648		–Giles		
F	0	11.9	-plot(C	COUNT~ TEMPC, data=Giles)	
			-### Lo	og Transform the independent variable (x+1)	
С	10.8823893	12.8	-Giles\$	SLcount<-log(Giles\$COUNT+1)	
F	43.5295571	13.1			
М	21.7647785	14.2	-### Pl	lot the log-transformed y against x	
Ν	61.6668725	12.9	– <mark>plot(</mark> L	.count ~ TEMPC, data=Giles)	
—		,			

Processing Script (R)

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#### 5. Preserve information (cont)

- Use a scripted language to process data
  - R Statistical package (free, powerful)
- MATLAB
- SAS
  - MATLAB



- Processing scripts are records of processing
  - Scripts can be revised, rerun
- Graphical User Interface-based analyses may seem easy, but don't leave a record

# 6. Perform basic quality assurance

- Assure that data are delimited and line up in proper columns
- Check that there no missing values (blank cells) for key parameters
- Scan for impossible and anomalous values
- Perform and review statistical summaries
- Map location data (lat/long) and assess errors
- No better QA than to analyze data



#### 6. Perform basic quality assurance (con't)

 $\uparrow$ Terrain ∈ & → Coordinates for site in Illinois are + incorrect Place geographic data on a map to ensure that coordinates are Coordinates for site in Brazil are incorrect POWERED BY Google

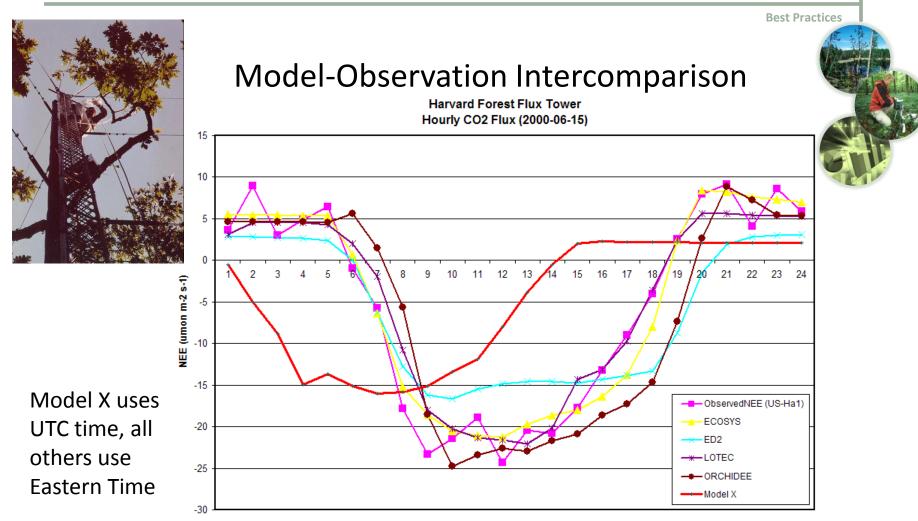
geographic

correct.

**Best Practices** 

#### 6. Perform basic quality assurance (con't)

#### **Plot information to examine outliers**

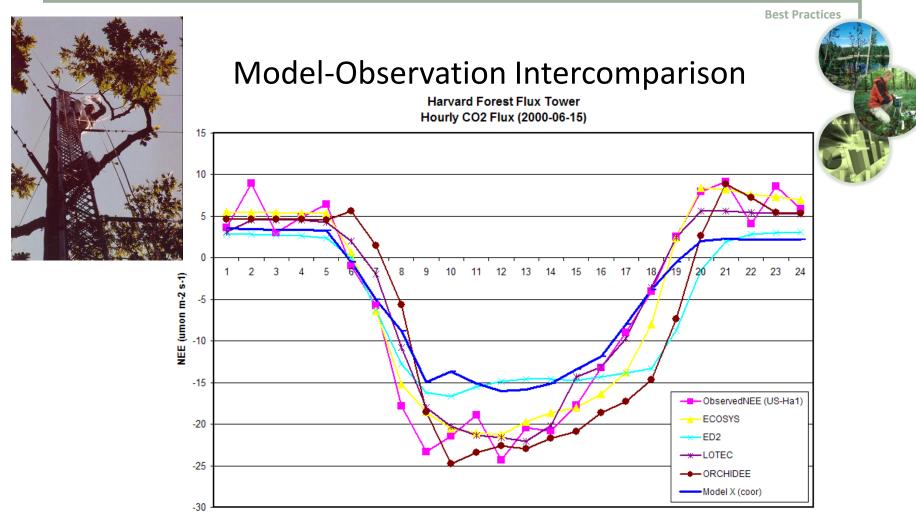


Hours

Data from the North American Carbon Program Interim Synthesis (Courtesy of Yaxing Wei, ORNL)

#### 6. Perform basic quality assurance (con't)

#### **Plot information to examine outliers**



Hours

Data from the North American Carbon Program Interim Synthesis (Courtesy of Yaxing Wei, ORNL)

# 7. Assign descriptive data set titles

- Data set titles should ideally describe the type of data, time period, location, and instruments used (e.g., Landsat 7).
- Titles should be concise (< 85 characters)
- Data set title should be similar to names of data files
  - Good: SAFARI 2000 Upper Air Meteorological Profiles, Skukuza, Dry Seasons 1999-2000"
  - Bad: "Productivity Data"



# 8. Provide Documentation / Metadata

- What does the data set describe?
- Why was the data set created?
- Who produced the data set and Who prepared the metadata?
- **How** was each parameter measured?
- What assumptions were used to create the data set?
- When and how frequently were the data collected?
- Where were the data collected and with what spatial resolution? (include coordinate reference system)
- **How** reliable are the data; what is the uncertainty; what problems remain in the data set?
- What is the use and distribution policy of the data set? How can someone get a copy of the data set?
- **Provide** any references to use of data in publication(s)?

**Best Practices** 

### 9. Protect data

- Create back-up copies often
  - Ideally two copies, one on-site and one off-site
  - Frequency based on need / risk
- Know that you can recover from a data loss
  - Periodically test your ability to restore information



# 9. Protect data (cont)

- Ensure that file transfers are done without error
  - Compare checksums before and after transfers
    - Example tools to generate checksums

http://www.pc-tools.net/win32/md5sums/

http://corz.org/windows/software/checksum/



#### **10. Acknowledge contributions**

- Who contributed data to your data set?
- How should your data be acknowledged / used by others?

**Best Practices** 

All data have been collected and curated by Dr. C. Hippocrepis at All Rotifers University.

Data may be freely downloaded for non-commercial uses. Please contact Dr. C. Hippocrepis (<u>chippocrepis@allrotifers.edu</u>) to let us know if you use these data. We report uses of the public data to our funders, and it is extremely helpful to know if others have been able to use these data in teaching or research.

# When your project is over, where should the data be archived?

- Part of project planning
- Contact archive / data center early to find out their requirements
  - What additional data management steps would they like you to do?
- Suggested data centers / archives:
  - Dryad
  - Ecological Archives
  - Knowledge Network for Biocomplexity (KNB)
- ORNL DAAC
- DataONE (Observation Network for Earth)
- National Biological Information Infrastructure





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#### **Best Practices: Conclusions**

- Data management is important in today's science
- Well organized data:
  - enables researchers to work more efficiently
  - can be shared easily by collaborators
  - can potentially be re-used in ways not imagined when originally collected



### **Bibliography**

- Ball, C. A., G. Sherlock, and A. Brazma. 2004. Funding high-throughput data sharing. Nature Biotechnology 22:1179-1183. doi:10.1038/nbt0904-1179.
- Borer, ET., EW. Seabloom, M.B. Jones, and M. Schildhauer. 2009. Some Simple Guidelines for Effective Data Management ,Bulletin of the Ecological Society of America. 90(2): 205-214.
- Christensen, S. W. and L. A. Hook. 2007. NARSTO Data and Metadata Reporting Guidance. Provides reference tables of chemical, physical, and metadata variable names for atmospheric measurements. Available on-line at: <a href="http://cdiac.ornl.gov/programs/NARSTO/">http://cdiac.ornl.gov/programs/NARSTO/</a>
- Cook, Robert B, Richard J. Olson, Paul Kanciruk, and Leslie A. Hook. 2001. Best Practices for Preparing Ecological Data Sets to Share and Archive. Bulletin of the Ecological Society of America, Vol. 82, No. 2, April 2001.
- Hook, L. A., T. W. Beaty, S. Santhana-Vannan, L. Baskaran, and R. B. Cook. June 2007. Best Practices for Preparing Environmental Data Sets to Share and Archive. <u>http://daac.ornl.gov/Pl/pi\_info.shtml</u>
- Kanciruk, P., R.J. Olson, and R.A. McCord. 1986. Quality Control in Research Databases: The US Environmental Protection Agency National Surface Water Survey Experience. In: W.K. Michener (ed.). Research Data Management in the Ecological Sciences. The Belle W. Baruch Library in Marine Science, No. 16, 193-207.
- Michener, W K. 2006. Meta-information concepts for ecological data management. Ecological Informatics. 1:3-7.
- Michener, W.K. and J.W. Brunt (ed.). 2000. Ecological Data: Design, Management and Processing, Methods in Ecology, Blackwell Science. 180p.
- Michener, W. K., J. W. Brunt, J. Helly, T. B. Kirchner, and S. G. Stafford. 1997. Non-Geospatial Metadata for Ecology. Ecological Applications. 7:330-342.
- U.S. EPA. 2007. Environmental Protection Agency Substance Registry System (SRS). SRS provides information on substances and organisms and how they are represented in the EPA information systems. Available on-line at: <u>http://www.epa.gov/srs/</u>
- USGS. 2000. Metadata in plain language. Available on-line at: <u>http://geology.usgs.gov/tools/metadata/tools/doc/ctc/</u>

