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University of Wisconsin-Madison  
Department of Geography  
GEOG 920:  
**CHARACTERIZING ORGANIC MATTER ON LAND AND WATER**  
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## **READING LIST**

### **1. REVIEWS**

#### **1.1. Chemical Composition**

- Kögel-Knabner, I. 2002. The macromolecular composition of plant and microbial residues as inputs to soil organic matter. *Soil Biology & Biochemistry* 34: 139-162. (Figures of molecular structures)
- Kleber, M. and M.G. Johnson. 2010. Advances in understanding the molecular structure of soil organic matter: Implications for interactions in the environment. *Advances in Agronomy* 106: 77-142.
- Hedges, J.I., G. Eglinton, P.G. Hatcher, D.L. Kichrman, C. Arnosti, S. Derenne, R.P. Evershed, I. Kögel-Knabner, J.W. de Leeuw, R. Littke, W. Michaelis, and J. Rullkötter. 2000. The molecularly-uncharacterized component of nonliving organic matter in natural environments. *Organic Geochemistry* 31: 945-958.
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- Grandy, A.S., and J.C. Neff. 2008. Molecular C dynamics downstream: the biochemical decomposition sequence and its impact on soil organic matter structure and function. *Science of the Total Environment* 404: 297-307.
- Lorenz, K., R. Lal, C.M. Preston, and K.G.J. Nierop. 2007. Strengthening the soil organic carbon pool by increasing contributions from recalcitrant aliphatic bio(macro)molecules. *Geoderma* 142: 1-10. See Table 1.
- Burdon, J. 2001. Are the traditional concepts of the structures of humic substances realistic? *Soil Science* 166: 752-769.
- Poirier, N., S.O. Sohi, J.L. Gaunt, N. Mahieu, E.W. Randall, D.S. Powlson, R.P. Evershed. 2005. The chemical composition of measurable soil organic matter pools. *Organic Geochemistry* 36: 1174-1189.
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### **1.2. Methods**

- Medeiros, P.M. and B.R.T. Simoneit. 2007. Gas chromatography coupled to mass spectrometry for analyses of organic compounds and biomarkers as tracers for geological, environmental, and forensic research. *Journal of Separation Science* 30: 1516-1536.
- Otto, A. and M.J. Simpson. 2007. Analysis of soil organic matter biomarkers by sequential chemical degradation and gas chromatography-mass spectrometry. *Journal of Separation Science* 30: 272-282.
- Amelung, W., S. Brodowski, A. Sandhage-Hofmann, and R. Bol. 2008. Combining biomarker with stable isotope analyses for assessing the transformation and turnover of soil organic matter. *Advances in Agronomy* 100: 155-249.
- Kögel-Knabner, I. 2000. Analytical approaches for characterizing soil organic matter. *Organic Geochemistry* 31: 609-625.
- Northcott, G.L. and K.C. Jones. 2000. Experimental approaches and analytical techniques for determining organic compound bound residues in soil and sediment. *Environmental Pollution* 108: 19-43.
- Simpson, M.J., A. Otto, and X. Feng. 2008. Comparison of solid-state Carbon-13 Nuclear Magnetic Resonance and organic matter biomarkers for assessing soil organic matter degradation. *Soil Science Society of America Journal* 72: 268-276.
- Shadkani, F. and R. Helleur. 2010. Review: Recent applications in analytical thermochemolysis. *Journal of Analytical and Applied Pyrolysis* 89: 2-16.
- Pena-Mendez, E.M., D. Gajdosova, J. Havel. 2010. Direct laser desorption ionisation time-of-flight (TOF) mass spectrometry of soil organic matter for fast soil fingerprints. *Chemistry and Ecology* 26: 167-175.

### **1.3. Technical Reviews**

- Sessions, A.L. 2006. Isotope-ratio detection for gas chromatography. *Journal of Separation Science* 29: 1946-1961.
- Brenna, J.T., T.N. Corso, H.J. Tobias, and R.J. Caimi. 1997. High-precision continuous-flow isotope ratio mass spectrometry. *Mass Spectrometry Reviews* 16: 227-258.
- Meier-Augenstein, W. 1999. Applied gas chromatography coupled to isotope ratio mass spectrometry. *Journal of Chromatography A*, 842: 351-371.
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## **2. APPLICATIONS: Multiple Methods**

- Guggenberger, G., B.T. Christensen, and W. Zech. 1994. Land-use effects on the composition of organic matter in particle-size separates of soil. I: Lignin and carbohydrate signature. *European Journal of Soil Science* 45: 449-458.
- Guggenberger, G., W. Zech, L. Haumaier, and B.T. Christensen. 1995. Land-use effects on the composition of organic matter in particle-size separates of soil. II: CPMAS and solution <sup>13</sup>C NMR analysis. *European Journal of Soil Science* 46: 147-158.
- Saiz-Jimenez, C., B. Hermosin, G. Guggenberger and W. Zech. 1996. Land-use effects on the composition of organic matter in particle-size separates of soil. III: Analytical pyrolysis. *European Journal of Soil Science* 47: 61-69.

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### **3. GENERAL Compound Classes**

#### **3.1. C-13-NMR and Molecular Mixing Model**

- Baldock, J.A., C.A. Masiello, Y. Gelinas, and J.I. Hedges. 2004. Cycling and composition of organic matter in terrestrial and marine ecosystems. *Marine Chemistry* 92: 39-64.
- Wilson, M.A., K.M. Goh, P.J. Collin and L.G. Greenfield. 1986. Origin of humus variation. *Organic Geochemistry* 9: 225-231.
- Wilson, M.A., R. J. Pugmire, K.W. Zilm, K.M. Goh, S. Heng and D.M. Grant. 1981. Cross-polarization  $^{13}\text{C}$ -NMR spectroscopy with 'magic angle' spinning characterizes organic matter in whole soils. *Nature* 294: 648-650.
- Kaal, J., J.A. Baldock, P. Buurman, K.G.J. Nierop, X. Ponteveda-Pombal, and A. Martinez-Cortizas. 2007. Evaluating pyrolysis-GC/MS and  $^{13}\text{C}$  CPMAS NMR in conjunction with a molecular mixing model of the Penido Vello peat deposit, NW Spain. *Organic Geochemistry* 38: 1097-1111.
- Preston, C.M. 2001. Carbon-13 solid-state NMR of soil organic matter – using the technique effectively. *Canadian Journal of Soil Science* 81: 255-270.
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- Baldock, J.A., J.M. Oades, P.N. Nelson, T.M. Skene, A. Golchin, and P. Clarke. 1997. Assessing the extent of decomposition of natural organic materials using solid-state  $^{13}\text{C}$  NMR spectroscopy. *Australian Journal of Soil Research* 35: 1061-83.
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#### **3.2. Pyrolysis**

- Parsi, Z., N. Hartog, T. Gorecki, and J. Poerschmann. 2007. Analytical pyrolysis as a tool for the characterization of natural organic matter--A comparison of different approaches. *Journal of Analytical and Applied Pyrolysis* 79: 9-15.
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- Leinweber, P. and H.-R. Schulten. 1999. Advances in analytical pyrolysis of soil organic matter. *Journal of Analytical and Applied Pyrolysis* 49: 359-383.
- Fabbri, D., M. Mongardi, L. Montanari, G.C. Galletti, G. Chiavari, and R. Scotti. 1998. Comparison between CP/MAS <sup>13</sup>C-NMR and pyrolysis-GC/MS in the structural characterization of humins and humic acids of soil and sediments. *Fresenius Journal of Analytical Chemistry* 362: 299-306.
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### **3.4. Carbohydrates- GC/C/IRMS**

- Derrien, D., C. Marol, M. Balabane, and J. Balesdent. 2006. The turnover of carbohydrate carbon in a cultivated soil estimated by <sup>13</sup>C natural abundances. *European Journal of Soil Science* 57: 547-557.

### **3.5. Proximate fractions: Chemical Extractions**

#### **3.5.1. Plant Litter**

- Ryan, M.G., J.M. Melillo, and A. Ricca. 1990. A comparison of methods for determining proximate carbon fractions of forest litter. *Canadian Journal of Forest Research* 20: 166-171.
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- Strickland, M.S., E. Osburn, C. Lauber, N. Fierer and M.A. Bradford. 2009. Litter quality is in the eye of the beholder: initial decomposition rates as a function of inoculum characteristics. *Functional Ecology* doi: 10.1111/j.1365-2435.2008.01515.x

#### **3.5.2. SOM**

- Entry, J.A., and W.H. Emmingham. 1998. Influence of forest age on forms of carbon in Douglas-fir soils in the Oregon Coast Range. *Canadian Journal of Forest Research* 28: 390-305.

### **3.6. Hydrophobicity (Solvent extractions and HPLC)**

- Marinari, S., K. Liburdi, D. Corradini, and S. Grego. 2010. Reversed-phase high performance liquid chromatographic profile of organic fractions extracted by solvents with different polarity as a tool to evaluate the hydrophobic character of soil under different management. *Soil & Tillage Research* 109: 36-40.

## **4. INDIVIDUAL Compounds: Biomarkers**

- Lichtfouse, E. 2000. Compound-specific isotope analysis. Application to archaeology, biomedical sciences, biosynthesis, environment, extraterrestrial chemistry, food science, forensic science, humic substances, microbiology, organic geochemistry, soil science and sport. *Rapid Communications in Mass Spectrometry* 14: 1337-1344.

- Glaser, B. 2005. Compound-specific stable-isotope ( $\delta^{13}\text{C}$ ) analysis in soil science. *Journal of Plant Nutrition and Soil Science* 168: 633-648.
- Feng, X. and M.J. Simpson. 2007. The distribution and degradation of biomarkers in Alberta grassland soil profiles. *Organic Geochemistry* 38: 1558-1570.
- Feng, X., A.J. Simpson, E.G. Gregorich, B. Elberling, D.W. Hopkins, A.D. Sparrow, P.M. Novis, L.G. Greenfield, and M.J. Simpson. 2010. Chemical characterization of microbial-dominated soil organic matter in the Garwood Valley, Antarctica. *Geochimica et Cosmochimica Acta* 74: 6485-6498.
- Feng, X., A.J. Simpson, K.P. Wilson, D.D. Williams, and M.J. Simpson. 2008. Increased cuticular carbon sequestration and lignin oxidation in response to soil warming. *Nature Geosciences* 1: 836-839.
- Evershed, R.P., S.N. Dudd, S. Charters, H. Mottram, A.W. Stott, A. Raven, P.F. van Bergen, and H.A. Bland. 1999. Lipids as carriers of anthropogenic signals from prehistory. *Philosophical Transactions of the Royal Society B*. 354: 19-31.

#### **4.1. Roots vs Shoots (Cutin and Suberin by GC/C/IRMS)**

- Mendez-Millan, M., M-F. Dignac, C. Rumpel and S. Derenne. 2010. Can cutin and suberin biomarkers be used to trace shoot and root-derived organic matter? A molecular and isotopic approach. *Biogeochemistry* DOI: 10.1007/s10533-010-9407-8

#### **4.2. Microbial**

- Guggenberger, G., S.D. Frey, J. Six, K. Paustian and E.T. Elliott. 1999. Bacterial and fungal cell-wall residues in conventional and no-tillage agroecosystems. *Soil Science Society of America Journal* 63: 1188-1198.
- Glaser, B., M-B. Turrion, and K. Alef. 2004. Amino sugars and muramic acid – biomarkers for soil microbial community structure analysis. *Soil Biology & Biochemistry* 36: 399-407.
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#### **4.4. Terrestrial Plants**

##### **4.4.1. Lignin Phenols- GC/C/IRMS**

- Dignac, M.-F., H. Bahri, C. Rumpel, D.P. Rasse, G. Bardoux, J. Balesdent, C. Girardin, 2C. Chenu and A. Mariotti. 2005. Carbon-13 natural abundance as a tool to study the dynamics of lignin monomers in soil: an appraisal at the Closeaux experimental field (France). *Geoderma* 128: 3-17.
- Preston, C.M., J.A. Trofymow, and L.B. Flanagan. 2006. Decomposition,  $\delta^{13}\text{C}$ , and the “lignin” paradox. *Canadian Journal of Soil Science* 86: 235-245.

##### **4.4.2. Lipids**

- Goossens, H., R.R. Duren, J.W. De Leeuw, and P.A. Schenck. 1989. Lipids and their mode of occurrence in bacteria and sediments – II. Lipids in the sediment of a stratified freshwater lake. *Organic Geochemistry* 14: 27-41.
- Almendros, G., P. Tinoco, F.J. González-Vila, H-D. Lüdemann, J. Sanz and F. Velasco. 2001.  $^{13}\text{C}$ -NMR of forest soil lipids. *Soil Science* 166: 186-196.

#### **4.5. Trees vs Grasses**

- Filley, T.R., T. W. Boutton, J.D. Liao, J.D. Jastrow, and D.E. Gamblin. 2008. Chemical changes to nonaggregated particulate soil organic matter following grassland-to-woodland transition in a subtropical savanna. *Journal of Geophysical Research* 113, G03009, doi:10.1029/2007JG000564, 2008
- Krull, E., D. Sachse, I. Mugler, A. Thiele, and G. Gleixner. 2006. Compound-specific  $\delta^{13}\text{C}$  and  $\delta^2\text{H}$  analyses of plant and soil organic matter: A preliminary assessment of the effects of vegetation change on ecosystem hydrology. *Soil Biology & Biochemistry* 38: 3211-3221.

#### **4.6. Animals (Lipids, Chitin and Proteins Steroids)**

- Stankiewicz, B.A., P.F. van Bergen, I.J. Duncan, J.F. Carter, D.E.G. Briggs, and R.P. Evershed. 1996. Recognition of chitin and proteins in invertebrate cuticles using analytical pyrolysis/gas chromatography and pyrolysis/gas chromatography/mass spectrometry. *Rapid Communications in Mass Spectrometry* 10: 1747-1757.
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- Gineys, N., B. Giroud, and E. Vulliet. 2010. Analytical method for the determination of trace levels of steroid hormones and corticosteroids in soil, based on PLE/SPE/LC-MS/MS. *Analytical and Bioanalytical Chemistry* 397: 2295-2302.

#### **4.7. Lignite/Coal**

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#### **4.8. Black Carbon**

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- Rodionov, A., W. Amelung, L. Haumaier, I. Urusevskaja, and W. Zech. 2006. Black carbon in the zonal steppe soils of Russia. *Journal of Plant Nutrition and Soil Science* 169: 363-369. DOI: 10.1002/jpln.200521813
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- Krull, E.S., J.O. Skjemstad, D. Graetz, K. Grice, W. Dunning, G. Cook, and JF Parr. 2003. <sup>13</sup>C-depleted charcoal from C4 grasses and the role of occluded carbon in phytoliths. *Organic Geochemistry* 34: 1337-1352.

## **5. ISOTOPES**

- Kelly, S., K. Heaton, K. and J. Hoogewerff. 2005. Tracing the geographical origin of food: the application of multi-element and multi-isotope analysis. *Trends in Food Science and Technology* 16: 555-567.
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- Boutton, T.W. 1996. Stable carbon isotope ratios of soil organic matter and their use as indicators of vegetation and climate change. In: T.W. Boutton and S. Yamasaki (eds). *Mass Spectrometry of Soils*. Marcel Dekker, Inc. NY, NY. Pp. 47-82.
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## **6. DISSOLVED Organic Matter**

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### **6.1. Marine vs Terrestrial**

- Mayer, L.M., L.L. Schick, T.S. Bianchi, and L. A. Wysocki. 2009. Photochemical changes in chemical markers of sedimentary organic matter source and age. *Marine Chemistry* 113: 123-128.
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### **6.2. Polarity (XAD Resins)**

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### **6.3. Microbial**

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## **6.4. Terrestrial vs Aquatic:**

### **6.4.1. Stable isotopes**

Finlay, J.C. and C. Kendall. 2007. Stable isotope tracing of temporal and spatial variability in organic matter sources to freshwater ecosystems. In: R. Michener and K. Lajtha. *Stable Isotopes in Ecology and Environmental Science*, 2nd Edition. Chapter 10. Wiley-Blackwell Pp 284-333.

### **6.4.2. Lignin Phenols**

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## **6.5. Humic acids**

Brunetti, G., C. Plaza, C.E. Clapp, and N. Senesi. 2007. Compositional and functional features of humic acids from organic amendments and amended soils in Minnesota, USA. *Soil Biology & Biochemistry* 39: 1355-1365.

## **6.6. Aromaticity (NMR and UV)**

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## **6.7. Fluorescence Spectroscopy (PARAFAC)**

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## **7. NANO-Scale**

### **7.1. NanoSIMS**

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### **7.2. NEXAFS**

Lehmann, J., D. Solomon, J. Kinyagi, L. Dathe, S. Wirick, and C. Jacobsen. 2008. Spatial complexity of soil organic matter forms at nanometre scales. *Nature Geosciences* 1: 238-242.

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### **8. PALEO Proxies and Biomarkers**

Meyers, P.A. 1997. Organic geochemical proxies of paleoceanographic, paleolimnologic, and paleoclimatic processes. *Organic Geochemistry* 27: 213-150.

Pancost, R.D., and C.S. Boot. 2004. The paleoclimatic utility of terrestrial biomarkers in marine sediments. *Marine Chemistry* 92: 239-261.

Hautevelle, Y., R. Michels, F. Malartre, and A. Trouiller. 2006. Vascular plant biomarkers as proxies for paleoflora and paleoclimatic changes at the Dogger/Malm transition of the Paris Basin (France). *Organic Geochemistry* 37:610-625.

Eglinton, T.I. and G. Eglinton. 2008. Molecular proxies for paleoclimatology. *Earth and Planetary Sciences Letters* 275: 1-16.

\*Brocks, J.J. and R.E. Summons. 2003. Sedimentary hydrocarbons, biomarkers for early life. *Treatise on Geochemistry* 8: 63-115.

### **9. ONLINE TECHNICAL Resources**

[http://www.cea.fr/var/cea/storage/static/gb/library/Clefs54/pdf-gb/EncadreD\\_54gb.pdf](http://www.cea.fr/var/cea/storage/static/gb/library/Clefs54/pdf-gb/EncadreD_54gb.pdf)

#### **NMR**

<http://www.cis.rit.edu/htbooks/nmr/>

<http://www.chem.queensu.ca/facilities/nmr/nmr/webcourse/>

<http://www.bruker-nmr.de/guide/>

<http://www2.chemistry.msu.edu:80/faculty/reusch/VirtTxtJml/Spectrpy/nmr/nmr1.htm>

<http://orgchem.colorado.edu/hndbksupport/nmrtheory/NMRtutorial.html>

#### **FTIR Spectroscopy**

<http://orgchem.colorado.edu/hndbksupport/irtutor/tutorial.html>

<http://mmrc.caltech.edu/FTIR/FTIRintro.pdf>

#### **Pv/GC/MS**

<http://www.bris.ac.uk/nerclsmsf/techniques/pyro.html>

#### **Chromatography**

<http://www.rpi.edu/dept/chem-eng/Biotech-Environ/CHROMO/chromintro.html>

<http://www.justchromatography.com/>