NEON USER GUIDE TO ROOT CHEMICAL PROPERTIES (NEON.DP1.10102) AND ROOT STABLE ISOTOPES (NEON.DP1.10099)

PREPARED BY	ORGANIZATION	DATE
Samantha Weintraub	FSU	01/22/2018

CHANGE RECORD

REVISION	DATE	DESCRIPTION OF CHANGE
A	01/22/2018	Initial Release

TABLE OF CONTENTS

LIST OF TABLES AND FIGURES

1 DESCRIPTION

1.1 Purpose

This document provides an overview of the data included in this NEON Level 1 data product, the quality controlled product generated from raw Level 0 data, and associated metadata. In the NEON data products framework, the raw data collected in the field - for example, soil temperature from a single collection event, are considered the lowest level (Level 0). Raw data that have been quality checked via the steps detailed herein, as well as simple metrics that emerge from the raw data, are considered Level 1 data products.

The text herein provides a discussion of measurement theory and implementation, data product provenance, quality assurance and control methods used, and approximations and/or assumptions made during L1 data creation.

1.2 Scope

This document describes the steps needed to generate the L1 data products Root chemical properties (NEON.DP1.10102) and Root stable isotopes (NEON.DP1.10099), which include carbon and nitrogen concentrations and stable isotope values in root biomass. This document also provides details relevant to the publication of the data products via the NEON data portal, with additional detail available in the files NEON Data Variables for Root chemical properties (NEON.DP1.10102) (AD[05]) and NEON Data Variables for Root stable isotopes (NEON.DP1.10099) (AD[06]), provided in the download package for this data product.

This document describes the process for ingesting and performing automated quality assurance and control procedures on carbon and nitrogen concentrations and stable isotope values measured in NEON root samples. How the Level 0 data are processed is detailed in the file, NEON Raw Data Validation for Carbon and nitrogen concentrations and stable isotopes in plants and soil (NEON.DP0.10103) (AD[04]), provided in the download package for this data product. Please note that raw data products (denoted by 'DP0') may not always have the same numbers (e.g., '10033') as the corresponding L1 data product.

2 RELATED DOCUMENTS AND ACRONYMS

2.1 Associated Documents

AD[01]	NEON.DOC.000001	NEON Observatory Design (NOD) Requirements
AD[02]	NEON.DOC.000913	TOS Science Design for Spatial Sampling
AD[03]	NEON.DOC.002652	NEON Level 1, Level 2 and Level 3 Data Products Catalog
AD[04]	NEON.DP0.10103.001 _dataValidation.csv	NEON Raw Data Validation for Carbon and nitrogen concentrations and stable isotopes in plants and soil (NEON.DP0.10103)
AD[05]	NEON.DP1.10102.001 _variables.csv	NEON Data Variables for Root chemical properties (NEON.DP1.10102)
AD[06]	NEON.DP1.10099.001 _variables.csv	NEON Data Variables for Root stable isotopes (NEON.DP1.10099)
AD[07]	NEON.DOC.000914	TOS Science Design for Plant Biomass, Productivity, and Leaf Area Index
AD[08]	NEON.DOC.000906	TOS Science Design for Terrestrial Biogeochemistry
AD[09]	NEON.DOC.014038	TOS Protocol and Procedure: Core Sampling for Plant Belowground Biomass
AD[10]	NEON.DOC.001708	TOS Protocol and Procedure: Soil Pit Sampling for Plant Belowground Biomass
AD[11]	NEON.DOC.000008	NEON Acronym List
AD[12]	NEON.DOC.000243	NEON Glossary of Terms
AD[13]	OS_Generic _Transitions.pdf	NEON Algorithm Theoretical Basis Document: OS Generic Transitions
AD[14]		NEON's Ingest Conversion Language (NICL) specifications

2.2 Acronyms

Acronym	Definition
δ13C	delta 13C, the stable carbon isotope ratio (13C:12C) in a sample compared to a reference material, reported in parts per thousand
δ15N	delta 15N, the stable nitrogen isotope ratio (15N:14N) in a sample compared to a reference material, reported in parts per thousand
C	Carbon
N	Nitrogen

3 DATA PRODUCT DESCRIPTION

The Root chemical properties (NEON.DP1.10102) and Root stable isotopes (NEON.DP1.10099) data products provide data about root samples collected using either TOS Protocol and Procedure: Core Sampling for Plant Belowground Biomass (AD[09]) or TOS Protocol and Procedure: Soil Pit Sampling for Plant Belowground Biomass (AD[10]). These procedures implement the guidelines and requirements described in the TOS Science Design for Plant Biomass, Productivity, and Leaf Area Index (AD[07]) and TOS Science Design for Terrestrial Biogeochemistry (AD[08]). All chemistry and isotope data are reported at the spatial resolution of a single root sample from a given depth and size class. The temporal resolution is that of a single collection date.

Measurements of root carbon and nitrogen concentrations and stable isotopes help to reveal drivers of variation in belowground carbon allocation and nutrient cycling at the plot, site, and continental scales. They also provide essential data for understanding change in belowground biogeochemical dynamics over time.

3.1 Spatial Sampling Design

There are two approaches by which NEON will sample and analyze plant belowground biomass. First, at each terrestrial NEON site, surface soil cores are periodically collected from all base plots that fall in the tower airshed ('Tower plots', Figure 1) to assess stocks of fine roots (< 10 mm diameter). This equates to either 20 or 30 plots, depending on the stature of site vegetation. This sampling enables estimation of plant belowground biomass within the same landsurface area where NEON Tower eddy covariance data are derived. At many sites this will also be in the dominant vegetation type(s). Belowground biomass sampling will not occur in Distributed base plots.

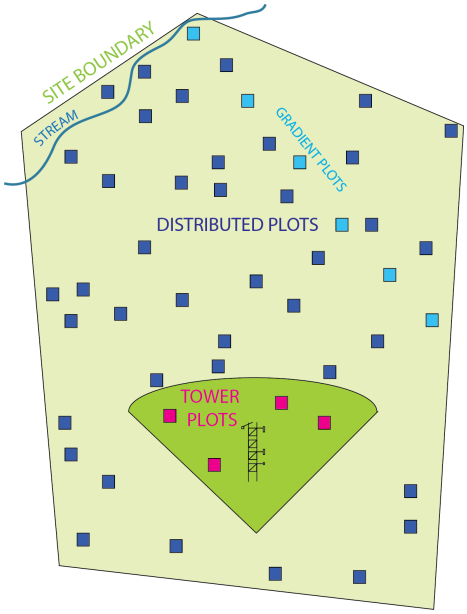

Figure 1: Representation of a NEON site with select Tower and Distributed plots shown

For Tower plot root sampling, one or two 0.5 x 3 m 'clip cells' are randomly chosen per plot. A large-diameter core (5-10 cm) is taken to 30 cm maximum depth from both the northern and southern end of the clip cell (Figure 2). After sieving soil material from roots, separating live and dead, sorting into four size classes, drying, and weighing, *live* root material from the two cores from a common clip cell will be composited by size class and sent for carbon and nitrogen concentration and stable isotope analyses via an external laboratory. See AD[02] for further details on the NEON spatial design and AD[09] for more information on Tower plot root core sampling specifically.

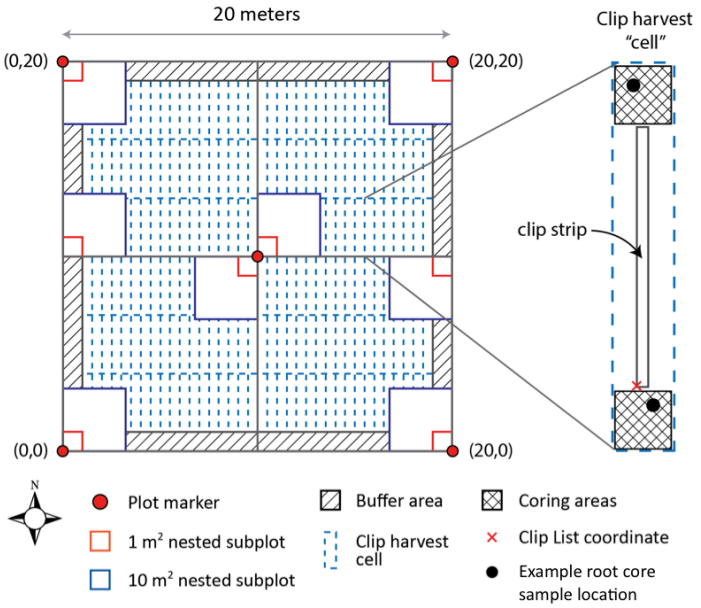

Figure 2: Example layout of a NEON plot divided into clip cells with locations of root core sampling

The other approach used by NEON to quantify belowground biomass stocks is one-time sampling of a 2 meter deep soil pit in the vicinity of the NEON tower. This soil pit is usually located within a few hundred meters of the NEON tower and soil sensor plots. Within each soil pit, three profiles are sampled (Figure 3). Soil samples are collected at 10 cm depth increments to the first 100 cm below the surface, then 20 cm depth increments thereafter to 200 cm. After sieving, separating samples by live and dead, sorting into two size classes, drying, and weighing, samples are sent for carbon and nitrogen concentration and stable isotope analyses via an external laboratory. See AD[10] for more information on soil pit sampling for belowground biomass. Note that prior to September 2017, nitrile gloves were not worn during laboratory processing of soil pit root samples, though forceps were generally used for the separating and sorting steps.

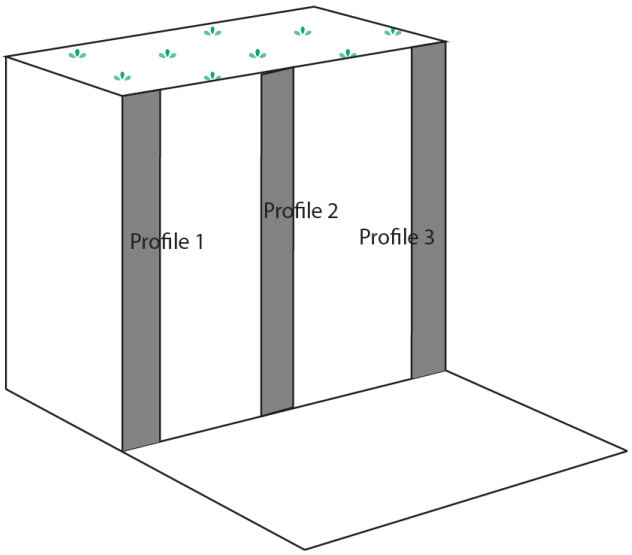

Figure 3: Representation of a NEON soil pit with three profiles for root sampling

3.2 Temporal Sampling Design

Root core sampling in Tower plots occurs once every five years at each NEON terrestrial site. Samples are collected during the growing season, roughly at the period of peak aboveground biomass. The exception is when peak biomass occurs during hot, dry parts of the year when soils are extremely hard and impenetrable, in which case the timing may be moved to earlier in the growing season when soil moisture is more conducive. For each sample with sufficient material, a subsample is archived for future analyses, available to the community upon request.

Soil pit root sampling occurs only once in the lifetime of a NEON site, during the growing season while the site is being constructed.

3.3 Theory of Laboratory Measurements

Concentrations of carbon and nitrogen in plant material are commonly measured via combustion and elemental analysis (EA). If stable isotope data are also desired, as is the case with NEON root samples, isotope ratio mass spectrometry (IRMS) can be coupled to elemental analysis, yielding simultaneous concentration and stable isotope data.

Isotopes are measured as the abundance ratio of a heavy, rare isotope (H) to a light, more common isotope (L), normalized by those same ratios in a standard reference material.

$$\delta = [(R_{sample}/R_{standard} - 1)] \times 1000$$

where R = H/L. For all NEON stable isotopic data, $\delta^{15}N$ values are expressed on the atmospheric N_2 scale and $\delta^{13}C$ values are expressed on the Vienna Pee Dee Belemite scale.

Standard operating procedures for laboratories performing root chemical and stable isotope analyses can be found in the NEON Data Portal document library (http://data.neonscience.org/documents), in the External Lab Protocols section.

3.4 Variables Reported

All variables reported from the laboratory (L0 data) are listed in the file, NEON Raw Data Validation for Carbon and nitrogen concentrations and stable isotopes in plants and soil (NEON.DP0.10103) (AD[04]). All variables reported in the published data (L1 data) are also provided separately in the files NEON Data Variables for Root chemical properties (NEON.DP1.10102) (AD[05]) and NEON Data Variables for Root stable isotopes (NEON.DP1.10099) (AD[06]).

Field names have been standardized with Darwin Core terms (http://rs.tdwg.org/dwc/; accessed 16 February 2014), the Global Biodiversity Information Facility vocabularies (http://rs.gbif.org/vocabulary/gbif/; accessed 16 February 2014), and the VegCore data dictionary (https://projects.nceas.ucsb.edu/nceas/projects/bien/wiki/VegCore; accessed 16 February 2014), where applicable. NEON TOS spatial data employs the World Geodetic System 1984 (WGS84) for its fundamental reference datum and GEOID09 for its reference gravitational ellipsoid. Latitudes and longitudes are denoted in decimal notation to six decimal places, with longitudes indicated as negative west of the Greenwich meridian.

Some variables described in this document may be for NEON internal use only and will not appear in downloaded data.

3.5 Spatial Resolution and Extent

For root core sampling in Tower plots, the finest resolution at which spatial data will be tracked is a unique sample collected from within a clip cell (two pooled core samples per cell) within a NEON plot.

cnSampleID (unique ID given to the individual root sample analyzed for carbon and nitogen) → **plotID** (ID of plot within site) → **siteID** (ID of NEON site) → **domainID** (ID of NEON domain.

For soil pit root sampling, the finest spatial resolution at which spatial data will be tracked is per sampling depth increment within a pit profile, with one pit per NEON site.

sampleID (unique ID given to the individual root sample) → **siteID** (ID of NEON site) → **domainID** (ID of NEON domain).

The basic spatial data included in the root chemistry and stable isotopes data products include domain, site, and plot (if applicable). For root core sampling in Tower plots, joining chemistry and stable isotope data to the field metadata present in the Root sampling tower plots (DP1.10067) data tables and following the instructions contained in the User Guide for that product allows for more precise geolocations for each sample to be calculated. For soil pit root sampling, joining chemistry and isotope data to the field metadata present in the Root sampling (Megapit) (NEON.DP1.10066) data tables allows for decimal latitude, decimal longitude, and elevation values

(as well as uncertainties) for each soil pit to be determined. Users can also access soil pit geolocation data using the NEON API (http://data.neonscience.org/data-api) or the def.extr.geo.os.R function in the geoNEON package (https://github.com/NEONScience/NEON-geolocation).

Shapefiles of all NEON Terrestrial Observation System sampling locations can be found in the Document Library: http://data.neonscience.org/documents.

3.6 Temporal Resolution and Extent

The finest temporal resolution that data are tracked is the **collectDate**. Root core sampling in Tower plot data are collected once every five years at each NEON site, while soil pit root sampling occurs only once. The NEON Data Portal currently provides data in monthly files for query and download efficiency. Code to stack files across months is available here: https://github.com/NEONScience/NEON-utilities.

3.7 Associated Data Streams

In order to make full utility of the data contained in Root chemical properties (NEON.DP1.10102) and Root stable isotopes (NEON.DP1.10099), users will most likely wish to download the field and internal laboratory metadata, including root biomass, for the parent root samples. For root core sampling in Tower plots, these can be found in the Root sampling tower plots (NEON.DP1.10067) data product, where **cnSampleID** in the bbc_chemistryPooling table can be used to join to **cnSampleID** in the chemistry and isotope tables. For soil pit root sampling, parent sample data can be found in the Root sampling (Megapit) (NEON.DP1.10066) data product, where **sampleID** in the mpr_perrootsample table can be used to join to **cnSampleID** in the chemistry and isotope tables

3.8 Product Instances

For root core sampling in Tower plots, each terrestrial NEON site will have one or two clip cells sampled from 20-30 plots. For each clip cell, roots are sorted into up to four size categories. Thus, on average, NEON will generate 120-160 unique root chemistry and isotope records per site per sampling year. Because root core sampling in Tower plots is conducted at a site once every five years, approximately 8-10 terrestrial NEON sites per year will be sampled. Thus, we expect between 960-1600 data records per year for these type of root samples.

For soil pit root sampling, there is one 2 meter soil pit for each NEON terrestrial site. There are three profiles per pit and 15 depth increments per profile, unless it is impossible to dig to the full prescribed depth of 200 cm. Roots are sorted into up to two size catagories and both live and dead roots are analyzed. Thus, we expect upto 180 records per site for these type of root samples, or 8,460 records across all 47 current Terrestrial NEON sites.

3.9 Data Relationships

Each record in the bbc_chemistryPooling table in Root sampling tower plots (NEON.DP1.10067) or mpr_perrootsample in Root sampling (Megapit) (NEON.DP1.10066) may appear from zero to two times in the bbc_rootStableIsotopes and bbc_rootChemistry tables, with its unique identifier recorded in the **cnSampleID**

field. Most **cnSampleID**s will appear once, but some may appear twice if analytical replicates were conducted by the laboratory. Duplicates and/or missing data may exist where protocol and/or data entry abberations have occurred; *users should check data carefully for anomalies before joining tables*.

bbc_rootStableIsotopes.csv - > One record expected per **cnSampleID** x **analyticalRepNumber** combination

bbc_rootChemistry.csv - > One record expected per **cnSampleID** x **analyticalRepNumber** combination

bgc_CNiso_externalSummary.csv - > One record expected per **laboratoryName** x **analyte** x **sampleType** x **labSpecificStartDate** combination. Can use corresponding variables in isotope and chemistry tables to associate sample data with relevant uncertainty values.

3.10 Special Considerations

None to report.

4 DATA QUALITY

4.1 Data Entry Constraint and Validation

Many quality control measures are implemented at the point of data entry within a mobile data entry application or web user interface (UI). For example, data formats are constrained and data values controlled through the provision of list-of-value options, which reduce the number of processing steps necessary to prepare the raw data for publication. An additional set of constraints are implemented during the process of ingest into the NEON database. The product-specific data constraint and validation requirements built into data entry and database ingest are described in the document NEON Raw Data Validation for Carbon and nitrogen concentrations and stable isotopes in plants and soil (NEON.DP0.10103), provided with every download of this data product. Contained within this file is a field named 'entryValidationRulesParser', which describes the validation rules for external labs that submit spreadsheets to the NEON database. Data entry constraints are described in Nicl syntax in the validation file provided with every data download, and the Nicl language is described in NEON's Ingest Conversion Language (NICL) specifications (AD[14]).

Note that field data collected prior to 2017 were processed using a paper-based workflow that did not implement the full suite of quality control features associated with the interactive digital workflow. Moreover, external laboratory data were also not subject to the same full suite of quality controls.

4.2 Automated Data Processing Steps

Following data entry into a mobile application or web user interface, the steps used to process the data through to publication on the NEON Data Portal are detailed in the NEON Algorithm Theoretical Basis Document: OS Generic Transitions (AD[13]).

4.3 Data Revision

All data are provisional until a numbered version is released; the first release of a static version of NEON data, annotated with a globally unique identifier, is planned to take place in 2020. During the provisional period, QA/QC is an active process, as opposed to a discrete activity performed once, and records are updated on a rolling basis as a result of scheduled tests or feedback from data users. The Change Log section of the data product readme, provided with every data download, contains a history of major known errors and revisions.

4.4 Quality Flagging

The **dataQF** field in each record is a quality flag for known issues applying to the record, added by NEON Science upon data review. At present, there are no dataQF entries for root chemistry and stable isotope data products.

4.5 Analytical Facility Data Quality

Analytical labs that generate root chemical and stable isotope data calibrate each run of NEON samples with primary reference materials, and include secondary reference materials analyzed as unknowns alongside NEON samples in order to gauge run acceptability. Labs communicate run-level issues with the accuracy of secondary reference materials, as well as record-level issues with samples or measurements, using the suite of quality flags described below. In general, an entry of 0 in a quality flag field means there is no issue to report.

In addition, long-term analytical precision and accuracy of secondary reference material analyses are reported for each lab to allow users to interpret and analyze root chemistry and stable isotope data in the context of their uncertainty ranges. The data table bgc_CNiso_externalSummary, which is available in the data product expanded package, contains the long-term precision and accuracy of lab analyses.

For further information about individual laboratory QA procedures, refer to the lab-specific SOPs found in the NEON Data Portal document library (http://data.neonscience.org/documents), External Lab Protocols section. NEON's Calibration/Validation department has regular procedures for auditing the quality assurance of external laboratories and their reports are also available to data users.

bbc_rootChemistry

fieldName	value	definition
cnPercentQF	0	Indicator for both percentNitrogen and percentCarbon in range
cnPercentQF	1	Indicator for percentNitrogen out of range
cnPercentQF	2	Indicator for percentCarbon out of range
cnPercentQF	3	Indicator for both percentNitrogen and percentCarbon out of range
percentAccuracyQF	0	Observed values of run QA material fall within acceptance criteria for percent concentration
percentAccuracyQF	1	Observed values of run QA material do not meet acceptance criteria for nitrogenPercent
percentAccuracyQF	2	Observed values of run QA material do not meet acceptance criteria for carbonPercent
percentAccuracyQF	3	Observed values of run QA material do not meet acceptance criteria for nitrogenPercent or carbonPercent

bbc_rootStableIsotopes

fieldName	value	definition
cnIsotopeQF	0	Indicator for both d15N and d13C in range
cnIsotopeQF	1	Indicator for d15N out of range
cnIsotopeQF	2	Indicator for d13C out of range
cnIsotopeQF	3	Indicator for both d15N and d13C out of range
isotopeAccuracyQF	0	Observed values of run QA material fall within acceptance criteria for stable isotopes
isotopeAccuracyQF	1	Observed values of run QA material do not meet acceptance criteria for d15N
isotopeAccuracyQF	2	Observed values of run QA material do not meet acceptance criteria for d13C
isotopeAccuracyQF	3	Observed values of run QA material do not meet acceptance criteria for d15N or d13C