MARS 2020
SHERLOC PDS Archive User’s Guide

Version 0.3

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1. Overview

This document is a quick start guide to the Mars 2020 SHERLOC data archive. This document is intended to give users a basic understanding of the SHERLOC archive, where to find relevant data products and information, and identify any caveats on data collection.

1.1. What is SHERLOC?

SHERLOC (Scanning Habitable Environments with Raman and Luminescence for Organics and Chemicals) is a robotic arm-mounted instrument on NASA's *Perseverance* rover. SHERLOC has two primary boresights. The Spectroscopy boresight generates spatially resolved chemical maps using fluorescence and Raman spectroscopy coupled to microscopic images (10.1 µm/pixel). The second boresight is the Wide Angle Topographic Sensor for Operations and eNgineering (WATSON); a copy of the Mars Science Laboratory (MSL) Mars Hand Lens Imager (MAHLI) that obtains color images from microscopic scales (~13 µm/pixel) to infinity. SHERLOC Spectroscopy focuses a 40 µs pulsed deep UV neon-copper laser (248.6 nm), to a ~100 µm spot on a target at a working distance of ~48 mm. Fluorescence emissions from organics, and Raman scattered photons from organics and minerals, are spectrally resolved with a single diffractive grating spectrograph with a spectral range of ~250 to ~354 nm. Because the fluorescence and Raman regions are naturally separated with deep UV excitation (<250 nm), the Raman region ~ 800 – 4000 cm^{-1} (250 to 275 nm) and the fluorescence region (275 to ~353 nm) are acquired simultaneously without time gating or additional mechanisms.

1.2. SHERLOC Operations

Although a detailed description of the SHERLOC instrument and its operation is described in Document [10], an overview is provided here, highlighting key points of the instrument necessary to understand before working with the data.

SHERLOC is mounted to a robotic arm, which positions the instrument 48 mm ± 7 mm above the target. The autofocus and contextual imager (ACI), laser illumination, and spectroscopy collection paths all share the same objective lenses, and image the same target. The WATSON color imager uses a separate boresight, requiring the robotic arm to be rotated for co-located measurements of a target. A photograph of SHERLOC, acquired before launch, is shown in Figure 1. The inside cover of the ACI/spectroscopy boresight shows the AlGaN calibration target, measured at the start and end of all SHERLOC activities.

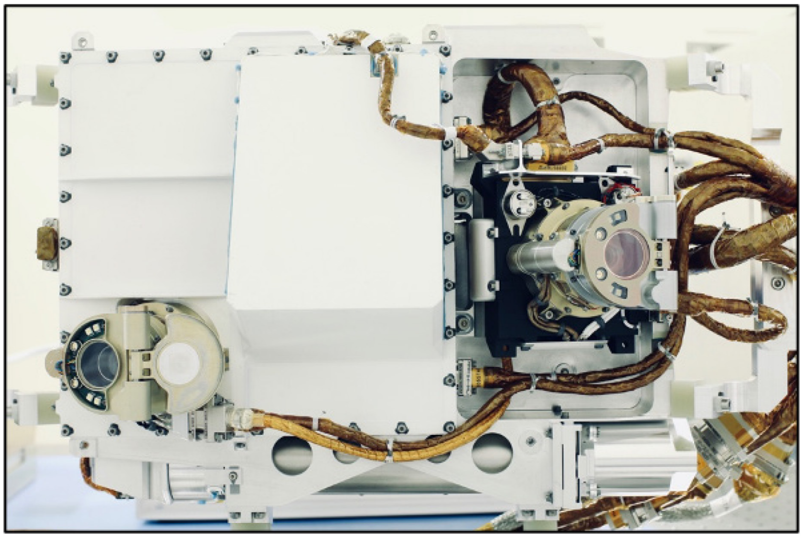


Figure 1: A photograph of the SHERLOC turret assembly before integration with the rover robotic arm. The right boresight is the WATSON color imager, and the left boresight is the ACI imager and spectrometer. The dust cover is open for the spectroscopy boresight in this image.

When in focus, the objective lens focuses the laser to a 100-110 µm diameter spot. Incident DUV laser pulses are focused on a target, using the moveable scanner mirror to sweep over an area to generate a map. The Raman and fluorescence photons excited by the laser are collected by the common-path ACI objective lens. The Raman scattered and fluoresced light is focused across the long axis of the 512-by-2048 pixel Spectrometer CCD (SCCD). The off-axis nature of the spectrometer's optical design causes a physical curving of the spectrum across the SCCD focal plane, which is referred to as a spectral smile, shown in Figure 2.

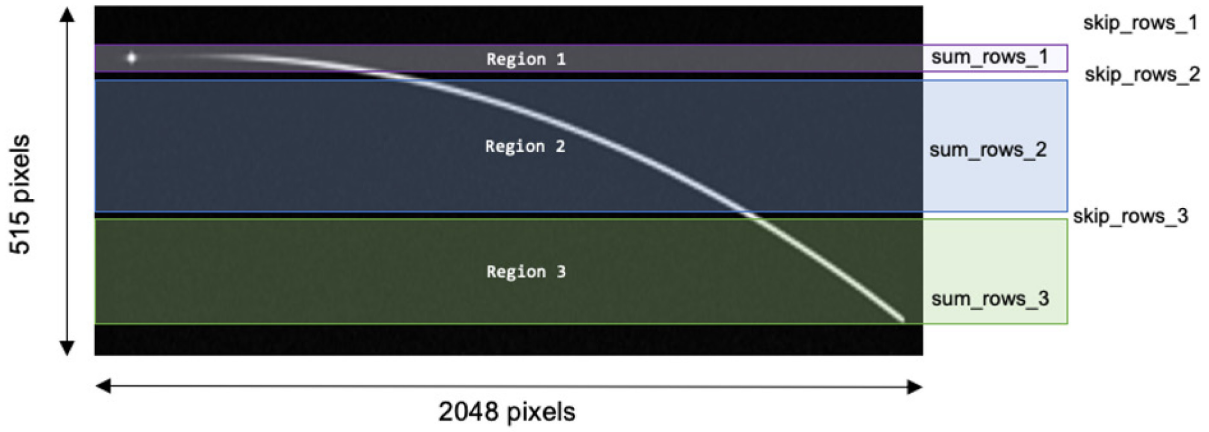


Figure 2: Illustration of the SCCD detector array overlayed with the spectrometer "smile" pattern and the on-chip integration patterns.

Data is read out in a columnar fashion, typically using three binned regions, as shown in Figure 1: Region 1 collects the Raman signal from 250 to 282 nm (225 to 4760 cm^{-1}), while Regions 2 and 3 collect fluorescence up to 355 nm. Dividing the SCCD into multiple regions minimizes noise and allows for configurable clock speeds and variable gain settings. These variable gain settings provide the flexibility to change the electrons/count for a binned region to accommodate the dynamic range necessary to acquire both low Raman signals, and the relatively more intense fluorescence signals, which may saturate the detector if a single gain setting were applied across the entire SCCD.

Each time a SHERLOC spectrum is collected, two frames are acquired: an active frame (with the laser firing at the target) and a dark/background frame (of the same duration as the active frame, but without the laser firing). The dark frame may be subtracted from the active frame to remove pixel-to-pixel variability in the SCCD.

The first and last 50 pixels on the SCCD are not light sensitive and do not contain spectral data. The intensity values for these channels are reported in the EDR and RDR products described below, and may be used for dark noise characterization. Typically, an end user would ignore these channels when generating a spectrum.

During spectroscopy map measurement collection, the laser intensity may decrease over time as the temperature increases due to use. The laser photodiode tracks the laser output, and may be used to normalize all spectra within a map to provide direct comparisons between spectral measurements.

1.3. Typical SHERLOC Activities

A typical SHERLOC mapping sequence runs through the following elements in order, described in detail below. Note, SHERLOC sequences may deviate from this typical plan to include additional ACI imaging and additional spectral map acquisitions observations following Process Data algorithm execution.

- Internal AlGaN calibration target measurement
- ACI image focus stack (subframes)
- ACI image focus
- SHERLOC spectroscopy map acquisition
- Process Data algorithm execution
- ACI image focus stack (subframes)
- ACI image focus
- Internal AlGaN calibration target measurement

A SHERLOC activity begins by using the Autofocus Context Imager (ACI) to obtain target focus and to acquire a 10.1 µm/pixel greyscale image. The ACI focus mechanism is stepped through a range of motor positions, with the ideal focus position determined by calculating the maximum compression ratio of all images acquired in the stack. A full frame ACI image is acquired at the best focus position, and the focus mechanism is offset ~150 µm to focus the spectrometer.

SHERLOC acquires a spectral map at the focus position with a defined map size, spacing, and number of laser shots per point. SHERLOC is not restricted to using pre-defined scanner tables, and may generate maps with irregularly spaced points. Default maps typically selected for reconnaissance of a target will generally include 7x7 mm survey mode scans (36 x 36 point grid or 10 x 10 point grid) and detailed-mode scans (5x5 mm or 1x1 mm grids with up to 1296 points) for follow-up measurements of regions of interest (ROIs). These ROIs may be selected autonomously by the on-board SHERLOC Process Data algorithm.

After the SHERLOC spectroscopy measurements have been collected, the data may be processed using on-board algorithms (called Process Data mode). This processed data will have a lower data volume, and may be downlinked for tactical decision-making before the full spectral map is available. On-board Process Data algorithms consist of:

[0] Copy Raw
[1] Background Subtraction: subtracting the dark frames from the active frames
[2] Laser Normalization: normalize all spectra to account for laser energy variability, as measured by the laser photodiode
[3] Raw Photodiode Dump: the returned data product includes all photodiode measurements
[4] Summary Photodiode Dump: the returned data product includes the average photodiode value for each map point
[5] Hot Pixel Removal
[6] Cosmic Ray Removal: (see Document [14] for details)
[7] Zone Specification: selection of up to six spectral ranges
[8] Spectral Binning: sum spectral channels in specified spectral zones
[9] Spatial Binning: sum spectral intensity values for all channels within pre-defined spatial regions of a default map
[10] Ranking: rank each spectrum based on the spectral zones, zone weights, and spectral intensity within each zone. Spatial locations with high ranking may be selected for autonomous follow-up detailed-mode spectral measurements.

After spectral acquisition and Process Data algorithms are applied, focused ACI subframe and full frame images are acquired. The initial and final ACI images and their focus positions may be used to characterize any robotic arm drift that may have occurred during the measurement. Additional images may be commanded during spectroscopy acquisition to provide finer resolution drift characterization, if necessary.

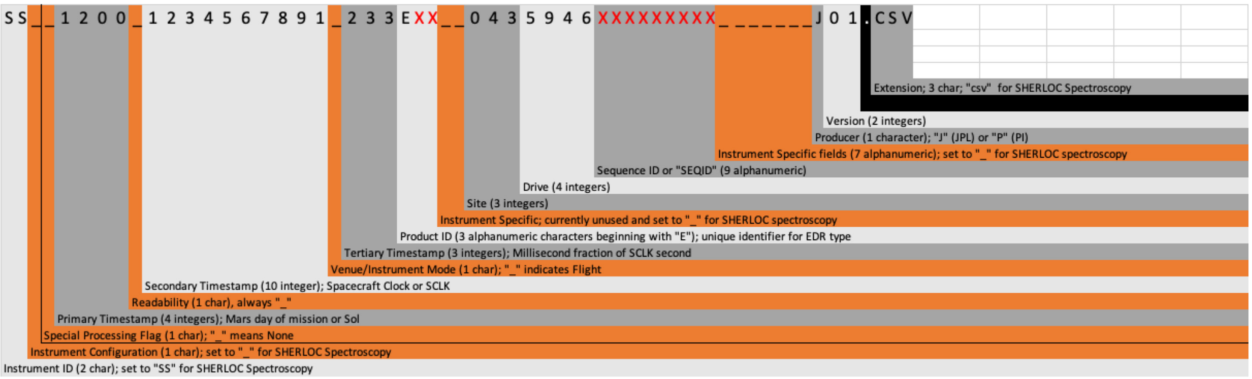
1.4. SHERLOC Data Products

The SHERLOC ground processing tools generate two types of data products that are archived in the PDS:

- EDRs (Engineering Data Records) – raw, un-calibrated data products
- RDRs (Reduced Data Records) – calibrated and/or processed data products. RDR products are generally the products a SHERLOC data user will use for analysis of a target.

Each of the SHERLOC EDR and RDR products are described in detail in the EDR/RDR SIS (Documents [6] and [7]) and summarized below in Section 3 and 4.

The SHERLOC data products follow the M2020 filename convention:


S S _ _ 1 2 0 0 _ 1 2 3 4 5 6 7 8 9 1 _ 2 3 3 E X X _ _ 0 4 3 5 9 4 6 X X X X X X X X X _ _ _ _ _ _ _ J 0 1 . C S V
Extension; 3 char; "csv" for SHERLOC Spectroscopy
Version (2 integers)
Producer (1 character); "J" (JPL) or "P" (PI)
Instrument Specific fields (7 alphanumeric); set to "_" for SHERLOC spectroscopy
Sequence ID or "SEQID" (9 alphanumeric)
Drive (4 integers)
Site (3 integers)
Instrument Specific; currently unused and set to "_" for SHERLOC spectroscopy
Product ID (3 alphanumeric characters beginning with "E"); unique identifier for EDR type
Tertiary Timestamp (3 integers); Millisecond fraction of SCLK second
Venue/Instrument Mode (1 char); "_" indicates Flight
Secondary Timestamp (10 integer); Spacecraft Clock or SCLK
Readability (1 char), always "_"
Primary Timestamp (4 integers); Mars day of mission or Sol
Special Processing Flag (1 char); "_" means None
Instrument Configuration (1 char); set to "_" for SHERLOC Spectroscopy
Instrument ID (2 char); set to "SS" for SHERLOC Spectroscopy

See Appendix A for a detailed description of each of these filename fields.

Filename Prefix:

- SS: SHERLOC Spectroscopy
- SC: SHERLOC Context Imager (ACI)
- SI: SHERLOC Imaging (WATSON)
- SE: SHERLOC Engineering (state-of-health information)

Product ID:

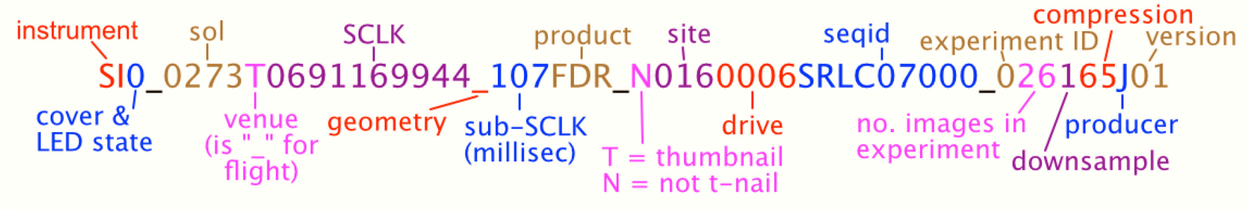
Values	Description
EDF	Engineering data in fault detection (cruise phase data only)
EDR	Science data frame (cruise phase data only)
ESH	Spectroscopy state of health in science mode
ECH	Spectroscopy state of health in calibration mode
EXH	Scanner position array (in pixel)
ERA	Full resolution active spectra in science mode
ERB	Full resolution background (dark) spectra in science mode
ECA	Full resolution active spectra in calibration mode
ECB	Full resolution background (dark) spectra in calibration mode
EPA	Photodiode array
ESP	Scanner position array (in millimeter unit of measurement)
RRA	Active frame, with or without processing (see instrument-specific filename field) in science mode
RRB	Dark frame, with or without processing (see instrument-specific filename field) in science mode

RCA	Active frame, with or without processing (see instrument-specific filename field) in calibration mode
RCB	Dark frame, with or without processing (see instrument-specific filename field) in calibration mode
RRS	Dark-subtracted spectrum – see instrument-specific field for processing applied in science mode
RCS	Dark-subtracted spectrum – see instrument-specific field for processing applied in calibration mode
RCC	Internal AlGaN peak assessment summary, used to determine spectral alignment
RLP	Scanner position table in scanner azimuth/elevation and target (mm) space
RLS	Laser shot positions for each ACI image
RLI	Laser intensity map
RM*	Spectral intensity map for pre-defined spectral ranges
RMO	Spectral intensity map and laser shot position summary

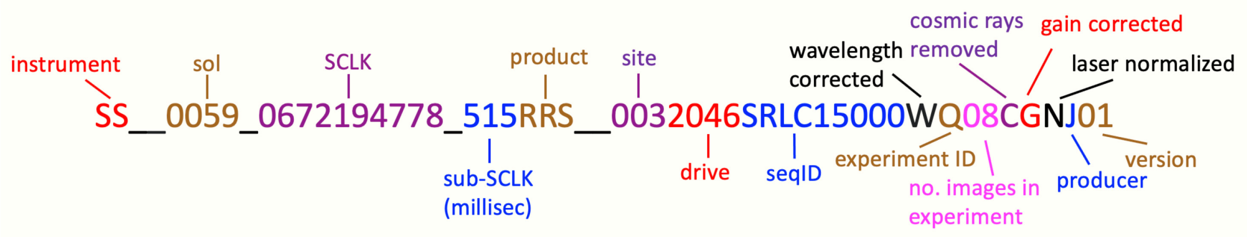
The instrument-specific field of the filename includes information on the processing performed and on linking the imaging and spectroscopy data files together. The SS* files use seven characters for this field, and SC* and SI* files use four characters. See the table above for an overview of valid values and the associated processing performed.

Example filenames:

The example below shows a SHERLOC imaging file name, along with descriptions of character groups.



The example below shows a SHERLOC spectroscopy file name, along with descriptions of character groups.



1.5. The SHERLOC Archive Bundle

The data acquired by SHERLOC is archived in the PDS within the **mars2020_sherloc** bundle. The bundle contains collections of SHERLOC products based on data processing level and type. Within data collections, products are sorted into subdirectories by Sol number. Products in the sub-directories are identified by the three-letter code found in positions 24-26 of the file name.

The structure of the **mars2020_sherloc** bundle is:

mars2020_pixl

data_raw_spectroscopy

sol_xxx

ECH, ESH – Spectroscopy state of health
ECA, ECB – Active and dark frame calibration spectra
ERA, ERB – Active and dark frame science spectra
ERP – Process_Data spectra
ESP – Scanner position
EPA – Laser photodiode

data_aci_imgops

sol_xxx

EDR – context image
ECM – companded images
ECZ, EZS – Z-stack images
EDM – focus merge image

data_watson_imgops

sol_xxx

EDR – context image
ECM – companded images
ECZ, EZS – Z-stack images
EDM – focus merge image

data_spectroscopy

sol_xxx

RCA, RCB – processed active and dark spectra (calibration target)
RRA, RRB – processed active and dark spectra (science target)
RCS – dark-subtracted spectra (calibration target)
RRS – dark- subtracted spectra (science target)
RAC, RBC, RAR, RBR – cosmic ray candidate lists
RCC – internal AlGaN calibration target fit results
RLS – laser shot position tables
RMO – laser shot and spectral position tables
RMx – selected integrated intensity maps

data_aci

sol_xxx

RAD – Radiometrically-corrected image

data_watson

sol_xxx

RAD – Radiometrically-corrected image

Document

SHERLOC EDR SIS

SHERLOC RDR SIS

SHERLOC Bundle SIS

2. Documents

These publications or websites describe the Planetary Data System Standards used to produce the SHERLOC archive. These documents are archived in the PDS system and are not found specifically in the SHERLOC archive. These documents are revised approximately every six months with each new release of the PDS Information Model. Current and previous versions may be found at the links below.

[1] PDS4 Concepts Document, https://pds.nasa.gov/datastandards/documents/concepts/.
[2] Planetary Data System Standards Reference, https://pds.nasa.gov/datastandards/documents/sr/.
[3] Planetary Data System Data Provider's Handbook, https://pds.nasa.gov/datastandards/documents/dph/.
[4] PDS4 Common Data Dictionary, Abridged, https://pds.nasa.gov/datastandards/documents/dd/.
[5] PDS4 Information Model Specification, https://pds.nasa.gov/datastandards/documents/im/.

These documents describe the specifics of the archive and the archive data products, and can be found in the SHERLOC document collection (i.e. mars2020_SHERLOC:document).

[6] <EDR SIS>
[7] <RDR SIS>
[8] <Camera SIS>
[9] <SHERLOC Bundle SIS>

These papers describe in detail the Mars 2020 mission and the SHERLOC instrument. These papers are published with open access and can be downloaded by following the DOI.

[10] Farley, K.A., et al. (2020), Mars 2020 Mission Overview, Space Sci. Rev. 216:142, doi:10.1007/s11214-020-00762-y.
[11] R. Bhartia, L.W. Beegle, L. DeFlores, et al. "Perseverance's Scanning Habitable Environments with Raman and Luminescence for Organics and Chemicals (SHERLOC) Investigation". Space Sci. Rev. 2021. *paper in press*.

[12] Uckert, K., Bhartia, R., Beegle, L. et al. (2021) "Calibration of the SHERLOC Deep UV Fluorescence/Raman Spectrometer on the Perseverance Rover". Applied Spectroscopy, accepted.
[13] Razzell Hollis, J., Abbey, W., Beegle, L., et al. (2021) "A Deep-Ultraviolet Raman and Fluorescence Spectral Library of 62 Minerals for the SHERLOC instrument onboard Mars 2020". Submitted to Planetary and Space Sciences.
[14] Uckert, K., Bhartia, R., Michel, J. "A semi-autonomous method to detect cosmic rays in Raman hyperspectral data sets." Applied spectroscopy 73.9 (2019): 1019-1027.

3. Raw Products

3.1. Raw Spectral Products

All EDR products contain several tables with instrument state-of-health (SOH) data, followed by spectral, laser photodiode, or scanner position data tables.

SOH data tables:
State of health data tables include data used by the SHERLOC operations team to evaluate the health of the instrument, and includes: temperatures for each SHERLOC subsystem, arguments used to command the instrument, SCCD configuration parameters, scanner configuration parameters, command timing information, instrument status flags (indicating the state of each subsystem at a specified time), and laser configuration parameters. See Document [7] for a full description of each table entry. This information may not be useful for an average science data product user.

ERA/ERB/ERS/ECA/ECB:

These products contain the raw spectral data for the active or dark frame, or dark-subtracted spectra, in the case of background-subtracted process data spectral products (ERS). Spectra from each region are listed, starting with a single line table header (e.g. DARK_SPECTRA_REGION_1:), followed by column headers (e.g. R1_Channel_0). All spectral information are listed in data tables of size N x 2148 x R, where N is the number of spectra (represented as a row in each table), 2148 represents the number of wavelength elements (represented by columns in each table), R represents the number of regions (represented by tables in the csv file – usually 3 regions are implemented).

EPA:

The laser photodiode data is listed in a table following the SOH entries. The table identifier (e.g. LASER_PHOTODIODE_DATA) precedes the table column headers (e.g. shot_number_0). The laser photodiode table is of size N x S, where N is the number of spectra (represented as a row in the table) and S is the number of shots in each spectrum (represented as columns in the table).

ESP:

The scanner data is listed in a table following the SOH entries. The scanner position data associated with the spectra is stored in a table of size N x 2, where N is the number of spectra (represented as a row in the table) and 2 is the number of position elements – azimuth and elevation (represented as columns in the table). If the LOAD_TABLE command is issued, a second table containing the commanded azimuth and elevation values will be present as a second table. The measured scanner position errors and scanner current tables are the last tables in the file.

3.2. Raw Image Products

ECM:

Contains companded data either as originally downlinked or JPEG decompressed.

ECZ:

A best-focus Z-stack image, **created onboard the instrument** from a combination of images at different focus settings, with a much greater depth of field.

EDM:

Second of two products produced by onboard focus merge (z-stacking). This single-band grayscale image provides information about which images the best-focus data came from, and can provide a crude measure of target surface relief.

DN of 255 indicates first image in the Z-stack, while the last is dependent on number of image-merge, with linear scaling between.

EDR:

Nominal data product.

EZS:

A best-focus Z-stack image, **created on the ground** from a combination of images at different focus settings, with a much greater depth of field.

4. Derived Products

4.1. Derived Spectral Products

RDR products do not contain the instrument state-of-health (SOH) data table present in the EDRs, but follow the same general format for spectral data.

It is anticipated that the primary data products needed by a SHERLOC data user will be the RRS (dark-subtracted spectra) and the RLS (laser shot position table) RDRs.

RRA/RRB/RRS:

The RRA and RRB products contain spectral products that have been processed in some way, which may include cosmic ray correction, gain correction, wavelength correction, and/or laser normalization. The instrument-specific field of the filename indicates the kind of processing that has been applied (see Appendix A). RRS products contain dark-subtracted spectra, and may also include aforementioned processing. If wavelength calibration has been performed, the first table will include wavelength (nm) assignments for each SCCD channel.

RCC:
This product contains a summary of the spectral alignment of SHERLOC based on fits to peaks in measurements of the internal AlGaN target.

RM*:
The integrated intensity within a specified wavelength region for each point is calculated and reported in a table with a single column. The wavelength regions are selected by the SHERLOC team, and may be used to automatically generate maps for Autolook and Quicklook product generation, however future science users may find it more convenient to generate their own maps from RRS product data.

Up to 35 RM* products may be generated for each RDR data set, with the first 6 reported in the Autolook report.

RLI:
This product contains the laser intensity map table – a single column with the average photodiode data. This product is used by the SHERLOC team during operations to map the laser power output.

RLS:
This product contains a table with all laser shot positions mapped to pixel positions in each ACI image.

RMO:
This product contains a summary of laser shot positions (present in the RLS product), and the spectral intensity maps (present in the RM* products), along with the wavelengths used for each spectral intensity map. The RMO product may be used to generate a multispectral image of the target with the pre-selected wavelength ranges, which may be useful for generating Quicklook products and rapid assessment for tactical decision-making.

4.2. Derived Imaging Products

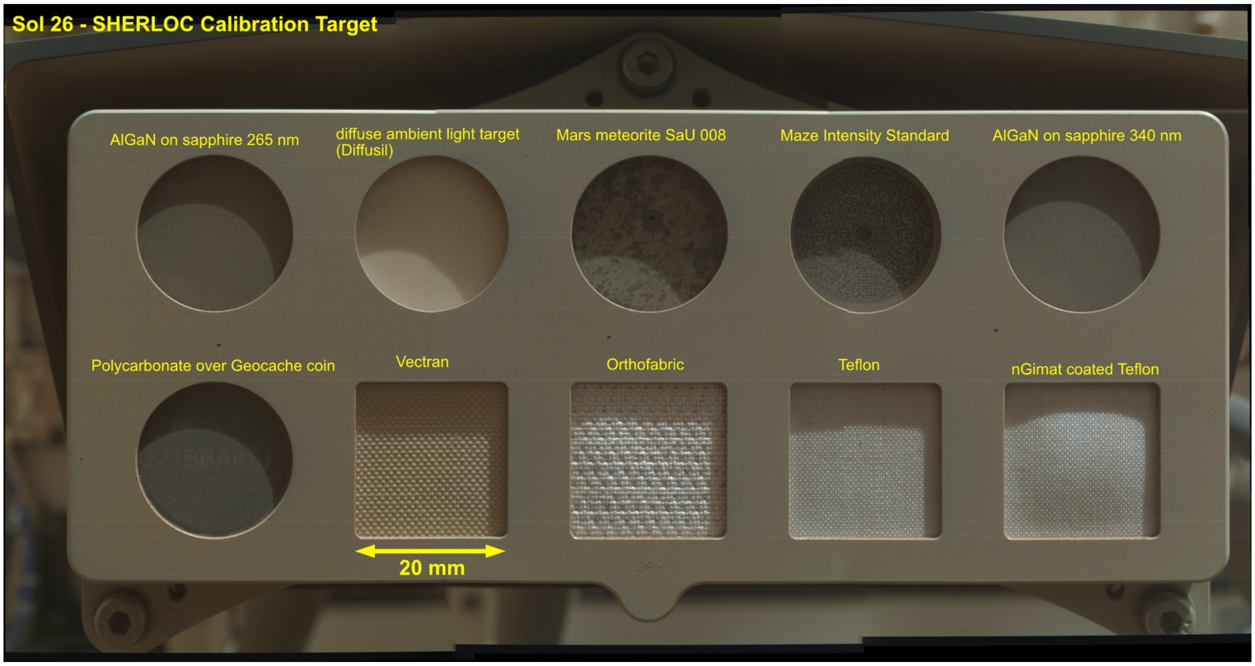
RAD:

Radiometrically-corrected images. Radiometric correction is the process of converting the image to a calibrated unit that represents the light entering the lens of the camera. It thus provides a representation of the scene as it exists, independent of the camera. It should not be confused with photometric correction, which takes into account lighting and geometry in order to describe the objects in the scene, independent of how they were observed. **As of this version of the SHERLOC User's Guide, a radiometric model for the SHERLOC cameras is not well-calibrated, and RAD products should not be considered in data analysis.**

5. Calibration Products

SHERLOC includes 11 calibration targets. Products associated with the internal AlGaN target are denoted with special EDR and RDR product IDs (ECA, ECB, RCA, RCB, RCS). External calibration targets will have Sequence ID fields that start with SRLC15*, with the external calibration target indicated in the LBL file under the CAL_TARGET_NAME field.

- An internal AlGaN target, with a central peak at ~277 nm. This target is measured after SHERLOC powers on to collect measurements and right before SHERLOC powers off.
- An external calibration palette, which will be measured less frequently, and includes the following targets:
    - 1) AlGaN on Sapphire (peak wavelength at 262.5 nm)
    - 2) Diffusil Diffuser
    - 3) Mars Meteorite SaU 008
    - 4) Intensity Target (maze, chrome on fused silica glass)
    - 5) AlGaN on Sapphire (peak wavelength at 335 nm)
    - 6) Polycarbonate visor material over Geocache opal glass
    - 7) Vectran spacesuit material
    - 8) Orthofabric spacesuit material
    - 9) Teflon spacesuit material
    - 10) nGimat-coated Teflon spacesuit material



6. Data Collection and Caveats

6.1. Data Acquisition and the SHERLOC DUV Laser

The SHERLOC laser configuration parameters should be noted when comparing SHERLOC datasets. The number of pulses per point, the laser rep rate, laser current, and the SCCD temperature may all be retrieved from the EDR SOH tables. The SCCD temperature is kept constant during a SHERLOC measurement through the use of a phase-change material, described in Document [2], however, operations outside of ideal times may cause some thermal variability to be observed during a measurement, which is usually in the order of 15 minutes for the largest maps.

Inherent to NeCu deep UV lasers are multiple laser lines that can be generated at different output energy levels. While most of these lines have been removed by SHERLOC's laser-conditioning optics, a small fraction of the 252.93 nm line reflected from a target may be observed at an intensity comparable with a strong Raman band. This line may obscure Raman features that coincide with this region of the spectrum (650 – 750 cm^{-1}).

6.2. Data Processing

The SHERLOC processing pipeline automatically removes cosmic ray noise spikes from spectra using the algorithm described in Document [14]. This algorithm is somewhat dependent on the tunable input parameters, including the threshold multiplier and the sigma clipping coefficient, which may be changed to improve performance. At the start of the mission, these parameters may not be fine-tuned, and many cosmic rays may still be present in the resulting RRA, RRB, and RRS RDR products.

The laser photodiode can be used to monitor the laser output energy level within a map, but should not be used to compare laser output energy for spectra collected on different Sols, or on different materials. The laser photodiode intensity may increase when measuring highly reflective targets (as is observed on the maze intensity calibration target), and has been observed to slightly depend on the optical bench temperature.

6.3. Processing Not Included in this Pipeline

RDRs generated as part of the SHERLOC PDS archive will not include baseline subtraction (which may be used to correct for variable fluorescence intensity) or Raman peak fitting. This processing usually requires a human-in-the-loop to be effectively implemented, and commercial and open-source tools exist to complete this processing, if desired. Document [13] contains an overview of baseline subtraction applied to SHERLOC data, and Document [14] contains information on fitting Raman peaks in SHERLOC data.

7. Acknowledgements:

The research was carried out at the Jet Propulsion Laboratory, California Institute of Technology, under a contract with the National Aeronautics and Space Administration (80NM0018D0004)

Appendix A:

Characters	Contents	Description
1-2	Instrument	SS: SHERLOC Spectroscopy SC: SHERLOC ACI SI: SHERLOC WATSON
3	Configuration	"_" for SHERLOC spectroscopy and engineering For image products, cover and LED state: 0 Cover closed, LEDs off 1 Cover open, LEDs off 2 Cover closed, LEDs on 4 Cover closed, LEDs on
4	Special Processing Flag	"_" (none for SHERLOC)
5-8	Sol	Sol number for flight surface data; see EDR SIS for other uses
9	Mission venue	"_" for Flight Mode
10-19	Spacecraft Clock Count (SCLK)	10-integer spacecraft clock count in seconds
20	Underscore	Always "_" for readability
21-23	Fractional SCLK	3-digit spacecraft clock count fractional seconds
24-26	Product Type	See SHERLOC Product Type in Table 1
27	Geometry	Not used for Spectroscopy, set to "_". For image products: denote for Geometry for WATSON and ACI: "_" indicates raw (non-linearized) geometry "L" indicates product has been linearized with nominal stereo partner "A" indicates product has been linearized with actual stereo partner
28	Thumbnail	"_" for non-image products "T": Product is a thumbnail images "N": Product is not a thumbnail image
29-31	Site	Site identifier from Rover Motion Counter
32-35	Drive	Drive identifier (position within a site location)

<table>
<tr><td><b>36-44</b></td><td>Sequence ID</td><td>Identifier indicating the command sequence from which the data were acquired</td></tr>
<tr><td colspan="3"><b>Start of Imaging vs Spectroscopy Instrument Specific Identifier Division</b></td></tr>
<tr><td colspan="3"><b>Image product only (Char 45-51)</b></td></tr>
<tr><td><b>45-48</b></td><td>Camera-specific identifier</td><td>For image products: Snnn where nnn is an observation number</td></tr>
<tr><td><b>49</b></td><td>Downsample resolution</td><td>“_” for non-image data products
For image products:
Resolution = 2^n x 2^n
<table>
<tr><th>Valid values</th><th>Resolution</th></tr>
<tr><td>0</td><td>1x1</td></tr>
<tr><td>1</td><td>2x2</td></tr>
<tr><td>2</td><td>4x4</td></tr>
<tr><td>3</td><td>8x8</td></tr>
<tr><td>…</td><td>…</td></tr>
</table></td></tr>
<tr><td><b>50-51</b></td><td>Compression</td><td>“__” for non-image data products
For image products:
<table>
<tr><th>Type</th><th>Valid values</th><th>Description</th></tr>
<tr><td>JPEG (lossy)</td><td>00
01-99
A0</td><td>Thumbnail
Jpeg quality level
Jpeg quality level 100</td></tr>
<tr><td>ICER (lossy)</td><td>I1, I2, …, I8
I9</td><td>1 bpp, 2 bpp, …, 8 bpp
Anything higher than 8 bpp</td></tr>
<tr><td>Lossless</td><td>LI
LL
LM
LU</td><td>ICER
LOCO
Malin
Uncompressed</td></tr>
</table></td></tr>
<tr><td colspan="3"><b>Spectroscopy Product only (Char 45-51)</b></td></tr>
<tr><td><b>45</b></td><td>Instrument-specific processing flag</td><td>For spectroscopy products:
“W” : denote Wavelength Correction algorithm performed
“B” : denote that the on-board process_data product is background-subtracted</td></tr>
<tr><td><b>46</b></td><td>Instrument specific identifier.</td><td>spectroscopy experiment ID designation.
<table>
<tr><th>Values</th><th>Range</th></tr>
</table></td></tr>
</table>

<table>
<tr><td></td><td></td><td><table><tr><td>0, 1, …, 9</td><td>0 thru 9</td></tr><tr><td>A, B, …, Z</td><td>10 thru 36</td></tr></table></td></tr>
<tr><td><b>47-48</b></td><td>Instrument specific identifier.</td><td>The valid value is the total number of ACI images acquired, in relation to the ExpID. The ACI image number can ranges between “00” thru “99”.</td></tr>
<tr><td><b>49</b></td><td>Instrument-specific processing flag</td><td>C : denote Cosmic Ray Correction algorithm performed
Z : denotes that Cosmic Ray Correction has been skipped, according to the algorithm configuration file
“_” : denote no Cosmic Ray Correction algorithm performed</td></tr>
<tr><td><b>50</b></td><td>Instrument-specific processing flag</td><td>G : denote Gain Correction algorithm performed
P : denotes that the on-board process_data algorithm has been applied
“_” : denote no Gain Correction algorithm performed</td></tr>
<tr><td><b>51</b></td><td>Instrument-specific processing flag</td><td>N : denote Normalization algorithm performed
Z : denotes that laser Normalization has been skipped, according to the algorithm configuration file
“_” : denote no Normalization Correction algorithm performed</td></tr>
<tr><td colspan="3"><b>End of Imaging vs Spectroscopy Instrument Specific Identifier Division</b></td></tr>
<tr><td>52</td><td>Provider</td><td>Provider institution ID
J: IDS at JPL
P: Instrument Principal Investigator
Other: Co-investigators as identified at discretion of PI</td></tr>
<tr><td>53-54</td><td>Product Version</td><td>Product version number. Increments by one whenever a previously generated file with an otherwise identical filename exists.<table><tr><th>Values</th><th>Range</th></tr><tr><td>00, 01, 02 …, 99</td><td>0 thru 99</td></tr><tr><td>A0, A1, …, A9</td><td>100 thru 109</td></tr><tr><td>AA, AB, …, AZ</td><td>110 thru 135</td></tr><tr><td>B0, B1, B2 …, B9</td><td>136 thru 145</td></tr><tr><td>BA, BB, …, BZ</td><td>146 thru 171</td></tr><tr><td>…</td><td>…</td></tr><tr><td>Z0, Z1, …, Z9</td><td>1000 thru 1009</td></tr><tr><td>ZA, ZB, …, ZZ</td><td>1010 thru 1035</td></tr><tr><td>_ _</td><td>Value is out of range</td></tr></table></td></tr>
</table>

55	Separator	Separator for filename and extension, always “.”
56-58	File name extension	"DAT" : Binary table "CSV" : ASCII comma-separated-value text file "IMG" : Image data

Appendix B

This section contains Python pseudo-code for reading RDR spectral data and storing the data in Numpy arrays or Pandas dataframes. In the examples below, the data contained within Pandas dataframes and numpy arrays are identical – both are presented here to enable users to work with either, depending on their preference.

Python dependencies required for using this pseudo-code:

- Python 3.7+ (any version of Python 3 will probably work, but has not been tested here). For Python installation instructions, see https://wiki.python.org/moin/BeginnersGuide/Download
- Pandas (`pip install pandas` on most systems): https://pandas.pydata.org/
- Numpy (`pip install numpy` on most systems): https://numpy.org/install/
- Matplotlib (used for plotting demonstrations in this example) (`pip install matplotlib` on most systems): https://matplotlib.org/

Read an RRS RDR file (with wavelength calibration included)

The RRS RDR file generally includes four tables: the wavelength assignment for each channel number, and three tables (one for each detector region) containing processed spectral intensity data. The following Python code will open an RRS file, save the spectral data as pandas dataframes and numpy arrays, and plot the median spectrum output for each region.

```python
"""
This Python script will:
    parse an example SHERLOC RRS RDR file
    store the contents in numpy arrays and Pandas dataframes
    plot the median spectrum

In an updated version of this code, the XML label file will be parsed to determine byte offsets
    (XML labels are not currently available)

To run this program, modify the lines bracketed by #### USER INPUT REQUIRED ####

Author: Kyle Uckert
Last Modified: June 26, 2020
Contact: kyle.uckert@jpl.nasa.gov
"""

import os
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

# a basic plotting function to generate a plot for all three spectral regions
def plot_basic_multiple(x, y, save_filename, color, alpha=0.7, x_title='', y_title='', title='', xrange=False, yrange=False):
    fig, ax1 = plt.subplots(figsize=(10, 4))
    fig.subplots_adjust(bottom=0.18)
    fig.patch.set_facecolor('#E0E0E0')
    for i in range(len(y)):
        plot = ax1.plot(x, y[i], color=color[i], linewidth=1, alpha = alpha)
    ax1.grid(b=True, which='major', linestyle='--')
    ax1.set_ylabel(y_title, fontsize=12)
    ax1.set_xlabel(x_title, fontsize=12)
    if xrange:
        ax1.set_xlim(left=xrange[0], right = xrange[1])
    if yrange:
        ax1.set_ylim(bottom=yrange[0], top = yrange[1])
    else:
        ax1.set_ylim(bottom = 0.9*min([min(y_i) for y_i in y]), top=1.1*max([max(y_i) for y_i in y]))
    plt.title(title)
    fig.tight_layout()
    fig.savefig(save_filename, transparent=False, dpi=300)
    ax1.cla()
    plt.clf()
    plt.close()


if __name__ == '__main__':
    #### USER INPUT REQUIRED ####
    # modify this line to point to a SHERLOC RRS RDR file located on your computer
    input_file = os.path.join('PDS_user_guide_example', 'input', 'SS__0059_0672194285_700RRS__0032046SRLC15020WS08CGNJ01.csv')
    # modify this line to point to the desired directory path for the output plot png file
    output_dir = os.path.join('PDS_user_guide_example', 'output', '')
    #### END USER INPUT ####

    # determine the number of spectra
    #### This information will be determined by parsing the PDS4 xml label, when it is available
    with open(input_file, 'r') as f:
        contents = f.readlines()
    # the number of lines in contents is n_spectra*n_regions (3) + 4 (headers) + 4 (column names) + 1 (wavelength table)
    n_spectra = int((len(contents) - 9)/3)

    # store each table in a pandas dataframe
    wavelength_df = pd.read_csv(input_file, nrows=1, skiprows=1)
    R1_spectra_df = pd.read_csv(input_file, nrows=n_spectra, skiprows=4)
    R2_spectra_df = pd.read_csv(input_file, nrows=n_spectra, skiprows=4+n_spectra+2)
    R3_spectra_df = pd.read_csv(input_file, nrows=n_spectra, skiprows=4+2*n_spectra+2+2)

    # store each table in a numpy array
    wavelength_np = np.array([float(w) for w in contents[2].split(',')])
    R1_spectra_np = np.genfromtxt(input_file, skip_header=5, max_rows=n_spectra, delimiter=',')
    R2_spectra_np = np.genfromtxt(input_file, skip_header=7+n_spectra, max_rows=n_spectra, delimiter=',')
    R3_spectra_np = np.genfromtxt(input_file, skip_header=9+2*n_spectra, max_rows=n_spectra, delimiter=',')

    # plot each region
    # dataframe example
    file_root = os.path.split(input_file)[-1].split('.')[0]
    save_file = os.path.join(output_dir, file_root+'_df_example.png')
    # the first and last 50 pixels on the SCCD are not illuminated, and should not be plotted
    x_df = wavelength_df[wavelength_df.columns[50:2098]].loc[0]
    y_df = [R1_spectra_df[R1_spectra_df.columns[50:2098]].median(axis=0),
            R2_spectra_df[R2_spectra_df.columns[50:2098]].median(axis=0),
            R3_spectra_df[R3_spectra_df.columns[50:2098]].median(axis=0)]
    plot_basic_multiple(x_df, y_df, save_file, ['b', 'g', 'r'],
                        alpha=0.7,
                        x_title='Wavelength (nm)',
                        title='Pandas DataFrame Example')

    # numpy example
    file_root = os.path.split(input_file)[-1].split('.')[0]
    save_file = os.path.join(output_dir, file_root+'_np_example.png')
    # the first and last 50 pixels on the SCCD are not illuminated, and should not be plotted
    x_np = wavelength_np[50:2098]
    y_np = [np.median(R1_spectra_np[:, 50:2098], axis=0),
            np.median(R2_spectra_np[:, 50:2098], axis=0),
            np.median(R3_spectra_np[:, 50:2098], axis=0)]
    plot_basic_multiple(x_np, y_np, save_file, ['b', 'g', 'r'],
                        alpha=0.7,
                        x_title='Wavelength (nm)',
                        title='Pandas Numpy Example')
```

Read an ERA EDR file

The ERA EDR file include a variable number of header rows containing state of health information, along with (typically) three tables (one for each detector region) of spectral intensity data. The following Python code will open an ERA file, save the spectral data as pandas dataframes and numpy arrays, and plot the median spectrum output for each region

```
"""
This Python script will:
    parse an example SHERLOC ERA EDR file
    store the contents in numpy arrays and Pandas dataframes
    plot the median spectrum

In an updated version of this code, the XML label file will be parsed to determine byte offsets
    (XML labels are not currently available)

To run this program, modify the lines bracketed by #### USER INPUT REQUIRED ####

Author: Kyle Uckert
Last Modified: June 26, 2020
Contact: kyle.uckert@jpl.nasa.gov
"""

import os
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

# a basic plotting function to generate a plot for all three spectral regions
def plot_basic_multiple(x, y, save_filename, color, alpha=0.7, x_title='', y_title='', title='', xrange=False, yrange=False):
    fig, ax1 = plt.subplots(figsize=(10, 4))
    fig.subplots_adjust(bottom=0.18)
    fig.patch.set_facecolor('#E0E0E0')
    for i in range(len(y)):
        plot = ax1.plot(x, y[i], color=color[i], linewidth=1, alpha = alpha)
    ax1.grid(b=True, which='major', linestyle='--')
    ax1.set_ylabel(y_title, fontsize=12)
    ax1.set_xlabel(x_title, fontsize=12)
    if xrange:
        ax1.set_xlim(left=xrange[0], right = xrange[1])
    if yrange:
        ax1.set_ylim(bottom=yrange[0], top = yrange[1])
    else:
        ax1.set_ylim(bottom = 0.9*min([min(y_i) for y_i in y]), top=1.1*max([max(y_i) for y_i in y]))
    plt.title(title)
    fig.tight_layout()
    fig.savefig(save_filename, transparent=False, dpi=300)
    ax1.cla()
    plt.clf()
    plt.close()


if __name__ == '__main__':
    #### USER INPUT REQUIRED ####
    # modify this line to point to a SHERLOC RRS RDR file located on your computer
    input_file = os.path.join('PDS_user_guide_example', 'input', 'SS__0059_0672194285_700ERA__0032046SRLC15020_S08___J01.csv')
    # modify this line to point to the desired directory path for the output plot png file
    output_dir = os.path.join('PDS_user_guide_example', 'output', '')
    #### END USER INPUT ####

    # determine the number of spectra
    #### This information will be determined by parsing the PDS4 xml label, when it is available
    with open(input_file, 'r') as f:
        contents = f.readlines()
    # the line number in the EDR file where each spectrum starts
    R1_start_line = [i for i in range(len(contents)) if 'R1_Channel_0' in contents[i]][0]
    R2_start_line = [i for i in range(len(contents)) if 'R2_Channel_0' in contents[i]][0]
    R3_start_line = [i for i in range(len(contents)) if 'R3_Channel_0' in contents[i]][0]
    # the number of lines in contents is n_spectra*n_regions (3) + 4 (headers) + 4 (column names) + 1 (wavelength table)
    n_spectra = R2_start_line-R1_start_line-2

    # store each table in a pandas dataframe
    R1_spectra_df = pd.read_csv(input_file, nrows=n_spectra, skiprows=R1_start_line)
    R2_spectra_df = pd.read_csv(input_file, nrows=n_spectra, skiprows=R2_start_line)
    R3_spectra_df = pd.read_csv(input_file, nrows=n_spectra, skiprows=R3_start_line)

    # store each table in a numpy array
    R1_spectra_np = np.genfromtxt(input_file, skip_header=R1_start_line+1, max_rows=n_spectra, delimiter=',')
    R2_spectra_np = np.genfromtxt(input_file, skip_header=R2_start_line+1, max_rows=n_spectra, delimiter=',')
    R3_spectra_np = np.genfromtxt(input_file, skip_header=R3_start_line+1, max_rows=n_spectra, delimiter=',')


    # plot each region
    # dataframe example
    file_root = os.path.split(input_file)[-1].split('.')[0]
    save_file = os.path.join(output_dir, file_root+'_df_example.png')
    # the first and last 50 pixels on the SCCD are not illuminated, and should not be plotted
    x_df = list(range(R1_spectra_df.shape[1]))[50:2098]
    y_df = [R1_spectra_df[R1_spectra_df.columns[50:2098]].median(axis=0),
            R2_spectra_df[R2_spectra_df.columns[50:2098]].median(axis=0),
            R3_spectra_df[R3_spectra_df.columns[50:2098]].median(axis=0)]
    plot_basic_multiple(x_df, y_df, save_file, ['b', 'g', 'r'],
                        alpha=0.7,
                        x_title='Channel Number',
                        title='Pandas DataFrame Example')

    # numpy example
    file_root = os.path.split(input_file)[-1].split('.')[0]
    save_file = os.path.join(output_dir, file_root+'_np_example.png')
    # the first and last 50 pixels on the SCCD are not illuminated, and should not be plotted
    x_np = list(range(R1_spectra_np.shape[1]))[50:2098]
    y_np = [np.median(R1_spectra_np[:, 50:2098], axis=0),
            np.median(R2_spectra_np[:, 50:2098], axis=0),
            np.median(R3_spectra_np[:, 50:2098], axis=0)]
    plot_basic_multiple(x_np, y_np, save_file, ['b', 'g', 'r'],
                        alpha=0.7,
                        x_title='Channel Number',
                        title='Pandas Numpy Example')
```