DEEDS

A Platform for Fully Integrating Data, Computations, and Scientific Workflows

CIF21 DIBBs: EI: Digital Environment for Enabling Data-driven Science (DEEDS)
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Award #1724728 | **Award Period** August 2017 – July 2021

Chandima HewaNadungodage
Gateways 2018
09-26-2018

PURDUE UNIVERSITY

National Science Foundation
WHERE DISCOVERIES BEGIN

Why Another Platform ???

Existing platforms

- Either supports data preservation/sharing or provides computing services
- Discipline specific and customized
- Lack of end-to-end support for the entire research investigation

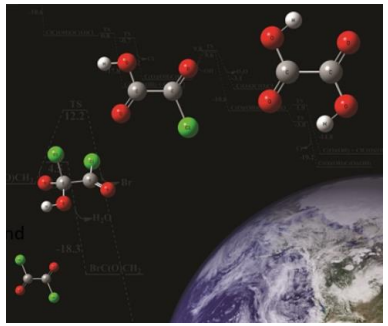
There is an emerging need for platforms that fully integrate data, computing, preservation, and sharing.

What DEEDS Offers

- Supports end-to-end research investigation
- Self-serve, cross-domain platform
- Fully integrate data with computations and workflows
- Systematic preservation and sharing
- Ease of discoverability and reuse
- Traceability and reproducibility

DEEDS USE CASES

Chemistry



Optimization of molecular structure and determination of properties

Joe Francisco - University of Pennsylvania

Nutrition Science

Effect of berries on net calcium retention & biochemical markers of polyphenol and bone metabolism

Connie Weaver - Purdue University

Environmental Science

Development of amphibian toxicity reference values for ecological risk assessment

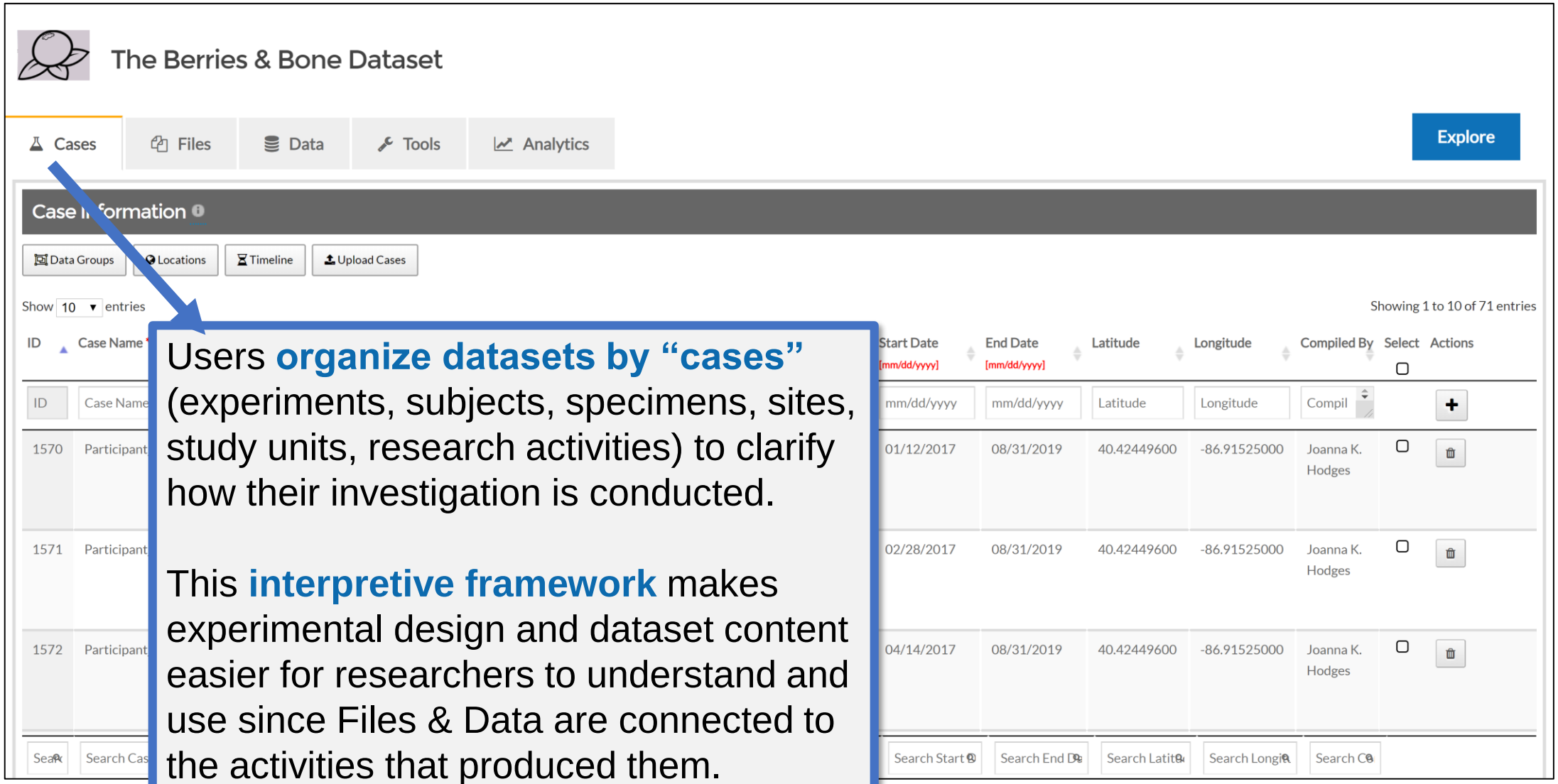
Marisol Sepúlveda - Purdue University

Electrical Engineering

Performance modeling of solar PV systems to determine efficiency degradation and predict system lifetime

Ashraf Alam - Purdue University

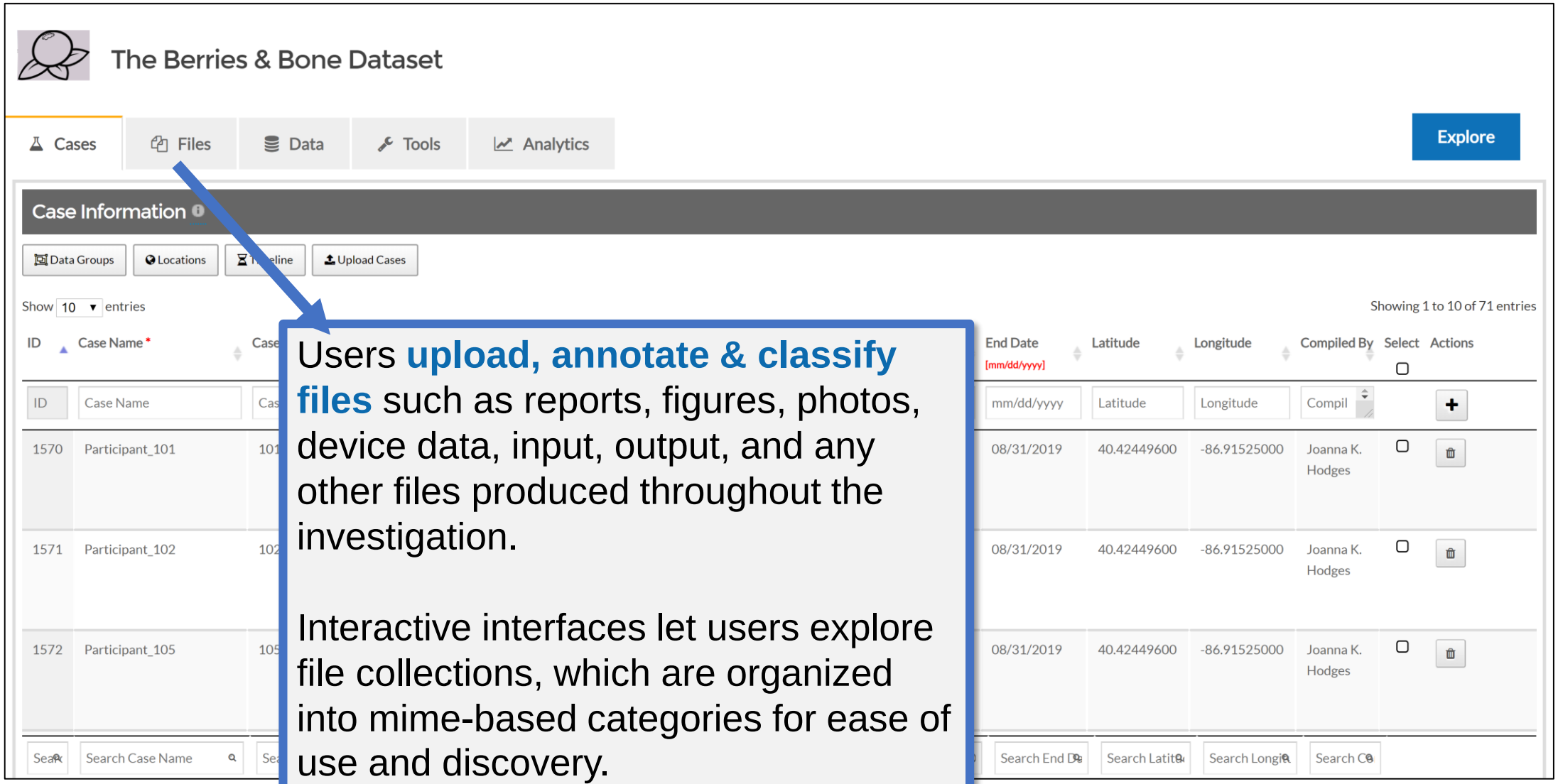
DEEDS DASHBOARD



Users **organize datasets by "cases"** (experiments, subjects, specimens, sites, study units, research activities) to clarify how their investigation is conducted.

This **interpretive framework** makes experimental design and dataset content easier for researchers to understand and use since Files & Data are connected to the activities that produced them.

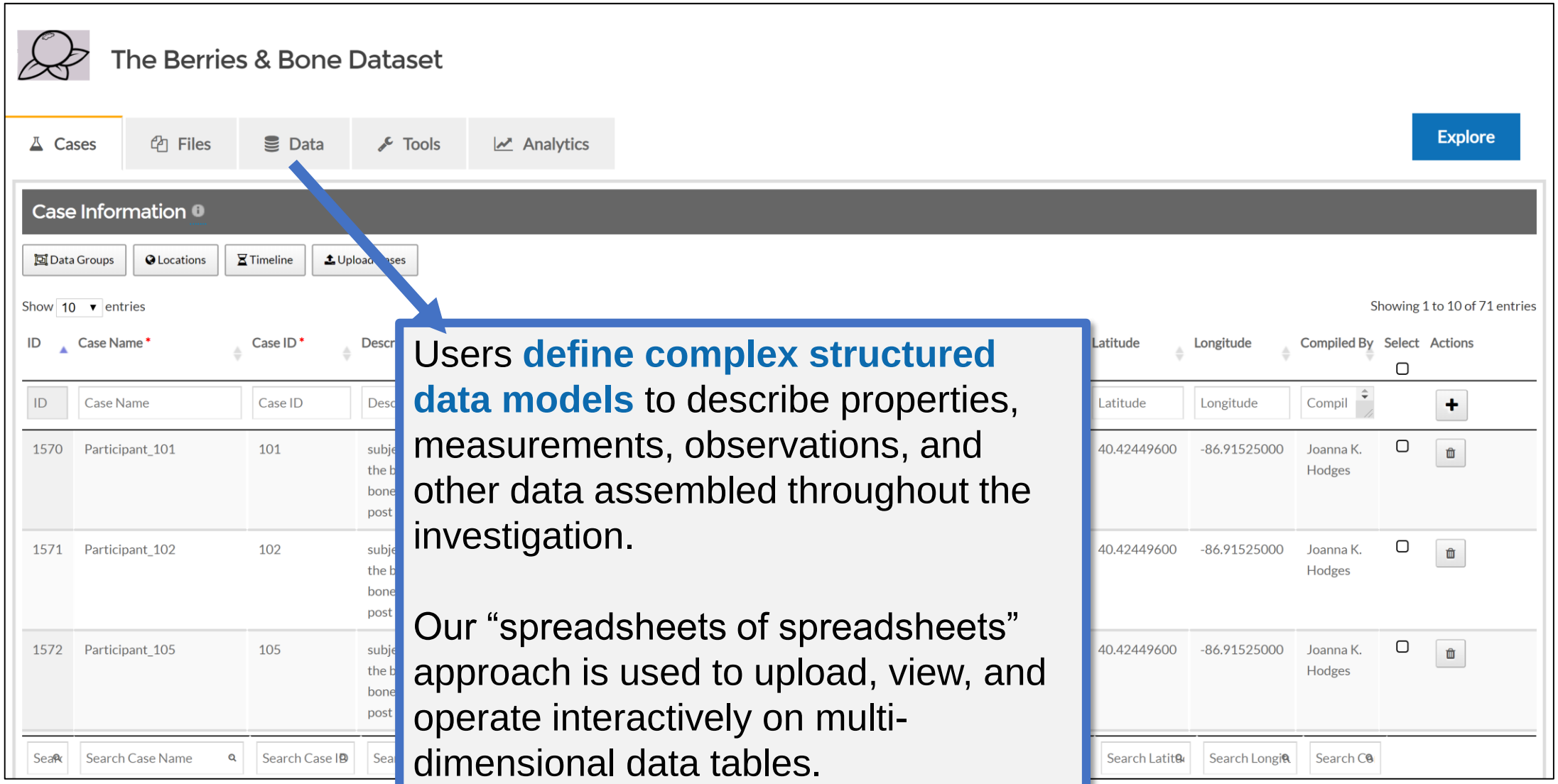
DEEDS DASHBOARD



Users **upload, annotate & classify files** such as reports, figures, photos, device data, input, output, and any other files produced throughout the investigation.

Interactive interfaces let users explore file collections, which are organized into mime-based categories for ease of use and discovery.

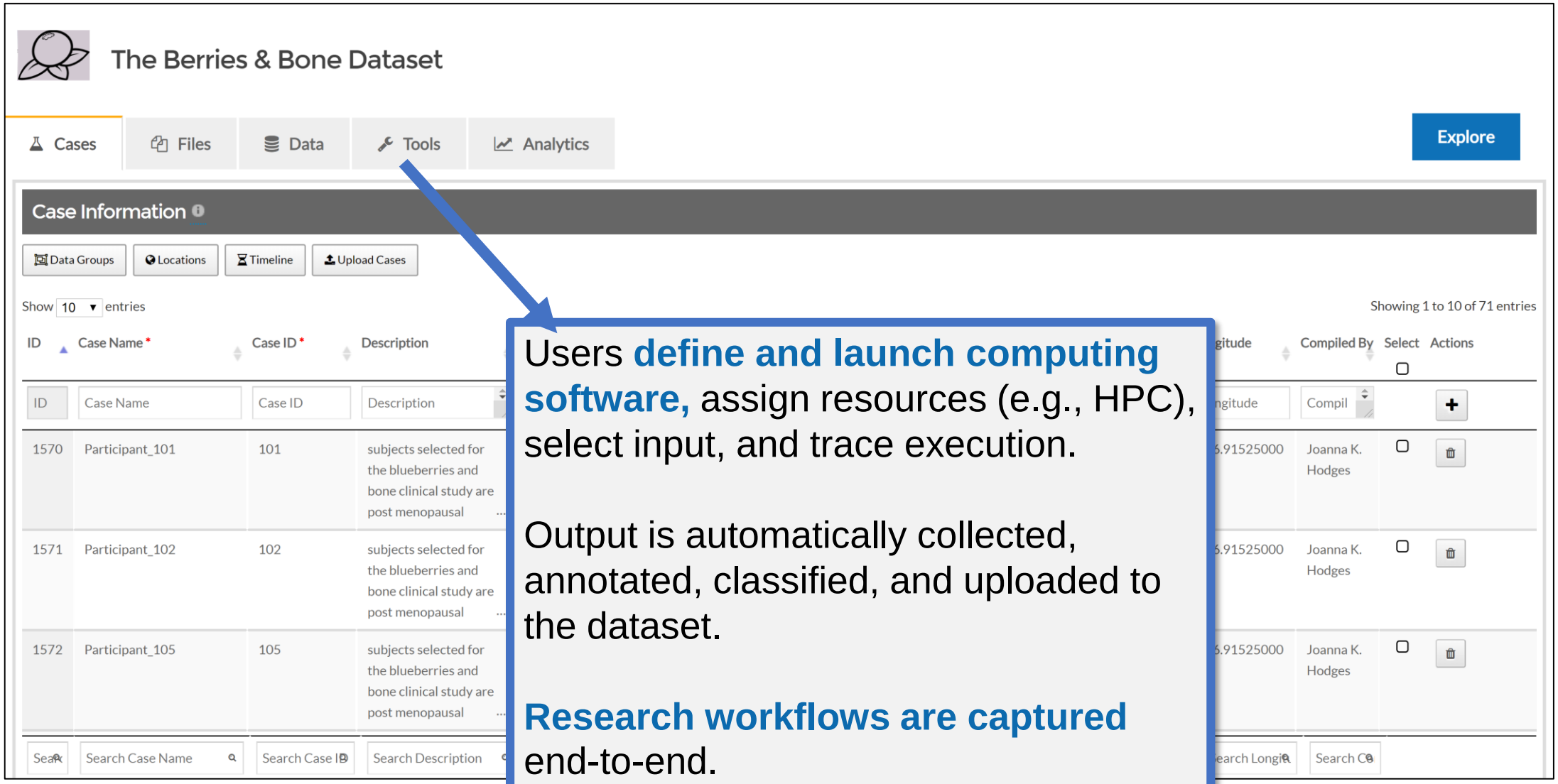
DEEDS DASHBOARD



Users **define complex structured data models** to describe properties, measurements, observations, and other data assembled throughout the investigation.

Our “spreadsheets of spreadsheets” approach is used to upload, view, and operate interactively on multi-dimensional data tables.

DEEDS DASHBOARD

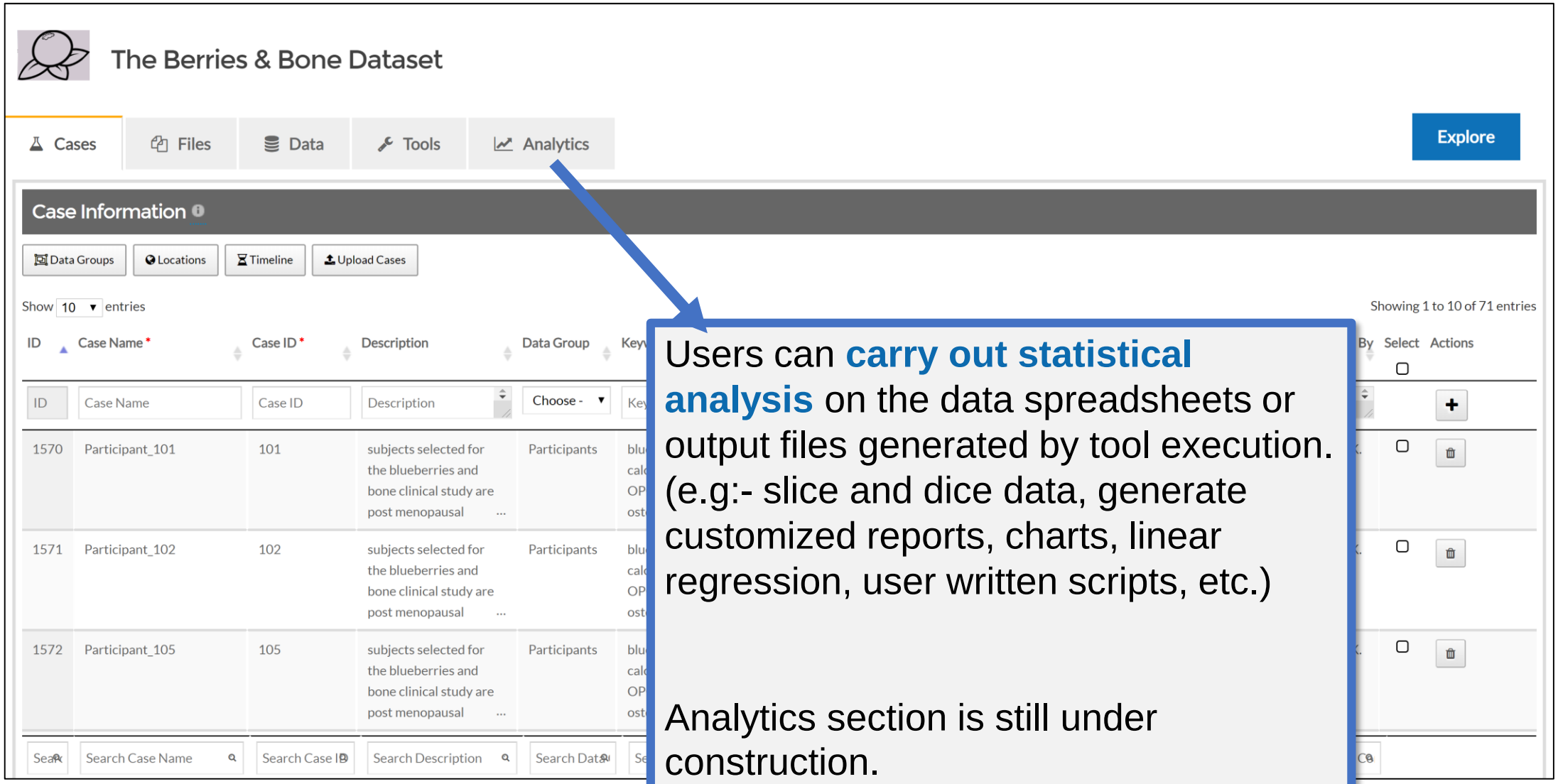


Users **define and launch computing software,** assign resources (e.g., HPC), select input, and trace execution.

Output is automatically collected, annotated, classified, and uploaded to the dataset.

Research workflows are captured end-to-end.

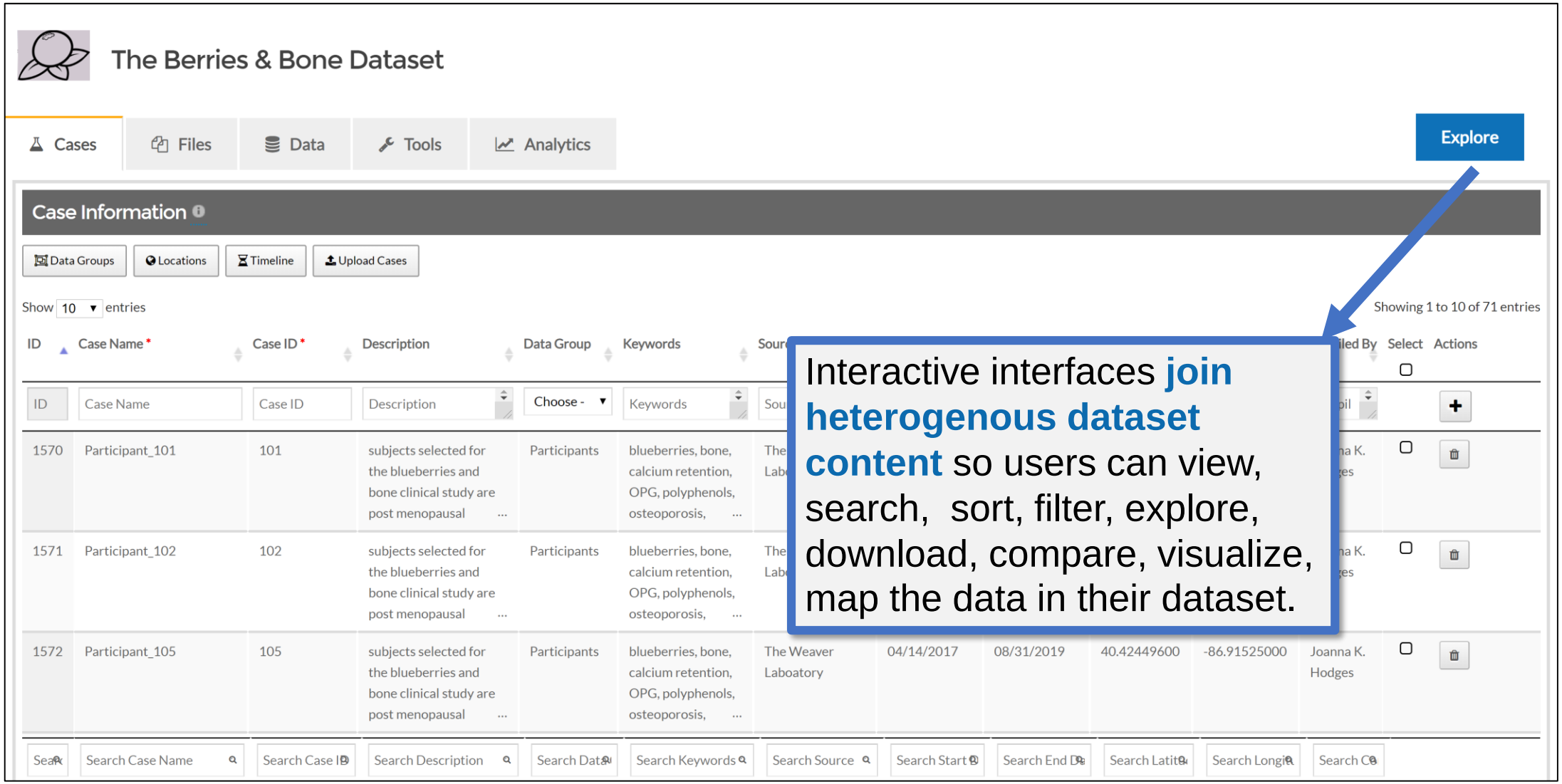
DEEDS DASHBOARD



Users can **carry out statistical analysis** on the data spreadsheets or output files generated by tool execution. (e.g:- slice and dice data, generate customized reports, charts, linear regression, user written scripts, etc.)

Analytics section is still under construction.

DEEDS DASHBOARD



Interactive interfaces **join heterogenous dataset content** so users can view, search, sort, filter, explore, download, compare, visualize, map the data in their dataset.

Research Computing Workflow

Solar PV Diagnosis: Real-time Monitoring of PV Systems using Suns-Vmp Method

CASES

Cases | Files | Data | Tools | Analytics

Explore

Case Information

Data Groups | Locations | Timeline | Upload Cases

Show 10 entries

Showing 1 to 2 of 2 entries

ID	Case Name *	Case ID *	Description	Keywords	Source	Start Date [mm/dd/yyyy]	End Date [mm/dd/yyyy]	Latitude	Longitude	Compiled By	Select	Actions
ID	Case Name	Case ID	Description	Keywords	Source	mm/dd/yyyy	mm/dd/yyyy	Latitude	Longitude	Compil		+
639	System #51	system-51	Solar farm in Golden Colorado, flat-plate photovoltaic (PV) modules deployed in a semi-arid climate. NREL ...	solar photovoltaic system, NREL, efficiency degradation, deconvolution of ...	The Alam Group	08/20/2017	12/31/2018	39.74160000	-105.23048400	Xingshu Sun, Tahir Patel, Reza ...		
640	System #50	system-50	Solar farm in Golden Colorado, flat-plate photovoltaic (PV) modules deployed in a semi-arid climate. NREL ...	solar photovoltaic system, NREL, efficiency degradation, deconvolution of ...	The Alam Group	05/10/2018	12/31/2019	39.74160000	-105.23048400	Tahir Patel, Reza Asadpour..		
Sea	Search Case Name	Search Case ID	Search Description	Search Keywords	Search Source	Search Start Da	Search End Da	Search Latitu	Search Longitu	Search Co		

Showing 1 to 2 of 2 entries

Previous 1 Next

Research Computing Workflow

Solar PV Diagnosis: Real-time Monitoring of PV Systems using Suns-Vmp Method

FILES

Files | Data | Tools | Analytics

Explore

Manage Case Files > System #51 > system-51

Back

Show 50 entries

Showing 1 to 50 of 54 entries

File ID	File Name	File Category	Description	Date and Time	Classification	Workflow	Shared File	Uploaded By	Select	Actions
			Description		Classificatic					
1025	Ini_Para.mat	Data	PV panel technology (module parameters) for solar farms #50, #51, MATLAB format.	06/12/2018 10:11:56	input		No	Muhammed Tahir Patel		
1026	Field_Data_232days.mat	Data	Field data for solar farms #51 and #50, 232 day simulation, MATLAB format.	06/12/2018 10:13:24	input		No	Muhammed Tahir Patel		
1027	Field_Data_963days.mat	Data	Field data for solar farms #51 and #50, 963 day simulation, MATLAB format.	06/12/2018 10:18:03	input		No	Muhammed Tahir Patel		
1028	Field_Data_7386days.mat	Data	Field data for solar farms #51 and #50, 7386 day simulation, MATLAB format.	06/12/2018 10:19:53	input		No	Muhammed Tahir Patel		
1029	232days_deconvolution_20180601-192442.jpg	Figures	System #51 output file generated by pvsuns-vmp r7. Tool workflow session mdtahirpatel_20180601-192442	06/12/2018 10:22:09	output		No	Muhammed Tahir Patel		
Search File	Search File Name	Search File	Search Description	Search Date	Search Cla	Search Wo	Search Sha	Search Up		

Research Computing Workflow

Solar PV Diagnosis: Real-time Monitoring of PV Systems using Suns-Vmp Method

Explore

Cases | File | TOOLS | Tools | Analytics

Tool Definitions

New Tool | Copy Tool | Save Tool | Import Tool

Show 10 entries

Search:

Tool Name	Tool Short Name	Version	Tool Description	Version Description	Date Tool Added	Developed By	Date Developed	Tool
Alam Group Solar PV Degradation Analyzer (Suns-Vmp Method)	pvsuns-vmp	r0	The solar PV tool uses Suns-Vmp method to analyze the performance of a module based on solar module technology and field data.	Initial version of code	2018-01-17	Yingshu Sun	2017-08-06	Co
Alam Group Solar PV Degradation Analyzer (Suns-Vmp Method)	pvsuns-vmp	r1	The solar PV tool uses Suns-Vmp method to analyze the performance of a module based on solar module technology and field data.		2018-01-17	Yingshu Sun	2017-09-25	Co
Alam Group Solar PV Degradation Analyzer (Suns-Vmp Method)	pvsuns-vmp	r2	The solar PV tool uses Suns-Vmp method to analyze the performance of a module based on solar module technology and field data.	New Features: Code generates JPG format figures.	2018-01-17	Yingshu Sun	2017-09-25	Co

Tool Launch

Show 5 entries

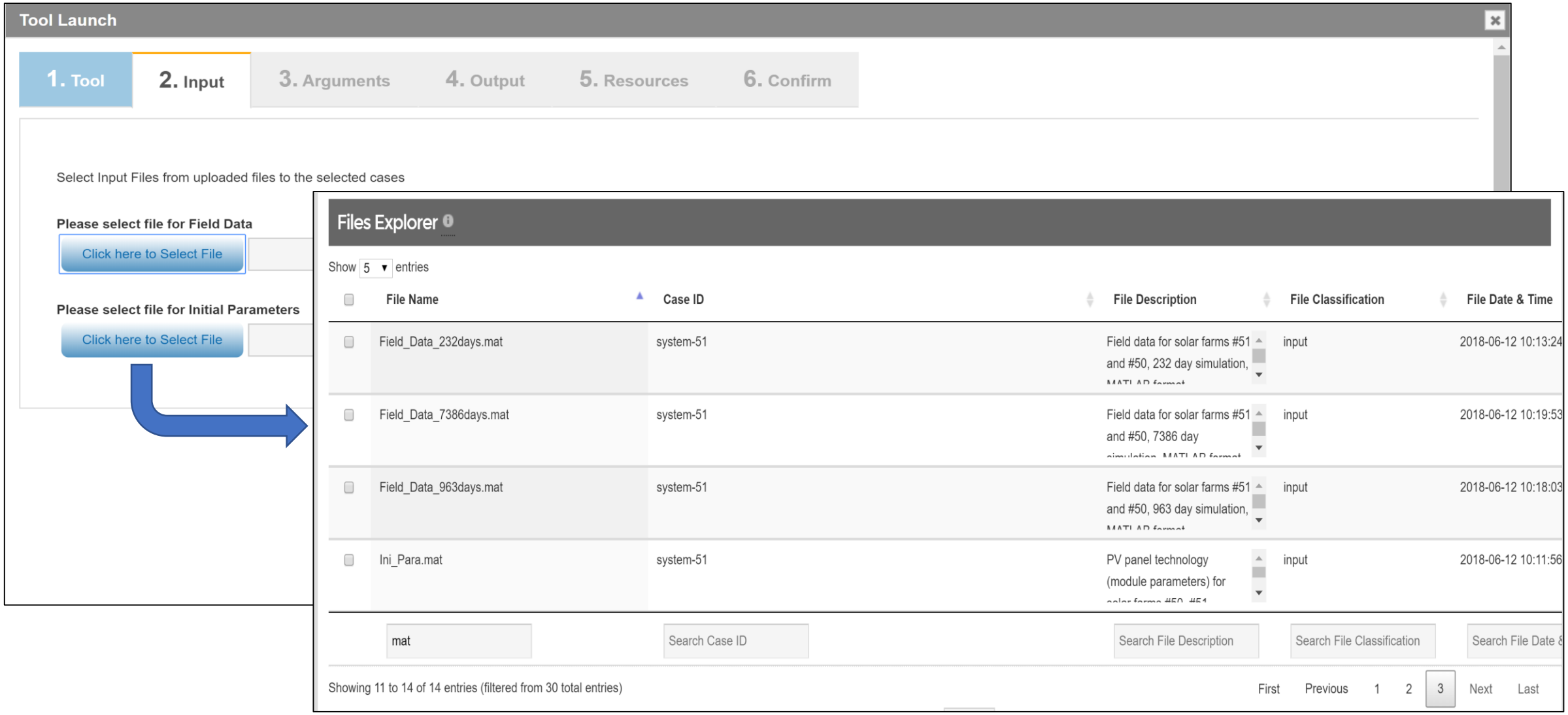
Tool Name	Tool Short Name	Latest Version	Description	Versions	Launch
Alam Group Solar PV Degradation Analyzer (Suns-Vmp Method)	pvsuns-vmp	r7	The solar PV tool uses Suns-Vmp method to analyze the performance of a module based on solar module technology and field data.	Versions	Launch
Search Tool Name	Search Tool Short Name	Search Latest Version	Search Description		

Showing 1 to 1 of 1 entries

First | Previous | 1 | Next | Last

Go to Page 1

Research Computing Workflow



Research Computing Workflow

Workflow

Show 20 entries

Search:

Session Id	Session Name	Status	Execution Trace	Tool	Version	Launched By	Launched Time	Input	Output	Execution Stats
104	mdtahirpatel_20180906-155822	Finished	View Execution Trace	pvsuns-vmp	r7	Muhammed Tahir Patel	20180906-155822	View Input	View Output	View Execution Sta
102	mdtahirpatel_20180906-002558	Finished	View Execution Trace	pvsuns-vmp	r7	Muhammed Tahir Patel	20180906-002558	View Input	View Output	View Execution Sta
88	sumudinie_20180903-020154	Aborted	View Execution Trace	pvsuns-vmp	r7	Sumudine Fernando	20180903-020154	View Input	View Output	View Execution Sta
85	sumudinie_20180902-211926	Aborted	View Execution Trace	pvsuns-vmp	r7	Sumudine Fernando	20180902-211926	View Input	View Output	View Execution Sta
82	acc_20180831-154733	Failed	View Execution Trace	pvsuns-vmp	r7	Ann Christine Catlin	20180831-154733	View Input	View Output	View Execution Sta
79	acc_20180830-224819	Aborted	View Execution Trace	pvsuns-vmp	r7	Ann Christine Catlin	20180830-224819	View Input	View Output	View Execution Sta
73	sumudinie_20180822-004648	Finished	View Execution Trace	pvsuns-vmp	r7	Sumudine Fernando	20180822-004648	View Input	View Output	View Execution Sta

Tool Launch Input

Download | Fullscreen | Clear Filters | No-Wrap

Show 25 entries

First Previous 1 Next Last

Session Id	Input Name	Description	Input Type	Value
104	Input Name	Description	Input Type	Value
104	Save Prefix	Output file prefix	text	System50
104	Field Data	Field data	file	Field_Data_Sys_50_1994_98.mat
104	Initial Parameters	Initial parameters	file	Ini_Para_Sys_50.mat
104	NS	Number of solar cells in series in a module	int	14
104	NP	Number of panels in parallel	int	5
104	NumofDay	Window of days spanning total number of days	int	3
104	DaiVar	Percent error in all the parameters	decimal	0.01

Show 25 entries

Showing 1 to 7 of 7 entries

Tool Launch Output

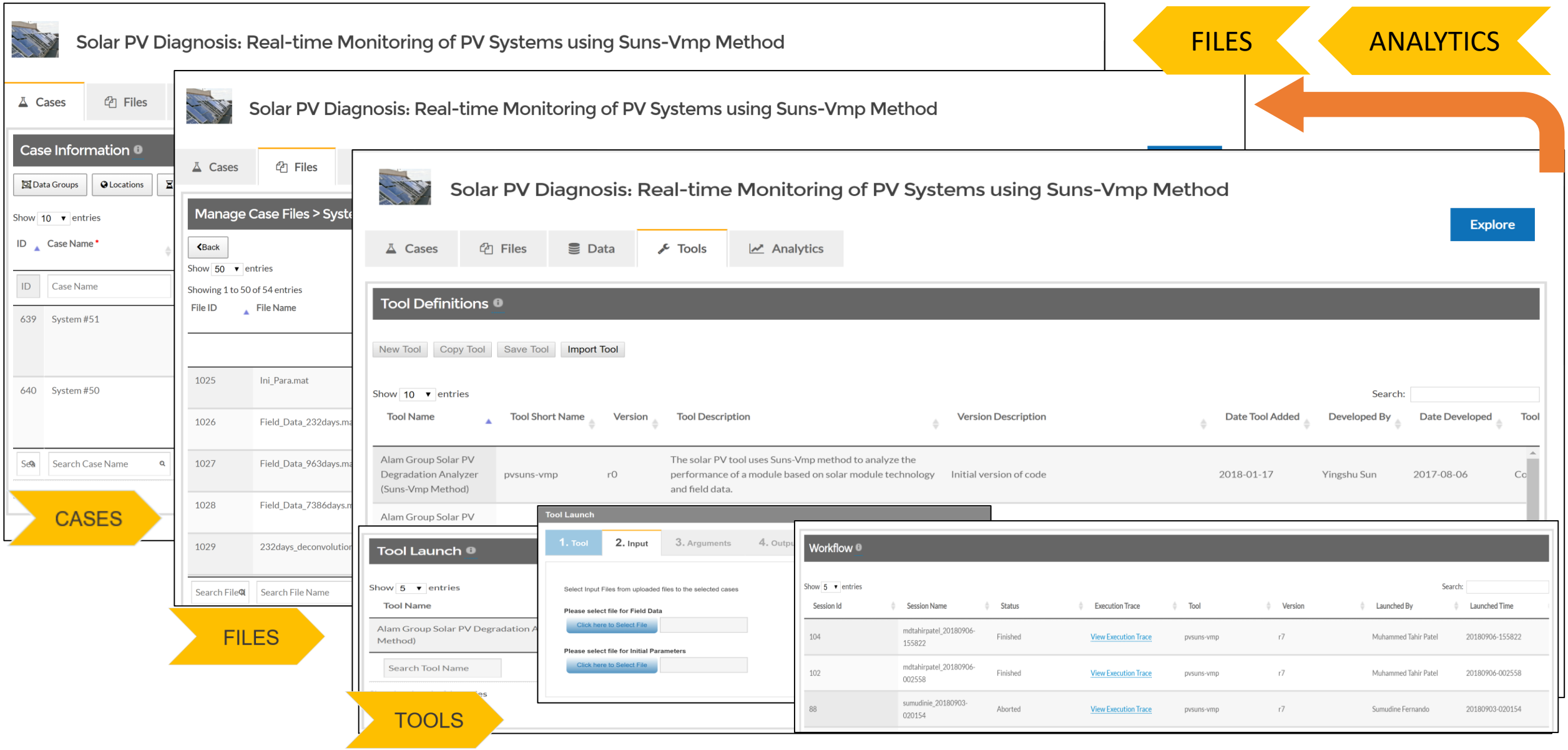
Download | Fullscreen | Clear Filters | No-Wrap

Show 25 entries

First Previous 1 Next Last

Session Id	Output File	File Size (kb)	Status
104	Output File	File Size (kb)	Status
104	System50_Input_Circuit_Parameter_20180906-155822.csv	154	Uploaded
104	System50_Results_20180906-155822.mat	2532847	Uploaded
104	System50_Output_Efficiency_20180906-155822.csv	5212	Uploaded
104	System50_temperature_coefficient_20180906-155822.jpg	50629	Uploaded
104	System50_Output_Circuit_Parameter_20180906-155822.csv	24483	Uploaded
104	System50_deconvolution_20180906-155822.jpg	62083	Uploaded
104	System50_efficiency_20180906-155822.jpg	45526	Uploaded
104	System50_Input_Field_Data_20180906-155822.csv	5034460	Uploaded
104	System50_circuit_parameter_20180906-155822.jpg	103355	Uploaded
104	System50_relative_error_20180906-155822.jpg	247436	Uploaded
104	submit.stdout	11306	Not Uploaded. [Will be removed on 2018-09-16]
104	submit.stderr	0	Not Uploaded. [Will be removed on 2018-09-16]
104	.submit.log	0	Not Uploaded. [Will be removed on 2018-09-16]
104	submit.metrics	156	Not Uploaded. [Will be removed on 2018-09-16]
104	submit.progress	402	Not Uploaded. [Will be removed on 2018-09-16]
104	00007740.stdout	34892	Not Uploaded. [Will be removed on 2018-09-16]

Research Computing Workflow



Statistical Computing Workflow

CASES

EcoTox X17-02 Dataset: Amphibian Per- and Polyfluoroalkyl Toxicity Reference Values for Ecological Risk Assessment

Cases | Files | Data | Tools | Analytics

Explore

Case Information

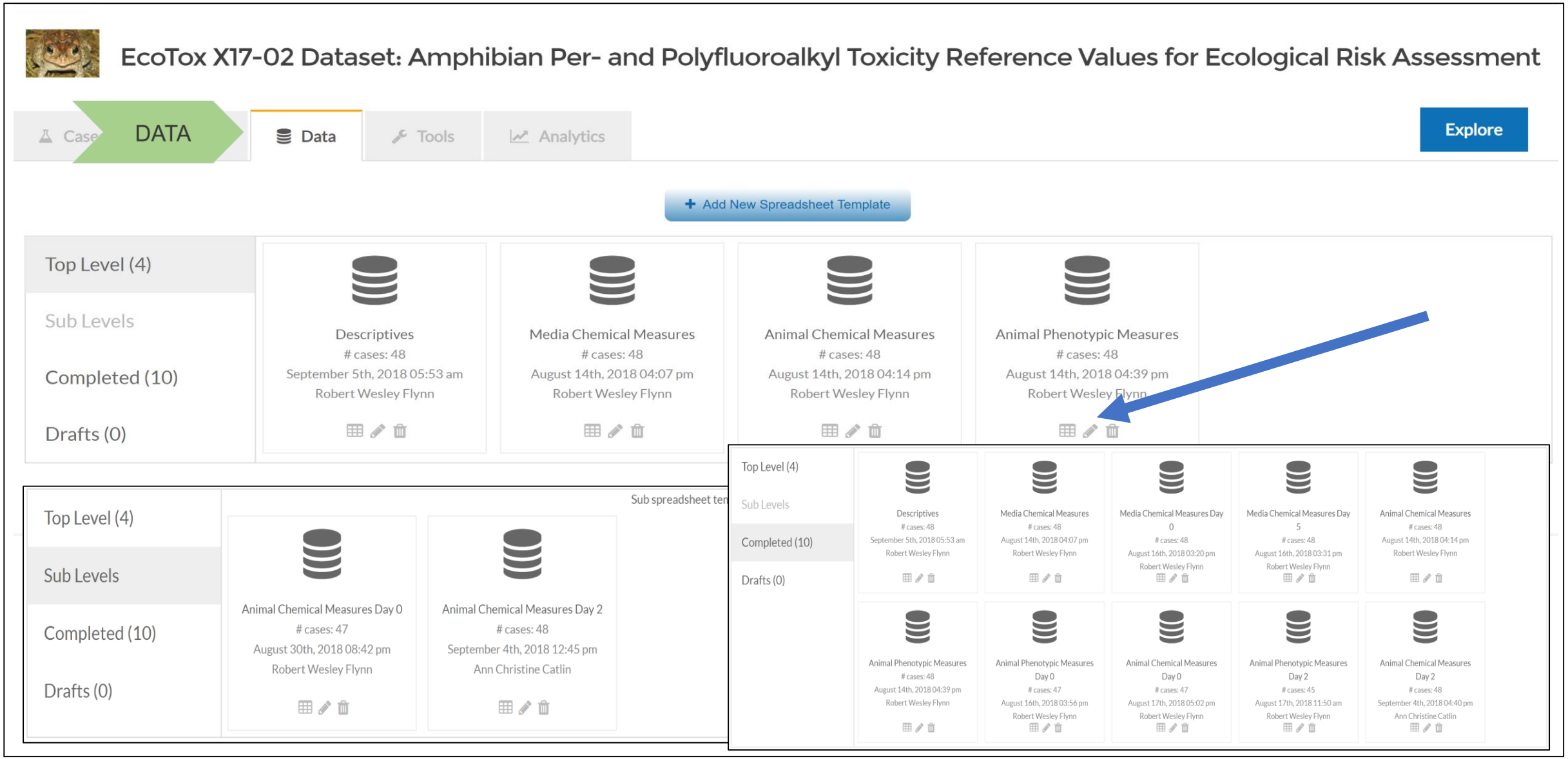
Data Groups | Locations | Timeline | Upload Cases

Show 10 entries

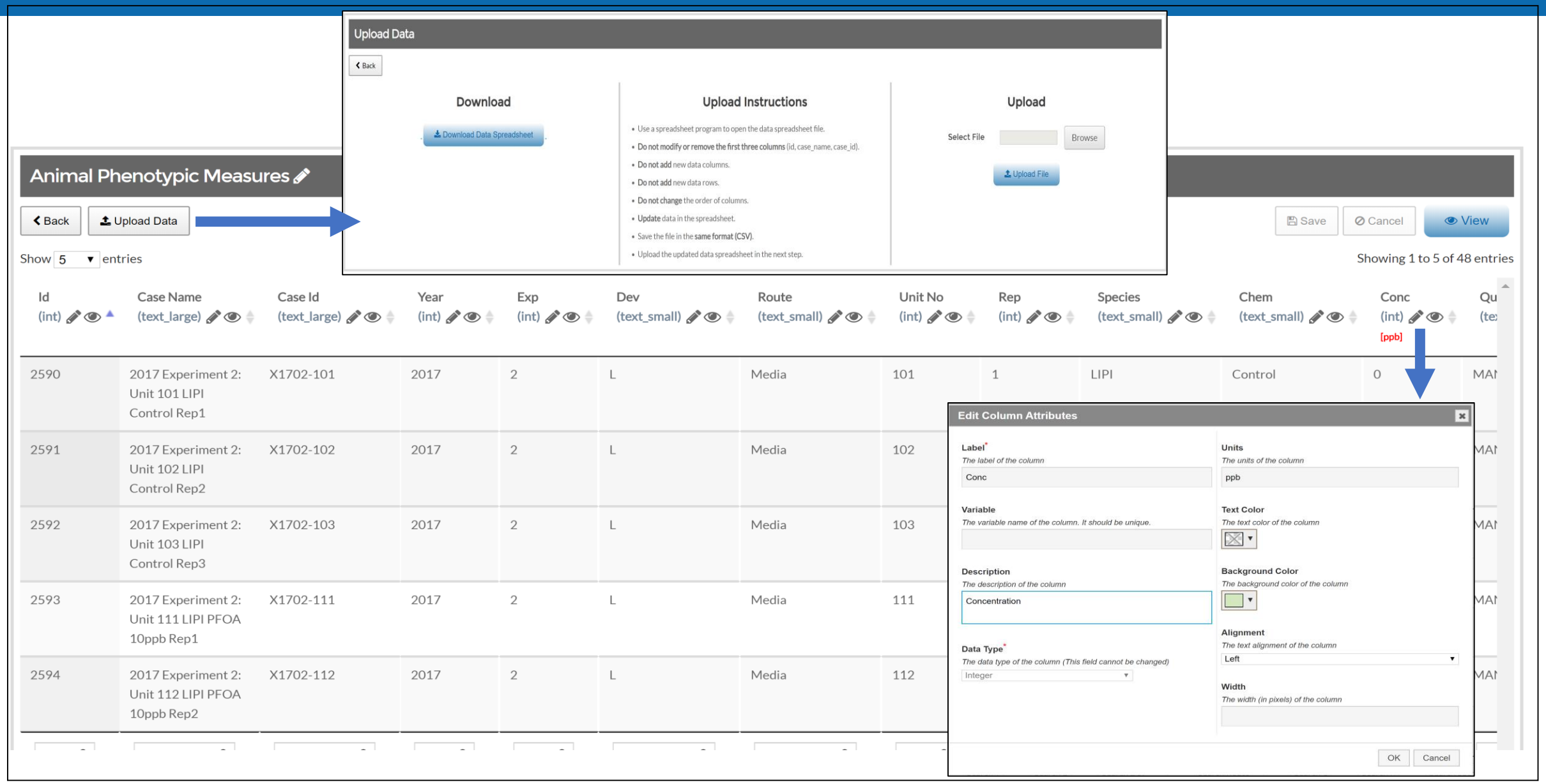
Showing 1 to 10 of 48 entries

ID	Case Name *	Case ID *	Description	Keywords	Source	Start Date [mm/dd/yyyy]	End Date [mm/dd/yyyy]	Latitude	Longitude	Compiled By	Select	Actions
ID	Case Name	Case ID	Description	Keywords	Source	mm/dd/yyyy	mm/dd/yyyy	Latitude	Longitude	Compil		+
2590	2017 Experiment 2: Unit 101 LIPI Control Rep1	X1702-101	Experiment #2 2017. Experimental unit 101 species=leopard frog, chemical=Control, concentration=0, route=dermal, ...	SERDP, ecotoxicology, poly- and perfluoroalkyl substances, ...	Sepulveda Lab	05/28/2018	06/29/2018	40.42809100	-86.92251000	Robert W. Flynn		
2591	2017 Experiment 2: Unit 102 LIPI Control Rep2	X1702-102	Experiment #2 2017. Experimental unit 102 species=leopard frog, chemical=Control, concentration=0, route=dermal, ...	SERDP, ecotoxicology, poly- and perfluoroalkyl substances, ...	Sepulveda Lab	05/28/2018	06/29/2018	40.42809100	-86.92251000	Robert W. Flynn		
2592	2017 Experiment 2: Unit 103 LIPI Control Rep3	X1702-103	Experiment #2 2017. Experimental unit 103 species=leopard frog, chemical=Control, concentration=0, route=dermal, ...	SERDP, ecotoxicology, poly- and perfluoroalkyl substances, ...	Sepulveda Lab	05/28/2018	06/29/2018	40.42809100	-86.92251000	Robert W. Flynn		
Sear	Search Case Name	Search Case ID	Search Description	Search Keywords	Search Source	Search Start D	Search End Da	Search Latit	Search Longi	Search Co		

Statistical Computing Workflow



Statistical Computing Workflow



Statistical Computing Workflow

Cases | Files | TOOLS | Tools | Ana

Tool Definitions

New Tool | Copy Tool | Save Tool | Import Tool

Show 10 entries

Tool Name	Tool Short Name	Version	Tool Description
spectrometry body burden measures across species and treatments	animalmassspec	v2	Plots generated for animal c spectrometry measures for
Animal phenotype plots from measurement data	animalphenotype	v1	Plots generated for animal phenotypic data, using

Workflow

Show 10 entries

Search:

Session Id	Session Name	Status	Execution Trace	Tool	Version	Launched By	Launched Time	Input	Output	Execution Stats
120	wflynn_20180919-145941	Executing	View Trace	animalmassspec	v2	Robert Wesley Flynn	20180919-145941	View Input		View Stats
101	wflynn_20180904-164800	Finished	View Trace	animalphenotype	v2	Robert Wesley Flynn	20180904-164800	View Input	View Output	View Stats
100	wflynn_20180904-102842	Finished	View Trace	animalphenotype	v2	Robert Wesley Flynn	20180904-102842	View Input	View Output	View Stats
97	acc_20180903-150033	Finished	View Trace	animalphenotype	v2	Ann Christine Catlin	20180903-150033	View Input	View Output	View Stats
96	hewanadun_20180903-124646	Aborted	View Trace	animalphenotype	v2	Chandima Hewanadungodage	20180903-124646	View Input	View Output	View Stats
95	hewanadun_20180903-114132	Finished	View Trace	animalmassspec	v2	Chandima Hewanadungodage	20180903-114132	View Input	View Output	View Stats

Tool Launch

Show 5 entries

Tool Name	Tool Short Name	Latest Version	Description	Versions	Launch
Animal chemical plots from mass spectrometry body burden measures across species and treatments	animalmassspec	v2	Plots generated for animal chemical measures using mass spectrometry measures for body burden	Versions	Launch
Animal phenotype plots from measurement data across species and treatments	animalphenotype	v2	Plots generated for animal phenotypic data, using replicated regression	Versions	Launch

Search Tool Name | Search Tool Short Name | Search Latest Version | Search Description

Showing 1 to 2 of 2 entries

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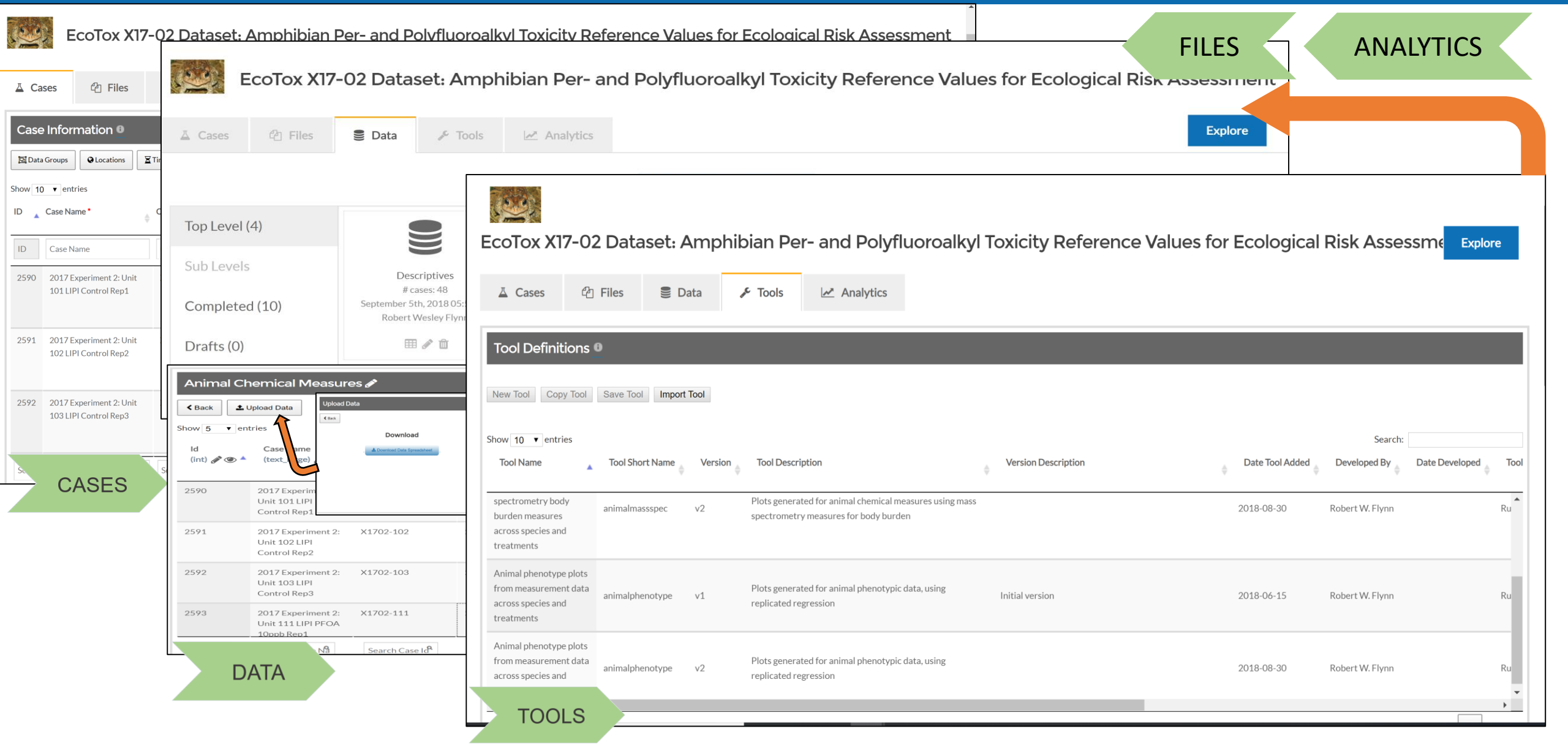
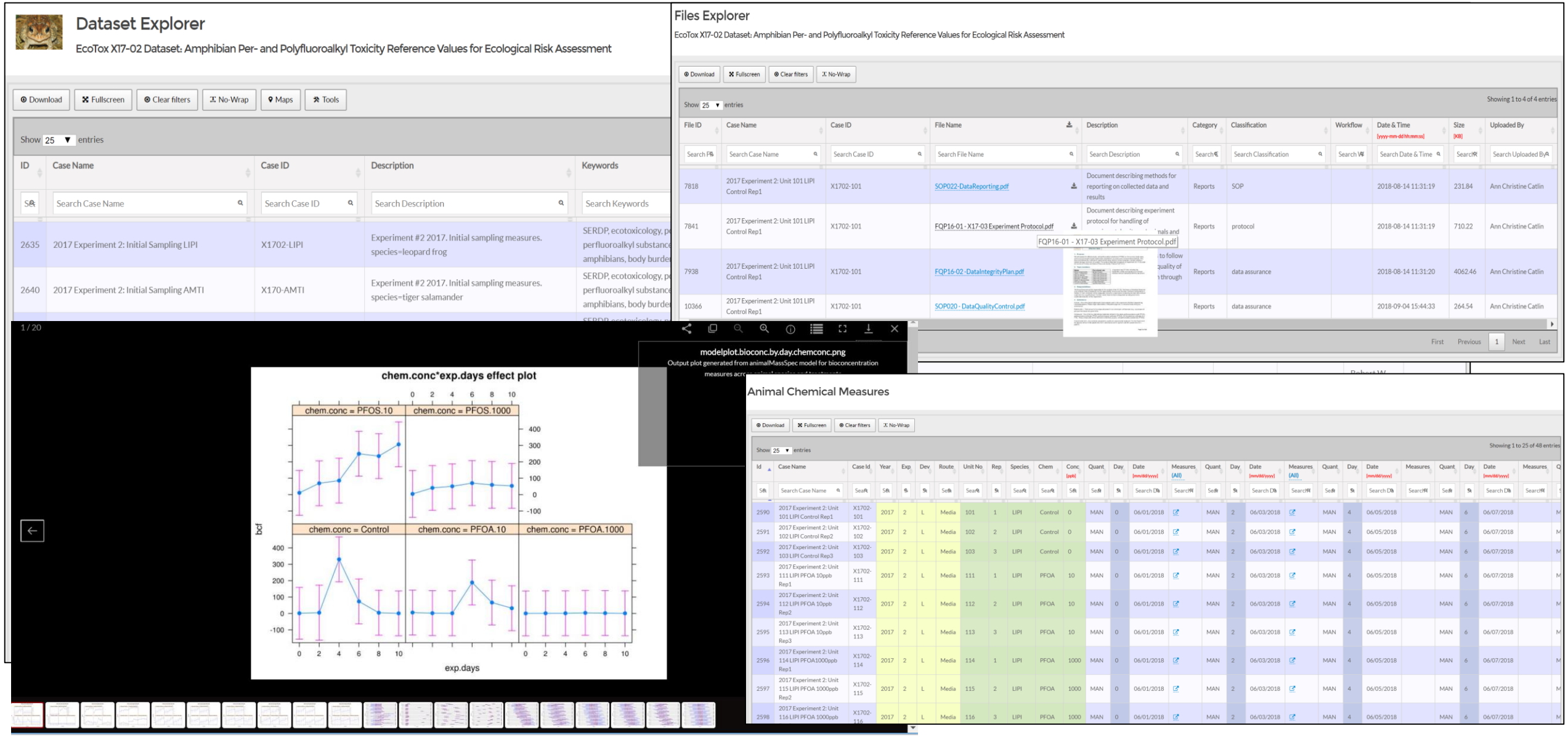
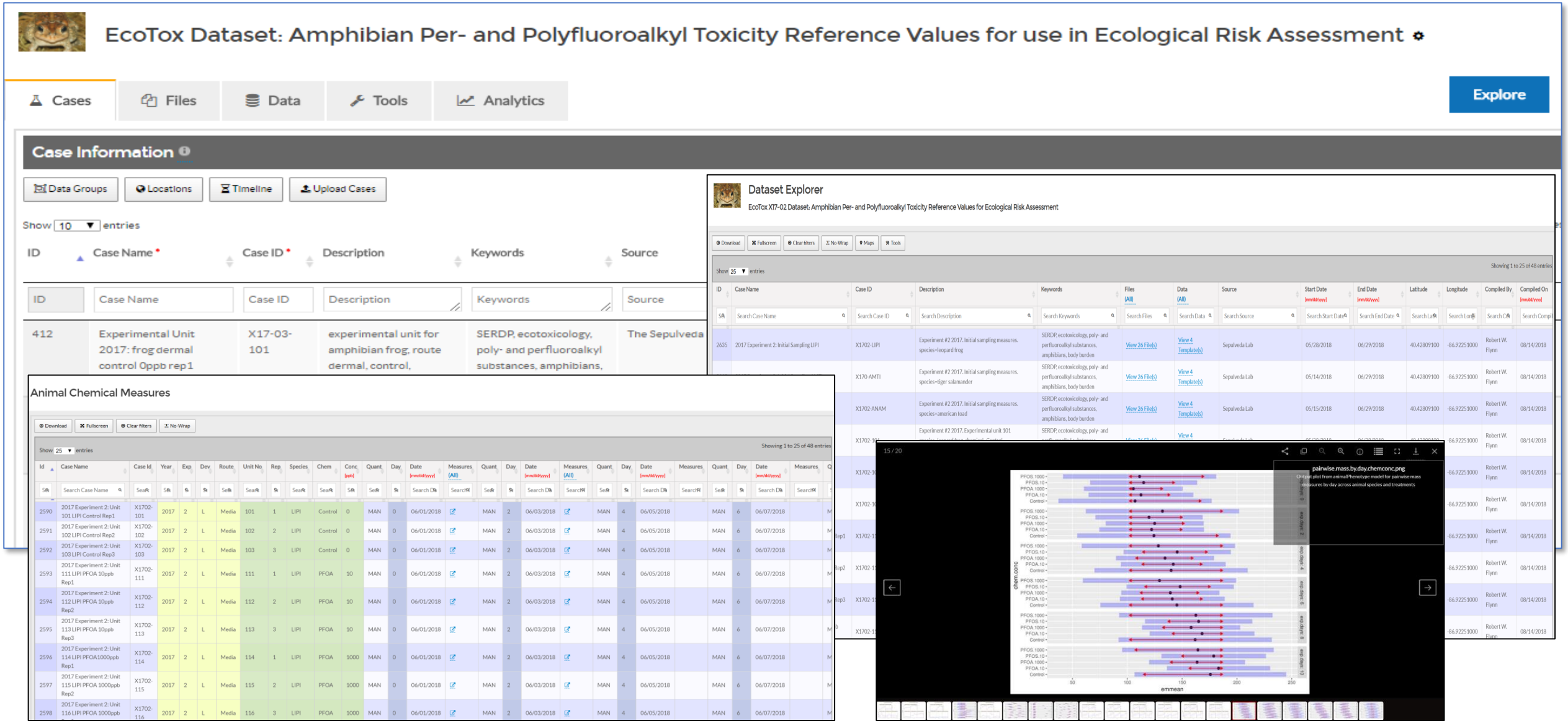
Statistical Computing Workflow



Discovery and Exploration



DEEDS DATASETS



DEEDS DATASETS

The Berries & Bone Dataset

Cases | Files | Data | Tools | Analytics

Case Information

Data Groups | Locations | Timeline | Upload Cases

Show 10 entries

ID	Case Name *	Case ID *	Description	Data Group	Keywords
1570	Participant_101	101	subjects selected for the blueberries and bone clinical study are post menopausal ...	Participants	blueberries, bone, calcium retention, OPG, polyphenols, osteoporosis, ...
1571	Participant_102	102	subjects selected for the blueberries and bone clinical study are post menopausal ...	Participants	blueberries, bone, calcium retention, OPG, polyphenols, osteoporosis, ...
1572	Participant_105	105	subjects selected for the blueberries and bone clinical study are post menopausal ...	Participants	blueberries, bone, calcium retention, OPG, polyphenols, osteoporosis, ...

Dataset Explorer

The Berries & Bone Dataset

Download | Fullscreen | Clear filters | No-Wrap | Maps | Tools

Show 25 entries — Showing 1 to 25 of 71 entries

ID	Case Name	Case ID	Description	Keywords	Files (All)	Data (All)	Source	Start Date [mm/dd/yyyy]	End Date [mm/dd/yyyy]
1570	Participant_101	101	subjects selected for the blueberries and bone clinical study are post menopausal women who will add blueberry powder to their regular diet to evaluate effect on calcium retention.	blueberries, bone, calcium retention, OPG, polyphenols, osteoporosis, RANKL	View 2 File(s)	View 3 Template(s)	The Weaver Laboatory	01/12/2017	08/31/2019
1571	Participant_102	102	subjects selected for the blueberries and bone clinical study are post menopausal women who will add blueberry powder to their regular diet to evaluate effect on calcium retention.	blueberries, bone, calcium retention, OPG, polyphenols, osteoporosis, RANKL	View 2 File(s)	View 3 Template(s)	The Weaver Laboatory	02/28/2017	08/31/2019
1572	Participant_105	105	subjects selected for the blueberries and bone clinical study are post menopausal women who will add blueberry powder to their regular diet to evaluate effect on calcium retention.	blueberries, bone, calcium retention, OPG, polyphenols, osteoporosis, RANKL	View 2 File(s)	View 3 Template(s)	The Weaver Laboatory	04/14/2017	08/31/2019
1573	Par		subjects selected for the blueberries and bone clinical						
1574	Par								
1575	Par								

Descriptives

Download | Fullscreen | Clear filters | No-Wrap

Show 25 entries — Showing 1 to 18 of 18 entries

Id	Case Name	Case Id	Study status	Date dropped	Reason dropped	Date of birth	Age [years]	Race	Ca-41 dose date	Height [cm]	Weight [kg]	BMI [kg/m2]	Blood draw time	Years past menopause [years]	Early menopause [yes/no]	Hysterectomy year	Medical conditions at screening [year]	Previous fracture [yes/no]
1570	Participant_101	101	participant	N/A	N/A	12/16/1953	63	White	03/16/2013	166.89	76.7	27.5	6:43 AM	9.5	Yes	N/A	None	No
1571	Participant_102	102	dropped out	9/21/2017	time contraints	08/22/1956	60.5	White	04/29/2017	160.26	58.9	22.9	7:18 AM	5	No	N/A	None	No
1572	Participant_105	105	dropped out	3/19/2018	too much food	05/22/1956	60	White	05/06/2017	160.23	65.7	25.6	9:14 AM	20	Yes	1997	Prediabetes 2012, chronic bronchitis 1973	No
1573	Participant_106	106	participant	N/A	N/A	10/31/1967	49	White	05/17/2017	163.56	59.6	22.3	9:58 AM	4	No	N/A	Osteopenia 2014, urinary tract infection 2013, hypothyroidism 2011	Yes
1574	Participant_107	107	participant	N/A	N/A	01/18/1964	53	White	05/17/2017	159.77	86.4	33.8	10:43 AM	5	Yes	2016	None	No
1575	Participant_110	110	participant	N/A	N/A	04/24/1958	59	White	05/26/2017	160.44	62.6	24.3	8:25 AM	5	No	N/A	None	No
1576	Participant_112	112	dropped out	1/3/2018	no reason given	11/26/1951	65	White	05/30/2017	157.39	82.3	33.2	8:42 AM	12	No	N/A	None	No
1577	Participant_114	114	dropped out	4/2/2018	constipation due to Ca supplement	03/17/1953	64	White	06/09/2017	156.25	50.7	20.8	11:01 AM	10	No	N/A	Autoimmune hepatits 2007, hepatitis 1976	Yes
1578	Participant_116	116	participant	N/A	N/A	05/13/1956	61	White	05/30/2017	165.55	74.3	27.1	8:22 AM	10	No	N/A	None	No
1579	Participant_117	117	participant	N/A	N/A	10/12/1962	54	White	05/30/2017	159.39	67.6	26.6	9:33 AM	5	No	N/A	Hypothyroidism 1997	No
1580	Participant_118	118	participant	N/A	N/A	06/19/1960	56	White	06/05/2017	170.56	71.6	24.6	10:38 AM	4	Yes	N/A	Hashimoto 2013, Factor V Leiden	Yes
1581	Participant_119	119	participant	N/A	N/A	11/25/1960	56	White	06/03/2017	158.22	59.3	23.7	8:57 AM	5	No	N/A	Hypothyroidism 2001, urinary tract infection	Yes
1582	Participant_124	124	participant	N/A	N/A	12/05/1961	55	White	06/09/2017	158.92	61.3	24.3	10:38 AM	4	No	N/A	Diverticulosis 2017, urinary tract infection 2017	Yes

DEEDS DATASETS

Quantum Post- Lock and Key Descriptor Dataset

Cases | Files | Data | Tools | Analytics

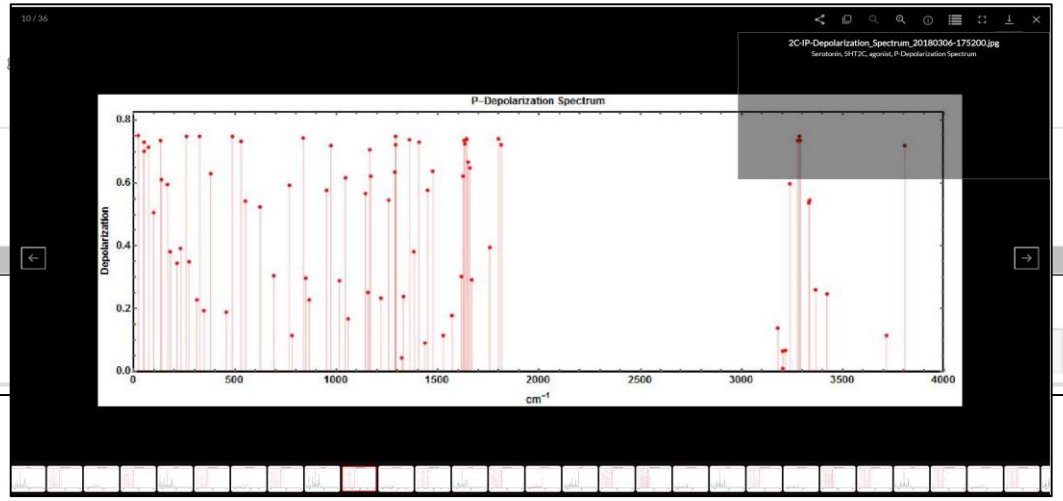
Tool Definitions

New Tool | Copy Tool | Save Tool | Import Tool

Show 10 entries

Tool Name	Tool Short Name	Version	Tool Description					
Gaussian09-E.01 computational chemistry software package	gaussian09	E.01 DEEDSv1	Gaussian is a licensed software package that provides state of the art capabilities for electronic structure modeling. This tool is the 2009 release of the Gaussian package.	Added pre-processing to replace "gjf" extension with ".com" and remove hard-coded checkpoint path. These are for handling input files generated by Gaussview.	Carnegie Mellon	Available at remote site	-	-
Gaussian16-A.03 computational chemistry software package								

Showing 1 to 2 of 2 entries



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Quantum Post- Lock and Key Descriptor Dataset

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Show 25 entries — Showing 1 to 3 of 3 entries

ID	Case Name	Case ID	Description	Keywords	Files (All)	Data (All)	Source	Start Date [mm/dd/yyyy]	End Date [mm/dd/yyyy]
712	5-HT2A	5-HT2A	Serotonin-class G-Protein Coupled Receptor (GPCR). Subclass 2A, typically non-hallucinogenic ,	Generic G-Protein Coupled Receptor, intercellular signaling, Receptor Binder, Antagonists	View 4 File(s)		Ross Douglas Hoehn	04/01/2018	04/23/2018
713	5-HT2C	5-HT2C	Serotonin-class G-Protein Coupled Receptor (GPCR). Subclass 2C,, typically involved in hallucinogenic activity.	Generic G-Protein Coupled Receptor, intercellular signaling, Receptor Binder, Agonist, 2C-X , DOX, Ergot	View 85 File(s)		Ross Douglas Hoehn	04/01/2018	04/23/2018
714	beta-Androgen	beta-Androgen	Generic G-Protein Coupled Receptor (GPCR). Androgenic receptor class.	Generic G-Protein Coupled Receptor, intercellular signaling, Receptor Binder, Antagonists, Agonists	View 36 File(s)		Ross Douglas Hoehn	04/01/2018	04/23/2018

Showing 1 to 3 of 3 entries — First | Previous | 1 | Next | Last

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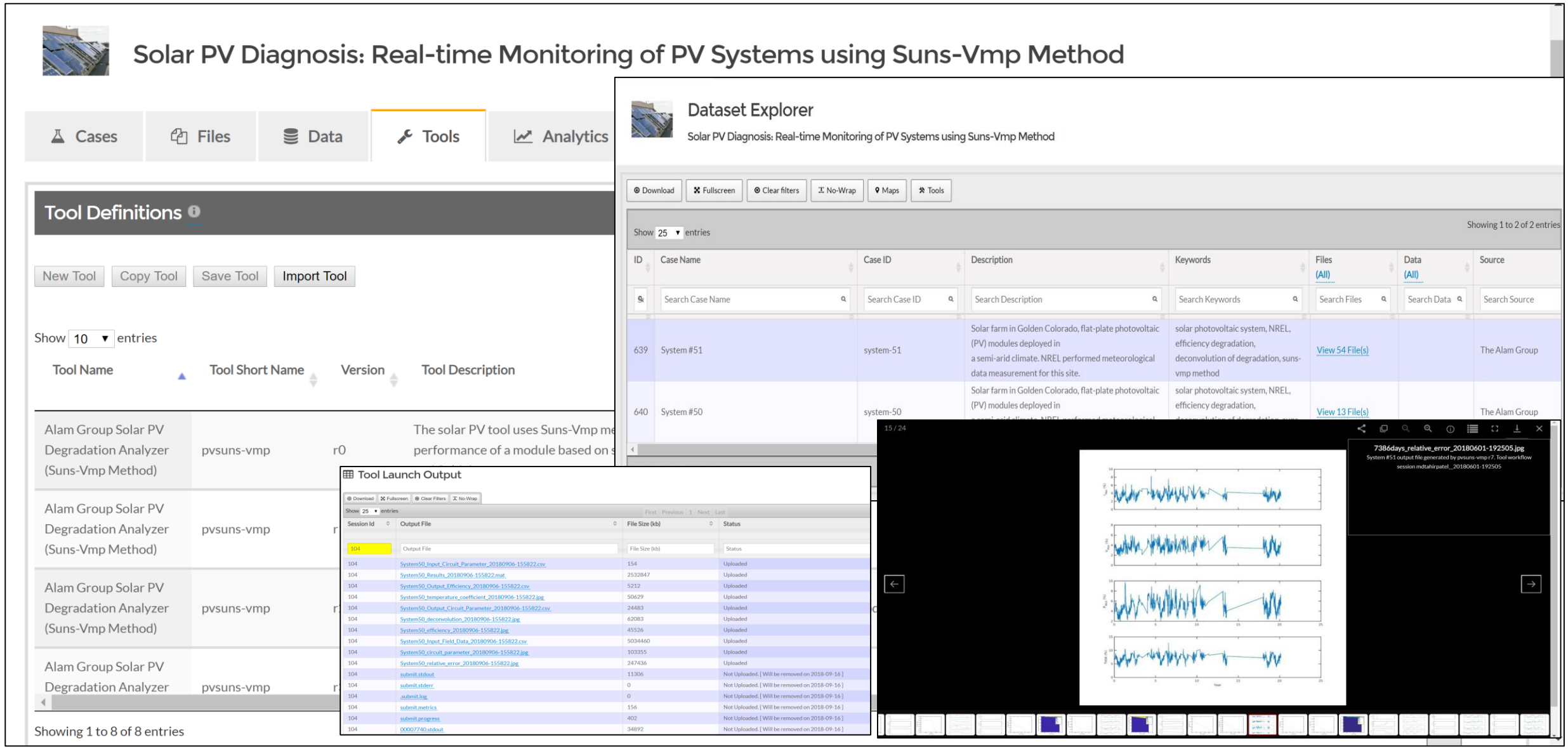
Show 25 entries — Showing 1 to 25 of 32 entries

File ID	Case Name	Case ID	File Name	Description	Category	Classification	Workflow
1244	5-HT2A	5-HT2A	Olanzapine.gjf	Serotonin, 5-HT2A, Antagonist	Data	GJF Input File - Gaussian Associated	
1245	5-HT2A	5-HT2A	MDL100907.gjf	Serotonin, 5-HT2A, Antagonist	Data	GJF Input File - Gaussian Associated	
1246	5-HT2A	5-HT2A	Risperidone.gjf	Serotonin, 5-HT2A, Antagonist	Data	GJF Input File - Gaussian Associated	
1247	5-HT2A	5-HT2A	Ly367265.gjf	Serotonin, 5-HT2A, Antagonist	Data	GJF Input File - Gaussian Associated	
1408	5-HT2A	5-HT2A	LY367265ChargeData_20100319-124412.csv	Serotonin, 5-HT2A, Antagonist, Charge data tables	Data	Post-processor output file	
1409	5-HT2A	5-HT2A	LY367265mol_20100319-124412.mol	Serotonin, 5-HT2A, Antagonist, MOL file	Data	Post-processor output file	

DEEDS DATASETS



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Pilot version of DEEDS currently available to use case groups at
www.datacenterhub.org

DEEDS platform will be available to general public in summer 2019

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Acknowledgements

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