SpecData™ User Manual

Document Date: 21 April 2022

Please report any errors or omissions to info@tellspec.com.

Preface

Thank you for subscribing to the Tellspec® SpecData™ system. We are here to help you be successful in collecting spectral data that can be used to build your calibration models. Feel free to contact us with any questions regarding this manual at info@tellspec.com or at +44 073 1239 6041.

The SpecData system has two parts, one that runs on the desktop and is used by the administrator (SpecData desktop app) and the other which runs on mobile devices for use by a team of workers (SpecData mobile app).

The SpecData desktop app is used to set up a project, allocate access to team workers, track work done, and plan work to be done. See 'Using the desktop SpecData app', below.

The SpecData mobile app has several purposes:

- To collect spectra of material samples along with the *label data* obtained from laboratory analysis of those samples;
- To make the data collected available to create chemometric or machine learning models for predicting label data from new spectra;
- Once those models are built and reside in Tellspec's cloud, to scan new samples, not previously seen, and obtain results for the label data of those samples, in order to test the models.

To use it you will need a Preemie Sensor™ or an Enterprise Sensor™.

If you are a new user and you still do not own a sensor, please visit us online for a Preemie Sensor or an Enterprise Sensor.

Chapter 1: The SpecData Mobile App

The mobile app works with both the Preemie Sensor and the Enterprise Sensor. They are described in later chapters of this manual:

The Preemie Sensor

The Enterprise Sensor

Using the mobile SpecData app

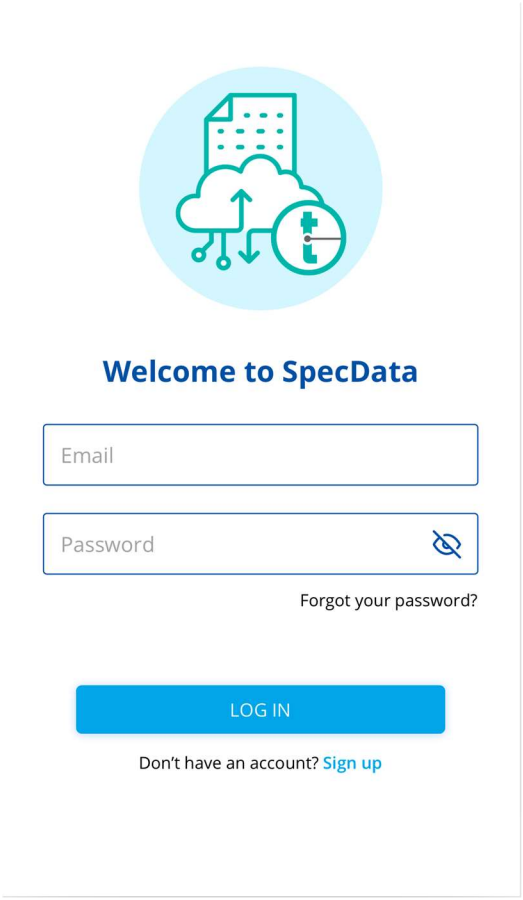
Downloading the app

The app is designed to work on iPhone® and iPad® models that are currently supported by Apple®. The minimum version of iOS® that the app will run on is 10.0. To download the app, please use the official App Store in iOS. You can find it by searching for SpecData.

The app also works on Android™-based devices which support Bluetooth® Low-Energy (BLE or Bluetooth 4). You can download the app from Google Play. You can find it by searching for SpecData. The minimum required version for Android OS is V7.

Logging In

When you launch the app, you are presented with the login screen, but only if you had not logged out last time. Logging out is optional.



If you have an account, enter your email address and password, then simply tap “Log in”. Tap the slashed eyeball icon to display the password.

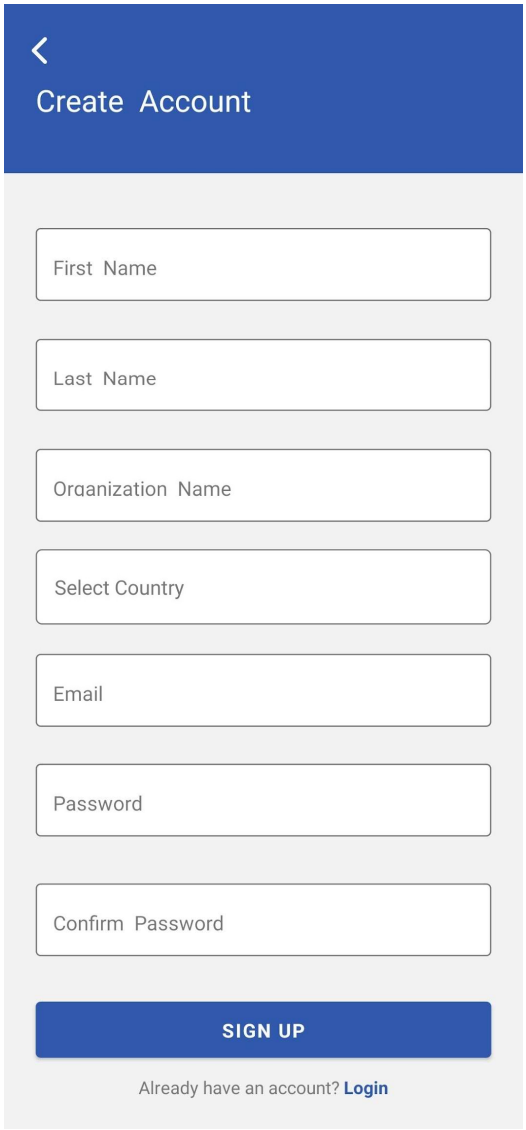
If you do not have an account with Preemie or Enterprise, see the section called “Registering with Us”.

If you have forgotten your password, you can tap the “Forgot your password?” button.

Registering With Us

Using this app requires a subscription; please contact info@tellspec.com. It also requires setting up a *project*, which defines the kinds of samples you intend to scan, and the data you will collect about them. We will work with your administrator to do that.

If you need to register an account with Preemie or Enterprise, on the login screen tap “Sign up”. You will be presented with the registration screen. **NB:** If you have registered in any other Preemie or Enterprise app you can log in with that email and password. You do not need to register again.



Simply fill in the form and tap “Sign up”.

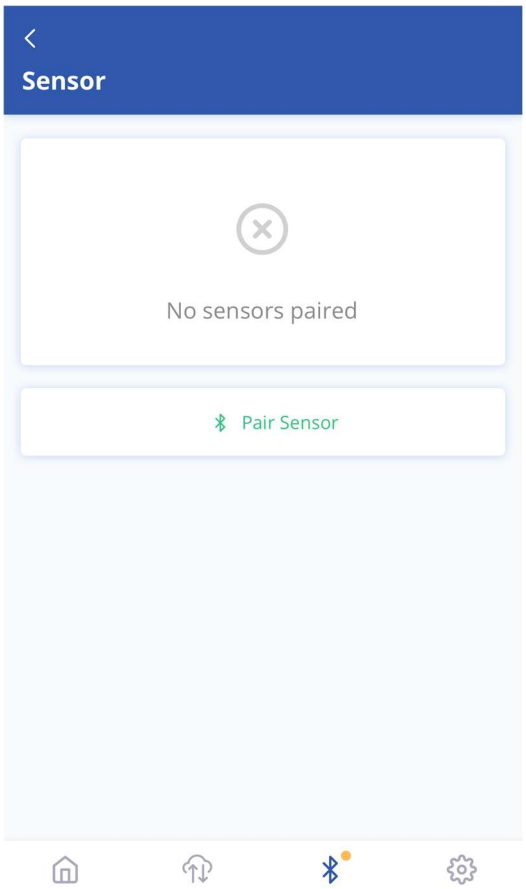
Tip: Users with phones that have a smaller screen, such as the iPhone 4S, can scroll the form up and down as necessary.

Shortly, you will receive an email asking you to verify your email address. Click the link and you are verified and ready to go.

Using the Preemie or Enterprise Sensor

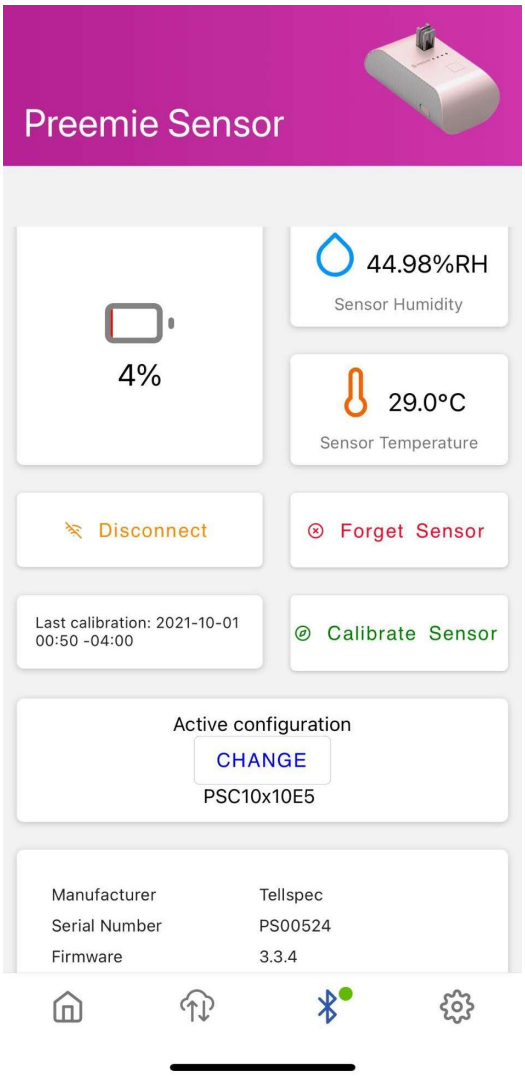
Bluetooth Pairing

When you intend to scan you need to pair your mobile device with your sensor. Tap the button at the bottom of the screen. That will take you to the sensor page. Tap “Pair Sensor”. You will see a list of nearby unconnected sensors’ serial numbers. (There may be only one.) Tap the serial number of your sensor. After downloading some data from the sensor and from the cloud, the sensor will be connected and ready to scan.



If you do not see your sensor, please make sure that you have Bluetooth enabled on your mobile device and in your Preemie or Enterprise sensor. (Refer to the section “Enabling/Disabling Bluetooth”.)

Sensor Information



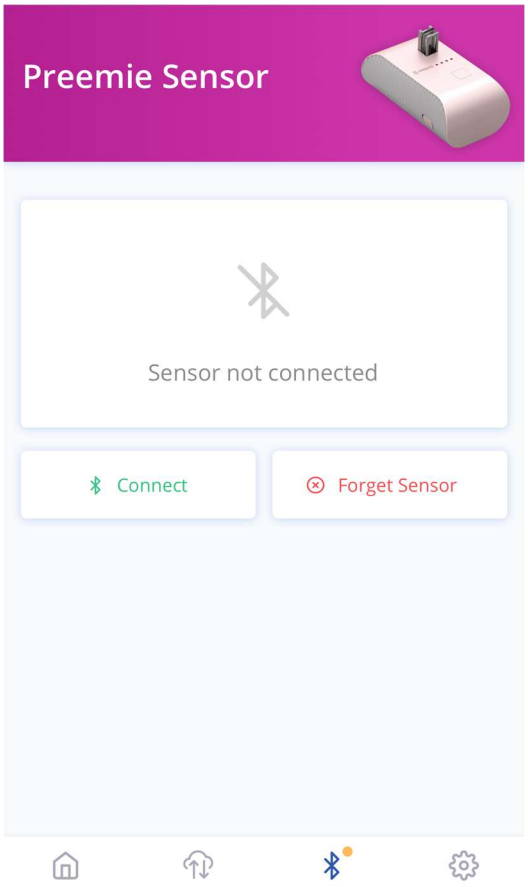
This shows a Preemie Sensor screen. An Enterprise Sensor screen shows the same information, but a different title and image.

When you pair with your sensor, and each time you connect to it, there will be a few seconds' delay while the app loads data from the sensor and the cloud, which it will need when doing scans.

Once you have paired your sensor you can connect immediately. If you tap 'Forget Sensor' then you will have to pair again. You should do this if the sensor needs to be paired with another mobile device.

If you disconnect the sensor, or close the app, your paired sensor will be remembered. You can connect again by tapping 'Connect' on the sensor screen, below. To release the sensor for use on another mobile device, tap 'Forget Sensor'. **NB:** Connection may involve a wait of as much as ten seconds with no activity on screen. If the word 'Connecting' with a "spinner" appears for

more than about five seconds with no other activity on screen, then quit the app and start it again.



Status LEDs

There are four colored LEDs on the top of the sensor.

Color	State	Meaning
Green	Steady	Power is on.
Green	Rapid flashing	Internal hardware check failed.
Blue	Steady	Bluetooth is on and ready to connect.
Blue	Slow flashing	Bluetooth is connected to a mobile device.
Blue	Rapid flashing	There was a Bluetooth communication error.
Orange	Steady	Scan in progress.
Orange	Rapid flashing	Scan error.

Red	Steady	Battery is charging.
Red	Rapid flashing	Battery is very low.
All Lights	Dark	Sensor is switched off, or battery is depleted.

Often, an error can be cleared by turning the sensor off and on again, and reconnecting to it.

Scan Configurations

The process of scanning has a number of parameters which can be varied. A stored set of parameter values is called a configuration. The sensors are shipped with a number of stored configurations, and one active configuration. The variable parameters are:

- The number of scans which are taken and averaged together to make the final result. More scans takes longer, but gives a more accurate spectrum.
- The approximate width, in nanometers of wavelength, of each point in the spectrum. Note that this affects the resolution of the spectrum, but not the number of points in it (which is 256 for all of our configurations). This means that there is some overlap in the wavelength range covered by each point, but the strongest contribution comes from the center of each point's range. A lower value passes less light, which might be a problem for some materials.
- In Preemie Sensors, the exposure time, in milliseconds, of each point in the spectrum. A shorter exposure takes less time, but may produce poorer results for darker or more absorptive materials.
- In Enterprise Sensors, there is column or Hadamard mode. Column scans a contiguous range of wavelengths (of the chosen width) for each point. Hadamard scans a number of nearby ranges, and combines them all in a way that provides more light with little loss of resolution. Very low-absorbance (i.e., bright) materials might do better with column scanning, but usually Hadamard gives better results.

The stored configurations are named with the following conventions:

For Enterprise Sensors the form is TSH20X9, meaning an Enterprise configuration (TS) in Hadamard mode (H), with 20 scans averaged, and each point about 9 nanometers wide.

For Preemie Sensors the form is PSC10X9E2, meaning a Preemie configuration (PS) in column mode (the usual empty-holder calibration does not work in Hadamard mode), with 10 scans averaged, each point about 9 nanometers wide, and exposed for a total of 2 milliseconds.

Changing the Configuration

The sensor screen shows the sensor's currently active configuration. To change it, tap the 'CHANGE' button. This shows a list of the available configurations, with one or more labelled 'Default', meaning that they are recommended for most uses. To change a different configuration scroll it into place and tap the 'CHOOSE' button. Note that changing the

configuration also changes the displayed 'Last calibration' date, and may require a calibration scan to be taken, if the existing one is out of date, or was never done.

Enabling/Disabling Bluetooth®

By default, Bluetooth is enabled when you switch on your sensor. You can confirm this by the blue LED lighting up.

NB: It is not normally necessary to disable Bluetooth on a sensor.

To manually enable/disable your sensor's Bluetooth radio, first make sure the sensor is turned on and charged. You should see the green power LED illuminated.

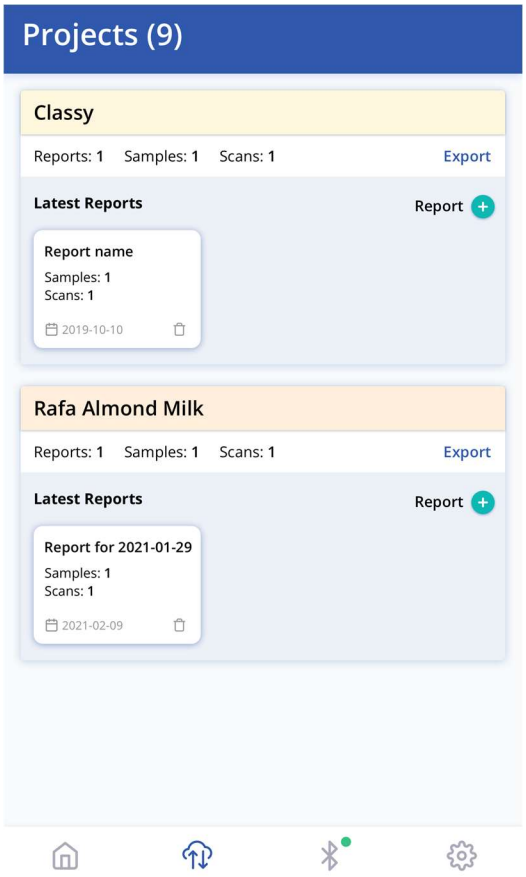
To disable Bluetooth, simply press and hold the scan button on the top of the sensor for five seconds and then release it. The blue LED will now be unilluminated, indicating that Bluetooth is not enabled.

To re-enable Bluetooth, press and hold the scan button on the top of the sensor for five seconds and then release it. The blue LED is now lit, indicating that Bluetooth is enabled again and the sensor is ready for your mobile device to connect. **When your mobile device is connected and paired to your sensor, the blue LED will flash**.

Note: The connection process between the device and the sensor takes about 5-6 seconds every time you connect. If the device does not reconnect, restart your device, then restart the app.

Home Screen

The home screen is the start of the app. It looks like this:



This screen shows two projects, each with one report.

You can work with existing reports or create new ones. You can not create or remove projects; that is done by the administrator. See 'Using the desktop SpecData app', below.

The Export button under each project title lets you export data from its reports. See Exporting Data, below.

The buttons at the bottom take you to various parts of the app:

Home. Shows information about the projects you are working on, and lets you choose one to work on now.

Testing of chemometric and machine learning models hosted or created in SpecAI, on new samples not used to build the models. See Testing models from SpecAI, below.

Sensor. Let's you connect to a Preemie or Enterprise Sensor, and displays information about it. The color of the dot indicates the sensor's state: Green for connected; Yellow for paired but not connected; Red for not paired. See Sensor Information, above.

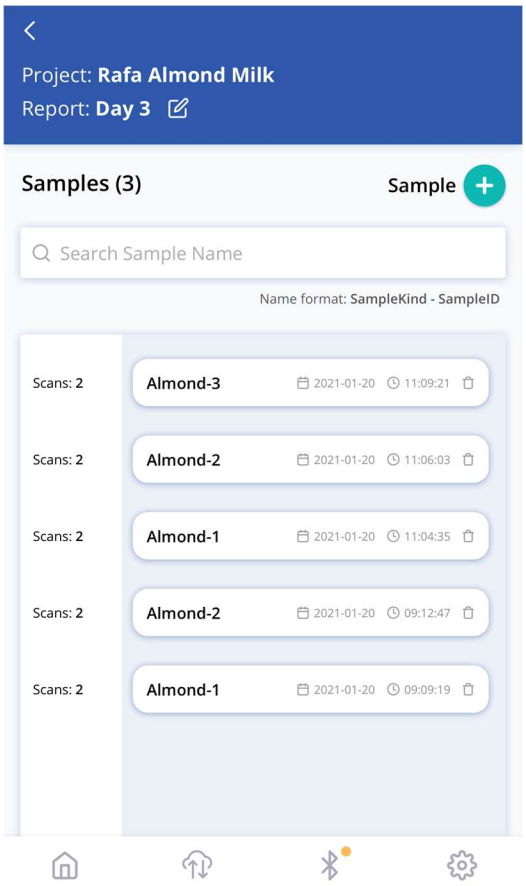
Settings. Let's you change various things about the operation of the app and about yourself. See Settings, below.

Reports

A report is a collection of scans of one or more samples, collected under a *project*. Below you see a report containing three different samples, scanned on five different occasions or *sessions*. The report name may be edited by tapping on the pencil icon. A scanning session may be deleted by tapping on its trash can icon.

The home screen shows the projects(s) you can work on, and any reports in them, starting with the most recent. You can work on an existing report by tapping its button in the list of reports (which you can scroll to the left as needed). You can start a new report by tapping on the button in its project's area.

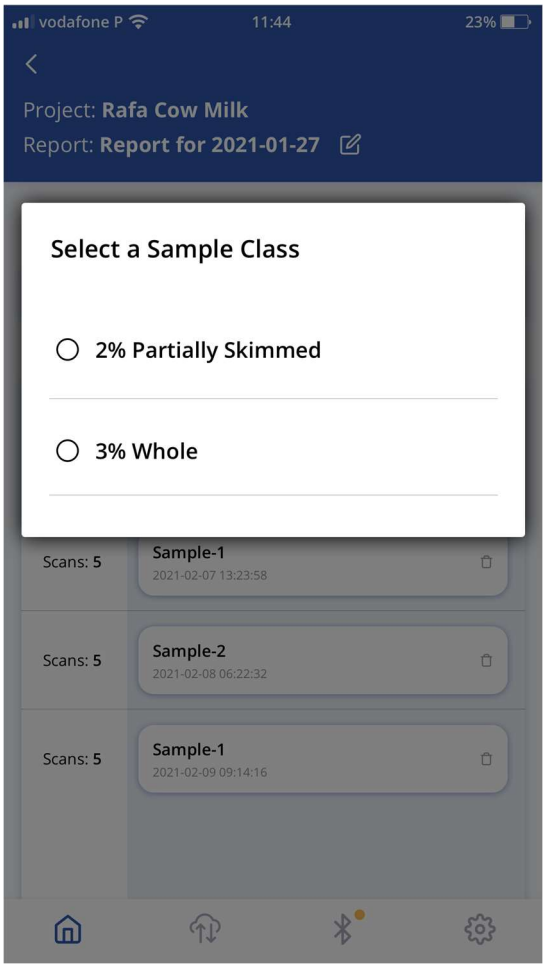
For an existing report, the next screen shows the scanning that has been done. If no scanning has been done then there will be no scans, but you can start by tapping the Sample button.



You should edit the automatically-assigned name of the report (Day 3 in this example) by tapping the pencil icon beside it, otherwise all of your reports will have the same name. A report is a collection of scans of samples. Each sample may be scanned many times. To add to the scans of an existing sample, tap its button, e.g. Almond-2 of 2021-01-20 11:06:03 in this example. The date and time are when that sample was created. The same sample may be scanned at different times, making different sessions. **NB:** In order to make this clear you must edit the sample names to be the same. The sessions will be distinguished by having different timestamps.

The list can get long. The search function can be used to show only a particular sample kind or sample ID, or both.

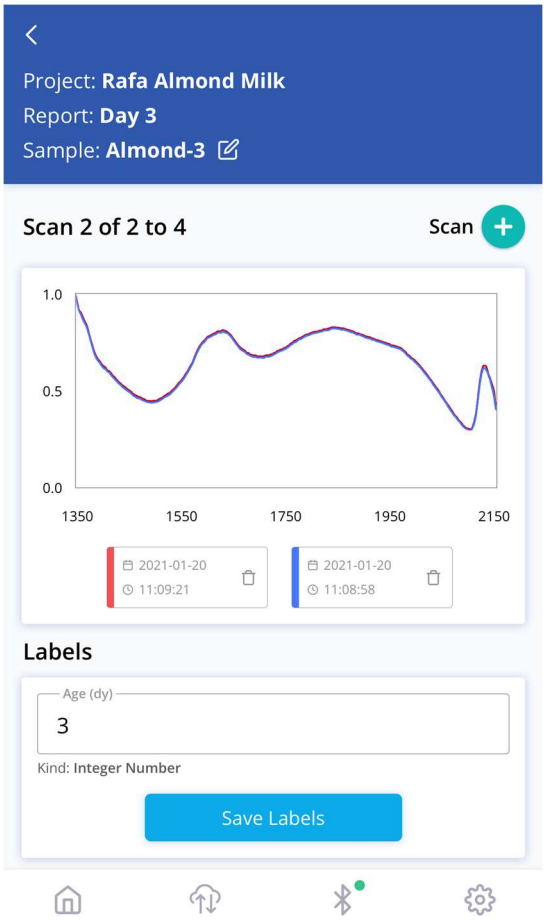
When you tap the Sample button you will see a dialog like the one below, which lets you choose what kind of sample you will scan. If the project has only one kind, then this step is skipped. The new sample will get an ID which is the next number in the sequence of existing IDs for that project.



Scanning

To scan with your sensor, first switch on the sensor and if necessary, enable Bluetooth. If you need help with this, please see "Turning your Preemie Sensor on and off" or "Turning your

Enterprise Sensor on and off" and the section titled "Enabling/Disabling Bluetooth".



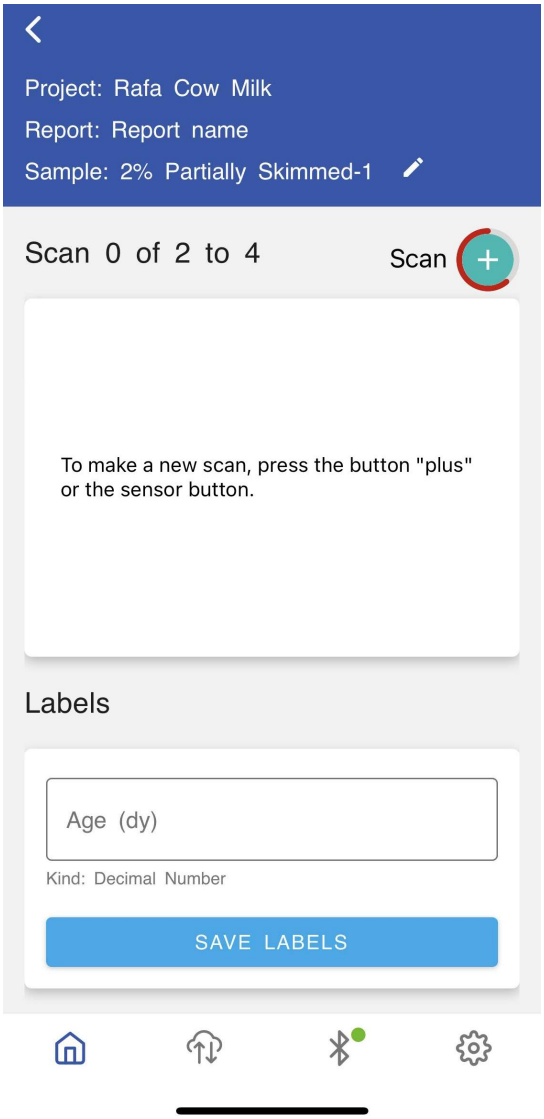
Load a sample into a clean empty cuvette, insert it into the sensor, then click the button on top of the sensor for one short press, or tap on the screen.

Sensor Warmup

The sensor needs to be warmed up for use. If it has been too long since the last warmup was done, another will be done in place of a new scan. After the warmup, you may proceed to take a sample scan. The countdown to the next warmup is indicated by the red circle around the button. When it is gone then a warmup will be done when you tap the button. **NB:** A warmup cycle does not perform a sample scan. **No sample should be in place during the warmup.**

The approach of a warmup cycle is shown by a red circle around the button. The circle gets smaller over time, and when it is gone, the next tap of the button or click of the sensor button will start a warmup cycle rather than a normal scan. Don't put a sample into place until the warmup has finished.

Note that warmups can be turned off with the "Periodic Warmup" option in the settings screen.



Sample Scan

After a warmup, if any, put your sample into place and tap or press the button on the sensor.

You will see the orange scanning light go on, and go off again after a few seconds. Several boxes will appear in the app showing the progress of the scanning process. When the scan has finished the screen shows the spectrum, along with its date and time. This spectrum is for visual confirmation of a good scan, and is not suitable for analysis.

You can add more scans of the sample, or you can tap the back button or any of the buttons at the bottom. Your scans and other data are saved automatically in your mobile device and in the cloud, where it is available to others working in the same project.

You can delete a scan by tapping its trash icon. You can also toggle a scan's presence in the plot by tapping its timestamp.

Labels

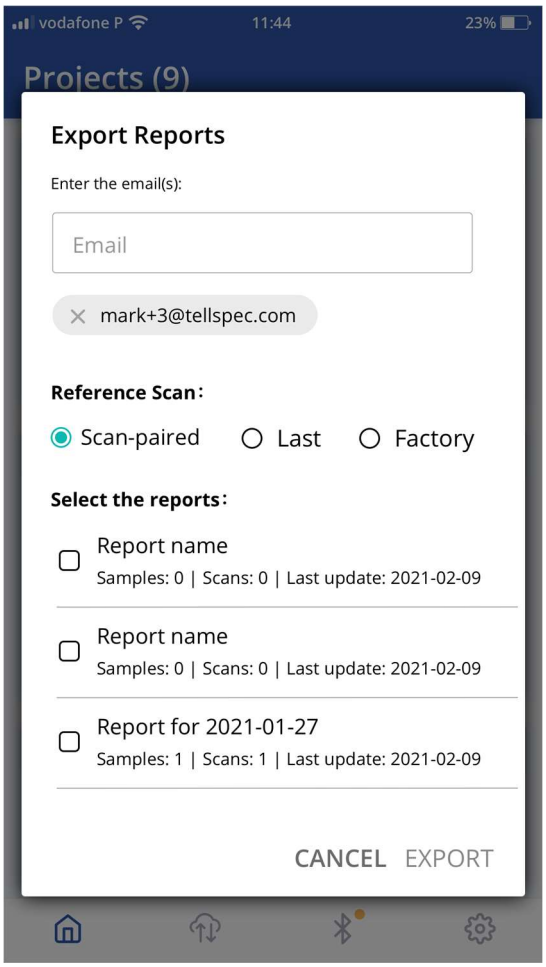
Data associated with this sample at this time is called “Labels”. There may be many labels, and they can be numerical, textual, or a choice of values. What labels exist is part of the project definition, as set by the administrator. Different sample kinds may have different sets of labels.

In the screen above there is just one label, a number called Age.

The label data may be added or edited at any time, before, during, or after scanning. Often it is added later when laboratory test results are available. The label data is stored in your mobile device and in the cloud, where it is available to others working in the same project.

Exporting Data

You can export spectral and label data for one or more reports in a project.



That screenshot shows no reports selected to be exported, yet. More than one report may be exported at once.

The emails which the report will be sent to appear below the email entry field. You can add

more emails by typing them into that field (one at a time), and you can delete emails by tapping them. The list of emails scrolls horizontally.

The reference (a.k.a. calibration) scan to be used to calculate the absorbance spectrum may be:

- 'Scan-paired' to use the last reference taken before each sample scan.
- 'Last' to use the most recent reference scan for the sensor.
- 'Factory' to use the reference scan taken at the time the sensor was manufactured.

This is (a part of) an export file:

	A	B	C	D	E	F	G	H	I	J	K
1	sample_name	sample_class	session_id	session	session_date_utc	scan	brix	scanner serial	scan configuration	900.682356944	904.639323881
2	Orange-3	orange	Orange-3:1	1	2021/02/09 11:39:08	1	12	TS10073	TSH20X9	0.5454005432	0.5464069204
3	Apple-2	apple	Apple-2:1	1	2021/02/09 11:36:04	1	13.2	TS10073	TSH20X9	0.6231688251	0.6265369471
4	Pear-1	pear	Pear-1:1	1	2021/02/09 11:35:02	1	15.3	TS10073	TSH20X9	1.8476182121	1.8316029311

Column E is the time the first scan of the sample was done, in UTC. In this case there was only one scan. Column G is label data for that row. In this project there was only one label, with the ID "brix". Columns H and I hold information about the sensor, and the rest are the scan data. The top row is wavelengths, in nanometres. The labelled rows under them are the spectrum in absorbance units.

If a report was created with a mix of sensors, then a wavelength row will be present for each spectrum row, because different sensors even of one type have slightly different wavelengths.

About exported data:

- It includes the saved label data for each scan.
- The scans are in absorbance units rather than raw intensity. Intensity spectra vary from one sensor to the next, and absorbance removes that variation.
- Each project has a list of default recipients of the export email. You can add or remove emails in that list for each export.
- You are given a choice of what reference scan to use to calculate the absorbance units:
    - "Paired" references are the last one taken before the sample scan. This allows a protocol where each sample scan is immediately preceded by a reference scan.
    - The "last" one is the most recently-taken scan stored in the cloud. If you have not taken your own reference then that will be the one which was stored in the cloud while preparing the sensor for shipping. This is normally what you should use.
    - The "factory" one was stored in the sensor's memory after manufacture. You could use this one if you suspect that there is a problem with the "last reference".

In addition to the spectral data in absorbance units this file includes the label data which was entered in the app or in the web application. The column called 'session_id' is a combination of 'sample_kind' and 'session'. It is provided for the convenience of scripts, which can use a single

string to select and group session data from a database. Session numbers are not currently implemented. They are there for backward compatibility with earlier apps.

Scanning Procedures

It is important to define and maintain consistency from day to day and lab to lab, when scanning. At the same time, one must keep in mind how the sensor will be operated by end users, especially in applications where it will be used by untrained personnel.

It's also important to consider the parameter (label) that you are analysing and treat it carefully, so that you can get better results. For example, if you are scanning a sample for its freshness, it's important to scan a fresh sample, to store it correctly before the scan and ensure consistency across different days. Temperature plays a crucial role in the acquired spectrum and needs to be kept constant in every scan. Small temperature variations (up to 5°C) won't negatively impact the collected spectrum.

The Preemie and Enterprise sensors are different in actual use. They are described in later chapters of this manual:

Using the Preemie Sensor

Using the Enterprise Sensor

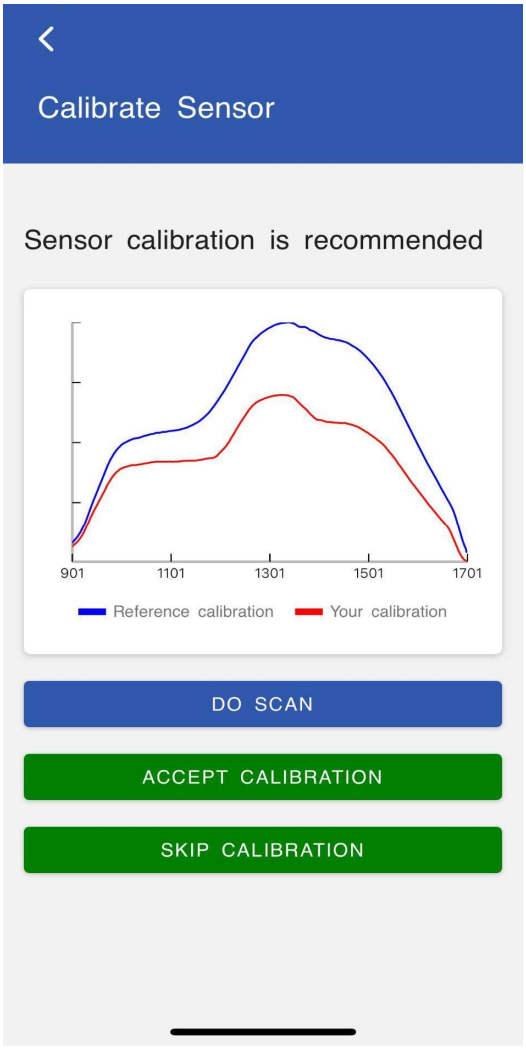
Reference (a.k.a. Calibration) Scans

A reference scan is used when exporting a report, to calculate absorbance values from the raw intensity data obtained from the sensor. The sensor comes with a reference scan built in at the factory, and also one stored in the cloud, which was taken when the sensor was prepared for shipment.

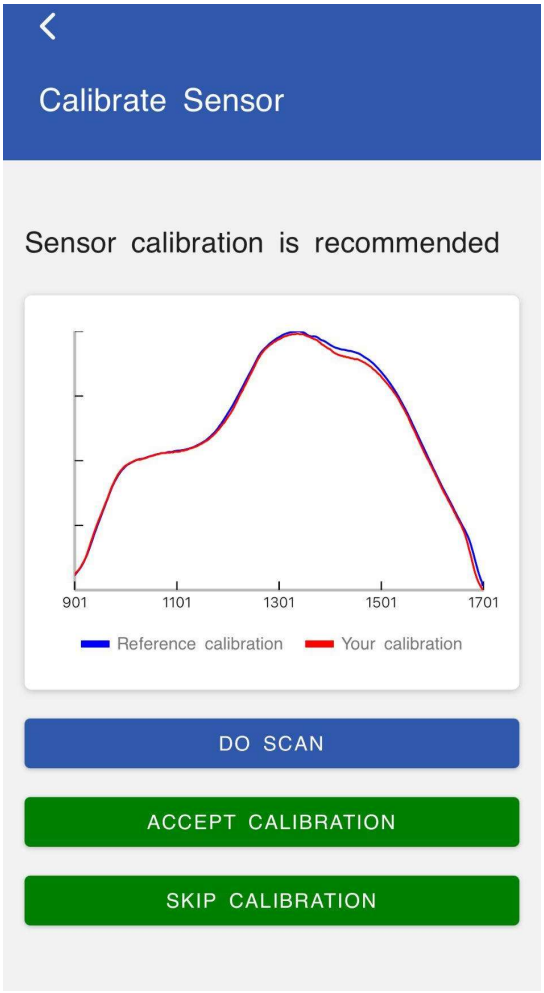
Each scan configuration has its own reference scan stored in the cloud. When the sensor is shipped only the active configuration's reference is present. If you change the configuration you will need to take a new reference scan.

If you wish to take periodic reference scans yourself:

1. Connect to the sensor.
2. Prepare the sensor, as described below for the Preemie Sensor or the Enterprise Sensor.
3. Tap the 'Calibrate Sensor' button on the sensor screen.
4. On the next screen, click the sensor's scan button, or tap the 'Do scan' button on the screen.
5. The screen will show the new reference spectrum with the built-in reference spectrum overlaid.
    a. If the two are similar in shape, then tap the 'Accept Reference' button. It is normal for them to be at slightly different levels.
    b. If the two are too different then tap 'Do Scan' and the app will scan again.
    c. To skip this reference and continue to use the previous reference tap the 'SKIP CALIBRATION' button.



An unacceptable reference scan.



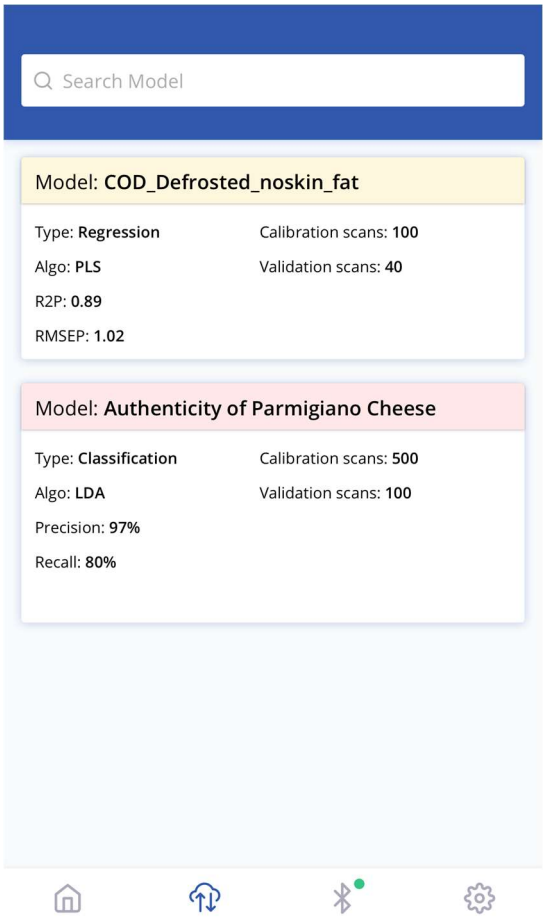
An acceptable reference scan.

If you choose a scan configuration which does not have a stored calibration then you will be presented with the calibration screen saying 'Sensor calibration is required', and with the 'SKIP CALIBRATION' button inactive. You must calibrate the sensor before you can take scans, or use the back button to return to the sensor screen and choose a different calibration.

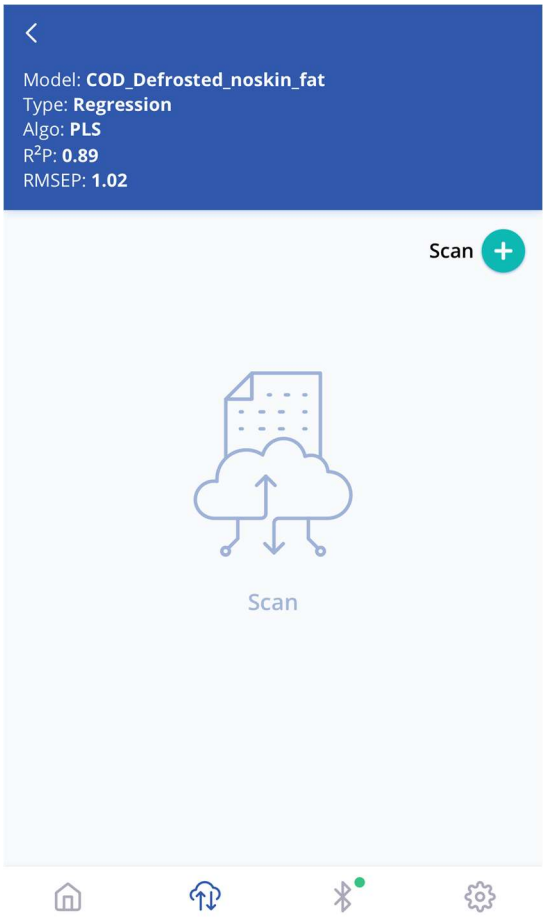
Testing Models from SpecAI

Tellspec's SpecAI system makes it possible to create machine learning models from data collected with the SpecData mobile app. Such models can be tested in the mobile app on new scans which were not used in the models' creation.

On any other screen, tap the SpecAI icon at the bottom of the screen. The next screen will be a list of models available for testing:



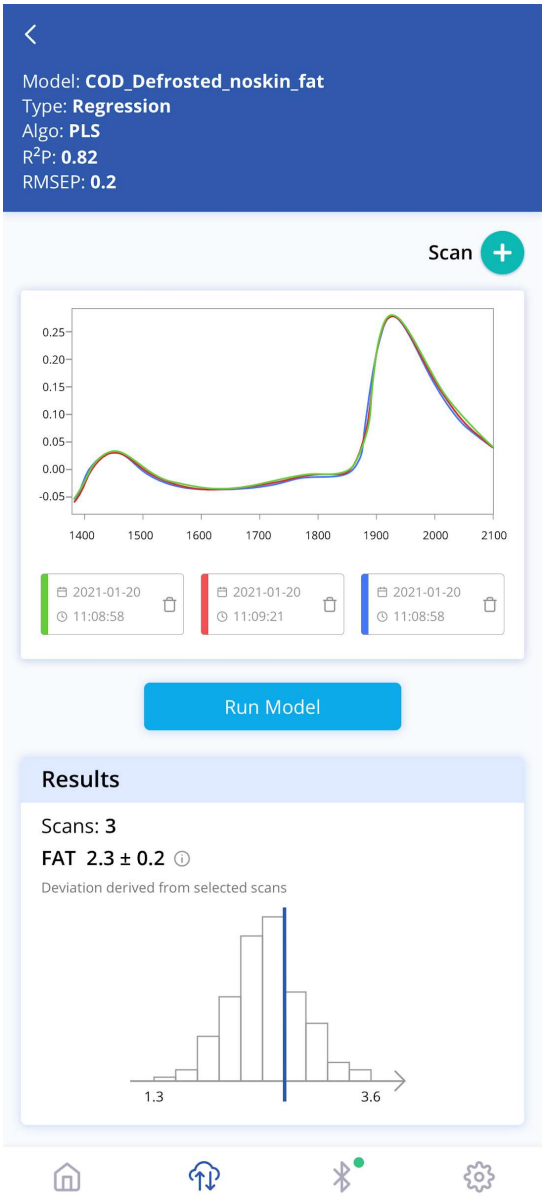
Tap the model that you wish to use to start scanning and testing.



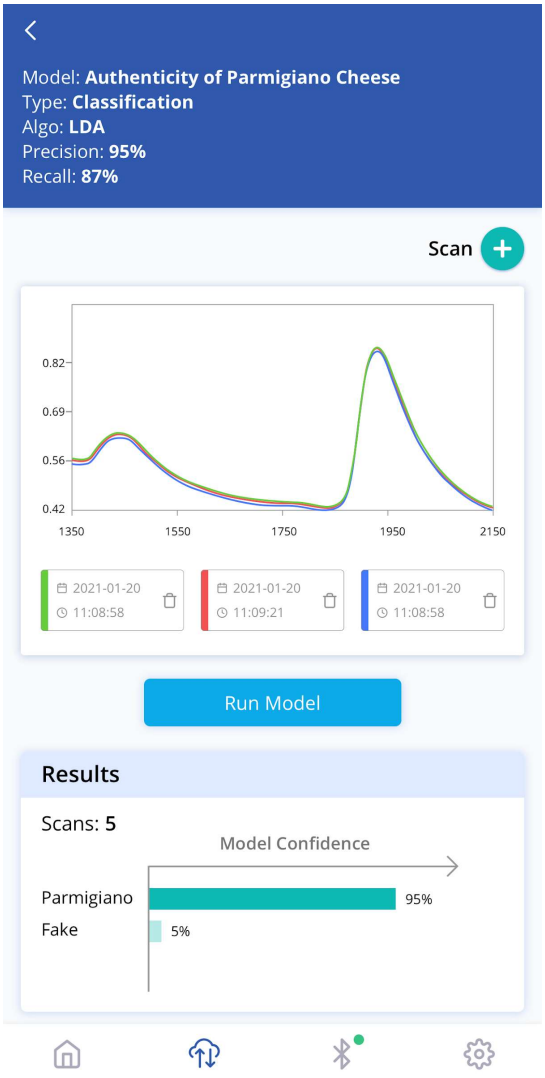
Ready to take the first test scan

The next two examples show models which are available for testing, of two types (regression and classification) with results from test scans.

Take a number of scans and tap the “Run Model” button. The average of their results is shown, numerically and also plotted on a histogram of the number of training data scans used:



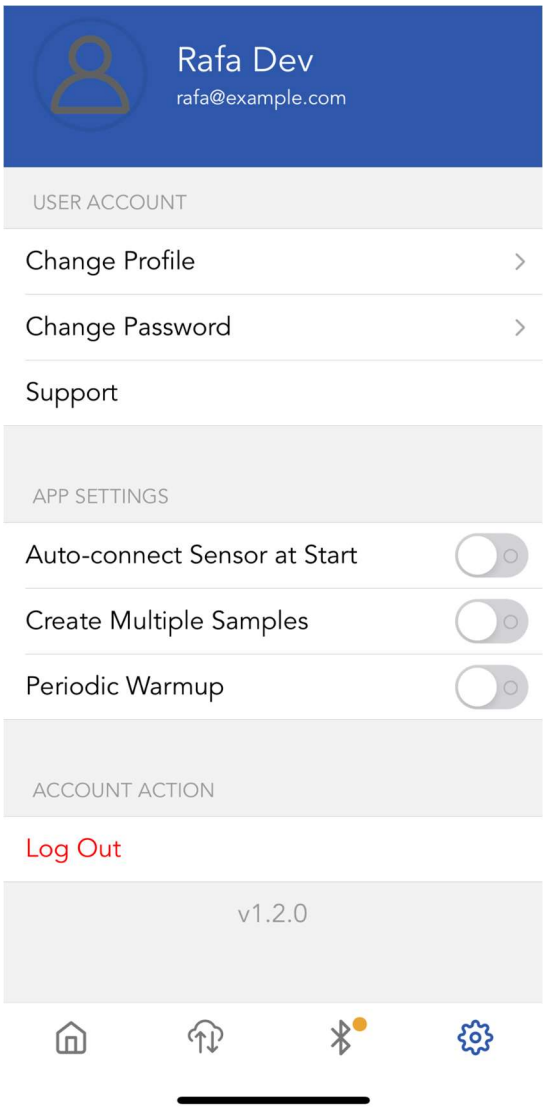
A regression model.



A classification model.

Settings

You can change information about yourself or about the use of the sensor here:



"Auto-connect Sensor at Start" means that when you launch the app it will immediately connect to the paired sensor, if any. If the sensor is not available or not needed, you can cancel the operation.

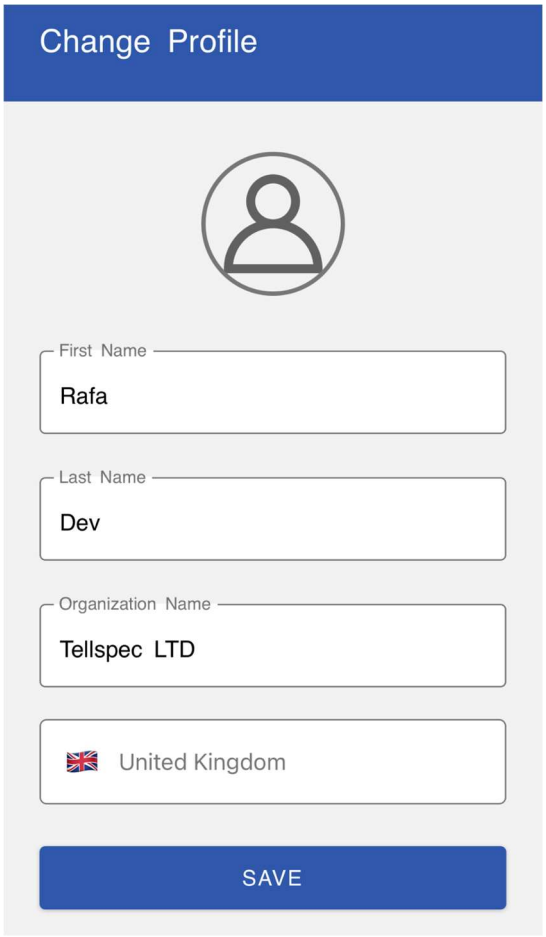
With "Create Multiple Samples" you will be asked how many samples to create at once when you tap the "Sample" button on a report screen.

"Periodic Warmup" means that when the sensor has not been used for a while, it will perform a warmup scan, rather than a sample scan, the next time a scan is done. See Sensor Warmup.

You can log out of the app here, but that is optional. You'll need to log out if someone else is going to use the app.

"Support" links you to Tellspec/Preemie personnel for help.

You can change your profile data here:



You can change your photo, name, organization, and country. You can't change your email address, which is used to log into the app.

Chapter 2: The SpecData Desktop App

Using the desktop SpecData app

Overview

Data collection is the process of scanning samples of a material for their spectrum, and collecting various parameters about the samples. The purpose is to use that data to create chemometric or machine learning models to predict the parameters' values for new samples of the same material.

Data collection happens in a *project*. A project has a name, information about the data to be collected, and about who is allowed to work on it. Many users will see only one project.

A project has *sample classes (or kinds)*, for example fish species. Every *sample* that will be scanned belongs to a class, which is the first choice a user makes when starting to work with a sample. Some projects may have only one or two sample classes.

Samples also have *intrinsic data*, which is inherent to the sample, rather than being measured in some way. In the case of fish that includes things like whether it is fresh, frozen, or defrosted. Not every project involves intrinsic data.

In addition to intrinsic data there is *external data*, things which are measured. There will usually be at least one. Data has a *data type*, and when users are scanning a sample, they may fill in the data in the app, but that can also be done later.

Samples get default names, with the class name and a serial number. The serial number may be edited by the user. The name may also include a team name, if teams are defined in the project. Sample scans are collected into *sessions*, and each session has associated parameter values, which apply to all the scans in the session. A sample may be scanned in multiple sessions, e.g. over days as it ages.

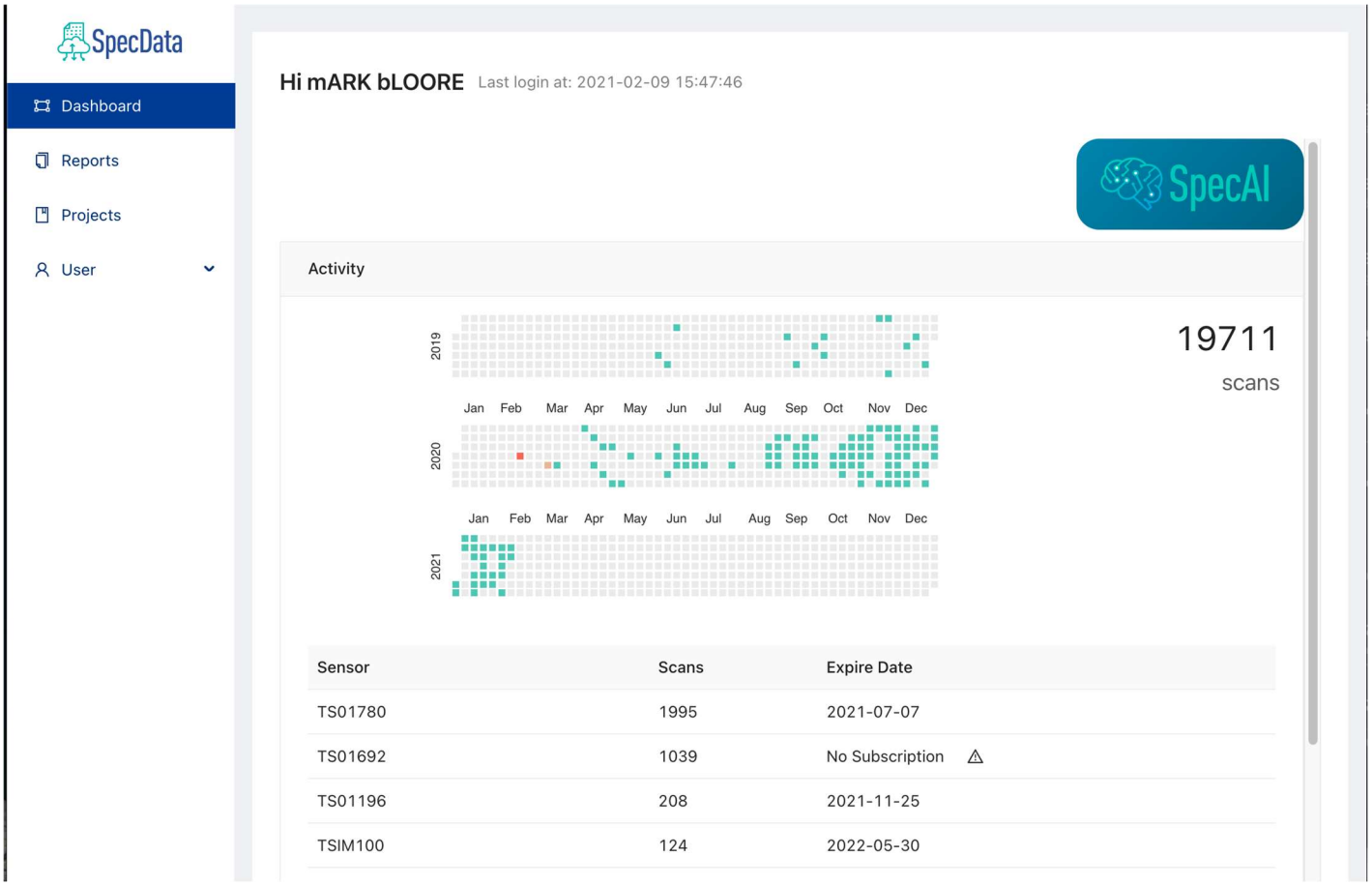
Each sample may be scanned a number of times in a session, and both a minimum and a maximum may be set for that number in the project definition. It is possible to create sessions ahead of time, to be scanned and have data added later. That can be handy to pre-define a scanning plan. The data can be added much later, e.g. when lab results come back.

Scanning sessions are collected together into *reports*. Some or all of the sessions may be chosen for export, which emails a CSV file of the sample info and data, along with the corresponding spectra, to the user. This may be used to create chemometric or machine learning models of the samples. Reports may also be imported directly into the SpecAI app for machine learning model creation.

Access

The SpecData desktop app is not downloaded. It may be reached at https://demo.tellspec.com/specdata/dashboard

Dashboard

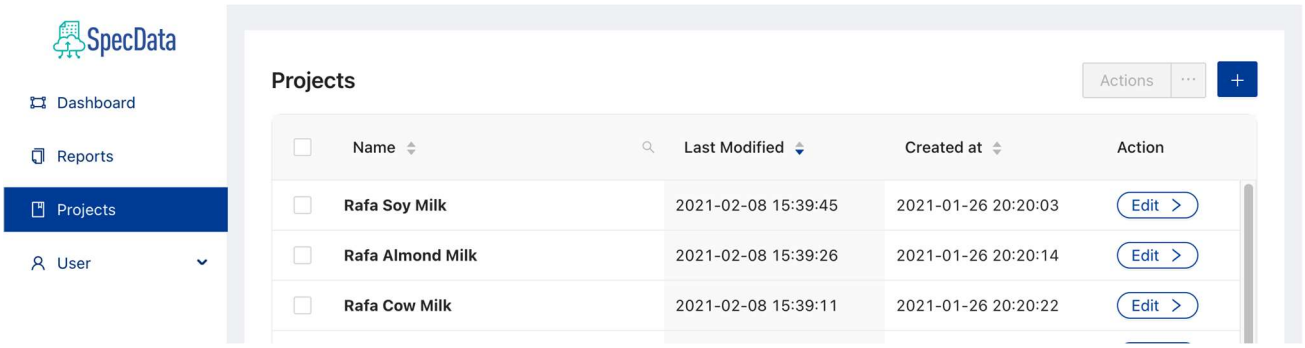


Upon login the dashboard appears. It shows some data about system activity, overall and per sensor. The expiration date refers to the subscription to the SpecData system associated with the particular sensor.

The SpecAI button takes you to that framework. It is separate from the SpecData system, but can interact with it through exported data and model testing.

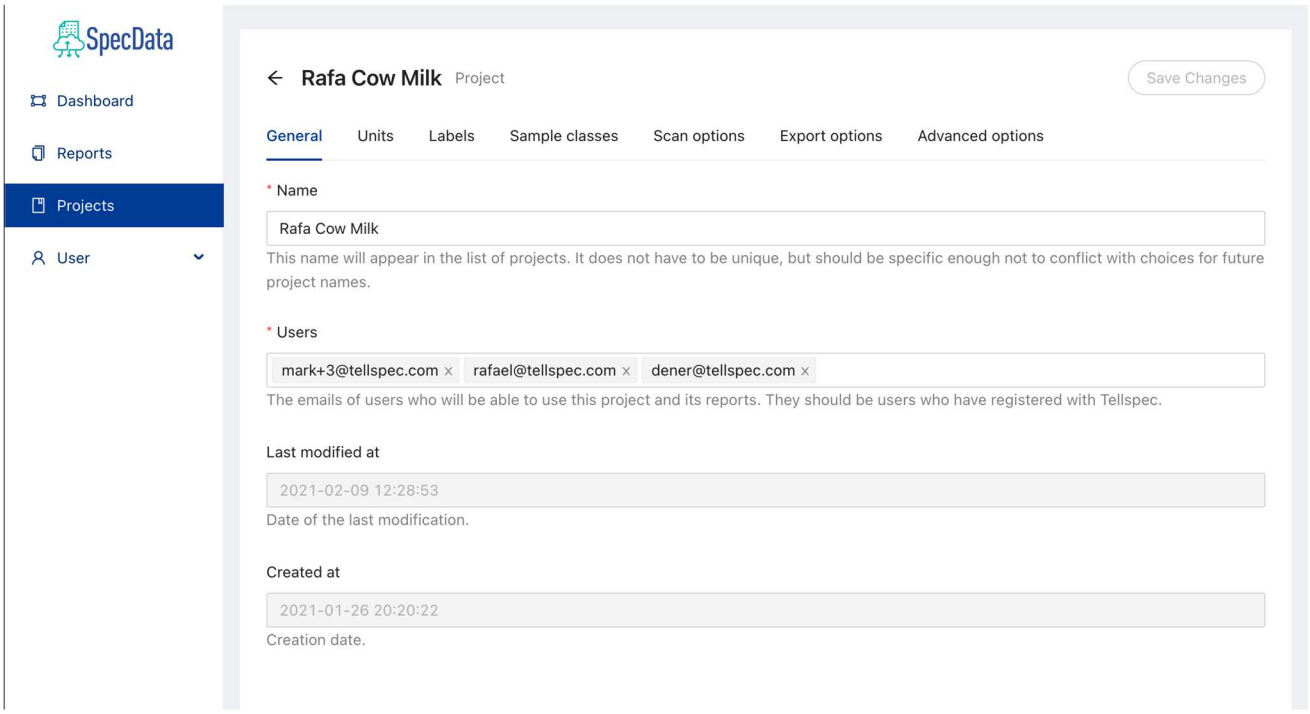
Projects Page

In the 'Projects' page of the Data Management app click the '+' icon in the top-right corner. You will be asked for a name, which must be unique, and then the project will appear in the list of projects. Click the 'Edit >' button at the right-hand edge of the page, and fill in the required information in a series of tabs.



Click 'Edit >' by Rafa Cow Milk:

General Tab



Go back to the list of projects by clicking the leftward arrow beside the project name.

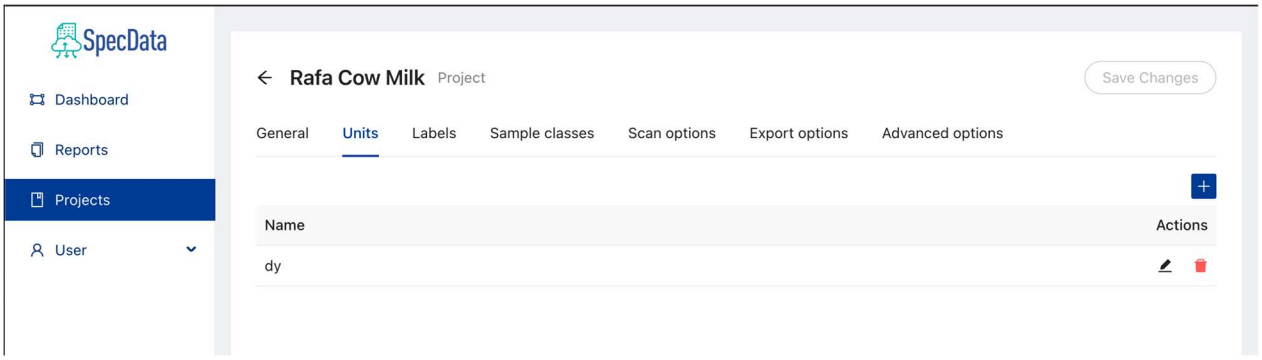
Name

To avoid confusion, each project must be given a name which is unique among all the projects which any of their users have access to. This is enforced by the system.

Users

Email addresses of users who may access the project. They should have registered with Tellspec, or be planning to do so. They must log in with that email. To add an email, click in the field and type it. End by hitting 'return'.

Units Tab

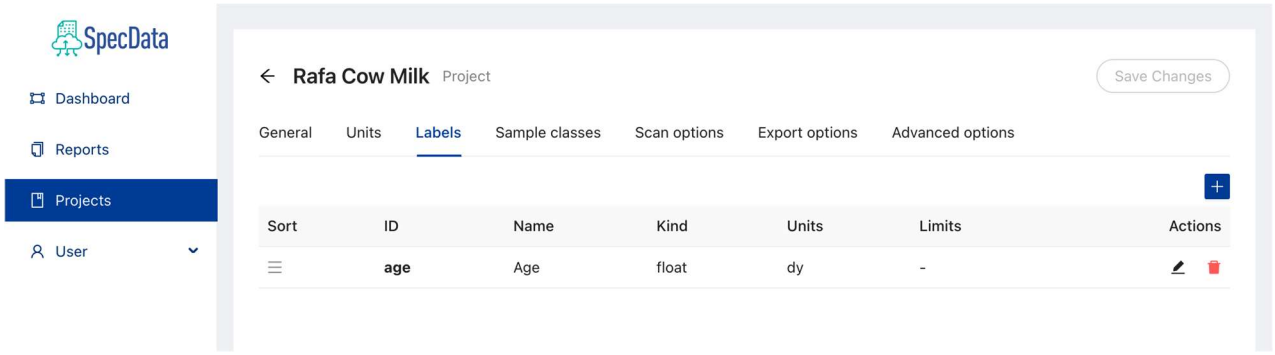


Numeric (Float and Integer) data types may have units of measurement, e.g. grams with a name of “g”. The units name appears in data entry screens, eg “Sample mass (g)”. The units have no other significance. In particular, the system does not do units conversions.

To add a units entry, click the ‘+’ icon in the top-right corner. Then fill in the name, which appears in the mobile app as mentioned above. It does not appear in exported data files, only the data type ID is there.

At the right-hand edge of the screen the pencil icon lets you edit the units entry, and the trashcan icon deletes it. Changes and deletions become permanent when you click the ‘Save Changes’ button at the top-right corner of the screen. If you go back to the main screen (left-arrow at top left of the screen) without saving you will be told that changes will be lost. Click OK to not save the changes, i.e. undo whatever was done.

Labels Tab



This shows a list of the labels which are used in the project. Each corresponds to a parameter about a sample which users of the SpecData mobile app will enter values for when preparing to scan or later, e.g. after receiving lab results for the sample.

At the right-hand edge of the screen the pencil icon lets you edit the label entry, and the trashcan icon deletes it. Changes and deletions become permanent when you click the ‘Save Changes’ button at the top-right corner of the screen. If you go back to the main screen (left-arrow at top left of the screen) without saving you will be told that changes will be lost. Click OK to not save the changes, i.e. undo whatever was done.

When creating or editing a label, a dialog with the following fields appears:

ID

Each label must be given an ID which is unique within the project. This is enforced by the system. That ID appears in exported data as a column header.

Name

A label's name appears in the data-entry screen of the mobile app, along with the units if it is a numeric type. The name does not have to be unique, though duplicates could be confusing to users of the mobile app.

Kind

A label has a *kind*, saying what sort of data it is. The available kinds are

- Float A number with a decimal point.
- Integer A whole number, with no fractional part.
- Classification A choice among predefined values. They are given by the limits.
- Text Free text to be entered by the user. Often used to add notes.

Units

A pop-up menu of the IDs of the units defined in the project. A label does not have to have units. Only numeric types have units.

Limits

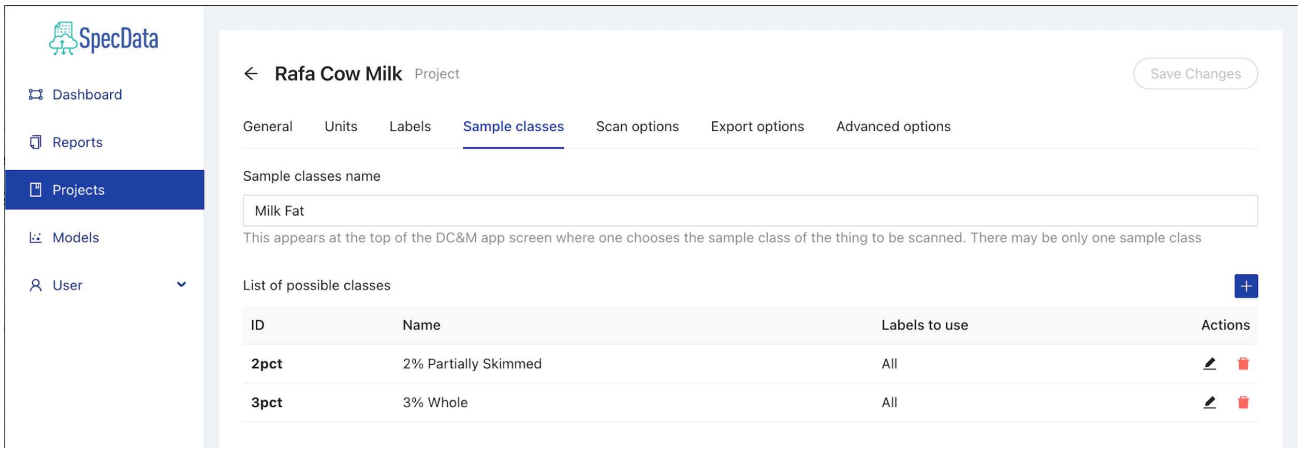
In the dialog, the appropriate data entry for the kind of the label appears. They are not labelled 'Limits' there, but that is the column name in the label list.

Numeric (Float and Integer) labels may have maximum and minimum allowed values. This is to reduce data-entry errors.

Classification types have a list of values which the user may choose among when entering data. The user is not forced to choose one. The values have ID and Name: the ID appears in exported data; the Name appears in the mobile app data-entry pages.

Text datatypes have no limits.

Sample Classes Tab



Samples may belong to different *classes*. This example uses the fat concentrations as class names. The 'Sample classes name' describes the classes as a group. That appears in the mobile app as a header on the screen where the user chooses the sample class.

It is not necessary for a project to define any classes, in which case the mobile app skips the step of choosing a class.

ID

Each sample class must be given an ID which is unique among the classes. This is enforced by the system. That ID appears in exported data in the 'sample_class' column.

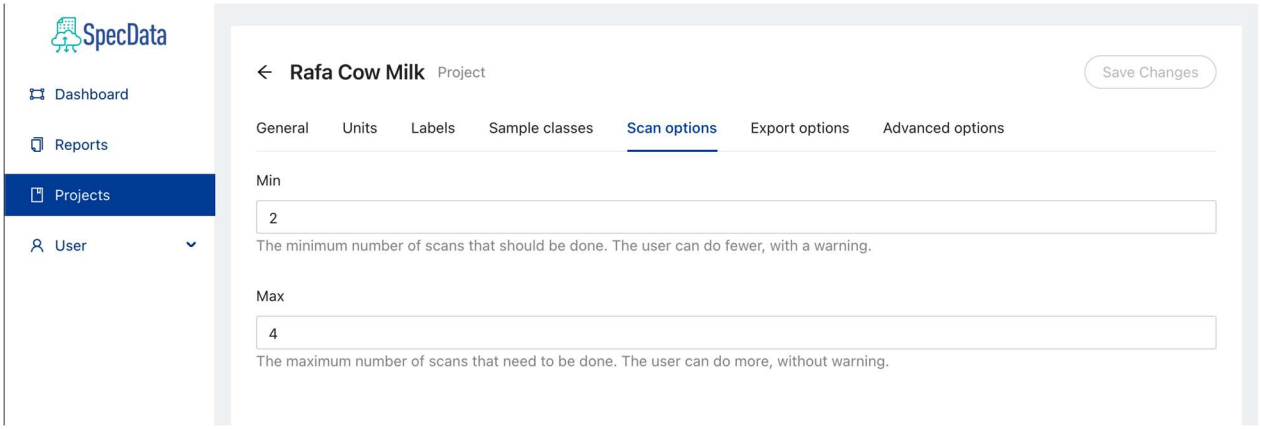
Name

A sample class's name appears in the mobile app when a user starts to scan a new sample.

Labels to use

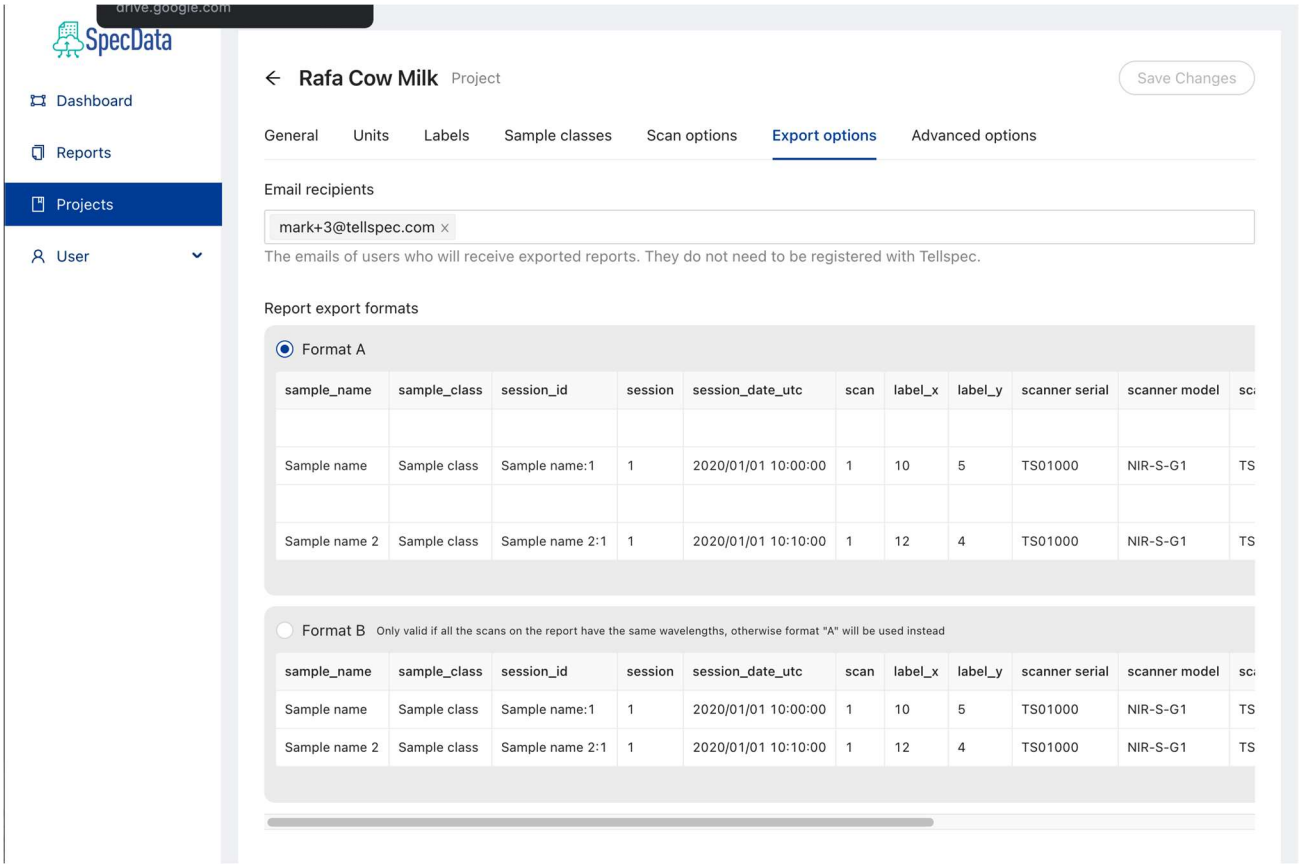
By default, a class presents all of the project's labels in the mobile app data-entry screen. By turning off this option, one may choose which labels are shown. (All of them will still appear in exported data, but without values.) When choosing a subset of labels, they can be moved between 'Selected', which is the set which will be used, and 'Available', which is those which exist but are not selected. **Note** that even if all are selected, if a label is later added to the project, it will not be added to that sample class's selected set.

Scan Options Tab



The user may be directed to do a minimum and/or a maximum number of scans in a session. The user is notified if the limits are exceeded, but may proceed regardless.

Export Options Tab

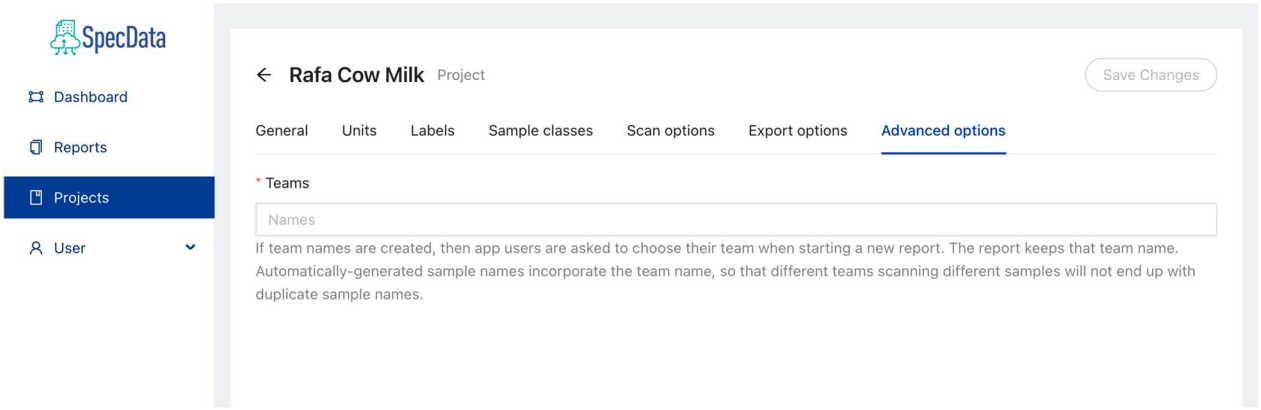


There is a list of email addresses of users who will receive exported data files. They need not be registered with Tellspec or Preemie. To add an email, click in the field and type it. End by hitting ‘return’.

The export file format A is good for reports that mix different sensors, which have slightly different wavelengths. It is also good for importing to software that needs wavelengths on every spectrum. Format B is good for reports done with a single sensor.

The format selected here will be the default in the mobile app, but can be changed when exporting reports. The emails to export to can also be changed there.

Advanced Options Tab

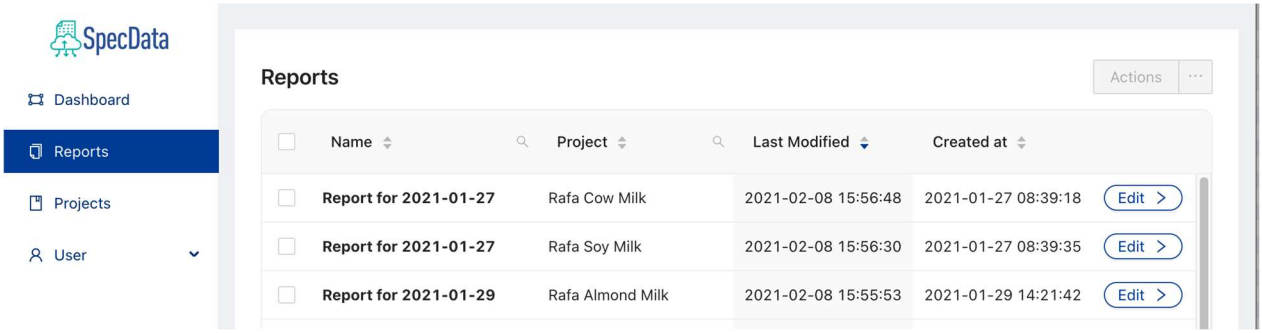


A project may optionally define *teams*, as a list of names. When a user adds a sample to a report it is given a default name, consisting of the sample class name and a serial number. Team names, if defined for the project, are added to that default, to prevent different users, working independently, from creating the same default name for different samples. Users choose their team when they start a new report, and that name remains attached to that report. Users will need to coordinate their choice of team, but they don’t have to always use the same team.

To add a team name, click in the field and type. End by hitting ‘return’ (or whatever your keyboard calls that key).

Reports Page

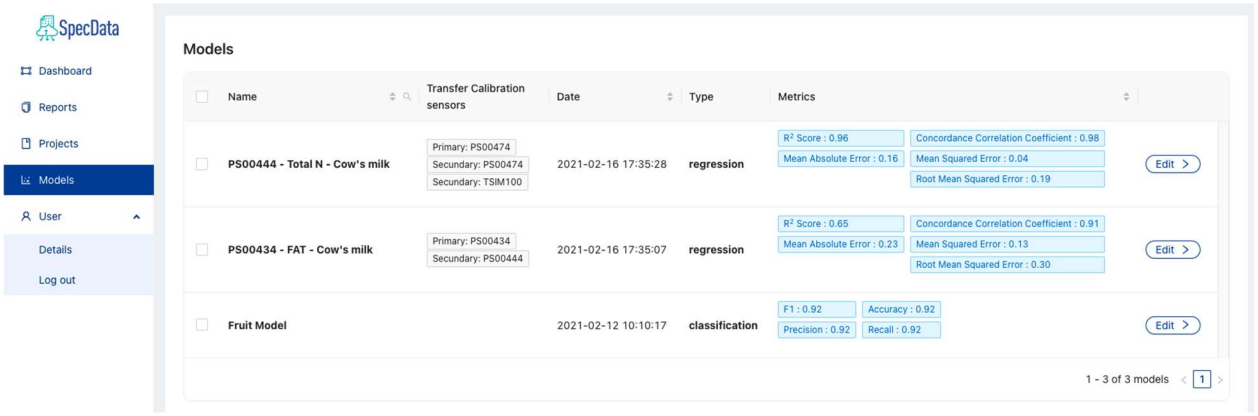
All scans belong to a report, and the user chooses the report to work in before starting to scan. A report actually contains scanning sessions, each with sample parameter values and some number of scans for a particular sample.



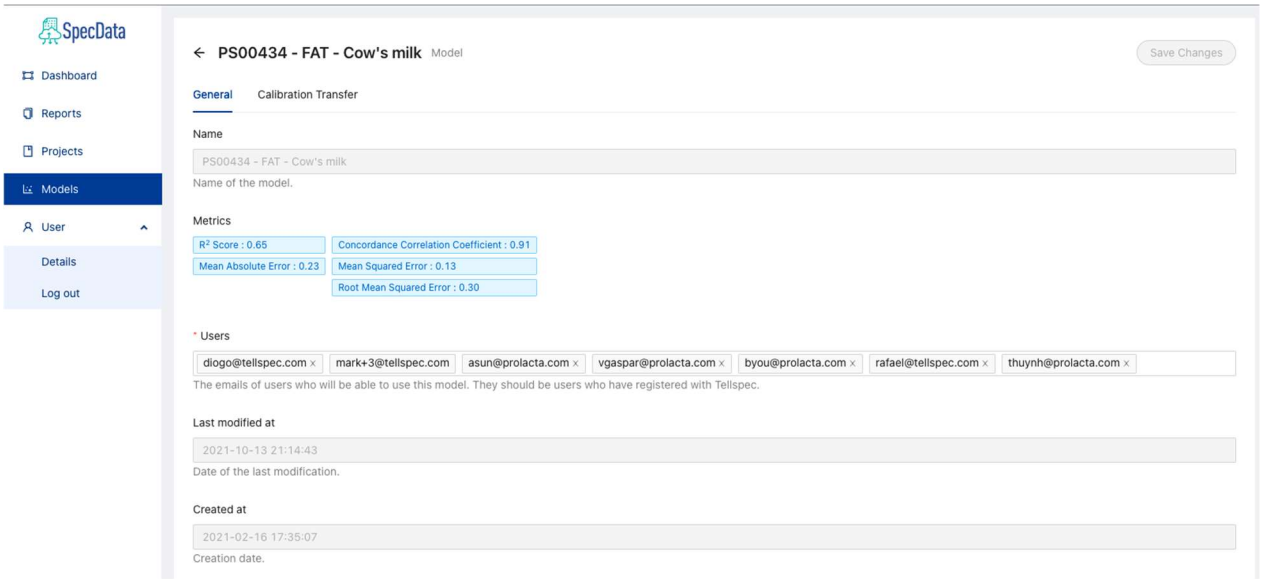
The Reports page of the Data Management app lists all the reports which you have access to. Clicking 'Edit' for one of them shows the report's name, which can be edited, and its project, which can't. The 'Data' tab of that page shows a spreadsheet-like interface in which the names and parameter values of all the samples can be edited. The spectra themselves are not shown, nor is there an indication of how many scans were taken. The 'Session Date' shown there is the date and time of the first scan done in that session. It is in the UTC time zone.

Models Page

The models which the logged-in user has access to are listed here, and certain data about them can be edited.



The data shown includes when the model was created, its type and related metrics, and any sensors for which a calibration transfer has been done. Clicking on an 'Edit' button brings up the details for that model.

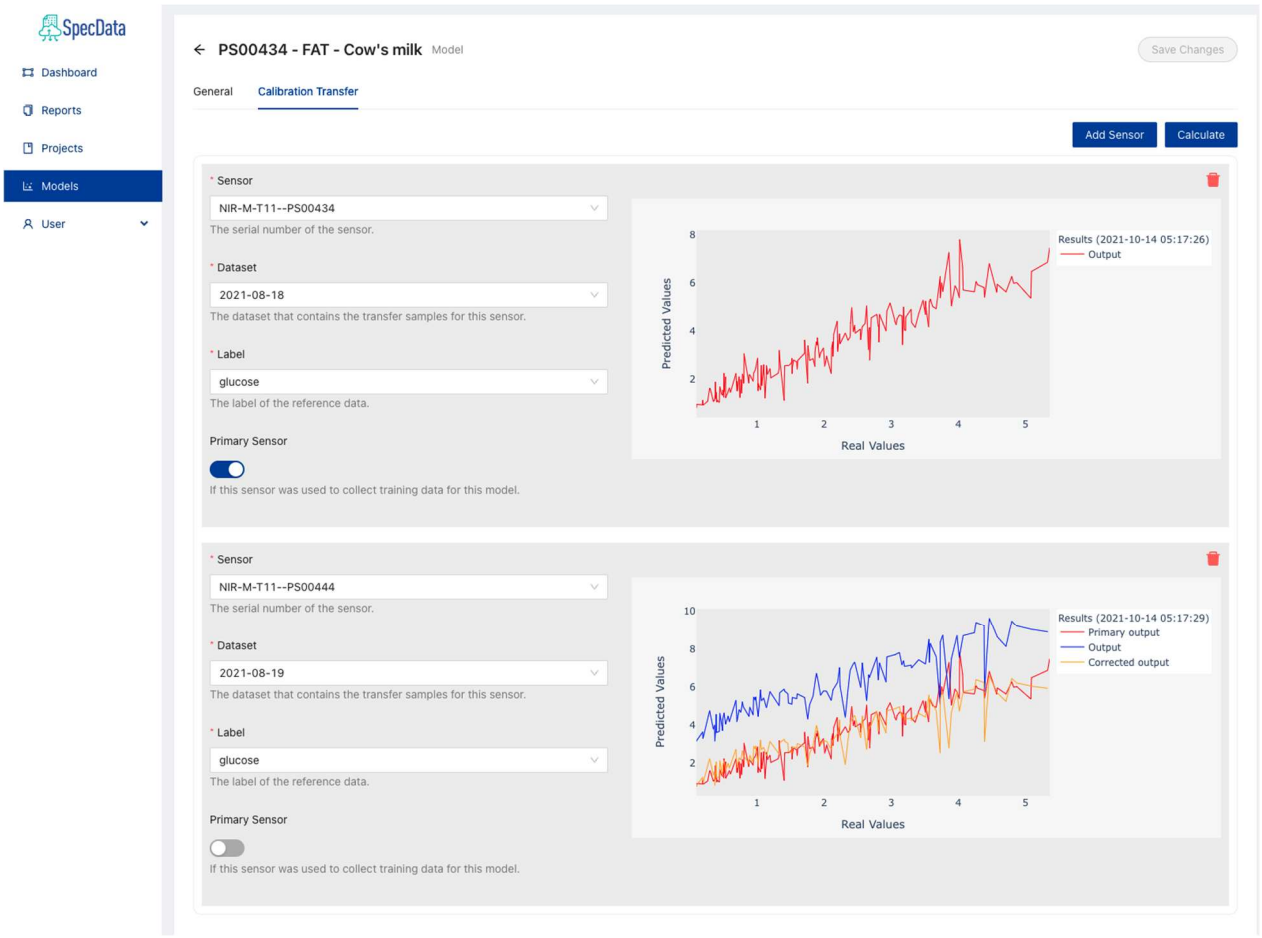


The information here includes the emails of the users who have access to the model. Existing users may be deleted, and new ones added by clicking in the blank space at the end of the list, typing the email, and pressing 'Return'. The other data can not be changed.

Calibration Transfer

Small physical differences between sensors and between different materials can affect a model's results. Therefore, there is a procedure for correcting results from scans taken with different sensors. This is called a "Calibration Transfer". (Not to be confused with a "Calibration Scan", which is performed with a sensor and is not related to models.) To view or create a calibration transfer, click on the 'Calibration Transfer' tab at the top of the model's page.

NB: Calibration transfer only applies to regression models. The tab does not appear for classification models.



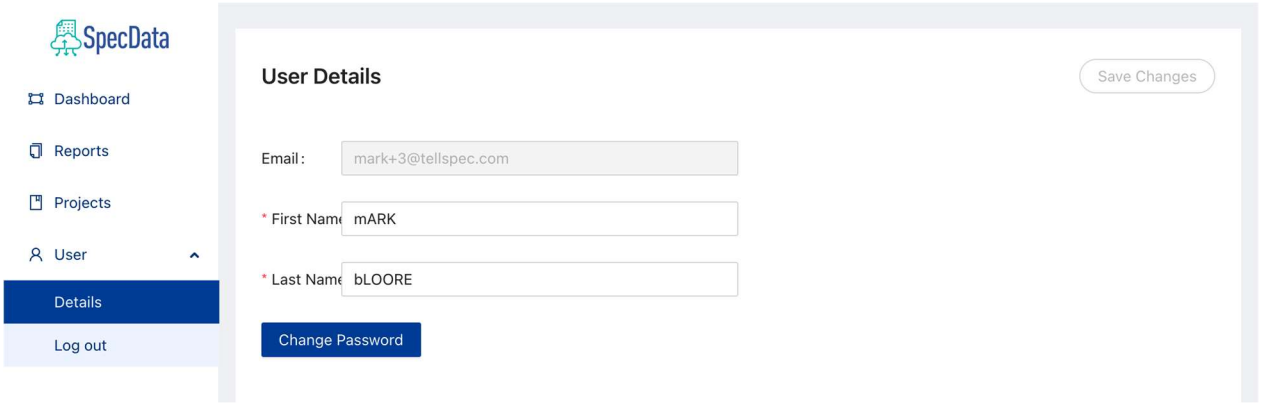
Calibration transfers run from “primary” sensors to “secondary” sensors. Primaries are those sensors which were used to collect the model’s training data. Secondaries are sensors which may be used with the model, and which need the calibration transferred to them. Each of the sensors must have been used to scan the same material, or at least a material with the same characteristics. Those scans are used to create the transfer data.

The process of creating a transfer is:

1. Add the sensors involved.
2. Click the ‘Primary’ button for those which were used to collect training data.
3. Choose the report, with all its sample scans, to be used for each sensor.
4. Click ‘Save’, just in case. This takes you back to the General tab.
5. Return to the Calibration Transfer tab.
6. Click ‘Calculate’. This process may take a while.
7. Click ‘Save’ again.

The primary sensors show the spectra of their samples. Once the calibration transfer has been calculated then each secondary shows the primary (or average of primaries) result function, the secondary result function, and the corrected result function. This correction will be applied to future scans from the secondary when used with this model.

User Page



Here you can change the name and password of the logged-in user. You can't change the email, since that is used to identify you for logging into the system.

You can also log out here.

Support

If you run into issues, please refer to the Troubleshooting section that follows. If you cannot resolve your problem, please contact info@tellspec.com.

Troubleshooting the mobile app

Symptom	Cause	Solution
Sensor will not turn on.	Discharged battery.	See Charging for instructions on how to charge your Preemie Sensor or Enterprise Sensor.
I do not see my sensor in the app.	Not connected.	See "Enabling/Disabling Bluetooth" for help on enabling Bluetooth.
My sensor works with my phone, but not with my tablet.	Your phone has kept communication open, stopping the tablet from seeing the sensor.	Turn off Bluetooth on the phone. The tablet will now be able to pair with the sensor.
The sensor performs a scan, but does not send data to the app.	The Bluetooth connection is not working.	Check that the blue light on the top of the sensor is flashing. If not, enable Bluetooth and wait five seconds. If the app still cannot receive scans, restart the app on your device.

Frequently Asked Questions about the mobile app

The following is a list of frequently asked questions about the app.

What mobile devices does the app run on?

The app runs on all iOS and Android devices that support Bluetooth Low Energy (BLE or Bluetooth 4). All current and recent Apple mobile devices support BLE. Most Android devices do, too.

Does the app support both Preemie and Enterprise sensors?

Yes, but the app is licenced for each sensor individually. That means that you can only connect the app to sensors for which you are licensed.

What iOS versions does the app run on?

The app works with iOS 10.0 and above.

What Android versions does the app run on?

The app works with Android 7 (Nougat) and above, depending on the particular model of mobile device.

Does the app support other date formats?

No. The app uses the ISO-standard date/time format: YYYY-MM-DD HH:MM:SS

Acknowledgements and Trademarks

Chapter 3: The Preemie Sensor

About the Preemie Sensor

The Preemie Sensor™ a transmissive spectrometer, for scanning liquids. Liquid samples go into a *cuvette*, a special tube or other device made for the purpose. For scanning, the sensor is connected by Bluetooth Low Energy to a mobile device running the SpecData app.

Using the Preemie Sensor

Your Preemie Sensor™ is a precision-engineered device, namely a spectrometer, that, if treated well, will provide you with trouble-free service for many years. The following outlines the basics of how to use it and how to care for it.

Charging the Preemie Sensor

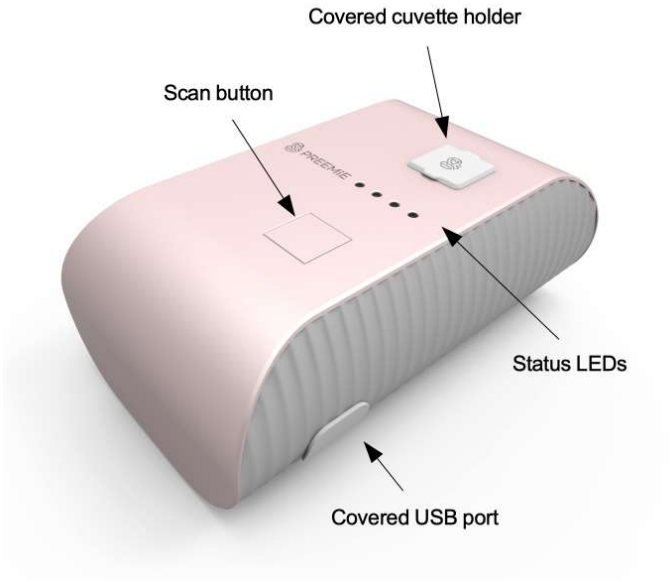
When you receive your Preemie Sensor, you may need to charge it. To do this, plug a micro-USB cable into the port at the side of the device. The red charge LED will light up on top of the device. When charging is complete, the LED will go out.

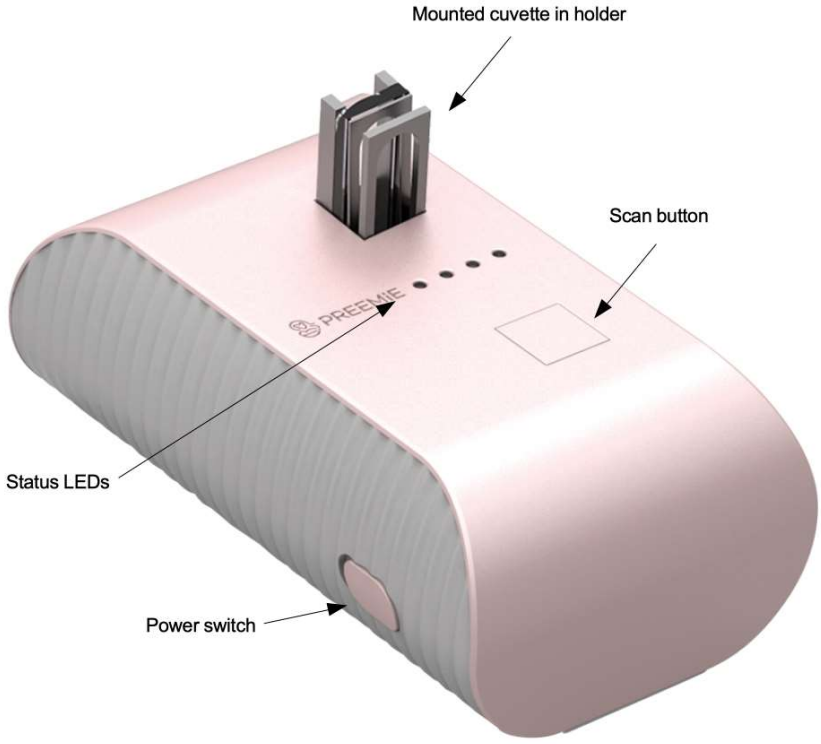
You should not scan with your sensor while it is plugged into a charger or computer that is plugged into the wall, as that may introduce electrical interference. Pure battery power is fine. You should not use it if the charge level is below 35 %, as that may affect scan quality.

Turning your Preemie Sensor on and off

To turn on your Preemie Sensor, locate the power switch on the side of the device. Slide the switch to the ON position (to the right). You will notice the green power LED illuminated on the top of the sensor. All of the LEDs flash briefly to show that they are working.

To turn off your Preemie Sensor, locate the power switch at the rear of the device. Slide the switch to the OFF position (to the left). All the LEDs should go out, except for the charging indicator if the sensor is plugged into USB and the battery is charging.





Caring for your Preemie Sensor

To maintain the life of your Preemie Sensor, do keep it clean with a lint-free cloth.

Do not do any of the following with your Preemie Sensor:

- Immerse it in liquid.
- Drop it onto a hard surface from any height.
- Expose it to excessive heat or cold.

- Puncture it, drill into it, or attempt to affix it to a permanent fixture.
- Modify it, disassemble it, or hardwire it to a permanent power source.

Please do the following with your Preemie Sensor:

- Keep it in a dry, dust-free environment away from direct sunlight, excessive heat, or low temperatures.
- Wipe your device with a damp lint-free cloth from time to time.

Protecting the Sensor

Please ensure you keep your sensor clean and clear of any debris, dust, and liquids.

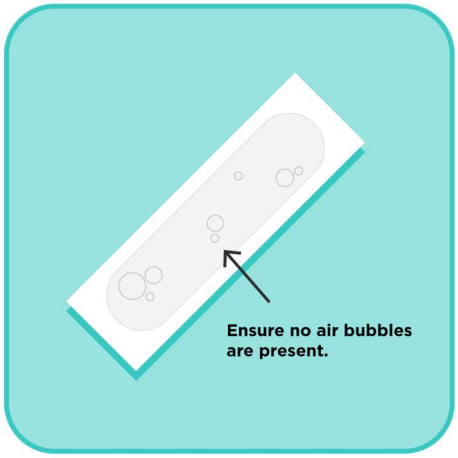
Make sure that there is no liquid outside the cuvette before inserting it into the sensor. Liquid which leaks into the sensor will not cause an immediate problem, but may cause trouble over time.

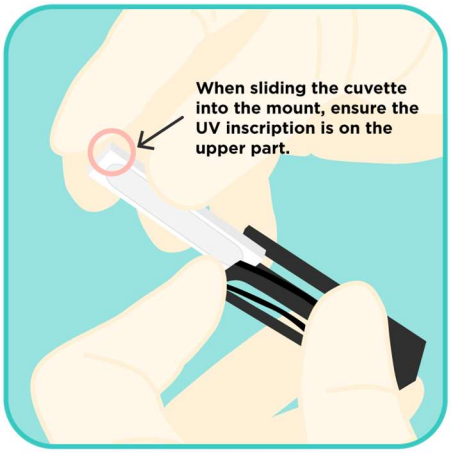
Scanning Liquids with Preemie Sensor

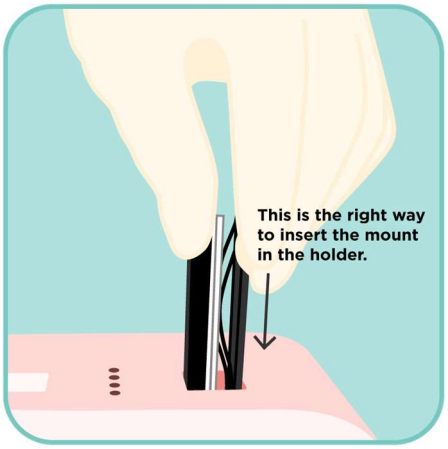
For high-absorbance liquids, such as milk, use a short pathlength demountable cuvette. Here, we are assuming a 0.1 mm pathlength, which affects the volume of sample needed.

Ensure that both cuvette windows are perfectly clean and free from lint. Then, place a small drop of liquid (*ca.* 40 µL) in the cuvette window with the sample chamber as depicted below. Place the drop at one end of the chamber.

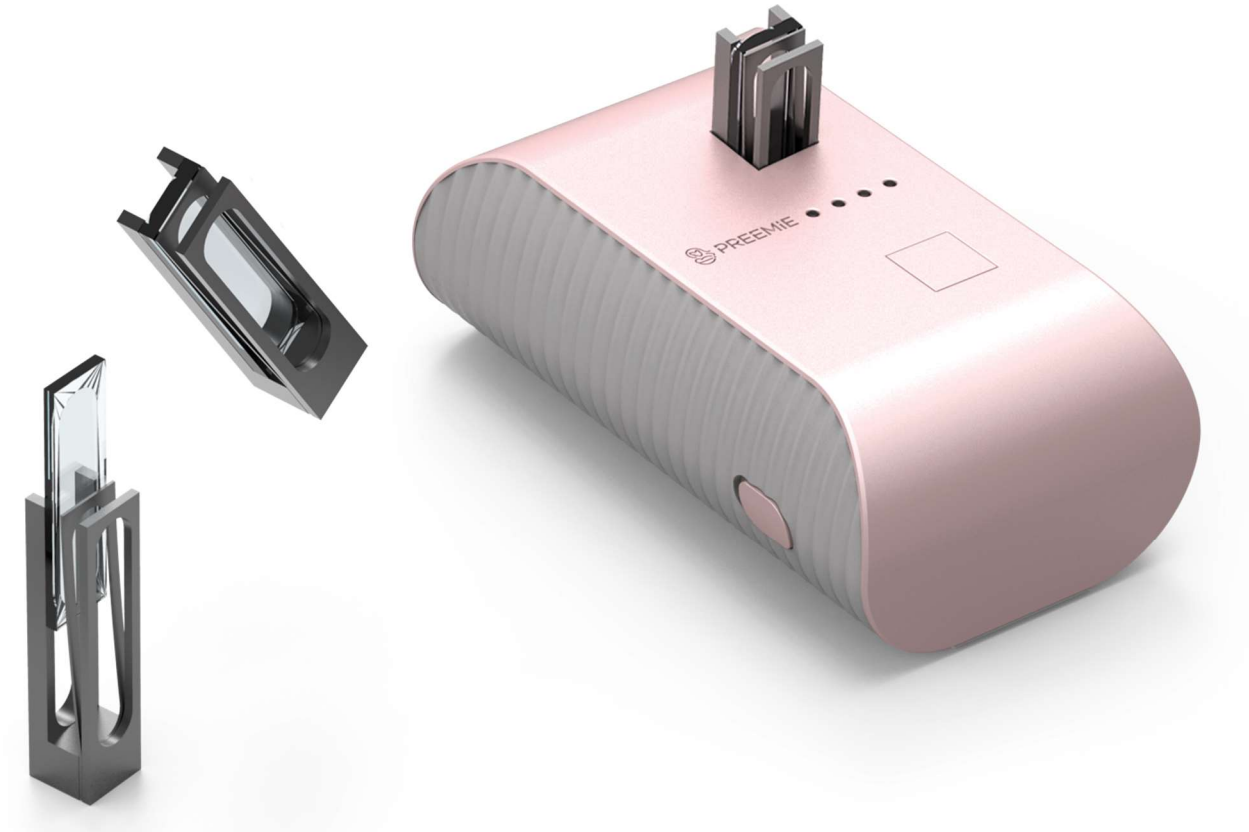
Slide the other window over the sample, starting at that end. Ensure that no bubbles form. It is OK if the sample does not reach the far end of the cuvette, so long as it reaches at least half way. The end with the sample slides into the cuvette mount first, and then into the sensor first.


Ensure no air bubbles
are present.


When sliding the cuvette
into the mount, ensure the
UV inscription is on the
upper part.



The following image shows loading a cuvette mount and inserting it into the cuvette holder of the Preemie Sensor.



After scanning, the cuvette slides should immediately be separated, cleaned with 99% isopropanol, and dried with a lint-free microfibre cloth. Inspect the slides for streaks or spots, and polish with a dry microfibre cloth as needed.

Preemie Sensor Reference Scans

For the Preemie Sensor a reference scan is taken with no cuvette or mount in place. Proceed to take a reference scan as described above.

Chapter 4: The Enterprise Sensor

About the Enterprise Sensor

Your Tellspec® Enterprise Sensor™ is a precision engineered device that, if treated well, will provide you with trouble-free service for many years. The following outlines the basics on how to use it and how to care for it.

The Enterprise Sensor is a reflectance spectrometer, for scanning solids, or suitably contained liquids. For scanning, the sensor is connected by Bluetooth Low Energy to a mobile device running the SpecData app.

In the box:

- The sensor itself;
- A micro-USB cable, used for charging the sensor's battery.

Using the Enterprise Sensor

Charging the Enterprise Sensor

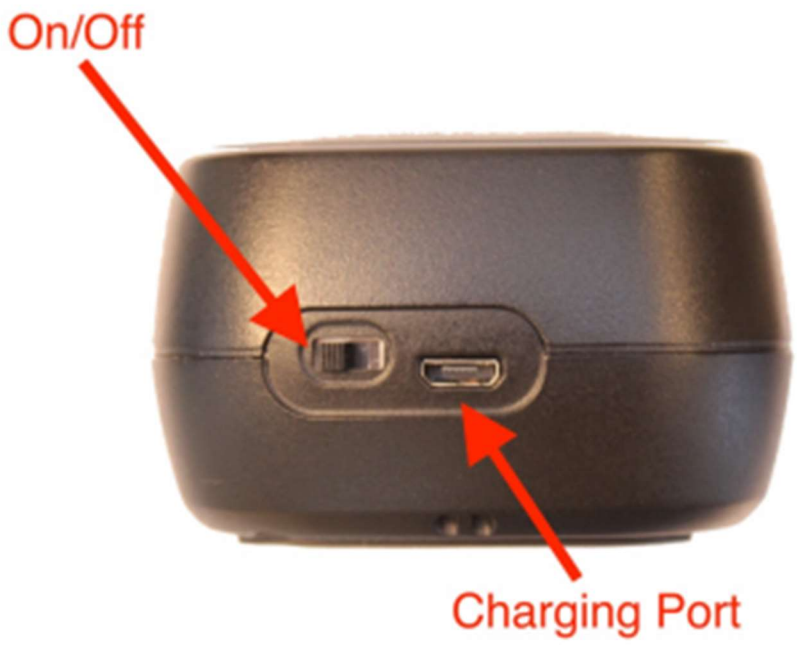
When you receive your Enterprise Sensor, you may need to charge it. To do this, plug a micro-USB cable into the port at the side of the device. The red charge LED will light up on top of the device. When charging is complete, the LED will go out.

You should not scan with your sensor while it is plugged into a charger or computer that is plugged into the wall, as that may introduce electrical interference. Pure battery power is fine. You should not use it if the charge level is below 35 %, as that may impact scan quality.

Turning your Enterprise Sensor on and off

To turn on your Enterprise Sensor, locate the power switch at the rear of the sensor. Slide the switch to the ON position (to the right). You will notice the green power LED illuminated on the top of the sensor.

To turn off your Enterprise Sensor, locate the power switch at the rear of the sensor. Slide the switch to the OFF position (to the left). All the LEDs should go out, except for the red charging indicator if the sensor is plugged into USB and the battery is charging.


On/Off
Charging Port


Power, Bluetooth,
Scanning, Charging
Scanning &
Bluetooth
tellspec®
Beam your health up

Caring for your Enterprise Sensor

To maintain the life of your Enterprise Sensor, do keep it clean with a lint-free cloth.

Do not do any of the following with your Enterprise Sensor:

- Immerse it in water.
- Drop it onto a hard surface from any height.
- Expose it to excessive heat or cold.
- Puncture it, drill into it, or attempt to affix it to a permanent fixture.
- Modify it, disassemble it, or hardwire it to a permanent power source.

Please do the following with your Enterprise Sensor.

- Keep it in a dry, dust-free environment away from direct sunlight, excessive heat or cold.
- Keep the scanning window clear of debris, dust, and other materials.
- Wipe your device with a damp lint-free cloth from time to time.

Safety Information

The light sources in the Enterprise Sensor are very low power, but to operate your scanner safely, please follow the following guidelines.

- Do not look directly into the scanner when it is illuminated.
- Do not shine the scanner light into other people's eyes.

Scanning with the Enterprise Sensor

Scanning Different Materials

The physical characteristics of a sample affect various aspects of how it should be scanned. Some considerations are:

Moisture, Oil, Dust

Protect the sensor as described above.

Powders and Fine Grains

Put such materials in a thin transparent plastic bag. How many different positions on the bag which you should scan depends on the homogeneity of the material. Also, if the grains are close to the size of the scanning window the number of positions should be enough to average out variations in the area of contact between scans and grains.

Liquids

Liquids need to be reflective in the sensor's spectral range. NIR-transparent liquids won't return any light for the sensor to measure. For those, the Preemie Sensor may be more suitable, with a cuvette of appropriate path length, up to 10 mm.

Liquids should be put into a thin transparent bag. A thin-walled bottle might work, but the sensor is focussed on the surface of the window, so too much distance from the sensor will return very little light.

How many different positions on the bag which you should scan depends on the homogeneity of the liquid.

Larger Objects

An object larger than the sensor window may be scanned in various positions, depending on how much it varies from place to place. Objects similar in size to the window could be scanned individually, or collected in a bag and scanned in various positions to average out variations.

Texture

A sample's surface may vary from smooth to rough to pitted, eg bread. Texture affects the spectrum, so it is best to choose scanning positions with common characteristics, or several different characteristics, each scanned separately. The number of positions scanned should be sufficient to average out variations.

Enterprise Sensor Reference Scans

For the Enterprise Sensor a reference scan is taken with an NIR diffuse-reflectance standard material in place of the sample. One such material is Spectralon 99 from Labsphere. A 1-inch uncalibrated 99% standard is suitable for this use. Proceed to take a reference scan as described above.