

User records experiment record in the same way as UF1, but for UF2 the analysis part is to be carried out by an external service provider

**Experiment**

Reaction: CC(=O)O + C1=CC=C(C=C1)O >> CC(=O)OC1=CC=C(C=C1)O Reaction ID: 7849

Author: [Name] Start: [Date] End: [Date] Project: [Project] Keywords: [Keywords] Laboratory/Instrument: [Lab/Inst] Status: [Status]

Materials: [List]

Safety Information: [List]

Steps: [List]

Samples: [List]

Data: [List]

Links: Plan, References, Similar Experiments

Comments: [Text]

Request Review, Share, Complete Experiment, Publish

Add Samples, generate IDs and configure properties. Some of these can be prepopulated from the plan.

**Samples**

Sample ID: [Field] Generate ID

Formula: [Field]

Structure: CC(=O)O

Properties: Melting Point, Air, Light, Thermal Stability, Solvent, Moisture, Mass, Appearance

Print Label, Request Analysis, Add Sample

Request an analysis from an external service. Choose analysis type.

Choose the analysis centre

Select Analysis Type

Select Analysis Service

Print barcode label to attach to sample

Print Barcode /QRCode

Content of the Analysis Request form based on requirements of the selected service. Much of the information required can be prepopulated from the user's profile, the experiment plan and the sample information already added.

**New Analysis Request Form**

Researcher's Details: Name, E-mail, Address, Project

Sample Information: Sample ID, Expected Formula, Expected Structure, Reaction Scheme, Materials

Properties: Melting Point, Air, Light, Thermal Stability, Solvent, Moisture, Mass, Appearance

Additional Comments

Full Structure Analysis, Data Collection Only, Temperature for Analysis: 120K, Reason if not 120K

Submit Analysis Request, Print Form & Label

The form can also be submitted online so that the sample can be recorded on the Analysis Centre system. A confirmation can be sent to the user

When form is complete user can print off the form and a label for the sample ready for packaging.

My Notebook

Analysis Request

Analysis Request Received

A sequence of notifications can be sent to indicate progress of the analysis. Data may be available only at the end or part way through the process

User can check the status of the Analysis request from within the notebook

Sample Received

Preparing Sample

Running Sample

The raw data can be imported into the notebook if desired

Important data into the experiment record. The sample ID should allow the correct data to be linked up with the correct experiment

Data Available

Calculating Structure

Data Collection Complete

View Data in an appropriate viewer, options to annotate and compare data from different sources

Data Viewer

Annotate

Compare Data

View Data in an appropriate viewer, options to annotate and compare data from different sources

Once the analysis results are returned user can add the data and interpretations into their record

**Experiment**

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Materials: [List]

Safety Information: [List]

Steps: [List]

Samples: [List]

Data: [List]

Spectrum Information: [Spectra]

Comments: [Text]

Request Review, Share, Complete Experiment, Publish

Add Comment

Request Approval

Approval Denied

Approval Granted

Some users may need to have their experiment reviewed