

fragmented system. A guarantee in this context means that description of an experiment protocol is complete, *i.e.*, all information needed to perform the experiment is included. In another aspect, the guarantee is that the experiment protocol is automatically linked to logs detailing actual experiment run, control logs, samples outputted, and data generated. In some embodiments, links are used to relate one experiment protocol to another. Instead of simply copying and pasting the original experimental protocol and then altering the input sample, a user can directly reference the original experiment and then specify only what the user wants to be done differently, *e.g.*, different sample input, different temperature, without limitation. This advantageously allows for very compact and easy to read code without any loss of completeness, precision, or reproducibility. In accordance with one embodiment of the present technology, the systems is configured to guarantee that when a user copies an experimental protocol, rerunning with new parameters or inputs can be accordingly adjusted and validated.

[0013] Another embodiment of the present disclosure relates to programmatically offering sensible default settings for an experiment. The user only needs to specify that which is different. This is not possible if the experiment is not represented in a machine computable form, *e.g.*, free text. Also, the default settings greatly improve ease of use by not forcing user to enter every single parameter an experiment requires. Yet in another embodiment, the experiment is automatically linked to logistical information about materials used in experiment, *e.g.*, age of stock solution used.

[0014] Another advantage of certain embodiments of the technology is that the analysis module can automatically understand output of the experiment, because in specifying experiment up front the system is contextually aware of definition of the output.

[0014a] In view of the above, according to an aspect of the present disclosure, there is provided a system for analyzing data obtained from a laboratory experiment. The system comprises a processor, memory, and program code that comprises: an experiment module configured to store values for experimental parameters for executing an experiment; a data module configured to store results from the experiment; an instrument module configured to store information about the instrument on which the experiment was run; an environment module configured to store environmental conditions under which the experiment was run; an analysis module configured to: determine whether it has sufficient information to resolve a parameter that is necessary to: display identification of a data set for which an analysis was

made and display an analysis summary or figure that represents a result of the analysis, determine, based on the determination of whether the analysis module has sufficient information, whether to access a link to a data object comprising data of the experiment, and access the link in response to the analysis module determining it does not have sufficient information; and a data visualization module configured to: select a visual representation of the results stored in the data module, configure at least one aspect of the visual representation based upon a reference data point, and generate the visual representation, wherein the reference data point is selected from the group consisting of the values for the experimental parameters, the information about the instrument and the environmental conditions.

[0014b] According to another aspect of the present disclosure, there is provided a system for analyzing data obtained from a laboratory experiment. The system comprises a processor, memory, and program code comprising: an experiment module configured to display identification of a sample used in an experiment, identification of an instrument for carrying out the experiment, identification of a data set generated from the experiment, and identification of an environmental record that comprises measurement of environmental conditions when and where the experiment was conducted, a data module configured to display data extract or visualization to represent a data set, identification of an experiment that generated the data set, and identification of an analysis performed on the data set; an instrument module configured to display a listing of experiments carried out on an instrument, a listing of control experiments run on the instrument, and a maintenance record for the instrument; an analysis module configured to determine whether it has sufficient information to resolve a parameter that is necessary to: display identification of a data set for which an analysis was made, and display an analysis summary or figure that represents a result of the analysis, determine, based on the determination of whether the analysis module has sufficient information, whether to access a link to a data object comprising data of the experiment, and access the link in response to the analysis module determining it does not have sufficient information; and an environment module configured to display environmental conditions when and where an experiment was conducted, wherein the system enables a user to explore information pertaining to an experiment while the user is presented with an experiment panel displayed by the experiment module, by: (1) allowing the user to click on the identification of a data set generated from the experiment on the experiment panel, and thereby invoking the data module to display identification of an analysis performed on the data set on a data panel, which allows the user to click on the identification of analysis performed on the data

set to invoke the analysis module to display an analysis summary or figure that represents a result of the analysis on an analysis panel; (2) allowing the user to click on the identification of an environmental record and thereby invoking the environment module to display environmental conditions when and where the experiment was conducted; and (3) allowing the user to click on the identification of an instrument for carrying out the experiment and thereby invoking the instrument module to display, on an instrument panel, a listing of control experiments run on the instrument, and a maintenance record for the instrument relevant to the experiment.

BRIEF DESCRIPTION OF THE DRAWINGS

[0015] The figures of the accompanying drawings describe provided embodiments by way of illustration only, in which:

[0016] FIG. 1 shows a user interface for selecting an experiment type to be run on a system of the present disclosure;

[0017] FIG. 2 shows that the user, after selecting an experiment type, is presented with an interface to choose samples;

CLAIMS:

1. A system for analyzing data obtained from a laboratory experiment, comprising a processor, memory, and program code that comprises:
 - an experiment module configured to store values for experimental parameters for executing an experiment;
 - a data module configured to store results from the experiment;
 - an instrument module configured to store information about the instrument on which the experiment was run;
 - an environment module configured to store environmental conditions under which the experiment was run;
 - an analysis module configured to:
 - determine whether it has sufficient information to resolve a parameter that is necessary to:
 - display identification of a data set for which an analysis was made and
 - display an analysis summary or figure that represents a result of the analysis,
 - determine, based on the determination of whether the analysis module has sufficient information, whether to access a link to a data object comprising data of the experiment, and
 - access the link in response to the analysis module determining it does not have sufficient information; and
 - a data visualization module configured to:
 - select a visual representation of the results stored in the data module,
 - configure at least one aspect of the visual representation based upon a reference data point, and
 - generate the visual representation,wherein the reference data point is selected from the group consisting of the values for the experimental parameters, the information about the instrument and the environmental conditions.
2. The system of claim 1, wherein the data visualization module is further configured to update the visual representation of the results based on the reference data point, wherein:
 - the reference data point indicates information not directly generated from the experiment, and

the updating comprises selectively representing the results by eliminating a portion of the results determined to be irrelevant, invalid, or not important based on a comparison of the results with the reference data point.

3. The system of claim 1, wherein the reference data point imposes a limitation on interpretation of the results.

4. The system of claim 1, wherein the reference data point comprises a result from a second experiment.

5. The system of claim 3, wherein the reference data point validates or invalidate the results.

6. The system of claim 3, wherein the reference data point serves as standard or control to the results.

7. A system for analyzing data obtained from a laboratory experiment, comprising a processor, memory, and program code comprising:

an experiment module configured to display identification of a sample used in an experiment, identification of an instrument for carrying out the experiment, identification of a data set generated from the experiment, and identification of an environmental record that comprises measurement of environmental conditions when and where the experiment was conducted,

a data module configured to display data extract or visualization to represent a data set, identification of an experiment that generated the data set, and identification of an analysis performed on the data set;

an instrument module configured to display a listing of experiments carried out on an instrument, a listing of control experiments run on the instrument, and a maintenance record for the instrument;

an analysis module configured to

determine whether it has sufficient information to resolve a parameter that is necessary to:

display identification of a data set for which an analysis was made, and display an analysis summary or figure that represents a result of the analysis,

determine, based on the determination of whether the analysis module has sufficient information, whether to access a link to a data object comprising data of the experiment, and

access the link in response to the analysis module determining it does not have sufficient information; and

an environment module configured to display environmental conditions when and where an experiment was conducted,

wherein the system enables a user to explore information pertaining to an experiment while the user is presented with an experiment panel displayed by the experiment module, by:

- (1) allowing the user to click on the identification of a data set generated from the experiment on the experiment panel, and thereby invoking the data module to display identification of an analysis performed on the data set on a data panel, which allows the user to click on the identification of analysis performed on the data set to invoke the analysis module to display an analysis summary or figure that represents a result of the analysis on an analysis panel;
- (2) allowing the user to click on the identification of an environmental record and thereby invoking the environment module to display environmental conditions when and where the experiment was conducted; and
- (3) allowing the user to click on the identification of an instrument for carrying out the experiment and thereby invoking the instrument module to display, on an instrument panel, a listing of control experiments run on the instrument, and a maintenance record for the instrument relevant to the experiment.

8. The system of claim 7, wherein the program code further comprises a sample module configured to display the identifications of a first experiment from which the sample is generated and a second experiment that is performed on the sample.

9. The system of claim 7, wherein the displayed analysis summary or figure on the analysis panel allows the user to make adjustment and access to the data set from which the analysis summary or figure is generated.

10. The system of claim 7, wherein the system allows the user to click on the listing of experiments on the instrument panel to view one or more other experiments conducted on the instrument for comparison.
11. The system of claim 1, wherein the data visualization module is further configured to dynamically update the visual representation based on a result stored in the experiment module, the instrument module, or the environment module.
12. The system of claim 1, wherein the data visualization module is further configured to dynamically update the visual representation without input from a user.
13. The system of claim 11, wherein the system is configured to dynamically update instructions generated for subsequent experiments based on the dynamically updated visual representation.
14. The system of claim 1, further comprising an orchestration module configured to use bar codes or RFID tags for tracking source materials and automatically linking information about the source materials to the results.
15. The system of claim 1, wherein the system determines whether to use a linear approach or a convergent approach in a synthesis process based on a complexity of a molecule to be synthesized.
16. The system of claim 1, wherein the system is configured to reference an original experiment protocol and to prompt the user to specify only changes in experiment setting for subsequent experiments.
17. The system of claim 1, wherein the system is configured to estimate the results based on the experimental parameters.
18. The system of claim 1, wherein the data visualization module is configured to dynamically adjust an upper bound of visualization based on a number of cycles of the experiment and to discard data outside the upper bound of visualization.

19. The system of claim 1, wherein the reference data point comprises a data result from a previous experiment.
20. The system of claim 7, wherein the data module determines a type of the data extract or visualization based on a type of experiment, and whether to generate multiple displays based on a complexity of the data.
21. The system of claim 7, wherein the analysis module is configured to access the link only in response to a determination that it does not have sufficient information.
22. The system of claim 1, wherein the data visualization module is configured to determine a type of the visual representation before generating the visual representation.