

A Tool to Link and Establish Confidence in Evidence Used to Construct Computer Simulations

Simomics



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Facilitating Knowledge Retention, Communication, Reusability, & Curation of Models

Modelling is being increasingly used to explore mechanisms of action within a system and offer reduced R&D costs. However, model design decisions, such as assumptions and simplifications, **can often be opaque to all but the model's author**, and should be justified and supported by evidence used to inform that decision process.

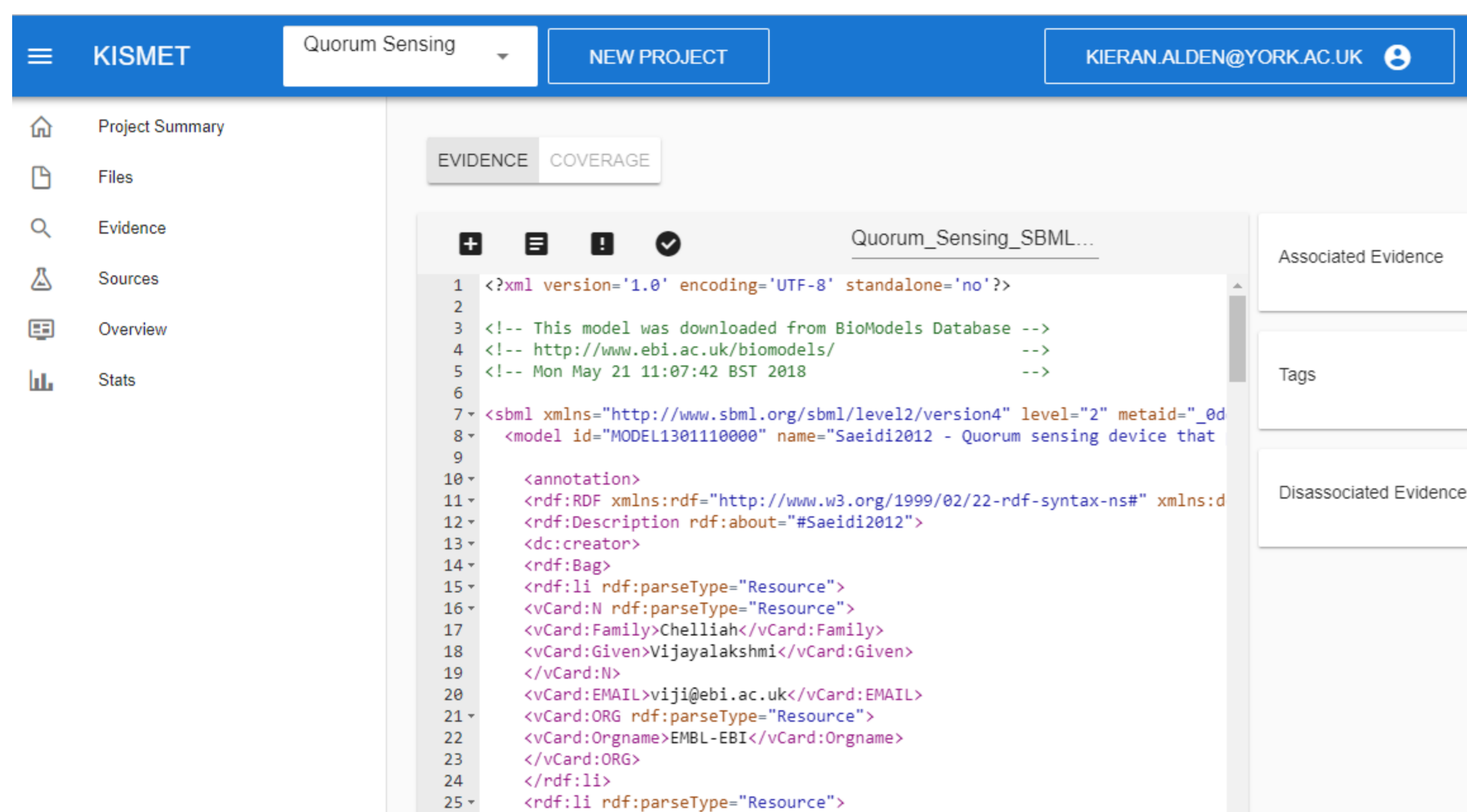
Our online platform **permits the attachment of sources of evidence**, including datasets, statistical calculations, images, and text, **to model file components**. Each attachment is accompanied by a value indicating confidence in that evidence, retaining the reasoning for model composition while identifying potential areas of deficiency.

Our tool is compatible with a range of model specification formats, including MATLAB, XML, and SBML. For SBML models, our platform **permits location and attachment of resources in the Minimum Information Required in the Annotation of Models (MIRIAM) registry**, using services provided by Identifiers.org

Overviews of evidence coverage and summary statistics are produced to assist in determining overall model confidence. Platform adoption **offers benefit in increasing model quality, auditability, and confidence in wider model application**, while reducing model maintenance effort and ensuring retention of IP within institutions.

Uploading Simulation Model File

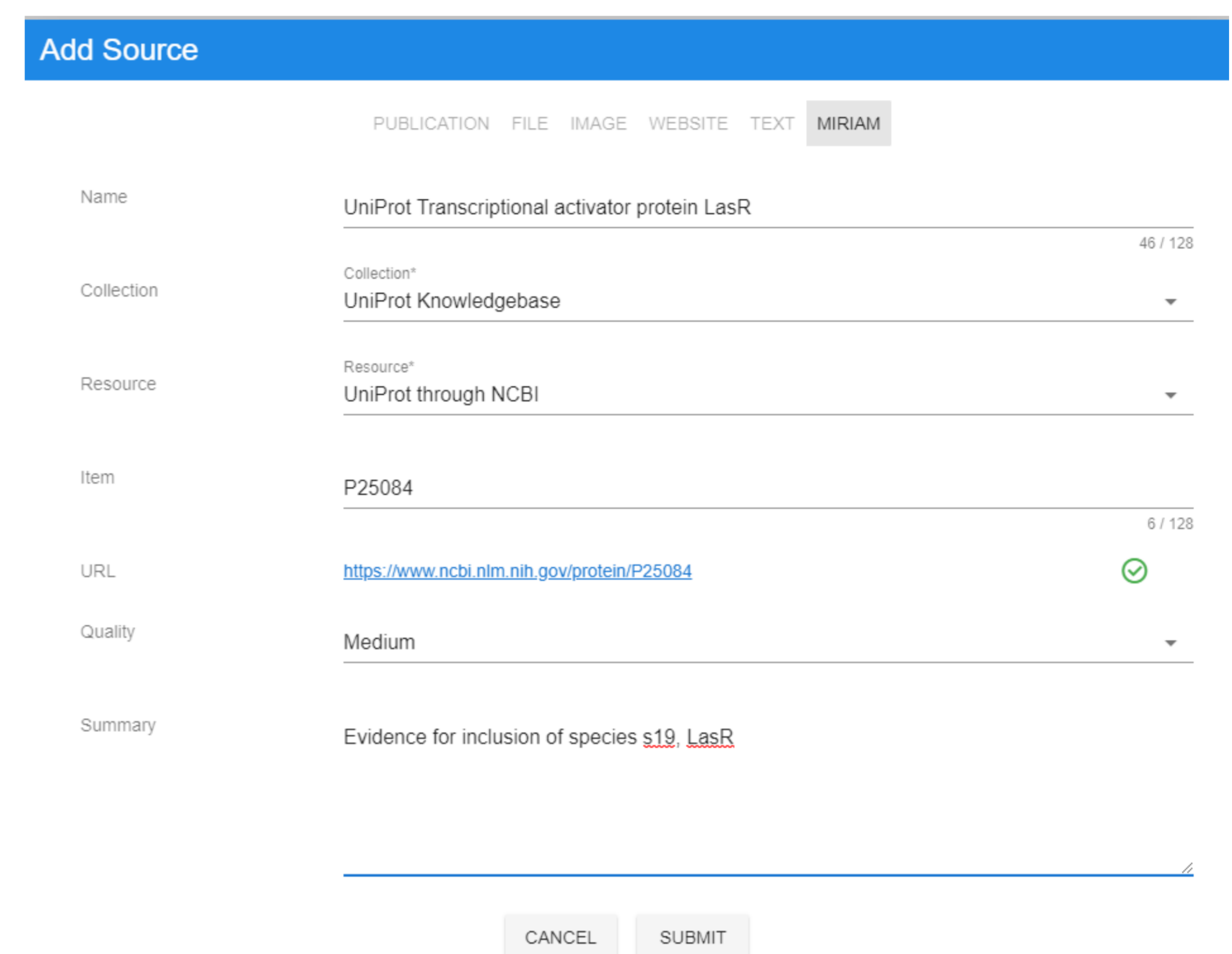
Compatibility Includes MATLAB, XML, and SBML Models



Models are managed in specific projects, each containing uploaded model files that can be viewed prior to attachment of evidence to lines of the code, and sources of evidence from which attached evidence is found. Platform compatibility to parse other model specification formats could be extended if appropriate.

Adding Sources of Evidence

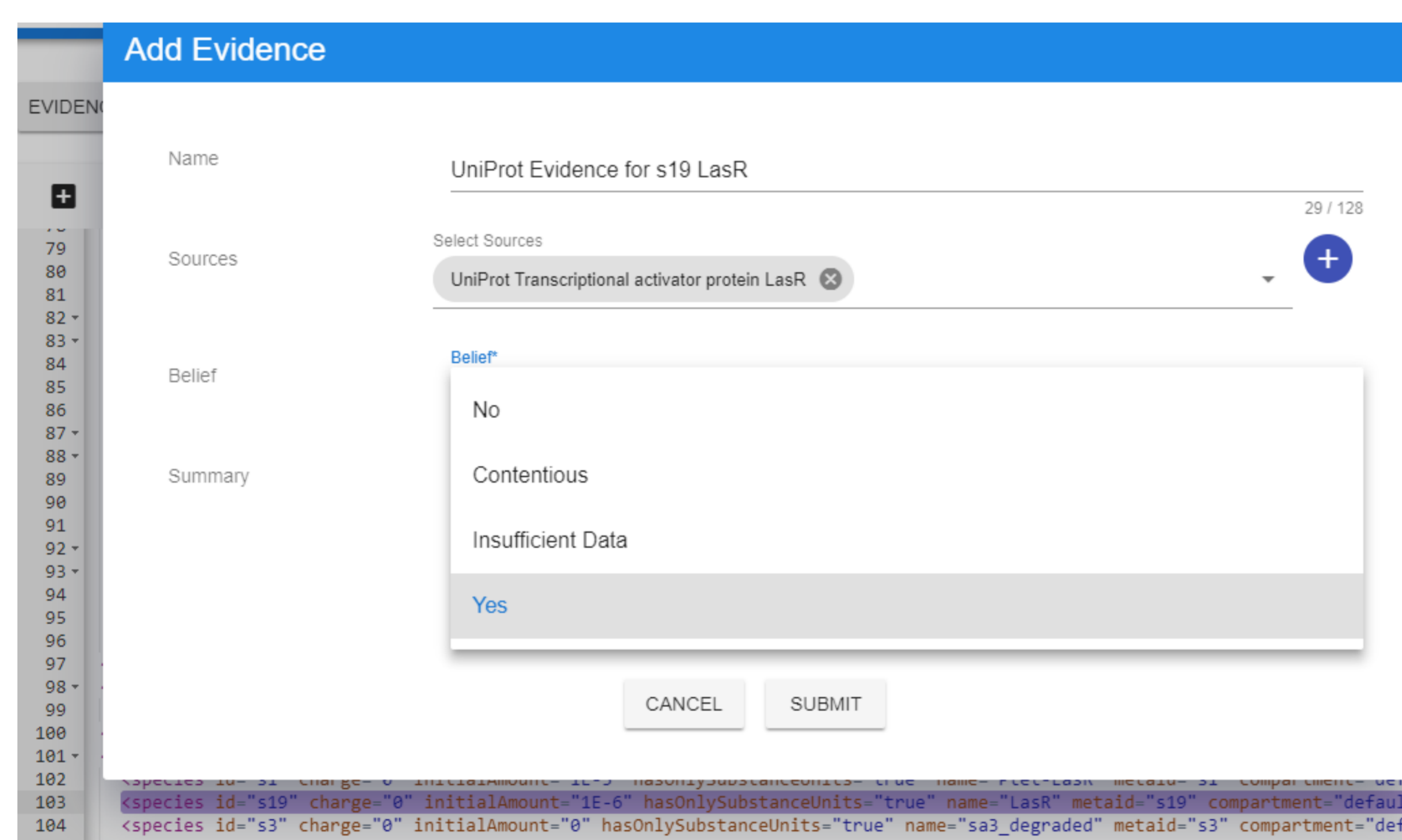
With Author Indicated Measure of Quality



Evidence sources may include publications, websites, files, and MIRIAM registry identifiers. Above: Evidence for species LasR in an SBML model of Quorum Sensing, showing link to persistent URL resource identifier, and author assessment of this evidence, rated from Low / Medium / High in this case)

Attaching of & Confidence in Evidence

Attachments to Selected Model Code with Author's Confidence Measure



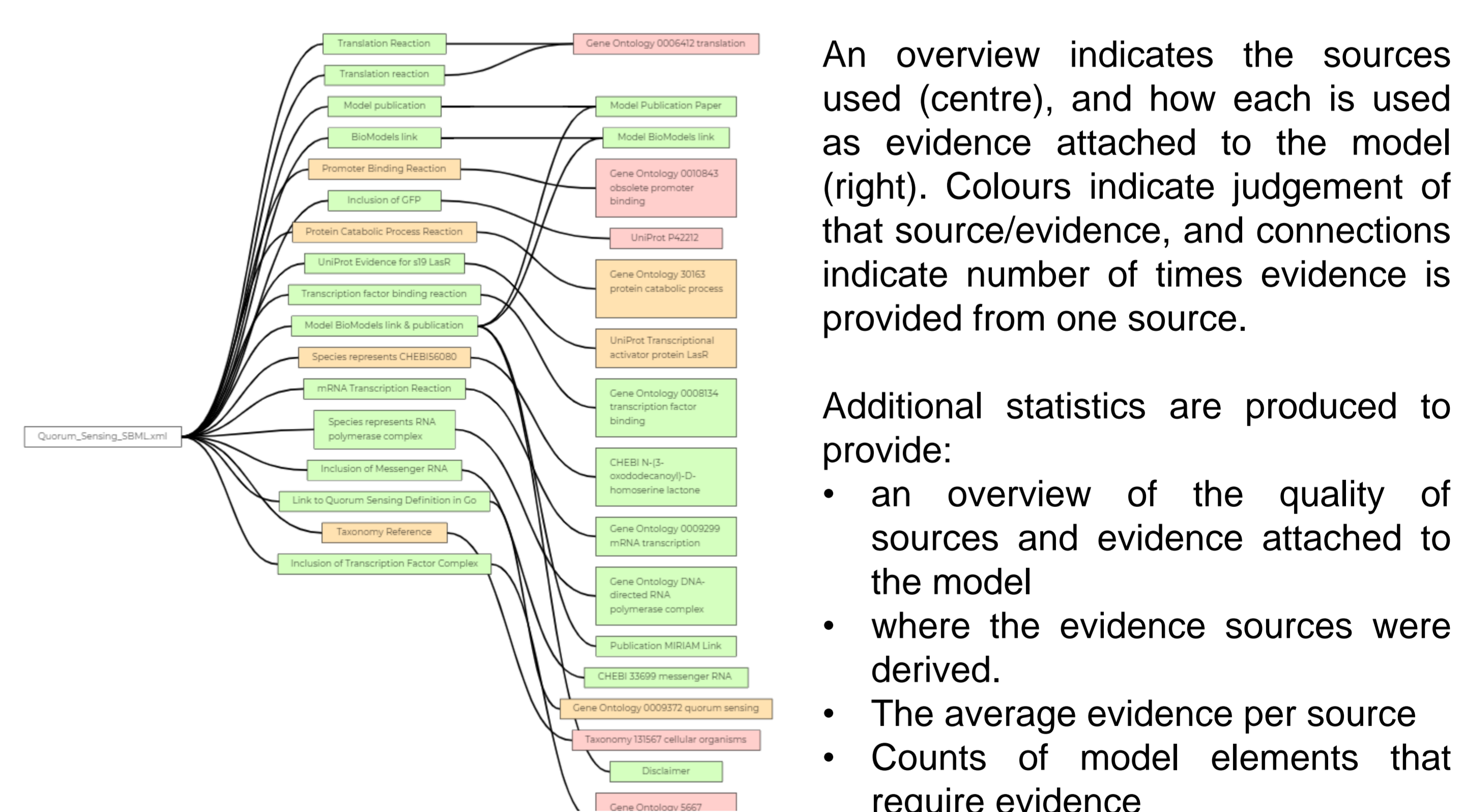
Evidence is attached by highlighting model elements in the editor (species s19 in this case), and selecting evidence from the sources added previously.



Model code with attached evidence is shown in blue. Alternatively, code that does not need evidence (grey), and is missing evidence (red), can also be indicated

Coverage & Overview

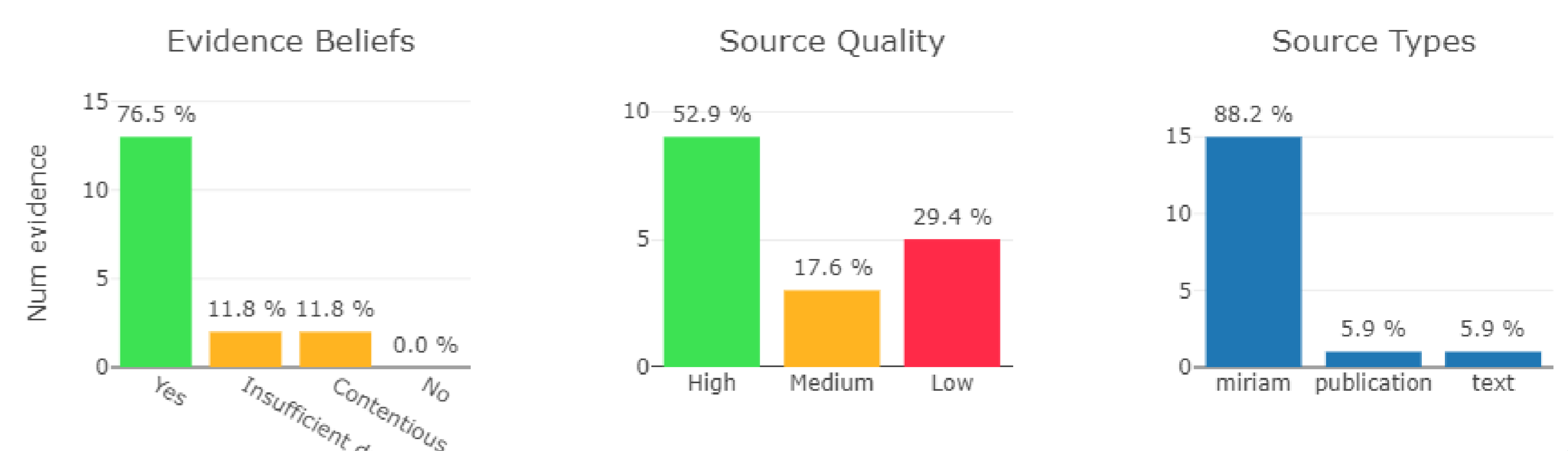
Statistics to Assist in Determining Overall Model Confidence



An overview indicates the sources used (centre), and how each is used as evidence attached to the model (right). Colours indicate judgement of that source/evidence, and connections indicate number of times evidence is provided from one source.

Additional statistics are produced to provide:

- an overview of the quality of sources and evidence attached to the model
- where the evidence sources were derived.
- The average evidence per source
- Counts of model elements that require evidence



Acknowledgements

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Innovate UK

Accessing the Platform

Access example model file with demonstrated attachment of and confidence in evidence used in model composition, at

<https://evidence.simomics.com>

