

FAIRifying Computational Models: Advancing Transparency and Reusability in the SSbD framework



Fairification Workshop
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FAIR data

- Build and deploy models at scale
- Effective collaboration of research communities
- Long-term data preservation



Guide to implement FAIR data and models

Box 2 | The FAIR Guiding Principles

To be Findable:

- F1. (meta)data are assigned a globally unique and persistent identifier
- F2. data are described with rich metadata (defined by R1 below)
- F3. metadata clearly and explicitly include the identifier of the data it describes
- F4. (meta)data are registered or indexed in a searchable resource

To be Accessible:

- A1. (meta)data are retrievable by their identifier using a standardized communications protocol
 - A1.1 the protocol is open, free, and universally implementable
 - A1.2 the protocol allows for an authentication and authorization procedure, where necessary
- A2. metadata are accessible, even when the data are no longer available

To be Interoperable:

- I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
- I2. (meta)data use vocabularies that follow FAIR principles
- I3. (meta)data include qualified references to other (meta)data

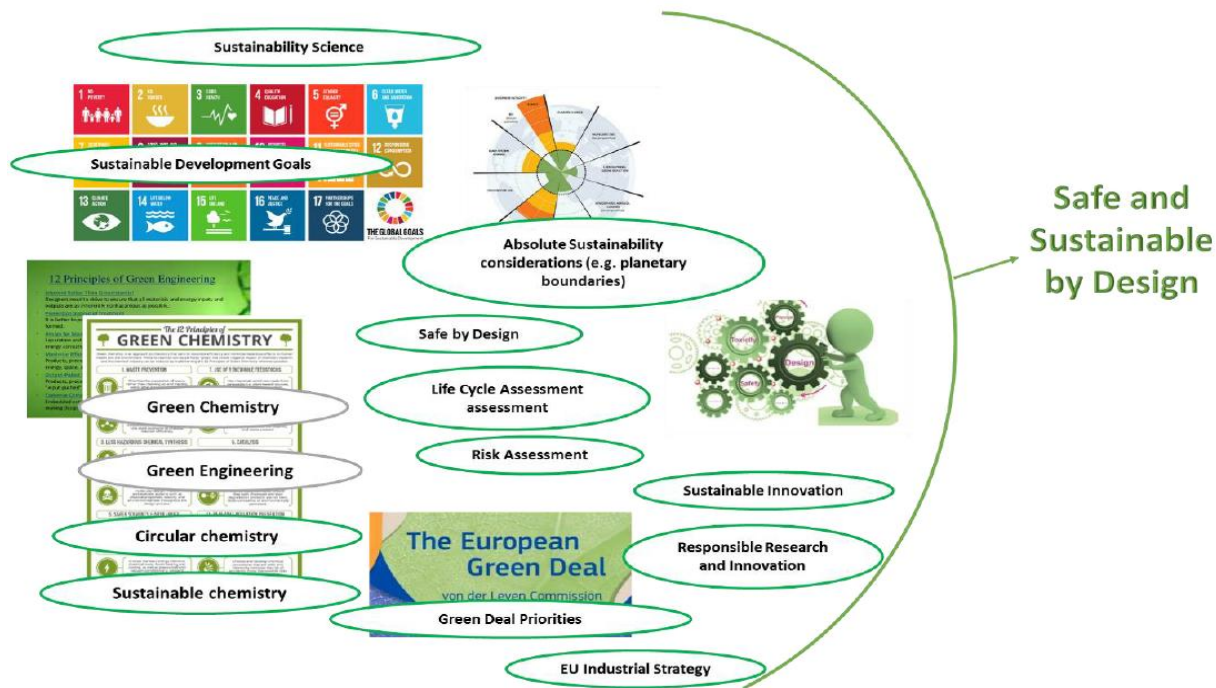
To be Reusable:

- R1. meta(data) are richly described with a plurality of accurate and relevant attributes
 - R1.1. (meta)data are released with a clear and accessible data usage license
 - R1.2. (meta)data are associated with detailed provenance
 - R1.3. (meta)data meet domain-relevant community standards



Wilkinson (2016)

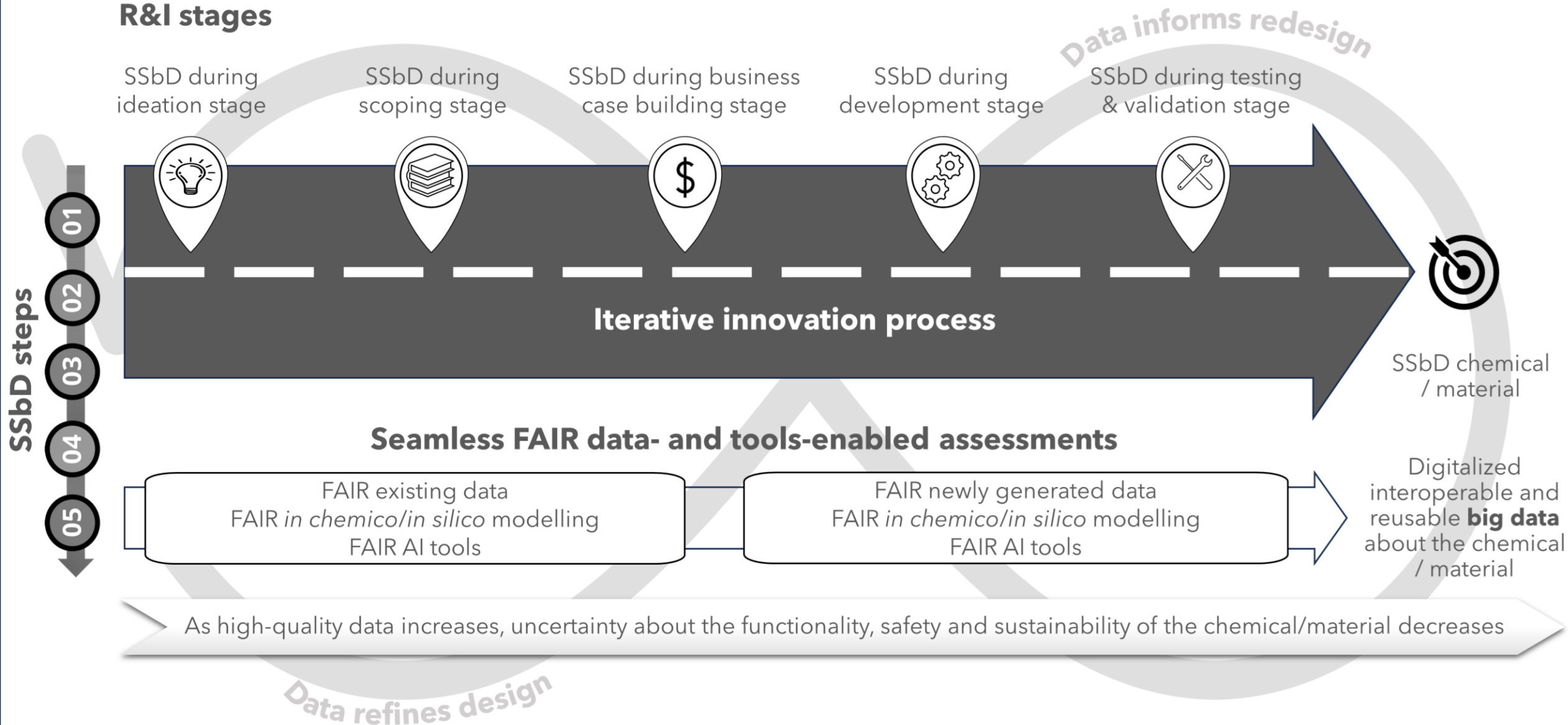
The FAIR Principles enable operationalization of SSbD



- (i) digitalization to leverage innovation towards a green transition;
- (ii) existing data sources and their interoperability;
- (iii) navigating SSbD with data from new scientific developments;
- (iv) transparency and trust through automated assessment of data quality and uncertainty; and
- (v) “seamless” integration of SSbD tools.



R&I stages



Seamless FAIR data- and tools-enabled operationalization of SSbD

FAIR principles



- ✓ (Meta)data and tools are persistent and not hidden away in silos (as open as possible, as restricted as necessary)
- ✓ (Meta)data and tools are made accessible to both humans and machines
- ✓ Data and tools are discoverable through standardized metadata and proper indexing and vocabularies
- ✓ Data is easily combined through data schemas with standardized templates
- ✓ Data and tools are well documented for reuse
- ✓ Data quality is transparent
- ✓ Tools provide transparent and robust high confidence outputs

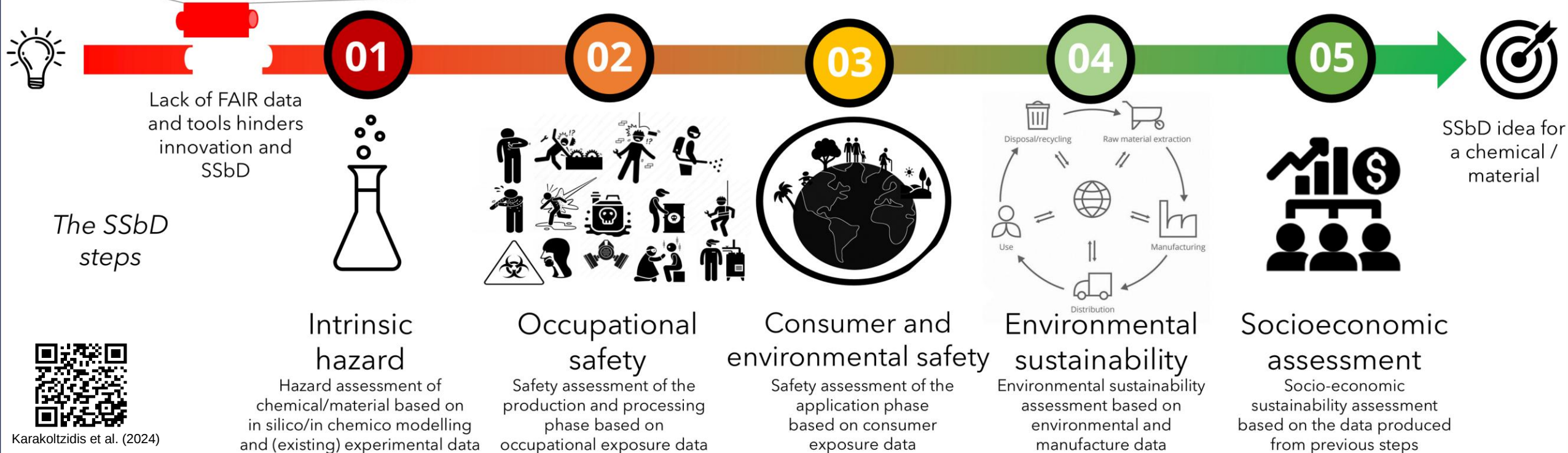
FAIR NAMs data and tools



FAIR sustainability and socioeconomic data



FAIR data infographic (CC-BY except F.A.I.R. logos CC-BY-SA by Sangya Pundir)



Karakoltzidis et al. (2024)

Findability

- F1. Are model and associated metadata assigned globally unique and persistent identifiers?
- F2. Are different versions of the software assigned distinct identifiers?
- F3. Is the model metadata publicly available in open access repositories?
- F4. Are the in-model implemented properties well described by ontological vocabularies? Explain.
- F5. Is the model conveniently identifiable through the common search engines (e.g., Google)?

Potential Responses: Not addressed yet; Partly addressed; Fully implemented

Accessibility

- A1. Are model and associated (meta)data retrievable by their identifier using a standardised communications protocol?
- A2. Is the protocol open, free, and universally implementable?
- A3. Does the protocol allow for an authentication and authorization procedure where necessary?
- A4. Does the model provide an API?
- A5. Is the model reachable through a DOI or other digital identifier?
- A6. Is the metadata of the model publicly available?

Potential Responses: Not addressed yet; Partly addressed; Fully implemented

Interoperability

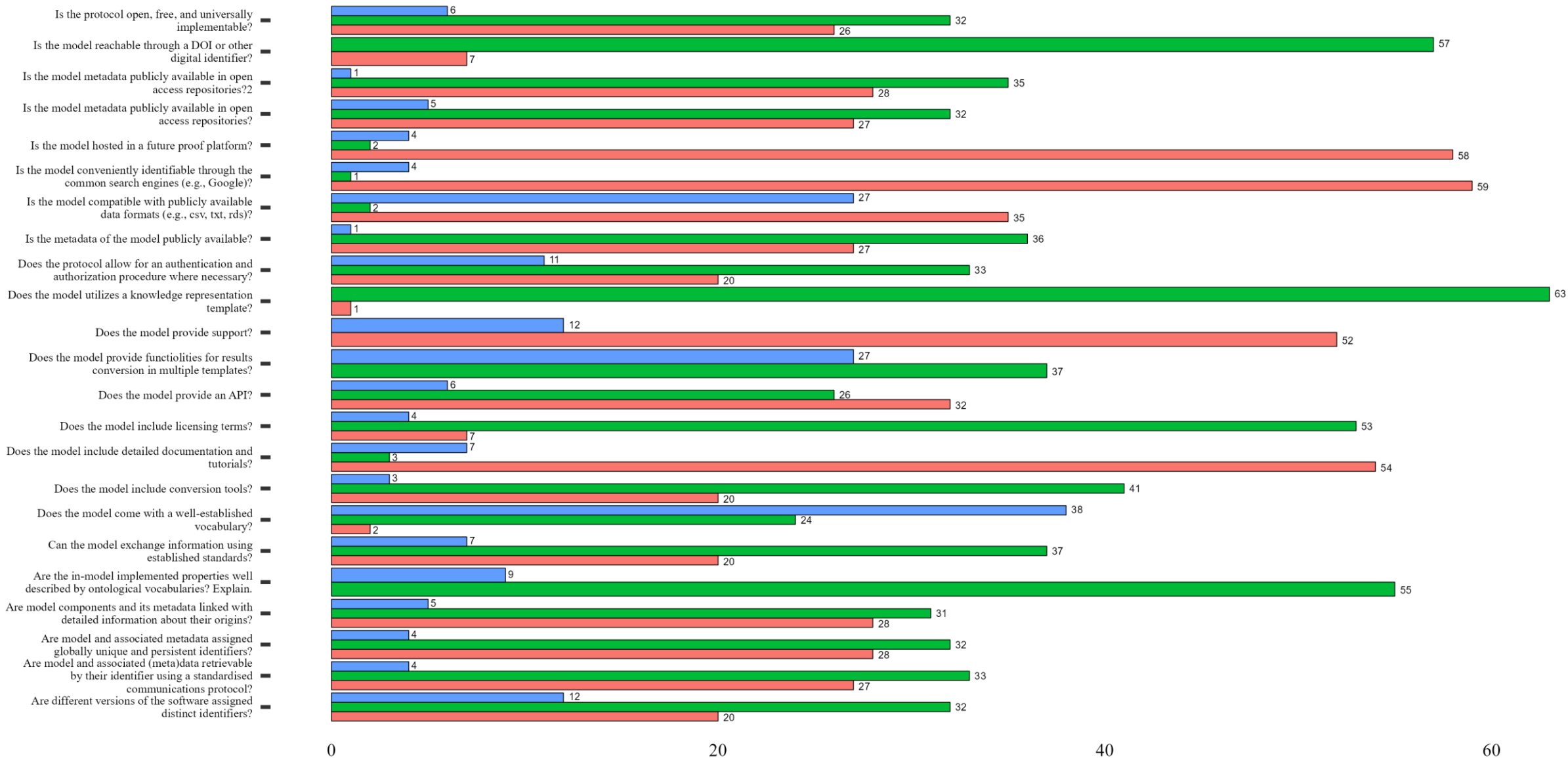
- I1. Can the model exchange information by using established standards?
- I2. Does the model utilize a knowledge representation template?
- I3. Does the model come with a well-established vocabulary?
- I4. Does the model provide functionalities for results conversion in multiple templates?
- I5. Is the model compatible with publicly available data formats (e.g., csv, txt, rds)?
- I6. Does the model provide an API?

Potential Responses: Not addressed yet; Partly addressed; Fully implemented

Reusability

- R1. Does the model include licensing terms?
- R2. Does the model include detailed documentation and tutorials?
- R3. Does the model provide support?
- R4. Is the model hosted in a future proof platform?
- R5. Does the model include conversion tools?
- R6. Is the model metadata publicly available in open access repositories?
- R7. Is the model metadata thoroughly described with relevant ontology-based vocabularies ?
- R8. Are model components and its metadata linked with detailed information about their origins?
- R9. Is the model compatible with publicly available data formats (e.g., csv, txt, rds)?

Potential Responses: Not addressed yet; Partly addressed; Fully implemented



Preliminary Results

■ Fully implemented
 ■ Not addressed yet
 ■ Partly addressed

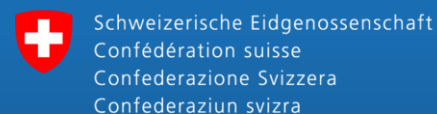
Next steps

- Raise people awareness regarding the importance of applying FAIR principles in the SSbD context
- Follow the “FAIR” gaps as identifies in the shared questionnaire
- Start by implementing the gaps and the models that are most closed to be characterized as FAIR
- Face challenges of INSIGHT FAIR implementation pipeline.

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THANK YOU

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