



## Sample Entity Changes

Rolf Krahel

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# Changes to SampleType

- Allow molecularFormula to be NULL and remove it from the uniqueness constraint.
- Allow for an InChI to be used in molecularFormula: widen the attribute from String [255] to String [1023] and adapt the attribute's description accordingly.
- Add a description attribute.
- Remove the relation with Facility.
- Rationale:
  - molecularFormula does not make sense for all samples, so it should be optional.
  - InChI provide a standardized representation for molecular formulas. The length constraint of 255 characters might be tight for some InChI.
  - A description is obviously useful.
  - It is not clear what the relation to Facility is supposed to mean.
- See: #239

# Make Relationship from Sample to Investigation many-to-many

- Rationale:
  - The same sample may be investigated independently in more than one investigation.
  - We should be able to search for all datasets / investigations related to a given sample.
  - At present this situation cannot be represented in the schema.
- Remove the many-to-one relation from Sample to Investigation.
- Add a new InvestigationSample class.
- Problem: the uniqueness constraint: the sample name will likely not be globally unique in all cases.
- Suggestion: add the pid to the constraint. That would change pid to be required (not NULL). Database update scripts would need to fill the field with some suitable default value.
- See: #231