Process Research & Development Ontology

# **Abstract**

# **Introduction**

## Why ontologies?

Standardization which:

Foundation of data interoperability ; facilitates data mining; enables machine learning

BFO

## What is process research & development?

= scope of the ontology

### standard operations and materials

unit operations

chemical roles – flocculants etc. (many roles are already defined elsewhere

### Workflow Domains



Figure 1 – review.

## Current State

What is already available

# **Workflows**

## Literature

## SINGLETON Reaction

Standard pattern of a reaction

## Reaction Screening

## Design of Experiment

## Fate and purge studies

## Mechanistic and kinetic determinations

## Polymorph screening

# **Use Cases**

Part of above – do we need to do all?

# **Conclusion**