



# Workflow based data integration for drug discovery

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**On behalf of the Open PHACTS Foundation**

**<http://www.openphactsfoundation.org>**

# Open PHACTS

Open Pharmacological Space





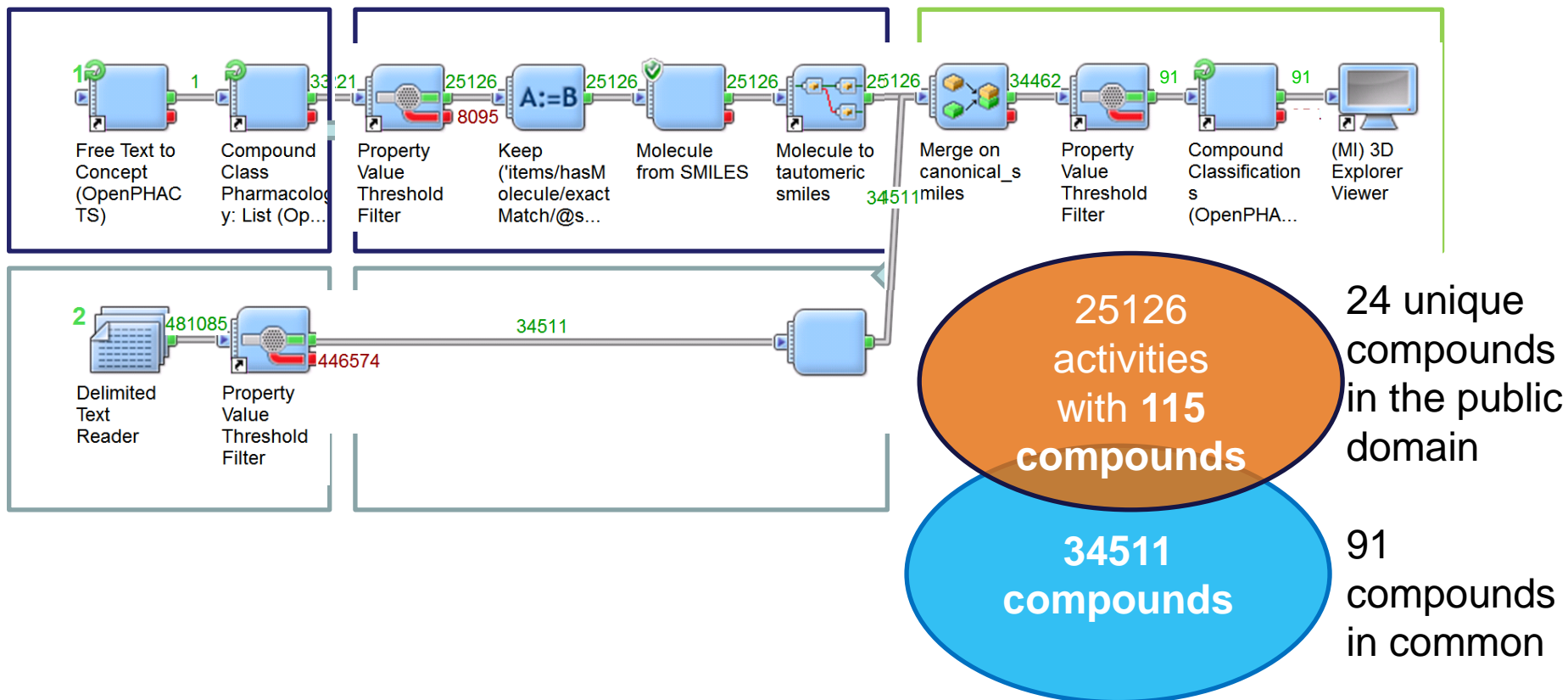
# Scientific Question

- ❖ What antiviral compounds and their classifications are available from public and proprietary compound activity databases ?
- ❖ Workflow Solution:
  - Run compound searches using Open PHACTS and in-house databases
  - Integrate results
  - View data



# Workflow Solution

## e.g. Knime, Pipeline Pilot









- ✦ Open PHACTS API documentation:  
<https://dev.openphacts.org/docs/1.5>
- ✦ Biovia Pipeline Pilot component collection:  
<https://exchange.sciencecloud.com>
- ✦ Knime nodes:  
<https://github.com/openphacts/OPS-Knime>
- ✦ Drug discovery FAQs: Workflows for answering multidomain drug discovery questions:  
<http://dx.doi.org/10.1016/j.drudis.2014.11.006>