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Implementation of automated processes at Philip Morris International R&D using Pipeline Pilot

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(Part of Philip Morris International group of companies)

Biovia London 8 June 2017

Pipeline Pilot use at PMI

We develop PP protocols to

- improve collecting data from smoke or aerosol complex matrices
- handle and calculate chemical structures
- automate analytical processes

and we post them for users on

Biovia Webport.

PMI R&D, Neuchatel, Switzerland

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Reduced-Risk Products

>800°C

Distillation / Pyrolysis / Combustion

more than 6000 constituents

<350°C

Heating not Burning

Aerosol

reduced level of constituents

Some of these constituents are categorized as harmful and potentially harmful constituents (HPHCs)

Reduced-Risk Products ("RRPs") is the term we use to refer to products that present, are likely to present, or have the potential to present less risk of harm to smokers who switch to these products versus continued smoking. We have a range of RRPs in various stages of development, scientific assessment and commercialization. Because our RRPs do not burn tobacco, they produce far lower quantities of harmful and potentially harmful compounds than found in cigarette smoke.

Integrated ChemoInformatics Platforms

Aerosol

Smoking machines generate aerosols that are trapped and collected.

Analytical chemistry

Aerosols are analyzed for HPHCs.

Computational chemistry

Constituents are deposited in database, clustered and calculated.

Systems Toxicology, Clinics

Studies to advance scientific and medical knowledge are performed. Toxicological and Clinical assessments are done.

PP used for:

CASI

Structural Identification

UCSD

Chemical and Spectra Registry

REPORTING

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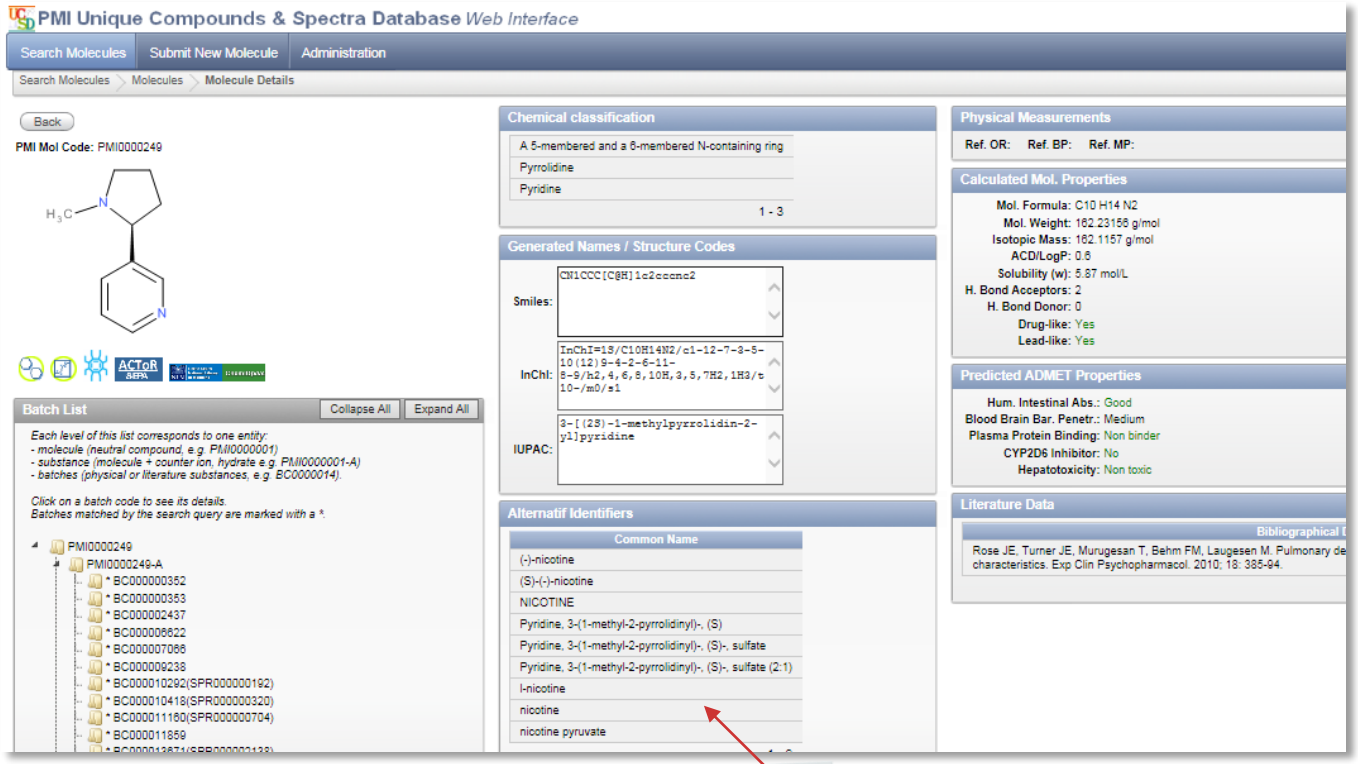
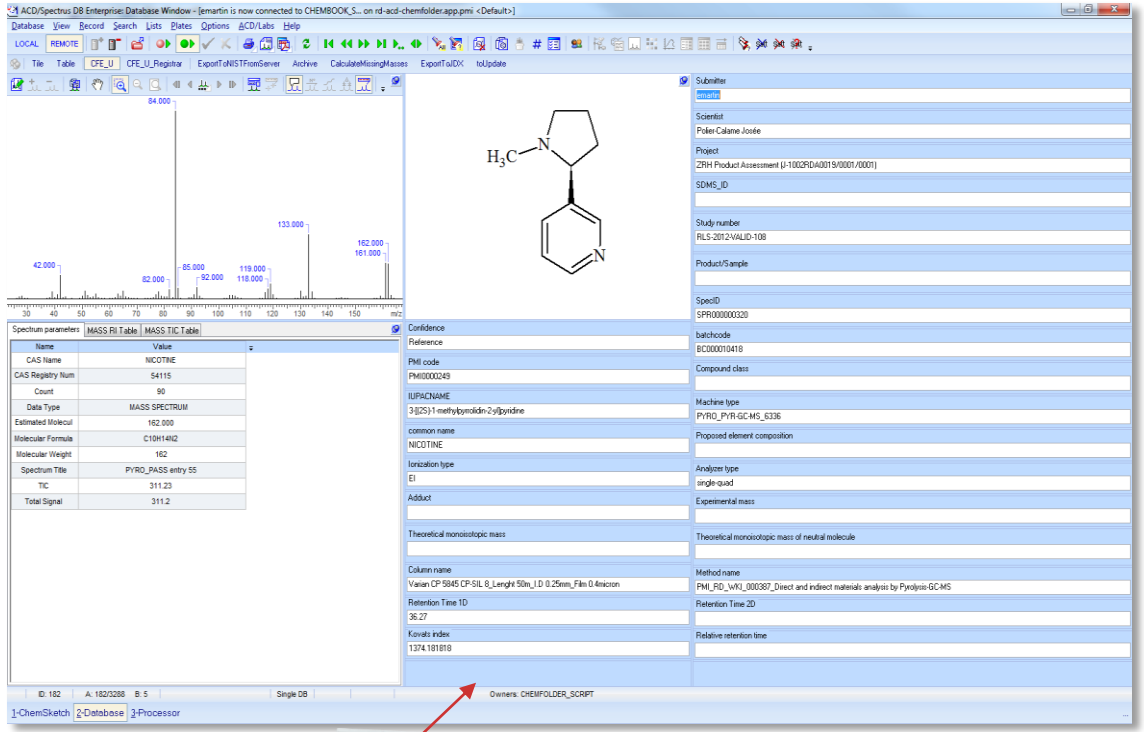
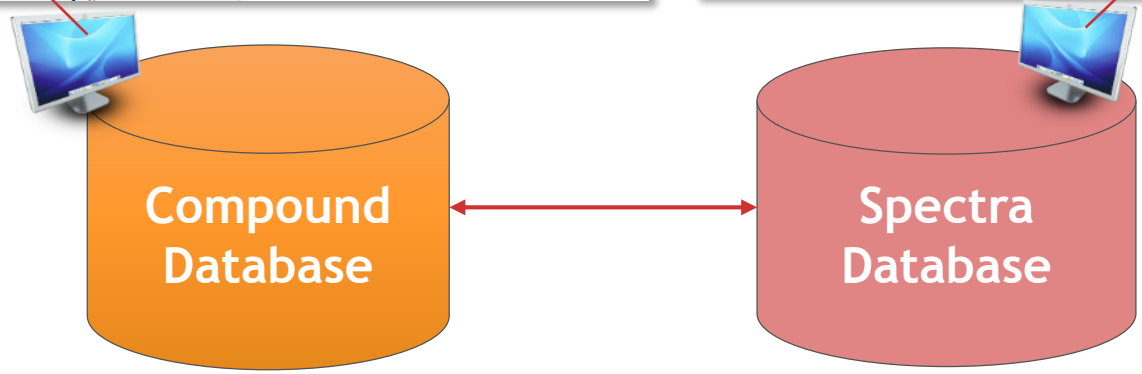
PMI Unique Compound & Spectra Database







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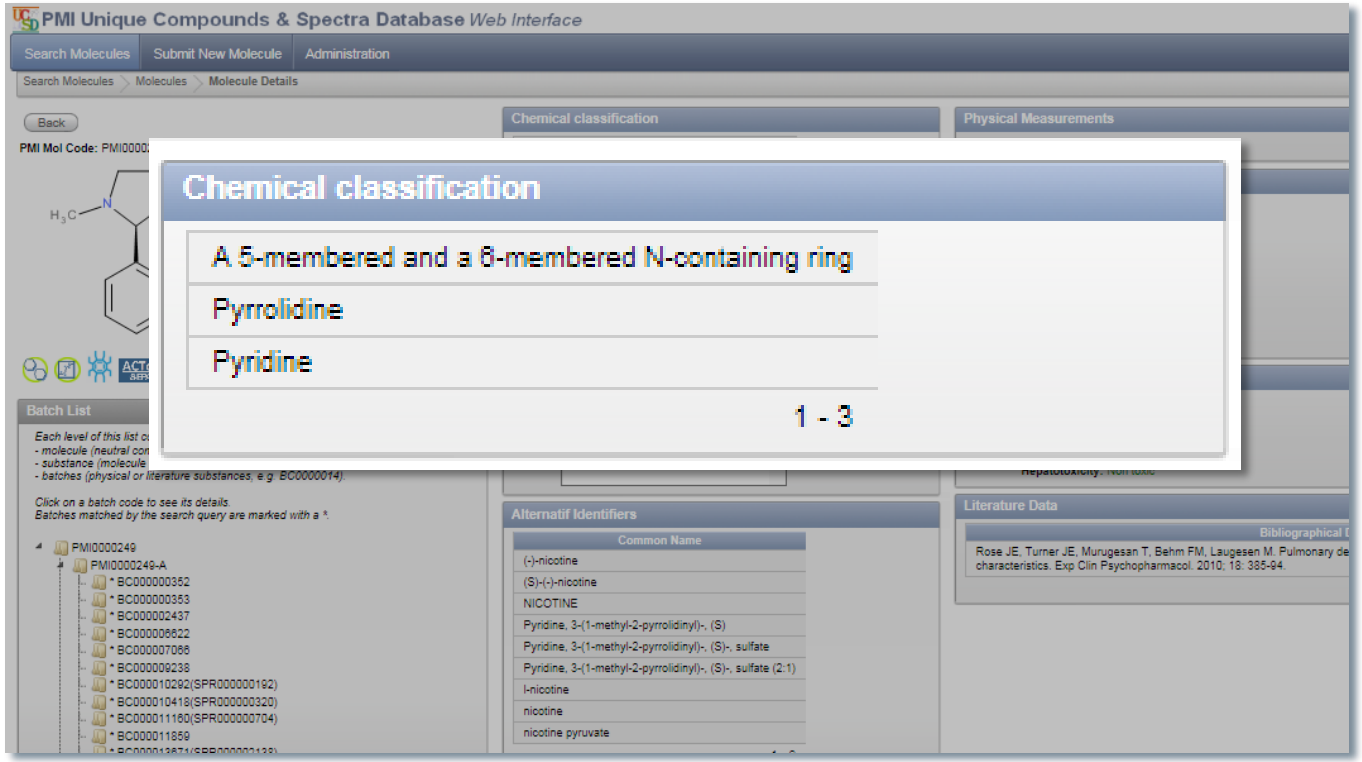
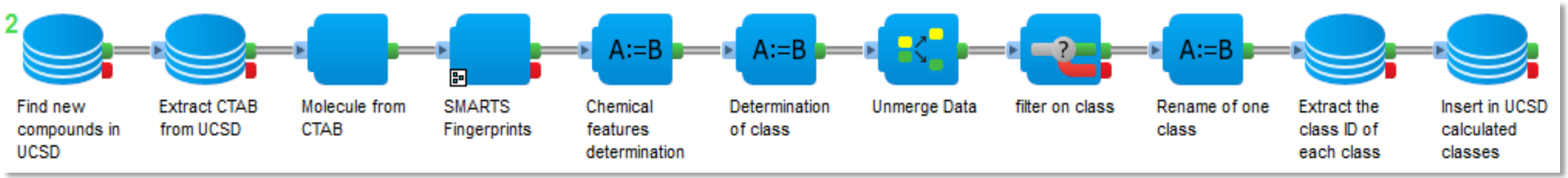
Martin et al., *J Cheminform*. 2012; 4(1)

Overnight protocols to fulfill UCSD

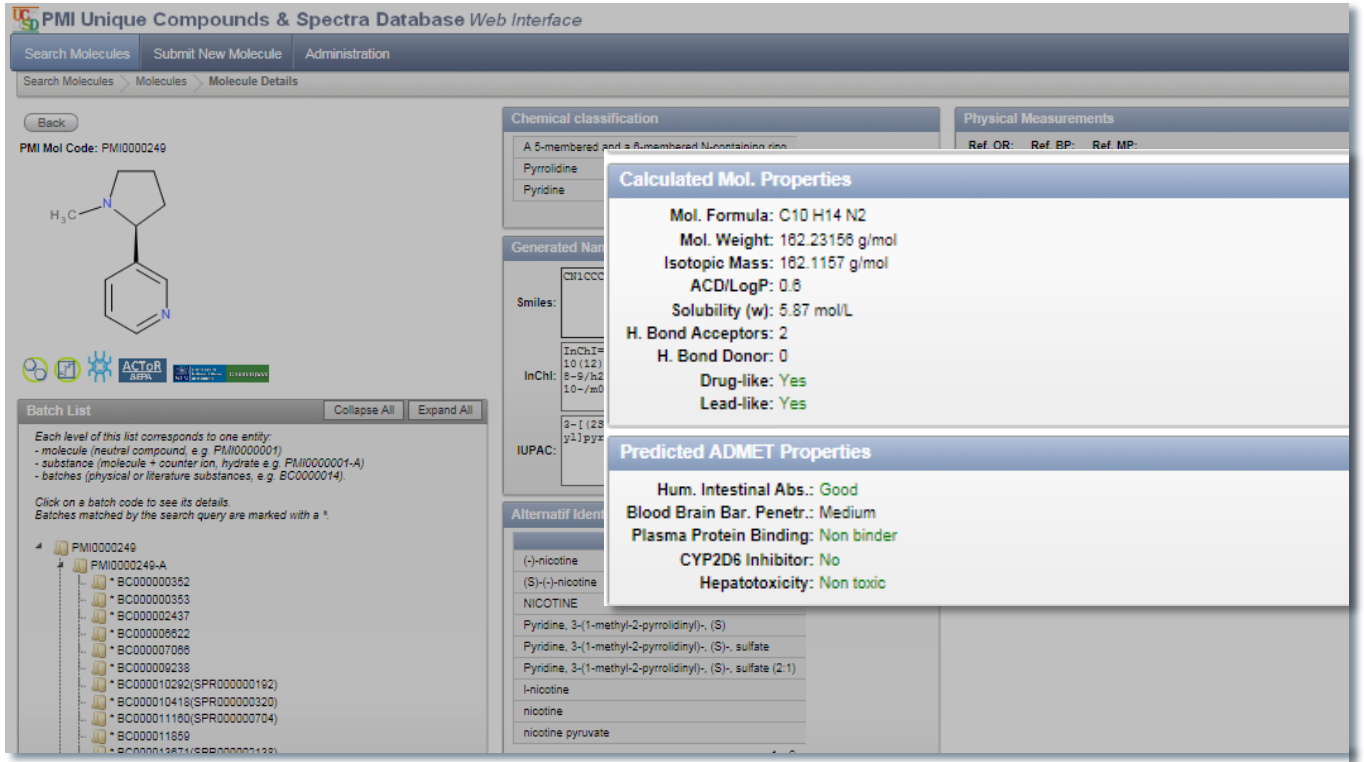
Protocol to determine to which chemical classes a compound belongs

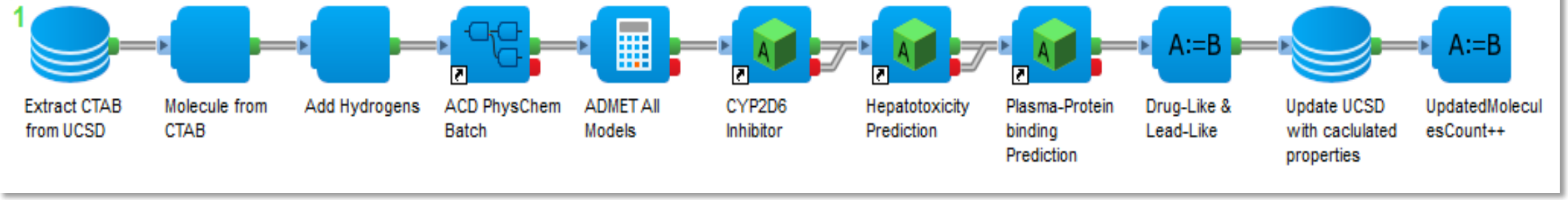




Compute physicochemical properties

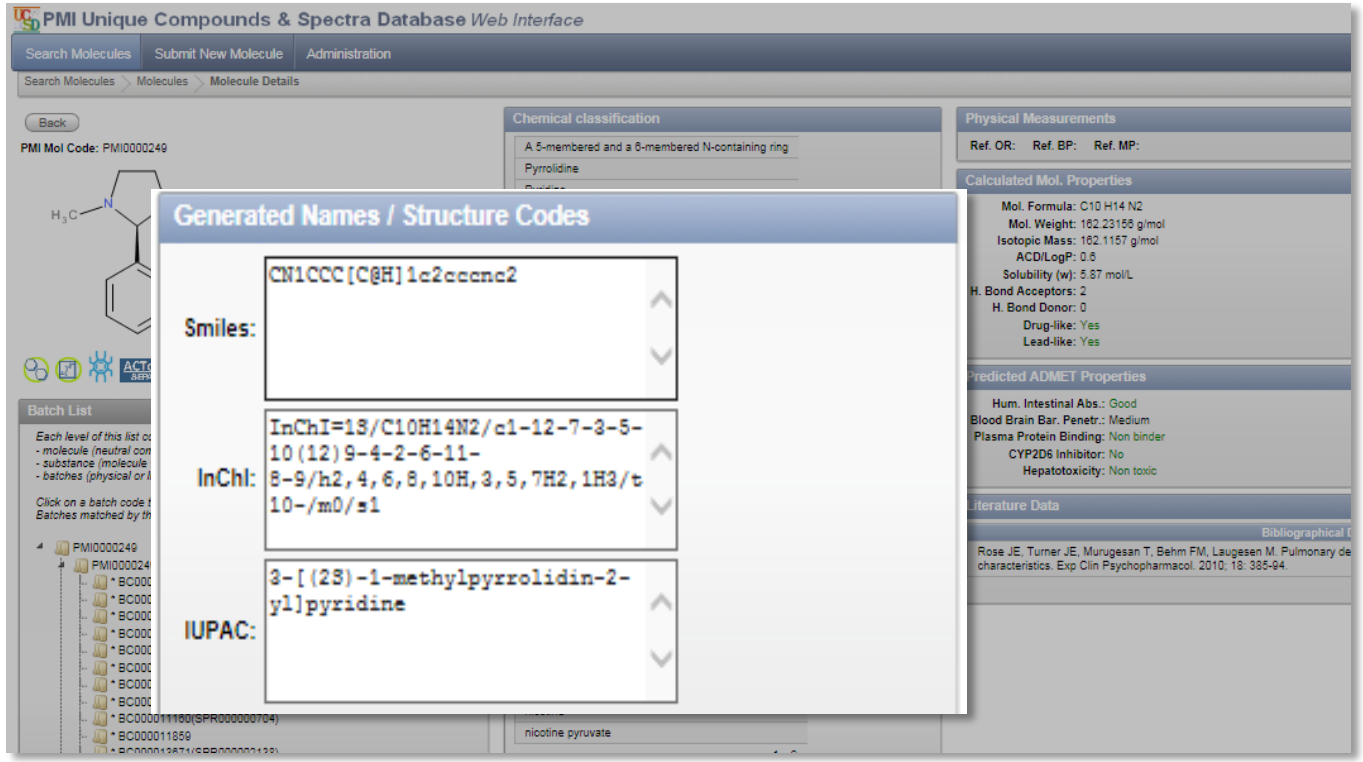
logP, water solubility, ADMET …

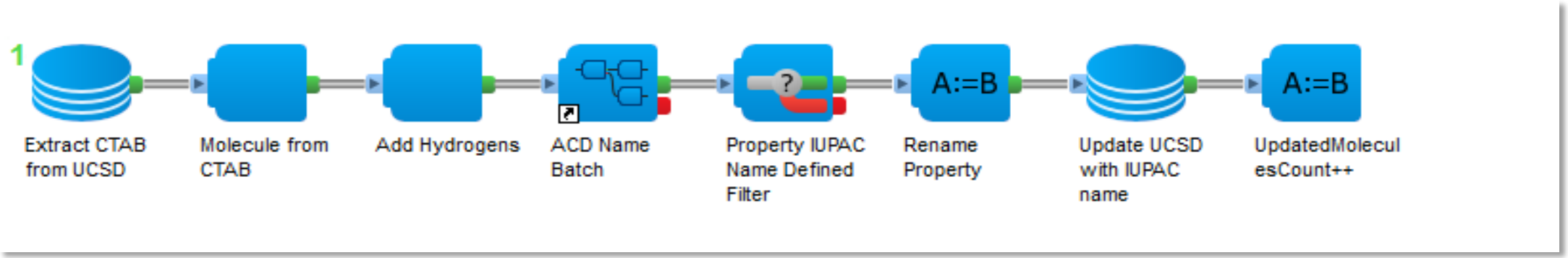




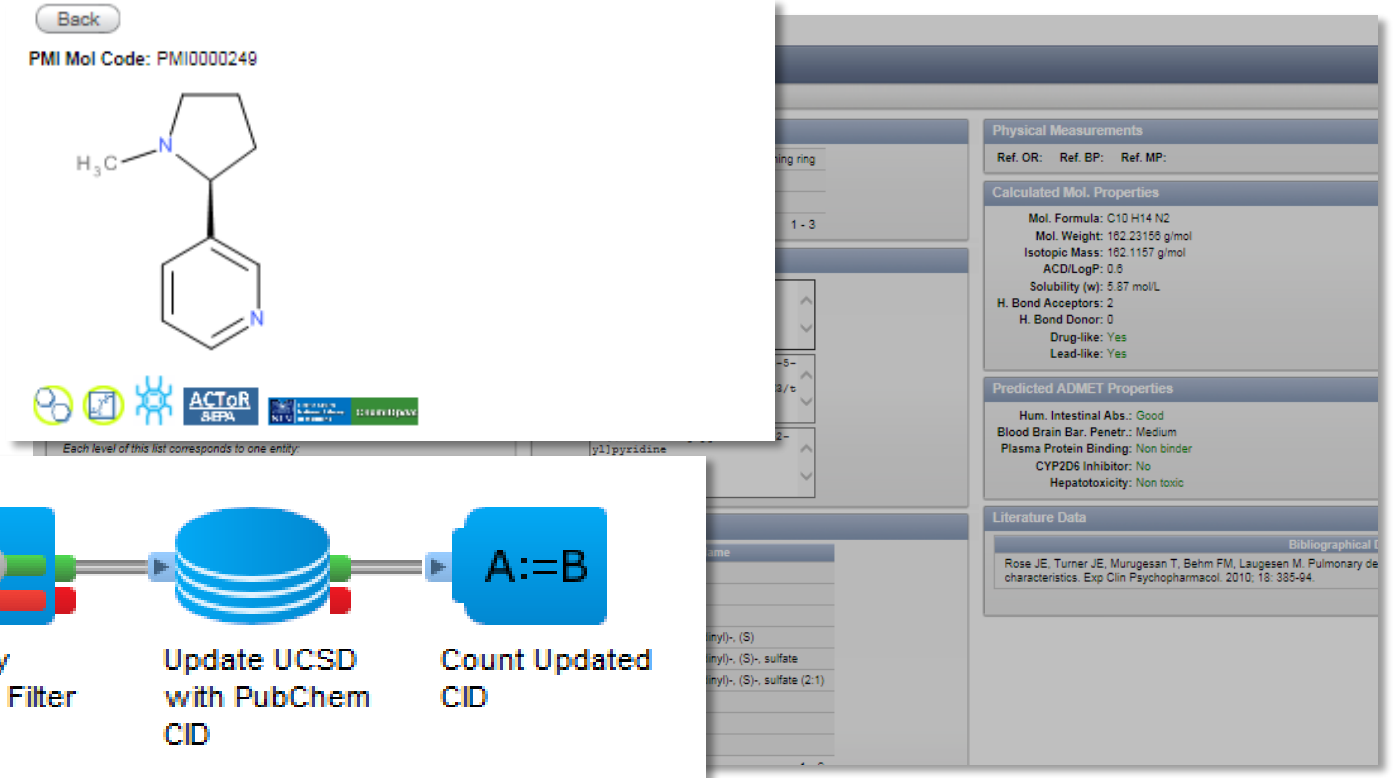
Naming

IUPAC name

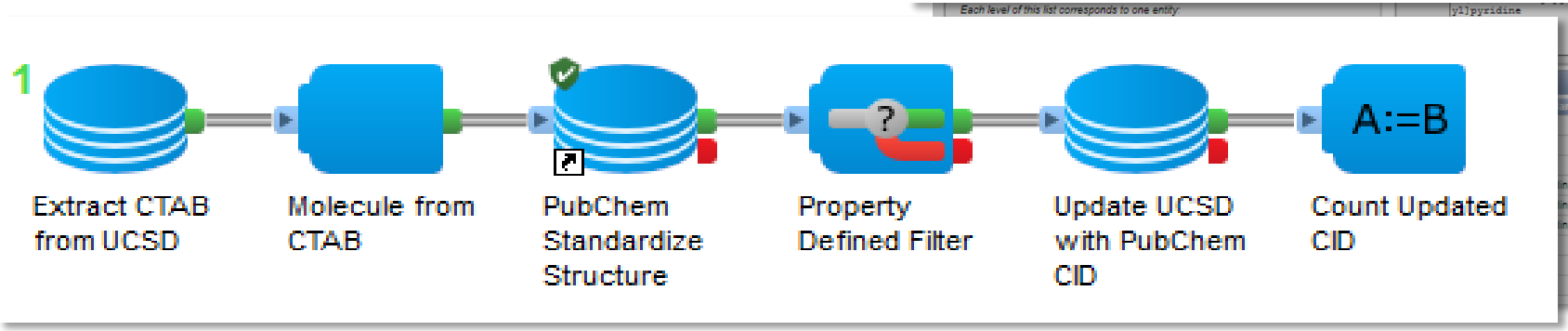




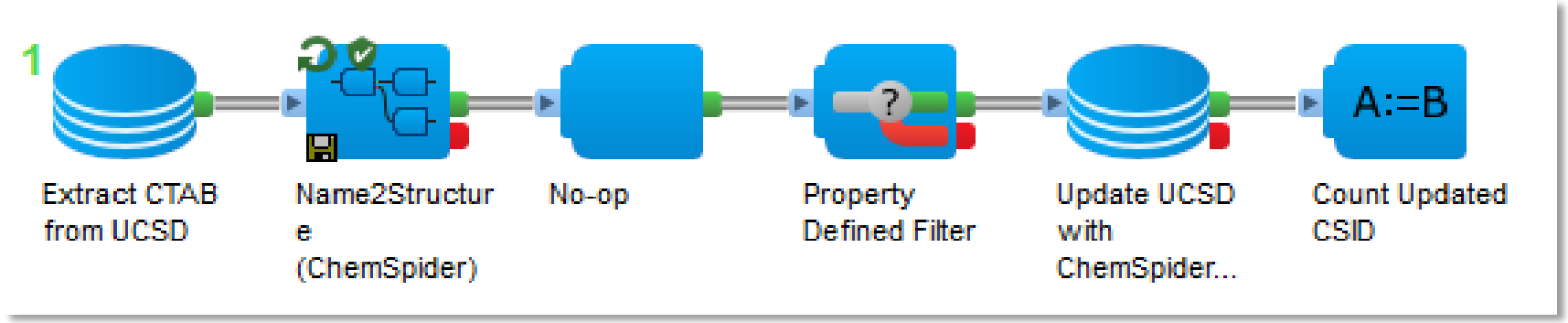
Links to other databases



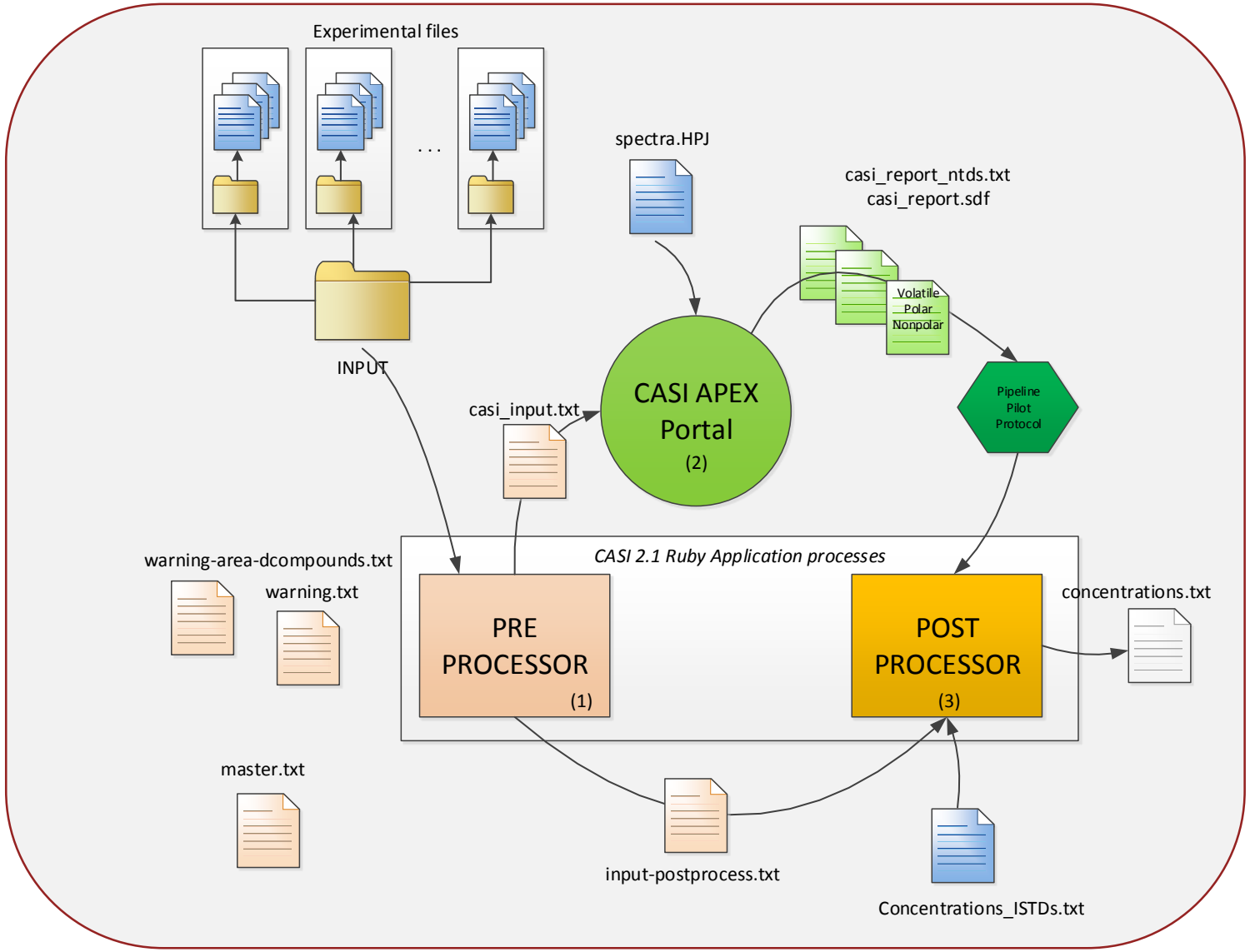
PubChem CID



ChemSpider CSID



PMI Computer-Assisted Structure Identification Platform



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Knorr et al., Anal Chem. 2013; 85(23)

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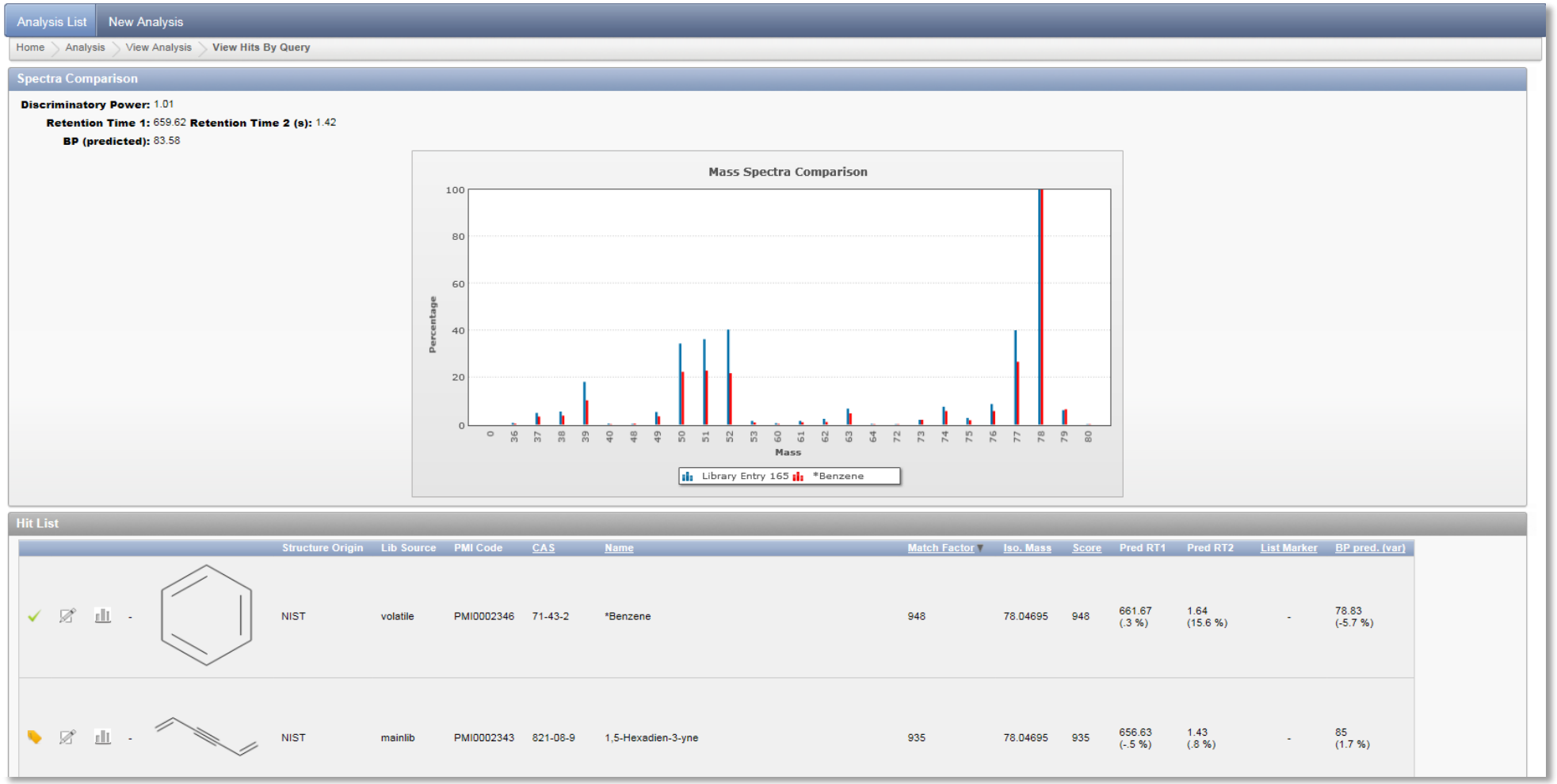

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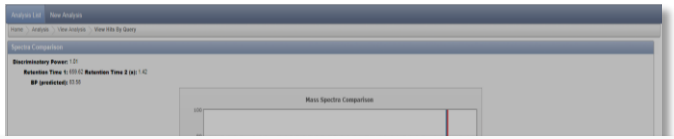
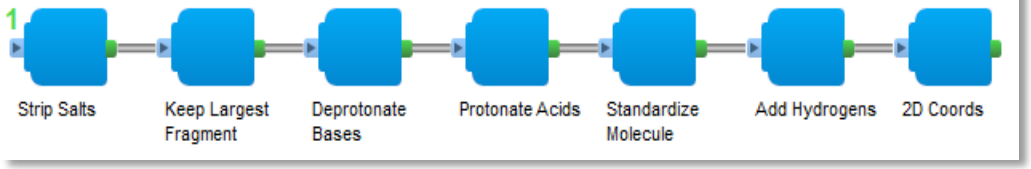
Protocols used in CASI process

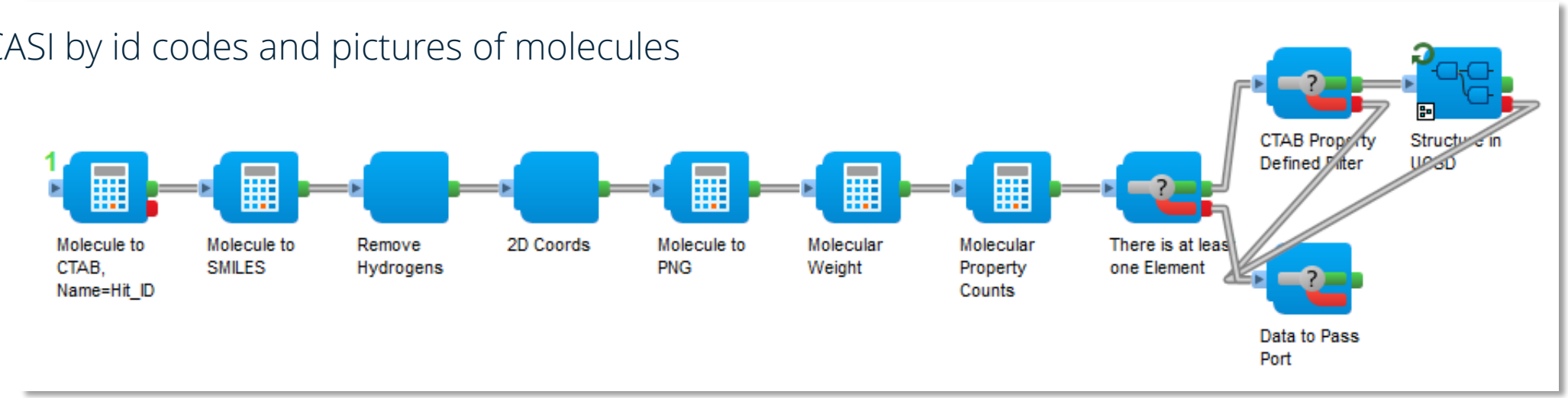


	Structure Origin	Lib Source	PMI Code	CAS	Name	Match Factor	Iso. Mass	Score	Pred RT1	Pred RT2	List Marker	BP pred. (var)
✓ -	NIST	volatile	PMI0002346	71-43-2	*Benzene	948	78.04695	948	661.67 (.3 %)	1.64 (15.6 %)	-	78.83 (-5.7 %)
-	NIST	mainlib	PMI0002343	821-08-9	1,5-Hexadien-3-yne	935	78.04695	935	656.63 (-.5 %)	1.43 (.8 %)	-	85 (1.7 %)

2D standardization of compounds



Updating data in CASI by id codes and pictures of molecules



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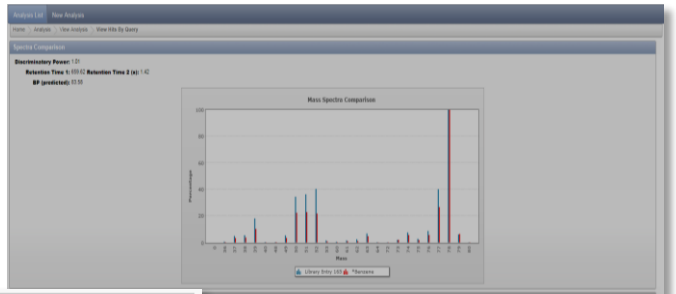
Protocols used in CASI process

Calculation of Boiling Point using PP and ACD/Labs



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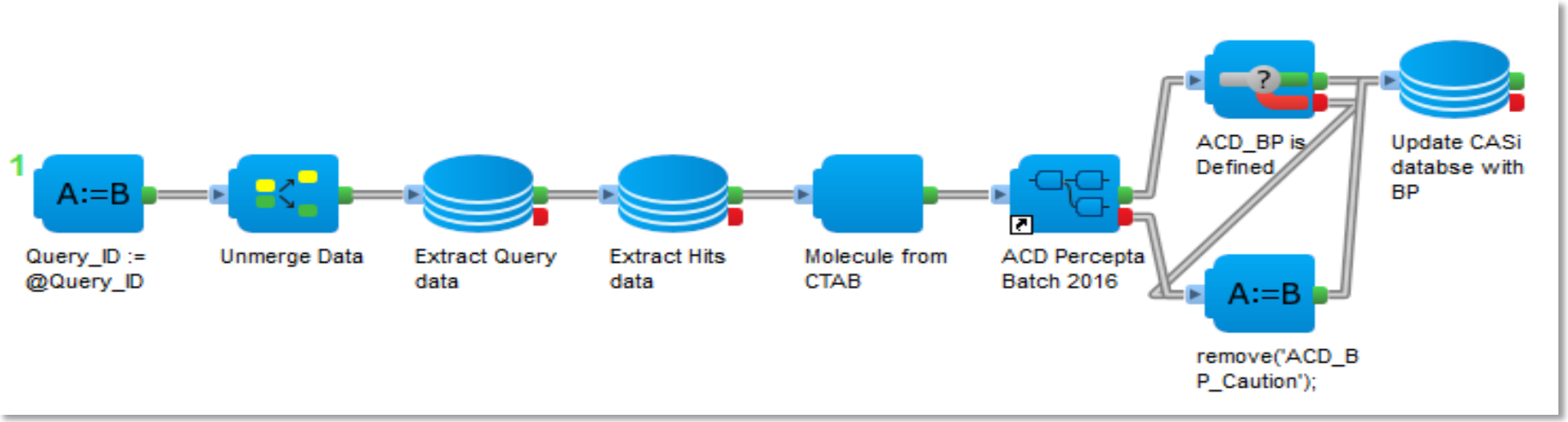

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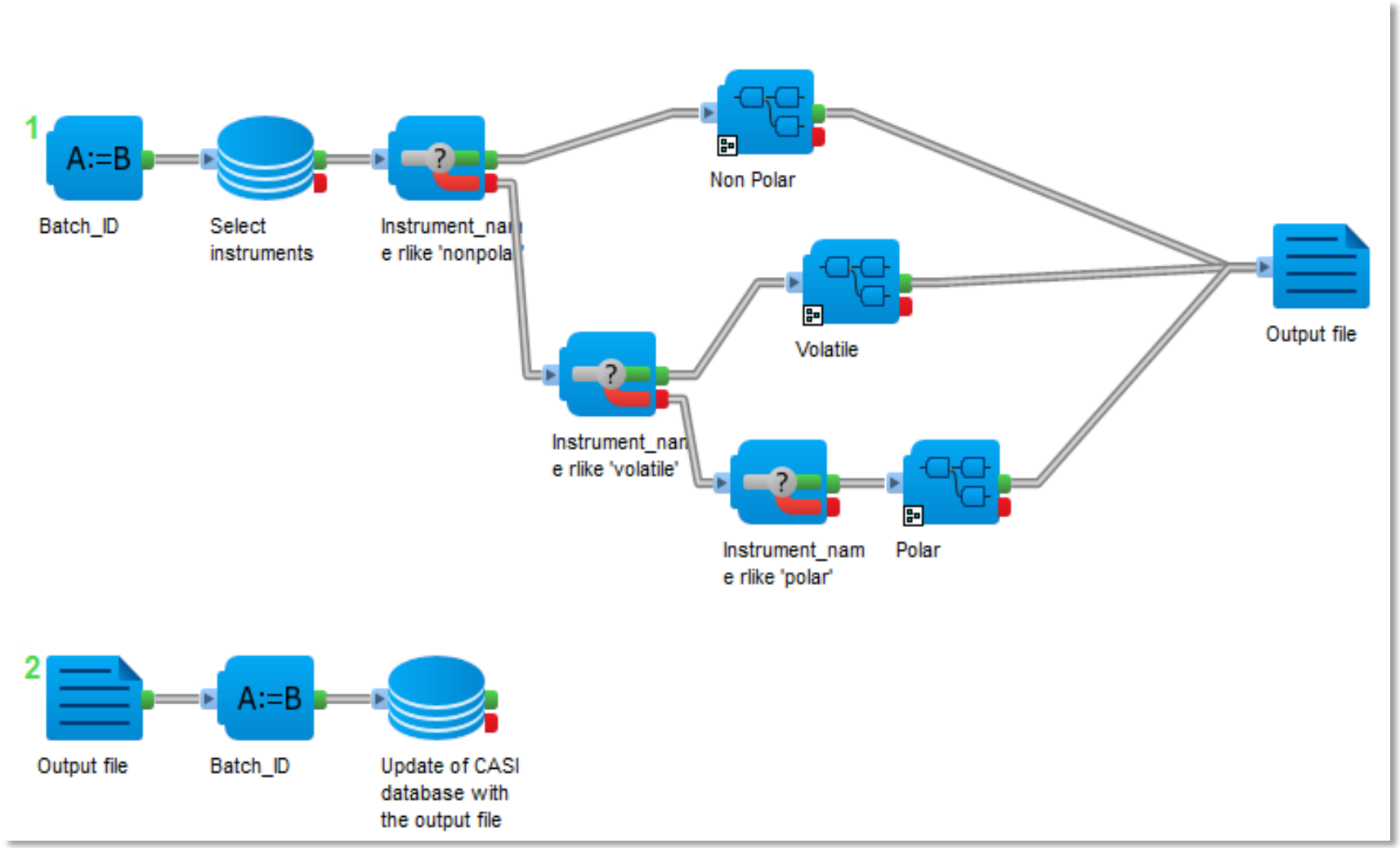
Protocols used in CASI process

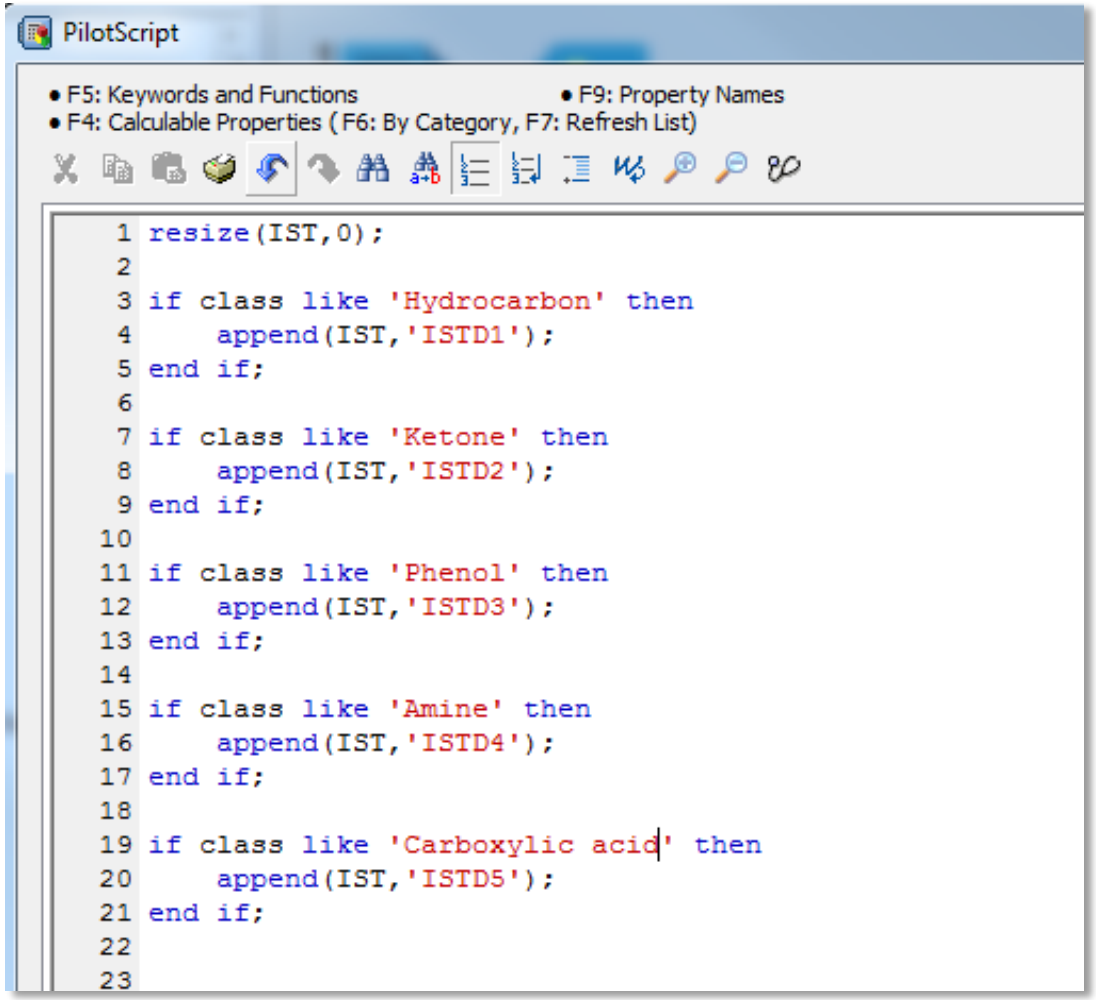
Determination of which internal standard to use to semi-quantify compounds concentrations



Protocols used in CASI process

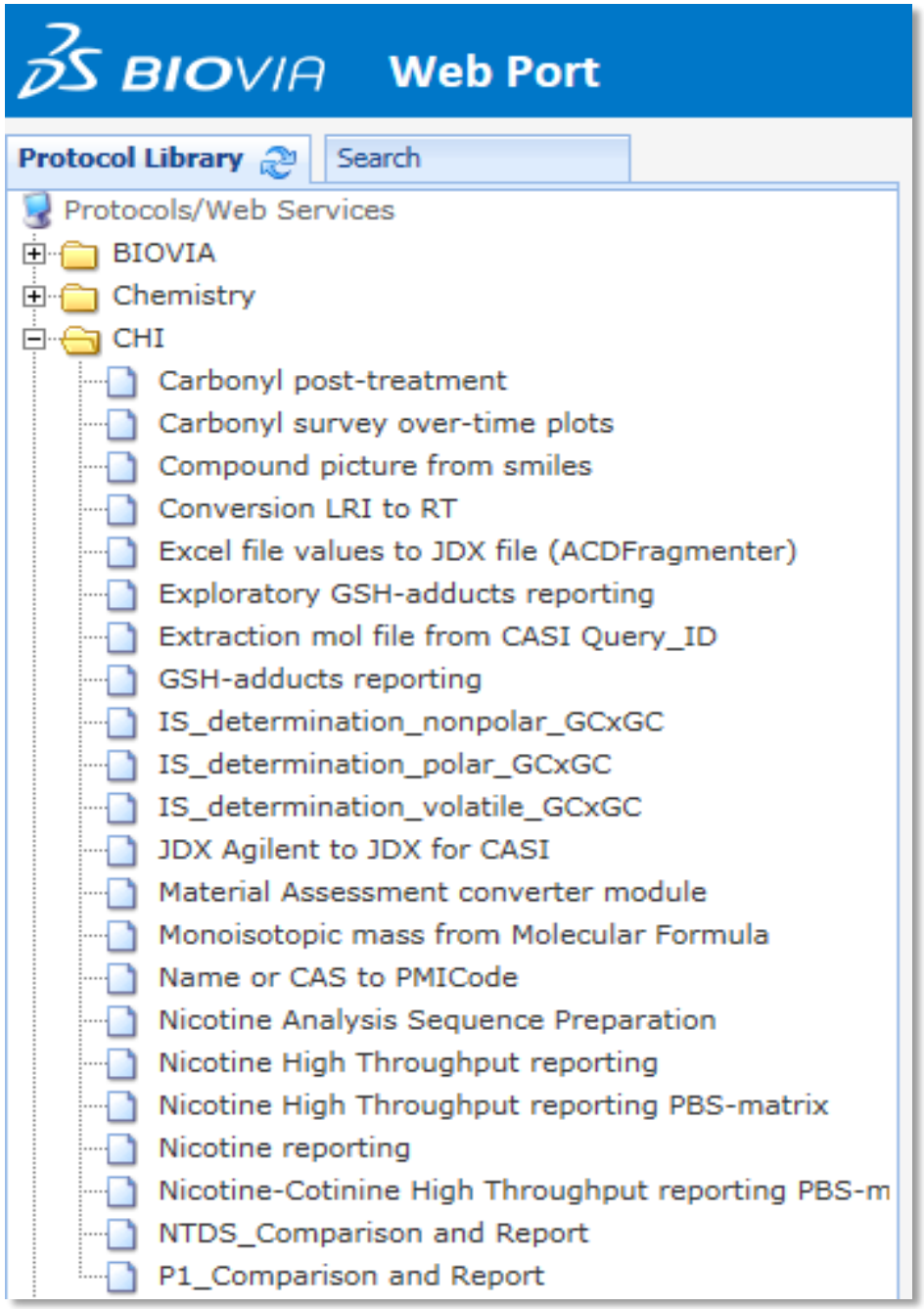
Example of script used in

Non Polar sub-protocol



Web Port applications

List of protocols used via webport



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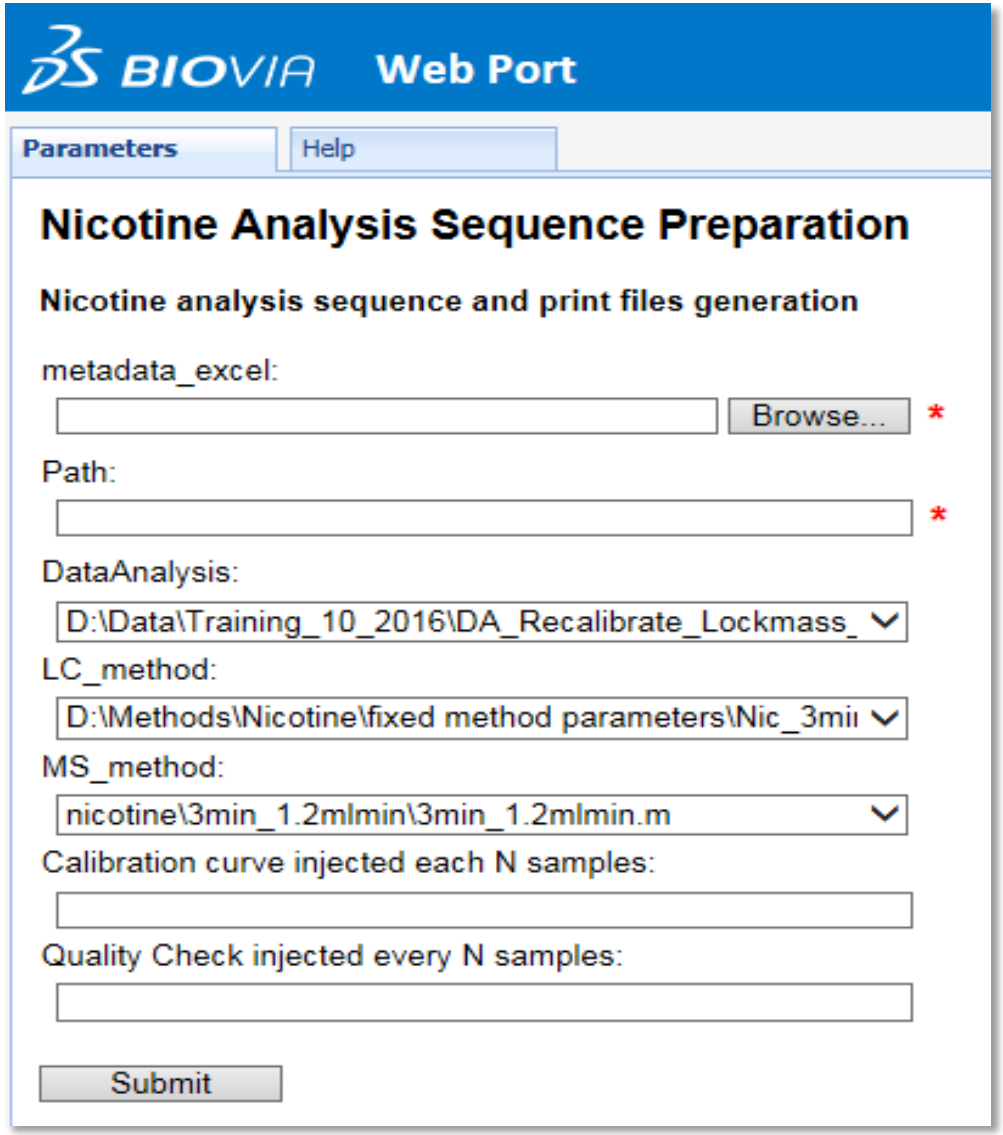
Nicotine Analysis Sequence Preparation

This protocol is used to prepare a sequence of input to the analytical instrument

and

to create a file to automatically print labels on vials



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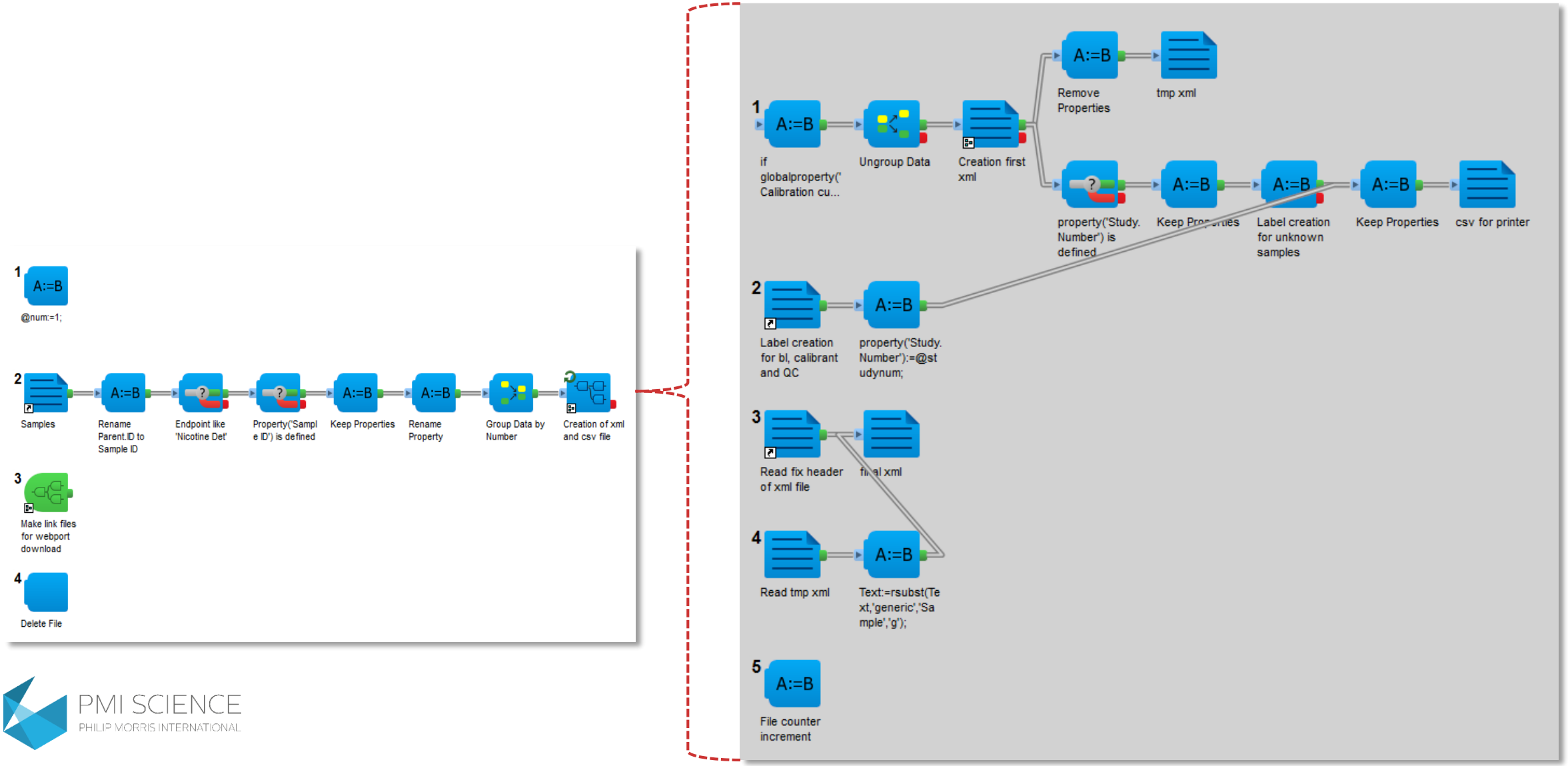
Nicotine Analysis Sequence Preparation



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Conclusion

At Philip Morris R&D we use Biovia Pipeline Pilot scripts to automate processes in analytical and computational chemistry.

We provide users with over 15 Webport scripts helping them sequence processing and reporting.

Thank you for your attention.

Questions?