Computing Stable Models for Nonmonotonic Existential Rules

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THE OWLS ARE NOT WHAT THEY SEEM

- OWL widely used for authoring biomedical ontologies

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GO the Gene Ontology

NCIthesaurus

BioPortal

SNOMED INTERNATIONAL

- Not marked for its ability to model cyclic structures
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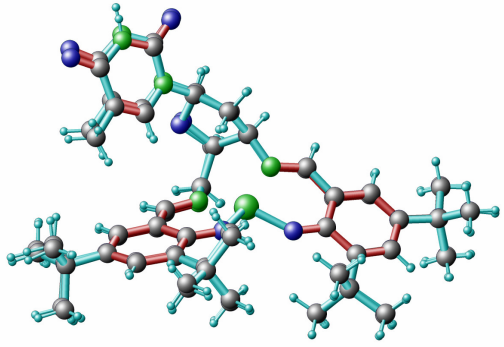

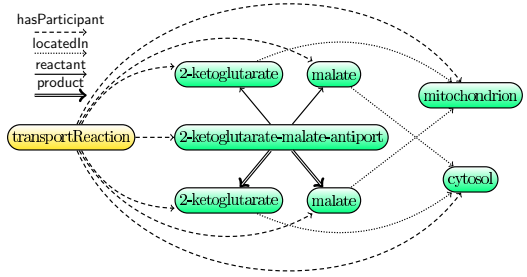

NONMONOTONIC EXISTENTIAL RULES

- Rules with nonmonotonic negation in the body and existentials in the head

$$B_1 \wedge \ldots \wedge B_n \wedge \ \mathbf{not}\ B_{n+1} \wedge \ldots \wedge \ \mathbf{not}\ B_m \rightarrow \exists \mathbf{y}.H_1 \wedge \ldots \wedge H_k$$

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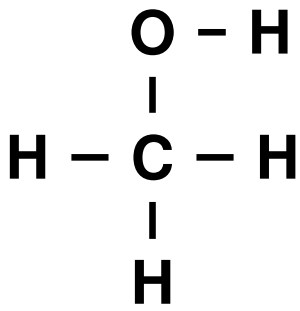
  - Stable model semantics supported by many tools: DLV, clasp, ...

Classification of Structured Objects I



Methanol molecule

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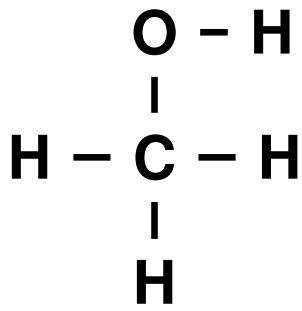

Methanol molecule

$$\text{methanol}(x) \rightarrow \exists_{i=1}^{6} y_i.\ \wedge_{i=1}^{6} \text{hasAtom}(x, y_i) \wedge c(y_1) \wedge o(y_2) \wedge \wedge_{i=3}^{6} h(y_i) \wedge \wedge_{i=2}^{5} \text{bond}(y_1, y_i) \wedge \text{bond}(y_2, y_6)$$

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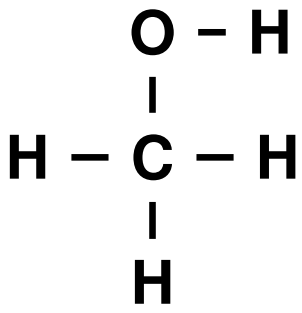

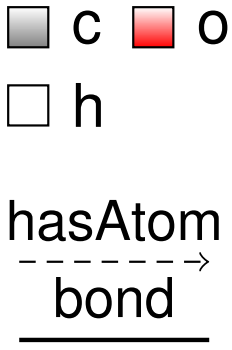

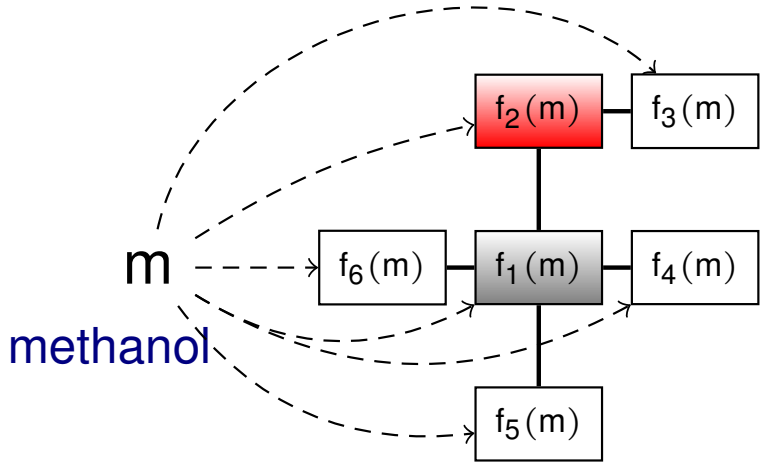

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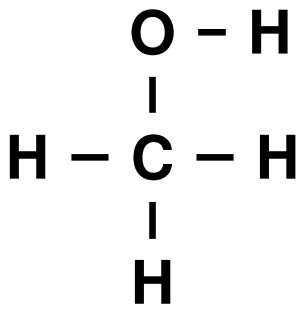

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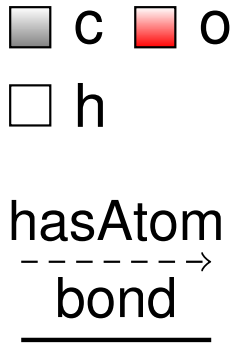

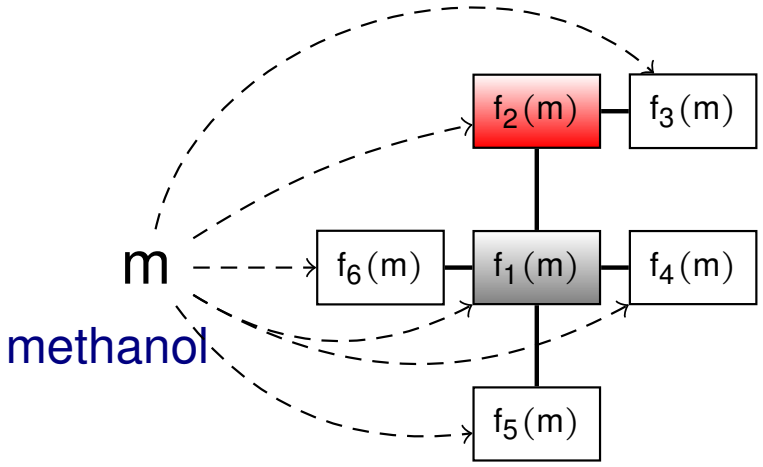

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$$\wedge_{i=1}^{3}\ \text{hasAtom}(x, z_i) \wedge c(z_1) \wedge o(z_2) \wedge h(z_3) \wedge \text{bond}(z_1, z_2) \wedge \text{bond}(z_2, z_3) \rightarrow \text{organicHydroxy}(x)$$

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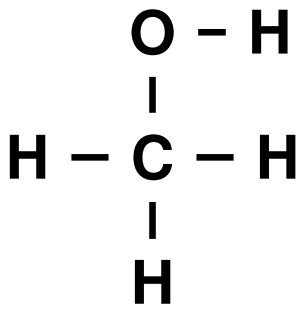

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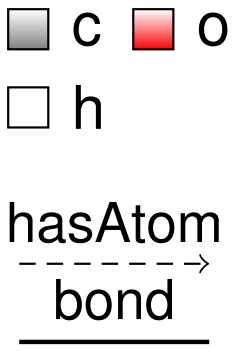

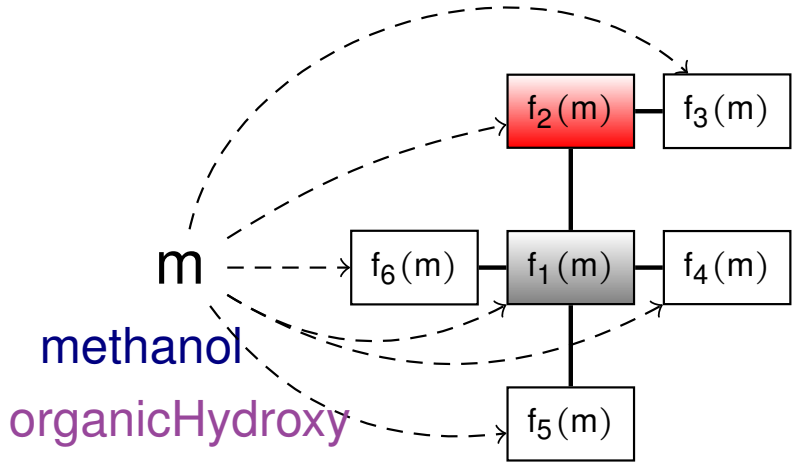

$$\text{methanol}(x) \rightarrow \exists^{6}_{i=1} y_i.\ \wedge^{6}_{i=1} \text{hasAtom}(x, y_i) \wedge c(y_1) \wedge o(y_2) \wedge \wedge^{6}_{i=3} h(y_i) \wedge \wedge^{5}_{i=2} \text{bond}(y_1, y_i) \wedge \text{bond}(y_2, y_6)$$

$$\wedge^{3}_{i=1} \text{hasAtom}(x, z_i) \wedge c(z_1) \wedge o(z_2) \wedge h(z_3) \wedge \text{bond}(z_1, z_2) \wedge \text{bond}(z_2, z_3) \rightarrow \text{organicHydroxy}(x)$$

$\text{methanol} \sqsubseteq \text{organicHydroxy}$ ✓

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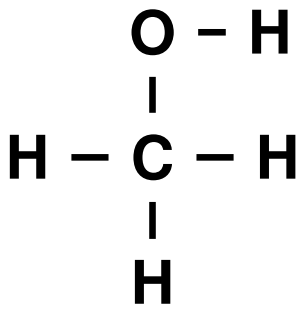

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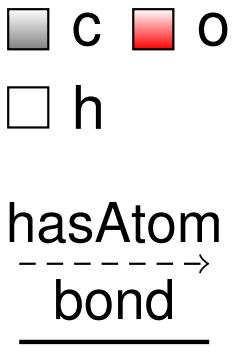

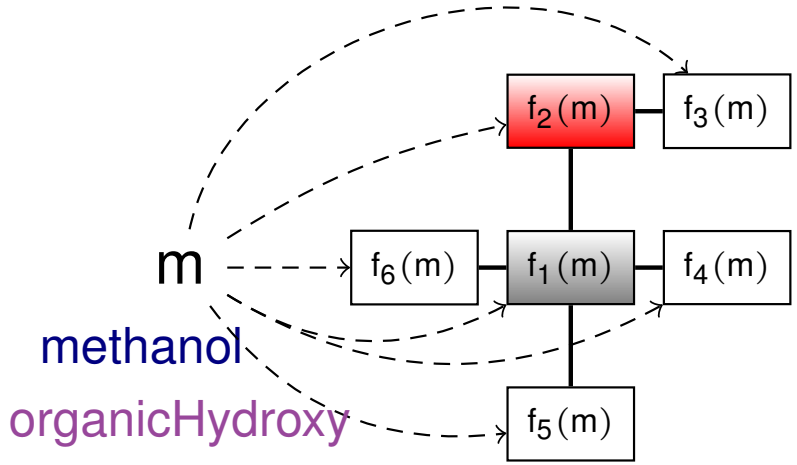

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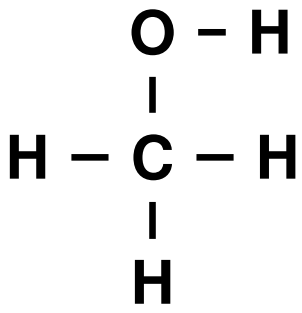

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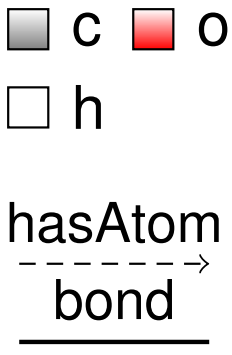

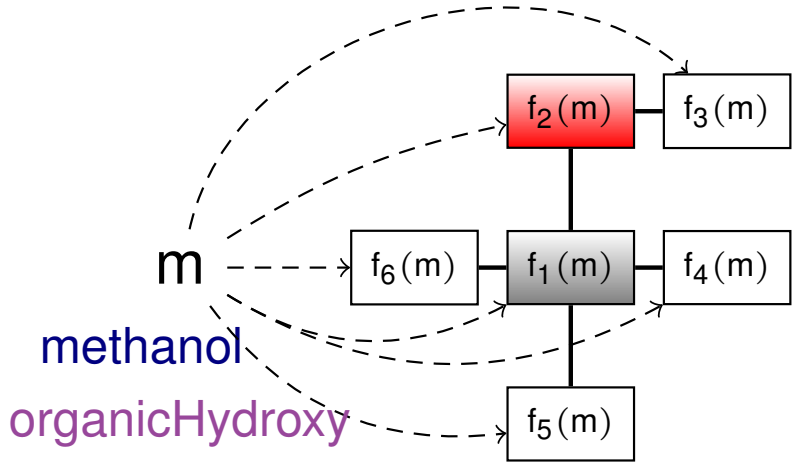

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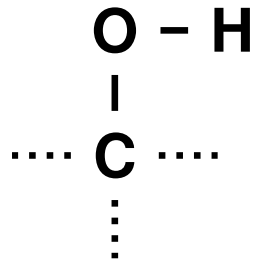
$$\text{hasAtom}(x, z) \wedge o(z) \rightarrow \text{hasOxygen}(x)$$

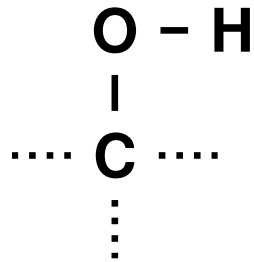
$\text{methanol} \sqsubseteq \text{organicHydroxy}$ ✓ $\text{methanol} \sqsubseteq \text{hasOxygen}$ ✓

CLASSIFICATION OF STRUCTURED OBJECTS II



Organic hydroxy group

Classification of Structured Objects II



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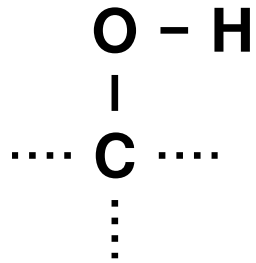
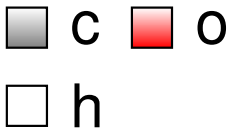
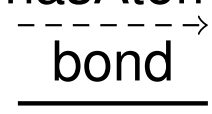
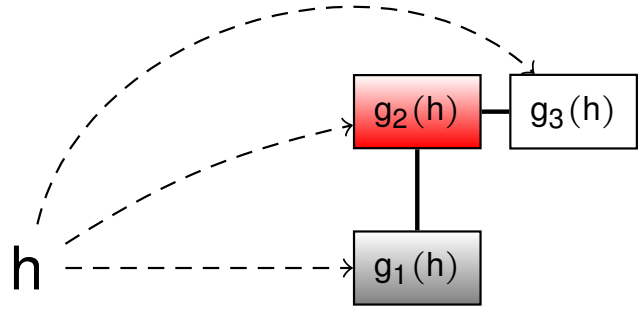


Organic hydroxy group



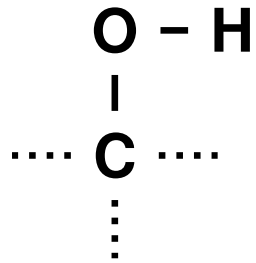




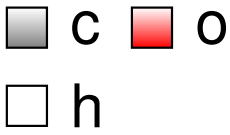
organicHydroxy

$$\text{organicHydroxy}(x) \rightarrow \exists_{i=1}^{3} y_i.\ \wedge_{i=1}^{3} \text{hasAtom}(x, y_i) \wedge \text{c}(y_1) \wedge \text{o}(y_2) \wedge \text{h}(y_3) \wedge \text{bond}(y_1, y_2) \wedge \text{bond}(y_2, y_3)$$

Classification of Structured Objects II

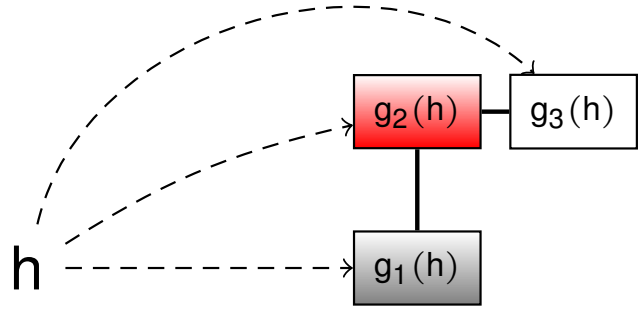


Organic hydroxy group



hasAtom

bond



organicHydroxy

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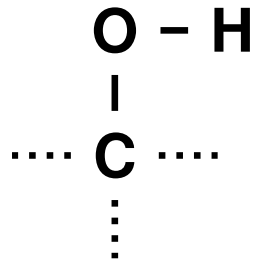
$$\text{hasAtom}(x, z) \wedge \text{o}(z) \rightarrow \text{hasOxygen}(x)$$

Classification of Structured Objects II



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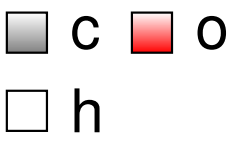

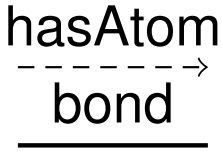

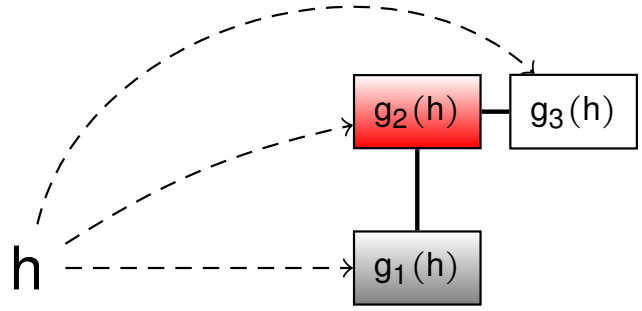

organicHydroxy

hasOxygen

$$\text{organicHydroxy}(x) \rightarrow \exists_{i=1}^{3} y_i.\ \wedge_{i=1}^{3} \text{hasAtom}(x, y_i) \wedge c(y_1) \wedge o(y_2) \wedge h(y_3) \wedge \text{bond}(y_1, y_2) \wedge \text{bond}(y_2, y_3)$$

$$\text{hasAtom}(x, z) \wedge o(z) \rightarrow \text{hasOxygen}(x)$$

$$\text{organicHydroxy} \sqsubseteq \text{hasOxygen}\ \checkmark$$

Incorrect Modelling

$$\text{methanol}(x) \rightarrow \exists_{i=1}^{6} y_i.\ \wedge_{i=1}^{6} \text{hasAtom}(x, y_i) \wedge \ldots \wedge \text{bond}(y_2, y_6)$$

$$\wedge_{i=1}^{3} \text{hasAtom}(x, z_i) \wedge \ldots \wedge \text{bond}(z_2, z_3) \rightarrow \text{organicHydroxy}(x)$$

$$\text{organicHydroxy}(x) \rightarrow \exists_{i=1}^{3} y_i.\ \wedge_{i=1}^{3} \text{hasAtom}(x, y_i) \wedge \ldots \wedge \text{bond}(y_2, y_3)$$

$$\text{hasAtom}(x, z) \wedge o(z) \rightarrow \text{hasOxygen}(x)$$

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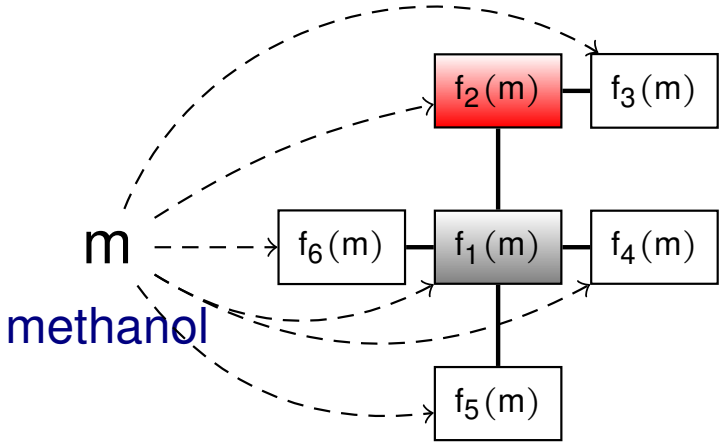


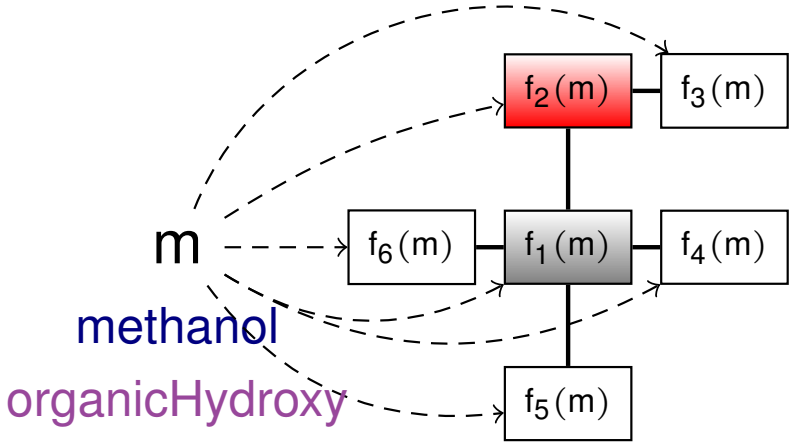
$$\text{methanol}(x) \rightarrow \exists_{i=1}^{6} y_i.\ \wedge_{i=1}^{6} \text{hasAtom}(x, y_i) \wedge \ldots \wedge \text{bond}(y_2, y_6)$$

$$\wedge_{i=1}^{3} \text{hasAtom}(x, z_i) \wedge \ldots \wedge \text{bond}(z_2, z_3) \rightarrow \text{organicHydroxy}(x)$$

$$\text{organicHydroxy}(x) \rightarrow \exists_{i=1}^{3} y_i.\ \wedge_{i=1}^{3} \text{hasAtom}(x, y_i) \wedge \ldots \wedge \text{bond}(y_2, y_3)$$

$$\text{hasAtom}(x, z) \wedge o(z) \rightarrow \text{hasOxygen}(x)$$

Incorrect Modelling



$$\text{methanol} \sqsubseteq \text{organicHydroxy}\ \checkmark$$

$$\text{methanol}(x) \rightarrow \exists_{i=1}^{6} y_i.\ \wedge_{i=1}^{6} \text{hasAtom}(x, y_i) \wedge \ldots \wedge \text{bond}(y_2, y_6)$$

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$$\text{hasAtom}(x, z) \wedge o(z) \rightarrow \text{hasOxygen}(x)$$

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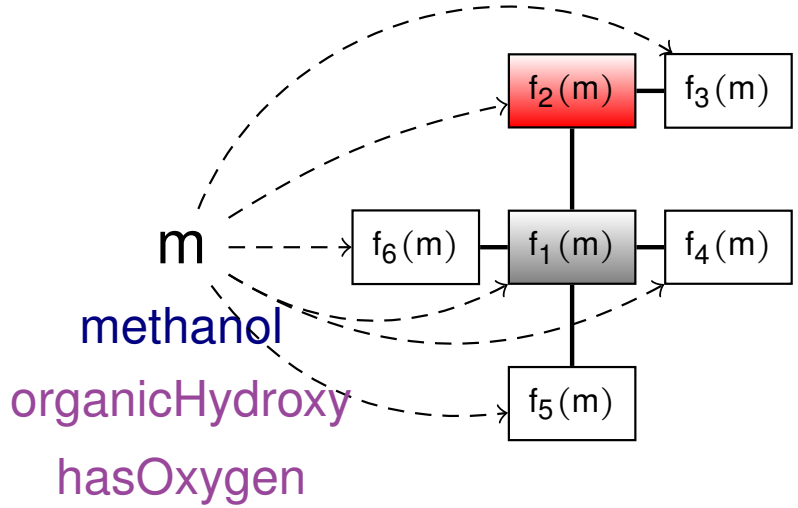

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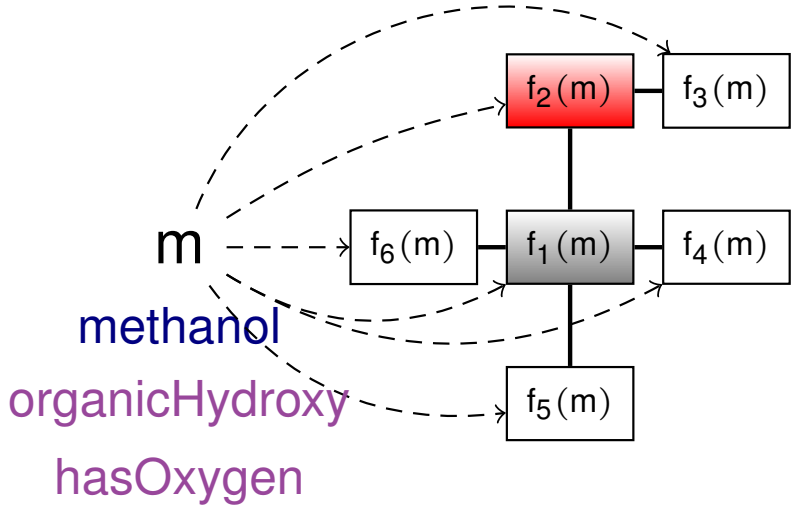

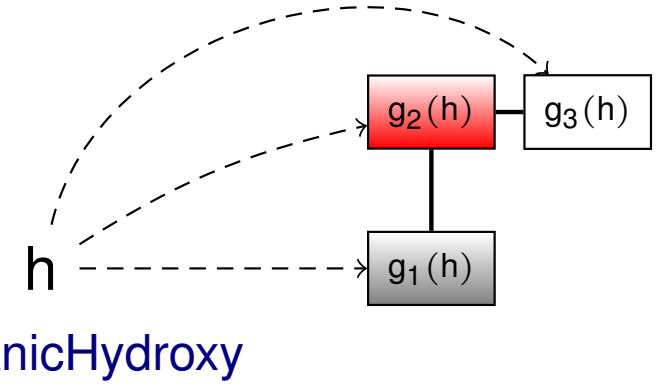

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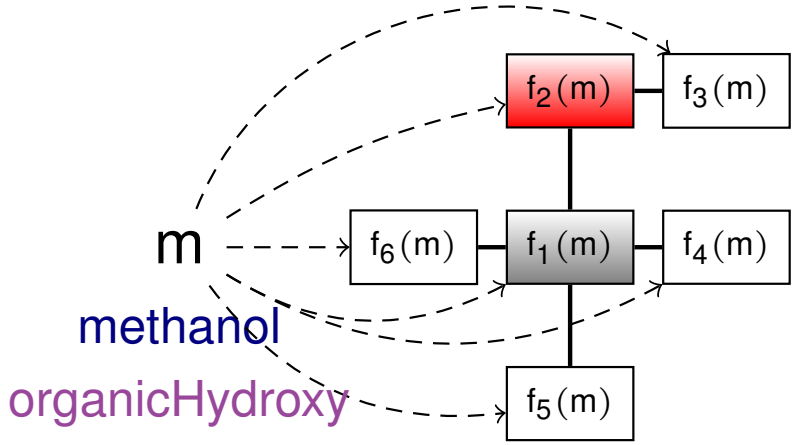

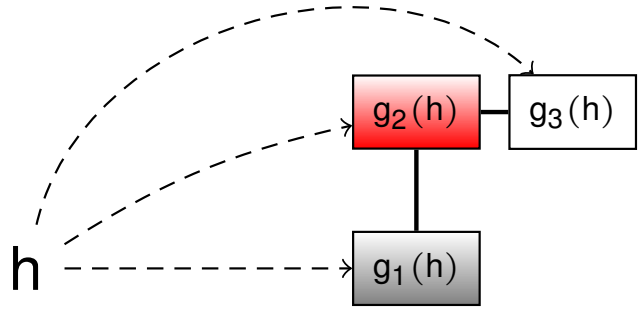

$$\text{organicHydroxy} \sqsubseteq \text{hasOxygen} \checkmark$$

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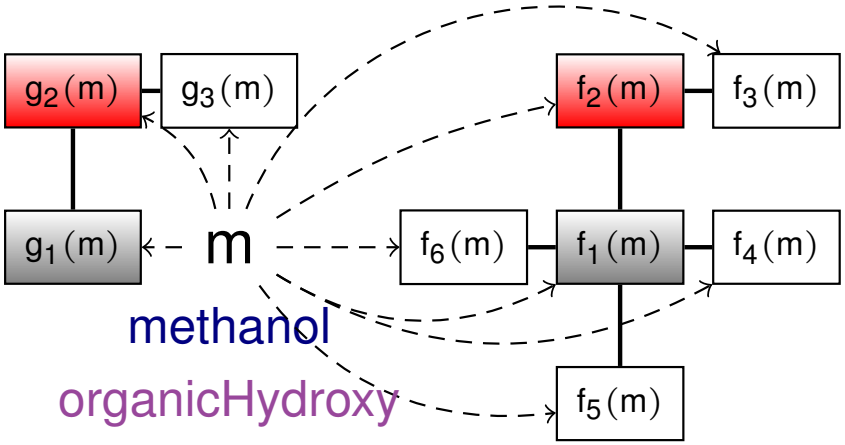

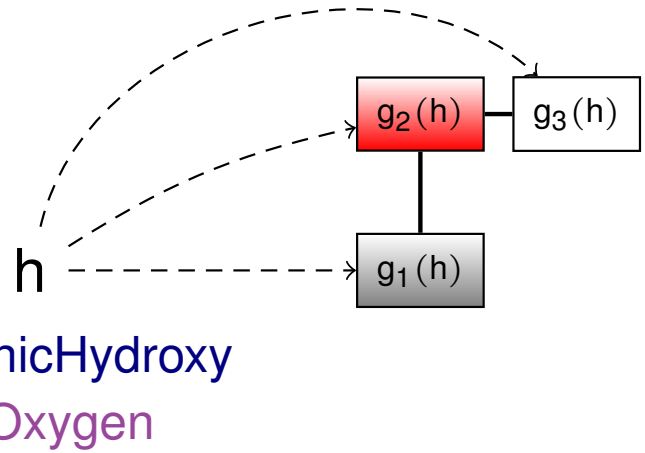

$$\text{methanol} \sqsubseteq \text{hasOneCarbon}\ \text{✘}$$

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Repair With Auxiliary Predicates

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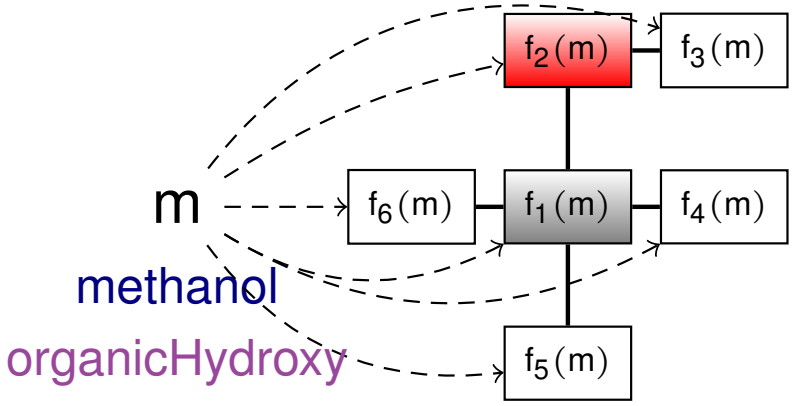

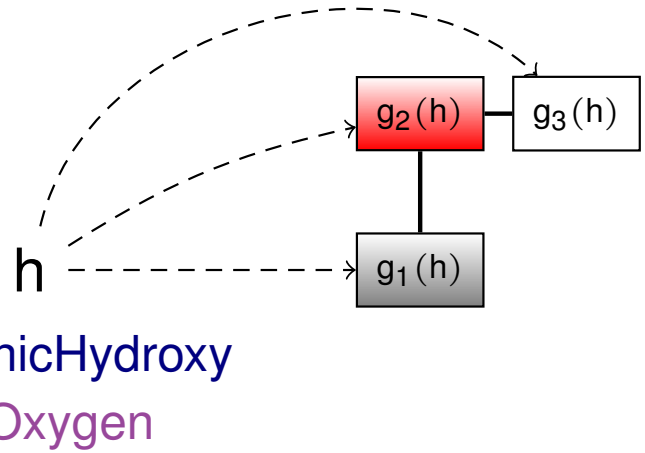

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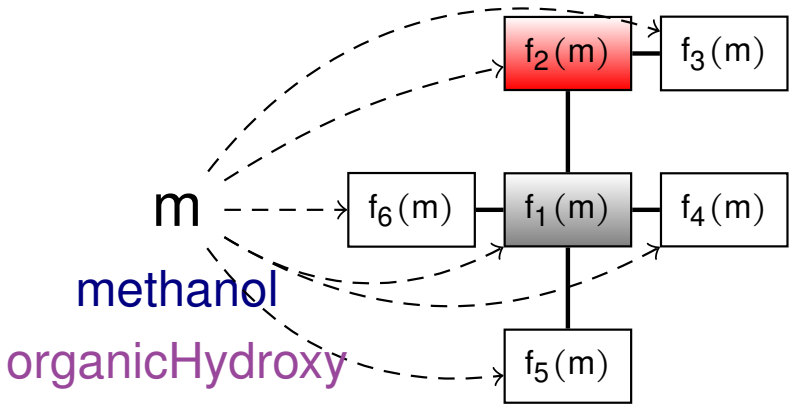

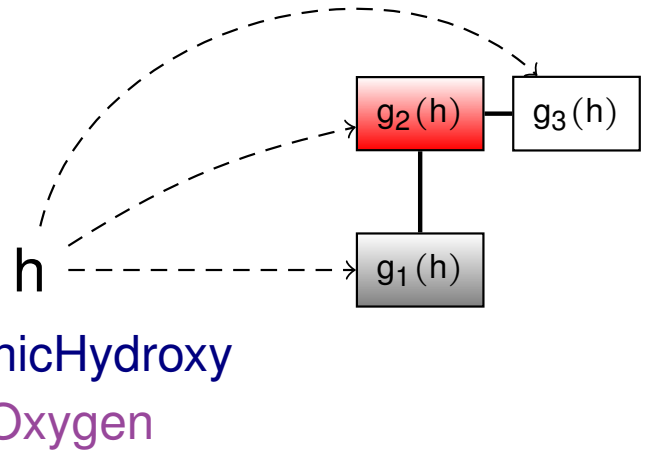

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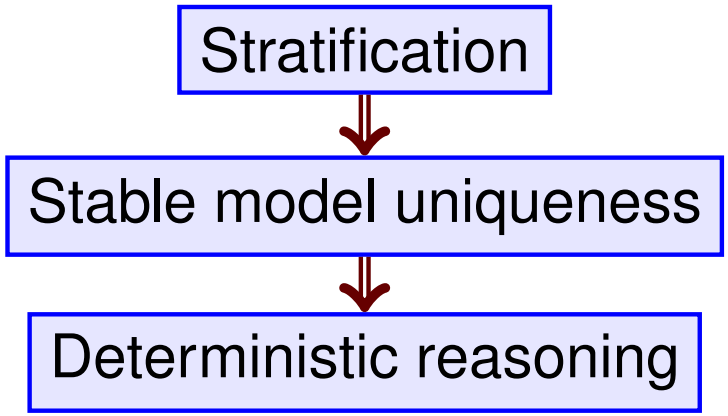

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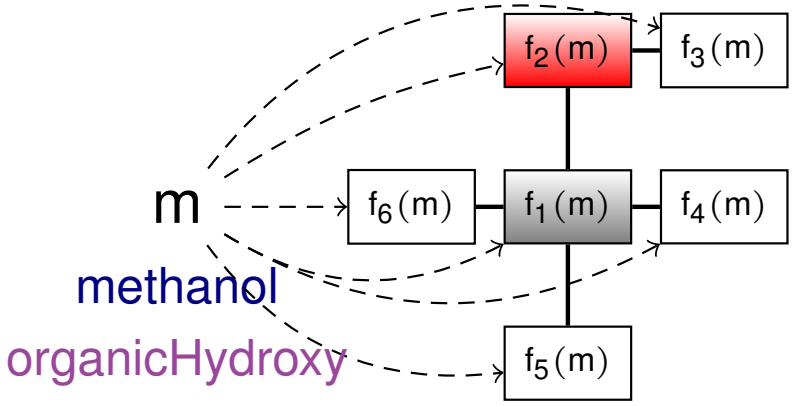

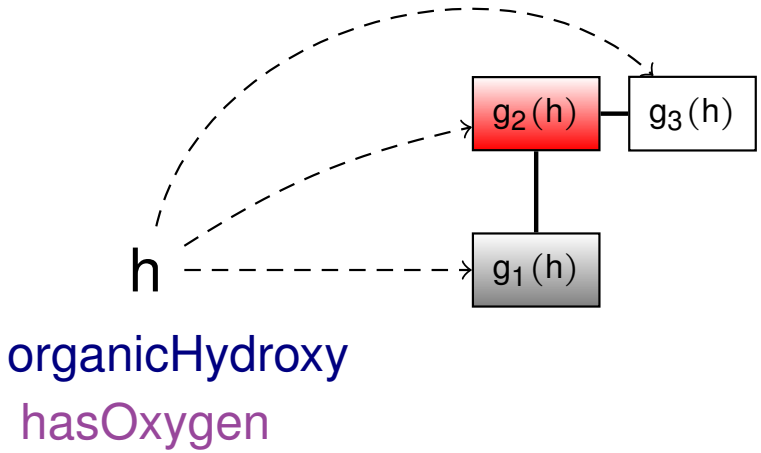

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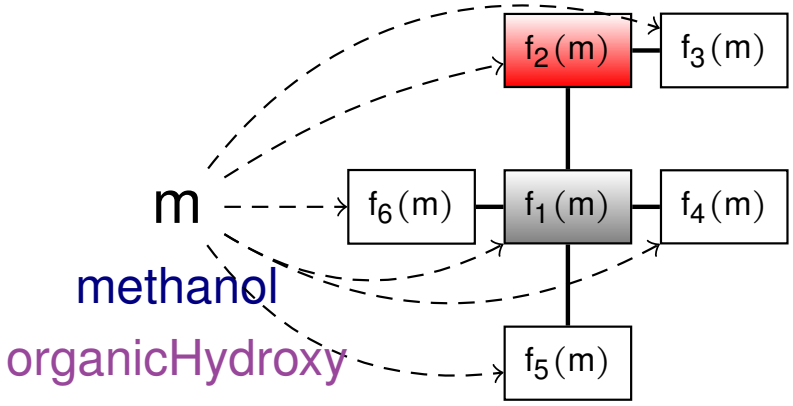

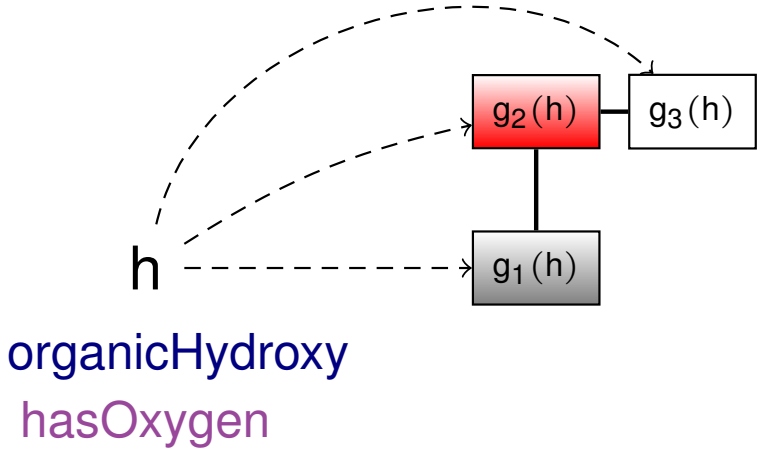

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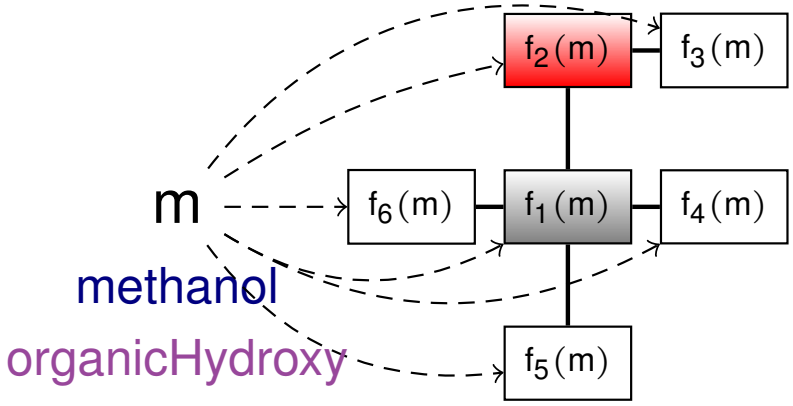

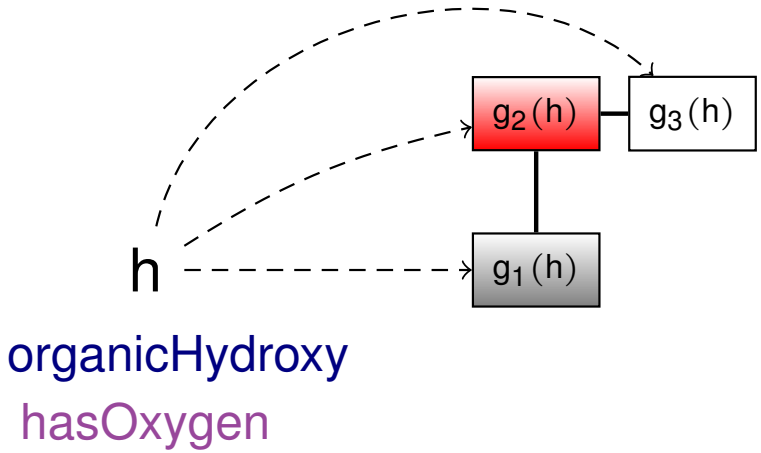

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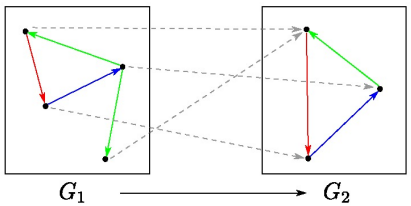
$r_1 \xrightarrow{+} r_2$ but $r_2 \not\xrightarrow{+} r_1$

- NP-complete to check

  (but only w.r.t. the size of the rules)



R-ACYCLICITY

- A program is R-acyclic: there is no cycle of positive reliances that involves a rule with an existential
  - Checking R-acyclicity is coNP-complete
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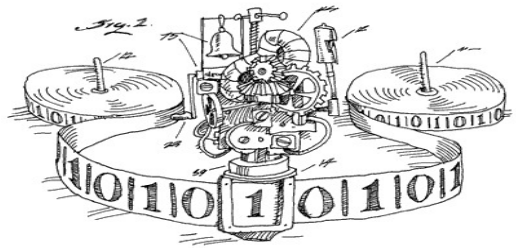

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- Polynomial time to check

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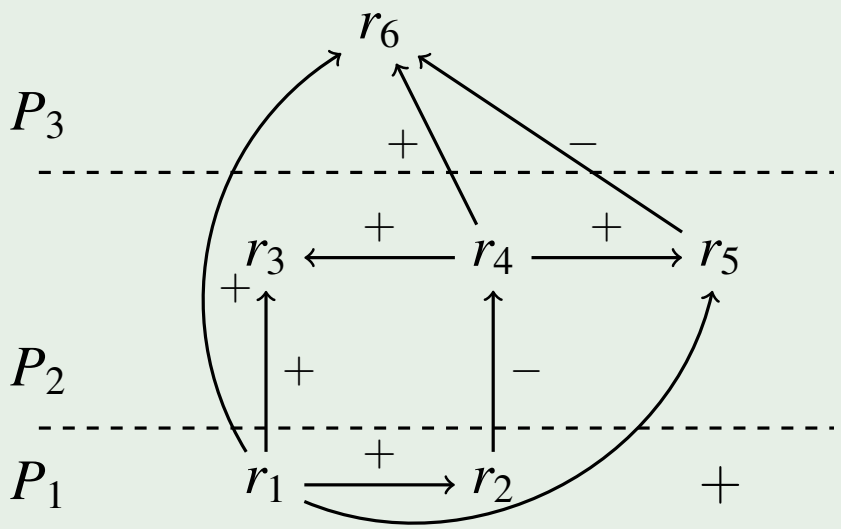

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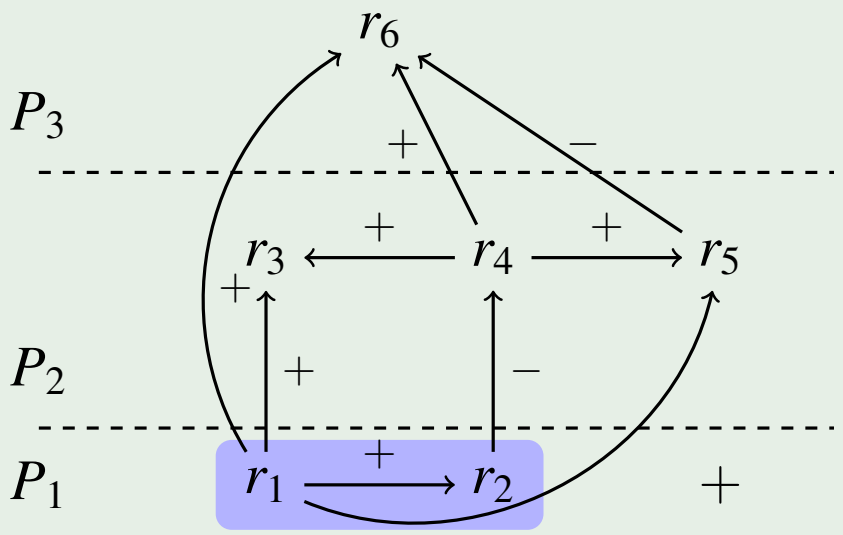

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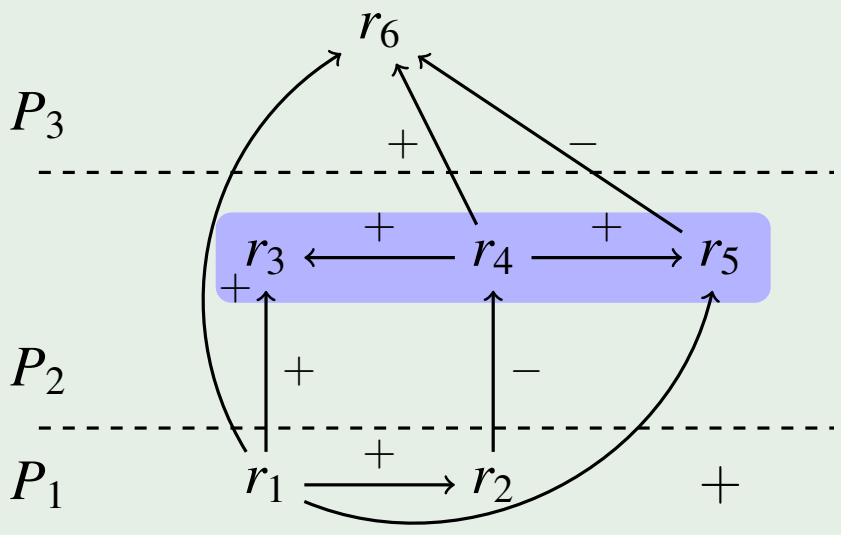

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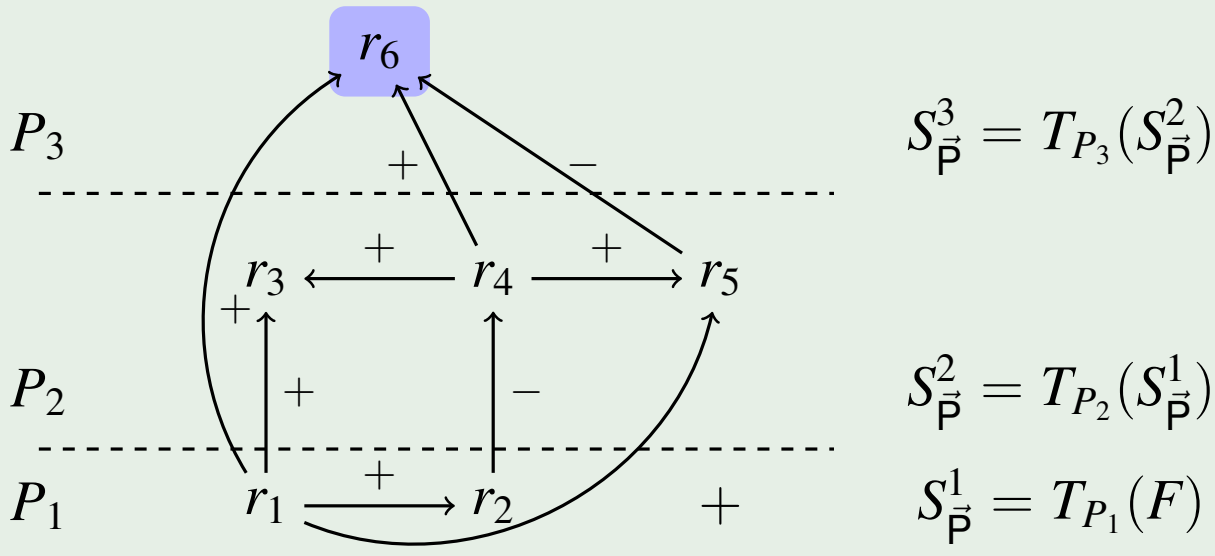

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- Slightly more complex to check:

Positive reliance	Negative reliance	R-acyclicity/R-stratification
Σ_2^P-complete	in Δ_2^P	Π_2^P-complete

$\rightsquigarrow$ Σ_2^P-hardness follows from satisfiability of a QBF $\exists\vec{p}.\forall\vec{q}.\varphi$

Experimental setup

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Example

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- Used DLV for stable model computation

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Split into lowest R-stratum P_1
and remaining four upper R-strata P_2^5

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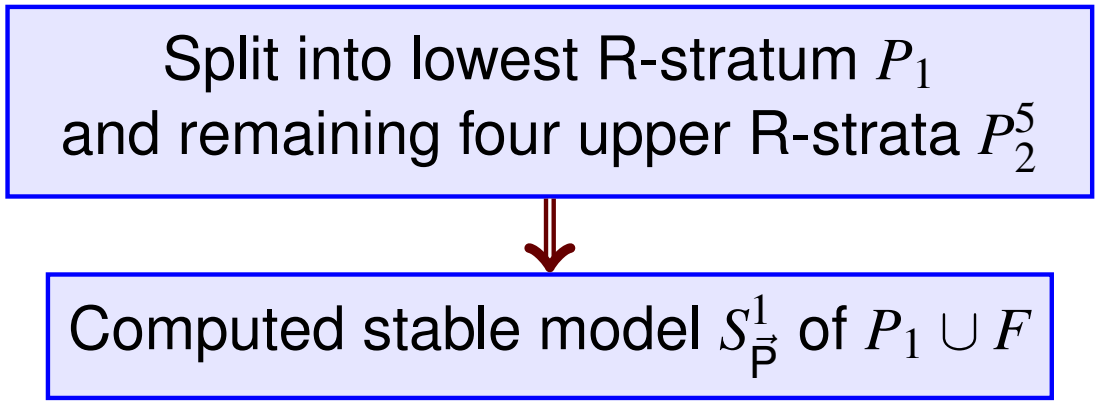

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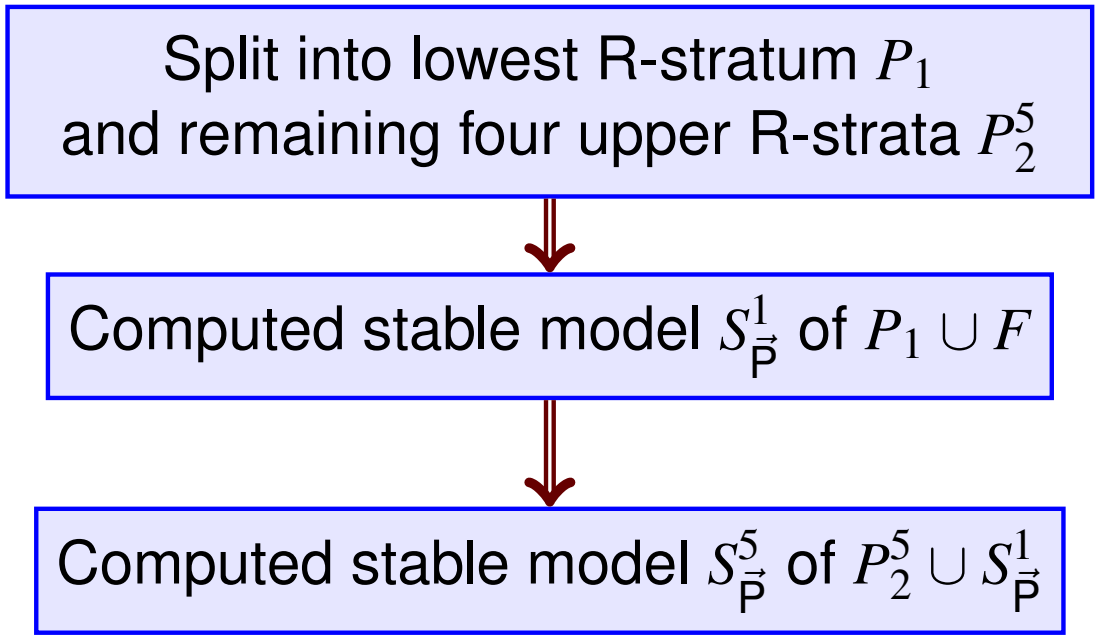

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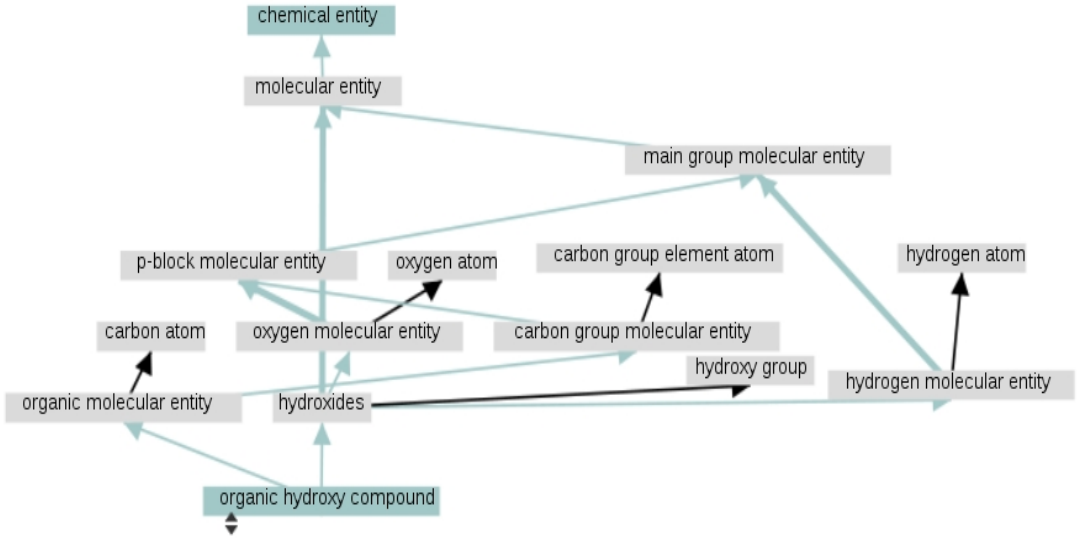
E.g. organicHydroxy $\sqsubseteq$ organoOxygenCompound ✓



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CONCLUSIONS

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Thank you! Questions?!?