# Metadata and Annotation Schema for PharmML DDMoRe Implementation: 0.5.0

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DDMoRe M66 – August 2016

## 5 ps:model-has-publication-source-external-id

- 6 label: source id.
- 7 Comment: link between a model and a publication identifier for a source of the model
- 8 Domain: pmlo:PHARMML\_0000001 .
- 9 Range: rdfs:Literal.

#### 10 ps:model-has-name

- label: name of model.
- Comment: link between a model and the name of this model; when automatically input
- per the model's PharmML source, the (string) value of ct:Name
- Domain: pmlo:PHARMML\_0000001 .
- Range: rdfs:Literal.

#### 16 ps:model-has-author

- label: author of model.
- 18 Comment: link between a model and the name (string) of the author of the PharmML
- 19 file for the model
- Domain: pmlo:PharmMLO\_0000001 .
- 21 Range: rdfs:Literal.

#### 22 ps:model-has-description

- label: description of model.
- 24 Comment: link between a model and the description of this model; when automatically
- 25 input per the model's PharmML source, the (string) value of ct:Description
- Domain: pmlo:PharmMLO\_0000001 .
- 27 Range: rdfs:Literal .

# 28 ps:model-has-description-short

- label: short description of model.
- Comment: link between a model and a description of this model; this description provides
- an account of the key features of the final model in the modeller's words
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

## 34 ps:model-has-description-long

- label: long description of model.
- 36 Comment: link between a model and a description of this model; this description includes
- 37 detailed discussions or material
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

## $_{ ext{\tiny 40}}$ wat:model-origin-of-code-in-literature-controlled

- label: model derived only from literature.
- 42 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

# $_{45}$ wat:model-implementation-conforms-to-literature-controlled

- label: model implements literature.
- 47 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- 49 Range: rdfs:Literal.

#### wat:model-implementation-source-discrepancies-freetext

- label: description of discrepancies between source and implementation.
- 52 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal .

#### $_{55}$ ps:model-modelling-question

- label: modelling question.
- 57 Comment: link between a model and a specific, possibly complex topic describing the
- specific question the model intends to address
- Domain: pmlo:PharmMLO\_0000001 .

Range: rdfs:Resource.

# 61 ps:model-research-stage

- label: nature of research.
- 63 Comment: link between a model and a type of research and/or development context in
- 64 which the model has been produced.
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

#### ps:model-field-purpose

- label: therapeutic area.
- 69 Comment: link between a model and a specific area of application for the model
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:model-related-to-disease-or-condition

- label: has disease or indications.
- 74 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

#### 77 ps:model-tasks-in-scope

- label: tasks in scope.
- Comment: link between a model and its relevant modelling tasks.
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# 82 ps:model-type-of-data-source

- label: data source type.
- <sup>84</sup> Comment: link between a data set and a generic type of data source
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## 87 ps:trialdesign-HasAssociatedDataOfType-DataPool

- label: .
- 89 Comment: A property links the trial design part of a model to a designated type of data
- 90 source.

- Domain: pmlo:PharmMLO\_0000006 .
- Range: rdfs:Resource .

# 93 ps:model-HasAssociatedDataOfType-DataPool

- 94 label: .
- Comment: A property links the model to the designated type of data source to which is
- 96 linked its data design part.
- 97 Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# 99 ps:trialdesign-HasAssociatedOrganismType-DataPool

- label: .
- Comment: A property links the trial design part of a model to designated species of animals to which the data relates.
- Domain: pmlo:PharmMLO\_0000006 .
- Range: rdfs:Literal.

## ps:trialdesign-HasAssociatedOrganismType-DataPool-freetext

- label: .
- Comment: A property links the trial design part of a model to designated species of animals to which the data relates as a freetext entry.
- Domain: pmlo:PharmMLO\_0000006 .
- Range: rdfs:Literal.

## ps:model-HasAssociatedOrganismType-DataPool

- label: .
- 113 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:model-HasAssociatedOrganismType-DataPool-freetext

- label: .
- 118 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal .

## ps:trialdesign-HasAssociatedHumanGroupByMedicalStatus-DataPool

- label: .
- 123 Comment: A property links the trial design part of a model to designated medical type
- of human to which the data relates.
- Domain: pmlo:PharmMLO\_0000006 .
- Range: rdfs:Resource.

# ${\tt ps:model-HasAssociatedHumanGroupByMedicalStatus-DataPool}$

- label: .
- 129 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:modellingstep-modelrun-uses-software

- label: software used to run model.
- 134 Comment:
- Domain: pmlo:PharmMLO\_0000007 .
- Range: rdfs:Resource.

# ps:model-modelrun-uses-software

- label: software used to run model.
- 139 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

#### ps:modellingstep-modelrun-uses-software-freetext

- label: software used to run model freetext variant.
- 144 Comment:
- Domain: pmlo:PharmMLO $_0000007$ .
- Range: rdfs:Literal.

#### ps:model-modelrun-uses-software-freetext

- label: software used to run model freetext variant.
- 149 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

## ps:model-HasAssumptions-freetext

- label: model assumptions.
- 154 Comment: A property allowing to record textual descriptions of modelling assumptions
- 155 made.
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

## ps:trialdesign-HasAssociatedRouteOfAdministration-datapool

- label: route of administration.
- 160 Comment:
- Domain: pmlo:PharmMLO\_0000006 .
- Range: rdfs:Resource.

# ${\scriptstyle 163} \quad ps: model-Has Associated Route Of Administration-data pools of the control of the co$

- label: route of administration.
- 165 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ${\tt ps:trialdesign-HasAssociatedRouteOfAdministration-datapool-free text}$

- label: route of administration.
- 170 Comment:
- Domain: pmlo:PharmMLO\_0000006 .
- Range: rdfs:Literal.

#### ps:model-HasAssociatedRouteOfAdministration-datapool-freetext

- label: route of administration.
- 175 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

#### ps:trialdesign-HasAssociatedDoseRegimen-DataPool

- label: dose regimen.
- 180 Comment:
- Domain: pmlo:PharmMLO\_0000006 .
- Range: rdfs:Resource.

## ps:model-HasAssociatedDoseRegimen-DataPool

- label: dose regimen.
- 185 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:trialdesign-HasAssociatedDoseAmount-DataPool

- label: dose regimen.
- 190 Comment:
- Domain: pmlo:PharmMLO\_0000006 .
- Range: rdfs:Resource.

## ps:model-HasAssociatedDoseAmount-DataPool

- label: dose regimen.
- 195 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# $_{198}$ ps:trialdesign-HasAssociatedDoseFrequency-DataPool

- label: dose frequency.
- 200 Comment:
- Domain: pmlo:PharmMLO\_0000006 .
- Range: rdfs:Resource.

# $_{203}$ ps:model-HasAssociatedDoseFrequency-DataPool

- label: dose frequency.
- 205 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# 208 ps:trialdesign-observed-variables-are-real-freetext

- label: observed variables are real.
- 210 Comment:
- Domain: pmlo:PharmMLO\_0000006 .
- Range: rdfs:Literal .

## ps:model-observed-variables-are-real-freetext

- label: observed variables are real.
- 215 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

## ps:trialdesign-HasAssociatedSamplingDesign-DataPool

- label: sampling design.
- 220 Comment:
- Domain: pmlo:PharmMLO\_0000006 .
- Range: rdfs:Resource.

## ps:model-HasAssociatedSamplingDesign-DataPool

- label: sampling design.
- 225 Comment:
- Domain: pmlo:PharmMLO\_0000006 .
- Range: rdfs:Resource.

# ${\tt ps:trialdesign-HasAssociatedNumberOfSubjects-DataPool}$

- label: number of subjects.
- 230 Comment:
- Domain: pmlo:PharmMLO\_0000006 .
- Range: rdfs:Literal.

# ${\tt ps:model-HasAssociatedNumberOfSubjects-DataPool}$

- label: number of subjects.
- 235 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal .

# ${\tt ps:trialdesign-HasAssociatedNumberOfModelledObservations-DataPool}$

- label: number of observations.
- 240 Comment:
- Domain: pmlo:PharmMLO\_0000006 .
- Range: rdfs:Literal .

## ps:model-HasAssociatedNumberOfModelledObservations-DataPool

- label: number of observations.
- 245 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

# ps:modeldefinition-HasAssociatedInputType

- label: type of input.
- 250 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Resource.

## ps:modeldefinition-HasAssociatedAbsorptionDelayModelType

- label: type of model for absorption delay.
- 255 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Resource .

## 258 ps:modeldefinition-HasAssociatedAbsorptionRateType

- label: type of modelled absorption rate.
- 260 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Resource.

## ps:model definition-Has Associated Bioavailability Type

- label: type of modelled bioavailability.
- 265 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Resource .

## 268 ps:modeldefinition-InputPresentsFormationFromOtherSubstance-string

- label: modelled formation from other stubstance.
- 270 Comment:
- Domain: pmlo:PharmMLO\_0000013.
- Range: rdfs:Resource.

## 273 ps:modeldefinition-InputPresentsFormationFromOtherSubstanceType

- label: modelled formation from type of susbtance.
- 275 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Resource.

# ${\tt ps:model definition-Input Presents Formation From Other Substance Model Type}$

- label: model for formation from another substance.
- 280 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Resource.

## ps:model-HasAssociatedInputType

- label: type of input.
- 285 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource .

## 288 ps:model-HasAssociatedAbsorptionDelayModelType

- label: type of model for absorption delay.
- 290 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

#### 293 ps:model-HasAssociatedAbsorptionRateType

- label: type of modelled absorption rate.
- 295 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## 298 ps:model-HasAssociatedBioavailabilityType

- label: type of modelled bioavailability.
- 300 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## 303 ps:model-InputPresentsFormationFromOtherSubstance-string

- label: modelled formation from other stubstance.
- 305 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ${\tt 308} \quad ps: model-Input Presents Formation From Other Substance Type$

- label: modelled formation from type of susbtance.
- 310 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ${\tt ps:model-InputPresentsFormationFromOtherSubstanceModelType}$

- label: model for formation from another substance.
- 315 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ${\tt ps:model definition-Has Associated Absorption Delay Model Type-free text}$

- label: .
- 320 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Literal.

# ${\tt ps:model definition-Has Associated Absorption Rate Type-free text}$

- label: .
- 325 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Literal.

## ps:modeldefinition-HasAssociatedBioavailabilityType-freetext

- label: .
- 330 Comment:
- Domain: pmlo:PharmMLO\_0000013.
- Range: rdfs:Literal.

# ${\tt ps:model definition-Input Presents Formation From Other Substance Type-free text}$

- label: .
- 335 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Literal.

# ${\tt 9338} \quad ps: model definition-Input Presents Formation From Other Substance Model Type-points and the property of the prop$

#### 339 freetext

- label: .
- 341 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Literal.

# ${}_{344}\quad ps: model-Has Associated Absorption Delay Model Type-free text$

- label: .
- 346 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

# $_{349}$ ps:model-HasAssociatedAbsorptionRateType-freetext

- label: .
- 351 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

#### ps:model-HasAssociatedBioavailabilityType-freetext

- label: .
- 356 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

## ps:model-InputPresentsFormationFromOtherSubstanceType-freetext

- label: .
- 361 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

# $_{364}$ ps:model-InputPresentsFormationFromOtherSubstanceModelType-freetext

- label: .
- 366 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

## ${\tt ps:model definition-Has Associated Number Of Modelled Compartments}$

- label: .
- 371 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Literal.

## $_{374}$ ps:model-HasHassociatedNumberOfModelledCompartments

- label: number of modelled compartments.
- 376 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

# ps:modeldefinition-HasAssociatedDistributionModellingAttribute-string

- label: .
- 381 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Literal.

# ps:model-HasAssociatedDistributionModellingAttribute-string

- label: .
- 386 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal .

# ${\tt 389} \quad ps: model definition-Has Associated Distribution Modelling Attribute-Enterohepatic Recycling Control of the control of the property of the control of the contr$

- label: enterohepatic recycling.
- 391 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Resource.

# ${\tt ps:model definition-Has Associated Distribution Modelling Attribute-Non Linear Transport}$

- label: non linear transport.
- 396 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Resource.

# ${\tt ps:model definition-Has Associated Distribution Modelling Attribute-Non Linear Protein Binder Binde$

- label: non linear protein binding.
- 401 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Resource.

## ps:model-HasAssociatedDistributionModellingAttribute-EnterohepaticRecycling

- label: enterohepatic recycling.
- 406 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ${\tt 99} \quad ps: model-Has Associated Distribution Modelling Attribute-Non Linear Transport to the property of t$

- label: non linear transport.
- 411 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ${}_{414} \quad ps: model-Has Associated Distribution Modelling Attribute-Non Linear Protein Binding \\$

- label: non linear protein binding.
- 416 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource .

# ps:modeldefinition-HasAssociatedEliminationModellingAttribute-CompartmentOfElimin

- label: .
- 421 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Resource.

# ps:model-HasAssociatedEliminationModellingAttribute-CompartmentOfElimination

- label: .
- 426 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ${\tt ps:model definition-Has Associated Elimination Modelling Attribute-Type Of Elimination}$

- label: .
- 431 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Resource.

## ps:model-HasAssociatedEliminationModellingAttribute-TypeOfElimination

- label: .
- 436 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ${\tt ps:model definition-Has Associated Modelled Drug Free System Type}$

- label: .
- 441 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Resource.

# ps:model-HasAssociatedModelledDrugFreeSystemType

- label: .
- 446 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:modeldefinition-HasShapeOfDrugEffectTypeAttribute

- label: shape of drug effect.
- 451 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Resource.

# $_{454}$ ps:modeldefinition-HasDriverOfDrugEffectTypeAttribute

- label: driver of drug effect.
- 456 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Resource.

# ${\tt ps:model definition-Has Temporal Relation Between Drug Effect And Response Type Attribute}$

- label: temporal relation between drug effect and response.
- 461 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Resource.

## ps:modeldefinition-HasModelForResponseType

- label: type of response.
- 466 Comment:
- Domain: pmlo:PharmMLO\_0000013 .
- Range: rdfs:Resource.

# $_{469}$ ps:model-HasShapeOfDrugEffectTypeAttribute

- label: shape of drug effect.
- 471 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:model-HasDriverOfDrugEffectTypeAttribute

- label: driver of drug effect.
- 476 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource .

## ps:model-HasTemporalRelationBetweenDrugEffectAndResponseTypeAttribute

- label: temporal relation between drug effect and response.
- 481 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource .

## ps:model-HasModelForResponseType

- label: type of response.
- 486 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:trialdesign-HasStudiedSubstanceAtttibute

- label: type of studied substance.
- 491 Comment: studied substance
- Domain: pmlo:PharmMLO $_00000006$ .
- Range: rdfs:Resource.

## ps:model-HasStudiedSubstanceAttribute

- label: type of studied substance.
- 496 Comment: studied substance
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# 499 ps:drug-ChebiIdOfDrug1

- label: CHEBI ID of drug 1.
- 501 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Resource.

## ps:drug-DrugBankIdOfDrug1

- label: DrugBank ID of drug 1.
- 506 Comment:
- 507 Domain: pkpd:PKPD\_0007172.
- Range: rdfs:Resource.

## ps:drug-NameOfDrug1-freetext

- label: name of drug 1.
- 511 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Literal.

# ps:drug-TypeOfDrug1

- label: type of drug 1.
- 516 Comment:
- Domain:  $pkpd:PKPD_0007172$ .
- Range: rdfs:Resource.

## ps:model-ChebiIdOfDrug1

- label: CHEBI ID of drug 1.
- 521 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:model-DrugBankIdOfDrug1

- label: DrugBank ID of drug 1.
- 526 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:model-NameOfDrug1-freetext

- label: name of drug 1.
- 531 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

# ps:model-TypeOfDrug1

- label: type of drug 1.
- 536 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:drug-ChebiIdOfDrug2

- label: CHEBI ID of drug 2.
- Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Resource.

# ps:drug-DrugBankIdOfDrug2

- label: DrugBank ID of drug 2.
- 546 Comment:
- 547 Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Resource.

# 549 ps:drug-NameOfDrug2-freetext

- label: name of drug 2.
- 551 Comment:
- Domain:  $pkpd:PKPD_0007172$ .
- Range: rdfs:Literal.

## ps:drug-TypeOfDrug2

- label: type of drug 2.
- 556 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Resource.

# ps:model-ChebiIdOfDrug2

- label: CHEBI ID of drug 2.
- 561 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:model-DrugBankIdOfDrug2

- label: DrugBank ID of drug 2.
- 566 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:model-NameOfDrug2-freetext

- label: name of drug 2.
- 571 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

# ps:model-TypeOfDrug2

- label: type of drug 2.
- 576 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:drug-ChebiIdOfDrug3

- label: CHEBI ID of drug 3.
- Comment:
- Domain:  $pkpd:PKPD_0007172$ .
- Range: rdfs:Resource.

## ps:drug-DrugBankIdOfDrug3

- label: DrugBank ID of drug 3.
- 586 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Resource .

# 589 ps:drug-NameOfDrug3-freetext

- label: name of drug 3.
- 591 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Literal.

## 594 ps:drug-TypeOfDrug3

- label: type of drug 3.
- 596 Comment:
- 597 Domain: pkpd:PKPD\_0007172.
- Range: rdfs:Resource.

## ps:model-ChebiIdOfDrug3

- label: CHEBI ID of drug 3.
- 601 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:model-DrugBankIdOfDrug3

- label: DrugBank ID of drug 3.
- 606 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:model-NameOfDrug3-freetext

- label: name of drug 3.
- 611 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

# ps:model-TypeOfDrug3

- label: type of drug 3.
- 616 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# $_{619}$ ps:drug-ChebiIdOfDrug4

- label: CHEBI ID of drug 4.
- 621 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Resource.

# ps:drug-DrugBankIdOfDrug4

- label: DrugBank ID of drug 4.
- 626 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Resource.

## ps:drug-NameOfDrug4-freetext

- label: name of drug 4.
- 631 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Literal.

# ps:drug-TypeOfDrug4

- label: type of drug 4.
- 636 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Resource.

## ps:model-ChebiIdOfDrug4

- label: CHEBI ID of drug 4.
- 641 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## 644 ps:model-DrugBankIdOfDrug4

- label: DrugBank ID of drug 4.
- 646 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:model-NameOfDrug4-freetext

- label: name of drug 4.
- 651 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

## 654 ps:model-TypeOfDrug4

- label: type of drug 4.
- 656 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:drug-ChebiIdOfDrug5

- label: CHEBI ID of drug 5.
- 661 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Resource.

## 664 ps:drug-DrugBankIdOfDrug5

- label: DrugBank ID of drug 5.
- 666 Comment:
- 667 Domain: pkpd:PKPD\_0007172.
- Range: rdfs:Resource.

## ps:drug-NameOfDrug5-freetext

- label: name of drug 5.
- 671 Comment:
- Domain:  $pkpd:PKPD_0007172$ .
- Range: rdfs:Literal.

## ps:drug-TypeOfDrug5

- label: type of drug 5.
- 676 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Resource.

# ps:model-ChebiIdOfDrug5

- label: CHEBI ID of drug 5.
- 681 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:model-DrugBankIdOfDrug5

- label: DrugBank ID of drug 5.
- 686 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:model-NameOfDrug5-freetext

- label: name of drug 5.
- 691 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

# 694 ps:model-TypeOfDrug5

- label: type of drug 5.
- 696 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# $_{699}$ ps:trialdesign-hasListOfInteractingDrugs-freetext

- label: has list of interacting drugs.
- 701 Comment:
- Domain: pmlo:PharmMLO\_0000006 .
- Range: rdfs:Literal.

## 704 ps:trialdesign-hasInteractorByNickname-freetext

- label: has interactor in drug interaction.
- 706 Comment:
- Domain: pmlo:PharmMLO\_0000006 .
- 708 Range: rdfs:Literal.

# $_{709}$ ps:trialdesign-hasInteracteeByNickname-freetext

- label: has interactee in drug interaction.
- 711 Comment:
- Domain: pmlo:PharmMLO\_0000006 .
- Range: rdfs:Literal.

# ${}_{714}\quad ps: trial design-has Type Of Model Component Impacted$

- label: has type of model component impacted.
- 716 Comment:
- Domain: pmlo:PharmMLO\_0000006 .
- Range: rdfs:Resource.

## ps:model-hasListOfInteractingDrugs-freetext

- label: has list of interacting drugs.
- 721 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal .

# ps:model-hasInteractorByNickname-freetext

- label: has interactor in drug interaction.
- 726 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

## ps:model-hasInteracteeByNickname-freetext

- label: has interactee in drug interaction.
- 731 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

## ps:model-hasTypeOfModelComponentImpacted

- label: has type of model component impacted.
- 736 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:drug-hasDoseAmountMin-Drug1

- label: has min dose amount for drug 1.
- 741 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Literal.

## 744 ps:drug-hasDoseAmountMax-Drug1

- label: has max dose amount for drug 1.
- 746 Comment:
- Domain: pkpd:PKPD\_0007172.
- Range: rdfs:Literal.

## 749 ps:drug-hasDoseAmountUnit-Drug1

- label: has doseamount unit for drug 1.
- 751 Comment:
- 752 Domain: pkpd:PKPD\_0007172.
- Range: rdfs:Resource.

## ps:drug-hasDoseAmountMin-Drug2

- label: has min dose amount for drug 2.
- 756 Comment:
- 757 Domain: pkpd:PKPD\_0007172.
- Range: rdfs:Literal.

## ps:drug-hasDoseAmountMax-Drug2

- label: has max dose amount for drug 2.
- 761 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Literal.

## 764 ps:drug-hasDoseAmountUnit-Drug2

- label: has doseamount unit for drug 2.
- 766 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Resource.

# ps:drug-hasDoseAmountMin-Drug3

- label: has min dose amount for drug 3.
- 771 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Literal.

## $_{774}$ ps:drug-hasDoseAmountMax-Drug3

- label: has max dose amount for drug 3.
- 776 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Literal.

## ps:drug-hasDoseAmountUnit-Drug3

- label: has doseamount unit for drug 3.
- 781 Comment:
- 782 Domain: pkpd:PKPD\_0007172.
- Range: rdfs:Resource.

## ps:drug-hasDoseAmountMin-Drug4

- label: has min dose amount for drug 4.
- 786 Comment:
- 787 Domain: pkpd:PKPD\_0007172.
- Range: rdfs:Literal.

## 789 ps:drug-hasDoseAmountMax-Drug4

- label: has max dose amount for drug 4.
- 791 Comment:
- Domain: pkpd:PKPD\_0007172.
- Range: rdfs:Literal.

## ps:drug-hasDoseAmountUnit-Drug4

- label: has doseamount unit for drug 4.
- 796 Comment:
- Domain: pkpd:PKPD\_0007172.
- Range: rdfs:Resource.

# 799 ps:drug-hasDoseAmountMin-Drug5

- label: has min dose amount for drug 5.
- 801 Comment:
- BO2 Domain: pkpd:PKPD\_0007172.
- Range: rdfs:Literal.

## ps:drug-hasDoseAmountMax-Drug5

- label: has max dose amount for drug 5.
- 806 Comment:
- Domain: pkpd:PKPD\_0007172 .
- 808 Range: rdfs:Literal.

## ps:drug-hasDoseAmountUnit-Drug5

- label: has doseamount unit for drug 5.
- 811 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Resource.

## ps:model-hasDoseAmountMin-Drug1

- label: has min dose amount for drug 1.
- 816 Comment:
- Domain: pkpd:PKPD\_0007172.
- Range: rdfs:Literal.

## ps:model-hasDoseAmountMax-Drug1

- label: has max dose amount for drug 1.
- 821 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Literal.

## ps:model-hasDoseAmountUnit-Drug1

- label: has doseamount unit for drug 1.
- 826 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Resource.

## ps:model-hasDoseAmountMin-Drug2

- label: has min dose amount for drug 2.
- 831 Comment:
- B32 Domain: pkpd:PKPD\_0007172.
- Range: rdfs:Literal.

#### ps:model-hasDoseAmountMax-Drug2

- label: has max dose amount for drug 2.
- 836 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Literal.

## ps:model-hasDoseAmountUnit-Drug2

- label: has doseamount unit for drug 2.
- 841 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Resource.

## ps:model-hasDoseAmountMin-Drug3

- label: has min dose amount for drug 3.
- 846 Comment:
- Domain: pkpd:PKPD\_0007172.
- Range: rdfs:Literal.

## ps:model-hasDoseAmountMax-Drug3

- label: has max dose amount for drug 3.
- 851 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Literal.

## ps:model-hasDoseAmountUnit-Drug3

- label: has doseamount unit for drug 3.
- 856 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Resource.

# ps:model-hasDoseAmountMin-Drug4

- label: has min dose amount for drug 4.
- 861 Comment:
- 862 Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Literal.

## ps:model-hasDoseAmountMax-Drug4

- label: has max dose amount for drug 4.
- 866 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Literal.

## ps:model-hasDoseAmountUnit-Drug4

- label: has doseamount unit for drug 4.
- 871 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Resource.

## ps:model-hasDoseAmountMin-Drug5

- label: has min dose amount for drug 5.
- 876 Comment:
- 877 Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Literal.

## ps:model-hasDoseAmountMax-Drug5

- label: has max dose amount for drug 5.
- 881 Comment:
- Domain:  $pkpd:PKPD_0007172$ .
- Range: rdfs:Literal.

## ps:model-hasDoseAmountUnit-Drug5

- label: has doseamount unit for drug 5.
- 886 Comment:
- Domain: pkpd:PKPD\_0007172 .
- Range: rdfs:Resource .

# ps:observed variable-OVLinks ToDrug-OV1

- label: links to drug.
- 891 Comment:
- 892 Domain: pkpd:PKPD\_0008106 .
- Range: rdfs:Literal.

## ps:observedvariable-OVHasNature-OV1

- label: has nature.
- 896 Comment:
- 897 Domain: pkpd:PKPD\_0008106.
- 898 Range: rdfs:Resource.

## ps:observedvariable-OVHasUnits-OV1

- 900 label: has units.
- 901 Comment:
- 902 Domain: pkpd:PKPD\_0008106 .
- 903 Range: rdfs:Resource.

# ps:observed variable-OVHasMatrixType-OV1

- 905 label: has matrix type.
- 906 Comment:
- 907 Domain: pkpd:PKPD\_0008106.
- 908 Range: rdfs:Resource.

# 909 ps:observedvariable-OVHasTypeOfObservedVariable-OV1

- 910 label: has type.
- 911 Comment:
- 912 Domain: pkpd:PKPD\_0008106.
- Page: rdfs:Resource .

## 914 ps:observedvariable-OVLinksToDrug-OV2

- 915 label: links to drug.
- 916 Comment:
- 917 Domain: pkpd:PKPD\_0008106 .
- 918 Range: rdfs:Literal.

# ps:observed variable-OVHas Nature-OV2

- 920 label: has nature.
- 921 Comment:
- 922 Domain: pkpd:PKPD\_0008106 .
- Page: rdfs:Resource .

# ps:observed variable-OVH as Units-OV 2

- label: has units.
- 926 Comment:
- 927 Domain: pkpd:PKPD\_0008106.
- Page: rdfs:Resource .

## 929 ps:observedvariable-OVHasMatrixType-OV2

- label: has matrix type.
- 931 Comment:
- 932 Domain: pkpd:PKPD\_0008106 .
- Range: rdfs:Resource .

# ps:observedvariable-OVHasTypeOfObservedVariable-OV2

- label: has type.
- 936 Comment:
- 937 Domain: pkpd:PKPD\_0008106 .
- Page: rdfs:Resource .

# 939 ps:observedvariable-OVLinksToDrug-OV3

- label: links to drug.
- 941 Comment:
- Domain:  $pkpd:PKPD_0008106$ .
- 943 Range: rdfs:Literal.

## 944 ps:observedvariable-OVHasNature-OV3

- label: has nature.
- 946 Comment:
- Domain: pkpd:PKPD\_0008106 .
- Range: rdfs:Resource .

# 949 ps:observedvariable-OVHasUnits-OV3

- 950 label: has units.
- 951 Comment:
- 952 Domain: pkpd:PKPD\_0008106 .
- Page: rdfs:Resource .

# ps:observed variable-OVH as Matrix Type-OV3

- label: has matrix type.
- 956 Comment:
- 957 Domain: pkpd:PKPD\_0008106.
- Page: rdfs:Resource .

# 959 ps:observedvariable-OVHasTypeOfObservedVariable-OV3

- 960 label: has type.
- 961 Comment:
- 962 Domain: pkpd:PKPD\_0008106 .
- 963 Range: rdfs:Resource.

# 964 ps:observedvariable-OVLinksToDrug-OV4

- label: links to drug.
- 966 Comment:
- 967 Domain: pkpd:PKPD\_0008106 .
- 968 Range: rdfs:Literal.

# 969 ps:observedvariable-OVHasNature-OV4

- 970 label: has nature.
- 971 Comment:
- 972 Domain: pkpd:PKPD\_0008106.
- Page: rdfs:Resource .

# 974 ps:observedvariable-OVHasUnits-OV4

- 975 label: has units.
- 976 Comment:
- Domain: pkpd:PKPD\_0008106 .
- Page: rdfs:Resource .

# ps:observed variable-OVH as Matrix Type-OV4

- label: has matrix type.
- 981 Comment:
- 982 Domain: pkpd:PKPD\_0008106 .
- Range: rdfs:Resource.

# ${\tt ps:} observed variable - OVHas Type OfObserved Variable - OV4$

- label: has type.
- 986 Comment:
- 987 Domain: pkpd:PKPD\_0008106.
- 988 Range: rdfs:Resource.

# ps:observed variable-OVLinks ToDrug-OV5

- 990 label: links to drug.
- 991 Comment:
- 992 Domain: pkpd:PKPD\_0008106 .
- 993 Range: rdfs:Literal.

## 994 ps:observedvariable-OVHasNature-OV5

- 995 label: has nature.
- 996 Comment:
- 997 Domain: pkpd:PKPD\_0008106.
- 998 Range: rdfs:Resource.

# $_{999}$ ps:observed variable-OVH as Units-OV $_{5}$

- label: has units.
- 1001 Comment:
- $_{1002}$  Domain: pkpd:PKPD\_0008106 .
- Range: rdfs:Resource.

## ps:observedvariable-OVHasMatrixType-OV5

- label: has matrix type.
- 1006 Comment:
- 1007 Domain: pkpd:PKPD\_0008106.
- Range: rdfs:Resource.

# ${\tt ps:observed Variable-OVHasTypeOfObserved Variable-OV5}$

- label: has type.
- 1011 Comment:
- 1012 Domain: pkpd:PKPD\_0008106.
- Range: rdfs:Resource.

## ps:model-OVLinksToDrug-OV1

- label: links to drug.
- 1016 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal .

# ps:model-OVHasNature-OV1

- label: has nature.
- 1021 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:model-OVHasUnits-OV1

- label: has units.
- 1026 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:model-OVHasMatrixType-OV1

- label: has matrix type.
- 1031 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:model-OVHasTypeOfObservedVariable-OV1

- label: has type.
- 1036 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ${\small 1039}\>\>\> ps:model-OVLinksToDrug-OV2$

- label: links to drug.
- 1041 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

## ps:model-OVHasNature-OV2

- label: has nature.
- 1046 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:model-OVHasUnits-OV2

- label: has units.
- 1051 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:model-OVHasMatrixType-OV2

- label: has matrix type.
- 1056 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:model-OVHasTypeOfObservedVariable-OV2

- label: has type.
- 1061 Comment:
- $_{1062}$  Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:model-OVLinksToDrug-OV3

- label: links to drug.
- 1066 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

# ps:model-OVHasNature-OV3

- label: has nature.
- 1071 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:model-OVHasUnits-OV3

- label: has units.
- 1076 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:model-OVHasMatrixType-OV3

- label: has matrix type.
- 1081 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:model-OVHasTypeOfObservedVariable-OV3

- label: has type.
- 1086 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:model-OVLinksToDrug-OV4

- label: links to drug.
- 1091 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

## ps:model-OVHasNature-OV4

- label: has nature.
- 1096 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:model-OVHasUnits-OV4

- label: has units.
- 1101 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:model-OVHasMatrixType-OV4

- label: has matrix type.
- 1106 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:model-OVHasTypeOfObservedVariable-OV4

- label: has type.
- 1111 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:model-OVLinksToDrug-OV5

- label: links to drug.
- 1116 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Literal.

## ps:model-OVHasNature-OV5

- label: has nature.
- 1121 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:model-OVHasUnits-OV5

- label: has units.
- 1126 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ps:model-OVHasMatrixType-OV5

- label: has matrix type.
- 1131 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

# ${\tt ps:model-OVHasTypeOfObservedVariable-OV5}$

- label: has type.
- 1136 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.

## ps:structuralmodel-HasComponentType

- label: has component type.
- 1141 Comment:
- Domain: pmlo:PharmMLO\_0000010 .
- Range: rdfs:Resource.

# ps:model-HasComponentType

- label: has component type.
- 1146 Comment:
- Domain: pmlo:PharmMLO\_0000001 .
- Range: rdfs:Resource.