

Controlled Values for PharmML Annotation Properties in DDMoRe Implementation version: 1.3.0

Pierre Grenon, University College London

DDMoRe M66 – August 2016

1 Namespace used

- **pkpd** <http://www.ddmore.org/ontologies/ontology/pkpd-ontology>

- **ncit** <http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl>

- **obo** obo <http://purl.obolibrary.org/obo/>

2 Controlled Annotating Values

wat:model-origin-of-code-in-literature-controlled

Yes

No

wat:model-implementation-conforms-to-literature-controlled

Yes

No

ps:model-modelling-question

Patient Population Selection and Bridging between Population (Pediatrics, Elderly, Obese),
pkpd_0006035

Candidate Comparison, Selection, Human Dose Prediction, pkpd_0006027

Mechanistic Understanding, pkpd_0006026

Therapeutic Drug Monitoring, pkpd_0006041

Pharmaco-economic, pkpd_0006038

Study Design Optimization, pkpd_0006028

25 Pharmacologic, pkpd_0006039
26 Diagnostic model, pkpd_0006042
27 Risk & Benefit Characterization, Outcome Prediction (Clinical & design Viability), pkpd_0006032
28 Disease Progression model, pkpd_0006036
29 Combination Therapy Dose Selection, pkpd_0006031
30 Similarity Assessment (MVC, Biosimilar, Formulation), pkpd_0006030
31 Dose & Schedule Selection and Label Recommendation, pkpd_0006034
32 Variability sources in PK and PD (CYP, Renal, Biomarkers), pkpd_0006029
33 Social-economic, pkpd_0006040
34 Comparator/Standard of Care Differentiation (Clinical & Commercial Viability), pkpd_0006033
35 Veterinary, pkpd_0006043
36 Clinical end-point, pkpd_0006037

37 **ps:model-research-stage**

38 1, Discovery stage, pkpd_0006003
39 1.1, Fundamental/Basic research, pkpd_0006004
40 1.2, Target selection & Validation, pkpd_0006005
41 1.3, Lead Generation & Optimization, pkpd_0006006
42 2, Preclinical development, pkpd_0000050
43 2.1, In silico, pkpd_0006007
44 2.2, In vitro, pkpd_0000051
45 2.3, In vivo, pkpd_0006008
46 3, Early clinical development (Phases I and II), pkpd_0006009
47 4, Approval phase/Registration trial (Phase III), pkpd_0006010
48 5, Life cycle management, pkpd_0006011
49 6, Clinical research & Therapeutic use, pkpd_0006012

50 **ps:model-field-purpose**

51 Respiratory, pkpd_0006018
52 CNS, pkpd_0001023
53 Gastroenterology, pkpd_0006021
54 Metabolism, pkpd_0006013
55 Cardiovascular, pkpd_0006016
56 Immunology, pkpd_0006023
57 Ophthalmology, pkpd_0006015
58 Vaccines, pkpd_00060025
59 Endocrinology, pkpd_0006020
60 Anti-infectives, pkpd_0001024
61 Rheumatology, pkpd_0006024

62 Diagnostics, pkpd_0006019
63 Haematology, pkpd_0006022
64 Oncology, pkpd_0000036

65 **ps:model-tasks-in-scope**

66 simulation, pkpd_0006000
67 estimation, pkpd_0006001
68 optimisation, pkpd_0006002

69 **ps:trialdesign-HasAssociatedDataOfType-DataPool**

70 Published data, pkpd_0000412
71 Observations, pkpd_0000411
72 Simulations, pkpd_0000413

73 **ps:model-HasAssociatedDataOfType-DataPool**

74 Published data, pkpd_0000412
75 Observations, pkpd_0000411
76 Simulations, pkpd_0000413

77 **ps:trialdesign-HasAssociatedOrganismType-DataPool**

78 dog, ncbi:9615
79 guinea pig, ncbi:10141
80 monkey, ncbi:9527
81 mouse, ncbi:10088
82 pig, ncbi:9823
83 rat, ncbi:10114
84 rabbit, ncbi:9986

85 **ps:model-HasAssociatedOrganismType-DataPool**

86 dog, ncbi:9615
87 guinea pig, ncbi:10141
88 monkey, ncbi:9527
89 mouse, ncbi:10088
90 pig, ncbi:9823
91 rat, ncbi:10114
92 rabbit, ncbi:9986

93 ps:trialdesign-HasAssociatedHumanGroupByMedicalStatus-DataPool

94 Healthy volunteer, pkpd_0008012

95 Patient, pkpd_0008011

96 ps:model-HasAssociatedHumanGroupByMedicalStatus-DataPool

97 Healthy volunteer, pkpd_0008012

98 Patient, pkpd_0008011

99 ps:modellingstep-modelrun-uses-software

100 Berkeley-Madonna, pkpd_0008000

101 Matlab, pkpd_0000390

102 Monolix, pkpd_0000391

103 NONMEM, pkpd_0000368

104 Openbugs, pkpd_0008001

105 R, pkpd_0001109

106 SAS, pkpd_0008002

107 Winbugs, pkpd_0008003

108 ps:model-modelrun-uses-software

109 Berkeley-Madonna, pkpd_0008000

110 Matlab, pkpd_0000390

111 Monolix, pkpd_0000391

112 NONMEM, pkpd_0000368

113 Openbugs, pkpd_0008001

114 R, pkpd_0001109

115 SAS, pkpd_0008002

116 Winbugs, pkpd_0008003

117 ps:trialdesign-HasAssociatedRouteOfAdministration-datapool

118 1, Parenteral, pkpd_0008016

119 1.1, Intravenous, pkpd_0008021

120 1.2, Subcutaneous, pkpd_0008022

121 1.3, Intra-muscular, pkpd_0008023

122 2, Enteral/Oral, pkpd_0008017

123 3, Topical, pkpd_0008018

124 3.1, Respiratory (i.e., inhalation), pkpd_0008020

125 3.2, Transdermal, pkpd_0008019

126 ps:model-HasAssociatedRouteOfAdministration-datapool

- 127 1, Parenteral, pkpd_0008016
- 128 1.1, Intravenous, pkpd_0008021
- 129 1.2, Subcutaneous, pkpd_0008022
- 130 1.3, Intra-muscular, pkpd_0008023
- 131 2, Enteral/Oral, pkpd_0008017
- 132 3, Topical, pkpd_0008018
- 133 3.1, Respiratory (i.e., inhalation), pkpd_0008020
- 134 3.2, Transdermal, pkpd_0008019

135 ps:trialdesign-HasAssociatedDoseRegimen-DataPool

- 136 Single dose, pkpd_0000423
- 137 Multiple doses, pkpd_0000424

138 ps:model-HasAssociatedDoseRegimen-DataPool

- 139 Single dose, pkpd_0000423
- 140 Multiple doses, pkpd_0000424

141 ps:trialdesign-HasAssociatedDoseAmount-DataPool

- 142 Fixed, pkpd_0008025
- 143 Flexible/adpted function of some criteria, pkpd_0008026

144 ps:model-HasAssociatedDoseAmount-DataPool

- 145 Fixed, pkpd_0008025
- 146 Flexible/adpted function of some criteria, pkpd_0008026

147 ps:trialdesign-HasAssociatedDoseFrequency-DataPool

- 148 QD (i.e. once per day), pkpd_0008028
- 149 BID (i.e. twice per day), pkpd_0008029
- 150 TID (i.e. Three times a day), pkpd_0008030
- 151 QOD (i.e. every other day), pkpd_0008031
- 152 Weekly, pkpd_0008032
- 153 QM (i.e. every month), pkpd_0008033

154 ps:model-HasAssociatedDoseFrequency-DataPool

155 QD (i.e. once per day), pkpd_0008028
156 BID (i.e. twice per day), pkpd_0008029
157 TID (i.e. Three times a day), pkpd_0008030
158 QOD (i.e. every other day), pkpd_0008031
159 Weekly, pkpd_0008032
160 QM (i.e. every month), pkpd_0008033

161 ps:trialdesign-observed-variables-are-real-freetext

162 Yes
163 No

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

165 Yes
166 No

167 ps:trialdesign-HasAssociatedSamplingDesign-DataPool

168 Assumed steady state, pkpd_0008035
169 Non steady state, pkpd_0008037

170 ps:model-HasAssociatedSamplingDesign-DataPool

171 Assumed steady state, pkpd_0008035
172 Non steady state, pkpd_0008037

173 ps:modeldefinition-HasAssociatedInputType

174 1, Direct input (e.g., intravenous), pkpd_0008050
175 1.1, Bolus, pkpd_0000043
176 1.2, Infusion, pkpd_0000044
177 2, Indirect input (e.g., oral), pkpd_0008051
178 2.1, Absorption delay, pkpd_0008052

179 ps:model-HasAssociatedInputType

180 1, Direct input (e.g., intravenous), pkpd_0008050
181 1.1, Bolus, pkpd_0000043
182 1.2, Infusion, pkpd_0000044
183 2, Indirect input (e.g., oral), pkpd_0008051

184 2.1, Absorption delay, pkpd_0008052

185 **ps:modeldefinition-HasAssociatedDistributionModellingAttribute**
186 **-EnterohepaticRecycling**

187 Yes, pkpd_0008044

188 No, pkpd_0008045

189 **ps:modeldefinition-HasAssociatedDistributionModellingAttribute**
190 **-NonLinearTransport**

191 Yes, pkpd_0008046

192 No, pkpd_0008047

193 **ps:modeldefinition-HasAssociatedDistributionModellingAttribute**
194 **-NonLinearProteinBinding**

195 Yes, pkpd_0008048

196 No, pkpd_0008049

197 **ps:model-HasAssociatedDistributionModellingAttribute**
198 **-EnterohepaticRecycling**

199 Yes, pkpd_0008044

200 No, pkpd_0008045

201 **ps:model-HasAssociatedDistributionModellingAttribute**
202 **-NonLinearTransport**

203 Yes, pkpd_0008046

204 No, pkpd_0008047

205 **ps:model-HasAssociatedDistributionModellingAttribute**
206 **-NonLinearProteinBinding**

207 Yes, pkpd_0008048

208 No, pkpd_0008049

209 **ps:modeldefinition-HasAssociatedAbsorptionDelayModelType**

210 Lag time, pkpd_0000075

211 Transit model, pkpd_0008054

212 ps:model-HasAssociatedAbsorptionDelayModelType

213 Lag time, pkpd_0000075

214 Transit model, pkpd_0008054

215 ps:modeldefinition-HasAssociatedAbsorptionRateType

216 Zero order, pkpd_0000071

217 Sequential (e.g., zero order then first order), pkpd_0008055

218 First order, pkpd_0000072

219 ps:model-HasAssociatedAbsorptionRateType

220 Zero order, pkpd_0000071

221 Sequential (e.g., zero order then first order), pkpd_0008055

222 First order, pkpd_0000072

223 ps:modeldefinition-InputPresentsFormationFromOtherSubstance-string

224 Yes

225 No

226 ps:model-InputPresentsFormationFromOtherSubstance-string

227 Yes

228 No

229 ps:modeldefinition-HasAssociatedBioavailabilityType

230 1, Constant, pkpd_0007016

231 2, Non constant, pkpd_0007017

232 2.1, with dose, pkpd_0007019

233 2.2, with concentration, pkpd_0007021

234 2.3, with hepatic extraction (i.e., first-pass effect), pkpd_0007022

235 2.4, with time, pkpd_0007020

236 ps:model-HasAssociatedBioavailabilityType

237 1, Constant, pkpd_0007016

238 2, Non constant, pkpd_0007017

239 2.1, with dose, pkpd_0007019

240 2.2, with concentration, pkpd_0007021

241 2.3, with hepatic extraction (i.e., first-pass effect), pkpd_0007022

242 2.4, with time, pkpd_0007020

243 **ps:modeldefinition-InputPresentsFormationFromOtherSubstanceType**

244 Administrated drug, pkpd_0007028

245 Other, pkpd_0007027

246 **ps:model-InputPresentsFormationFromOtherSubstanceType**

247 Administrated drug, pkpd_0007028

248 Other, pkpd_0007027

249 **ps:modeldefinition-InputPresentsFormationFromOtherSubstanceModelType**

250 Linear, pkpd_0007030

251 Nonlinear, pkpd_0007031

252 Time-dependent, pkpd_0007032

253 **ps:model-InputPresentsFormationFromOtherSubstanceModelType**

254 Linear, pkpd_0007030

255 Nonlinear, pkpd_0007031

256 Time-dependent, pkpd_0007032

257 **ps:modeldefinition-HasAssociatedEliminationModellingAttribute**
258 **-CompartmentOfElimination**

259 Central, pkpd_0007043

260 Other than central, pkpd_0007044

261 **ps:model-HasAssociatedEliminationModellingAttribute**
262 **-CompartmentOfElimination**

263 Central, pkpd_0007043

264 Other than central, pkpd_0007044

265 **ps:modeldefinition-HasAssociatedEliminationModellingAttribute**
266 **-TypeOfElimination**

267 1, Linear with drug concentration, pkpd_0000054

268 2, Michaelis-Menten (MM), pkpd_0000055

269 3, Target Mediated Drug Disposition (TMDD), pkpd_0000500

270 4, Time dependent, pkpd_0007046

271 4.1, Induction, pkpd_0007047

272 4.2, Inhibition, pkpd_0007048

273 4.3, Other, pkpd_0008056

274 **ps:model-HasAssociatedEliminationModellingAttribute**
275 **-TypeOfElimination**

276 1, Linear with drug concentration, pkpd_0000054

277 2, Michaelis-Menten (MM), pkpd_0000055

278 3, Target Mediated Drug Disposition (TMDD), pkpd_0000500

279 4, Time dependent, pkpd_0007046

280 4.1, Induction, pkpd_0007047

281 4.2, Inhibition, pkpd_0007048

282 4.3, Other, pkpd_0008056

283 **ps:modeldefinition-HasAssociatedModelledDrugFreeSystemType**

284 1, Baseline, pkpd_0008058

285 1.1, Constant, pkpd_0008059

286 1.2, Non constant, pkpd_0008060

287 2, Model for physiological system (description of some systems of physiology in healthy
288 state), pkpd_0008061

289 3, Disease model (physiology system perturbed by the disease), pkpd_0008062

290 4, Other, pkpd_0008063

291 **ps:model-HasAssociatedModelledDrugFreeSystemType**

292 1, Baseline, pkpd_0008058

293 1.1, Constant, pkpd_0008059

294 1.2, Non constant, pkpd_0008060

295 2, Model for physiological system (description of some systems of physiology in healthy
296 state), pkpd_0008061

297 3, Disease model (physiology system perturbed by the disease), pkpd_0008062

298 4, Other, pkpd_0008063

299 **ps:modeldefinition-HasDriverOfDrugEffectTypeAttribute**

300 1, Dose, pkpd_0008065

301 2, Concentration profile, pkpd_0008066

302 3, Summary measure, pkpd_0008067

303 3.1, Average concentration, pkpd_0008068

304 3.2, Minimal concentration or Through or pre-dose, pkpd_0008069

- 305 3.3, Maximal concentration, pkpd_0008070
306 3.4, AUC Over Dosing Interval, pkpd_0008071
307 3.5, Time over a threshold concentration, pkpd_0008072
308 3.6, Other, pkpd_0008073
- 309 **ps:model-HasDriverOfDrugEffectTypeAttribute**
- 310 1, Dose, pkpd_0008065
311 2, Concentration profile, pkpd_0008066
312 3, Summary measure, pkpd_0008067
313 3.1, Average concentration, pkpd_0008068
314 3.2, Minimal concentration or Through or pre-dose, pkpd_0008069
315 3.3, Maximal concentration, pkpd_0008070
316 3.4, AUC Over Dosing Interval, pkpd_0008071
317 3.5, Time over a threshold concentration, pkpd_0008072
318 3.6, Other, pkpd_0008073
- 319 **ps:modeldefinition-HasShapeOfDrugEffectTypeAttribute**
- 320 Linear relation, pkpd_0008075
321 Emax/Imax, pkpd_0008076
322 Sigmoid Emax/Imax, pkpd_0008077
323 Other, pkpd_0008078
- 324 **ps:model-HasShapeOfDrugEffectTypeAttribute**
- 325 Linear relation, pkpd_0008075
326 Emax/Imax, pkpd_0008076
327 Sigmoid Emax/Imax, pkpd_0008077
328 Other, pkpd_0008078
- 329 **ps:modeldefinition-HasTemporalRelationBetweenDrugEffect**
330 **AndResponseTypeAttribute**
- 331 1, Direct, pkpd_0008080
332 2, Indirect, pkpd_0008081
333 2.1, Affecting production of response (kin), pkpd_0008082
334 2.2, Affecting elimination of response (kout), pkpd_0008083
335 3, Effect compartment, pkpd_0008084
336 4, Binding model (i.e., to enzyme/receptor), pkpd_0008085
337 5, Tolerance phenomena, pkpd_0008086
338 6, Other, pkpd_0008087

339 **ps:model-HasTemporalRelationBetweenDrugEffect**
340 **AndResponseTypeAttribute**

- 341 1, Direct, pkpd_0008080
- 342 2, Indirect, pkpd_0008081
- 343 2.1, Affecting production of response (kin), pkpd_0008082
- 344 2.2, Affecting elimination of response (kout), pkpd_0008083
- 345 3, Effect compartment, pkpd_0008084
- 346 4, Binding model (i.e., to enzyme/receptor), pkpd_0008085
- 347 5, Tolerance phenomena, pkpd_0008086
- 348 6, Other, pkpd_0008087

349 **ps:modeldefinition-HasModelForResponseType**

- 350 1, Binary categorical observed variable , pkpd_0007051
- 351 1.1, Logistic regression model, pkpd_0007052
- 352 1.2, Markov model, pkpd_0007053
- 353 2, Ordered categorical observed variable, pkpd_0007054
- 354 2.1, Proportional odds model, pkpd_0007055
- 355 2.2, Differential odds model, pkpd_0007056
- 356 2.3, Markov model, pkpd_0007057
- 357 3, Non-ordered categorical observed variable, pkpd_0007058
- 358 3.1, Markov model, pkpd_0007059
- 359 4, Count or frequency categorical observed variable, pkpd_0007060
- 360 4.1, Poisson distribution model, pkpd_0007061
- 361 4.2, Zero-inflated Poisson distribution model, pkpd_0007062
- 362 4.3, Truncated poisson model, pkpd_0007063
- 363 4.4, Generalized poisson model, pkpd_0007064
- 364 4.5, Negative binomial model, pkpd_0007065
- 365 4.6, Zero-inflated negative binomial model, pkpd_0007066
- 366 4.7, Markov model, pkpd_0007067
- 367 5, Time-to-event observed variable, pkpd_0007068
- 368 5.1, Time-to-event single event observed variable, pkpd_0007069
- 369 5.1.1, Semi-parametric survival model , pkpd_0007070
- 370 5.1.1.1, Cox model, pkpd_0007071
- 371 5.1.2, Parametric survival model, pkpd_0007072
- 372 5.1.2.1, Exponential distribution model, pkpd_0007073
- 373 5.1.2.2, Weibull distribution model, pkpd_0007074
- 374 5.1.2.3, Log-normal distribution model, pkpd_0007075
- 375 5.1.2.4, Gamma distribution model, pkpd_0007076
- 376 5.1.2.5, Gompertz model, pkpd_0007077

377 5.2, Time-to-event repeated event observed variable, pkpd_0007078
378 5.2.1, Markov model, pkpd_0007079

379 **ps:model-HasModelForResponseType**

380 1, Binary categorical observed variable , pkpd_0007051
381 1.1, Logistic regression model, pkpd_0007052
382 1.2, Markov model, pkpd_0007053
383 2, Ordered categorical observed variable, pkpd_0007054
384 2.1, Proportional odds model, pkpd_0007055
385 2.2, Differential odds model, pkpd_0007056
386 2.3, Markov model, pkpd_0007057
387 3, Non-ordered categorical observed variable, pkpd_0007058
388 3.1, Markov model, pkpd_0007059
389 4, Count or frequency categorical observed variable, pkpd_0007060
390 4.1, Poisson distribution model, pkpd_0007061
391 4.2, Zero-inflated Poisson distribution model, pkpd_0007062
392 4.3, Truncated poisson model, pkpd_0007063
393 4.4, Generalized poisson model, pkpd_0007064
394 4.5, Negative binomial model, pkpd_0007065
395 4.6, Zero-inflated negative binomial model, pkpd_0007066
396 4.7, Markov model, pkpd_0007067
397 5, Time-to-event observed variable, pkpd_0007068
398 5.1, Time-to-event single event observed variable, pkpd_0007069
399 5.1.1, Semi-parametric survival model , pkpd_0007070
400 5.1.1.1, Cox model, pkpd_0007071
401 5.1.2, Parametric survival model, pkpd_0007072
402 5.1.2.1, Exponential distribution model, pkpd_0007073
403 5.1.2.2, Weibull distribution model, pkpd_0007074
404 5.1.2.3, Log-normal distribution model, pkpd_0007075
405 5.1.2.4, Gamma distribution model, pkpd_0007076
406 5.1.2.5, Gompertz model, pkpd_0007077
407 5.2, Time-to-event repeated event observed variable, pkpd_0007078
408 5.2.1, Markov model, pkpd_0007079

409 **ps:trialdesign-HasStudiedSubstanceAttribute**

410 Drug/Investigational agent/Hypothetical drug, C1909
411 No drug, C14165
412 Placebo, C753
413 Stimulus (ex: glucose tolerance test), C41210

414 ps:model-HasStudiedSubstanceAtttribute

415 Drug/Investigational agent/Hypothetical drug, C1909

416 No drug, C14165

417 Placebo, C753

418 Stimulus (ex: glucose tolerance test), C41210

419 ps:drug-TypeOfDrug1

420 Antibody or other biological drug, pkpd_0007173

421 Small molecule, pkpd_0007174

422 ps:drug-TypeOfDrug2

423 Antibody or other biological drug, pkpd_0007173

424 Small molecule, pkpd_0007174

425 ps:drug-TypeOfDrug3

426 Antibody or other biological drug, pkpd_0007173

427 Small molecule, pkpd_0007174

428 ps:drug-TypeOfDrug4

429 Antibody or other biological drug, pkpd_0007173

430 Small molecule, pkpd_0007174

431 ps:drug-TypeOfDrug5

432 Antibody or other biological drug, pkpd_0007173

433 Small molecule, pkpd_0007174

434 ps:trialdesign-hasInteractorByNickname-freetext

435 Drug1

436 Drug2

437 Drug3

438 Drug4

439 Drug5

440 OV1

441 OV2

442 OV3

443 OV4

444 OV5

445 **ps:trialdesign-hasInteracteeByNickname-freetext**

446 Drug1

447 Drug2

448 Drug3

449 Drug4

450 Drug5

451 OV1

452 OV2

453 OV3

454 OV4

455 OV5

456 **ps:trialdesign-hasTypeOfModelComponentImpacted**

457 1, PK, pkpd_0000006

458 1.1, Drug metabolism or transport, pkpd_0008101

459 1.1.1, Inhibition - reversible or irreversible, pkpd_0008102

460 1.1.2, Induction of enzymes or transporters, pkpd_0008103

461 1.2, Binding to plasma protein(s), pkpd_0008104

462 2, PD, pkpd_0000007

463 **ps:model-hasTypeOfModelComponentImpacted**

464 1, PK, pkpd_0000006

465 1.1, Drug metabolism or transport, pkpd_0008101

466 1.1.1, Inhibition - reversible or irreversible, pkpd_0008102

467 1.1.2, Induction of enzymes or transporters, pkpd_0008103

468 1.2, Binding to plasma protein(s), pkpd_0008104

469 2, PD, pkpd_0000007

470 **ps:model-hasInteractorByNickname-freetext**

471 Drug1

472 Drug2

473 Drug3

474 Drug4

475 Drug5

476 OV1

477 OV2

478 OV3

479 OV4

480 OV5

481 **ps:model-hasInteracteeByNickname-freetext**

482 Drug1

483 Drug2

484 Drug3

485 Drug4

486 Drug5

487 OV1

488 OV2

489 OV3

490 OV4

491 OV5

492 **ps:drug-hasDoseAmountUnit-Drug1**

493 mg, C28253

494 ug, C48152

495 IU (international unit), C48579

496 ml, C28254

497 **ps:drug-hasDoseAmountUnit-Drug2**

498 mg, C28253

499 ug, C48152

500 IU (international unit), C48579

501 ml, C28254

502 **ps:drug-hasDoseAmountUnit-Drug3**

503 mg, C28253

504 ug, C48152

505 IU (international unit), C48579

506 ml, C28254

507 **ps:drug-hasDoseAmountUnit-Drug4**

508 mg, C28253

509 ug, C48152

510 IU (international unit), C48579
511 ml, C28254

512 **ps:drug-hasDoseAmountUnit-Drug5**

513 mg, C28253
514 ug, C48152
515 IU (international unit), C48579
516 ml, C28254

517 **ps:model-hasDoseAmountUnit-Drug1**

518 mg, C28253
519 ug, C48152
520 IU (international unit), C48579
521 ml, C28254

522 **ps:model-hasDoseAmountUnit-Drug2**

523 mg, C28253
524 ug, C48152
525 IU (international unit), C48579
526 ml, C28254

527 **ps:model-hasDoseAmountUnit-Drug3**

528 mg, C28253
529 ug, C48152
530 IU (international unit), C48579
531 ml, C28254

532 **ps:model-hasDoseAmountUnit-Drug4**

533 mg, C28253
534 ug, C48152
535 IU (international unit), C48579
536 ml, C28254

537 ps:model-hasDoseAmountUnit-Drug5

538 mg, C28253

539 ug, C48152

540 IU (international unit), C48579

541 ml, C28254

542 ps:model-OVLinksToDrug-OV1

543 Drug1

544 Drug2

545 Drug3

546 Drug4

547 Drug5

548 ps:model-OVHasNature-OV1

549 Concentration, PATO_0000033

550 Score, C25338

551 ps:model-OVHasMatrixType-OV1

552 Blood, FMA_9670

553 Cerebrospinal Fluid (CSF), FMA_20935

554 Plasma, FMA_62970

555 Serum, FMA_63083

556 Urine, FMA_12274

557 ps:model-OVHasTypeOfObservedVariable-OV1

558 1, Continuous, pkpd_0000415

559 2, Categorical, pkpd_0000416

560 3, Count, pkpd_0000418

561 4, Frequency, pkpd_0008105

562 5, Time-to-event, pkpd_0000417

563 ps:model-OVLinksToDrug-OV2

564 Drug1

565 Drug2

566 Drug3

567 Drug4

568 Drug5

569 ps:model-OVHasNature-OV2

570 Concentration, PATO_0000033

571 Score, C25338

572 ps:model-OVHasMatrixType-OV2

573 Blood, FMA_9670

574 Cerebrospinal Fluid (CSF), FMA_20935

575 Plasma, FMA_62970

576 Serum, FMA_63083

577 Urine, FMA_12274

578 ps:model-OVHasTypeOfObservedVariable-OV2

579 1, Continuous, pkpd_0000415

580 2, Categorical, pkpd_0000416

581 3, Count, pkpd_0000418

582 4, Frequency, pkpd_0008105

583 5, Time-to-event, pkpd_0000417

584 ps:model-OVLinksToDrug-OV3

585 Drug1

586 Drug2

587 Drug3

588 Drug4

589 Drug5

590 ps:model-OVHasNature-OV3

591 Concentration, PATO_0000033

592 Score, C25338

593 ps:model-OVHasMatrixType-OV3

594 Blood, FMA_9670

595 Cerebrospinal Fluid (CSF), FMA_20935

596 Plasma, FMA_62970

597 Serum, FMA_63083

598 Urine, FMA_12274

599 ps:model-OVHasTypeOfObservedVariable-OV3

- 600 1, Continuous, pkpd_0000415
- 601 2, Categorical, pkpd_0000416
- 602 3, Count, pkpd_0000418
- 603 4, Frequency, pkpd_0008105
- 604 5, Time-to-event, pkpd_0000417

605 ps:model-OVLinksToDrug-OV4

- 606 Drug1
- 607 Drug2
- 608 Drug3
- 609 Drug4
- 610 Drug5

611 ps:model-OVHasNature-OV4

- 612 Concentration, PATO_0000033
- 613 Score, C25338

614 ps:model-OVHasMatrixType-OV4

- 615 Blood, FMA_9670
- 616 Cerebrospinal Fluid (CSF), FMA_20935
- 617 Plasma, FMA_62970
- 618 Serum, FMA_63083
- 619 Urine, FMA_12274

620 ps:model-OVHasTypeOfObservedVariable-OV4

- 621 1, Continuous, pkpd_0000415
- 622 2, Categorical, pkpd_0000416
- 623 3, Count, pkpd_0000418
- 624 4, Frequency, pkpd_0008105
- 625 5, Time-to-event, pkpd_0000417

626 ps:model-OVLinksToDrug-OV5

- 627 Drug1
- 628 Drug2
- 629 Drug3
- 630 Drug4

631 Drug5

632 **ps:model-OVHasNature-OV5**

633 Concentration, PATO_0000033

634 Score, C25338

635 **ps:model-OVHasMatrixType-OV5**

636 Blood, FMA_9670

637 Cerebrospinal Fluid (CSF), FMA_20935

638 Plasma, FMA_62970

639 Serum, FMA_63083

640 Urine, FMA_12274

641 **ps:model-OVHasTypeOfObservedVariable-OV5**

642 1, Continuous, pkpd_0000415

643 2, Categorical, pkpd_0000416

644 3, Count, pkpd_0000418

645 4, Frequency, pkpd_0008105

646 5, Time-to-event, pkpd_0000417

647 **ps:structuralmodel-HasComponentType**

648 PK, pkpd_0000006

649 PD, pkpd_0000007

650 PBPK, pkpd_0000012

651 Drug-Drug Interaction, pkpd_0008100

652 **ps:model-HasComponentType**

653 PK, pkpd_0000006

654 PD, pkpd_0000007

655 PBPK, pkpd_0000012

656 Drug-Drug Interaction, pkpd_0008100

657 **ps:model-OVHasUnits-OV1**

658 1, concentration, C48207

659 1.1, nM, C48517

660 1.2, uM, C48509

661 1.3, ng/mL, C67306

662 1.4, mg/mL, C42576
663 1.5, mg/dL, C67015
664 1.6, ug/mL, C67305
665 1.7, g/L, C42576
666 1.8, mg/L, C67306
667 1.9, number/L, C105515
668 "1.10", number/mL, C103452
669 1.11, IU/mL, C67377
670 1.12, IU/L, C67376
671 1.13, mIU/L, C67405
672 2, volume, C44279
673 2.1, L, C48505
674 2.2, mL, C28254
675 2.3, mm3, C48153
676 2.4, cm3, C28254
677 3, length, C42578
678 3.1, mm, C28251
679 3.2, cm, C49668
680 3.2, m, C41139
681 4, area, C48037
682 4.1, mm2, C65104
683 4.2, cm2, C48460
684 5, clearance, C48568
685 5.1, L/h, C69160
686 5.2, L/min, C67388
687 5.3, mL/h, C66962
688 6, rate, C25636
689 6.1, h-1, C66966
690 6.2, min-1, C66967
691 6.3, day-1, C66968
692 6.4, week-1, C67069
693 6.5, year-1, C74924
694 7, time, C42574
695 7.1, h, C25529
696 7.2, min, C48154
697 7.3, day, C25301
698 7.4, week, C29844
699 7.5, year, C29848
700 8, amount, C42579
701 8.1, g, C48155
702 8.2, mg, C28253

703 8.3, kg, C28252
704 8.4, International Unit (IU), C48579

705 **ps:model-OVHasUnits-OV2**

706 1, concentration, C48207
707 1.1, nM, C48517
708 1.2, uM, C48509
709 1.3, ng/mL, C67306
710 1.4, mg/mL, C42576
711 1.5, mg/dL, C67015
712 1.6, ug/mL, C67305
713 1.7, g/L, C42576
714 1.8, mg/L, C67306
715 1.9, number/L, C105515
716 "1.10", number/mL, C103452
717 1.11, IU/mL, C67377
718 1.12, IU/L, C67376
719 1.13, mIU/L, C67405
720 2, volume, C44279
721 2.1, L, C48505
722 2.2, mL, C28254
723 2.3, mm3, C48153
724 2.4, cm3, C28254
725 3, length, C42578
726 3.1, mm, C28251
727 3.2, cm, C49668
728 3.2, m, C41139
729 4, area, C48037
730 4.1, mm2, C65104
731 4.2, cm2, C48460
732 5, clearance, C48568
733 5.1, L/h, C69160
734 5.2, L/min, C67388
735 5.3, mL/h, C66962
736 6, rate, C25636
737 6.1, h-1, C66966
738 6.2, min-1, C66967
739 6.3, day-1, C66968
740 6.4, week-1, C67069
741 6.5, year-1, C74924

742 7, time, C42574
743 7.1, h, C25529
744 7.2, min, C48154
745 7.3, day, C25301
746 7.4, week, C29844
747 7.5, year, C29848
748 8, amount, C42579
749 8.1, g, C48155
750 8.2, mg, C28253
751 8.3, kg, C28252
752 8.4, International Unit (IU), C48579

753 **ps:model-OVHasUnits-OV3**

754 1, concentration, C48207
755 1.1, nM, C48517
756 1.2, uM, C48509
757 1.3, ng/mL, C67306
758 1.4, mg/mL, C42576
759 1.5, mg/dL, C67015
760 1.6, ug/mL, C67305
761 1.7, g/L, C42576
762 1.8, mg/L, C67306
763 1.9, number/L, C105515
764 "1.10", number/mL, C103452
765 1.11, IU/mL, C67377
766 1.12, IU/L, C67376
767 1.13, mIU/L, C67405
768 2, volume, C44279
769 2.1, L, C48505
770 2.2, mL, C28254
771 2.3, mm3, C48153
772 2.4, cm3, C28254
773 3, length, C42578
774 3.1, mm, C28251
775 3.2, cm, C49668
776 3.2, m, C41139
777 4, area, C48037
778 4.1, mm2, C65104
779 4.2, cm2, C48460
780 5, clearance, C48568

781 5.1, L/h, C69160
782 5.2, L/min, C67388
783 5.3, mL/h, C66962
784 6, rate, C25636
785 6.1, h-1, C66966
786 6.2, min-1, C66967
787 6.3, day-1, C66968
788 6.4, week-1, C67069
789 6.5, year-1, C74924
790 7, time, C42574
791 7.1, h, C25529
792 7.2, min, C48154
793 7.3, day, C25301
794 7.4, week, C29844
795 7.5, year, C29848
796 8, amount, C42579
797 8.1, g, C48155
798 8.2, mg, C28253
799 8.3, kg, C28252
800 8.4, International Unit (IU), C48579

801 **ps:model-OVHasUnits-OV4**

802 1, concentration, C48207
803 1.1, nM, C48517
804 1.2, uM, C48509
805 1.3, ng/mL, C67306
806 1.4, mg/mL, C42576
807 1.5, mg/dL, C67015
808 1.6, ug/mL, C67305
809 1.7, g/L, C42576
810 1.8, mg/L, C67306
811 1.9, number/L, C105515
812 "1.10", number/mL, C103452
813 1.11, IU/mL, C67377
814 1.12, IU/L, C67376
815 1.13, mIU/L, C67405
816 2, volume, C44279
817 2.1, L, C48505
818 2.2, mL, C28254
819 2.3, mm3, C48153

820 2.4, cm3, C28254
821 3, length, C42578
822 3.1, mm, C28251
823 3.2, cm, C49668
824 3.2, m, C41139
825 4, area, C48037
826 4.1, mm2, C65104
827 4.2, cm2, C48460
828 5, clearance, C48568
829 5.1, L/h, C69160
830 5.2, L/min, C67388
831 5.3, mL/h, C66962
832 6, rate, C25636
833 6.1, h-1, C66966
834 6.2, min-1, C66967
835 6.3, day-1, C66968
836 6.4, week-1, C67069
837 6.5, year-1, C74924
838 7, time, C42574
839 7.1, h, C25529
840 7.2, min, C48154
841 7.3, day, C25301
842 7.4, week, C29844
843 7.5, year, C29848
844 8, amount, C42579
845 8.1, g, C48155
846 8.2, mg, C28253
847 8.3, kg, C28252
848 8.4, International Unit (IU), C48579

849 **ps:model-OVHasUnits-OV5**

850 1, concentration, C48207
851 1.1, nM, C48517
852 1.2, uM, C48509
853 1.3, ng/mL, C67306
854 1.4, mg/mL, C42576
855 1.5, mg/dL, C67015
856 1.6, ug/mL, C67305
857 1.7, g/L, C42576
858 1.8, mg/L, C67306

859 1.9, number/L, C105515
860 "1.10", number/mL, C103452
861 1.11, IU/mL, C67377
862 1.12, IU/L, C67376
863 1.13, mIU/L, C67405
864 2, volume, C44279
865 2.1, L, C48505
866 2.2, mL, C28254
867 2.3, mm3, C48153
868 2.4, cm3, C28254
869 3, length, C42578
870 3.1, mm, C28251
871 3.2, cm, C49668
872 3.2, m, C41139
873 4, area, C48037
874 4.1, mm2, C65104
875 4.2, cm2, C48460
876 5, clearance, C48568
877 5.1, L/h, C69160
878 5.2, L/min, C67388
879 5.3, mL/h, C66962
880 6, rate, C25636
881 6.1, h-1, C66966
882 6.2, min-1, C66967
883 6.3, day-1, C66968
884 6.4, week-1, C67069
885 6.5, year-1, C74924
886 7, time, C42574
887 7.1, h, C25529
888 7.2, min, C48154
889 7.3, day, C25301
890 7.4, week, C29844
891 7.5, year, C29848
892 8, amount, C42579
893 8.1, g, C48155
894 8.2, mg, C28253
895 8.3, kg, C28252
896 8.4, International Unit (IU), C48579