

pHUBpk: Pharmacokinetics on the pharmaHUB

Stephen D. Stamatis¹, Michael J. McLennan², and Lee E. Kirsch¹

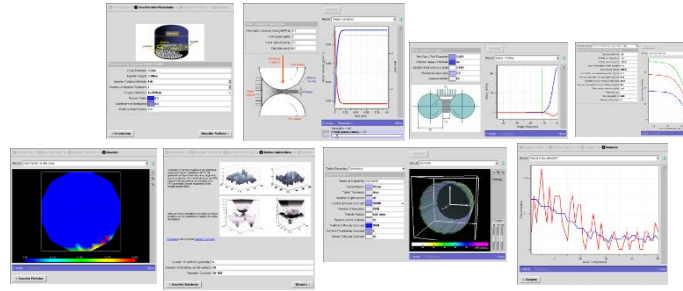
HUBbub 2013

¹The University of Iowa College of Pharmacy

²Purdue University



pharmaHUB



22 simulation tools

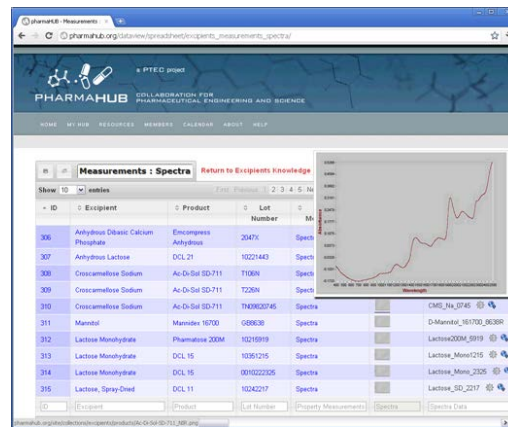
23,000

Users Worldwide



Collaboration for
Pharmaceutical
Engineering and Science


\$1.9M NSF CDI award
Purdue University
Rutgers University
University of Iowa



NIPTE-FDA
Excipients
Knowledge Base

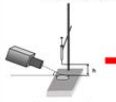
Visualizing the Interaction of Light & Particles

- No sample preparation in NIR spectroscopy.
- Light interactions with particles.
- Need to learn to visualize the particles and their interaction with light.



J.L. Koenig, M. B. Sauer, R.J. Rowell, A.425
PharmTech, 2013, 23, whole 11.

Formulation Characterization



Water penetration time (w-Gabapentin + HPC K10)

Experiments were performed with 22 Gauge needle. The drop penetration time for the drop sizes of interest are calculated by:

$$t_{p,2} = \frac{d_{p,2}^2}{g}$$

Drop Size (µm)	Penetration time (sec)
2.51	75.4 ± 4.8*
3.17	6.10
3.75	6.86
4.50	334

* measured

Toward intelligent decision support for pharmaceutical product development

Chunhua Shan, Anwar Ajan, Laxmi Halderman, Prabang Suruch, Parvatharam Akshaya, Ghosh, Jagdish, Venkat Venkateshramanian, Gireesh V. Reddy, Ken Morris, and Prabh Basu

Journal of Pharmaceutical Innovation, 2014, 3(1), 1-10

100 other

pharmaHUB Community

Tools

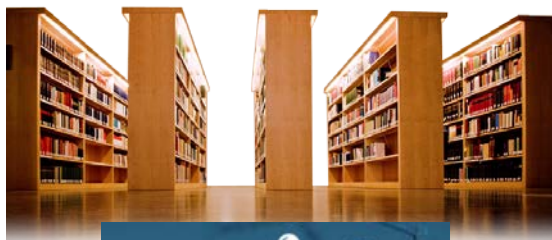
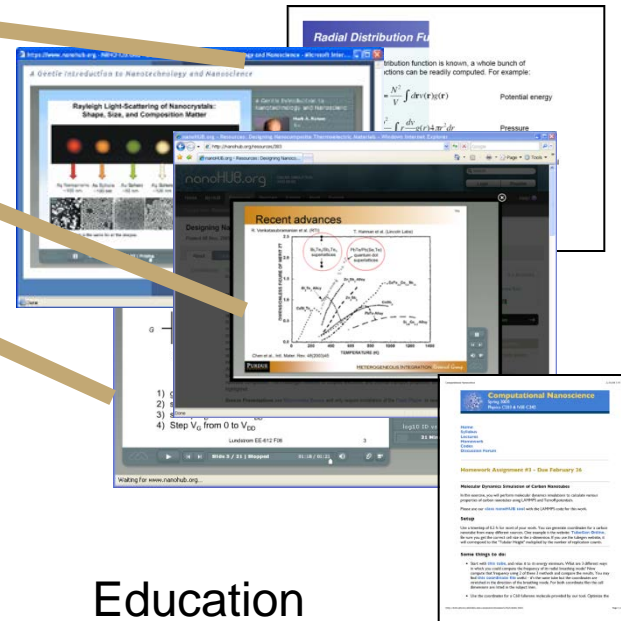
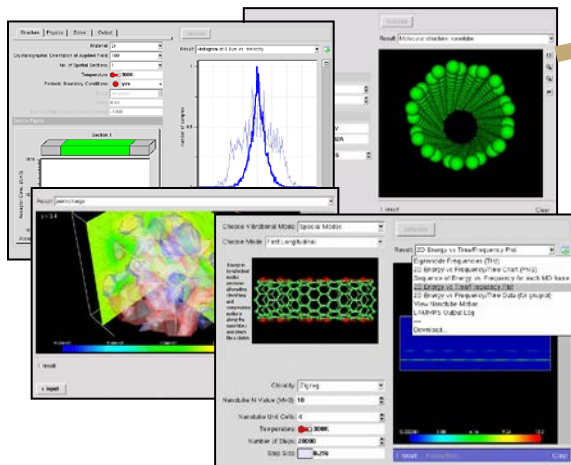
Tags

Supporting Resources

Crystallization

Particle Size Distribution

Dissolution



Research

Education

Reviews

- ★★★★ James k fodor said: 26 Jan, 2006 10:24 AM This is a great learning module. Simply because it would help...
- ★★★★ Jing Guo said: 26 Jan, 2006 09:12 AM It's an excellent material to learn...

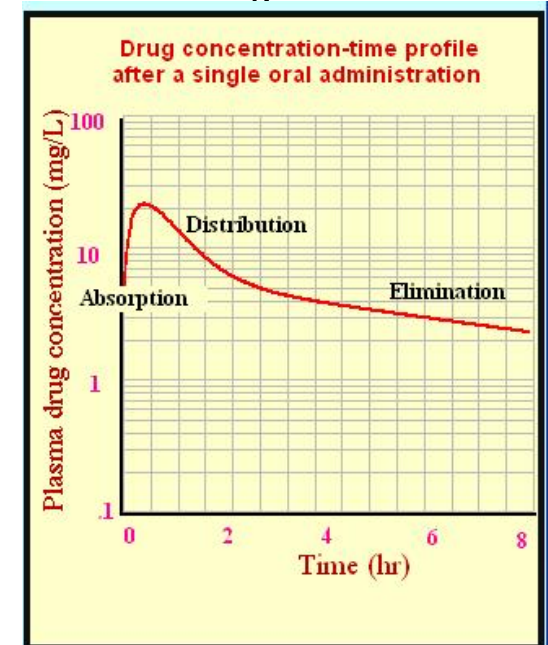
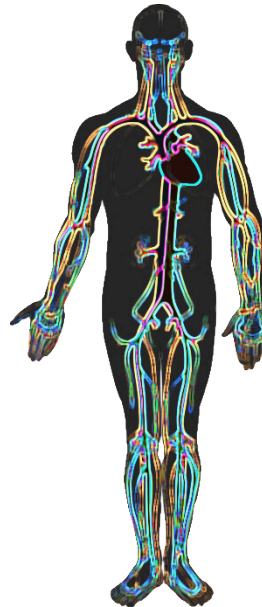


Reviews

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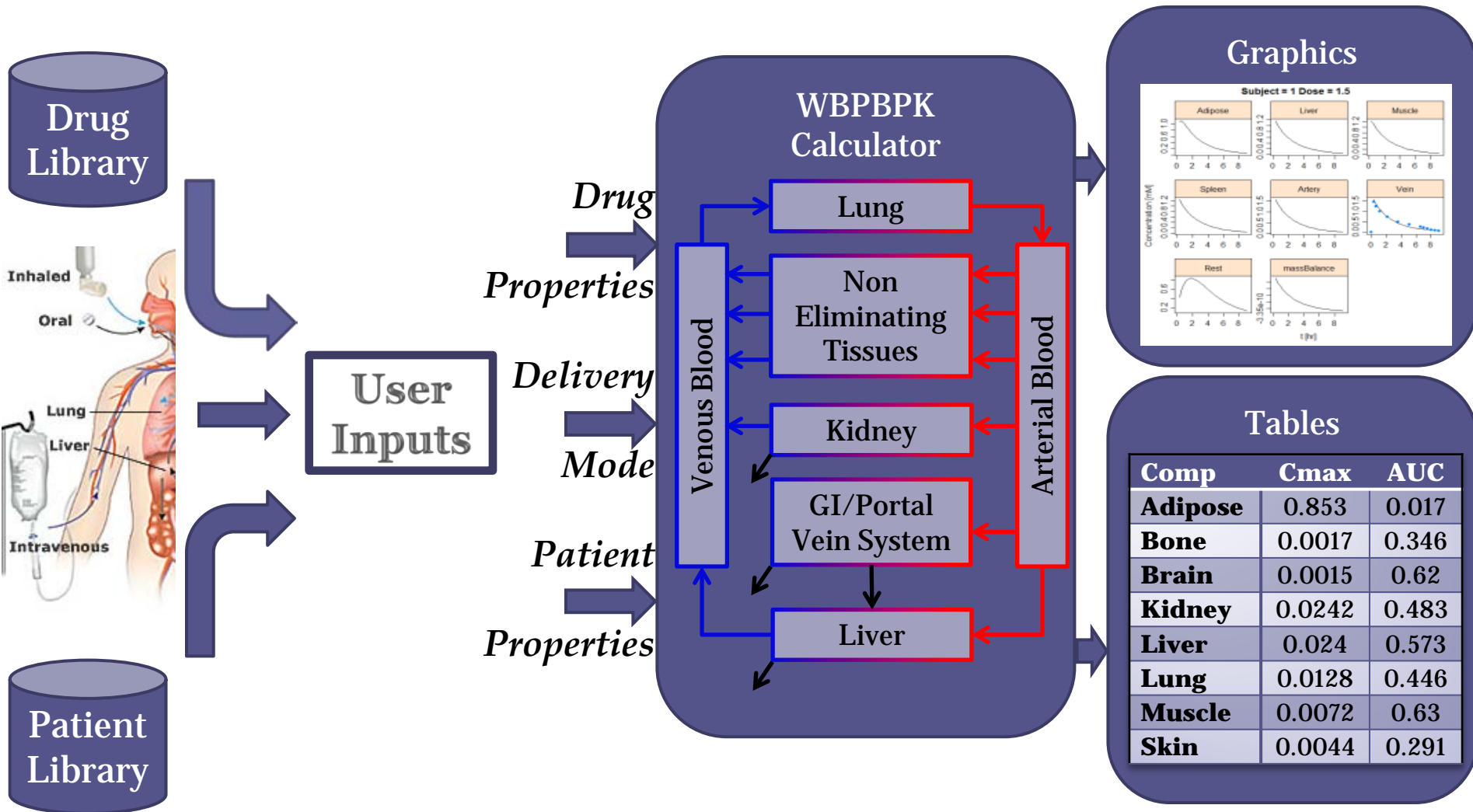
Pharmacokinetics

- Loosely speaking: the study of what the body does to a drug

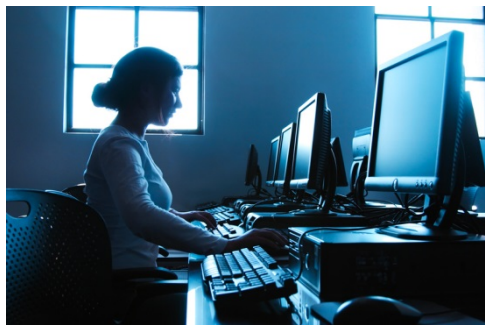
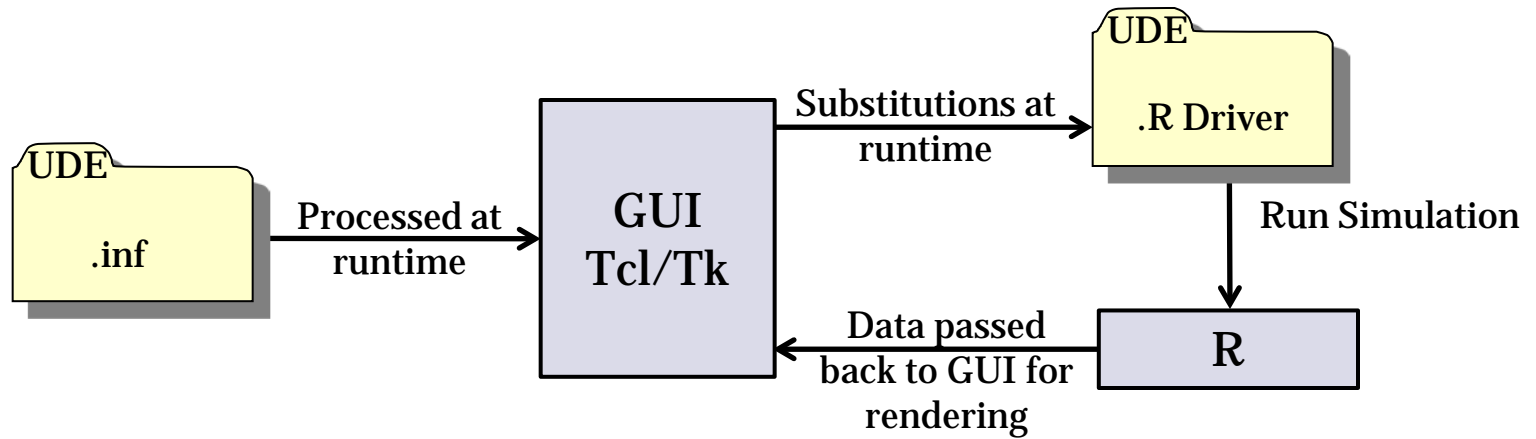


- Whole Body Physiologically Based Models provide a unique opportunity to learn about PK actively

pHUBpk



Implementation



All code runs on the PharmaHUB





Understanding Drug Distribution

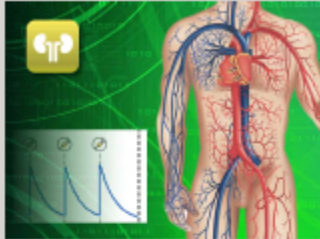
UDD: Understanding Drug Distribution

In this Active Learning Environment you can explore aspects of drug distribution including:

- How molecular properties like pK_a and $\log P$ influence the volume of distribution
- How Patient properties like body composition change drug distribution

The paper by [Rodgers and Rowland](#) is an excellent review of the subject and presents some of the equations used in this tool.

Start >



Understanding Drug Elimination



UDE: Understanding Drug Elimination

In this Active Learning Environment you can explore aspects of drug elimination including:

- How clearance parameters affect the plasma concentration time profile
- The effect of different dosing strategies on the concentration time profile
- and the approach to steady state following multiple IV boluses or constant rate IV infusion

Start >

[< Back](#)*pHUBpk: Understanding Drug Elimination***Drug Properties**

Molecule	Alfentanil	▼
Ion Class	Weak Base	▼

	MEAN	CV
pKa	6.5	0
LogP _{ow}	2.16	0
LogP _{vow}	1.07	0

Patient Characteristics

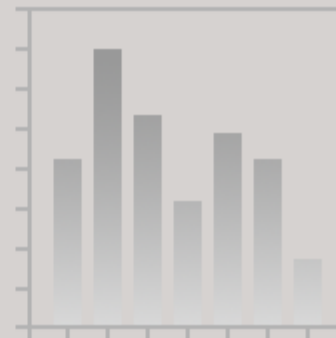
Subject	Man	▼
---------	-----	---

	MEAN	CV
Mass (kg)	70	0
Cardiac Output (L/hr)	312	0
Hematocrit	0.434	0
fV _{Adipose} (frac)	0.2	0
fV _{Bone} (frac)	0.144	0
fV _{Brain} (frac)	0.0199	0
fV _{Heart} (frac)	0.00452	0
fV _{Kidney} (frac)	0.00425	0
fV _{Liver} (frac)	0.0247	0
fV _{Lung} (frac)	0.00685	0

Drug Subject**Administration Variables****Compute**

Clear All

Download

*Simplify this tool...*

< Back

Drug Properties

Molecule	Alfentanil
Ion Class	Weak Base

pKa	
LogP _{ow}	2.16
LogP _{vow}	1.07

Patient Characteristics

Subject
Mass (kg)
Cardiac Output (L/hr)
Hematocrit
fV _{Adipose} (frac)
fV _{Bone} (frac)
fV _{Brain} (frac)
fV _{Heart} (frac)
fV _{Kidney} (frac)
fV _{Liver} (frac)
fV _{Lung} (frac)

Drug Subject**Administration Variables**

pKa

pKa is the logarithmic measure of the acid dissociation constant. The larger the value, the less acidic the compound, and the smaller the extent of dissociation.

If the drug is known to be a base at physiologic pH, the pKa refers to the conjugate acid of the base.

< Back

*pHUBpk: Understanding Drug Elimination***Drug Properties**

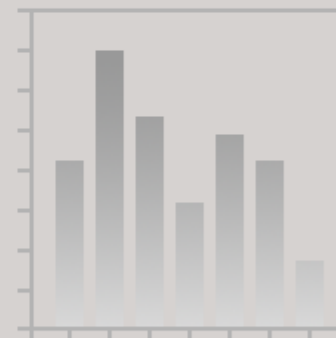
Molecule	Alfentanil
Ion Class	W
pKa	6.
LogP _{ow}	2.
LogP _{vow}	1.
Patient Char	
Subject	Diazepam

	MEAN	CV
Mass (kg)	70	0
Cardiac Output (L/hr)	312	0
Hematocrit	0.434	0
fV_Adipose (frac)	0.2	0
fV_Bone (frac)	0.144	0
fV_Brain (frac)	0.0199	0
fV_Heart (frac)	0.00452	0
fV_Kidney (frac)	0.00425	0
fV_Liver (frac)	0.0247	0
fV_Lung (frac)	0.00685	0

Drug Subject**Administration Variables****Compute**

✖ Clear All

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< Back

pHUBpk: Understanding Drug Elimination

Drug Properties

Molecule	Chlorpheniramine	▼
Ion Class	Strong Base	▼

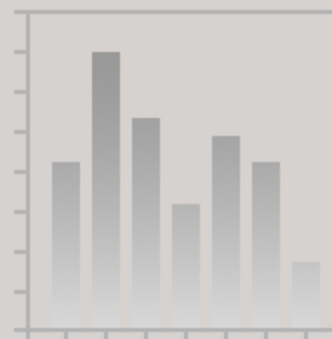
	MEAN	CV
pKa	9.13	0
LogP _{ow}	3.07	0
LogP _{vow}	2.08	0

Patient Characteristics

Subject	Man	▼
---------	-----	---

	MEAN	CV
Mass (kg)	70	0
Cardiac Output (L/hr)	312	0
Hematocrit	0.434	0
fV _{Adipose} (frac)	0.2	0
fV _{Bone} (frac)	0.144	0
fV _{Brain} (frac)	0.0199	0
fV _{Heart} (frac)	0.00452	0
fV _{Kidney} (frac)	0.00425	0
fV _{Liver} (frac)	0.0247	0
fV _{Lung} (frac)	0.00685	0

Drug Subject**Administration Variables****Compute**
 Clear All

 Download
*Simplify this tool...*

< Back

*pHUBpk: Understanding Drug Elimination***Drug Properties**

Molecule	Chlorpheniramine	▼
Ion Class	Strong Base	▼

	MEAN	CV
pKa	9.13	0
LogP _{ow}	3.07	0
LogP _{vow}	2.08	0

Patient Characteristics

Subject	Man	▼	▲
---------	-----	---	---

Drug Subject

	MEAN	CV
fu,p	0.28	0
B:P	1.34	0

Liver Function	First Order	▼
----------------	-------------	---

	MEAN	CV
Liver CL (L/hr)	75.4	0

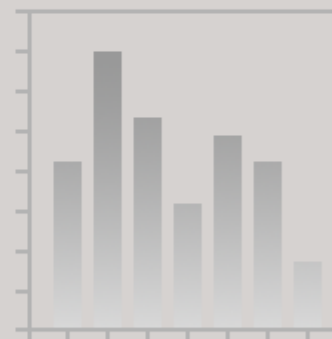
Kidney Function	First Order	▼
-----------------	-------------	---

	MEAN	CV
Kidney CL (L/hr)	22.5	0

Administration Variables**Compute**

✖ Clear All

📄 Download

*Simplify this tool...*

< Back

*pHUBpk: Understanding Drug Elimination***Drug Properties**

Molecule	Chlorpheniramine	▼
Ion Class	Strong Base	▼

	MEAN	CV
pKa	9.13	0
LogP _{ow}	3.07	0
LogP _{vow}	2.08	0

Patient Characteristics

Subject	Man	▼	↕
---------	-----	---	---

Drug Subject

	MEAN	CV
fu,p	0.28	0.05
B:P	1.34	0.05

Liver Function	First Order	▼
----------------	-------------	---

	MEAN	CV
Liver CL (L/hr)	75.4	0.05

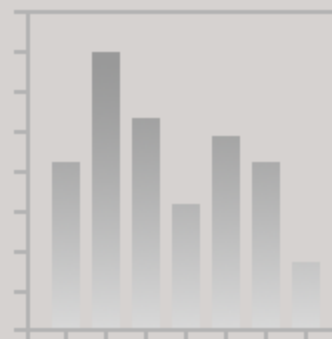
Kidney Function	First Order	▼
-----------------	-------------	---

	MEAN	CV
Kidney CL (L/hr)	22.5	0.05

Administration Variables**Compute**

✖ Clear All

⬇ Download

*Simplify this tool...*

< Back

*pHUBpk: Understanding Drug Elimination***Drug Properties**

Molecule	Chlorpheniramine	▼
Ion Class	Strong Base	▼

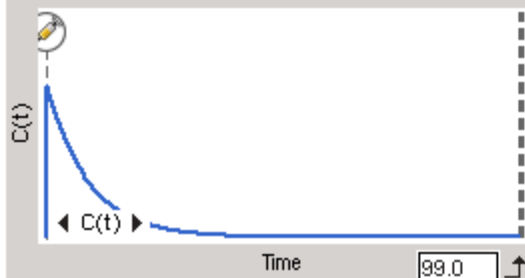
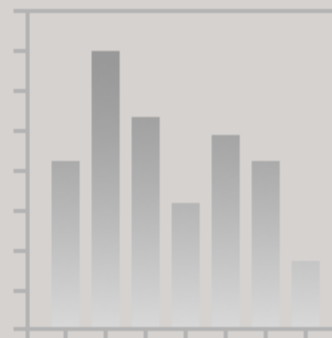
	MEAN	CV
pKa	9.13	0
LogP _{ow}	3.07	0
LogP _{vow}	2.08	0

Patient Characteristics**Drug Subject**

	MEAN	CV
fu,p	0.28	0.05

Administration Variables

Doses

Regimen: *Simplify this tool...***Compute**

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pHUBpk: Understanding Drug Elimination

Drug Properties

Molecule	Chlorpheniramine	▼
Ion Class	Strong Base	▼

	MEAN	CV
pKa	9.13	0
LogP _{ow}	3.07	0
LogP _{vow}	2.08	0

Compute

✖ Clear All

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Patient Characteristics

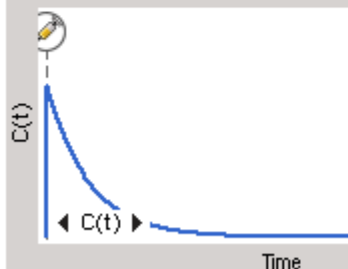
Drug Subject

	MEAN	
fu,p	0.28	0.05

Administration Variables

Doses

Regimen: Set



Specify a Regimen

Route: IV Bolus



Dose per kg: 10 (mg/kg)

Duration: 1 (hr)

Total Dose: 700 (mg)



70 kg

◆ Single dose

◇ Multiple doses

Number of doses: 4

Interval: 4 (hrs)

Extend simulation: 5 (half-lives)

Apply

Simplify this tool...

< Back

pHUBpk: Understanding Drug Elimination

Drug Properties

Molecule	Chlorpheniramine	▼
Ion Class	Strong Base	▼

	MEAN	CV
pKa	9.13	0
LogP _{ow}	3.07	0
LogP _{vow}	2.08	0

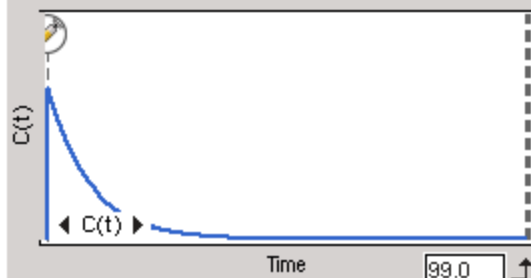
Patient Characteristics

Drug Subject

	MEAN	CV
fu,p	0.28	0.05

Administration Variables

Doses

Regimen: 

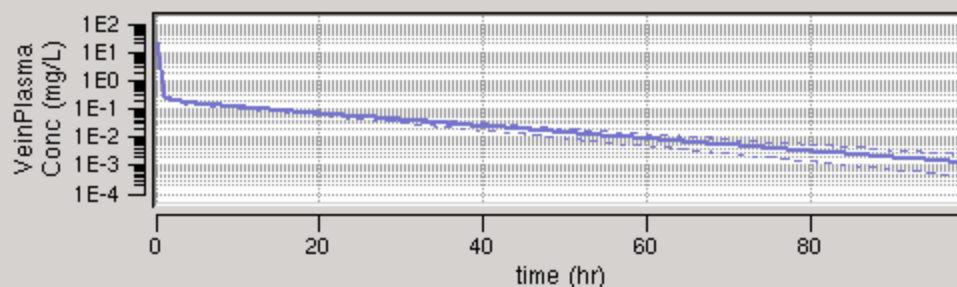
Simplify this tool...

Compute

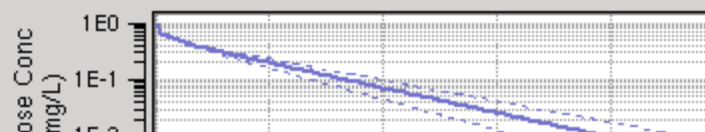
✖ Clear All

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View: Concentration Time Profiles ▼



AUC _{0-t1}	AUC _{t1-extInf}	AUC _{0-extInf}	Vd _{uss}	Vd _{ss}
1.18	0.025	1.205	1508.717	420.245



◀ AUC_{0-t1} ▶
11.053

■ Case #1

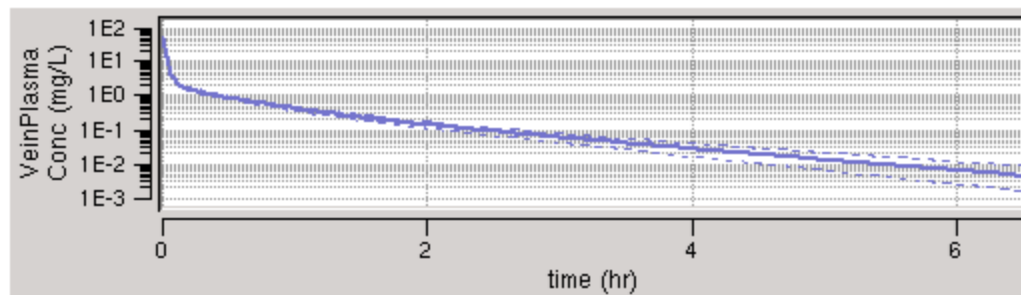
Molecule	Chlorpheniramine	
Ion Class	Strong Base	
	MEAN	CV
pKa	9.13	0
LogP _{ow}	3.07	0
LogP _{vow}	2.08	0

< Back

Concentration Time Profile

Compute

View: Conc

 VeinPlasma
 Conc (mg/L)
 1E2
 1E1
 ?
 1E-3
 1E-4


In this image, we show how the plasma drug concentration changes as a function of time. The solid line represents the expected value of the concentration at each time. The dashed lines represent the 95% confidence interval for the mean, giving a sense of the uncertainty that follows in the concentration caused by uncertainty in the parameters.

 ose Conc
 (mg/L)
 1E0
 1E-1
 1E-2

Molecule

Ion Class

pKa

LogP_ow

LogP_vow

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pHUBpk: Understanding Drug Elimination

Drug Properties

Molecule Chlorpheniramine

Ion Class Strong Base

	MEAN	CV
pKa	9.13	0
LogP _{ow}	3.07	0
LogP _{vow}	2.08	0

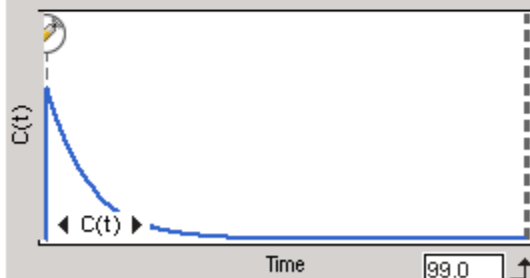
Patient Characteristics

Drug Subject

	MEAN	CV
fu,p	0.28	0.05

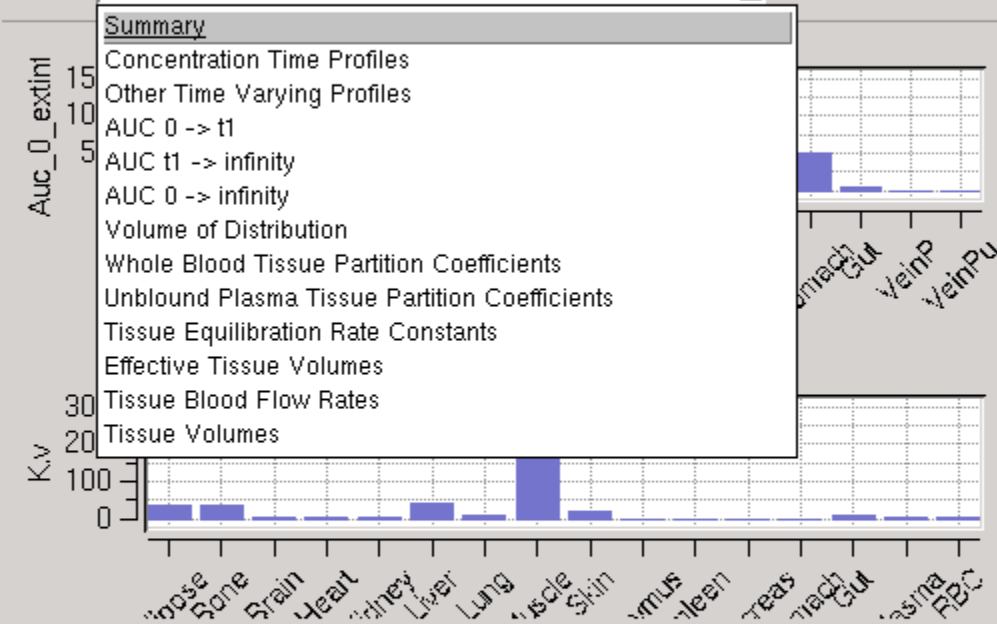
Administration Variables

Doses

Regimen: 

Simplify this tool...

Compute

View: 

Case #1

Molecule	Chlorpheniramine	
Ion Class	Strong Base	
	MEAN	CV
pKa	9.13	0
LogP _{ow}	3.07	0
LogP _{vow}	2.08	0

< Back

pHUBpk: Understanding Drug Elimination

Drug Properties

Molecule	Chlorpheniramine	▼
Ion Class	Strong Base	▼

	MEAN	CV
pKa	9.13	0
LogP _{ow}	3.07	0
LogP _{vow}	2.08	0

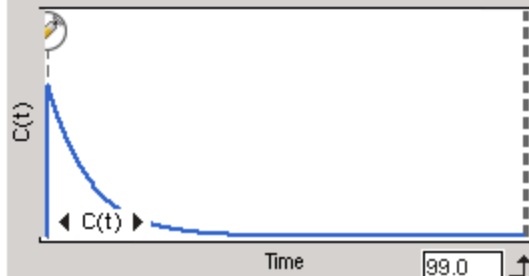
Patient Characteristics

Drug Subject

	MEAN	CV
fu,p	0.28	0

Administration Variables

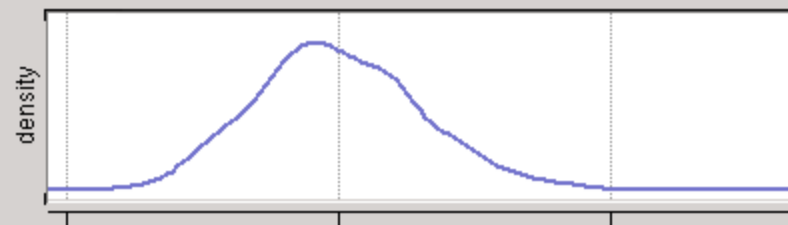
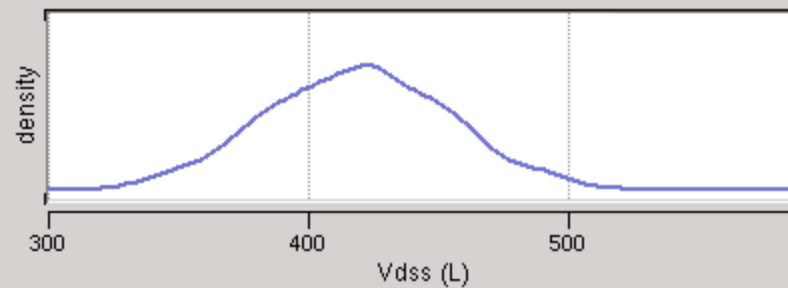
Doses

Regimen: 

Simplify this tool...

Compute

View: Volume of Distribution ▼



■ Case #1

Molecule	Chlorpheniramine	
Ion Class	Strong Base	
	MEAN	CV
pKa	9.13	0
LogP _{ow}	3.07	0
LogP _{vow}	2.08	0

< Back

pHUBpk: Understanding Drug Elimination

Drug Properties

Molecule	Chlorpheniramine	▼
Ion Class	Strong Base	▼

	MEAN	CV
pKa	9.13	0
LogP _{ow}	3.07	0
LogP _{vow}	2.08	0

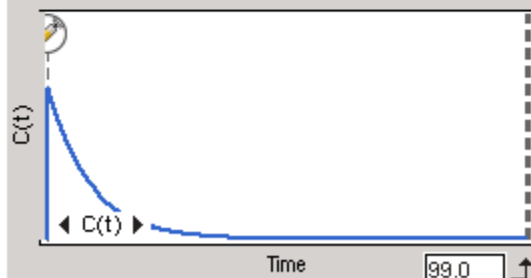
Patient Characteristics

Drug Subject

	MEAN	CV
fu,p	0.28	0.05

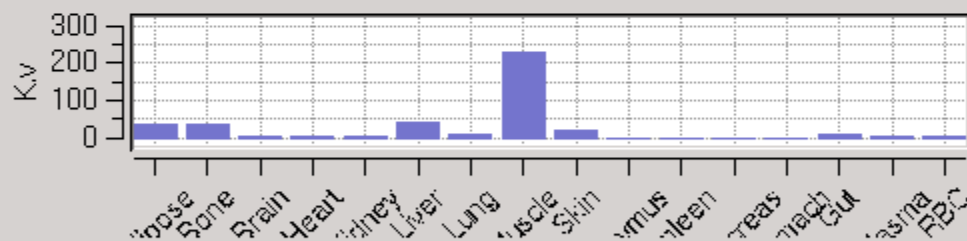
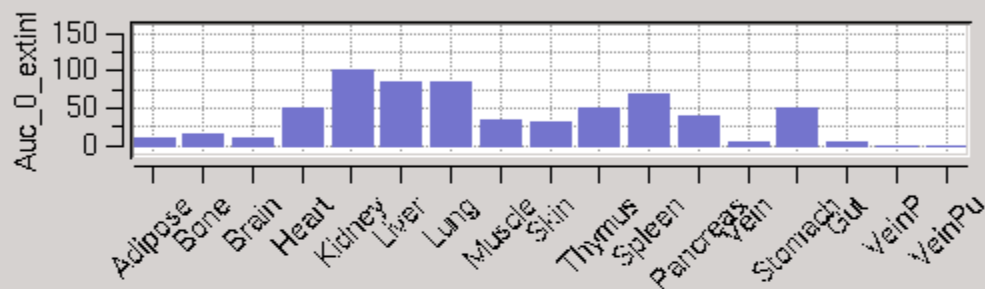
Administration Variables

Doses

Regimen: 

Simplify this tool...

Compute

View: 

■ Case #1

Molecule	Chlorpheniramine	
Ion Class	Strong Base	
	MEAN	CV
pKa	9.13	0
LogP _{ow}	3.07	0
LogP _{vow}	2.08	0

Case Comparison

- To explore and discover how the various properties influence interface is interactive, we allow users to compare different cases
- Cases can be different
 - Drugs
 - Subjects
 - Regimens
- We highlight the differences in the case browser

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pHUBpk: Understanding Drug Elimination

Drug Properties

Molecule	Ibuprofen	▼
Ion Class	Acid	▼

	MEAN	CV
pKa	4.7	0
LogP _{ow}	4.06	0
LogP _{vow}	3.19	0

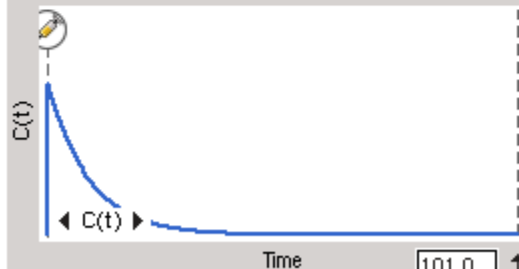
Patient Characteristics

Drug Subject

	MEAN	CV
fu,p	0.0061	0.05

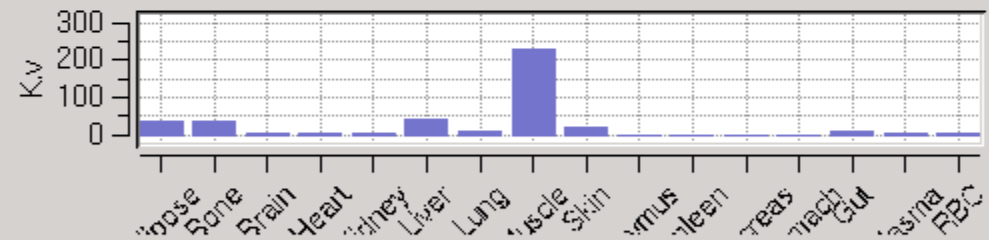
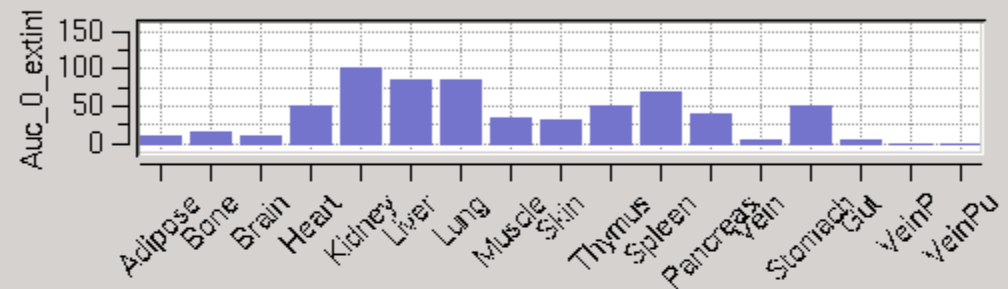
Administration Variables

Doses

Regimen: 

Simplify this tool...

Compute

View: 

fu,p	0.28	0.05
B:P	1.34	0.05
Liver Function	First Order	
	MEAN	CV
Liver CL (L/hr)	75.4	0.05
Kidney Function	First Order	
	MEAN	CV

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pHUBpk: Understanding Drug Elimination

Drug Properties

Molecule	Ibuprofen	▼
Ion Class	Acid	▼

	MEAN	CV
pKa	4.7	0
LogP _{ow}	4.06	0
LogP _{vow}	3.19	0

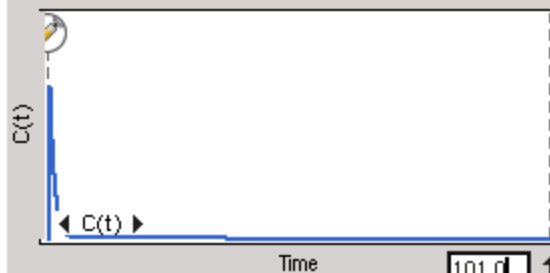
Patient Characteristics

Drug Subject

	MEAN	CV
fu,p	0.0061	0.05

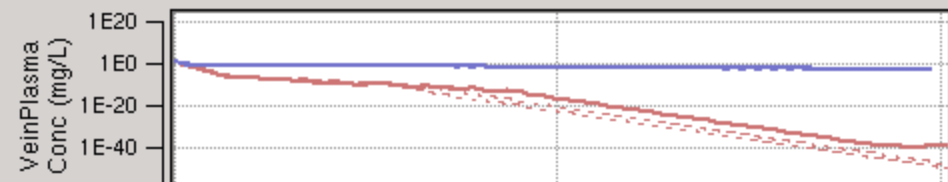
Administration Variables

Doses

Regimen: 

Simplify this tool...

Compute

View:  Case #1 Case #2

	Chlorpheniramine		Ibuprofen	
	MEAN	CV	MEAN	CV
Molecule	Chlorpheniramine		Ibuprofen	
Ion Class	Strong Base		Acid	
pKa	9.13	0	4.7	0
LogP _{ow}	3.07	0	4.06	0
LogP _{vow}	2.08	0	3.19	0
fu,p	0.28	0.05	0.0061	0.05
B:P	1.34	0.05	0.55	0.05
Liver CL (L/hr)	75.4	0.05	5780	0.05
Kidney CL (L/hr)	22.5	0.05	584	0.05

Doses



< Back

pHUBpk: Understanding Drug Elimination

Drug Properties

Molecule
 Ion Class

	MEAN	CV
pKa	4.7	0
LogP_ow	4.06	0
LogP_vow	3.19	0

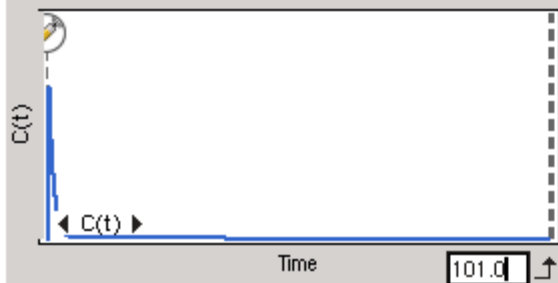
Patient Characteristics

Drug Subject

	MEAN	CV
fu,p	0.0061	0.05

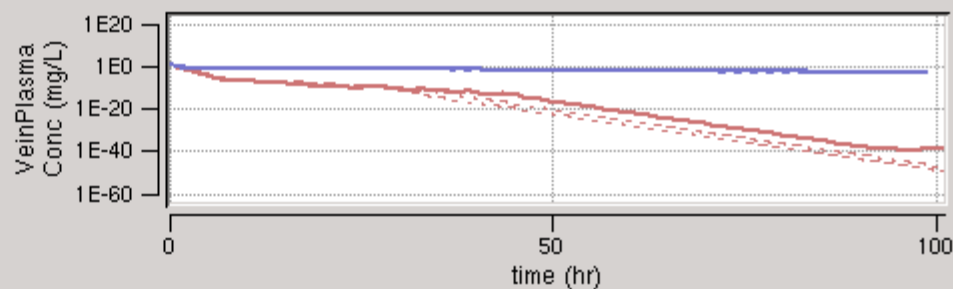
Administration Variables

Doses Regimen:

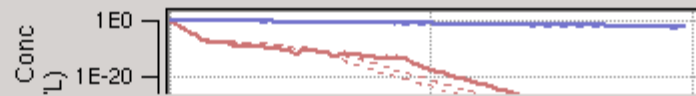


Compute

View:



AUC_0_t1	AUC_t1_extInf	AUC_0_extInf	Vduss	Vdss
1.18	0.024	1.205	1498.055	418.062
0.026	0	0.026	1374.336	8.335



AUC_0_t1
11

fQ_Blood (frac)	0.000	0	0.000	0
fQ_Bone (frac)	0.053	0	0.053	0
fQ_Brain (frac)	0.128	0	0.128	0
fQ_Heart (frac)	0.043	0	0.043	0
fQ_Kidney (frac)	0.201	0	0.201	0
fQ_Muscle (frac)	0.181	0	0.181	0
fQ_Skin (frac)	0.053	0	0.053	0

Simplify this tool...

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pHUBpk: Understanding Drug Elimination

Drug Properties

Molecule	Ibuprofen	
Ion Class	Acid	
	MEAN	CV
pKa	4.7	0
LogP _{ow}	4.06	0
LogP _{vow}	3.19	0

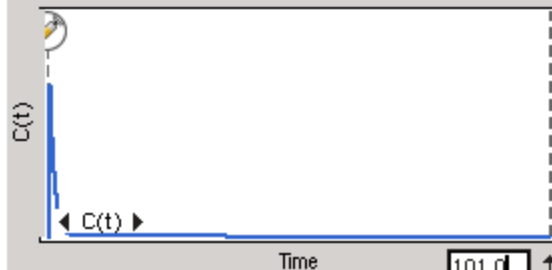
Patient Characteristics

Drug Subject

	MEAN	CV
fu,p	0.0061	0.05

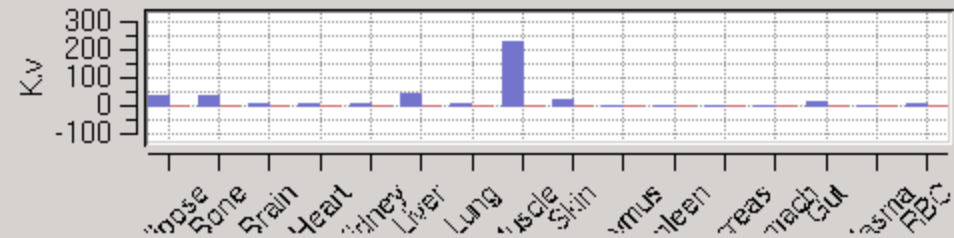
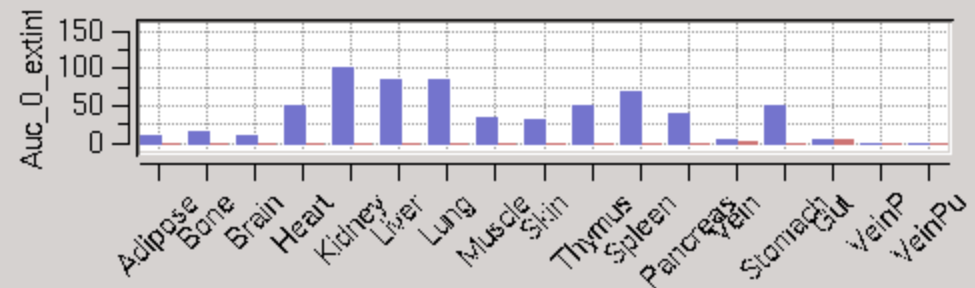
Administration Variables

Doses

Regimen: 

Simplify this tool...

Compute

View: 

fQ_Adipose (frac)	0.000	0	0.000	0
fQ_Bone (frac)	0.053	0	0.053	0
fQ_Brain (frac)	0.128	0	0.128	0
fQ_Heart (frac)	0.043	0	0.043	0
fQ_Kidney (frac)	0.201	0	0.201	0
fQ_Muscle (frac)	0.181	0	0.181	0
fQ_Skin (frac)	0.053	0	0.053	0



Wizards simplify

- **The input libraries contain all the relevant quantities**
- **There is no need to show the default values to new users**
- **Similarly, new users need not be overwhelmed with all of the output**
- **Instructors can use a GUI to hide fields and output for simple laboratory class assignments**

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pHUBpk: Understanding Drug Elimination

Drug Properties

Molecule 
 Ion Class 

	MEAN	CV
pKa	4.7	0
LogP _{ow}	4.06	0
LogP _{vow}	3.19	0

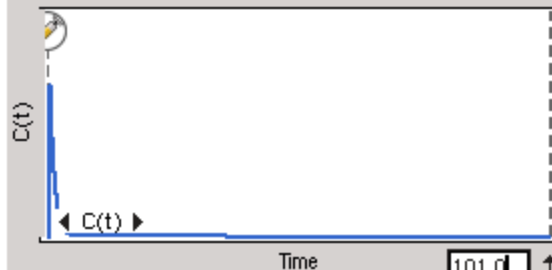
Patient Characteristics

Drug Subject

	MEAN	CV
fu,p	0.0061	0.05


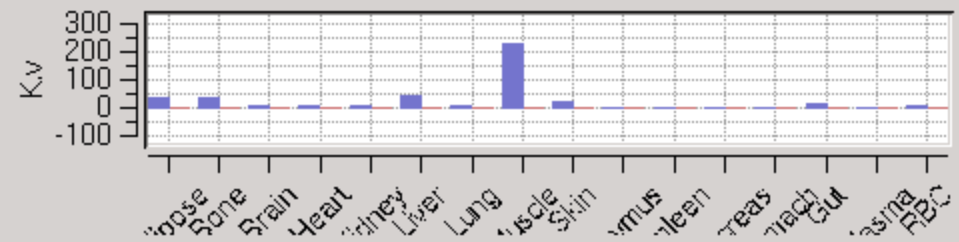
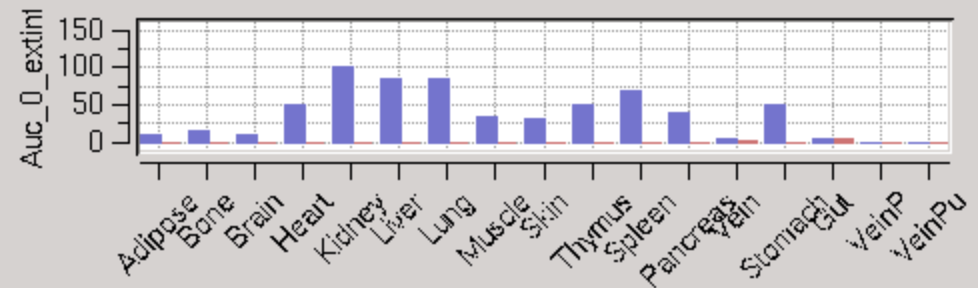
Administration Variables

Doses

Regimen: 

Simplify this tool...

Compute

 Clear All DownloadView: 

fQ_Adipose (frac)	0.000	0	0.000	0
fQ_Bone (frac)	0.053	0	0.053	0
fQ_Brain (frac)	0.128	0	0.128	0
fQ_Heart (frac)	0.043	0	0.043	0
fQ_Kidney (frac)	0.201	0	0.201	0
fQ_Muscle (frac)	0.181	0	0.181	0
fQ_Skin (frac)	0.053	0	0.053	0

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Simplify this tool

Use this editor to create a simpler version of this tool for classroom use. Hide various inputs and outputs. Then, click the Save button to save your configuration and create a URL that can be used to launch the simplified tool.

Drug Properties

Molecule	<input type="text" value="Keep as a n"/>	<input type="text" value="Alfentanil"/>
Ion Class	<input type="text" value="Keep as a n"/>	<input type="text" value="Weak Base"/>
		Original
		MEAN CV
pKa	<input type="text" value="Keep as a n"/>	<input type="text" value="6.5"/> <input type="text" value="0"/>
pKa_Base	<input type="text" value="Keep as a n"/>	Original
pKa_Acid	<input type="text" value="Keep as a n"/>	Original
		MEAN CV
LogP_ow	<input type="text" value="Keep as a n"/>	<input type="text" value="2.16"/> <input type="text" value="0"/>
		MEAN CV
LogP_vow	<input type="text" value="Keep as a n"/>	<input type="text" value="1.07"/> <input type="text" value="0"/>

Patient Characteristics

Subject

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Simplify this tool

Save

Close

Use this editor to create a simpler version of this tool for classroom use. Hide various inputs and outputs. Then, click the Save button to save your configuration and create a URL that can be used to launch the simplified tool.

Drug Properties

Molecule	Keep as a normal parameter	Alfentanil	
Ion Class	<input type="checkbox"/> Hide, and hard-code to this value >> <input type="checkbox"/> Show, but hard-code to this value >> <input checked="" type="checkbox"/> Keep as a normal parameter		Original
pKa	Keep as a normal parameter	6.5	0
		MEAN	CV
pKa_Base	Keep as a normal parameter		Original
pKa_Acid	Keep as a normal parameter		Original
LogP_ow	Keep as a normal parameter	2.16	0
		MEAN	CV
LogP_vow	Keep as a normal parameter	1.07	0
		MEAN	CV

Patient Characteristics

Subject Keep as a normal parameter Man

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Simplify this tool

Use this editor to create a simpler version of this tool for classroom use. Hide various inputs and outputs. Then, click the Save button to save your configuration and create a URL that can be used to launch the simplified tool.

Drug Properties

Molecule	Show, but hide	Alfentanil
Ion Class	Hide, and hide	Weak Base
		Original
		MEAN CV
pKa	Hide, and hide	6.5 0
pKa_Base	Hide, and hide	Original
pKa_Acid	Hide, and hide	Original
		MEAN CV
LogP_ow	Hide, and hide	2.16 0
		MEAN CV
LogP_vow	Hide, and hide	1.07 0

Patient Characteristics

Subject	Keep as a normal	Man
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Simplify this tool

Save

Close

Use this editor to create a simpler version of this tool for classroom use. Hide various inputs and outputs. Then, click the Save button to save your configuration and create a URL that can be used to launch the simplified tool.

Doses Keep as a no

Time

Outputs

Summary Keep this group**Auc_0_extinf** Keep this output**K.v** Keep this output**Kt** Keep this output**K** Keep this output**Kpu** Keep this output**Q** Keep this output**V** Keep this output**Auc_0_t1** Keep this output

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pHUBpk: Understanding Drug Elimination

Simplify this tool

Save

Close

Use this editor to create a simpler version of this tool for classroom use. Hide various inputs and outputs. Then, click the Save button to save your configuration and create a URL that can be used to launch the simplified tool.

Doses Keep as a no

Time

Outputs

Summary Keep this group**Auc_0_extinf** Keep this output**K.v** Keep this output**Kt** Keep this output**K** Keep this output**Kpu** Hide this output
Keep this output**Q** Keep this output**V** Keep this output**Auc_0_t1** Keep this output

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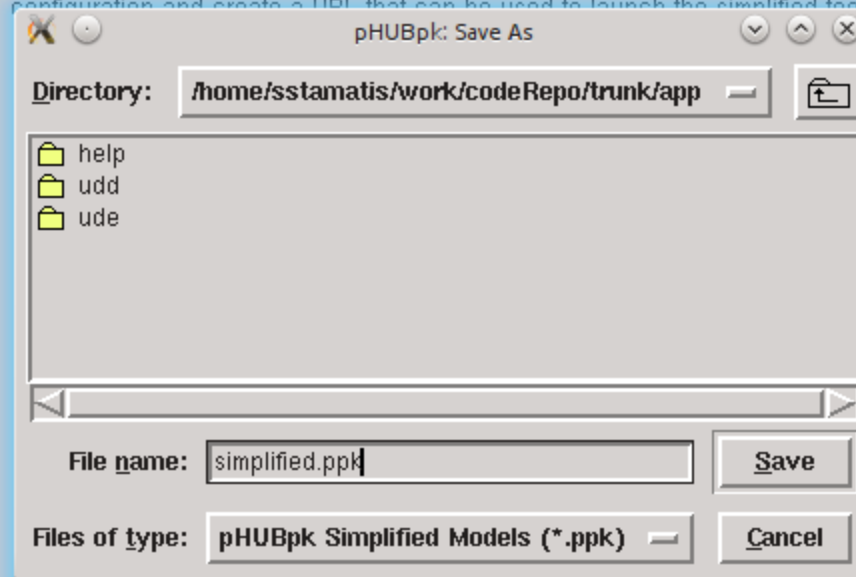
pHUBpk: Understanding Drug Elimination

Simplify this tool

Save

Close

Use this editor to create a simpler version of this tool for classroom use. Hide various inputs and outputs. Then, click the Save button to save your configuration and create a URL that can be used to launch the simplified tool.



Drug Properties

Molecule ▼

Patient Characteristics

Subject ▼

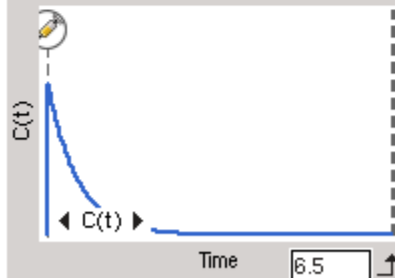
Drug Subject

	MEAN	CV
fu,p	0.077	0
B:P	0.63	0
Liver CL (L/hr)	3020	0
Kidney CL (L/hr)	30.5	0

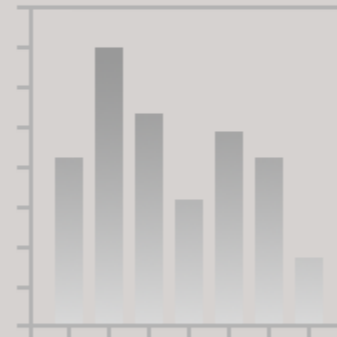
Administration Variables

Doses

Regimen:



Compute



Drug Properties

Molecule Alfentanil

Patient Characteristics

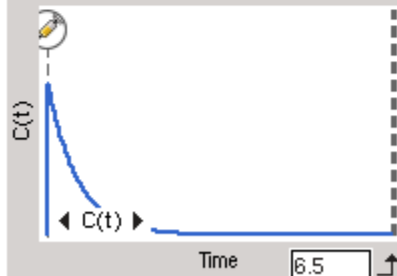
Subject Man

Drug Subject

	MEAN	CV
fu,p	0.077	0
B:P	0.63	0
Liver CL (L/hr)	3020	0
Kidney CL (L/hr)	30.5	0

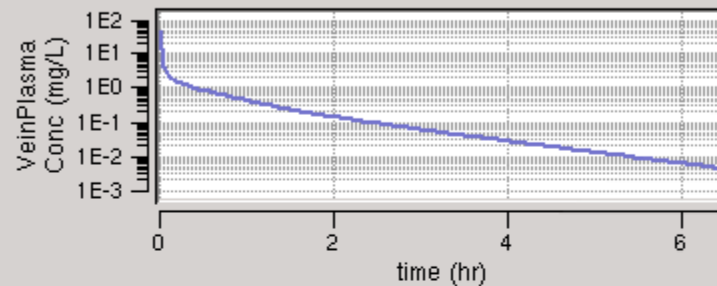
Administration Variables

Doses

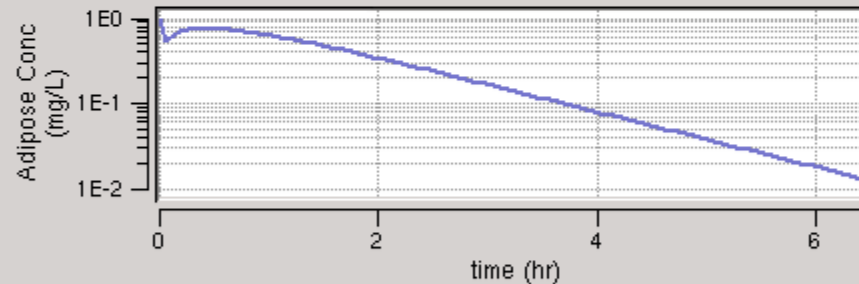
Regimen: 

Compute

View: Concentration Time Profiles



AUC_0_extInf	Vd _{lss}	Vd _{ss}
0.174	377.699	29.083



AUC_0_extInf
1.626

Case #1

Subject	Man	
	MEAN	CV
fu,p	0.077	0
B:P	0.63	0
Liver CL (L/hr)	3020	0
Kidney CL (L/hr)	30.5	0

Drug Properties

Molecule Alfentanil

Patient Characteristics

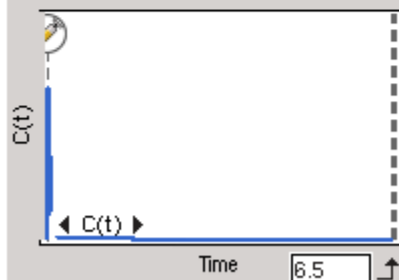
Subject Man

Drug Subject

	MEAN	CV
fu,p	0.77	0
B:P	0.63	0
Liver CL (L/hr)	3020	0
Kidney CL (L/hr)	30.5	0

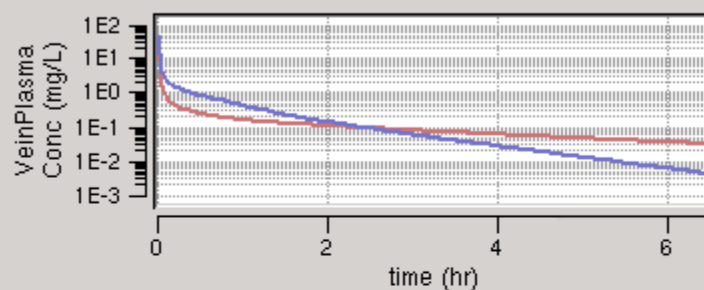
Administration Variables

Doses

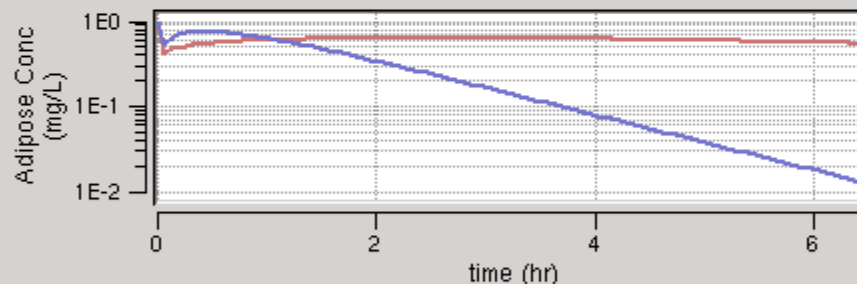
Regimen: 

Compute

View: Concentration Time Profiles



AUC_0_extInf	Vduss	Vdss
0.174	377.699	29.083
1.127	280.443	215.941



AUC_0_extInf
1.626
12.58

■ Case #1

■ Case #2

	MEAN	CV	MEAN	CV
fu,p	0.077	0	0.77	0
Subject	Man		Man	
	MEAN	CV	MEAN	CV
B:P	0.63	0	0.63	0
Liver CL (L/hr)	3020	0	3020	0

Summary

- <http://pharmaHUB.org>
 - No cost to users
 - Community tools
- pHUBpk
 - A collection of active learning environments for pharmacokinetics
 - Users discover trends with simulated empiricism