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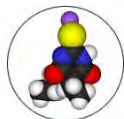
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Thursday, November 5, 2015

“From Truth Serum to Anesthesia: The Discovery and Uses of Sodium Thiopental”

Michael Matson, Reservoir Engineer, Kinder Morgan CO²

Dave Harwell, Assistant Manager of Industry Member Programs, The American Chemical Society



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“Chemistry of Addiction”

Anthony Rappé, Professor of Chemistry, Colorado State University

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Preformulation in Drug Discovery and Development
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Lecture 1: Preformulation and Biopharmaceutical Considerations in Drug Product Design and Development

Lecture 2: Drug Substance Physical Form Selection

Lecture 3: Drug Substance Physical Form Characterization

Lecture 4: Solubility: General Principles and Practical Considerations

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Jan 29	Designing Better Drug Candidates	Dr. Paul Leeson
Feb 26	Strategies to Improve Solubility of Drug Candidates	Dr. Michael Walker
Module 2: Activity/Potency Screening for Drug Lead & Candidate Optimization		
Mar 19	Fragment-Based Drug Design Strategies	Dr. Dan Erlanson
April 30	Screening Strategies	Dr. David Swinney
May 28	PAINS (Pan-Assay Interference Compounds)	Dr. Jonathan Baell
June 25	Positron Emission Tomography (PET) Labeling in Drug Discovery & Development	Dr. Lei Zhang
July 30	X-Ray Crystallography in Drug Discovery	Dr. Jon Mason & Dr. Miles Congreve
Module 3: Enabling Drug Discovery		
Aug 27	Choices and Trends in Solid Dosage Form Section	Dr. Scott Trzaska & Dr. Ron Smith
Sept 24	Delivery Options to Support Dose Escalation in Preclinical Toxicology and Pharmacodynamic Activity Studies	Dr. Evan Thackaberry
Module 4: Pharmacokinetics		
Oct 29	Pharmacokinetic Considerations in Drug Design and Development	Dr. Punit Marathe
Nov 19	Prodrugs in Drug Discovery	Dr. John Higgins

12

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13



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“Pharmacokinetic Considerations in Drug Design and Development”



Punit H. Marathe, Ph.D.



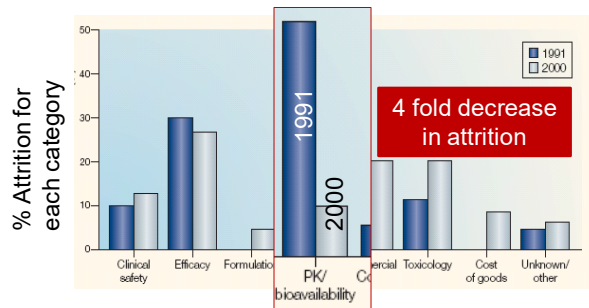
Executive Director, Bristol-Myers Squibb

Objectives

- **What are the key pharmacokinetic parameters?**
- **How are these parameters inter-related?**
- **How do we interpret preclinical pharmacokinetic parameters for achieving desirable clinical exposure?**



Importance of Pharmacokinetics on Clinical Drug Attrition



Attrition of drugs due to poor pharmacokinetic properties has significantly decreased.



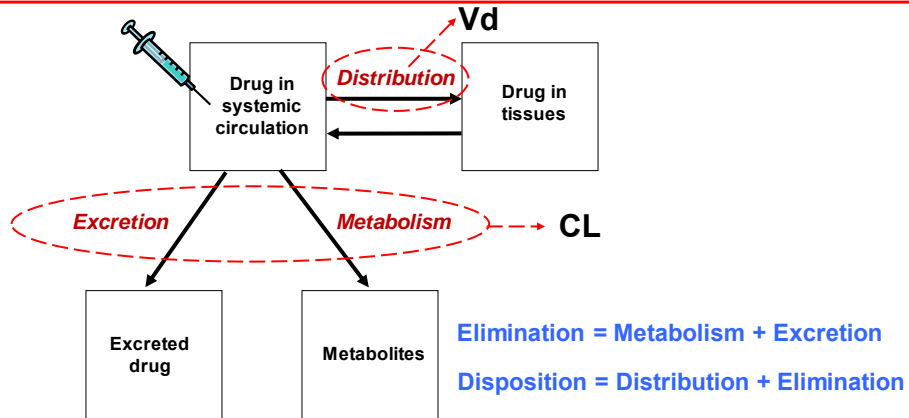
Audience Survey Question 

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

What role can DMPK scientists play?

- Work with medicinal chemists to optimize SAR
- Work with biologists to understand target biology
- Try to achieve a balance of potency, selectivity and ADME properties
- All of the above

Basic Concepts in Pharmacokinetics



- **Primary pharmacokinetic parameters:** Clearance and Volume of distribution
- **Secondary pharmacokinetic parameters:** Half-life, Bioavailability



Important Pharmacokinetic Parameters

- Clearance (CL)
- Volume of distribution (V_d)
- Half-life ($t_{1/2}$)
- Bioavailability ($F\%$)
- Protein binding (f_u)



Clearance Concepts

- Clearance describes how efficiently or rapidly a drug is eliminated from the body

Elimination { Metabolism: liver, intestine, lung, kidney, etc.
Excretion: urine, bile, saliva, milk, etc.

- Clearance is defined as:

$$CL \text{ (mL/min)} = \frac{\text{Rate of Elimination } (\mu\text{g/min})}{\text{Blood or Plasma Conc } (\mu\text{g/mL})}$$

In Practice:

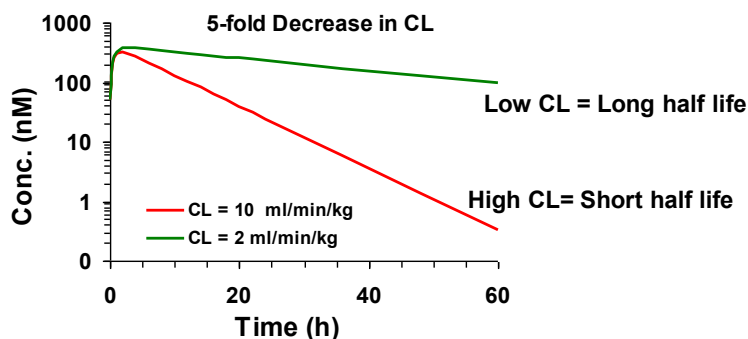
✓ $CL = \text{Dose}_{iv} / AUC_{iv}$ (Need to dose IV to estimate CL of compound)

✓ After PO dose CL is apparent clearance (CL/F)

$CL/F = \text{Dose}_{po} / AUC_{po}$, Where F = oral bioavailability



Effects of Change in CL on Plasma Concentration-Time Profile

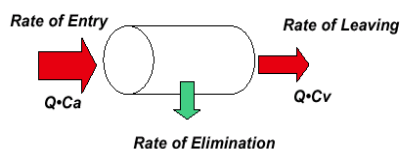


- $t_{1/2}$ changes in inverse proportion to CL
 - Decrease in CL results in a proportional increase in $t_{1/2}$ and vice versa
- CL is the only parameter that affects both $t_{1/2}$ and AUC
 - 5-fold reduction in CL resulted in 5-fold increase in $t_{1/2}$ and AUC



Organ Clearance and Extraction Ratio

Clearance - Organ CL



- Rate of Entry = $Q * C_a$
 - Rate of Leaving = $Q * C_v$
- where Q = organ blood flow

Now,

Rate of Entry = Rate of Leaving + Rate of Elimination

Rate of Elimination = Rate of Entry – Rate of Leaving = $Q * C_a - Q * C_v$

$$\therefore CL = \frac{\text{Rate of Elimination}}{C_a} = Q \cdot \frac{(C_a - C_v)}{C_a}$$

$CL = Q \cdot \text{Extraction Ratio}$

Extraction ratio is commonly used to triage compounds in discovery



Example: Calculating Extraction Ratio in Preclinical Species

Blood Flow to the Liver in Various Species

Blood flow	Mouse (0.02 kg)	Rat (0.25 kg)	Monkey (5 kg)	Dog (10 kg)	Human (70 kg)
mL/min	1.8	13.8	218	309	1450
mL/min/kg	90	65	44	31	21

Calculating ER

- If NCE has systemic blood clearance of 25 mL/min/kg in Cyno
- Hepatic Extraction ratio in Cyno = $CL/Q_{liver} = 25 / 44 = 0.56$
- This is considered intermediate clearance
- Useful criterion to triage molecules in discovery
- Prefer compounds with ER < 0.3
- Classification
 - Low CL (ER < 0.3), Intermediate CL (ER: 0.3 - 0.7) and High CL (ER > 0.7)



24

Assessing the Contribution of Individual Pathways to Total Clearance

- ✓ For a drug that undergoes hepatic and renal CL

$$CL_{\text{total}} = CL_{\text{hepatic}} + CL_{\text{renal}}$$

- ✓ Estimating individual pathways

- a. Renal CL: Measure fraction of drug excreted unchanged in urine (f_e)

f_e = Amount of drug in urine/Dose

$CL_R = f_e * CL$ (Difficult to optimize in discovery setting)

- b. Hepatic CL = $CL_{\text{total}} - CL_{\text{renal}}$

- ✓ *In vitro* microsomal/hepatocyte turnover can be correlated to *in vivo* clearance establishing IVIVC
- ✓ Following IVIVC, liver microsomes can used to optimize *in vivo* CL
- ✓ Microsomal turnover can be further extended to establish common metabolic pathways in preclinical species and human



25

Example: Interpretation of Interspecies Differences in Clearance

Compound A

Mouse CL:	19 mL/min.kg	Bioavailability: 78%
Rat CL:	11 mL/min.kg	Bioavailability: >100%
Dog CL:	9.5 mL/min.kg	Bioavailability: 62%
Monkey CL:	40 mL/min/kg	Bioavailability: 8%

- *In vivo* CL could be predicted from *in vitro* CL in liver microsomes
 - Based on human *in vitro* CL, *in vivo* CL predicted to be 7.8 mL/min/kg
 - Allometric scaling predicted human CL of 16.4 mL/min/kg
- Compound advanced to development based on understanding of differences in metabolic CL and pathways



26

Important Pharmacokinetic Parameters

- Clearance (CL)
- **Volume of distribution (V_d)**
- Half-life ($t_{1/2}$)
- Bioavailability (F%)
- Protein binding (f_u)



Volume of Distribution - Definition

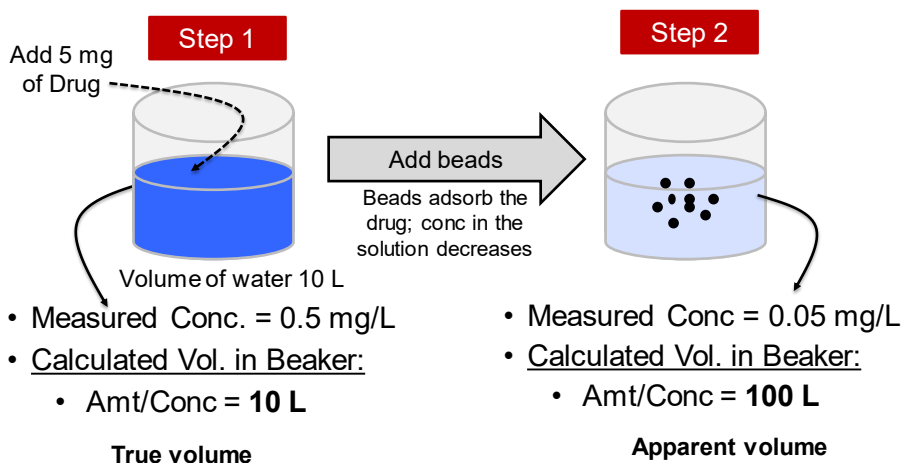
- The apparent volume of distribution (V_d) measures how well a drug is distributed outside the vascular space and is defined as:

$$V_d (mL) = \frac{\text{Amount in Body } (\mu\text{g})}{\text{Blood or Plasma Conc } (\mu\text{g/mL})}$$

- Why is V_d an apparent volume?
 - Because V_d is a term that relates blood or plasma concentration of a drug to its amount in the body
 - It rarely reflects true physiologic volume, such as plasma or total body water



Why is Volume of Distribution “Apparent” ?



In the same beaker the calculated Volume can be different

29

Volume of Distribution in Relation to Physiologic Volumes

Physiologic volumes

Total body water = Intracellular fluid + Extracellular fluid

Extracellular fluid = Plasma + Interstitial fluid

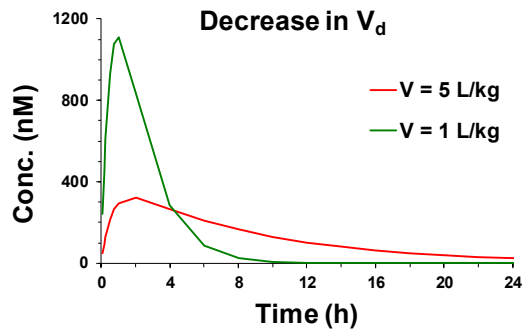
	Plasma	Extracellular Fluid	Total body Water
70-kg Human	3 L	18 L	42 L
	(0.04 L/kg)	(0.3 L/kg)	(0.6 L/kg)

- **Vd scales very well with body weight - similar volumes for preclinical animal species**
- Preclinical studies are valuable in estimating Vd in humans



30

Effects of Changes in Volume of Distribution on PK Profile



- $t_{1/2}$ changes in direct proportion to V_d
 - Increase in V_d results in a proportional increase in $t_{1/2}$ and vice versa
- Change in V_d does not lead to change in AUC



31

Relationship of V_d with Protein Binding

$V_{d,ss}$ can be related to true physiologic volume

$$V_{d,ss} = V_p + V_{tw} \cdot \frac{f_{u,p}}{f_{u,t}}$$

Where,

V_p - plasma volume

V_{tw} - volume of tissue water outside plasma

$f_{u,p}$ - unbound fraction in plasma

$f_{u,t}$ - unbound fraction in tissues

- $\uparrow f_{u,p} \Rightarrow \uparrow V_{d,ss}$
- $\downarrow f_{u,t} \Rightarrow \uparrow V_{d,ss}$



32

Classification of Volume of Distribution

- **When $V_{dss} < 0.3$ L/kg, a drug is considered to have a small volume of distribution**

Indicates the drug could be highly protein bound in plasma and/or does not distribute to tissues

- **When is this desirable?** For vascular or extracellular targets

- **When $V_{dss} > 0.7$ L/kg, a drug is said to have a relatively large volume of distribution**

Indicates that the drug is distributed outside the vascular space

- May be well distributed in the body OR
- May not distribute throughout the body but only concentrates in certain tissues

- **When is this desirable?** For intracellular targets



Audience Survey Question 

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

Which of the following is a TRUE statement about V_{dss} ?

- A)** A small volume of distribution indicates the drug is not highly protein bound in plasma.
- B)** A large volume of distribution is desirable for vascular or extracellular targets.
- C)** A small volume of distribution is desirable for intracellular targets.
- D)** A large volume of distribution indicates the drug is inside the vascular space.
- E)** A large vol. of distribution indicates the drug is outside the vascular space.

| 34

Important Pharmacokinetic Parameters

- Clearance (CL)
- Volume of distribution (V_d)
- **Half-life ($t_{1/2}$)**
- Bioavailability (F%)
- Protein binding (f_u)



Half-life - Definition

- **Defined as the time taken for the concentration of drug in blood or plasma to decline to half of its original value**
- **$t_{1/2}$ is a hybrid pharmacokinetic parameter and is determined by the V_d and CL**
- **$t_{1/2}$ can be predicted from the predicted CL and V_{ss} values in preclinical species**

$$t_{1/2} \text{ (min)} = \frac{0.693 \cdot V_d \text{ (mL/kg)}}{CL \text{ (mL/min/kg)}}$$

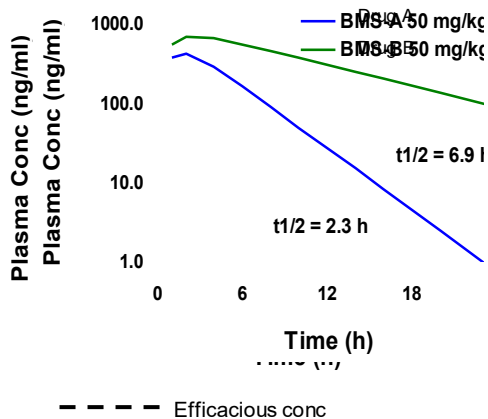
- $\uparrow V_d \Rightarrow \uparrow t_{1/2}$
- $\downarrow CL \Rightarrow \uparrow t_{1/2}$

- If V_d is restricted to extracellular volume, CL needs to be dramatically reduced in order to have a decent $t_{1/2}$
e.g. $V_d=0.3$ L/kg, $CL=1$ mL/min/kg will lead to $t_{1/2}$ of 3.5 h



Why is Half-life Useful?

- $t_{1/2} \sim 10-20$ h enables once-a-day dosing
- Compounds with short $t_{1/2}$ ($\sim 2-3$ h) will require frequent daily dosing (poor compliance)
- Extremely long $t_{1/2}$ ($>50 - 100$ h) is problematic
- Also useful for calculating extent of accumulation following multiple dosing
- Half-life enables estimation of "coverage" over a dosing interval



Important Pharmacokinetic Parameters

- Clearance (CL)
- Volume of distribution (V_d)
- Half-life ($t_{1/2}$)
- **Bioavailability (F%)**
- Protein binding (f_u)



Bioavailability - Definition and Estimation

- Oral bioavailability (F_{po}) measures the **extent of absorption** into the systemic circulation
- Absolute bioavailability is defined as:

$$F_{po} = \frac{\left(\frac{AUC_{po}}{Dose_{po}} \right)}{\left(\frac{AUC_{iv}}{Dose_{iv}} \right)}$$

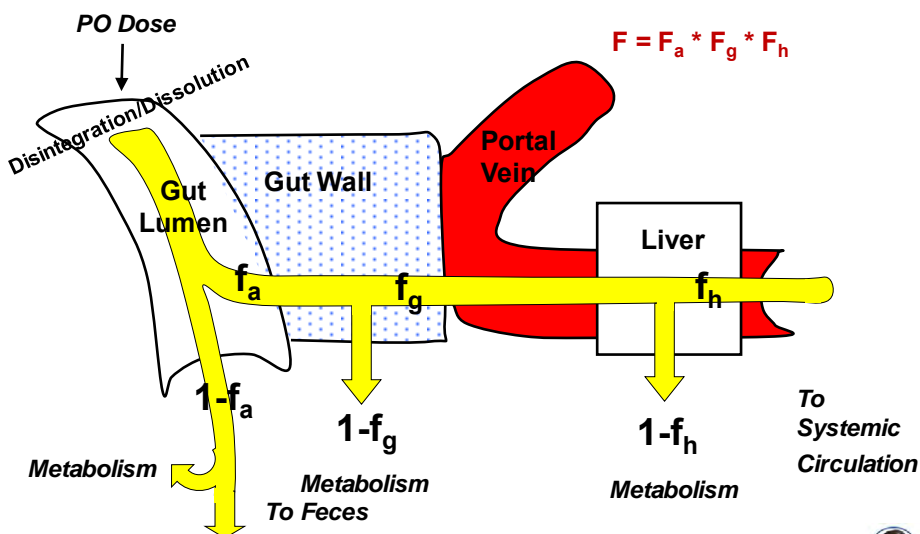
- Relative Bioavailability: Compares the AUC of two dosage forms (tablet vs. solution)

$$F_{Relative} = \frac{AUC_{PO,Tablet}}{AUC_{PO,Solution}}$$



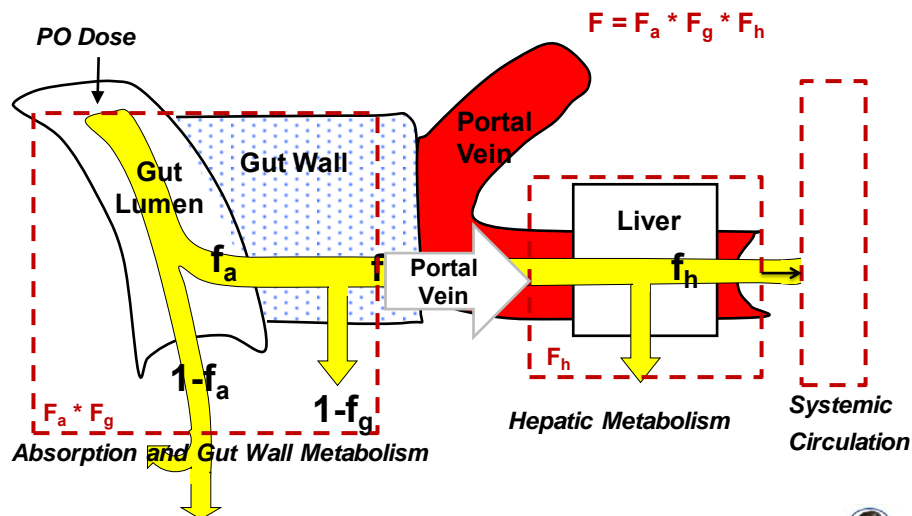
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Determinants of Oral Bioavailability



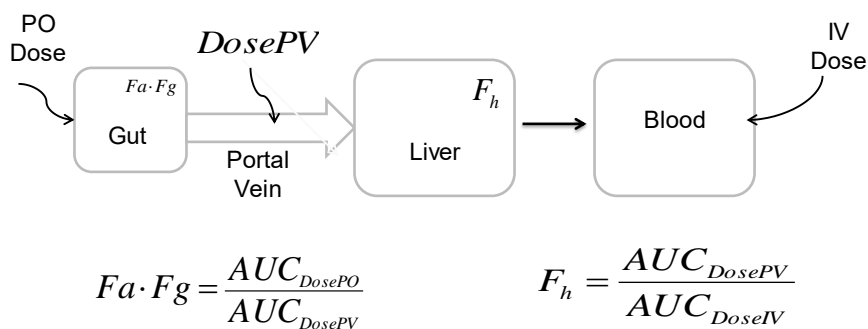
40

Determinants of Oral Bioavailability



41

Estimation of Gut vs. Liver First Pass



- Dose via different routes and measure systemic concentration
- Remember

$$F = \frac{AUC_{DosePO}}{AUC_{DoseIV}}$$



42

Important Pharmacokinetic Parameters

- Clearance (CL)
- Volume of distribution (V_d)
- Half-life ($t_{1/2}$)
- Bioavailability (F%)
- **Protein binding (f_u)**

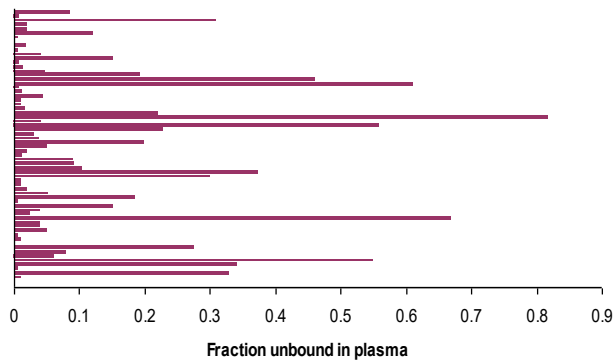


Protein Binding

- **Free-drug hypothesis- Only non protein-bound drug can exert therapeutic effect**
- **Only unbound drug can pass through most cell membranes; hence unbound drug concentration is more closely related to activity of drug than is total concentration**
- $f_u = C_u/C$
- **Representative proteins to which drugs bind in plasma:**
 - ✓ **albumin (35-50 g/L)**
 - ✓ **a1- acid glycoprotein (0.4-1 g/L)**
 - ✓ **lipoproteins (variable)**



Example: Plasma protein binding of BMS development candidates



N= 62
 $f_u < 0.02 = 23$
 $f_u < 0.01 = 14$

- > Most compounds have small $f_{u,p}$
- > Difficult to measure accurately
- > Small changes in protein binding may become significant



Protein Binding and V_d

$V_{d,ss}$ can be related to true physiologic volume

$$V_{d,ss} = V_p + V_{tw} \cdot \frac{f_{u,p}}{f_{u,t}}$$

Where,

- V_p - plasma volume
- V_{tw} - volume of tissue water outside plasma
- $f_{u,p}$ - unbound fraction in plasma
- $f_{u,t}$ - unbound fraction in tissues

- > $\uparrow f_{u,p} \Rightarrow \uparrow V_{d,ss}$
- > $\downarrow f_{u,t} \Rightarrow \uparrow V_{d,ss}$

Protein Binding and Hepatic Clearance

$$CL = \frac{Q_H f_{u,B} CL_{int}}{Q_H + f_{u,B} CL_{int}}$$

Where,

Q_H = hepatic blood flow;

CL_{int} = intrinsic clearance

For drugs with low extraction ratio: $CL = f_{u,B} CL_{int}$

$\uparrow f_{u,B} \Rightarrow \uparrow CL$; $\downarrow C_{ss}$; assuming no change in CL_{int}

For drugs with high extraction ratio:

$CL = Q_H$; CL independent of plasma protein binding

Hepatic clearance is a function of plasma protein binding for low ER drugs



47

Protein Binding and Half-life

For low extraction ratio drugs

$$t_{1/2} = 0.693 \times \left[\frac{V_B}{f_{u,B} CL_{int}} + \frac{V_T}{f_{u,T} CL_{int}} \right]$$

$\uparrow f_{u,B} \Rightarrow \downarrow t_{1/2}$; depending on relative magnitude of $\frac{V_B}{f_{u,B} CL_{int}}$ compared to $\frac{V_T}{f_{u,T} CL_{int}}$

When V is large, half-life is independent of $f_{u,B}$

For high extraction ratio drugs

$$t_{1/2} = 0.693 \times \left[\frac{V_B + V_T \frac{f_{u,B}}{f_{u,T}}}{Q} \right]$$

Changes in half-life as a function of protein binding depend on the magnitude of V and CL



48

Does Change in Plasma Protein Binding Change Efficacy?

Efficacy is determined by unbound drug concentrations at the active site

Common misconception:

- When plasma protein binding is reduced, increased unbound concentrations will cause increase in drug effect and potential toxicity
- Focus on drugs administered orally and cleared by liver

$$AUC_{oral} = \frac{F_a \times F_G \times F_H \times Dose}{CL} \quad F_H = 1 - ER = 1 - \frac{f_{u,B} CL_{int}}{Q_H + f_{u,B} CL_{int}} \quad \text{and} \quad CL = \frac{Q_H \times f_{u,B} CL_{int}}{Q_H + f_{u,B} CL_{int}}$$

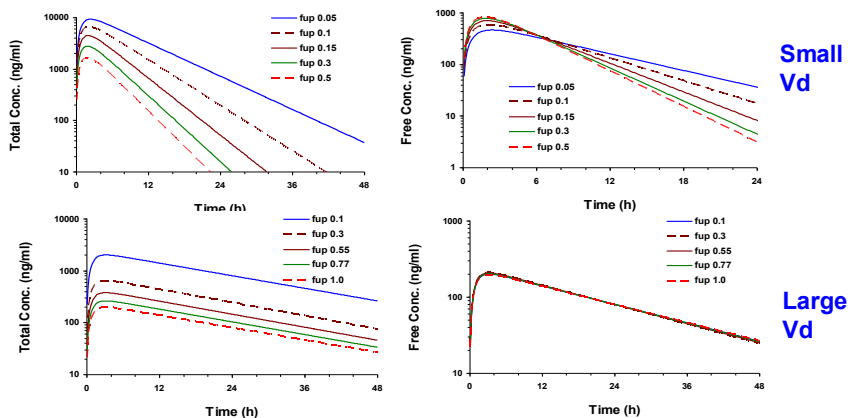
$$AUC_{oral} = \frac{F_a \times F_G \times Dose}{f_{u,B} CL_{int}} \quad \Rightarrow \quad AUC_{u,oral} = \frac{f_{u,B} \times F_a \times F_G \times Dose}{f_{u,B} CL_{int}}$$

Plasma protein binding has no effect
on unbound AUC and hence in vivo efficacy



49

Going beyond AUC: Effect of fu on PK Profile for low CL compounds



With decreased protein binding

- No change in unbound AUC and C_{trough} ;
- decreased unbound C_{trough} for compounds with small Vss



50

Summary: Lessons Learned

- **CL and V_d are primary PK parameters for drug design optimization**
- **Small structural changes can have large effects on PK**
- **Protein binding affects many PK parameters *but does not alter unbound AUC* (neither efficacy nor toxicity) for drugs administered orally and eliminated by liver**



Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

Does change in plasma protein binding change efficacy?

- A)** Yes, when plasma protein binding is reduced, increased unbound concentrations will cause increase in drug effect.
- B)** No, change in plasma protein binding has no effect on unbound AUC and hence in vivo efficacy.
- C)** Yes, when plasma protein binding is reduced, increased unbound concentrations will cause increase potential toxicity.
- D)** No, efficacy is determined by fraction unbound at the active site.



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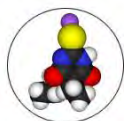


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54

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Michael Matson, Reservoir Engineer, Kinder Morgan CO²

Dave Harwell, Assistant Manager of Industry Member Programs, The American Chemical Society



Thursday, November 12, 2015

“Chemistry of Addiction”

Anthony Rappé, Professor of Chemistry, Colorado State University

Darren Griffen, Professor of Genetics, University of Kent

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“2015 Drug Design and Delivery Symposium: Pharmacokinetic Considerations in Drug Design and Development”



Shane Roller

Co-founded Phoundry
Pharmaceuticals and Director
of DMPK



Punit Marathe

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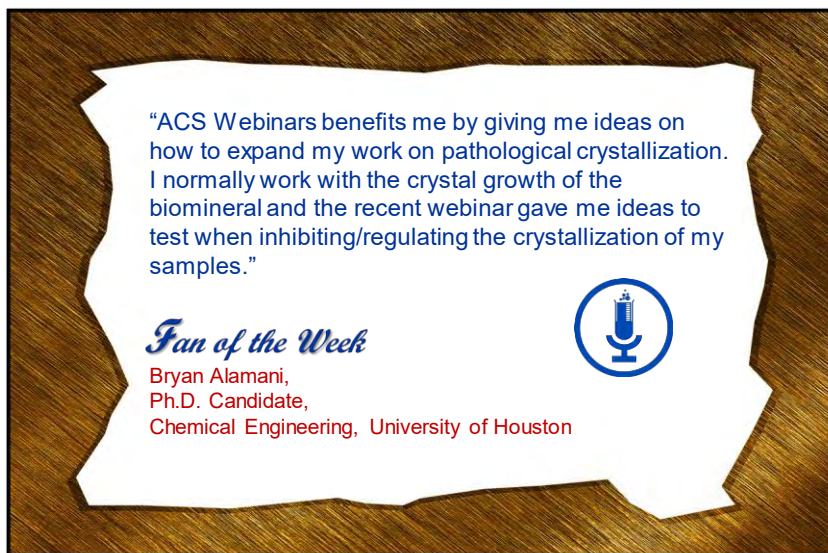
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62



2015 Drug Design & Delivery Symposium



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Co-produced by
ACS Division of Medicinal Chemistry
American Association of Pharmaceutical
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Module 1: Improving Drug Design Efficiency and Efficacy

Jan 29	Designing Better Drug Candidates	Dr. Paul Leeson
Feb 26	Strategies to Improve Solubility of Drug Candidates	Dr. Michael Walker

Module 2: Activity/Potency Screening for Drug Lead & Candidate Optimization

Mar 19	Fragment-Based Drug Design Strategies	Dr. Dan Erlanson
April 30	Screening Strategies	Dr. David Swinney
May 28	PAINS (Pan-Assay Interference Compounds)	Dr. Jonathan Baell
June 25	Positron Emission Tomography (PET) Labeling in Drug Discovery & Development	Dr. Lei Zhang
July 30	X-Ray Crystallography in Drug Discovery	Dr. Jon Mason & Dr. Miles Congreve

Module 3: Enabling Drug Discovery

Aug 27	Choices and Trends in Solid Dosage Form Section	Dr. Scott Trzaska & Dr. Ron Smith
Sept 24	Delivery Options to Support Dose Escalation in Preclinical Toxicology and Pharmacodynamic Activity Studies	Dr. Evan Thackaberry

Module 4: Pharmacokinetics

Oct 29	Pharmacokinetic Considerations in Drug Design and Development	Dr. Punit Marathe
Nov 19	Prodrugs in Drug Discovery	Dr. John Higgins

63