ACS Webinars
CLICK · WATCH · LEARN · DISCUSS

ACS Chemistry for Life®

We will begin momentarily at 2pm ET

Recordings will be available to ACS members after one week

www.acs.org/acswebinars

Have Questions?

ACS Chemistry for Life®

"Why am I muted?"
Don't worry. Everyone is muted except the presenter and host. Thank you and enjoy the show.

Type them into questions box!

ACS Webinars
CLICK • WATCH • LEARN • DISCUSS

ACS Chemistry for Life®

Have you discovered the missing element?

www.acs.org/2joinACS

Find the many benefits of ACS membership!

3

ACS Webinars
CLICK • WATCH • LEARN • DISCUSS

ACS Chemistry for Life®

Benefits of ACS Membership

C&EN
CHEMICAL & ENGINEERING NEWS

Chemical & Engineering News (C&EN)
The preeminent weekly news source.

ACS Presentations on Demand™
YOUR SOURCE FOR RECORDED MEETING CONTENT

NEW! Free Access to ACS Presentations on Demand®
ACS Member only access to over 1,000 presentation recordings from recent ACS meetings and select events.

NEW! ACS Career Navigator
Your source for leadership development, professional education, career services, and much more.

www.acs.org/2joinACS

4

Like us on Facebook!

facebook.com/acswebinars

5

How has ACS Webinars® benefited you?

"For me these are really fun events, with surprisingly broad benefits. There are so many issues I am trying to learn more about, and these ACS Webinars have covered many of them! It is especially helpful to hear what questions other participants have and also appreciate having access to the slides BEFORE the presentation."

Fan of the Week

Susan K Lamontagne
Senior Coordinator, Public Affairs
Pfizer

Be a featured fan on an upcoming webinar! Write to us @ acswebinars@acs.org

6

ACS Webinars®
CLICK · WATCH · LEARN · DISCUSS

ACS Chemistry for Life®

7

ACS Webinars®
CLICK · WATCH · LEARN · DISCUSS

ACS Chemistry for Life®

All recordings of ACS Webinars® will be available to current ACS members one week after the Live broadcast date.

Live weekly ACS Webinars ®will continue to be available to the general public.

Contact ACS Webinars ® at acswebinars@acs.org

8

Upcoming ACS Webinars®

www.acs.org/acswebinars

Thursday, February 5, 2015

"**Natural Product Chemistry:** Benefits of Pterostilbene on Health, Memory, and Anxiety"

Dr. Agnes Rimando, Research Chemist, U.S. Department of Agriculture

Dr. Dave Harwell, Assistant Director of Industry Member Programs, American Chemical Society

Thursday, February 12, 2015

"**Sweet Science:** Chocolate Chemistry for Valentine's Day"

Dr. Richard Hartel, Professor Food Engineering, University of Wisconsin-Madison

Dr. Gregory Ziegler, Professor of Food Science, Penn State University

Contact ACS Webinars ® at acswebinars@acs.org

9

Join the ACS Division of Medicinal Chemistry Today!

Division of Medicinal Chemistry

The MEDI Division is one of the largest ACS Divisions having ~9,600 members from 79 countries. The Division prepares and publishes Annual Reports in Medicinal Chemistry. This is a **600+ page volume containing timely reviews of progress in many therapeutic areas and on important new technologies, written by expert medicinal chemists**. This volume is provided free to members each year, and members have on-line access to previous volumes in the series.

Find out more about the ACS MEDI Division! www.acsmedchem.org

10

DEVELOPING SCIENCE. IMPACTING HEALTH.

A professional, scientific association with approximately 11,000 members employed in industry, academia, and government worldwide from diverse scientific backgrounds such as pharmaceutics, biopharmaceutics, chemistry, biology, engineering, and medicine..

A Robust Networking Community and Countless Opportunities Await within AAPS

AAPS offers Nine Sections to Concentrate Your Experience

- **Unite** scientific disciplines into forums to share experiment results
- **Explore** and disseminate research finding
- **Exchange** ideas
- **Examine** regulatory and ethical concerns

Find out more about AAPS and membership today!

AAPS Scientific Sections:

- **Analysis and Pharmaceutical Quality**
- **Biotechnology**
- **Clinical Pharmacology and Translational Research**
- **Drug Discovery and Development Interface**
- **Formulation Design and Development**
- **Manufacturing Science and Engineering**
- **Physical Pharmacy and Biopharmaceutics**
- **Pharmacokinetics, Pharmacodynamics, and Drug Metabolism**
- **Regulatory Sciences**

Find out more at the AAPS website


AAPS eLEARNING
AAPS eCourses
Available Now:
Coming in 2015:
AAPS Regulatory Affairs 101
Essentials of Regulatory Affairs for Pharmaceutical Scientists eLearning Series
AAPS Biotechnology 101
Fundamentals of Biotherapeutics Development eLearning Series
AAPS Translational Sciences 101
Drug Discovery, Development, and Pharmacotherapy eLearning Series
AAPS Immunogenicity 101
Immunogenicity of Biologically Based Therapeutics eLearning Series
AAPS Good Oral Candidates 101
Selecting Candidates with Optimal Oral Exposure eLearning Series
AAPS Preformulation 101
Preformulation in Drug Discovery and Development eLearning Series
AAPS Stability Testing 101
Stability Testing of Pharmaceutical Products eLearning Series
Visit www.aaps.org/eCourses to find out more!
aaps


YOUR NOVEL RESULTS DESERVE
Distinction and Extra Speed
Journal of Medicinal Chemistry
MOST CITED IN MEDICINAL CHEMISTRY
ACS Medicinal Chemistry Letters
PUBLICATION SPEED OF 9 WEEKS OR LESS
Submit Your Research Today!
Pubs.acs.org
ACS Publications
Most Trusted. Most Cited. Most Read.

2015 Drug Design & Delivery Symposium

#ACSWebinars

Co-produced by
ACS Division of Medicinal Chemistry
American Association of Pharmaceutical Scientists (AAPS)

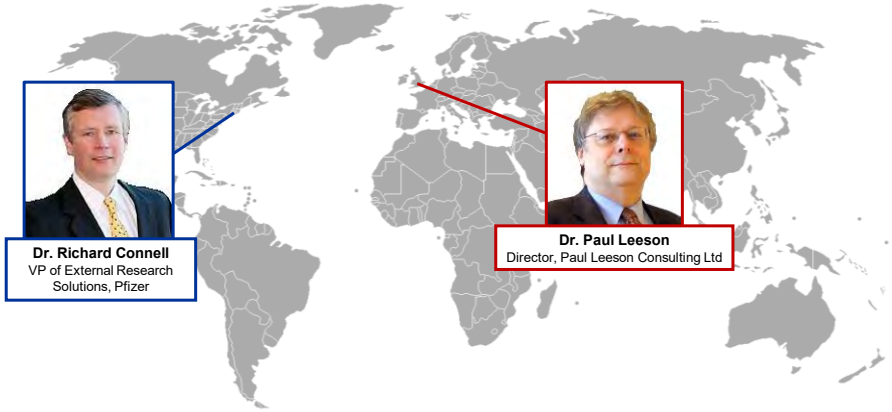
Module 1: Improving Drug Design Efficiency and Efficacy		
Jan 29	Designing Better Drug Candidates	*Dr. Paul Leeson*
Feb 26	Strategies to Improve Solubility of Drug Candidates	*Dr. Michael Walker*
Module 2: Activity/Potency Screening for Drug Lead & Candidate Optimization		
Mar 19	Fragment-Based Drug 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*

15

ACS Webinars
CLICK · WATCH · LEARN · DISCUSS

ACS Chemistry for Life®

"2015 Drug Design and Delivery Symposium: Designing Better Drug Candidates"



Dr. Richard Connell
VP of External Research Solutions, Pfizer

Dr. Paul Leeson
Director, Paul Leeson Consulting Ltd

Slides available Now! Recordings will be available to ACS members after one week

www.acs.org/acswebinars

This session of the 2015 Drug Design and Delivery Symposium is sponsored by ACS Publications
This Symposium is co-produced by ACS Webinars, the ACS Division of Medicinal Chemistry and AAPS

16

Designing Better Drug Candidates

Paul D Leeson
paul.leeson@virgin.net

- Attrition and Compound Quality
- Druglike & Leadlike molecular properties
- Ligand efficiency metrics in optimisation

Root Causes of Clinical Efficacy Attrition

Evidence for progression of unoptimised compounds

- **Pfizer: '4 Pillars' for phase II success** (Morgan et al, *Drug Discovery Today* 2012, **17**, 419; Bunnage, et al *Nat. Chem. Biol*. 2013, **9**, 195)
  - **Exposure at target; Binding to target; Pharmacological response; Target linked clinically to disease modification**
  - Low confidence in *exposure* amongst failed candidates: **"cannot conclude mechanism tested adequately in 43% of cases"**

18

Root Causes of Clinical Efficacy Attrition

Evidence for progression of unoptimised compounds

- **AstraZeneca: '5Rs'** (Cook et al, *Nat. Revs. Drug Disc.* 2014, **13**, 419)
  - **'Right': Target & Tissue (4Ps); Safety; Patient; Commercial potential**
  - 29% Clinical efficacy failures **"dose limited by compound characteristics or tissue exposure not established"**
  - **Decision making process:** 38% projects advanced to clinic had *low confidence in safety* & 78% of these eventually failed due to toxicity

19

Root Causes of Clinical Efficacy Attrition

Evidence for progression of unoptimised compounds

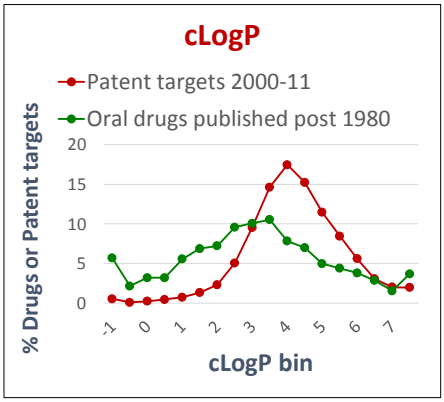
- **FDA submissions** (Sacks et al, *JAMA* 2014, **311**, 378)
  - 50% unsuccessful 1st time, 29% of which had **dose or clinical end point issues**

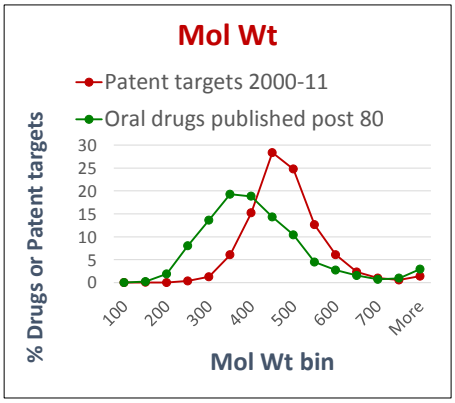
- ***Medicinal Chemist's accountability: compound-related failure***

20

Fundamental Assertion

Physicochemical properties of molecules drive all aspects of compound quality: from target affinity to ADME & toxicity





Compounds patented by the leading 18 Companies carry increased ADME & toxicity risk versus recently marketed drugs

Drug data: Leeson et al*, Med. Chem. Comm*. 2011, **2**, 91, *oral drugs updated to 2014*;
Patent targets 2000-11 from 18 companies: Leeson & St-Gallay, *NRDD* 2011, **10**, 749

21

Inflation of 'Druglike' Physical Properties

LogP: 1-octanol/ water partition coefficient

Mol Wt / HA: molecular weight/heavy atom count

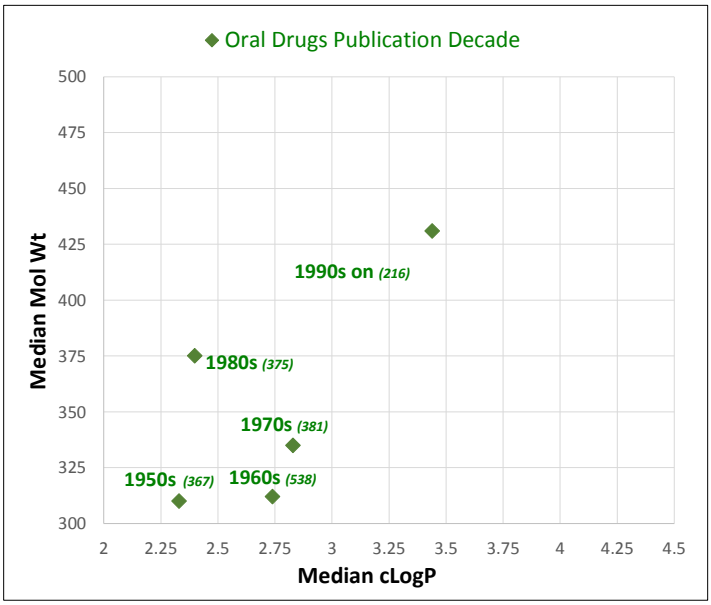
HBD / HBA: # hydrogen bond donors/acceptors

Fsp3: fraction of Csp3 atoms/total C atoms

Ar: # aromatic rings or atoms

RotB: # freely rotating bonds

PSA: polar surface area



Drug data: Leeson et al*, Med. Chem. Comm*. 2011, **2**, 91, *oral drugs updated to 2014*;
Patent targets 2000-11 from 18 companies: Leeson & St-Gallay, *NRDD* 2011, **10**, 749

22

Inflation of 'Druglike' Physical Properties

LogP: 1-octanol/ water partition coefficient

Mol Wt / HA: molecular weight/heavy atom count

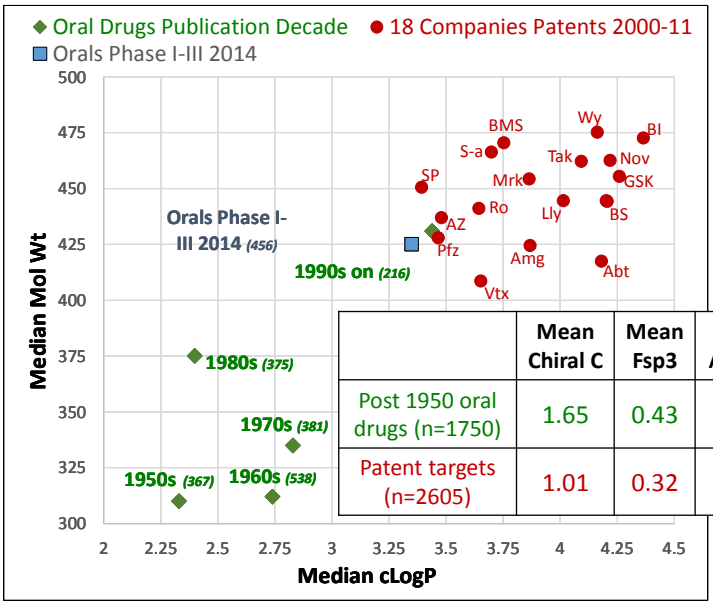
HBD / HBA: # hydrogen bond donors/acceptors

Fsp3: fraction of Csp3 atoms/total C atoms

Ar: # aromatic rings or atoms

RotB: # freely rotating bonds

PSA: polar surface area



	Mean Chiral C	Mean Fsp3	Mean Ar ring
Post 1950 oral drugs (n=1750)	1.65	0.43	1.77
Patent targets (n=2605)	1.01	0.32	2.55

Oral drugs vs time

Least change: cLogP, HBD, Fsp3, # chiral atoms

Most change: Mol Wt, HBA, RotB, PSA, Ar; *all increasing*

23

Audience Survey Question

ANSWER WITH THE CORRECT LETTER IN THE QUESTIONS BOX

Will the probability of success in a portfolio of drug candidates increase when its physicochemical & experimental properties more closely resemble those of marketed drugs?

a) Yes
b) No
c) Don't know

24

Some Causes of 'Molecular Obesity'

- **Increasing potency:** by adding atoms in optimisation?
- **HTS:** hit selection? *Mean published HTS hit ~ 1µM & cLogP ~ 4*
- **Synthesis:** choosing hits suitable for parallel chemistry?
- **Newer targets:** eg protein-protein interactions
- **Target product profile:** disease risk/benefit can lead to acceptance of greater safety risk & dosing inconvenience

Post 1990 oral drugs (n=216)	**Median cLogP**	**Median Mol Wt**
Kinase, HIV prot., HCV (n=45)	4.64	556
Others (n=171)	3.07	420

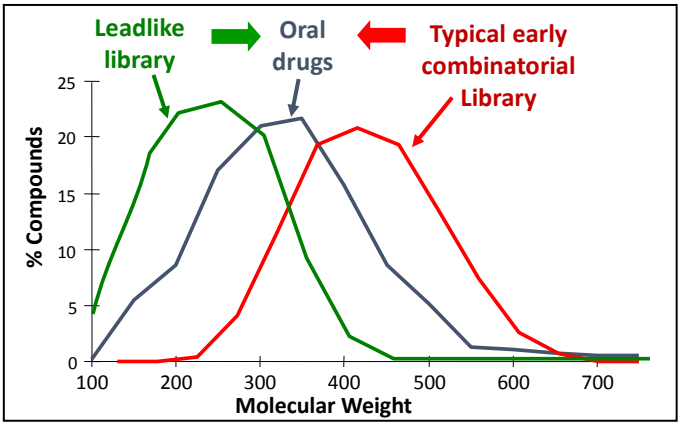
- **Local culture:** company physical property differences *not* driven by target & comparable to target class variation

Potency 'obsession': Hann, *MedChemComm.* 2011, **2**, 349; **HTS hit selection:** Keserű & Makara, *Nat. Rev. Drug Disc.* 2009, **8**, 203; Dahlin & Walters, *Future Med. Chem.* 2014, 6, 1265; **Synthetic pragmatism:** Keserű et al, *Chem. Soc. Rev*., 2014, **43**, 5387; **Company culture:** Leeson & St-Gallay, *Nat. Rev. Drug Disc.* 2011, **10,** 749; Leeson & Springthorpe, *Nat. Rev. Drug Disc.* 2007, **6**, 881

25

Optimisation: the 'Leadlike' Hypothesis

Mol Wt & LogP tend to increase in optimisation

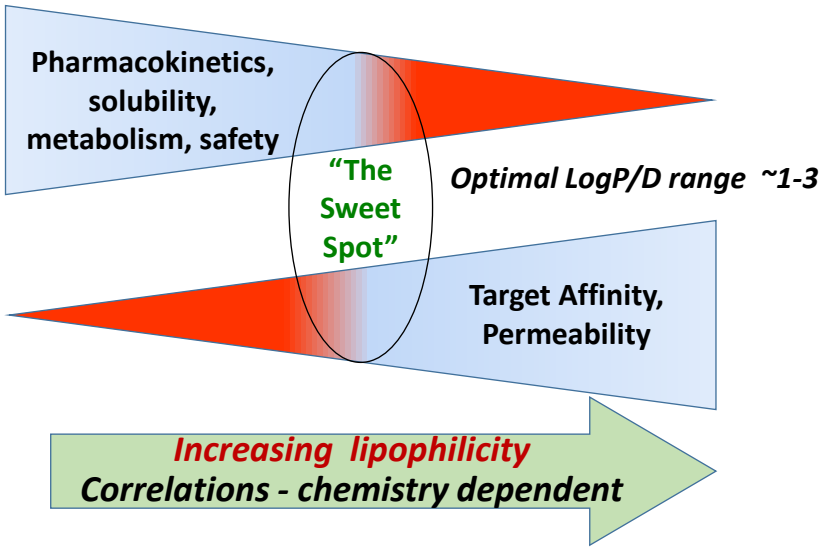


'Leadlike' lead: Affinity >0.1µM; Mol Wt 100-350; cLogP 1-3

Leadlikeness: Teague et al, *Angew. Chem. Int . Ed.* 1999, **38**, 3743; Oprea et al, *J. Chem. Inf. Comput. Sci.* 2001, **41**, 1308; Hann et al, *J. Chem. Inf. Comput. Sci.* 2001, **41**, 856; **Synthetic challenges:** Doveston et al., *Org. Biomol. Chem.* 2015, **13**, 859)

26

Lipophilicity - LogP & $LogD_{7.4}$ - a Key Property



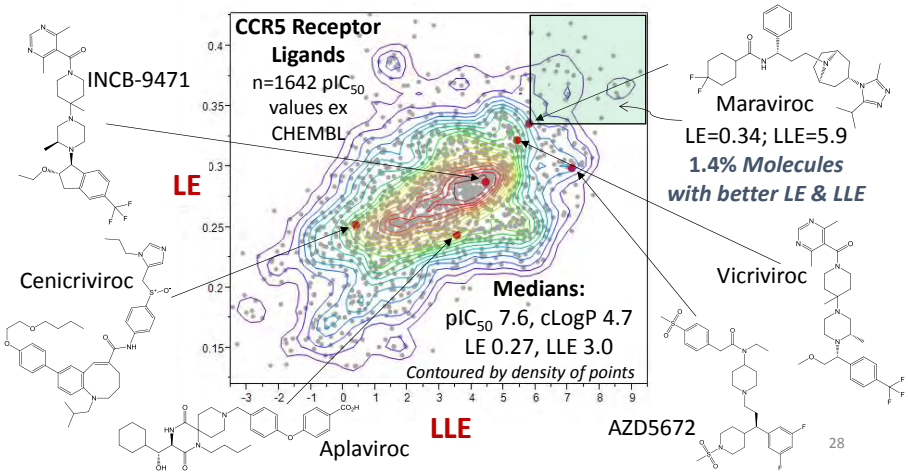
Lipophilicity: Waring, *Exp. Op. Drug Disc*. 2010, **5**, 235; **ADME/potency balanc**e: Hann & Keserű, *Nat. Rev. Drug Disc*. 2012, **11**, 355; Gleeson et al. *Nat. Rev. Drug Disc.* 2011, **10**, 197

27

Ligand Efficiency Metrics - *'Bang for Your Buck'*

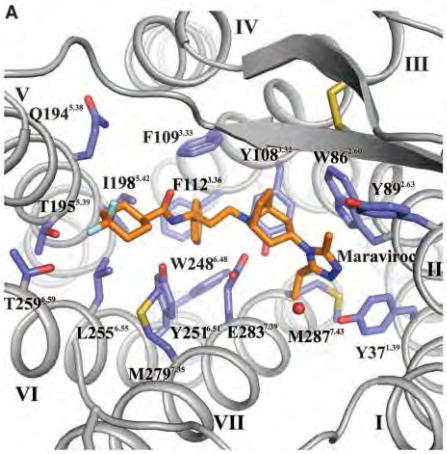
Hopkins et al, *Nat. Rev. Drug Disc.*, 2014, **13**, 105

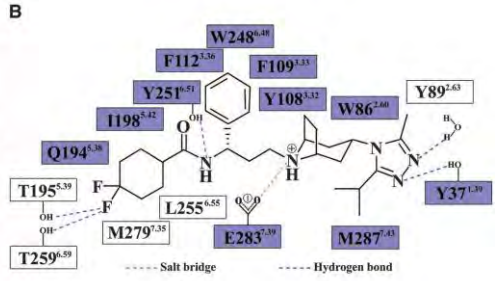
Ligand Efficiency - *kcal/mol/atom*	**Lipophilic Ligand Efficiency** - *Specificity*
LE = p(Activity) x 1.37 / # Heavy Atoms	**LLE or LipE = p(Activity) – cLogP**
Mean oral drug LE = 0.45	Mean oral drug LLE = 4.4
Lead optimisation: *conserve/increase*	Lead optimisation: *increase*



28

Structure of Maraviroc Bound to CCR5





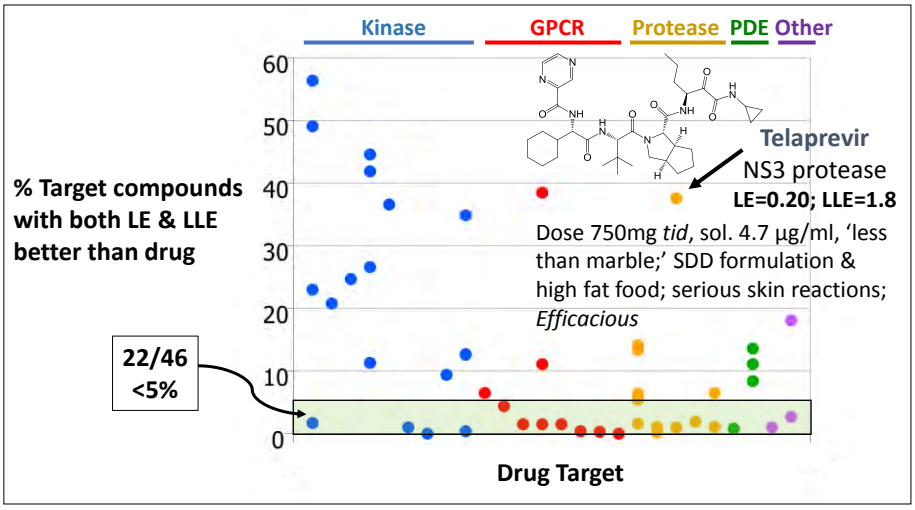
- **Efficient use of H-bonding atoms**
  - **7 Polar atoms make 6 polar interactions**
- **Efficient local hydrophobic interactions**
  - **Phenyl, isopropyl, tropane & cyclohexyl binding pockets**

Tan et al, *Science*, 2013, **341**, 1387
Polar contact review: Higueruelo et al, *PLoS ONE* 2012, 7(12): e51742

29

Oral Drug Ligand Efficiencies: 46 Drugs, 25 Targets

% LE + LLE better vs drug: kinases 22%; other targets 2.7%;
Only in class 1.5%. LE & LLE contribute equally to % score

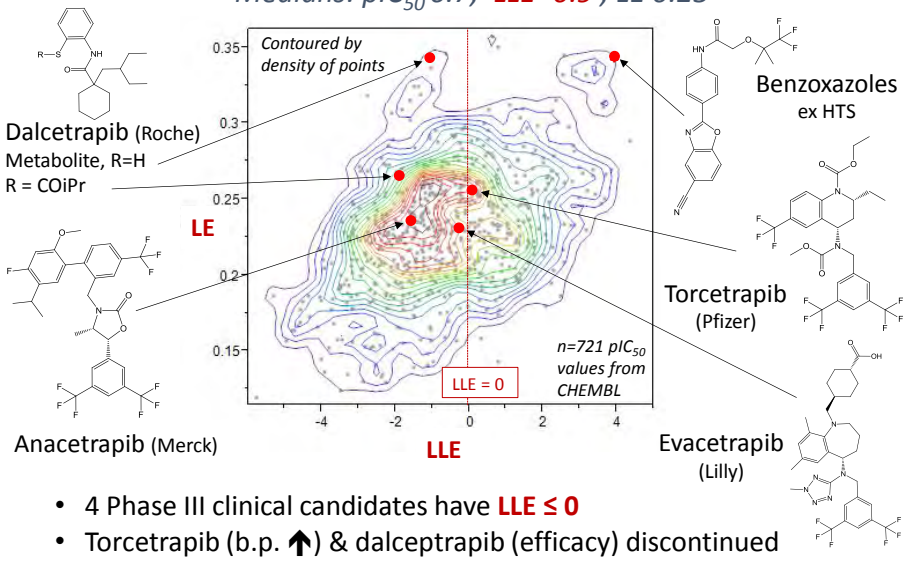


Details of Drugs & Targets: Hopkins et al, *Nat. Rev. Drug Disc.*, 2014, **13**, 105
Telaprevir: Kwong et al, *Nat. Biotech.* 2011, **29**, 993

30

CETP: A High Value 'Lipophilic' Target

Medians: pIC_{50} 6.7; LLE -0.9 ; LE 0.23



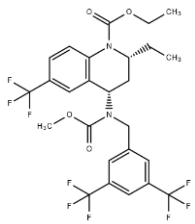
- 4 Phase III clinical candidates have **LLE ≤ 0**
- Torcetrapib (b.p. ↑) & dalceptrapib (efficacy) discontinued
- Anacetrapib: levels are ~40% of treatment after 12 weeks; detectable in plasma four years after last dose

31

CETP: Less Lipophilic Inhibitors

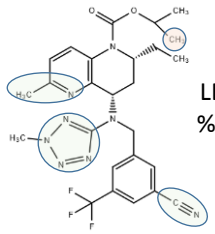
C → N & O, hydrophilic substituents, control HA

Fernandez et al (Lilly), *Bioorg. Med. Chem. Lett*. 2012, **22**, 3056



Torcetrapib (Pfizer) pIC_{50} 7.7
cLogP 7.6; HA 41; **LE 0.1; LE 0.26**

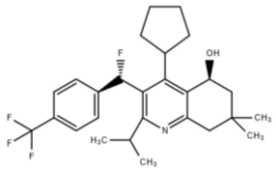
'Mitigate lipophilicity'
LogP values not cited
Δ LLE = 3.8
Δ LE = 0.01



LE + LLE % better **1.4%**

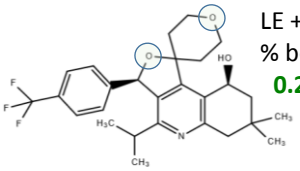
Lilly lead pIC_{50} 7.7
cLogP 3.8; HA 39; **LLE 3.9 LE 0.27**

Trieselmann et al (BI), *J. Med. Chem.* 2014, **57**, 8766



BI hit pIC_{50} 6.6
cLogP 7.6; HA 33; **LLE -1.0; LE 0.27**

'Reduce lipophilicity'
LogP values tracked
Δ LLE = 4.1
Δ LE = 0.04



LE + LLE % better **0.28%**

BI lead pIC_{50} 7.7
cLogP 4.6; HA 34; **LLE 3.1; LE 0.31**

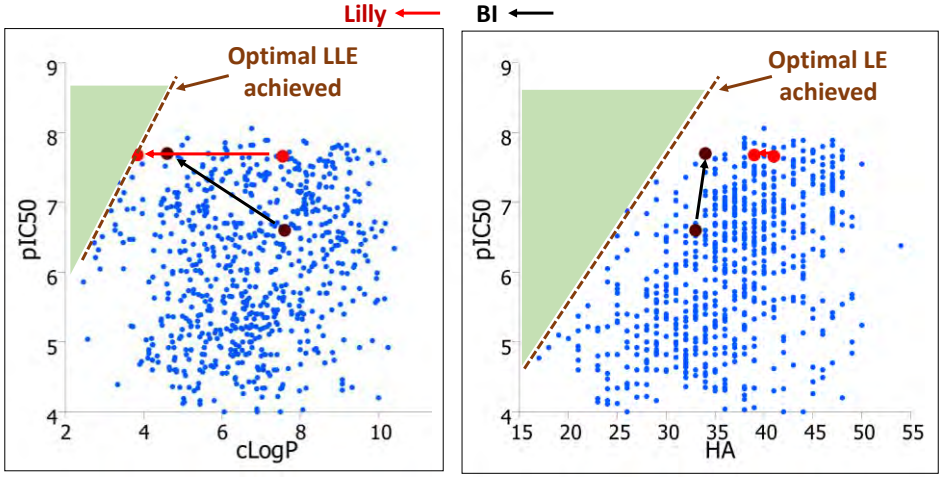
32

Tracking Optimisation Trajectories

CETP illustrated - applicable to any target

LLE or LipE = p(Activity) – cLogP **LE = p(Activity) x 1.37 / # Heavy Atoms**

Lilly ← BI ←



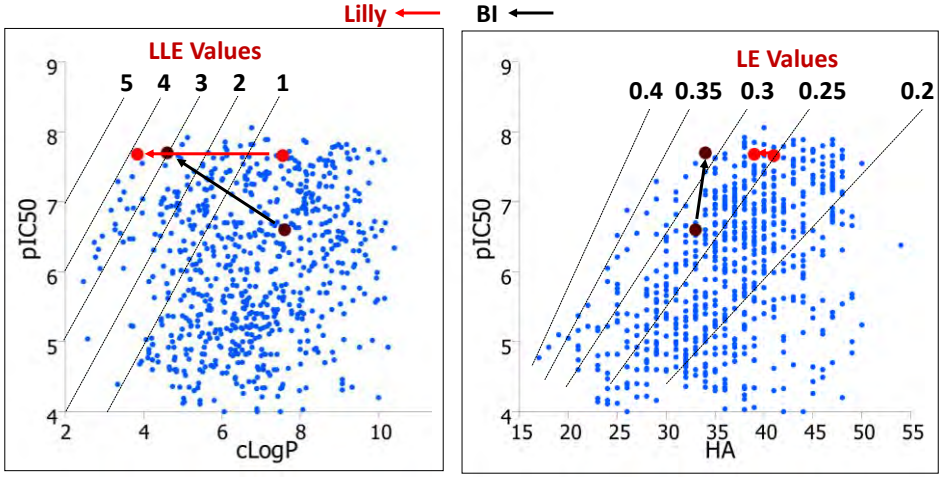
33

Tracking Optimisation Trajectories

CETP illustrated - applicable to any target

LLE or LipE = p(Activity) – cLogP **LE = p(Activity) x 1.37 / # Heavy Atoms**

Lilly ← BI ←



- **Plus LE vs LLE, LE vs HA, LLE vs cLogP*….etc***
- **Easy to do & you will learn something**

34

Audience Survey Question

ANSWER WITH THE CORRECT LETTER IN THE QUESTIONS BOX

What viable strategies, other than seeking druglike physicochemical properties, can medicinal chemists apply to increase the output of new drugs?

a) Invest in novel synthetic methods to expand chemical space of parallel synthesis (eg greater Csp3 content) & produce improved leadlike screening collections
b) Employ predictive multi-parameter computational tools (eg, clearance, permeability, dose, solubility, LogD, hERG, Cyp inhibition etc) from hit i.d. onwards
c) Ensure excellent collaboration with ADME & safety scientists
d) Ensure timely terminations of compound series or projects making little/slow progress
e) Others….?

35

Designing Better Candidates: Lessons Learned

- Compound quality contributes to clinical attrition
- The physicochemical property spaces occupied by patented molecules and marketed drugs are different
- In optimisation, lead molecules often increase in size and lipophilicity
- Ligand efficiencies, measures of potency per unit of lipophilicity & size, are frequently optimised for the targets of marketed drugs
- Tracking potency vs lipophilicity & size in optimisation can help steer projects towards drug like space, even with challenging targets

36

Acknowledgements

GlaxoSmithKline	AstraZeneca	Academia & Industry
Martin Bayliss	Andy Davis	Paul Gleeson
James Butler	John Dixon	Andrew Hopkins
Paul Feldman	David Payling	György Keserű
Darren Green	Jan-Erik Nyström	Jonathan Mason
Mike Hann	Brian Springthorpe	Tudor Oprea
Alan Hill	Steve St-Gallay	David Rees
Mike Palovich	Simon Teague	Chuck Reynolds
Anthony Taylor	Mark Wenlock	
Rob Young	**AZ Global Chemistry Forum**	
GSK Chemistry Council	**AZ Scientists**	
GSK Scientists		

"Without convincing evidence to the contrary, drugs should be made as hydrophilic as possible without loss of efficacy."

Hypothesis proposed by: Hansch et al, *J. Pharm. Sci.* 1987, **76**, 663

37

Slide Titles & References

- Inflation of 'Druglike' Physical Properties
  - Phase I-III orals: http://www. citeline.com/; **Drug properties vs time:** Leeson & Davis, *J. Med. Chem* 2004, **47**, 6338; Leeson & Springthorpe, *Nat. Rev. Drug Disc.* 2007, **6**, 881; Proudfoot, *Bioorg. Med. Chem. Lett.* 2005, **15**, 1087; Leeson et al, *Med. Chem. Comm*. 2011, **2**, 91; Walters et al, *J. Med. Chem*. 2011, **54**, 6405; **Phase I-III properties:** Wenlock et al, *J. Med. Chem.* 2003, **46,** 1250; Blake, *Medicinal Chemistry*, **2005**, 1, 649; Oprea, *J. Comp.-Aid. Mol. Des*. **2002**, 16, 325
- Optimisation: the 'Leadlike' Hypothesis
  - **Optimisation, lead-drug pairs:** Hann, *J.Chem. Inf. Comput. Sci.* 2001, **41**, 856; Oprea, *J. Chem. Inf. Comput. Sci.* 2001, **41**, 1308; Perola, *J. Med. Chem*. 2010, **53**, 2986; Giordanetto, *Drug Disc. Today* 2011**,16**, 722**; Optimisation, literature start-finish pairs**: Morphy, *J. Med. Chem.* 2006, **49**, 2969; Keseru, *Nat. Rev. Drug Disc.* 2009, **8**, 203; Macarron, *Nat. Rev. Drug Disc.* 2011, **10**, 188; Ferenczy *J. Med. Chem.* 2013, **56**, 2478; **LLE optimisations**: Hopkins, *Nat. Rev. Drug Disc.,* 2014, **13**, 105
- Ligand Efficiency Metrics - *'Bang for Your Buck'*
  - **Debate:** Shultz, *ACS Med. Chem. Lett.* 2014, **5**, 2; Murray et al, *ACS Med. Chem. Lett.* 2014, **5**, 616; Kenny et al, *J. Comput. Aided Mol. Des.* 2014, **28**, 699

Slide Titles & References

- CETP: A High Value 'Lipophilic' Target
  - **LE & LLE data:** Hopkins et al*, Nat. Rev. Drug Disc.*, 2014, **13**, 105; **CETP review:** Mantlo & Escribano. *J. Med. Chem.* 2014, **57**, 1; **Anacetrapib:** Gotto et al, *Am. J. Cardiol.* 2014*,* **113**, 76; **Benzoxazole**s, eg *Bioorg. Med. Chem. Lett*. 2010, **20**, 1019
- Tracking Optimisation Trajectories
  - **Lipophilic efficiency:** Leeson & Springthorpe, *Nat. Rev. Drug Disc.* 2007*,* **6***,* 881; Freeman-Cook et al, *Fut. Med. Chem.* 2013, **5**, 113; Shultz, *Bioorg. Med. Chem. Lett*. 2013, **23**, 5992; Tarcsay et al, *J. Med. Chem.* 2012*,* **55**, 1252; Hopkins et al*, Nat. Rev. Drug Disc*, 2014, **13**, 105
- Controlling Risk: Compound Quality Guidance
  - **Multi-parameter optimisation schemes & scoring: eg,** Wager et al*, ACS Chem. Neurosci.* 2010*,* **1**, 435; Bickerton et al *Nature Chem.*2012, **4**, 90

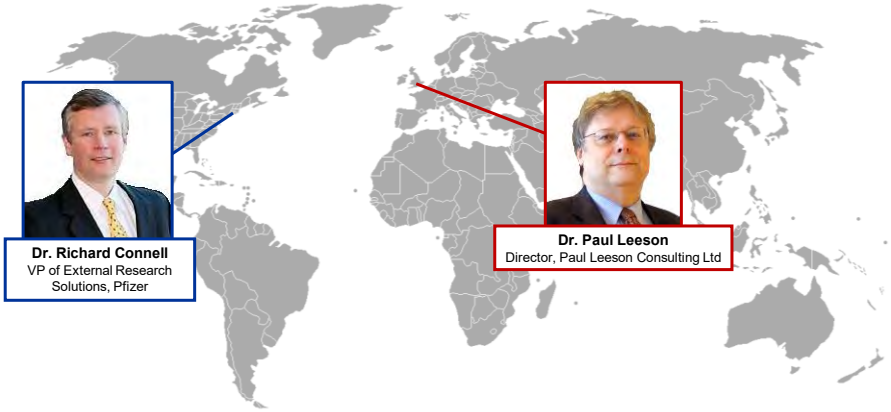
Additional References

- **DMPK data.** Gleeson, *J. Med. Chem.*, 2008, **51**, 817; Waring, *Bioorg. Med. Chem. Lett.,* 2009*,* **19***,* 2844; Johnson et al, *Bioorg. Med. Chem. Le*tt., 2009, **19**, 55; Varma et al, *J. Med. Chem.* 2010, 53, 1098
- **Toxicity. Phys props:** Hughes et al, *Bioorg. Med. Chem. Lett.* 2008, **18**, 4872; Peters et al, *Drug Discovery Today* 2012, **17**, 325; Sutherland et al*, J. Med. Chem.* 2012, **55**, 6455; Luker et al, *Bioorg. Med. Chem. Lett.*, 2011, **21**, 5673; **Critique:** Muthas et al, *Med. Chem. Commun*. 2013, **4**, 1058; **dose/exposure:** Wager et al, *J. Med. Chem.* 2013, **56**, 9771; Stepan et al, *Chem. Res. Toxicol.* 2011**, 24***,* 1345; Sakatakis et al, *Chem. Res. Toxicol*. 2012, **25**, 2067; Chen et al, *Hepatology* 2014, **58**, 388;
- **Ionisation.** Charifson & Walters, *J. Med. Chem.* 2014, **57,** 9701
- **Aromaticity.** Ritchie & Macdonald, *J. Med. Chem.* 2014, **57***,* 7206; Young et al, *Drug Disc. Toda*y 2011, **16**, 822
- **Drug targets**. Paolini et al, *Nature Biotechnology* 2006, **7**, 805
- **Beyond Ro5.** Doak et al, *Chemistry & Biology* 2014, **21**, 1115
- **Critique.** Kenny & Montanari, *Comput Aided Mol Des*. 2013, **27**, 1
- **Review.** Meanwell, *Chem. Res. Toxicol*. 2011, **24**, 1420

ACS Webinars
CLICK • WATCH • LEARN • DISCUSS

ACS Chemistry for Life®

"2015 Drug Design and Delivery Symposium: Designing Better Drug Candidates"



Dr. Richard Connell
VP of External Research Solutions, Pfizer

Dr. Paul Leeson
Director, Paul Leeson Consulting Ltd

Slides available Now! Recordings will be available to ACS members after one week

www.acs.org/acswebinars

This session of the 2015 Drug Design and Delivery Symposium is sponsored by ACS Publications
This Symposium is co-produced by ACS Webinars, the ACS Division of Medicinal Chemistry and AAPS

41

YOUR NOVEL RESULTS DESERVE
Distinction and Extra Speed

Journal of Medicinal Chemistry
MOST CITED IN MEDICINAL CHEMISTRY

ACS Medicinal Chemistry Letters
PUBLICATION SPEED OF 9 WEEKS OR LESS

Submit Your Research Today!

Pubs.acs.org

ACS Publications
Most Trusted. Most Cited. Most Read.

Join us February 26, 2015 for the 2nd Session!

www.acs.org/content/acs/en/events/upcoming-acs-webinars/drug-design-2015.html

43

Upcoming ACS Webinars®

www.acs.org/acswebinars

Thursday, February 5, 2015

"**Natural Product Chemistry:** Benefits of Pterostilbene on Health, Memory, and Anxiety"

Dr. Agnes Rimando, Research Chemist, U.S. Department of Agriculture

Dr. Dave Harwell, Assistant Director of Industry Member Programs, American Chemical Society

Thursday, February 12, 2015

"**Sweet Science:** Chocolate Chemistry for Valentine's Day"

Dr. Richard Hartel, Professor Food Engineering, University of Wisconsin-Madison

Dr. Gregory Ziegler, Professor of Food Science, Penn State University

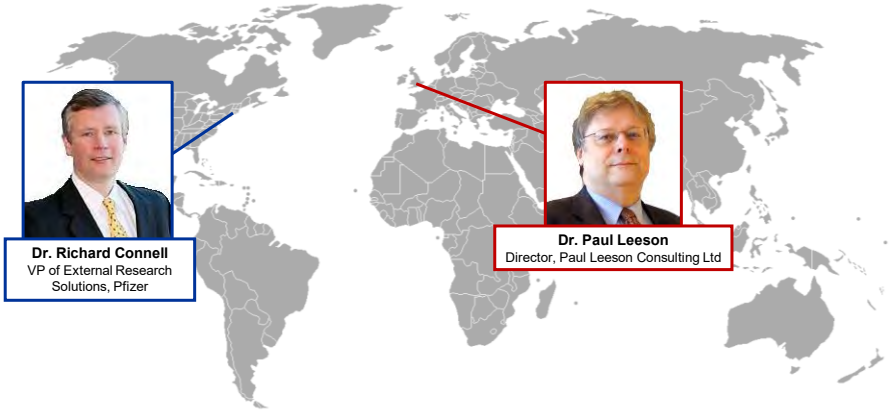
Contact ACS Webinars ® at acswebinars@acs.org

44

ACS Webinars
CLICK • WATCH • LEARN • DISCUSS

ACS Chemistry for Life®

"2015 Drug Design and Delivery Symposium:
Designing Better Drug Candidates"



Dr. Richard Connell
VP of External Research Solutions, Pfizer

Dr. Paul Leeson
Director, Paul Leeson Consulting Ltd

Slides available Now! Recordings will be available to ACS members after one week
www.acs.org/acswebinars

This session of the 2015 Drug Design and Delivery Symposium is sponsored by ACS Publications
This Symposium is co-produced by ACS Webinars, the ACS Division of Medicinal Chemistry and AAPS

45

aaps **American Association of Pharmaceutical Scientists**

DEVELOPING SCIENCE. IMPACTING HEALTH.

A professional, scientific association with approximately 11,000 members employed in industry, academia, and government worldwide from diverse scientific backgrounds such as pharmaceutics, biopharmaceutics, chemistry, biology, engineering, and medicine..

A Robust Networking Community and Countless Opportunities Await within AAPS

AAPS offers Nine Sections to Concentrate Your Experience

- **Unite** scientific disciplines into forums to share experiment results
- **Explore** and disseminate research finding
- **Exchange** ideas
- **Examine** regulatory and ethical concerns

Find out more about AAPS and membership today! aaps

Join the ACS Division of Medicinal Chemistry Today!

ACS Chemistry for Life®

Division of Medicinal Chemistry

The MEDI Division is one of the largest ACS Divisions having ~9,600 members from 79 countries. The Division prepares and publishes Annual Reports in Medicinal Chemistry. This is a **600+ page volume containing timely reviews of progress in many therapeutic areas and on important new technologies, written by expert medicinal chemists**. This volume is provided free to members each year, and members have on-line access to previous volumes in the series.

Find out more about the ACS MEDI Division! www.acsmedchem.org

47

How has ACS Webinars® benefited you?

ACS Chemistry for Life®

"For me these are really fun events, with surprisingly broad benefits. There are so many issues I am trying to learn more about, and these ACS Webinars have covered many of them! It is especially helpful to hear what questions other participants have and also appreciate having access to the slides BEFORE the presentation."

Fan of the Week

Susan K Lamontagne
Senior Coordinator, Public Affairs
Pfizer

Be a featured fan on an upcoming webinar! Write to us @ acswebinars@acs.org

48

ACS Webinars
CLICK · WATCH · LEARN · DISCUSS

ACS Chemistry for Life®

49

ACS Webinars
CLICK · WATCH · LEARN · DISCUSS

ACS Chemistry for Life®

Benefits of ACS Membership

C&EN CHEMICAL & ENGINEERING NEWS

Chemical & Engineering News (C&EN)
The preeminent weekly news source.

ACS Presentations on Demand™
YOUR SOURCE FOR RECORDED MEETING CONTENT

NEW! Free Access to ACS Presentations on Demand®
ACS Member only access to over 1,000 presentation recordings from recent ACS meetings and select events.

NEW! ACS Career Navigator
Your source for leadership development, professional education, career services, and much more.

www.acs.org/2joinACS

50

ACS Webinars® does not endorse any products or services. The views expressed in this presentation are those of the presenter and do not necessarily reflect the views or policies of the American Chemical Society.

Contact ACS Webinars ® at acswebinars@acs.org

51

2015 Drug Design & Delivery Symposium

#ACSWebinars

Co-produced by
ACS Division of Medicinal Chemistry
American Association of Pharmaceutical Scientists (AAPS)

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*

52