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"As a budding medicinal chemist in the academia, our research is often too focused to appreciate the vast field out there. ACS Webinars help us gain knowledge and insight in diverse topics which are out of curriculum in our university, yet could be applied to everyday chemistry performed in our labs."

Fan of the Week

Akul Y. Mehta, Ph.D.
Department of Medicinal Chemistry
Virginia Commonwealth University

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Upcoming ACS Webinars®

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Thursday, April 2, 2015

"Talking About Polymers, Detecting Explosives"

Jennifer Novotney, PhD Student, Cornell University, 2014 Chemistry Champions Competition Winner

Dr. Darcy Gentleman, Manager of Engagement and Science Communications, The American Chemical Society

Thursday, April 9, 2015

"Active vs. Passive Voice in Scientific Writing"

Dr. Kristin Sainani, Associate Professor, Stanford

Ms. Celia Elliott, Science Writer and Technical Editor, University of Illinois at Urbana-Champaign

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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*

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Join us April 30, 2015 for the 4th Session!

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

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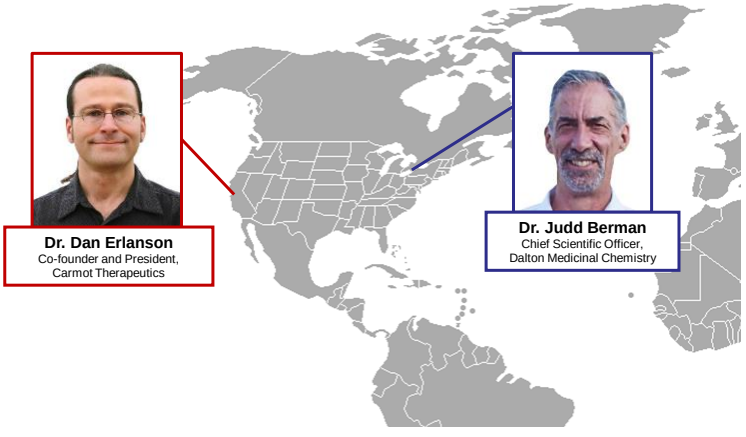
"2015 Drug Design and Delivery Symposium: Fragment-Based Drug Design Strategies"



This Symposium is co-produced by ACS Webinars, the ACS Division of Medicinal Chemistry and AAPS

Fragment-Based Drug Design Strategies

Daniel A. Erlanson
Carmot Therapeutics, Inc.

derlanson@carmot.us

ACS 2015 Drug Design and Delivery Symposium
Session 3
19 March 2015

What You Will Learn:

1) Why FBLD can be useful

2) How to find fragments – and avoid pitfalls

3) What you can do with fragments

From Fragment to Clinic: 30+ and Counting

Approved
- **Vemurafenib (PLX-4032) Plexxikon B-Raf (V600E)**

Phase 3
- **ABT-199 Abbott Bcl-2**
- **MK-8931 Merck BACE1**

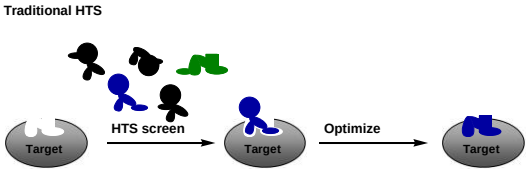
Phase 2
- **AT13387 Astex HSP90**
- **AT7519 Astex CDK1,2,4,5**
- **AT9283 Astex Aurora, Janus Kinase 2**
- **AUY-922 Novartis/Vernalis HSP90**
- **AZD5363 AstraZeneca/Astex AKT**
- Indeglitazar Plexxikon PPAR agonist
- **Linifanib (ABT-869) Abbott VEGF & PDGFR**
- LY2886721 **Lilly BACE1**
- LY517717 Lilly/Protherics Fxa
- **Navitoclax (ABT 263) Abbott Bcl-2/Bcl-xL**
- **PLX3397 Plexxikon FMS, KIT, and FLT-3-ITD**

Phase 1
- ABT-518 Abbott MMP-2 & 9
- ABT-737 Abbott Bcl-2/Bcl-xL
- **AT13148 Astex AKT, p70S6K**
- AZD3839 AstraZeneca BACE1
- AZD5099 AstraZeneca Bacterial Topo II
- DG-051 deCODE LTA4H
- IC-776 Lilly/ICOS LFA-1
- **JNJ-42756493 J&J/Astex FGFr**
- LP-261 Locus Tubulin
- LY2811376 Lilly BACE1
- PLX5568 Plexxikon Kinase
- SGX-393 SGX Bcr-Abl
- SGX-523 SGX Met
- SNS-314 Sunesis Aurora
- **Undisclosed Roche BACE1**
- **Undisclosed Vernalis/Servier Bcl-2**

Practical Fragments 5 January 2015
http://practicalfragments.blogspot.com/2015/01/fragments-in-clinic-2015-edition.html
Also Baker *Nature Reviews Drug Discovery* 2013 12(1) 5-7

Slide 17

HTS vs. Fragment Approaches:



Slide 18

"Chemical Space" is Unimaginably Large:

- ~ 10^{63} possible molecules with up to 30 C, N, O, S atoms
  Bohacek, McMartin, & Guida, *Med. Res. Rev.,* 16: 3-50 (1996)

- Global screening collection ~ 10^{8} different molecules
  Hann & Oprea, *Curr. Opin. Chem. Biol.,* 8: 255-263 (2004)

∴ Even largest libraries sample an insignificant fraction of diversity space

Audience Survey Question

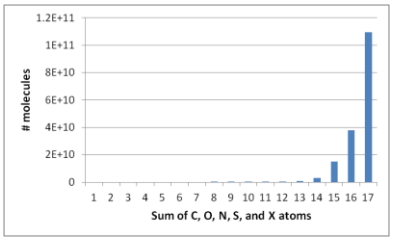
ANSWER THE QUESTION ON SCREEN

How many possible molecules can be made with up to 11 non-hydrogen atoms (C, N, O, and F only)?

- ~100,000
- ~1,000,000
- ~10,000,000
- ~100,000,000

Smaller Number of Smaller Fragments:

- 1.11 x 10^8 molecules with up to 11 non-hydrogen atoms (MW < 160; C, N, O, and F only)
  6.4 x 10^5 reported molecules of this size (0.06%)
- 9.77 x 10^8 molecules with up to 13 atoms
- 1.66 x 10^{11} molecules with up to 17 atoms



Reymond, *Angew. Chem. Int. Ed. Engl.*, 44: 1504-1508 (2005)
J. Chem. Inf. Mod., 47: 342-353 (2007); *J. Am. Chem. Soc.*, 131: 8732-8733 (2009)
J. Chem. Inf. Mod., 52: 2864-2875 (2012)

Slide 21

Other Advantages of Fragments:

- Small fragments less likely to have interfering functionality ("molecular complexity")

Hann et al. *J. Chem. Inf. Comput. Sci.*, 41, 856-864 (2001); Leach & Hann *Curr. Opin. Chem. Biol.*, 15, 489-496 (2011)

- Smaller libraries allow more up-front attention to purity and drug-like properties
- Smaller libraries easier for universities and small companies to get started
- Fragments can tackle new classes of targets

Slide 22

What is a Fragment?

- **Lipinski's "Rule of 5" for orally active drugs**
  C.A. Lipinski et al. (1997) *Adv Drug Del Rev* 23: 3–25

  < 500 Da (~38 heavy atoms)*
  < 5 H-bond donors
  < 10 H-bond acceptors
  < 5 octanol-water partition coefficient (logP)

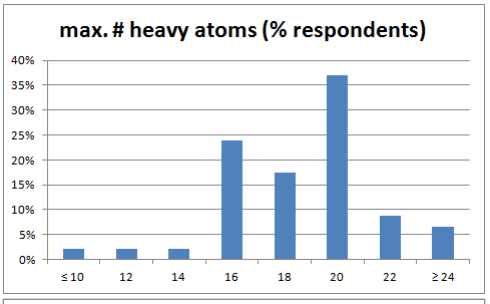
- **Astex's "Rule of 3" for fragments**
  M. Congreve et al. (2003) *Drug Discovery Today* 8: 876-877

  < 300 Da (~23 heavy atoms)*
  < 3 H-bond donors
  < 3 H-bond acceptors
  < 3 ClogP

* Hopkins, AL et al., *Drug Discovery Today*, 9(10), 430-431 (2004)
Mean molecular mass of a non-hydrogen (or "heavy") atom is 13.286 Da (Pfizer)

Slide 23

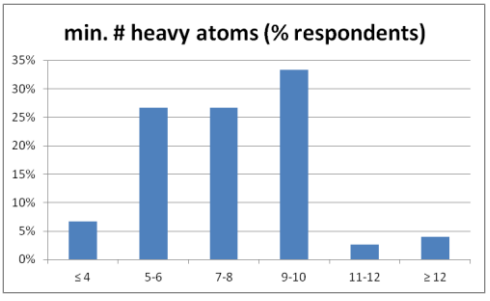
How Large (and Small) are Fragments?



Poll on *Practical Fragments* May 2012:

"What is the largest number of atoms you would allow in a fragment?"

46 responses



Poll on *Practical Fragments* May 2013

"What is the smallest number of atoms you would allow in a fragment?"

75 responses

Most fragments have between 5 and 20 non-hydrogen atoms

Slide 24

Small Fragments Give High Hit Rates!

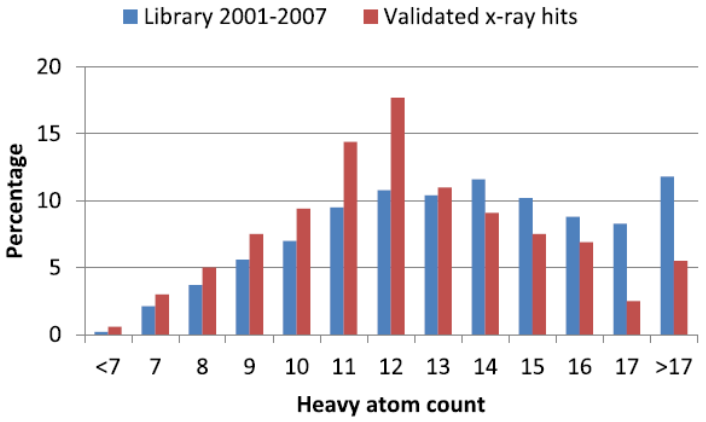


Fig. 6. Percentage of compounds with specified heavy atom count (i.e. the number of non-hydrogen atoms) for compounds in Astex screening libraries from 2001 to 2007 compared with X-ray hits.

Hall, RJ et al. *Prog. Biophys. Mol. Biol.* 2014, *116*, 82-91.

Slide 25

Pitfalls in Fragment Screening

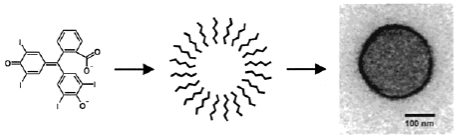
Davis & Erlanson
Bioorg Med Chem Lett 2013 2844
http://dx.doi.org/10.1016/j.bmcl.2013.03.028

Learning from our mistakes:
the 'unknown knowns' in fragment screening

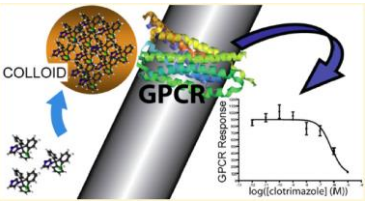
- Solubility
- Reactive molecules (electrophiles, oxidizers, etc.)
  - not always obvious (PAINS, May 28)
  - at high concentrations, low-level impurities can be more problematic
- Aggregators

Slide 26

Compounds Can Form Aggregates that Non-specifically Inhibit:

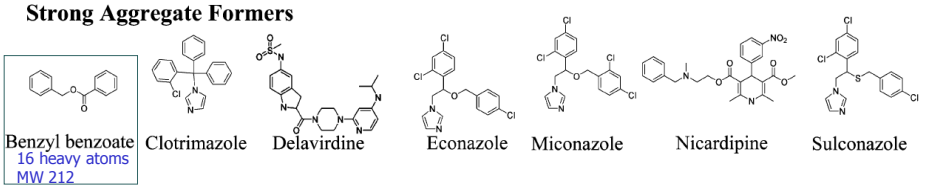


→ Inhibit enzymes, PPIs, GPCRs, etc.



Even approved drugs can inhibit nonspecifically at micromolar concentrations

Strong Aggregate Formers



McGovern, SL et al. *J. Med. Chem.* 2002, *45*, 1712-1722; Seidler, J et al. *J. Med. Chem.* 2003, *46*, 4477-4486; Shoichet, BK *Drug Discovery Today* 2006, *11*, 607-615; Sassano et al. *J. Med. Chem.* 2013, *56*, 2406-2414

Slide 27

Protecting Yourself From Aggregators:

- Add non-ionic detergent to the assay (Triton X-100, Tween-20, CHAPS, others)
- Increase protein concentration – this should have no effect on genuine binders (within limits)
- Characterize the mechanism of inhibition (competitive, noncompetitive, or uncompetitive): competitive inhibitors are normally not promiscuous
- Centrifuge your samples and retest them – this can sometimes remove aggregators
- Examine your samples with DLS or flow cytometry – aggregators can sometimes be directly observed as 50-1000 nm particles
- Look closely at your dose-response curve - unusually steep slopes can signal aggregation

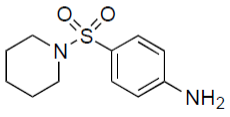
Feng, BY and Shoichet, BK *Nature Protocols* 2006, *1*, 550-553.
Shoiceht, BK *Drug Discovery Today* 2006, 11, 607-615.

Slide 28

Audience Survey Question

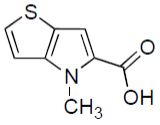
ANSWER THE QUESTION ON SCREEN

Which two of these fragments are aggregators?



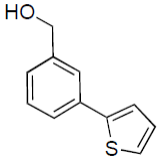
2

IC_{50} = 65 µM



3

40 µM



4

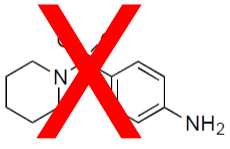
226 µM

- 2 and 3
- 2 and 4
- 3 and 4

Vom, et al. *Aus. J. Chem.* 2013, *66*, 1518-1524.

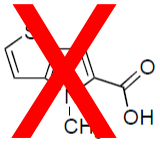
29

Aggregators Can't Be Recognized A Priori:



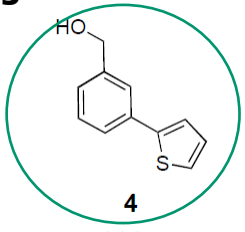
2

IC_{50} = 65 µM



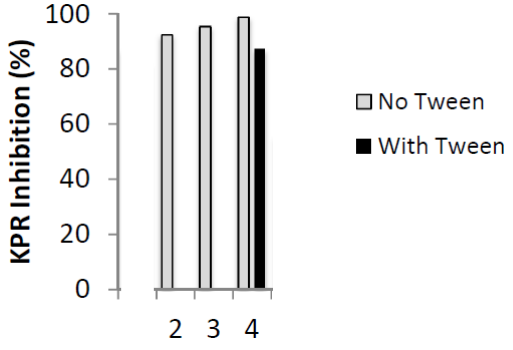
3

40 µM



4

226 µM



Vom, et al. *Aus. J. Chem.* 2013, *66*, 1518-1524.

Slide 30

The first principle is that you must not fool yourself– and you are the easiest person to fool.

So you have to be very careful about that.

Richard Feynman
1974 Caltech commencement address

Slide 31

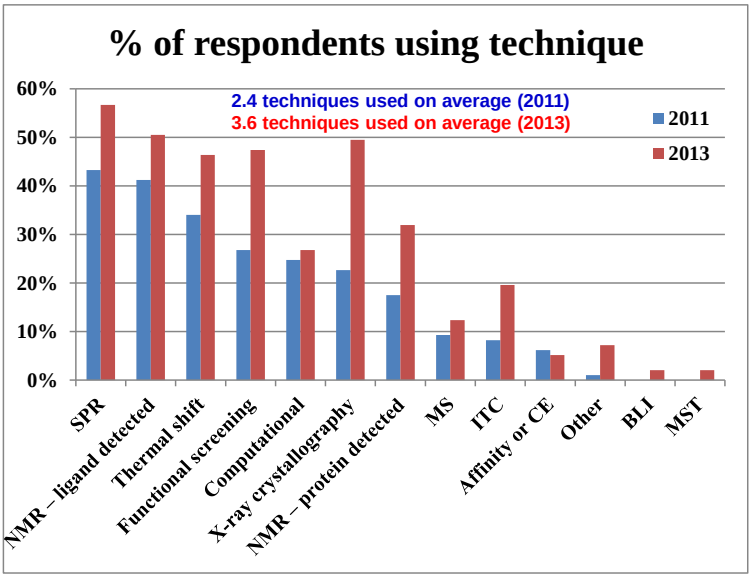
So How Do You Find Fragments?

- NMR
  - Protein detected (ie, SAR by NMR) — *Structural information*
  - Ligand detected (ie, STD, TINS)
- X-ray crystallography — *Structural information*
- Surface plasmon resonance (SPR) — *Increasingly common*
- Functional screening
  - High concentration screening — *Keep eyes open!*
- Computational — *Especially as filter*
- Thermal shift
- Isothermal titration calorimetry
- Mass spectrometry: non-covalent or covalent
- Affinity chromatography / capillary electrophoresis

Combinations of above

Slide 32

What Methods are People Using?



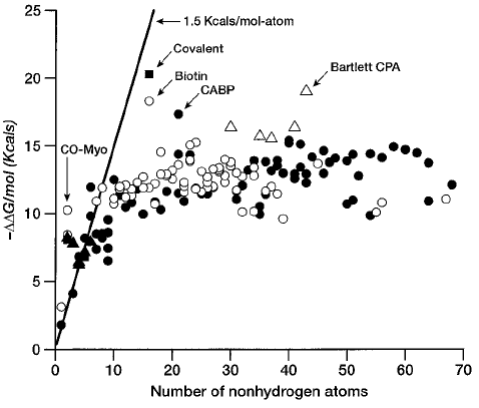
Polls on *Practical Fragments* September 2011 and December 2013, 97 responses (each)

Ligand Efficiency (LE): Binding Energy Per Non-hydrogen Atom

Binding energy:

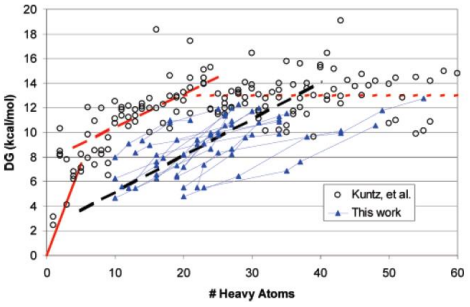
$\Delta G = -RT\ln(K)$

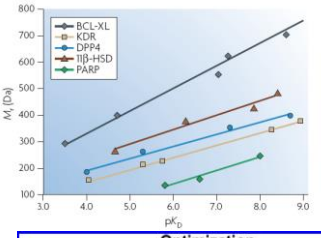
$$LE = \frac{\Delta G}{(\#\ \text{heavy atoms})}$$

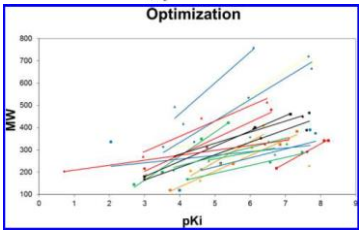


Kuntz, ID et al. *Proc. Acad. Nat. Acad. Sci. USA, 96*, 9997-1002 (1999)
Hopkins, AL et al., *Drug Discovery Today*, 9(10), 430-431 (2004)

Some Predictability in Fragment Optimization:





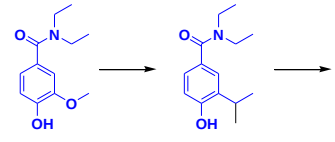


Each atom adds ~0.3 kcal/mol (or)
Each 10x increase in potency adds ~64 Da

Hajduk, PJ *J. Med. Chem.* 2006, *49*, 6972-6976.
Hajduk, PJ and Greer, P *Nature Reviews Drug Discovery* 2007, *6*, 211-219.
Ferenczy, GG and Keserü, GM *J. Med. Chem.* 2013, *56*, 2478-2486.

Slide 35

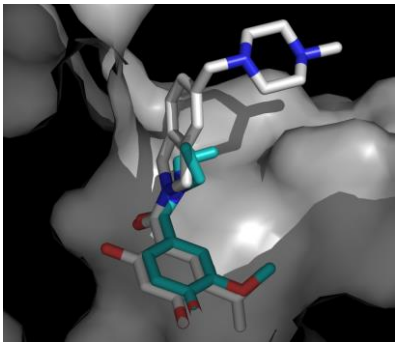
Fragment Growing: Hsp90 Clinical Compound from Astex



Compound 3
K_d = 790 µM
LE = 0.26

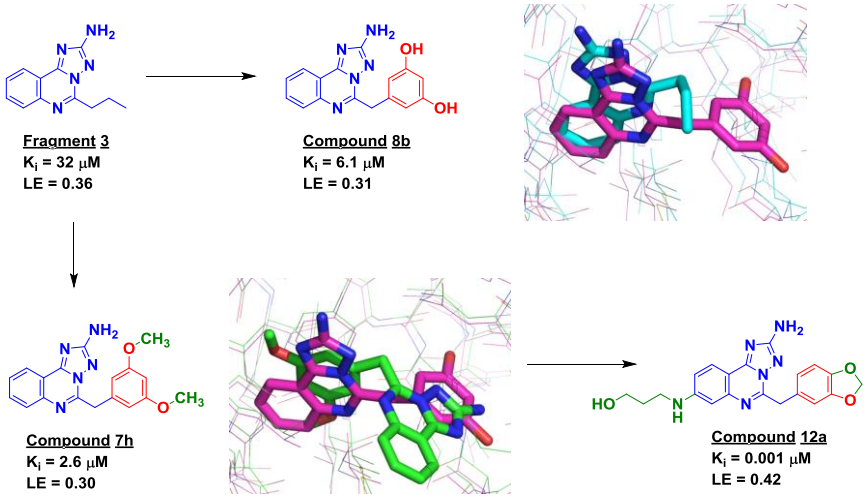
Compound 17
K_d = 7 µM
LE = 0.41

AT13387
Phase 1: solid tumors
Phase 2: GIST



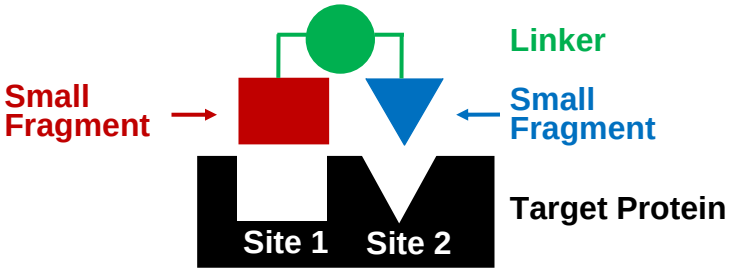
Murray et al. *J. Med. Chem.* 2010, *53,* 5942-5955
Woodhead et al. *J. Med. Chem.* 2010, *53,* 5956-5969

But Don't Assume Binding Mode Remains The Same!



Casale et al. *Bioorg. Med. Chem.* 2014, *22*, 4135-5150

The Dream of Fragment Linking:



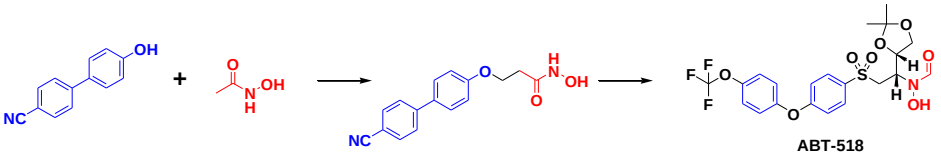
$$\Delta G_{(\text{linked fragments})} = \Delta G_{(\text{Frag A})} + \Delta G_{(\text{Frag B})} + \Delta G_{\text{linker}}$$

$$\therefore K_{D(\text{linked fragments})} = K_{D\ (\text{Frag A})} * K_{D(\text{Frag B})} * L_{(\text{linker coefficient})}$$

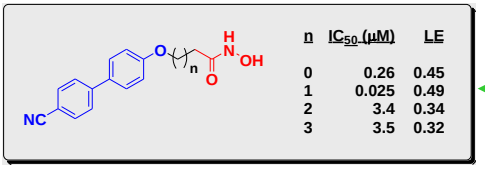
Huge combinatorial advantage:
10^4 x 10^4 = 10^8 virtual compounds

Proc. Natl. Acad. Sci. USA
Vol. 78, No. 7, pp. 4046–4050, July 1981
Biochemistry

The Dream of Linking:
Synergy SAR by NMR to Develop an MMP-2 Inhibitor



K_d = 20 µM LE = 0.43	K_d = 17,000 µM LE = 0.48	IC_{50} = 0.025 µM LE = 0.49	ABT-518 IC_{50} = 0.00078 µM LE = 0.37
15 heavy atoms MW 195	5 heavy atoms MW 75	21 heavy atoms MW 282	34 heavy atoms MW 505



n	IC_{50} (µM)	LE
0	0.26	0.45
1	0.025	0.49
2	3.4	0.34
3	3.5	0.32

Hajduk, PJ et al. *J. Am. Chem. Soc.* 1997, *119*, 5818-5827
Wada, CK *Curr. Top. Med. Chem.* 2004, *4*, 1255-1267

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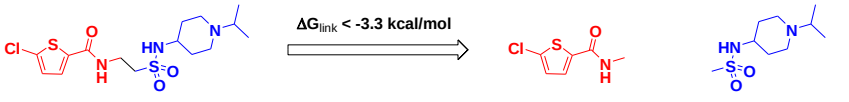
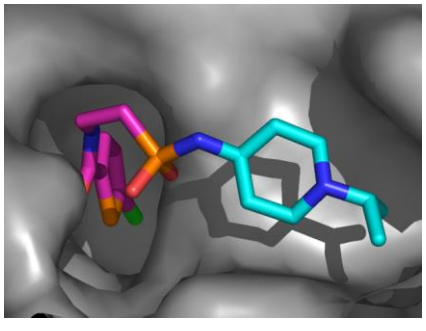
Superadditivity from Extremely Weak Fragments



Compound 1a
K_i = 0.002 µM
LE = 0.49
ΔG = -11.8 kcal/mol

Compound 1g
K_i = 58 µM
LE = 0.58
ΔG = -5.8 kcal/mol

Compound 1d
K_i > 10,000 µM
LE < 0.19
ΔG > -2.7 kcal/mol



M Nazaré, H Matter, et al. *Angew. Chem. Int. Ed.* 2012, 51, 905-911

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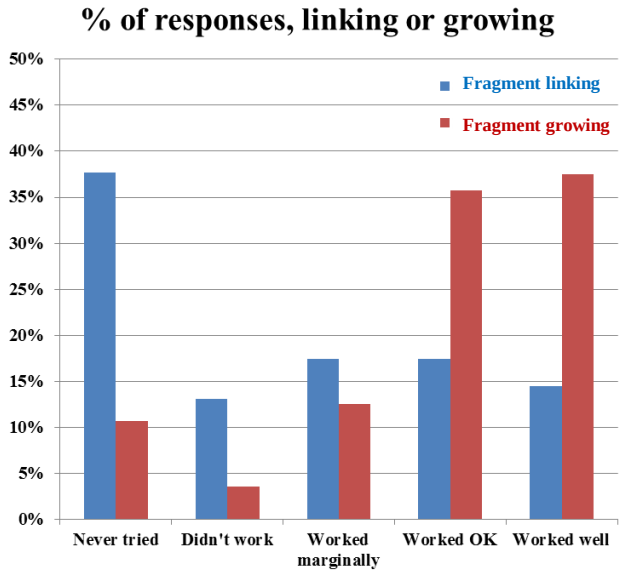
Growing versus Linking



Poll on *Practical Fragments* July-August 2014: 69 responses (linking), 56 responses (growing)
http://practicalfragments.blogspot.com/2014/09/fragment-growing-vs-fragment-linking.html

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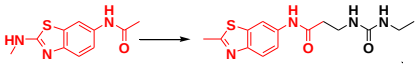
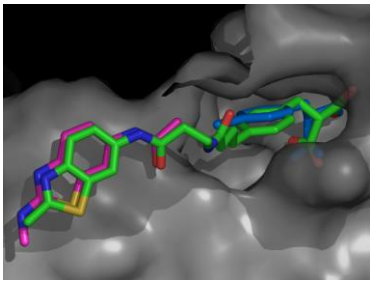
Fragment Linking for LDHA: AstraZeneca



Compound 12
K_D = 770 µM
LE = 0.28
Enzyme IC_{50} > 500 µM

Compound 24
K_D = 160 µM
LE = 0.25
Enzyme IC_{50} > 500 µM



Ward et al. *J. Med. Chem.* 2012, *55*, 3285

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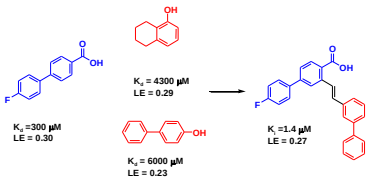
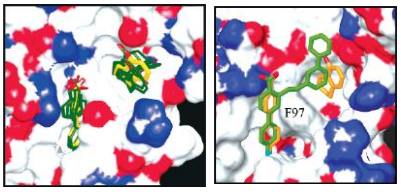
Fragment linking? Abbott's Bcl Family Inhibitors





Nature 2005, *435*, 677-681.
J. Med. Chem. 2006, *49*, 656-663.
J. Med. Chem. 2008, 51, 6902-6915.
Nat. Med. 2013 19, 202-208.

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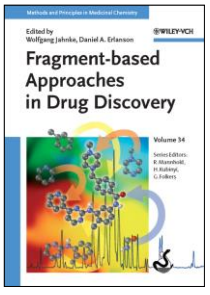
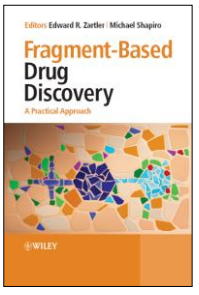
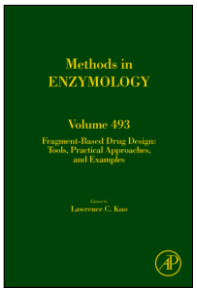
Resources – books:



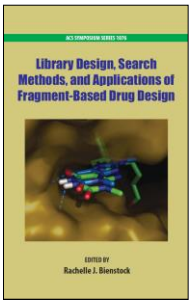
2006



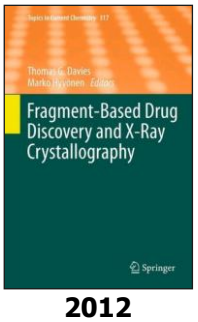
2008



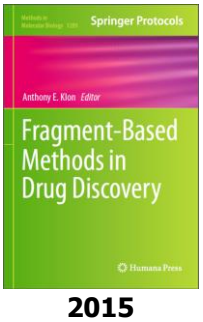
2011



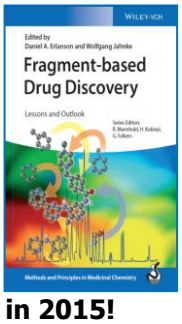
2012



2012



2015



Coming soon in 2015!

Resources from the Web

- **Practical Fragments** (http://practicalfragments.blogspot.com/)
- **LinkedIn** (http://www.linkedin.com/groups?gid=121172)
- **Carmot Therapeutics** (www.carmot.us)

Please contact me (derlanson@carmot.us)

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Upcoming Events in 2015

- Fragments 2015, Cambridge, UK, March 22-24
- CHI's Protein-Protein Interactions and Fragment-Based Drug Discovery, San Diego, CA, April 21-23
- NovAlix's Biophysics in Drug Discovery, Strasbourg, France, June 9-12
- OMICS Group's Drug Discovery and Designing, Frankfurt, Germany, August 11-13
- Pacifichem 2015, Honolulu, Hawaii, December 15-20
  http://www.pacifichem.org/technical-program/abstracts/

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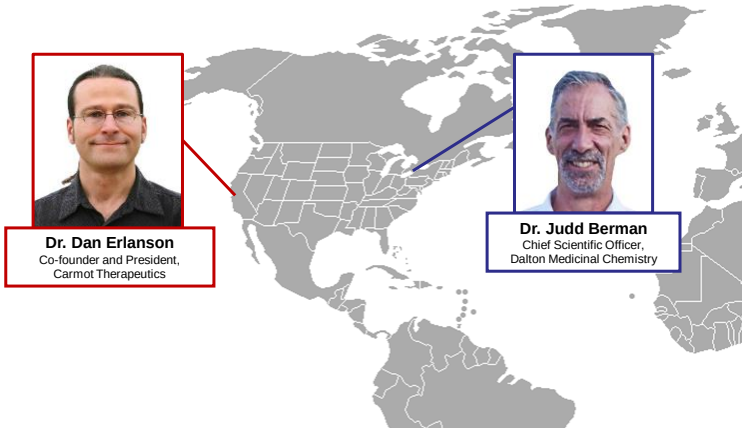

Dr. Dan Erlanson
Co-founder and President,
Carmot Therapeutics

Dr. Judd Berman
Chief Scientific Officer,
Dalton Medicinal Chemistry

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

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Thursday, April 2, 2015

"Talking About Polymers, Detecting Explosives"

Jennifer Novotney, PhD Student, Cornell University, 2014 Chemistry Champions Competition Winner

Dr. Darcy Gentleman, Manager of Engagement and Science Communications, The American Chemical Society

Thursday, April 9, 2015

"Active vs. Passive Voice in Scientific Writing"

Dr. Kristin Sainani, Associate Professor, Stanford

Ms. Celia Elliott, Science Writer and Technical Editor, University of Illinois at Urbana-Champaign

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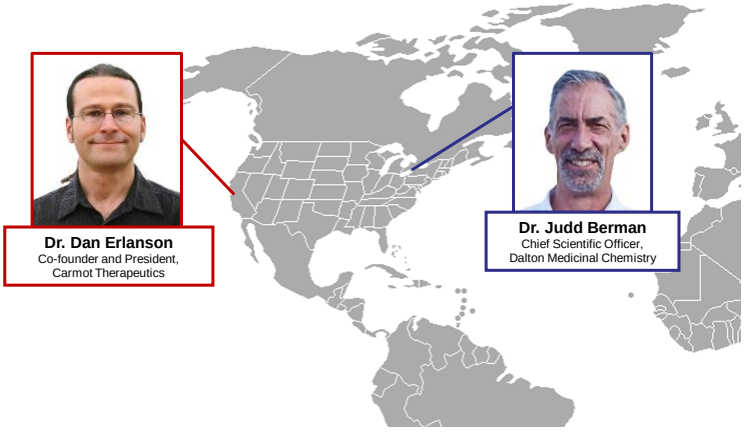

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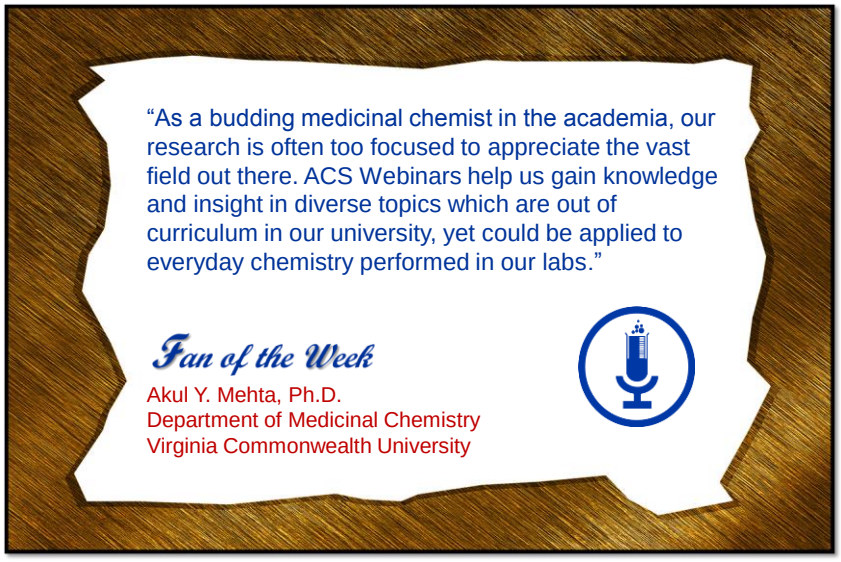

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Mar 19	Fragment-Based Drug Design Strategies	*Dr. Dan Erlanson*
April 30	Screening Strategies	*Dr. David Swinney*
May 28	PAINS (Pan-Assay Interference Compounds)	*Dr. Jonathan Baell*
June 25	Positron Emission Tomography (PET) Labeling in Drug Discovery & 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*

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