

Journal Club Presentations/Discussions

Summer 2023

JC1 - WEEK 2

Zolli-Juran, M.; Cechetto, J. D.; Hartlen, R.; Daigle, D. M.; Brown, E. D., High throughput screening identifies novel inhibitors of Escherichia coli dihydrofolate reductase that are competitive with dihydrofolate. *Bioorganic & Medicinal Chemistry Letters* 2003, 13 (15), 2493-2496.

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- [Zolli_JuranDHFRbacteriaHTSBioorgMedChemLett2003.pdf](#)

JC2 - WEEK 3 (now week 4)

Park, H.; Kim, Y. J.; Hahn, J. S., A novel class of Hsp90 inhibitors isolated by structure-based virtual screening. *Bioorganic & Medicinal Chemistry Letters* **2007**, 17 (22), 6345-6349.

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- [ParkHsp90drugVirtualScreenBioorgMedChemLett2007.pdf](#)

JC3 - WEEK 6 (week after 4th of July week)

Prasannan, P.; Suliman, H. S.; Robertus, J. D., Kinetic analysis of site-directed mutants of methionine synthase from Candida albicans. *Biochem Biophys Res Commun* **2009**, 382 (4), 730-4.

[PrasannanPriya_MetSynthaseKinetic_RobertusBiochemBiophysResComm2009.pdf](#)

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Reading Strategies for Journal Articles

First pass - Skim Abstract, Conclusions, Figures

Second pass - Read Introduction, Methods, Results

---- Underline – only up to 10%. Make notes in margin, draw sketches

- ----Look up reaction mechanism of enzyme, Circle unfamiliar words

----- Then go back afterwards and look up definitions

Take a break (couple of hours - to a day or so) - Coffee break !

Third pass - Read for comprehension

JC4 - WEEK 5

JC5 - WEEK 6

OTHERS

NDM-1 variants paper (Fast) - ?

- [Fast_NDM1_MutantZincStability_JBiolChem2018.pdf](#)

DSF Kinetic vs Thermodynamic paper

- [Wu, et. al. DSF kinetic vs. thermodynamic paper](#)

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Presentation Order:

DHFR paper -JC1 -

Hsp90 - JC2 -

HisG - JC3 -

MetSynthase - JC4

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JC3

Cho, Y.; Ioerger, T.; Sacchettini, J., Discovery of novel nitrobenzothiazole inhibitors for Mycobacterium tuberculosis ATP phosphoribosyl transferase (HisG) through virtual screening. *J Med Chem* **2008**, 51 (19), 5984-92.

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JC4

UPCOMING PAPERS

- We will meet on the week before (or earlier) to discuss initial questions on paper
- Then, show me a draft of your slides by at least two days before
- We will meet again on the day before to review final
- Upload your presentation before class to the
[/GroupMeetingSlides/StudentPresentations](#) folder on **Google Docs**
 - give it a super awesome VDS style filename so that we can tell what it is.

[Guidelines For Presentations \(technical, journal clubs, research\)](#)

- Read this before preparing your presentation

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Zhang, Y.; White, S.; Rock, C., Inhibiting bacterial fatty acid synthesis. *J Biol Chem* **2006**, 281 (26), 17541-4.

[Google Drive Folder of Journal Club Papers as PDFs for Summer](#)

Herschhorn, A.; Hizi, A., Virtual screening, identification, and biochemical characterization of novel inhibitors of the reverse transcriptase of human immunodeficiency virus type-1. *J Med Chem* **2008**, 51 (18), 5702-13.

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Extra

Covid-19 papers?

N/A

6th Week -Candida - JC6 -

7th Week -

Hirayama, K.; Aoki, S.; Nishikawa, K.; Matsumoto, T.; Wada, K., Identification of novel chemical inhibitors for ubiquitin C-terminal hydrolase-L3 by virtual screening. **Bioorg Med Chem** 2007, 15 (21), 6810-8.

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Potential Papers:

Singh, J.; Chuaqui, C.; Boriack-Sjodin, P.; Lee, W.; Pontz, T.; Corbley, M.; Cheung, H.; Arduini, R.; Mead, J.; Newman, M.; Papadatos, J.; Bowes, S.; Josiah, S.; Ling, L., Successful shape-based virtual screening: the discovery of a potent inhibitor of the type I TGFbeta receptor kinase (TbetaRI). **Bioorg Med Chem Lett** 2003, 13 (24), 4355-9.

Li, Z.; Garner, A. L.; Gloeckner, C.; Janda, K. D.; Carlow, C. K., Targeting the Wolbachia cell division protein FtsZ as a new approach for antifilarial therapy. **PLoS Negl Trop Dis** 2011, 5 (11), e1411.

Henriksson, L. M.; Unge, T.; Carlsson, J.; Aqvist, J.; Mowbray, S. L.; Jones, T. A., Structures of Mycobacterium tuberculosis 1-deoxy-D-xylulose-5-phosphate reductoisomerase provide new insights into catalysis. **J Biol Chem** 2007, 282 (27), 19905-16.

Tomlinson, S.; Malmstrom, R.; Watowich, S., New approaches to structure-based discovery of dengue protease inhibitors. **Infect Disord Drug Targets** 2009, 9 (3), 327-43.

Sacchettini, J.; Rubin, E.; Freundlich, J., Drugs versus bugs: in pursuit of the persistent predator *Mycobacterium tuberculosis*. *Nat Rev Microbiol* **2008**, 6 (1), 41-52.

Mochalkin, I.; Miller, J.; Narasimhan, L.; Thanabal, V.; Erdman, P.; Cox, P.; Prasad, J.; Lightle, S.; Huband, M.; Stover, C., Discovery of antibacterial biotin carboxylase inhibitors by virtual screening and fragment-based approaches. *ACS Chem Biol* 2009, 4 (6), 473-83.

Bai, Y.; Monzingo, A.; Robertus, J., The X-ray structure of ricin A chain with a novel inhibitor. *Arch Biochem Biophys* **2009**, 483 (1), 23-8.

COMPLETED PAPERS 2019 Summer:

JC?

Zhang, Y.; White, S.; Rock, C., Inhibiting bacterial fatty acid synthesis. *J Biol Chem* **2006**, 281 (26), 17541-4.

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JC?

Cho, Y.; Ioerger, T.; Sacchettini, J., Discovery of novel nitrobenzothiazole inhibitors for Mycobacterium tuberculosis ATP phosphoribosyl transferase (HisG) through virtual screening. *J Med Chem* **2008**, 51 (19), 5984-92.

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