From Lab Bench to Your Medicine Cabinet

Week 3 – Fragment based screening
Fragment screening of inhibitors for MIF tautomerase reveals a cryptic surface binding site.
Larry R. McLean, Ying Zhang, Hua Li, Yong-Mi Choi, Zuoning Han, Roy J. Vaz, Yi Li.

Helpful Review
A decade of fragment-based drug design: strategic advances and lessons learned
Philip J. Hajduk and Jonathan Greer
And
Recent progress in fragment-based lead discovery
Michele N Schulz and Roderick E Hubbard

In-class Discussion Questions

1. What general class of therapeutics is the author’s investigating? Why?
2. What specific scaffolding is being used? Why?
3. What are the properties of the scaffold?
4. How were the derivatives selected?
5. What is your assessment of the inhibitory results of the synthesized compounds?
6. Can you propose an analog based on their results that might be better?
7. Do you think knowing what the target (e.g. mechanism of action) would help design a better derivative? Why?