

# Overall performance in the solubility challenge

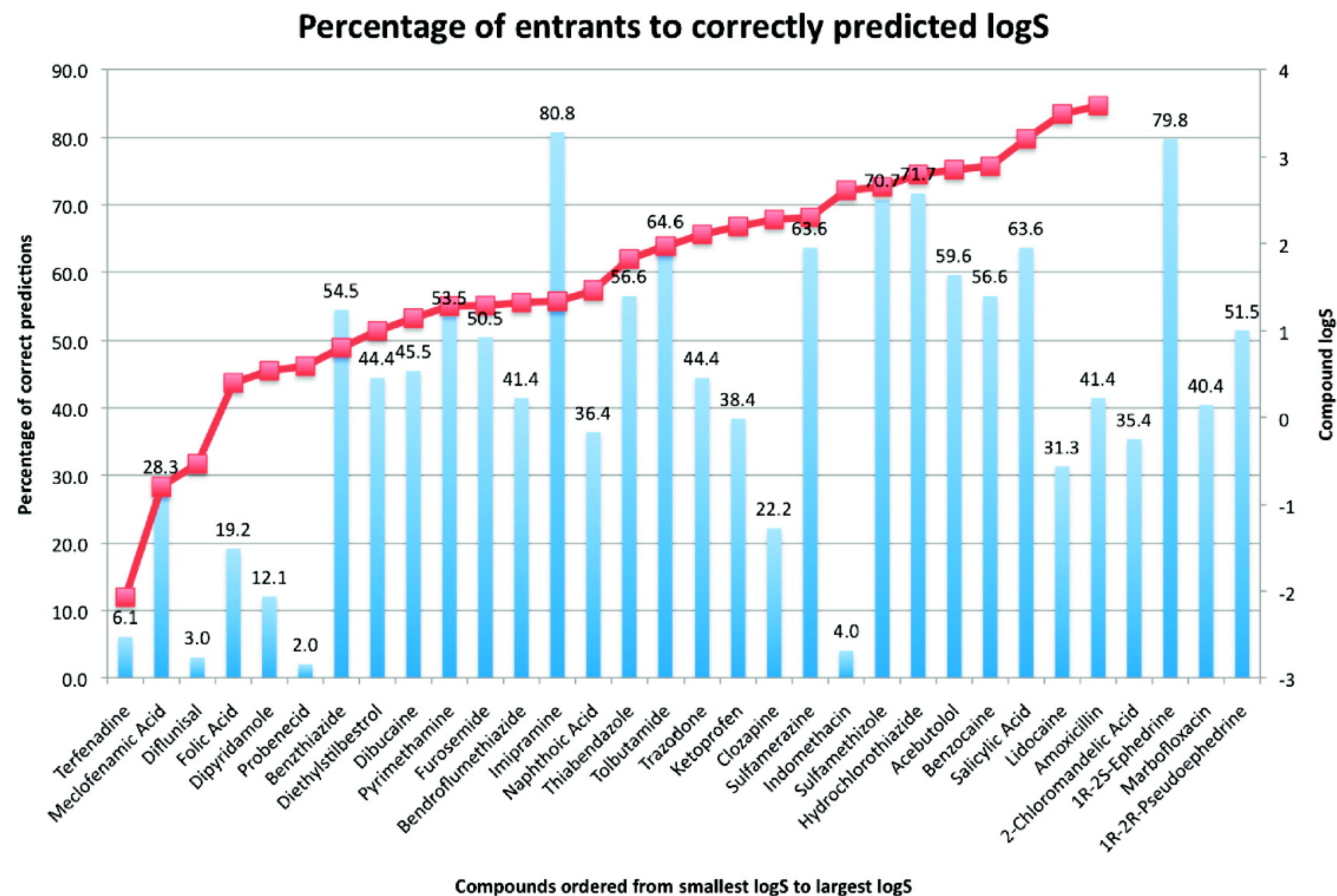


Figure 2 from ref [3]  
“Correct” is within 0.5 logS  
Blue bars are percentage correct  
Red is actual logS

# Stated major findings [3]

- For measured set of 28 compounds, percent correct on
  - absolute S ( $\pm 10\%$ ) ranges from 0%-18%
  - logS ( $\pm 0.5$  logS) ranges from 10-61%
  - Worst two compounds 2% and 4% correct by logS
- $R^2$  ranges from 0 to 0.65
- No polymorph predictions
- Compounds with “normal” solubility (logS = 0.5 to 3) were easiest
- Many methods, but none clearly the best