

Overall performance in the solubility challenge

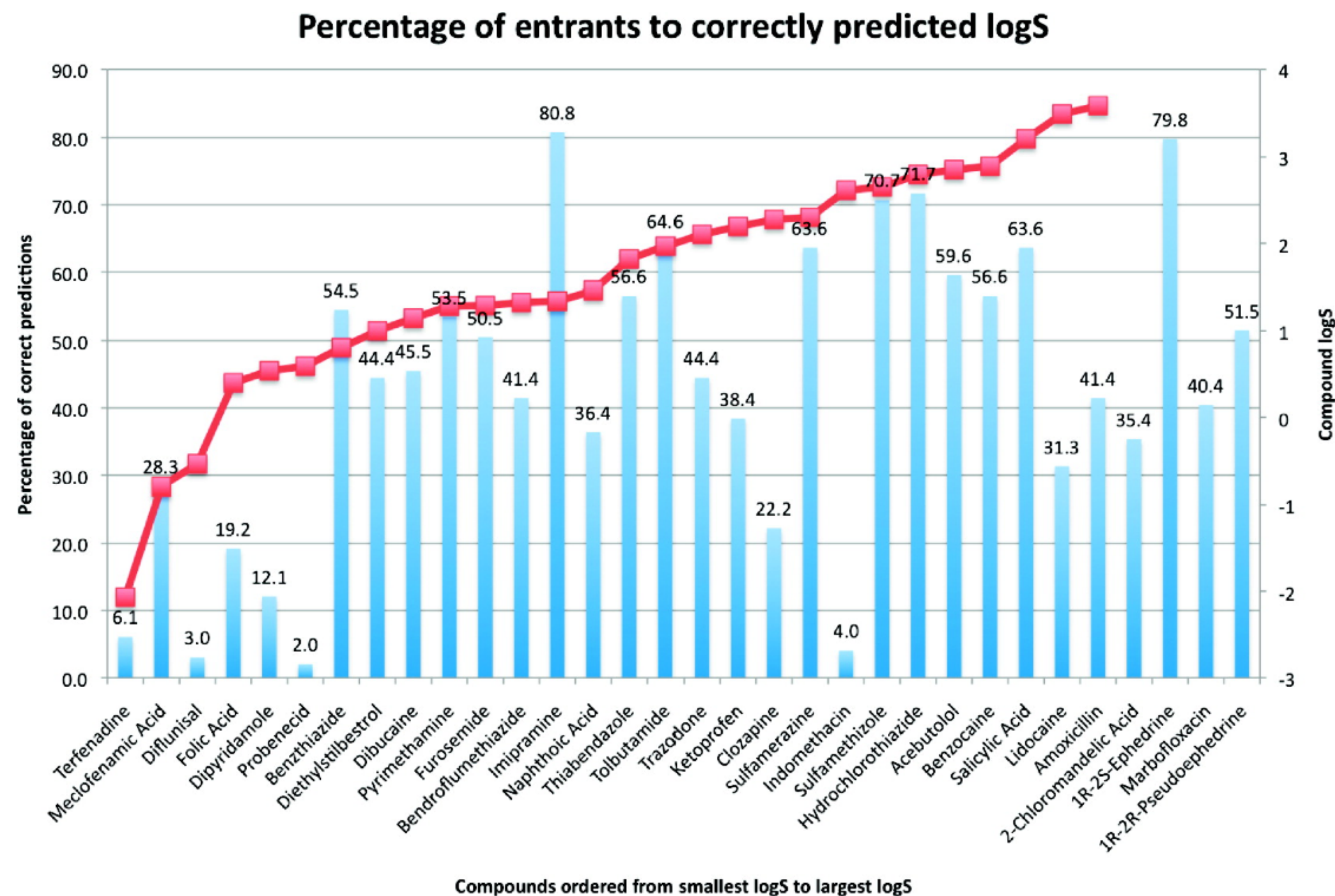


Figure 2 from ref [3]
“Correct” is within 0.5 logS
Blue bars are percentage correct
Red is actual logS

Stated major findings [3]

- For measured set of 28 compounds, percent correct on
 - absolute S ($\pm 10\%$) ranges from 0%-18%
 - logS (± 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