Stated major findings [3]

- For measured set of 28 compounds, percent correct on
  - absolute S (±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

QSPR prediction of solubility