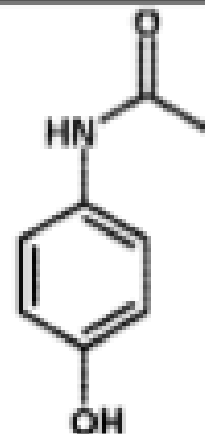
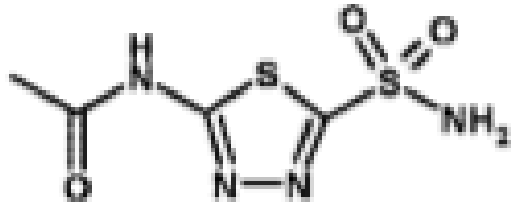
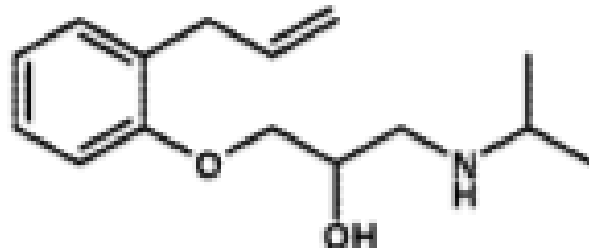
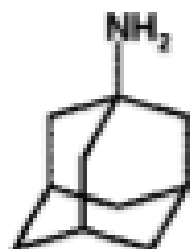


# Examples from the dataset [2]

| Structure   | Name          | MW<br>Neutral Form | pKa              | Kinetic Solubility<br>$\mu\text{M}$<br>$\mu\text{g/ml}$ | Intrinsic Solubility<br>$\mu\text{M}$<br>$\mu\text{g/ml}$ |
|---|---------------|--------------------|------------------|---|---|
|    | Acetaminophen | 151.17             | $9.52 \pm 0.01$  | $161700 \pm 7000 \mu\text{M}$                           | $86300 \pm 7000 \mu\text{M}$                              |
|   |               |                    |                  | $24400 \pm 1060 \mu\text{g/ml}$                         | $13000 \pm 1060 \mu\text{g/ml}$                           |
|  | Acetazolamide | 222.25             | $8.75 \pm 0.02$  | $6100 \pm 3840 \mu\text{M}$                             | $3670 \pm 80 \mu\text{M}$                                 |
|   |               |                    | $7.31 \pm 0.04$  | $1360 \pm 850 \mu\text{g/ml}$                           | $816 \pm 18 \mu\text{g/ml}$                               |
|  | Alprenolol    | 249.36             | $9.47 \pm 0.01$  | $5080 \pm 50 \mu\text{M}$                               | $2320 \pm 40 \mu\text{M}$                                 |
|   |               |                    |                  | $1266 \pm 12 \mu\text{g/ml}$                            | $580 \pm 10 \mu\text{g/ml}$                               |
|  | Amantadine    | 151.25             | $10.48 \pm 0.01$ | $17300 \pm 3960 \mu\text{M}$                            | $14000 \pm 1180 \mu\text{M}$                              |
|   |               |                    |                  | $2620 \pm 600 \mu\text{g/ml}$                           | $2120 \pm 180 \mu\text{g/ml}$                             |

# Overall performance in the solubility challenge

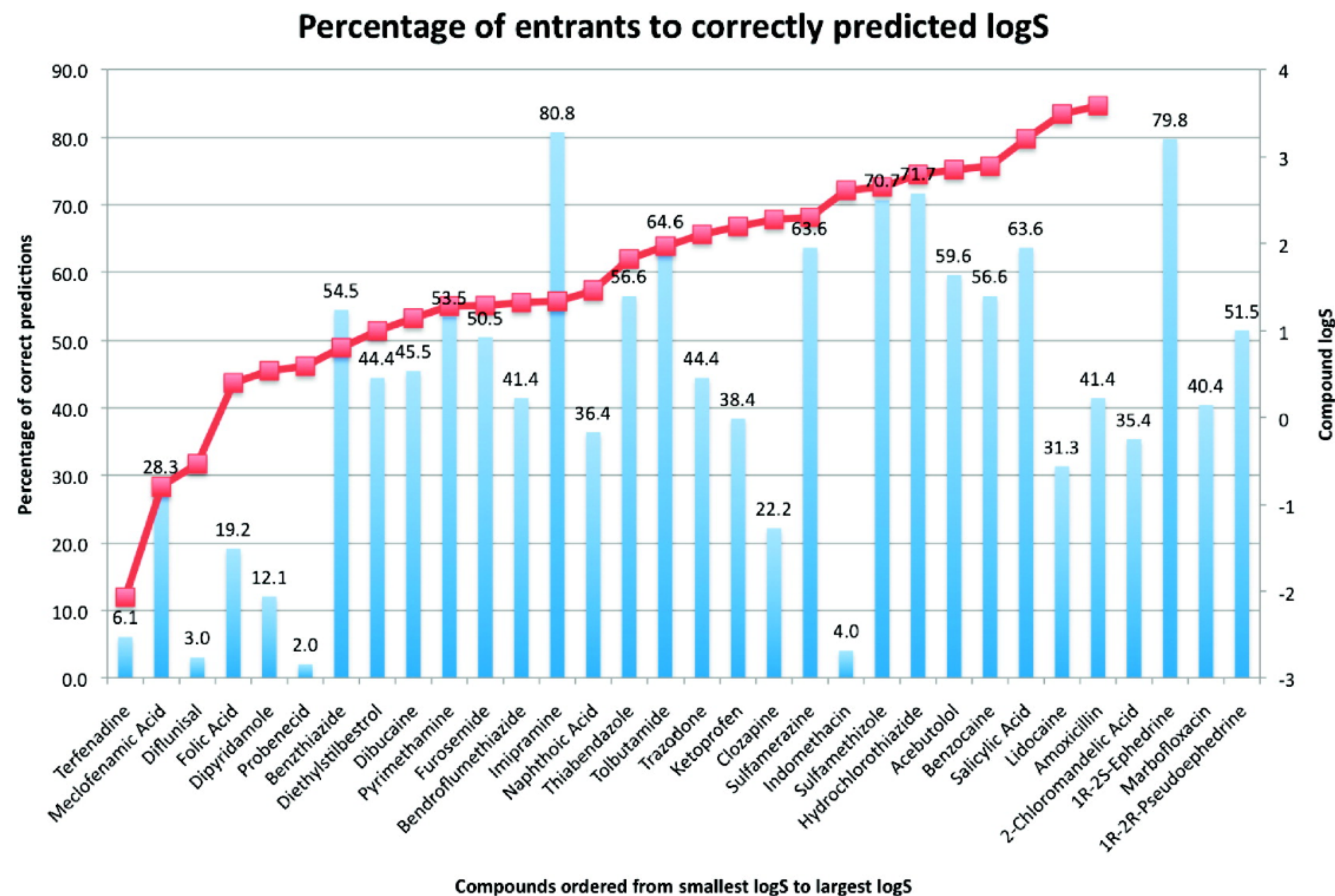


Figure 2 from ref [3]  
“Correct” is within 0.5 logS  
Blue bars are percentage correct  
Red is actual logS