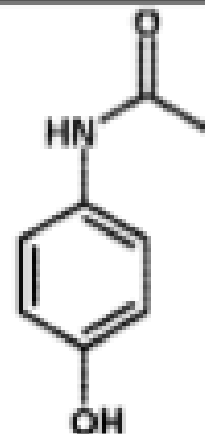
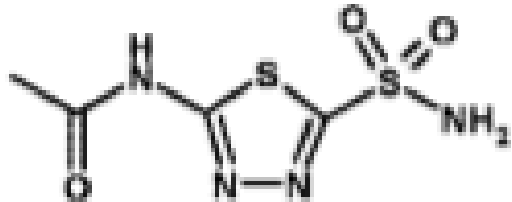
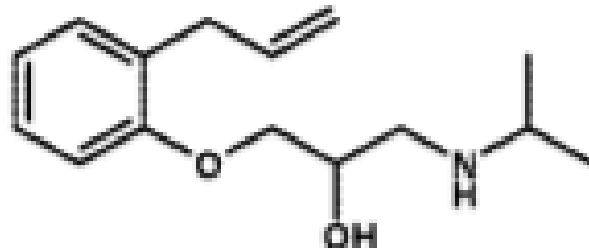
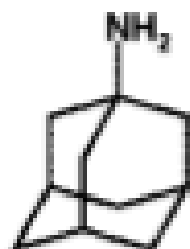


Solubility Challenge (2008) [2, 3]

- measured
 - intrinsic solubility (free acid/free base)
 - highly reproducible (thermodynamic versus kinetic solubility)
- published 100 solubilities
- challenged researchers to predict 32 more
- received >100 entries between July and September 2008

Examples from the dataset [2]

Structure	Name	MW Neutral Form	pKa	Kinetic Solubility μM $\mu\text{g/ml}$	Intrinsic Solubility μM $\mu\text{g/ml}$
	Acetaminophen	151.17	9.52 ± 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 ± 0.02	$6100 \pm 3840 \mu\text{M}$	$3670 \pm 80 \mu\text{M}$
			7.31 ± 0.04	$1360 \pm 850 \mu\text{g/ml}$	$816 \pm 18 \mu\text{g/ml}$
	Alprenolol	249.36	9.47 ± 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 ± 0.01	$17300 \pm 3960 \mu\text{M}$	$14000 \pm 1180 \mu\text{M}$
				$2620 \pm 600 \mu\text{g/ml}$	$2120 \pm 180 \mu\text{g/ml}$