Chemistry 5.46
Organic Structure Determination
Major Points Summary

Entry points based on…

- Chemical shifts
- Integrals and intensities
- J-couplings and multiplet analysis

HMQC/HSQC

- Identifies methyl ^{13}C's
- Pairs methylene ^{1}H's with $\Delta\delta$'s on ^{13}C's
- Reveals methine ^{1}H/^{13}C pairs

Miscellaneous

- 2-D plotting: t_1 ridges and snow-capped peaks

- 2-D plotting: threshold and noise floor

- HMBC: consequence of no X-decoupling

- Norbornane: methine bridgehead ^3J to exo is bigger than to endo

gCOSY

- $^3J_{HH}$'s most useful
- $^4J_{HH}$'s and $^5J_{HH}$'s should be plausible
- Helps improve ^1H δ determinations

HMBC

- $^2J_{HC}$'s stronger through sp^3 and than sp^2 ^{13}C's

- $^3J_{HC}$'s 0-12+ Hz as function of dihedral angle

- $^4J_{HC}$'s and $^5J_{HC}$'s found in rigid systems