Week 7

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7.1 Office Hours (Moe)

2/13:

- Use chemical shift as your x-axis in NMR plots.
- Hexylamine is our substance.
- Interpreting NMR data files: Column E is chemical shift; column C is peak intensity. Column D is hertz (not chemical shift).
  - Chemical shift is in the rightmost column.
- Fitting tutorial: If solver still isn't helping (you get an error message and no convergence), divide the absolute intensities by a million. You can also do this from the get-go.
- M_z should be calculated for each carbon; it is the absolute integral value in the all-integrals spreadsheet.
- Don't let the peaks overlap in the plot of multiple vertically offset T_1 values.
  - Use 3 plots.
- R outputs standard error values automatically.
  - In Excel, it's much more difficult.
  - A residuals plot is a good thing to include, but there won't be points for it. Standard error also isn't worth points. Sarah will have them upload the rubric. Sarah opened the door to email her.
  - We need standard error for all 6 regressions.
- Sarah will send a source for literature values.