Virtual Spectroscopy[1]

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You will use the Integrated Spectral Database System for Organic Compounds (SDBS)[2] for this assignment. Compound numbers refer to the internal reference number for each compound on SDBS.

You have been assigned the primary compound number 2379 and five companion compounds numbered 1942, 2292, 3439, 3450 and 5702.

1. Look up the primary compound on SDBS.
2. Draw the structure (given on SDBS).
3. Print the four spectra: MS, IR, ^{1}H NMR and ^{13}C NMR.
4. For each companion compound:
   a) Look up the compound on SDBS.
   b) Identify structural features that would be expected to spectroscopically distinguish the companion compound from your primary compound. For example, the companion may have a carbonyl group where the primary does not.
   c) View the spectra of the companion compound. Choose one distinguishing spectroscopic feature, and write a brief explanation of how that feature is inconsistent with the structure of your primary compound. You are expected to choose a feature that would convincingly differentiate the companion from the primary compound. For this reason, it is most likely that you will need to use several different spectroscopies for your different compounds. See the examples below.

      Example. The IR of compound #2428 1,4-benzodioxane shows no peak in the carbonyl region 1680-1740 cm^{-1}. My compound #1725 benzyl formate has a C=O group which absorbs strongly at 1725 cm^{-1}.

      Example. The ^{1}H NMR of compound #1448 *para*-toluic acid has a methyl group at δ = 2.375. My compound does not have a methyl group and shows no peaks in that region.

      Example. The MS of compound #725 methyl benzoate shows the base peak at 105, which is 31 mass units from the molecular ion peak at 136. This corresponds to loss of a methoxy group. My compound does not have any methoxy groups and shows only a small peak at 105.[3]

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[1] Kandel, M.; Tonge, P.J. *J. Chem. Ed.* **2001**, *78*, 1208-1209.

[2] http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/cre_index.cgi, maintained by the Japanese National Institute of Materials and Chemical Research.

[3] Lest you think this is an easy way out, be advised that all your compounds are constitutional isomers!