

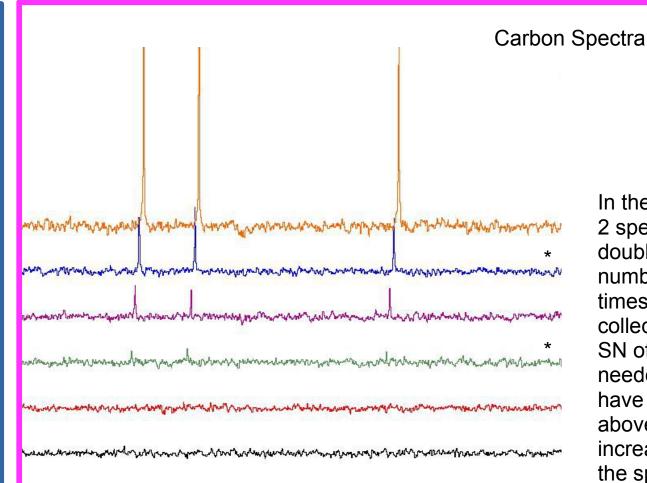
Above: Overlay of 1H spectra of 2-Ethyl-1-Indanone increasing from 4mM to 128mM by factors of 2. Expanded to show signal-to-noise, and scaled to solvent peak.

| ·  |                             |        |        |  |
|--|-----------------------------|--------|--------|--|
| Variable Name  | Variable<br>(Bruker/Varian) | Proton | Carbon |  |
| Number of Scans  | ns/nt                       | 16     | 256    |  |
| Relaxation Delay<br>(sec)  | d1/d1                       | 1      | 3      |  |
| Aquisition Time (sec)  | aq/at                       | 3.99   | 1.37   |  |
| Sweep Width (ppm)  | sw/sw*                      | 20.48  | 236.58 |  |
| Spectral Center<br>(ppm)   | o1p/tof*                    | 6.17   | 100    |  |
| Standard Paramters Used. * Varian parameters are in Hz by default to put them in ppm put a p at the end of the command line entry ie. sw=100p. |                             |        |        |  |

Below: Overlay of 1H spectra of 2-Ethyl-1-Indanone increasing from 4mM to 128mM by factors of 2. Expanded to show noise, and scaled to methylene peak.

1H Spectra of 2-Ethyl-1-Indanone in decreasing concentration. Acquired with standard 1H paramters on Waltz. Spectra scaled to solvent peak (\*).

## Signal-to-Noise versus Concentration



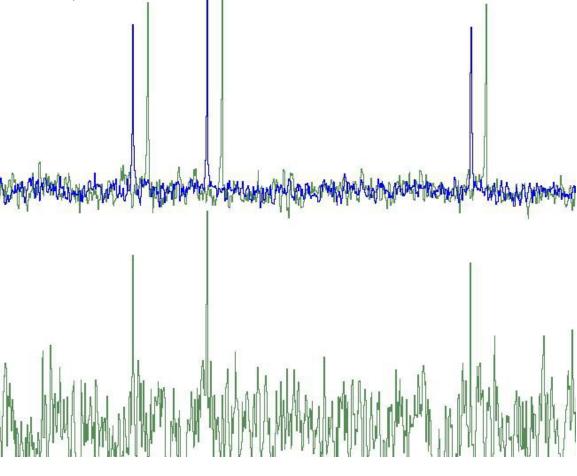
Above: Overlay of 13C spectra of 2-Ethyl-1-Indanone increasing from 4mM to 128mM by factors of 2. Expanded to show signal-to-noise, and scaled to solvent peak.

| # of<br>Scans | Time<br>(hrs)                                  |
|---------------|--|
| 256           | 0.32   |
| 1024          | 1.26   |
| 4096          | 5.01   |
| 16384         | 20.03  |
| 65536         | 80.10  |
| 262144        | 320.40   |
|               | Scans<br>256<br>1024<br>4096<br>16384<br>65536 |

Table: This table shows the number of scans required to get the same signal to noise that standard sample has in 256 scans. It is easy to see that the time it takes to improve the spectral SN quickly becomes very large.

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In the Figure to the left the \*'s indicate the 2 spectra of interest. To theoretically double the SN ratio of a spectra the number of scans needs to be increased 4 times. Each of these spectra were collected for 256 scans, so to double the SN of the green spectra 1024 scans are needed. This would make the spectra have a SN similar to the purple one right above it. If the number of scans is increase, by 4 times again, to 4096 scans the specta would now be similar to the blue spectra. This is demonstrated in the Figure Below.



Left: Overlay of 13C spectra of 2-Ethyl-1-Indanone increasing from 16mM to 128mM by factors of 2. Expanded to show noise, and scaled to methylene peak. 4 and 8 mM excluded on account of unobserved signals.