## General approach for structure determination:

### *How to assign structure when all the required spectral data are provided?*

1. Molecular formula from MS: If odd mass, may be odd no of nitrogen is present
   Calculate DBE
2. From IR find out the important functional groups present (e.g., carbonyl, alcohol, aldehyde, alkyne, NH, Cyanide etc.
3. From $^{13}C$ NMR: Find out how many carbon signal are present in the spectra. Then subtract it from total no of carbon present in the molecular formula to get how many symmetrical carbons present. In a crude way, relative intensity of the $^{13}C$-signals will also provide you information to identify symmetrical carbon signals present in the spectra (especially if comparison is made over similar type of $^{13}C$ nuclei, i.e., CH, $CH_2$, $CH_3$, C).
4. From DEPT: Identify how many quaternary, CH, $CH_2$ and $CH_3$ carbon are present.
5. Find out how many aliphatic, aromatic, etc $^{1}H$ nuclei are present in the molecule.
6. Fit all data to propose a structure. If you think it is not matching, then try to alter and repeat the procedure of correlating all the data with the structure.
7. For more complex structure, COSY, HMQC, HMBC, NOE data need to match if they are provided.