**Table S1.** Commonly used IR and Raman spectroscopy spectral regions for protein structure analysis *.

| **Spectral Region ($cm^{-1}$)** | **Notes** | **Application** |
|---|---|---|
| Amide I (~1700-1600) | Mainly CO stretching vibrations<br>Strong signals in both IR and Raman. | Primarily used to obtain backbone structure information, hardly influenced by the nature of side chains. Reveals prevalence of α-helices, β-sheets, disordered regions and turns. Raman excels in aqueous samples due to the weak water absorption in this region. |
| Amide II (~1600-1500) | Mainly a combination of NH bending and CN stretching.<br>Weaker signals observed in Raman vs IR. | Limited secondary structure information compared to Amide I. Minimally affected by the nature of side chains. |
| Amide III (~1400-1200) | Mainly a combination of NH bending and CN stretching.<br>Stronger signals observed in Raman vs IR. | Greater influence by the side chain environment compared to Amide I and Amide II regions. Provides complementary structural information. |
| Skeletal (~950-900) | Backbone CC stretching.<br>Skeletal vibrations prominent in Raman. | Provides complementary information on α-helix identification. |
| Disulphide bond (~550-500) | SS stretch very weak in IR, strong in Raman | Information on tertiary structure and folding. |
| Side Chains (~1000-1600) | Aromatic residue signal weak in IR, but strong in Raman due to high polarisability. | Information on tertiary structure and folding. Raman can provide information on Tyr, Trp and Phe environment. |

*Top-level summary table compiled using information from [45–48,68–70].

**Supplementary Figure S1**

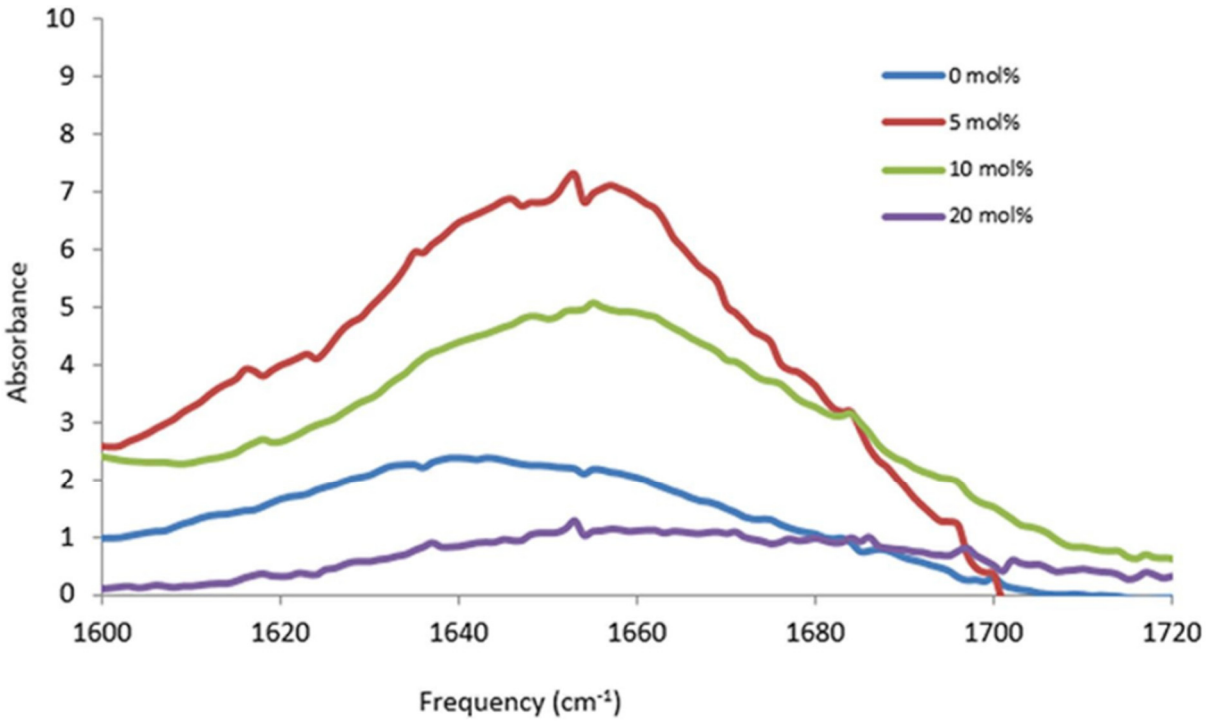


**Figure S1.** Amide I region of FTIR spectra of α-amylase in aqueous solutions of 0, 5, 10 and 20 mol% of ethylammonium nitrate, showing progressive changes in secondary structure. Reproduced from [44] under Creative Commons Attribution License (CC BY). Copyright © 2019 Arunkumar, Drummond and Greaves.

**Supplementary Figure S2**

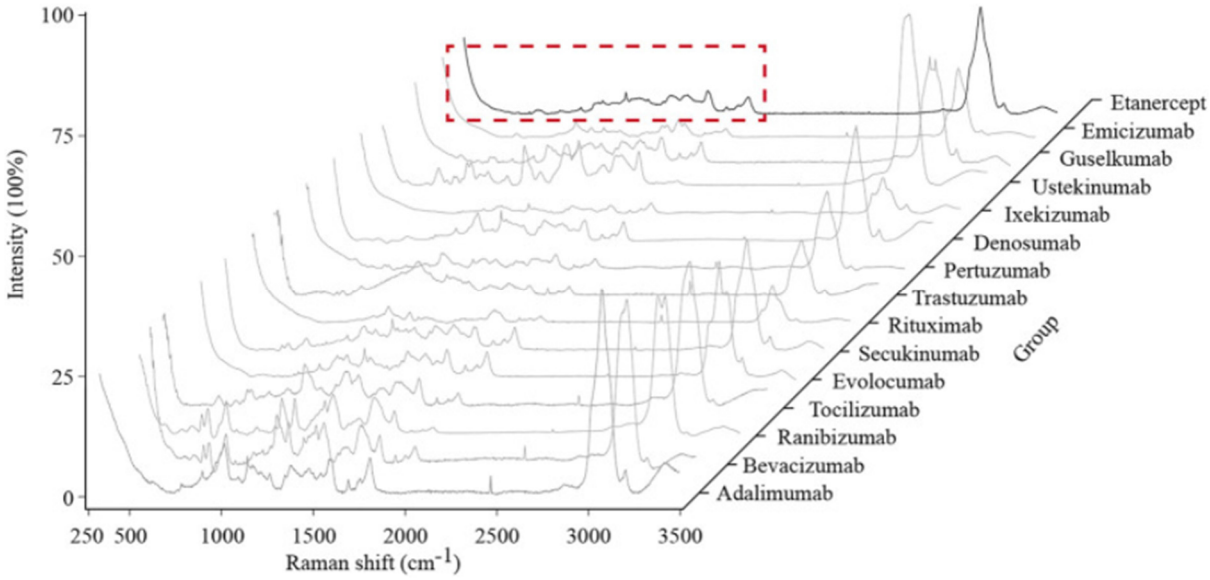


**Figure S2.** Raman spectra of 15 therapeutic monoclonal antibodies, with the characteristic spectral region highlighted by a red dashed box. Reproduced from [89] under Creative Commons Attribution License (CC BY). Copyright © 2022 Ling, Zheng, Xu, Chen, Wang, Mao and Shao.