Ring vibrations to sense anionic Ibuprofen in aqueous solution as revealed by Resonance Raman

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Supplementary Material

Contents

1 Clustering Methodology
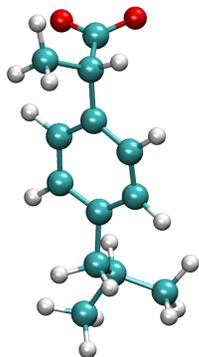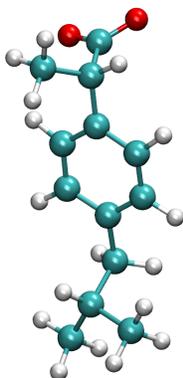
Ibu1 (47%) **Ibu2 (34%)** **Ibu3 (10%)** **Ibu4 (8%)**
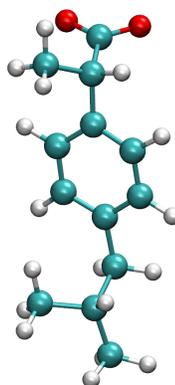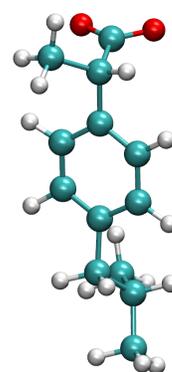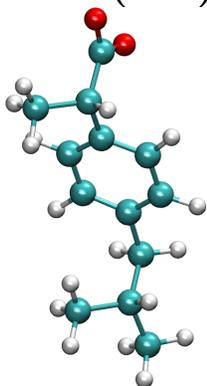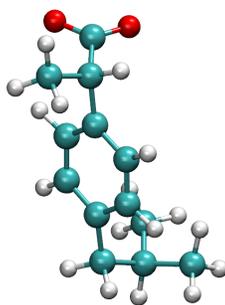
**Ibu5 (1%)** **Ibu6 (≈0%)** **Ibu7 (≈0%)**
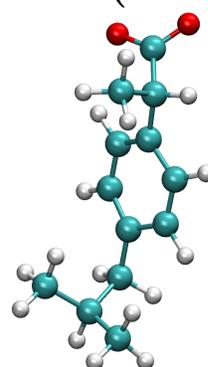
Figure S1: The 7 most populated conformers obtained from a 30 ns MD simulation of a anionic Ibuprofen in aqueous solution at 298 K; clustering performed with a 0.13 nm cut-off with the GROMOS method.
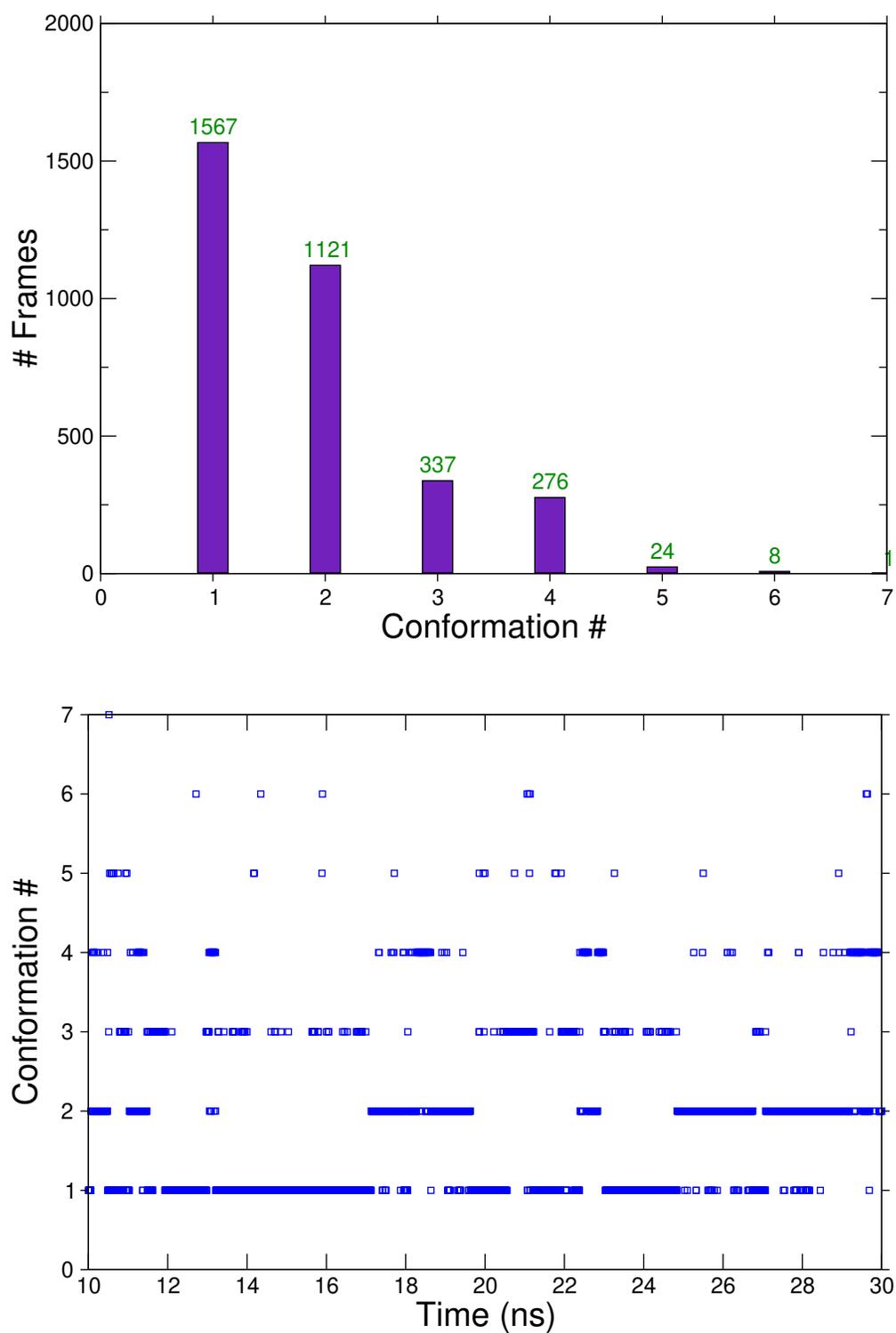
Figure S2: Top panel: Number of frames exhibiting a similar conformation of Ibu$^-$. Bottom panel: the occurrence along the MD simulation of the seven most populated structures. The corresponding conformations are displayed in Figure S1.

2 Additional plots regarding UV-Vis
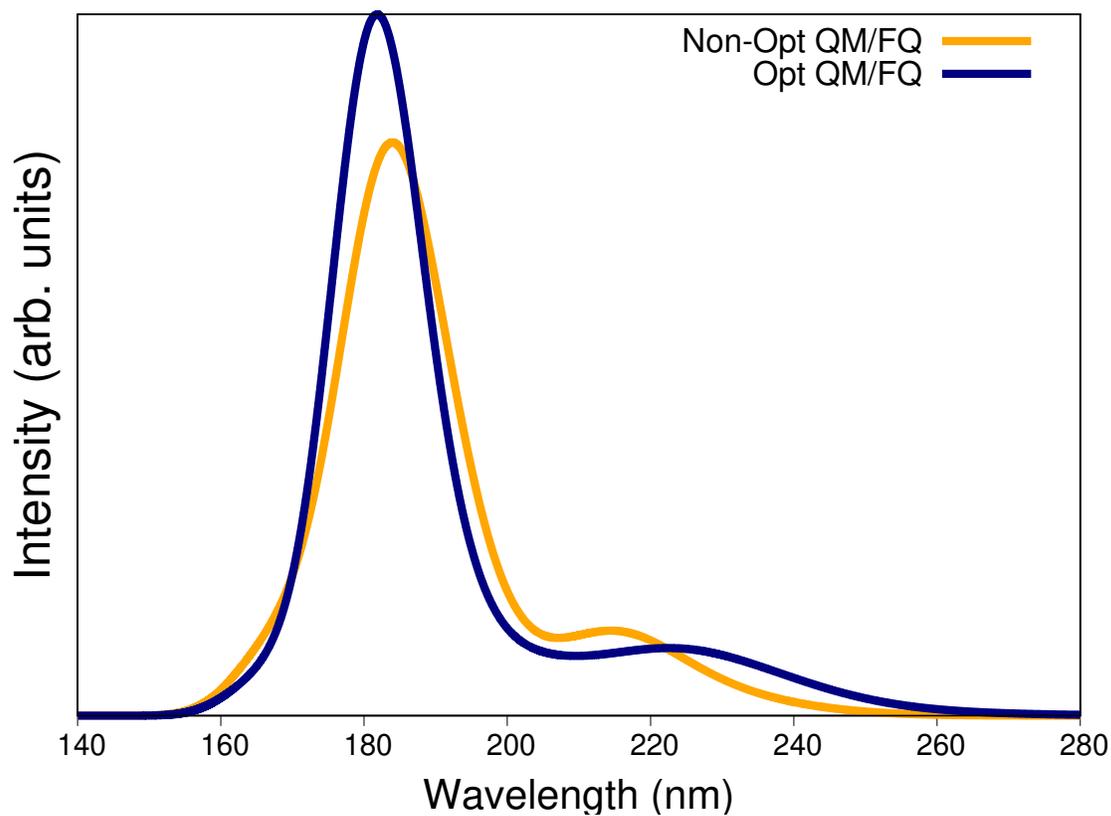
Figure S3: Effect of the optimization on the final UV–Vis spectra of anionic Ibuprofen in water. 200 structures were optimized at the QM/FQ level, with B3LYP/6–311++G(d, p) and then the absorption spectra were calculated in the TD–DFT framework.

3   Additional plots regarding RR
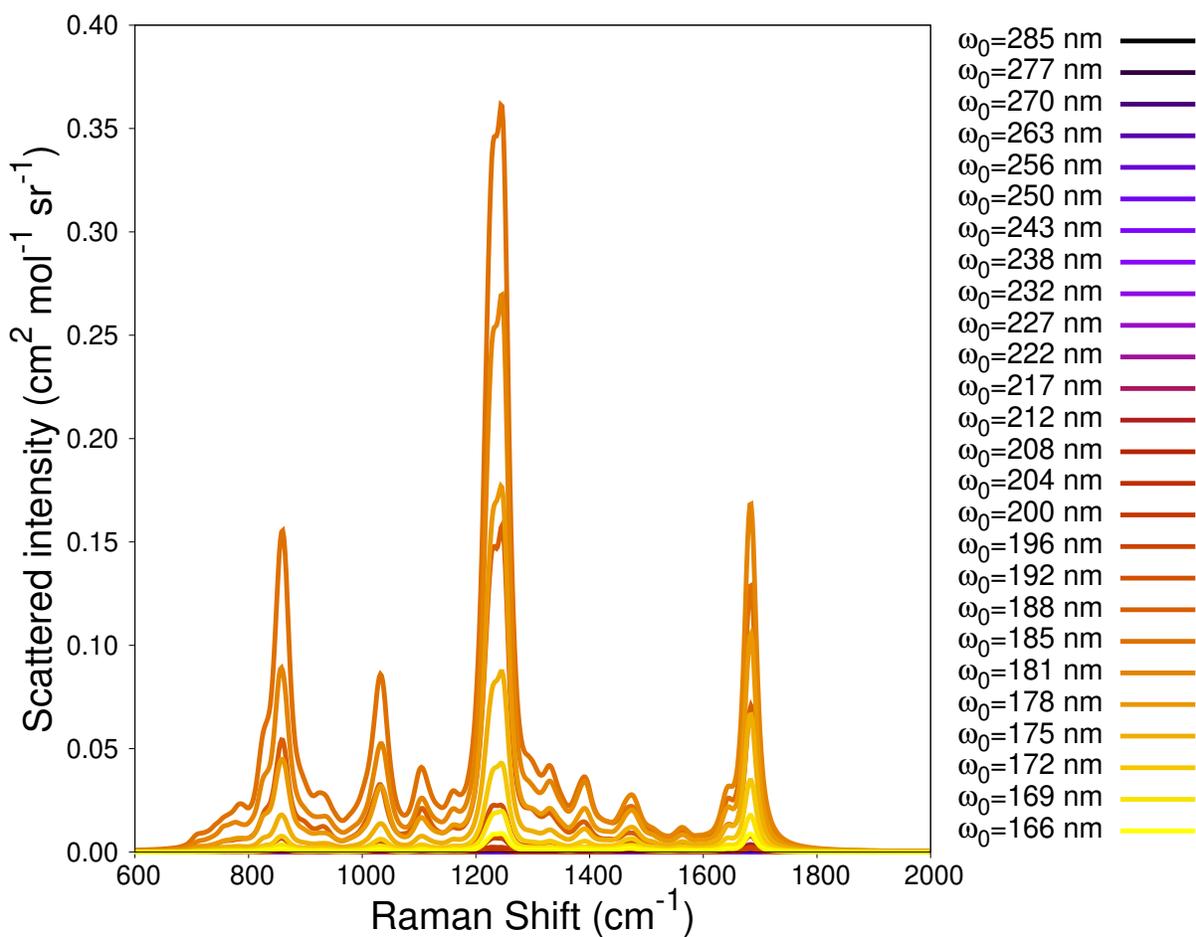
Figure S4: Resonance Raman spectra of anionic Ibuprofen in water, computed at different incident wavelengths.
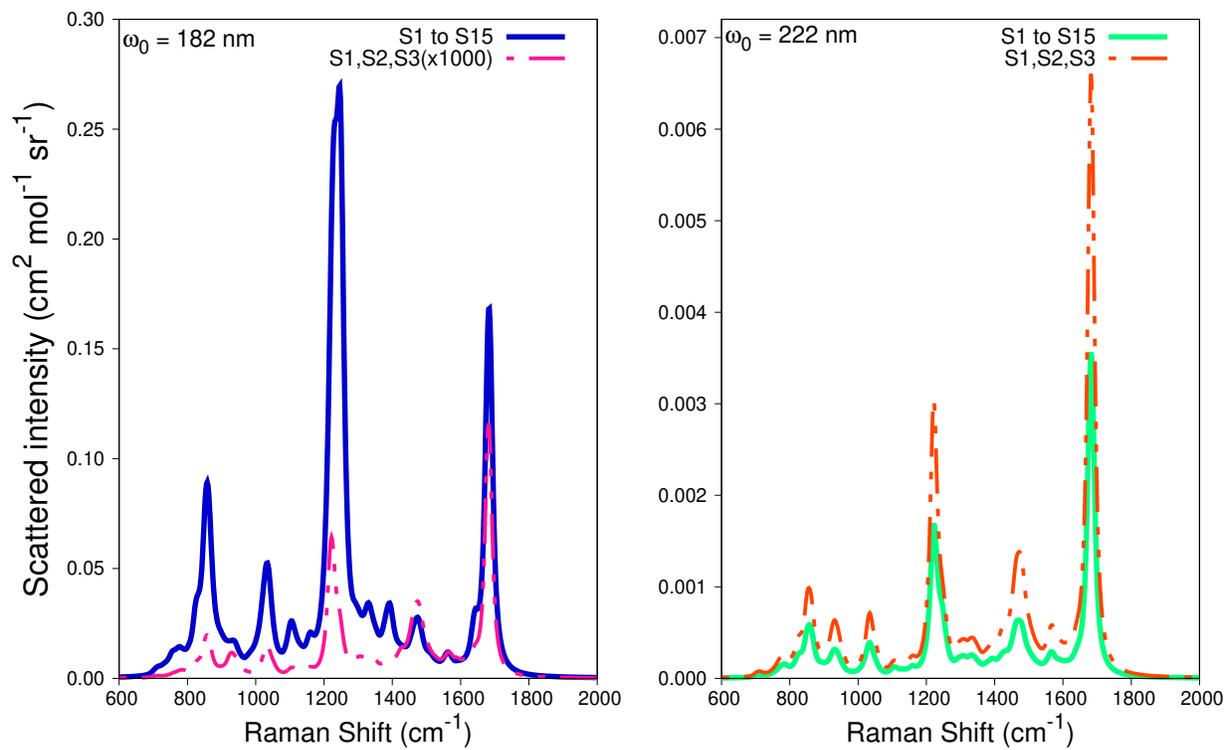
Figure S5: Effect of specific excited states on the selectivity and intensity seen in Resonance Raman spectra of anionic Ibuprofen in aqueous solution.

4 Convergence plots
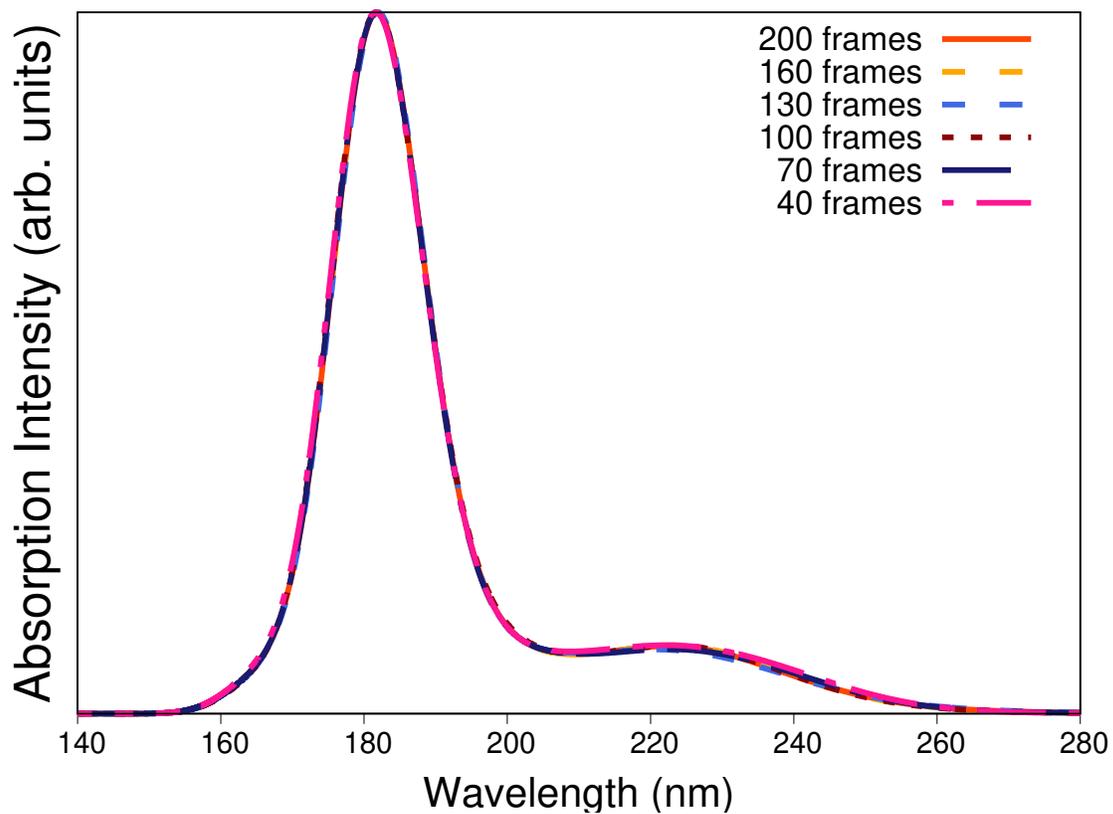
Figure S6: Comparison between the QM/FQ absorption spectra of anionic Ibuprofen in aqueous solution obtained by averaging an increasing number of snapshots.
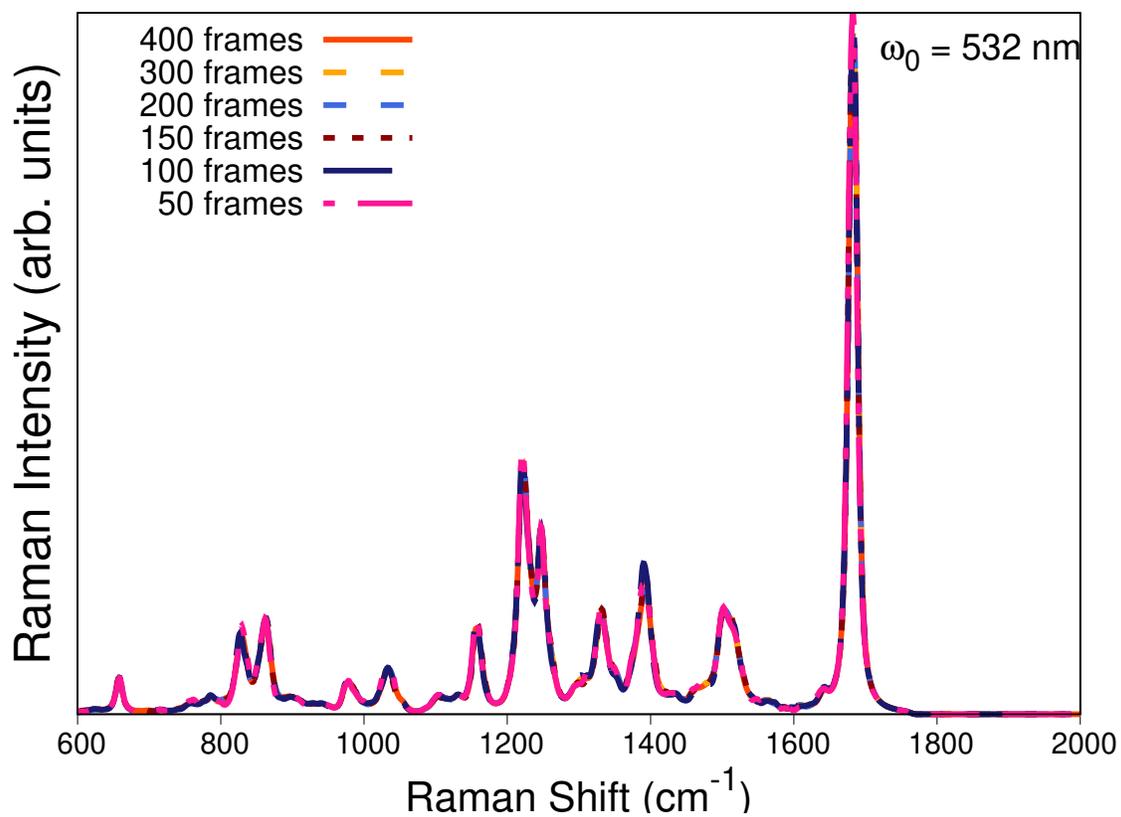
Figure S7: Comparison between the QM/FQ Raman spectra of anionic Ibuprofen in aqueous solution obtained by averaging an increasing number of snapshots.
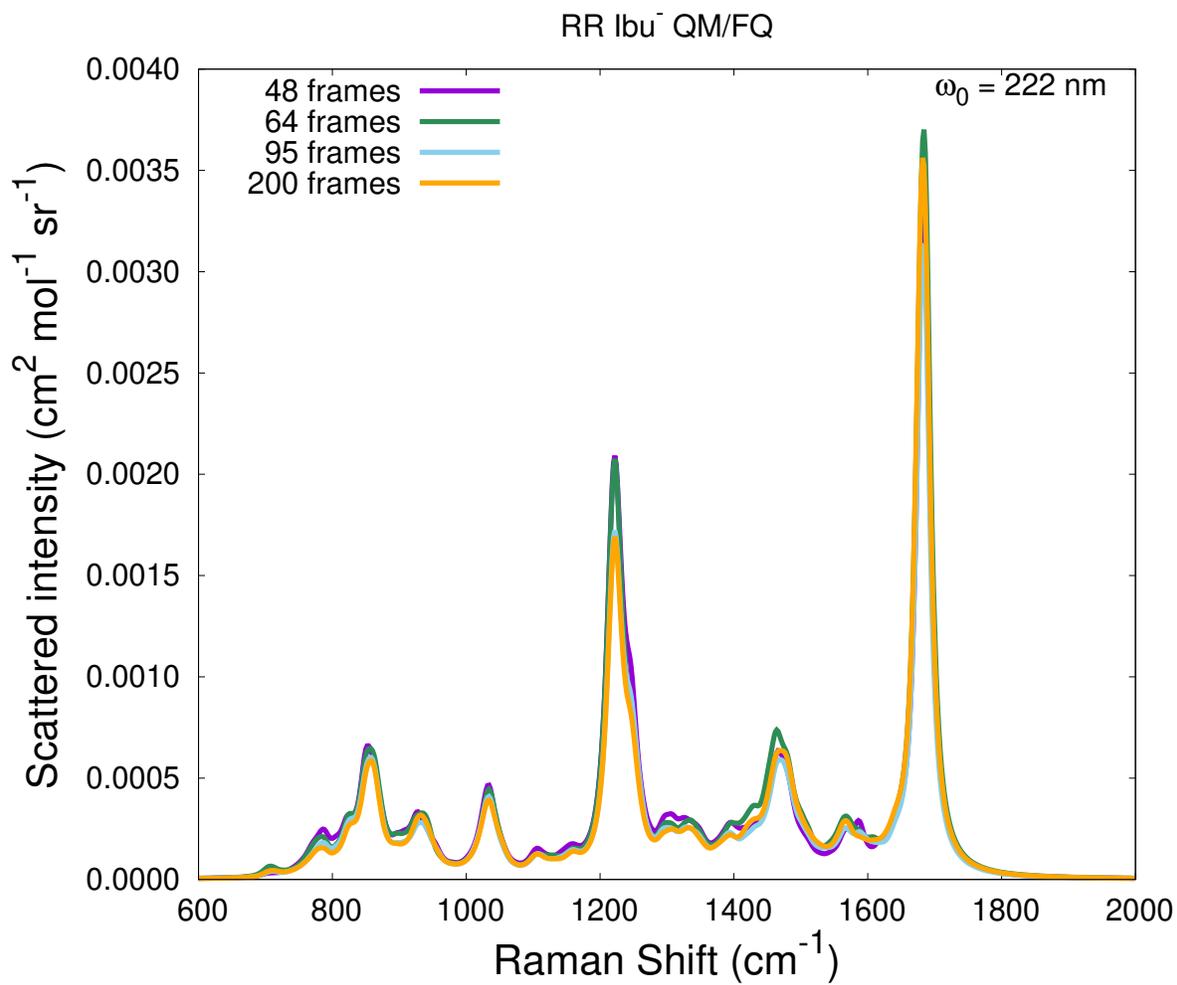
Figure S8: Comparison between the QM/FQ Resonance Raman spectra of anionic Ibuprofen in aqueous solution obtained by averaging an increasing number of snapshots.