

Appendix A. Supplementary Material

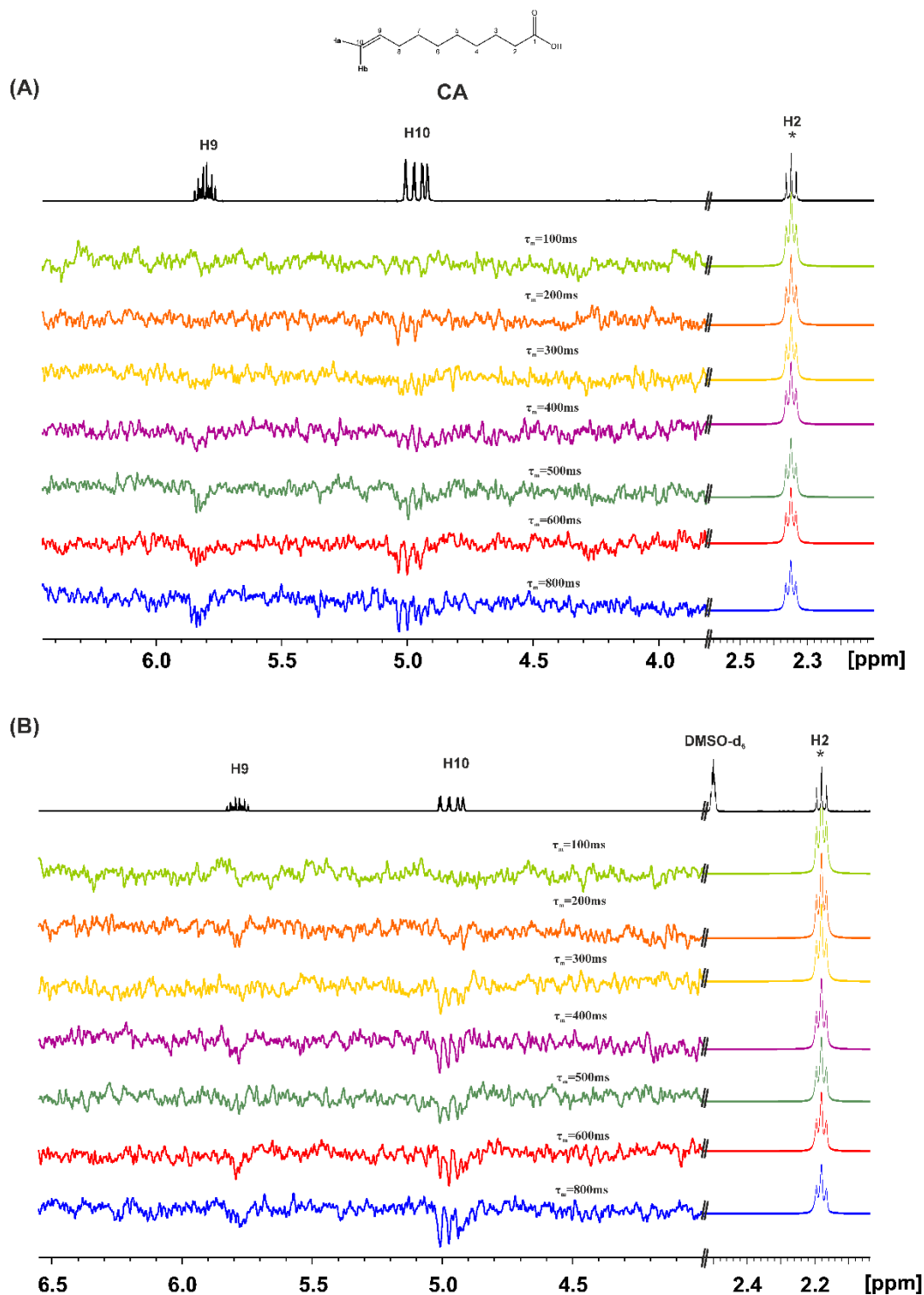


Figure S1. 1D transient NOE (500 MHz) NMR spectra of caproic acid (CA), $c = 20$ mM in CDCl₃ solution (A) and $c = 20$ mM in DMSO-d₆ solution (B) (number of scans=512, $T=298$ K, $T_{\text{acq}}=4.09$ s, relaxation delay=4s) using various mixing times (τ_m). The excited α -CH₂ group (denoted with the asterisk (*)), is reduced by a factor of 30, relative to the amplitude of the NOE signals in the region up to 5.9 ppm.

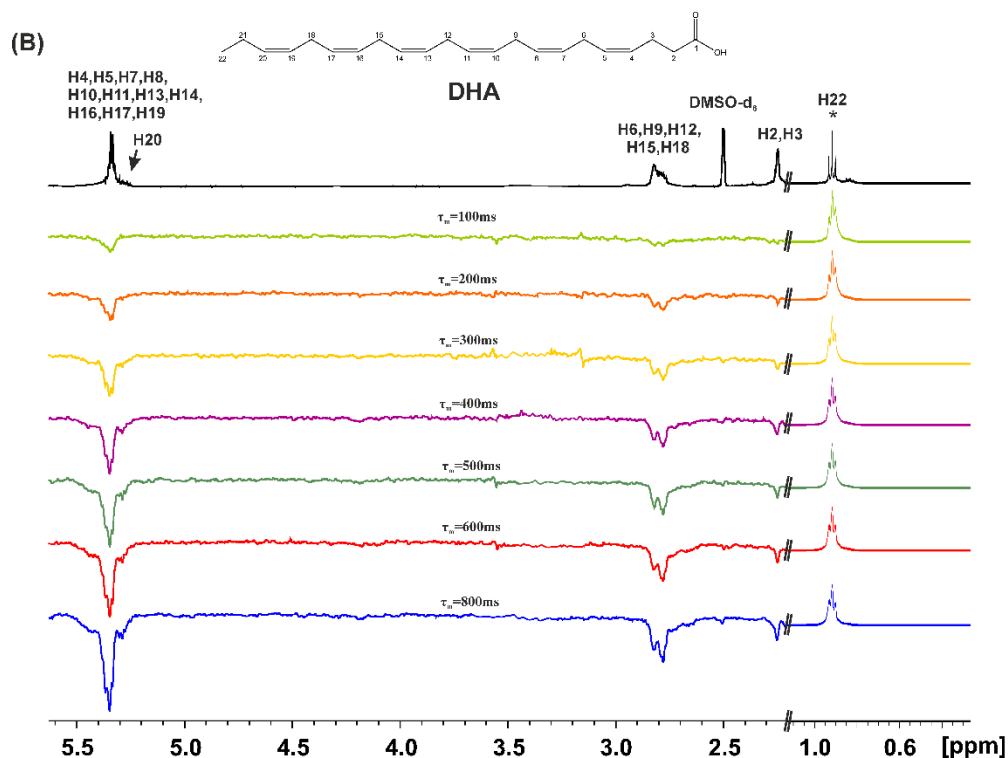
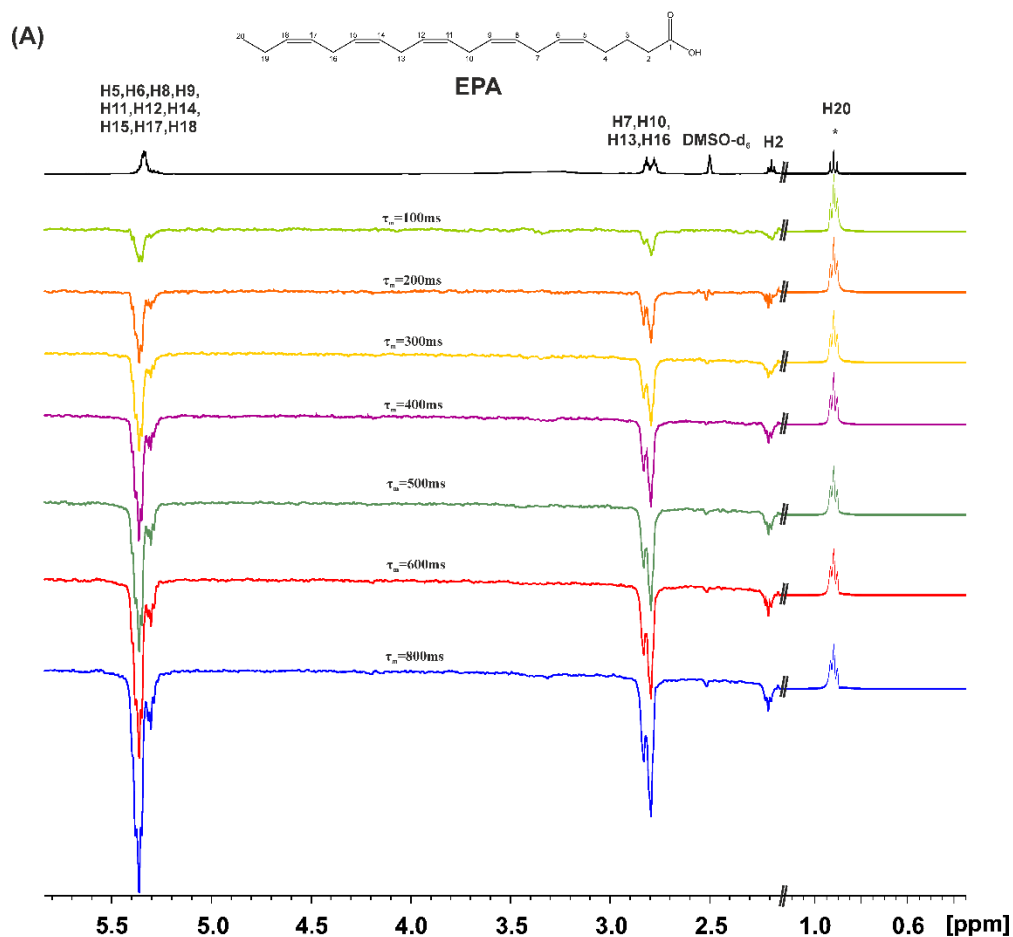


Figure S2. 1D transient NOE NMR spectra of: (A) EPA and (B) DHA, concentration = 20 mM in DMSO- d_6 at 298 K (number of scans = 512, T_{acq} =4.09s, relaxation delay=4s), using various τ_m values. The amplitude of the excited CH_3 - group (denoted with the asterisk (*)), is reduced by a factor of 30, relative to the amplitude of the rest of the NOE signals.

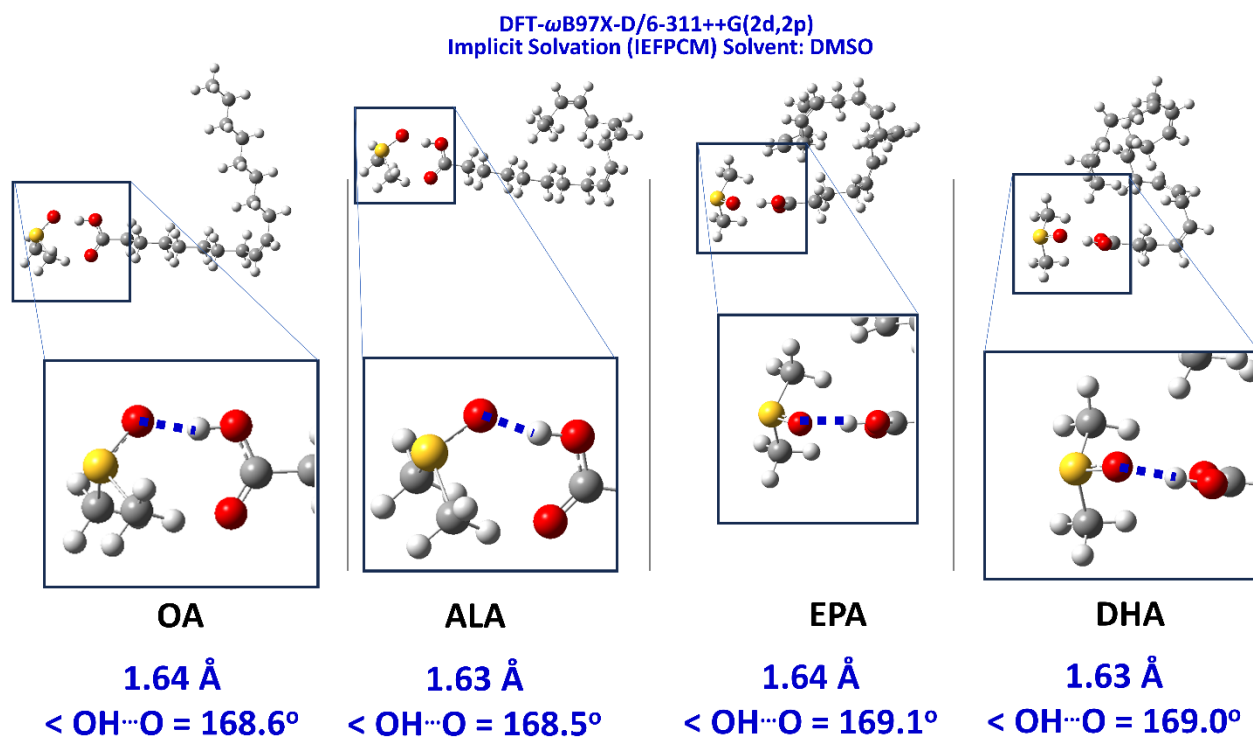


Figure S3. Optimized structures of oleic acid (OA), α -linolenic acid (ALA), EPA and DHA with a discrete solvation molecule of DMSO on the carboxylic group.