**Appendix A. Supplementary Material**



**Figure S1**. 1D transient NOE (500 MHz) NMR spectra of caproleic acid (CA), c = 20 mM in CDCl3 solution (A) and c = 20 mM in DMSO-d6 solution (B) (number of scans=512, T=298K, Tacq=4.09s, relaxation delay=4s) using various mixing times (τm). 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**. Optimized structure of α-linolenic acid (ALA) with a discrete solvation molecule of DMSO on the carboxylic group.