

Abstract Submitted  
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**The Effect of *Trans* Unsaturation on Molecular Organization in a Phospholipid Membrane** SMITA SONI, IUPUI1, JENNIFFER RUNYAN, GARRISON BRICH, IUPUI2, JESSE WARD, Wabash, STEPHANIE SEN, IUPUI2, SCOTT FELLER, Wabash, STEPHEN WASSALL, IUPUI1 — The ingestion of *trans* fatty acids (TFA) formed during the partial hydrogenation of vegetable oils has been linked to a detrimental impact on health by an, as yet, unknown mechanism. We synthesized deuterated analogs of 1-elaidoyl-2-stearoylphosphatidylcholine (*t*18:1-18:0PC) that contains a single “unnatural” *trans* double bond and 1-oleoyl-2-stearoylphosphatidylcholine (*c*18:1-18:0PC) that contains a single “natural” *cis* double bond. Solid state  $^2\text{H}$  NMR spectra for model membranes prepared from these phospholipids reveal a higher chain melting temperature for the *trans* isomer, indicating tighter molecular packing in the gel state. In the liquid crystalline, however, the difference between the *trans* and *cis* isomers is subtle. Order as probed by the perdeuterated  $[\text{}^2\text{H}_{31}]18:0$  *sn*-2 chain, and corroborated by molecular dynamics (MD) simulation, coincides within <5%.

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