

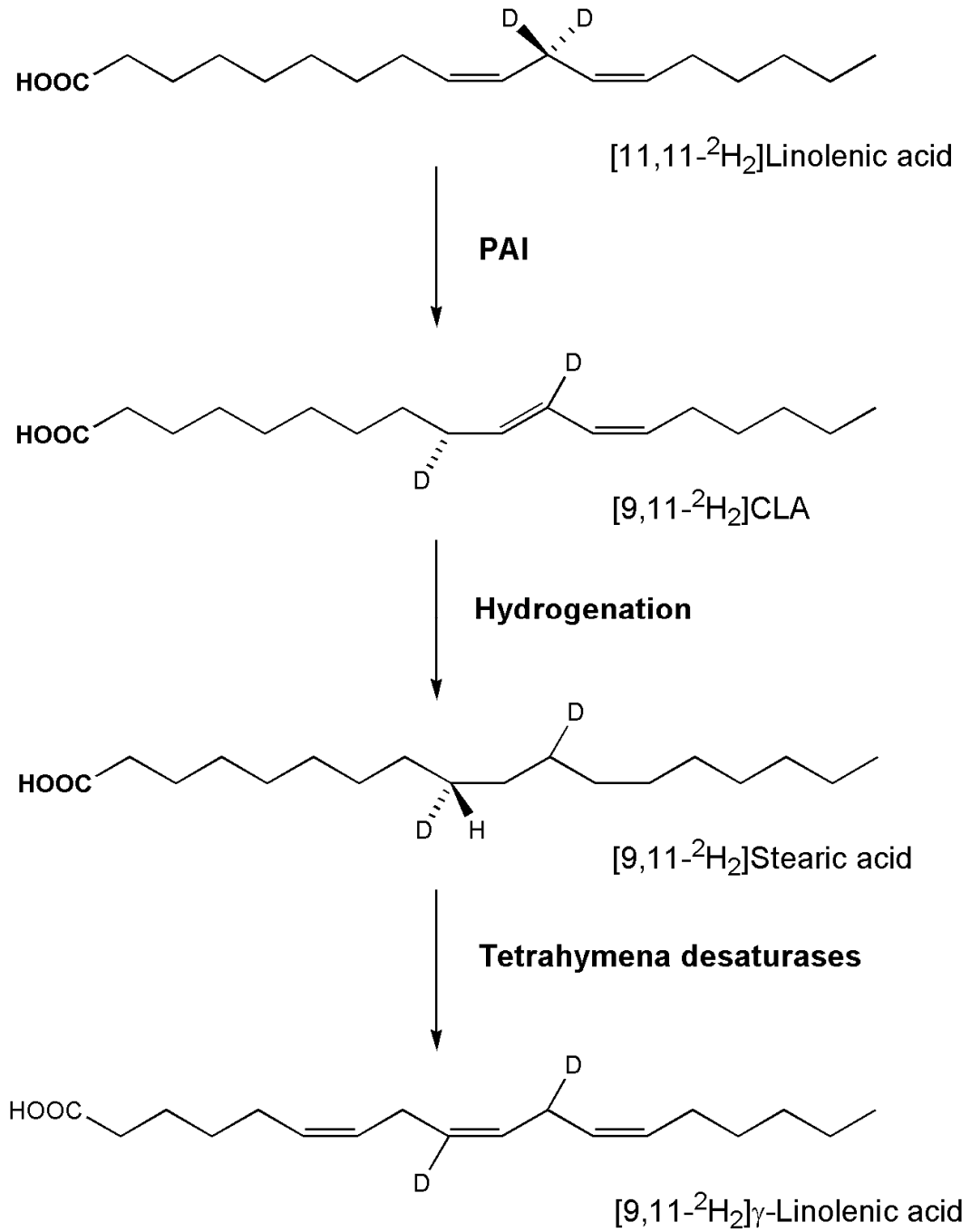
Supplemental Figure 1. Scheme explaining the experimental strategy to identify the absolute configuration of the hydrogen atom at C-9.

Supplemental Figure 2. Absorption spectra of WT PAI (red) and Phe-168-Ile mutant (black). The spectra shown are representative for all mutants analyzed.

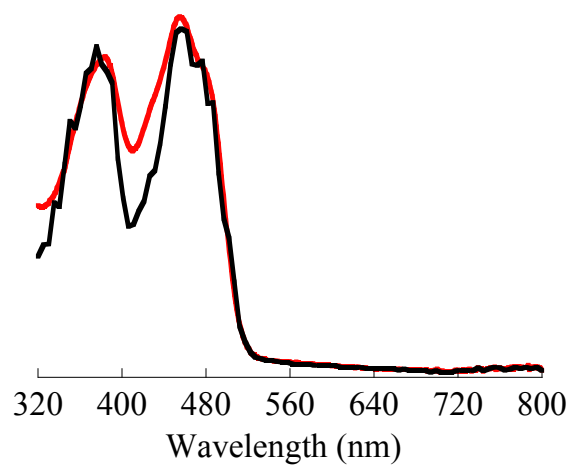
Supplemental Figure 3. Pulse EPR spectra of PAI with LA recorded at X-Band for freeze quenching the sample at 23 s, 60 s and 120 s after mixing. A reference spectrum of an empty EPR tube is also shown and the expected signal position for $g = 2.0023$ is indicated by a dashed line. No change in the EPR signal is observed. Similar results were obtained in CW modus using deuterated substrate.

Experimental conditions: All spectra were measured at a temperature of 20 K using a Hahn-Echo pulse sequence of 12 ns - 136 ns - 24 ns at 4 dB TWT attenuation and a receiver gain of 60 dB over a field range of 1000 G.

SUPPLEMENTAL FIGURE 1



SUPPLEMENTAL FIGURE 2



SUPPLEMENTAL FIGURE 3

