Kinetic simulation results with the final detailed model for n-heptane developed in this work

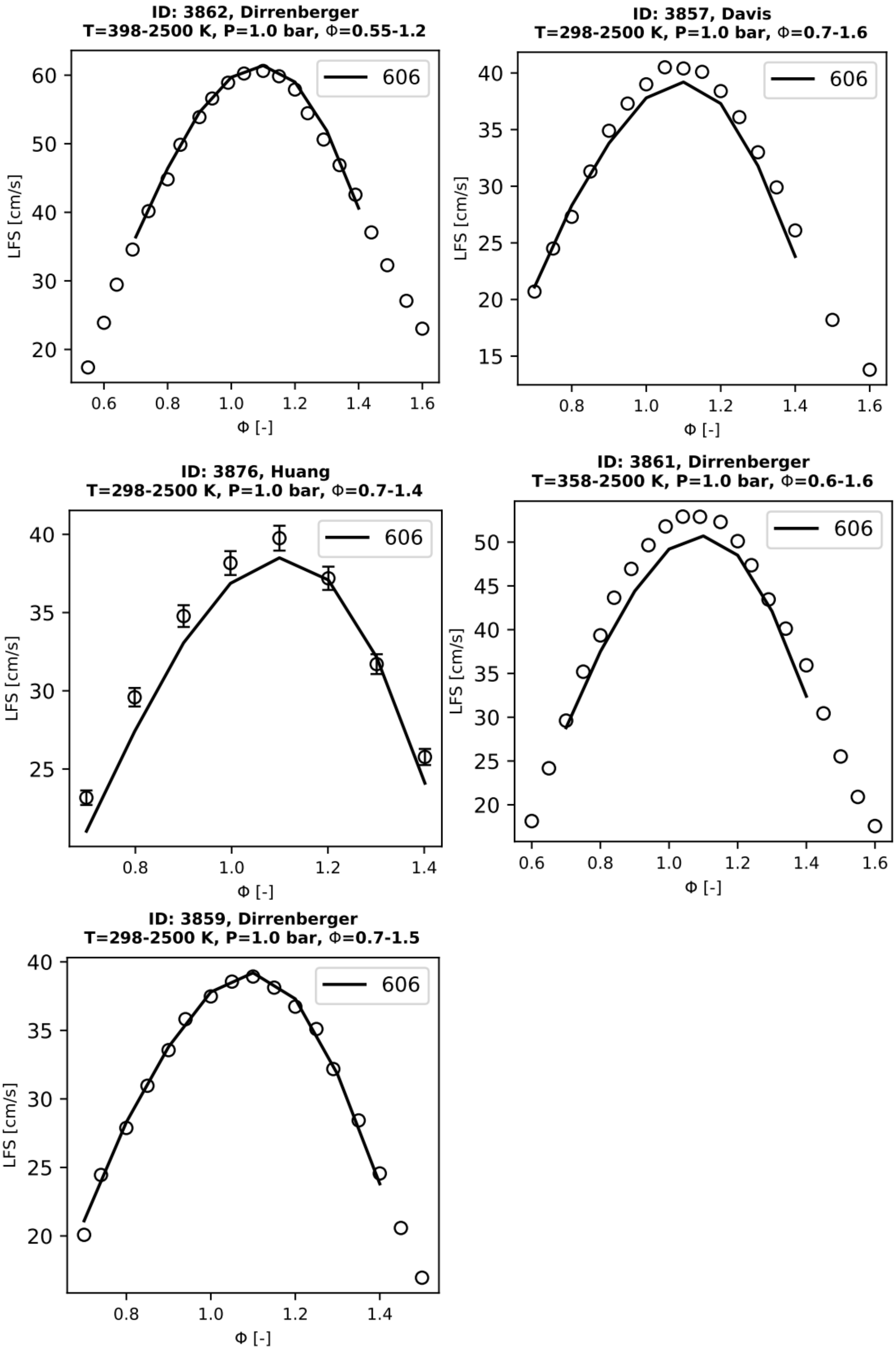


Figure S1: Simulated (solid line) and experimental (empty symbols, from [1,2]*) laminar burning velocities of n-heptane measured at different operating conditions (see plot titles for details).*

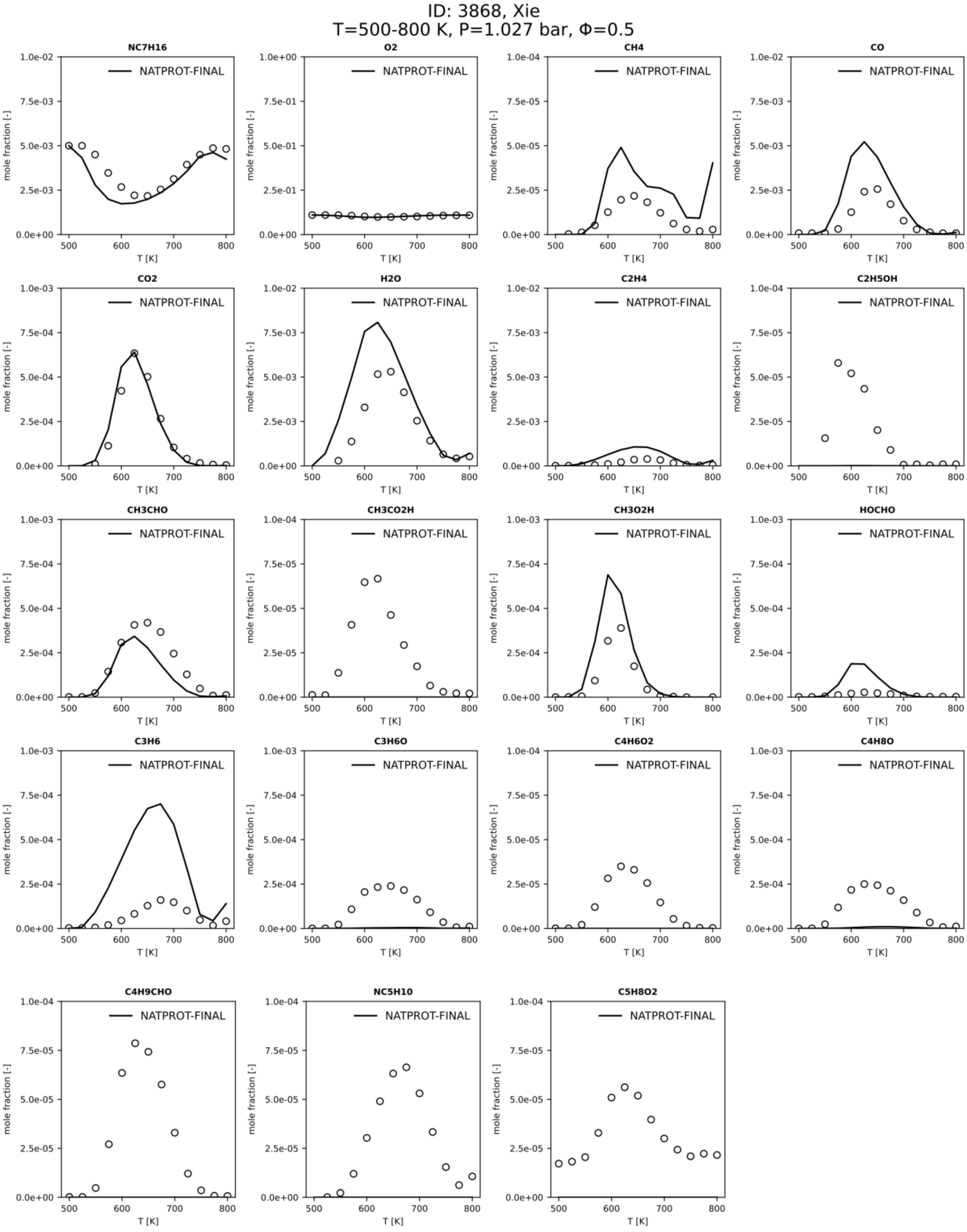
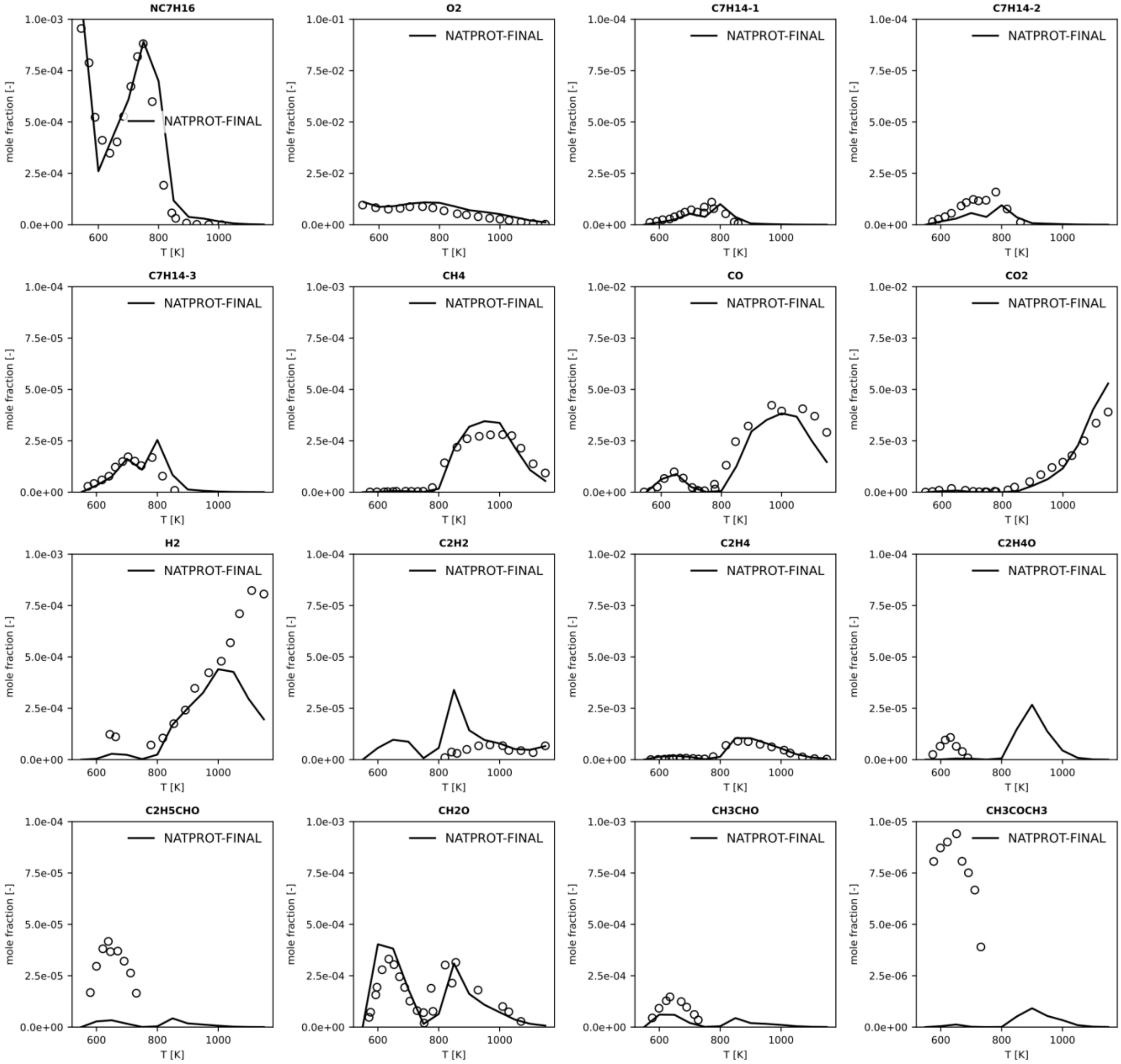


Figure S2: Simulated (solid line) and experimental (empty symbols) speciation profiles in the JSR experiments of n-heptane oxidation of Xie et al. [3]. *Detailed experimental conditions are reported in the figure title.*

ID: 3877, Dagaut
T=543-1150 K, P=10.133 bar, Φ=1.0



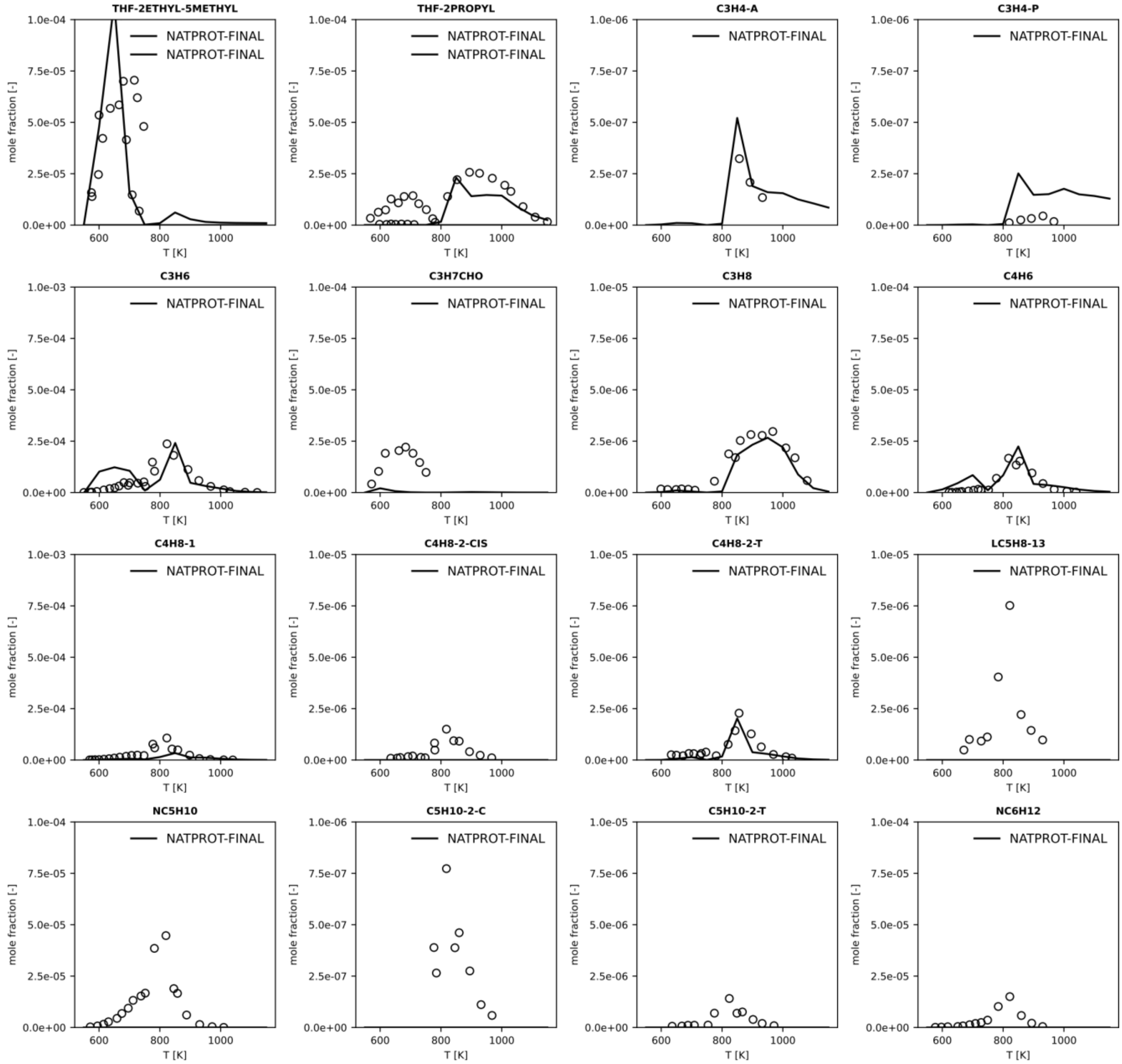


Figure S3: Simulated (solid line) and experimental (empty symbols) speciation profiles in the JSR experiments of n-heptane oxidation of Dagaut et al.[4]*. Detailed experimental conditions are reported in the figure title.*

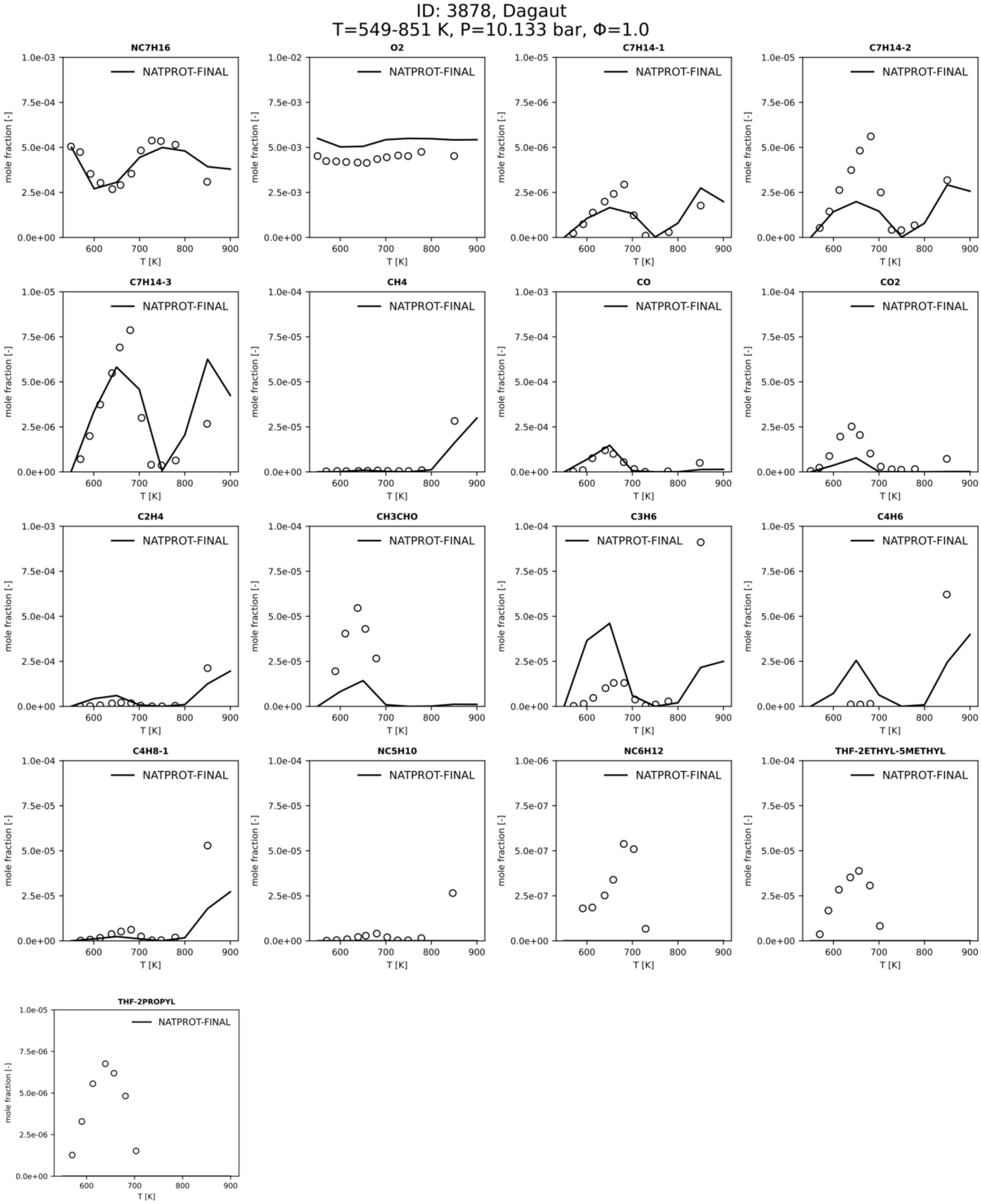
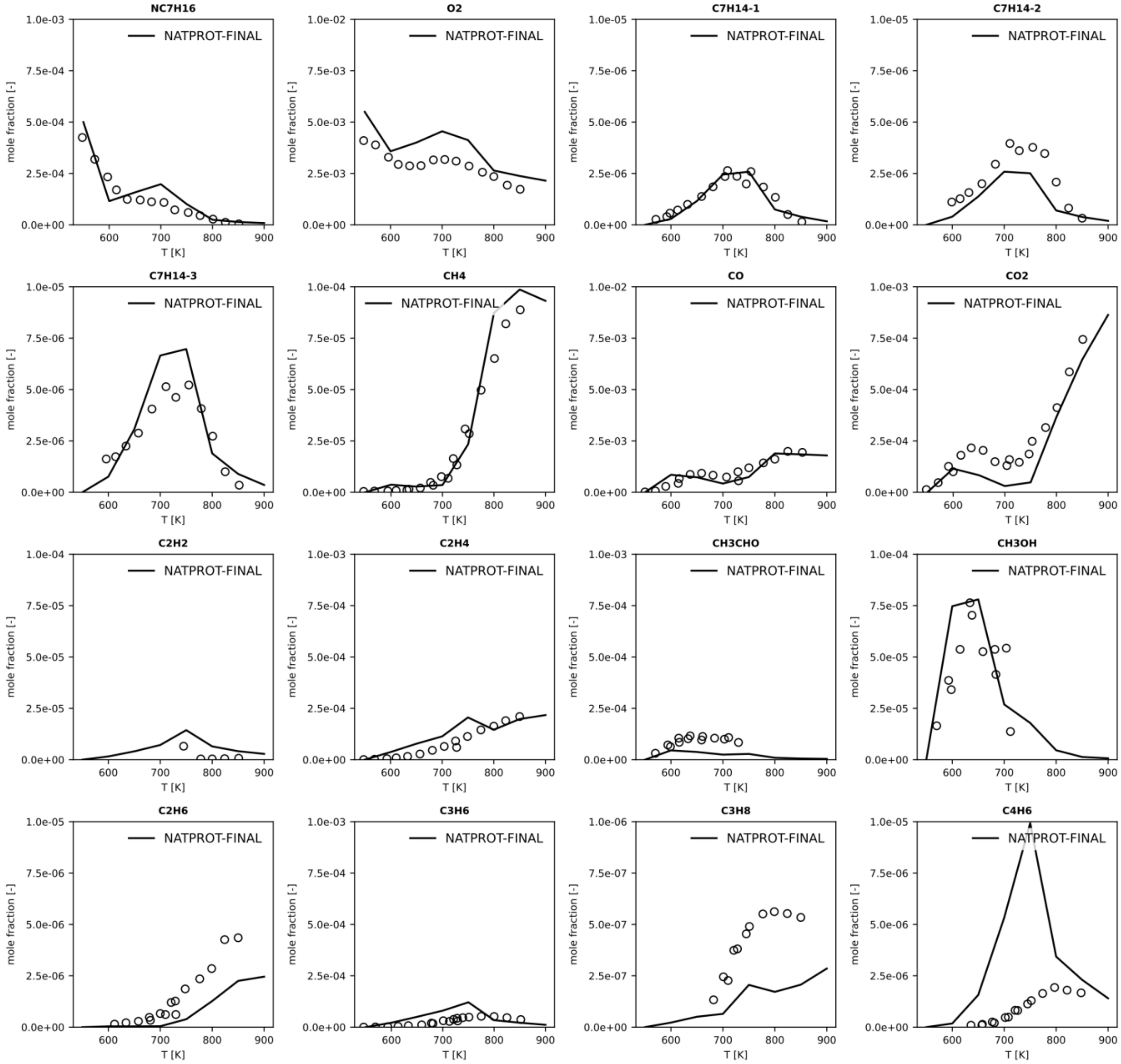


Figure S4: Simulated (solid line) and experimental (empty symbols) speciation profiles in the JSR experiments of n-heptane oxidation of Dagaut et al.[4]*. Detailed experimental conditions are reported in the figure title.*

ID: 3879, Dagaut
T=546-853 K, P=40.53 bar, Φ=1.0



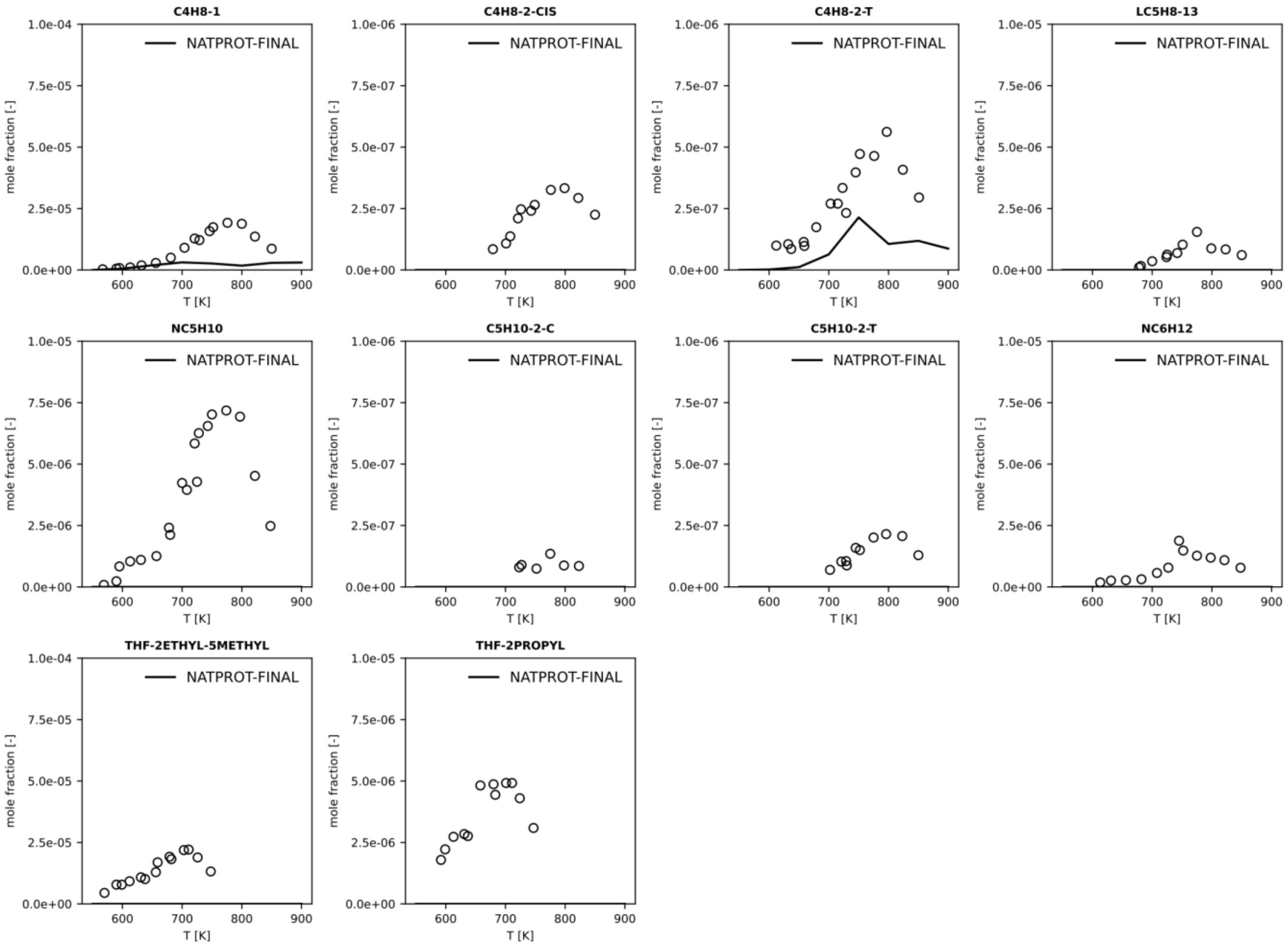


Figure S5: Simulated (solid line) and experimental (empty symbols) speciation profiles in the JSR experiments of n-heptane oxidation of Dagaut et al.[4]*. Detailed experimental conditions are reported in the figure title.*

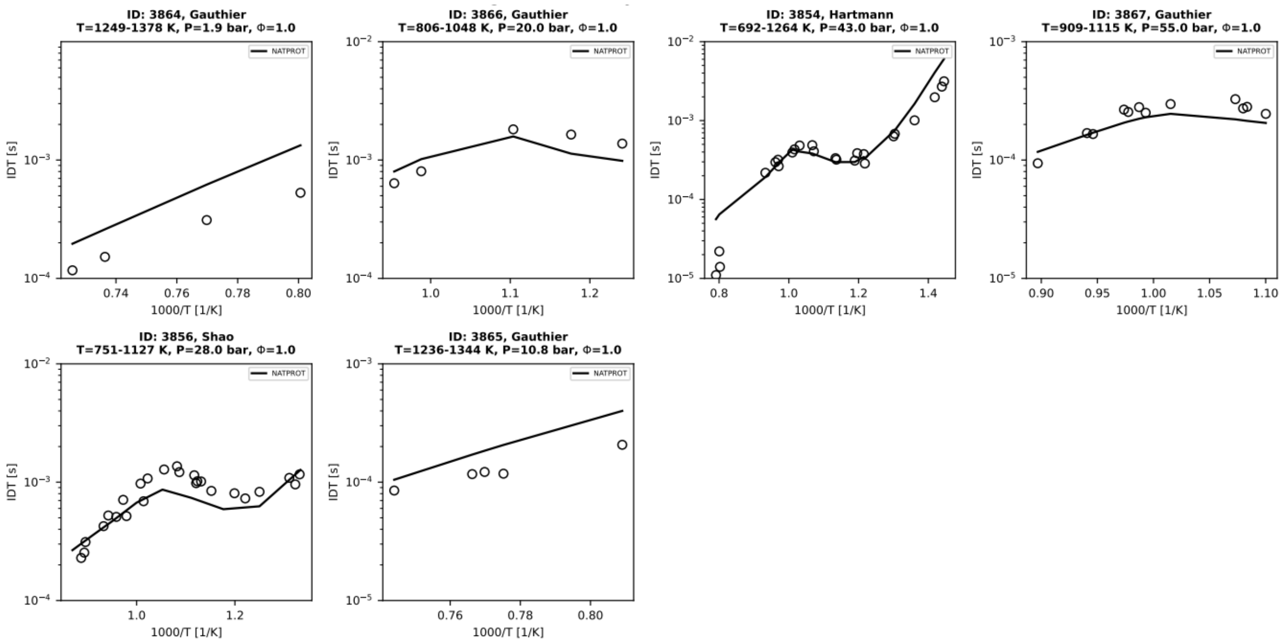


Figure S6: Simulated (solid line) and experimental (empty symbols [5–7]*) ignition delay times for n-heptane oxidation. Experimental conditions and the corresponding references are reported in the title of each plot.*

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