

Table S3 The nomenclatures, formulas, and structures of important species in the present model.

Formulas	Nomenclatures	IUPAC names	Structure	Formulas	Nomenclatures	IUPAC names	Structure
C ₇ H ₁₆ O	FUEL	<i>n</i> -Heptanol		C ₇ H ₁₅ O	FUEL1J	1-Hydroxy-1-heptyl radical	
C ₇ H ₁₅ O	FUEL2J	1-Hydroxy-2-heptyl radical		C ₇ H ₁₅ O	FUEL3J	1-Hydroxy-3-heptyl radical	
C ₇ H ₁₅ O	FUEL4J	1-Hydroxy-4-heptyl radical		C ₇ H ₁₅ O	FUEL5J	1-Hydroxy-5-heptyl radical	
C ₇ H ₁₅ O	FUEL6J	1-Hydroxy-6-heptyl radical		C ₇ H ₁₅ O	FUEL7J	1-Hydroxy-7-heptyl radical	
C ₇ H ₁₅ O	C ₇ H ₁₅ OJA	<i>n</i> -Heptyloxy radical		C ₇ H ₁₄ O	C ₆ H ₁₃ HCO	Heptanal	
C ₇ H ₁₄ O	FUEL1E	1-Hepten-1-ol		C ₇ H ₁₄ O	FUEL2E	2-Hepten-1-ol	
C ₇ H ₁₄ O	FUEL3E	3-Hepten-1-ol		C ₇ H ₁₄ O	FUEL4E	4-Hepten-1-ol	
C ₇ H ₁₄ O	FUEL5E	5-Hepten-1-ol		C ₇ H ₁₄ O	FUEL6E	6-Hepten-1-ol	
C ₇ H ₁₅ O ₂	FUEL1O ₂	Heptyl-1-ol-1-peroxyl radicals		C ₇ H ₁₅ O ₂	FUEL2O ₂	Heptyl-1-ol-2-peroxyl radicals	
C ₇ H ₁₅ O ₂	FUEL3O ₂	Heptyl-1-ol-3-peroxyl radicals		C ₇ H ₁₅ O ₂	FUEL4O ₂	Heptyl-1-ol-4-peroxyl radicals	
C ₇ H ₁₅ O ₂	FUEL5O ₂	Heptyl-1-ol-5-peroxyl radicals		C ₇ H ₁₅ O ₂	FUEL6O ₂	Heptyl-1-ol-6-peroxyl radicals	
C ₇ H ₁₅ O ₂	FUEL7O ₂	Heptyl-1-ol-7-peroxyl radicals		C ₇ H ₁₆ O ₃	FUEL1O ₂ H	1-Hydroperoxyl-heptan-1-ol-	
C ₇ H ₁₆ O ₃	FUEL2O ₂ H	2-Hydroperoxyl-heptan-1-ol-		C ₇ H ₁₆ O ₃	FUEL3O ₂ H	3-Hydroperoxyl-heptan-1-ol-	
C ₇ H ₁₆ O ₃	FUEL4O ₂ H	4-Hydroperoxyl-heptan-1-ol-		C ₇ H ₁₆ O ₃	FUEL5O ₂ H	5-Hydroperoxyl-heptan-1-ol-	
C ₇ H ₁₆ O ₃	FUEL6O ₂ H	6-Hydroperoxyl-heptan-1-ol-		C ₇ H ₁₆ O ₃	FUEL7O ₂ H	7-Hydroperoxyl-heptan-1-ol-	
C ₇ H ₁₅ O ₃	FUEL3J1O ₂ H	1-Hydroperoxyl-1-ol-hept-2-yl		C ₇ H ₁₅ O ₃	FUEL3J1O ₂ H	1-Hydroperoxyl-1-ol-hept-3-yl	

C ₇ H ₁₅ O ₃	FUEL4J2O ₂ H	1-Hydroperoxyl-1-ol-hept-4-yl		C ₇ H ₁₅ O ₃	FUEL5J2O ₂ H	1-Hydroperoxyl-1-ol-hept-5-yl	
C ₇ H ₁₅ O ₃	FUEL1J3O ₂ H	3-Hydroperoxyl-1-ol-hept-1-yl		C ₇ H ₁₅ O ₃	FUEL5J3O ₂ H	3-Hydroperoxyl-1-ol-hept-5-yl	
C ₇ H ₁₅ O ₃	FUEL6J3O ₂ H	3-Hydroperoxyl-1-ol-hept-6-yl		C ₇ H ₁₅ O ₃	FUEL1J4O ₂ H	4-Hydroperoxyl-1-ol-hept-1-yl	
C ₇ H ₁₅ O ₃	FUEL2J4O ₂ H	4-Hydroperoxyl-1-ol-hept-2-yl		C ₇ H ₁₅ O ₃	FUEL6J4O ₂ H	4-Hydroperoxyl-1-ol-hept-6-yl	
C ₇ H ₁₅ O ₃	FUEL2J5O ₂ H	5-Hydroperoxyl-1-ol-hept-2-yl		C ₇ H ₁₅ O ₃	FUEL3J5O ₂ H	5-Hydroperoxyl-1-ol-hept-3-yl	
C ₇ H ₁₅ O ₃	FUEL3J6O ₂ H	6-Hydroperoxyl-1-ol-hept-3-yl		C ₇ H ₁₅ O ₃	FUEL4J6O ₂ H	6-Hydroperoxyl-1-ol-hept-4-yl	
C ₇ H ₁₅ O ₃	FUEL4J7O ₂ H	7-Hydroperoxyl-1-ol-hept-4-yl		C ₇ H ₁₅ O ₃	FUEL5J7O ₂ H	7-Hydroperoxyl-1-ol-hept-5-yl	
C ₇ H ₁₄ O ₂	FUELCY3O1	2-Butyl-4-ol-oxetane		C ₇ H ₁₄ O ₂	FUELCY4O1	2-Propyl-5-ol-tetrahydrofuran	
C ₇ H ₁₄ O ₂	FUELCY4O2	2-Propyl-4-hydroxymethyl-oxetane		C ₇ H ₁₄ O ₂	FUELCY5O2	2-Ethyl-5-hydroxymethyl-tetrahydrofuran	
C ₇ H ₁₄ O ₂	FUELCY5O3	2-Ethyl-4-hydroxyethyl-oxetane		C ₇ H ₁₄ O ₂	FUELCY6O3	2-Methyl-5-hydroxyethyl-tetrahydrofuran	
C ₇ H ₁₄ O ₂	FUELCY6O4	2-Methyl-4-hydroxypropyl-oxetane		C ₇ H ₁₄ O ₂	FUELCY7O4	2-Hydroxypropyl-tetrahydrofuran	
C ₇ H ₁₄ O ₂	FUELCY7O5	2-Hydroxybutyl-oxetane		C ₇ H ₁₅ O ₅	FUEL1O ₂ H3O ₂	1-Hydroperoxyl-heptyl-1-ol-3-peroxyl radical	
C ₇ H ₁₅ O ₅	FUEL1O ₂ H4O ₂	1-Hydroperoxyl-heptyl-1-ol-4-peroxyl radical		C ₇ H ₁₅ O ₅	FUEL2O ₂ H4O ₂	2-Hydroperoxyl-heptyl-1-ol-4-peroxyl radical	

C ₇ H ₁₅ O ₅	FUEL2O ₂ H5O ₂	2-Hydroperoxyl-heptyl-1-ol-5-p eroxyl radical		C ₇ H ₁₅ O ₅	FUEL3O ₂ H1O ₂	3-Hydroperoxyl-heptyl-1-ol-1-p eroxyl radical	
C ₇ H ₁₅ O ₅	FUEL3O ₂ H5O ₂	3-Hydroperoxyl-heptyl-1-ol-5-p eroxyl radical		C ₇ H ₁₅ O ₅	FUEL3O ₂ H6O ₂	3-Hydroperoxyl-heptyl-1-ol-6-p eroxyl radical	
C ₇ H ₁₅ O ₅	FUEL4O ₂ H1O ₂	4-Hydroperoxyl-heptyl-1-ol-1-p eroxyl radical		C ₇ H ₁₅ O ₅	FUEL4O ₂ H2O ₂	4-Hydroperoxyl-heptyl-1-ol-2-p eroxyl radical	
C ₇ H ₁₅ O ₅	FUEL4O ₂ H6O ₂	4-Hydroperoxyl-heptyl-1-ol-6-p eroxyl radical		C ₇ H ₁₅ O ₅	FUEL5O ₂ H2O ₂	5-Hydroperoxyl-heptyl-1-ol-2-p eroxyl radical	
C ₇ H ₁₅ O ₅	FUEL5O ₂ H3O ₂	5-Hydroperoxyl-heptyl-1-ol-3-p eroxyl radical		C ₇ H ₁₅ O ₅	FUEL6O ₂ H3O ₂	6-Hydroperoxyl-heptyl-1-ol-3-p eroxyl radical	
C ₇ H ₁₅ O ₅	FUEL6O ₂ H4O ₂	6-Hydroperoxyl-heptyl-1-ol-4-p eroxyl radical		C ₇ H ₁₅ O ₅	FUEL7O ₂ H4O ₂	7-Hydroperoxyl-heptyl-1-ol-4-p eroxyl radical	
C ₇ H ₁₅ O ₅	FUEL7O ₂ H5O ₂	7-Hydroperoxyl-heptyl-1-ol-5-p eroxyl radical		C ₇ H ₁₅ O ₅	FUEL1*O3O ₂ H	1-Carbonyl-3-hydroperoxyl-hep tyl-1-ol	
C ₇ H ₁₄ O ₄	FUEL1*O4O ₂ H	1-Carbonyl-4-hydroperoxyl-hep tyl-1-ol		C ₇ H ₁₄ O ₄	FUEL2*O4O ₂ H	2-Carbonyl-4-hydroperoxyl-hep tyl-1-ol	
C ₇ H ₁₄ O ₄	FUEL2*O5O ₂ H	2-Carbonyl-5-hydroperoxyl-hep tyl-1-ol		C ₇ H ₁₄ O ₄	FUEL3*O5O ₂ H	3-Carbonyl-5-hydroperoxyl-hep tyl-1-ol	
C ₇ H ₁₄ O ₄	FUEL3*O6O ₂ H	3-Carbonyl-6-hydroperoxyl-hep tyl-1-ol		C ₇ H ₁₄ O ₄	FUEL4*O1O ₂ H	4-Carbonyl-1-hydroperoxyl-hep tyl-1-ol	
C ₇ H ₁₄ O ₄	FUEL4*O2O ₂ H	4-Carbonyl-2-hydroperoxyl-hep tyl-1-ol		C ₇ H ₁₄ O ₄	FUEL4*O6O ₂ H	4-Carbonyl-6-hydroperoxyl-hep tyl-1-ol	

C ₇ H ₁₄ O ₄	FUEL5*O ₂ O ₂ H	5-Carbonyl-2-hydroperoxyl-heptyl-1-ol		C ₇ H ₁₄ O ₄	FUEL5*O ₃ O ₂ H	5-Carbonyl-3-hydroperoxyl-heptyl-1-ol	
C ₇ H ₁₄ O ₄	FUEL6*O ₃ O ₂ H	6-Carbonyl-3-hydroperoxyl-heptyl-1-ol		C ₇ H ₁₄ O ₄	FUEL6*O ₄ O ₂ H	6-Carbonyl-4-hydroperoxyl-heptyl-1-ol	
C ₇ H ₁₄ O ₄	FUEL7*O ₄ O ₂ H	4-Hydroperoxyl-7-ol-heptanal		C ₇ H ₁₄ O ₄	FUEL7*O ₅ O ₂ H	5-Hydroperoxyl-7-ol-heptanal	
C ₇ H ₁₅ O ₂	FUEL1O	Heptyl-1-ol-1-oxy radical		C ₇ H ₁₅ O ₂	FUEL2O	Heptyl-1-ol-2-oxy radical	
C ₇ H ₁₅ O ₂	FUEL3O	Heptyl-1-ol-3-oxy radical		C ₇ H ₁₅ O ₂	FUEL4O	Heptyl-1-ol-4-oxy radical	
C ₇ H ₁₅ O ₂	FUEL5O	Heptyl-1-ol-5-oxy radical		C ₇ H ₁₅ O ₂	FUEL6O	Heptyl-1-ol-6-oxy radical	
C ₇ H ₁₅ O ₂	FUEL7O	Heptyl-1-ol-7-oxy radical		C ₇ H ₁₆ O ₃	FUEL1O ₂ H	1-Hydroperoxyl-heptyl-1-ol	
C ₇ H ₁₆ O ₃	FUEL2O ₂ H	2-Hydroperoxyl-heptyl-1-ol		C ₇ H ₁₆ O ₃	FUEL3O ₂ H	3-Hydroperoxyl-heptyl-1-ol	
C ₇ H ₁₆ O ₃	FUEL4O ₂ H	4-Hydroperoxyl-heptyl-1-ol		C ₇ H ₁₆ O ₃	FUEL5O ₂ H	5-Hydroperoxyl-heptyl-1-ol	
C ₇ H ₁₆ O ₃	FUEL6O ₂ H	6-Hydroperoxyl-heptyl-1-ol		C ₇ H ₁₆ O ₃	FUEL7O ₂ H	7-Hydroperoxyl-heptyl-1-ol	
C ₆ H ₁₃ O	HXOL6J	<i>n</i> -Hexanol-6-yl radical		C ₅ H ₁₁ O	PE1OL5J	<i>n</i> -Pentanol-5-yl radical	
C ₄ H ₉ O	B1OL4J	<i>n</i> -Butanol-4-yl radical					