Thermochemical Properties of Jet Fuels

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July 6, 2015

Two types of fuels are investigated in National Jet Fuel Combustion Program (NJFCP):

1) Category A: conventional petroleum-derived fuels
2) Category C: alternative fuels having properties outside the "experience base."

Nine fuels are considered in this report. They are listed in Table 1. The composition of these fuels may be found in the Appendix. The average molecular formula is calculated from the molecular weight and hydrogen mass fraction.

Table 1. List of fuels considered.

Name	POSF#	Description	Average Formula	MW (g/mol)
A1	10264	JP8 (best case)	$C_{10.8}H_{21.6}$	151.9
A2	10325	Jet A (middle case)	$C_{11.4}H_{21.7}$	158.6
A3	10289	JP5 (worse case)	$C_{12.0}H_{22.3}$	166.1
C1	11498	Gevo ATJ	$C_{12.5}H_{27.1}$	178.0
C2	12223	Bimodal fuel C14/TMB	$C_{12.3}H_{24.6}$	173.0
C3	12341	High viscosity	$C_{12.8}H_{25.0}$	179.6
C4	12344	Low cetane, broad boiling	$C_{11.4}H_{24.7}$	162.2
C5	12345	Flat boiling	$C_{9.7}H_{18.7}$	135.4
C6	10279-2	Virent HDO SK	$C_{11.9}H_{23.7}$	166.8

The standard enthalpy of formation is determined from the lower heating value (LHV), enthalpy of evaporation (H_v) and molecular weight. Unfortunately, the latent enthalpy of evaporation is unavailable and has to be estimated based on literature data. Chickos et al.[1] determined the H_v values for several representative jet fuels. Figure 1 shows these values as a function of molecular weight of four multicomponent aviation and rocket fuels along with some representative pure hydrocarbon compounds. Clearly, H_v increases almost linearly with molecular weight for each type of hydrocarbon compounds. Aromatic compounds tend to have a larger enthalpy of evaporation than paraffins and cycloparaffins of comparable molecular weight. The data may be correlated by

$$H_v \text{ (kJ/mol)} = 2.6 + 0.333 \text{ MW (g/mol)} + 10.9\, y_A \quad (1)$$

where y_A is the total mass fraction of the aromatic compounds.

[1] Chickos, J. S., Zhao, H. "Measurement of the vaporization enthalpy of complex mixtures by correlation-gas chromatography. The vaporization enthalpy of RP-1, JP-7, and JP-8 rocket and jet fuels at T= 298.15 K." Energy & fuels 19 (2005) 2064-2073.

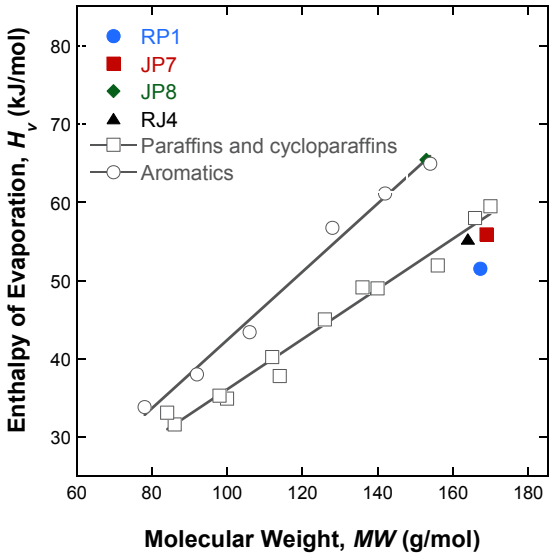

Figure 1. Enthalpy of evaporation versus molecular weight.

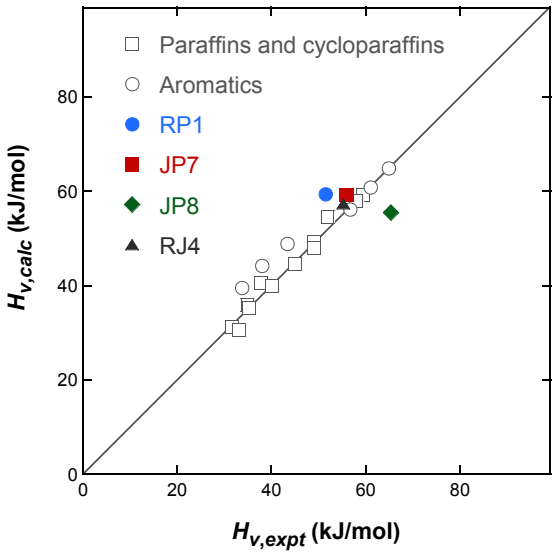

Figure 2. Calculated versus experimental enthalpy of evaporation.

Table 2 summarizes the enthalpy of evaporation estimated from the above equation for fuels listed in Table 1, along with the LHV values, approximate integer molecular formula, and the standard enthalpy of formation. The use of approximate integer molecular formula is necessary because many existing computer codes can only take such a formula as the input. When using the integer formula, one must consider the difference of the actual and approximate molecular weight when determining the unburned fuel-oxidizer composition, as will be discussed later. Table 2 shows that the H_v values are no larger than 1% of the LHV value. For this reason, the maximum error of 15% in an estimated H_v value by equation (1) leads to a negligible difference in the enthalpy of combustion of vapor-phase fuels (approximately 0.05 MJ/kg or < 0.15%).

Table 2. Some key thermochemical properties.

Fuel	POSF#	Approximate Integer Formula	MW_{app} [a] (g/mol)	LHV (MJ/kg)	H_v [b] (MJ/kg)	$\Delta_f H^o_{298}$ [c] (kcal/mol)	$\Delta_f H^o_{298}$/#C (kcal/mol)
A1	10264	$C_{11}H_{22}$	154.3	43.17	0.36	–65.1	–5.92
A2	10325	$C_{11}H_{22}$	154.3	43.12	0.36	–66.8	–6.08
A3	10289	$C_{12}H_{23}$	167.3	42.94	0.36	–61.7	–5.14
C1	11498	$C_{13}H_{28}$	184.4	43.90	0.35	–81.9	–6.30
C2	12223	$C_{13}H_{26}$	182.3	43.46	0.36	–64.5	–4.96
C3	12341	$C_{13}H_{25}$	181.3	43.22	0.36	–56.6	–4.35
C4	12344	$C_{11}H_{24}$	156.3	43.79	0.35	–79.0	–7.18
C5	12345	$C_{10}H_{19}$	139.3	42.98	0.38	–46.6	–4.66
C6	10279-2	$C_{12}H_{24}$	168.3	43.30	0.35	–66.2	–5.51

[a] Approximate molecular weight based on the integer formula. [b] Estimated from eq (1). [c] Derived from LHV, approximate integer formula and H_v.

The specific heat and entropy may be estimated by defining a thermochemical surrogate, as shown in Table 3. For each fuel, a neat reference compound of molecular weight similar to the mean molecular weight of a class of similar compounds (e.g., *n*-alkane) is assigned to that class. Only major compound classes are considered. Attention has been placed on matching the mean molecular weight of the thermodynamic surrogate with that of the real fuel. Table 4 lists the thermochemical property values for the reference compounds considered. The thermochemical properties of the jet fuels are listed in Tables 5 through 13, and the property data are presented in the form of NASA polynomials in Table 14.

The adiabatic flame temperature (T_{ad}) is calculated for the nine fuels in air at 1 atm pressure. Figures 3-11 shows the adiabatic flame temperature plotted as a function of the equivalence ratio. Figure 12 collects all curves into one plot. Clearly, the T_{ad} values of all nine fuels are similar over the entire range of equivalence ratio, and peak within 2280-2300 K. Given the small difference in the adiabatic flame temperature, it is unlikely that differences observed in the combustion behavior of these fuels, if any, is attributable to the difference in their thermochemical properties.

The use of the thermochemical properties requires a careful consideration of the actual molecular weight of the fuel and approximate molecular weight due to the use of integer molecular formula. The rule is always to use the actual mass of the fuel in the calculation of composition and convert the masses of fuel and oxidizer to their respective mole fractions using the approximate molecular weight of the fuel.

Table 3. Thermochemical surrogate composition in mole fractions.

Name	POSF#	Composition	Average Formula
A1	10264	16.40% 1,2,4-trimethylbenzene (C_9H_{12}) + 37.33% *iso*-undecane ($iC_{11}H_{24}$) + 25.22% *n*-undecane ($nC_{11}H_{24}$) + 21.05% butyl-cyclohexane ($MC_{10}H_{20}$)	$C_{10.5}H_{21.2}$
A2	10325	23.42% 1,2,4-trimethylbenzene (C_9H_{12}) + 26.09% *iso*-dodecane ($iC_{12}H_{26}$) + 19.33% *n*-undecane ($nC_{11}H_{24}$) + 31.16% pentyl-cyclohexane ($MC_{11}H_{22}$)	$C_{10.8}H_{21.1}$
A3	10289	27.35% 1,2,4-trimethylbenzene (C_9H_{12}) + 15.71% *iso*-tridecane ($iC_{13}H_{28}$) + 13.02% *n*-dodecane ($nC_{12}H_{26}$) + 29.72% hexyl-cyclohexane ($MC_{12}H_{24}$) + 14.21% methyl-dicyclohexane ($DC_{13}H_{24}$)	$C_{11.5}\ H_{21.6}$
C1	11498	86.49% *iso*-dodecane ($iC_{12}H_{26}$) + 13.51% *iso*-hexadecane ($iC_{16}H_{34}$)	$C_{12.5}\ H_{27.1}$
C2	12223	28.45% 1,2,4-trimethylbenzene (C_9H_{12}) + 71.55% *iso*-tetradecane ($iC_{14}H_{30}$)	$C_{12.6}\ H_{24.9}$
C3	12341	19.85% 1,2,4-trimethylbenzene (C_9H_{12}) + 37.56% *iso*-pentadecane ($iC_{15}H_{32}$) + 9.44% *n*-dodecane ($nC_{12}H_{26}$) + 22.43% hexyl-cyclohexane ($MC_{12}H_{24}$) + 10.72% dicyclohexane ($DC_{12}H_{22}$)	$C_{12.5}\ H_{24.6}$
C4	12344	8.72% *iso*-nonane (iC_9H_{20}) + 17.85% *iso*-denane ($iC_{10}H_{22}$) + 24.70% *iso*-undecane ($iC_{11}H_{24}$) + 43.85% *iso*-dodecane ($iC_{12}H_{26}$) + 4.88% *iso*-hexadecane ($iC_{16}H_{34}$)	$C_{11.3}\ H_{24.7}$
C5	12345	34.38% 1,2,4-trimethylbenzene (C_9H_{12}) + 48.90% *iso*-denane ($iC_{10}H_{22}$) + 16.72% *n*-denane ($iC_{10}H_{22}$)	$C_{9.7}\ H_{18.6}$
C6	10279-2	16.18% *iso*-dodecane ($iC_{12}H_{26}$) + 60.73% hexyl-cyclohexane ($MC_{12}H_{24}$) + 23.09% dicyclohexane ($DC_{12}H_{22}$)	$C_{12.0}H_{23.9}$

Table 4. Thermochemical data of reference species.

Species	S^o_{298} (cal/mol-K)	C_p (cal/mol-K)					Reference/ comments
		300 K	500 K	1000 K	1500 K	2000 K	
n-undecane	139.8	61.8	93.1	143.4	162.8	174.7	Burcat & Ruscic[2]
n-dodecane	149.3	67.3	101.3	156.0	177.0	189.9	Burcat & Ruscic[2]
iso-octane	101.1	45.3	70.0	108.7	129.1	142.0	Burcat & Ruscic[2]
iso-nonane	110.5	50.8	78.3	121.3	143.2	157.2	Group additivity[a]
iso-denane	119.9	56.2	86.5	133.9	157.4	172.4	Group additivity[a]
iso-undecane	129.4	61.7	94.8	146.5	171.6	187.5	Group additivity[a]
iso-dodecane	138.8	67.2	103.0	159.0	185.8	202.7	Group additivity[a]
iso-tridecane	148.2	72.7	111.3	171.6	200.0	217.9	Group additivity[a]
iso-tetradecane	157.6	78.2	119.6	184.2	214.2	233.1	Group additivity[a]
iso-pentadecane	167.0	83.7	127.8	196.7	228.4	248.3	Group additivity[a]
iso-hexadecane	176.4	89.1	136.1	209.3	242.6	263.5	Group additivity[a]
butyl-cyclohexane	105.0	47.0	76.9	122.1	143.3	153.9	JetSurf 2.0[3]
pentyl-cyclohexane	114.4	52.5	85.2	134.6	157.5	169.1	Group additivity[b]
hexyl-cyclohexane	123.8	57.9	93.4	147.2	171.7	184.3	Group additivity[b]
dicyclohexane	94.3	48.6	85.5	138.4	166.3	178.6	Group additivity[c]
methyl-dicyclohexane	99.1	53.8	92.7	147.5	179.8	193.0	Group additivity[c]
1,2,4-Trimethylbenzene	94.6	37.1	56.7	87.2	99.9	107.2	Burcat & Ruscic[2]

[a] Drived from iso-octane. [b] Derived from butyl-cyclohexane. [c] Derived from cyclohexane and butyl-cyclohexane.

[2] Burcat, A., Ruscic, B. *Third millenium ideal gas and condensed phase thermochemical database for combustion with updates from active thermochemical tables*. Argonne, IL: Argonne National Laboratory, 2005.

[3] Wang, H., Dames, E., Sirjean, B., Sheen, D. A., Tangko, R., Violi, A. et al. (2010). A high temperature chemical kinetic model of n-alkane (up to n-dodecane), cyclohexane, and methyl-, ethyl-, n-propyl and n-butyl-cyclohexane oxidation, JetSurF version 2.0; September 19, 2010. URL (http://melchior.usc.edu/JetSurF/JetSurF2.0).

Table 5. Thermochemical properties of POSF10264 (A1)

POSF10264 = 11 C(S) + 11 H2

T (K)	Cp (cal/mol-K)	S (cal/mol-k)	H(T)-H(298) (kcal/mol)	Hf (kcal/mol)	Gf (kcal/mol)
298.	54.325	121.203	0.000	-65.114	5.628
300.	54.646	121.567	0.109	-65.201	6.103
400.	70.216	139.447	6.362	-69.298	30.505
500.	84.305	156.662	14.102	-72.747	55.869
600.	96.474	173.139	23.158	-75.530	81.865
700.	106.672	188.800	33.331	-77.719	108.278
800.	115.244	203.619	44.438	-79.415	134.970
900.	122.926	217.640	56.350	-80.682	161.848
1000.	130.845	230.993	69.031	-81.490	188.844
1100.	135.847	243.702	82.369	-81.894	215.899
1200.	140.409	255.721	96.185	-82.066	242.981
1300.	144.555	267.126	110.437	-82.037	270.068
1400.	148.310	277.979	125.083	-81.836	297.146
1500.	151.700	288.329	140.087	-81.489	324.205
1600.	154.750	298.218	155.412	-81.021	351.237
1700.	157.485	307.684	171.026	-80.452	378.236
1800.	159.931	316.756	186.899	-79.802	405.199
1900.	162.115	325.462	203.004	-79.088	432.125
2000.	164.064	333.828	219.314	-78.324	459.011
2100.	165.803	341.876	235.809	-77.525	485.858
2200.	167.361	349.626	252.469	-76.699	512.667
2300.	168.766	357.097	269.277	-75.855	539.437
2400.	170.044	364.307	286.218	-74.999	566.171
2500.	171.224	371.272	303.282	-74.134	592.868

Table 6. Thermochemical properties of POSF10325 (A2)

POSF10325 = 11 C(S) + 11 H2

T (K)	Cp (cal/mol-K)	S (cal/mol-k)	H(T)-H(298) (kcal/mol)	Hf (kcal/mol)	Gf (kcal/mol)
298.	54.187	121.061	0.000	-66.867	3.917
300.	54.518	121.425	0.109	-66.955	4.392
400.	70.421	139.319	6.367	-71.046	28.808
500.	84.683	156.600	14.138	-74.465	54.182
600.	96.982	173.157	23.238	-77.204	80.180
700.	107.323	188.908	33.469	-79.335	106.586
800.	116.042	203.823	44.648	-80.959	133.263
900.	123.801	217.944	56.645	-82.141	160.116
1000.	131.594	231.385	69.409	-82.865	187.077
1100.	136.718	244.172	82.829	-83.187	214.089
1200.	141.328	256.269	96.736	-83.269	241.119
1300.	145.466	267.748	111.079	-83.148	268.148
1400.	149.171	278.666	125.814	-82.859	295.161
1500.	152.480	289.073	140.900	-82.430	322.148
1600.	155.432	299.010	156.298	-81.888	349.103
1700.	158.061	308.513	171.976	-81.256	376.021
1800.	160.403	317.615	187.901	-80.553	402.900
1900.	162.492	326.345	204.048	-79.797	429.738
2000.	164.359	334.728	220.392	-79.000	456.535
2100.	166.037	342.789	236.913	-78.174	483.292
2200.	167.556	350.548	253.594	-77.327	510.008
2300.	168.945	358.027	270.420	-76.465	536.686
2400.	170.231	365.245	287.380	-75.590	563.326
2500.	171.442	372.219	304.464	-74.706	589.930

Table 7. Thermochemical properties of POSF10289 (A3)

POSF10289 = 12 C(S) + 11.5 H2

T (K)	Cp (cal/mol-K)	S (cal/mol-k)	H(T)-H(298) (kcal/mol)	Hf (kcal/mol)	Gf (kcal/mol)
298.	54.860	119.480	0.000	-61.720	14.596
300.	55.213	119.848	0.110	-61.818	15.109
400.	72.055	138.077	6.487	-66.383	41.457
500.	87.090	155.807	14.461	-70.266	68.881
600.	100.078	172.865	23.836	-73.455	97.021
700.	111.039	189.141	34.408	-76.020	125.644
800.	120.251	204.586	45.986	-78.057	154.598
900.	128.247	219.220	58.418	-79.646	183.780
1000.	135.820	233.124	71.621	-80.798	213.115
1100.	141.431	246.336	85.488	-81.559	242.546
1200.	146.455	258.862	99.887	-82.052	272.034
1300.	150.931	270.765	114.761	-82.321	301.553
1400.	154.897	282.098	130.056	-82.406	331.086
1500.	158.395	292.907	145.725	-82.344	360.620
1600.	161.466	303.230	161.721	-82.166	390.146
1700.	164.154	313.101	178.005	-81.902	419.658
1800.	166.503	322.552	194.541	-81.575	449.152
1900.	168.559	331.611	211.296	-81.207	478.627
2000.	170.369	340.304	228.244	-80.813	508.082
2100.	171.982	348.656	245.363	-80.404	537.516
2200.	173.447	356.690	262.636	-79.989	566.931
2300.	174.815	364.431	280.049	-79.571	596.328
2400.	176.139	371.899	297.597	-79.147	625.705
2500.	177.472	379.116	315.278	-78.713	655.065

Table 8. Thermochemical properties of POSF11498 (C1)

POSF11498 = 13 C(S) + 14 H2

T (K)	Cp (cal/mol-K)	S (cal/mol-k)	H(T)-H(298) (kcal/mol)	Hf (kcal/mol)	Gf (kcal/mol)
298.	69.823	143.887	0.000	-81.899	10.819
300.	70.232	144.355	0.140	-82.005	11.442
400.	89.906	167.295	8.161	-86.910	43.352
500.	107.546	189.295	18.053	-90.943	76.403
600.	122.788	210.287	29.590	-94.097	110.183
700.	135.650	230.210	42.531	-96.466	144.427
800.	146.528	249.052	56.654	-98.178	178.964
900.	156.204	266.876	71.796	-99.323	213.681
1000.	165.837	283.827	87.893	-99.887	248.496
1100.	172.339	299.942	104.806	-99.940	283.339
1200.	178.333	315.198	122.344	-99.670	318.173
1300.	183.843	329.693	140.456	-99.112	352.973
1400.	188.896	343.505	159.097	-98.299	387.720
1500.	193.516	356.697	178.221	-97.263	422.400
1600.	197.729	369.323	197.787	-96.032	457.005
1700.	201.559	381.427	217.754	-94.632	491.528
1800.	205.031	393.048	238.087	-93.086	525.964
1900.	208.168	404.219	258.749	-91.417	560.311
2000.	210.994	414.969	279.710	-89.646	594.567
2100.	213.533	425.326	300.939	-87.789	628.732
2200.	215.807	435.314	322.408	-85.864	662.808
2300.	217.839	444.952	344.092	-83.884	696.794
2400.	219.652	454.262	365.968	-81.864	730.693
2500.	221.266	463.262	388.016	-79.816	764.508

Table 9. Thermochemical properties of POSF12223 (C2)

POSF12223 = 13 C(S) + 13 H2

T (K)	Cp (cal/mol-K)	S (cal/mol-k)	H(T)-H(298) (kcal/mol)	Hf (kcal/mol)	Gf (kcal/mol)
298.	66.122	139.691	0.000	-64.495	20.167
300.	66.509	140.135	0.133	-64.594	20.735
400.	85.087	161.852	7.726	-69.232	49.897
500.	101.732	182.667	17.085	-73.097	80.143
600.	116.094	202.520	27.996	-76.177	111.093
700.	128.190	221.352	40.228	-78.556	142.502
800.	138.405	239.153	53.571	-80.343	174.210
900.	147.497	255.986	67.871	-81.618	206.111
1000.	156.590	271.991	83.070	-82.360	238.126
1100.	162.704	287.208	99.040	-82.631	270.191
1200.	168.224	301.605	115.591	-82.612	302.267
1300.	173.209	315.271	132.667	-82.344	334.330
1400.	177.712	328.275	150.217	-81.867	366.366
1500.	181.784	340.677	168.195	-81.210	398.360
1600.	185.469	352.528	186.561	-80.402	430.306
1700.	188.809	363.874	205.277	-79.466	462.197
1800.	191.840	374.753	224.312	-78.422	494.030
1900.	194.593	385.201	243.636	-77.287	525.803
2000.	197.097	395.247	263.223	-76.075	557.513
2100.	199.373	404.919	283.048	-74.798	589.161
2200.	201.442	414.242	303.090	-73.468	620.747
2300.	203.316	423.239	323.330	-72.095	652.272
2400.	205.006	431.928	343.747	-70.687	683.736
2500.	206.517	440.328	364.325	-69.255	715.141

Table 10. Thermochemical properties of POSF12341 (C3)

POSF12341 = 13 C(S) + 12.5 H2

T (K)	Cp (cal/mol-K)	S (cal/mol-k)	H(T)-H(298) (kcal/mol)	Hf (kcal/mol)	Gf (kcal/mol)
298.	62.976	133.501	0.000	-56.568	25.285
300.	63.368	133.924	0.126	-56.667	25.834
400.	82.148	154.766	7.416	-61.260	54.048
500.	98.955	174.943	16.490	-65.061	83.331
600.	113.458	194.303	27.130	-68.062	113.304
700.	125.668	212.737	39.105	-70.348	143.722
800.	135.939	230.207	52.199	-72.032	174.425
900.	144.969	246.747	66.251	-73.199	205.307
1000.	153.801	262.474	81.186	-73.846	236.292
1100.	159.863	277.422	96.874	-74.035	267.318
1200.	165.348	291.571	113.139	-73.934	298.348
1300.	170.291	305.005	129.925	-73.583	329.358
1400.	174.730	317.790	147.180	-73.022	360.334
1500.	178.703	329.983	164.856	-72.285	391.263
1600.	182.246	341.632	182.907	-71.403	422.138
1700.	185.400	352.777	201.292	-70.406	452.955
1800.	188.201	363.455	219.975	-69.316	483.710
1900.	190.689	373.699	238.922	-68.155	514.402
2000.	192.902	383.537	258.103	-66.940	545.032
2100.	194.881	392.997	277.494	-65.687	575.599
2200.	196.665	402.105	297.073	-64.405	606.107
2300.	198.293	410.884	316.822	-63.102	636.556
2400.	199.806	419.355	336.728	-61.783	666.947
2500.	201.245	427.541	356.781	-60.449	697.284

Table 11. Thermochemical properties of POSF12344 (C4)

POSF12344 = 11 C(S) + 12 H2

T (K)	Cp (cal/mol-K)	S (cal/mol-k)	H(T)-H(298) (kcal/mol)	Hf (kcal/mol)	Gf (kcal/mol)
298.	63.180	132.475	0.000	-78.972	-2.282
300.	63.556	132.899	0.127	-79.055	-1.767
400.	81.519	153.684	7.395	-82.832	24.587
500.	97.556	173.636	16.366	-85.751	51.798
600.	111.426	192.682	26.833	-87.822	79.516
700.	123.179	210.766	38.580	-89.138	107.519
800.	133.156	227.883	51.410	-89.815	135.666
900.	141.992	244.084	65.173	-89.943	163.864
1000.	150.610	259.487	79.800	-89.523	192.048
1100.	156.661	274.129	95.168	-88.624	220.165
1200.	162.233	288.003	111.117	-87.399	248.185
1300.	167.350	301.194	127.600	-85.885	276.090
1400.	172.041	313.770	144.573	-84.114	303.870
1500.	176.330	325.788	161.994	-82.115	331.514
1600.	180.241	337.295	179.826	-79.917	359.019
1700.	183.798	348.330	198.031	-77.544	386.381
1800.	187.026	358.929	216.575	-75.019	413.598
1900.	189.947	369.120	235.426	-72.363	440.672
2000.	192.582	378.932	254.554	-69.597	467.603
2100.	194.953	388.386	273.933	-66.736	494.392
2200.	197.081	397.505	293.537	-63.797	521.044
2300.	198.986	406.309	313.342	-60.795	547.561
2400.	200.687	414.814	333.327	-57.741	573.946
2500.	202.203	423.038	353.473	-54.649	600.203

Table 12. Thermochemical properties of POSF12345 (C5)

POSF12345 = 10 C(S) + 9.5 H2

T (K)	Cp (cal/mol-K)	S (cal/mol-k)	H(T)-H(298) (kcal/mol)	Hf (kcal/mol)	Gf (kcal/mol)
298.	49.444	112.998	0.000	-46.572	12.247
300.	49.725	113.329	0.099	-46.645	12.642
400.	63.448	129.533	5.765	-50.040	32.930
500.	75.979	145.065	12.749	-52.878	54.013
600.	86.844	159.905	20.905	-55.135	75.612
700.	95.944	173.998	30.058	-56.870	97.547
800.	103.558	187.320	40.043	-58.172	119.700
900.	110.341	199.913	50.742	-59.099	141.994
1000.	117.324	211.892	62.118	-59.625	164.370
1100.	121.864	223.291	74.081	-59.792	186.779
1200.	125.992	234.074	86.477	-59.744	209.194
1300.	129.741	244.309	99.267	-59.512	231.597
1400.	133.142	254.051	112.413	-59.119	253.976
1500.	136.224	263.343	125.884	-58.589	276.323
1600.	139.016	272.226	139.649	-57.942	298.630
1700.	141.542	280.731	153.679	-57.197	320.893
1800.	143.825	288.887	167.949	-56.367	343.110
1900.	145.888	296.719	182.436	-55.469	365.279
2000.	147.750	304.250	197.120	-54.512	387.399
2100.	149.428	311.500	211.980	-53.509	409.470
2200.	150.939	318.487	227.000	-52.467	431.492
2300.	152.296	325.227	242.163	-51.397	453.467
2400.	153.511	331.735	257.454	-50.305	475.394
2500.	154.594	338.024	272.861	-49.200	497.275

Table 13. Thermochemical properties of POSF10279-2 (C6)

POSF10279 = 12 C(S) + 12 H2

T (K)	Cp (cal/mol-K)	S (cal/mol-k)	H(T)-H(298) (kcal/mol)	Hf (kcal/mol)	Gf (kcal/mol)
298.	56.917	119.435	0.000	-66.160	14.823
300.	57.315	119.817	0.114	-66.261	15.367
400.	76.285	138.951	6.811	-70.854	43.291
500.	93.148	157.826	15.301	-74.571	72.276
600.	107.755	176.135	25.365	-77.422	101.927
700.	120.143	193.703	36.778	-79.496	131.993
800.	130.532	210.444	49.327	-80.913	162.309
900.	139.324	226.339	62.831	-81.787	192.770
1000.	147.106	241.427	77.158	-82.174	223.301
1100.	153.468	255.752	92.192	-82.131	253.850
1200.	159.182	269.355	107.830	-81.754	284.379
1300.	164.279	282.301	124.008	-81.091	314.865
1400.	168.789	294.644	140.666	-80.192	345.291
1500.	172.752	306.428	157.747	-79.100	375.645
1600.	176.208	317.690	175.199	-77.855	405.922
1700.	179.204	328.464	192.973	-76.493	436.117
1800.	181.791	338.782	211.026	-75.047	466.229
1900.	184.022	348.673	229.320	-73.544	496.259
2000.	185.958	358.162	247.821	-72.003	526.209
2100.	187.662	367.277	266.504	-70.443	556.081
2200.	189.201	376.043	285.348	-68.872	585.879
2300.	190.649	384.486	304.341	-67.293	615.605
2400.	192.080	392.630	323.477	-65.705	645.262
2500.	193.577	400.501	342.759	-64.095	674.853

Table 14. NASA Polynomials for fuels considered.

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POSF10264          S07/15C  11H  22    0    0G   298.000  3000.000               1
 0.25897423E+02 0.55462092E-01-0.17337738E-04 0.17582452E-08 0.63971899E-13    2
-0.46337805E+05-0.11004780E+03 0.47049127E+01 0.58911327E-01 0.10500014E-03    3
-0.18501088E-06 0.82238431E-10-0.37391863E+05 0.13439449E+02                   4
POSF10325          S07/15C  11H  22    0    0G   298.000  3000.000               1
 0.21357891E+02 0.66589087E-01-0.25967469E-04 0.44775001E-08-0.23607152E-12    2
-0.45796996E+05-0.86136086E+02 0.25785518E+01 0.72624832E-01 0.73236370E-04    3
-0.15115444E-06 0.68935579E-10-0.38029855E+05 0.22533735E+02                   4
POSF10289          S07/15C  12H  23    0    0G   298.000  3000.000               1
 0.20115053E+02 0.69181815E-01-0.23171997E-04 0.19519781E-08 0.27041864E-12    2
-0.42549684E+05-0.79951393E+02 0.40264606E-01 0.88749342E-01 0.42724278E-04    3
-0.11716354E-06 0.53996904E-10-0.35190535E+05 0.32478203E+02                   4
POSF11498          S07/15C  13H  28    0    0G   298.000  3000.000               1
 0.33643040E+02 0.67928091E-01-0.20546000E-04 0.24969564E-08-0.69632051E-13    2
-0.58361672E+05-0.14804048E+03 0.42177753E+01 0.93084201E-01 0.80710743E-04    3
-0.17453084E-06 0.79970509E-10-0.47017836E+05 0.18436749E+02                   4
POSF12223          S07/15C  13H  26    0    0G   298.000  3000.000               1
 0.23490032E+02 0.85596524E-01-0.38567501E-04 0.92140393E-08-0.93389261E-12    2
-0.46210473E+05-0.94542419E+02 0.41502266E+01 0.87146208E-01 0.78981066E-04    3
-0.16891829E-06 0.77439957E-10-0.37970086E+05 0.18512276E+02                   4
POSF12341          S07/15C  13H  25    0    0G   298.000  3000.000               1
 0.26887732E+02 0.71930587E-01-0.24302843E-04 0.28183538E-08 0.61754170E-13    2
-0.43089531E+05-0.11438541E+03 0.18479576E+01 0.91500171E-01 0.69557325E-04    3
-0.15754647E-06 0.72036557E-10-0.33425066E+05 0.27544807E+02                   4
POSF12344          S07/15C  11H  24    0    0G   298.000  3000.000               1
 0.28867313E+02 0.64736143E-01-0.20546313E-04 0.28714062E-08-0.13840350E-12    2
-0.54667609E+05-0.12421461E+03 0.24618831E+01 0.93917467E-01 0.48512080E-04    3
-0.13020244E-06 0.61101103E-10-0.44851785E+05 0.23525198E+02                   4
POSF12345          S07/15C  10H  19    0    0G   298.000  3000.000               1
 0.20425438E+02 0.57119373E-01-0.22741666E-04 0.46415480E-08-0.40493837E-12    2
-0.34667656E+05-0.81659836E+02 0.59423847E+01 0.44303942E-01 0.11181572E-03    3
-0.18200340E-06 0.78981086E-10-0.27845352E+05 0.62907639E+01                   4
POSF10279          S07/15C  12H  24    0    0G   298.000  3000.000               1
 0.22479706E+02 0.69448672E-01-0.17031076E-04-0.17819028E-08 0.91128515E-12    2
-0.45737859E+05-0.94360107E+02-0.40326195E+01 0.11361472E+00 0.75787307E-05    3
-0.81596667E-07 0.38462480E-10-0.37068410E+05 0.49526718E+02                   4
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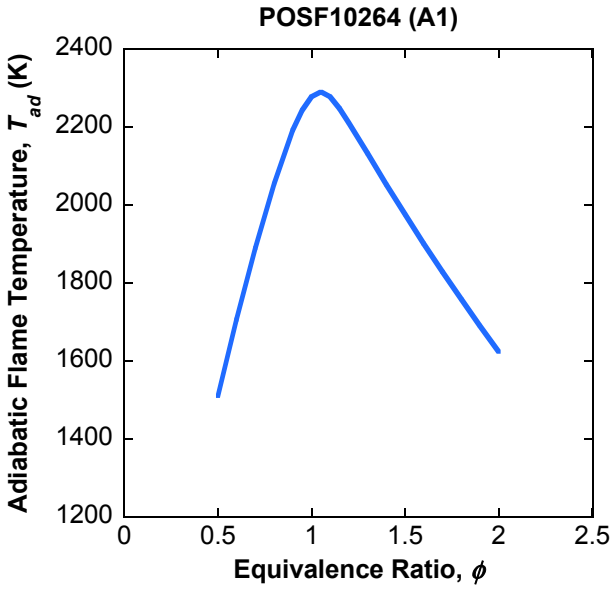

Figure 3. Adiabatic flame temperature of POSF10264 (A1) in air (p = 1 atm, T_0 = 298 K).

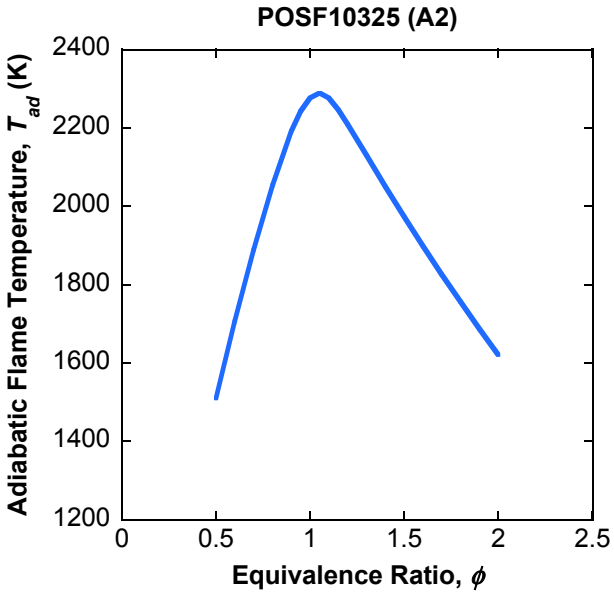

Figure 4. Adiabatic flame temperature of POSF10325 (A2) in air (p = 1 atm, T_0 = 298 K).

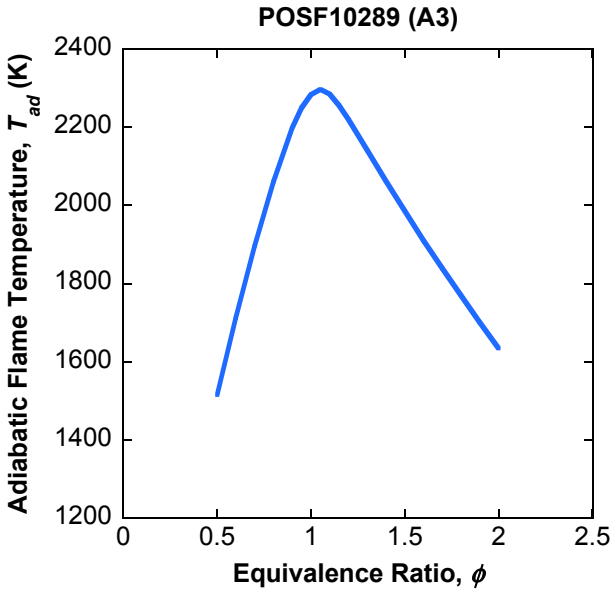

Figure 5. Adiabatic flame temperature of POSF10289 (A3) in air (p = 1 atm, T_0 = 298 K).

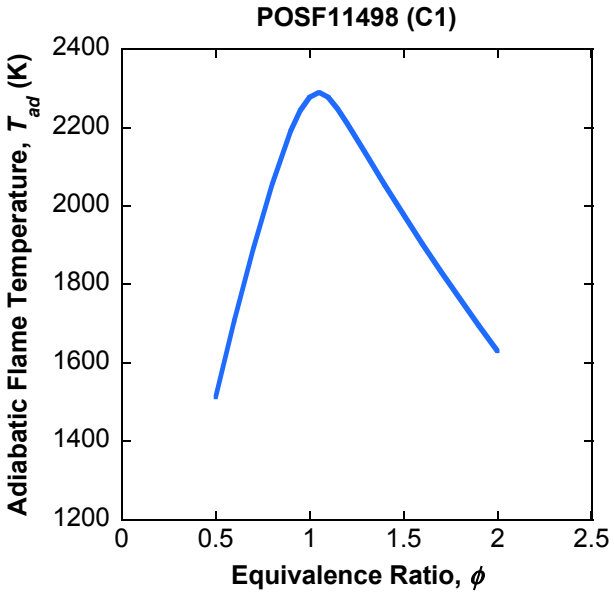

Figure 6. Adiabatic flame temperature of POSF11498 (C1) in air (p = 1 atm, T_0 = 298 K).

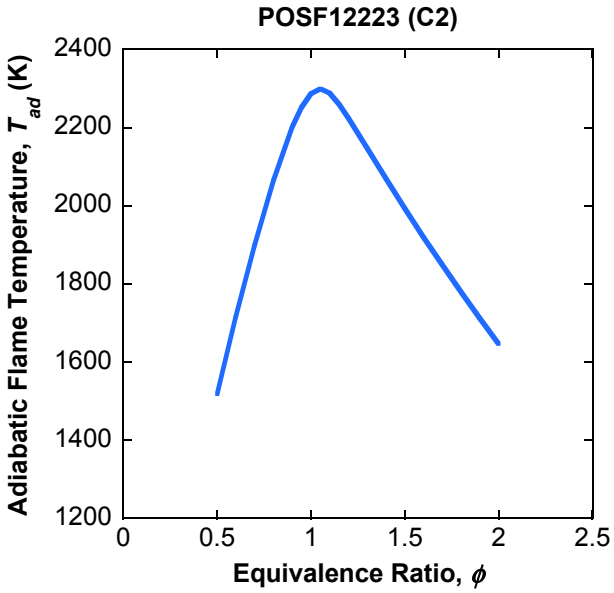

Figure 7. Adiabatic flame temperature of POSF12223 (C2) in air (p = 1 atm, T_0 = 298 K).

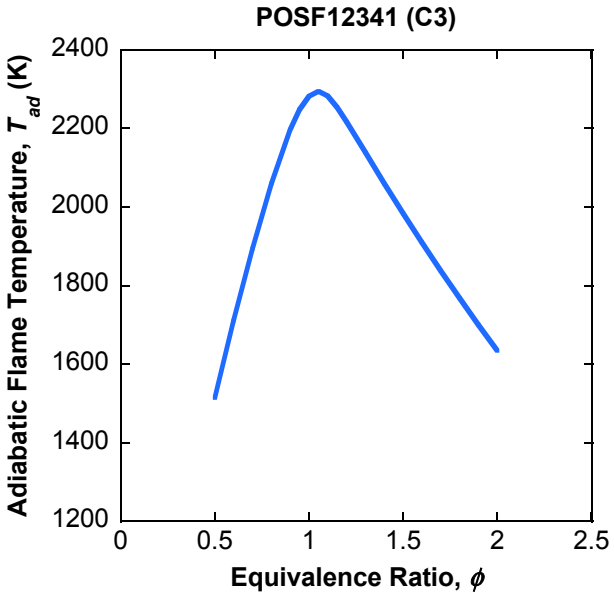

Figure 8. Adiabatic flame temperature of POSF12341 (C3) in air (p = 1 atm, T_0 = 298 K).

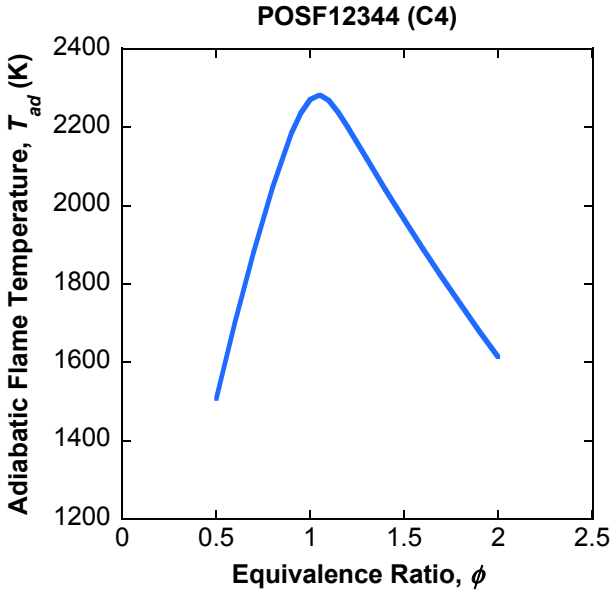

Figure 9. Adiabatic flame temperature of POSF12344 (C4) in air (p = 1 atm, T_0 = 298 K).

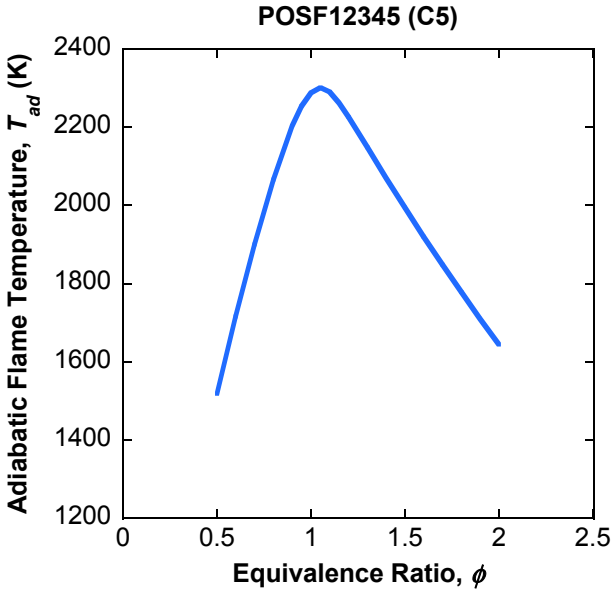

Figure 10. Adiabatic flame temperature of POSF12345 (C5) in air (p = 1 atm, T_0 = 298 K).

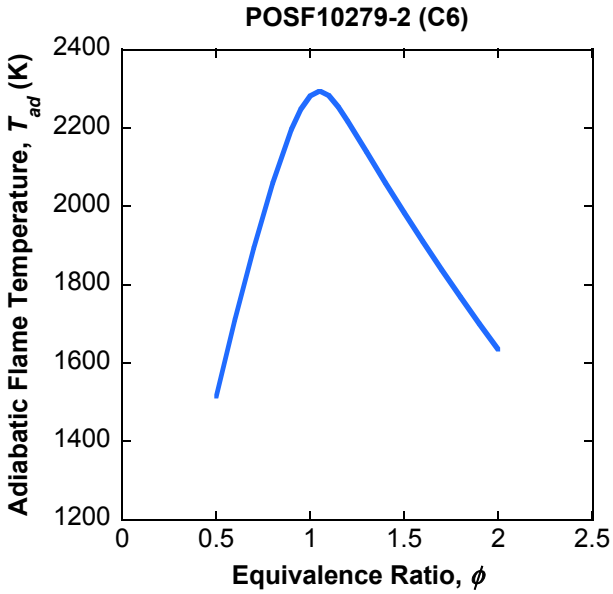

Figure 11. Adiabatic flame temperature of POSF10279-2 (C6) in air (p = 1 atm, T_0 = 298 K).

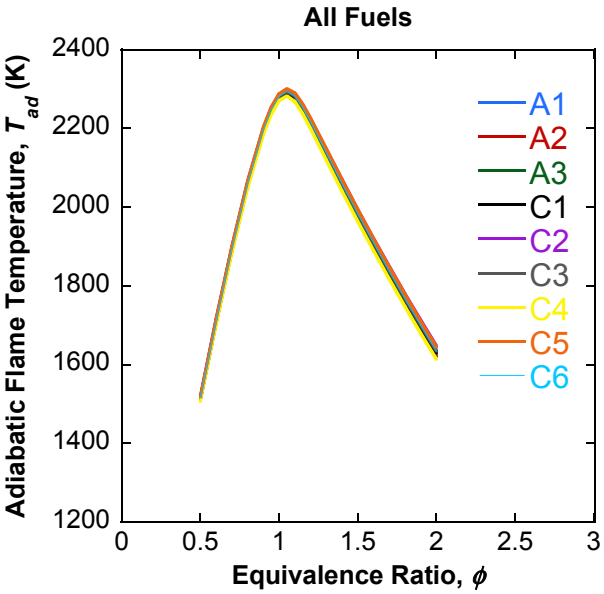

Figure 12. Comparison of adiabatic flame temperatures of selected jet fuels in air (p = 1 atm, T_0 = 298 K).

Appendix

Composition pie charts of selected fuels

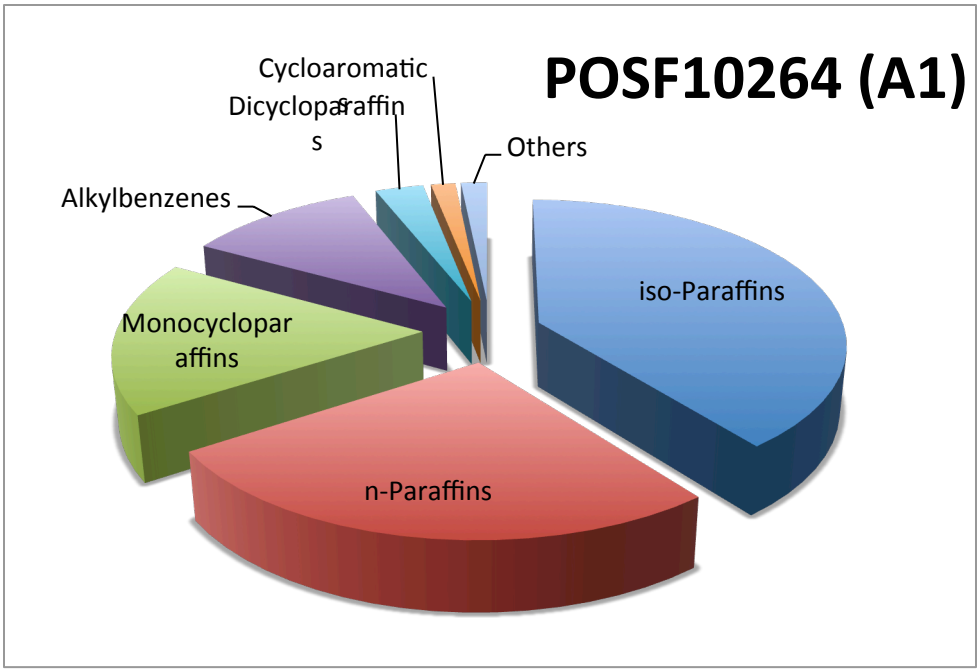

Figure A1. Composition pie chart of POSF10264 (A1)

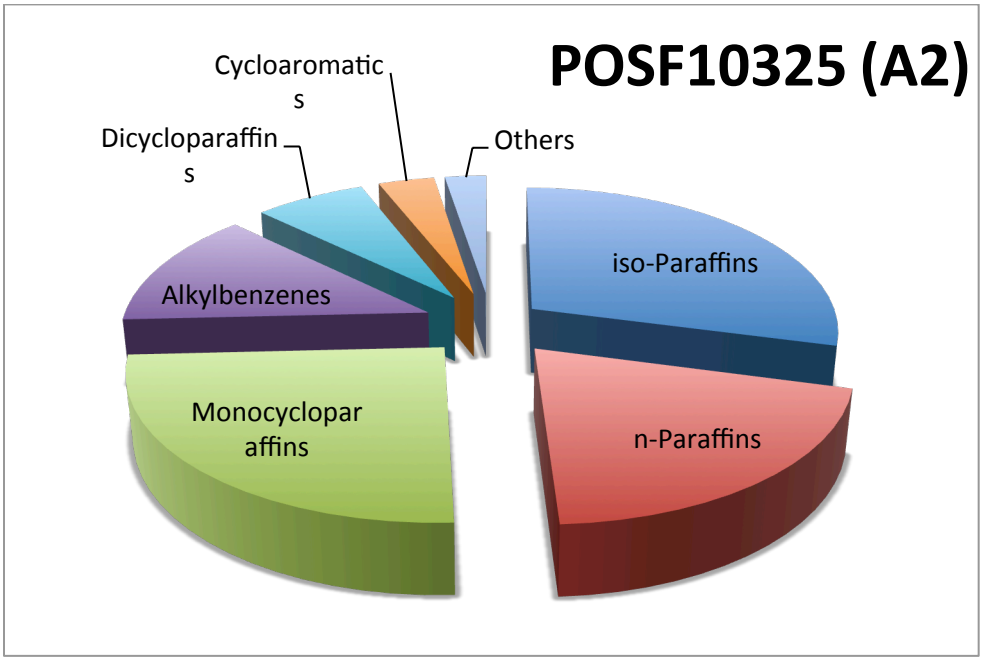

Figure A2. Composition pie chart of POSF10325 (A2)

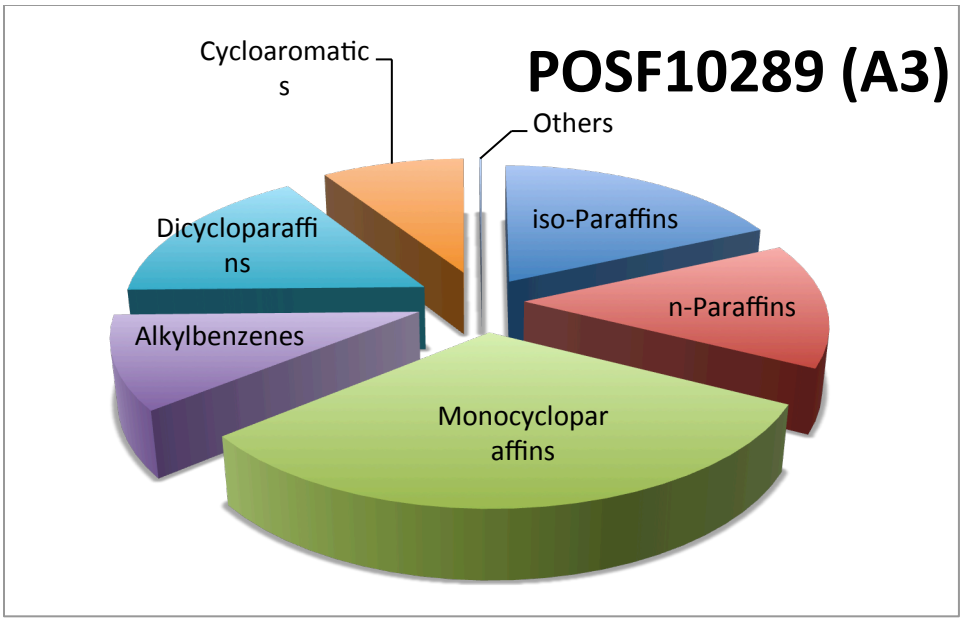

Figure A3. Composition pie chart of POSF10289 (A3)

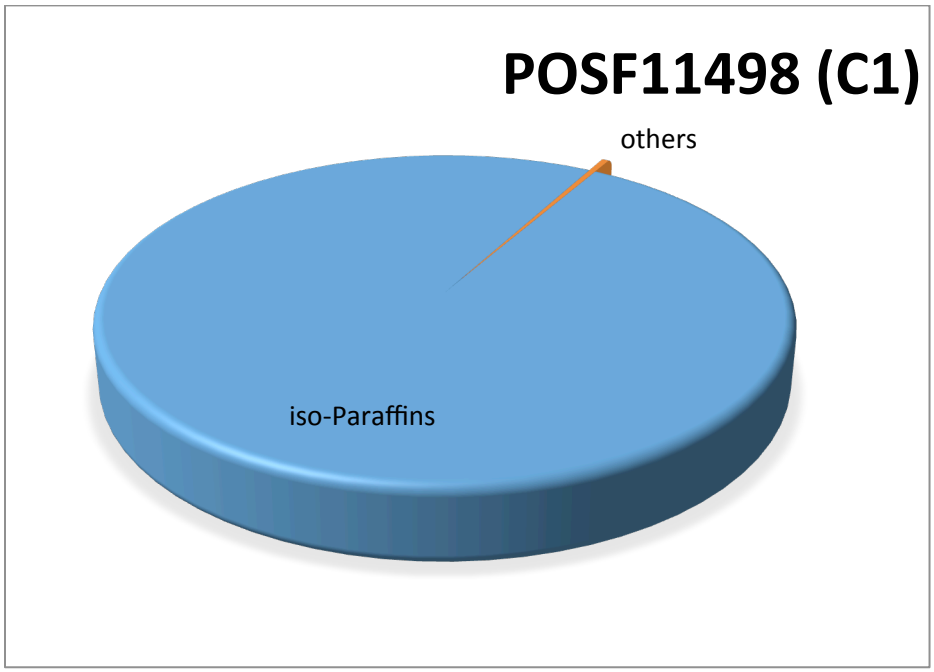

Figure A4. Composition pie chart of POSF11498 (C1)

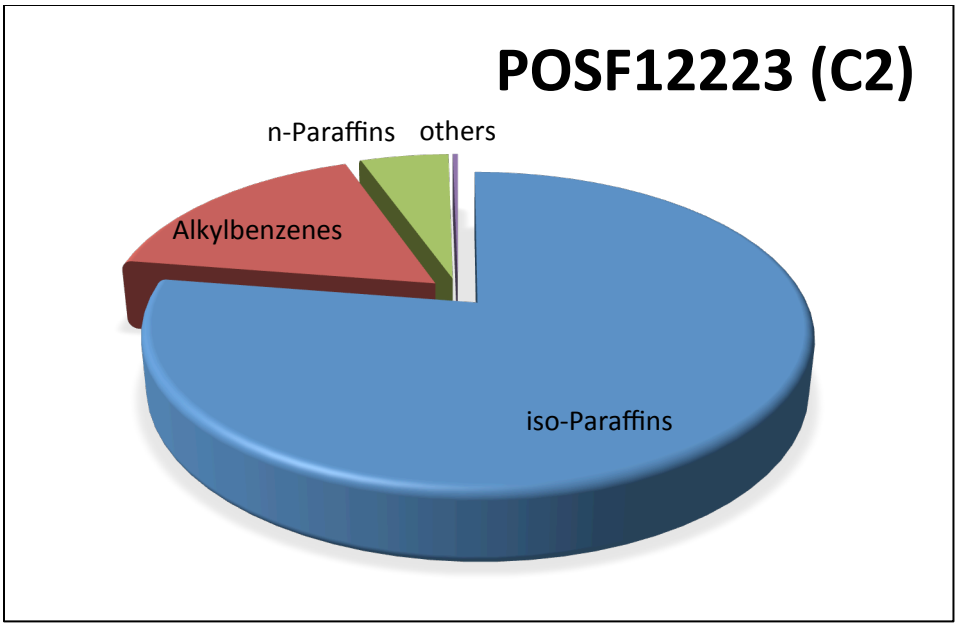

Figure A5. Composition pie chart of POSF12223 (C2)

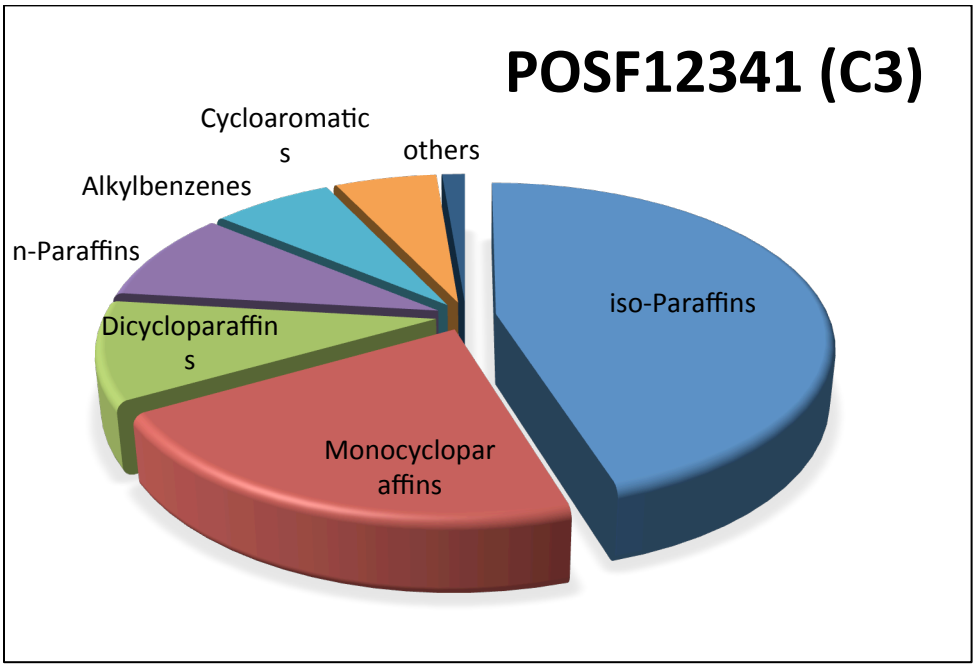

Figure A6. Composition pie chart of POSF12341 (C3)

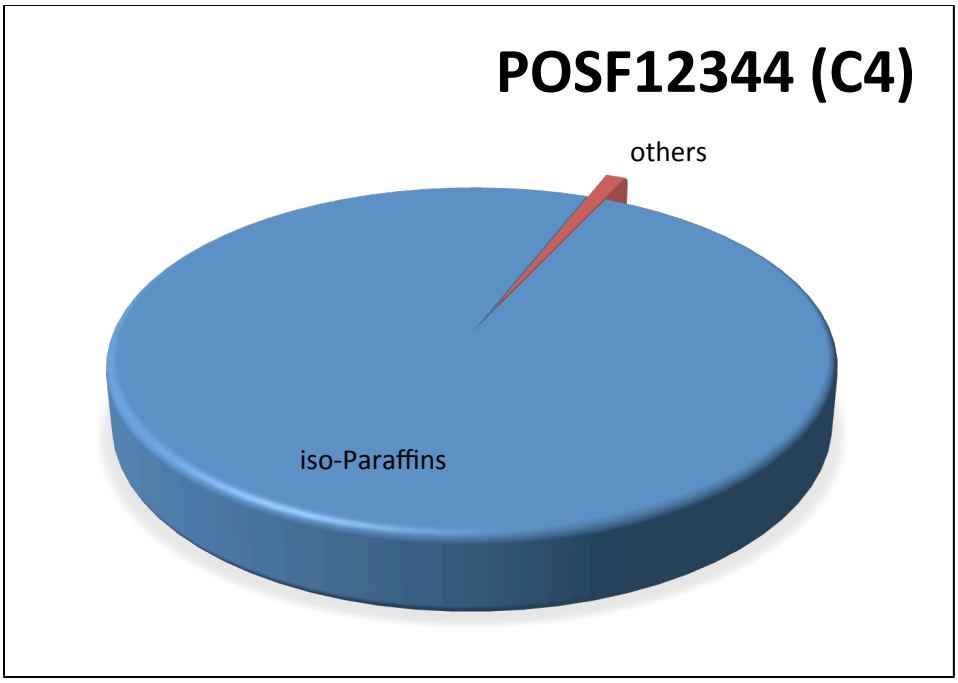

Figure A7. Composition pie chart of POSF12344 (C4)

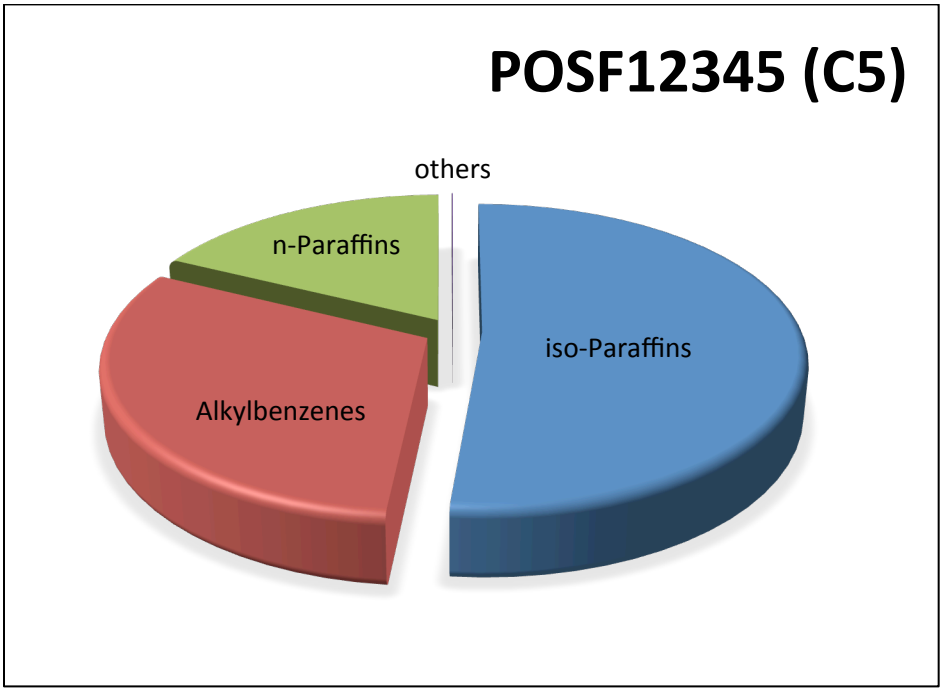

Figure A8. Composition pie chart of POSF12345 (C5)

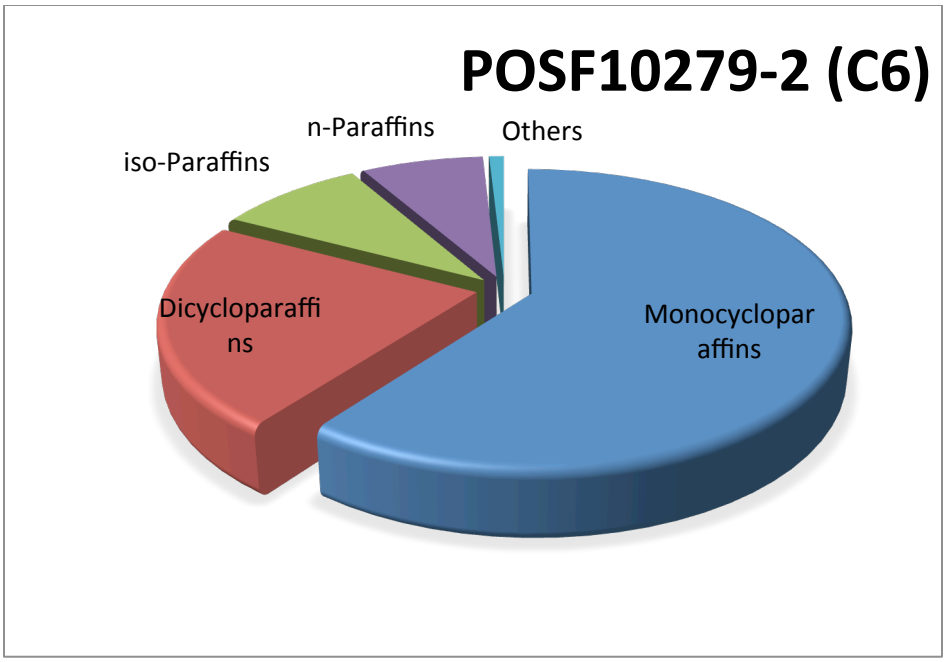

Figure A9. Composition pie chart of POSF10279-2 (C6)