Electronic Supplementary Material (ESI) for RSC Sustainability.

Supplementary material for:

Upcycling Mixed-Material Waste with Elemental Sulfur: Applications to Plant Oil, Unseparated Biomass, and Raw Post-Consumer Food Waste

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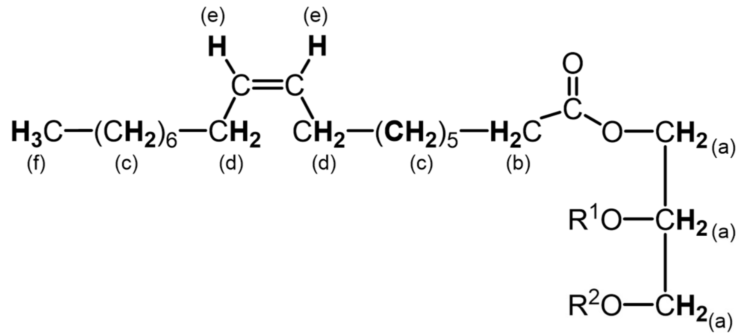
A)



B)

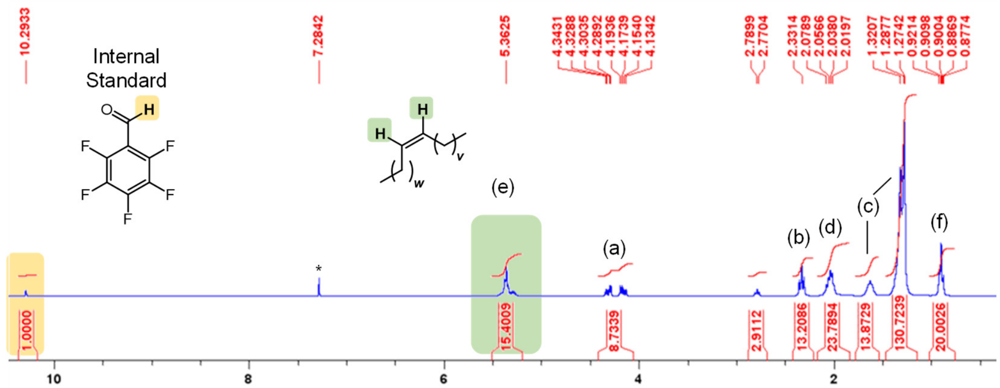


Figure S1. A) Representative unsaturated fatty acid chain in peanut oil triglycerides (A) and proton NMR spectrum (300 MHz, $CDCl_3$) of peanut oil with 2,3,4,5,6–pentafluorobenzaldehyde added as internal standard (B). The yellow- and green-highlighted peaks were those used in calculation of the olefin content of the oil. The peak labeled with the asterisk is a residual solvent signal.

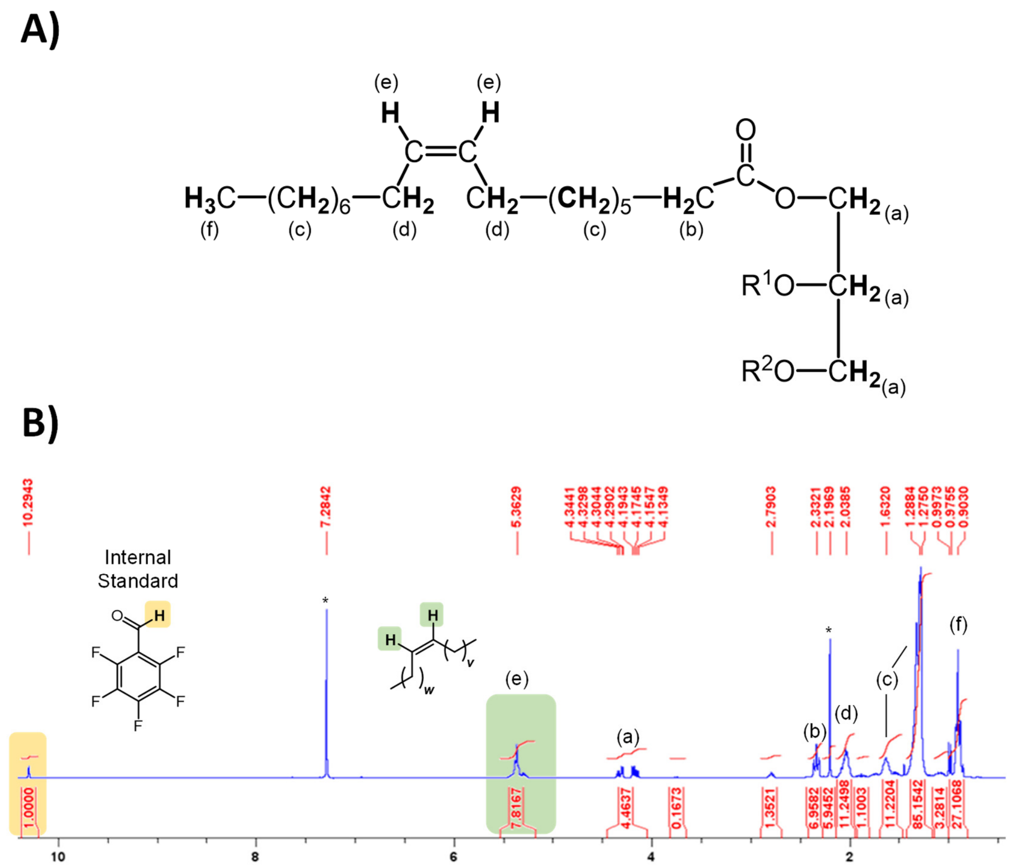


Figure S2. Representative unsaturated fatty acid chain in peanut oil triglycerides from French fries (A) and proton NMR spectrum (300 MHz, $CDCl_3$) of peanut oil with 2,3,4,5,6–pentafluorobenzaldehyde added as internal standard (B). The yellow- and green-highlighted peaks were those used in calculation of the olefin content of the oil. The peaks labeled with the asterisks are residual solvent signals.

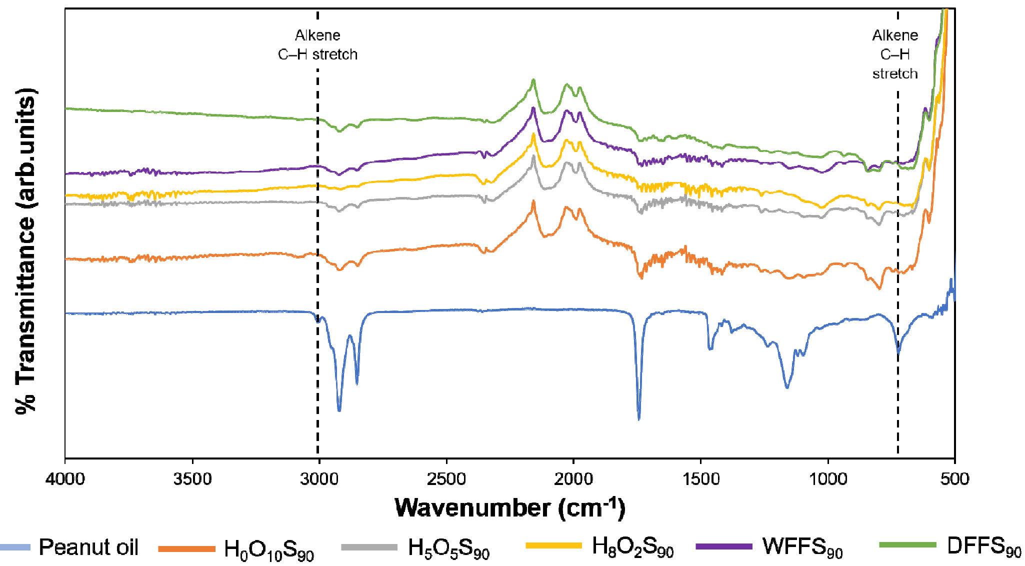


Figure S3 Full Infrared spectrum of peanut oil, **$H_0O_{10}S_{90}$**, **$H_5O_5S_{90}$**, **$H_8O_2S_{90}$**, **$WFFS_{90}$**, and **$DFFS_{90}$**. Alkene C-H stretch is highlighted at ~3000 cm^{-1}, and cis C-H bend at ~720 cm^{-1}.

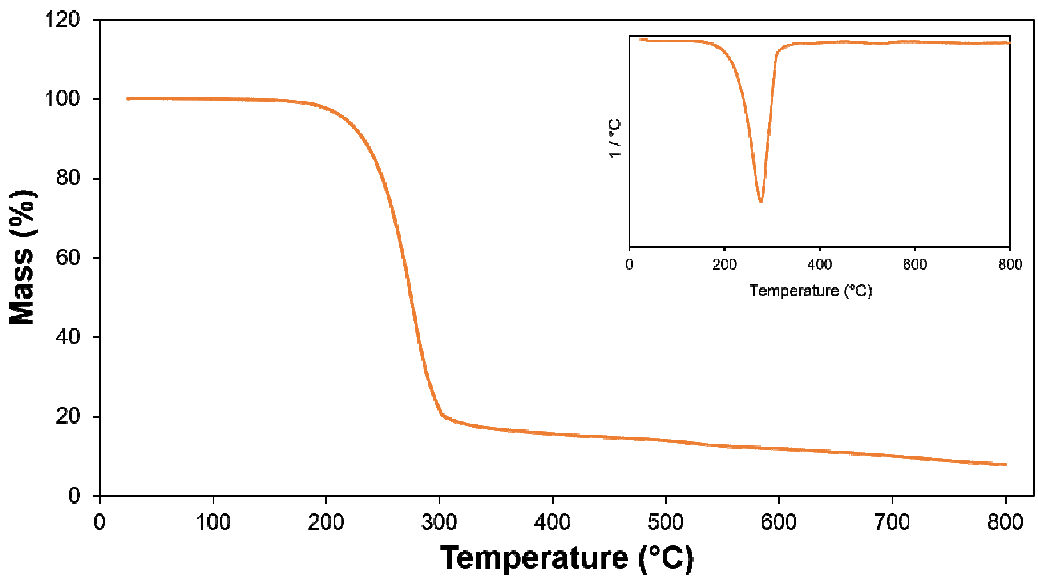


Figure S4 Mass loss curve and dTGA from thermogravimetric analysis for the **$H_0O_{10}S_{90}$**

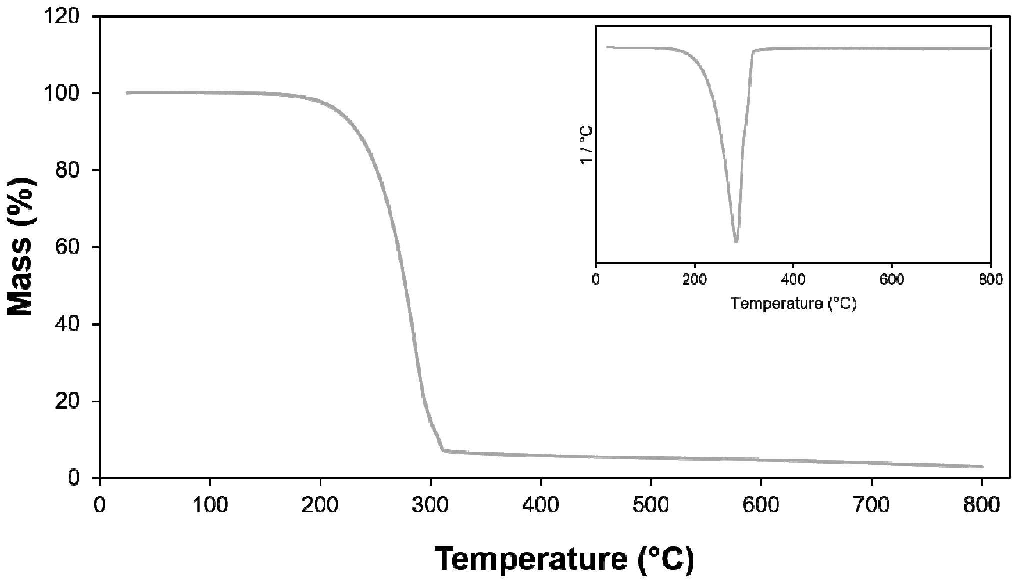


Figure S5 Mass loss curve and dTGA from thermogravimetric analysis for the $\mathbf{H_5O_5S_{90}}$

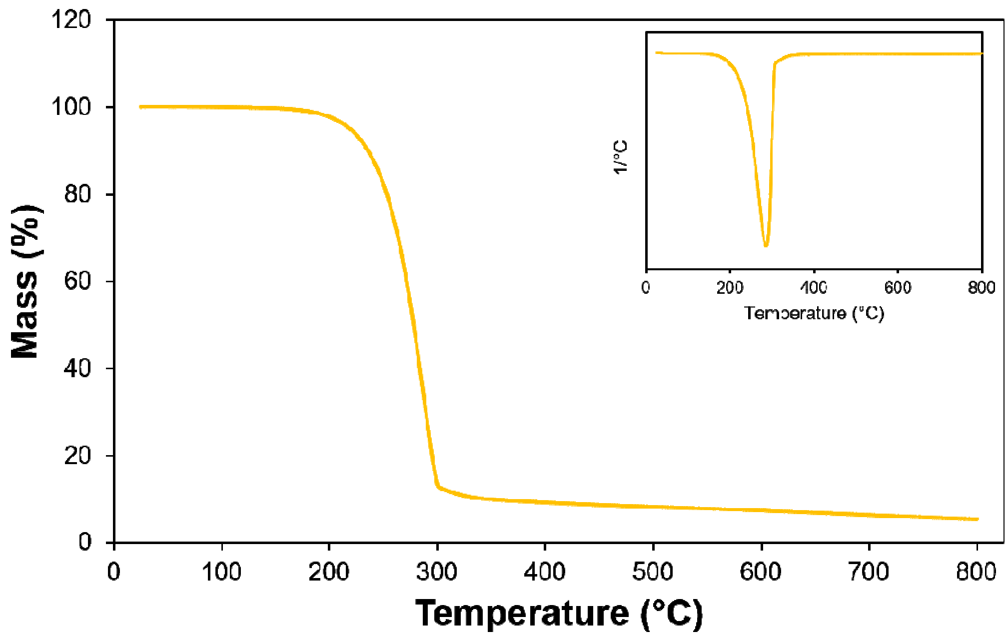


Figure S6 Mass loss curve and dTGA from thermogravimetric analysis for the $\mathbf{H_8O_2S_{90}}$.

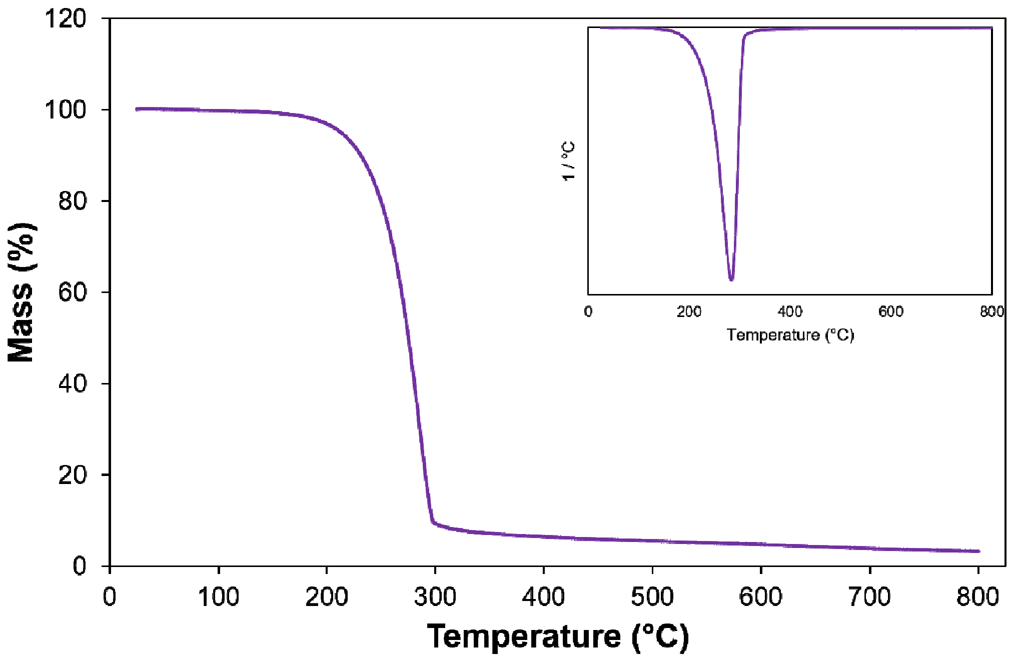


Figure S7 Mass loss curve and dTGA from thermogravimetric analysis for the **WFFS$_{90}$**.

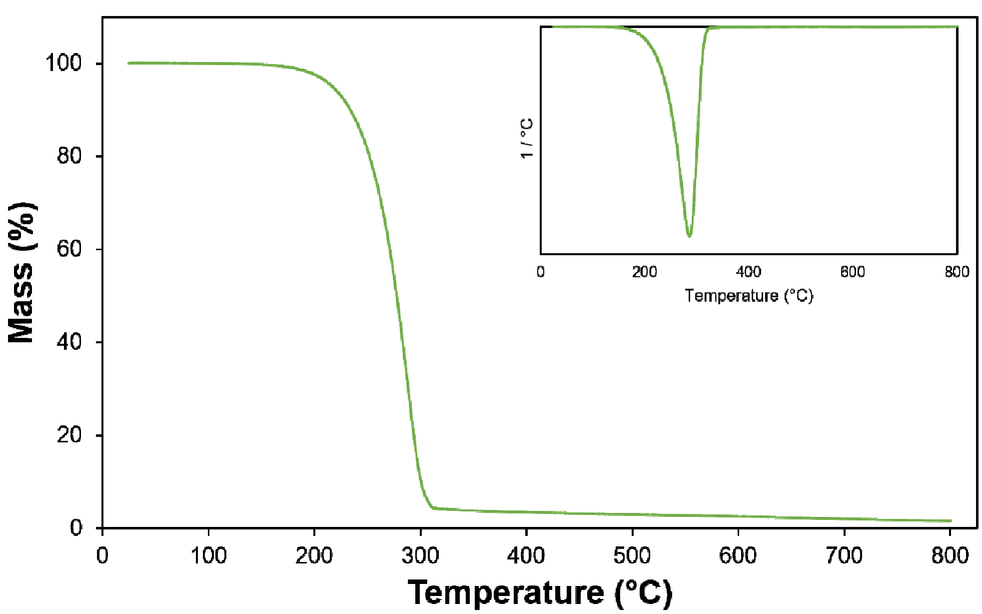


Figure S8 Mass loss curve and dTGA from thermogravimetric analysis for the **DFFS$_{90}$**.

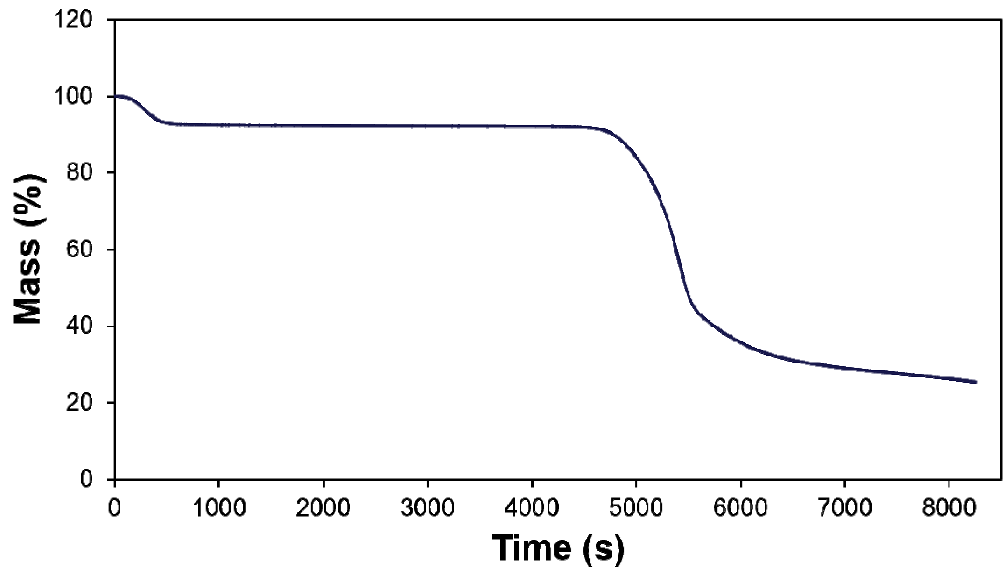


Figure S9 Mass loss curve for peanut hulls from thermogravimetric analysis. Two dynamic ranges were 25-120 and 120-800 °C and isothermal analysis was performed at 120°C for 60 min.

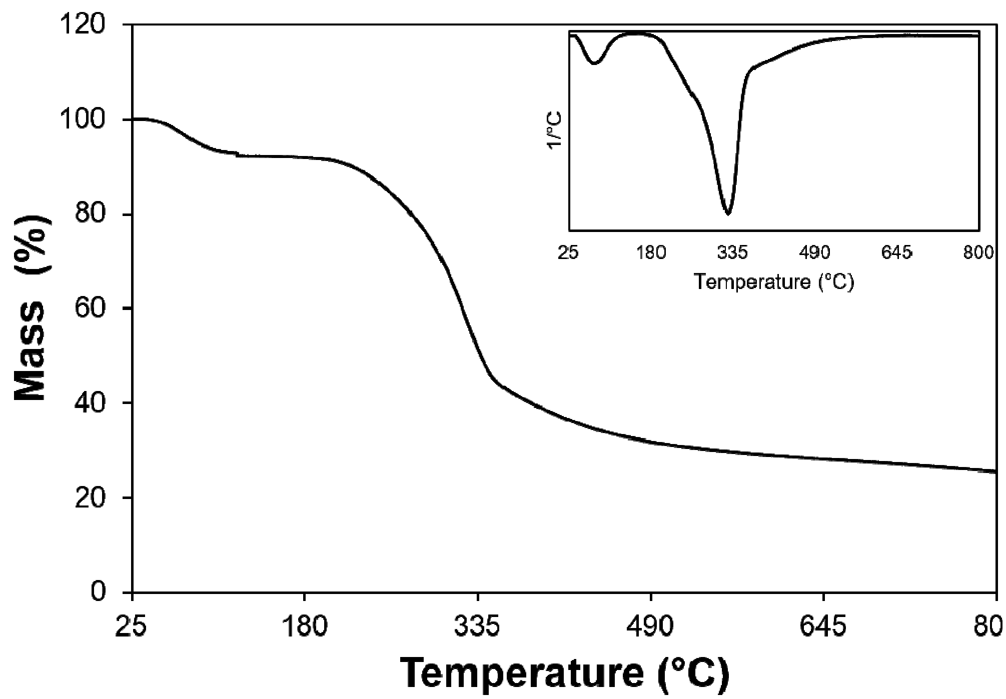


Figure S10 Mass loss curve and dTGA from thermogravimetric analysis for the peanut hulls.

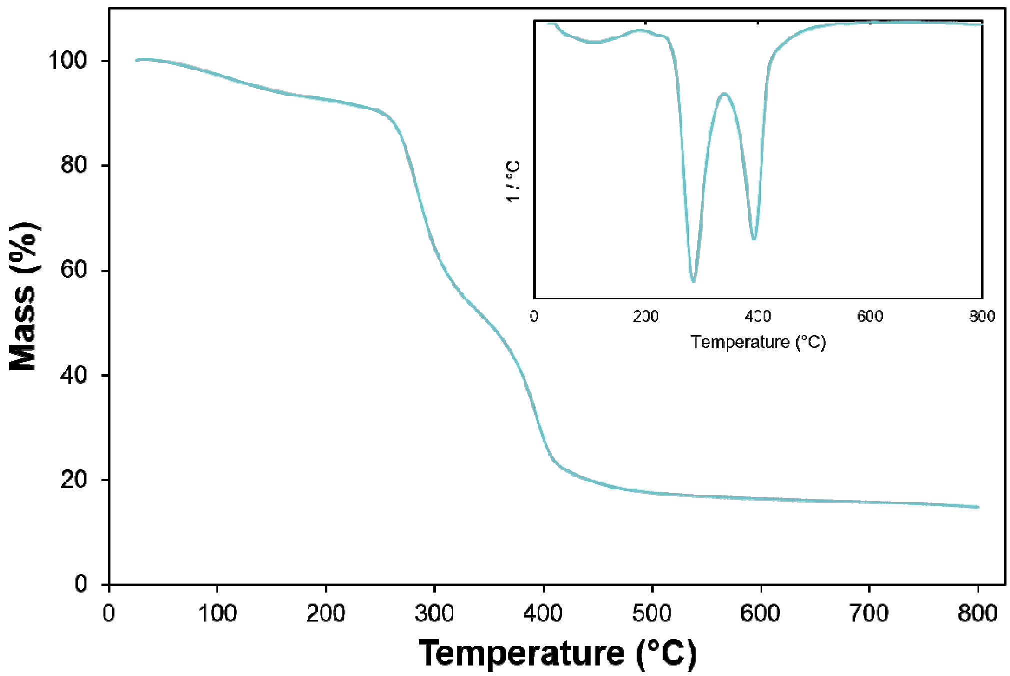


Figure S11 Mass loss curve and dTGA from thermogravimetric analysis for the wet French fries.

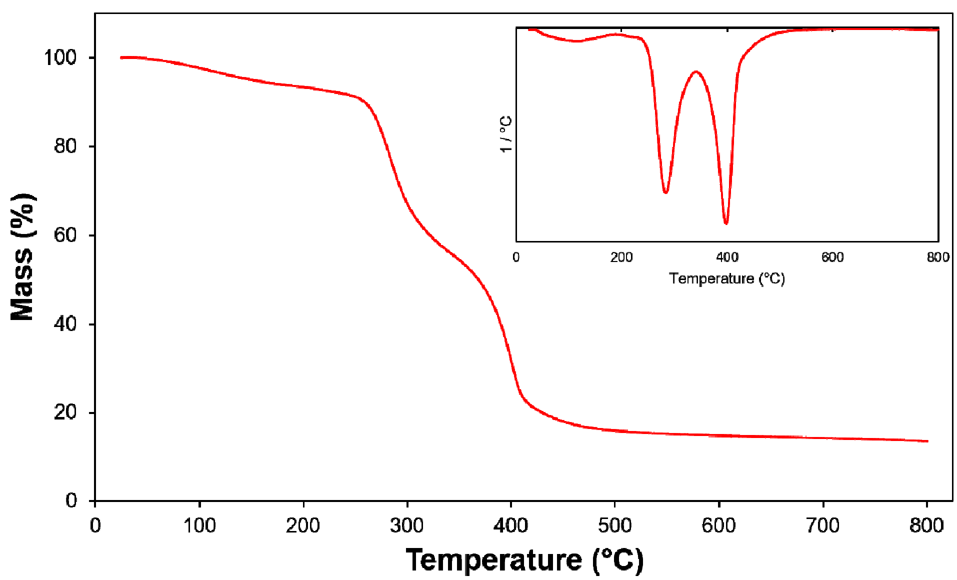


Figure S12 Mass loss curve and dTGA from thermogravimetric analysis for the dry French fries.

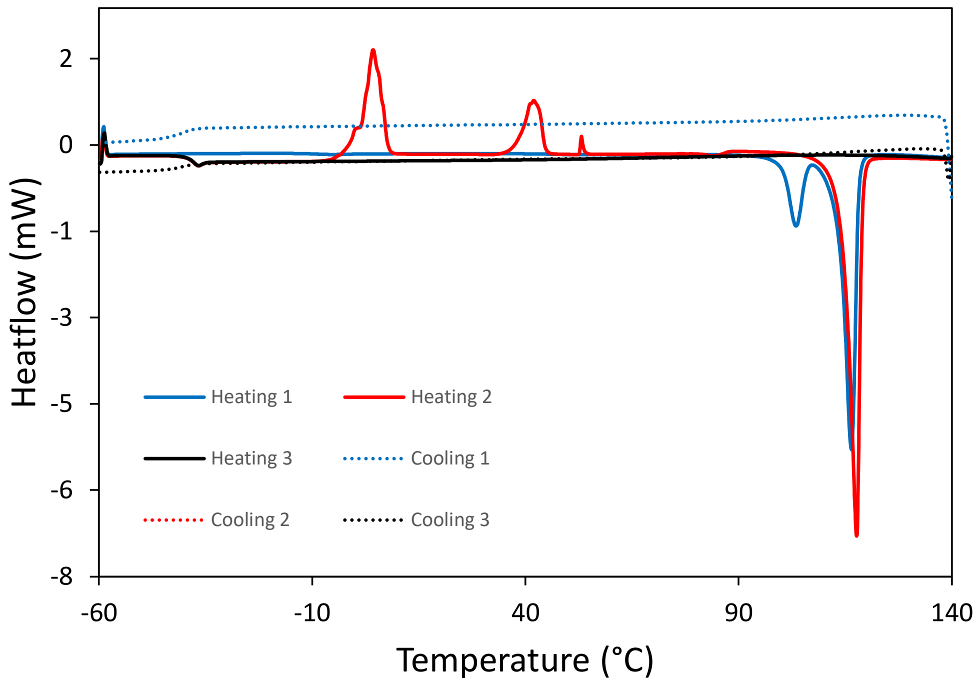


Figure S13 Differential scanning calorimetry (DSC) traces for $\mathbf{H_0O_{10}S_{90}}$. Heating cycles are shown as solid lines and and cooling cycles as dotted lines.

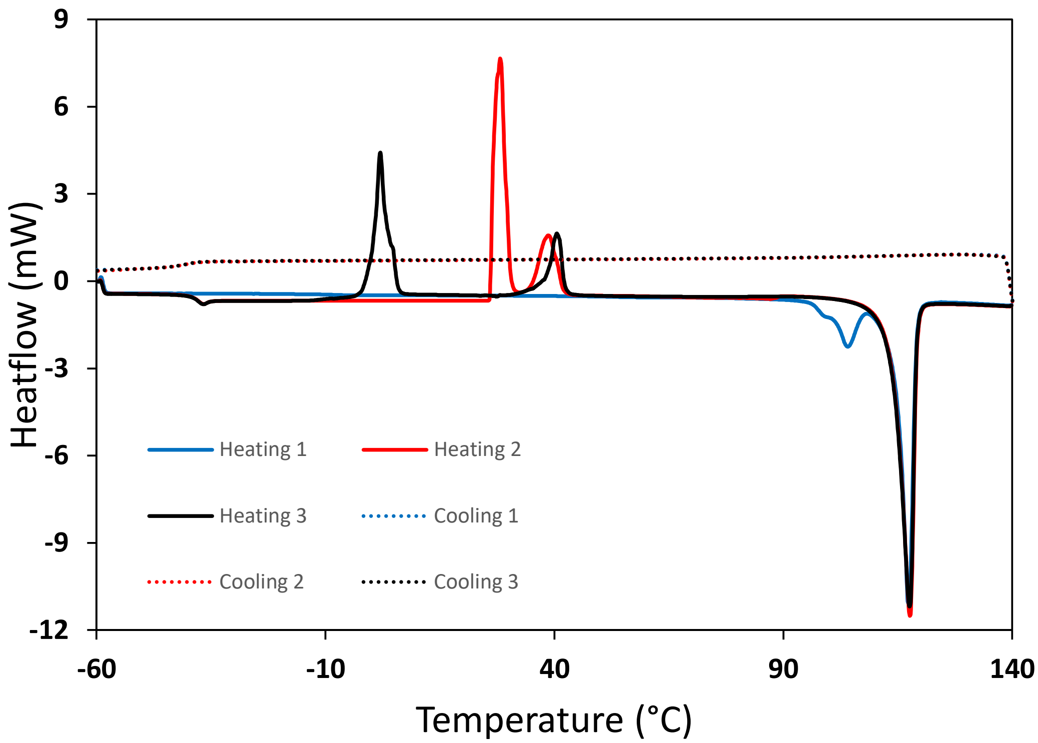


Figure S14 Differential scanning calorimetry (DSC) traces for $\mathbf{H_5O_5S_{90}}$. Heating cycles are shown as solid lines and, cooling cycles as dotted lines.

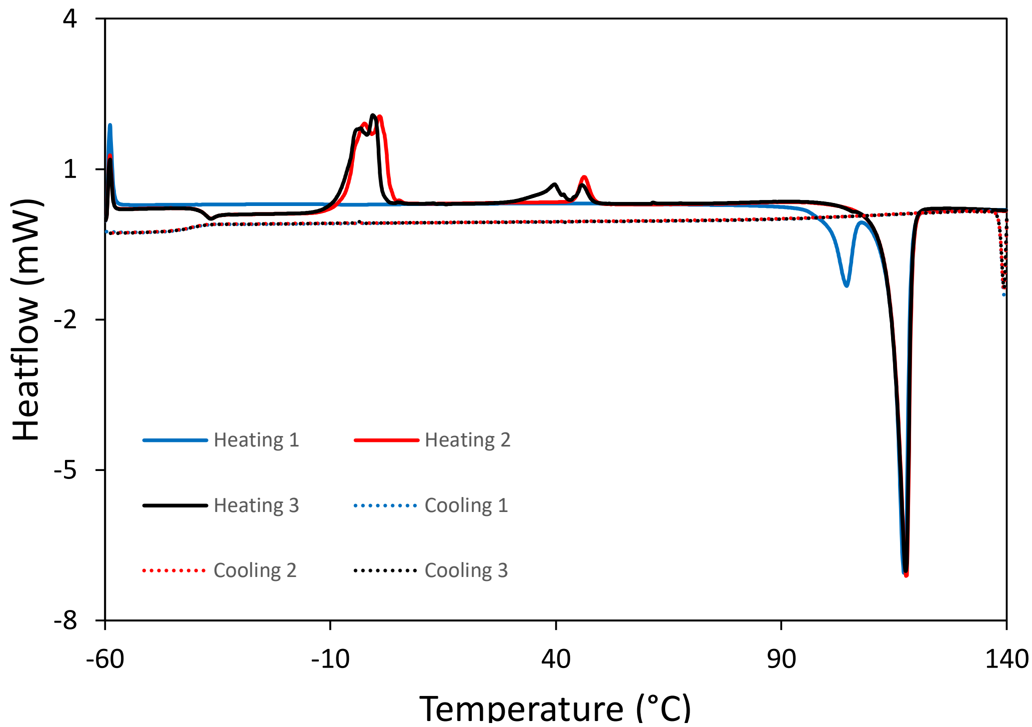


Figure S15 Differential scanning calorimetry (DSC) traces for **$H_8O_2S_{90}$**. Heating cycles are shown as solid lines and, cooling cycles as dotted lines.

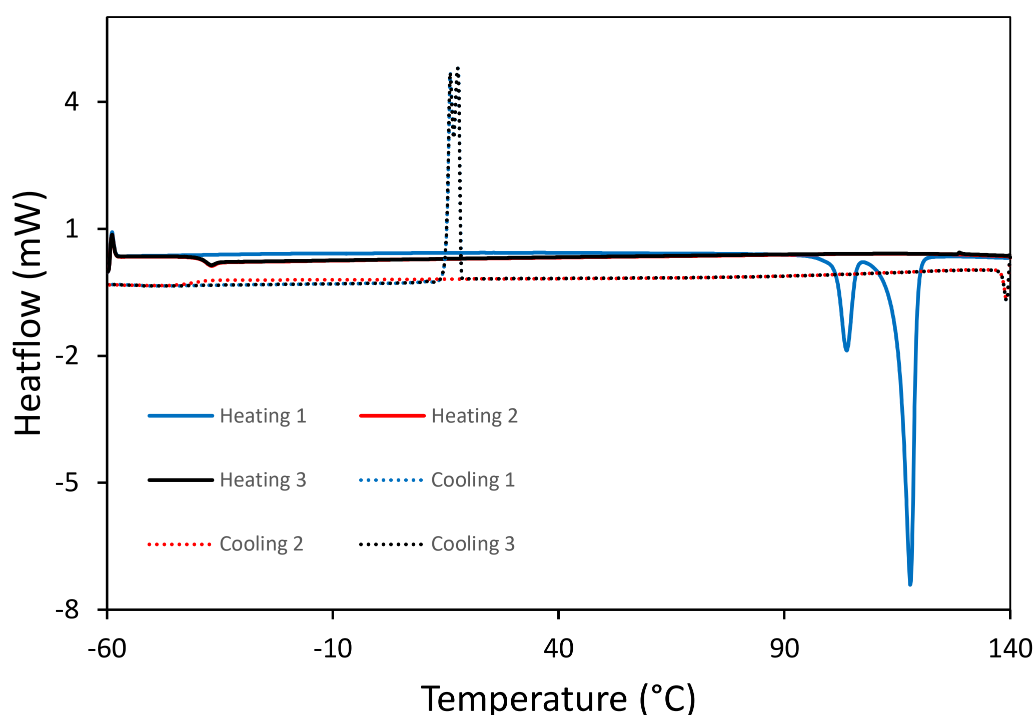


Figure S16 Differential scanning calorimetry (DSC) traces for W**FFS_{90}**. Heating cycles are shown as solid lines and, cooling cycles as dotted lines.

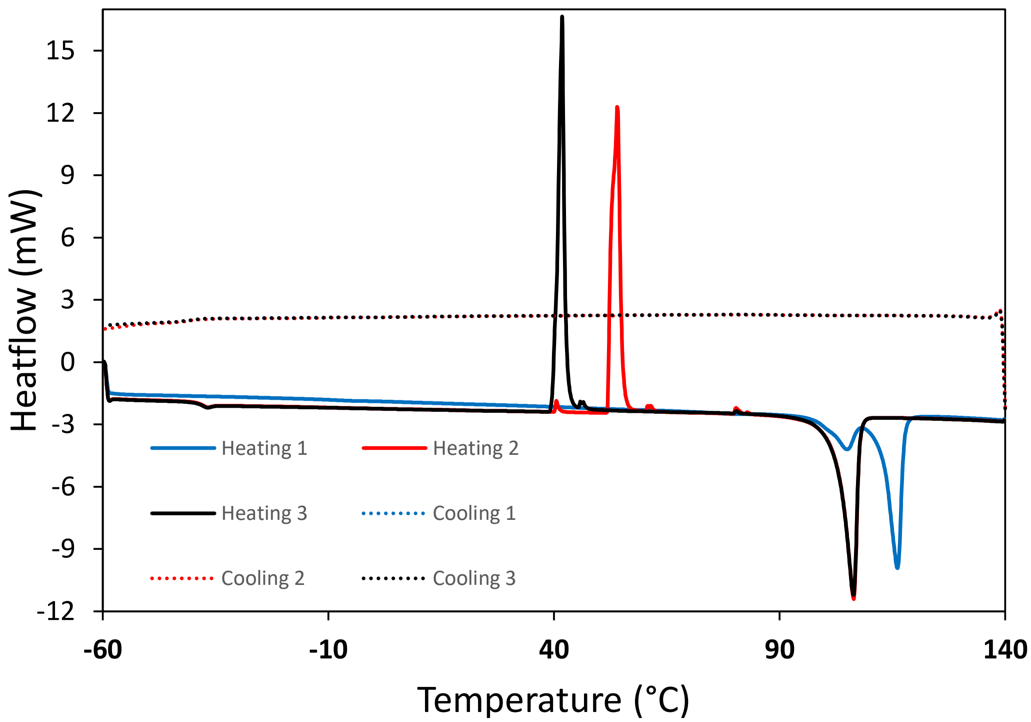


Figure S17 Differential scanning calorimetry (DSC) traces for **$DFFS_{90}$**. Heating cycles are shown as solid lines and, cooling cycles as dotted lines.

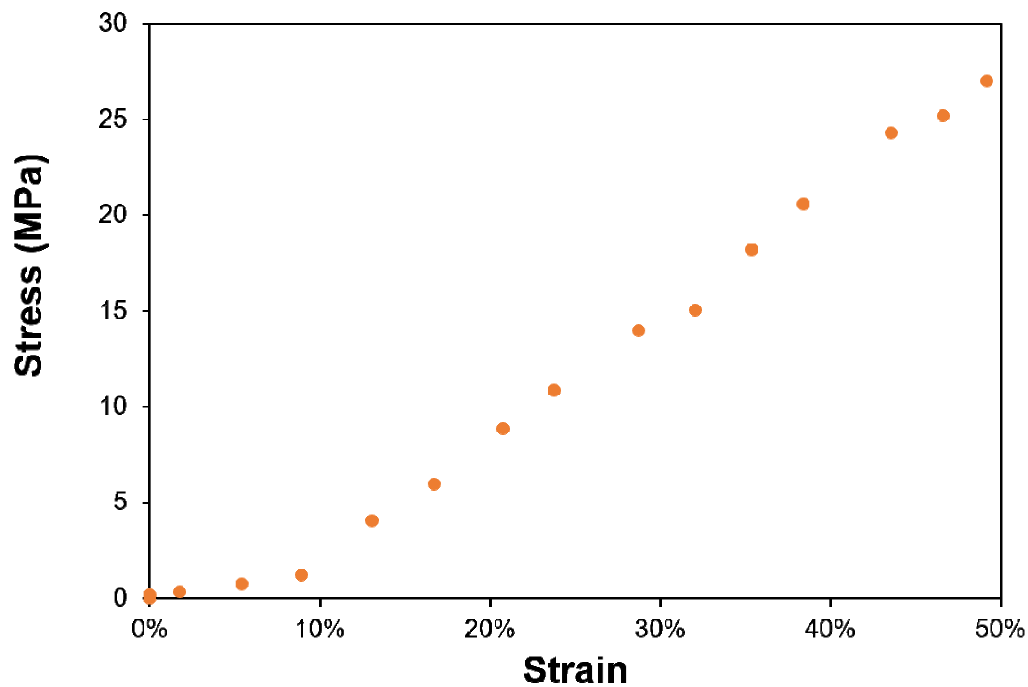


Figure S18 Stress-strain plots for measurements of the compressive strength of **$H_0O_{10}S_{90}$** after 4d at room temperature.

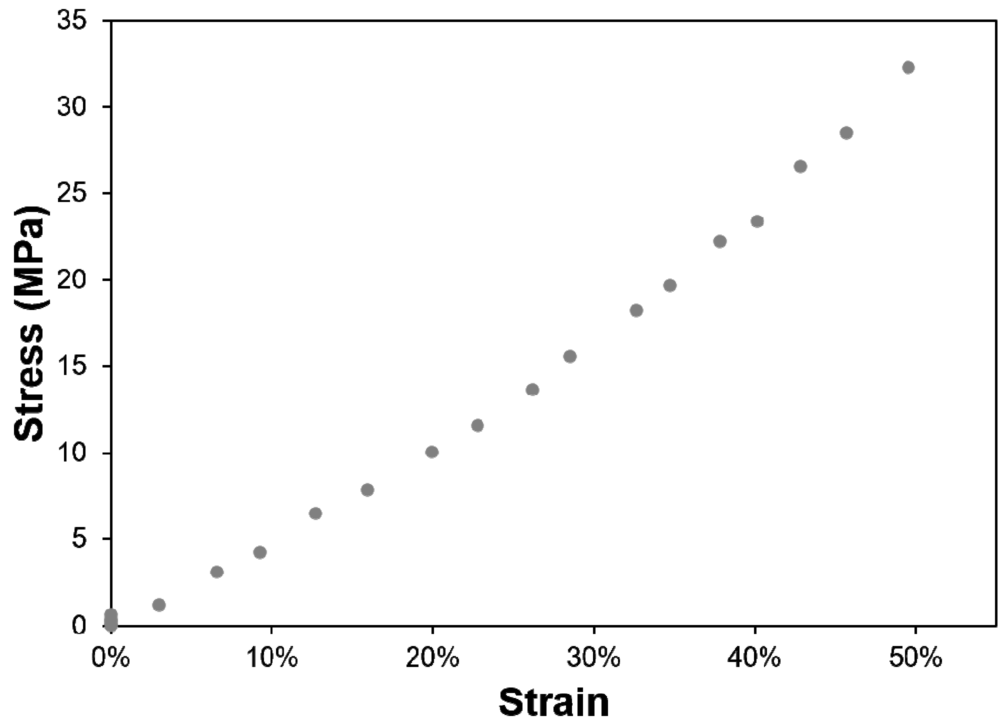


Figure S19 Stress-strain plots for measurements of the compressive strength of **$H_5O_5S_{90}$** after 4d at room temperature.

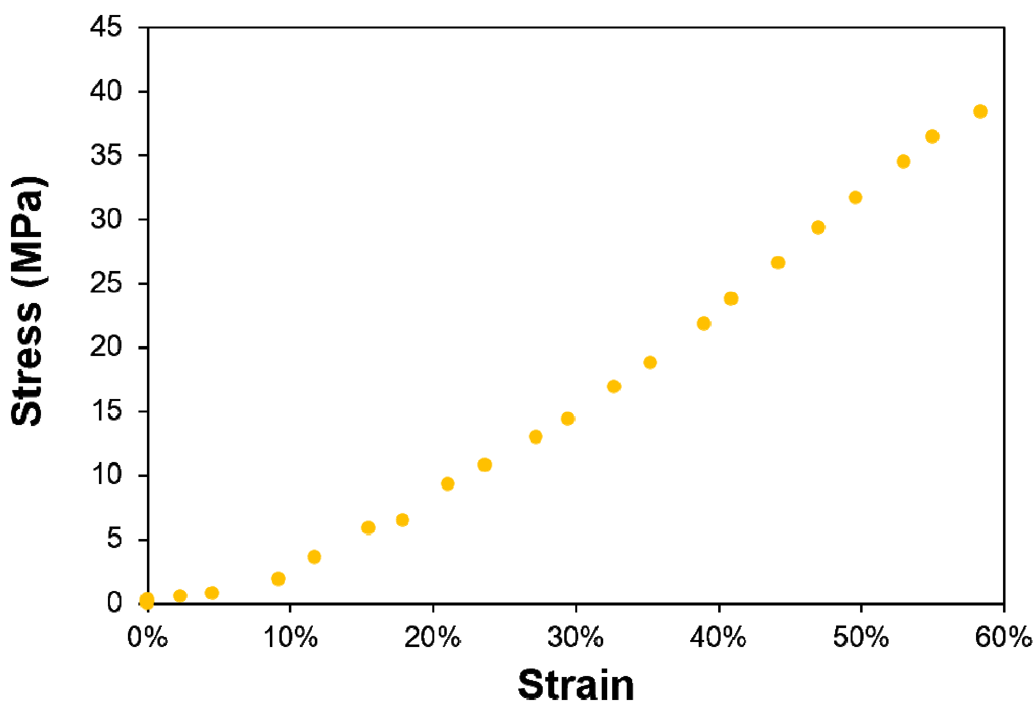


Figure S20 Stress-strain plots for measurements of the compressive strength of **$H_8O_2S_{90}$** after 4d at room temperature.

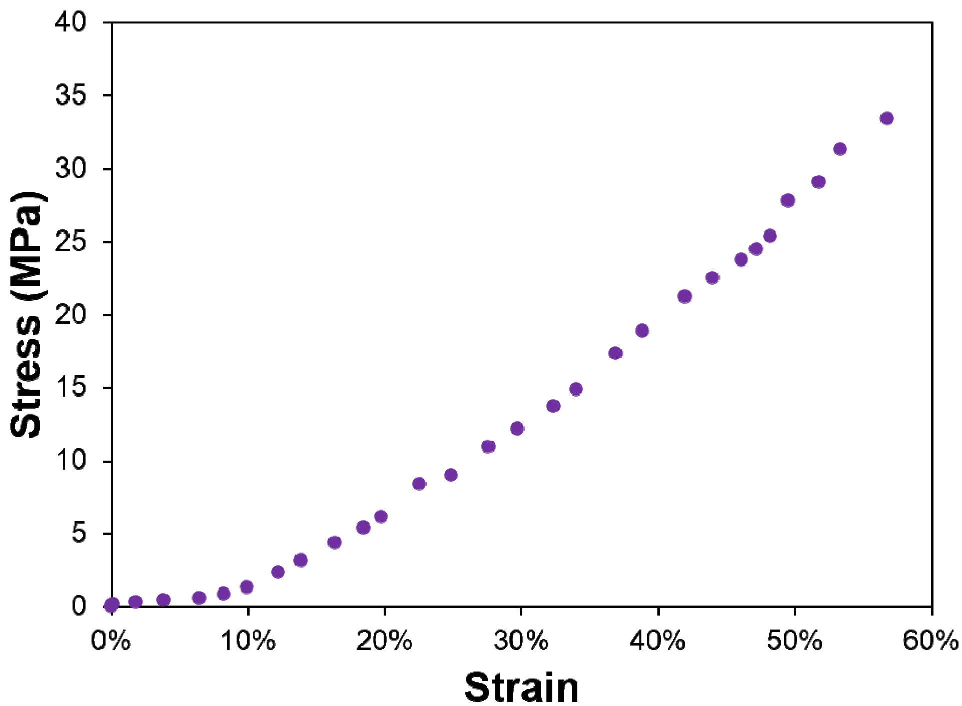


Figure S21 Stress-strain plots for measurements of the compressive strength of **WFFS$_{90}$** after 4d at room temperature.

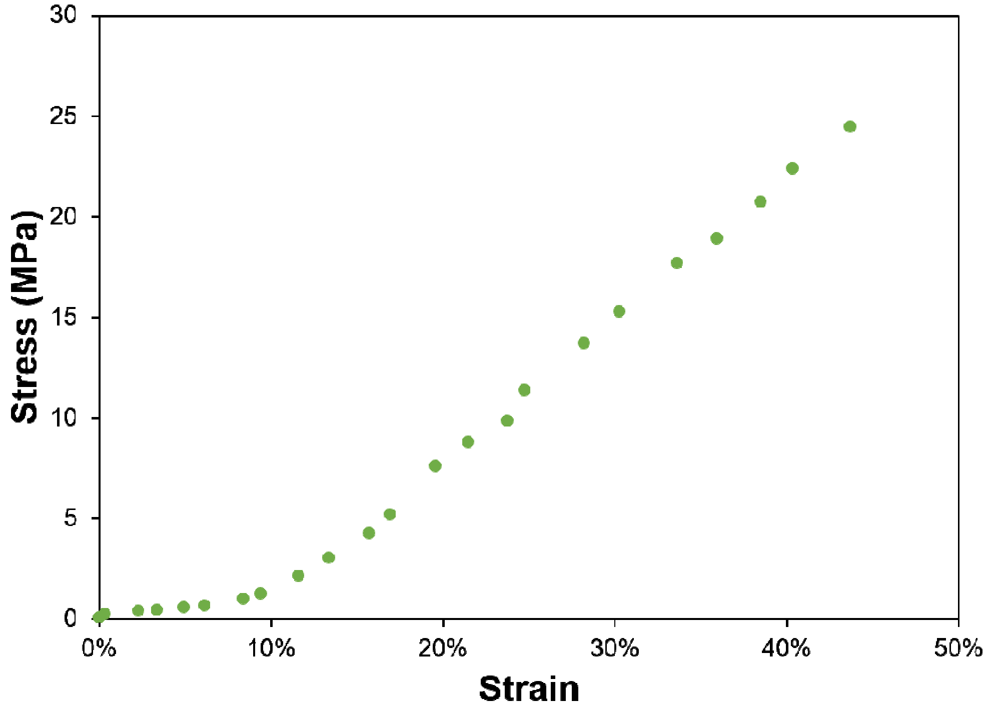


Figure S22 Stress-strain plots for measurements of the compressive strength of **DFFS$_{90}$** after 4d at room temperature.

Calculating the Global Warming Potential of ***$H_xO_yS_{90}$***

For this current calculation it was assumed that the sulfur would remain landfilled if it were not used in this process, so its use does not in itself count for or against the synthesis of **$H_xO_yS_{90}$** in terms of carbon content of constituents, but sulfur will factor into heat requirements for the process as described below. The organic components of **$H_xO_yS_{90}$** factored into the calculation are thus peanut oil and peanut hulls. The calculation assumes that these materials would be incinerated if they were not used to prepare **$H_xO_yS_{90}$**, with values of 1.62 kg CO_2 e/kg for the incineration of the hulls or oils, when the carbon content of these constituents is taken as a conservative estimate of 50%. The amount of CO_2 required to make the peanut oil is 7.54 kg CO_2 e/kg[1] and for peanut hulls it is 1.47 kg CO_2 e/kg.[2] Use of the hulls are treated as a waste product whose recovery offsets the CO_2 cost of making the peanuts from which the hulls were derived, while the use of peanut oil, a useful commodity, is treated as a carbon cost. To estimate the amount of energy needed to heat the **$H_xO_yS_{90}$** reaction mixture from 20 °C to 180 °C and to hold it at that temperature for 24 h, we use metrics for sulfur, which makes up 90 wt. % of the mixture. The energy needed to accomplish heating was thus calculated to be 0.016 kg CO_2e/kg on the basis of the heat capacity and heat of fusion of sulfur [3] over the range of 20 °C to 180 °C and assuming a 90% efficiency for heat retention during the 24 h holding period (thus holding contributes negligibly to the overall heat), and taking an average carbon intensity of 0.500 kg CO_2e/kWh for the electricity source.[4-9] The tables below summarize the calculations of global warming potentials for the **$H_xO_yS_{90}$** composites.

$H_0O_{10}S_{90}$

Process	**Cost (+) or Credit (–)?**	**Value (kg CO_2e)**
Make Peanut Oil (0.1 kg × 7.54 kg CO_2e/kg)	+	0.754
Heating (1.00 kg of sulfur × 0.016 kg CO_2e/kg)	+	0.016
Prevent Incineration of Peanut Oil (0.1 kg × 1.62 kg CO_2e/kg)	–	0.162
	TOTAL	**+0.608 kg CO_2e/kg**

$H_5O_5S_{90}$

Process	**Cost (+) or Credit (–)?**	**Value (kg CO_2e)**
Make Peanut Oil (0.05 kg × 7.54 kg CO_2e/kg)	+	0.377
Make Peanut Hull (0.05 kg × 1.47 kg CO_2e/kg)	–	0.0735
Heating (1.00 kg of sulfur × 0.016 kg CO_2e/kg)	+	0.016
Prevent Incineration of Oil/Hulls (0.05 kg × 1.62 kg CO_2e/kg)	–	0.162
	TOTAL	**+0.158 kg CO_2e/kg**

$H_8O_2S_{90}$

Process	**Cost (+) or Credit (–)?**	**Value (kg CO_2e)**
Make Peanut Oil (0.02 kg × 7.54 kg CO_2e/kg)	+	0.151
Make Peanut Hull (0.08 kg × 1.47 kg CO_2e/kg)	–	0.118
Heating (1.00 kg of sulfur × 0.016 kg CO_2e/kg)	+	0.016
Prevent Incineration of Oil/Hulls (0.05 kg × 1.62 kg CO_2e/kg)	–	0.162
	TOTAL	**–0.113 kg CO_2e/kg**

$H_{10}O_0S_{90}$

Process	**Cost (+) or Credit (–)?**	**Value (kg CO_2e)**
Make Peanut Hull (0.1 kg × 1.47 kg CO_2e/kg)	–	0.147
Heating (1.00 kg of sulfur × 0.016 kg CO_2e/kg)	+	0.016
Prevent Incineration of Peanut Hull (0.05 kg × 1.62 kg CO_2e/kg)	–	0.162
	TOTAL	**–0.293 kg CO_2e/kg**

Calculating the Global Warming Potential of ***WFFS90*** *and* ***DFFS90***

The calculation is carried out as described above for the **$H_xO_yS_{90}$** composites, but instead of hulls and oil the fries were employed as the organic materials, using a value of 3.62 kg CO_2e/kg for production of French fries[2] before drying and taking their use as a feedstock for a valuable product as an offset that would otherwise have been lost in a landfill. The amount of heat needed to drive off the water found in the fries is also included as an energy cost, taking the average carbon intensity of 0.500 kg CO_2e/kWh for the electricity source used to apply the heat.[4-9] We assume that the fry waste would not have been incinerated if they were not used in this process. The tables below summarize the calculations of global warming potentials for the **$WFFS_{90}$** and **$DFFS_{90}$** composites.

$WFFS_{90}$

Process	**Cost (+) or Credit (–)?**	**Value (kg CO_2e)**
Make Fries (0.1 kg × 3.62 kg CO_2e/kg)	–	0.362
Heating and Evaporating 0.041 kg water	+	0.015
Heating (1.00 kg of sulfur × 0.016 kg CO_2e/kg)	+	0.016
	TOTAL	**–0.331 kg CO_2e/kg**

$DFFS_{90}$

Process	**Cost (+) or Credit (–)?**	**Value** (kg CO_2e)
Make Fries (0.17 kg × 3.62 CO_2e/kg)	–	0.615
Heating and Evaporating 0.069 kg water	+	0.025
Heating (1.00 kg of sulfur × 0.016 kg CO_2e/kg)	+	0.016
	TOTAL	**–0.574 kg CO_2e/kg**

Author Contributions

Conceptualization, R.C.S.; methodology, R.C.S.; formal analysis, R.C.S, B.G.S.G. and A.G.T.; investigation, B.G.S.G., P.Y.S., N.L.K.D., K.M.D., and S.K.W.; resources, R.C.S. and A.G.T.; data curation, B.G.S.G., P.Y.S., N.L.K.D., K.M.D., and S.K.W.; writing—original draft preparation, all authors; writing—review and editing, all authors; supervision, R.C.S. and A.G.T.; funding acquisition, R.C.S. All authors have read and agreed to the published version of the manuscript.

Supporting Information References

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