Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supplementary Information for:

Evaluating the Bis-isoxazole Core for Energetic Heterocyclic-Based Oligomers

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Experimental Data and Crystallographic Refinement Details

For **2**, a clear colorless block crystal of dimensions 0.208 x 0.117 x 0.030 mm^3 was mounted on a MiteGen MicroMesh using a small amount of Cargille Immersion Oil. Data were collected on a Bruker three-circle platform diffractometer equipped with a PHOTON II CPAD detector. The crystals were irradiated using a 1 μs microfocus CuKα source (λ= 1.54178) with Montel optics. Data was collected at room temperature (20 °C).

Data collection was performed, and the unit cell was initially refined using *APEX3* [v2015.5-2].[1] Data Reduction was performed using *SAINT* [v8.34A][2] and *XPREP* [v2014/2][3]. Corrections were applied for Lorentz, polarization, and absorption effects using *SADABS* [v2014/2].[4] The structure was solved and refined with the aid of the program SHELXL-2014/7.[5] The full-matrix least-squares refinement on F^2 included atomic coordinates and anisotropic thermal parameters for all non-H atoms. Hydrogen atoms were located from the difference electron-density maps and added using a riding model. Crystallographic data for the structure was deposited with the Cambridge Crystallographic Data Centre as publication no. CCDC 2010533. Copies of the data can be obtained free of charge by e-mail: deposit@ccdc.cam.ac.uk.

	2
Formula	$C_{22}H_{18}N_4O_6$
FW	434.4
Habit	Block
Color	Clear Colorless
T	293(2) K
λ	1.54178 Å
Lattice	Triclinic
Space group	P-1
a (Å)	9.4021(3)
b (Å)	13.6517(3)
c (Å)	24.7468(6)
α (°)	95.6130(14)
β (°)	95.4022(15)
γ (°)	91.5873(15)
V ($Å^3$)	3144.91(14)
Z	6
d_{calc} (g/cm^3)	1.376
μ (mm^{-1})	0.860
Size (mm^3)	0.208 x 0.117 x 0.030
GOF on F^2	1.033
Final R indices [I>2σ(I)]	R_1 = 0.0524 wR_2 = 0.1474
R indices (all data)	R_1 = 0.0905 wR_2 = 0.1668

Table S1. Unit cell and crystal data for the crystal structure of **2**.

Analytical Spectroscopy of 2, 3, 5, and 6

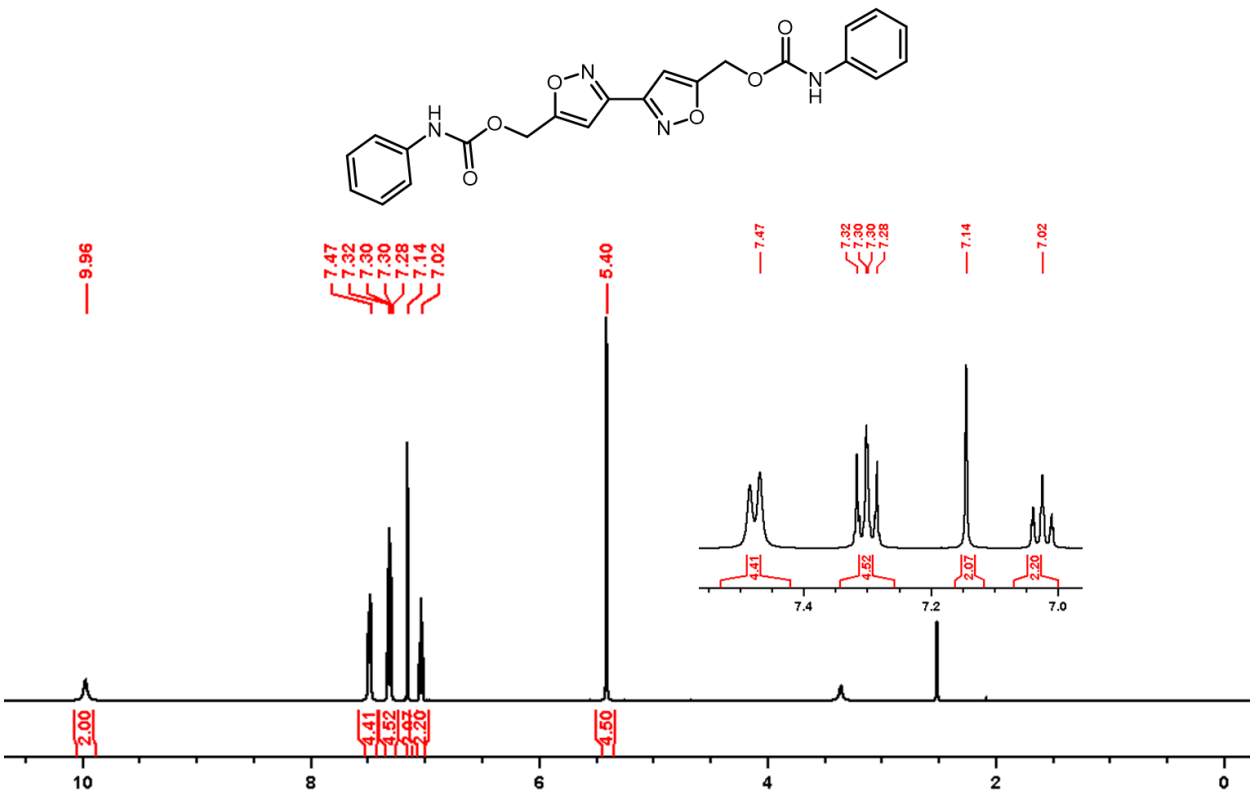

Figure S1. ^{1}H NMR spectra of **2**. Solvent: DMSO-d_6, 500 MHz, δ in ppm.

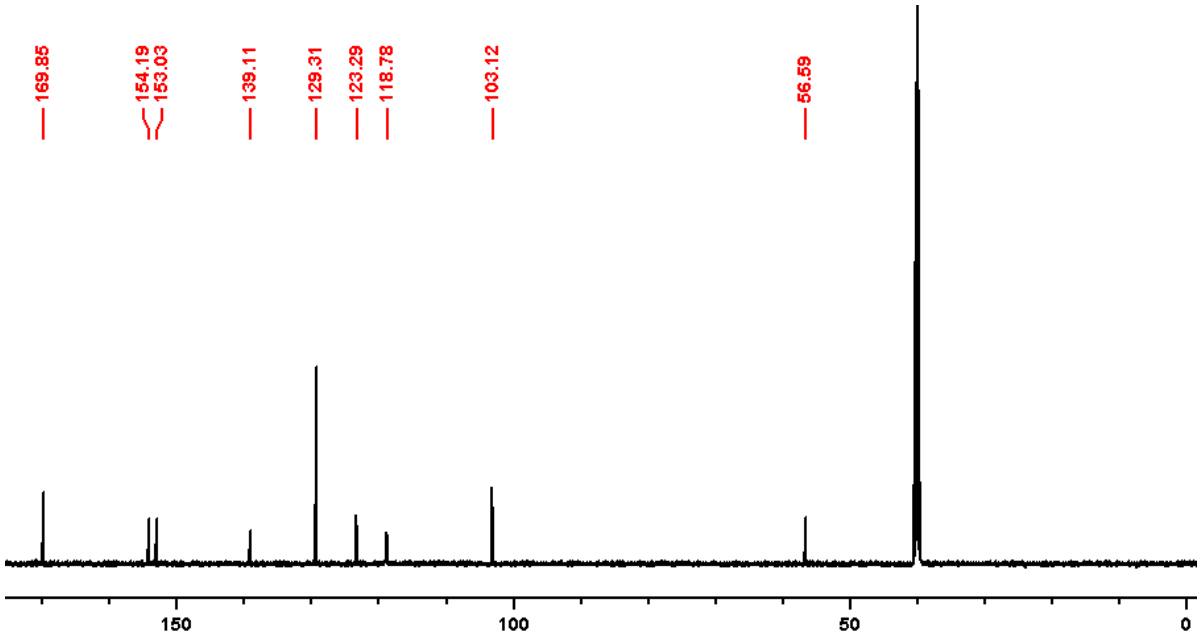

Figure S2. ^{13}C NMR spectrum of **2**. Solvent: DMSO-d_6, 500 MHz, δ in ppm.

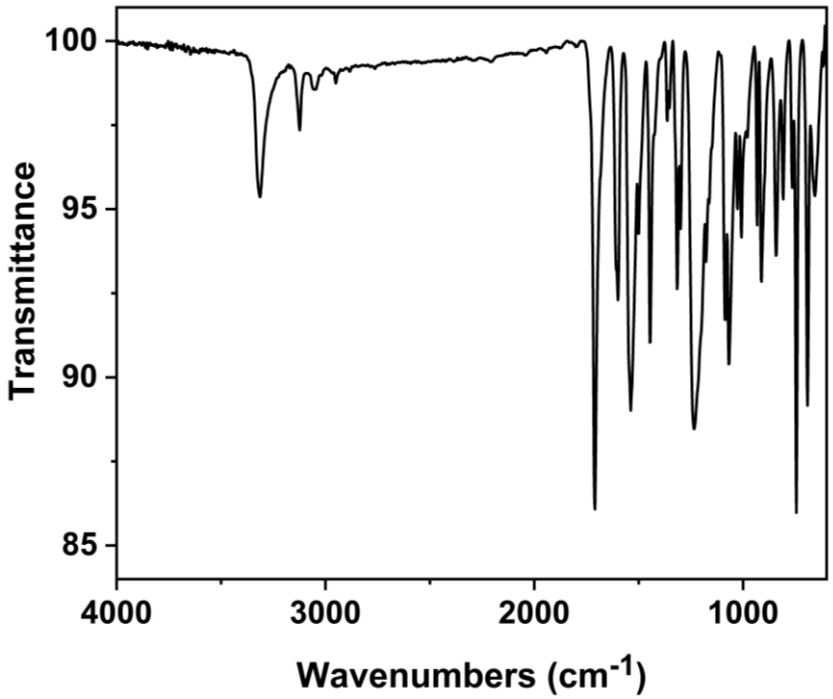

Figure S3. Infrared spectrum of **2**.

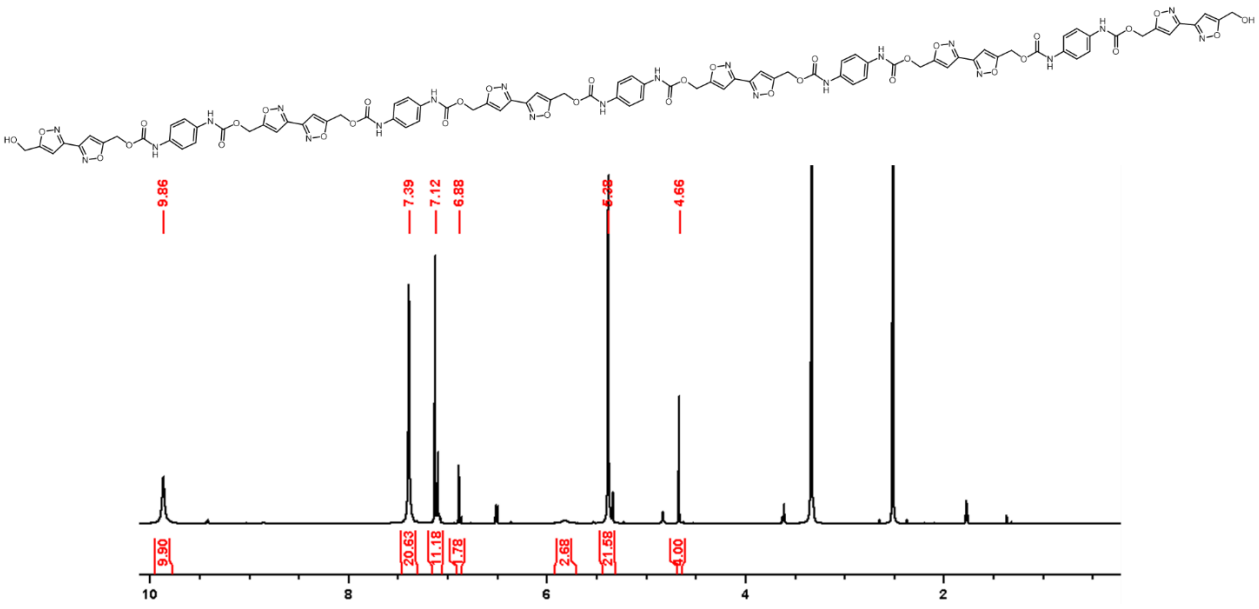

Figure S4. ^{1}H NMR of **3**. Solvent: DMSO-d_6, 500 MHz, δ in ppm.

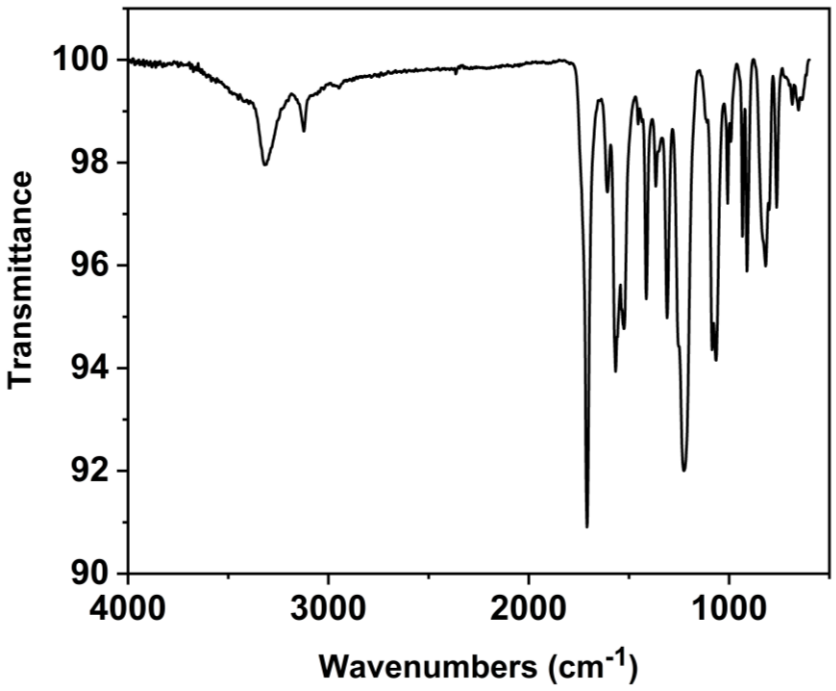

Figure S5. Infrared spectrum of **3**.

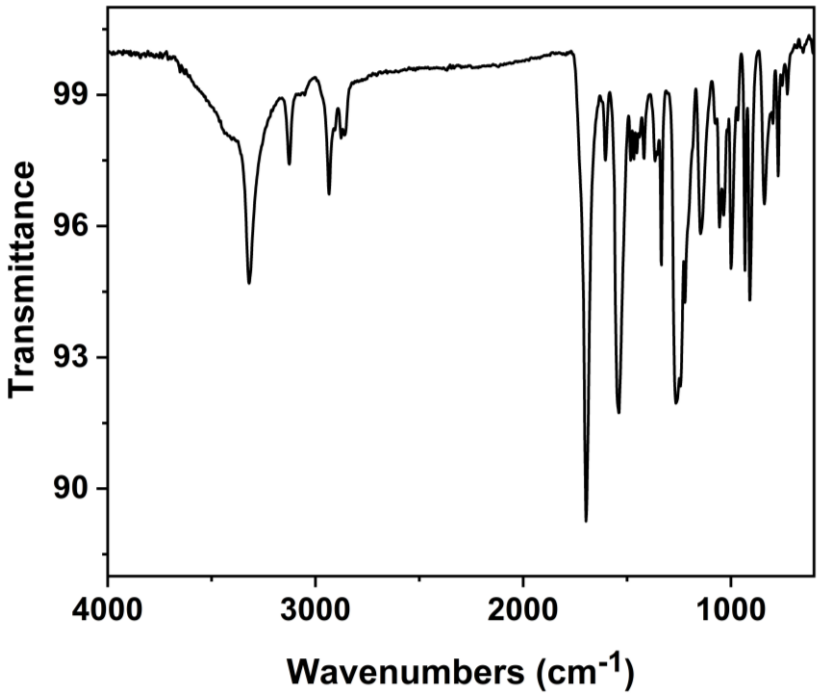

Figure S6. Infrared spectrum of **4**.

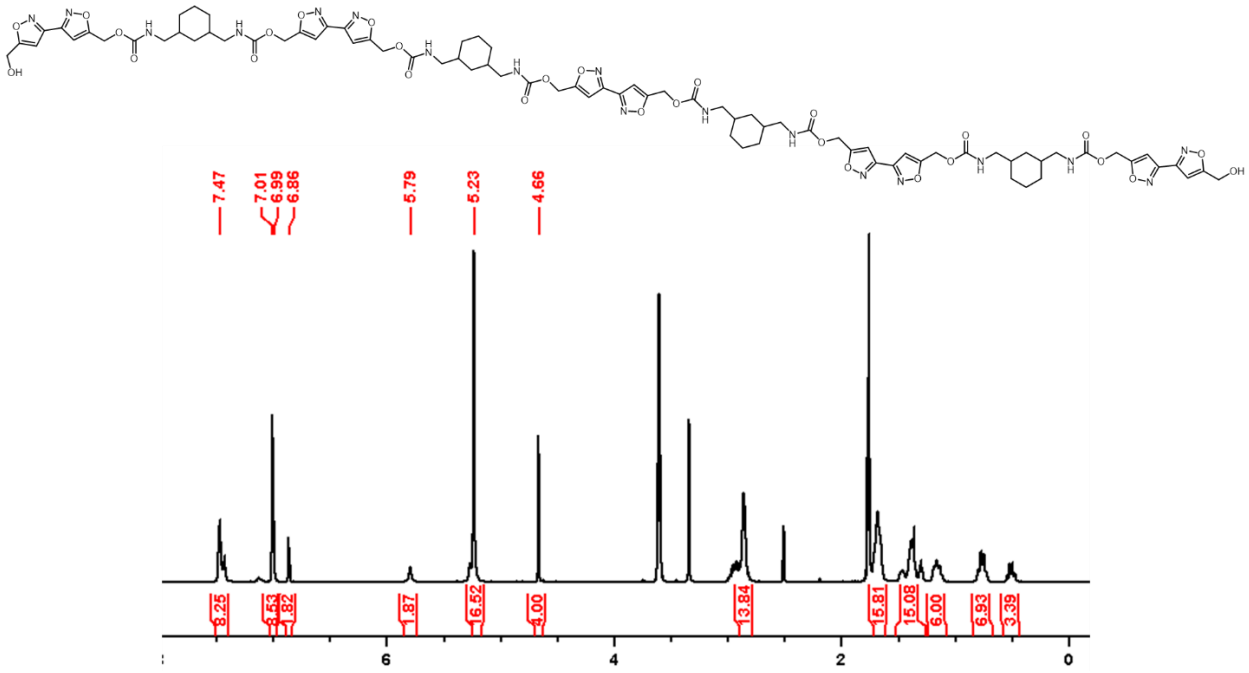

Figure S7. ^{1}H NMR of **5**. Solvent: DMSO-d_6, 500 MHz, δ in ppm.

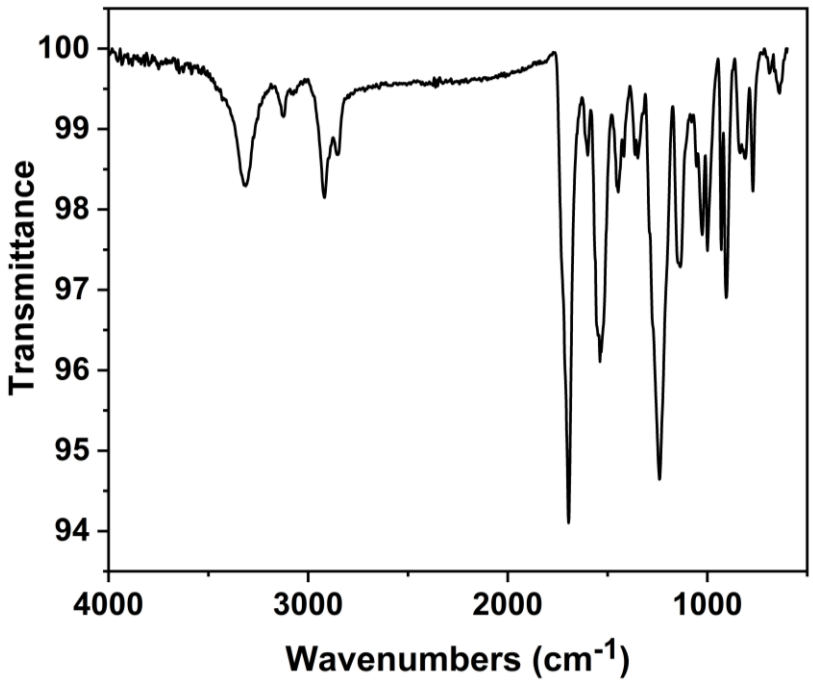

Figure S8. Infrared spectrum of **5**.

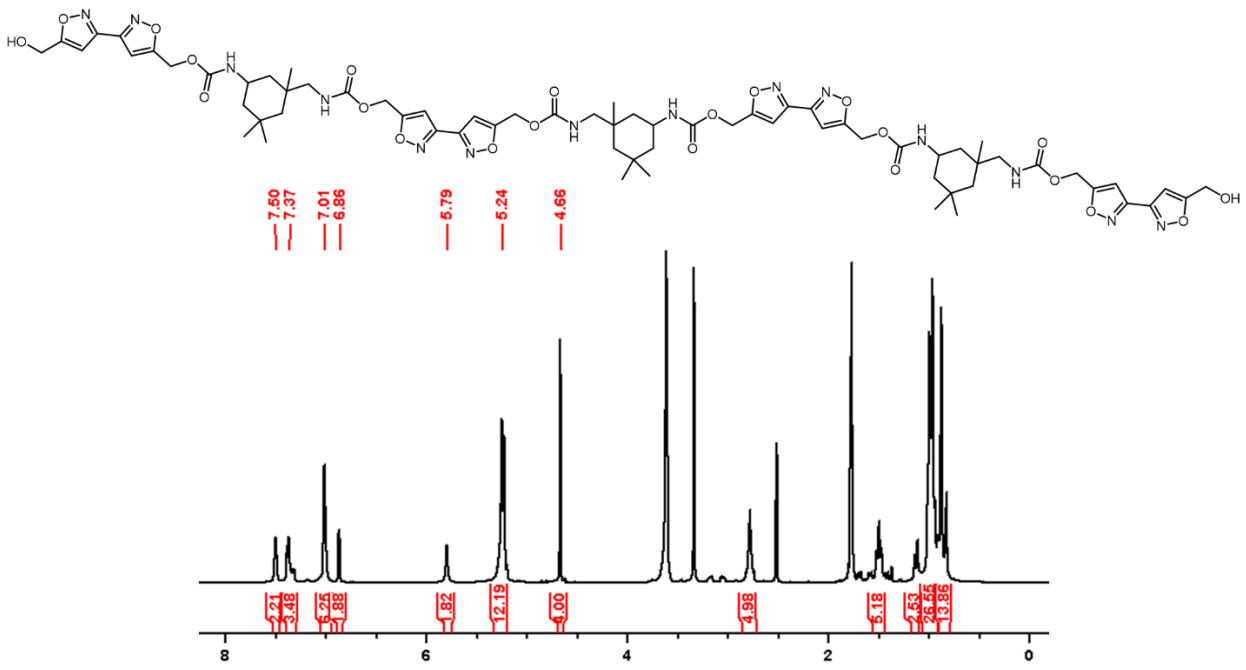

Figure S9. ^{1}H NMR of **6**. Solvent: DMSO-d_6, 500 MHz, δ in ppm.

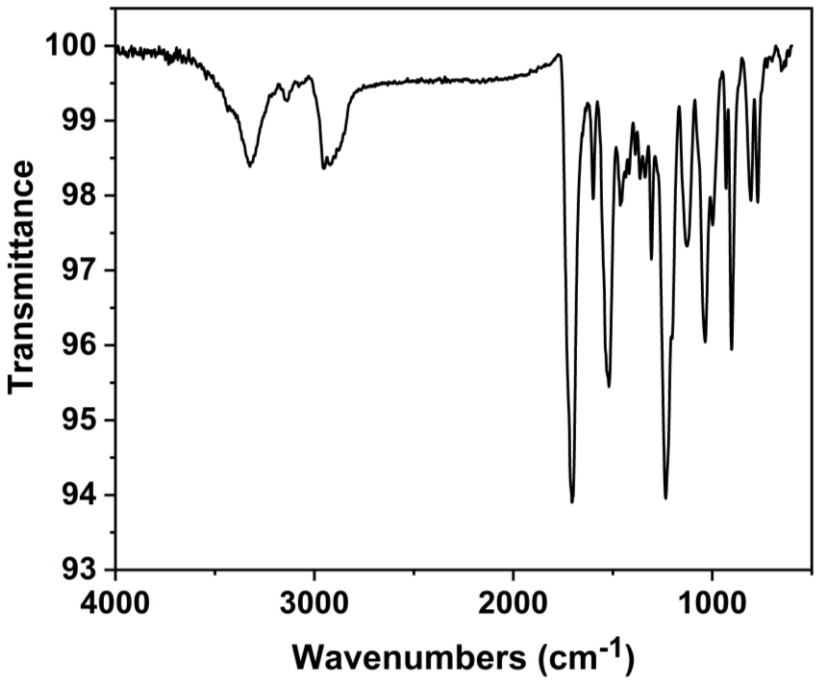

Figure S10. Infrared spectrum of **6.**

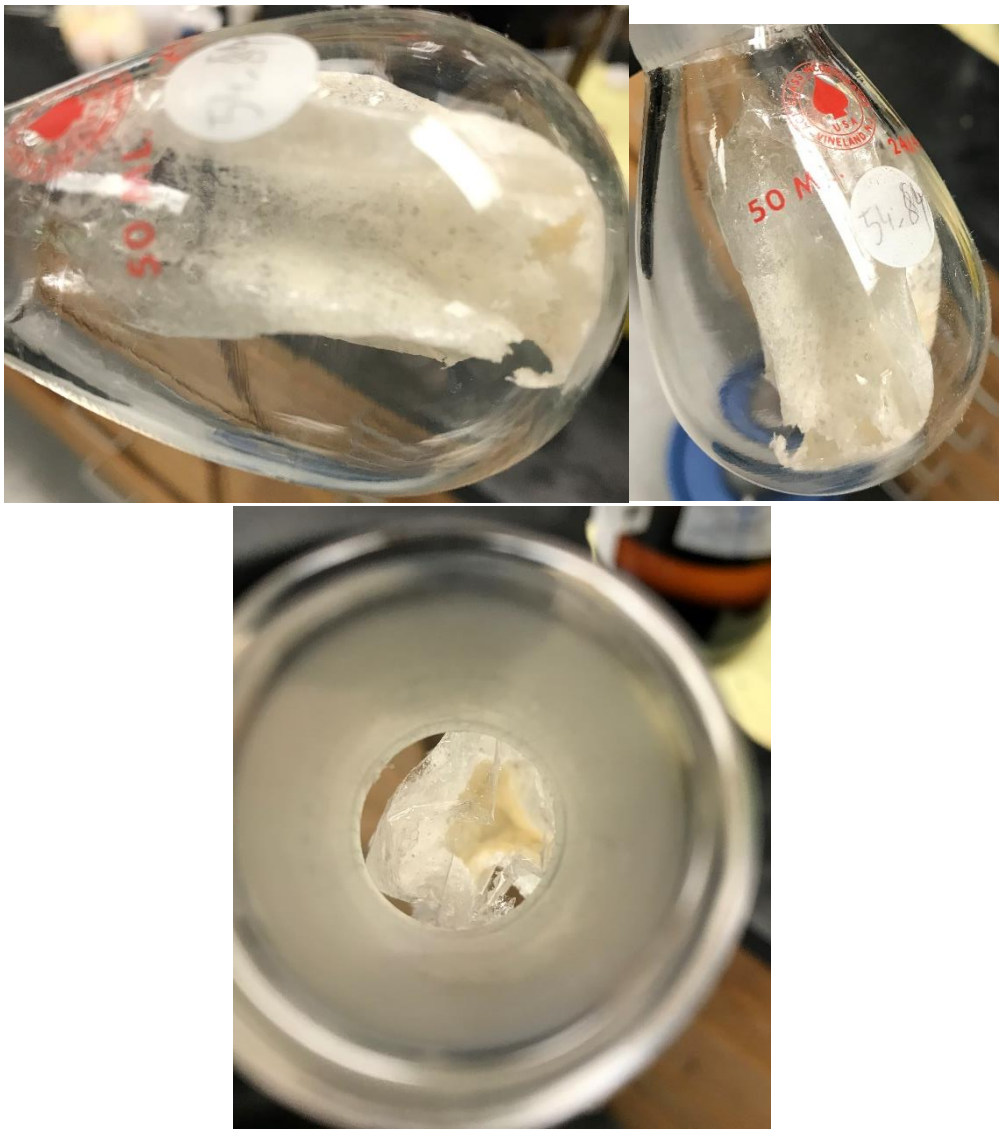

Figure S11. Images of the product of a high temperature reaction resulting in a plastic. Reaction input ratio 10:9. Reaction output ratio 25:24.

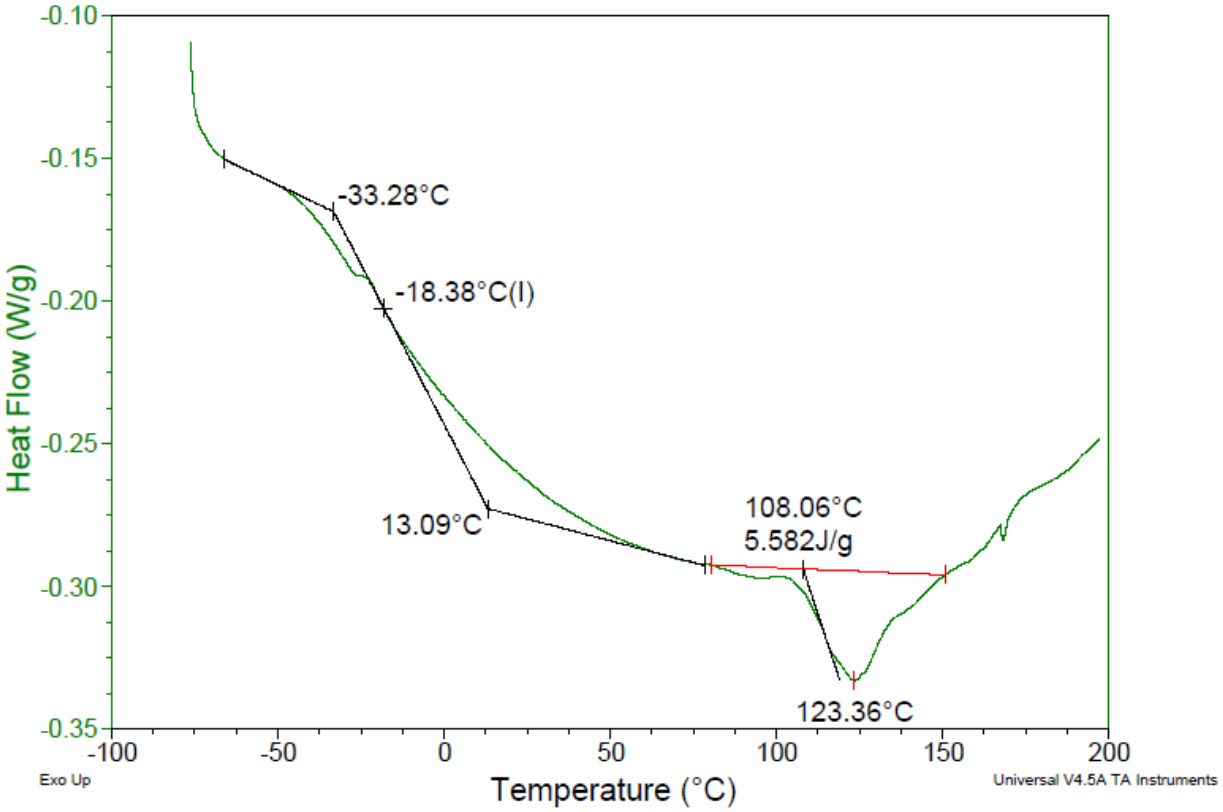

Figure S12. DSC trace of **7** showing T_g and crystalline region melting points.

References

1. Bruker (2015). APEX3 v2015.5-2. Bruker AXS Inc., Madison, Wisconsin, USA.
2. Bruker (2013). SAINT v8.34A. Bruker AXS Inc., Madison, Wisconsin, USA.
3. Bruker (2014). XPREP v2014/2. Bruker AXS Inc., Madison, Wisconsin, USA.
4. Bruker (2014). SADABS v2014/5, Bruker AXS Inc., Madison, Wisconsin, USA.
5. Sheldrick, G. M. (2014). SHELXL-2014/7. University of Göttingen, Germany.

Acknowledgements

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