

Supporting Information for:
Antimicrobial Dye-Conjugated Polyglobalide-Based Organogels

Jason V. Rowley,[†] Patrick Wall,[†] Huayang Yu,[†] Giuseppe Tronci,^{‡§} Deirdre A.

Devine,^{||} Jonathan J. Vernon^{||} and Paul D. Thornton^{†}*

[†]School of Chemistry, [§]Clothworkers' Centre for Textile Materials Innovation for

Healthcare, School of Design, ^{||}Division of Oral Biology, School of Dentistry,

University of Leeds, Leeds LS2 9JT, U.K. [‡]Biomaterials and Tissue Engineering

Research Group, School of Dentistry, St. James's University Hospital, University of

Leeds, Leeds LS9 7TF, U.K.

* P.D.Thornton@leeds.ac.uk

Materials, equipment and settings

All chemicals used were purchased from Sigma-Aldrich and used as received unless otherwise stated. Globalide was received from Symrise and used as received. 3-Mercaptopropionic acid was purchased from Alfa Aesar and used as received. Advanced Polymer Chromatography (APC) was conducted on a Waters Acquity APC system using an Acquity column (Acquity APC TM 200 2.5 µm, 4.5 x 150 mm). The

APC instrument was calibrated against standard poly(methyl methacrylate) samples in tetrahydrofuran (THF). Differential Scanning Calorimetry (DSC) curves were collected using a TA Instruments DSC Q20 instrument with a heating rate of 10 °C min⁻¹ and an inert gas flow of N₂ at a rate of 50 mL min⁻¹. FTIR spectra were recorded on a Perkin Elmer Spectrum One spectrometer equipped with a Specac Golden Gate Attenuated Total Reflectance attachment. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker AVANCE III HD-400 spectrometer; chemical shifts were referenced to trimethylsilane at 0 ppm. Rheological data were obtained on a TA Instruments AR1500ex rheometer fitted with a 40 mm 3° steel cone and operating an oscillation procedure at 25 °C. Scanning Electron Microscopy (SEM) samples were prepared on conductive tape and sputter-coated with a thin layer of gold in a Quorum Q150RS sputter-coater. Images were then collected using a Jeol JSM-6610LV instrument and analyzed on ImageJ. UV-vis spectroscopic analyses were conducted using a Varian Cary 50 UV-visible spectrophotometer with quartz cuvettes.

Supplementary figures

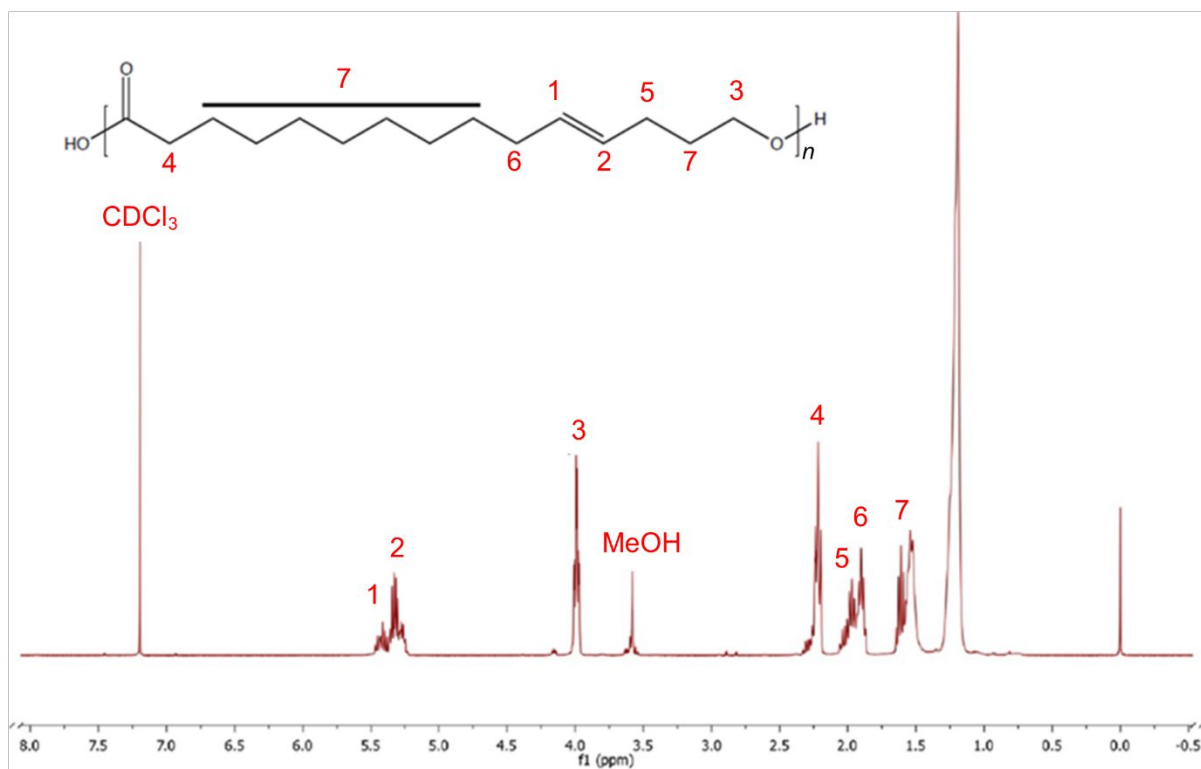


Figure S1. ^1H NMR spectrum of PGI (400 MHz, CDCl_3).

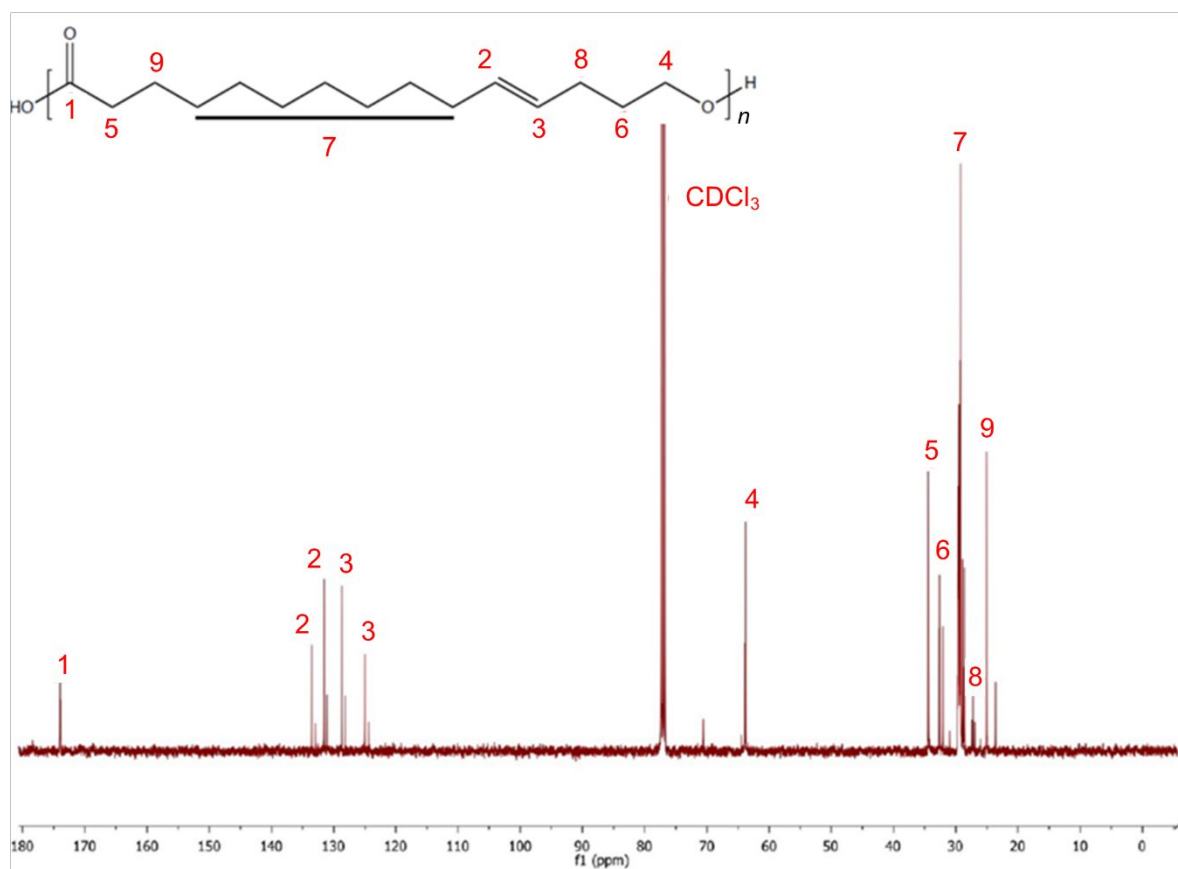


Figure S2. ^{13}C NMR spectrum of PGI (100 MHz, CDCl_3).

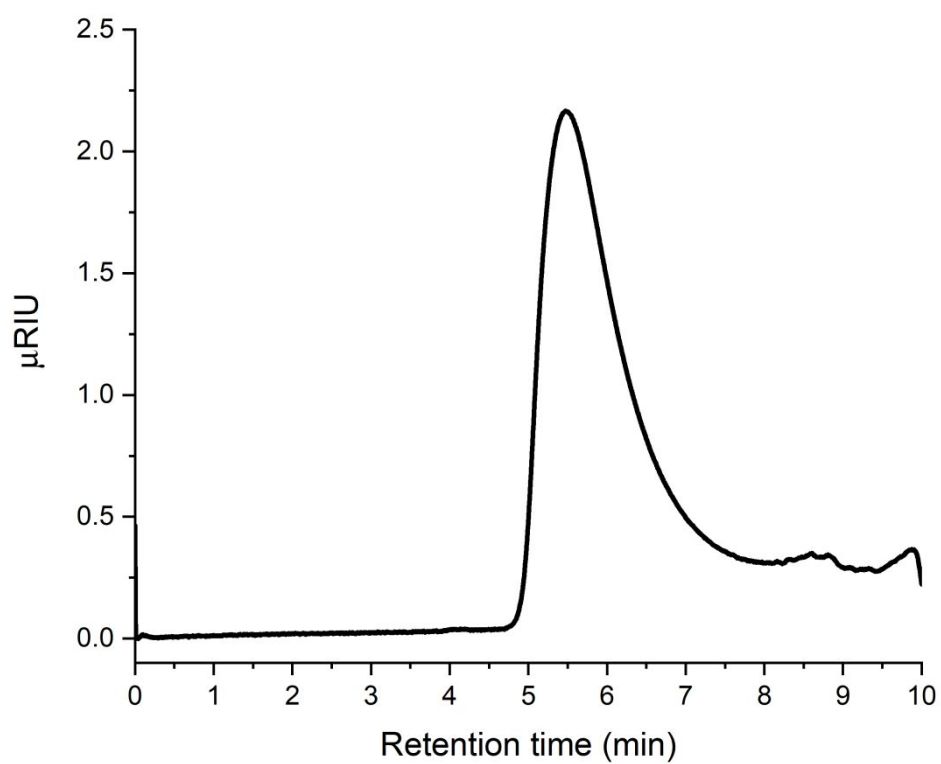


Figure S3. APC chromatogram of PGL.

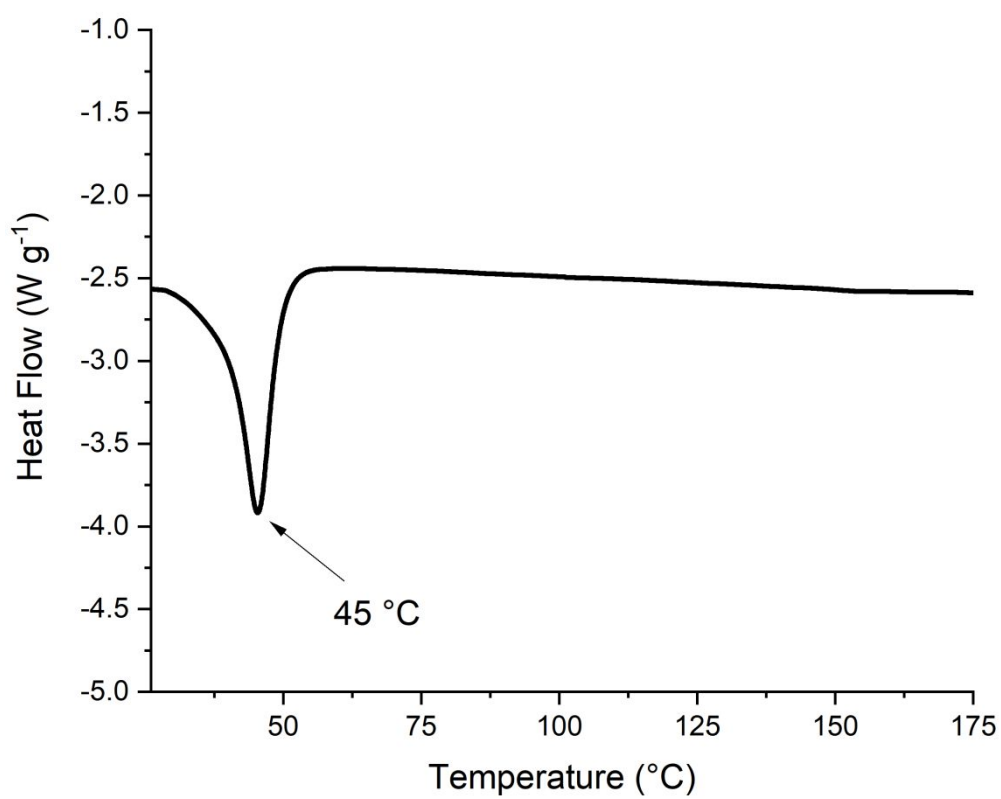


Figure S4. DSC thermogram for PGL.

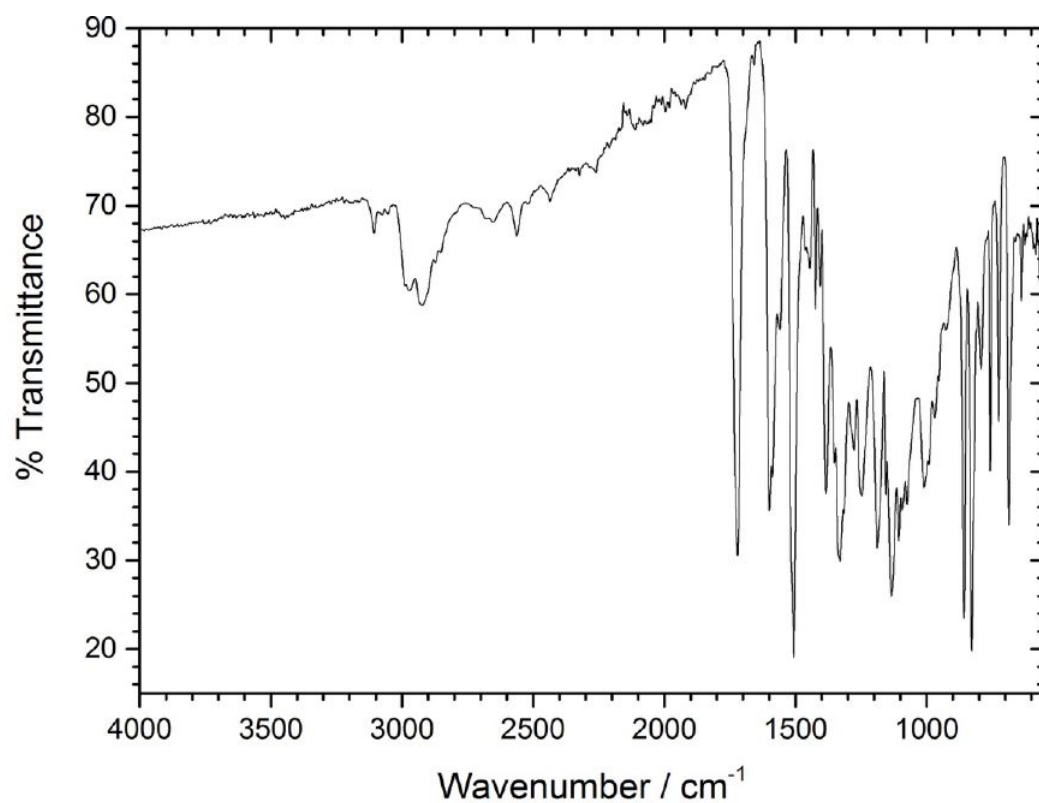


Figure S5. FTIR spectrum corresponding to DR1 3-mercaptopropionate.

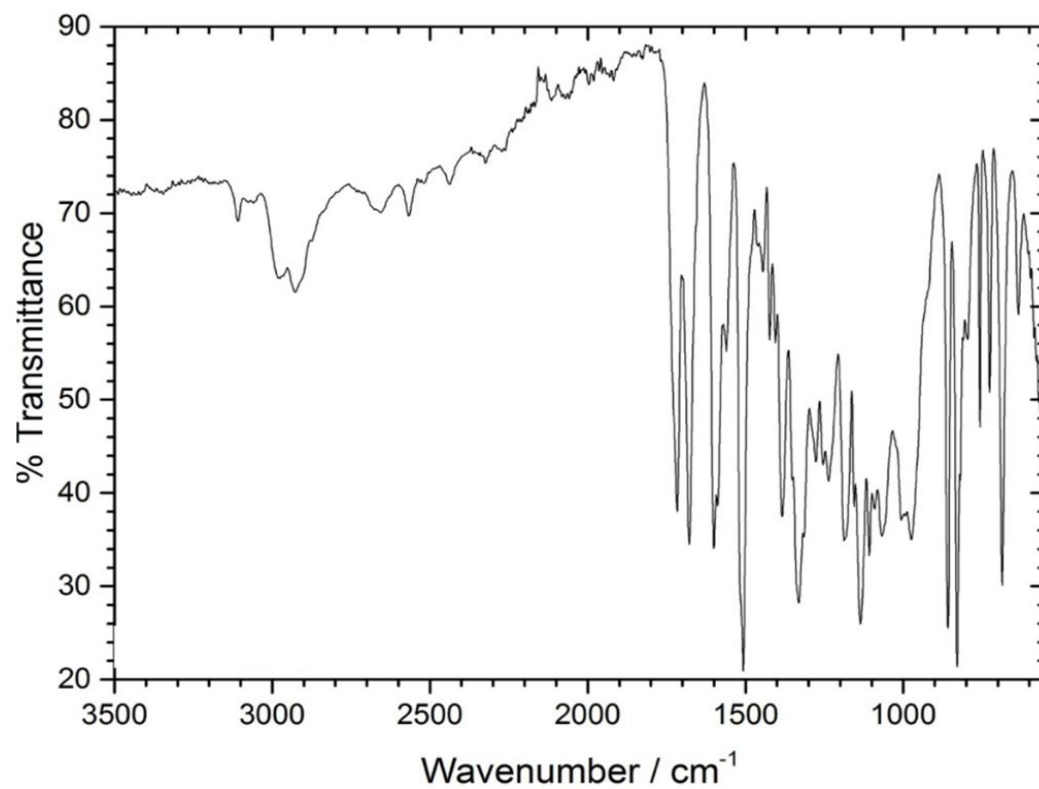


Figure S6. FTIR spectrum corresponding to DR1 bis(3-mercaptopropionate).

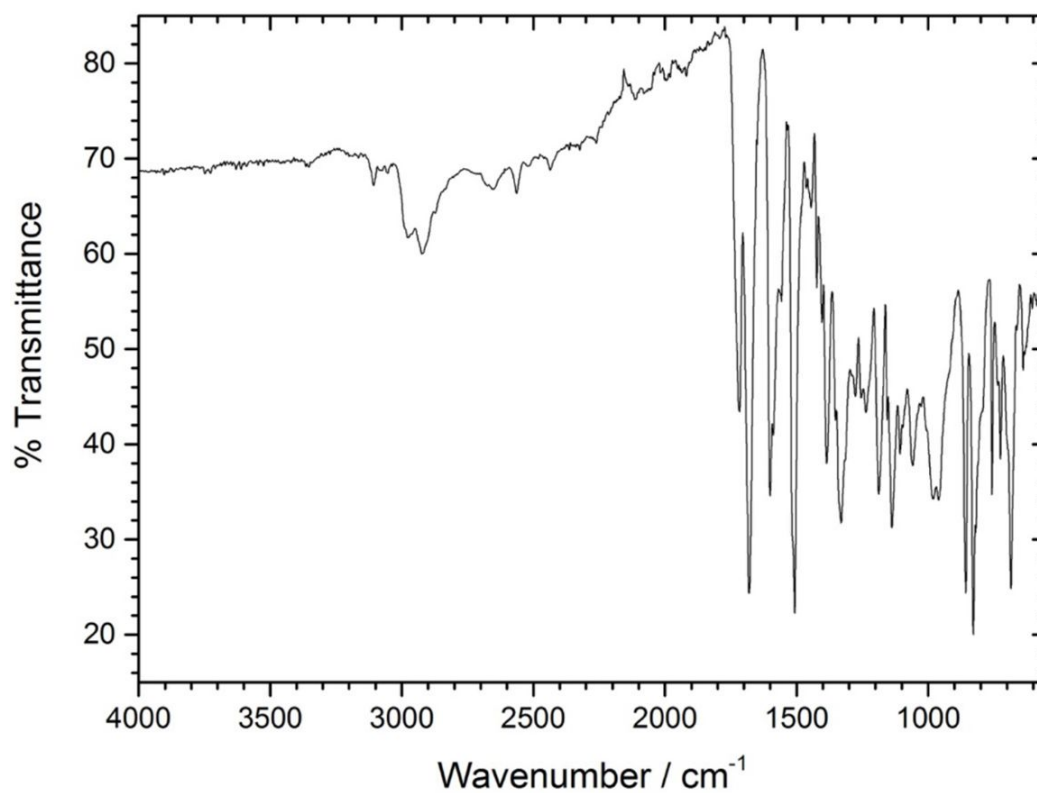


Figure S7. FTIR spectrum corresponding to DR1 tris(3-mercaptopropionate).

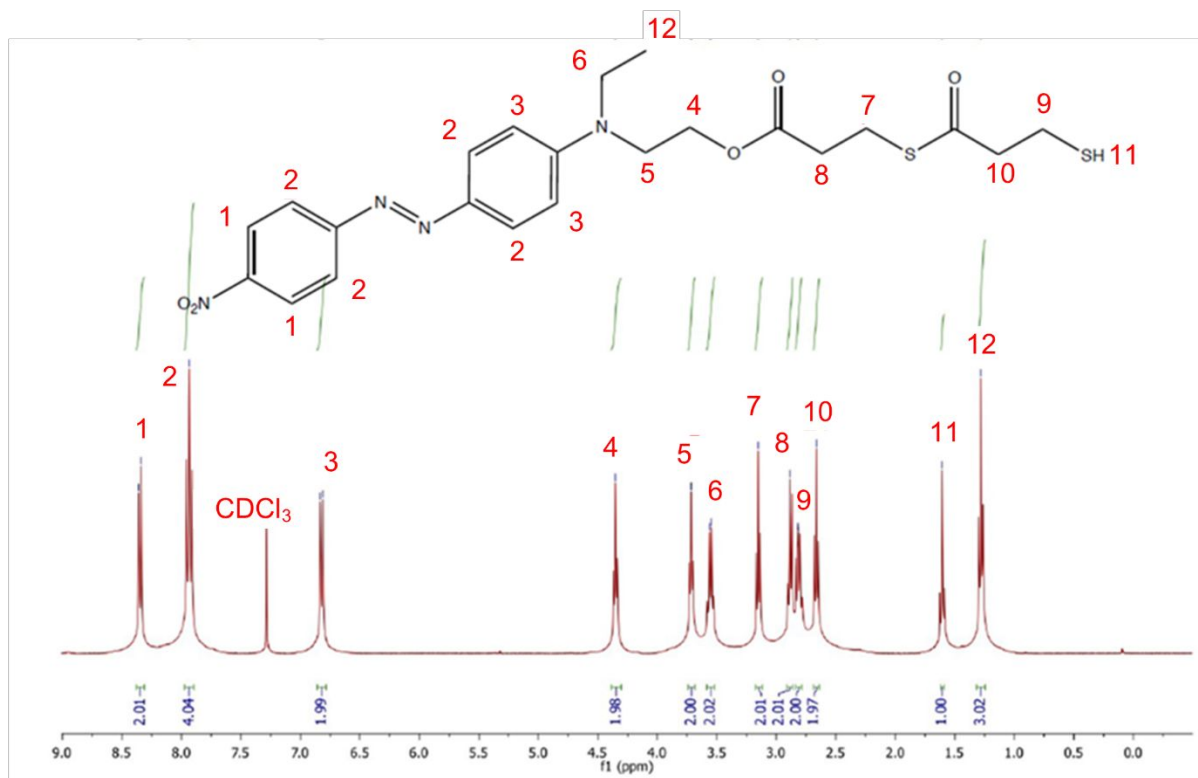


Figure S8. ¹H NMR spectrum corresponding to DR1 bis(3-mercaptopropionate) (400 MHz, CDCl₃).

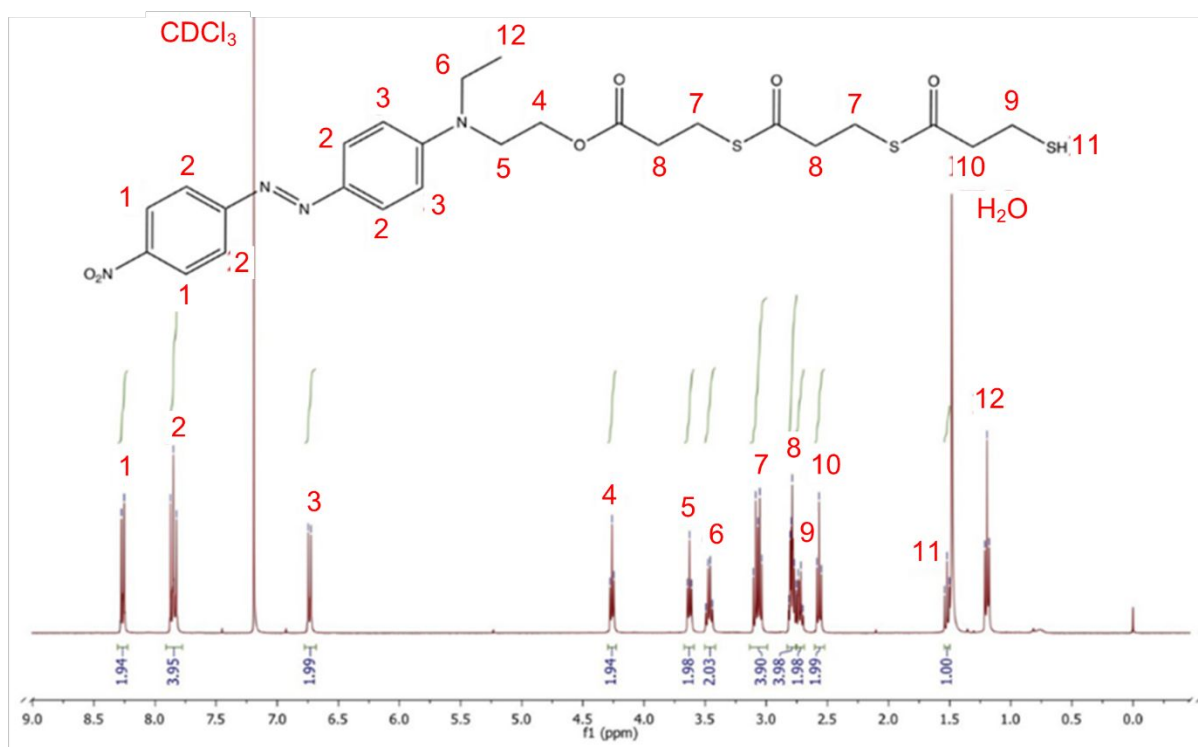


Figure S9. ^1H NMR spectrum corresponding to DR1 tris(3-mercaptopropionate) (400 MHz, CDCl_3).

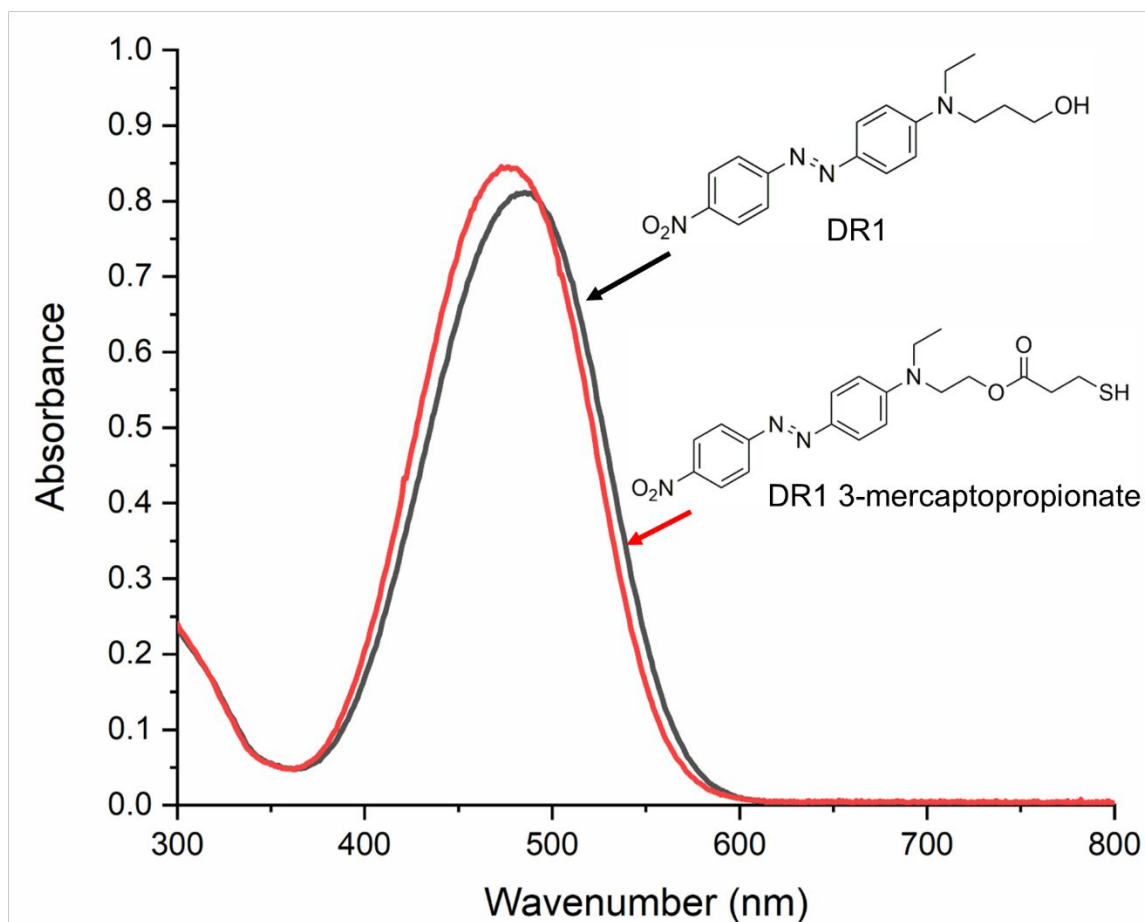


Figure S10. UV-vis absorption spectra of DR1 and DR1 3-mercaptopropionate.

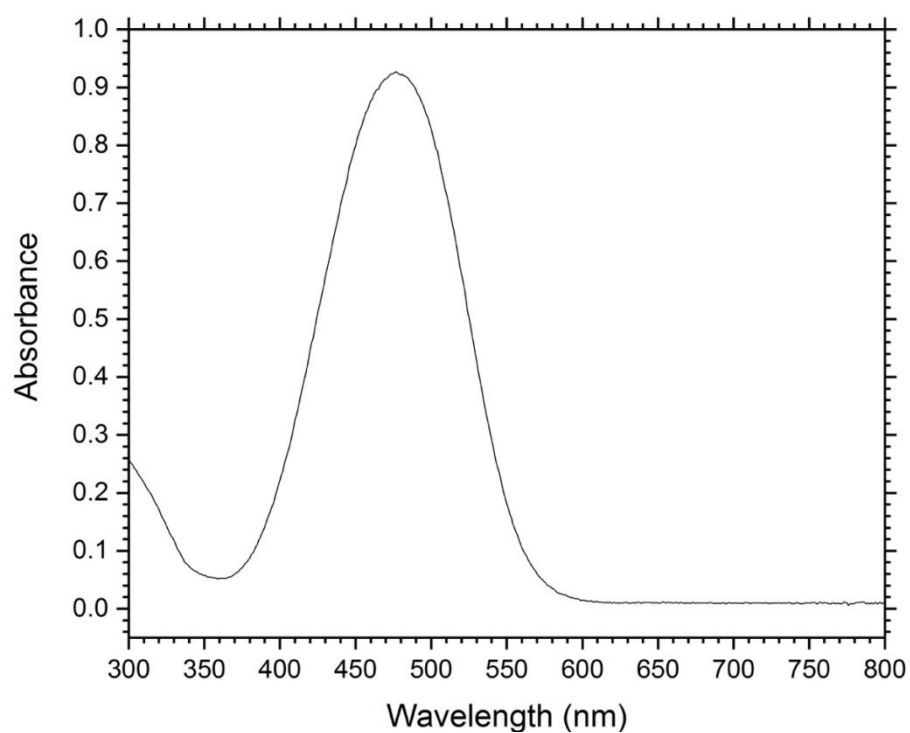


Figure S11. UV-vis absorption spectrum of DR1 bis(3-mercaptopropionate).

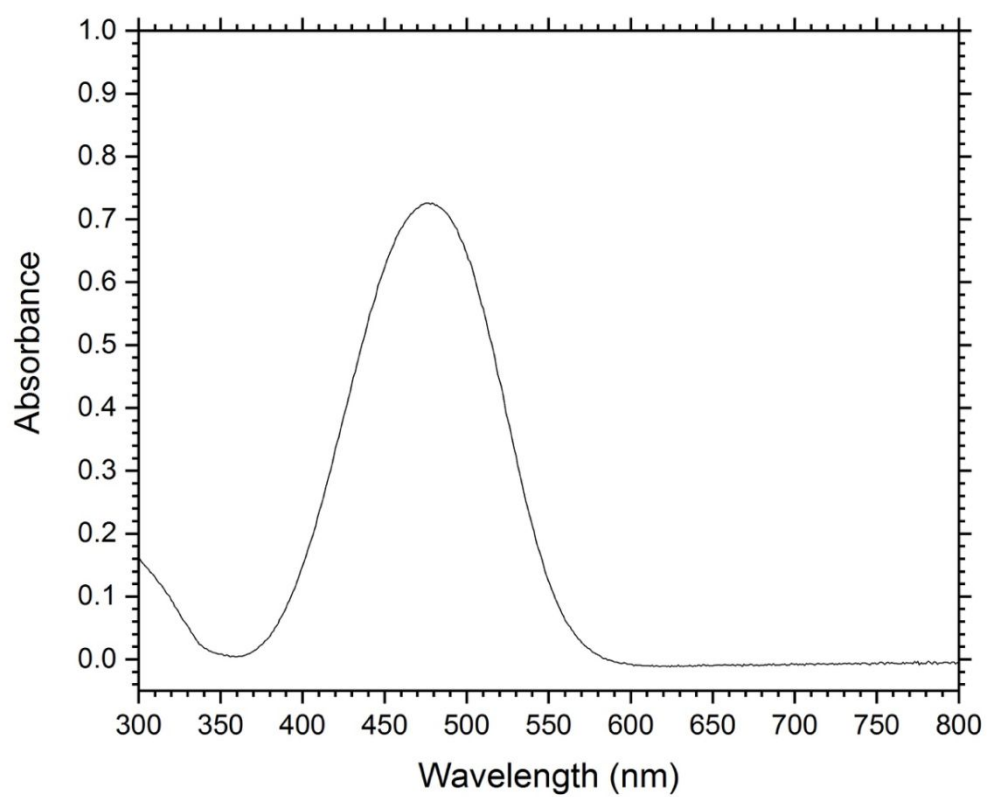


Figure S12. UV-vis absorption spectrum of DR1 tris(3-mercaptopropionate).

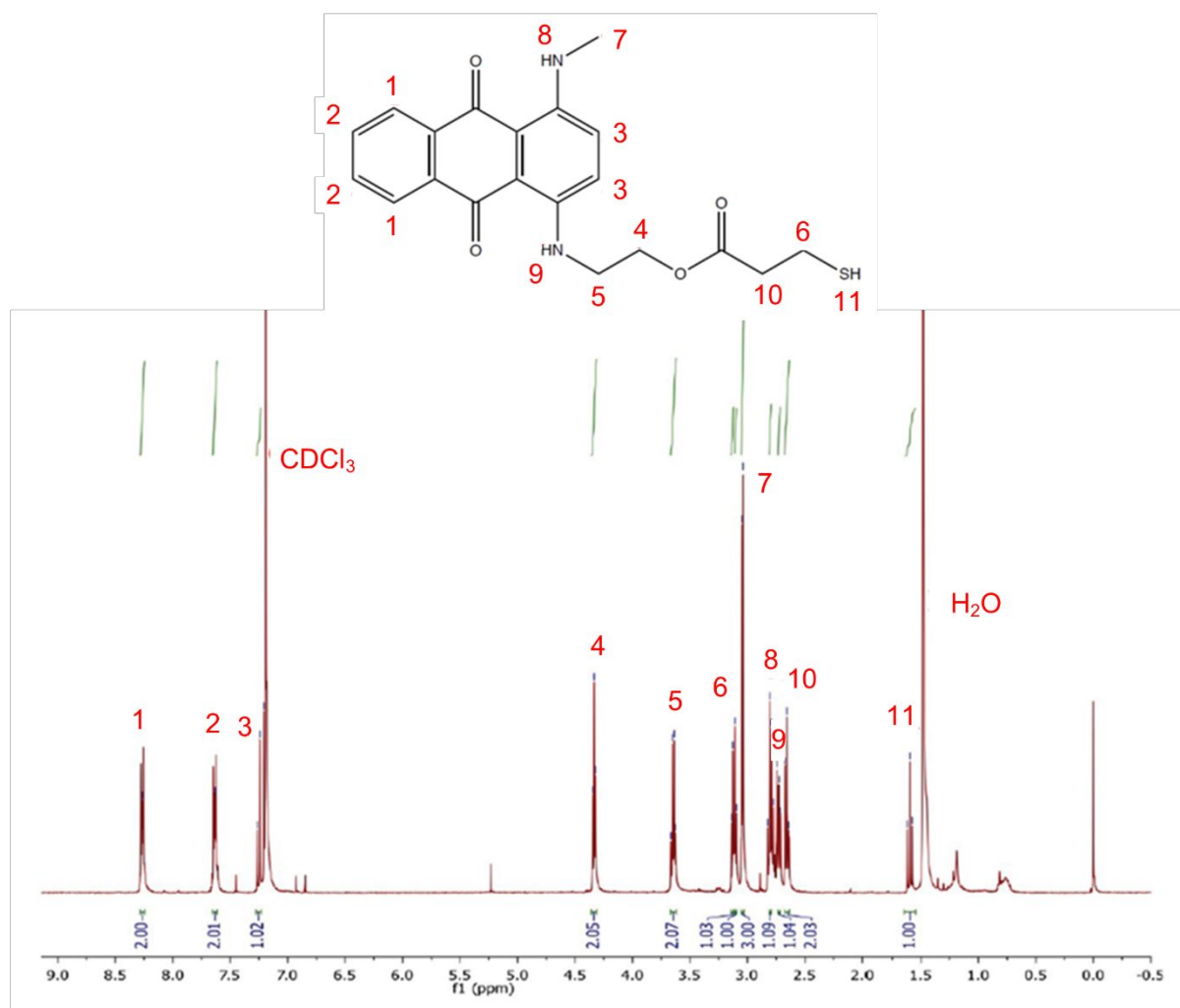


Figure S13. ¹H NMR spectrum corresponding to DB3 3-mercaptopropionate (400 MHz, CDCl₃).

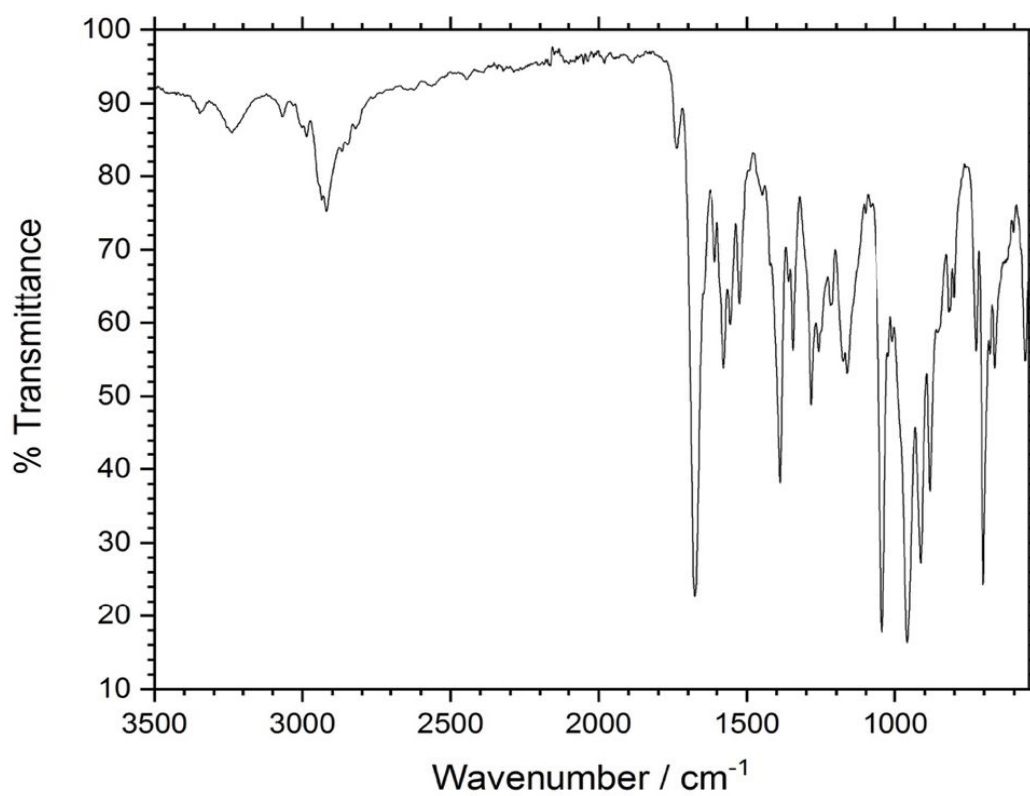


Figure S14. FTIR spectrum corresponding to DB3 3-mercaptopropionate.

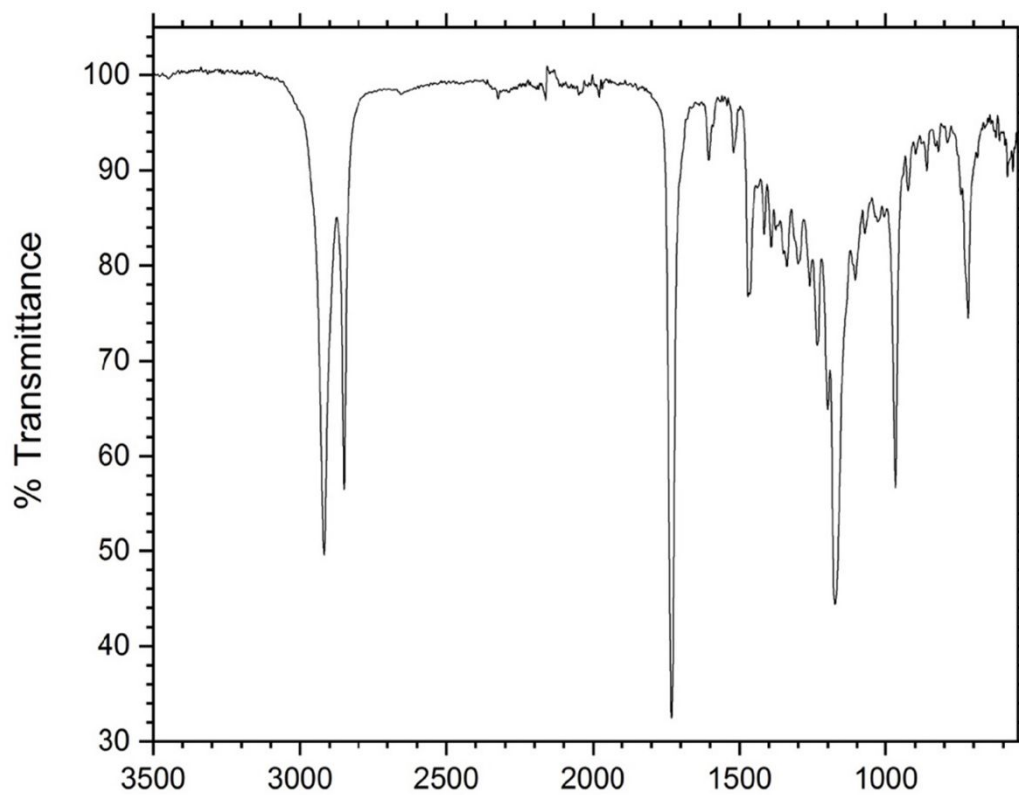


Figure S15. FTIR spectrum corresponding to DR1 3-mercaptopropionate dyed PGL.

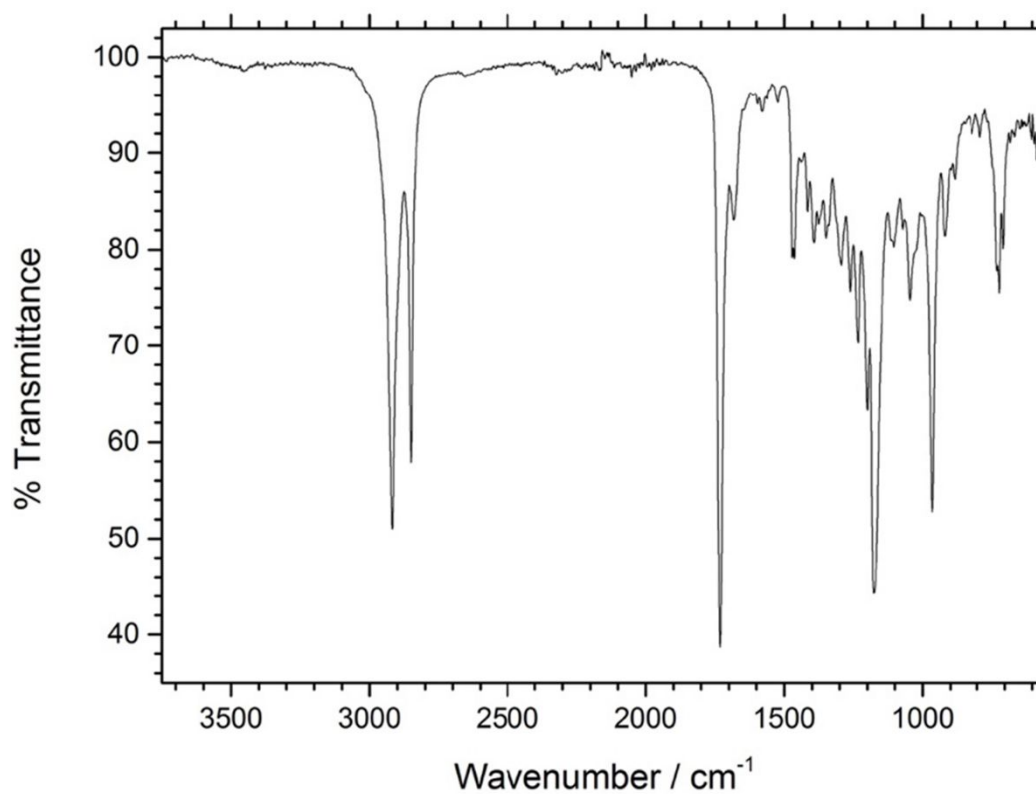


Figure S16. The FTIR spectrum corresponding to DB3 3-mercaptopropionate dyed PGI.

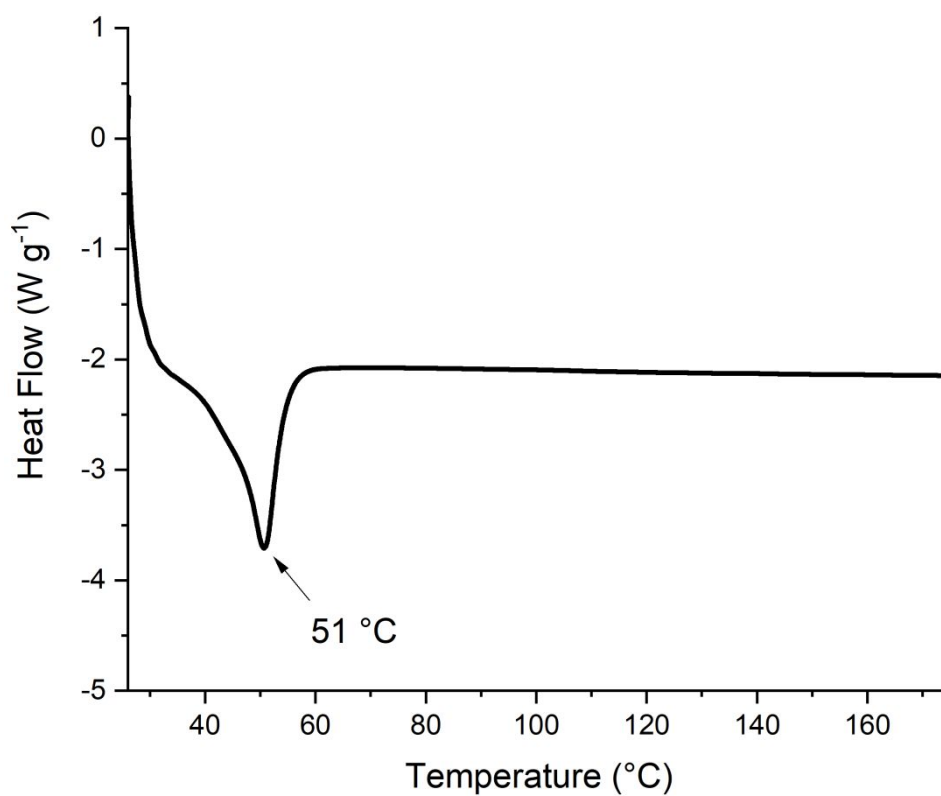


Figure S17. DSC thermogram for DR1 3-mercaptopropionate dyed PGI.

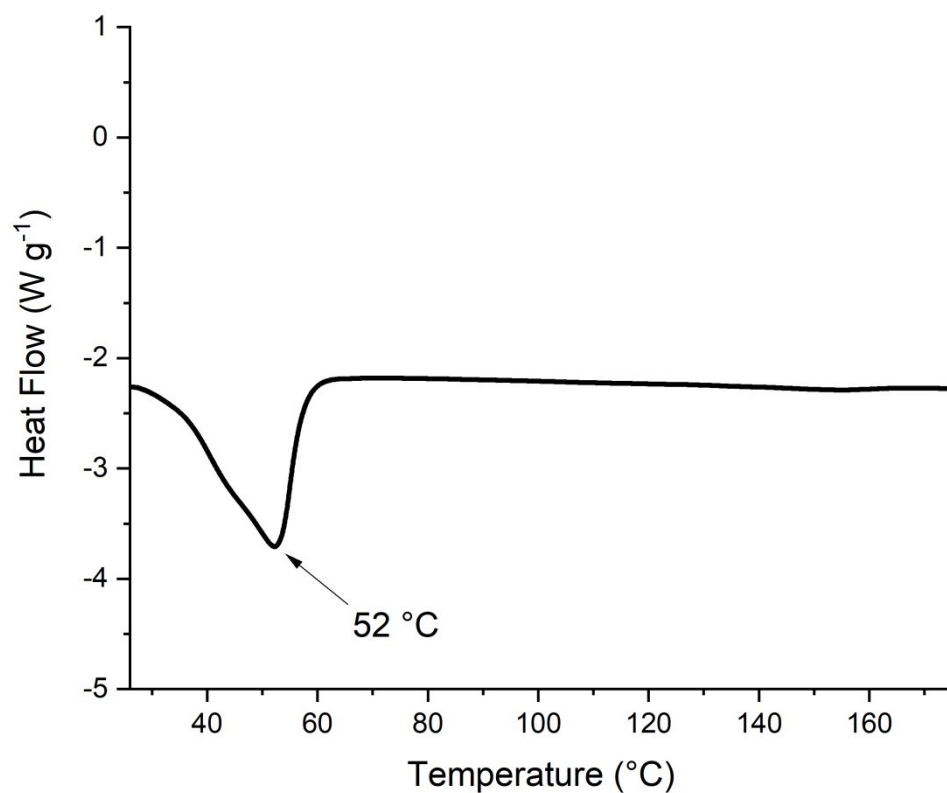


Figure S18. DSC thermogram for DB3 3-mercaptopropionate dyed PGI.

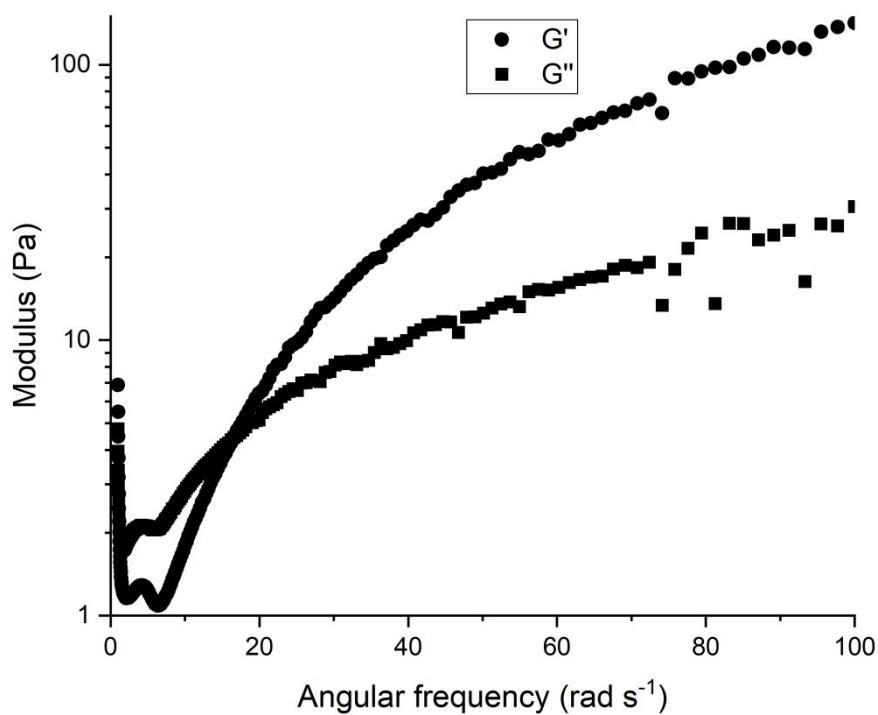


Figure S19. Elastic (G') and viscous modulus (G'') against angular frequency for PGI swollen in 2-phenylethanol.

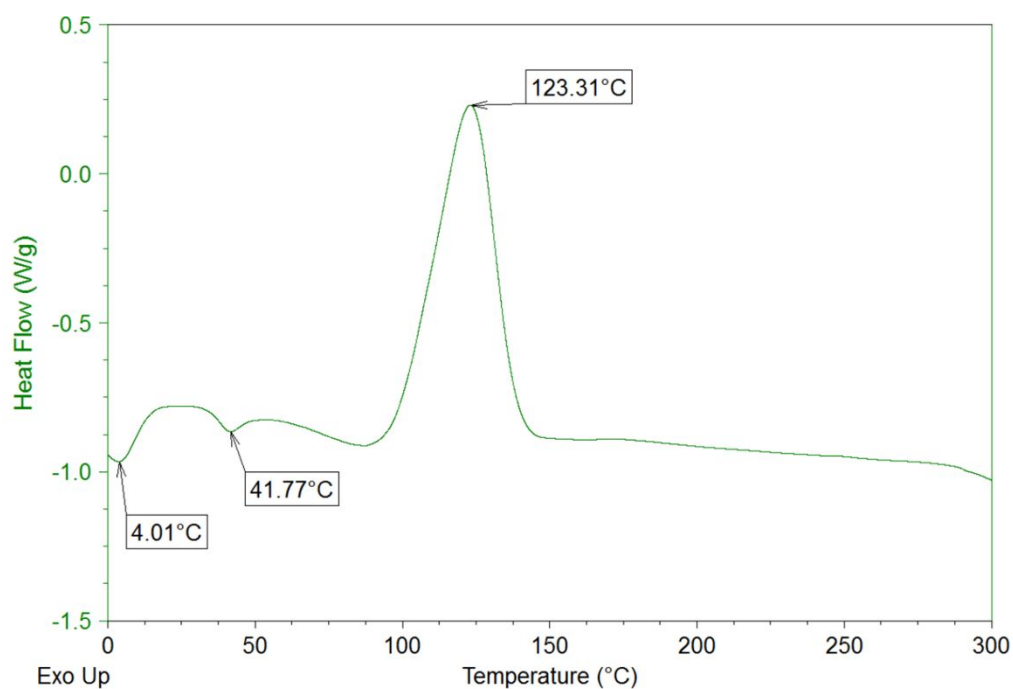


Figure S20. DSC thermogram for PGI crosslinked with 2,2'-(ethylenedioxy)diethanethiol.

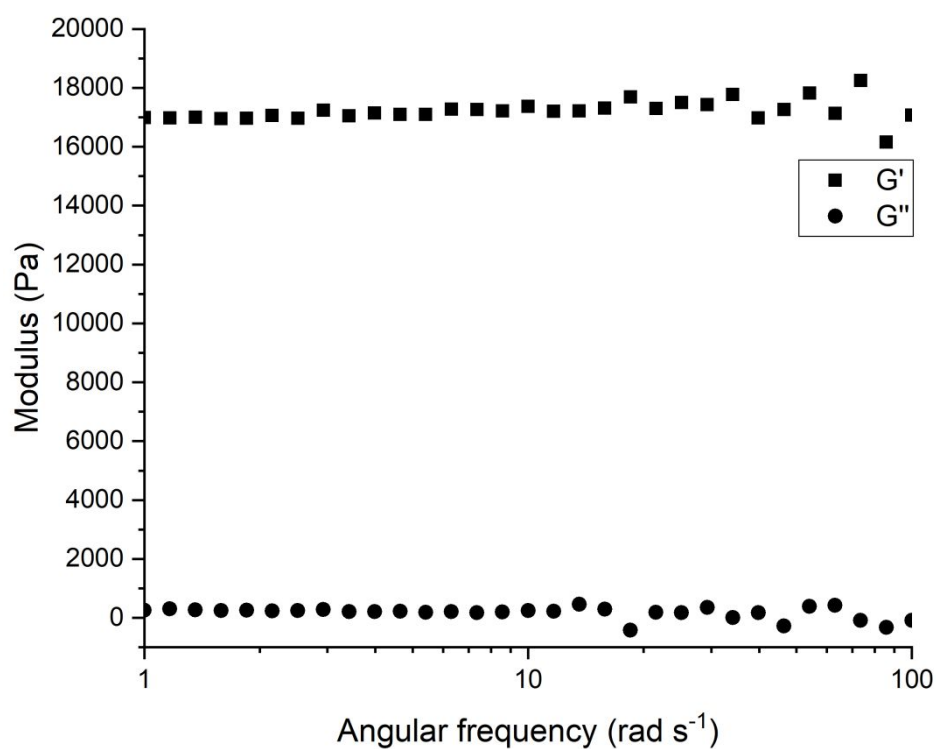


Figure S21. Average (n=6) elastic (G') and viscous modulus (G'') against angular frequency for PGI crosslinked with 2,2'-(ethylenedioxy)diethanethiol and swollen in 2-phenylethanol.

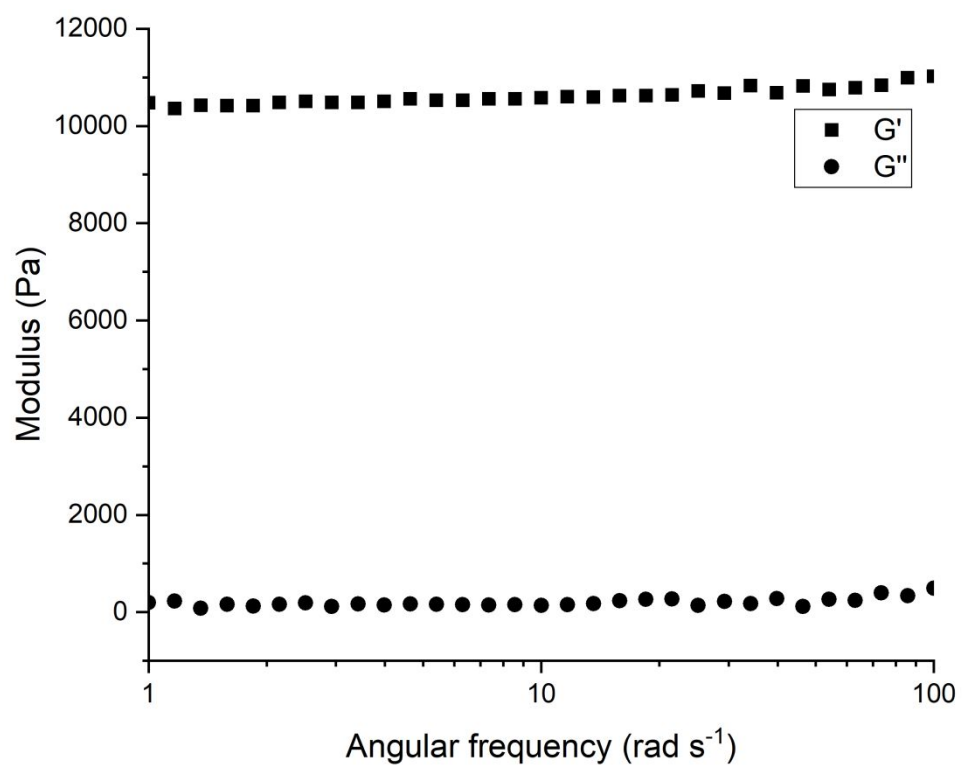


Figure S22. Average ($n=7$) elastic (G') and viscous modulus (G'') against angular frequency for PGI crosslinked with 2,2'-(ethylenedioxy)diethanethiol, covalently dyed with DB3 3-mercaptopropionate and swollen in 2-phenylethanol.