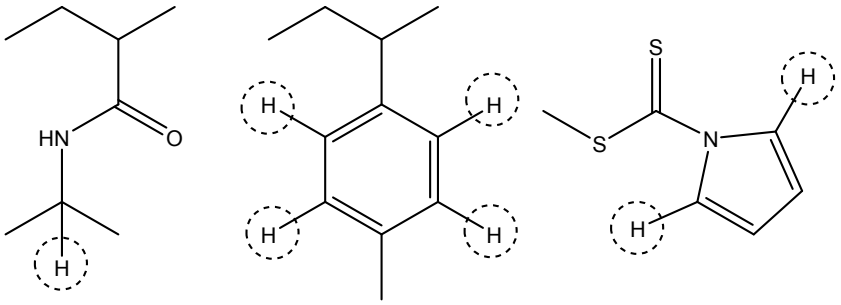
NMR functionality calculations

For ^{1}H NMR functionality calculations the integrals of the NIPAM isopropyl functional unit, the benzyl unit and the N-pyrrole hydrogens were compared, fixing the isopropyl NIPAM functionalities to 1 (results shown in Table SI 2). The ^{1}H values were calculated by dividing the integrals of the isopropyl NIPAM by 6, Benzyl by 4 and N-pyrrole by 2.

The distal hydrogen from the pyrrole functional unit overlaps the benzyl peak and so was removed from the benzyl integrals prior to calculations being made. For this reason distal pyrroles were not used in functionality calculations.

Fig SI. 1 – Protons used in 1H NMR functionality calculations for isopropyl NIPAM, benzyl and N-pyrrole



Calculations for functionality were used to calculate the % pyrrole and acid (via TAI) ends per branch point and the degree of branching (number of branch points per number of monomers).

$$\%\ Pyrrole\ Functionality = \frac{1H\ Pyrrole}{1H\ Benzyl} \times 100$$

$$Degree\ of\ Branching = \frac{1H\ Benzyl}{(1H\ NIPAM + 1H\ Benzyl + 1H\ Pyrrole)}$$

TAI CHAIN END NMR REACTION

The presence of Acid Chain Ends were determined by reacting the sample with 200 µl trichloroacetyl isocyanate (TAI) to 50 mg polymer in the 1H NMR flask. The Imide peak was found at 11.1 ppm and compared to the isopropyl integral of that spectra; this was confirmed by addition of a small amount of D_2O after which the peak disappeared.

$$\%\ Acid\ Functionality = \frac{1H\ Imide}{1H\ Benzyl} \times 100$$