



Figure S1. (a) Solvent Accessible Surface Area (SASA) plots of the hydrogels crosslinked with maleic acid (γ -CDPVAHMA), malic acid (γ -CDPVAHMLA) and glutamic (γ -CDPVAHGLU), at acid (0-50 ns) and neutral-basic pH (51-100 ns), respectively. (b) Number of NFD molecules retained by γ -CDPVAHMA, γ -CDPVAHMLA and γ -CDPVAHGLU during the three simulations: in methanol (0-50 ns), at acid pH (51-100 ns) and at neutral-basic pH (101-150 ns).