

New types of hyperbranched 1,2,3-triazole-alkoxysiloxane functional polymers for metal embedded nanocomposite surface coatings

Supplementary information

Hyperbranched poly-3-azidopropylethoxysiloxane

^1H -NMR (300 MHz, CDCl_3) δ : 3.79 (m, 2H), 3.25 (m, 2H), 1.67 (m, 2H), 1.20 (m, 3H), 0.67 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 58.24, 53.55, 22.50, 18.03, (10.31, 9.61, 9.45, 9.24, 9.19, 9.13, 9.07, 8.97, 8.44, 8.16); ^{29}Si -NMR (60 MHz, CDCl_3), δ : (-49.3) – (-51.6) ($\text{R-Si}(\text{OCH}_2\text{CH}_3)_2\text{O}_{0.5}$), (-52.1) – (54.4), ($\text{R-Si}(\text{OCH}_2\text{CH}_3)\text{O}$), (-65.4) – (-70.0) ($\text{R-SiO}_{1.5}$). GPC: M_w =1696 g/mol, M_w/M_n =1.2.

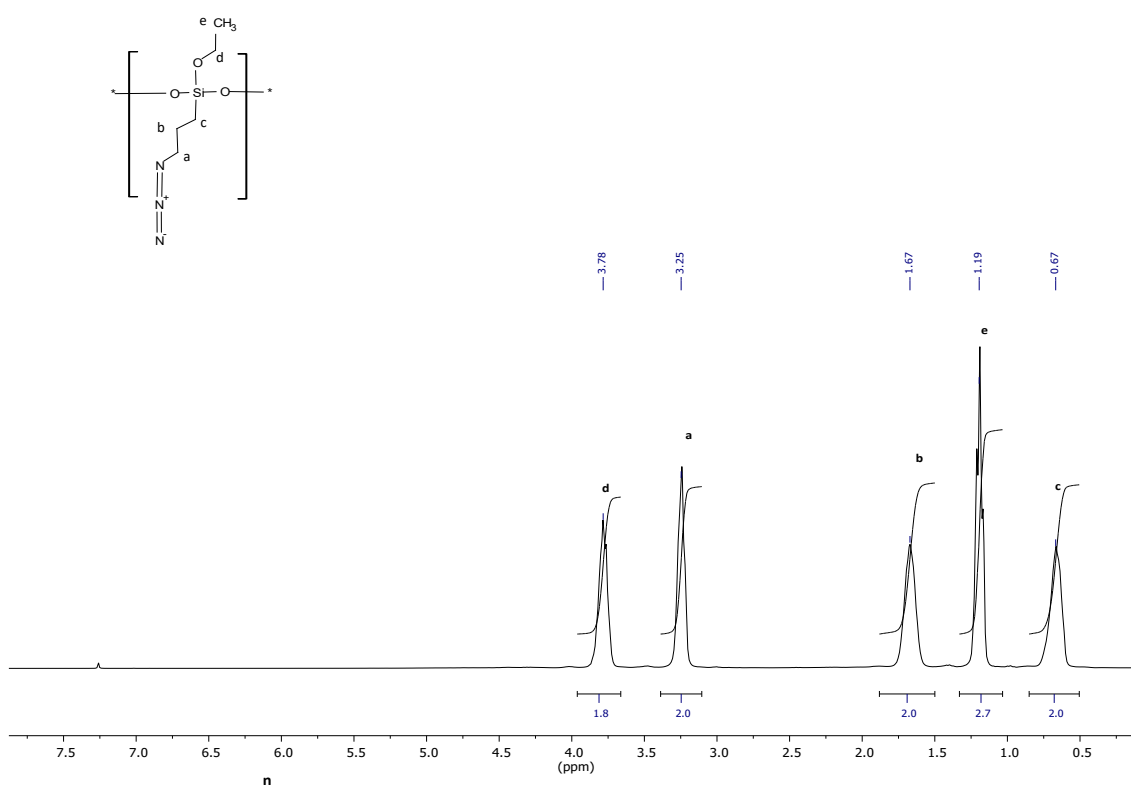


Fig. S1 ^1H NMR Spectra of hyperbranched poly-3-azidopropylethoxysiloxane

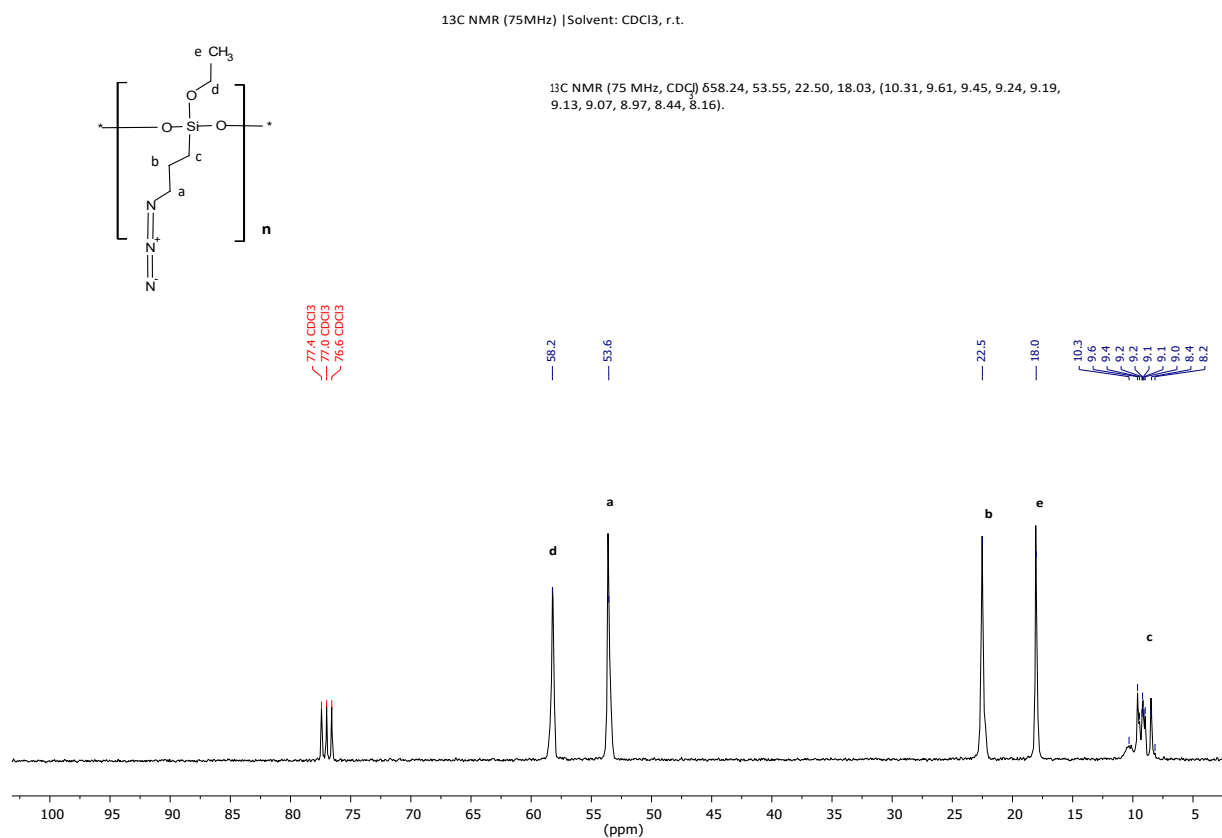


Fig. S2 ¹³C NMR Spectra of hyperbranched poly-3-azidopropylethoxysiloxane

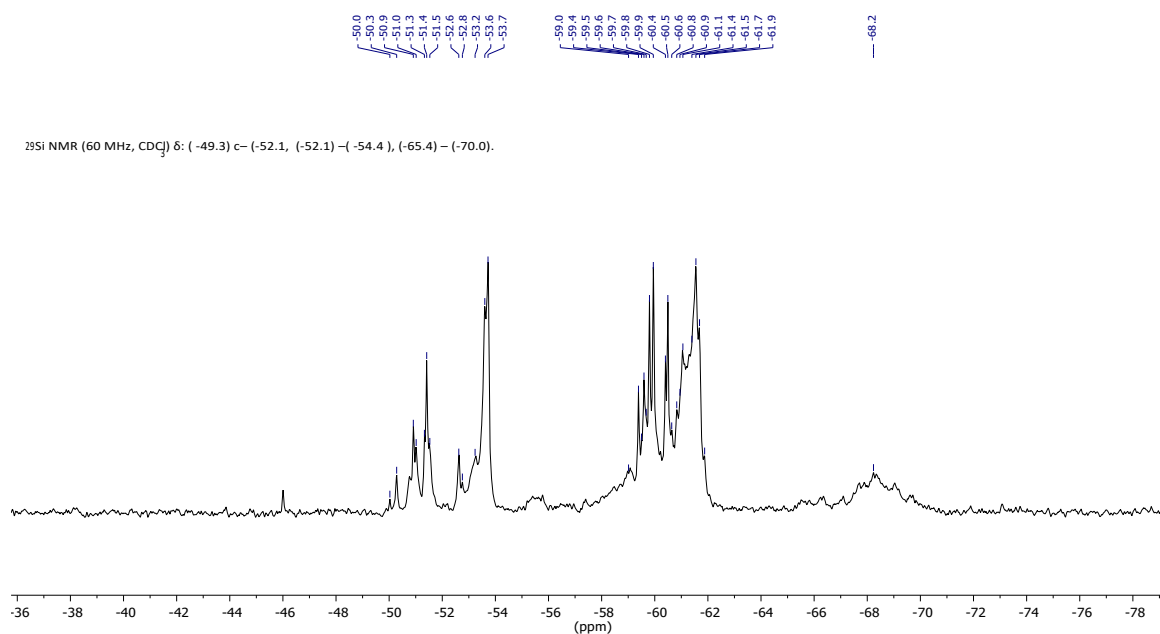


Fig. S3 ²⁹Si NMR Spectra of hyperbranched poly-3-azidopropylethoxysiloxane

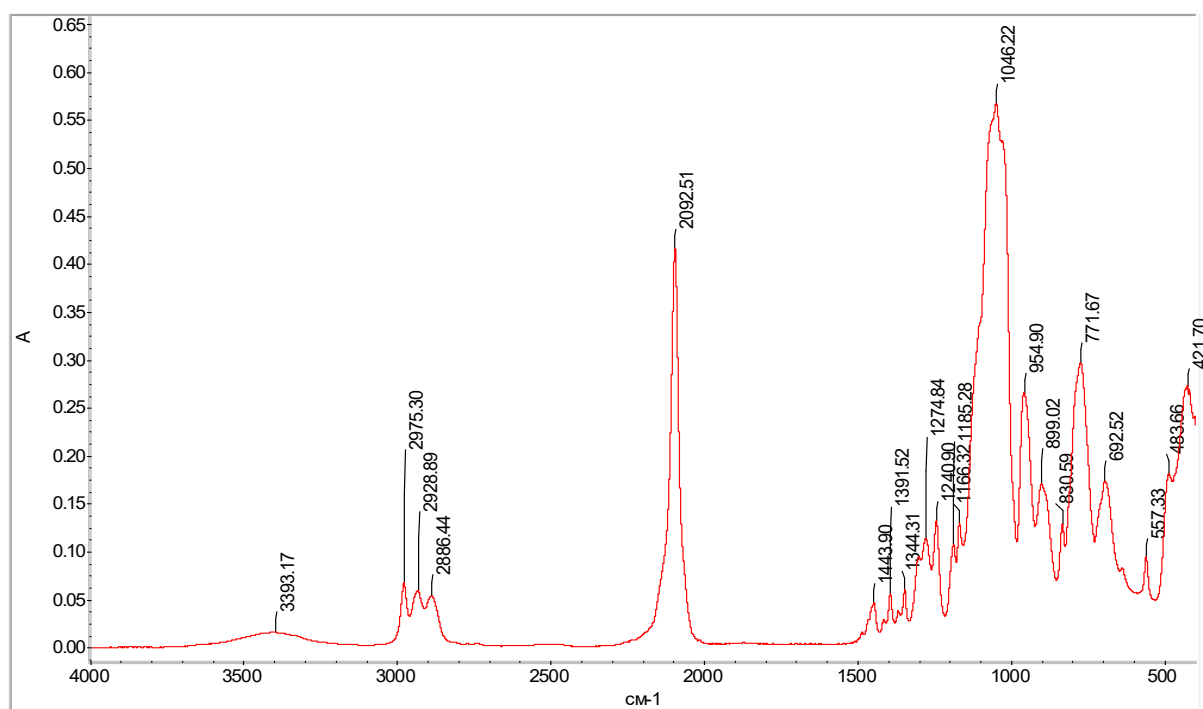


Fig. S4 FTIR Spectra of hyperbranched poly-3-azidopropylethoxysiloxane

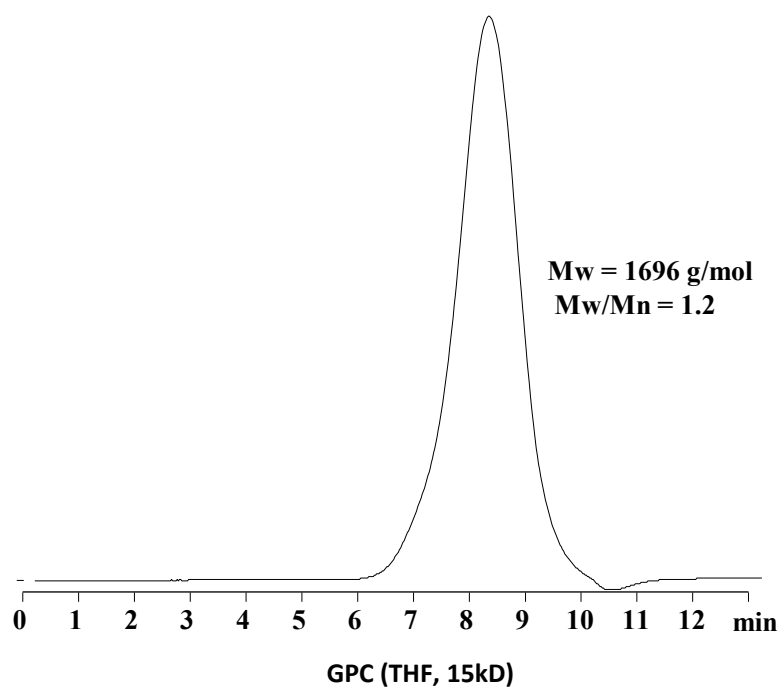


Fig. S5 GPC curve of poly-3-azidopropylethoxysiloxane

Hyperbranched poly(3-(4-(((dimethylamino)methyl)-1H-1,2,3-triazol-1-yl)propyl)ethoxysiloxane (DMA-1,2,3-triazole-siloxane).

^1H NMR (300 MHz, CDCl_3) δ 7.7-7.4 (m, 1H), 4.3-4.1 (m, 2H), 3.7- 3.5 (m, 1.5H), 3.6 -3.3 (m, 2H), 2.1 (br.s, 3H), 1.9 - 1.7 (m, 2H), 1.0-0.8 (m, 2H), 0.6-0.3 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 144.4, 122.5, 58.0, 53.9, 51.9, 44.8, 25.2, 23.8, 17.8, 9.9, 9.2, 8.7, 8.0; ^{29}Si NMR (60 MHz, CDCl_3) δ : (-53.6) - (-54.5) (R-Si(OCH_2CH_3) $_2\text{O}_{0.5}$), (-59.0) - (-62.6) (R-Si(OCH_2CH_3)O), (-64.0) - (-70.0) (R-SiO $_{1.5}$). MALDI: M_w =2348 g/mol, M_w/M_n =1.1.

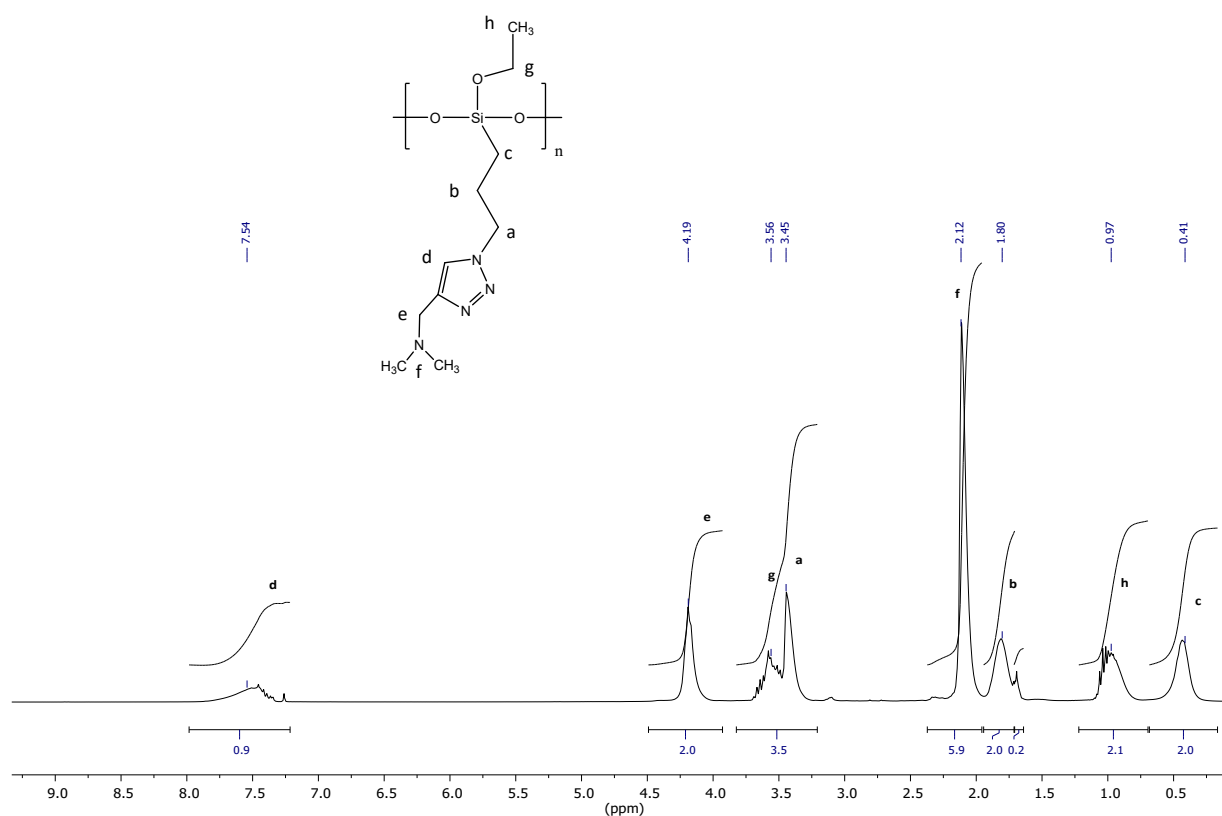


Fig. S6 ^1H NMR Spectra of DMA-1,2,3-triazole-siloxane

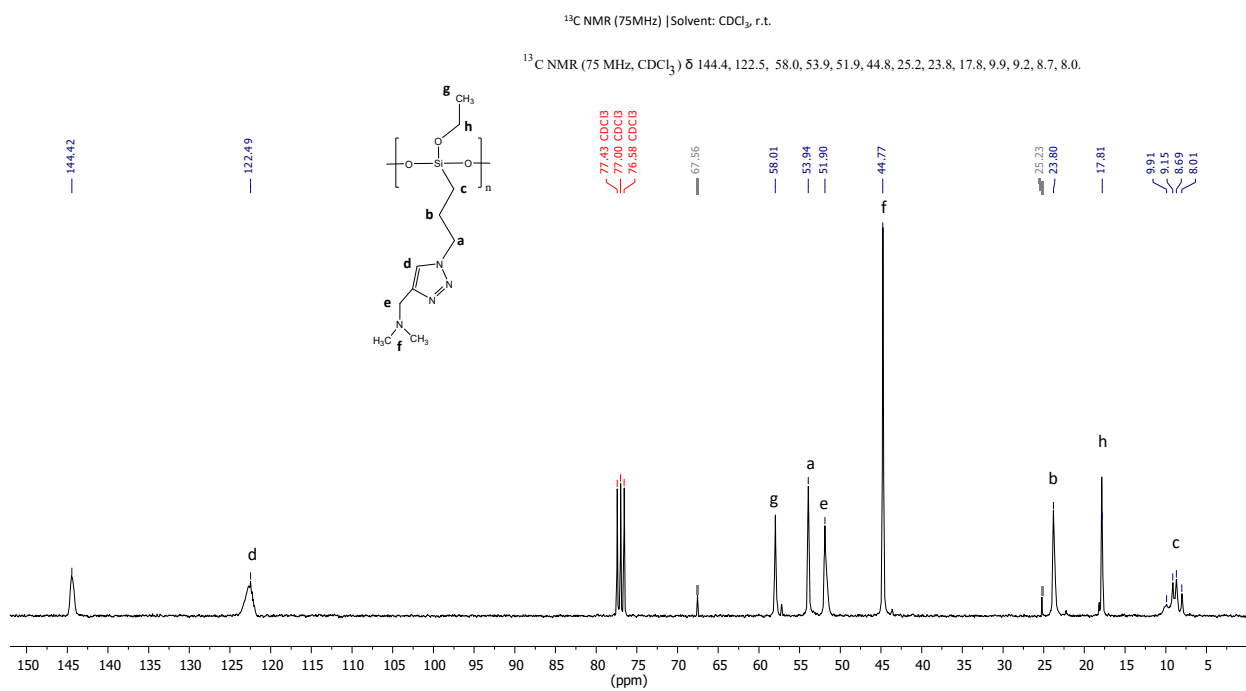


Fig. S7 ^{13}C NMR Spectra of DMA-1,2,3-triazole-siloxane

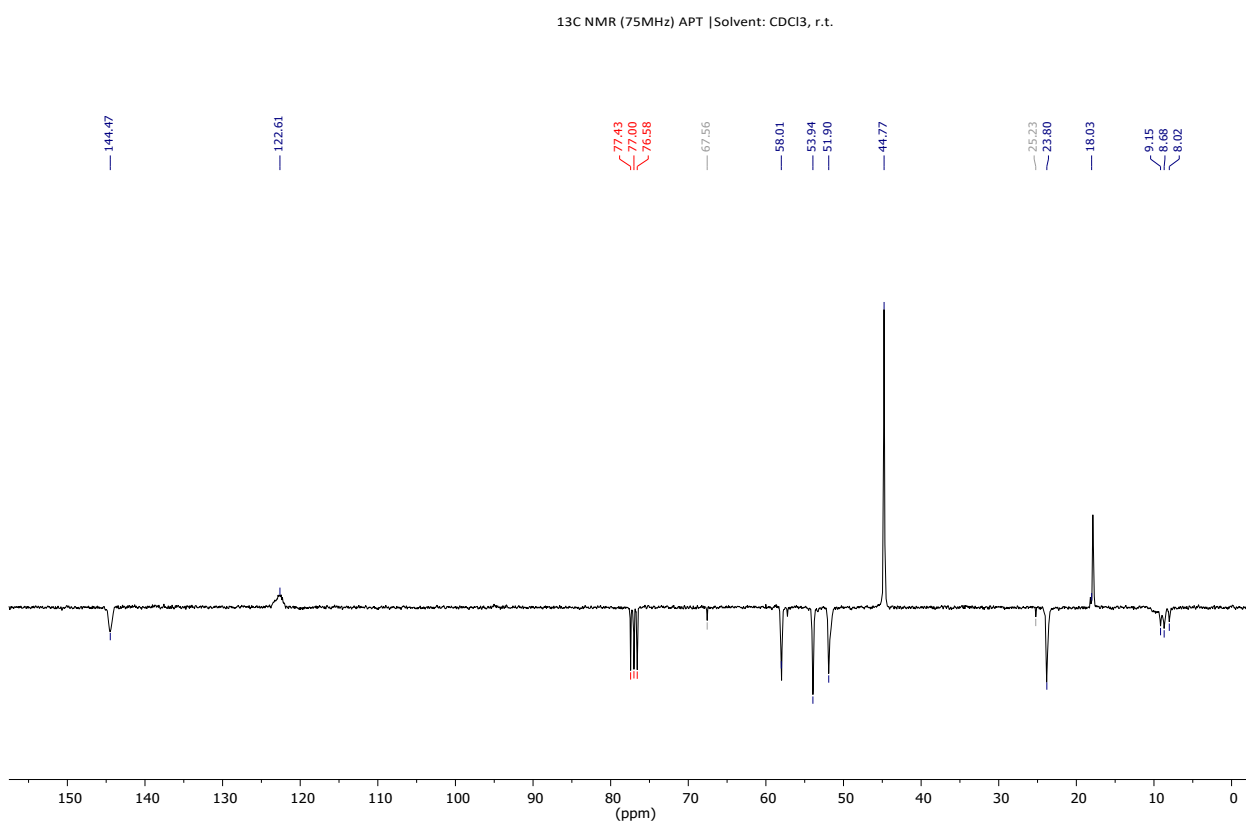


Fig. S8 ^{13}C NMR APT Spectra of DMA-1,2,3-triazole-siloxane

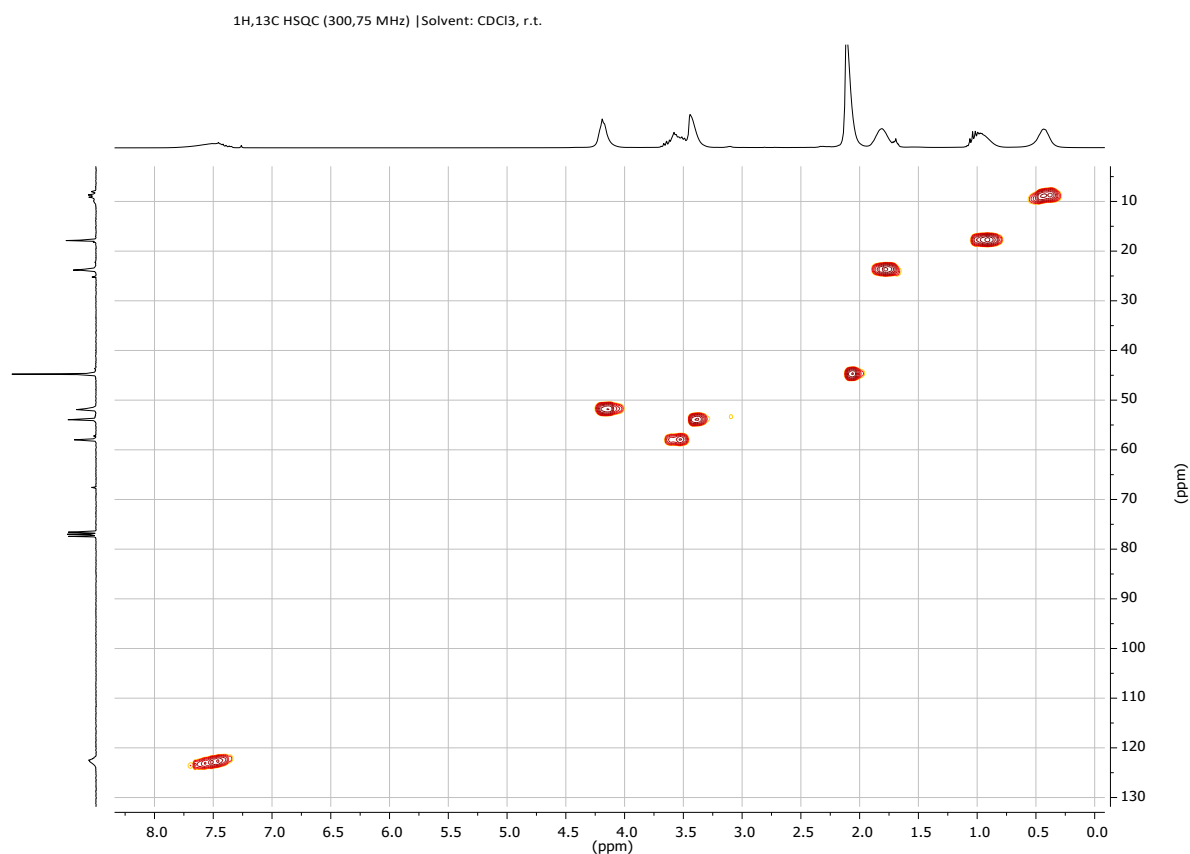


Fig. S9 ^1H , ^{13}C NMR HSQC Spectra of DMA-1,2,3-triazole-siloxane

MHz) | Solvent: CDCl_3 , r.t.

^{29}Si NMR (60 MHz, CDCl_3) δ : (-53.6) - (-54.5), (-59) - (-62.6), (-64) - (-70).

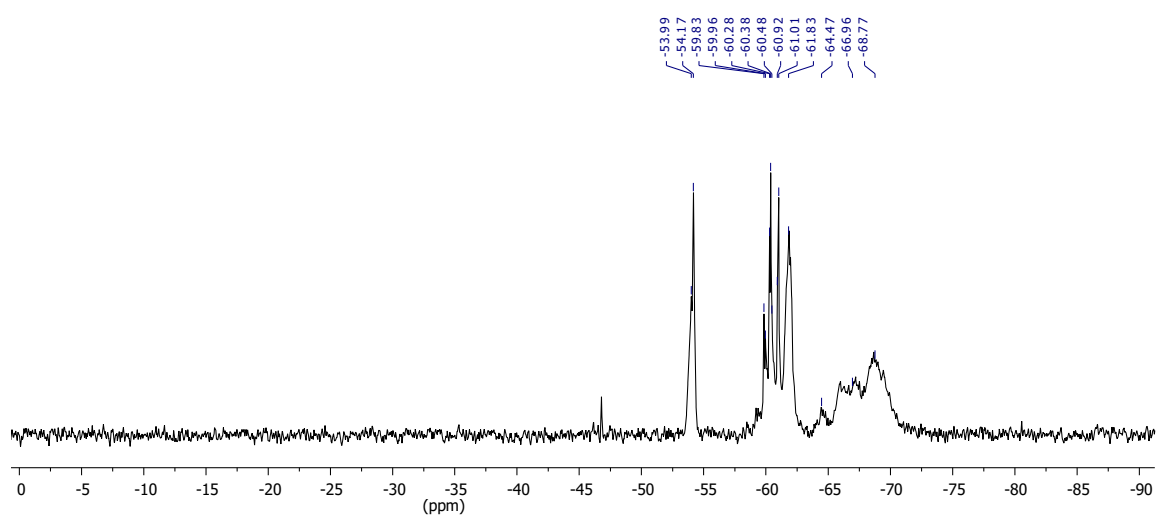


Fig. S10 ^{29}Si NMR Spectra of DMA-1,2,3-triazole-siloxane

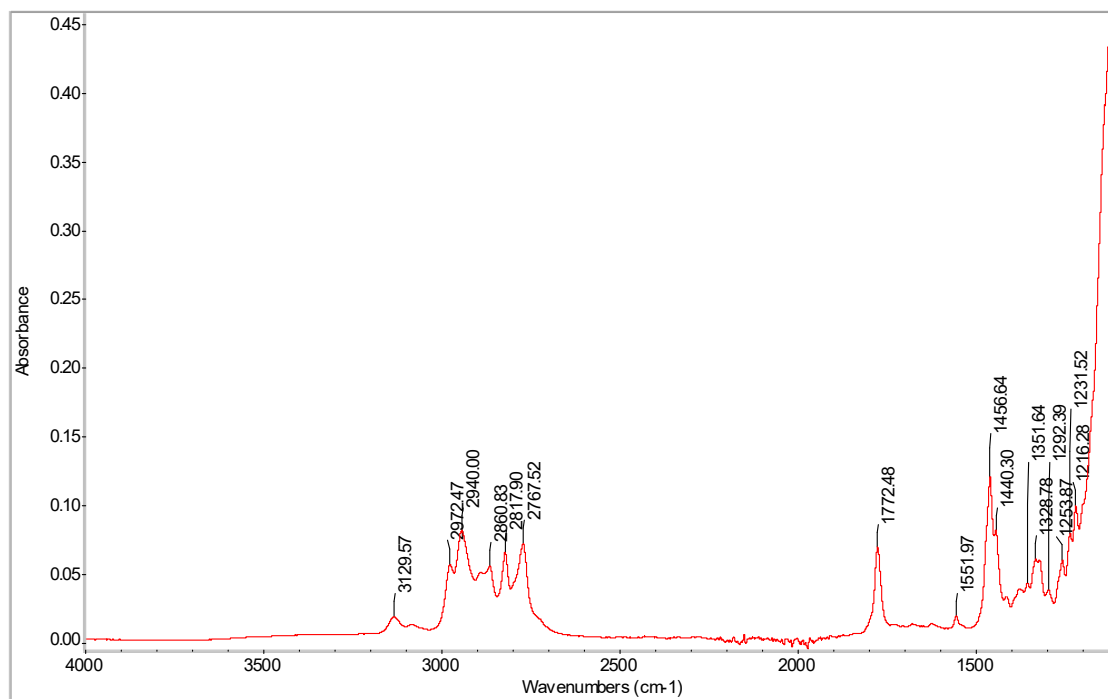


Fig. S11 FTIR Spectra of DMA-1,2,3-triazole-siloxane

Due to the specific interactions of amino groups in amino-containing polymers with GPC column fillers and metal tubing, leading to the adsorption of such polymers on the column, and thus making impossible to detect and determine their molecular weight characteristics investigation of M_w and M_n of DMA-1,2,3-triazole-siloxane polymer was done by MALDI method)

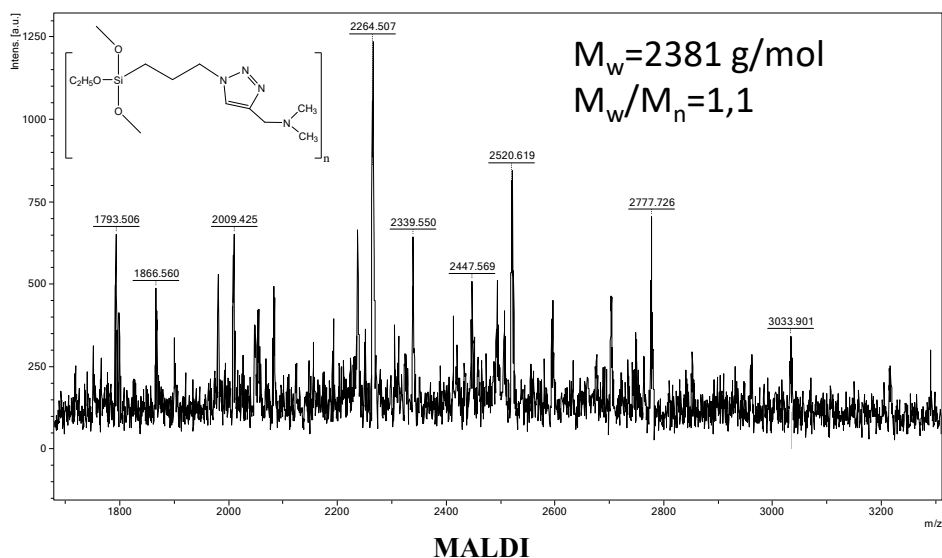


Fig. S12 MALDI spectra of DMA-1,2,3-triazole-siloxane

Hyperbranched poly(3-(4-(pyridin-2-yl)-1H-1,2,3-triazol-1-yl)propyl)ethoxysiloxane (PY-1,2,3-triazole-siloxane).

^1H NMR (300 MHz, CDCl_3) δ : 8.57 – 8.34 (m, 1H), 8.31 – 8.10 (m, 2H), 7.7-7.5, 1H), 7.2 – 6.9 (m, 1H), 4.46 – 4.18 (m, 2H), 3.79 – 3.45 (m, 1.8H), 2.1 – 1.8 (m, 2H), 1.2-0.9 (m, 2.8H), 0.7 – 0.4 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ : 150.11, 149.15, 147.95, 136.62, 122.53, 122.25, 119.88, 67.72, 58.27, 58.16, 52.27, 25.37, 23.90, 17.99, 17.92, 10.11, 9.23, 8.85, 8.18; ^{29}Si NMR (60 MHz, CDCl_3) δ : (-51) – (-55) ($\text{R-Si}(\text{OCH}_2\text{CH}_3)_2\text{O}_{0.5}$), (-58) – (-63) ($\text{R-Si}(\text{OCH}_2\text{CH}_3)\text{O}$), (-65) – (-71) ($\text{R-SiO}_{1.5}$); GPC: $M_w=2855$ g/mol, $M_w/M_n=1.2$.

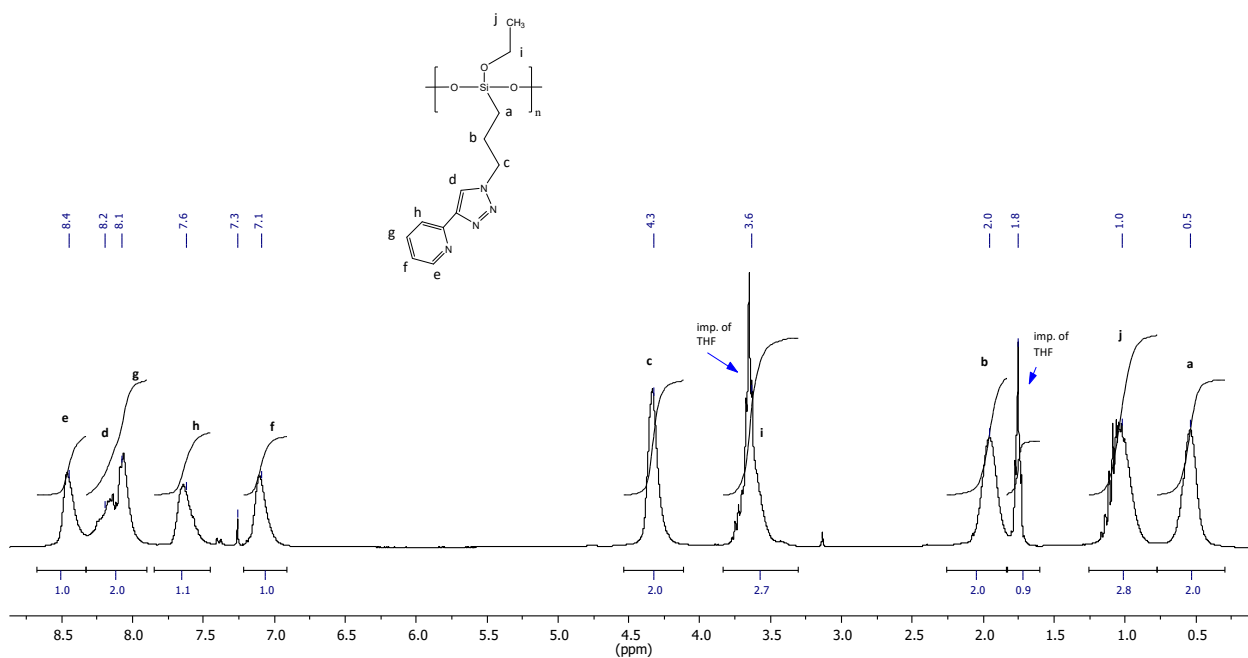


Fig. S13 ^1H NMR Spectra of PY-1,2,3-triazole-siloxane

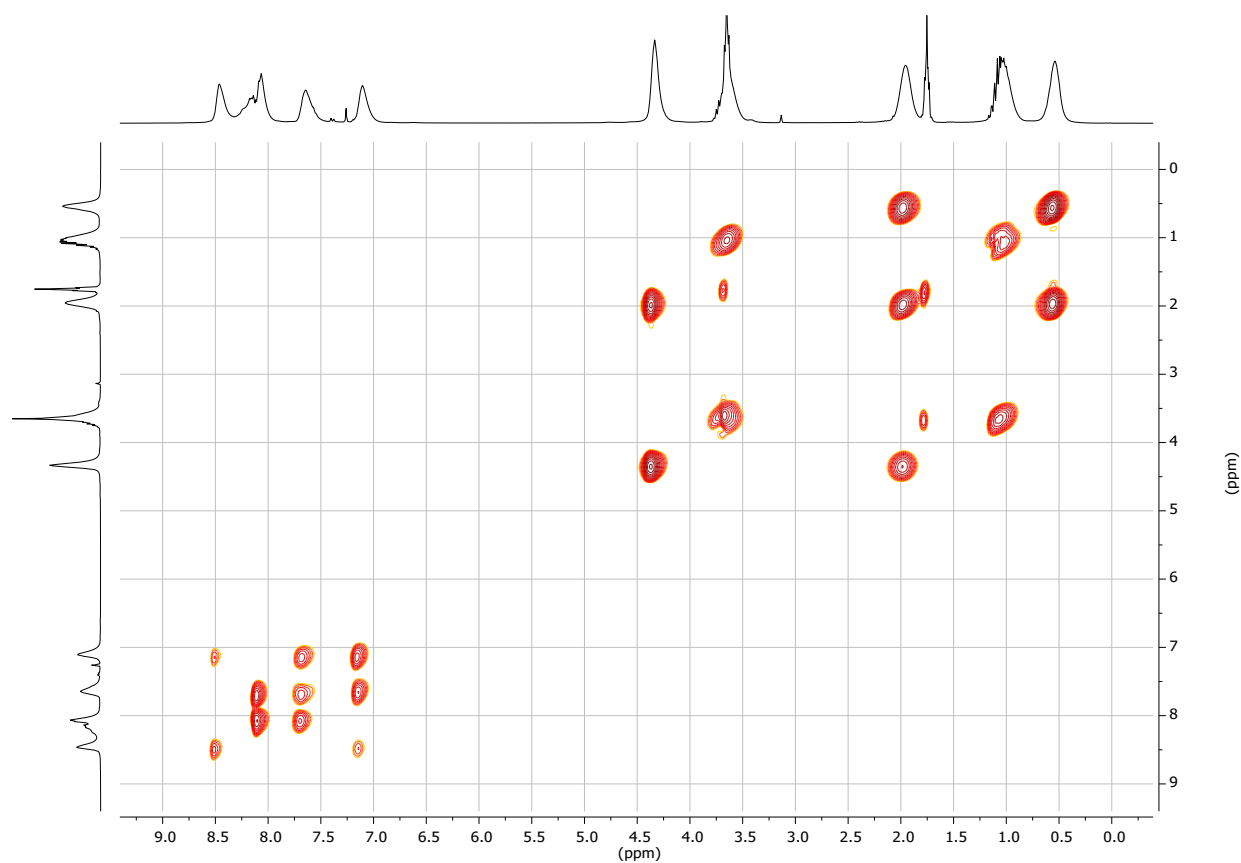


Fig. S14 ^1H COSY Spectra of PY-1,2,3-triazole-siloxane

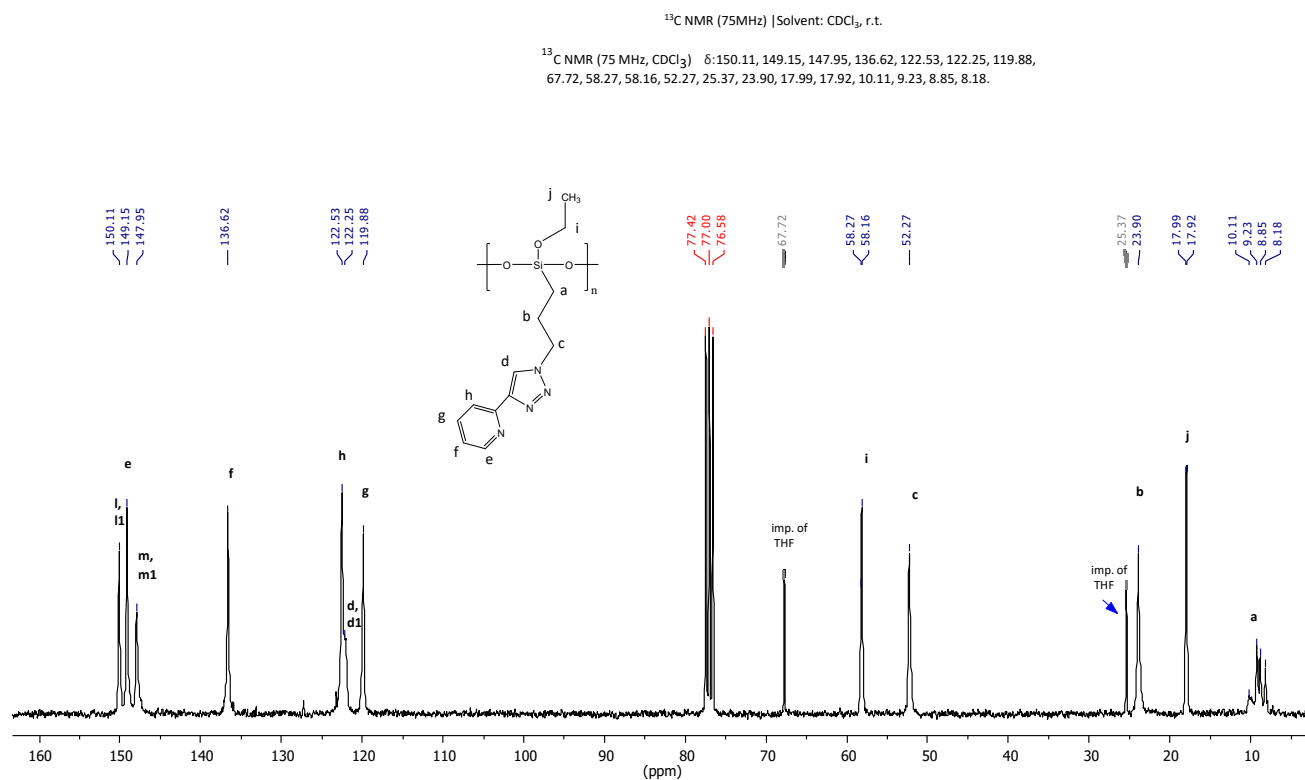


Fig. S15 ^{13}C NMR Spectra of PY-1,2,3-triazole-siloxane

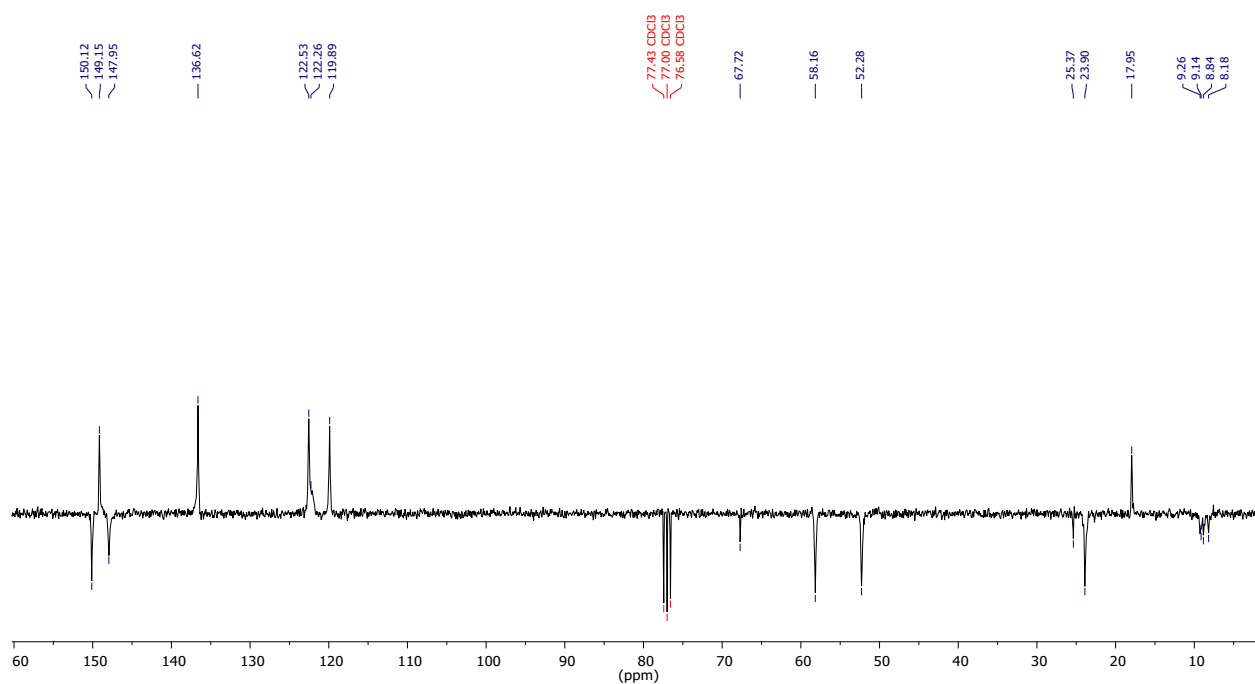


Fig. S16 ¹³C NMR APT Spectra of PY-1,2,3-triazole-siloxane

Si NMR (60 MHz, CDCl₃) δ: (-51)–(-55), (-58)–(-63), (-65)–(-71).

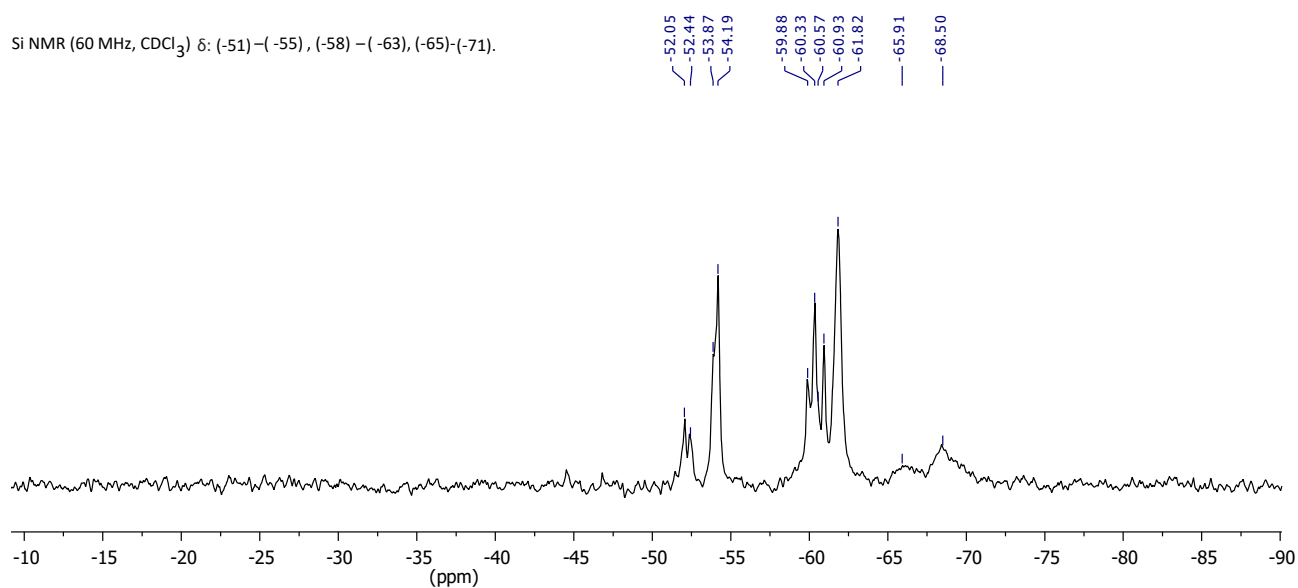


Fig. S17 ²⁹Si NMR Spectra of PY-1,2,3-triazole-siloxane

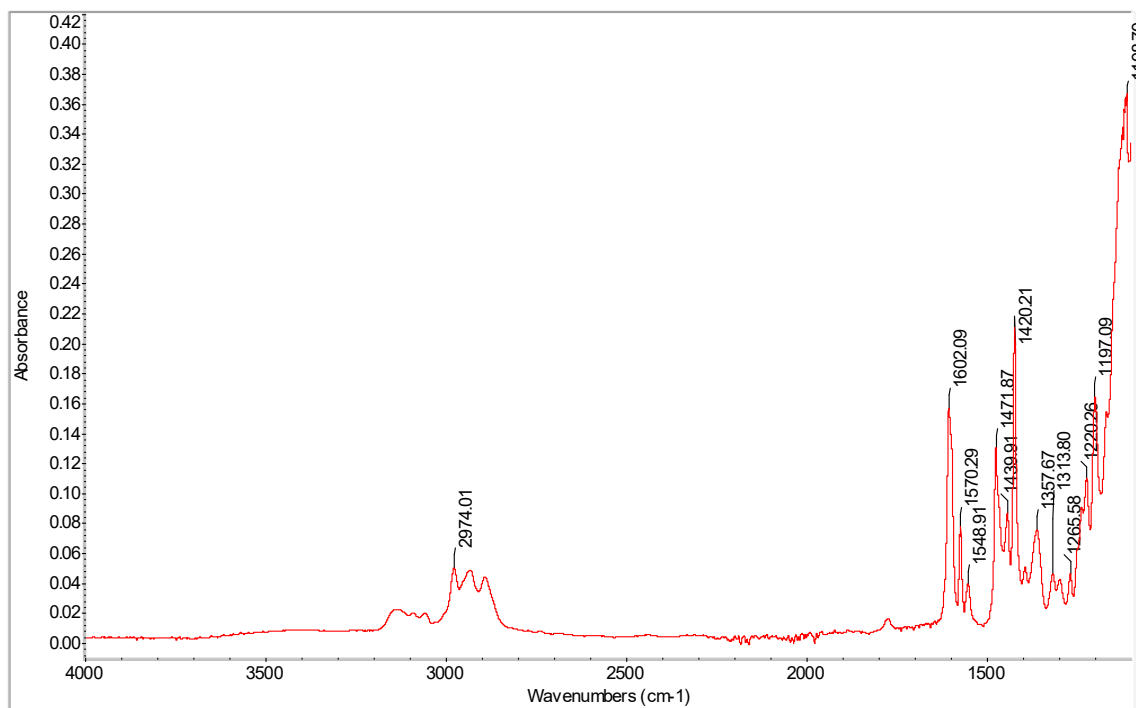


Fig. S18 FTIR spectra of PY-1,2,3-triazole-siloxane

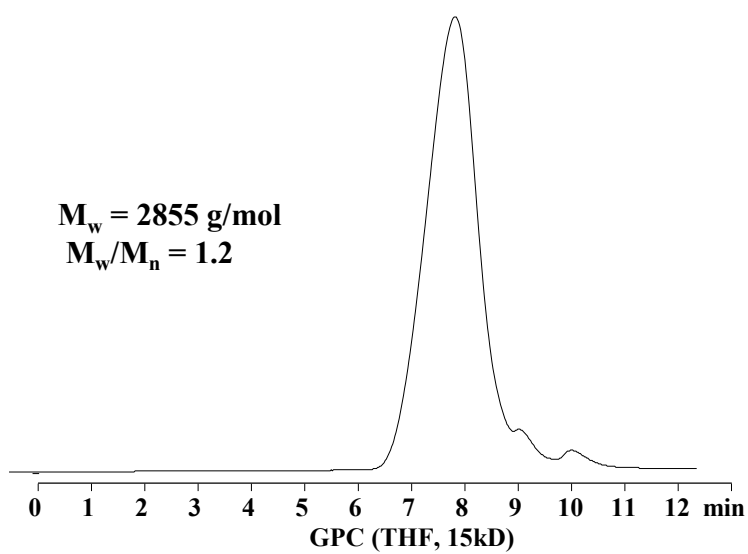


Fig. S19 GPC curve of PY-1,2,3-triazole-siloxane

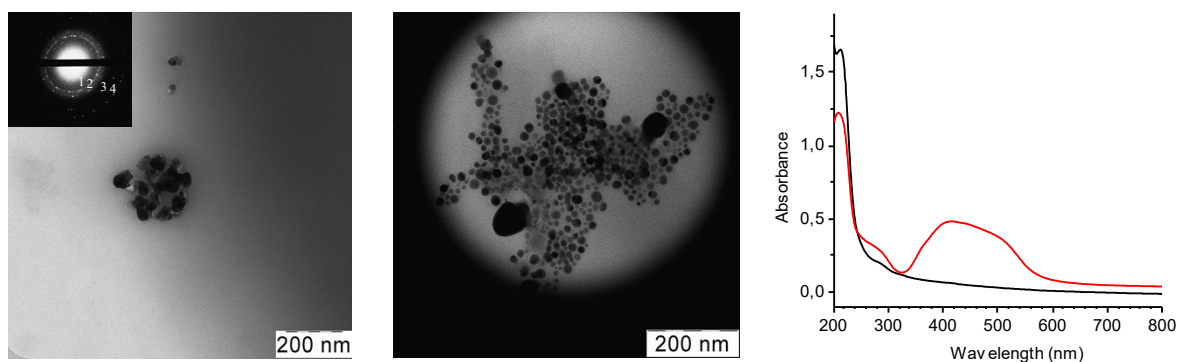


Fig. S20 TEM images with microdiffraction patterns (1,2,3,4 Debye rings correspond to crystalline silver lattice interplanar distances of 2.36, 2.04, 1.45 and 1.23 Å relatively) of DMA-1,2,3-triazole-siloxane/Ag-NPs (6:1) obtained with a 30 kGy X-ray irradiation dose of 0.2% ethanol solutions.

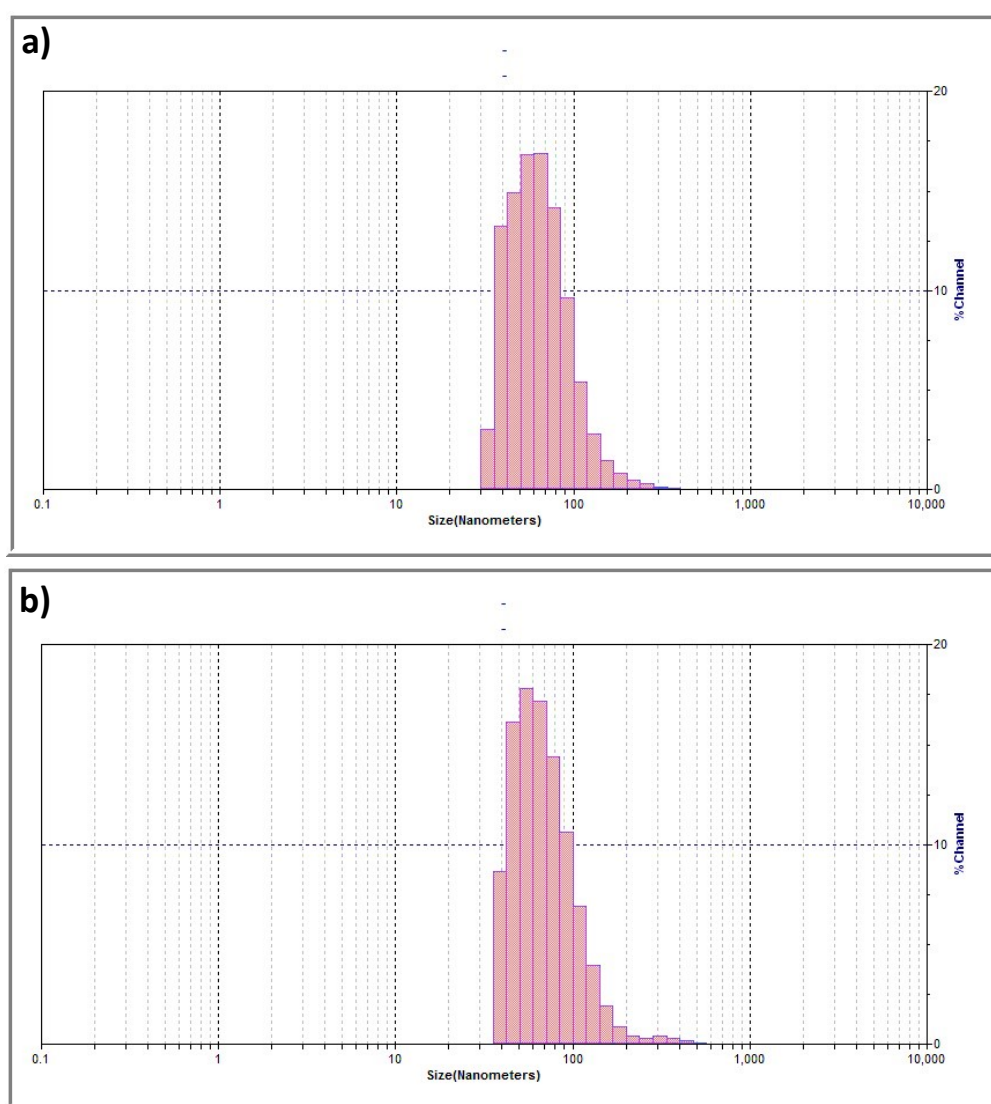


Fig. S21 DLS data for size distribution of DMA-1,2,3-triazole siloxane/Ag-NPs water solutions before (a) and after 2 months of storage (b)

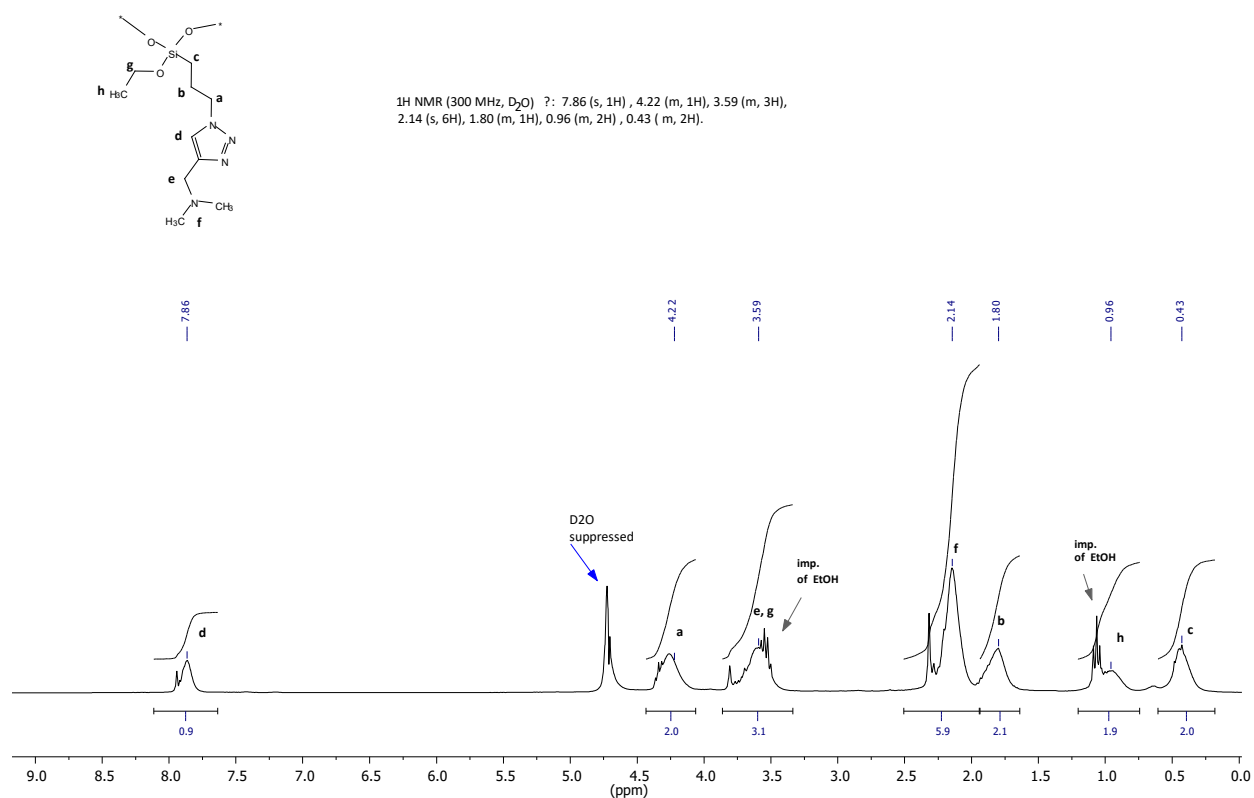


Fig. S22 ^1H NMR Spectra of DMA-1,2,3-triazole-siloxane/Ag-NPs composite in D_2O

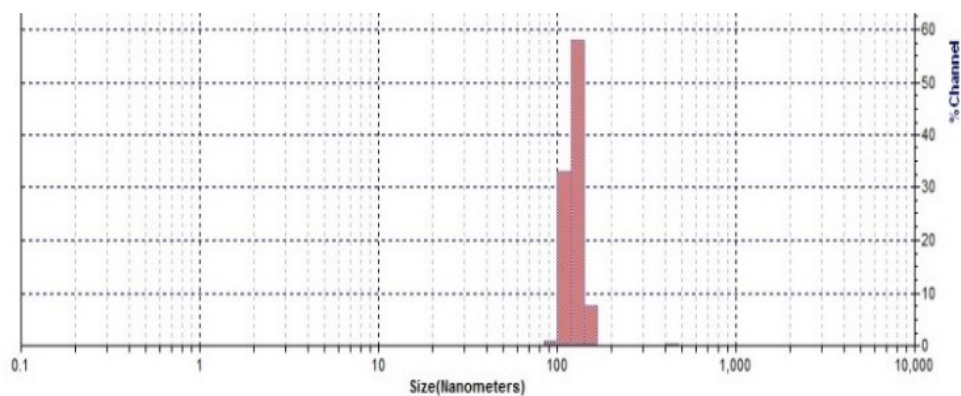
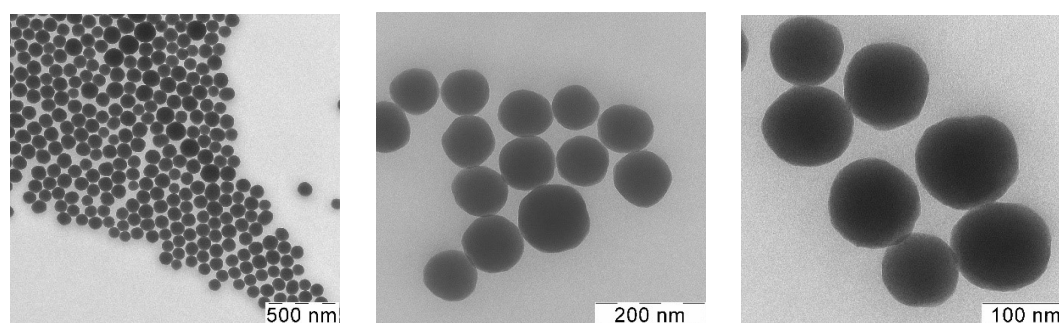


Fig. S23 TEM images and DLS data for size distribution of Stober silica in H_2O

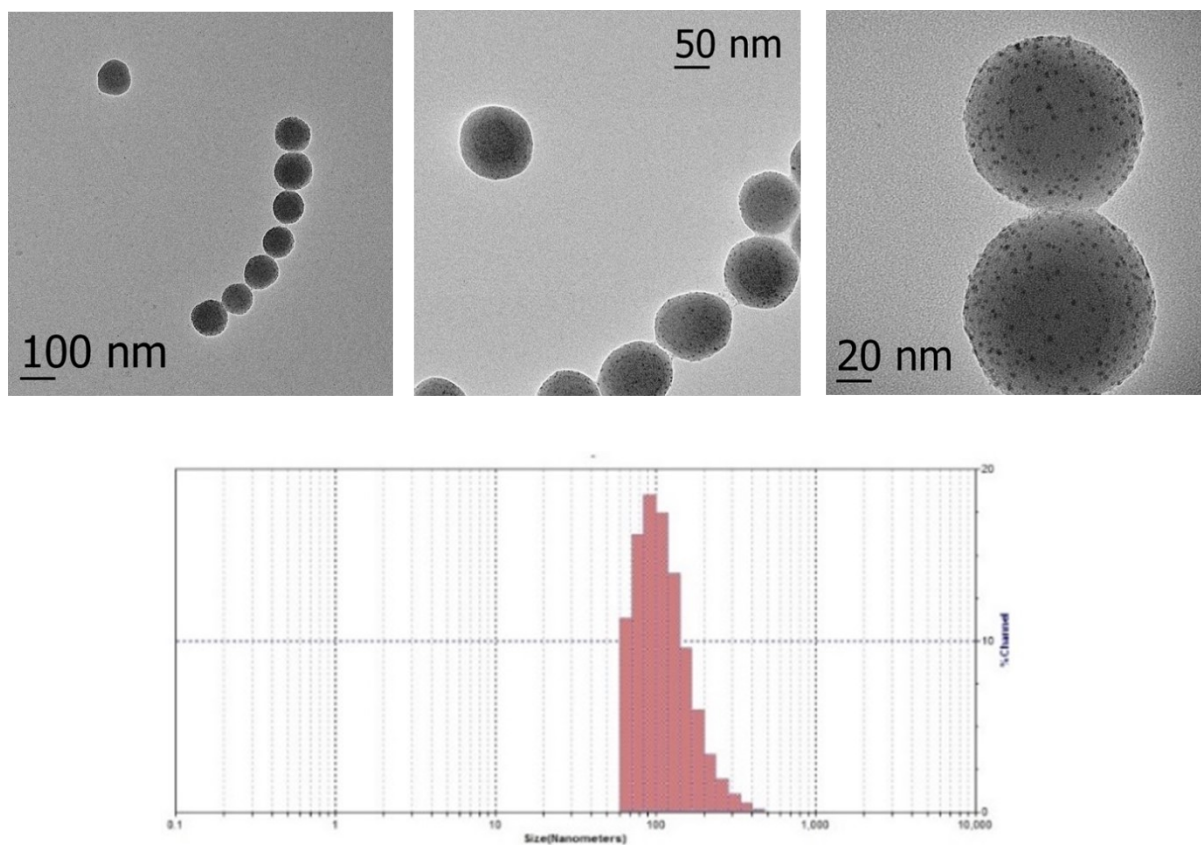


Fig. S24 TEM images and DLS data for size distribution of Stöber silica modified with DMA-1,2,3-triazole-siloxane/Ag-NPs