Electronic Supplementary Information

for

The effect of organosilicon modifiers structure on efficiency of polybutadiene hydrosilylation process

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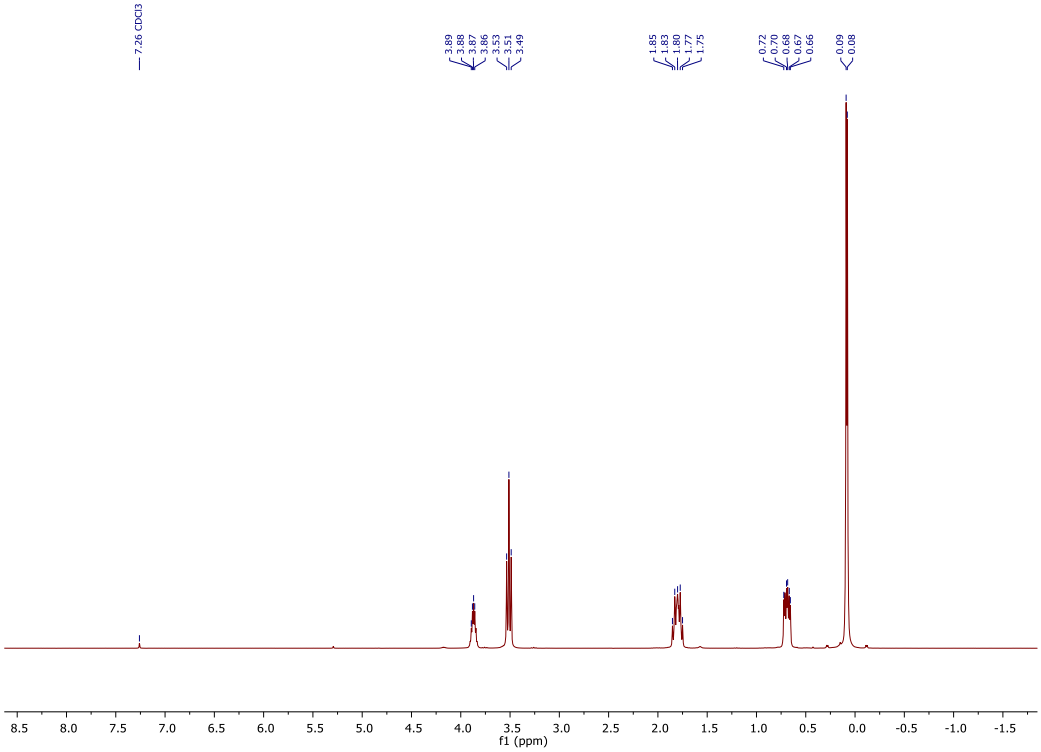
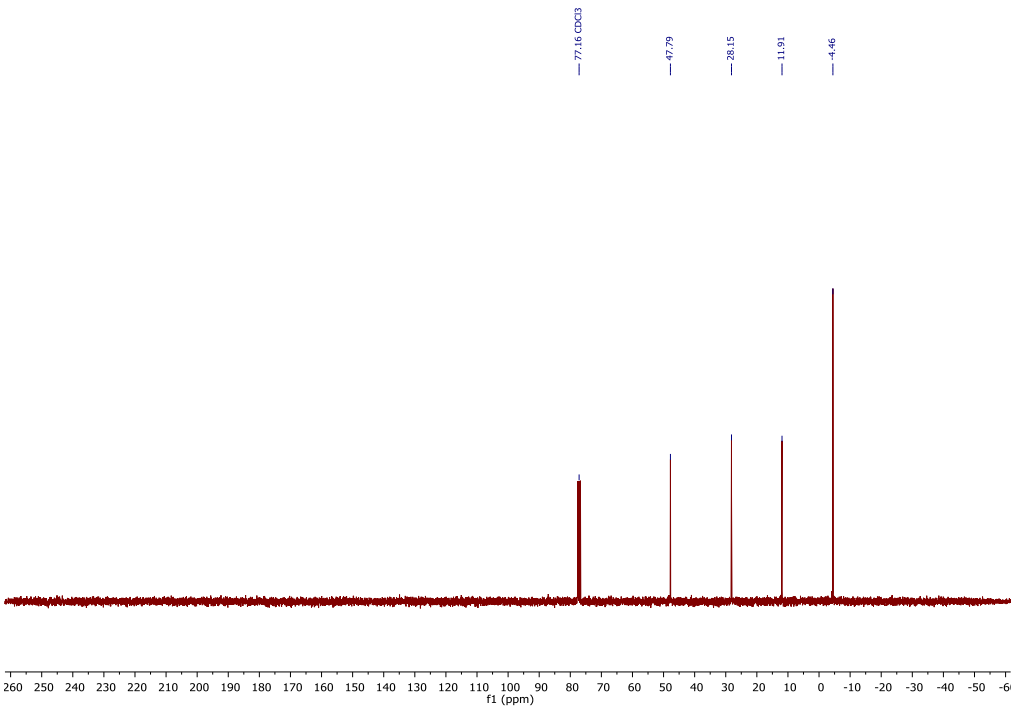
NMR spectra of synthesized silanes

a) 3- chloropropyldimethylsilane

^{1}H NMR:

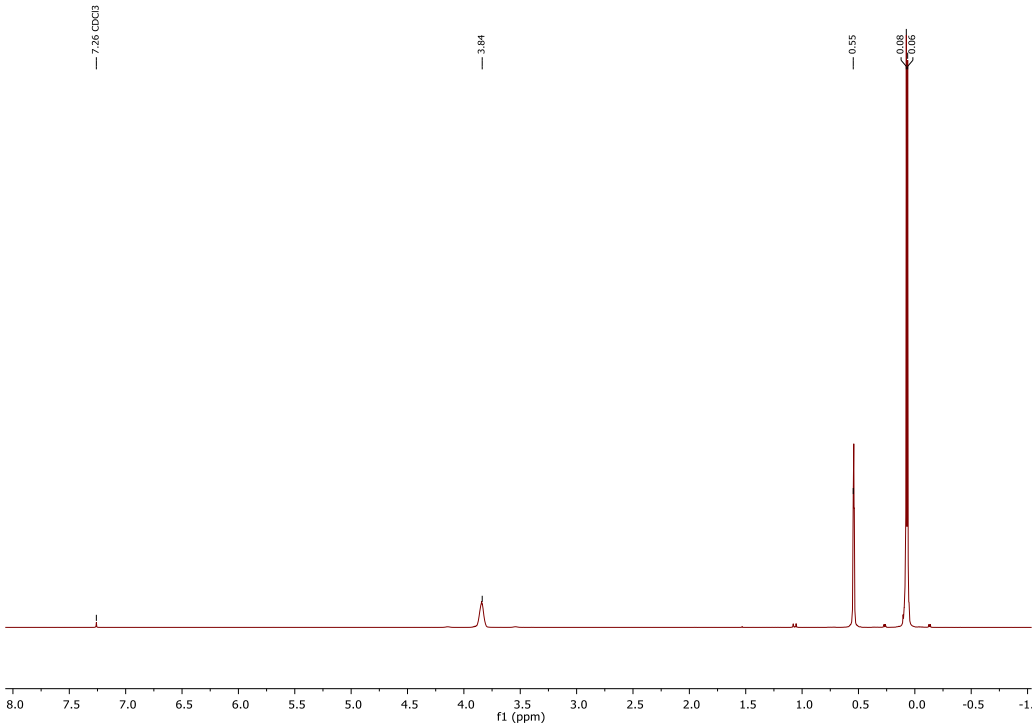


^{13}C NMR:

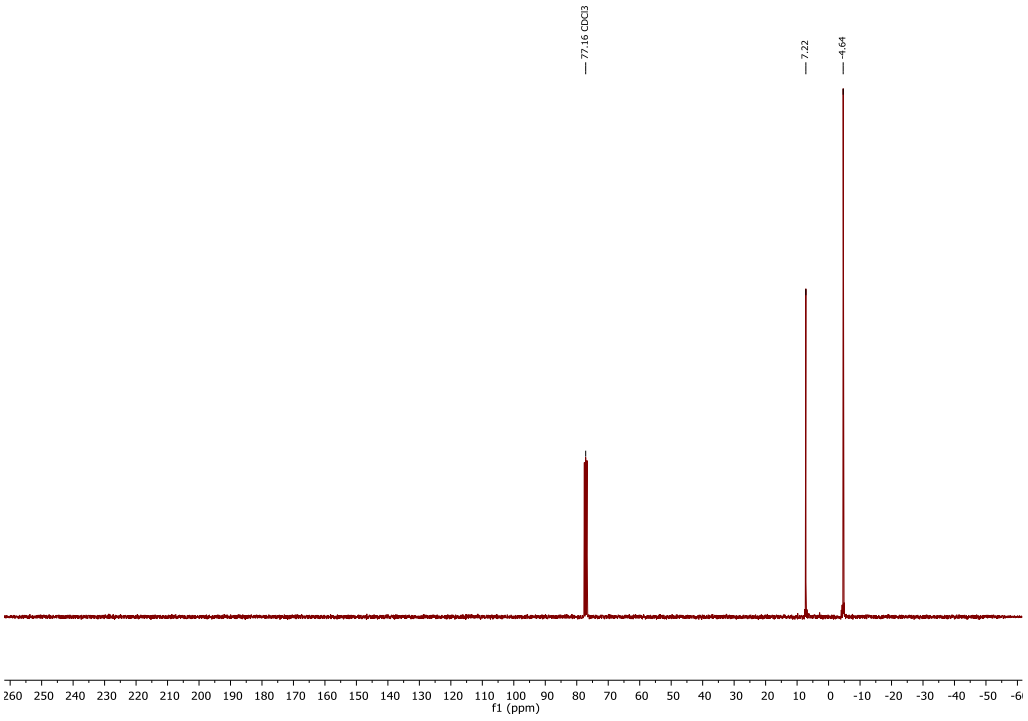


b) 1,2-bis(dimethylchlorosilyl)ethane

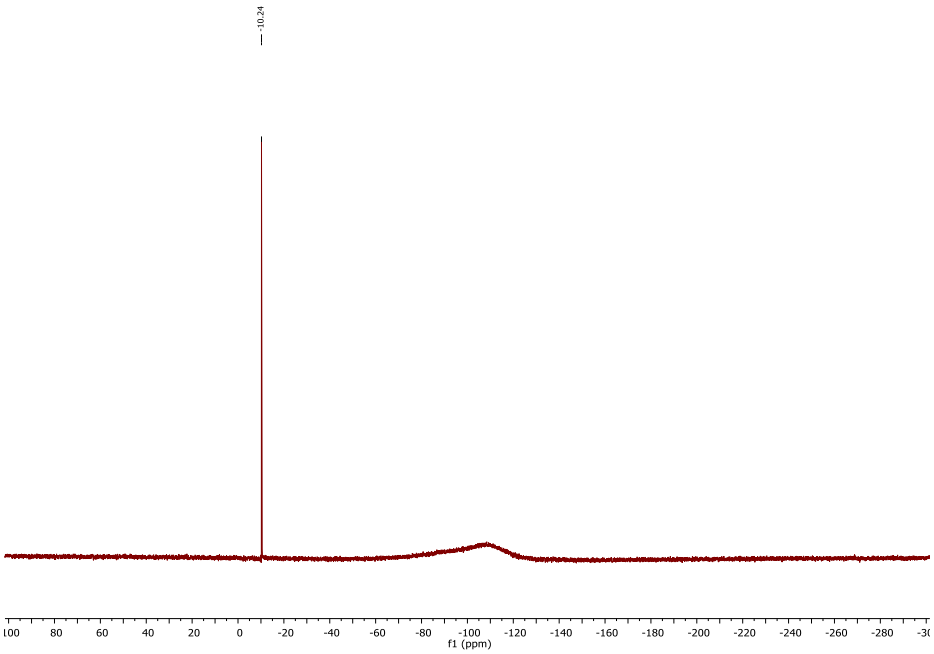
^{1}H NMR:



^{13}C NMR:

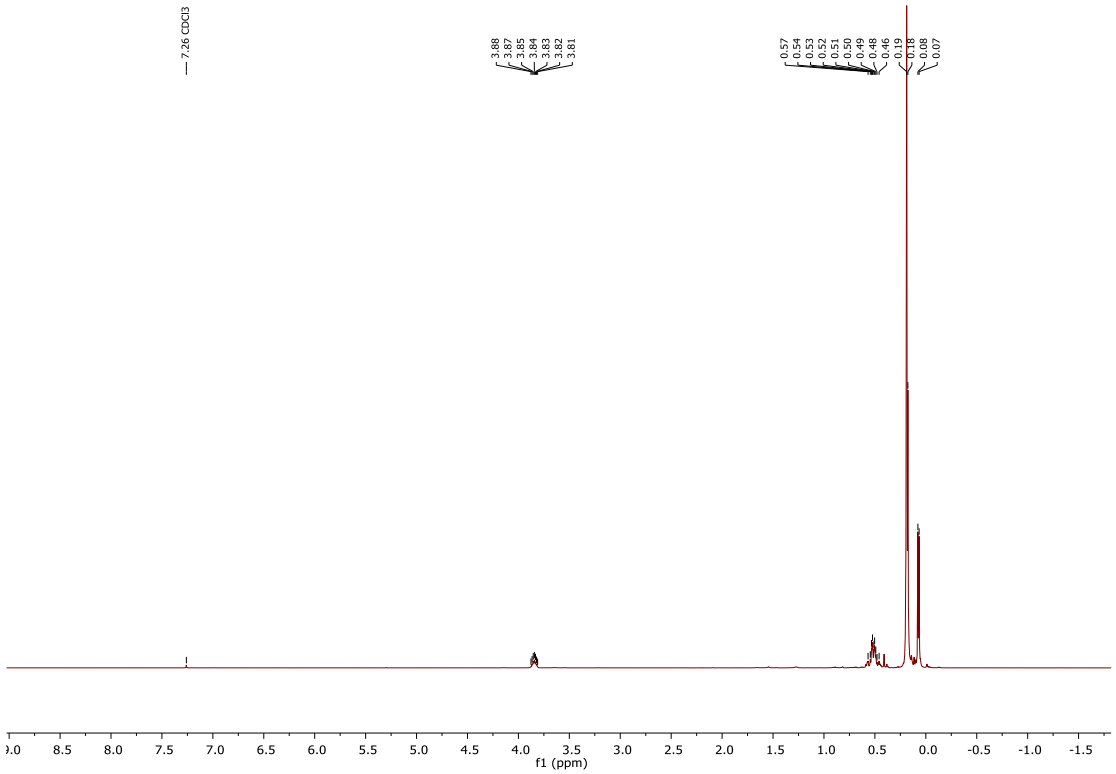


^{29}Si NMR:

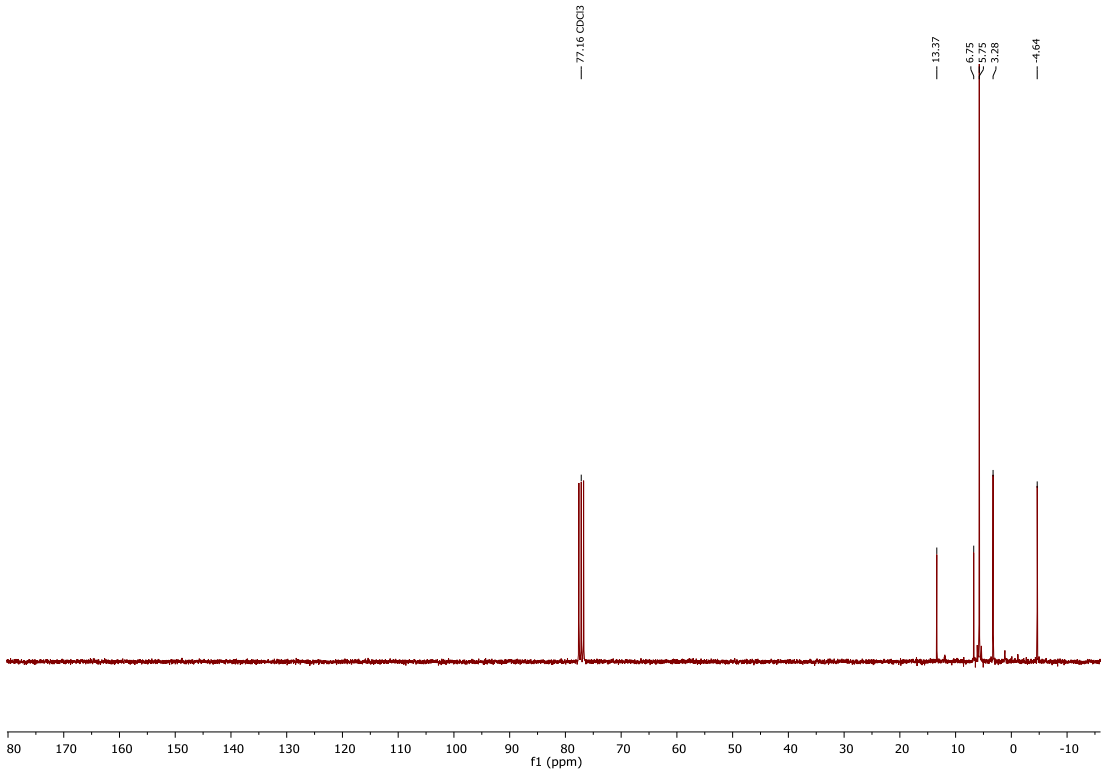


c) dimethyl{ethyl[dimethysilylbis(trimethylsilyl)amine]}silane

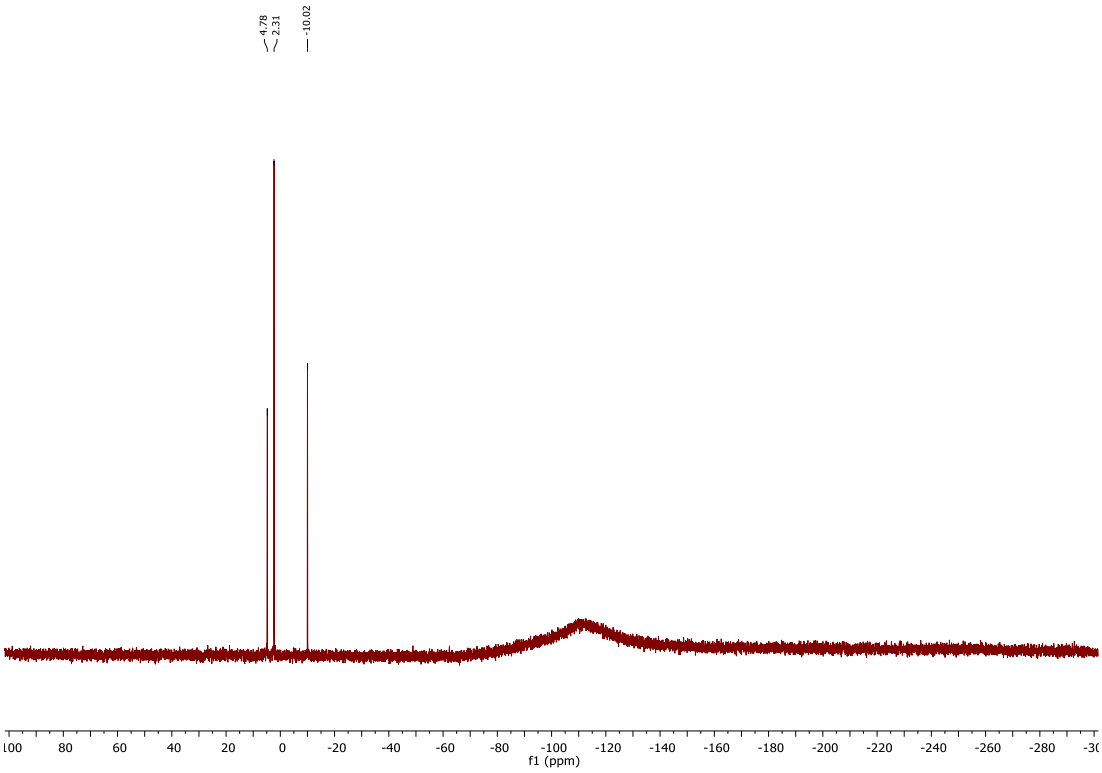
^{1}H NMR:



^{13}C NMR:

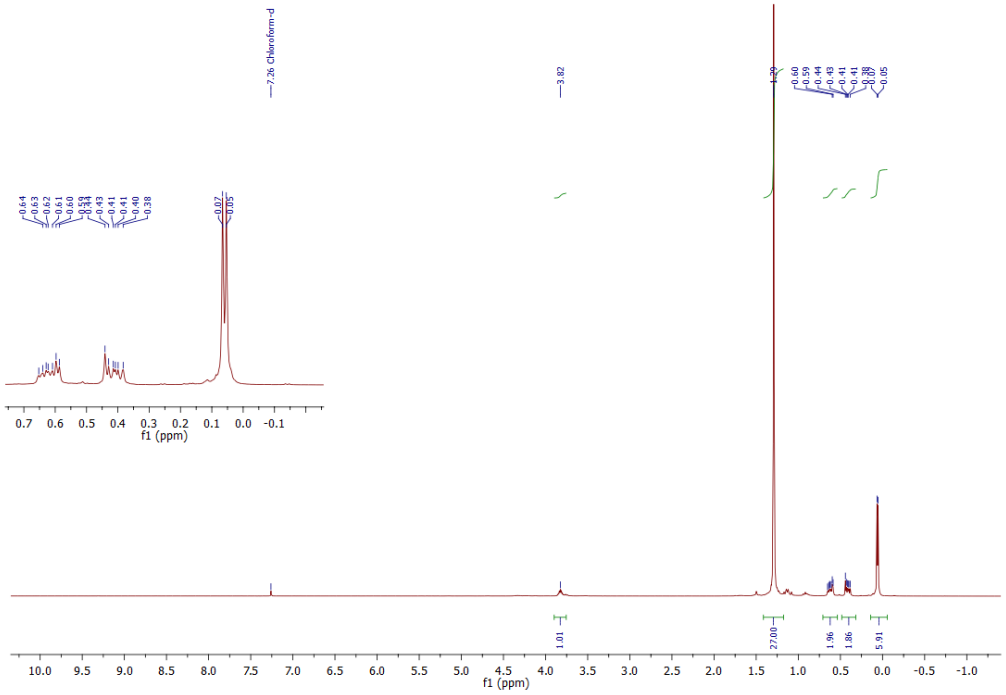


^{29}Si NMR:

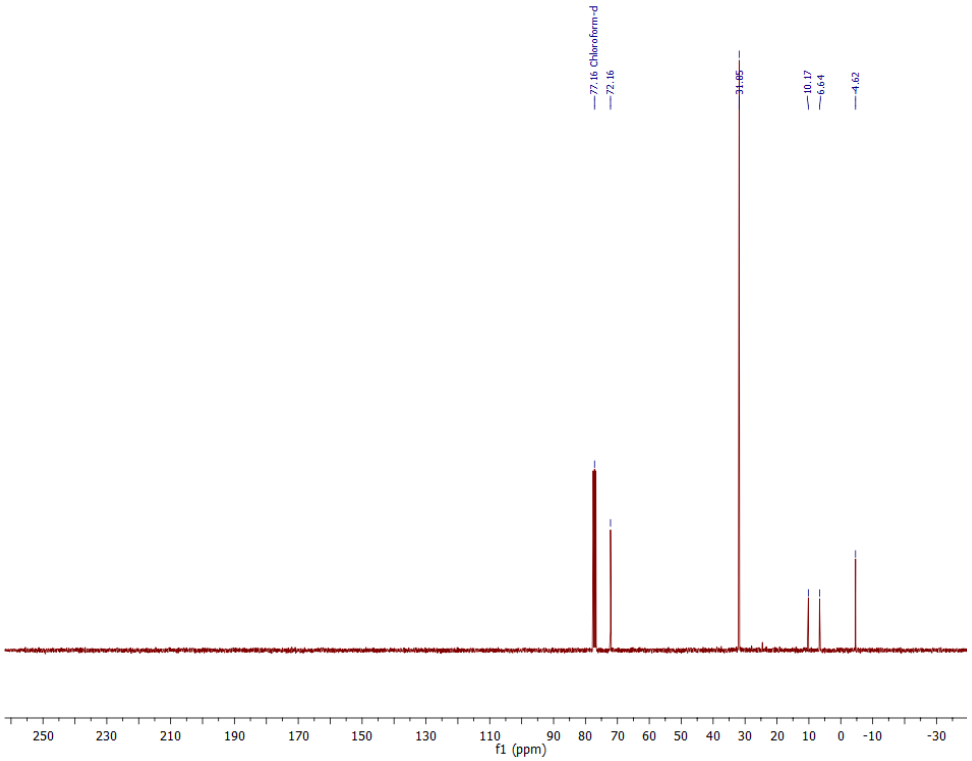


d) dimethyl[2-ethyltris(tertbutoxysilane)]

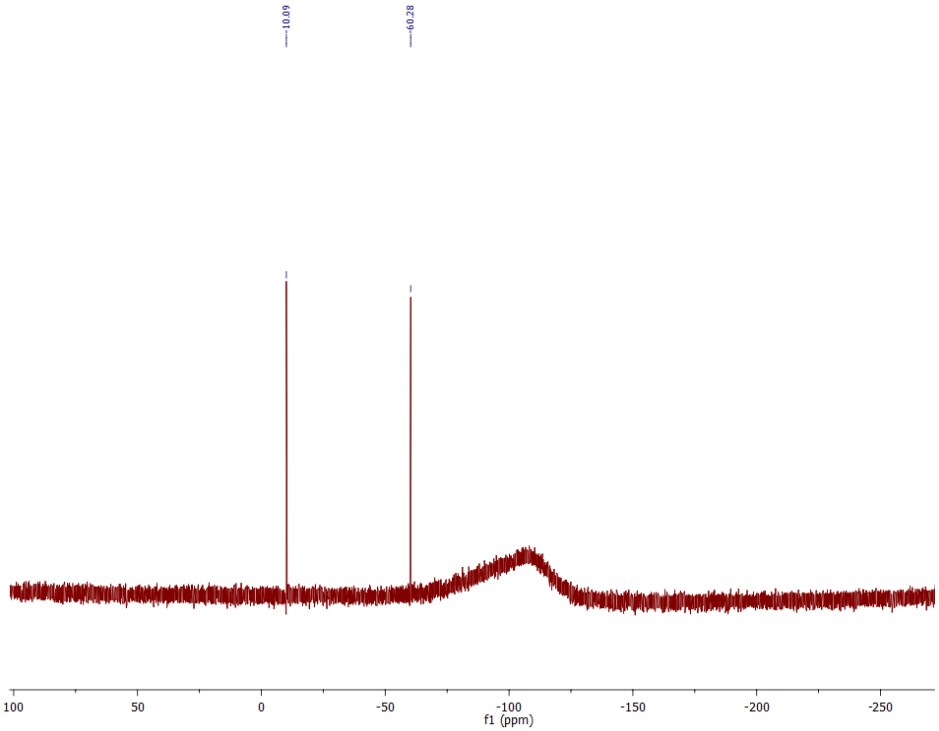
^{1}H NMR



^{13}C NMR:

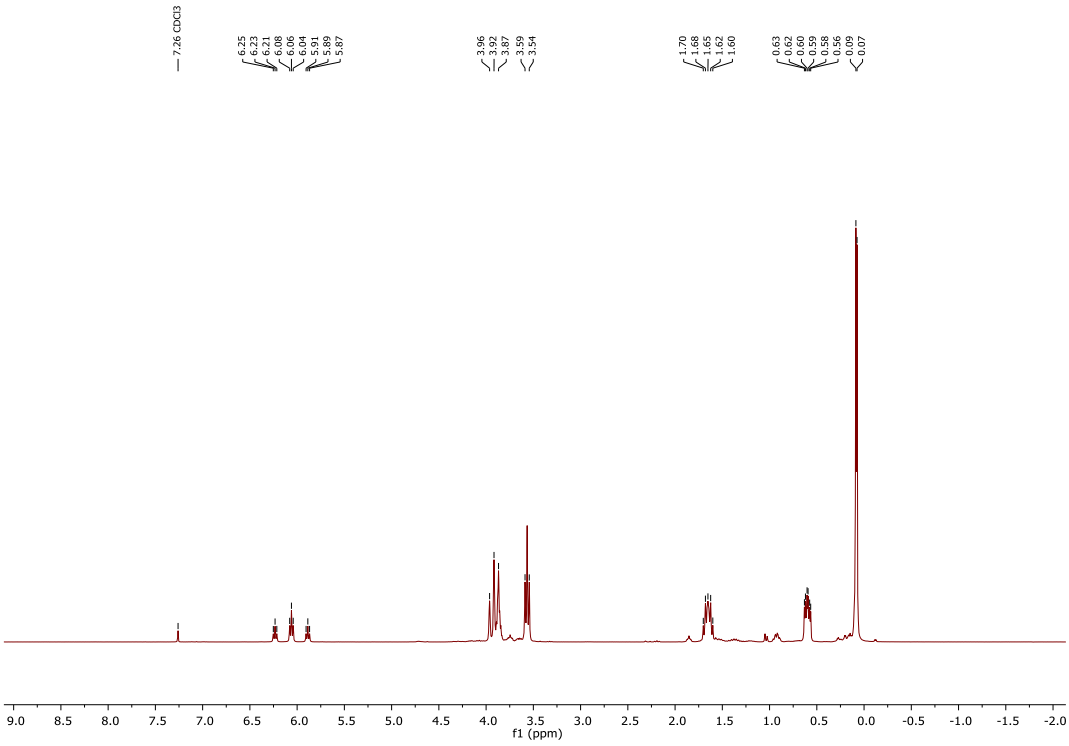


^{29}Si NMR:

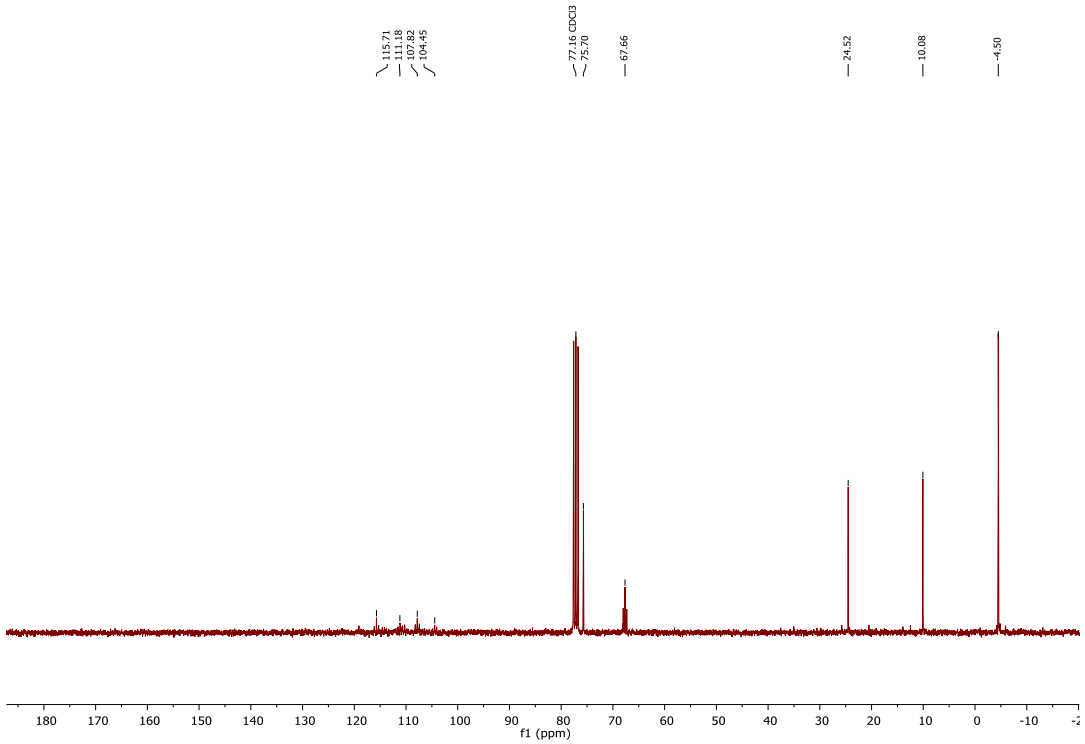


e) dimethyl(3-oktafluoropentyloxy)propylsilane

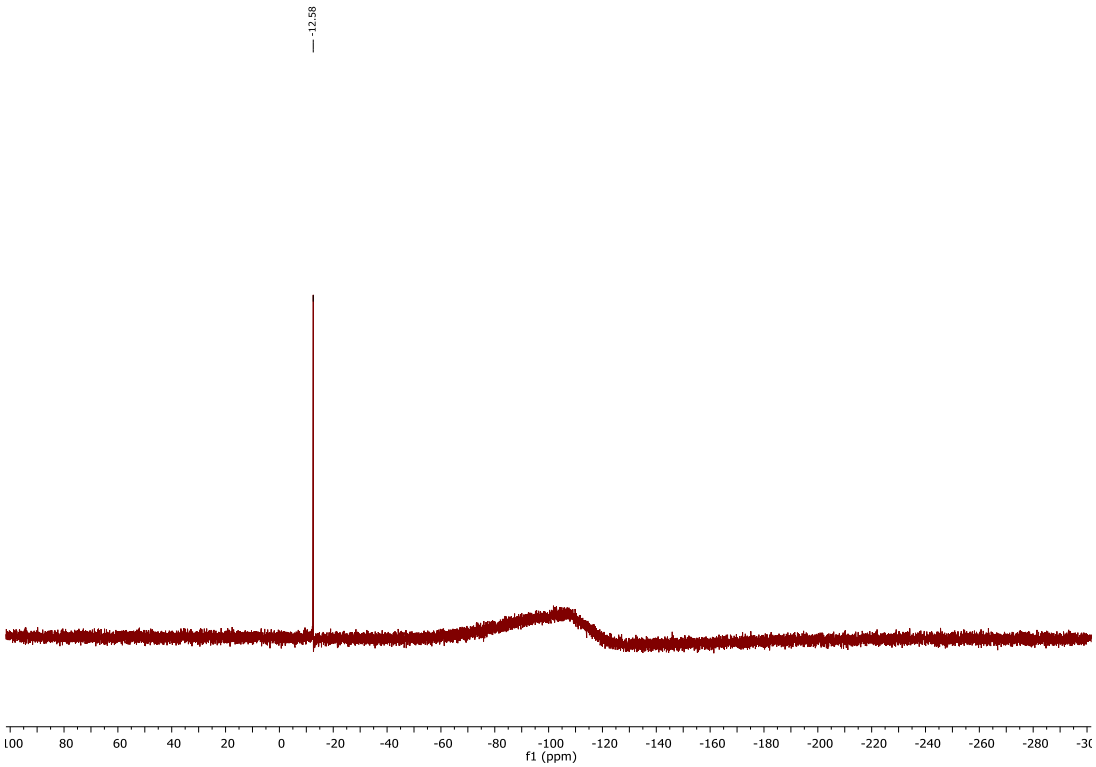
^{1}H NMR:



^{13}C NMR:

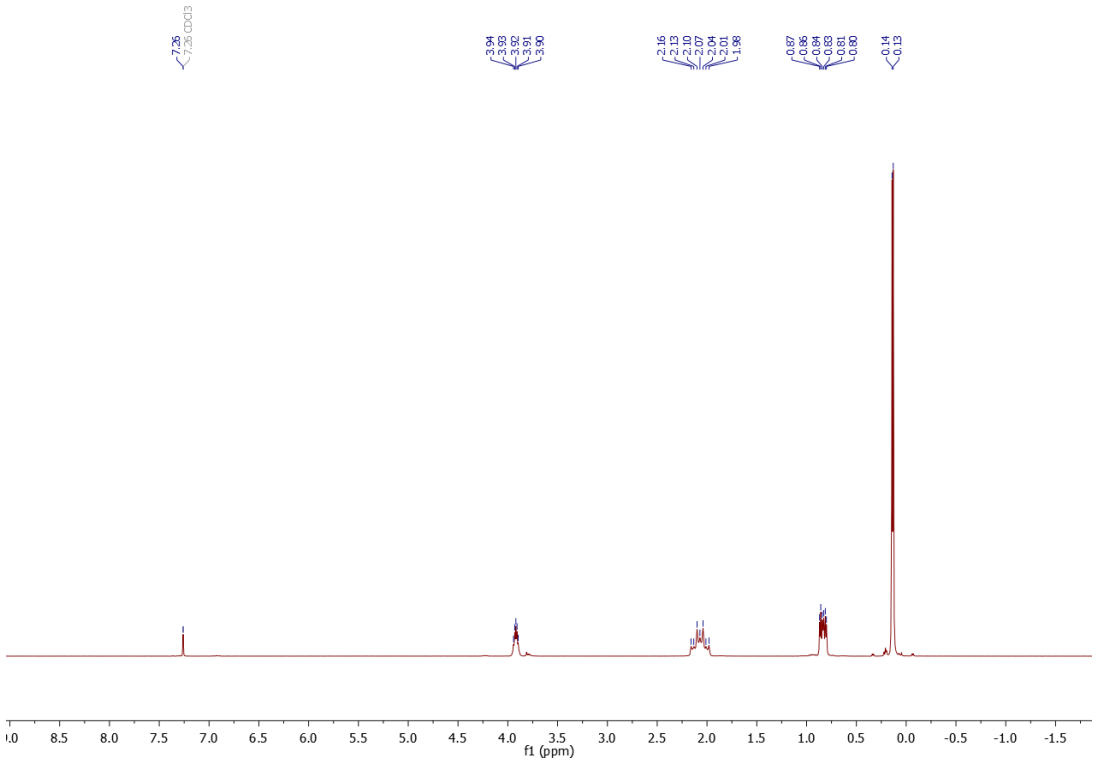


^{29}Si NMR:

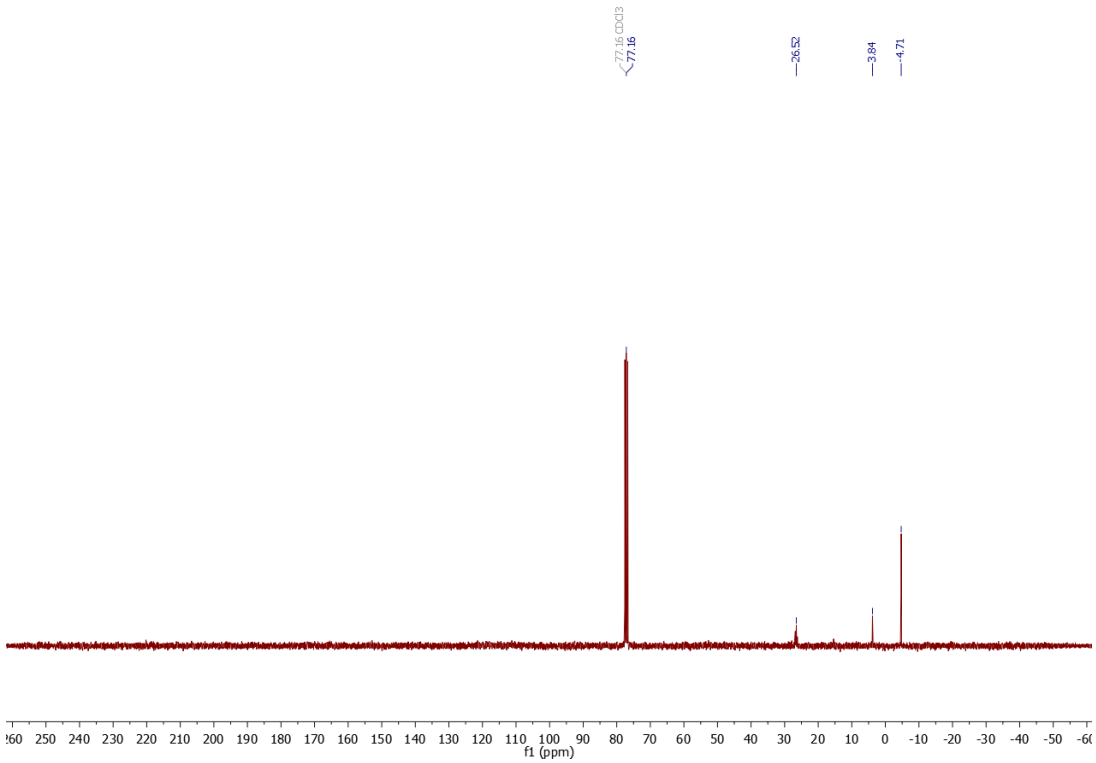


f) (tridecafluoro-1,1,2,2-tetrahydrooctyl)dimethylsilane

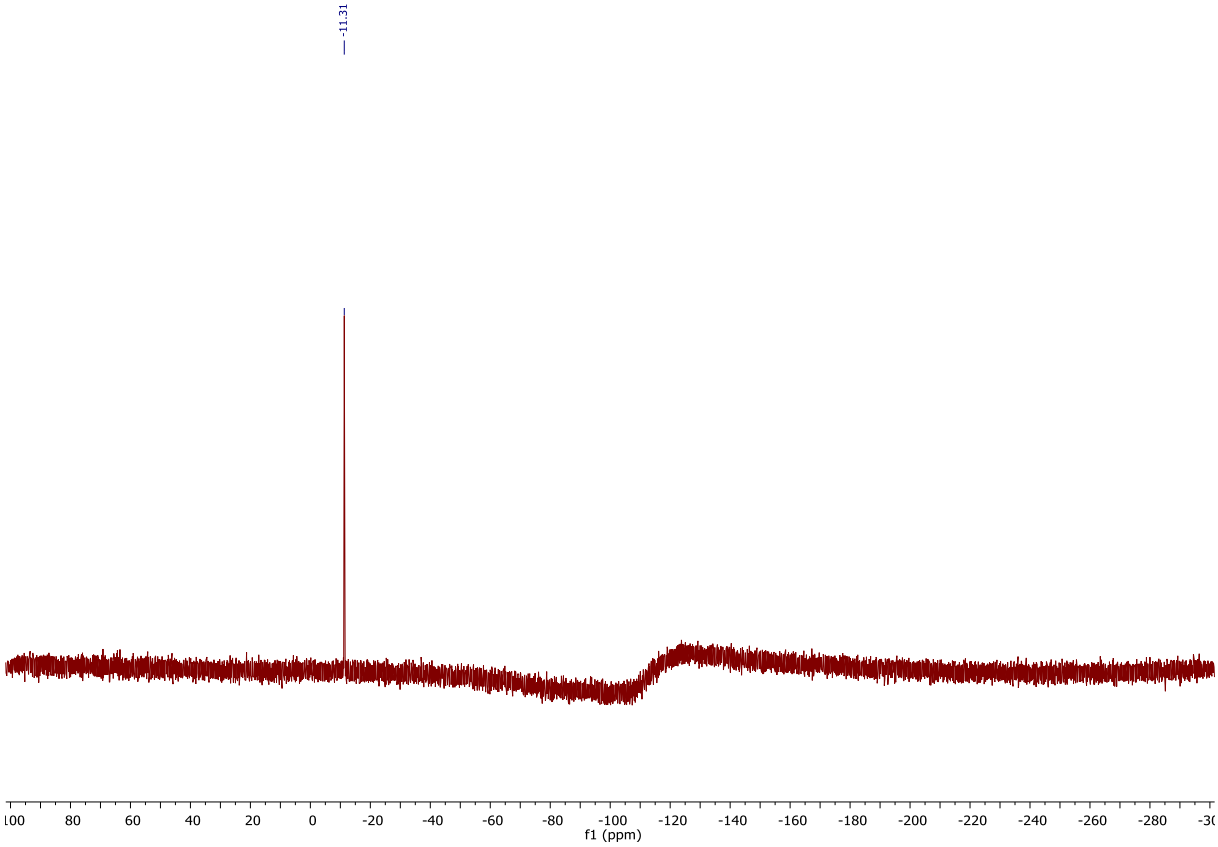
^{1}H NMR:



^{13}C NMR:

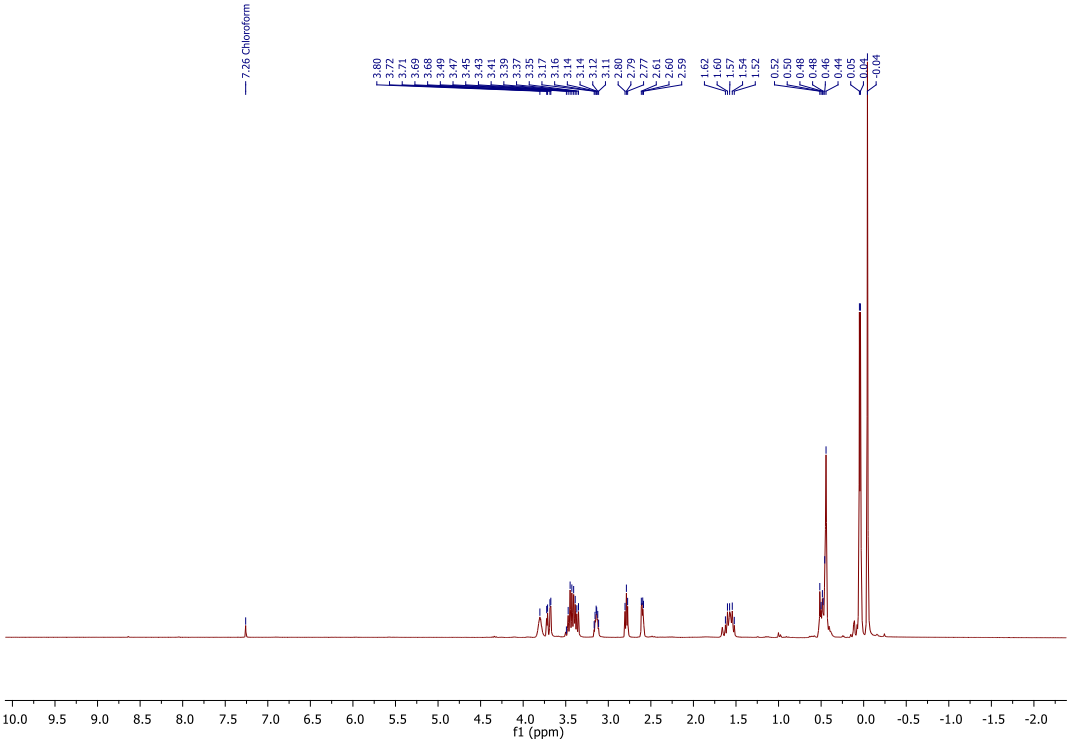


^{29}Si NMR:

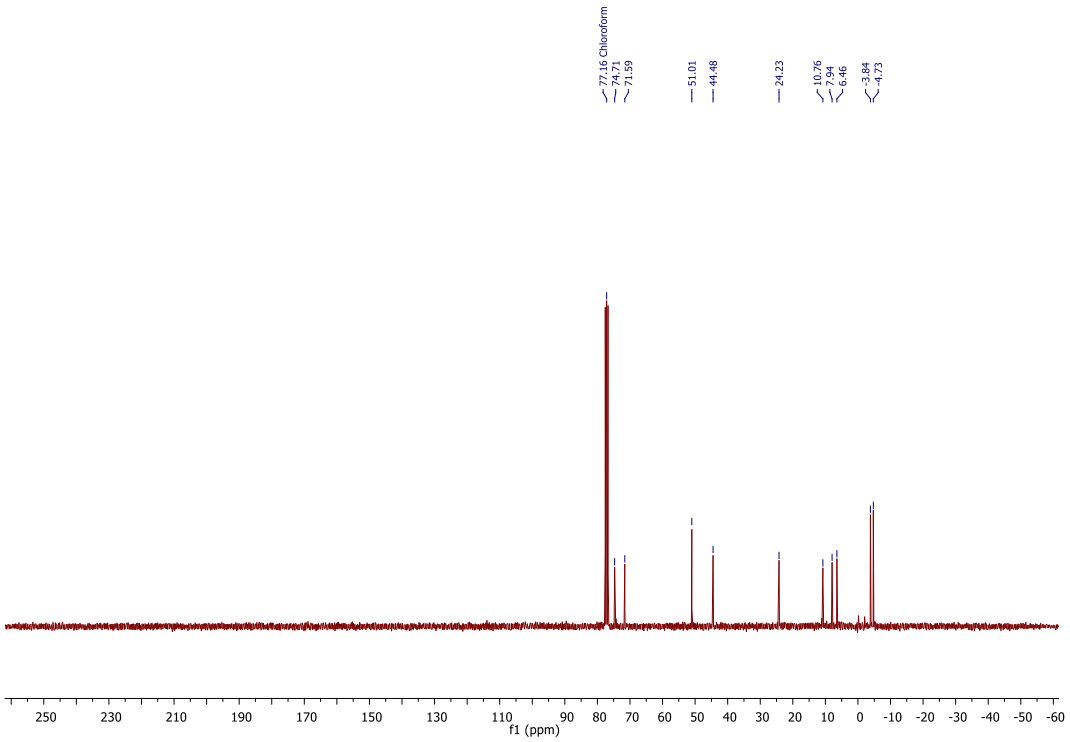


g) dimethyl{ethyl[2-dimethyl(3-glycidylpropyl)silyl]}silane

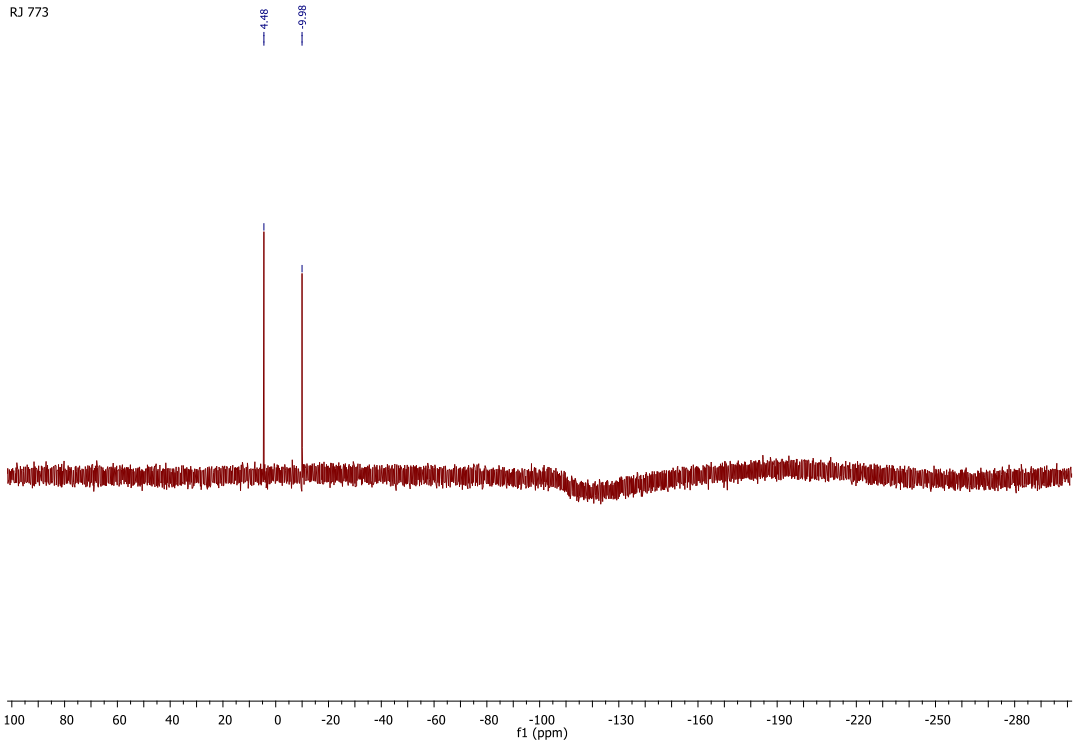
^{1}H NMR:



^{13}C NMR:



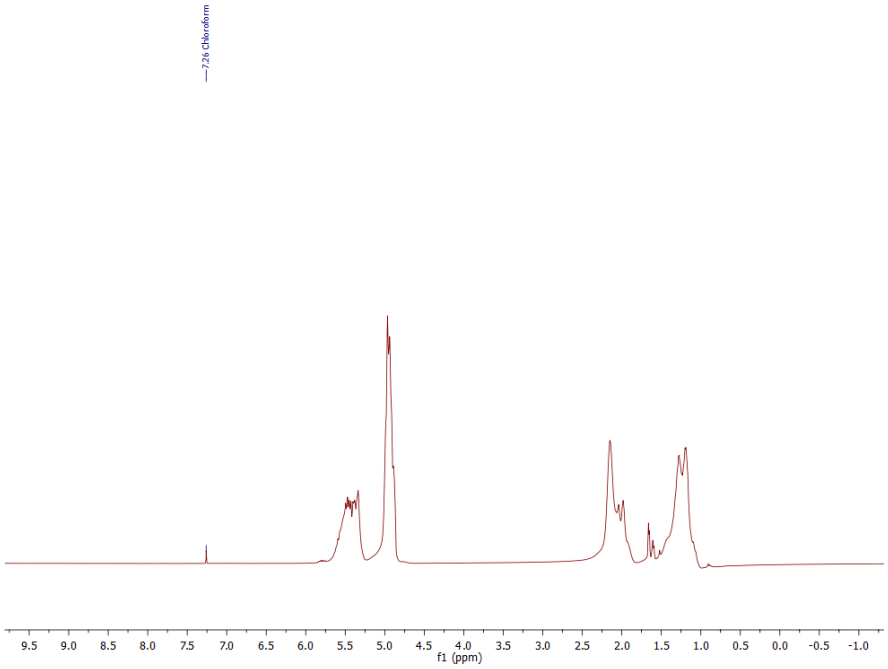
^{29}Si NMR:



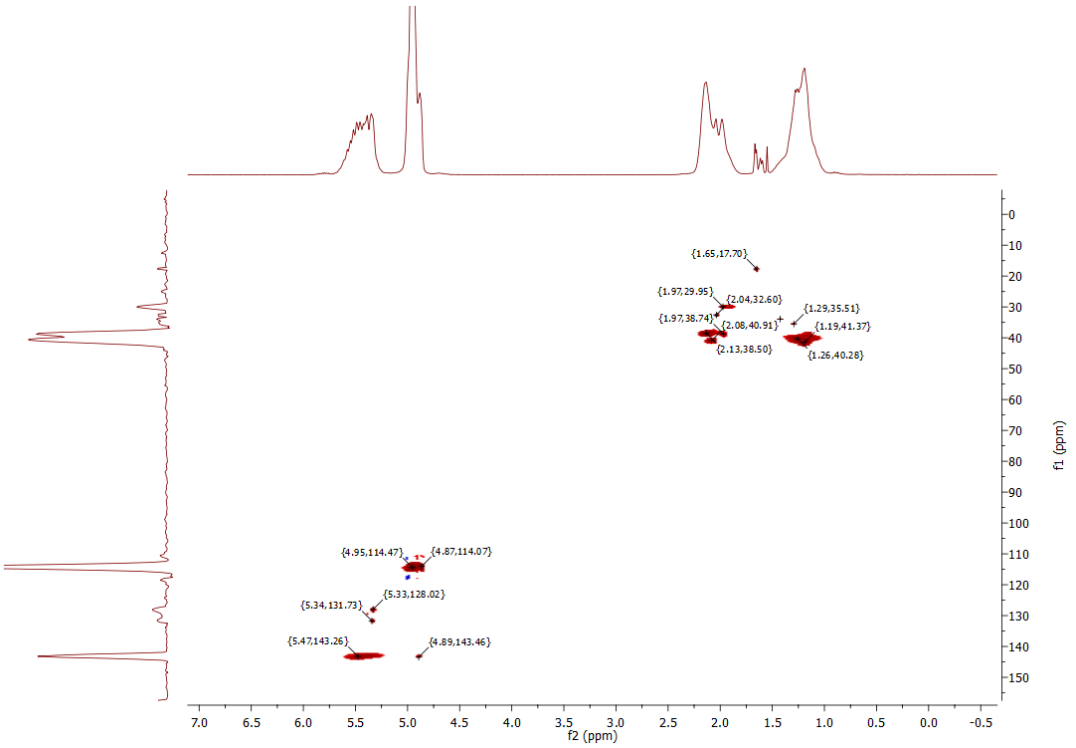
Analytical data of obtained polymers

a) polybutadiene (PB)

^{1}H NMR spectrum of polybutadiene containing 90% of 1,2-units:



2D HSQC NMR spectrum of 1,2-polybutadiene

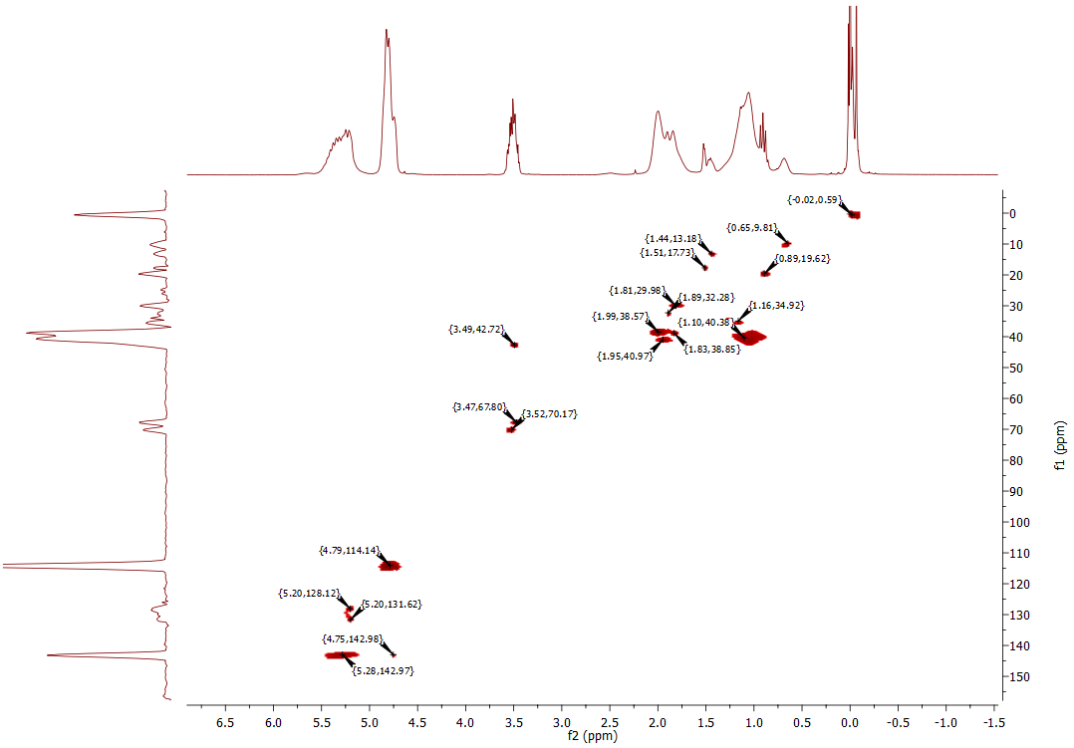


b) PB1A

^{1}H NMR ($CDCl_3$, 298K, δ): 0.06 ($SiCH_3$); 0.78; 1,02 ($SiCH_2$); 0.92-2.26 (CH, CH_2); 3.62-3.65 ($CH_2OCH_2CH_2Cl$); 4.85-5.53 ($CH=CH_2$); 5.44-5.34 (CH=CH);

^{13}C NMR ($CDCl_3$, 298K, δ): 0.67 ($SiCH_3$), 10.51; 19.78 ($SiCH_2$); 13.18-41.37 (CH, CH_2); 42.69; 67.81; 70.10 ($CH_2OCH_2CH_2Cl$); 114.28-143.41($CH=CH_2$); 128.13-131.63 (CH=CH);

GPC: Mn = 5989 [g•mol^{-1}], Mw = 8782 [g•mol^{-1}], PD=1.46.

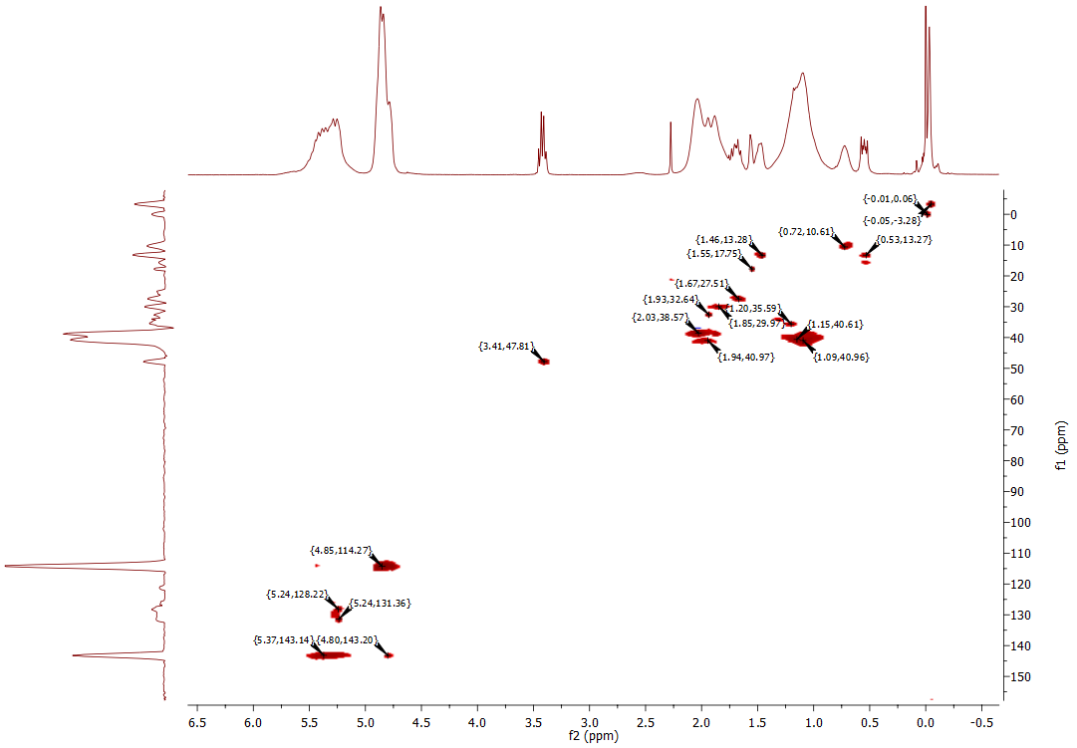


c) **PB1B**

^{1}H NMR ($CDCl_3$, 298K, δ): 0.06 ($SiCH_3$); 0.53; 0.72 ($SiCH_2$); 0.90-2.28 (CH, CH_2); 3.41 (CH_2Cl); 4.88-5.45 ($CH=CH_2$); 5.33-5.34 (CH=CH);

^{13}C NMR ($CDCl_3$, 298K, δ): -3.28 ($SiCH_3$); 10.61; 13.27 ($SiCH_2$); 13.28-40.96 (CH, CH_2); 47.81 (CH_2Cl); 114.27-143.20 ($CH=CH_2$); 128,22-131.36 (CH=CH);

GPC: Mn =5615 [g•mol^{-1}], Mw =8581 [g•mol^{-1}], PD=1.52.

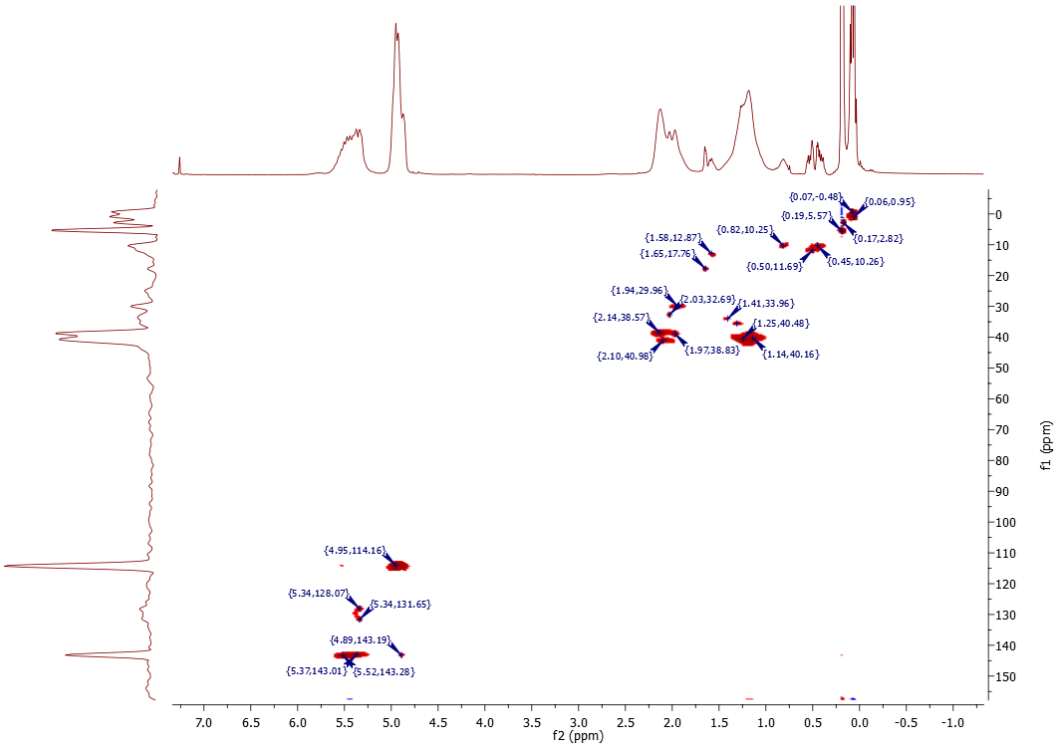


d) **PB2A**

^{1}H NMR ($CDCl_3$, 298K, δ): 0.08; 0.17; 0.19 ($SiCH_3$); 0.45; 0.50; 0.82 ($SiCH_2$); 0.95-2.28 (CH, CH_2); 4.89-5.53 ($CH=CH_2$); 5.34-5.35 (CH=CH);

^{13}C NMR ($CDCl_3$, 298K, δ): 0.77; 2.79; 5.27 ($SiCH_3$); 10.23; 10.25; 11.67 ($SiCH_2$); 13.25-40.82 (CH, CH_2); 114.06-143.32 ($CH=CH_2$); 128.10-131.61 (CH=CH);

GPC: Mn =6424 [g•mol^{-1}], Mw = 9507 [g•mol^{-1}], PD=1.48.

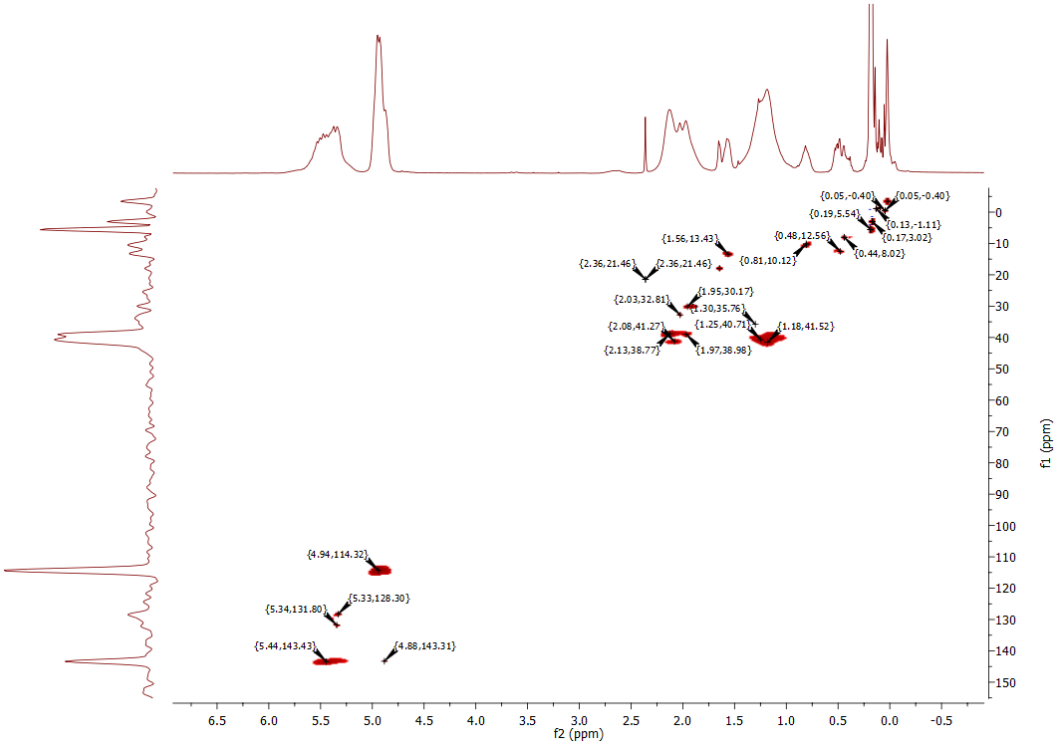


e) PB2B

^{1}H NMR ($CDCl_3$, 298K, δ): 0.02-0.19 ($SiCH_3$); 0.44; 0.48; 0.81 ($SiCH_2$); 0.91-2.31 (CH, CH_2); 4.88-5.44 ($CH=CH_2$); 5.34-5.34 (CH=CH);

^{13}C NMR ($CDCl_3$, 298K, δ): -3.45-5.54 ($SiCH_3$); 8.02; 10.12; 12.56 ($SiCH_2$); 13.43-41.52 (CH, CH_2); 114.32-143.43 ($CH=CH_2$); 128.30-131.80 (CH=CH);

GPC: Mn =5701 [g•mol^{-1}], Mw = 8323 [g•mol^{-1}], PD=1.46.

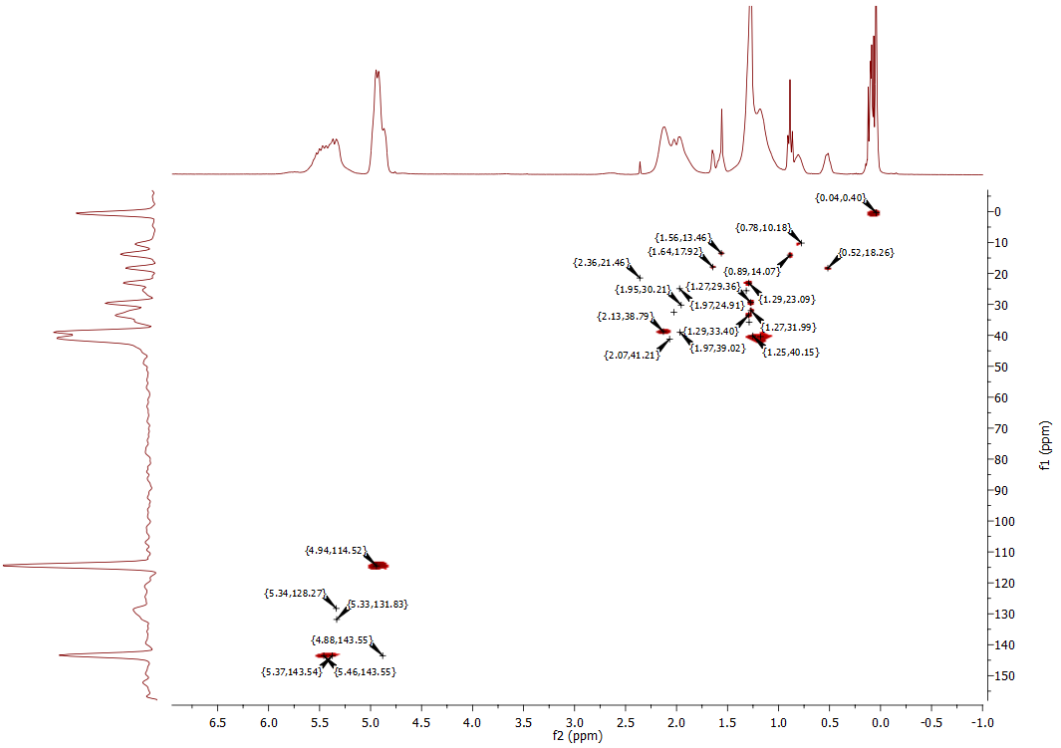


f) PB3A

^{1}H NMR ($CDCl_3$, 298K, δ): 0.40 ($SiCH_3$); 0.52; 0.78 ($SiCH_2$); 0.89 (CH_3); 0.95-2.24 (CH, CH_2); 4.88-5.46 ($CH=CH_2$); 5.33-5.34 (CH=CH);

^{13}C NMR ($CDCl_3$, 298K, δ): 0.40 ($SiCH_3$); 10.18; 18.26 ($SiCH_2$); 14.07 (CH_3); 13.46-41.21 (CH, CH_2); 114.52-143.55 ($CH=CH_2$); 128.27-131.83(CH=CH);

GPC: Mn =6002 [g•mol^{-1}], Mw = 8792 [g•mol^{-1}], PD=1.46.

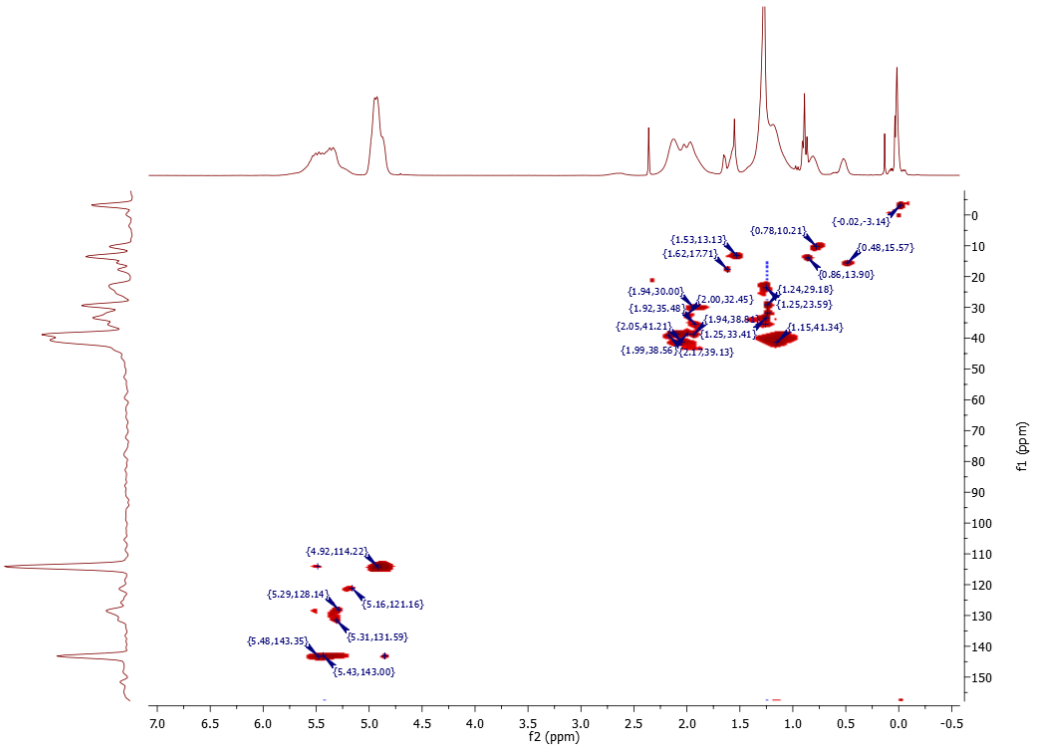


g) PB3B

^{1}H NMR ($CDCl_3$, 298K, δ): -0.02 ($SiCH_3$); 0.48; 0.78 ($SiCH_2$); 0.86 (CH_3); 0.99-2.45 (CH, CH_2); 4.93-5.44 (-CH=CH_2); 5.18-5.33 (CH=CH);

^{13}C NMR ($CDCl_3$, 298K, δ): -3.14 ($SiCH_3$); 10.52; 15.58 ($SiCH_2$); 13.90 (CH_3); 13.07-41.20 (CH, CH_2); 114.22-143.39 (CH=CH_2); 120.90-131.60 (CH=CH);

GPC: Mn = 6012 [g•mol^{-1}], Mw = 9491 [g•mol^{-1}], PD=1.58.

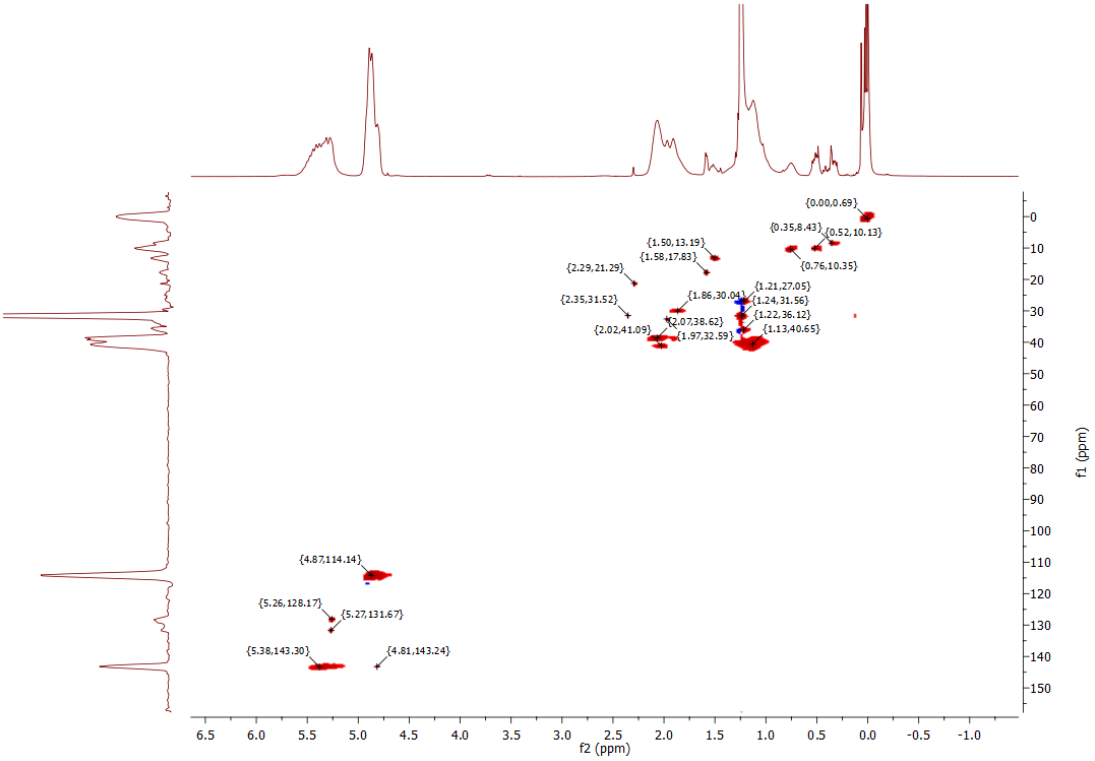


h) PB4A

^{1}H NMR ($CDCl_3$, 298K, δ): 0.00; 0.11 ($SiCH_3$); 0.35; 0.52; 0.76 ($SiCH_2$); 0.92-2.35 (CH, CH_2); 1.24 ($C(CH_3)_3$); 4.87-5.39 ($CH=CH_2$); 5.26-5.27 (CH=CH);

^{13}C NMR ($CDCl_3$, 298K, δ): 0.69 ($SiCH_3$); 8.43; 10.13; 10.35 ($SiCH_2$); 13.19-41.09 (CH, CH_2); 31.56 ($C(CH_3)_3$); 114.14-143.30 ($CH=CH_2$); 128.17-131.67 (CH=CH);

GPC: Mn =6507 [g•mol^{-1}], Mw =9500 [g•mol^{-1}], PD=1.46.

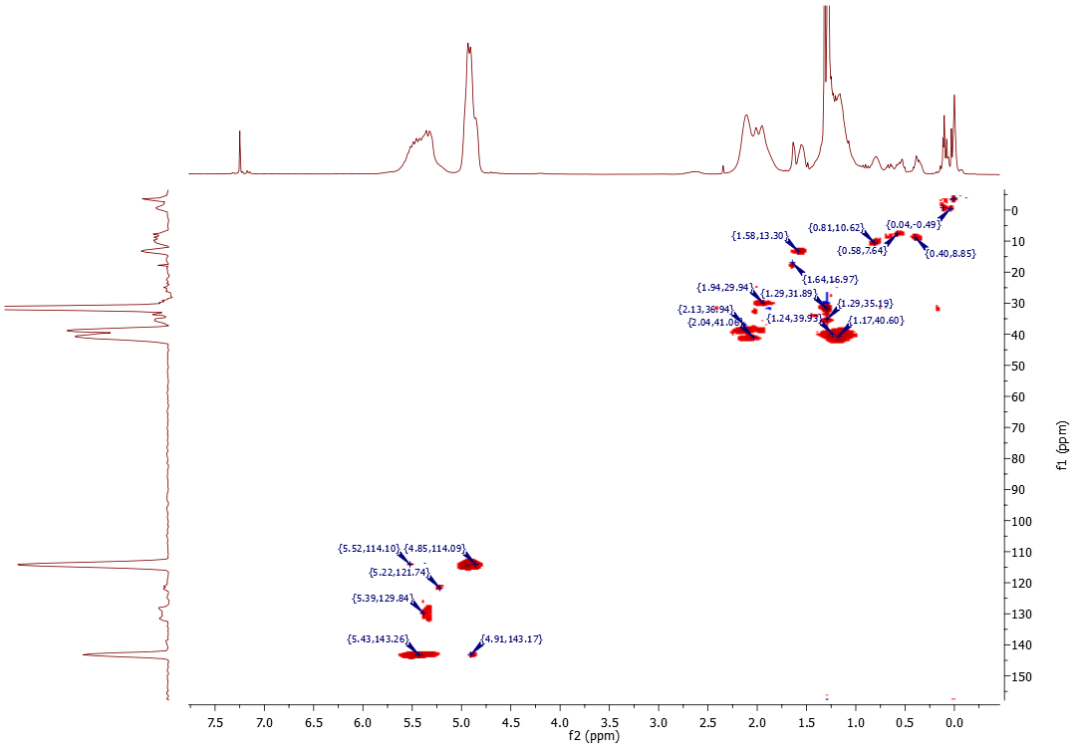


PB4B

^{1}H NMR ($CDCl_3$, 298K, δ): 0.12 ($SiCH_3$); 0.40; 0.58; 0.82 ($SiCH_2$); 1.29 (CH_3); 0.94-2.31 (CH, CH_2); 4.85-5.43 ($CH=CH_2$); 5.32-5.34 (CH=CH);

^{13}C NMR ($CDCl_3$, 298K, δ): -0.60 ($SiCH_3$); 7.64; 8.85; 10.62 ($SiCH_2$); 35.19 (CH_3); 13.05-40.96 (CH, CH_2); 113.59-143.34 ($CH=CH_2$); 128.10-131.60 (CH=CH);

GPC: Mn =5983 [g•mol^{-1}], Mw =8757 [g•mol^{-1}], PD=1.46.

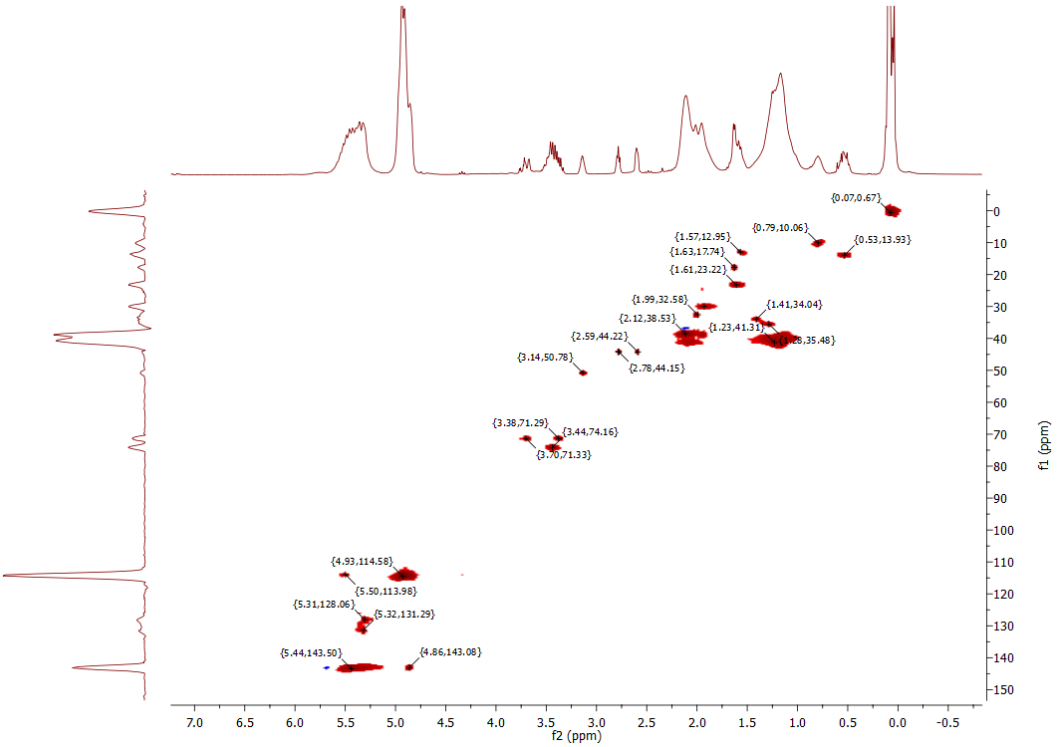


i) PB5A

^{1}H NMR ($CDCl_3$, 298K, δ): 0.07 ($SiCH_3$); 0.53; 0.79 ($SiCH_2$); 0.94-2.32 (CH, CH_2); 2.59; 2.78; 3.14; 3.70 (CH_2OCH_2); 3.38; 3.44 ($CH(O)CH_2$); 4.86-5.50 ($CH=CH_2$); 5.31-5.32 (CH=CH);

^{13}C NMR ($CDCl_3$, 298K, δ): 0.67 ($SiCH_3$); 10.06; 13.93 ($SiCH_2$); 12.95-41.31 (CH, CH_2); 44.22; 50.78 (CH_2OCH_2); 71.30; 74.16 ($CH(O)CH_2$); 113.98-143.50 ($CH=CH_2$); 128.08-131.29 (CH=CH);

GPC: Mn = 6311 [g•mol^{-1}], Mw = 9084 [g•mol^{-1}], PD= 1.44.

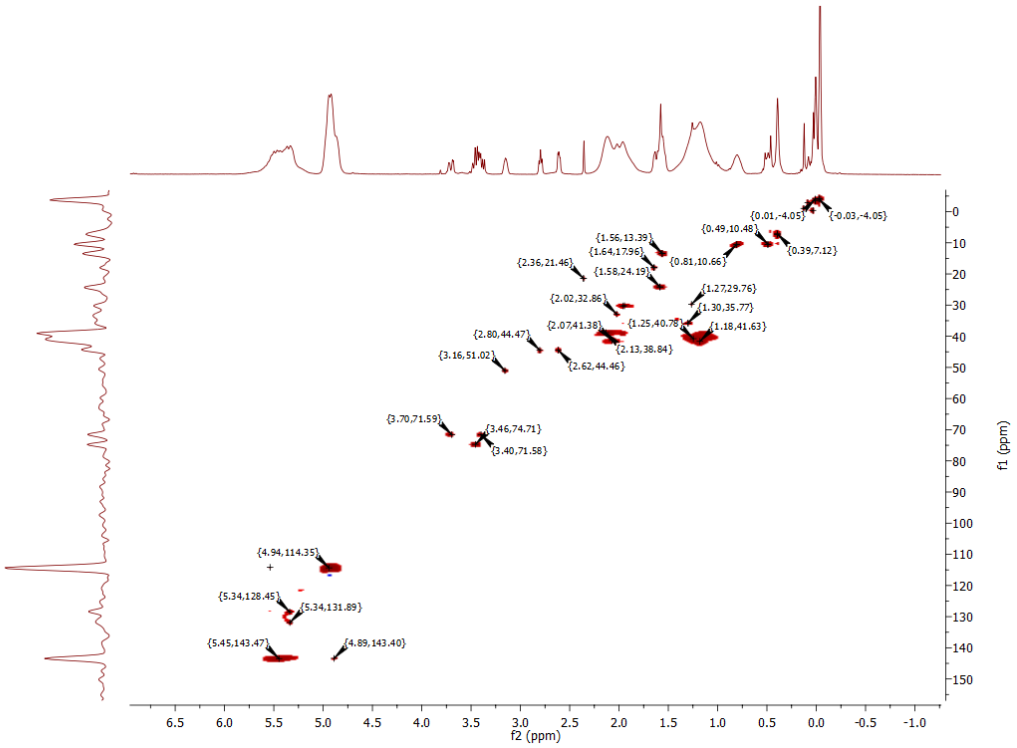


j) **PB5B**

^{1}H NMR ($CDCl_3$, 298K, δ): -0.03 ($SiCH_3$); 0.39; 0.49; 0.81 ($SiCH_2$); 0.90-2.28 (CH, CH_2); 2.62; 2.80; 3.16; 3.70 (CH_2OCH_2); 3.40; 3.46 ($CH(O)CH_2$); 4.94-5.45 ($CH=CH_2$); 5.33-5.34 (CH=CH);

^{13}C NMR ($CDCl_3$, 298K, δ): -4.05 ($SiCH_3$); 7.12; 10.48; 10.66 ($SiCH_2$); 13.39-41.63 (CH, CH_2); 44.46; 51.02 (CH_2OCH_2); 71.59; 74.71 ($CH(O)CH_2$); 114.35-143.47 ($CH=CH_2$); 128.45-131.89 (CH=CH);

GPC: Mn = 6435 [g•mol^{-1}], Mw = 9201 [g•mol^{-1}], PD= 1,43.

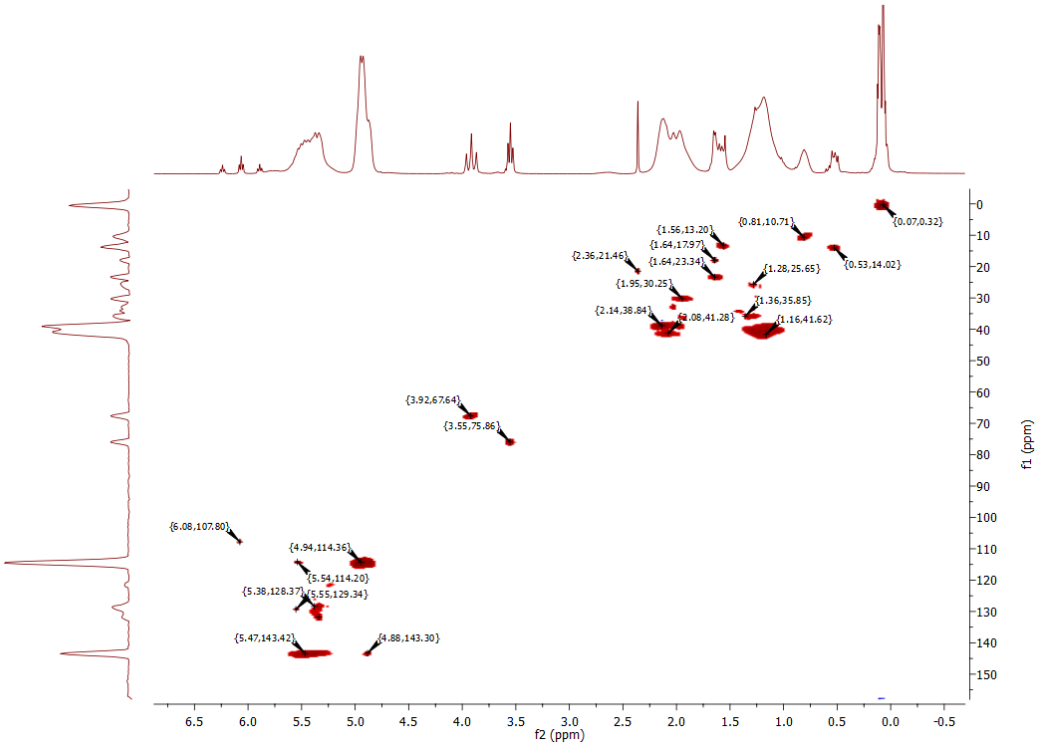


k) PB6A

^{1}H NMR ($CDCl_3$, 298K, δ): 0.07 ($SiCH_3$); 0.53, 0.81 ($SiCH_2$); 0.97-2.30 (CH, CH_2); 3.55, 3.92 (CH_2OCH_2); 4.88-5.47 ($CH=CH_2$); 5.38-5.55 (CH=CH); 6.08 (CF_2H);

^{13}C NMR ($CDCl_3$, 298K, δ): 0.32 ($SiCH_3$); 10.71; 14.02 ($SiCH_2$); 14.20-41.62 (CH, CH_2); 67.64; 75.86 (CH_2OCH_2); 114.36-143.30 ($CH=CH_2$); 128.37-129.34 (CH=CH); 107.80 (CF_2H);

GPC: Mn =7302 [g•mol^{-1}], Mw =10645 [g•mol^{-1}], PD=1.46.

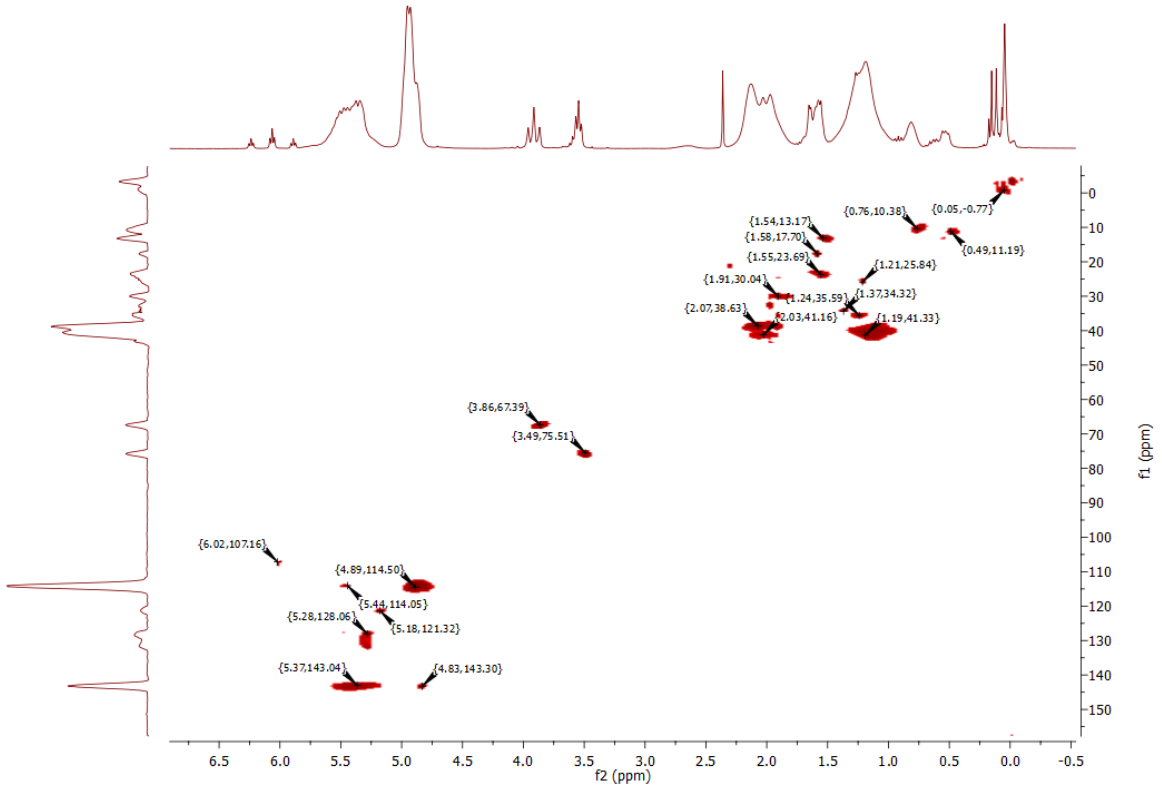


l) PB6B

^{1}H NMR ($CDCl_3$, 298K, δ): -0.04-0.10 ($SiCH_3$); 0.49; 0.76 ($SiCH_2$); 0.91-2.25 (CH, CH_2); 3.49; 3.86 (CH_2OCH_2); 4.89-5.37 ($CH=CH_2$); 5.28-5.34 (CH=CH); 6.02 (CHF_2);

^{13}C NMR ($CDCl_3$, 298K, δ): -0.77 ($SiCH_3$); 10.38; 11.19 ($SiCH_2$); 13.49-41.61 (CH, CH_2); 67.39; 75.51 (CH_2OCH_2); 107.16 (CHF_2); 114.05-143.30 ($CH=CH_2$); 128.06-131.86 (CH=CH);

GPC: Mn = 6395 [g•mol^{-1}], Mw = 8932 [g•mol^{-1}], PD= 1.39.



m) PB7B

^{1}H NMR ($CDCl_3$, 298K, δ): 0.09 ($SiCH_3$); 0.78-0.81 ($SiCH_2$); 0.93-2.31 (CH, CH_2); 4.87-5.44 ($CH=CH_2$); 5.33-5.38 (CH=CH);

^{13}C NMR ($CDCl_3$, 298K, δ): -3.13 ($SiCH_3$); 5.25; 10.69 ($SiCH_2$); 13.60-41.78 (CH, CH_2); 114.52-143.68 ($CH=CH_2$); 126.60-132.05 (CH=CH);

GPC: Mn = 7140 [g•mol^{-1}], Mw = 9739 [g•mol^{-1}], PD= 1.36.