

## Supporting Information

### Self-Assembly Supramolecular Structure through Complementary Multiple Hydrogen Bonding of Heteronucleobase-Multifunctionalized Polyhedral Oligomeric Silsesquioxanes (POSS) Complexes

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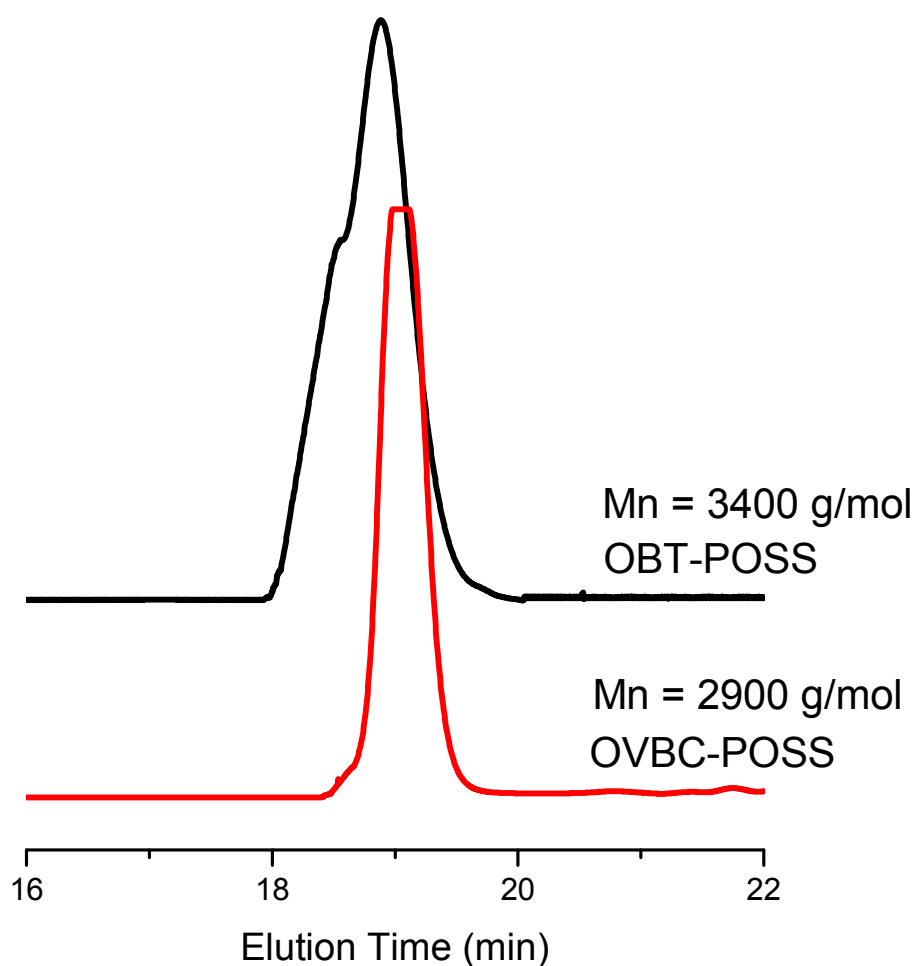


Figure S1: GPC analyses of OBT-POSS and OVBC-POSS

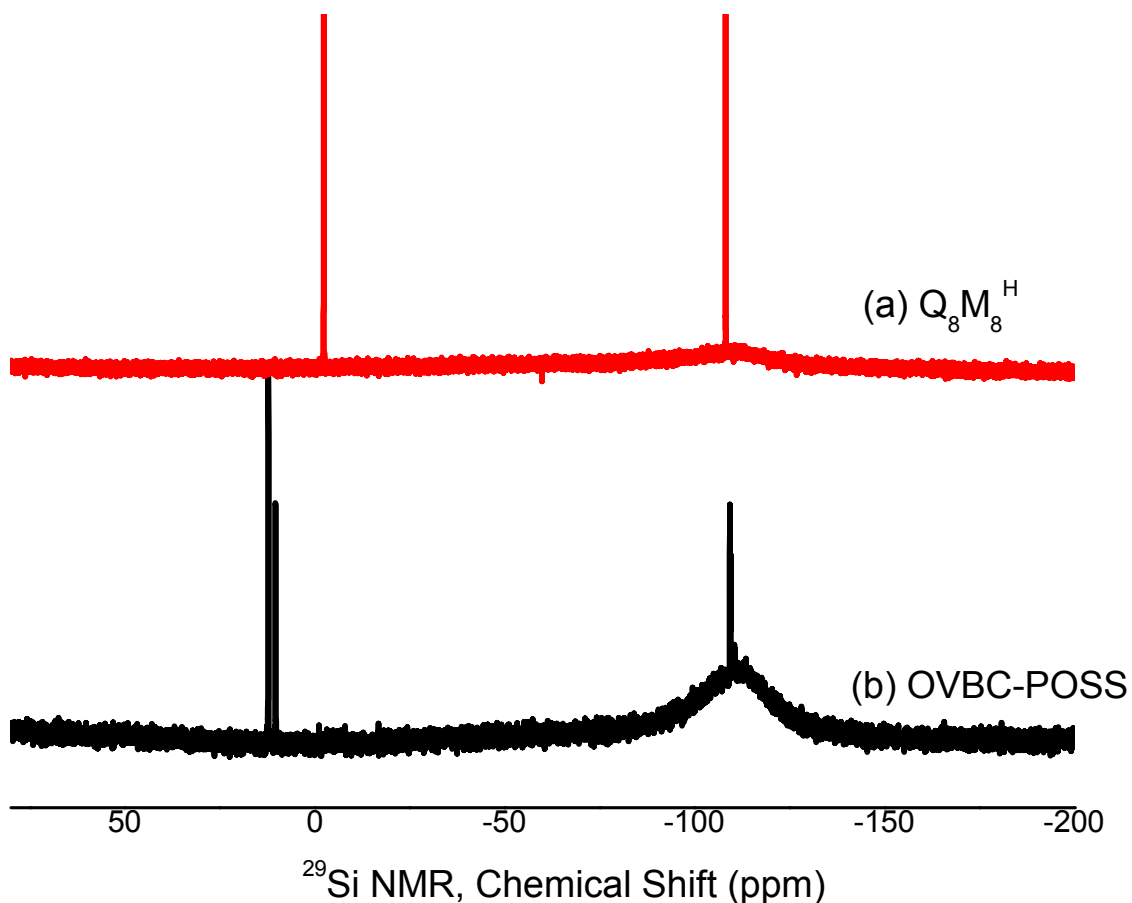


Figure S2:  $^{29}\text{Si}$  NMR of (a)  $\text{Q}_8\text{M}_8^{\text{H}}$ , and (b) OVBC-POSS.

The  $^{29}\text{Si}$  NMR spectrum of  $\text{Q}_8\text{M}_8^{\text{H}}$  in Figure S1 shows two peaks at  $(\text{CH}_3)_2\text{Si-H}$ : -2.1 ppm and  $\text{Si-O-Si}(\text{CH}_3)_2\text{H}$ : -109.3 ppm. In addition, the  $^{29}\text{Si}$  NMR spectrum of OVBC-POSS shows three peaks at 10.28 ppm for  $(\text{CH}_3)_2\text{Si}-(\text{CHCH}_3)$  and 12.16 ppm for  $(\text{CH}_3)_2\text{Si-CH}_2\text{-CH}_2\text{-}$  and -109.2 ppm for  $\text{Si-O-Si}(\text{CH}_3)_2\text{H}$ . The chemical shift clearly indicates that the hydrosilylation reaction occurred to completion under the reaction conditions.

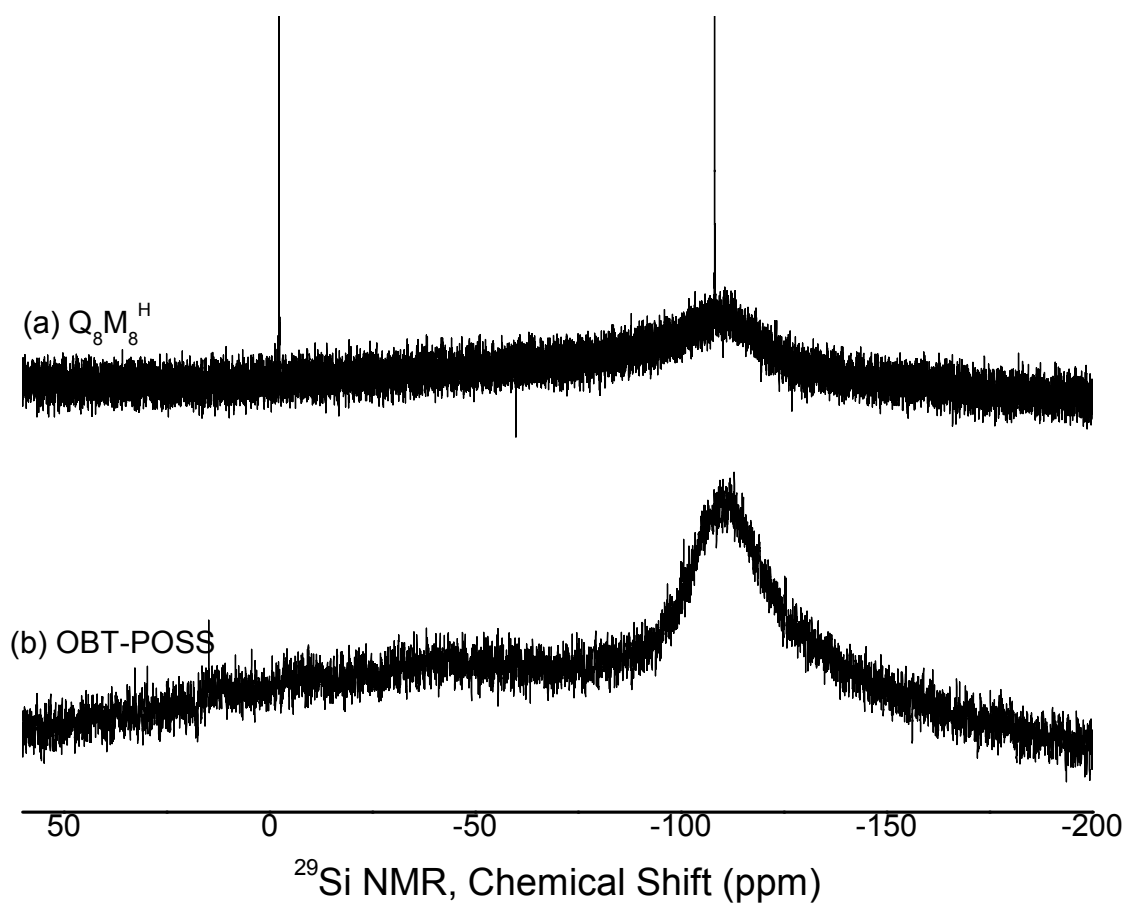


Figure S3:  $^{29}\text{Si}$  NMR of (a)  $\text{Q}_8\text{M}_8^{\text{H}}$ , and (b) OBT-POSS.

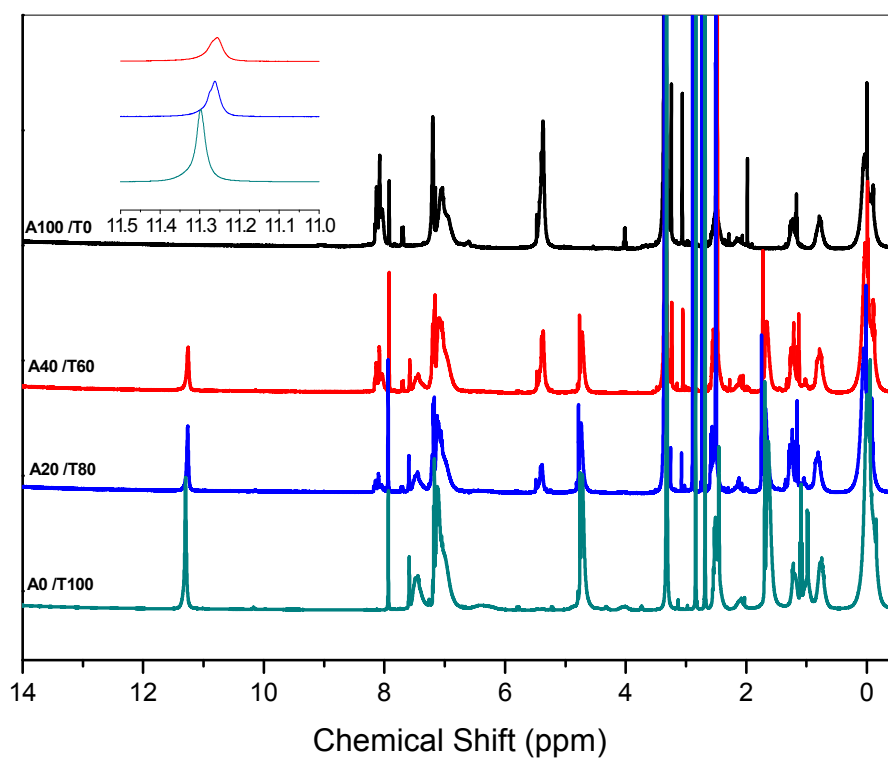


Figure S4:  $^1\text{H}$  NMR of OBA-POSS/OBT-POSS mixtures with different compositions at room temperature in *d*-DMSO.