Supplemental Information

Nanoreactors for the non-enzymatic introduction of ortho or para-hydroxyl groups to aromatic molecules.

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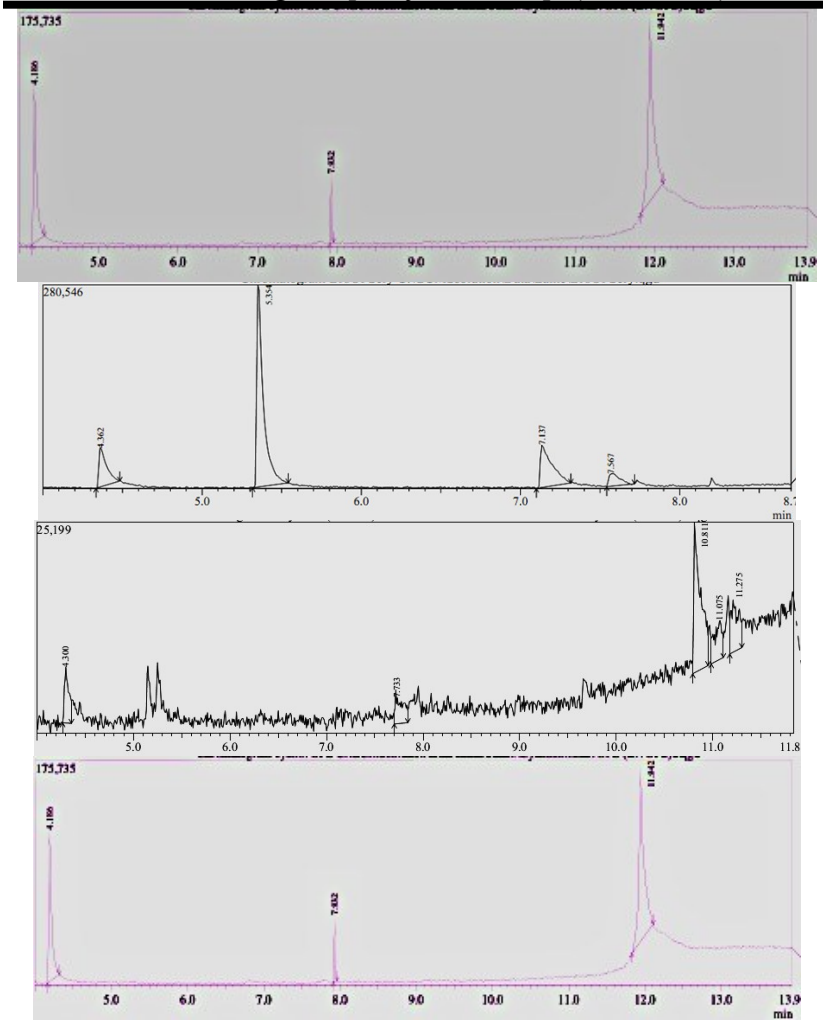
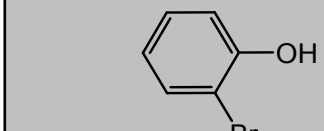
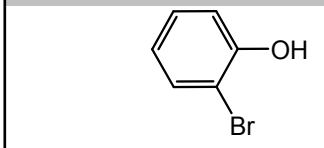
Table S1. GC data for cleavage of different Ortho, Meta, and Para derivatives of PhSQs.

GC of cleavage of $[RStyrPhSiO_{1.5}]_x$ (X=8,10,12)

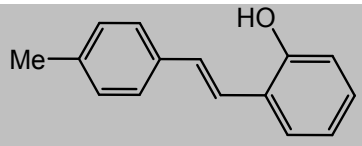




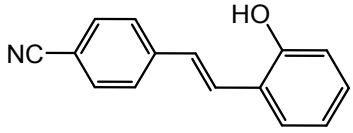
$[BrPhSiO_{1.5}]_8$



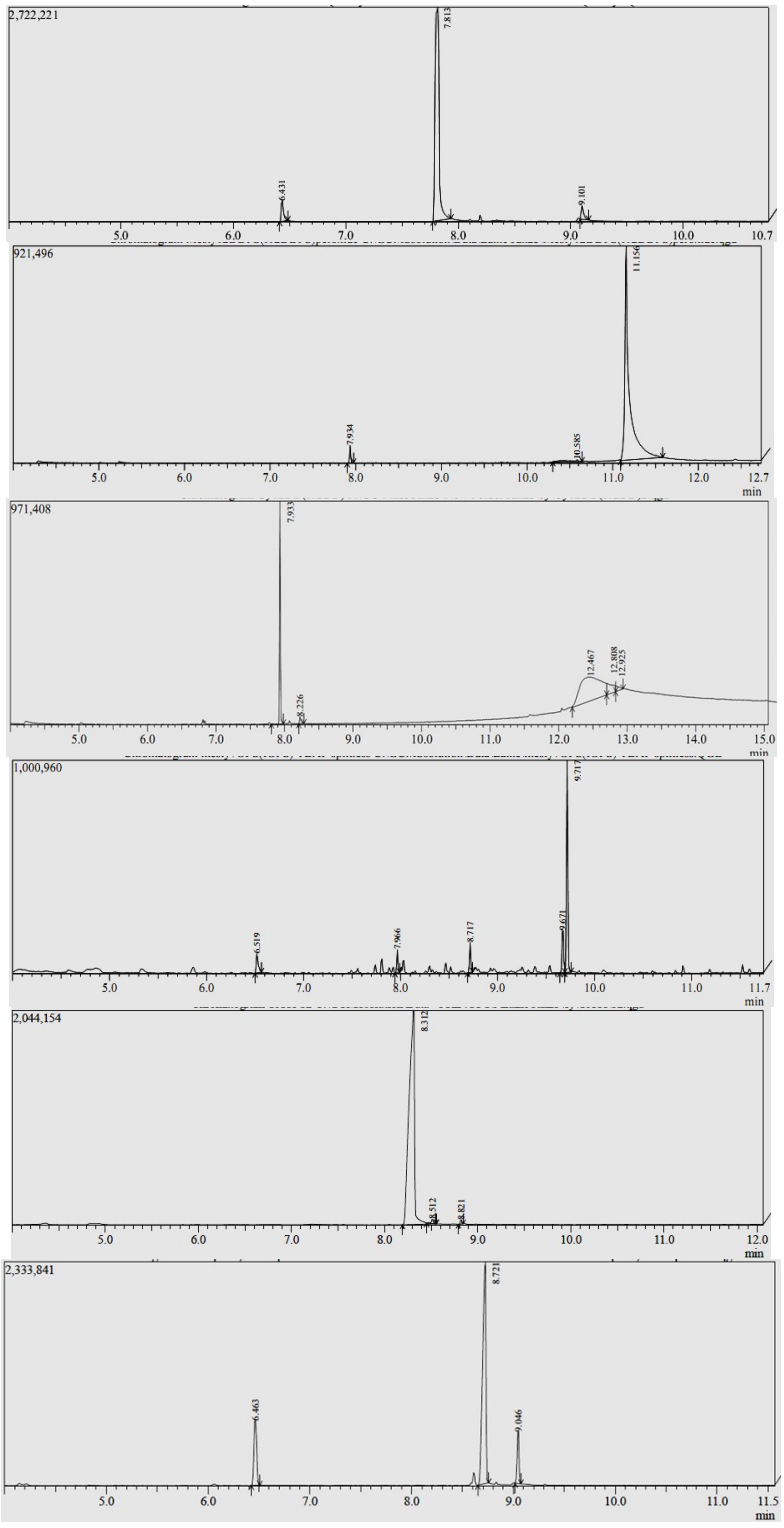
$[o\text{-}BrPhSiO_{1.5}]_8$
(After recrystallization)

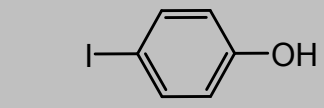


$[o\text{-}MeStyr_7Ph_8Si_8O_{12}]$

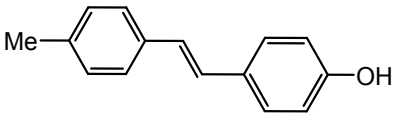


$[o\text{-}cyanoStyr_7Ph_8Si_8O_{12}]$

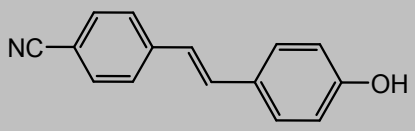




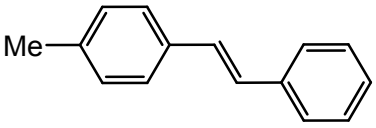
[*p*-IPhSiO$_{1.5}$]$_{12}$



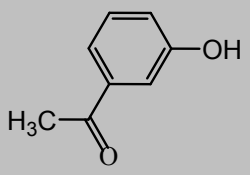
[*p*-MeStyrPhSiO$_{1.5}$]$_{12}$



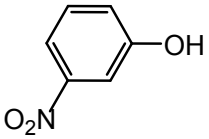
[*p*-cyanoStyrPhSiO$_{1.5}$]$_{12}$



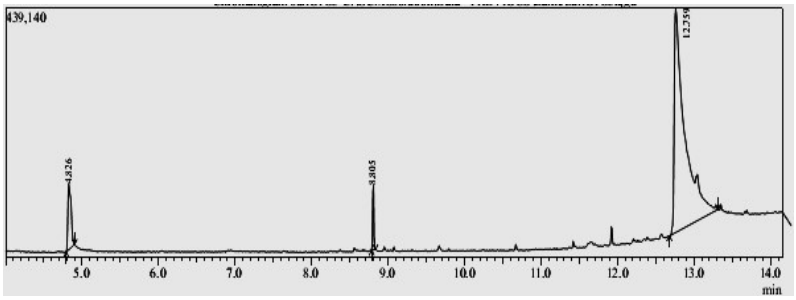
[*p*-MeStyr$_7$Ph$_8$Si$_8$O$_{12}$]
F$^-$ cleaved

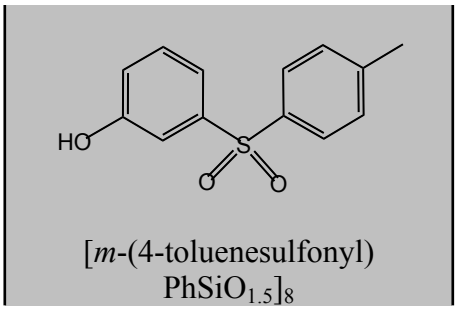


[*m*-AcetylPhSiO$_{1.5}$]$_8$



[*m*-NitroPhSiO$_{1.5}$]$_8$





[*m*-(4-toluenesulfonyl) $PhSiO_{1.5}]_8$

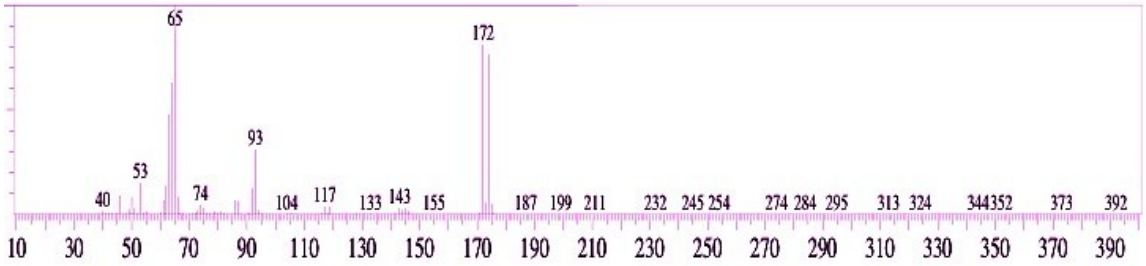


Figure S1. Mass spec of peroxide cleavage of $[BrPhSiO_{1.5}]_8$ residence time 5.4 m.

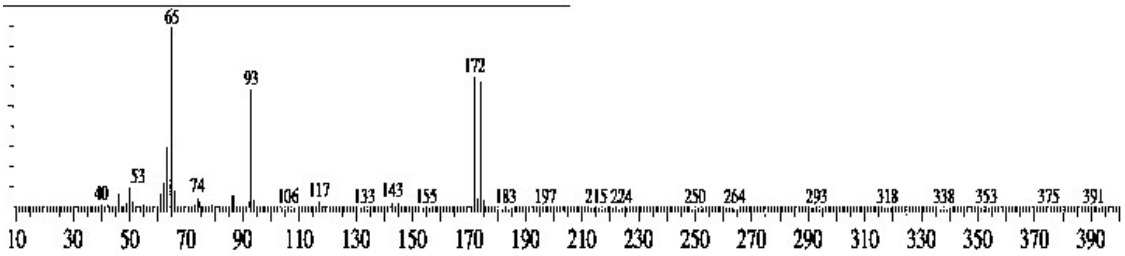


Figure S2. Mass spec of peroxide cleavage of $[BrPhSiO_{1.5}]_8$ residence time 7.1 m.

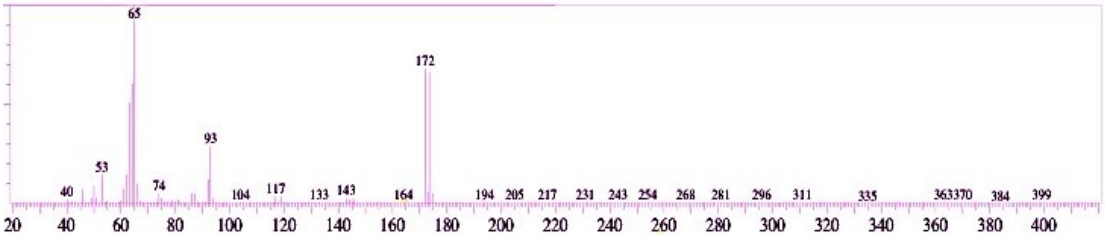


Figure S3. Mass spec of peroxide cleavage of $[BrPhSiO_{1.5}]_{10}$ residence time 5.4 min.

Figure S4. Mass spec of peroxide cleavage of $[BrPhSiO_{1.5}]_{10}$ residence time 7.1 min.

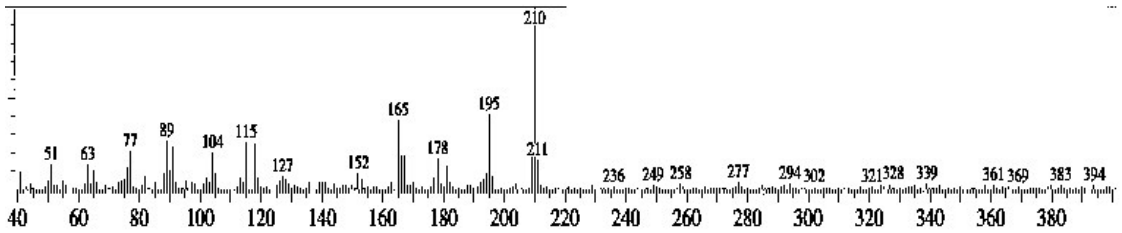


Figure S5. Mass spec of peroxide cleavage of [*o*-MeStyr$_7$Ph$_8$Si$_8$O$_{12}$] for peak with R = 10.8 min.

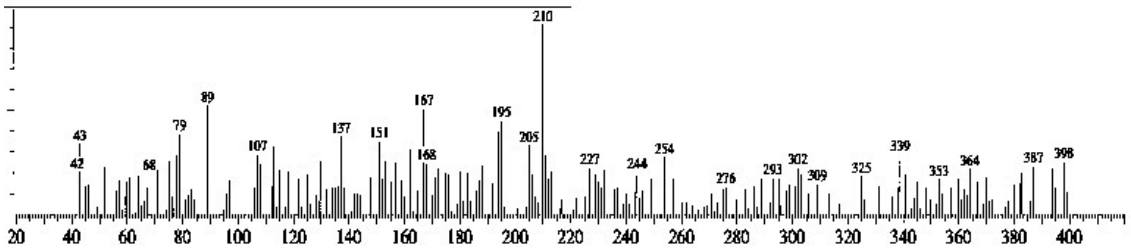


Figure S6. Mass spec of peroxide cleavage of [*p*-MeStyr$_7$Ph$_8$Si$_8$O$_{12}$] for peak with R = 11.3 min.

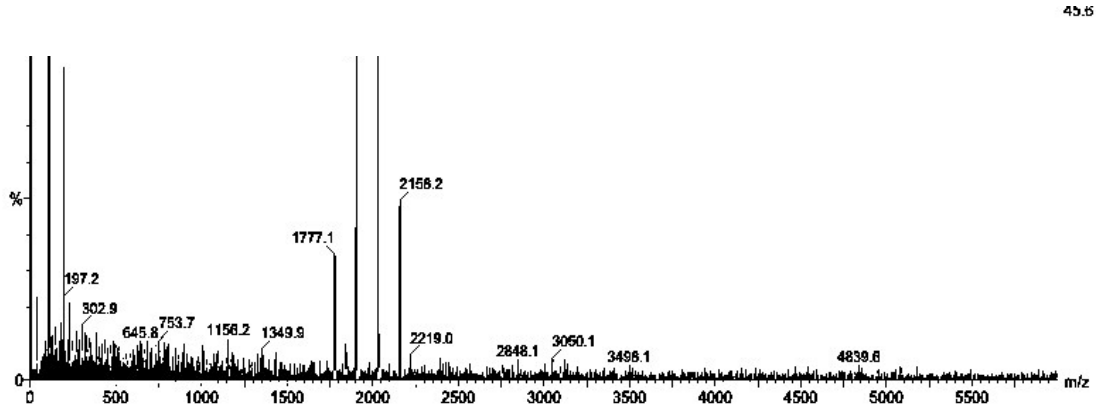


Figure S7. MALDI of mixture of [*o*-cyanoStyr$_6$Ph$_8$Si$_8$O$_{12}$] + Ag m/z = 1906, [*o*-cyanoStyr$_7$Ph$_8$Si$_8$O$_{12}$] + Ag m/z = 2032 and [*o*-cyanoStyrPhSiO$_{1.5}$]$_8$ + Ag parent m/z = 2158.

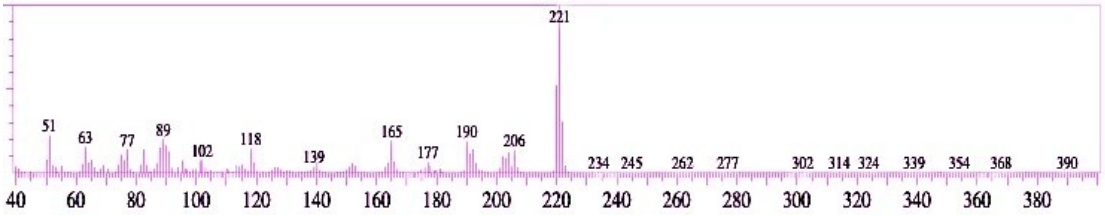


Figure S8. Mass spec of peroxide cleavage of [*o*-cyanoStyr$_7$Ph$_8$Si$_8$O$_{12}$]. residence time 12 min 4-cyano-2'-OH-stilbene.

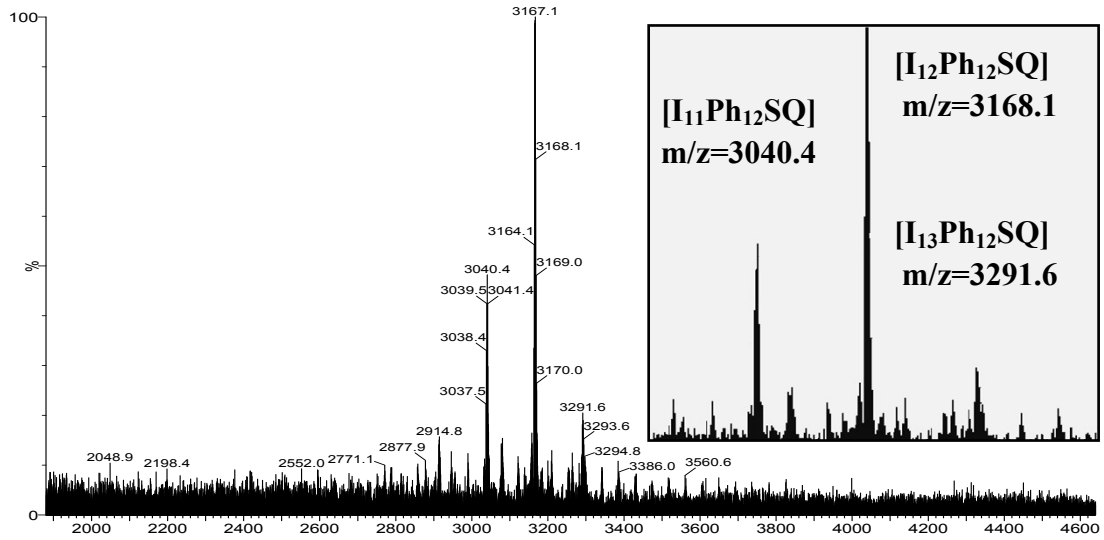


Figure S9. MALDI of [*p*-IPhSiO$_{1.5}$]$_{12}$ + Ag. Cal mass spec m/z =3168.9,
Experimental m/z = 3168.1.

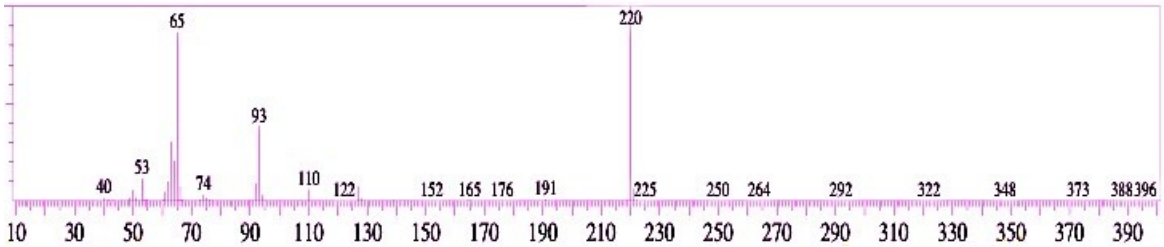


Figure S10. Mass spec of peroxide cleavage of [IPhSiO$_{1.5}$]$_{12}$ residence time 6.4 m.

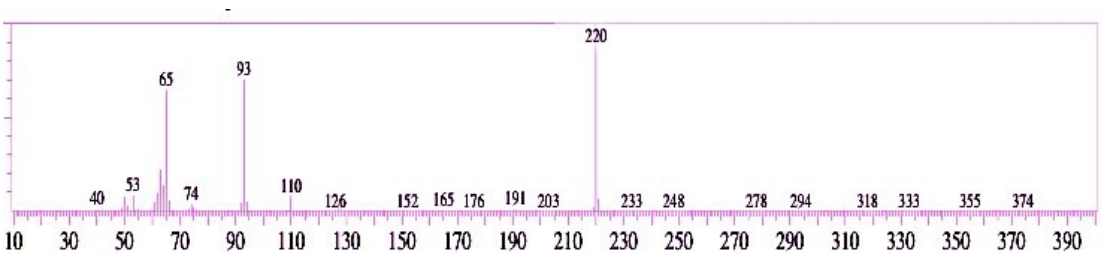


Figure S11. Mass spec of peroxide cleavage of [IPhSiO$_{1.5}$]$_{12}$ residence time 7.8 m.

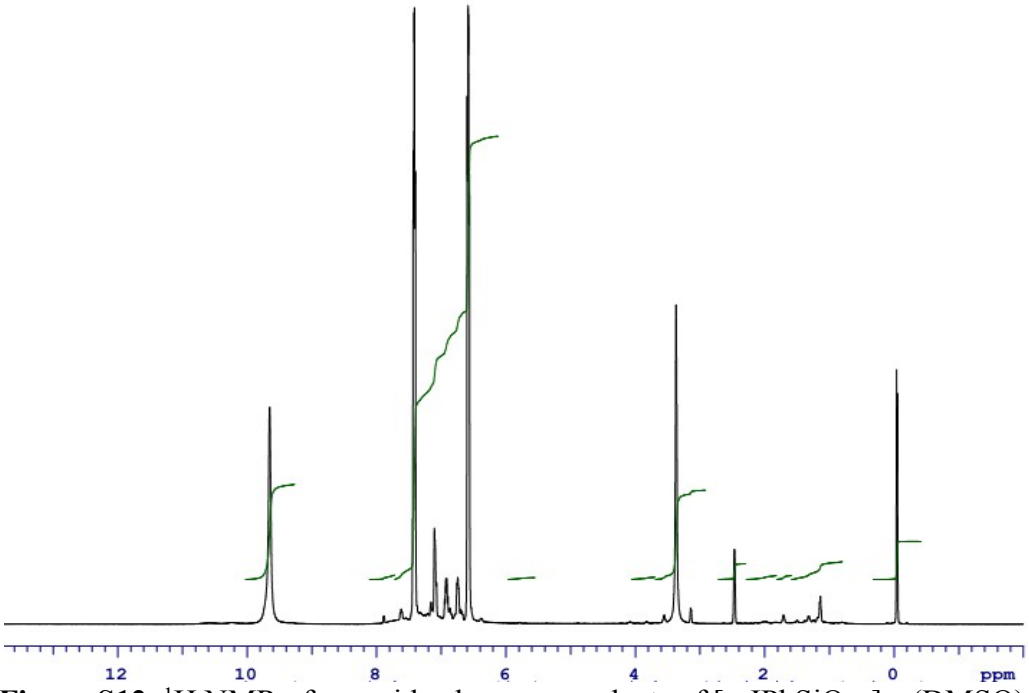


Figure S12. ^{1}H NMR of peroxide cleavage products of [*p*-IPhSiO$_{1.5}$]$_{12}$ (DMSO).

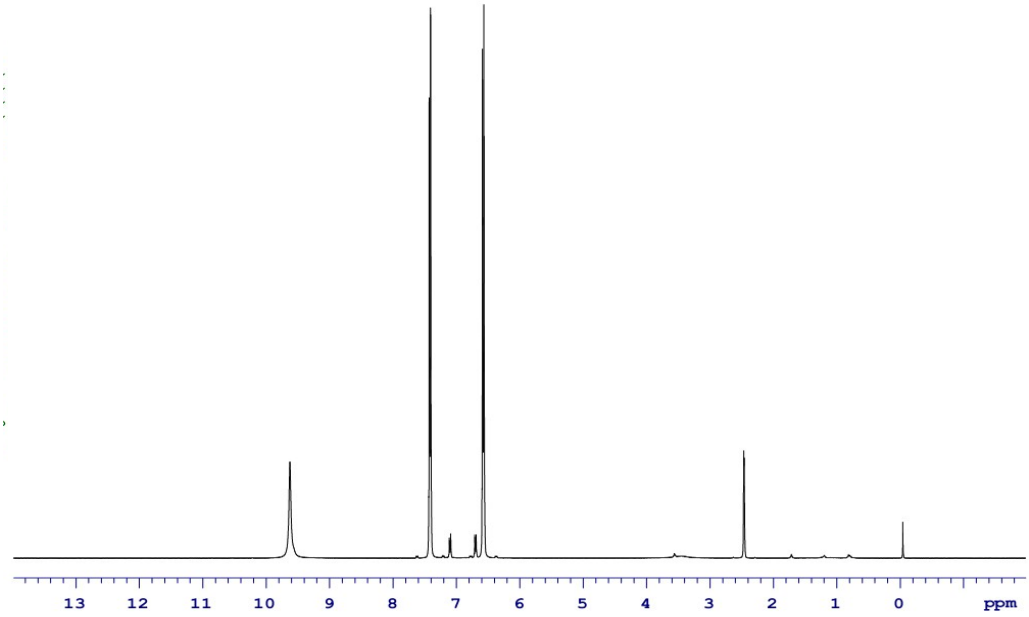


Figure S13. ^{1}H NMR of 4-iodophenol (pure sample, DMSO).

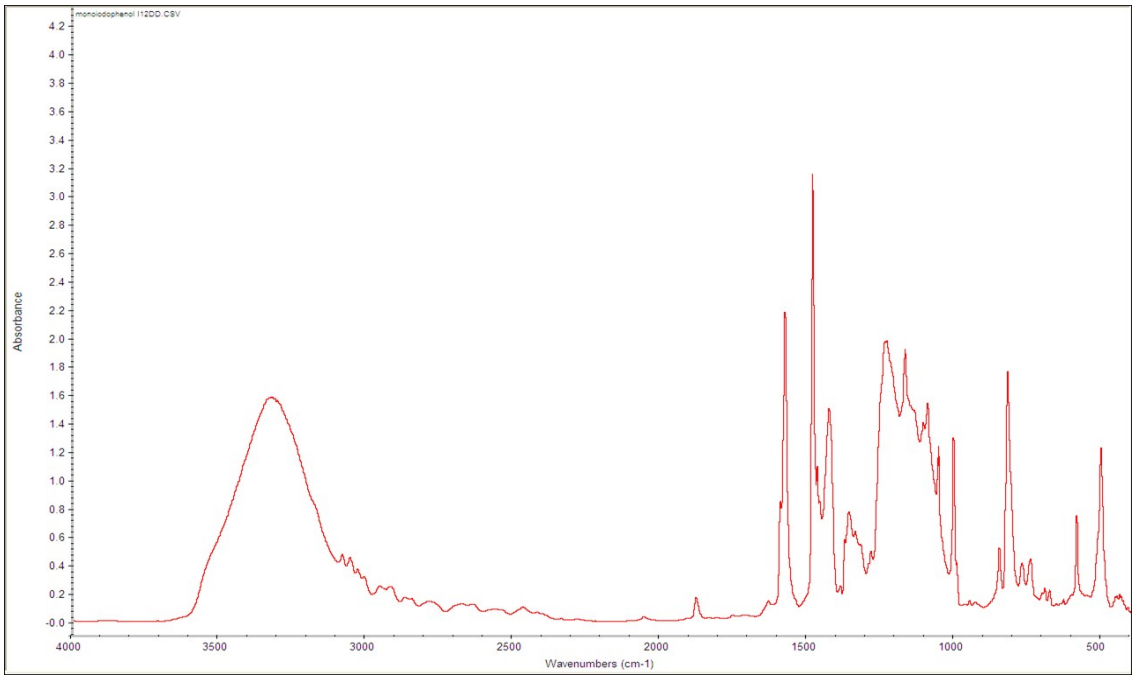


Figure S14. FT-IR of peroxide cleavage of [*p*-IPhSiO$_{1.5}$]$_{12}$.

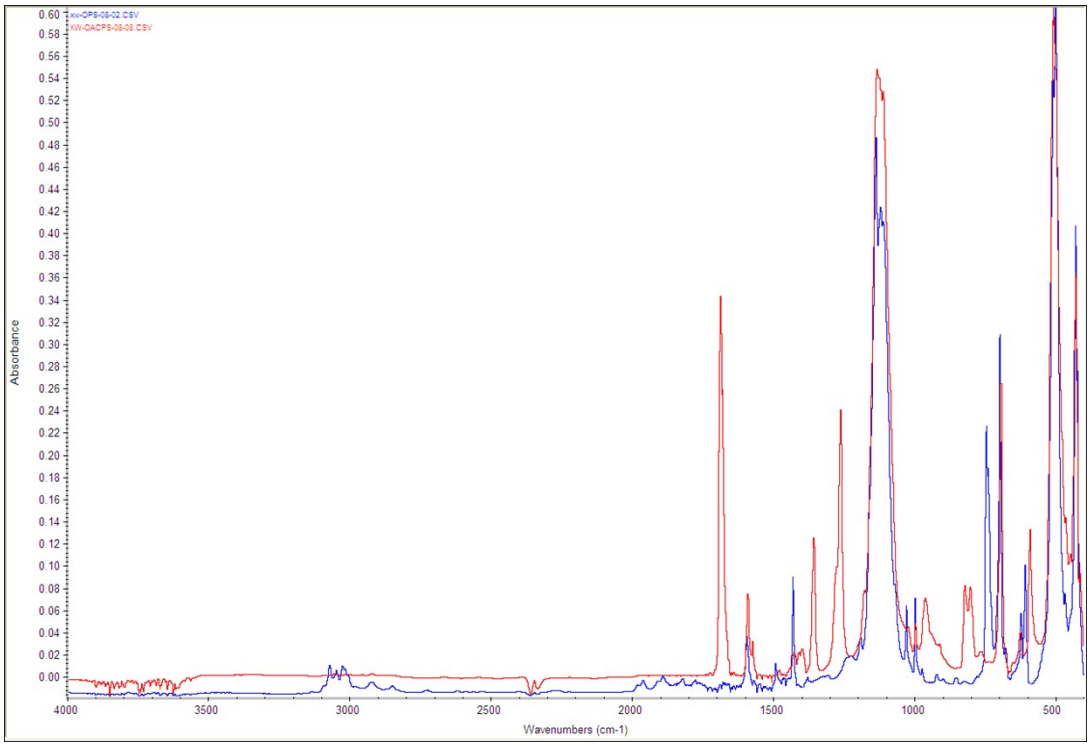


Figure S15. FTIR of OPS (blue) and OAcPS (red).

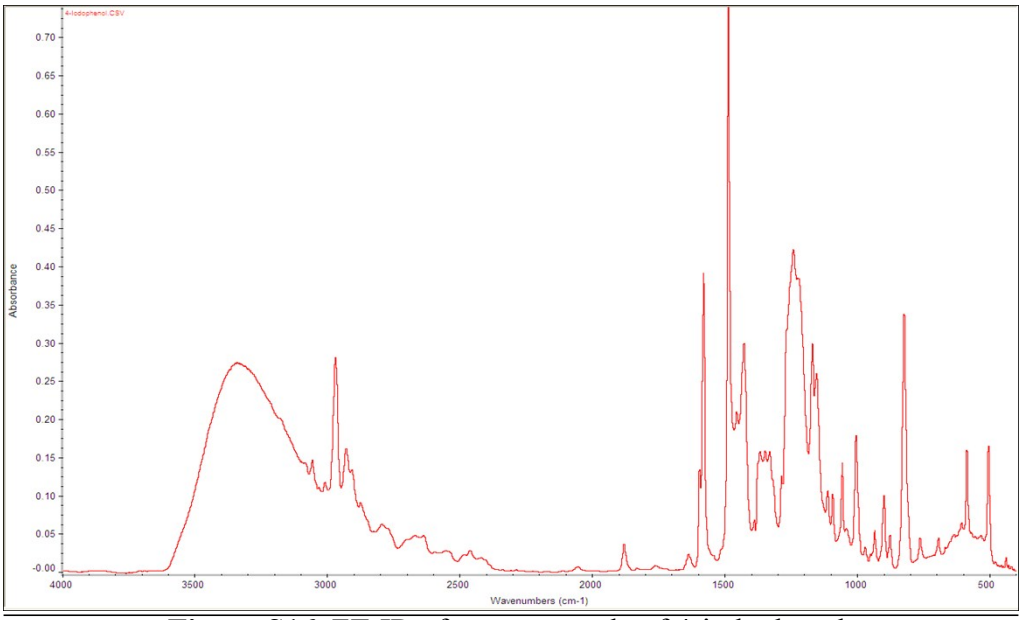


Figure S16. FT-IR of a pure sample of 4-iodophenol.

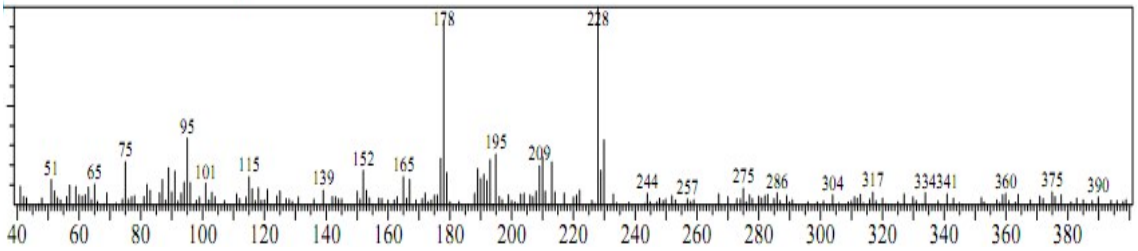


Figure S17. Mass spec of peroxide cleavage of [*p*-MeStyrPhSiO$_{1.5}$]$_{12}$ residence time 10.6 min suggesting an epoxidized derivative.

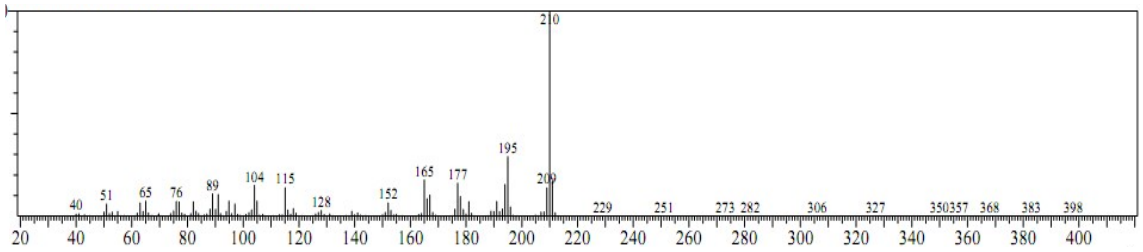


Figure S18. Mass spec of *4,4'*- Me,OH-stilbene with a residence time 11.2 min.

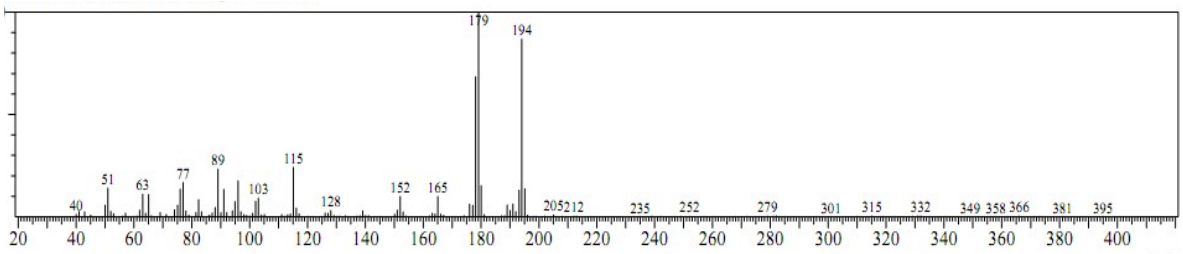


Figure S19. Mass spec of F$^-$ cleaved [*p*-MeStyr$_7$Ph$_8$Si$_8$O$_{12}$] time R=8.7 min.

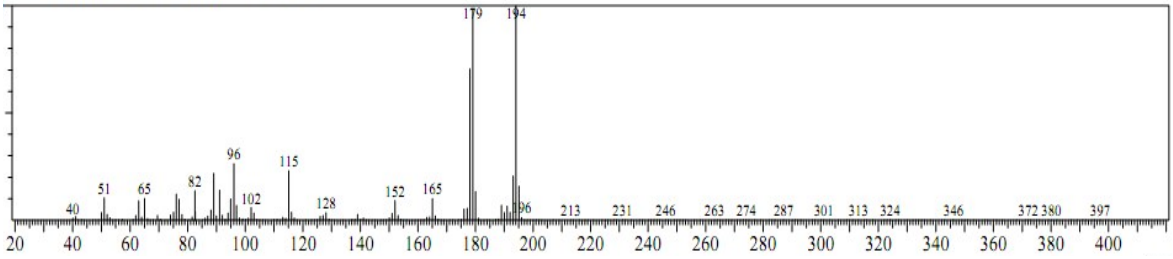


Figure S20. Mass spec of F^- cleaved [*o*-MeStyr$_7$Ph$_8$Si$_8$O$_{12}$] residence time 9.7 min.

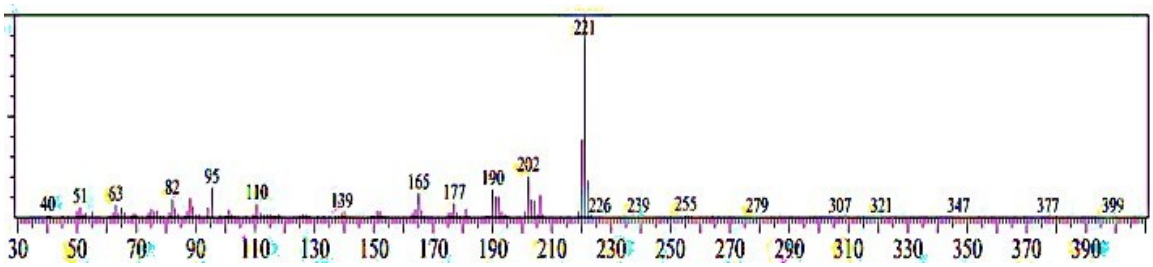


Figure S21. Mass spec of peroxide cleavage of [*p*-cyanoStyrPhSiO$_{1.5}$]$_{12}$ residence time 12.5 min.

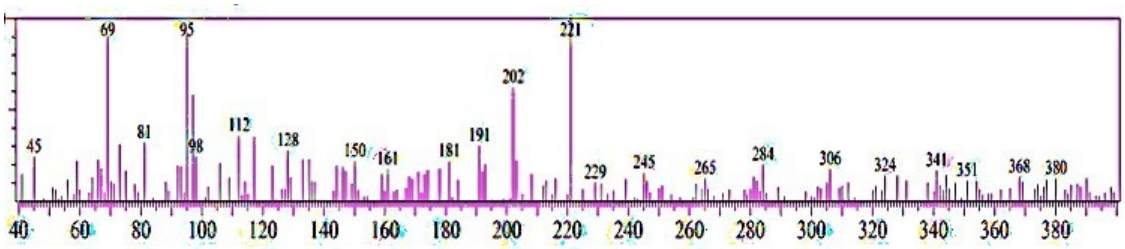


Figure S22. Mass spec peroxide cleavage of [*p*-cyanoStyrPhSiO$_{1.5}$]$_{12}$ residence time 12.8 min.

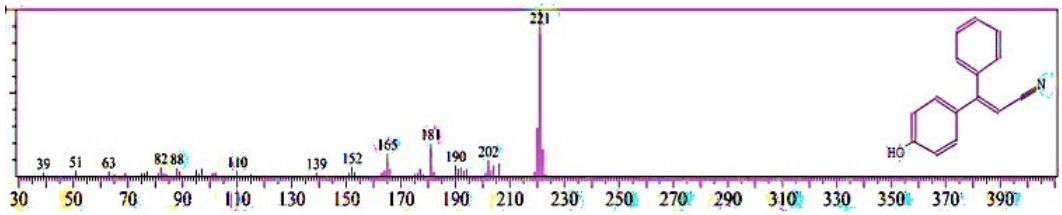


Figure S23. Library prediction for 4-hydroxy-beta-phenylcinnamononitrile mass spec.

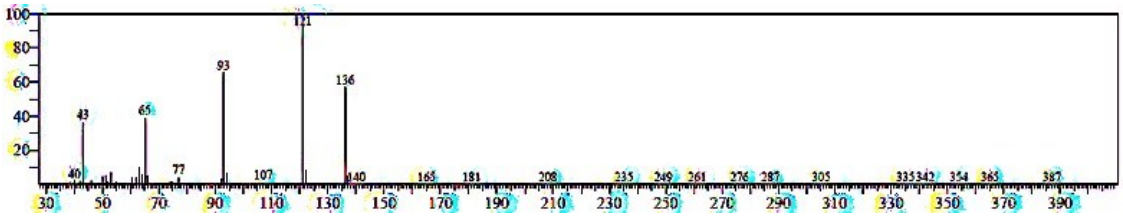


Figure S24. Mass spec peroxide cleavage of [*m*-AcetylPhSiO$_{1.5}$]$_8$ residence time 8.3 min.

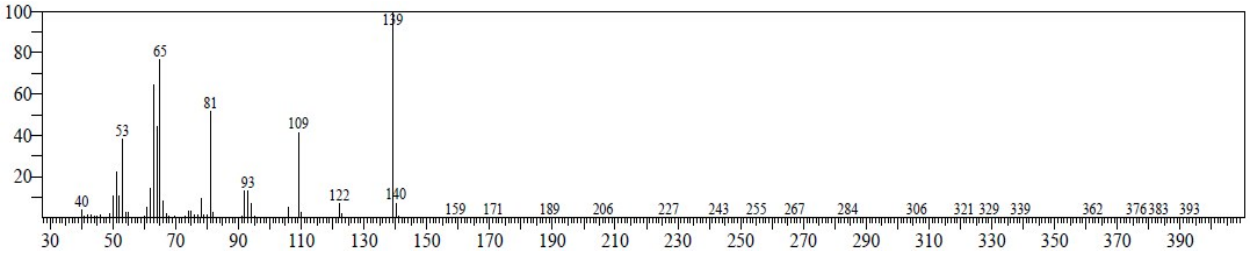


Figure S25. Mass spec peroxide cleavage of [*m*-NitroPhSiO$_{1.5}$]$_8$ residence time 6.5 min.

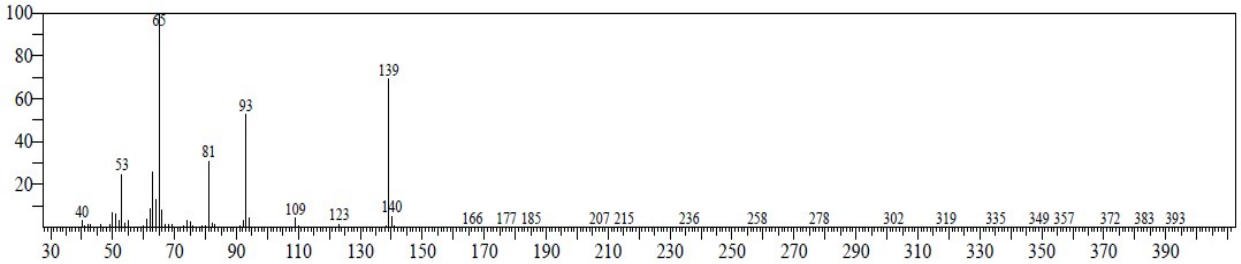


Figure S26. Mass spec peroxide cleavage of [*m*-NitroPhSiO$_{1.5}$]$_8$ residence time 8.7 min.

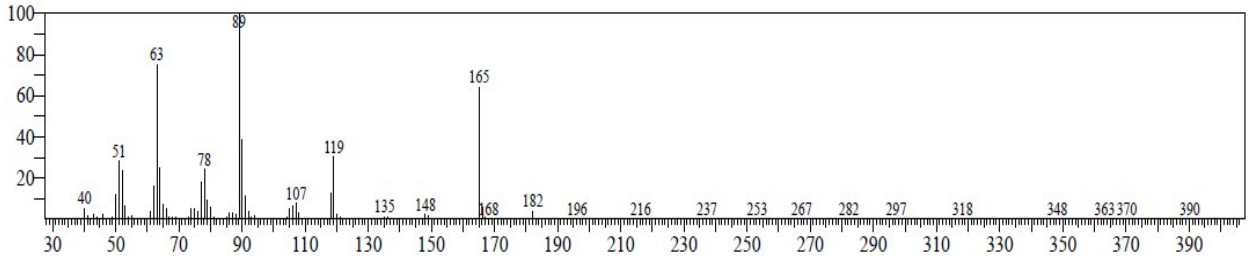


Figure S27. Mass spec peroxide cleavage of [*m*-NitroPhSiO$_{1.5}$]$_8$ residence time 9 min.

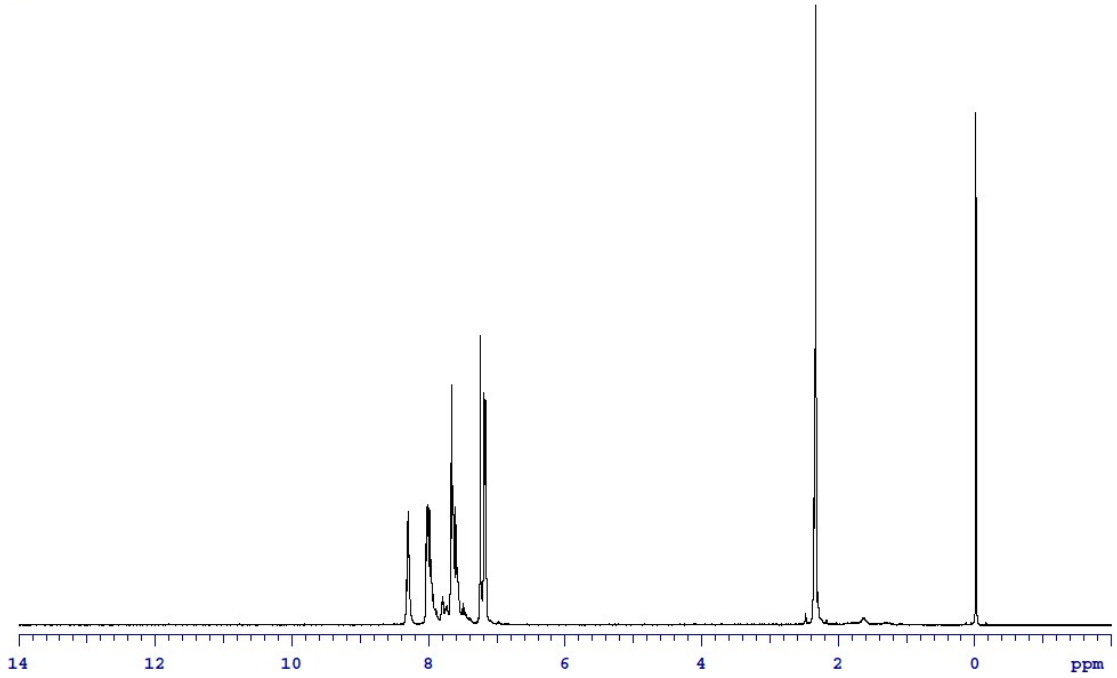


Figure S28. H-NMR of [*m*-(4-toluenesulfonyl)PhSiO$_{1.5}$]$_8$.

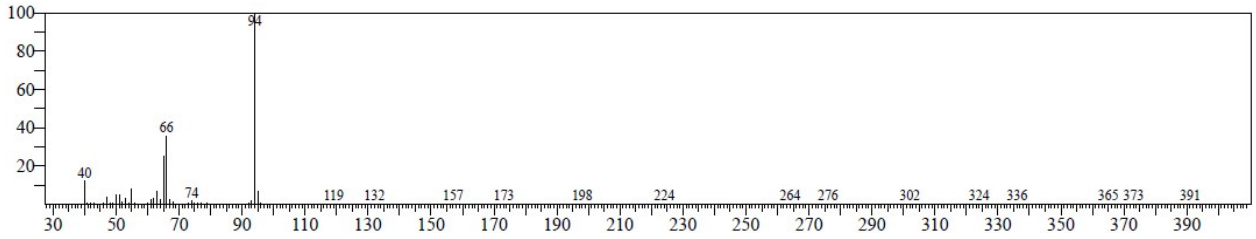


Figure S29. Mass spec peroxide cleavage of [*m*-(4-toluenesulfonyl)$PhSiO_{1.5}$]$_8$ residence time 4.8 min.

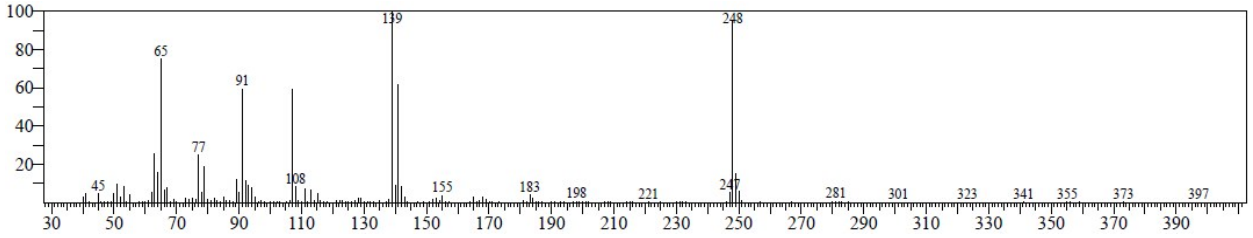


Figure S30. Mass spec peroxide cleavage of [*m*-(4-toluenesulfonyl)$PhSiO_{1.5}$]$_8$ residence time 12.8 min.

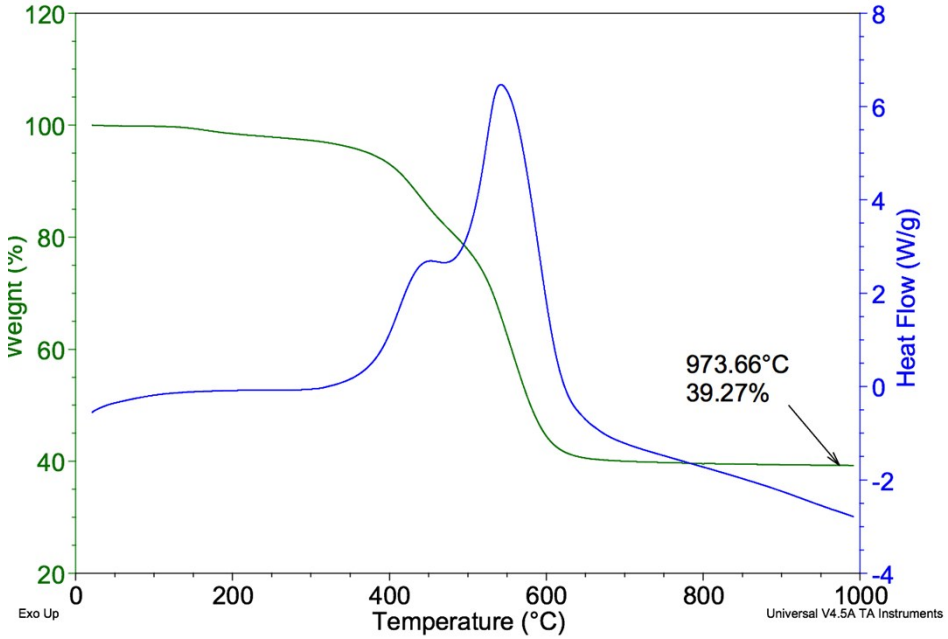


Figure S31. TGA of sample [$AcPhSiO_{1.5}$]$_{12}$ representative of TGAs for all acetyl cages.

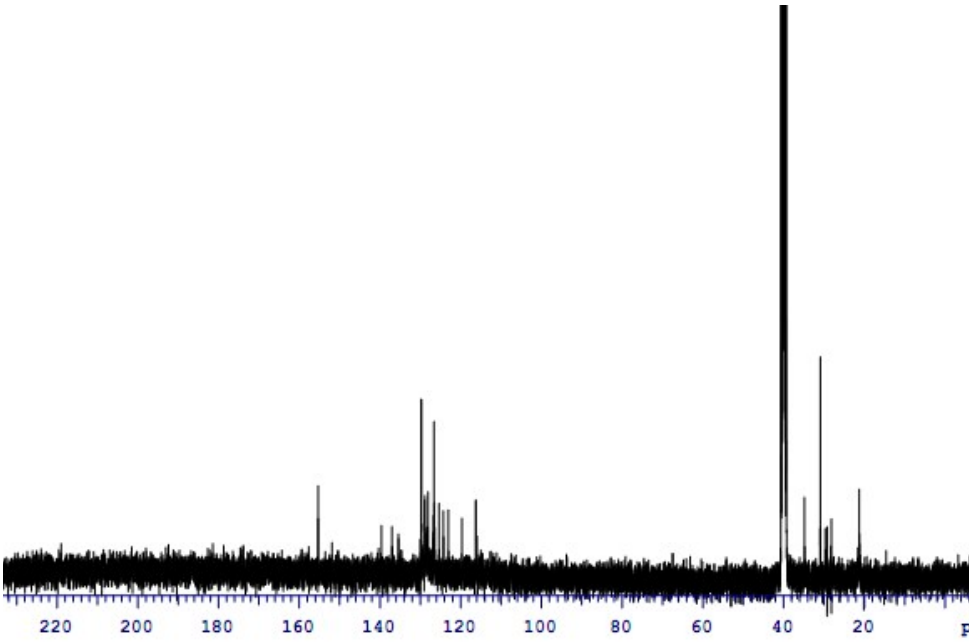


Figure S32. ^{13}C-NMR of *4,2'*-Me,OH-stilbene.

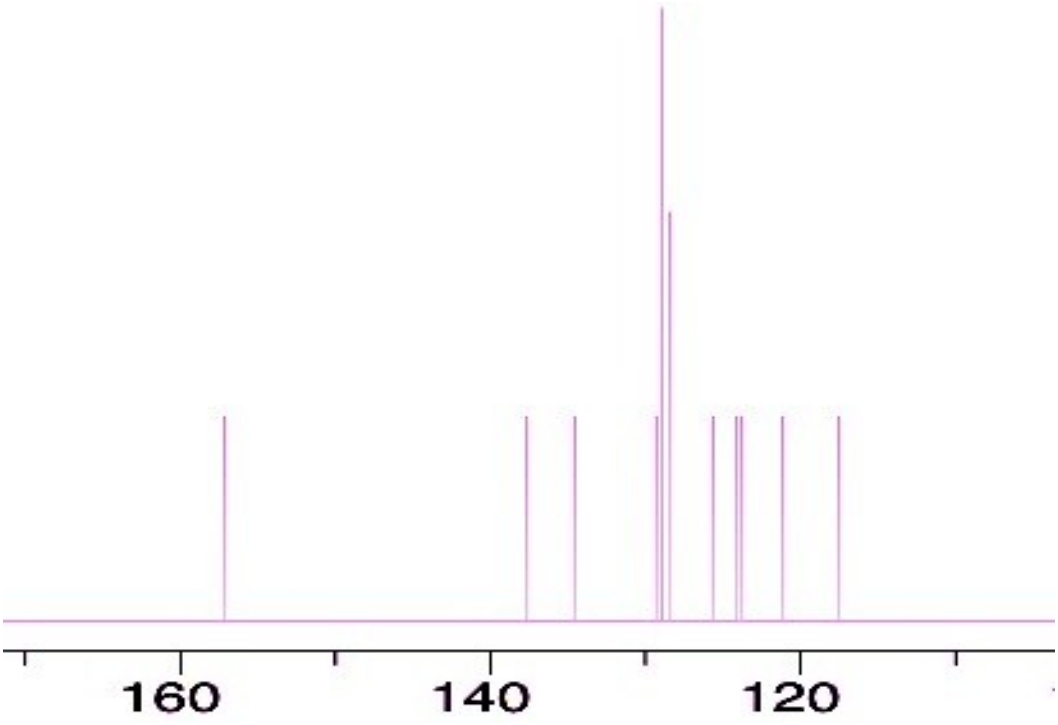


Figure S33. Predicted ^{13}C-NMR of *4,2'*-Me,OH-stilbene.

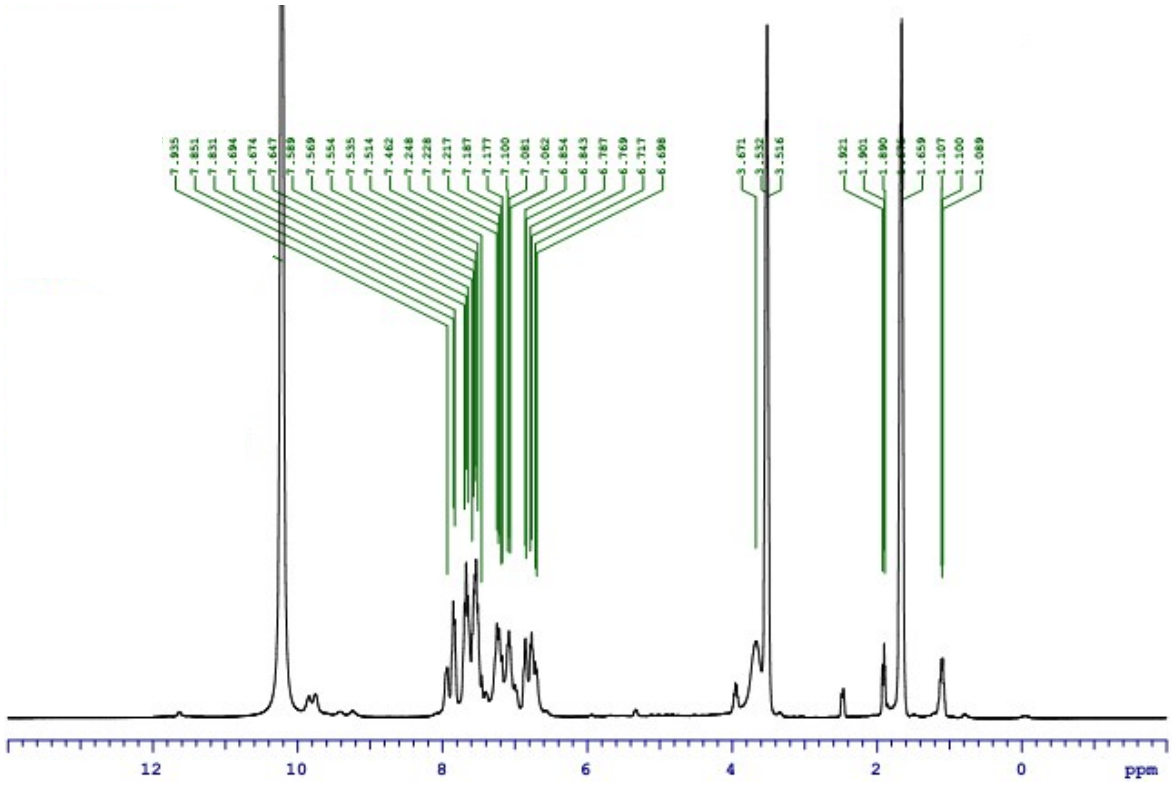


Figure S34. The ^{1}H-NMR of *o*-phenol derivative of [*o*-cyanostilbene$SiO_{1.5}$]$_7$[$PhSiO_{1.5}$].

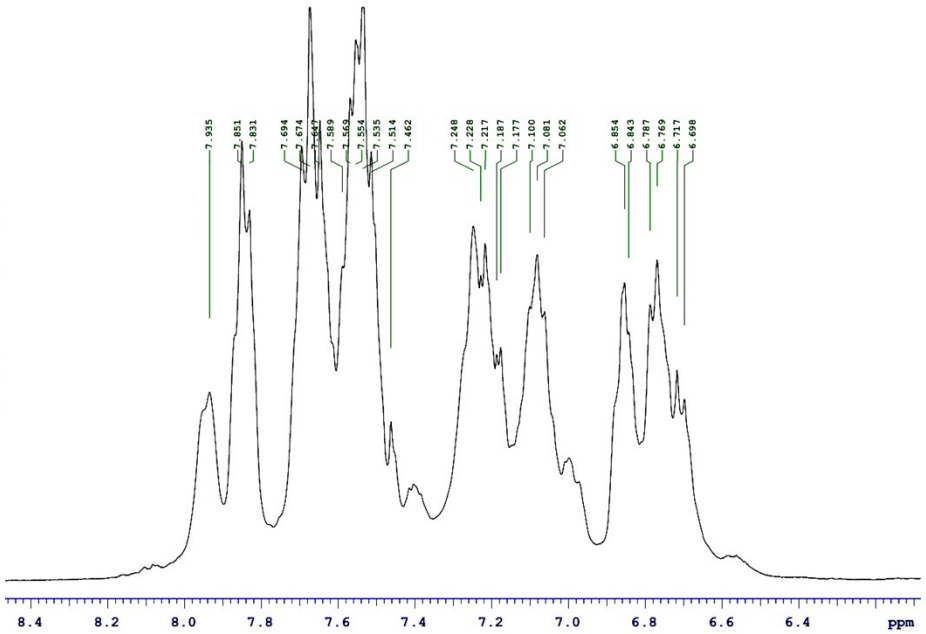


Figure S35. Blow up of ^{1}H-NMR of *o*-phenol derivative of [*o*-cyanostilbene$SiO_{1.5}$]$_7$[$PhSiO_{1.5}$].

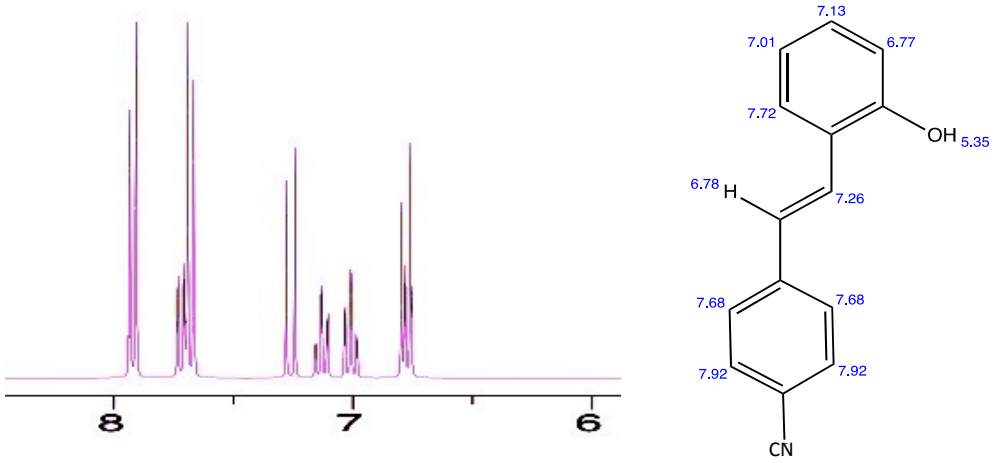


Figure S36. Blow up of predicted ^{1}H-NMR of *o*-phenol derivative of [o-cyanostilbene$SiO_{1.5}$]$_7$[$PhSiO_{1.5}$].

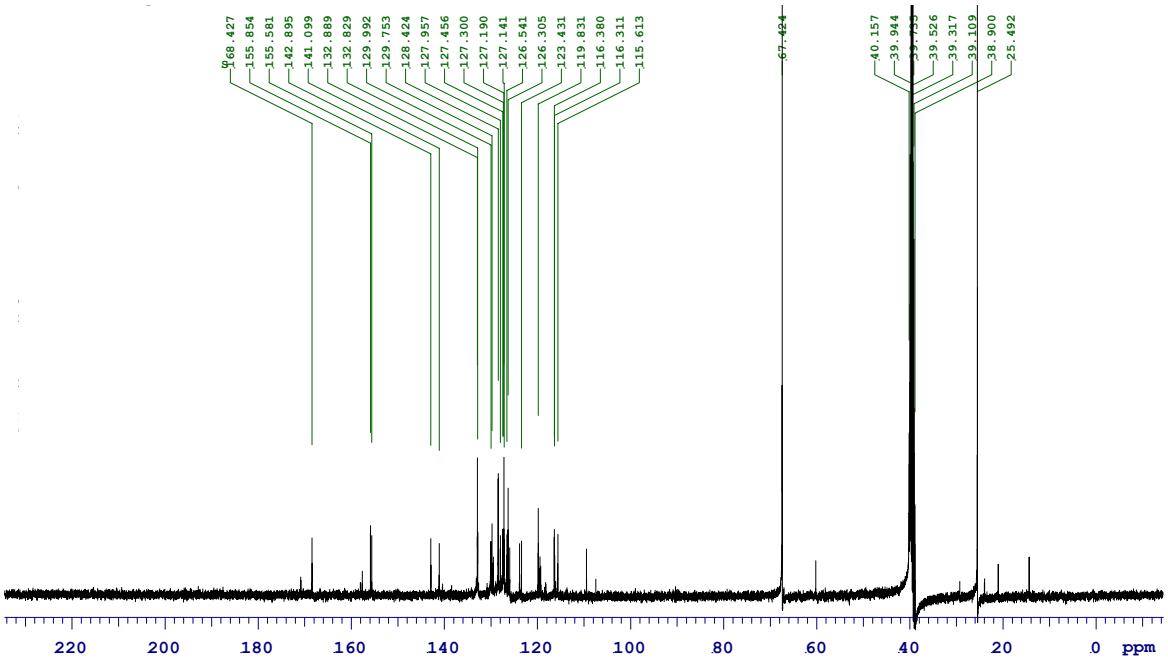


Figure S37. The ^{13}C-NMR of *o*-phenol derivative of [*o*-cyanostilbene-$SiO_{1.5}$]$_7$[$PhSiO_{1.5}$].

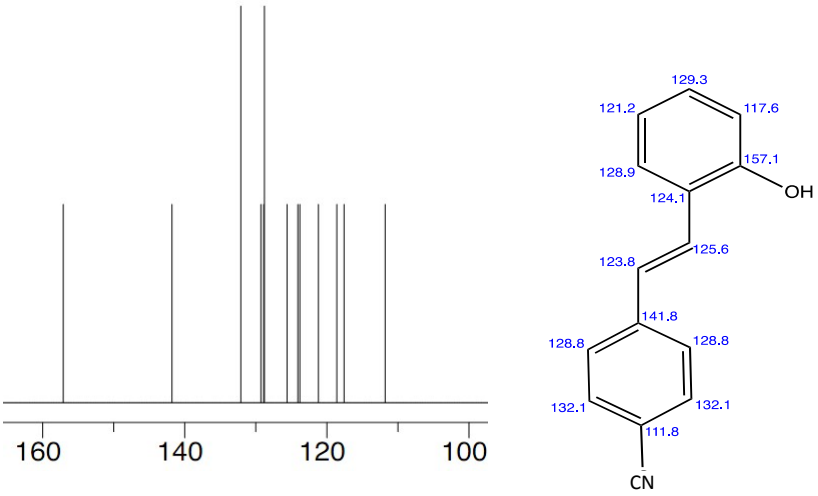


Figure S38. Blow up of predicted ^{13}C-NMR of *o*-phenol derivative of [*o*-cyanostilbene-$SiO_{1.5}$]$_7$[$PhSiO_{1.5}$].

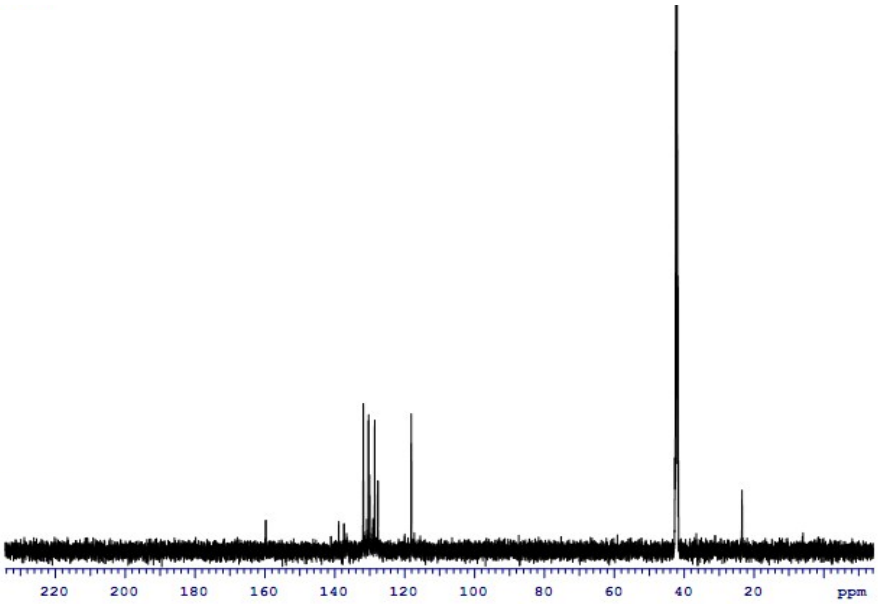


Figure S39. ^{13}C-NMR of *4,4'*-Me,OH-stilbene from I_{12}.

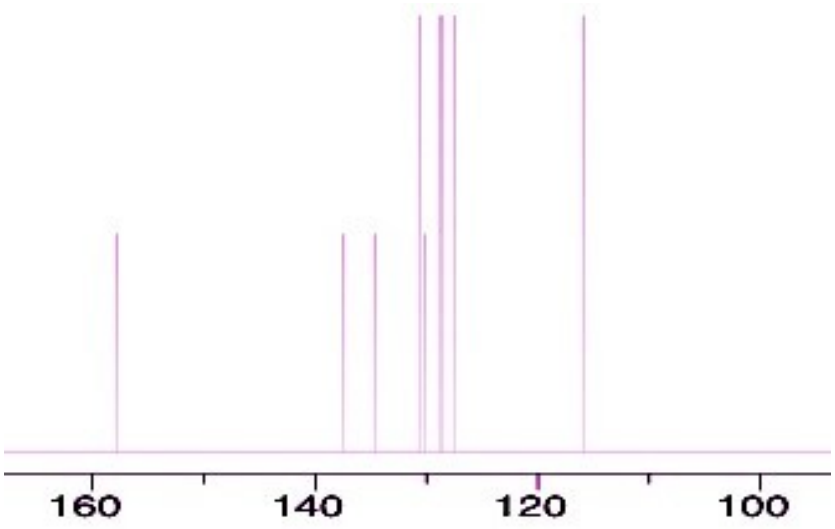


Figure S40. Predicted ^{13}C-NMR of *4,4'*-Me,OH-stilbene.

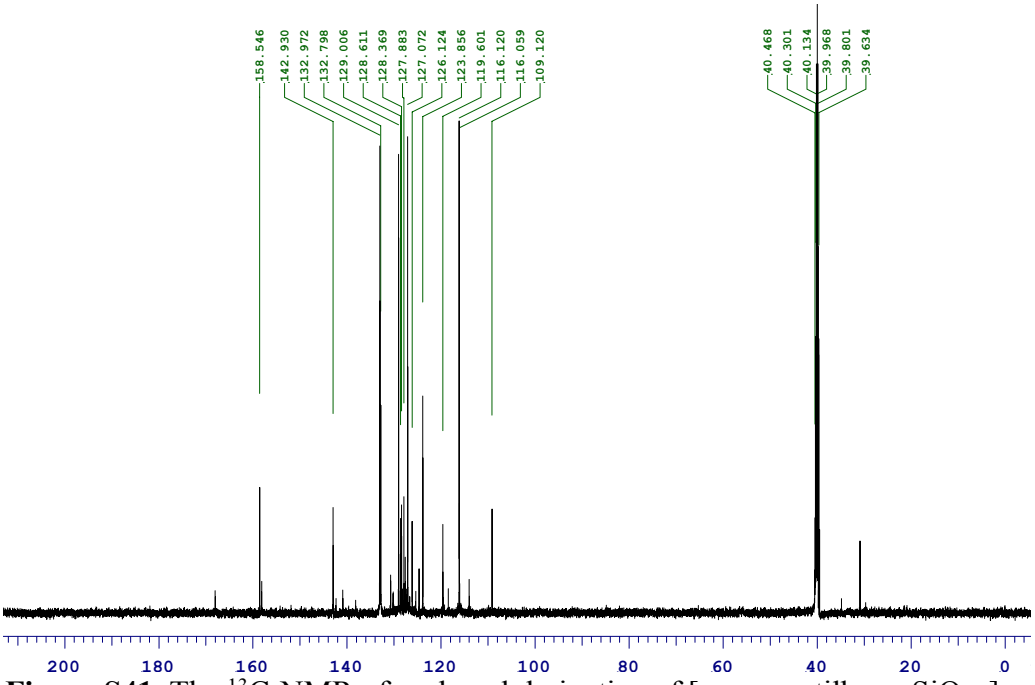


Figure S41. The ^{13}C-NMR of *p*-phenol derivative of [*p*-cyanostilbene-$SiO_{1.5}$]$_{12}$.

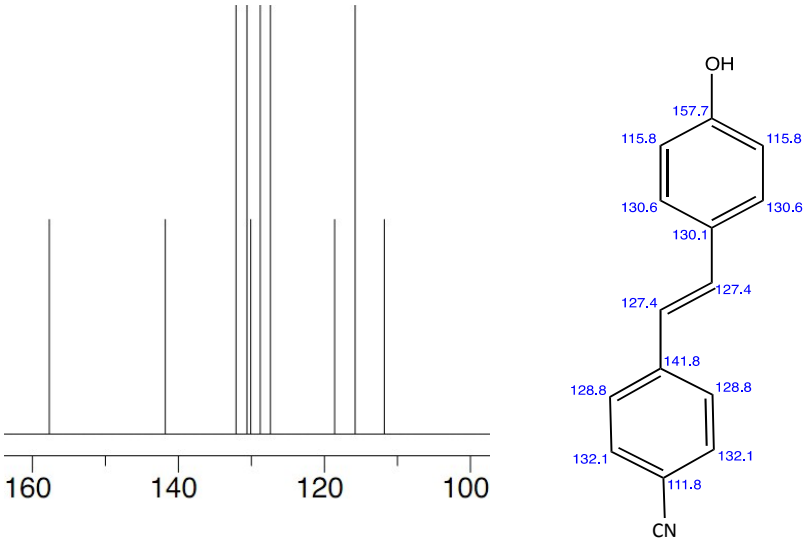


Figure S42. Predicted ^{13}C-NMR of *p*-Cyanostilbene.

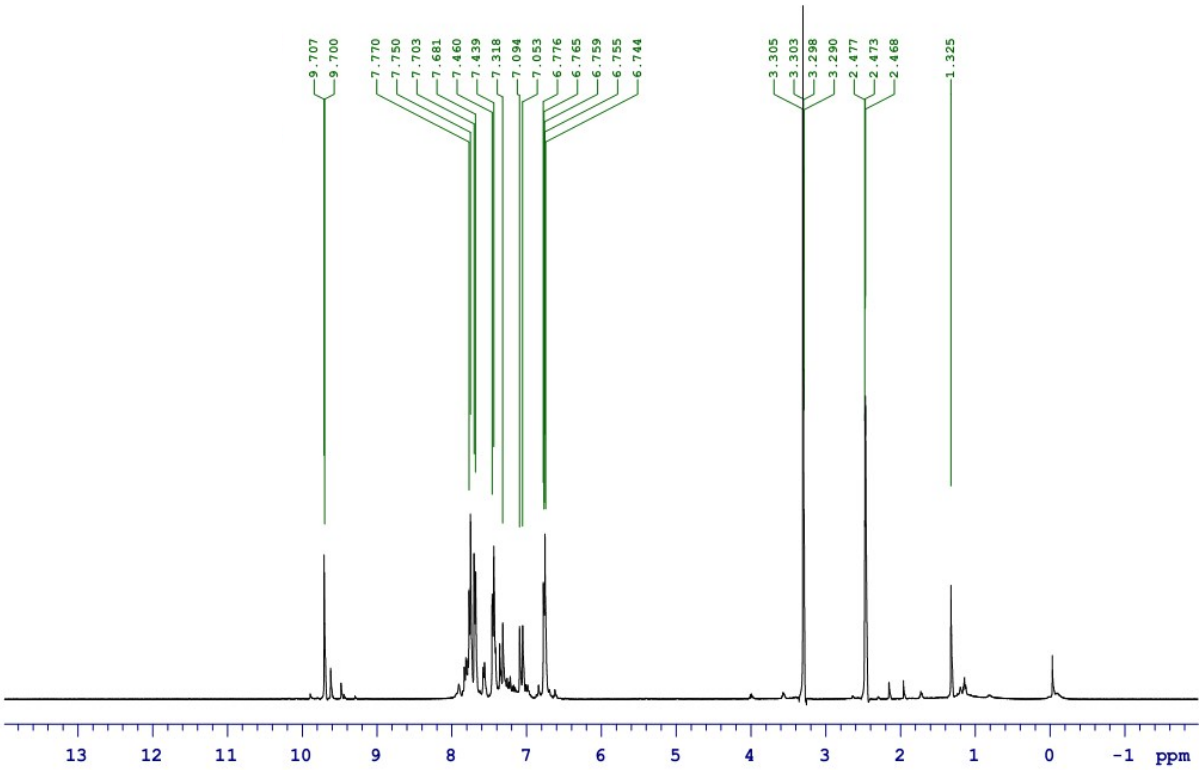


Figure S43. The ^{1}H-NMR of *p*-phenol derivative of [*p*-cyanostilbene$SiO_{1.5}$]$_{12}$.

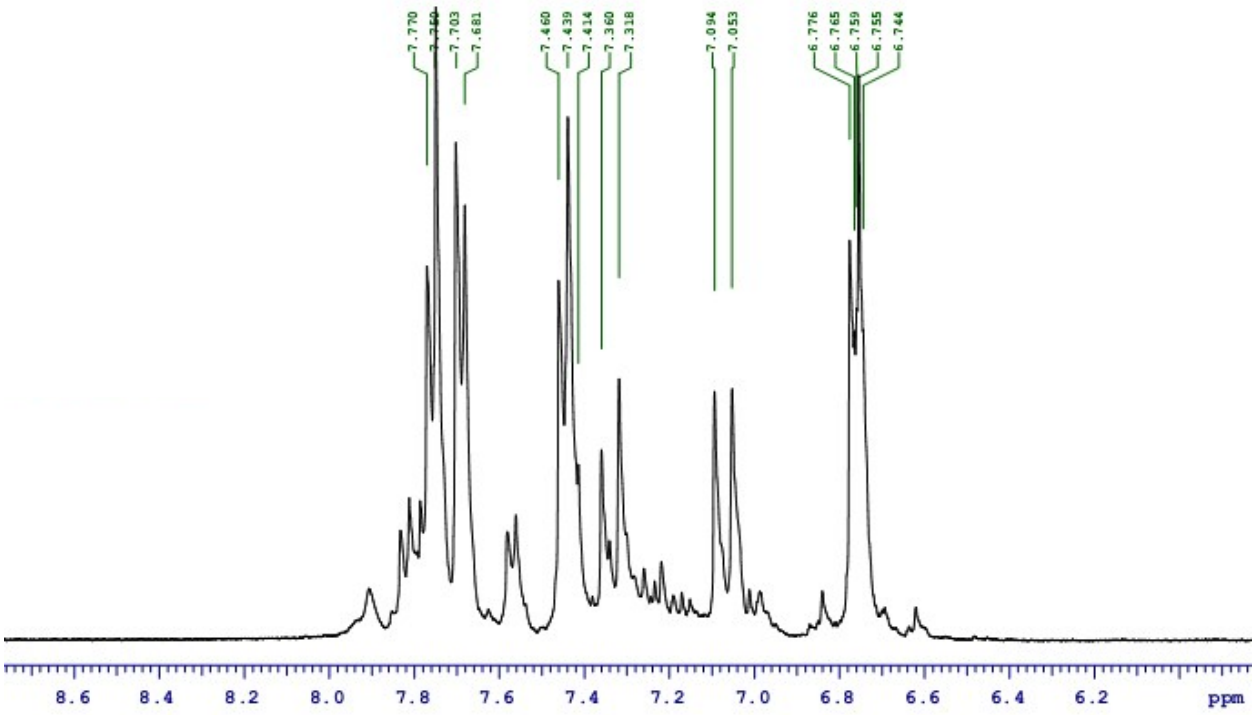


Figure S44. Blow up of ^{1}H-NMR of *p*-phenol derivative of [*p*-cyanostilbene$SiO_{1.5}$]$_{12}$.

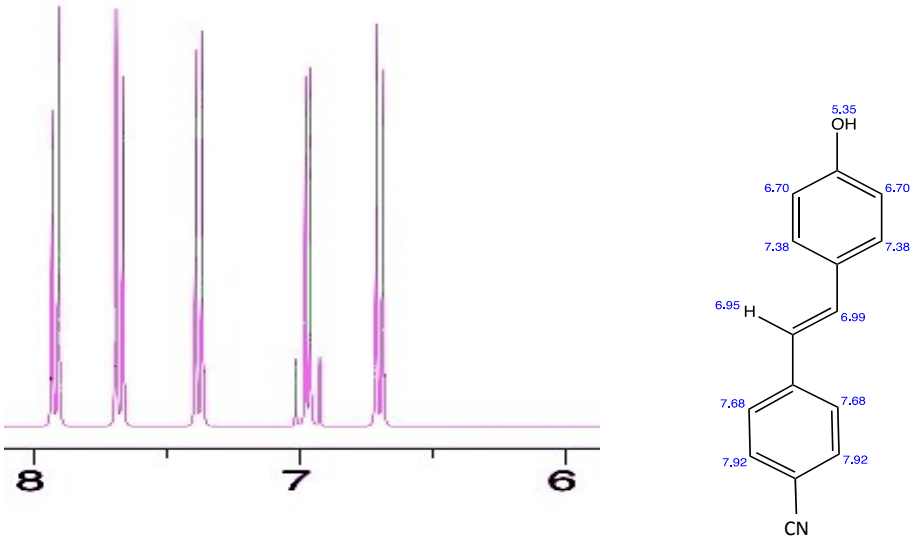


Figure S45. Blow up of predicted ^{1}H-NMR of *p*-cyanophenol from [*p*-cyanostilbene-$SiO_{1.5}$]$_{12}$.