SUPPLEMENTARY INFORMATION 2

Synthesis of self-assembling glycerotriazolophanes

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Supporting Information

S1 Computational details

All the Density Functional Theory (DFT)[1] calculations were carried out using the Gaussian03 package[2] utilizing gradient geometry optimization. Geometry optimizations were performed using the B3LYP functional with the 6-31+G(d) basis set.[3,4] Initially, the geometries of monomers (**5a** and **6a**) were optimized using the same basis set. The optimized geometries of the monomers were utilized in constructing the geometries of dimers (**D-5a** and **D-6a**), which were further optimized. Further, polymeric arrangements of **5a** and **6a** were obtained using many optimized geometries of dimers. The different polymeric arrangements of **5a** and 6a were observed owing to different inter- and intramolecular interactions as described in the results-section. The vibrational frequency calculations for all structures at the same level of geometry optimization were performed to characterize them as minima on the potential energy surface.[5] The estimates of zero point energy values were scaled by 0.9806 before employing them in correcting the absolute energies.[6] The charge analysis was carried out using the Natural Bond Orbital (NBO) method.[7] Atoms in molecules (AIM) method[8] was employed to trace the bond paths associated with intra- and intermolecular interactions, using AIM2000 software package. The energy and geometric parameters used in the discussion are from B3LYP/6-31+G(d) method unless otherwise specifically mentioned.

1 (a) Parr, R. G. *Density Functional Theory of Atoms and Molecules*; Oxford University Press: New York, 1989. (b) Pople, J. A.; Beveridge, D. L. *Approximate Molecular Orbital Theory*; McGraw-Hill Book, New York, 1970.
2 Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.
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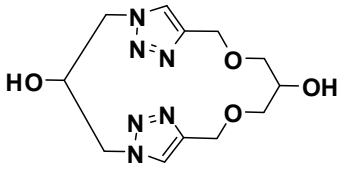
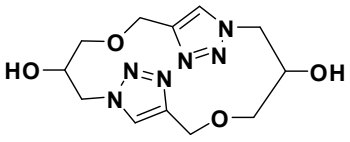
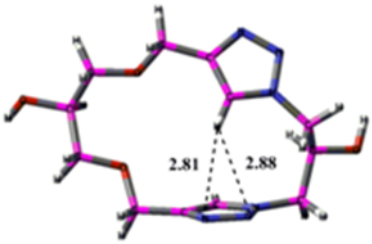
8 Bader, R. Chem. Rev. 1991, 91, 893–928.

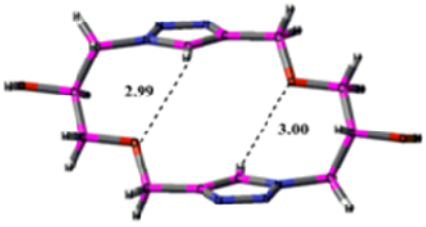
S2 Procedure for DFT calculation in flowchart-form



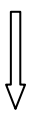


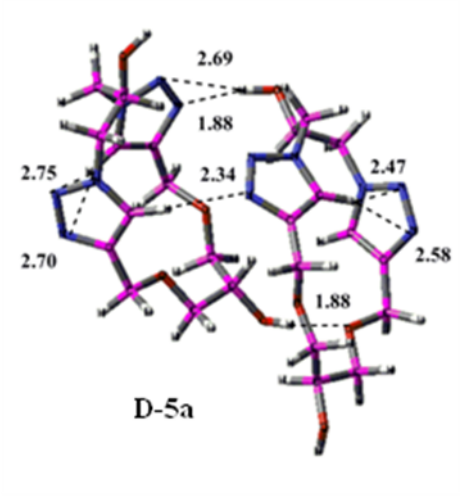


5a

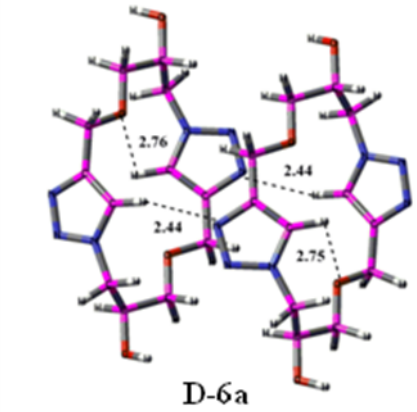


6a





D-5a



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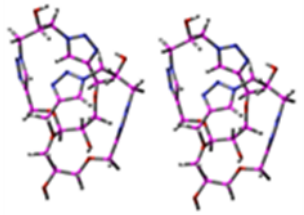
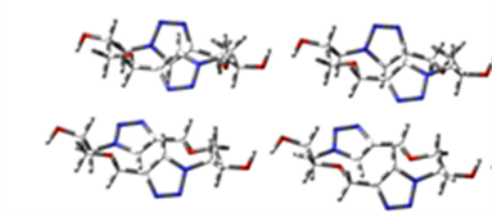


Tetrameric arrangement of 5a



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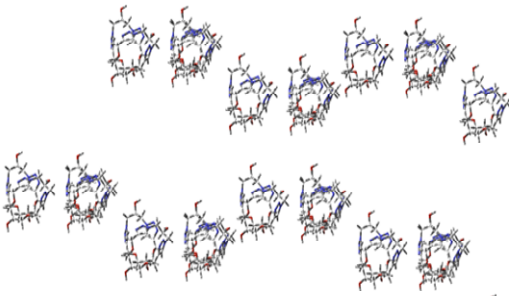
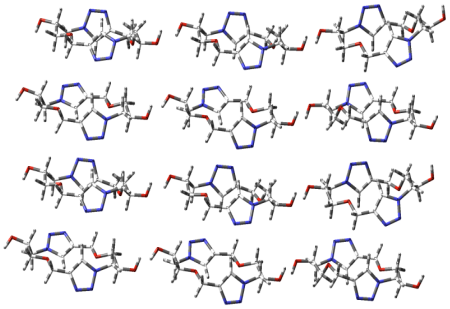
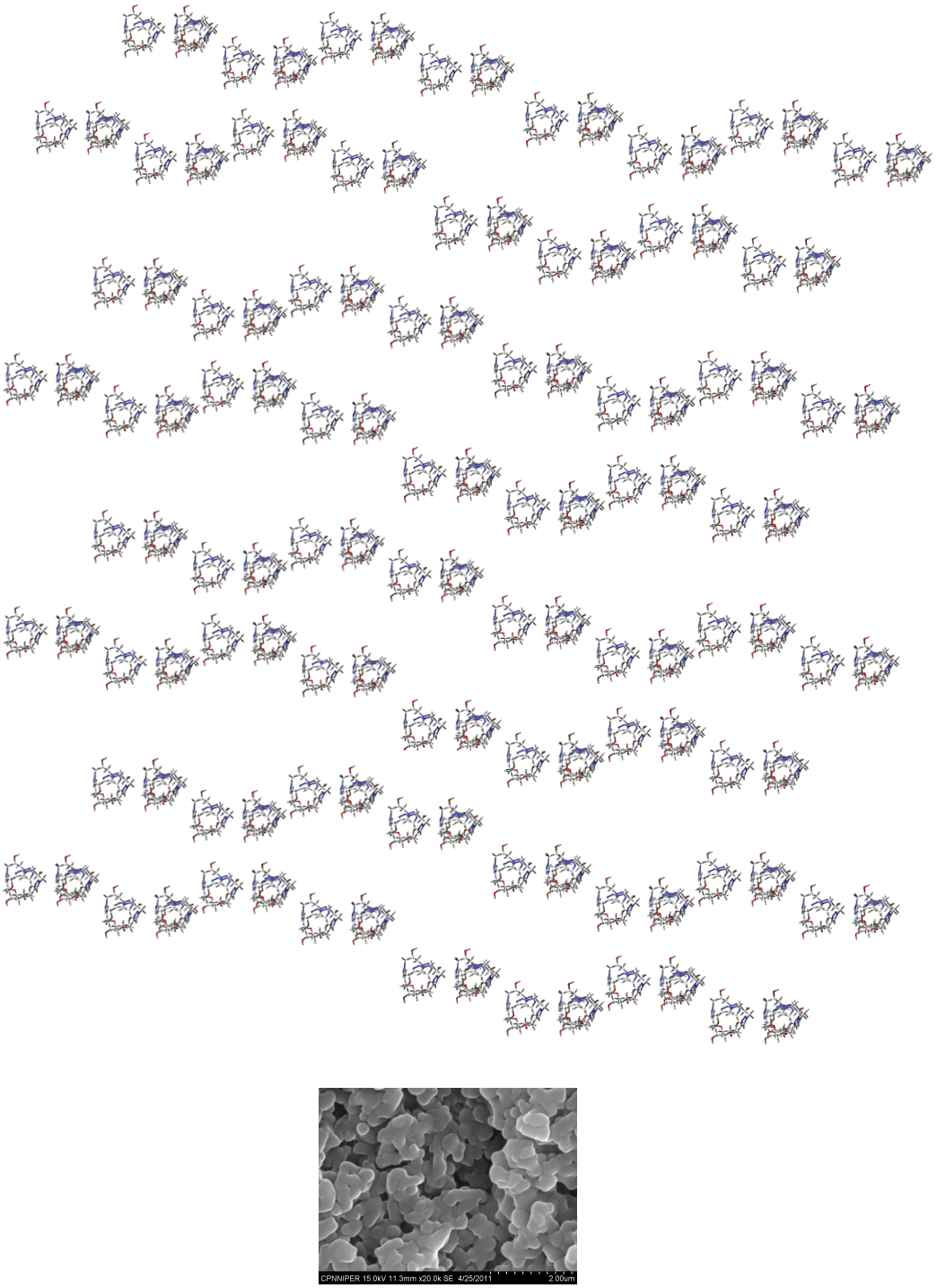
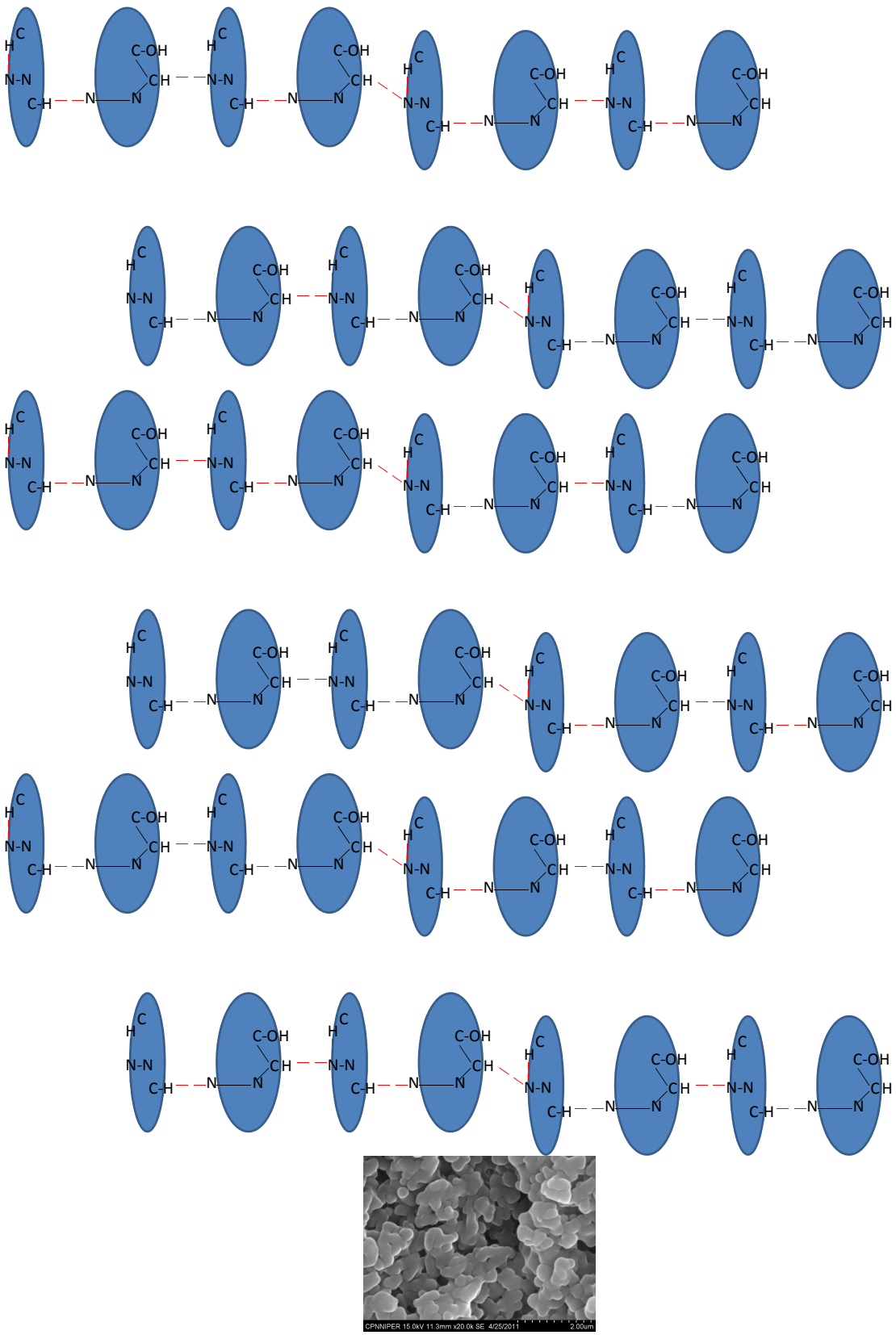




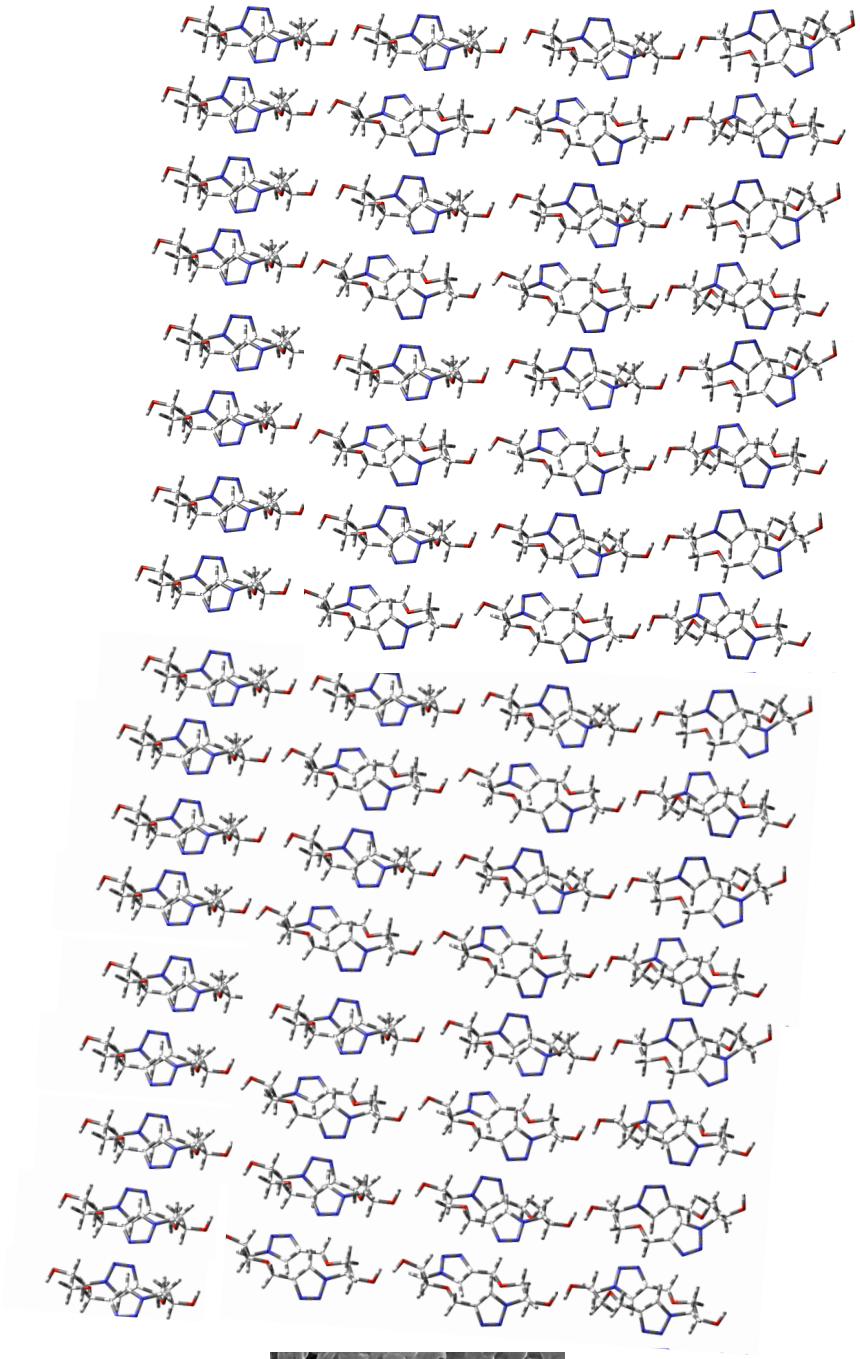
Extending further to get polymeric arrangement of 5a and 6a

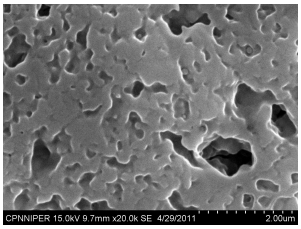
Figure S1 The polymeric arrangement of macromolecules **5a** and **6a** and correlation with their SEM analysis

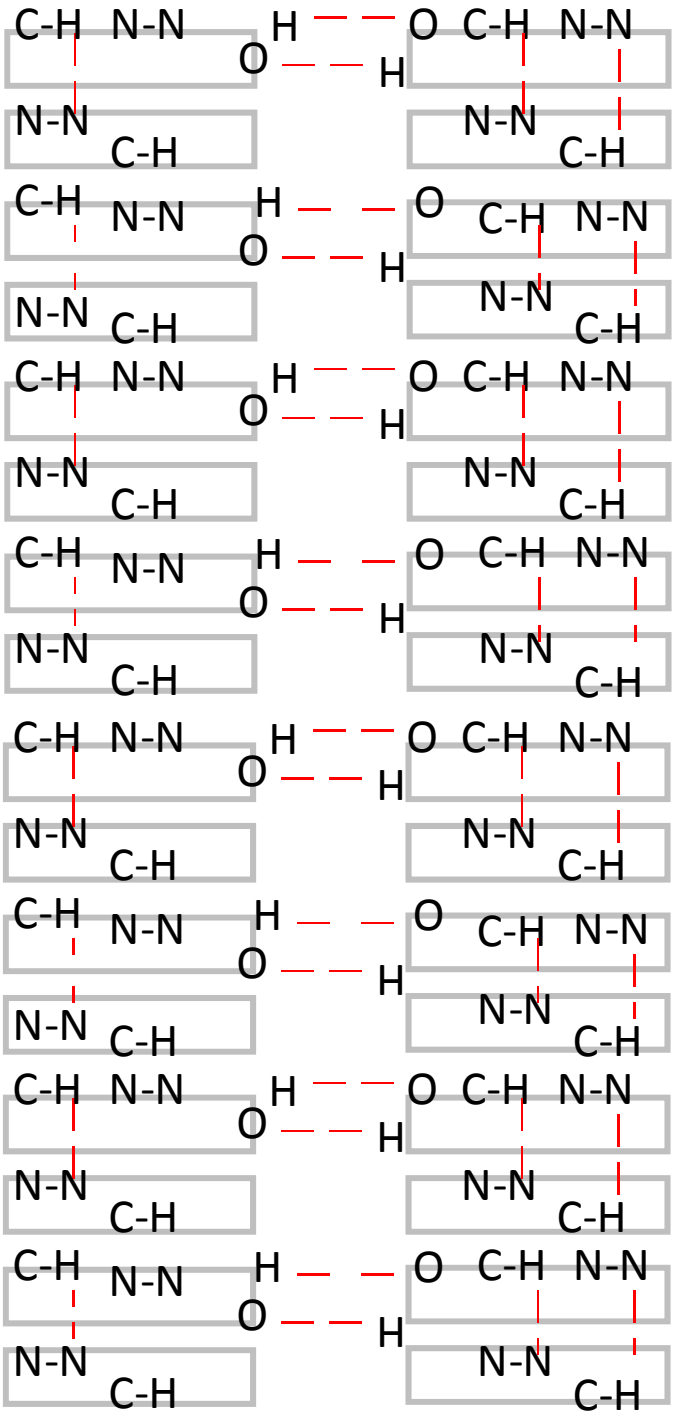


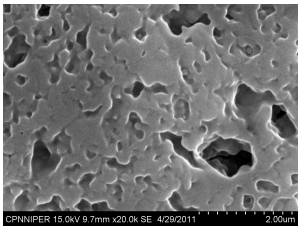


Cs-Pseudosymmetric arrangement (polymeric) of macromolecule **5a**: Aggregates and globules with spaces in between as seen in the SEM



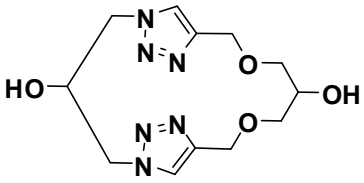




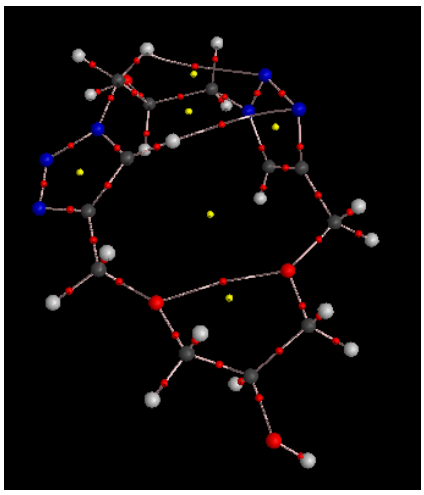


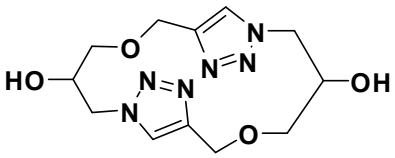
C2-Pseudosymmetric arrangement (polymeric) of macromolecule **6a**: Flat and diffused SEM.

Figure S2 The AIM analysis of monomeric and dimeric structures of macromolecules **5a** and **6a** showing the presence of different interactions (Yellow points**:** Ring critical points**;** Red points**:** Bond critical points)

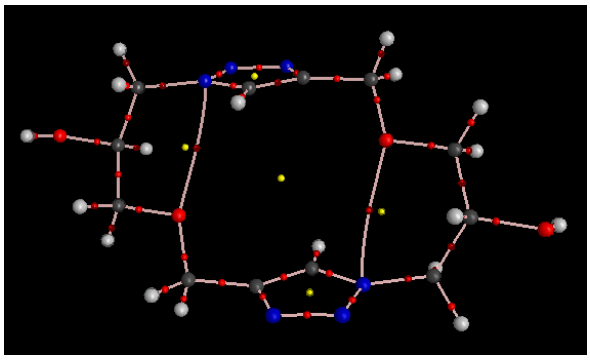


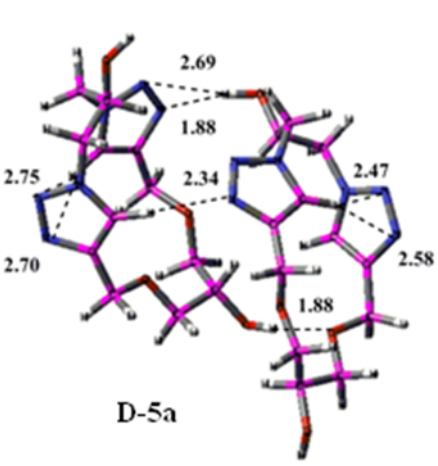
5a



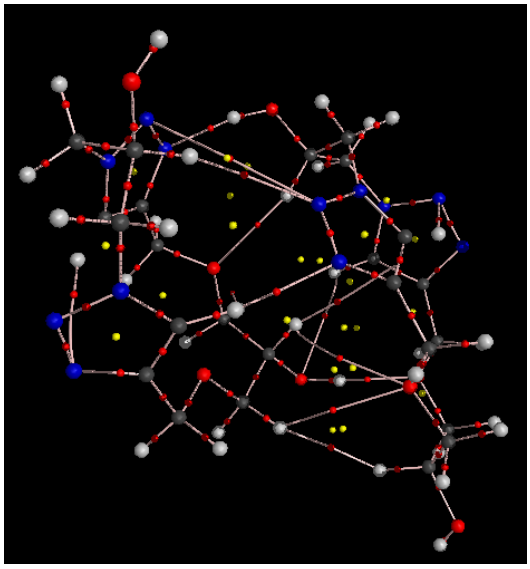


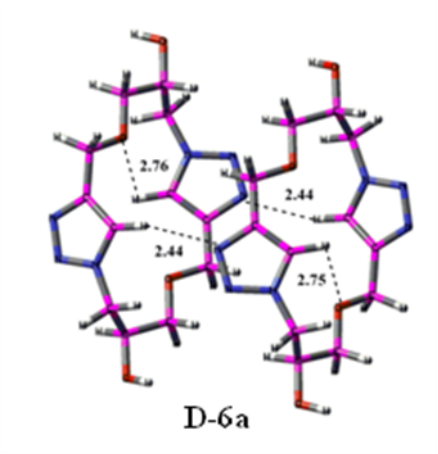
6a

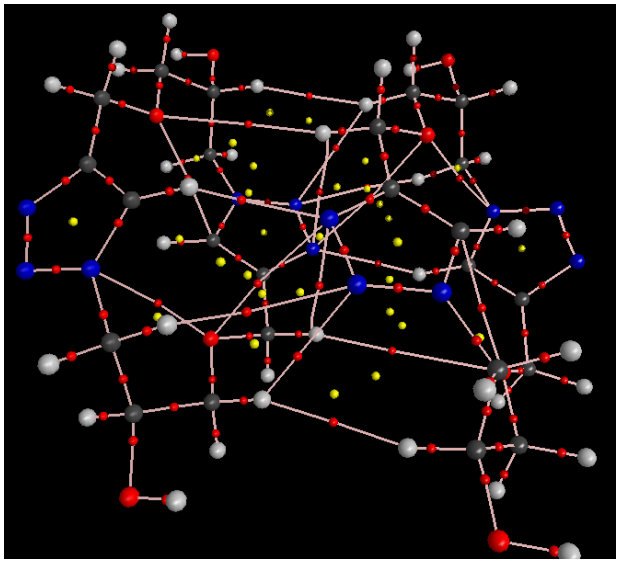




D-5a







S3 Archive-entries of all the optimized geometries, along with absolute energies and frequencies

Monomer **5a**

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,-0.8622916571,-0.3040786539\C,3.6017707127,0.939378734,-1.1407574077\
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Monomer **6a**

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Dimer **5a**

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Dimer **6a**

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