

Supplementary Information

Selectivity and bio-compatibility of self-assembled chiral flower-like and helical nanostructures

Sopan M. Wagalgave,^{a,f} Sachin D. Padghan,^a Mohammad Al Kobaisi,^c Duong Duc La,^d Keerti Bhamidipati,^{f,g} Nagaprasad Puvvada,^{f,g} Rajesh S. Bhosale,^e Sidhanath V. Bhosale,^{a,f*} Sheshanath V. Bhosale^{b*}

^aPolymers and Functional Materials Division CSIR-Indian Institute of Chemical Technology, Hyderabad 500007, Telangana, India.

^bSchool of Chemical Sciences, Goa University, Taleigao Plateau, Goa-403206, India.

^cDepartment of Chemistry and Biotechnology, FSET, Swinburne University of Technology, Hawthorn VIC 3122, Australia.

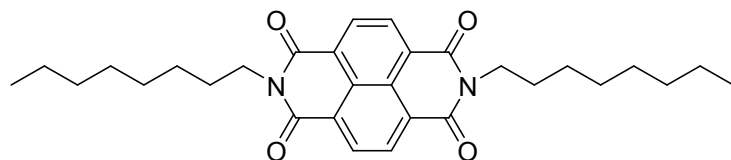
^dInstitute of Chemistry and Materials, 17 Hoang Sam, Cay Giay, Hanoi, Vietnam.

^eDepartment of Chemistry, Indrashil University, Kadi, Mehsana-382740, Gujarat, India.

^fAcademy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, India.

^gApplied Biology Division, CSIR-Indian Institute of Chemical Technology, Hyderabad 500007, Telangana, India.

*Correspondence addressed to S.V.B. (G.U.) svbhosale@unigoa.ac.in or S.V.B. (CSIR-IICT): bhosale@iict.res.in



Scheme S1. Structure of NDI control molecule

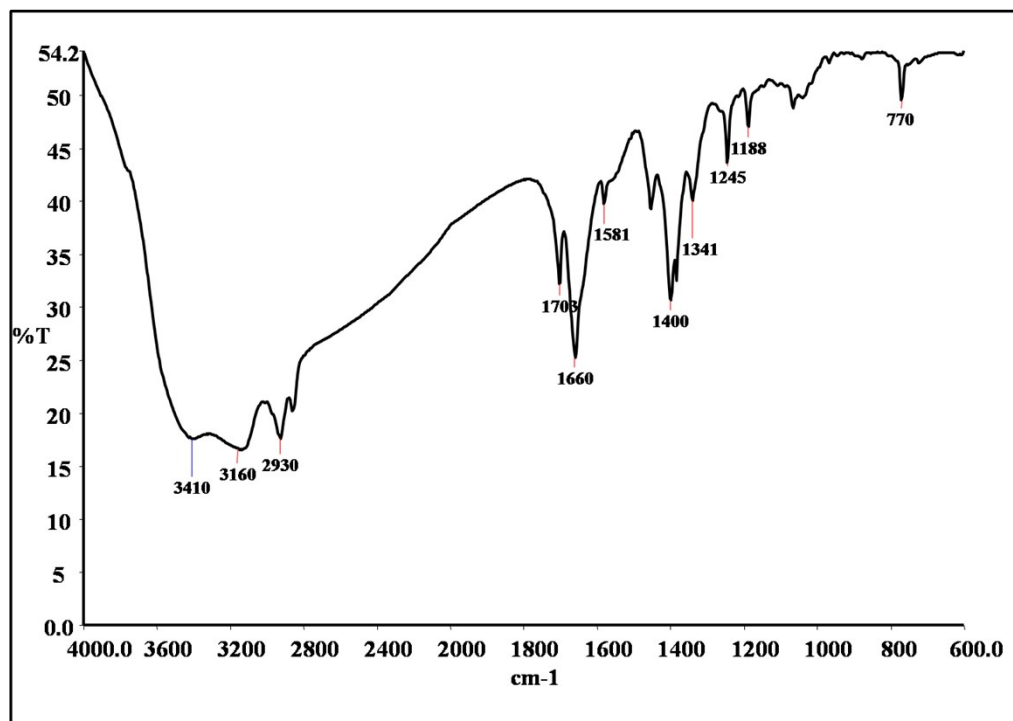


Fig. S1FT-IR spectra of **NDI-LCA**.

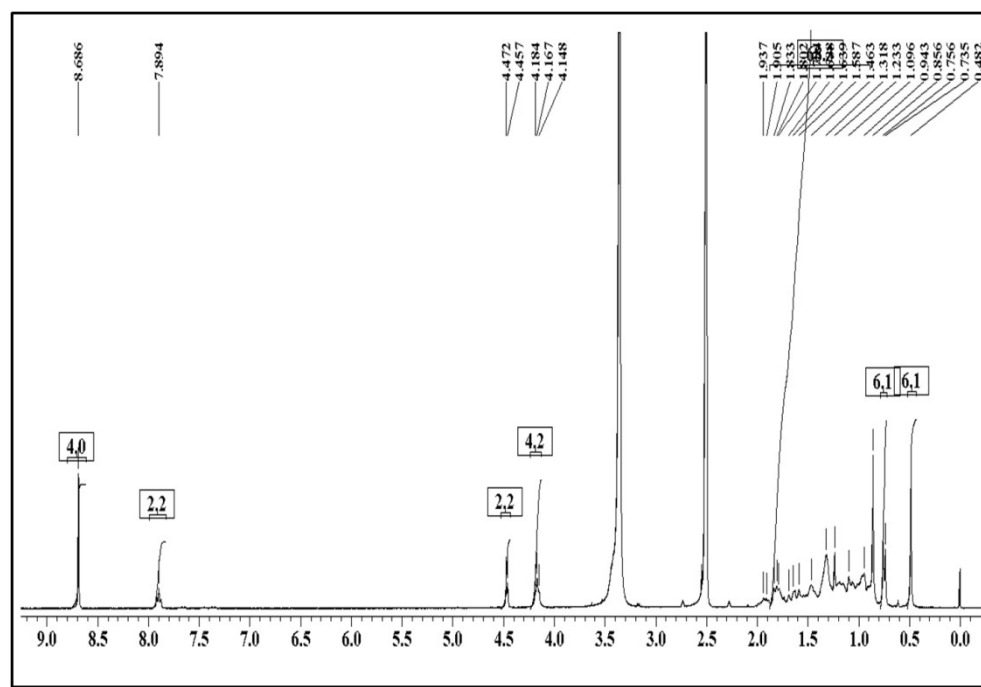


Fig. S2 ^1H NMR spectra of **NDI-LCA**.

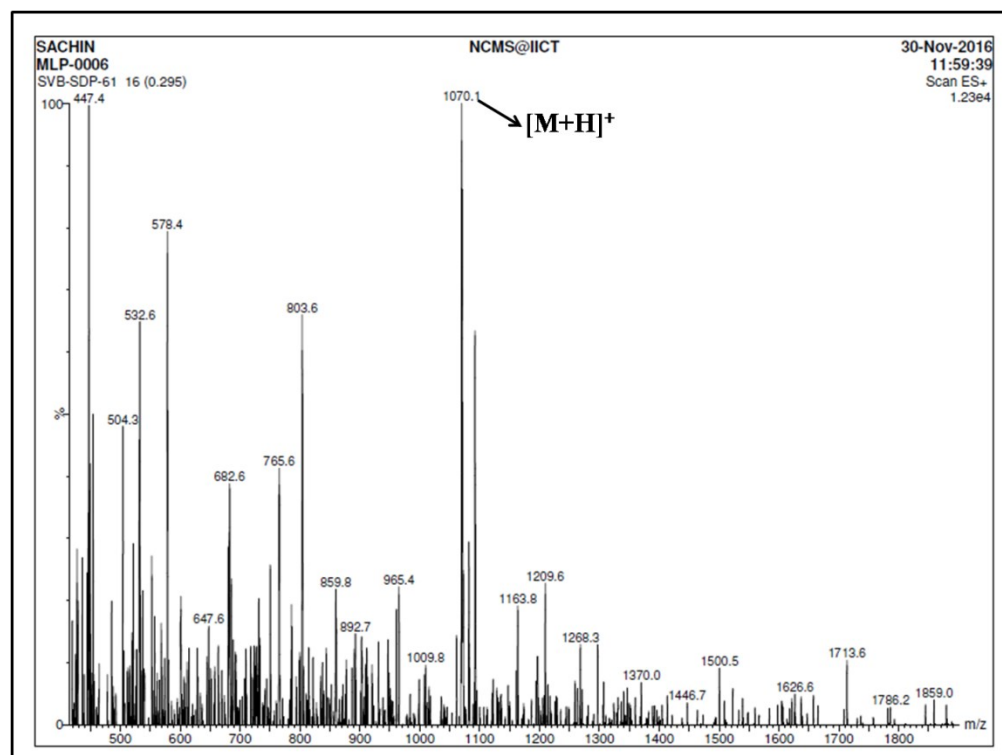


Fig. S3 ESI mass spectra of **NDI-LCA**.

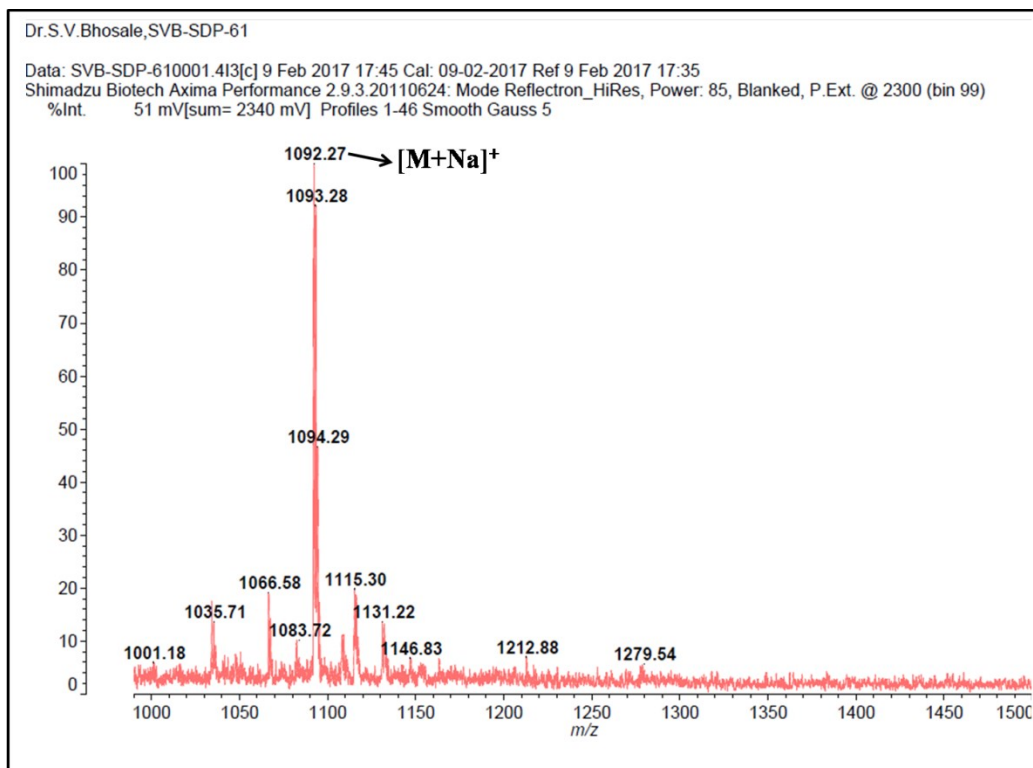


Fig. S4 MALDI-TOF spectra of **NDI-LCA**.

Scanning Electron Microscopic Properties

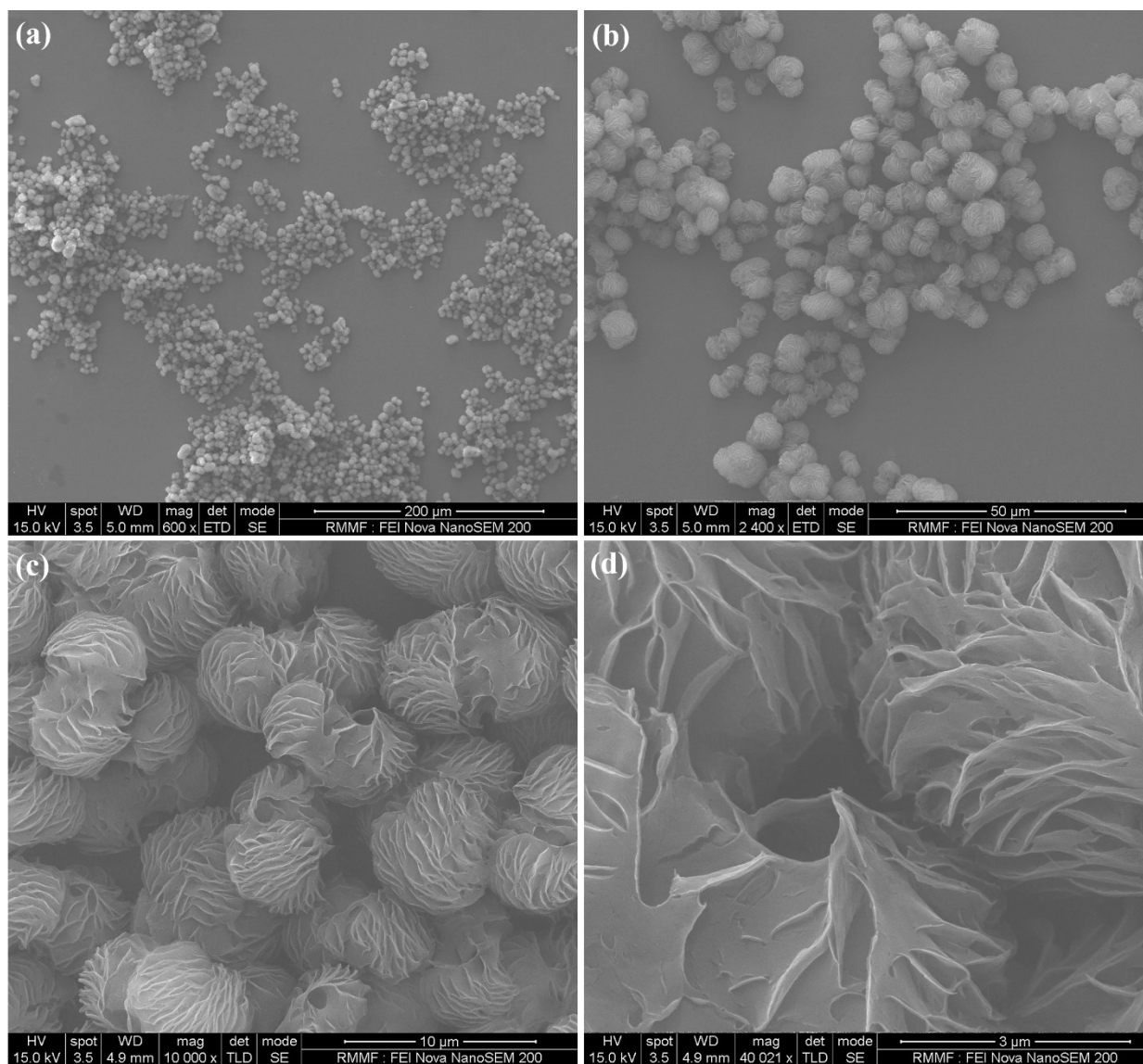


Fig. S5 SEM images of NDI-LCA in THF:MCH (20:80%, v/v ratio).

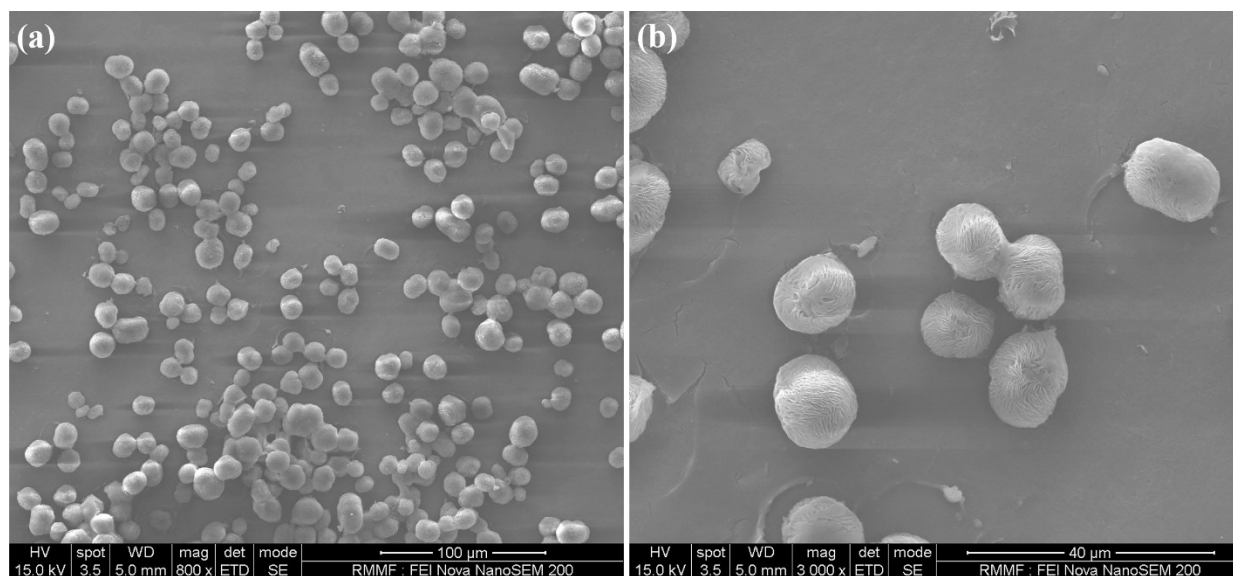


Fig. S6 SEM images of NDI-LCA in THF:MCH (30:70%, v/v ratio).

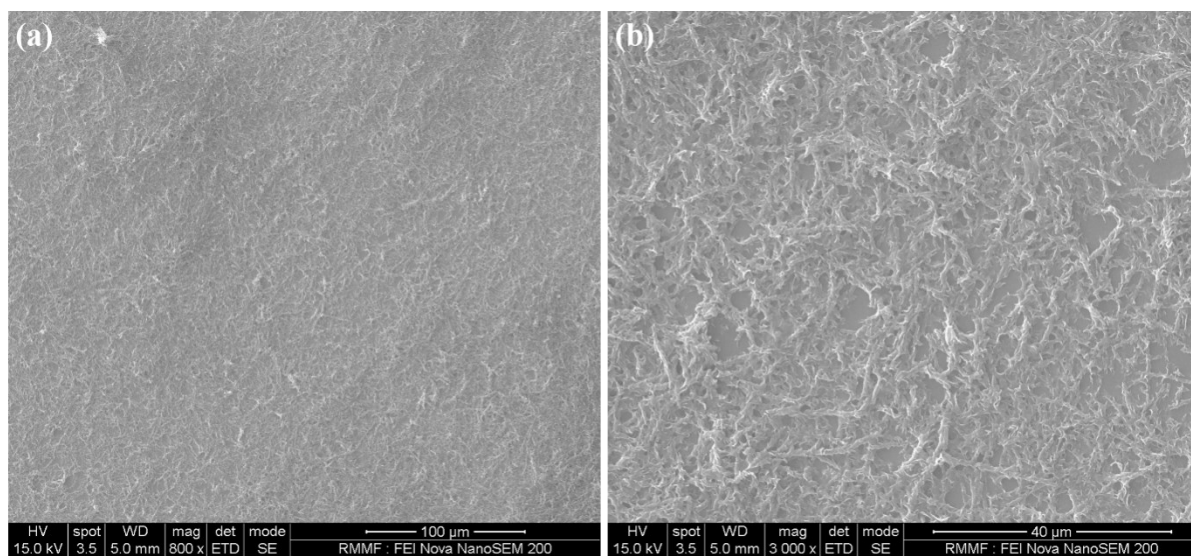


Fig. S7 SEM images of NDI-LCA in THF:H₂O (30:70%, v/v ratio).

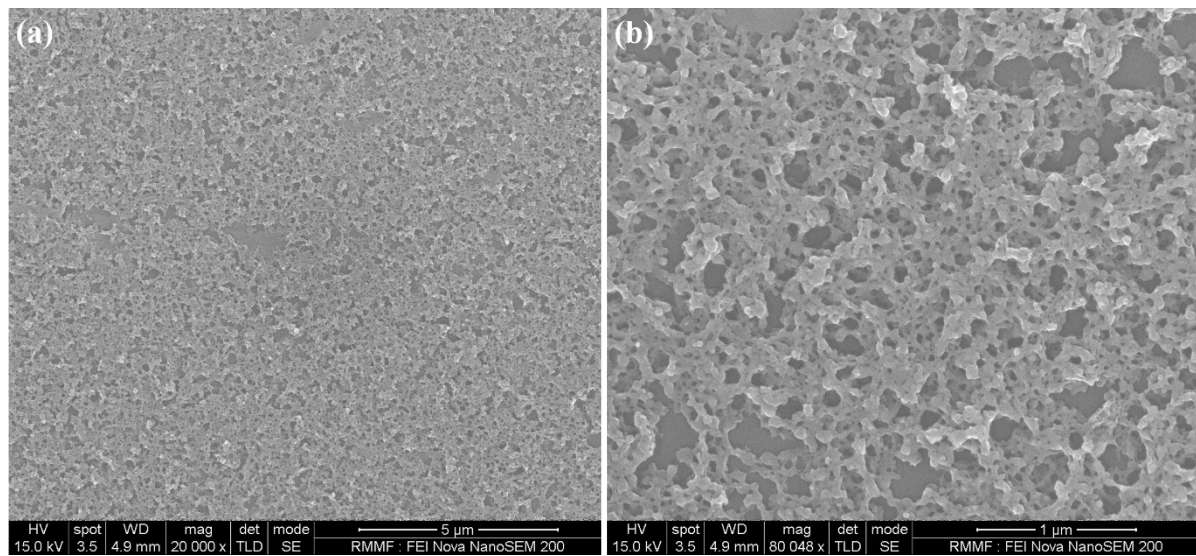


Fig. S8 SEM images of NDI-LCA in THF:H₂O (20:80%, v/v ratio).

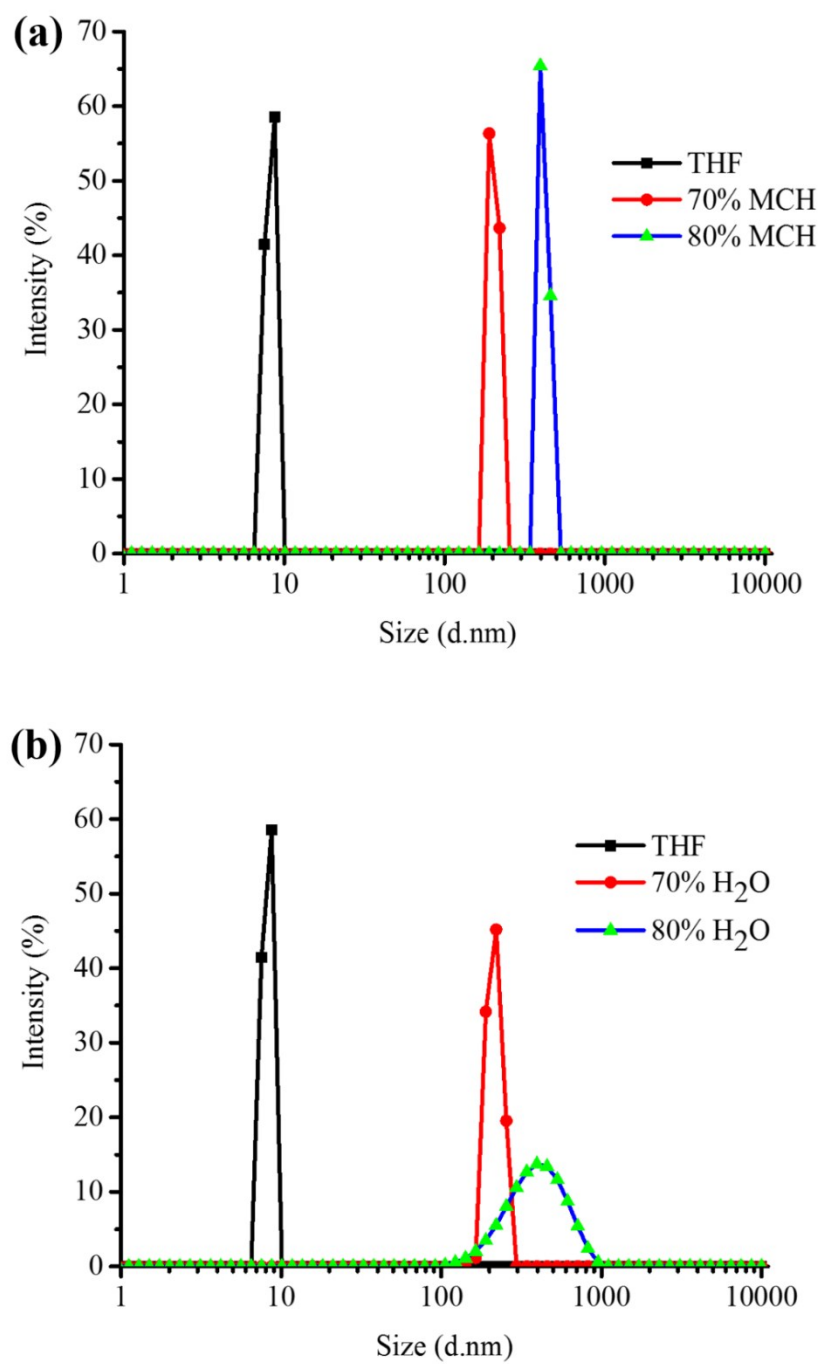


Fig. S9 Dynamic light scattering measurements of **1** in (a) THF:MCH and (b) THF:H₂O.

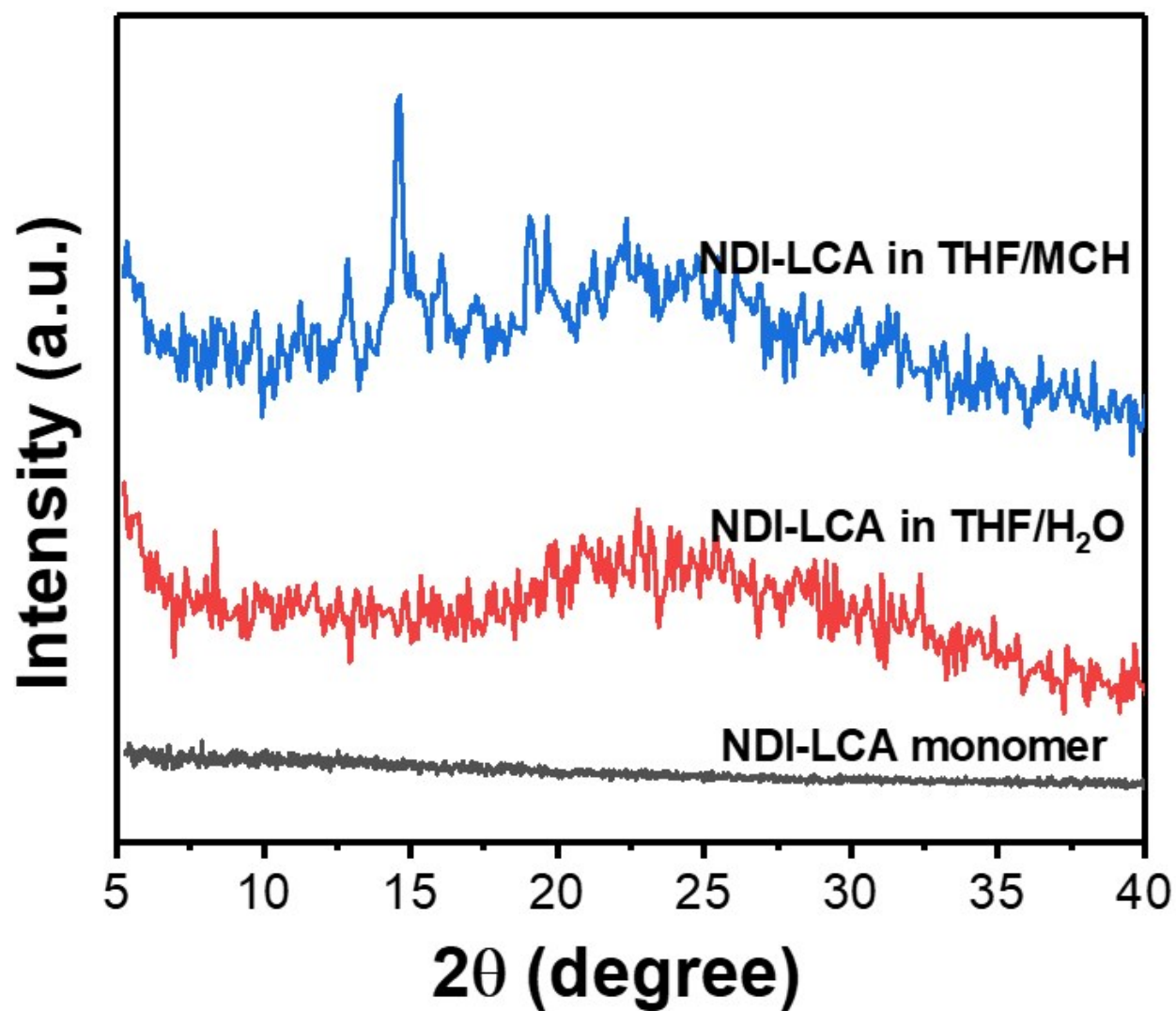


Fig. S10 XRD patterns of the NDI-LCA monomer (grey line), the microstructures of self-assembled NDI-LCA in THF/H₂O (red line) and THF/MCH (blue line) with water fraction of 30%.

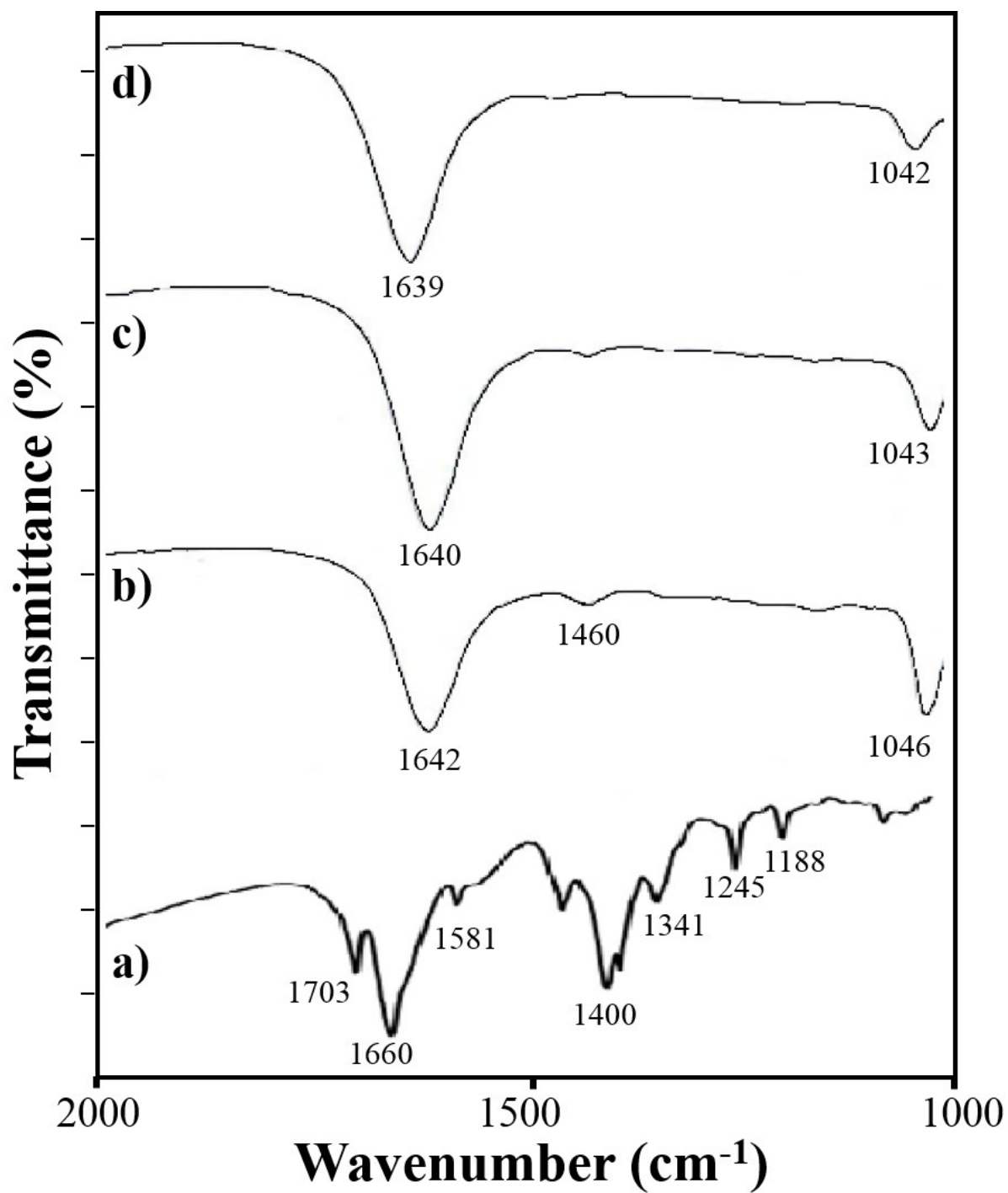


Fig.S11 FT-IR spectra of NDI-LCA in (a) THF, (b) THF:H₂O (30:70%, v/v ratio), (c) THF: H₂O (20:80%, v/v ratio); (d) THF: H₂O (10:90%, v/v ratio)

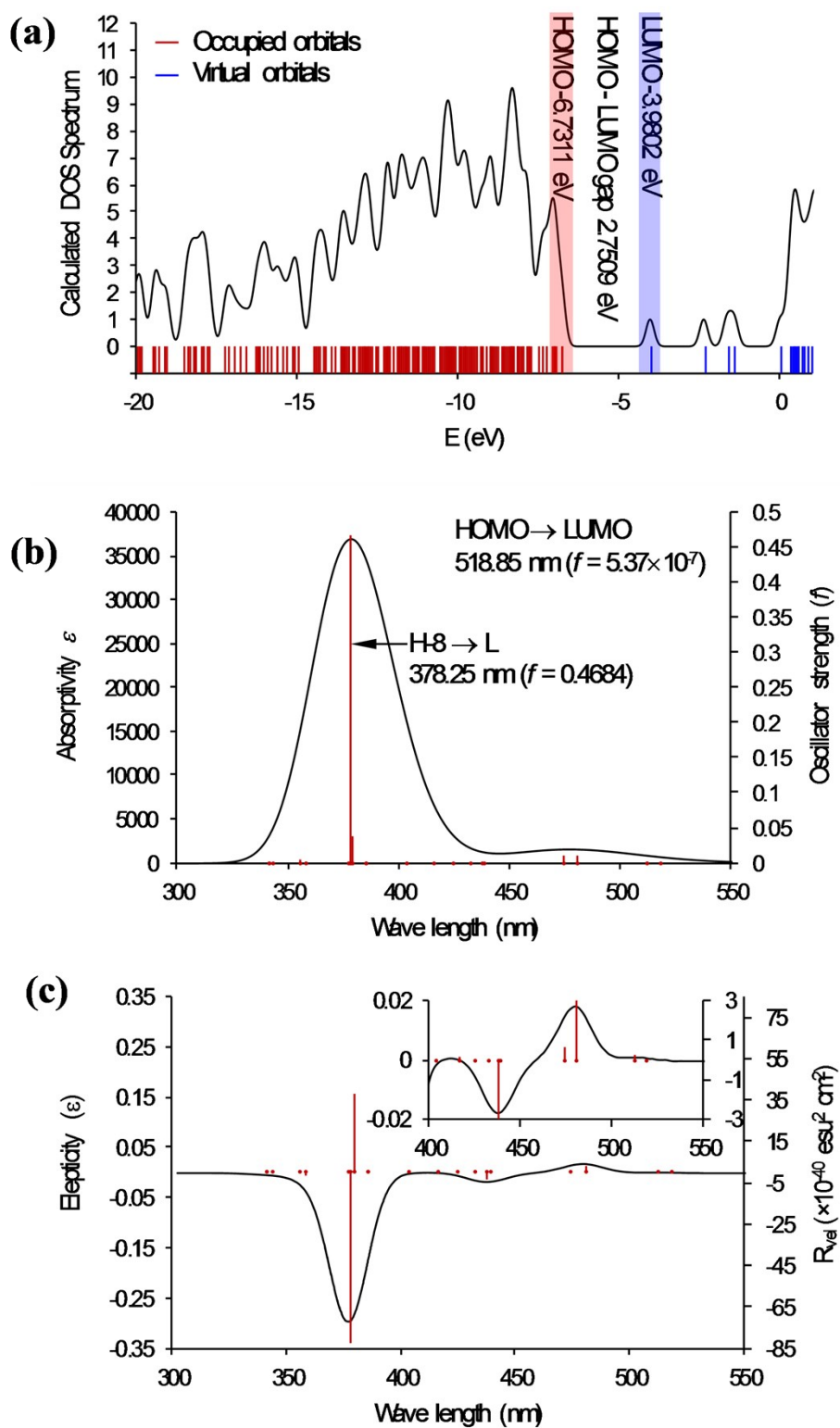


Fig. S12(a) DOS, (b) absorbance, and (c) CD spectra of NDI-LCA as calculated using TDDFT at B3LYP/def2-TZVP basis set.