Electronic Supplementary Information

Solvent Effect on the Production of Spherical Lignin Nanoparticles

Ya Ma[a,b], Yuhe Liao[c], Zhicheng Jiang[a,b]*, Qingyong Sun[a,b], Xingjie Guo[a,b], Wenhua Zhang[a,b], Changwei Hu[a,b,d], Rafael Luque[e]*, Bi Shi[a,b], Bert F. Sels[f]

[a] College of Biomass Science and Engineering, Sichuan University, Chengdu 610065, China

[b] National Engineering Research Center of Clean Technology in Leather Industry, Sichuan University, Chengdu 610065, China

[c] Guangzhou Institute of Energy Conversion, Chinese Academy of Sciences, Guangzhou 510640, China

[d] Key Laboratory of Green Chemistry and Technology, Ministry of Education, College of Chemistry, Sichuan University, Chengdu 610065, China

[e] Departamento de Química Orgánica, Universidad de Córdoba, Ctra Nnal IV-A, Km 396, E14014, Cordoba, Spain

[f] Center for sustainable catalysis and Engineering, KU Leuven, 3001 Heverlee, Belgium

*Corresponding Authors:

Zhicheng Jiang, E-mail: zhichengjiang@scu.edu.

Rafael Luque, E-mail: rafael.luque@uco.es.

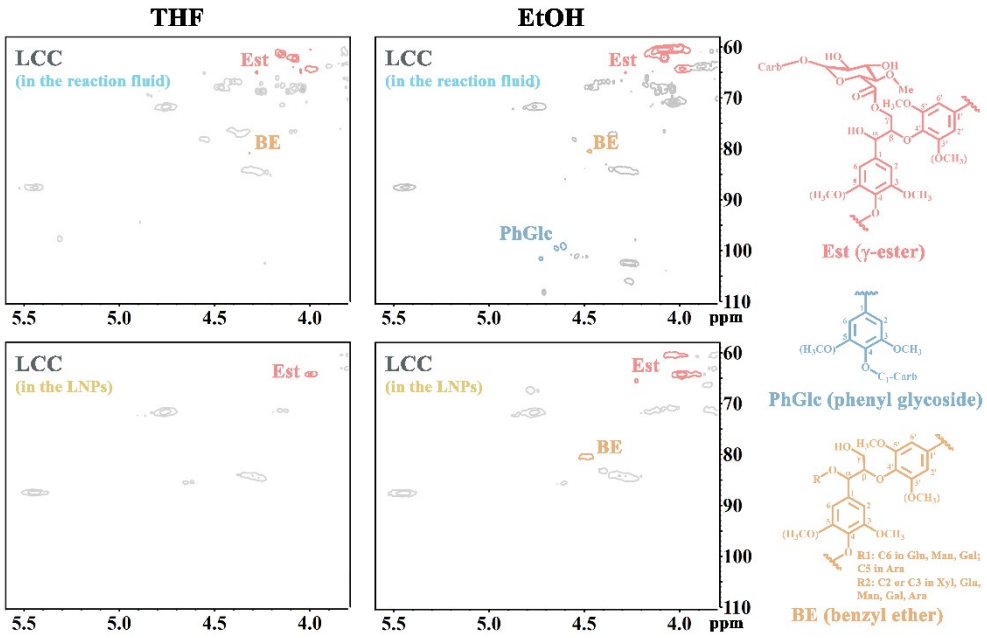

Fig. S1. 2D HSQC NMR spectra of the lignin carbohydrate complex (LCC).

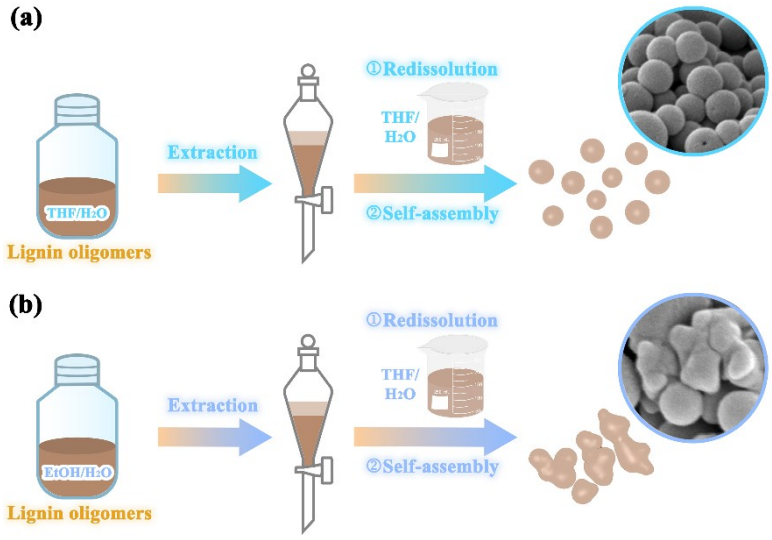

Fig. S2. The morphology of LNPs using different lignin oligomers generated from the same co-solvents. (a) Lignin oligomers were obtained from THF reaction system. (b) Lignin oligomers were obtained from EtOH reaction system.

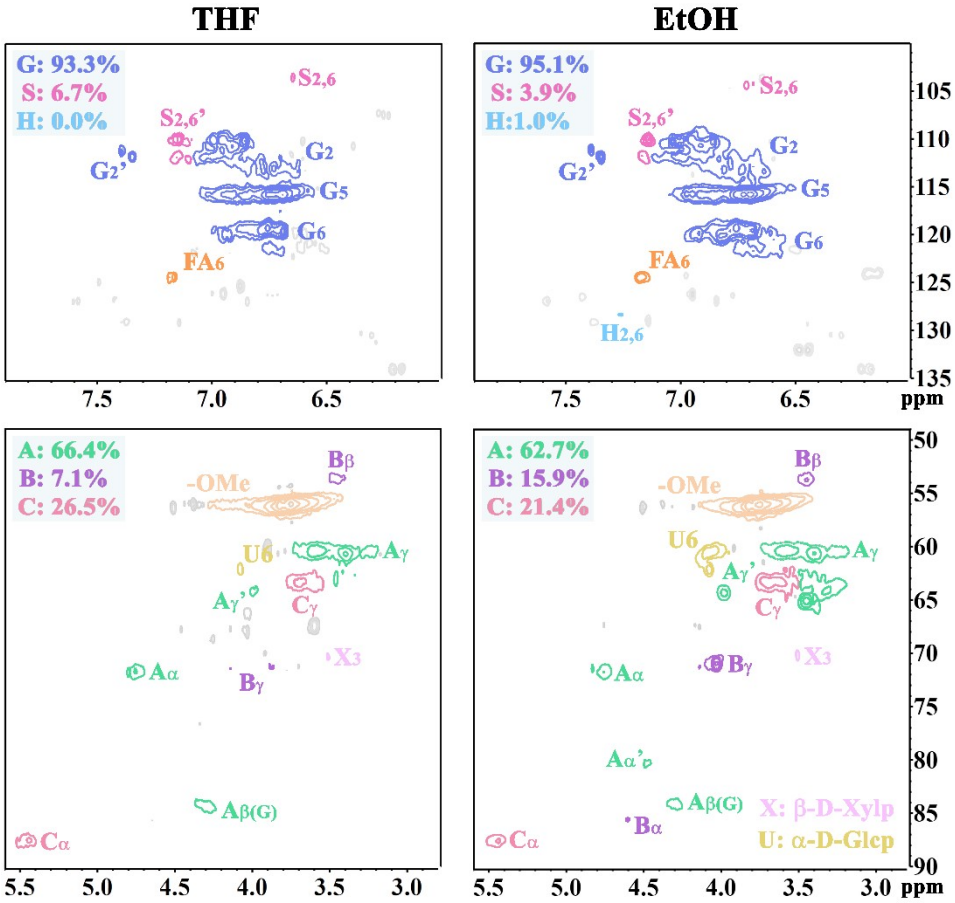

Fig. S3. 2D HSQC NMR spectra of the extracted oligomers.

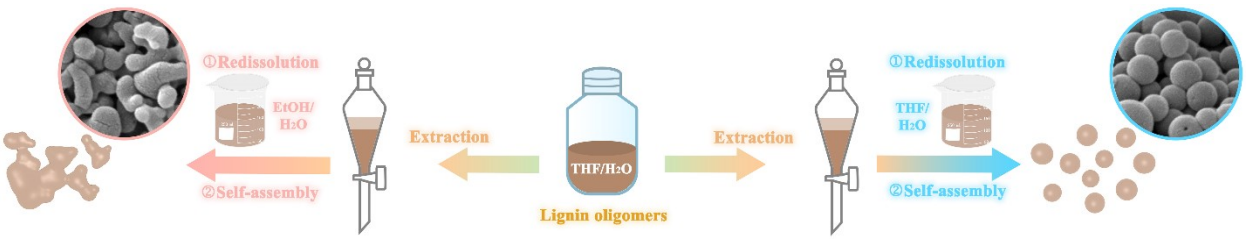

Fig. S4. The morphology of LNPs using the same extracted lignin oligomers generated from different co-solvents.

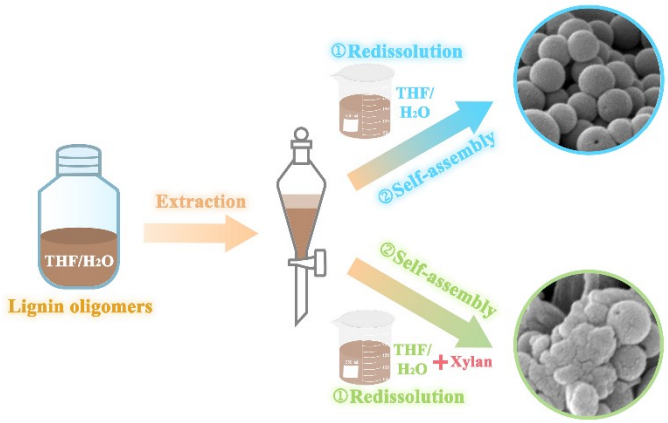

Fig. S5. The morphology of LNPs using the same lignin oligomers with/without additional xylo-oligosaccharides added generated from the same co-solvents.

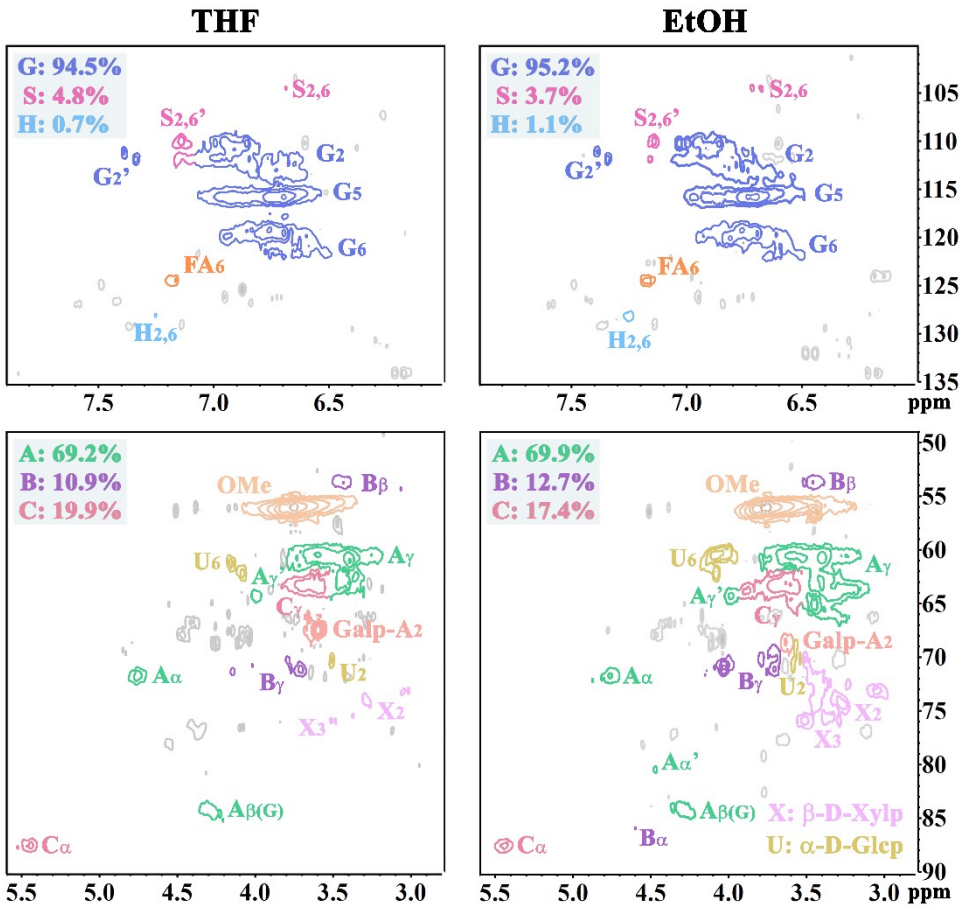

Fig. S6. 2D HSQC NMR spectra of the oligomers originally dissolved in reaction fluids.

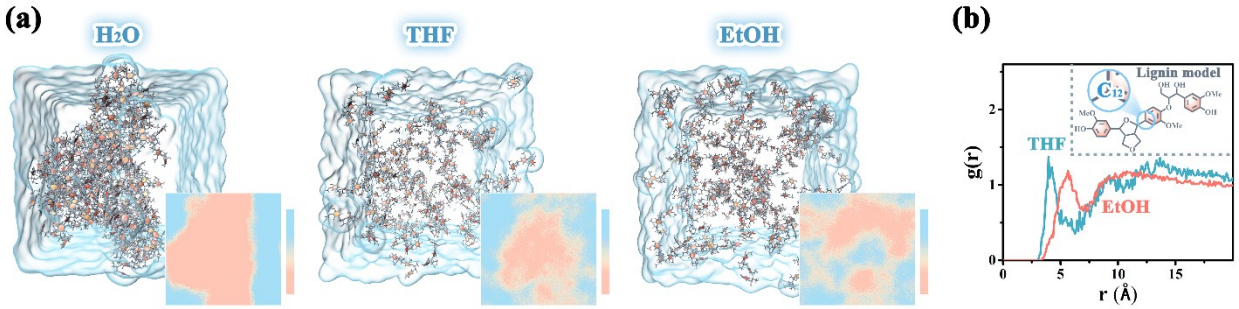

Fig. S7. MD simulation of lignin oligomer model compound (G-B-G-A-G). (a) Snapshots and density maps of the lignin oligomers after self-assembly from MD simulation. (b) The model compound of lignin molecule and C_{12}-C_{12} site-site radical distribution functions from different systems.