Supporting Information for

Enantioseparation Characteristics of Chiral Stationary Phases Based on Derivatives of Cellulose and Chitin

Xiao-Chen Wang¹[†], Juan Zhang²[†], Xiao-Qin Xu¹, Wei Chen¹, Yong-Gang Yang^{3*} and Zheng-Wu Bai^{1*}

¹School of Chemistry and Environmental Engineering, ²School of Chemical Engineering and Pharmacy, Wuhan Institute of Technology, Wuhan 430073, China ³College of Chemistry, Chemical Engineering and Materials Science, Soochow University, Suzhou 215123, China

*Corresponding authors at:

School of Chemistry and Environmental Engineering, Wuhan Institute of Technology, Wuhan 430073, China. Tel.: +86 27 87195680, Fax: +86 27 87194560, E-mail address: <u>zwbai@wit.edu.cn</u> (Z.-W. Bai);

College of Chemistry, Chemical Engineering and Materials Science, Soochow University, Suzhou 215123, China. Tel.: +86 512 65880047, Fax: +86 512 65882052, E-mail: <u>ygyang@suda.edu.cn</u> (Y.-G. Yang)

[†]The first two authors contributed equally to this work.

Preparation of the derivatives

Microcrystalline cellulose (2.5g) and 4-*N*,*N*-dimethylaminopyridine (DMAP) (28.9mg) were suspended in pyridine (40ml) at 110°C and then 4-methylbenzoyl chloride (10ml) was added. The mixture was refluxed for 48 h. After being cooled to 60°C, the mixture was dropped into methanol (300 ml) under vigorous stirring. The resulting precipitant was collected by sucking filtration. Then the solid was dissolved in CH_2Cl_2 (100 ml) and was re-precipitated by the addition of methanol (500 ml) and washed with methanol. Cellulose tris(4-methylbenzoate) (CMB) (7.6 g) was obtained

in a yield of 95%, after the removal of the volatiles in vacuo. IR(KBr, cm⁻¹): 1729 (- CO_2 -), 1611, 1507 (-CONH-, Ph-); Elemental analysis [(EA), %]: Calculated for: C 69.77, H 5.43, found C 69.73, H 5.58.

Cellulose tris(3,5-dimethylphenylcarbamate) (CDMPC) (7.6g) was prepared with microcrystalline cellulose (2.5g) and 3,5-dimethylphenyl isocyanate (12ml) in a yield of 82%. The preparation manner was same as the one described above. IR(KBr, cm⁻¹): 3316 (-NH-), 1731 (-CO₂-), 1611, 1545 (-CONH-, Ph-); EA (%): Calculated for: C 64.69, H 6.25, N 6.86, found C 64.29, H 6.22, N 6.74.

Chitin bis(3,5-dimethylphenylcarbamate) (Chi-DMPC) (1.6g) was prepared by the reaction between 3,5-dimethylphenyl isocyanate and chitin (1.0g). The chitin was pre-activated in N,N-dimethylacetamide (DMAc) (30ml) at ca. 160°C for 1 h. After being cooled to ambient temperature, the chitin was collected by sucking filtration and washed with acetone. After being dried in vacuo at 60 °C, the chitin was stirred with a solution of LiCl (1.5g) in DMAc (15ml) at 80 °C for 24 h, and then an excess of 3,5-dimethylphenyl isocyanate (5ml) and DMAP (30mg) were added. The resulting solution was continuously stirred for 24 h. After the completion of the reaction, the mixture was dropped into methanol (150 ml) with vigorous stirring. The solid was collected by sucking filtration and dissolved in DMAc (150ml). The viscous solution was centrifuged for 5min under 4000r/m. The supernatant liquor was poured into water. The resulting solid was washed with ethanol till no organic compound was detected by thin-layer chromatography. After removing the volatiles, Chi-DMPC was obtained in a yield of 81%. IR(KBr, cm⁻¹): 3287 (-NH-), 1721 (-CO₂-), 1611, 1549 (-CONH-, Ph-); EA (%): Calculated for: C 60.57, H 6.45, N 8.15, found C 60.05, H 6.57, N 8.69.