Supporting Information
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Supporting Information (SI)

A Facile Route to Ursodeoxycholic Acid based on Stereocontrolled Conversion and Aggregation Behavior Research

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1. Determination of CMC

Pyrene was purchased from 9 Ding Chemicals and recrystallized from hot EtOH. The solution of pyrene in freshly distilled acetone was added to a 10 mL flask and the bile salt dissolved in distilled water was poured after acetone was volatized completely. The mixture was sonicated for 15 mins and set aside overnight. Concentration of pyrene kept about 0.3 μM and sample was excited at 338 nm. The intensity of I₃ and I₁ vibronic bands of pyrene fluorescence was recorded at 543 nm to 480 nm, followed by the calculation of I₃/I₁ ratio. The whole fluorescence spectra were recorded on Hitachi F-7000.
2. NMR spectral data of compounds 2-11 and 1b

Methyl 3α,6α-dihydroxy-cholan-24-oate (2)

$^1$H NMR

$^{13}$C NMR
Methyl 3α-hydroxy-6-oxo-cholan-24-oate (3)

$^1$H NMR

$^{13}$C NMR
Methyl 3α-acetoxy-6-oxo-cholan-24-oate (4)

\(^1\)H NMR

\(^{13}\)C NMR
Methyl 3α-acetoxy-6-[(4-methylphenyl)sulfonyl]hydrazinylidene]cholan-24-oate (5)

$^1$H NMR

$^{13}$C NMR
Methyl 3α-acetoxy-chol-6-en-24-oate (6)

$^1$H NMR

$^{13}$C NMR
Methyl 3α-acetoxy-6,7-epoxy-cholan-24-oate (7)

$^1$H NMR

$^{13}$C NMR
Methyl 3α-acetoxy-7α-hydroxyl-cholan-24-oate (8)

$^1$H NMR

$^{13}$C NMR
Methyl 3α-acetoxy-7-oxo-cholan-24-oate (9)

$^1$H NMR

$^{13}$C NMR
UDCA (1b)

$^1$H NMR

$^{13}$C NMR
Methyl 3α-acetoxy-6-trimethylsilyloxy-chol-6-en-24-oate (10)

$^1$H NMR

$^{13}$C NMR
Methyl 3α-acetoxy-7α-hydroxyl-6-oxo-cholan-24-oate (11)

$^1$H NMR

$^{13}$C NMR
3. References
