Supporting Information

Nanoparticles based on lipidyl-β-cyclodextrins: synthesis, characterization and experimental and computational biophysical studies for encapsulation of atazanavir

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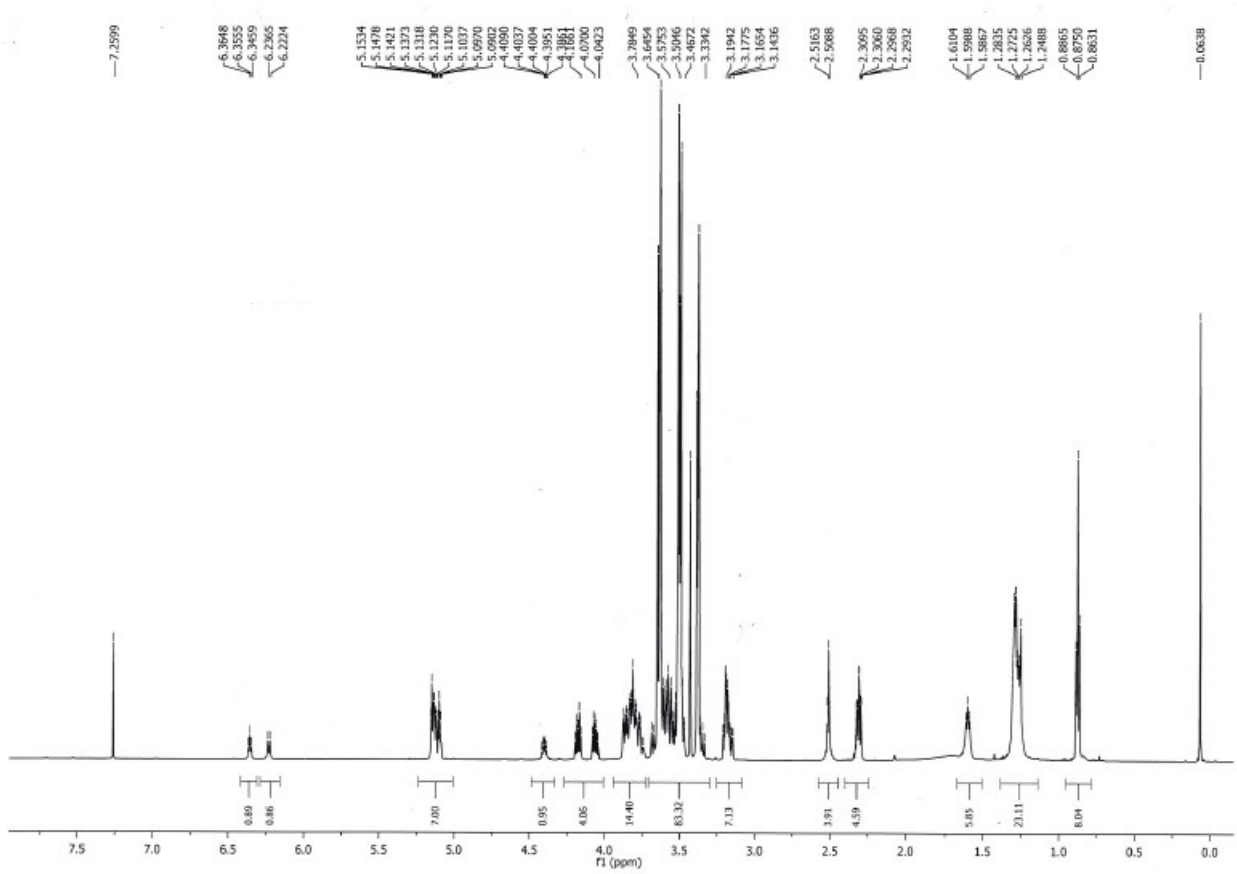


Fig S1 ^{1}H NMR of DCCD 600MHz in $CDCl_3$

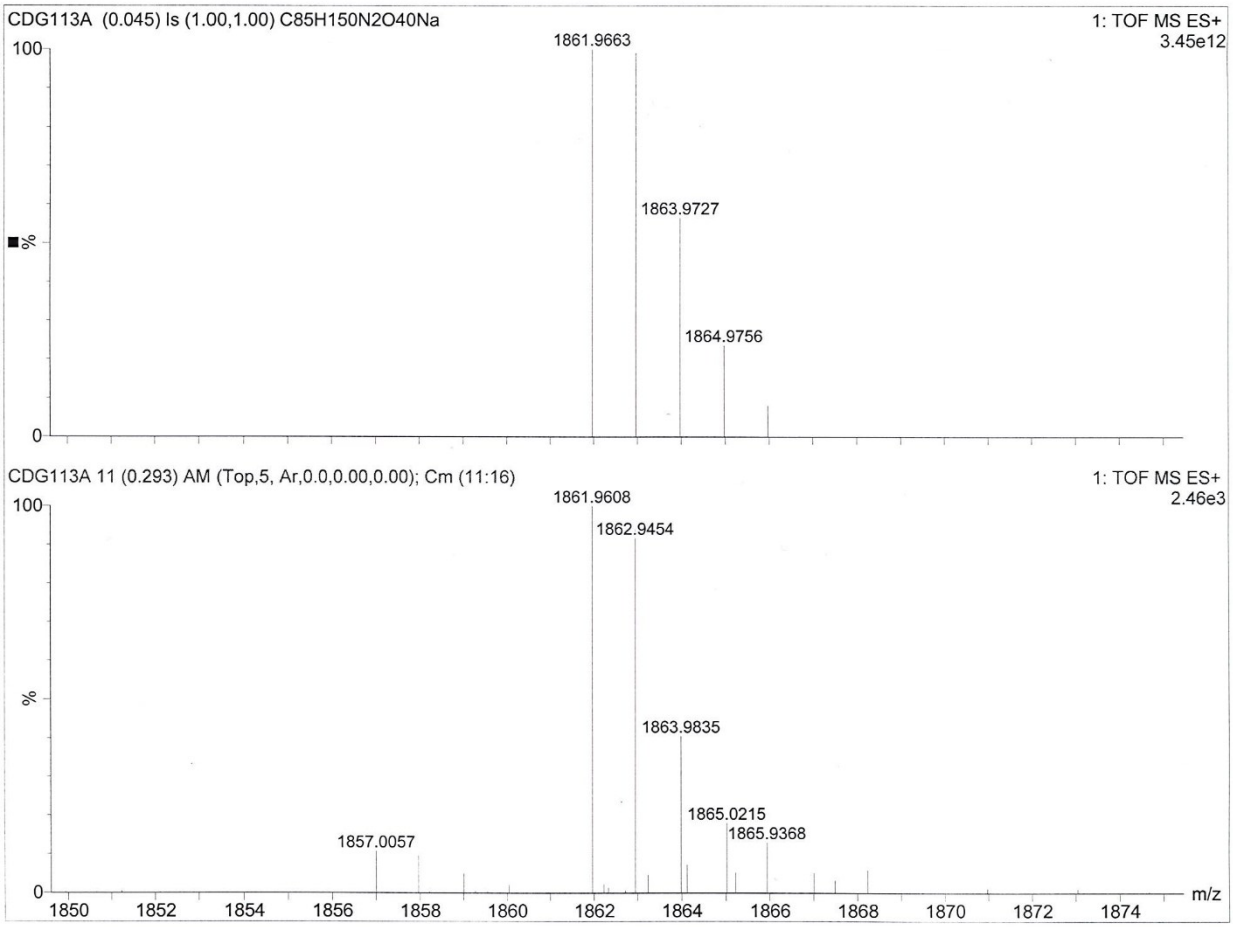


Fig S2 Isotopic pattern of $[M+Na]^+$ of DCCD

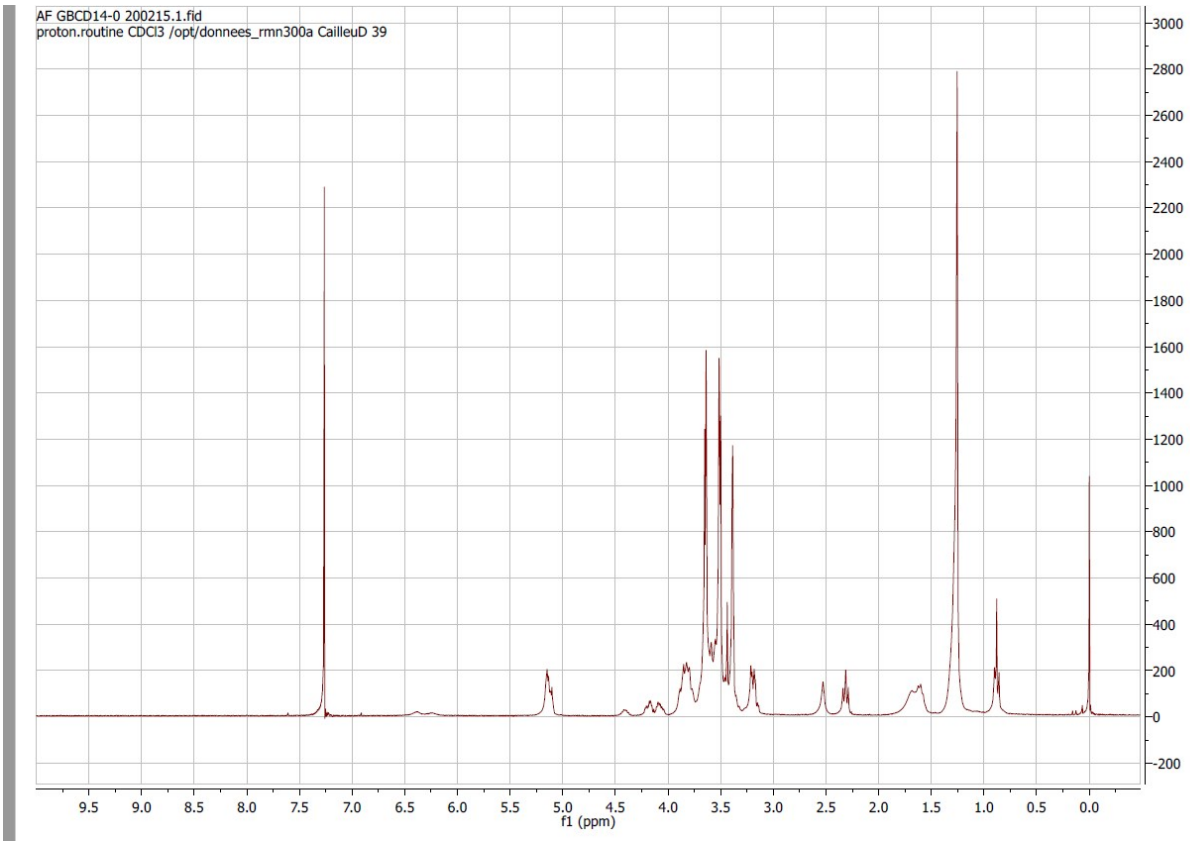


Fig S3 ^{1}H NMR of DMCD 300MHz in $CDCl_3$

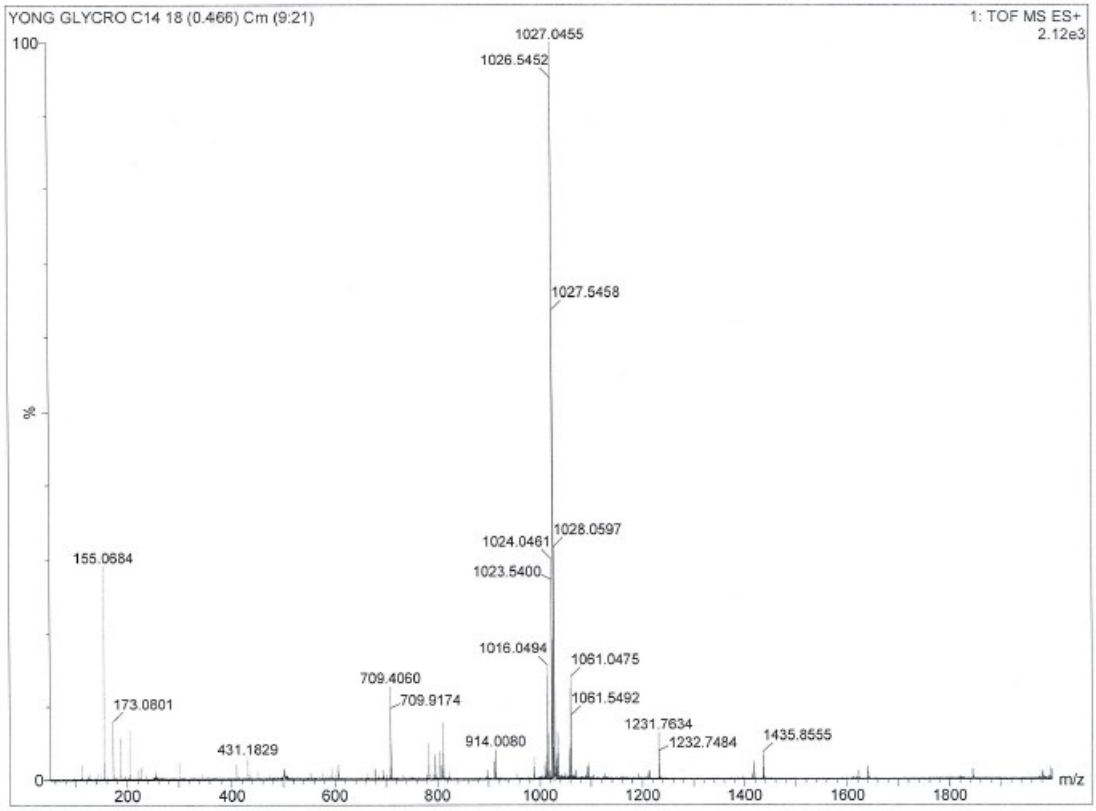


Fig S4 Mass spectra of DMCD (1027.0455 m/z of $[M+2Na]^{2+}$)

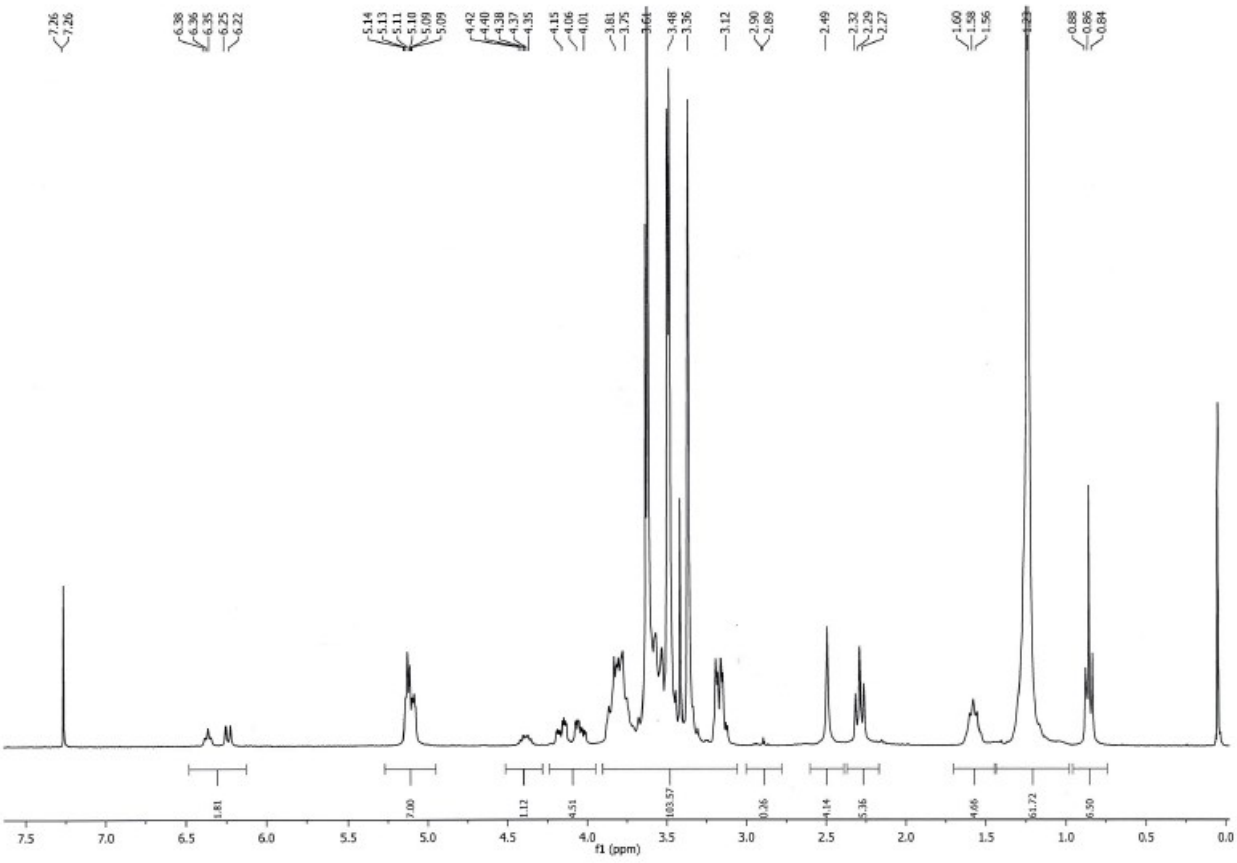
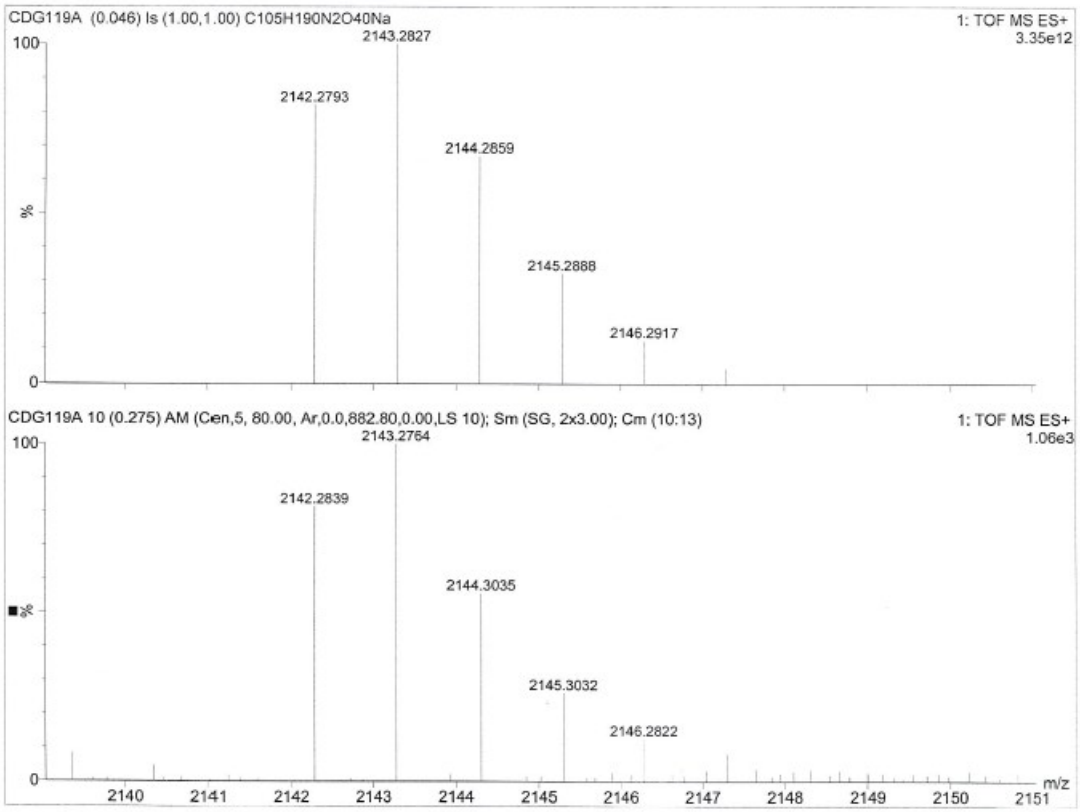


Fig S5 ^{1}H NMR of DSCD 600MHz in $CDCl_3$

a)


CDG119A (0.046) Is (1.00,1.00) C105H190N2O40Na
1: TOF MS ES+
3.35e12
100
%
0
2143.2827
2142.2793
2144.2859
2145.2888
2146.2917
CDG119A 10 (0.275) AM (Cen,5, 80.00, Ar,0.0,882.80,0.00,LS 10); Sm (SG, 2x3.00); Cm (10:13)
1: TOF MS ES+
1.06e3
100
%
0
2143.2764
2142.2839
2144.3035
2145.3032
2146.2822
2140
2141
2142
2143
2144
2145
2146
2147
2148
2149
2150
2151
m/z

b)

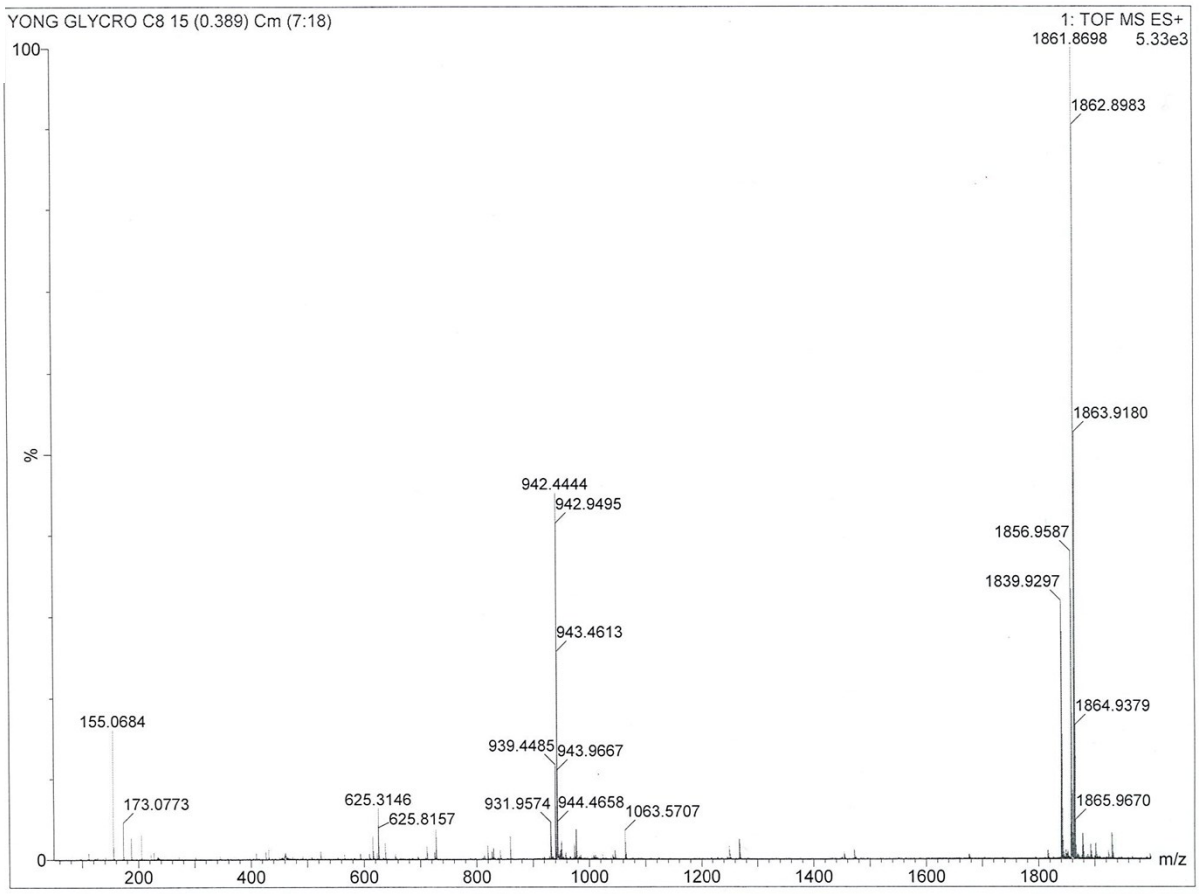


Fig S6 a) Isotopic pattern of $[M+Na]^+$ of DSCD and b) Mass spectrum of DOCD

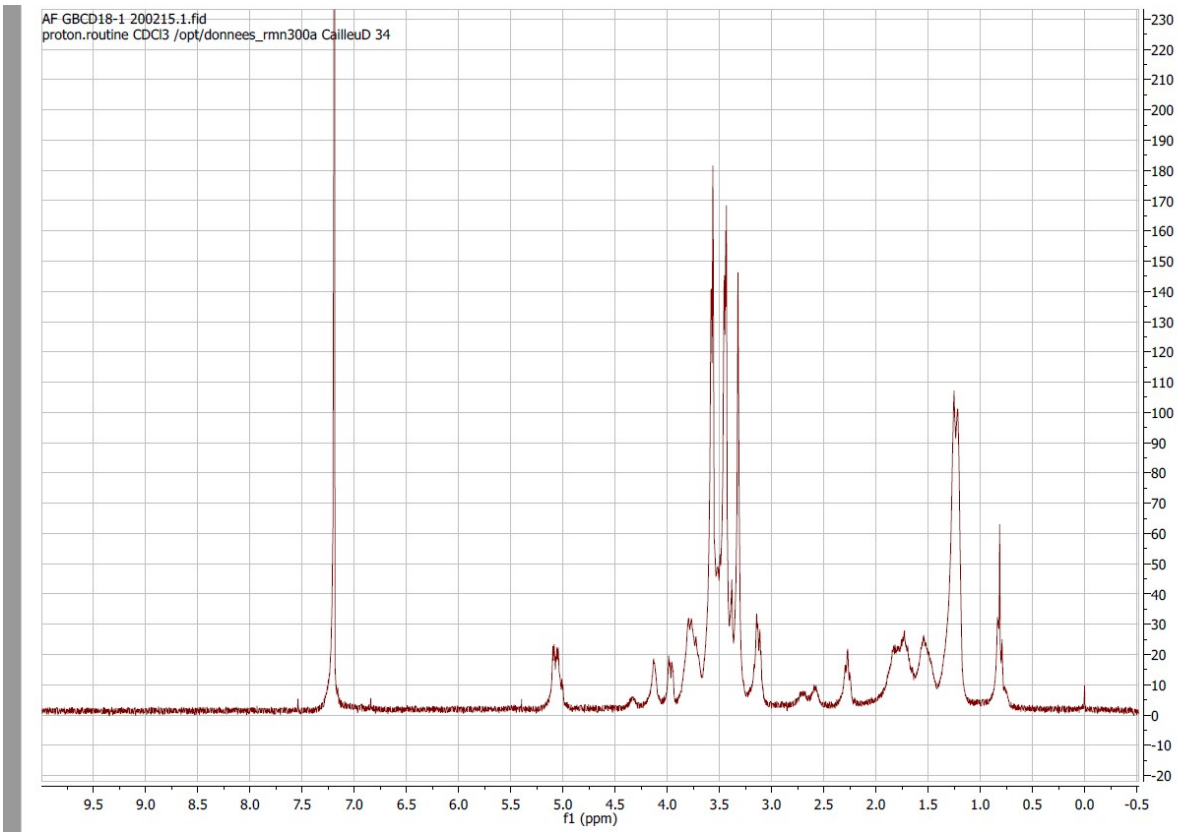


Fig S7 ^{1}H NMR of DOCD 300MHz in $CDCl_3$

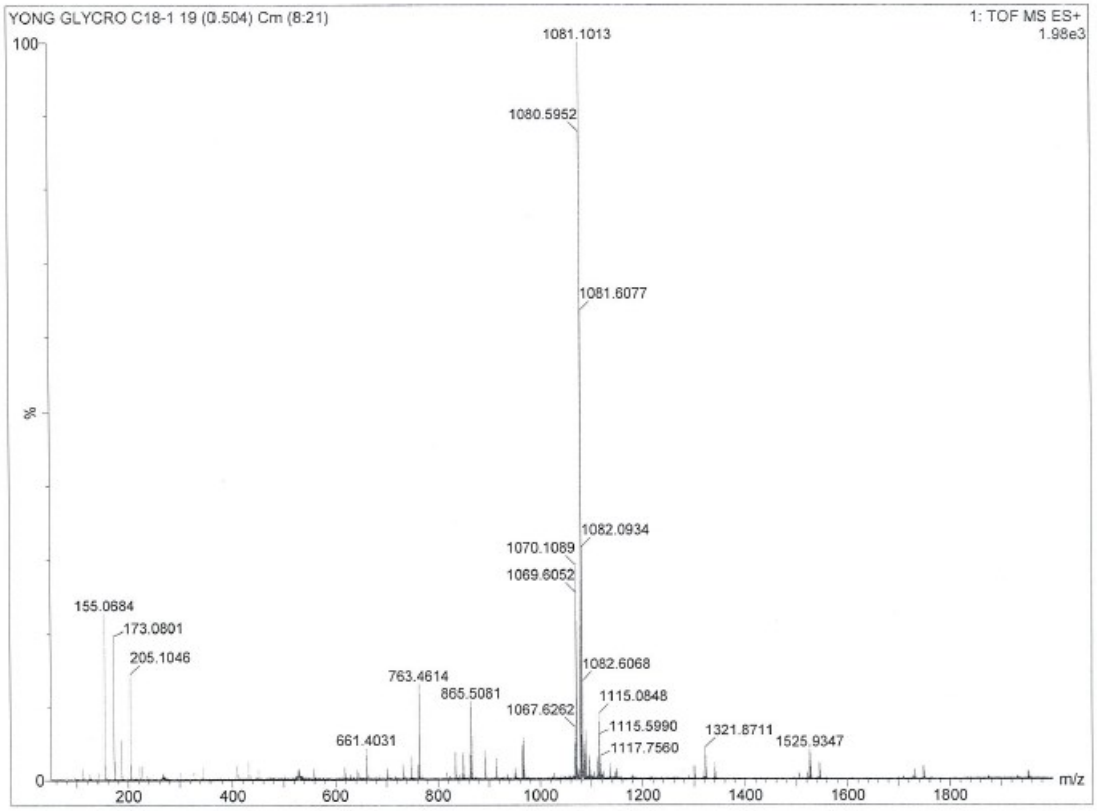


Fig S8 Mass spectrum of DOCD (1081.1013 m/z of $[M+2Na]^{2+}$)

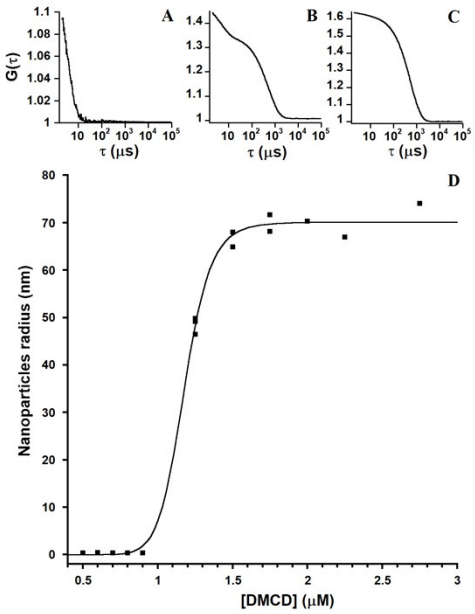


Figure S9: Autocorrelation functions of DMCD at 0.7 (A), 1.25 (B) and 2 mmol/L (C). (D) Variation of the nanoparticles radius for the same sample. These nanoparticles have been hydrated by a 5% glucose buffer solution. T = 25 °C.

Figure S10 TLC (CH_2Cl_2/MeOH 95:5) of fractions 5-13 of size exclusion chromatography of NPs prepared in pure water mixing DSCD and ATAZ. (Red: UV 254nm, Black: Vanillin/H_2SO_4 followed by heating) : fractions 6-8 = NPs containing ATAZ encapsulated, fractions 9-10: free CDs, fractions 12-13: free ATAZ.

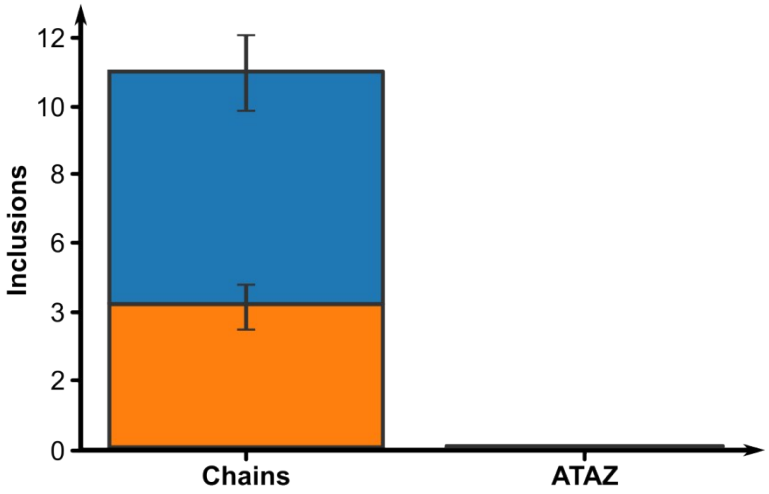


Figure S11: Average number of moieties included inside DOCD hydrophobic cavities. Left bar represents the inclusions of lipids chains from either the same DOCD (ie "self-inclusion", orange) or from other DOCD molecules (blue). Right bar represents the inclusions of ATAZ molecules. An inclusion is considered when the moiety stays at least 0.4 ns inside the hydrophobic cavity. The last 100 ns of the DOCD36/ATAZ18 simulation were used for averaging, allowing computation of standard deviations (represented by error bars). As no ATAZ inclusion was observed, the corresponding standard deviation is 0 (hence no visible error bar).