Cyclodextrin Modified with Different Groups to Enhance the Drug Delivery Efficiency of Gold Nanoparticles to Treat Cancer

Cao-Hien Nguyen[1,2†], Kien-Sam Banh[3†], Tran Nguyen Minh An[4], Nguyen Thi Hong Anh[1], Chi-Hien Dang[2,3]*, Van-Dat Doan[4], Tran Thi Kim Chi[5], Hieu Vu-Quang[6], and Thanh-Danh Nguyen[2,3]*

[1]Department of Chemical Technology, Ho Chi Minh City University of Food Industry, 140 Le Trong Tan, Tan Phu District, Ho Chi Minh 72000, Viet Nam

[2]Graduate University of Science and Technology, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Cau Giay, Hanoi 11000, Viet Nam

[3]Institute of Chemical Technology, Vietnam Academy of Science and Technology, 1A, TL 29 Thanh Loc Ward, District 12, Ho Chi Minh City 700000, Viet Nam

[4]Faculty of Chemical Engineering, Industrial University of Ho Chi Minh City, Ho Chi Minh City 71420, Vietnam

[5]Institute of Materials Science, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Cau Giay District, Hanoi 11000, Vietnam.

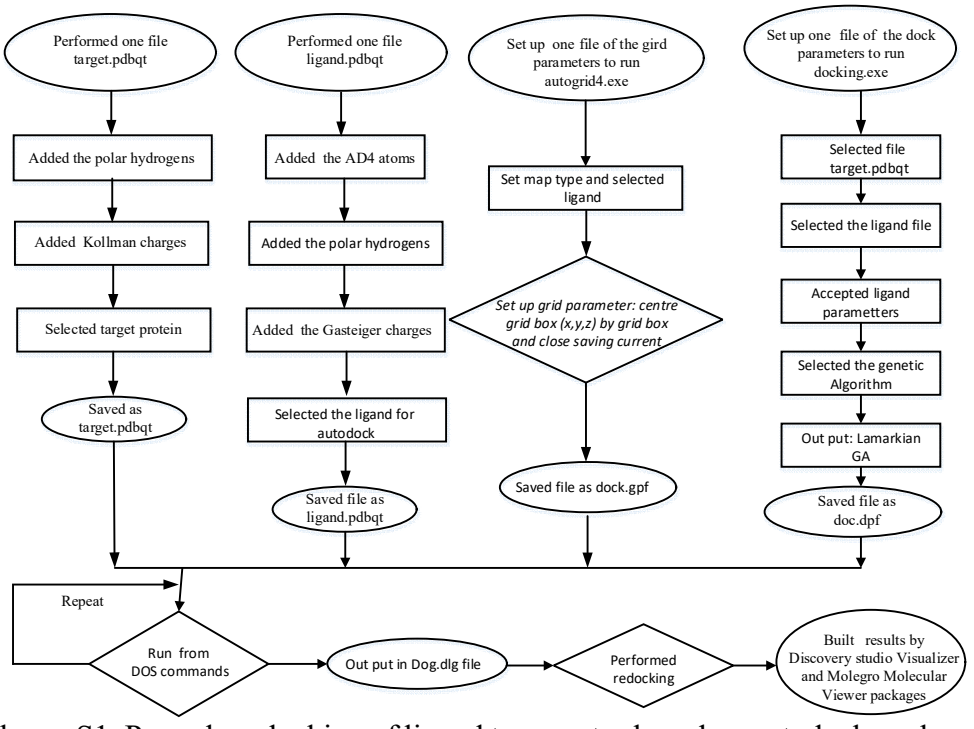
[6]NTT Hi-Tech Institute, Nguyen Tat Thanh University, Ho Chi Minh City 700000, Vietnam.

***Corresponding author:** dangchihien@gmail.com (C.H. Dang), ntdanh@ict.vast.vn (T.D. Nguyen)

Keywords: breast anticancer; modified β-cyclodextrin; gold nanoparticles; 5-fluorouracil; drug delivery, molecular docking model.

†These authors contributed equally to this study.

Supporting Information



Scheme S1. Procedure docking of ligand to receptor based on autodock package and built model by DSC software.

Table S1. Profile of thermal behavior and percent of mass loss for drug, the blank composites and the drug loaded nanocomposites.

Samples	**Variables***	**Stages**		
		First	Second	Third
5-FU	T_d (ºC)/m_{loss} (%)	273-318/98.5	-	
AuNPs/CD	T_d (ºC)/m_{loss} (%)	30-100/2.6	100-530/73.8	530-790/4.3
AuNPs/HPCD	T_d (ºC)/m_{loss} (%)	258-540/78.6	-	-
AuNPs/TMACD	T_d (ºC)/m_{loss} (%)	30-100/2.7	100-530/65.5	398-790/5.1
5-FU@AuNPs/CD	T_d (ºC)/m_{loss} (%)	30-100/7.4	100-530/77.4	530-790/4.1
5-FU@AuNPs/HPCD	T_d (ºC)/m_{loss} (%)	30-100/2.3	100-530/75.1	530-790/14.1
5-FU@AuNPs/TMACD	T_d(ºC)/m_{loss} (%)	30-100/2.7	100-530/52.7	500-790/6.7

*T_d is decomposition temperature collected and m_{loss} is overall mass loss

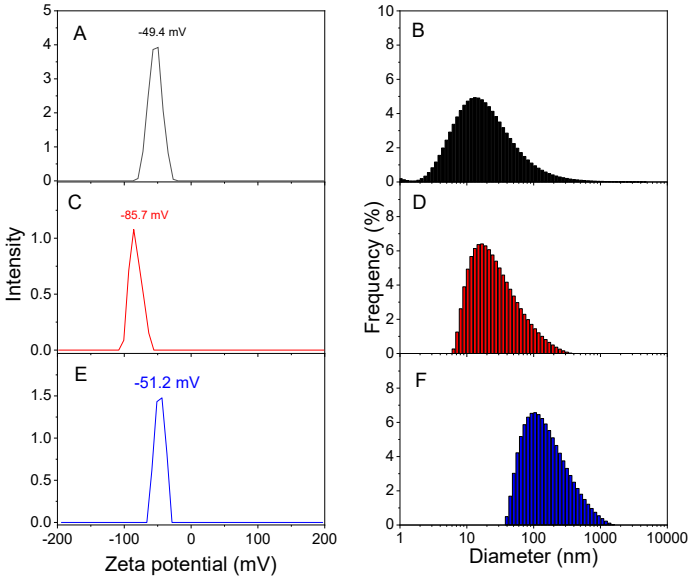


Figure S1. Zeta potential (left) and DLS (right) spectra of AuNPs@CD (A and B), AuNPs@HPCD (C and D), AuNPs@TMACD (E and F).

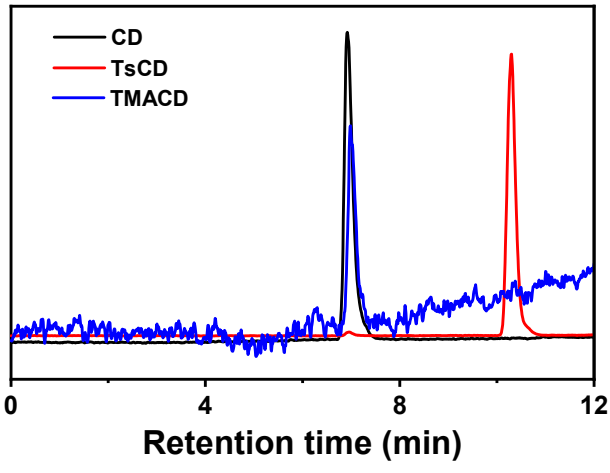


Figure S2. HPLC spectra of β-CD (RT = 6.920, purity = 99.9%) and synthesized TsCD (RT = 10.2970, purity = 99%) and TMACD (RT = 6.983, purity = 99.9%).

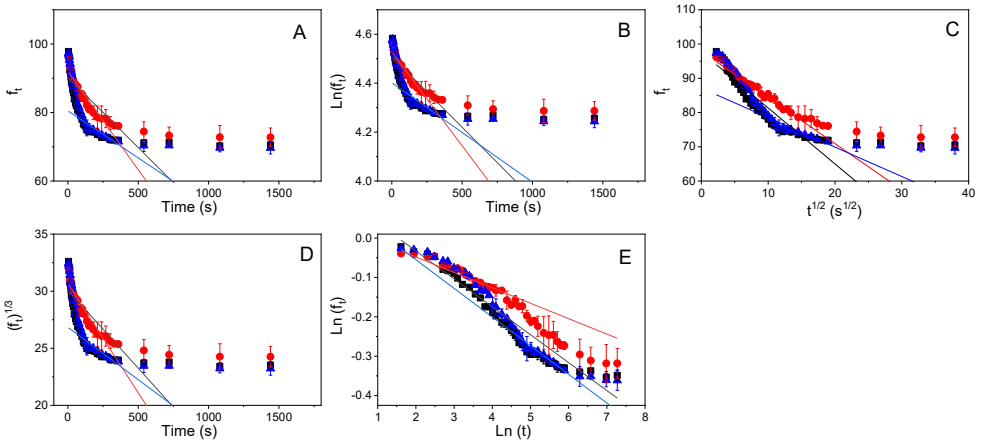


Figure S3. The fitting of kinetic data to various models: (A) zero order; (B) first order; (C) Higuchi, (D) Hixson-Crowell and (E) Korsmeyer-Peppas.

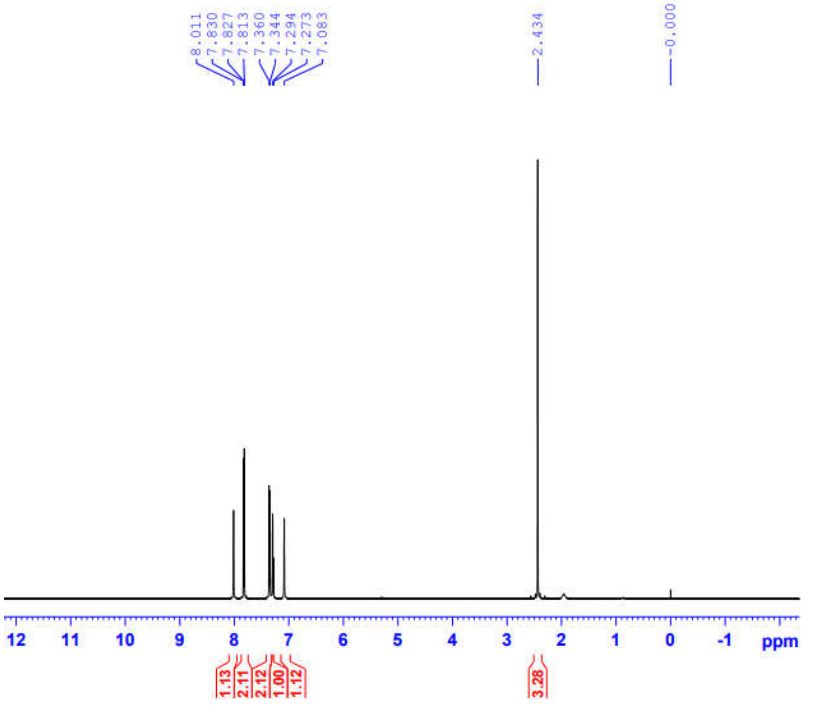


Figure S4. ^{1}H NMR spectrum of TsIm ($CDCl_3$, 500 MHz)

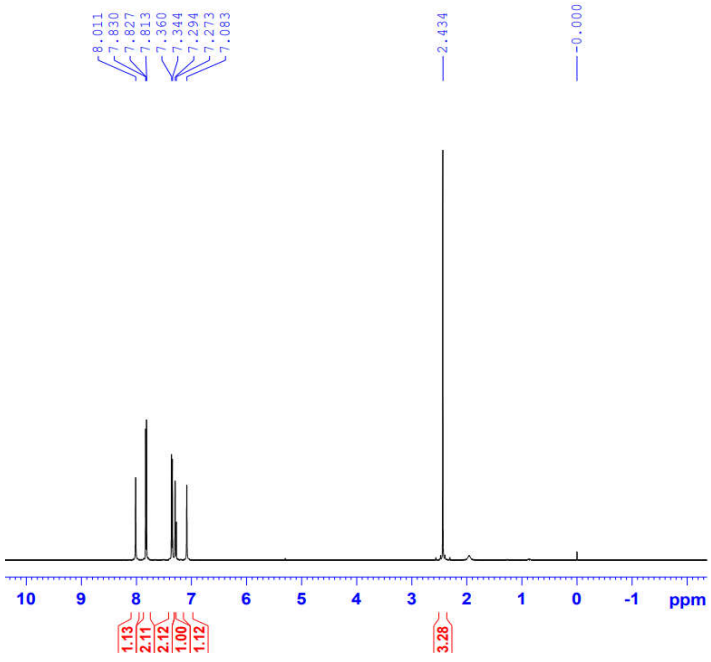


Figure S5. ^{13}C NMR spectrum of TsIm ($CDCl_3$, 125 MHz)

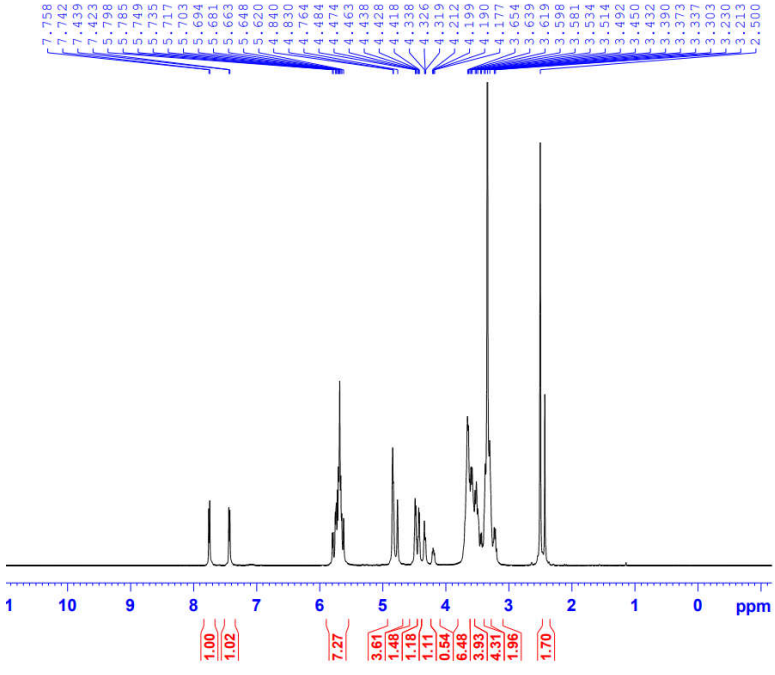


Figure S6. ^{1}H NMR spectrum of TsCD (DMSO, 500 MHz)

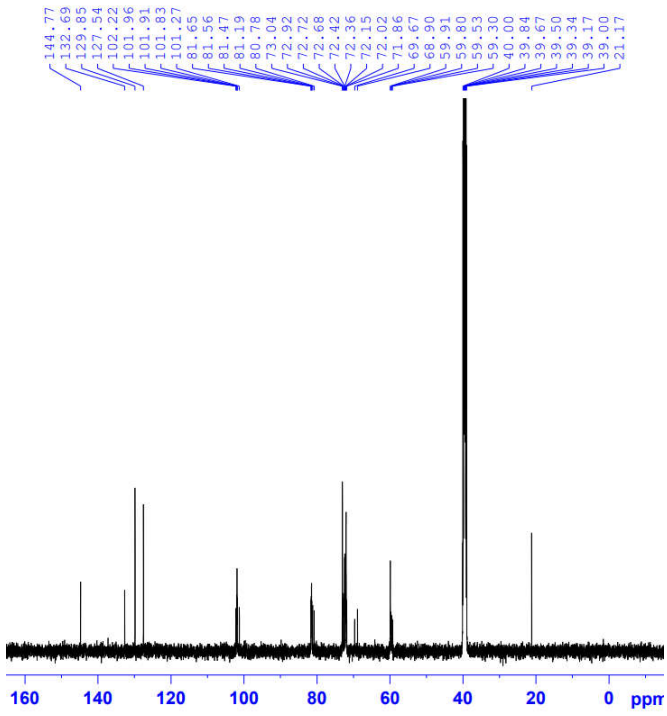


Figure S7. ^{13}C NMR spectrum of TsCD (DMSO, 125 MHz)

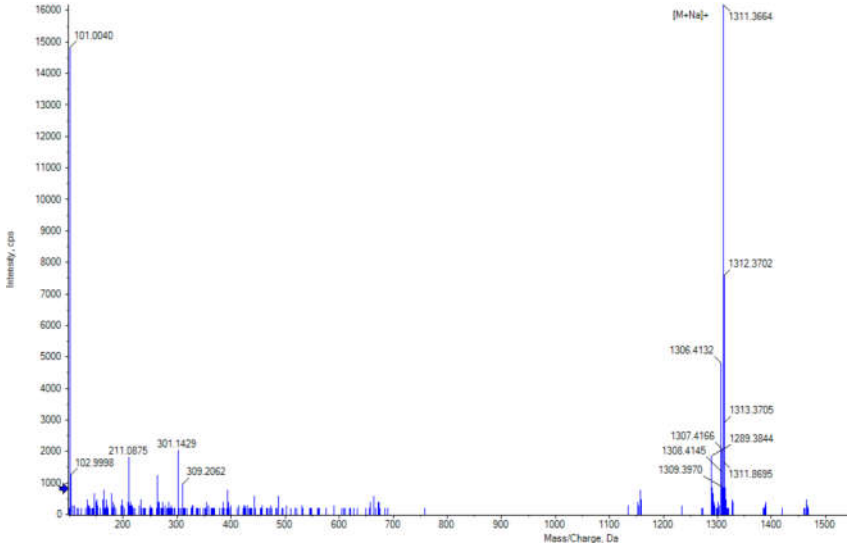


Figure S8. QTOF-MS spectrum of TsCD

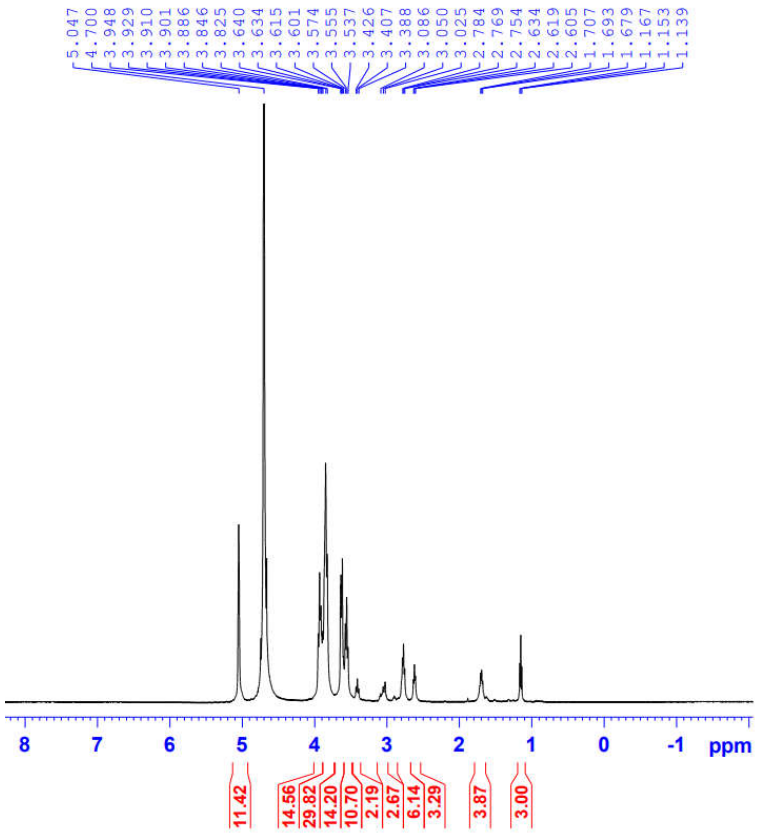


Figure S9. ^{1}H NMR spectrum of TMACD (D_2O, 500 MHz).

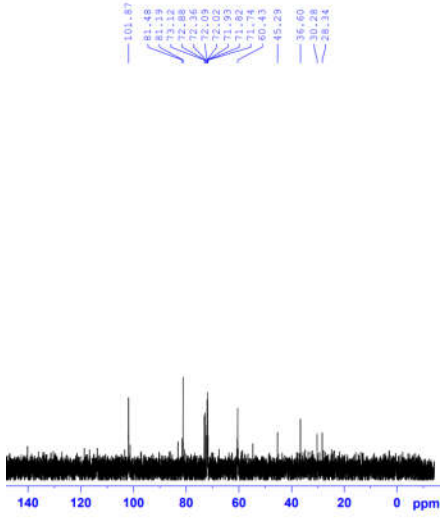


Figure S10. ^{13}C NMR spectrum of TMACD (D_2O, 125 MHz)

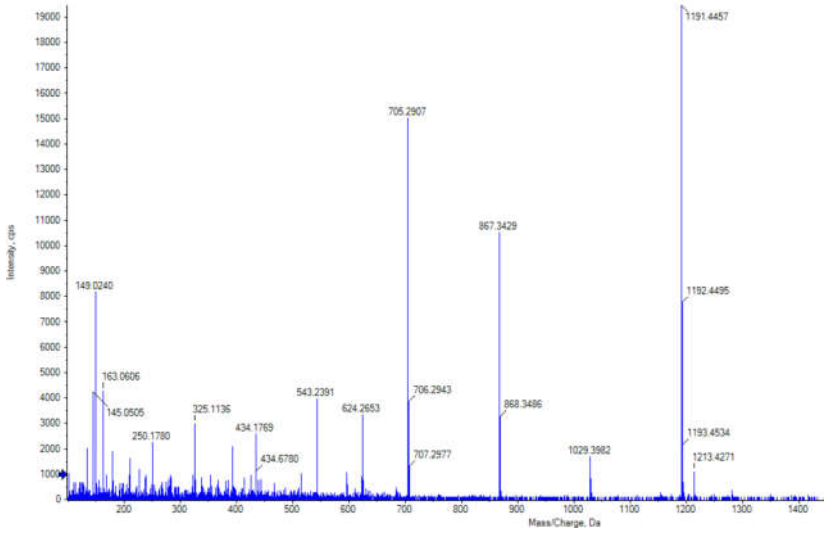


Figure S11. QTOF-MS spectrum of TMACD