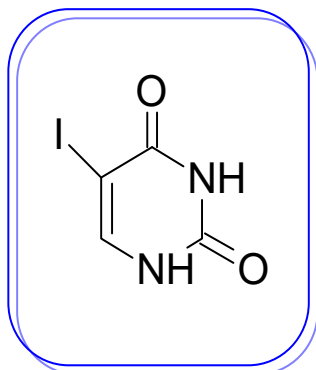


Supporting Information for A green chemistry approach for iodination of pyrimidine derivatives by mechanical grinding under solvent-free conditions

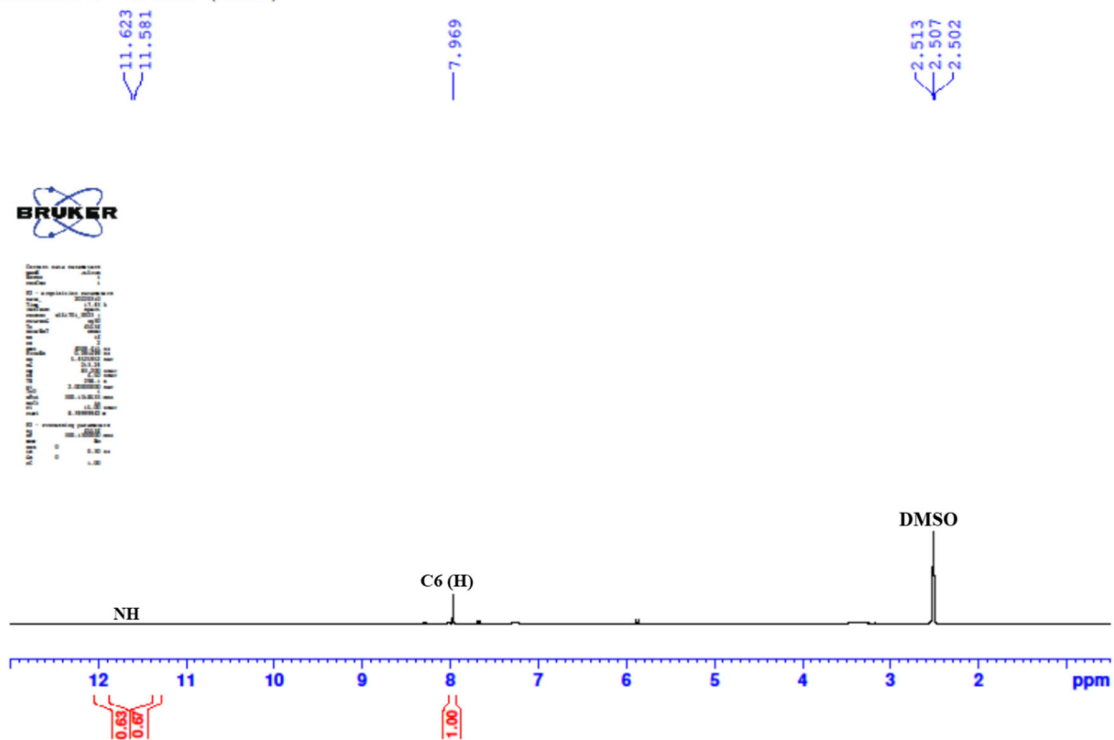
Thananjeyan Balasubramaniam^{1,§}, Byeong-Seon Kim^{2,§}, Badvel Pallavi², Ho-seong Jin¹, Sung Kuk Kim^{1,*} and Joon-Hwa Lee^{1,*}

(A)

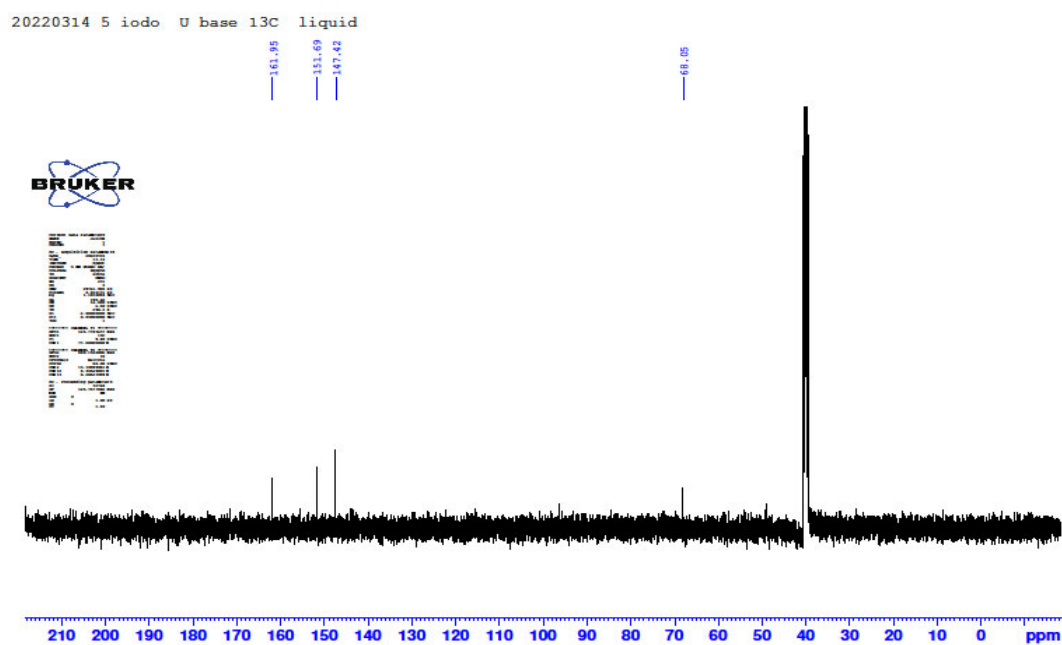


(B)

20220310 5- C BASE (SOLID)



(C)



(D)

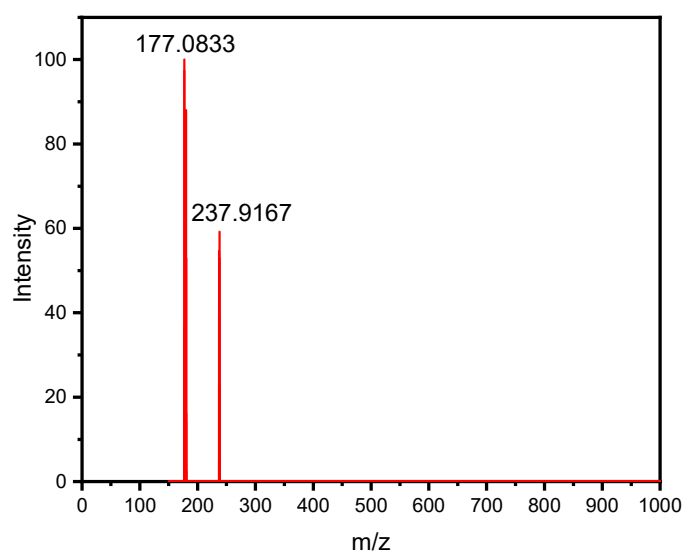
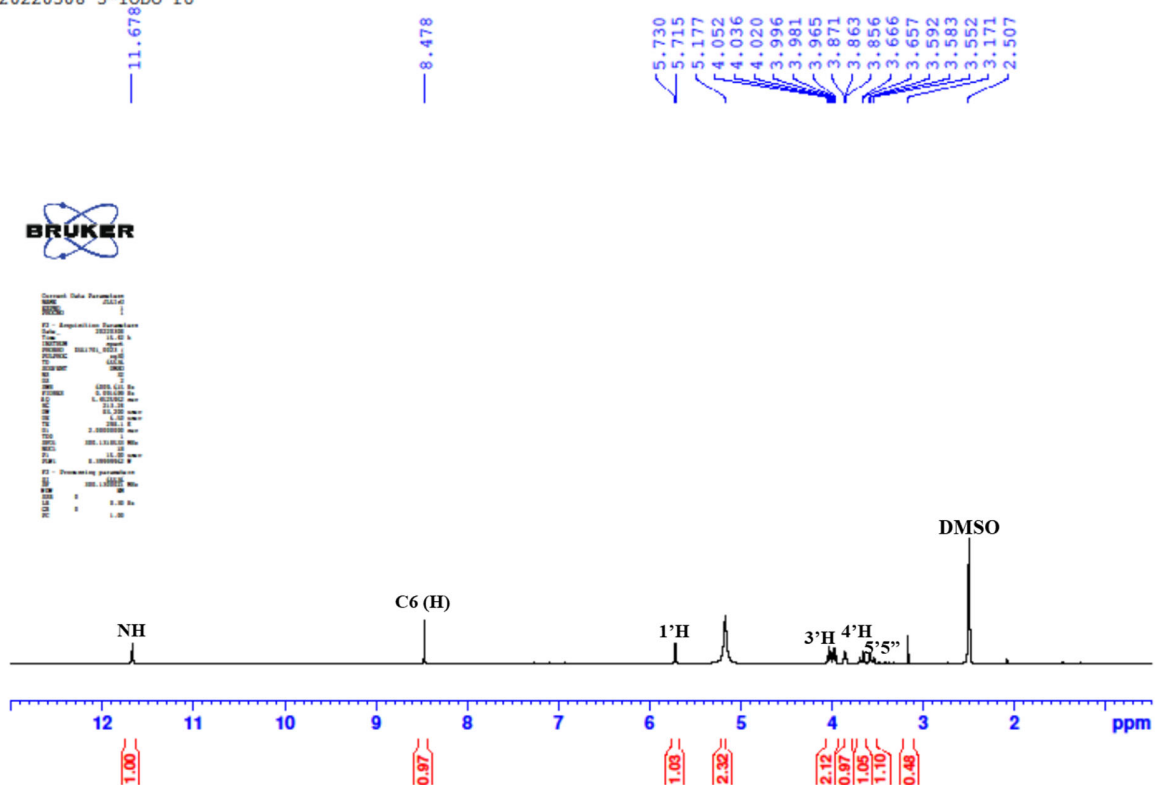


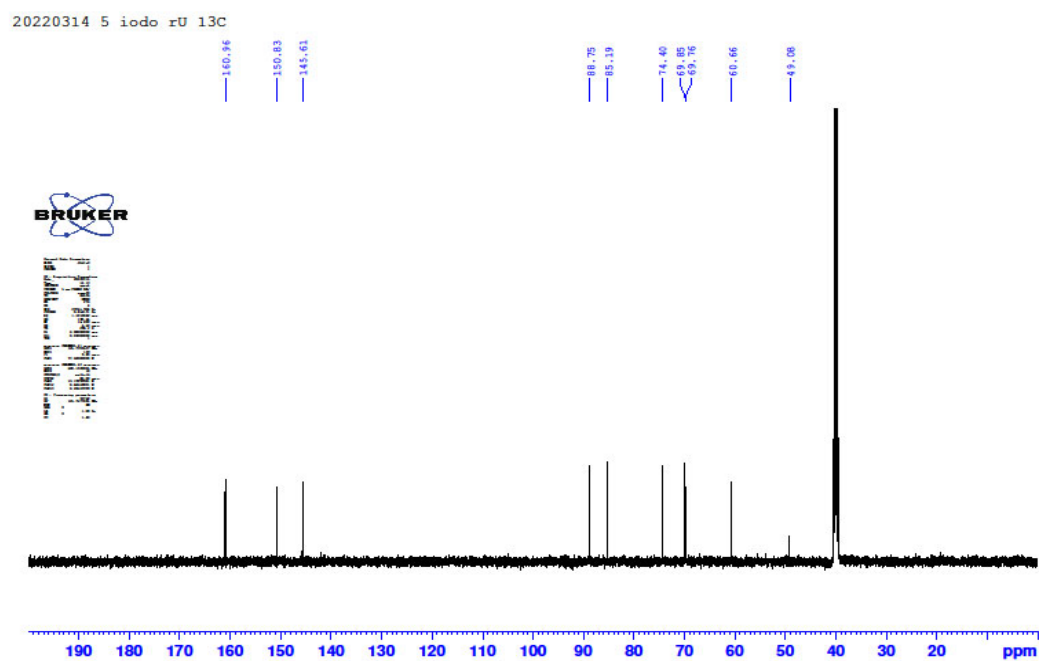
Figure S1. (A) Chemical structure and (B) ¹H NMR, (C) ¹³C NMR, and (D) ESI-Mass spectra of 5-iodo-uracil (5I-U).

O=C1NC(=O)C(I)=CN1[C@H]2O[C@H](CO)[C@@H](O)[C@H]2O

20220308 5-IDO rU



(C)



(D)

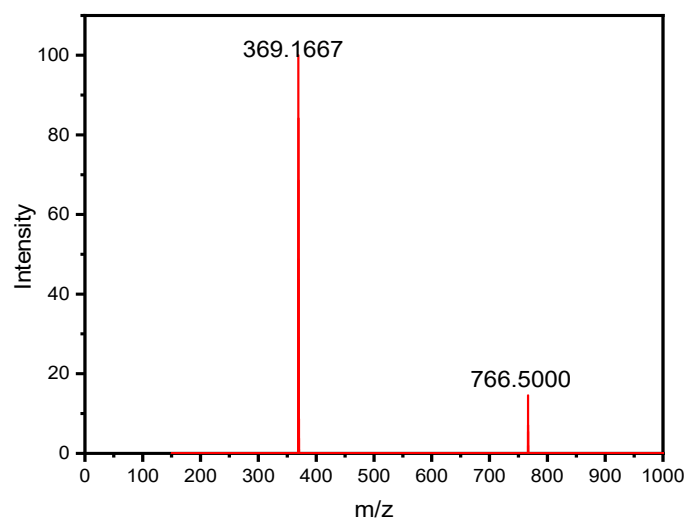
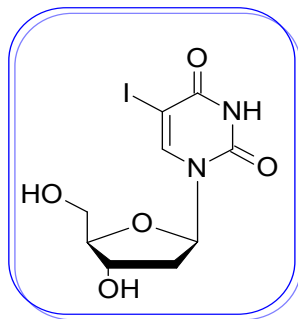


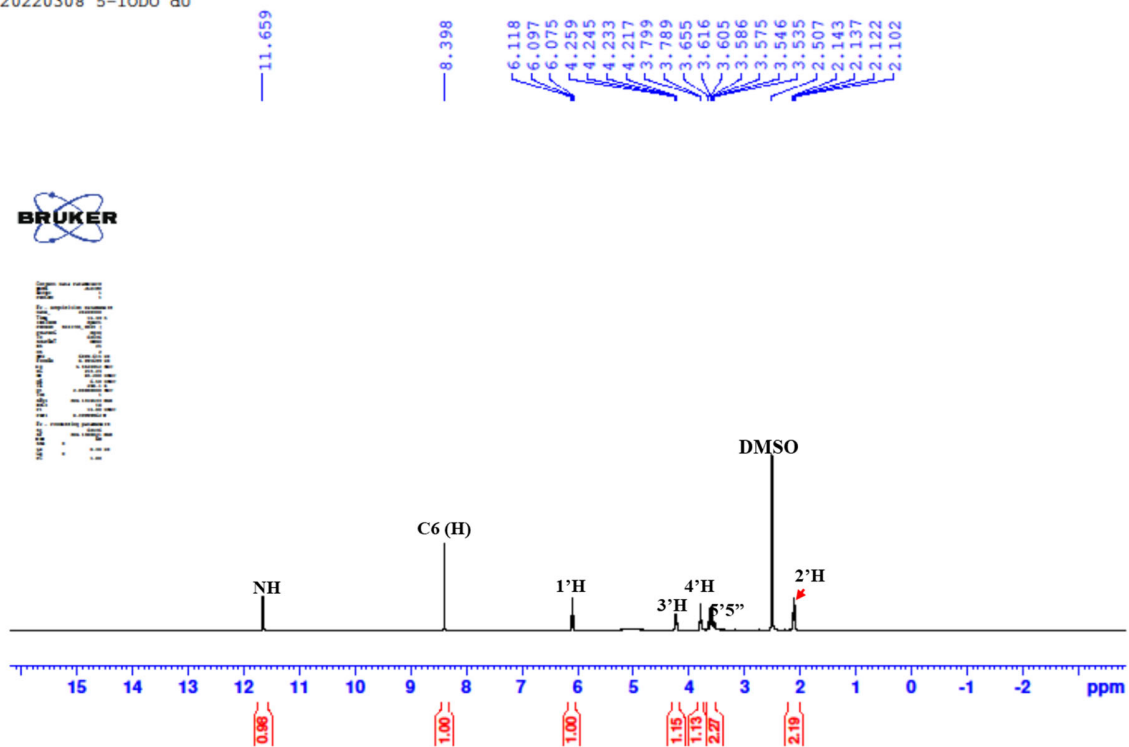
Figure S2. (A) Chemical structure and (B) ^1H NMR, (C) ^{13}C NMR, and (D) ESI-Mass spectra of 5-iodo-uridine (5I-rU).

(A)

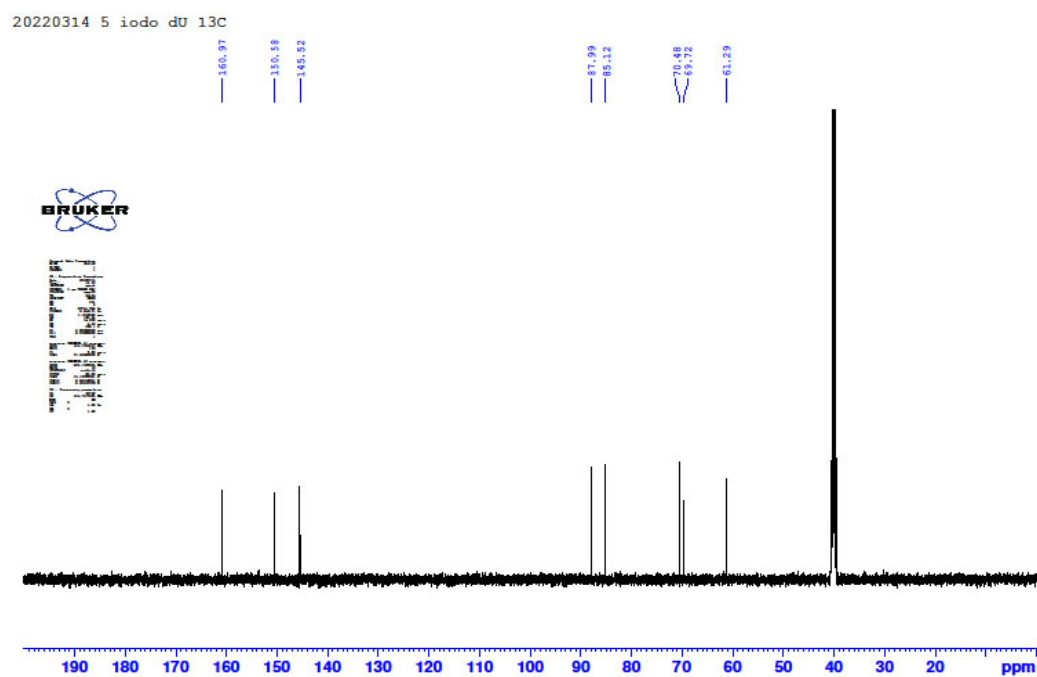


(B)

20220308 5-IODO du



(C)



(D)

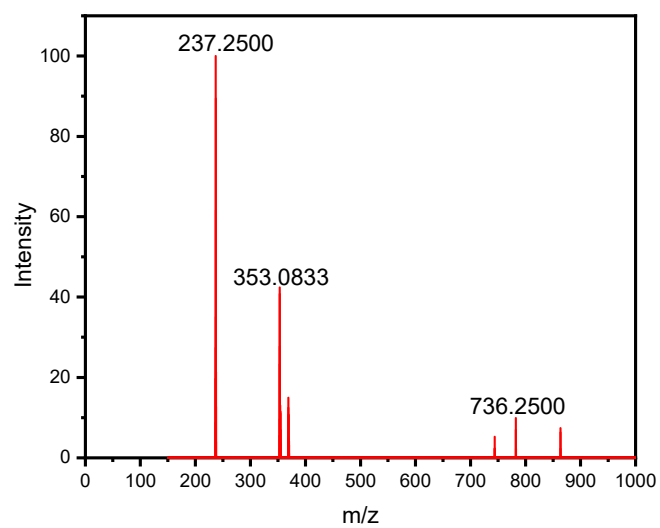
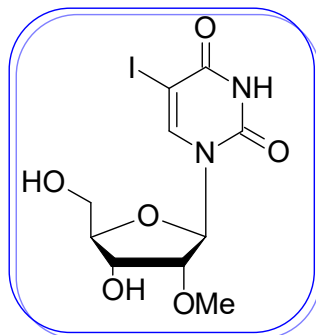
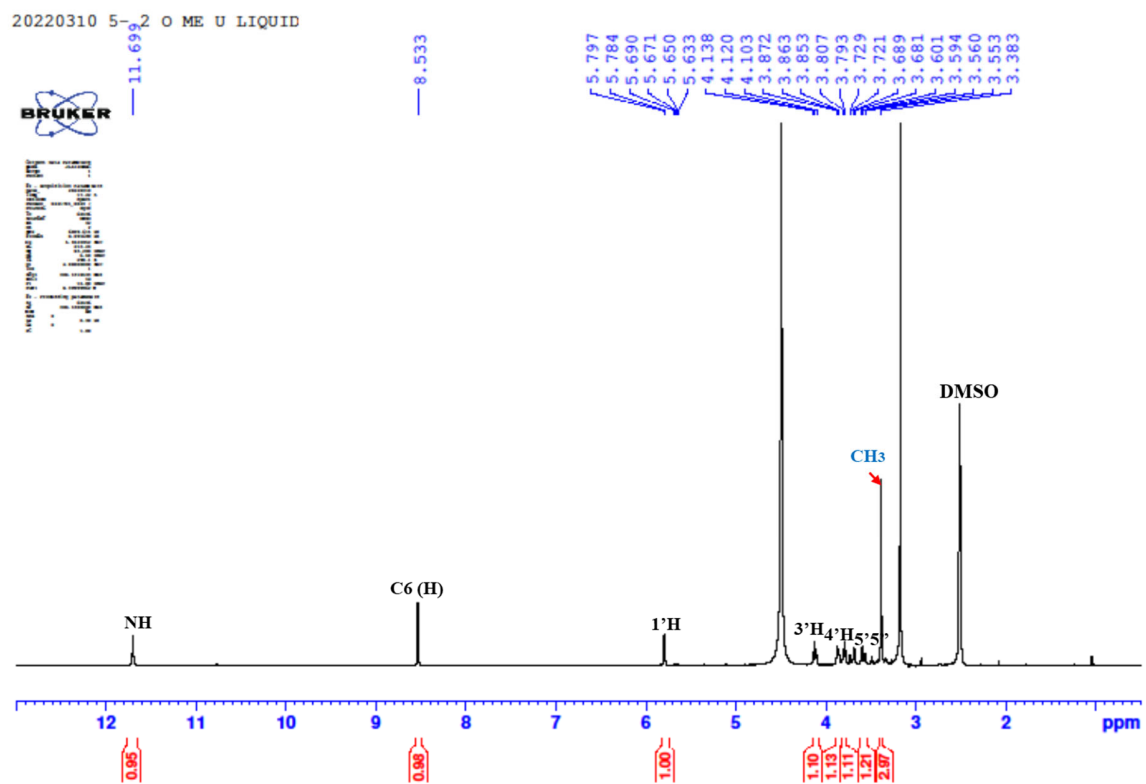


Figure S3. (A) Chemical structure and (B) ^1H NMR, (C) ^{13}C NMR, and (D) ESI-Mass spectra of 5-iodo-2'-deoxyuridine (5I-dU).

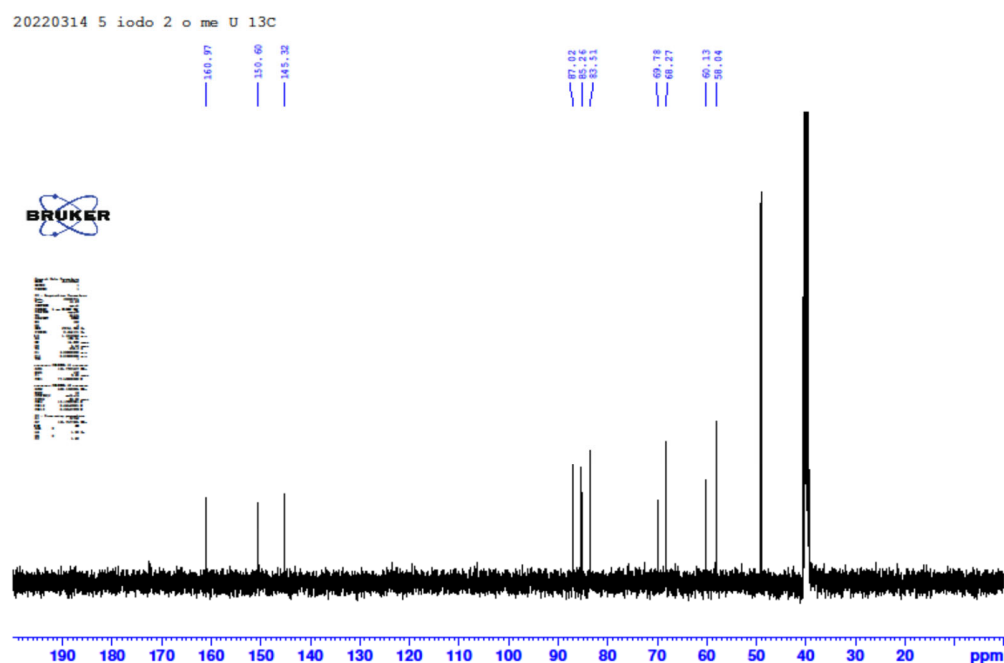
(A)



(B)



(C)



(D)

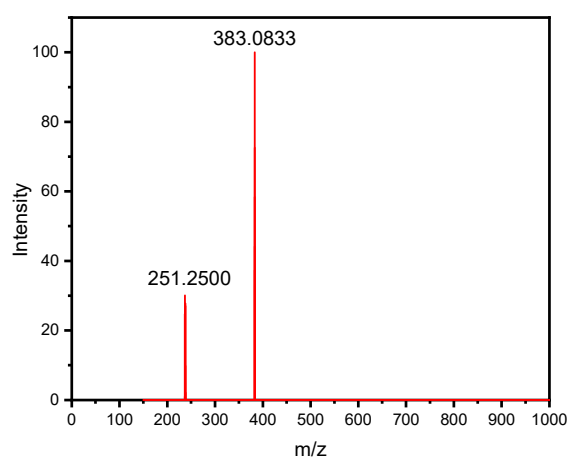
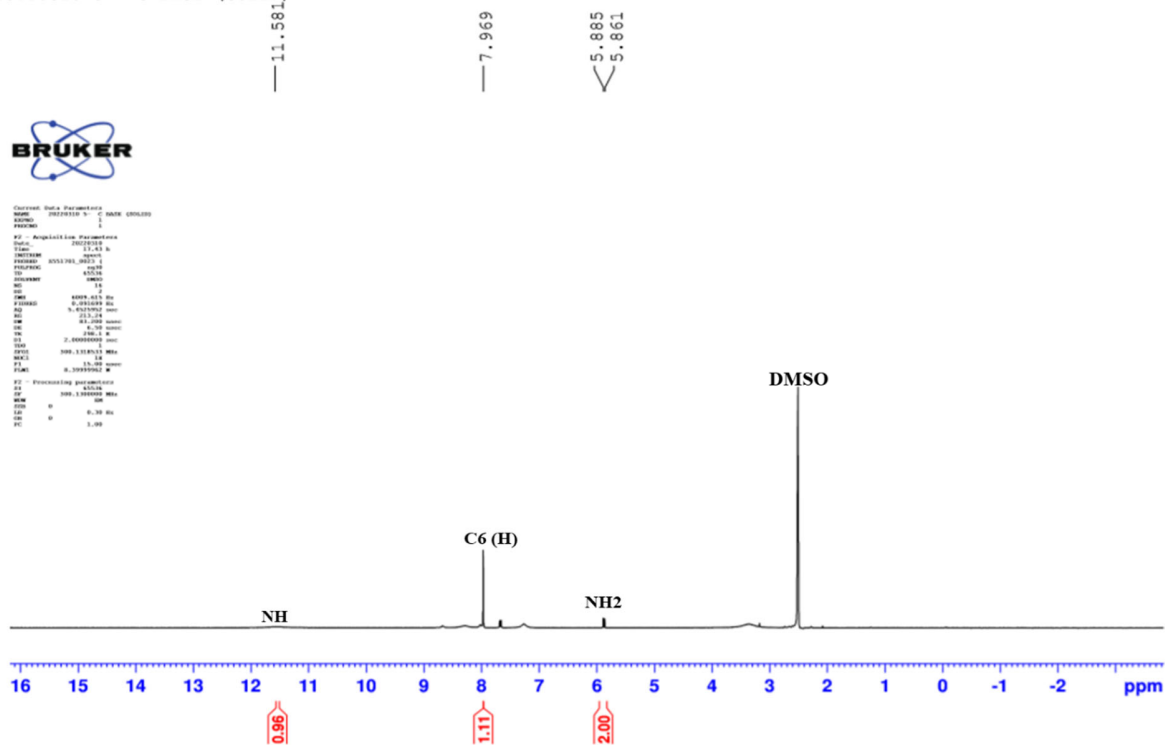


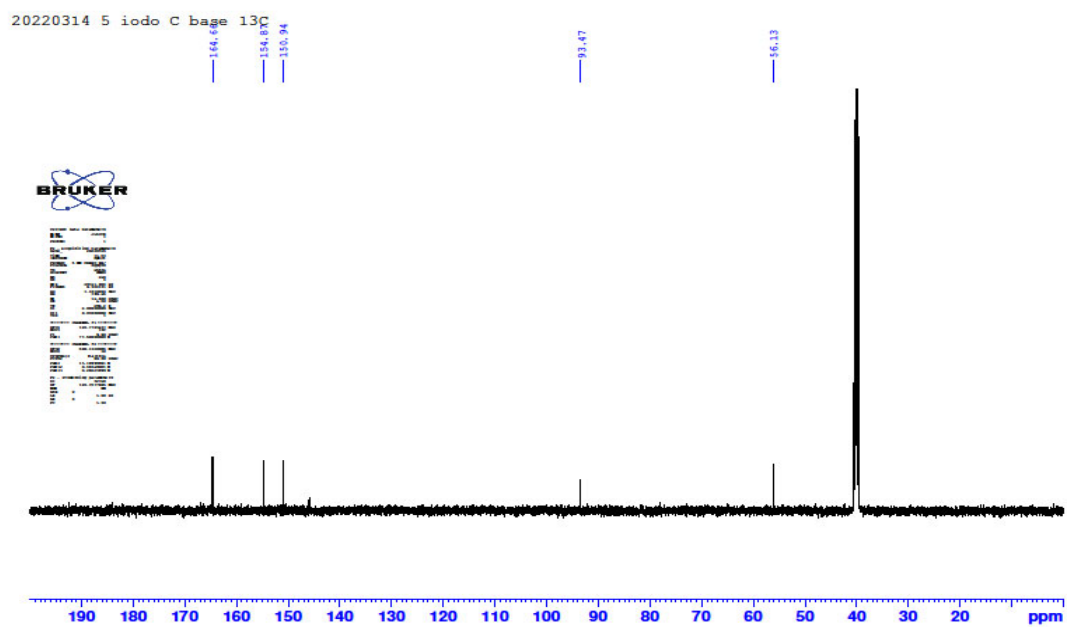
Figure S4. (A) Chemical structure and (B) ^1H NMR, (C) ^{13}C NMR, and (D) ESI-Mass spectra of 5-iodo-2'-OMe-uridine (5I-mU).

NC1=NC(=O)C=CI

20220310 5- C BASE (SOLID)



(C)



(D)

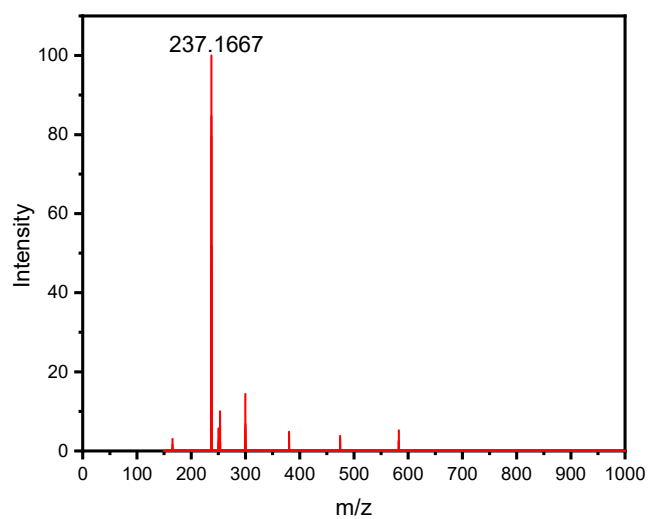
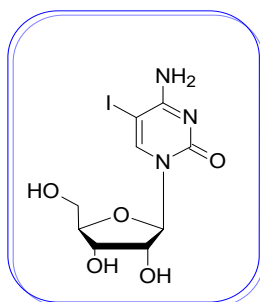


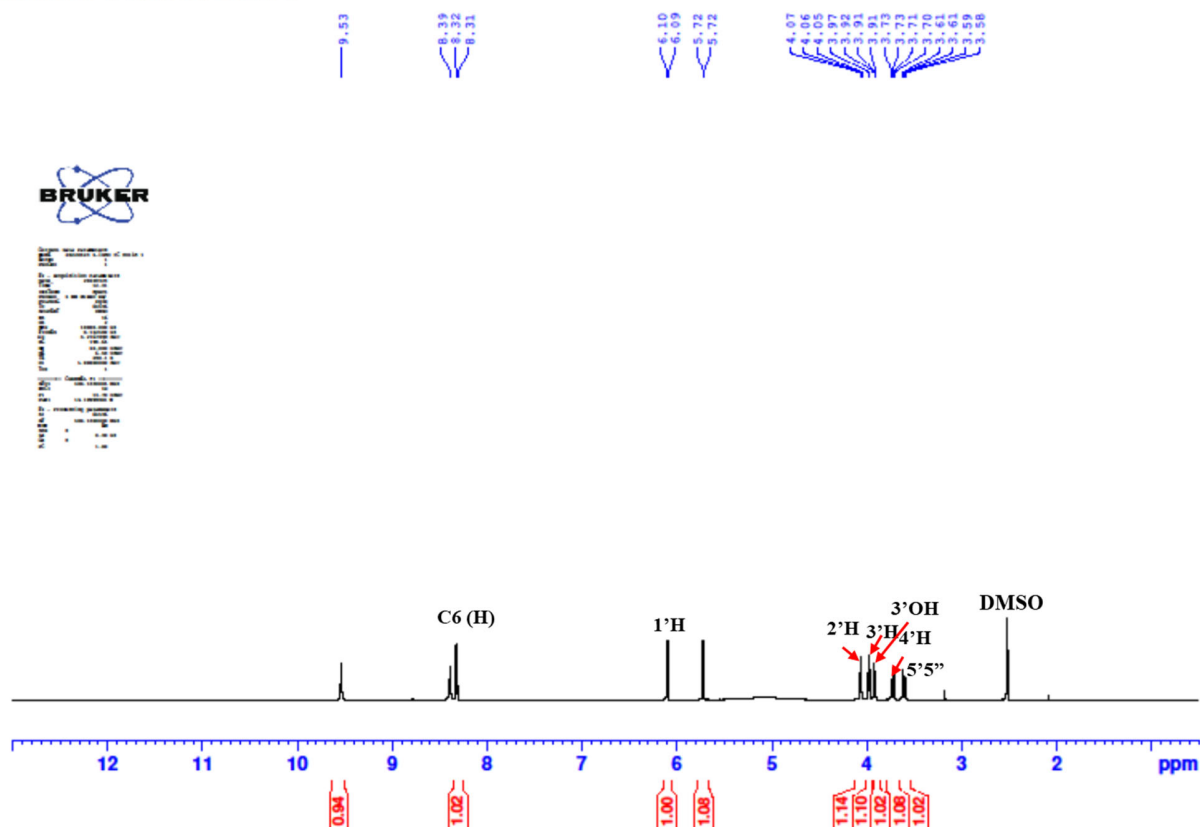
Figure S5. (A) Chemical structure and (B) ^1H NMR, (C) ^{13}C NMR, and (D) ESI-Mass spectra of 5-iodo-cytosine (5I-C).

(A)

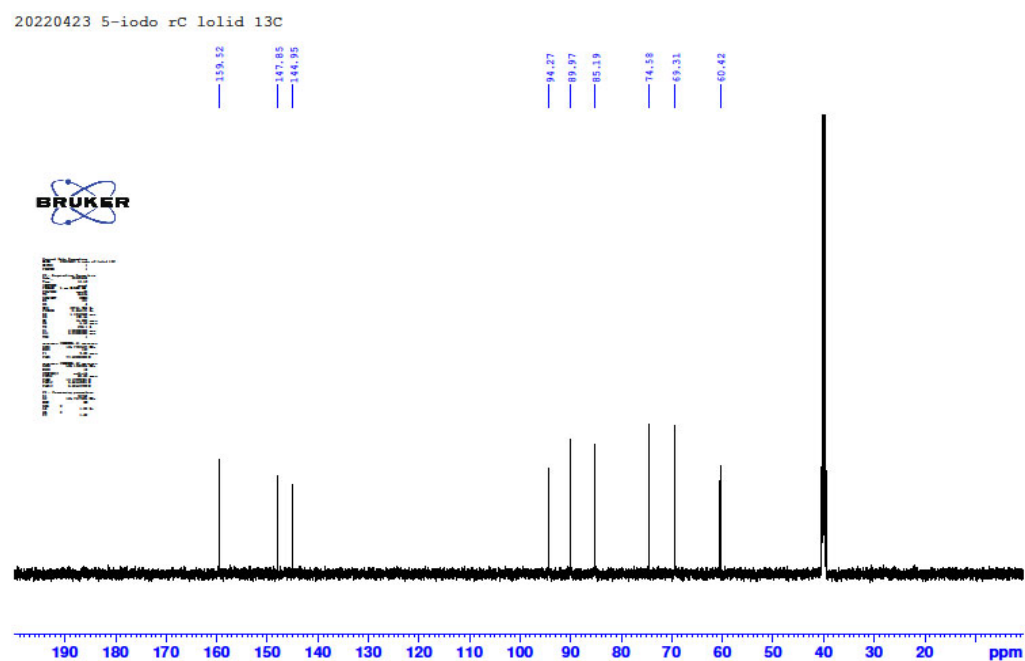


(B)

20220423 5-iodo rC solid 1



(C)



(D)

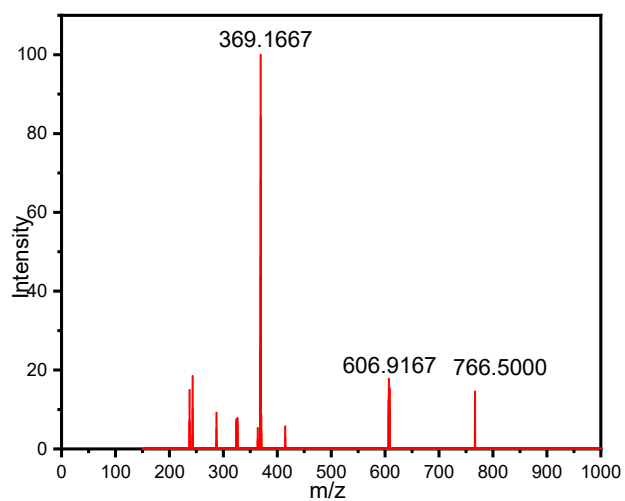
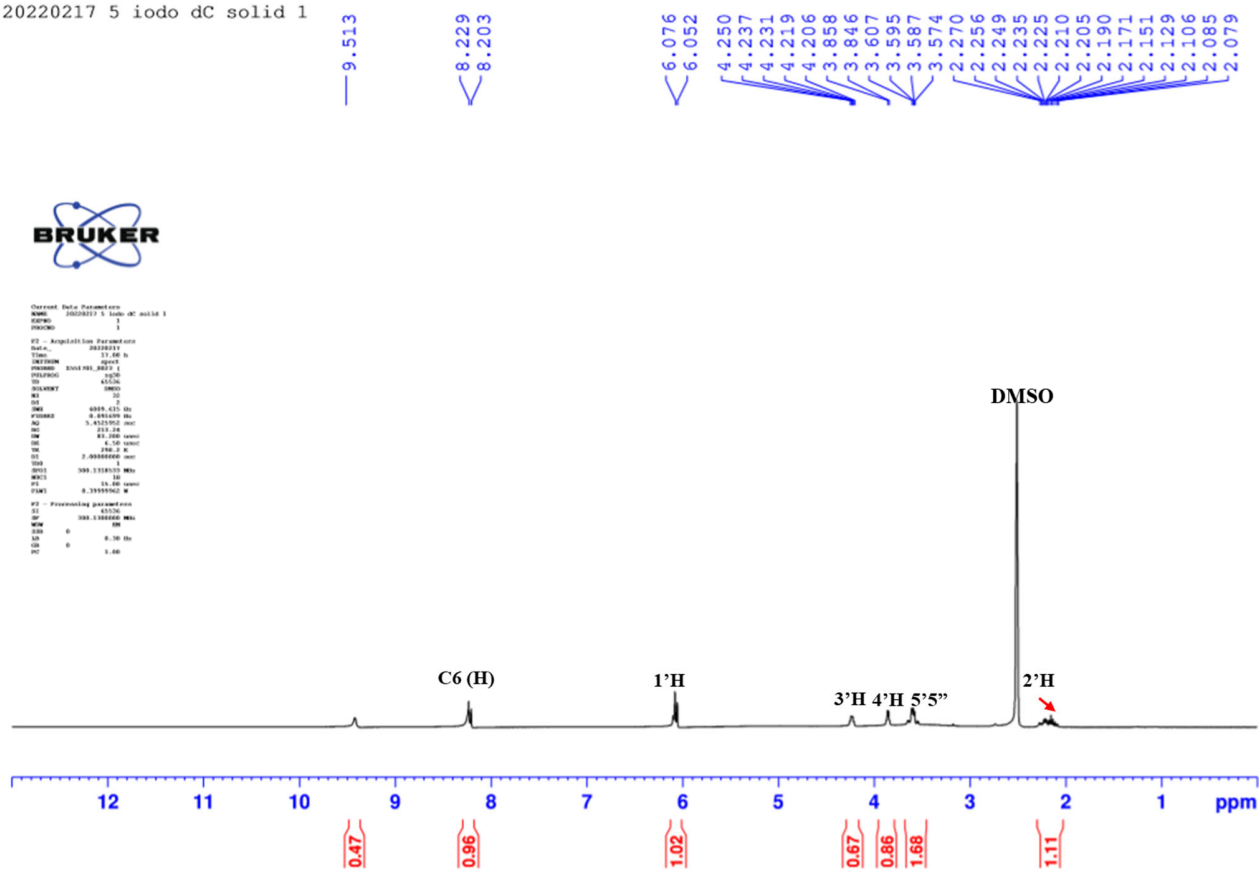


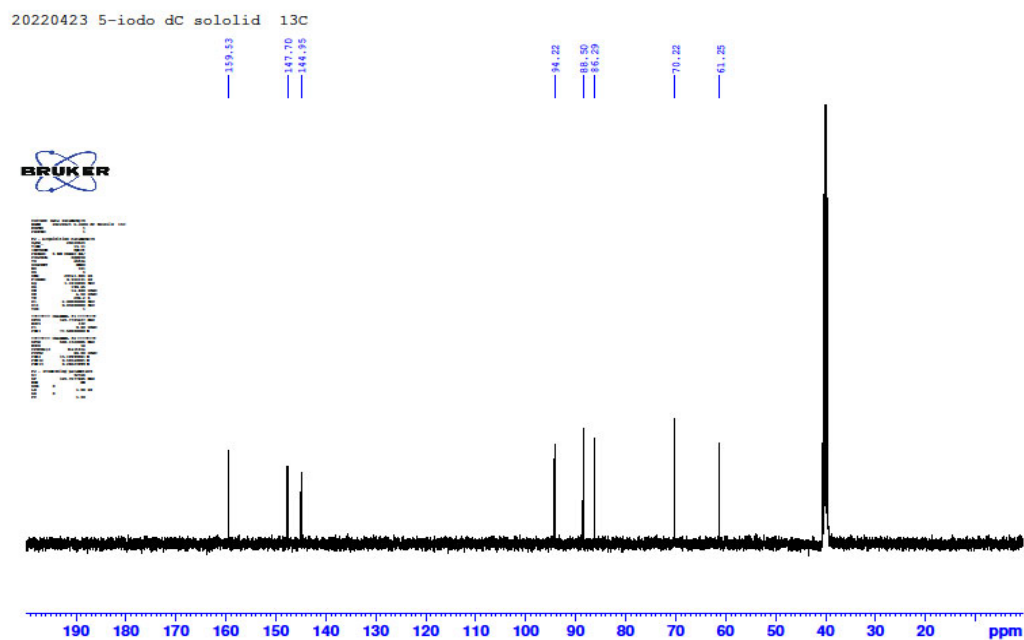
Figure S6. (A) Chemical structure and (B) ^1H NMR, (C) ^{13}C NMR, and (D) ESI-Mass spectra of 5-iodo-cytidine (5I-rC).

NC1=NC(=O)N(C1[C@H]2O[C@H](CO)[C@@H](O)[C@H]2O)C=C(I)C1=CC=CC=C1

20220217 5 iodo dC solid 1



(C)



(D)

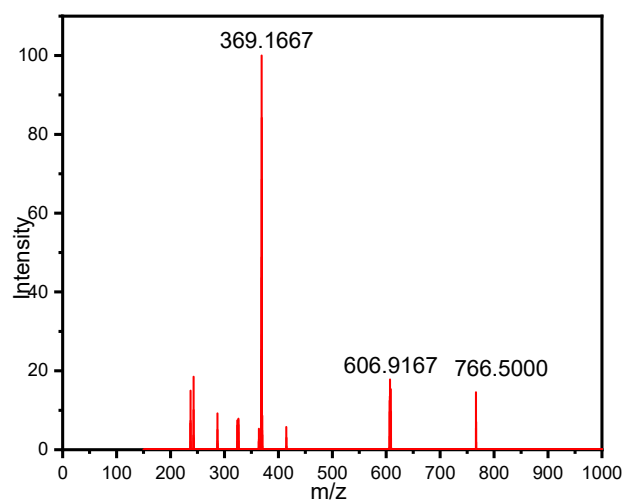
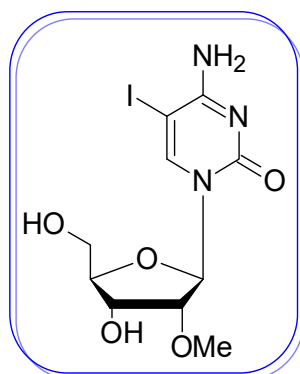
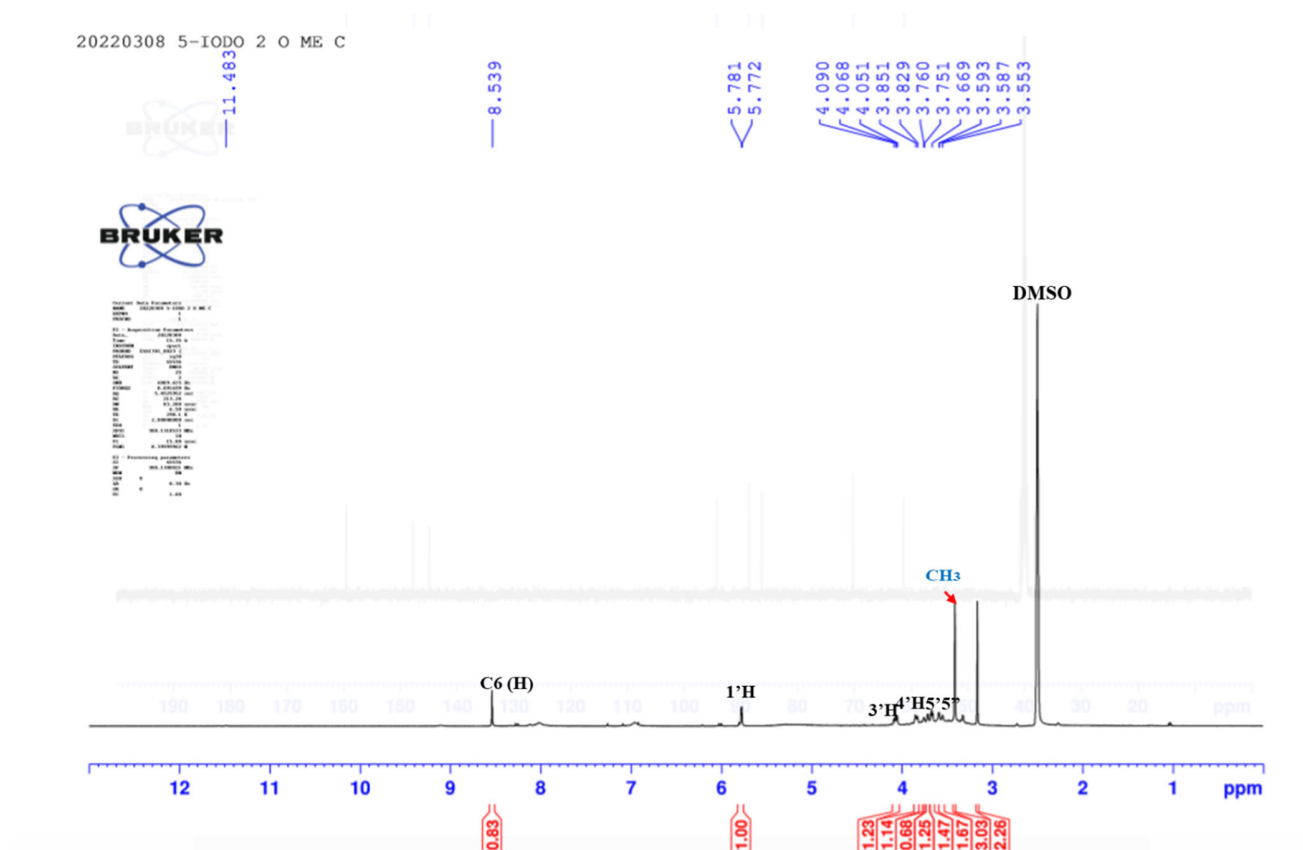


Figure S7. (A) Chemical structure and (B) ^1H NMR, (C) ^{13}C NMR, and (D) ESI-Mass spectra of 5-iodo-2'-deoxycytidine (5I-dC).

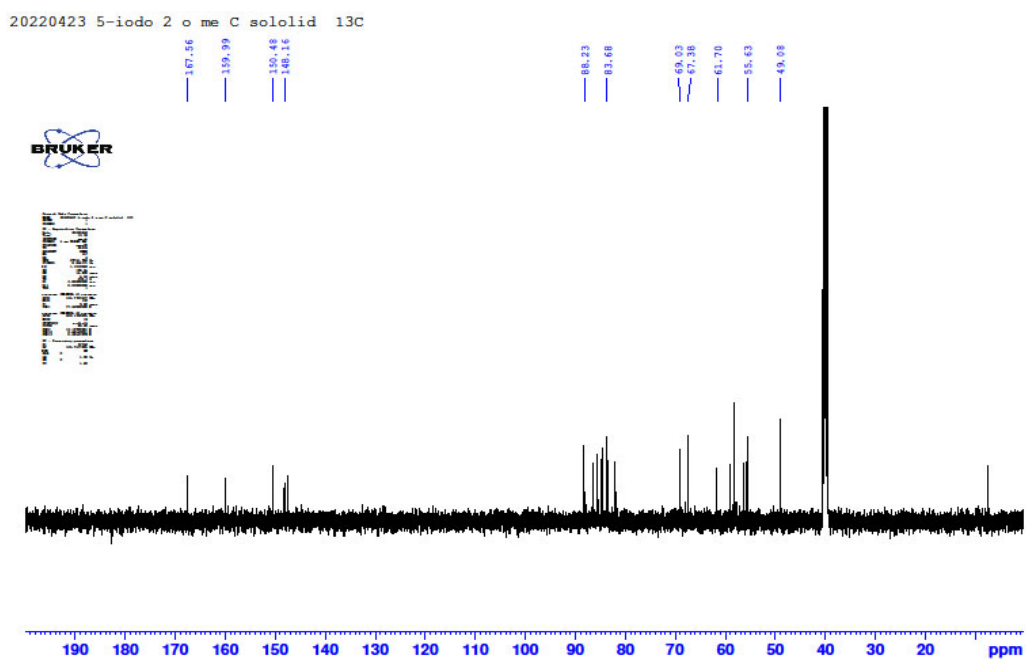
(A)



(B)



(C)



(D)

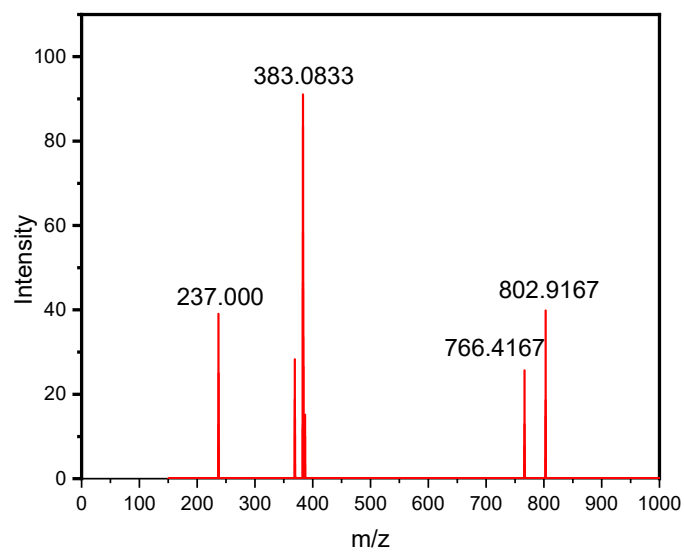


Figure S8. (A) Chemical structure and (B) ^1H NMR, (C) ^{13}C NMR, and (D) ESI-Mass spectra of 5-iodo-2'-OMe-cytidine (5I-mC).

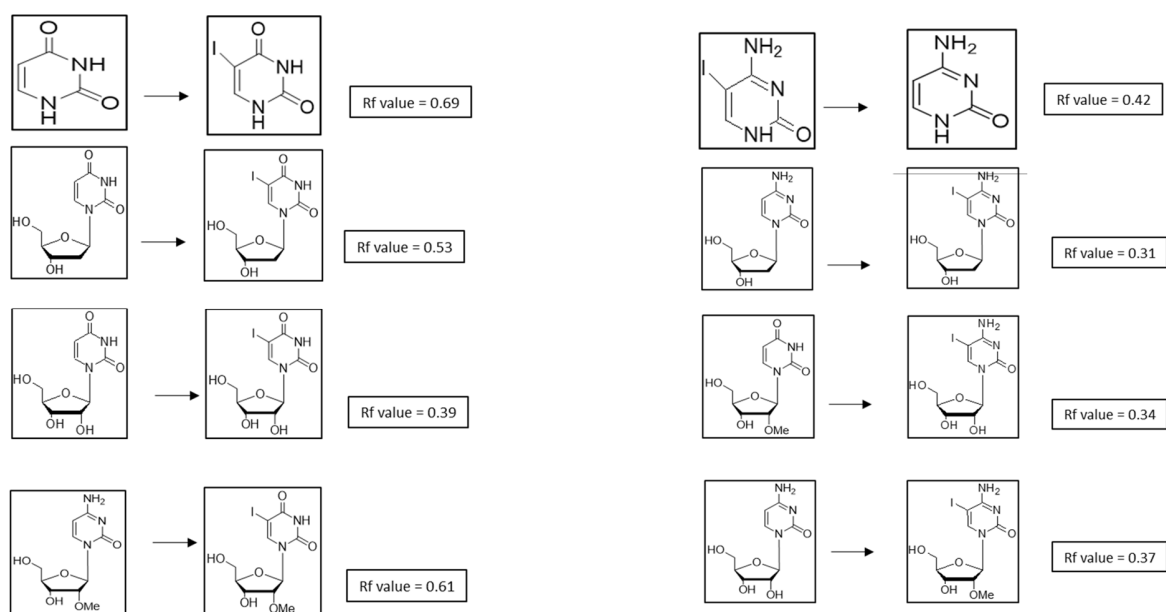


Figure S9. The TLC Rf values of fractions of 5-iodo pyrimidine derivatives (solvent $\text{CH}_2\text{Cl}_2:\text{MeOH}$ (5:1)).