

Supplementary Materials for

**Chemical Synthesis of
Oligodeoxyribonucleotides Containing *N*3- and
*O*4-carboxymethylthymidine and Their Formation
in DNA” (NAR-01852-M-2008).**

Jianshuang Wang and Yinsheng Wang

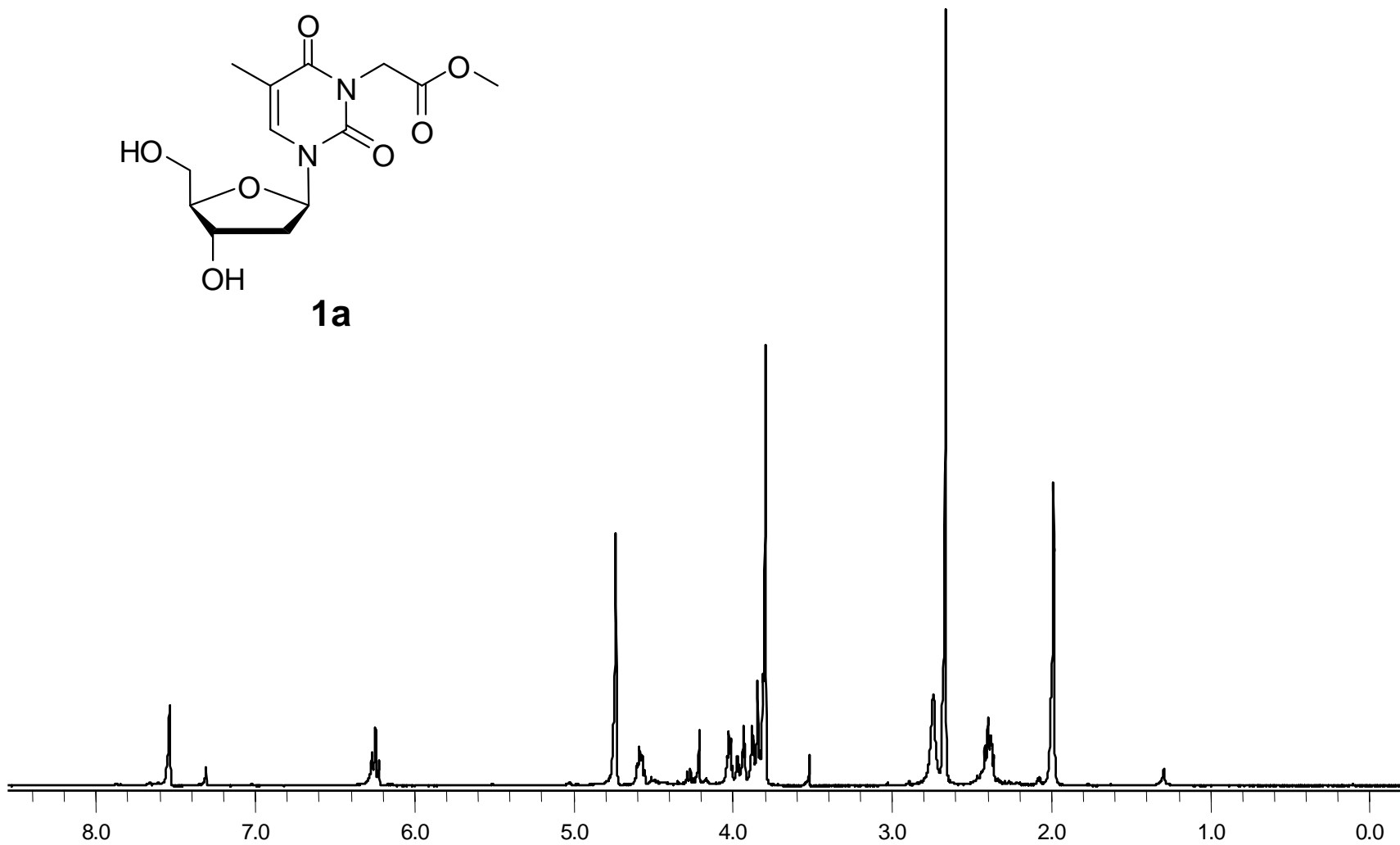
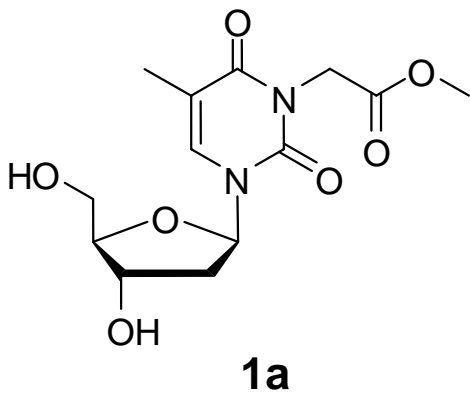


Figure S1. ^1H NMR of *N*3-methoxycarbonylmethylthymidine (300 MHz, CDCl_3 , 25 $^\circ\text{C}$).

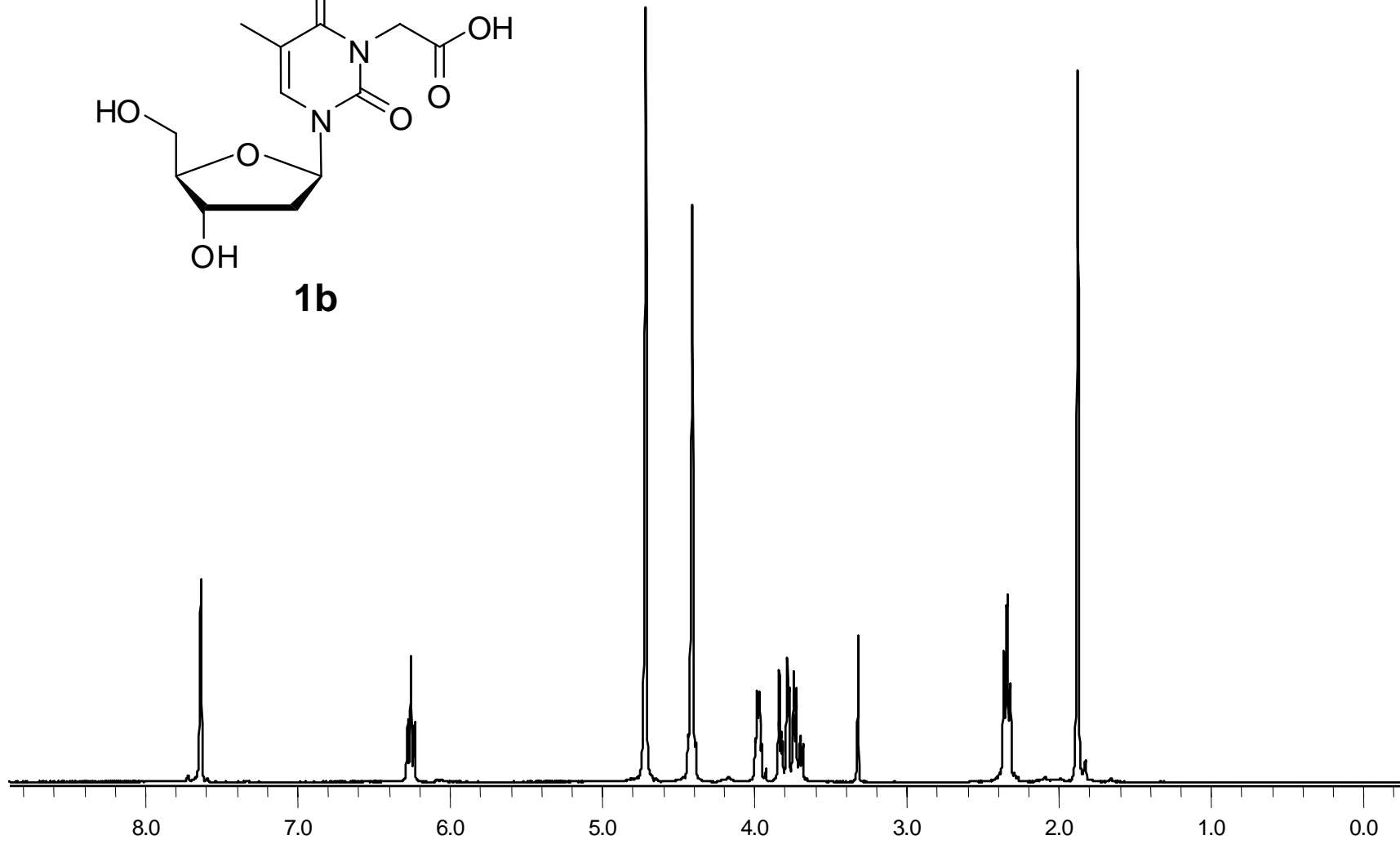
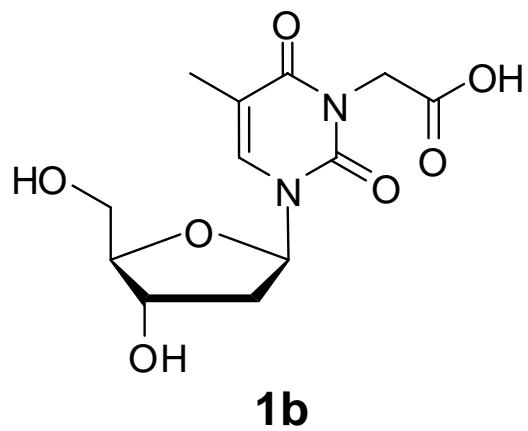


Figure S2. ¹H NMR of *N*³-carboxymethylthymidine (300 MHz, D₂O, 25 °C).

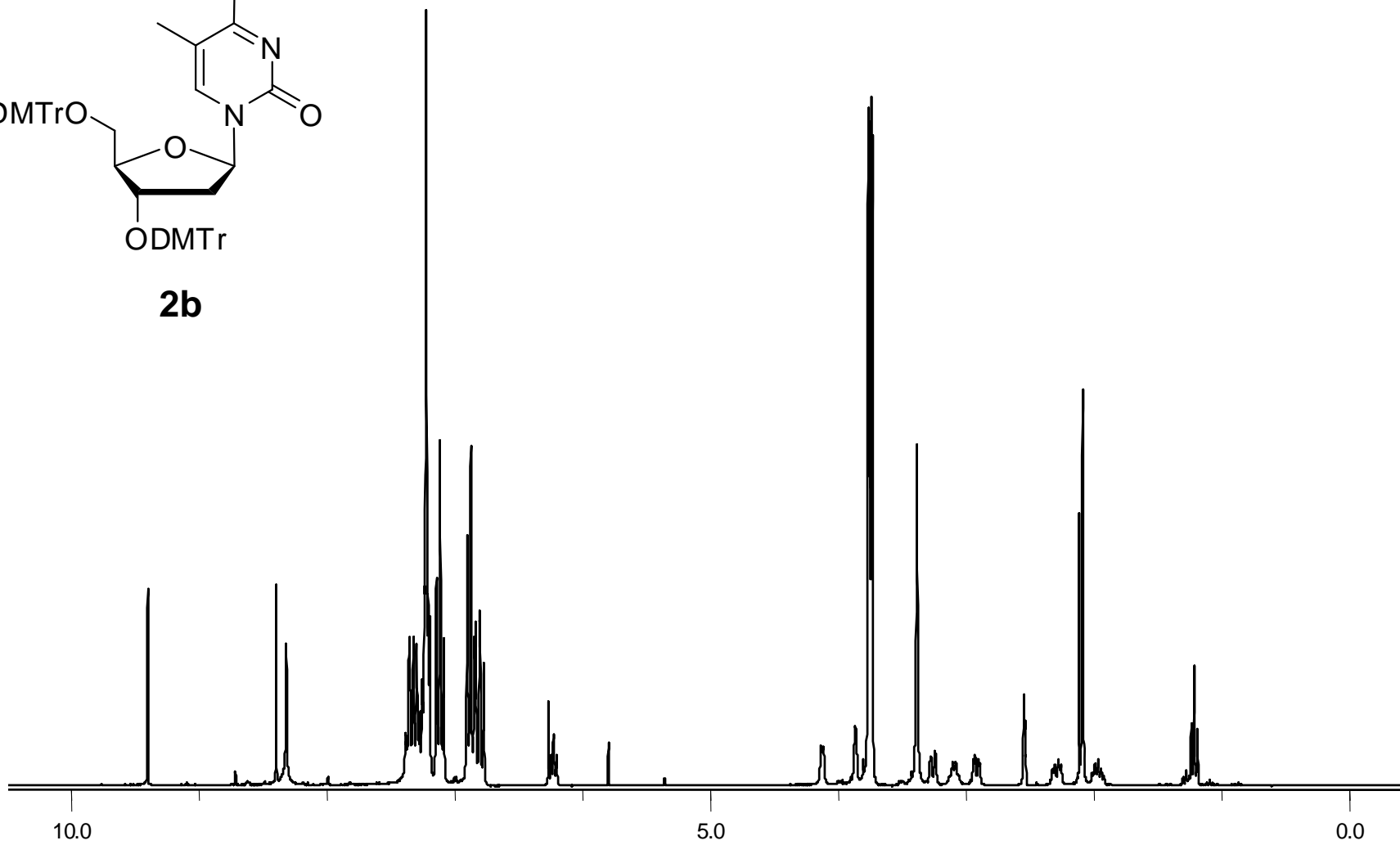
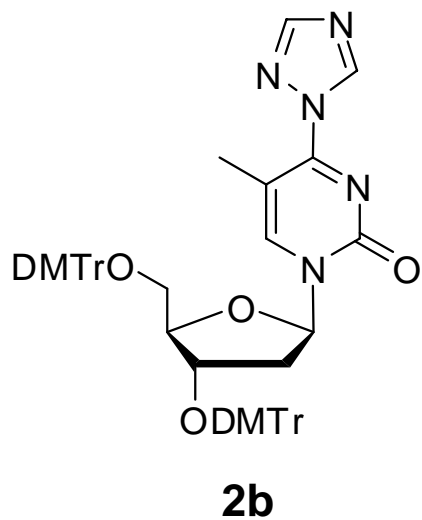
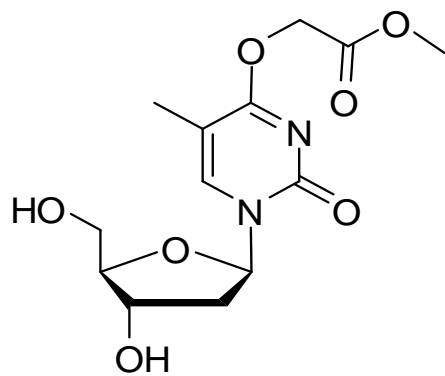


Figure S3. ^1H NMR spectrum of 3',5'-O-di(4,4'-dimethoxytrityl)-4-O-triazolylthymidine (300 MHz, $\text{DMSO-}d_6$, 25 $^\circ\text{C}$).



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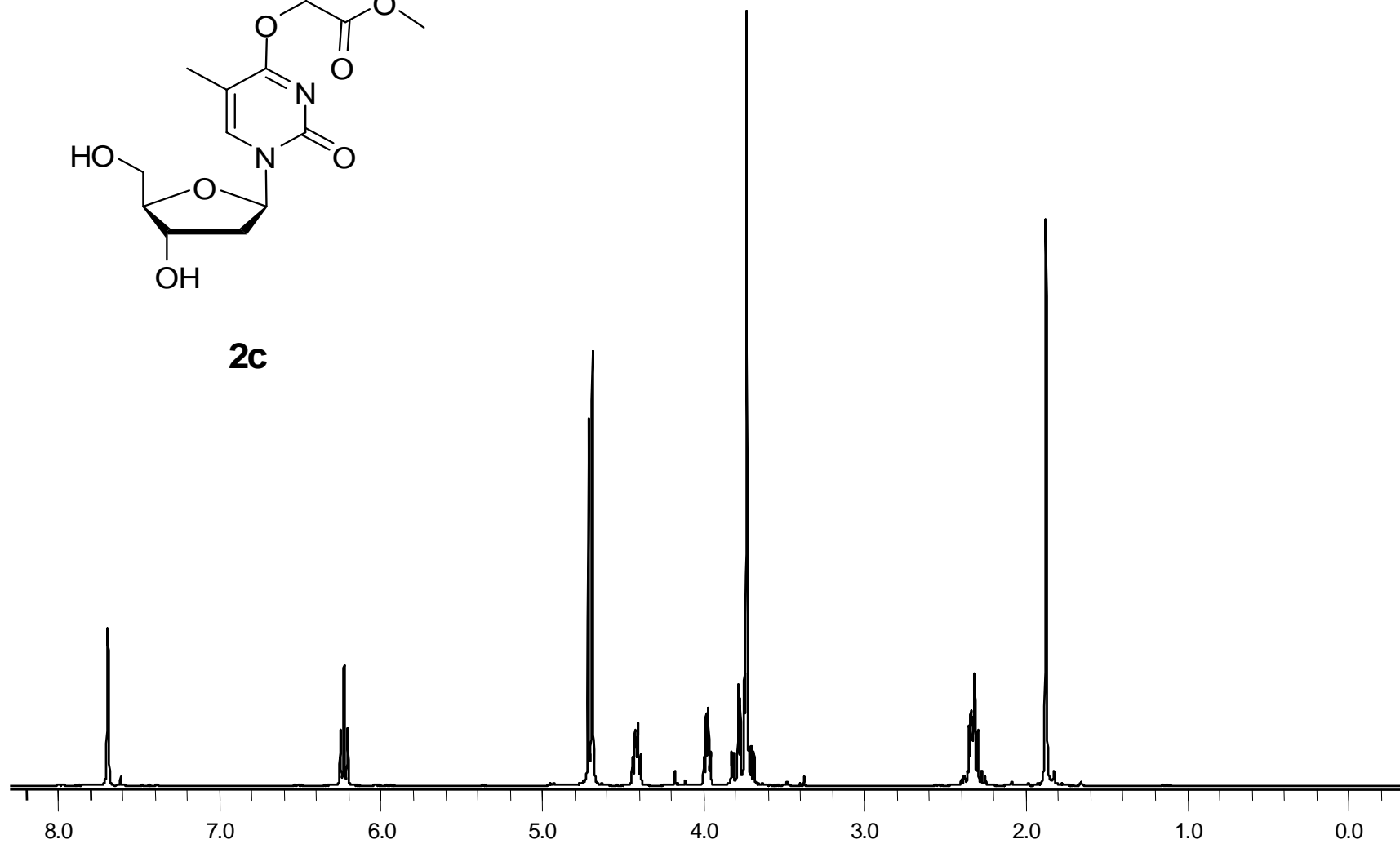


Figure S4. ¹H NMR spectrum of *O*⁴-methoxycarbonylmethylthymidine (300 MHz, D₂O, 25 °C).

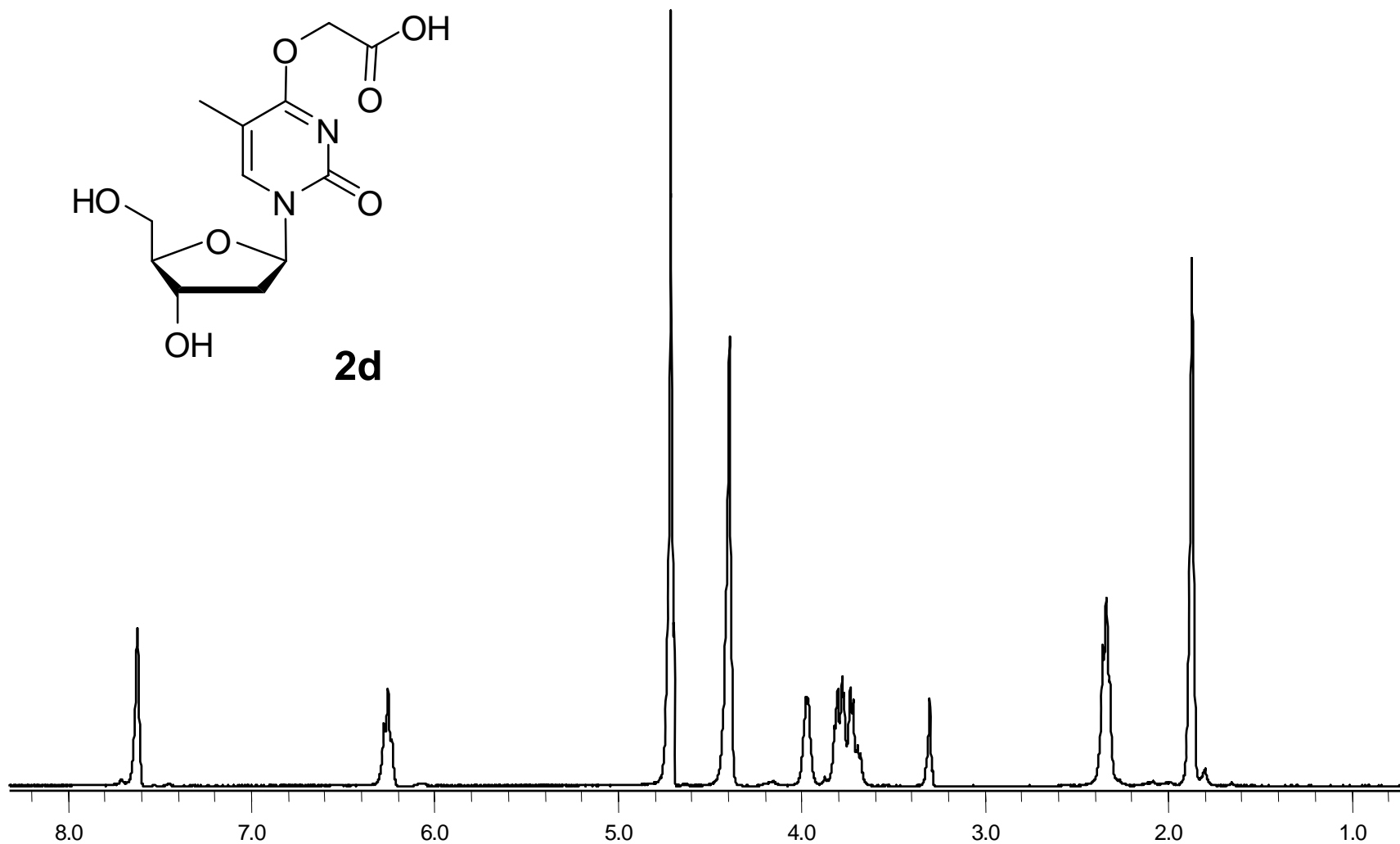
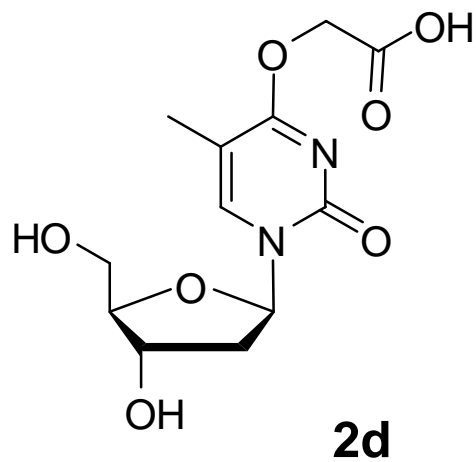


Figure S5. ^1H NMR spectrum of *O*⁴-carboxymethylthymidine (300 MHz, D_2O , 25 °C).

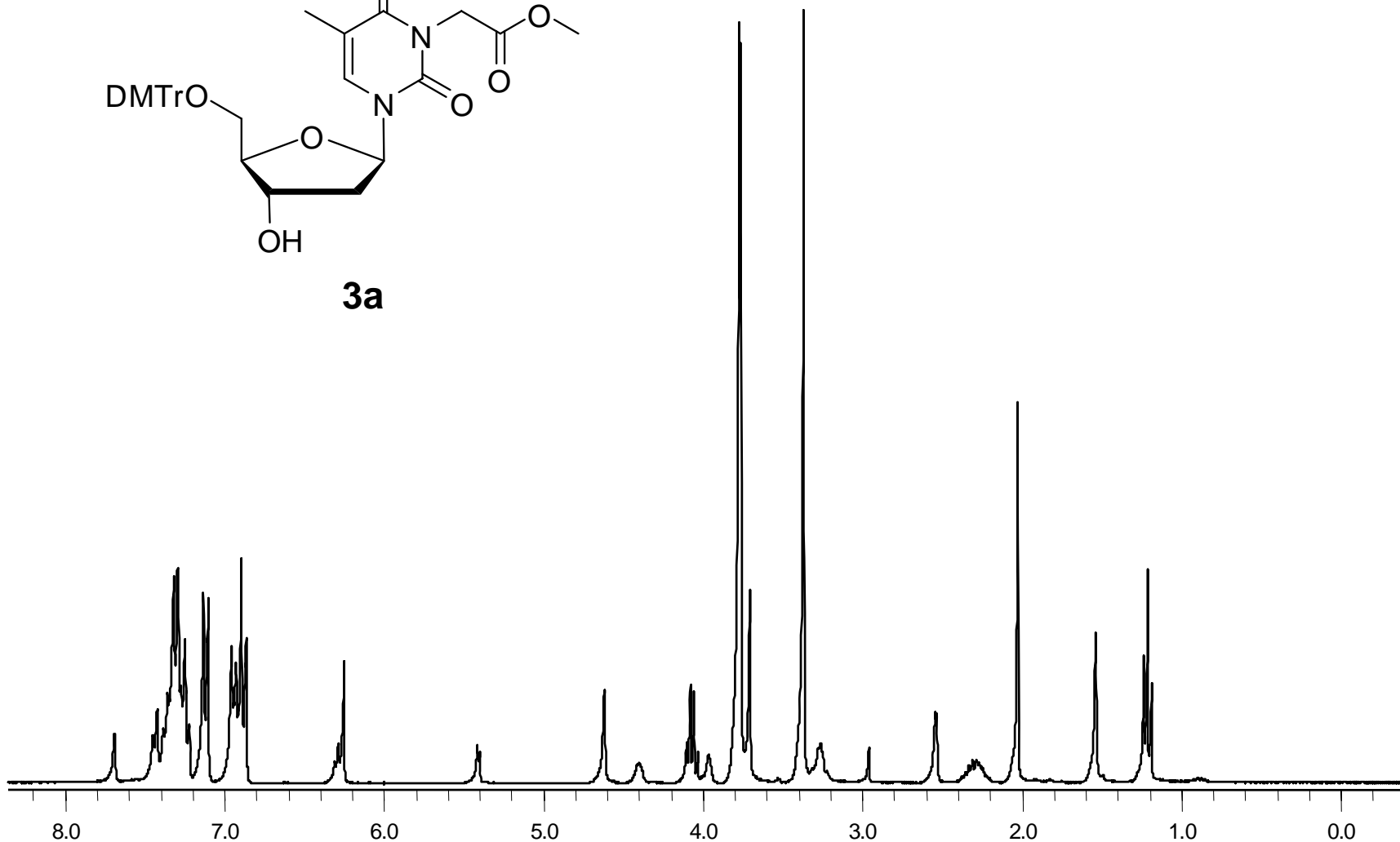
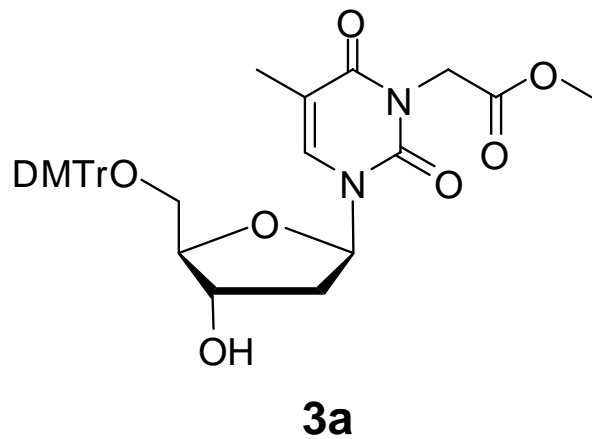


Figure S6. ^1H NMR spectrum of 5'-O-(4,4'-dimethoxytrityl)-*N*3-methoxycarbonylmethylthymidine (300 MHz, $\text{DMSO-}d_6$, 25°C).

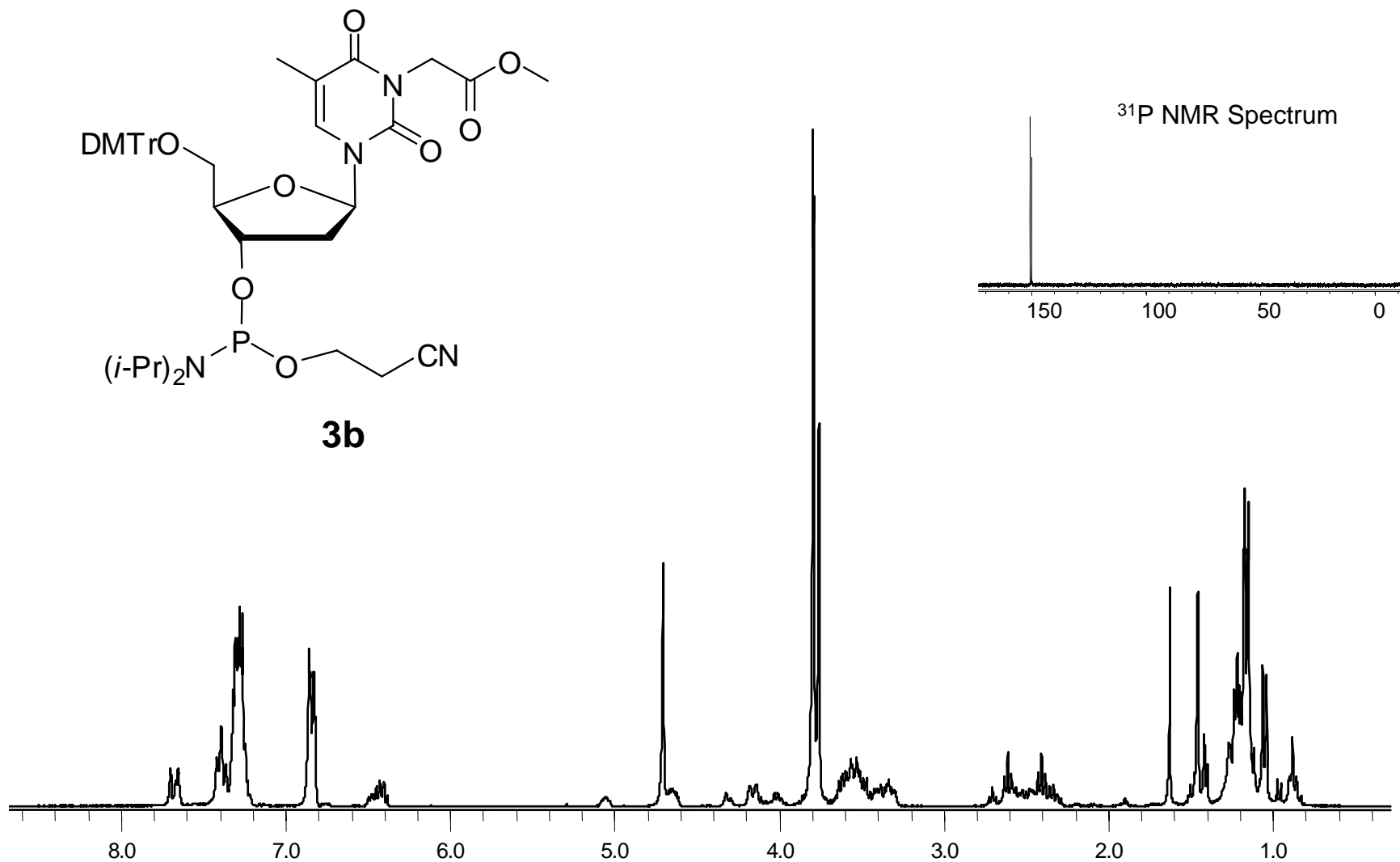


Figure S7. ¹H NMR spectrum of 5'-O-(4,4'-dimethoxytrityl) thymidine-3'-O-[(2-cyanoethyl)-N,N-diisopropylphosphoramidite] (300 MHz, CDCl₃, 25 °C). The insert is a ³¹P NMR spectrum of this compound at 80 MHz.

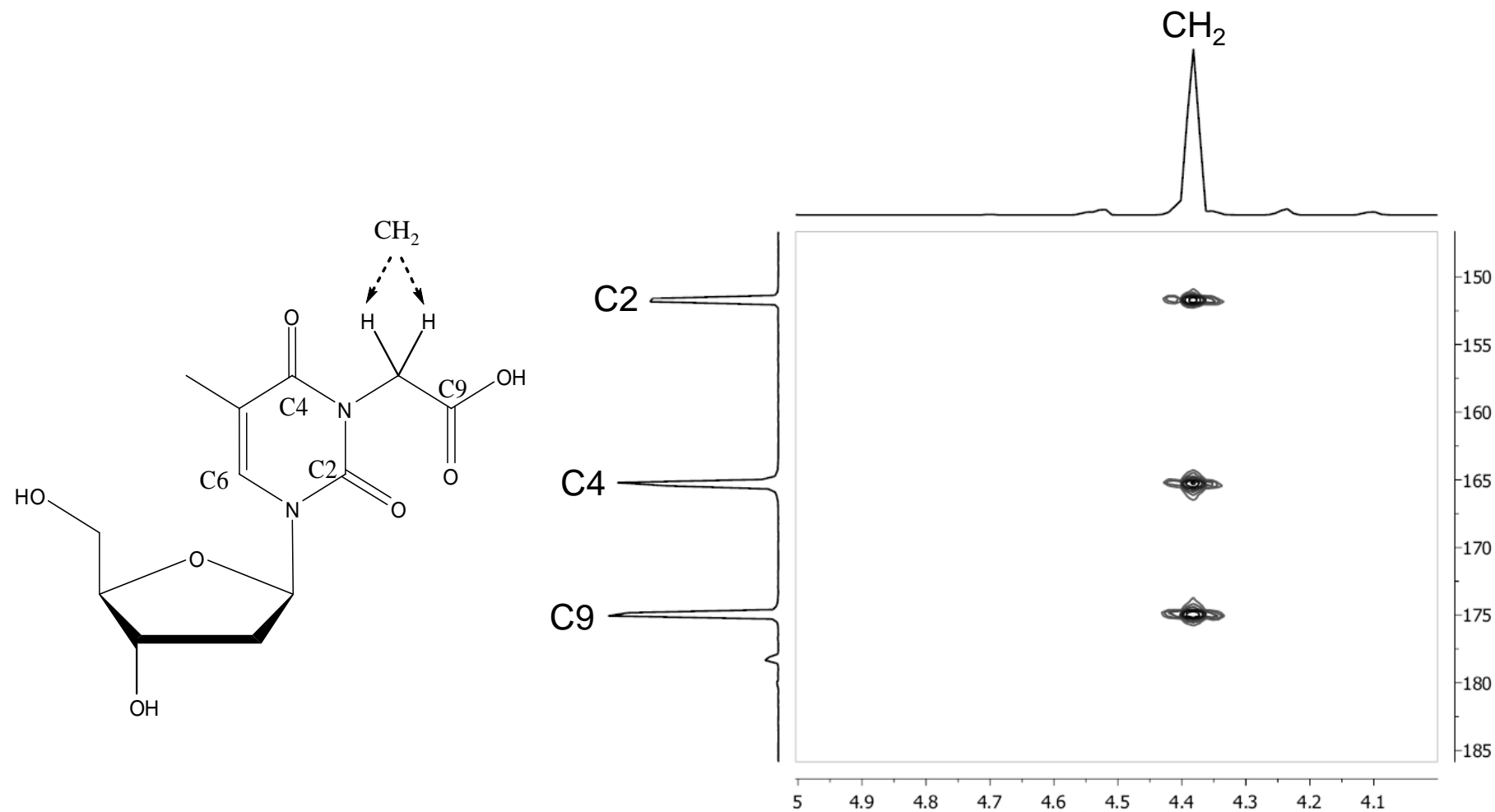


Figure S8. A portion of the 2-D HMBC spectrum of *N*³-carboxymethylthymidine (500 MHz, D₂O, 25 °C) showing the correlation between the methylene protons of the carboxymethyl functionality and the carbon atoms of the thymine ring.

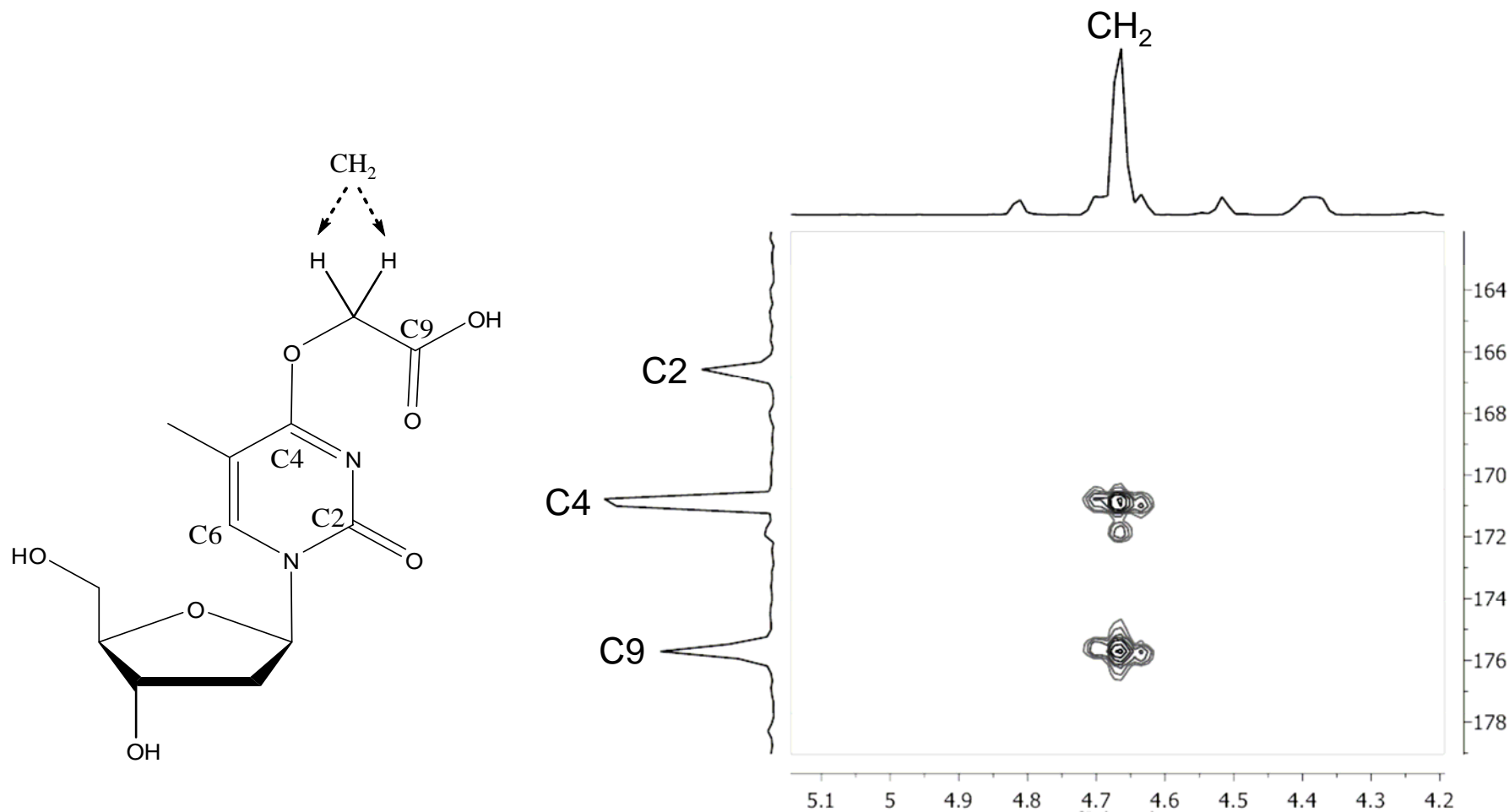


Figure S9. A portion of the 2-D HMBC spectrum of *O*⁴-carboxymethylthymidine (500 MHz, D₂O, 25 °C) showing the correlation between the methylene protons of the carboxymethyl functionality and the carbon atom of the thymine ring.