Supporting Information

to the manuscript:

Design, synthesis, and characterization of an amphiphilic lipoic acid-based Ru(III) complex as a versatile tool for the functionalization of different nanosystems

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Table of contents

Figure S1. Chemical structures of previously reported Ru(III) complexes.

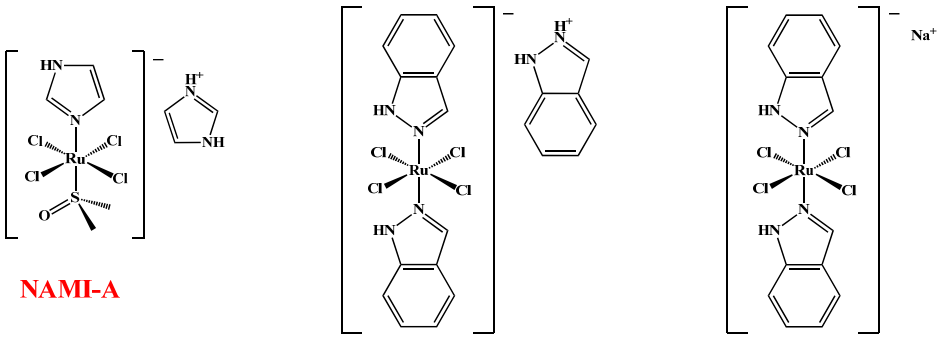
Figure S2. NMR and ESI-MS spectra of final LipThyRu Ru(III) complex.

Figure S3. ^{1}H-NMR spectrum of compound **2**.

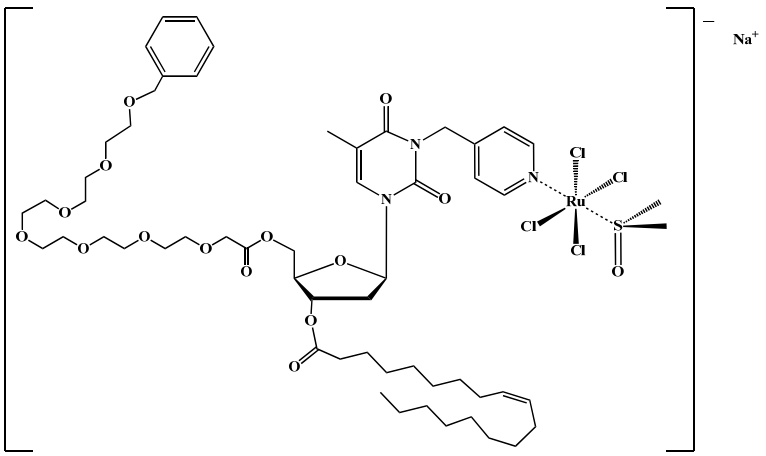
Figure S4-S6. ^{1}H-NMR, ^{13}C-NMR and ESI-MS spectra of compound **3**.

Figure S7-S9. ^{1}H-NMR, ^{13}C-NMR and ESI-MS spectra of compound **4**.

Figure S10-S12. ^{1}H-NMR, ^{13}C-NMR and ESI-MS spectra of compound **5**.



NAMI-A KP1019 NKP1339



HoThyRu

Figure S1. Chemical structures of NAMI-A, KP1019, NKP-1339 and HoThyRu, as indicated.

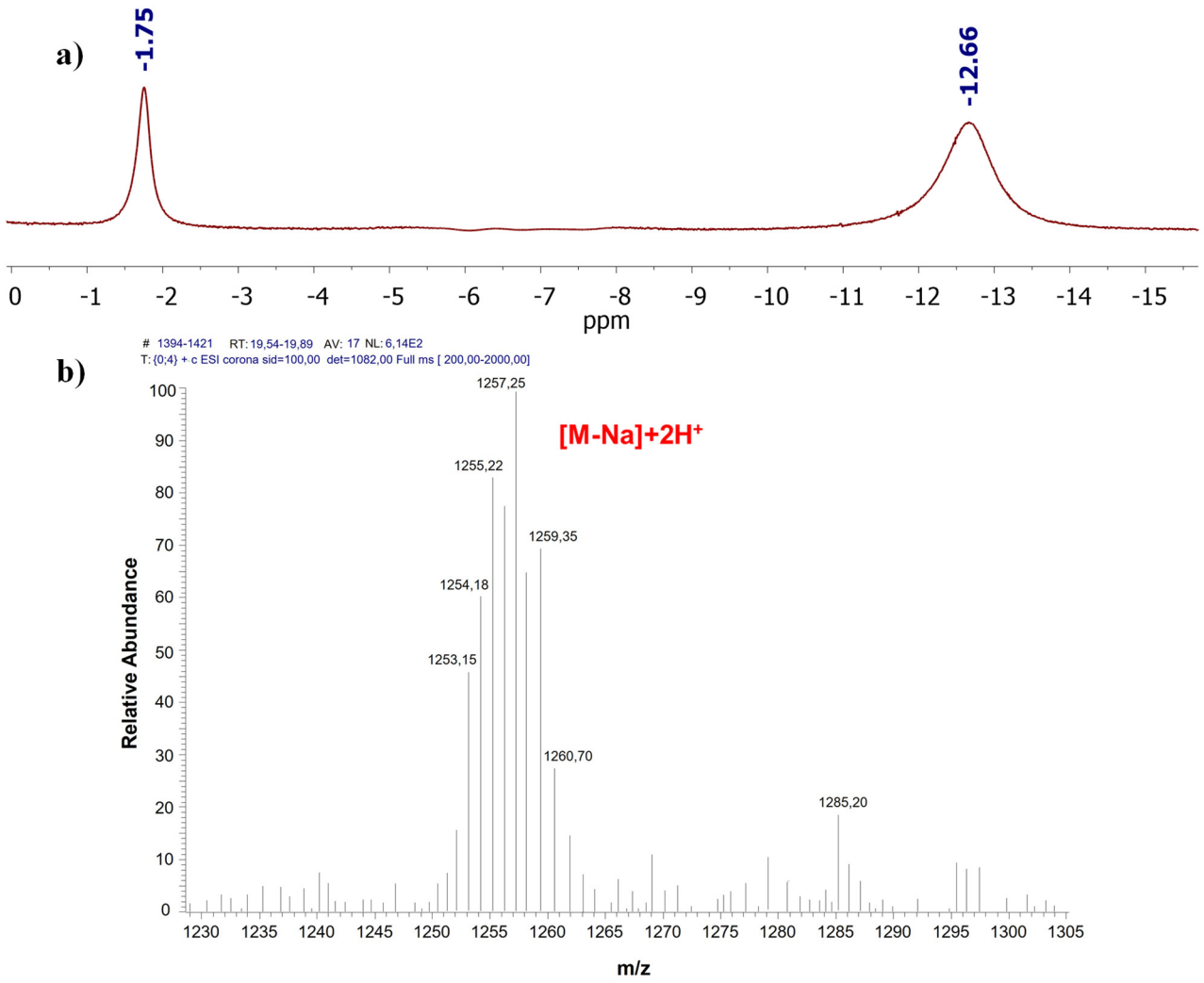
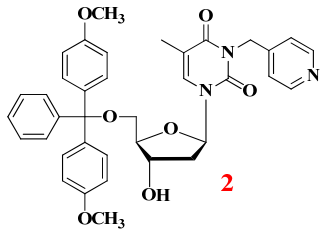


Figure S2. a) Expansion of the upfield region of the ^{1}H NMR spectrum of the nucleolipid-based Ru(III) complex LipThyRu [400 MHz, $(CD_3)_2CO$]; **b**) ESI-MS spectrum (positive ions) of LipThyRu.



3-(4-pyridylmethyl)-5′-O-(4,4′-dimethoxytriphenylmethyl)-thymidine

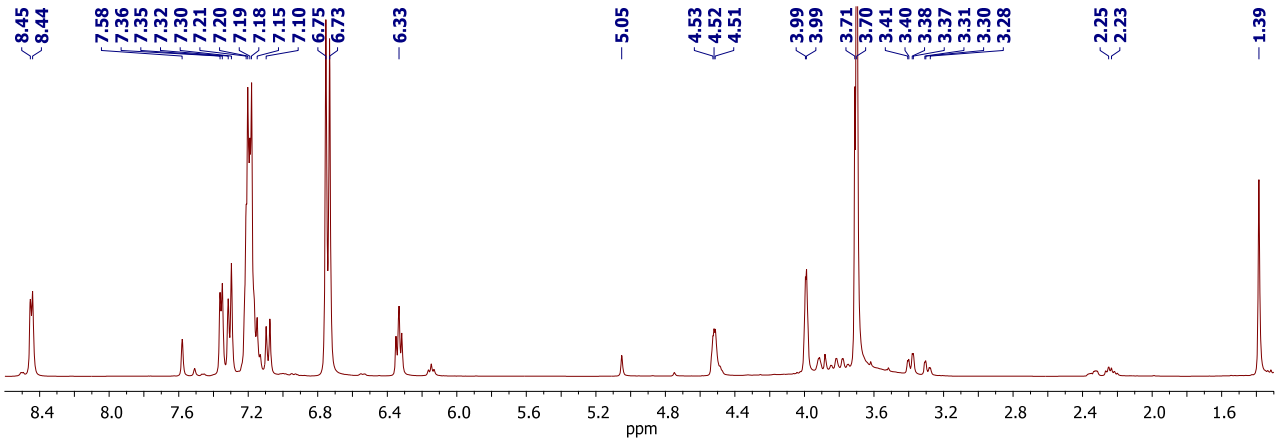
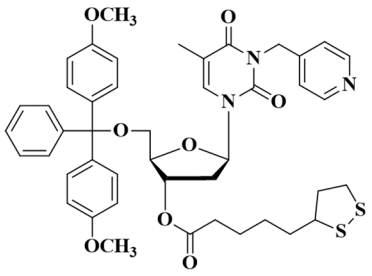


Figure S3. ^{1}H-NMR spectrum of compound **2** (400 MHz, $CDCl_3$).



3

Synthesis of 3-(4-pyridylmethyl)-3′-O-lipoyl-5′-O-(4,4′-dimethoxytriphenylmethyl)-thymidine

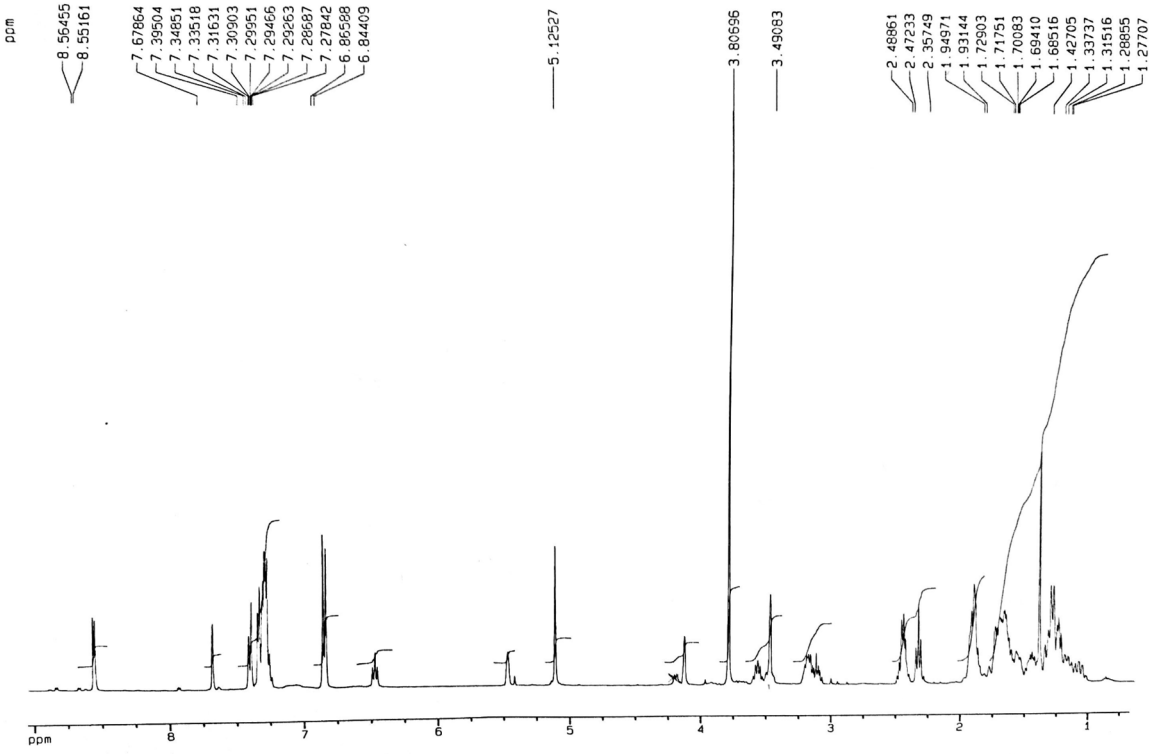


Figure S4. ^{1}H-NMR spectrum of compound **3** (400 MHz, $CDCl_3$).

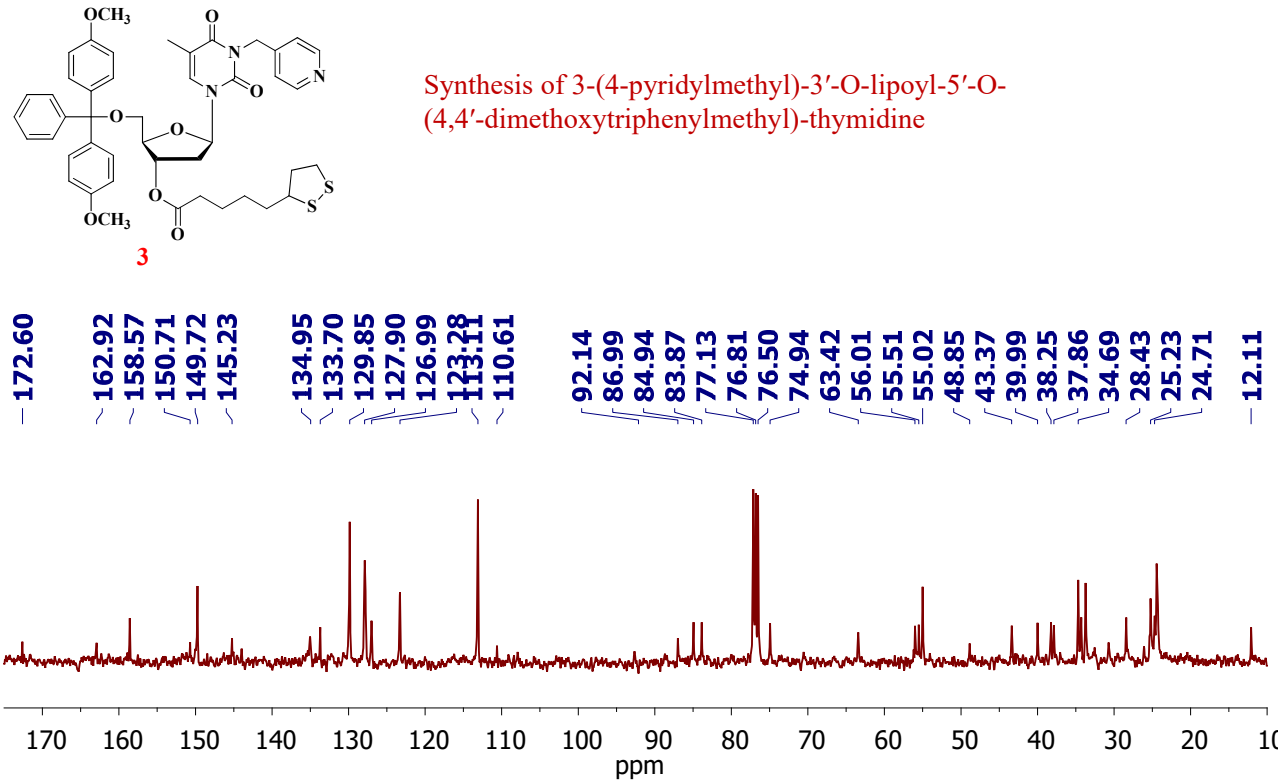


Figure S5. ^{13}C-NMR spectrum of compound **3** (100 MHz, $CDCl_3$).

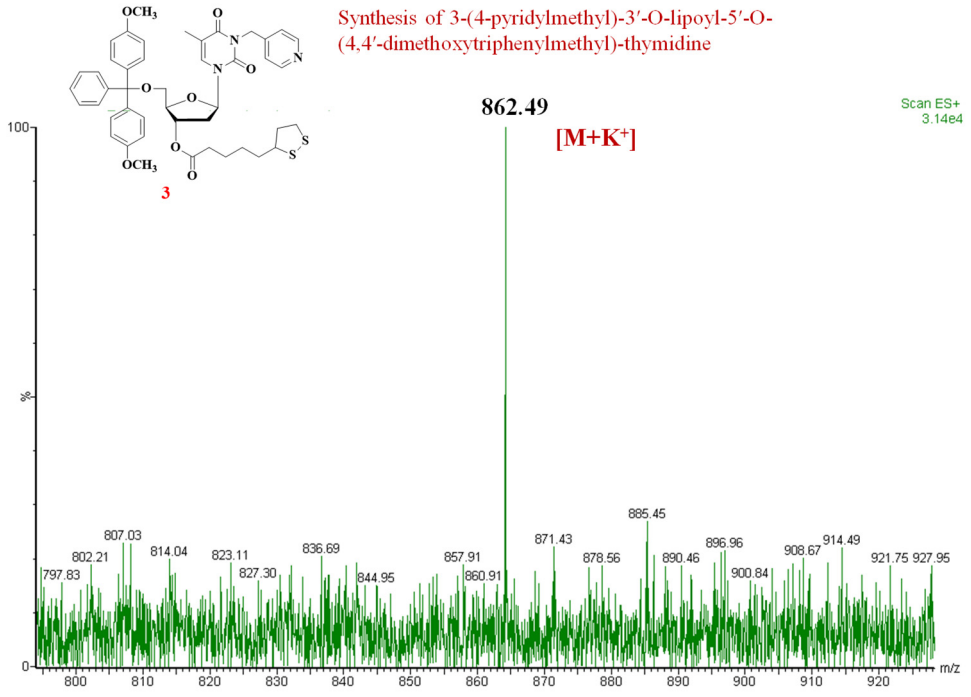


Figure S6. ESI-MS spectrum of compound **3** (positive ions).

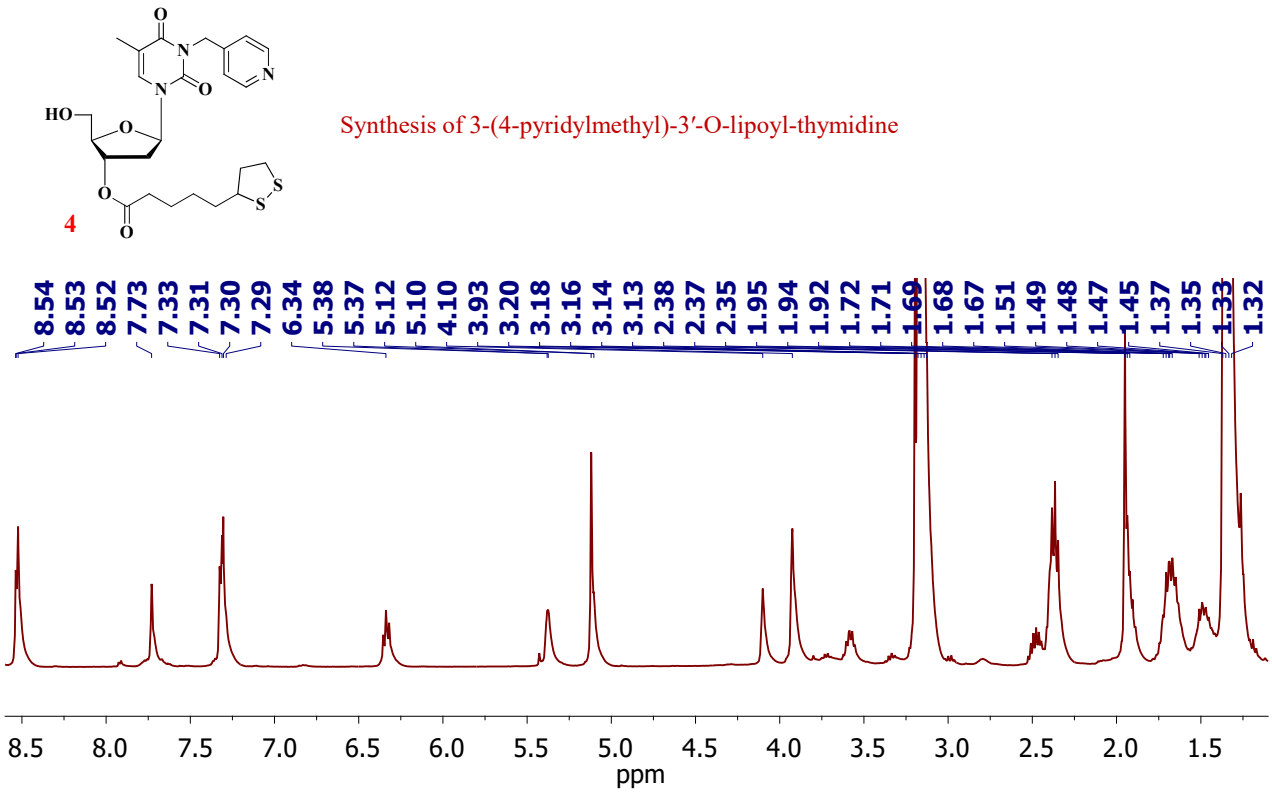


Figure S7. ^{1}H-NMR spectrum of compound **4** (400 MHz, $CDCl_3$).

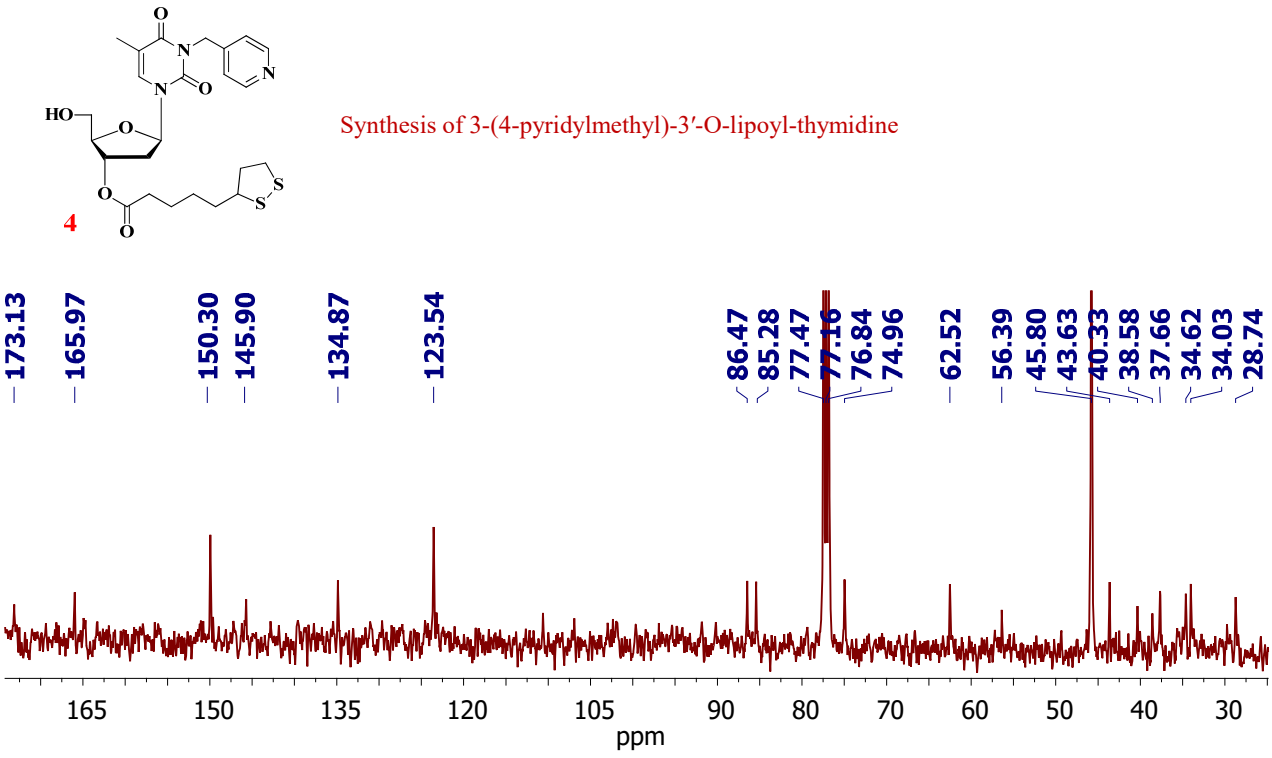
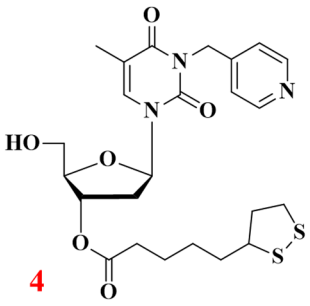


Figure S8. ^{13}C-NMR spectrum of compound **4** (100 MHz, $CDCl_3$).



Synthesis of 3-(4-pyridylmethyl)-3′-O-lipoyl-thymidine

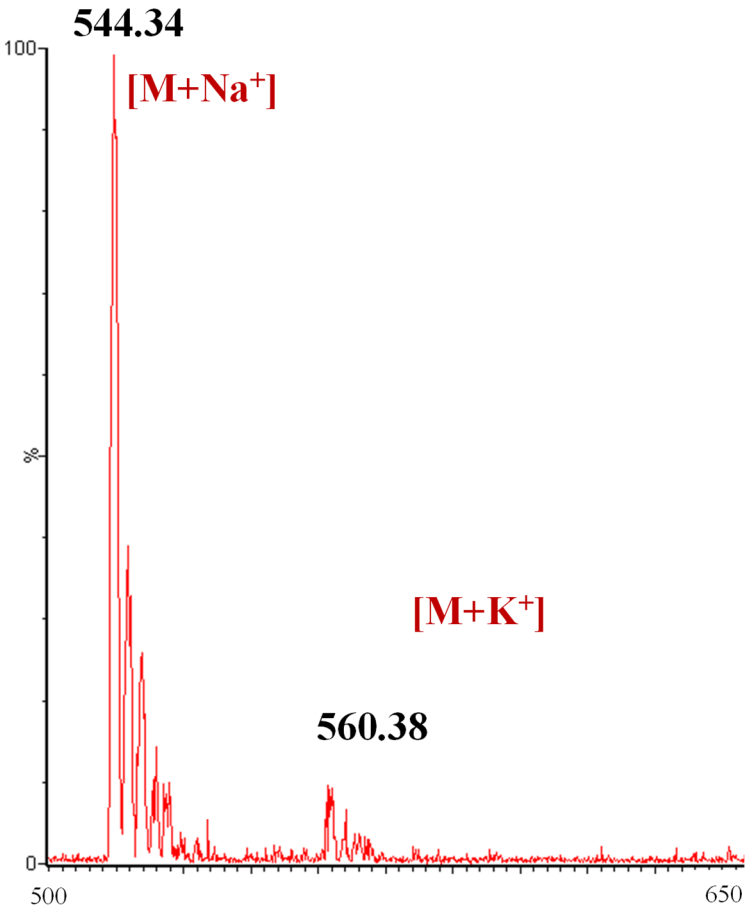
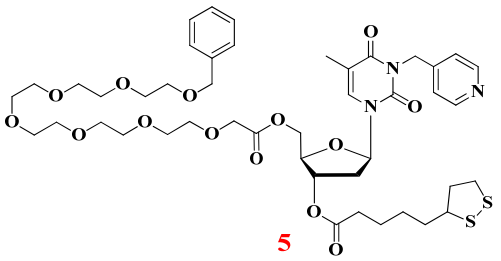


Figure S9. ESI-MS spectrum of compound **4** (positive ions).



Synthesis of 3-(4-pyridylmethyl)-3′-O-lipoyl-5′-O-(benzyloxy)hexaethylene glycol acetyl-thymidine

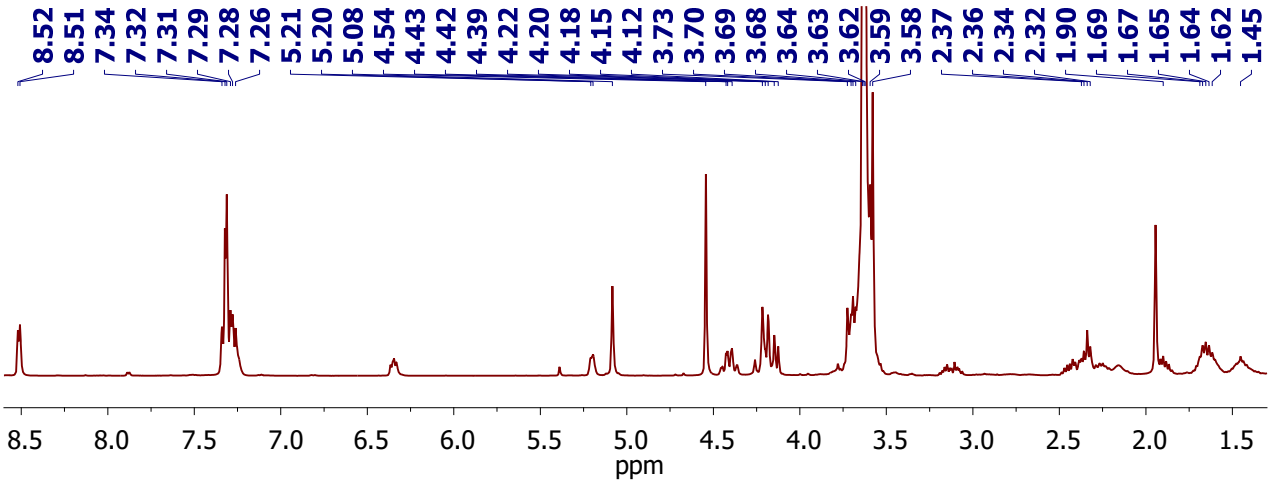
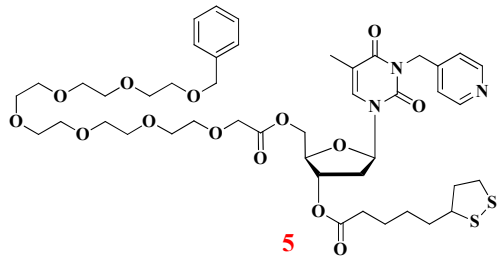


Figure S10. ^{1}H-NMR spectrum of compound **5** (400 MHz, $CDCl_3$).



Synthesis of 3-(4-pyridylmethyl)-3′-O-lipoyl-5′-O-(benzyloxy)hexaethylene glycol acetyl-thymidine

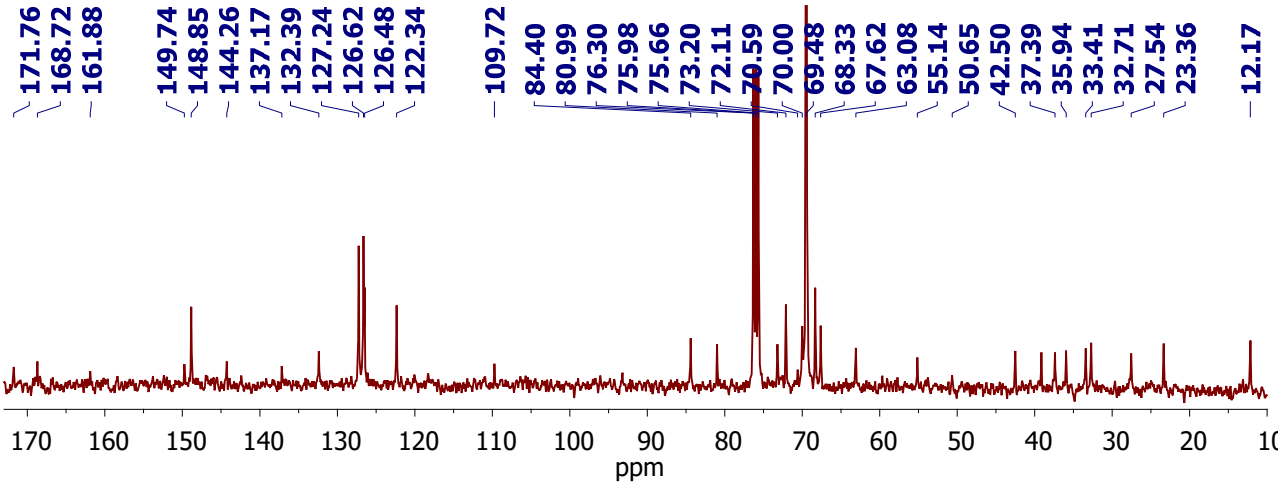


Figure S11. ^{13}C-NMR spectrum of compound **5** (100 MHz, $CDCl_3$).

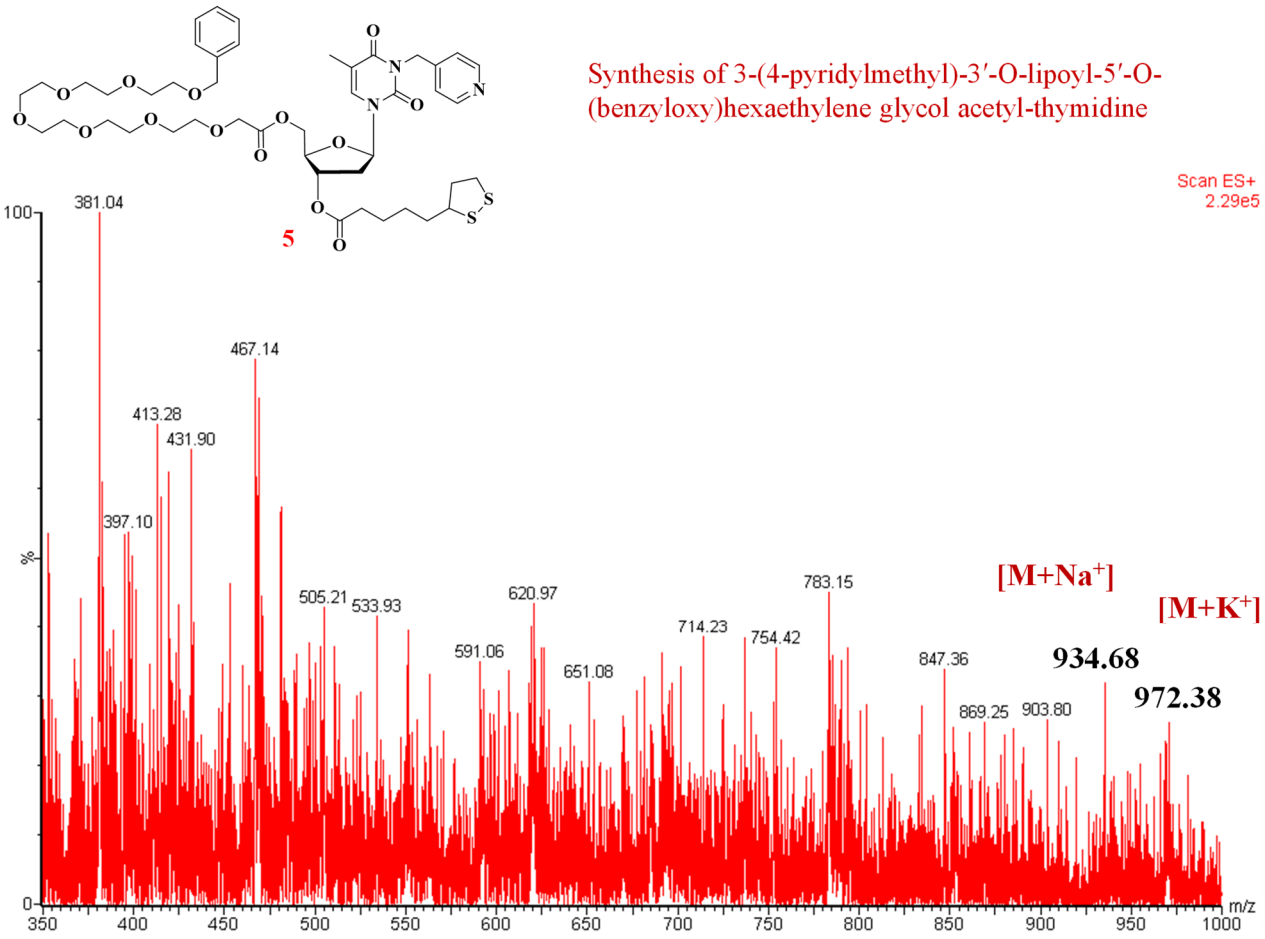


Figure S12. ESI-MS spectrum of compound **5** (positive ions).