

Supplementary Information

Synthesis of process related impurities of Citicoline and Citicoline sodium[#]

Amit H Pakhurde, Priyanka S More, Nilesh L Bonde & Sandeep A Kotharkar*

Embio Research Centre, Embio Limited, Plot No. E-22/1, MIDC Industrial Estate, Mahad, Dist. Raigad, Maharashtra 402 309, India

E-mail: sandeep.kotharkar@embio.co.in, amit@embio.co.in, synthetic@embio.co.in

Received 11 November 2023; accepted (revised) 26 February 2024

Contents	Page no.
Fig. S1: ¹ H NMR Cytidine 5'-monophosphomorpholidate (III)	2
Fig. S2: ¹³ C NMR Cytidine 5'-monophosphomorpholidate (III)	2
Fig. S3: ¹ H NMR Cytidine 5'-monophosphate methyl ester (IV)	3
Fig. S4: ¹³ C NMR Cytidine 5'-monophosphate methyl ester (IV)	3
Fig. S5: ¹ H NMR Desmethyl cytidine -5'-diphosphocholine (V)	4
Fig. S6: ¹³ C NMR Desmethyl cytidine -5'-diphosphocholine (V)	4
Fig. S7: ¹ H NMR Cytidine -5'-diphosphoethanolamine (VI)	5
Fig. S8: ¹³ C NMR Cytidine -5'-diphosphoethanolamine (VI)	5
Fig. S9: ¹ H NMR Uridine 5'-diphosphocholine (VII)	6
Fig. S10: ¹³ C NMR Uridine 5'-diphosphocholine (VII)	6

Sample Code: CIT-2022-101-94-1

Solvent: dmsd
SA-ACILANT 400MHz NMR
Date: Nov 25 2022

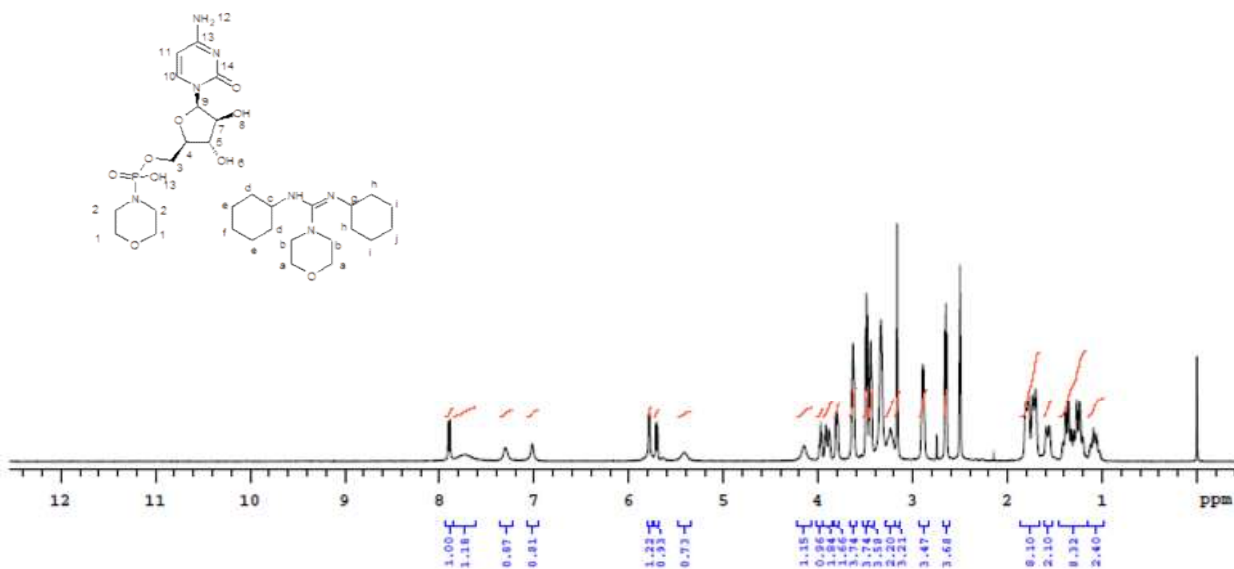


Fig.S1: ^1H NMR Cytidine 5'-monophosphomorpholidate (III)

Sample Code: CIT-2022-101-94-1-13C-NMR

Solvent: dmsd
SA-Varian 400MHz NMR
Date: Nov 25 2022

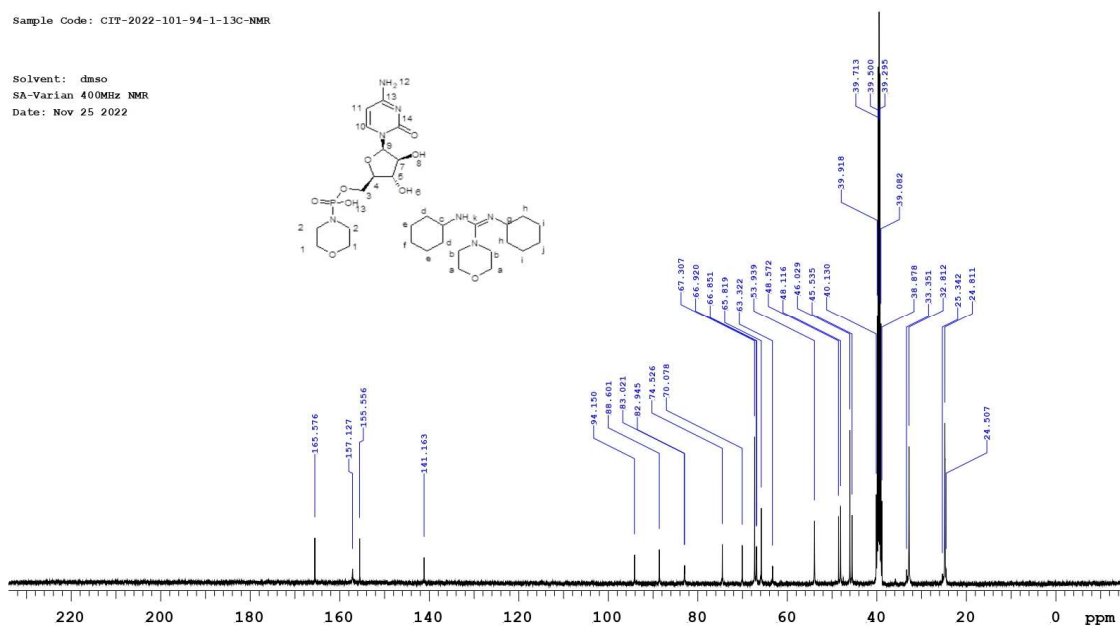


Fig.S2: ^{13}C NMR Cytidine 5'-monophosphomorpholidate (III)

Sample Code: CIT-2023-102-99-5

CYTIDINE-5'-MONOPHOSPHATE METHYL ESTER
EMBIO LABS

Solvent: d2o
SA-Varian 400MHz NMR
Date: Mar 8 2023

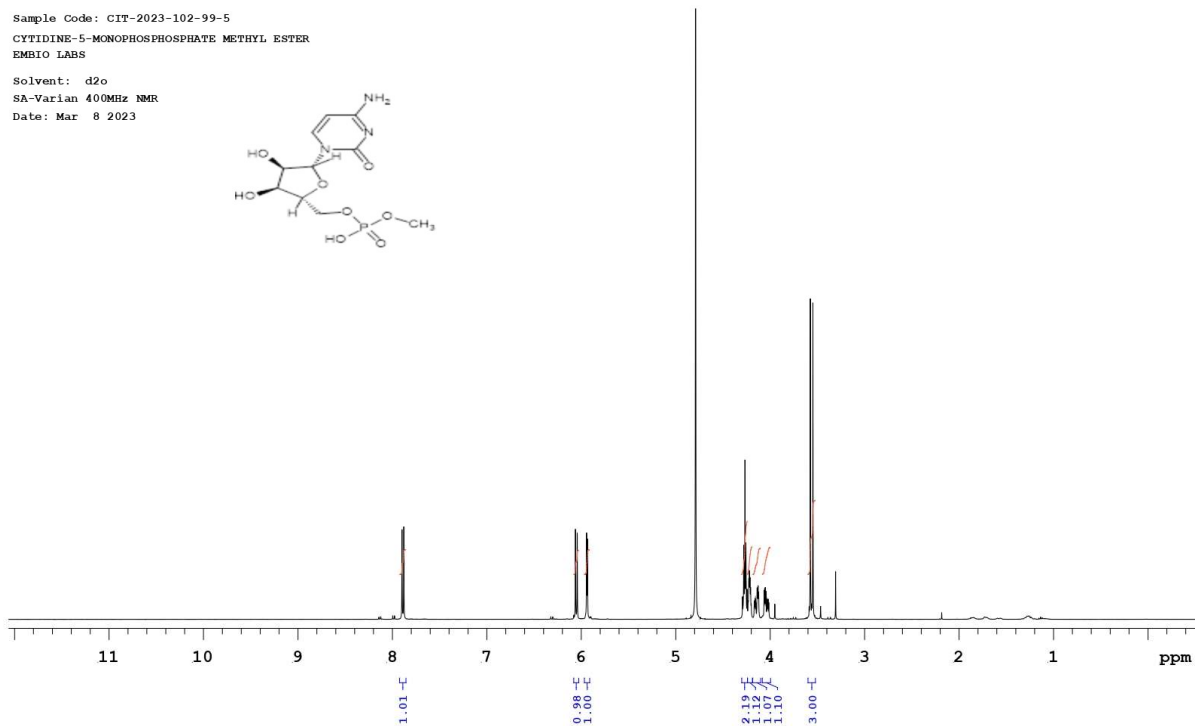
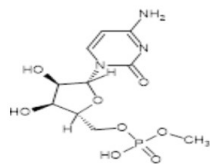


Fig.S3: ¹H NMR Cytidine 5'-monophosphate methyl ester (IV)

Sample Code: CIT-2023-102-99-5-13C-NMR
CYTIDINE-5'-MONOPHOSPHATE METHYL ESTER
13C NMR

Solvent: d2o
SA-AGILENT 400MHz NMR
Date: Mar 9 2023

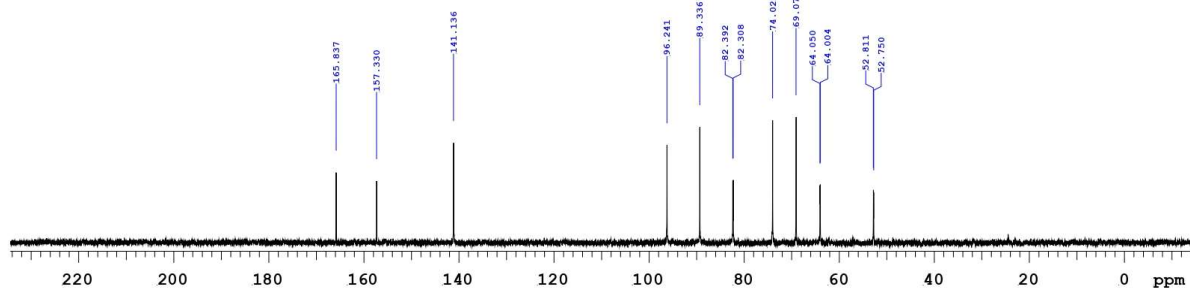
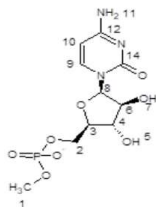


Fig.S4: ¹³C NMR Cytidine 5'-monophosphate methyl ester (IV)

Sample Code: CIT-2023-104-21-1

Solvent: d2o
SA-Varian 400MHz NMR
Date: May 31 2023

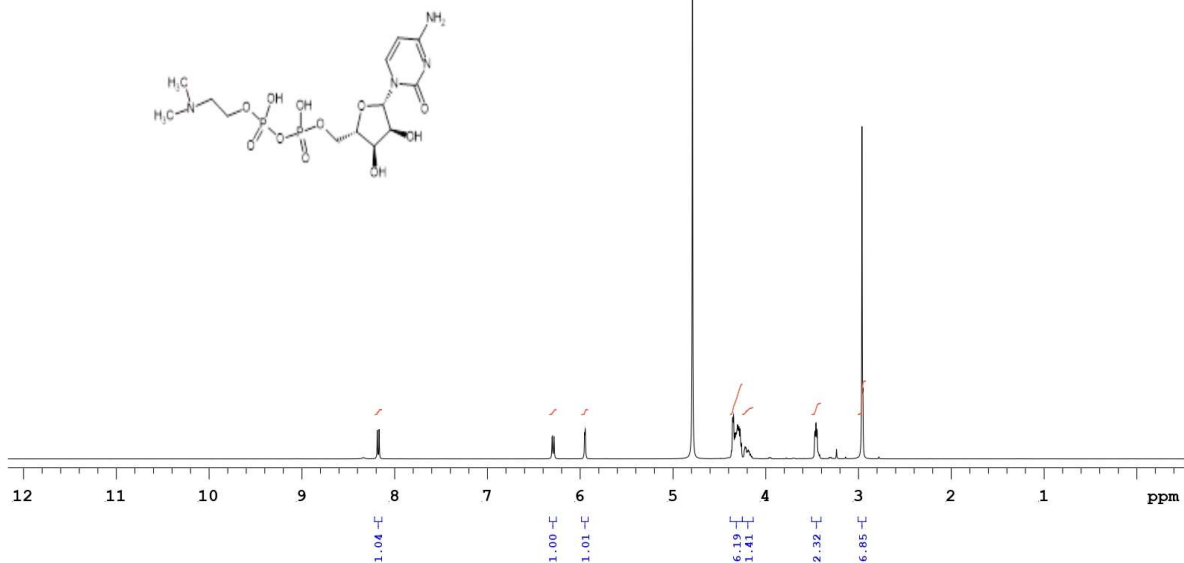


Fig.S5: ¹H NMR Desmethyl cytidine -5'-diphosphocholine (V)

Sample Code: CIT-2023-104-21-1-13C-NMR

Solvent: d2o
SA-Varian 400MHz NMR
Date: Jun 2 2023

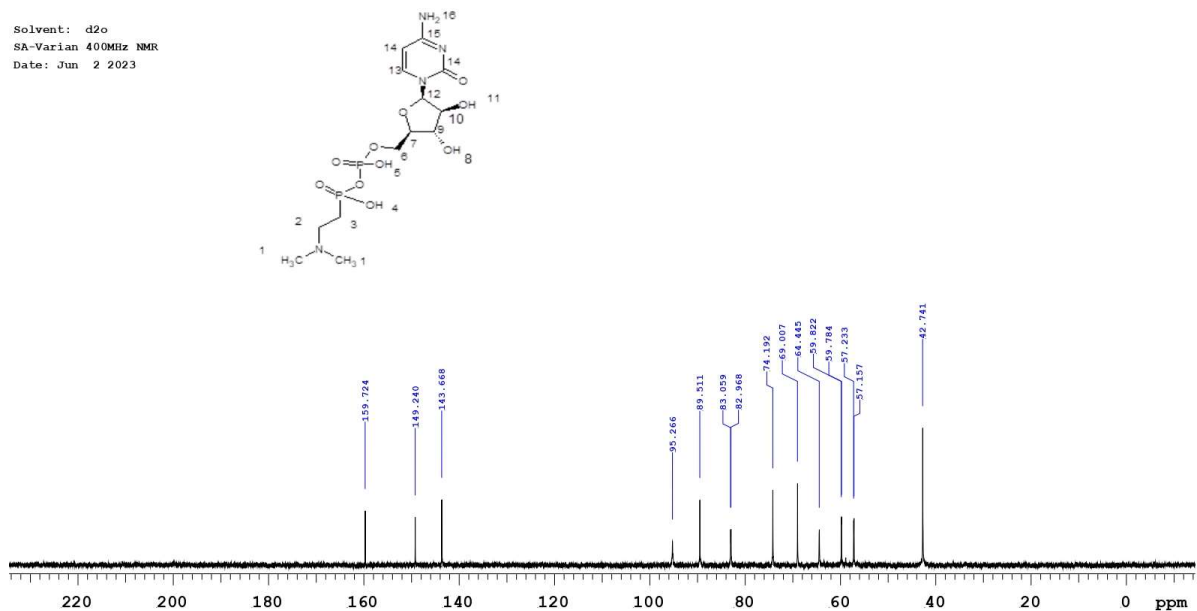


Fig.S6: ¹³C NMR Desmethyl cytidine -5'-diphosphocholine (V)

Sample Code: CIT-2023-104-13-2

Solvent: d2o
SA-Varian 400MHz NMR
Date: May 31 2023

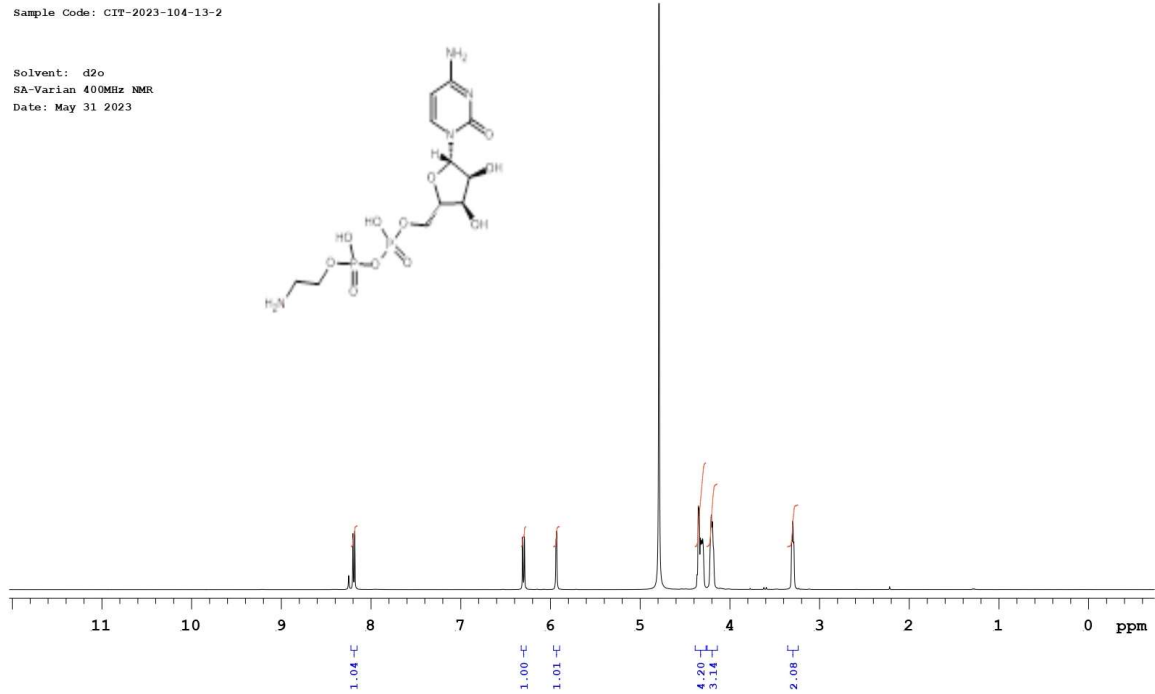


Fig.S7: ¹H NMR Cytidine -5'-diphosphoethanolamine (VI)

Sample Code: CIT-2023-104-13-2-13C-NMR

Solvent: d2o
SA-Varian 400MHz NMR
Date: Jun 2 2023

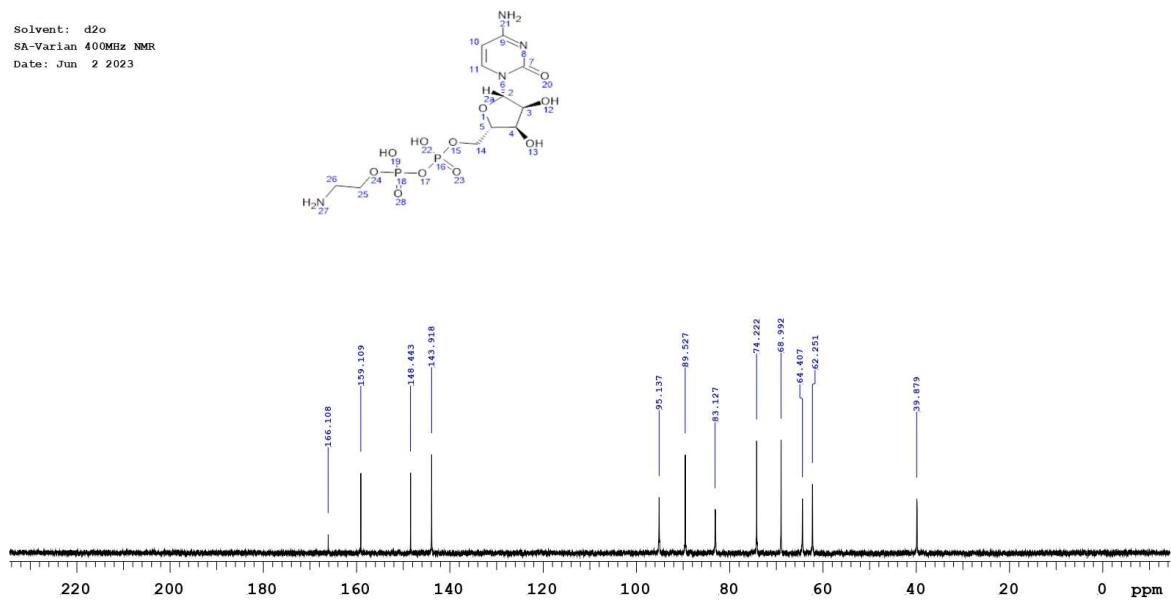


Fig.S8: ¹³C NMR Cytidine -5'-diphosphoethanolamine (VI)

Sample Code: CIT-2023-103-50-1

Solvent: d2o
SA-Varian 400MHz NMR
Date: May 17 2023

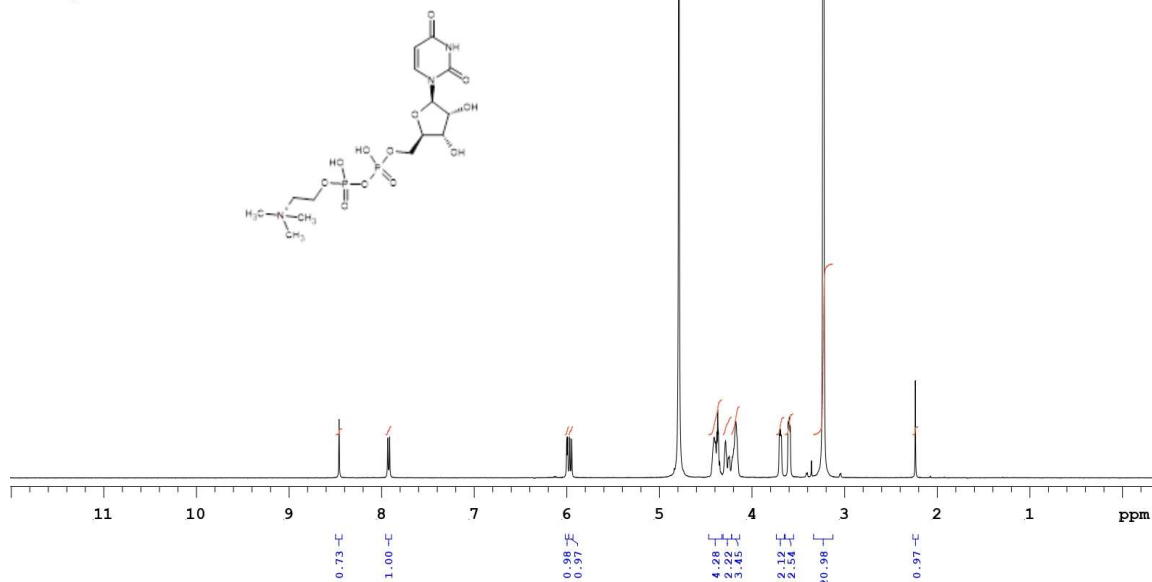


Fig.S9: ^1H NMR Uridine 5'-diphosphocholine (VII)

Sample Code: CIT-2023-103-50-1-13C-NMR

Solvent: d2o
SA-Varian 400MHz NMR
Date: May 20 2023

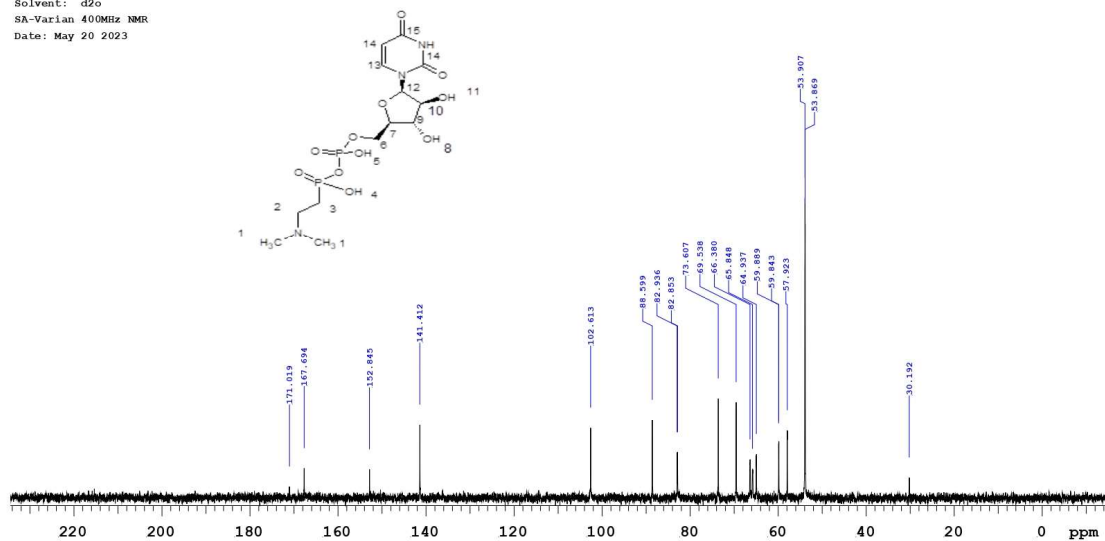


Fig.S10: ^{13}C NMR Uridine 5'-diphosphocholine (VII)