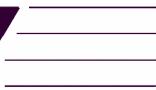


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Supporting Information

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Self-Assembly of N²-Modified Guanosine Derivatives: Formation of Discrete G-Octamers

Sanela Martić, Xiangyang Liu, Suning Wang,* and Gang Wu*

Figure 1. ^1H spectrum of p-pyrenyliodophenyl (**1**).

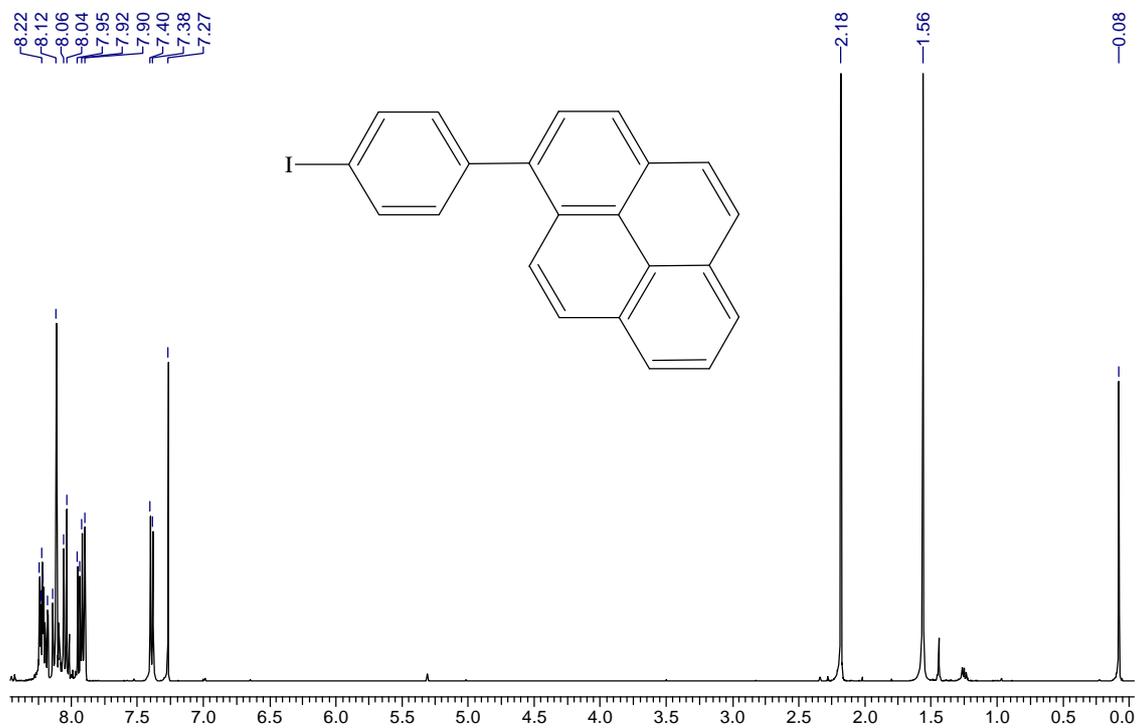


Figure 2. ^{13}C spectrum of p-pyrenyliodophenyl (**1**).

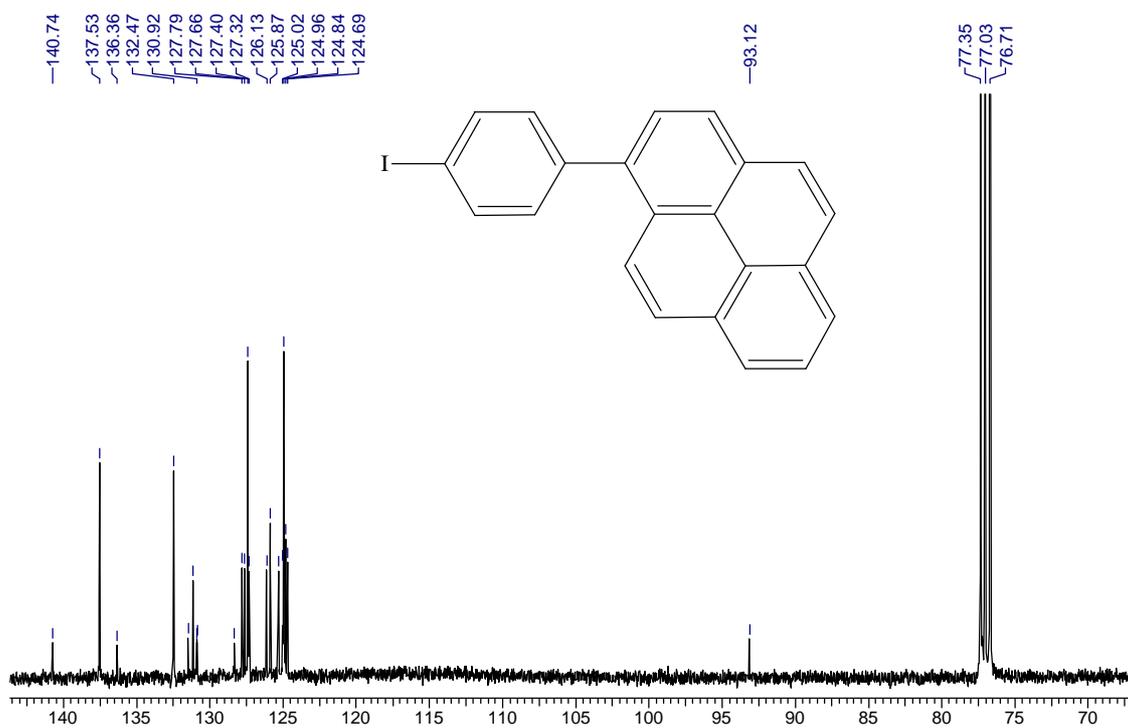


Figure 3. ^1H spectrum of N^2 -(4-pyrenylphenyl) guanosine (**2**).

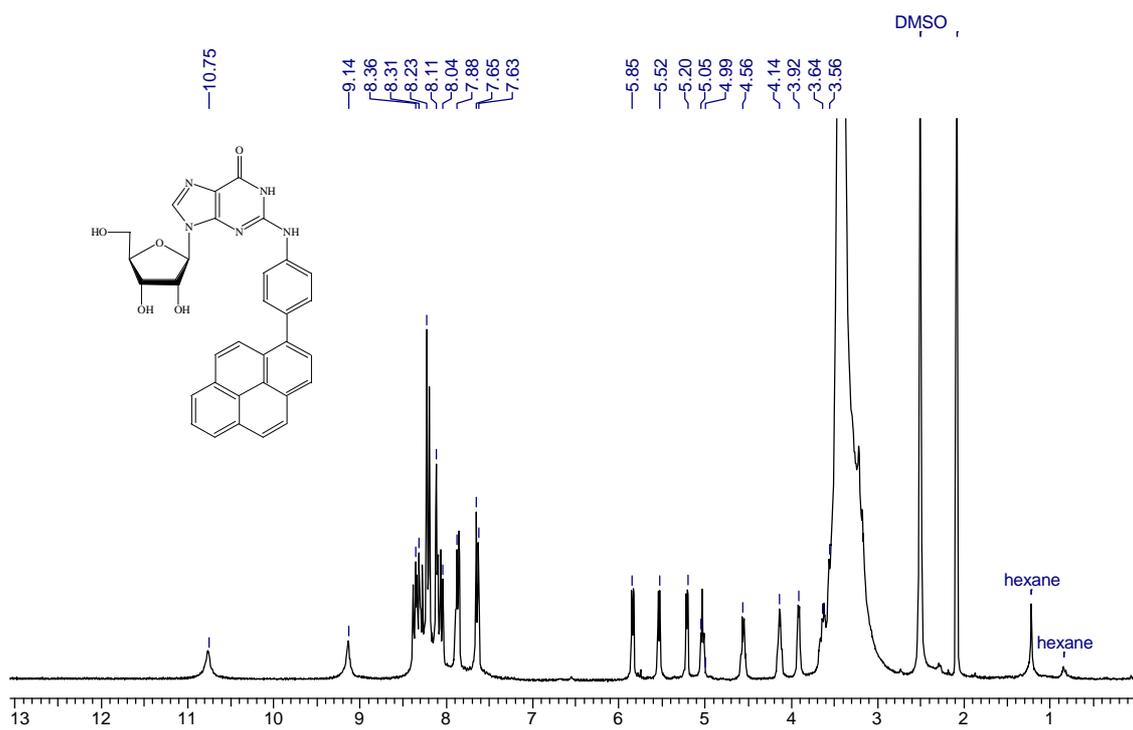


Figure 4. ^{13}C spectrum of N^2 -(4-pyrenylphenyl) guanosine (**2**).

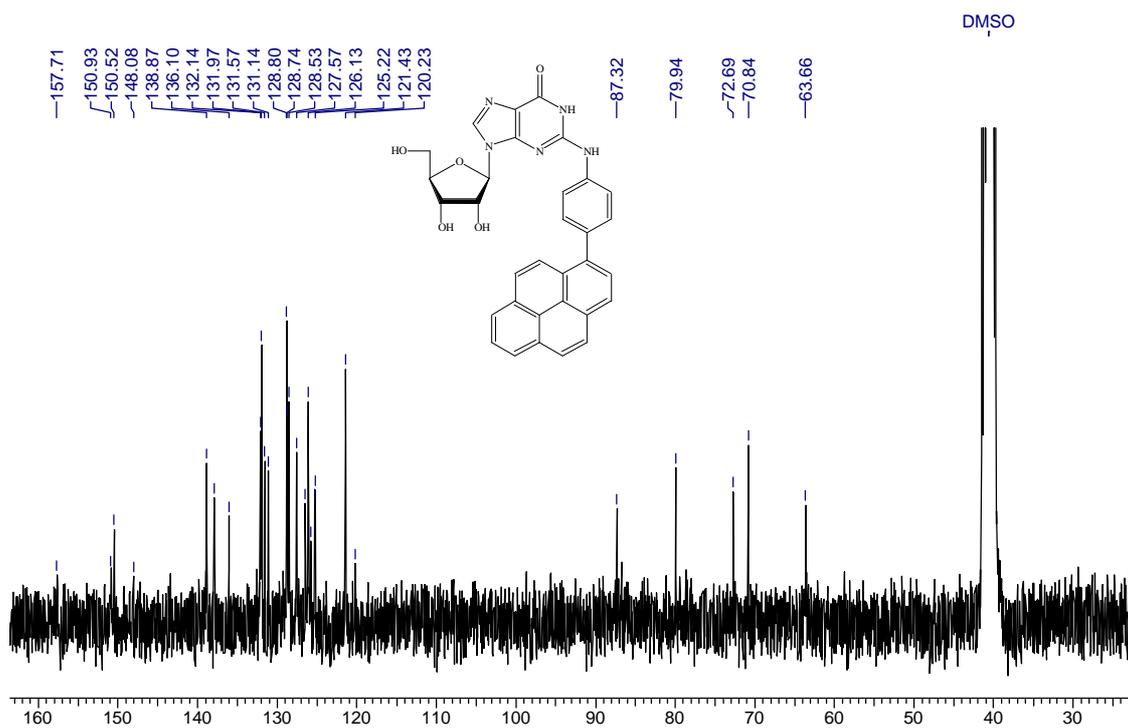


Figure 5. COSY spectrum of N²-(4-pyrenylphenyl) guanosine (**2**).

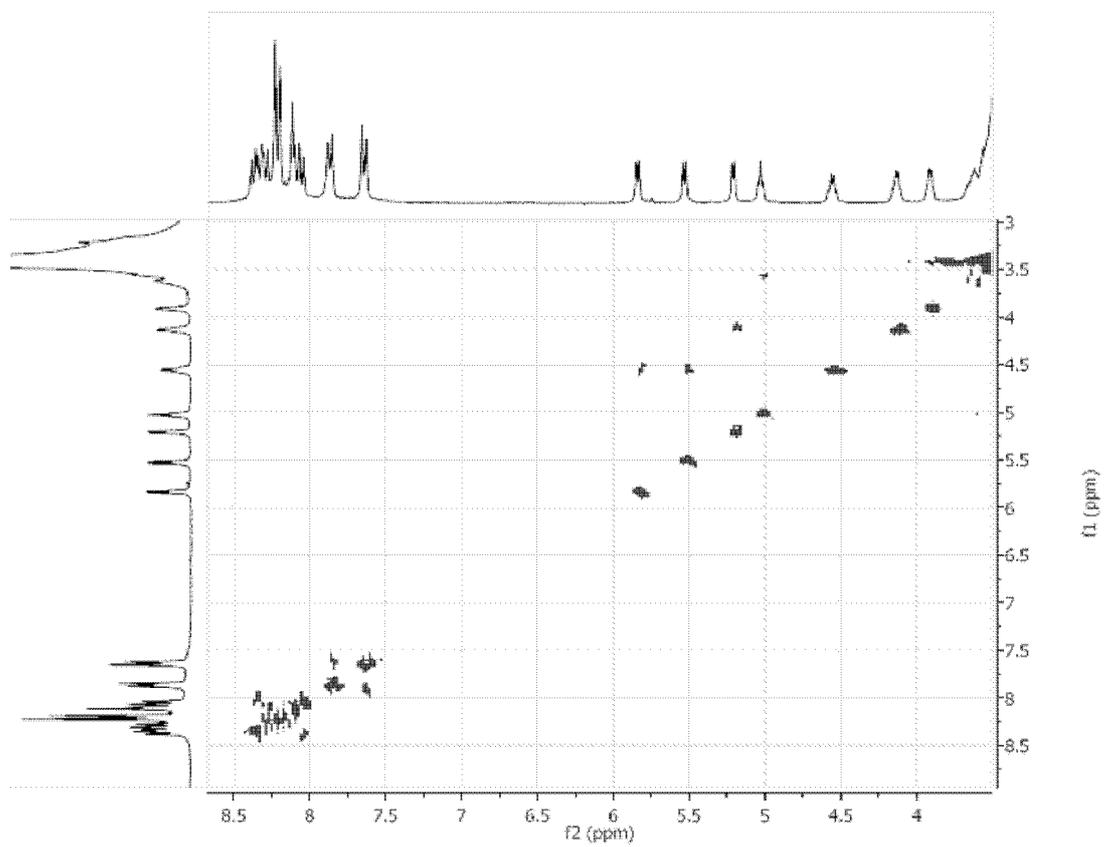


Figure 6. ^1H spectrum of N^2 -(4-pyrenylphenyl)-(2',3',5'-*O*-triacetyl) guanosine (**G2**).

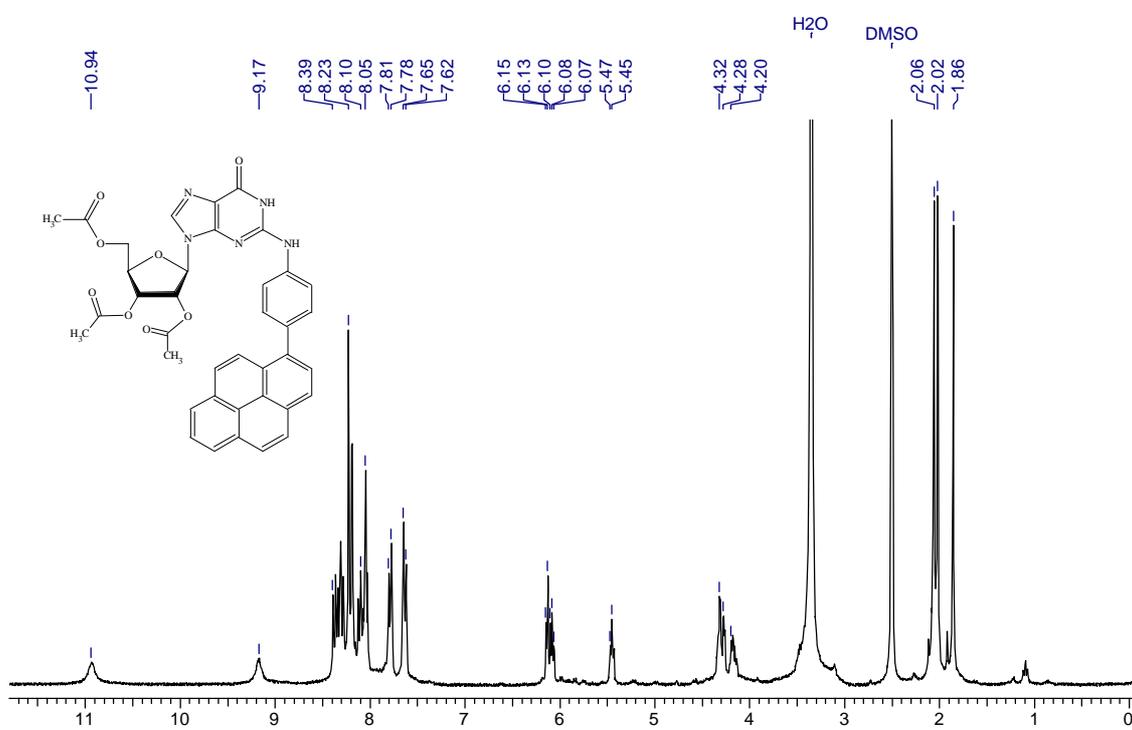


Figure 7. ^{13}C spectrum of N^2 -(4-pyrenylphenyl)-(2',3',5'-*O*-triacetyl) guanosine (**G2**).

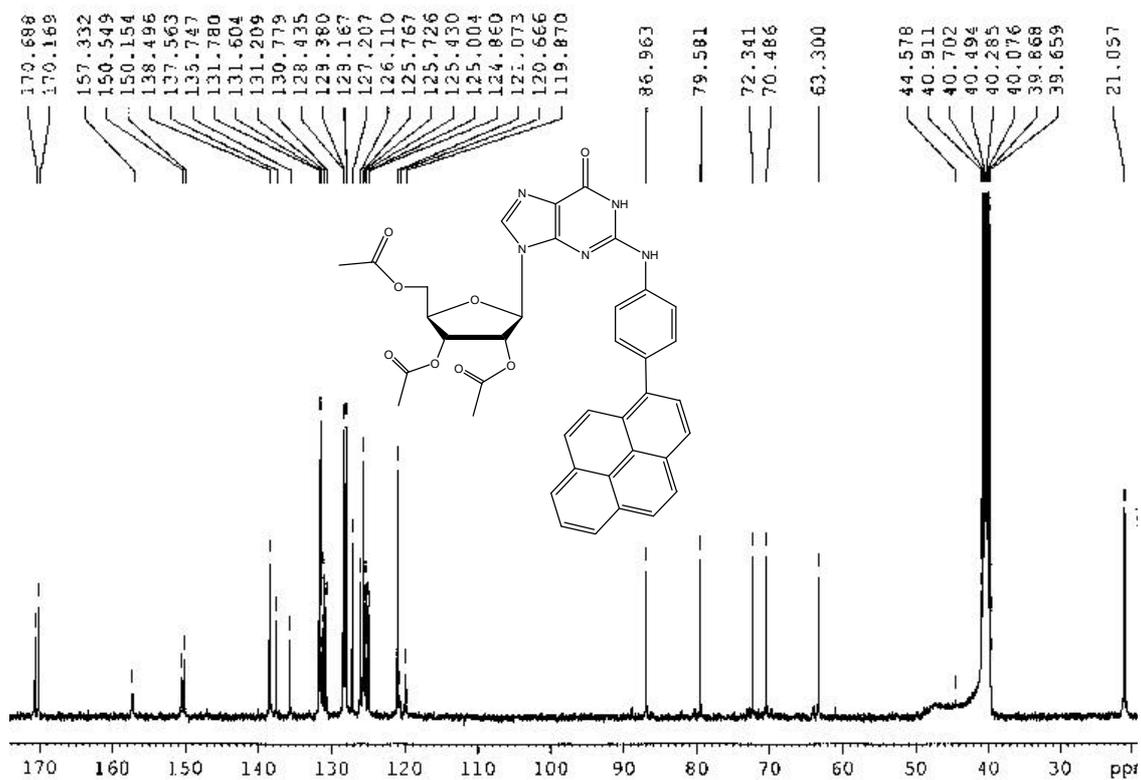


Figure 8. Portions of ^1H NMR spectra of **G2** in CD_2Cl_2 , CDCl_3 , CD_3CN and CD_2COCD_3 at 298 K.

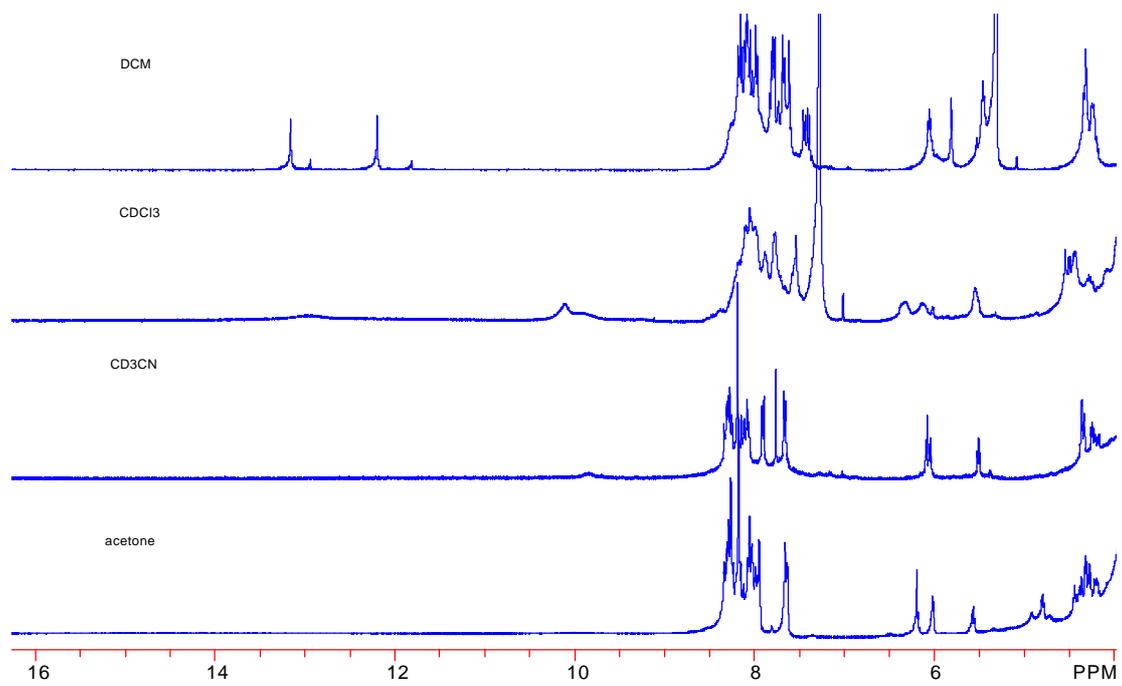


Figure 9. NOESY 2D NMR spectrum of **G2** in CD₂Cl₂ at 298 K.

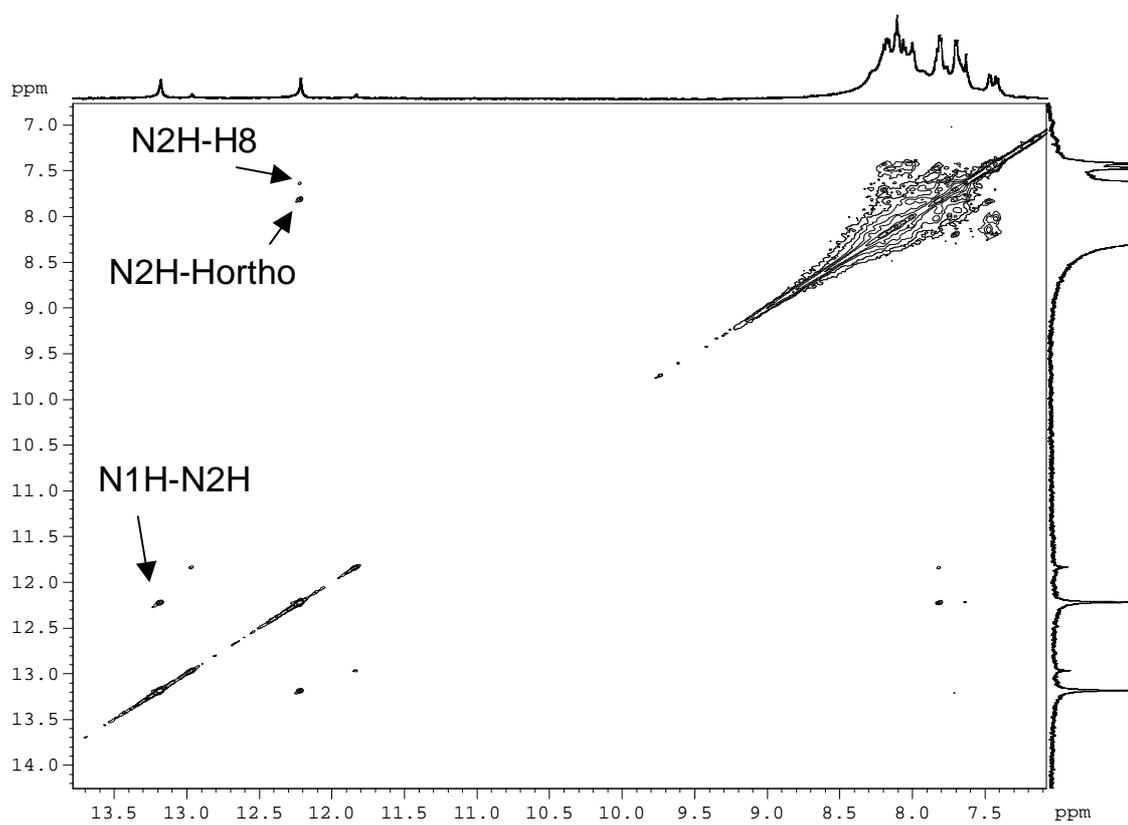


Figure 10. ^{23}Na NMR spectrum of **G1** in CD_3CN at 278 K.

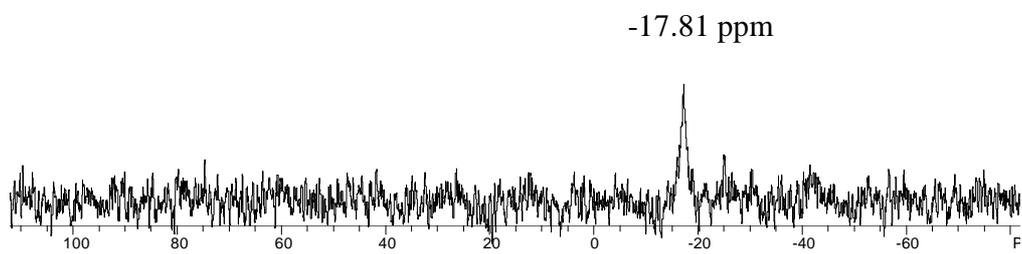


Figure 11. Portions of 1D ^1H NMR spectra of **G1** in CD_2Cl_2 , CD_3CN and $\text{CD}_2\text{Cl}_2/\text{CD}_3\text{CN}$ (1:1) at 298 K.

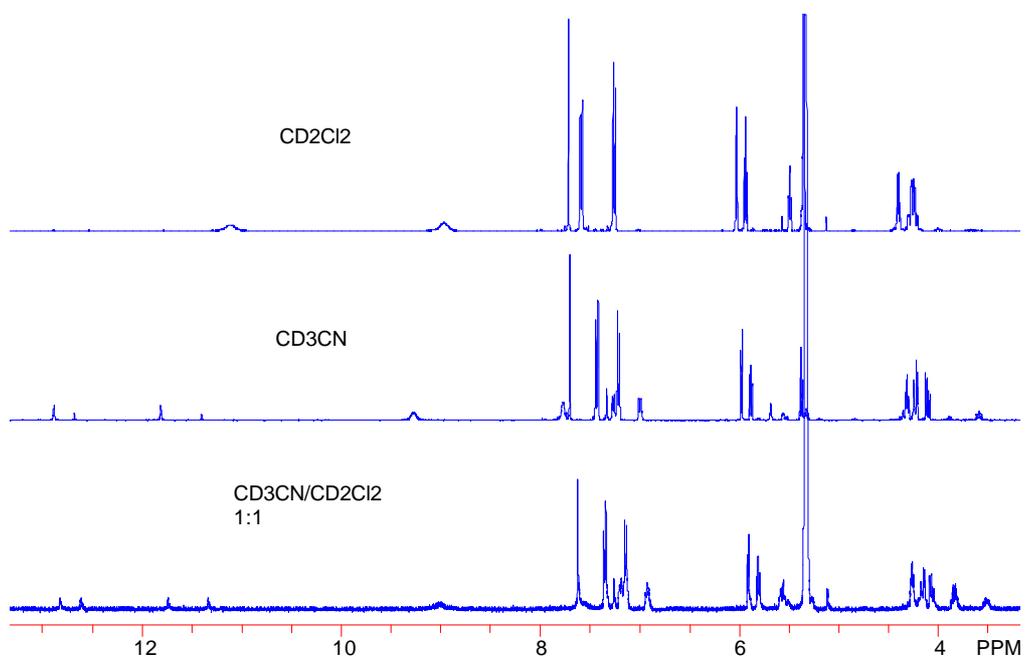


Figure 12. NOESY 2D NMR spectrum of **G1** in CD₃CN at 298 K (negative NOE peaks are in black and positive NOE peaks are in red).

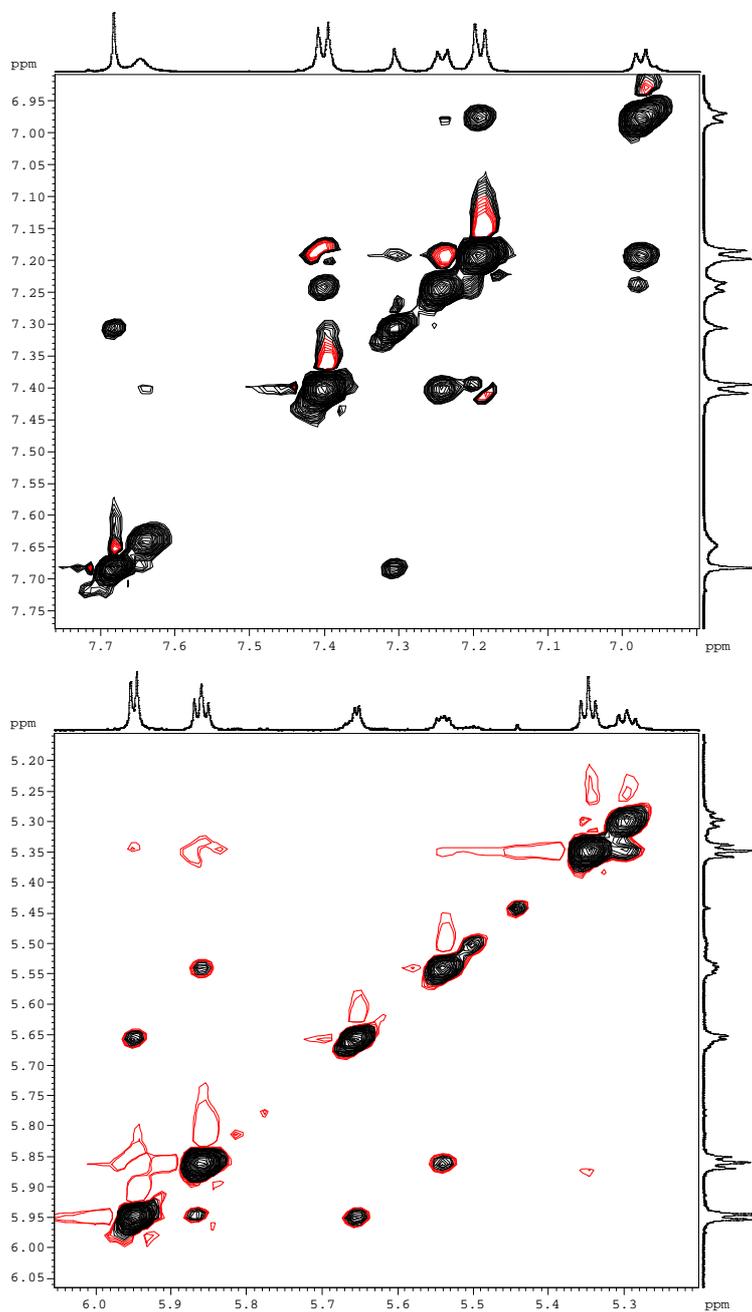


Figure 13. NOESY 2D NMR spectrum of **G1** in CD₃CN at 218 K.

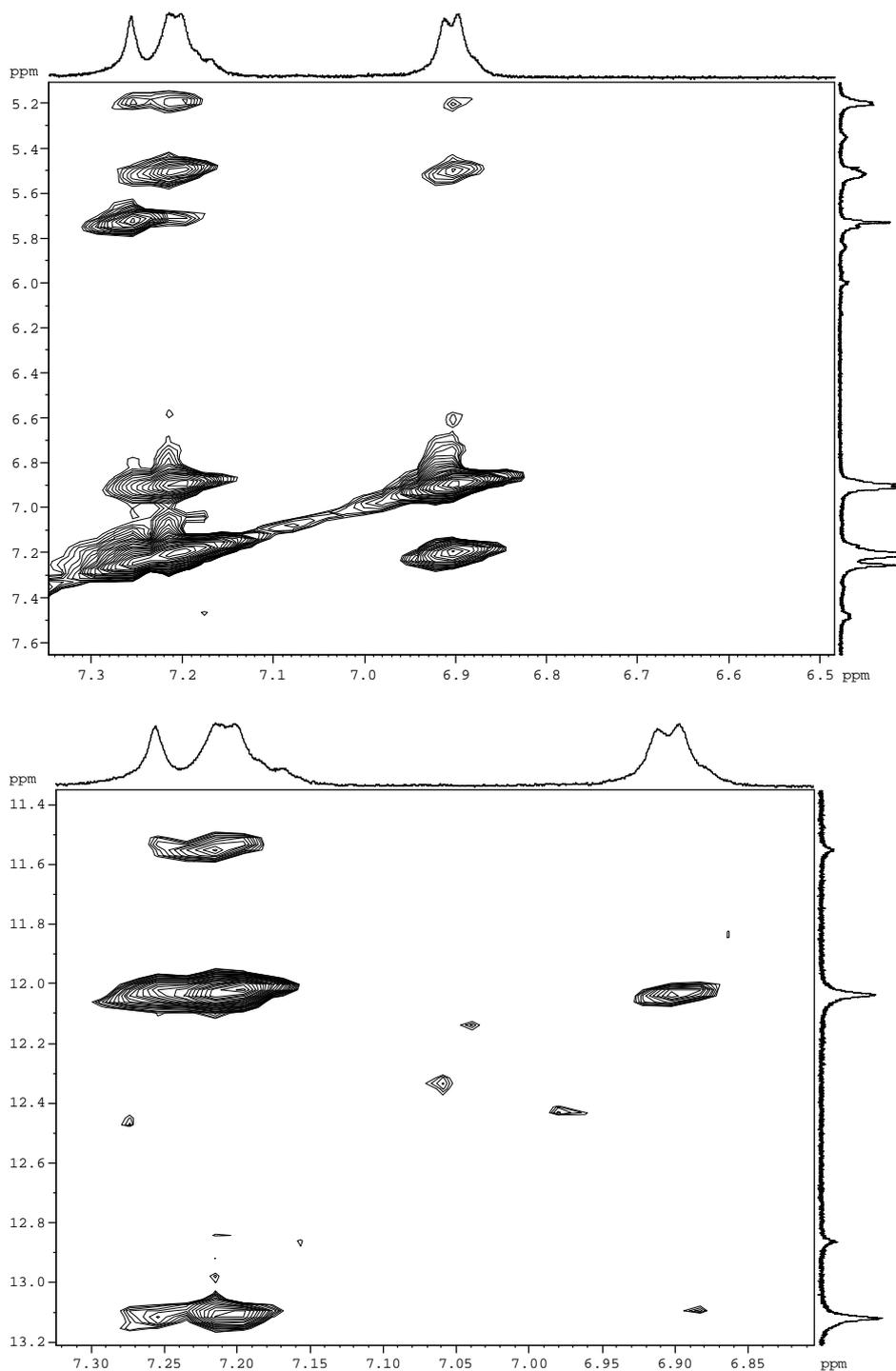


Figure 14. Variable temperature ^1H NMR spectra of **G1** in CD_3CN (star-**G1** monomer, arrow – **G1** octamer; temperature is given in Kelvin).

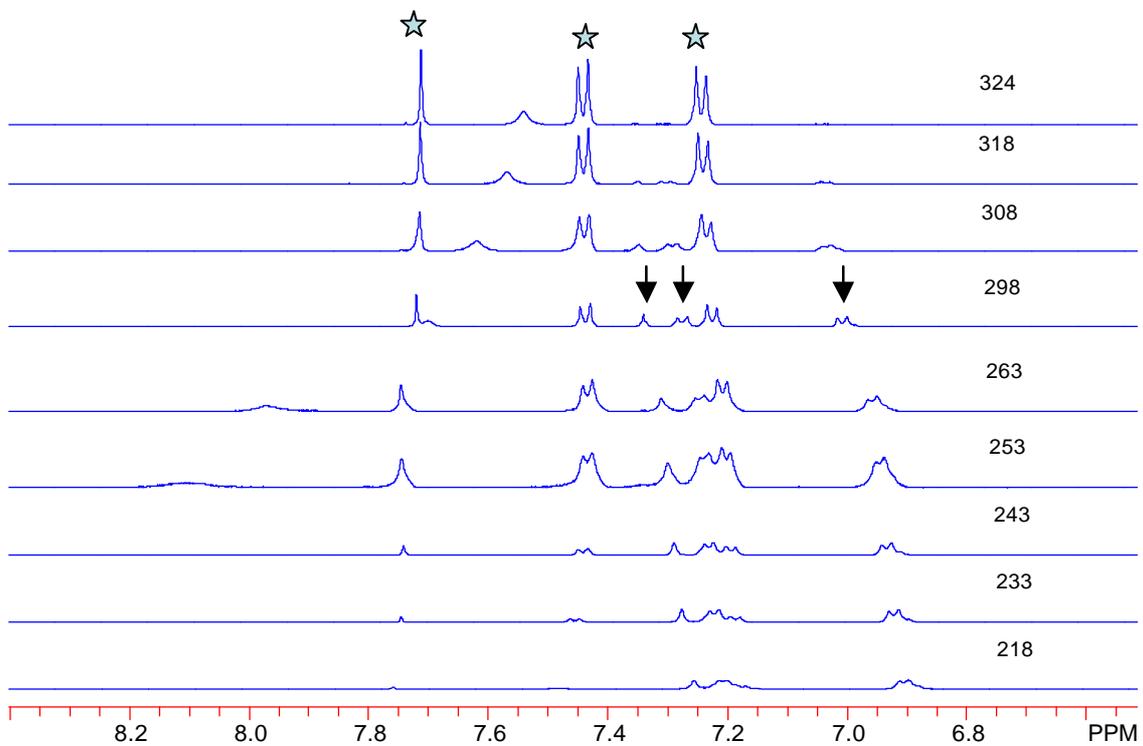


Figure 15. Full ESI-MS spectrum of **G1** in nitromethane.

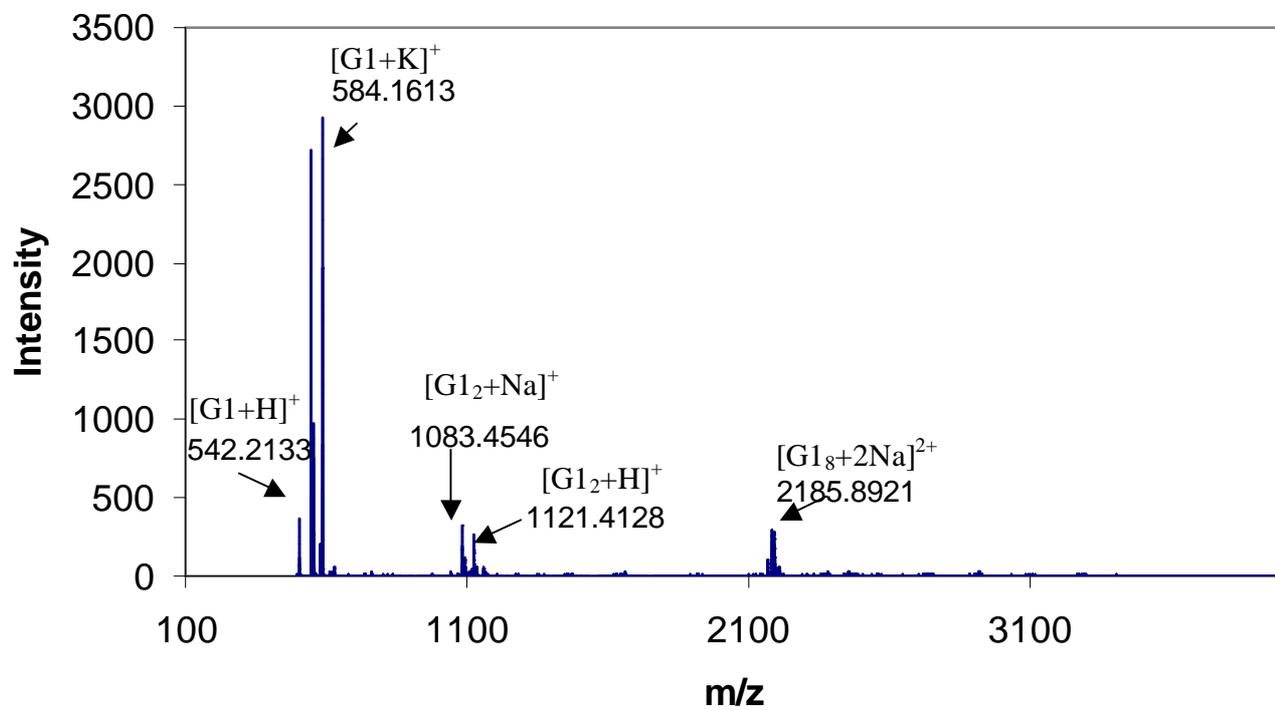


Figure 16. CD spectra of **G1** in acetonitrile at various temperatures shown in Kelvin ([G1]=250 μ M).

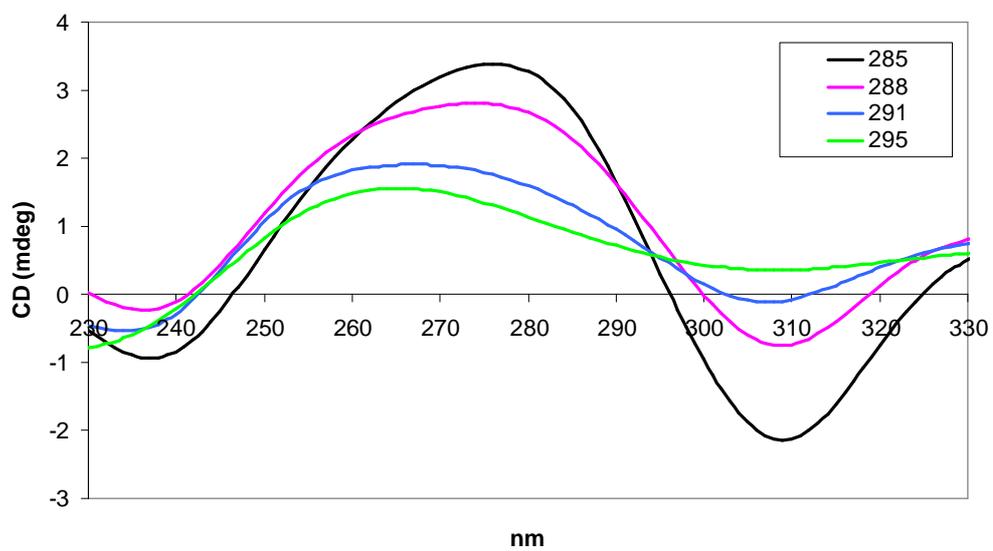
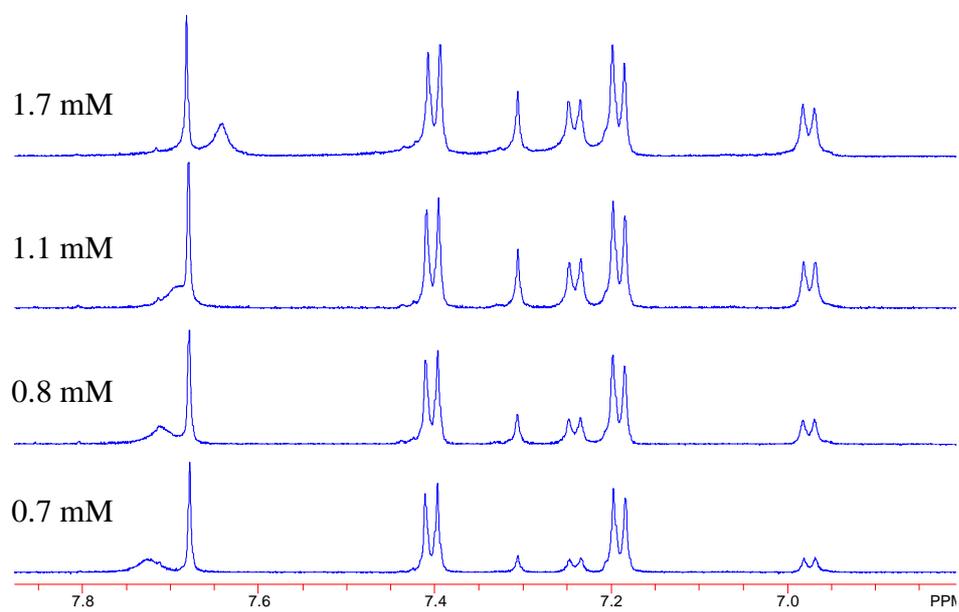


Figure 17. NMR dilution experiments of **G1** in CD₃CN at a) 298 K and b) 283 K

a)



b)

