

## SUPPLEMENTARY INFORMATION

### **Rationally designed squaryldiamides – a novel class of sugar-nucleotide mimics?**

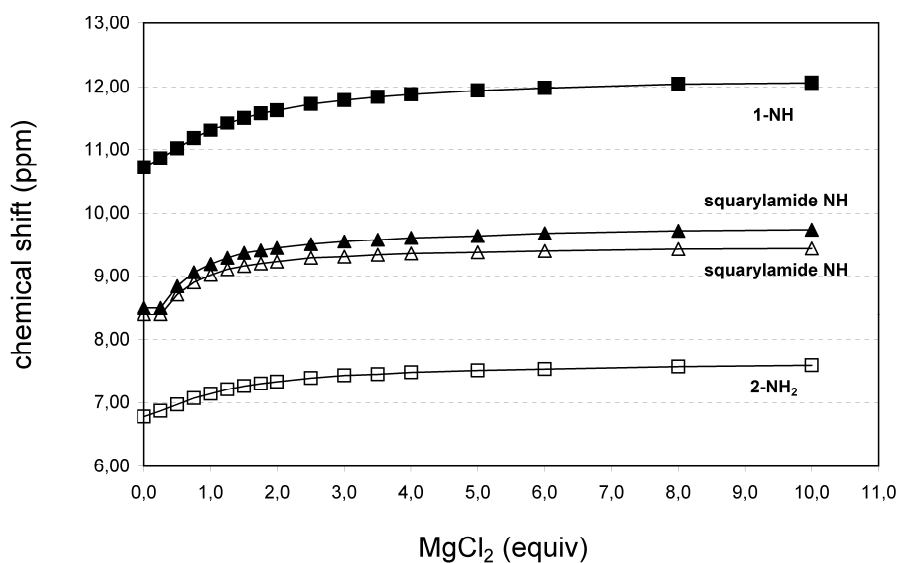
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Richard J. Morris;<sup>3</sup> Gerd K. Wagner<sup>1,\*</sup>

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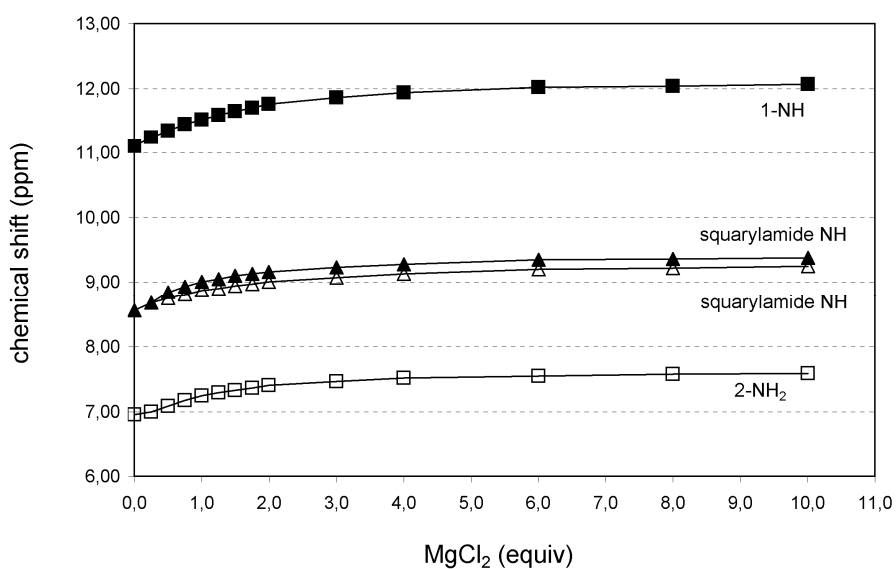
*\*Correspondence should be addressed to G.K.W.*

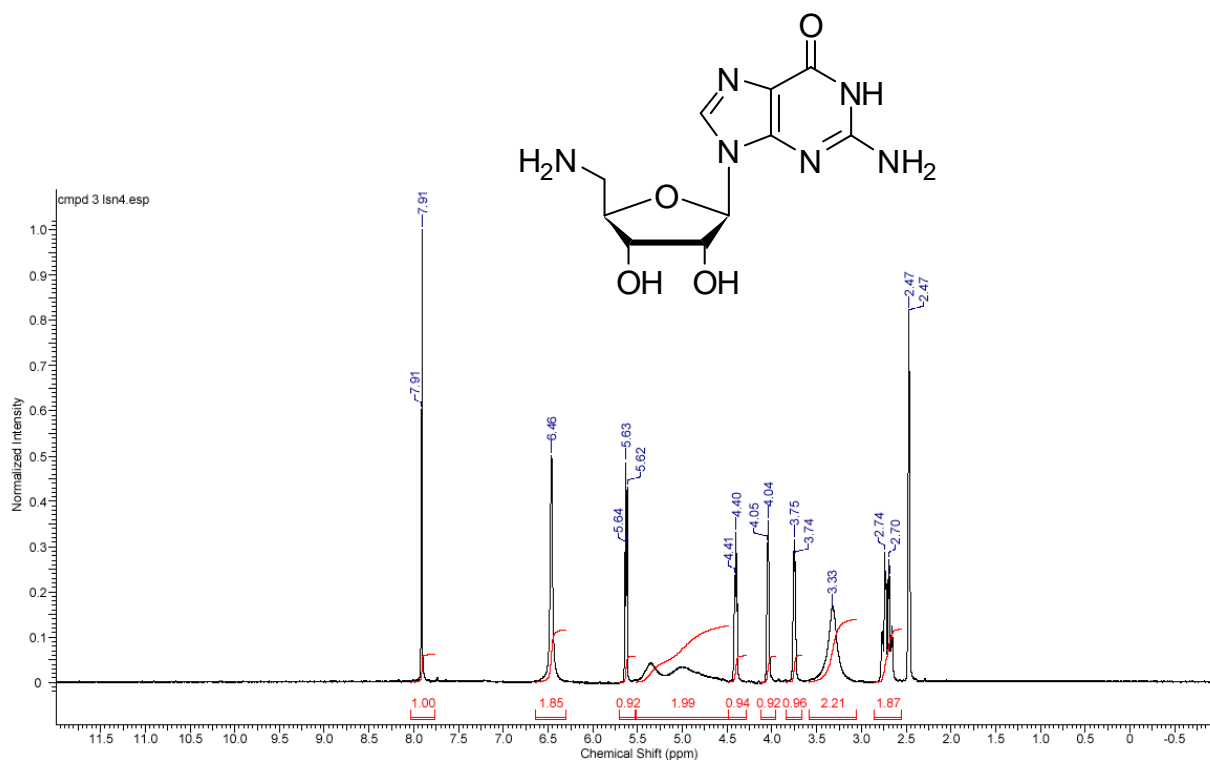
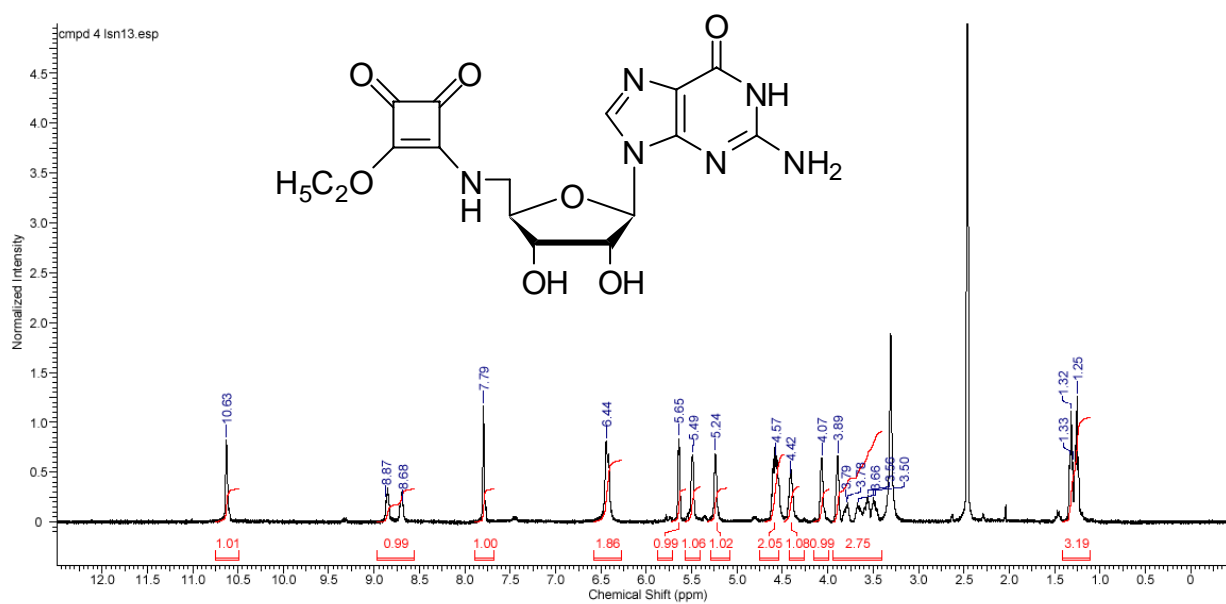
- (i) .....<sup>1</sup>H-NMR titration curves for compounds **5c** and **5g**
- (ii) .....<sup>1</sup>H-NMR spectra of compounds **3**, **4**, **5a-g** and **6a-g**
- (iii) .....<sup>1</sup>H-NMR spectra for titration of **5g** with MgCl<sub>2</sub>

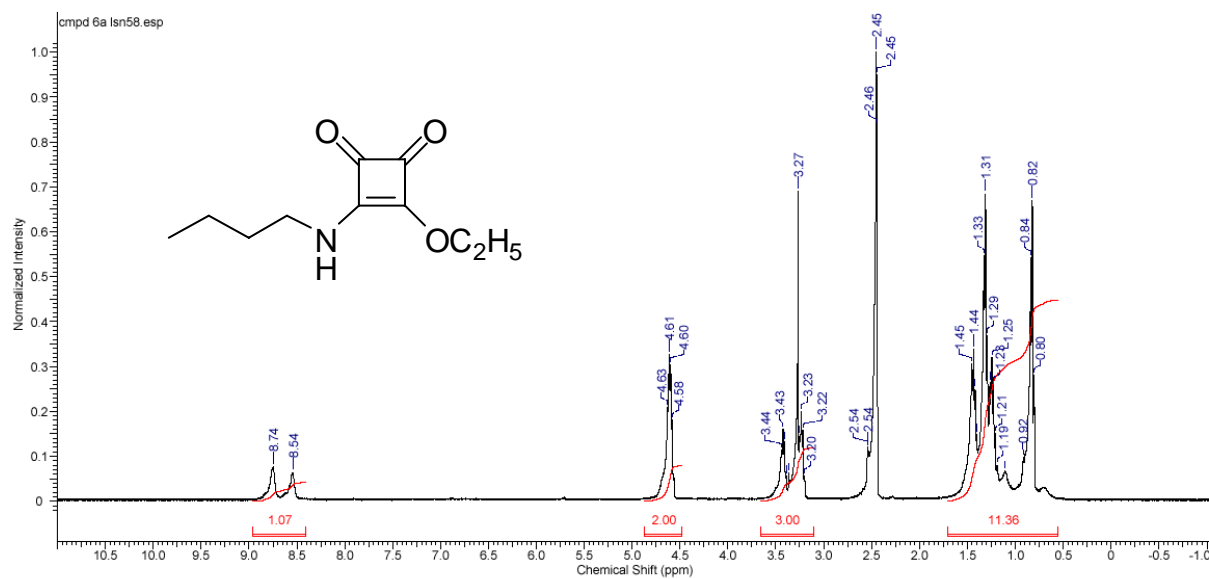
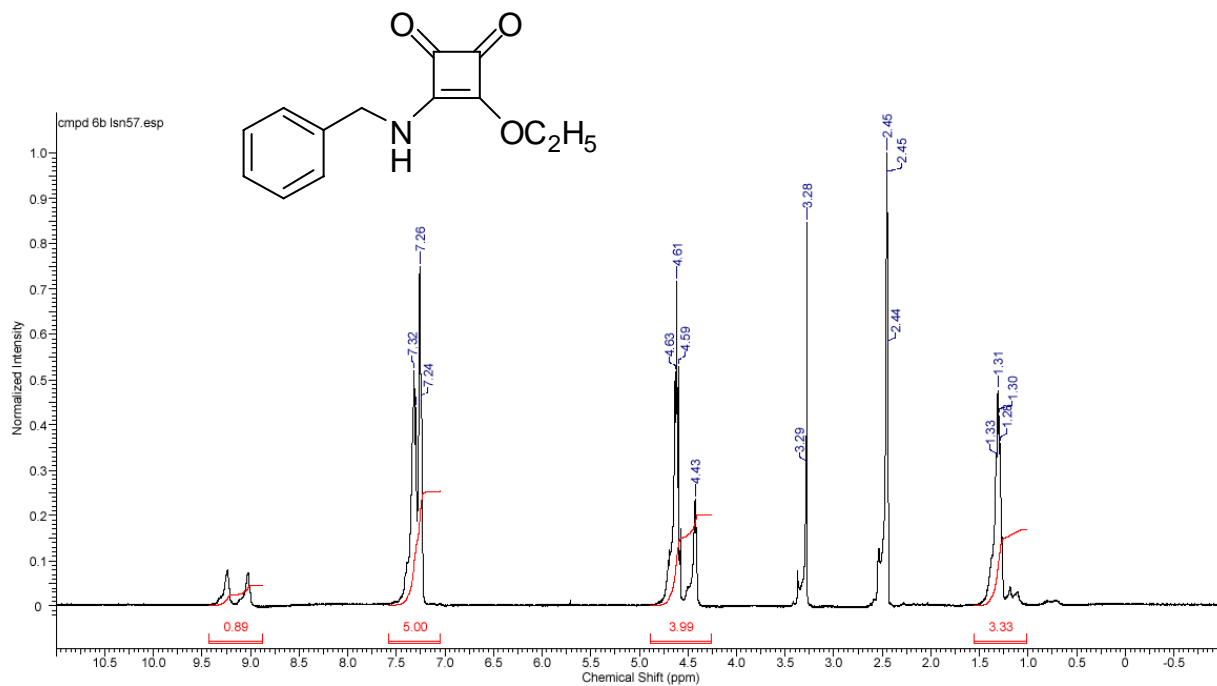
Chemical shifts ( $^1\text{H-NMR}$ ) for diagnostic protons upon titration of **5c** with  $\text{MgCl}_2$

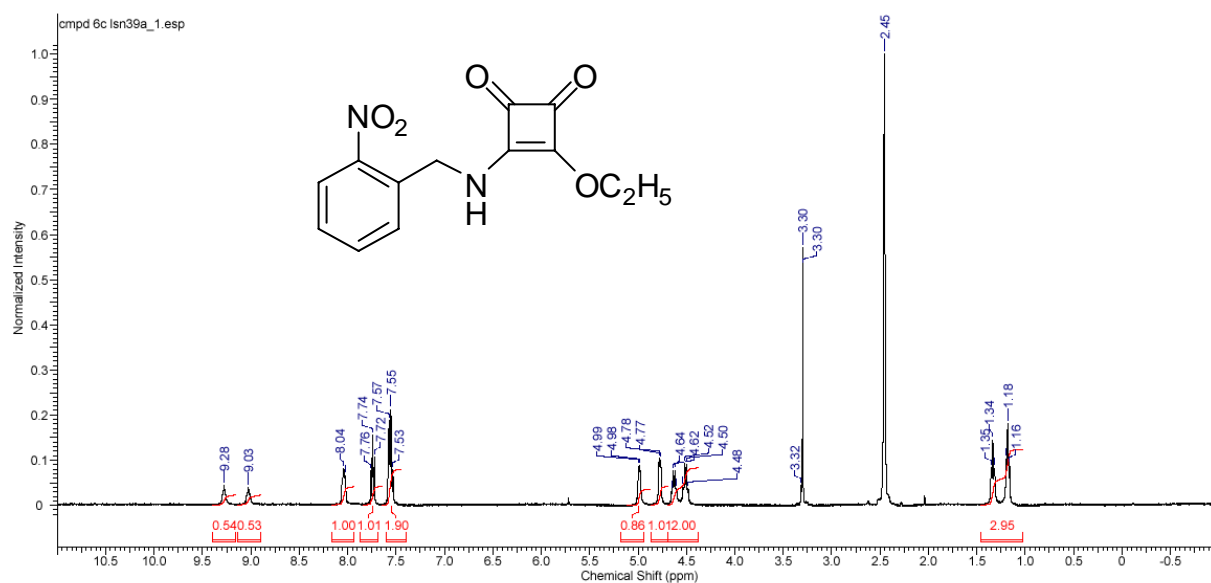
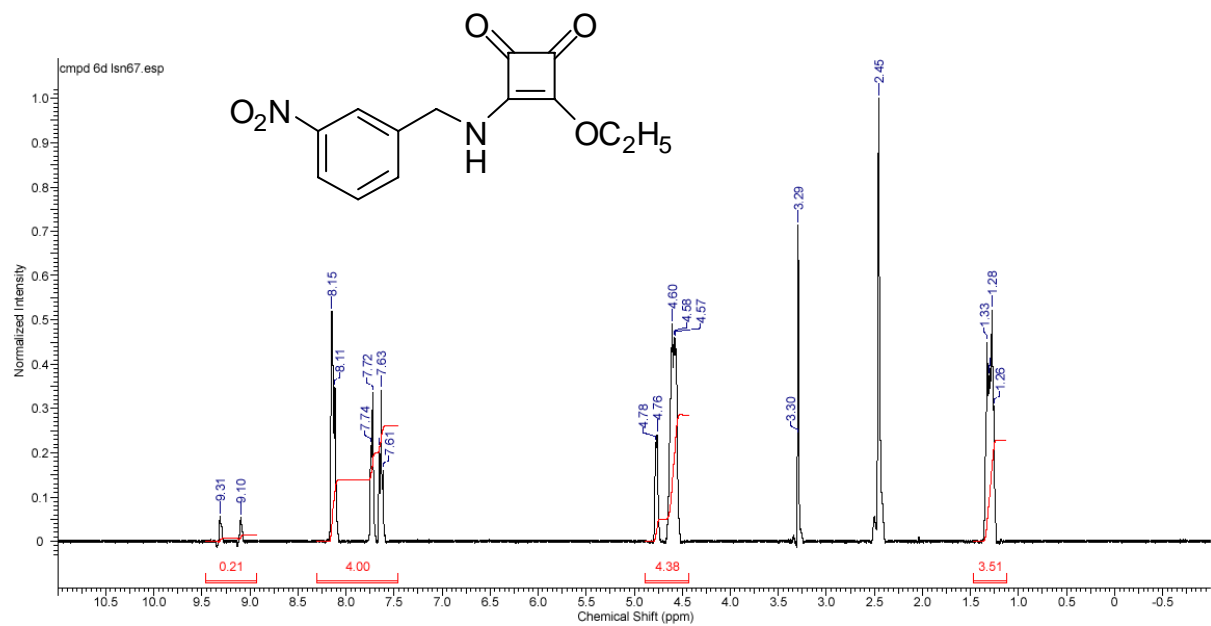


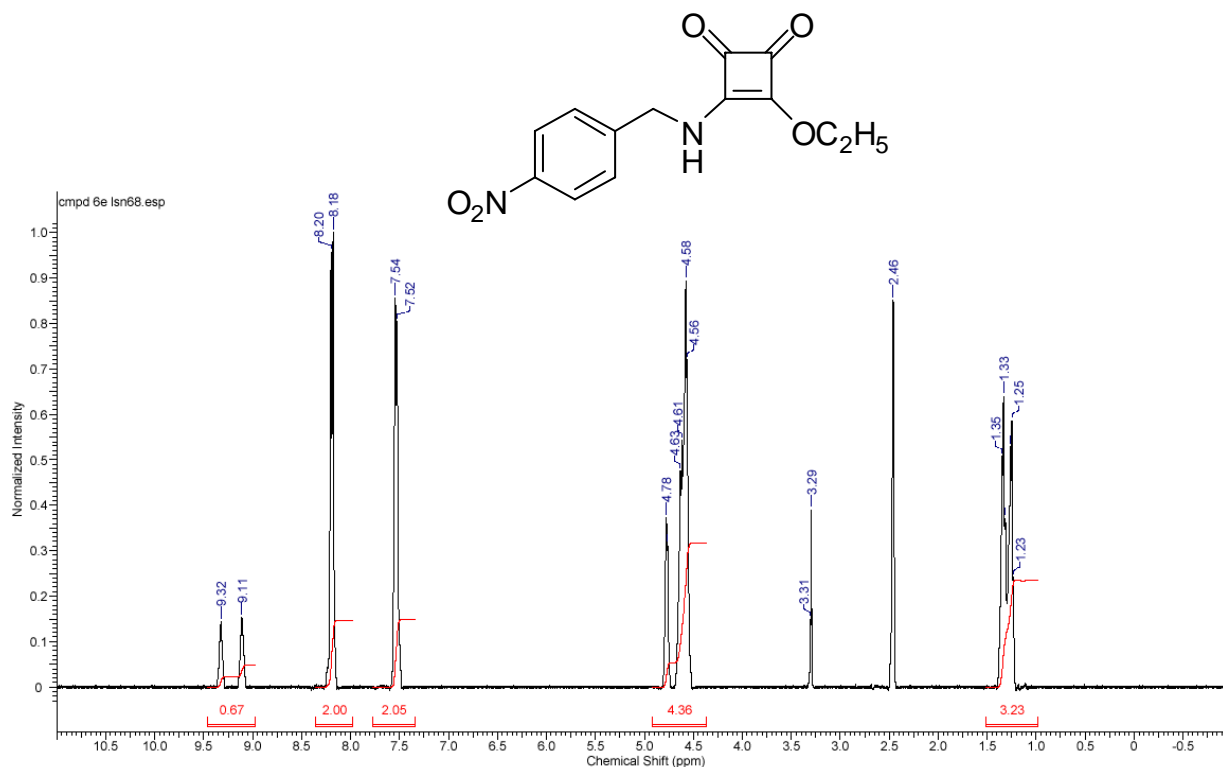
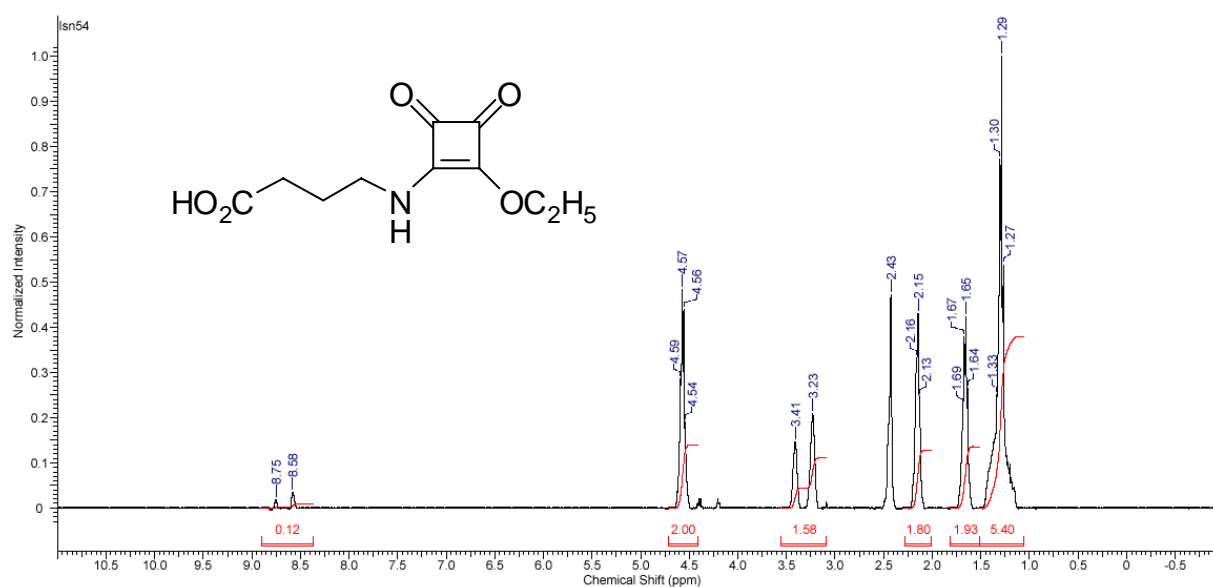
Chemical shifts ( $^1\text{H-NMR}$ ) for diagnostic protons upon titration of **5g** with  $\text{MgCl}_2$

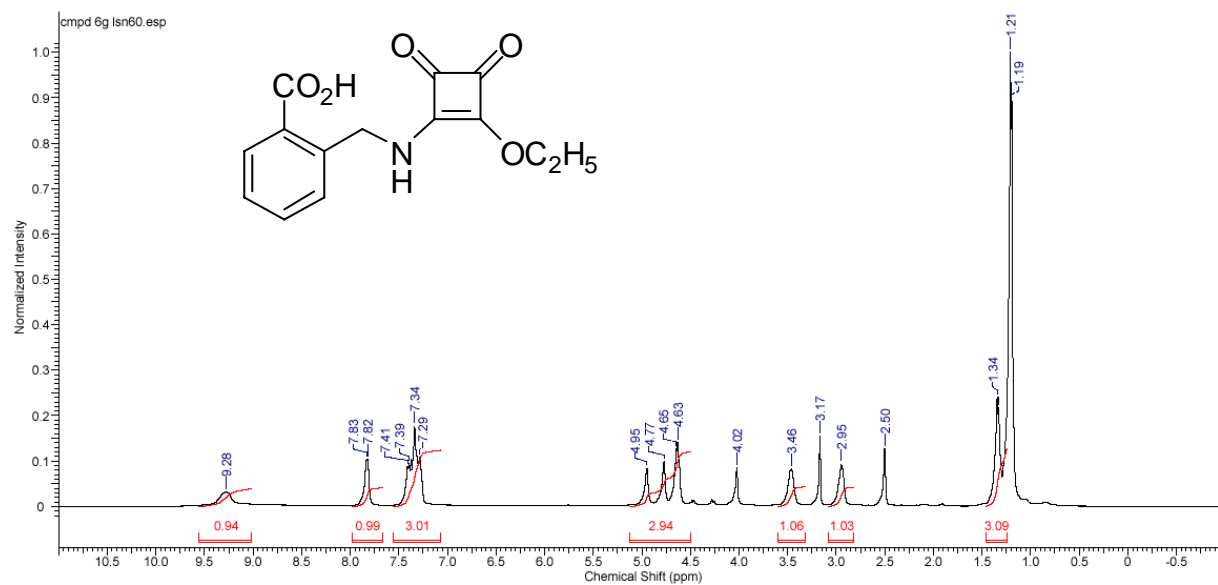
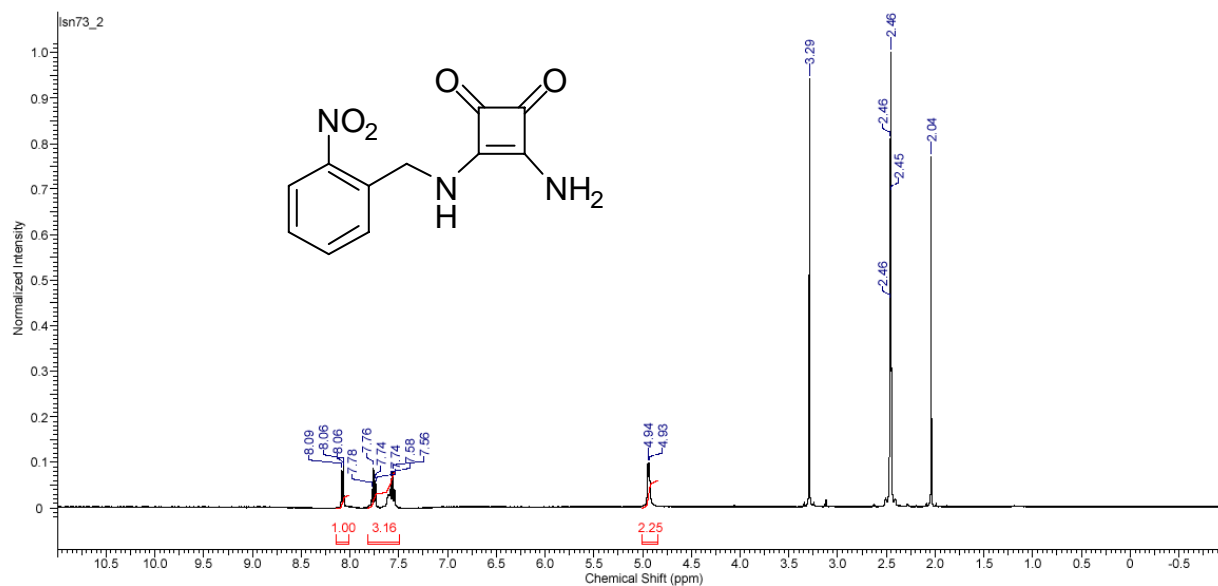


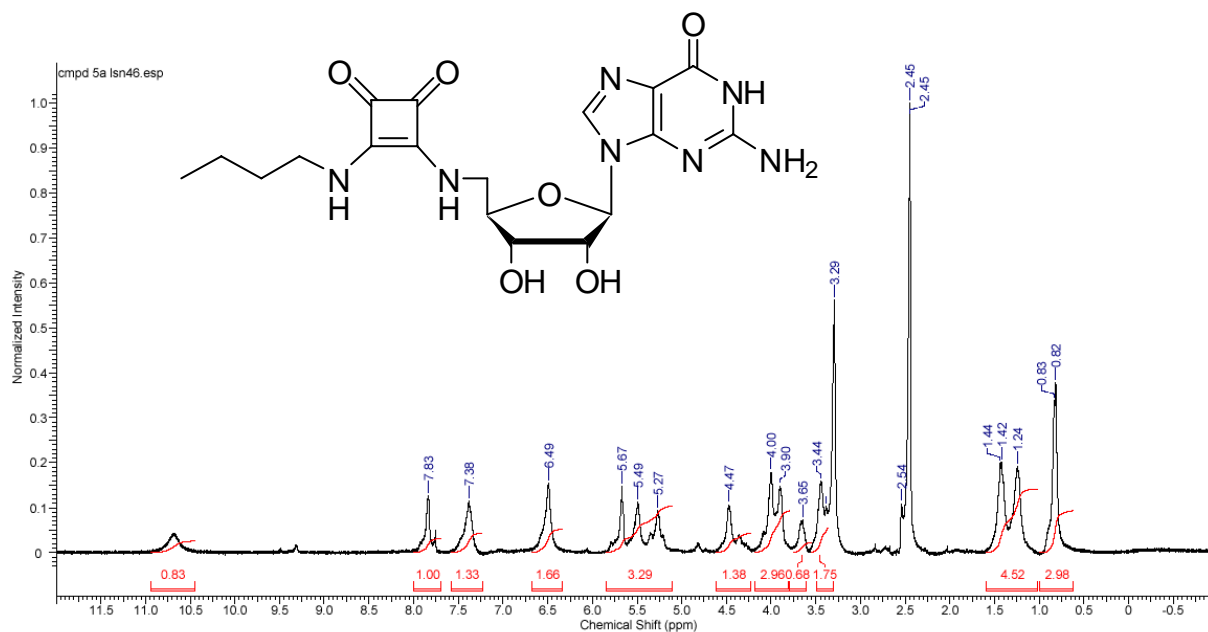
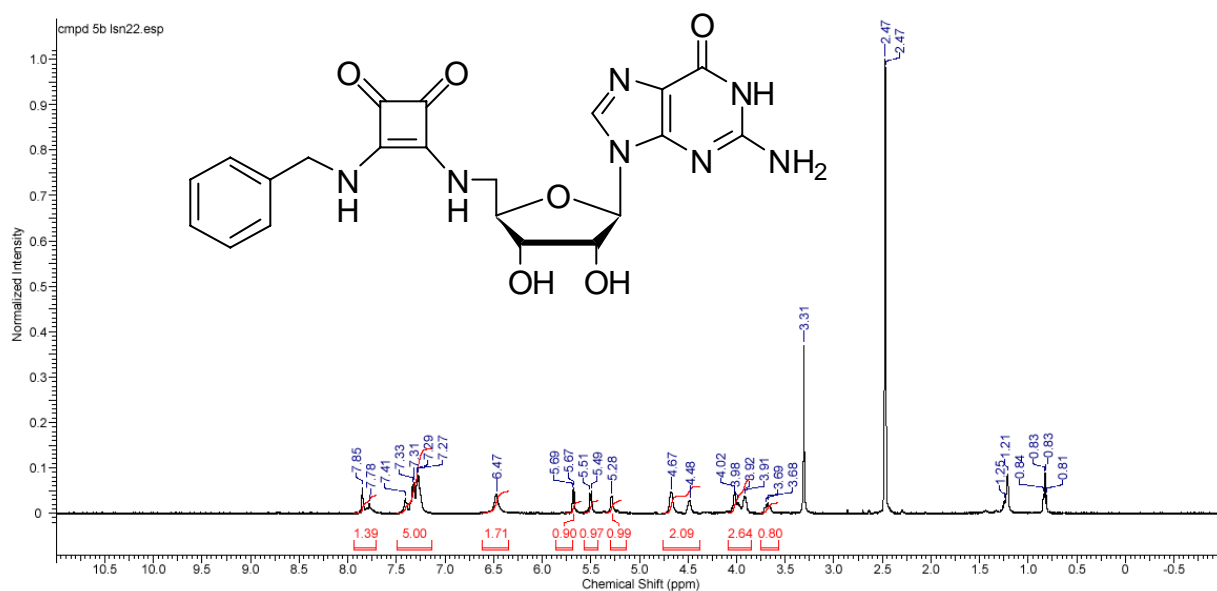
<sup>1</sup>H-NMR spectrum (400 MHz, d6-DMSO) – 3<sup>1</sup>H-NMR spectrum (400 MHz, d6-DMSO) – 4

<sup>1</sup>H-NMR spectrum (400 MHz, d6-DMSO) – **6a**<sup>1</sup>H-NMR spectrum (400 MHz, d6-DMSO) – **6b**

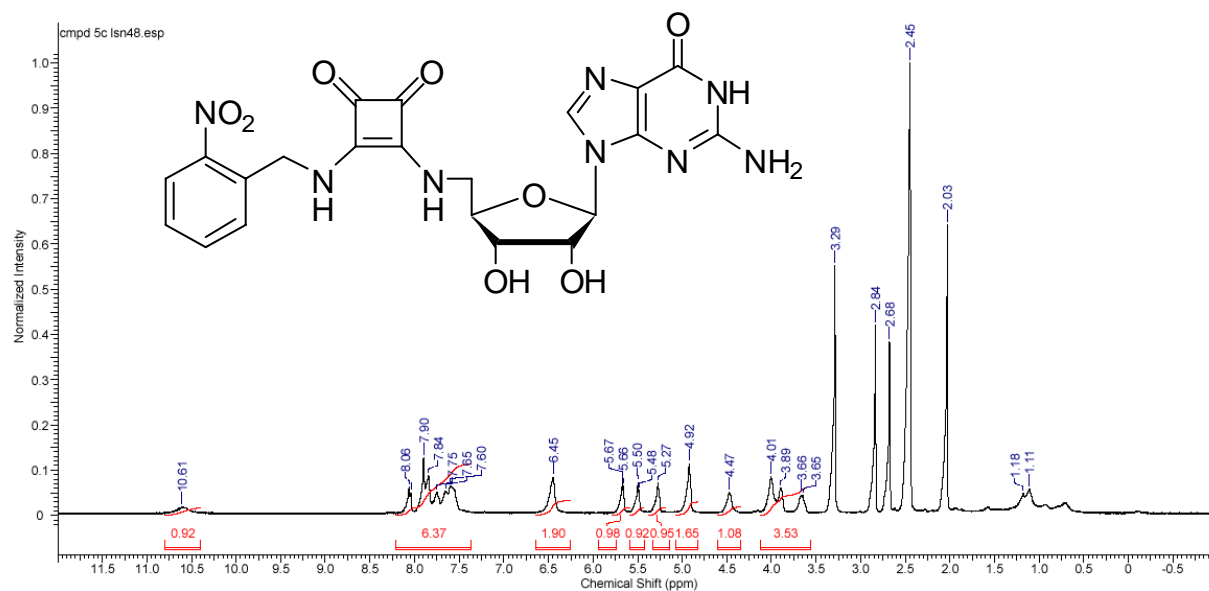
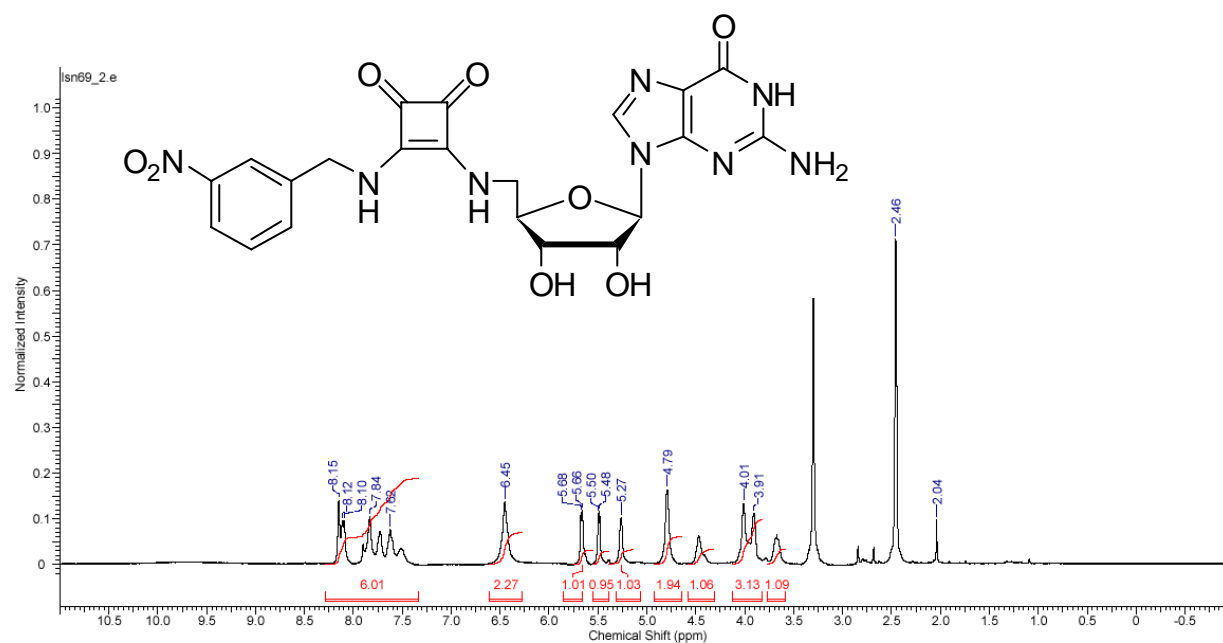
$^1\text{H-NMR}$  spectrum (400 MHz,  $d_6$ -DMSO) – **6c** $^1\text{H-NMR}$  spectrum (400 MHz,  $d_6$ -DMSO) – **6d**

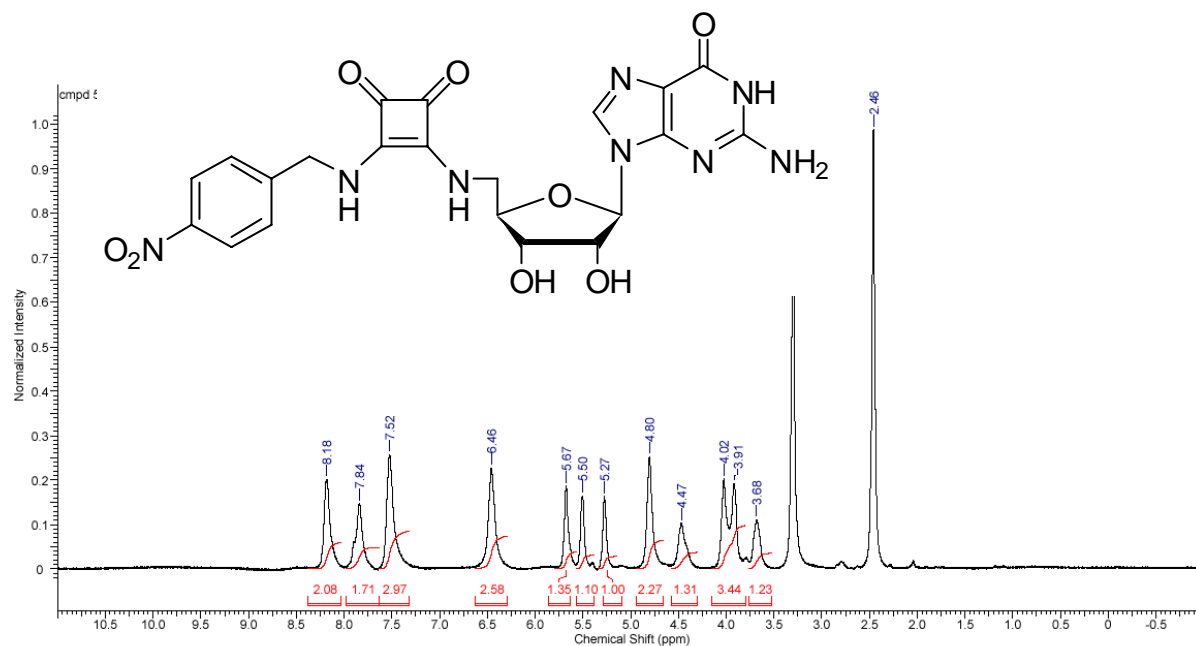
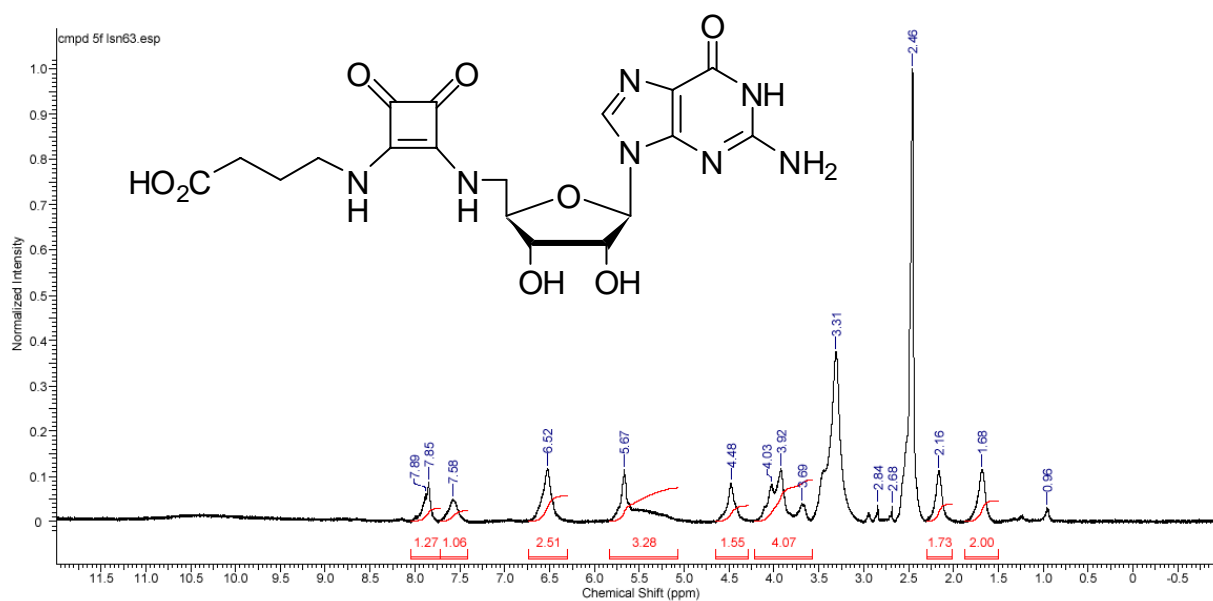
$^1\text{H-NMR}$  spectrum (400 MHz,  $d_6$ -DMSO) – **6e** $^1\text{H-NMR}$  spectrum (400 MHz,  $d_6$ -DMSO) – **6f**

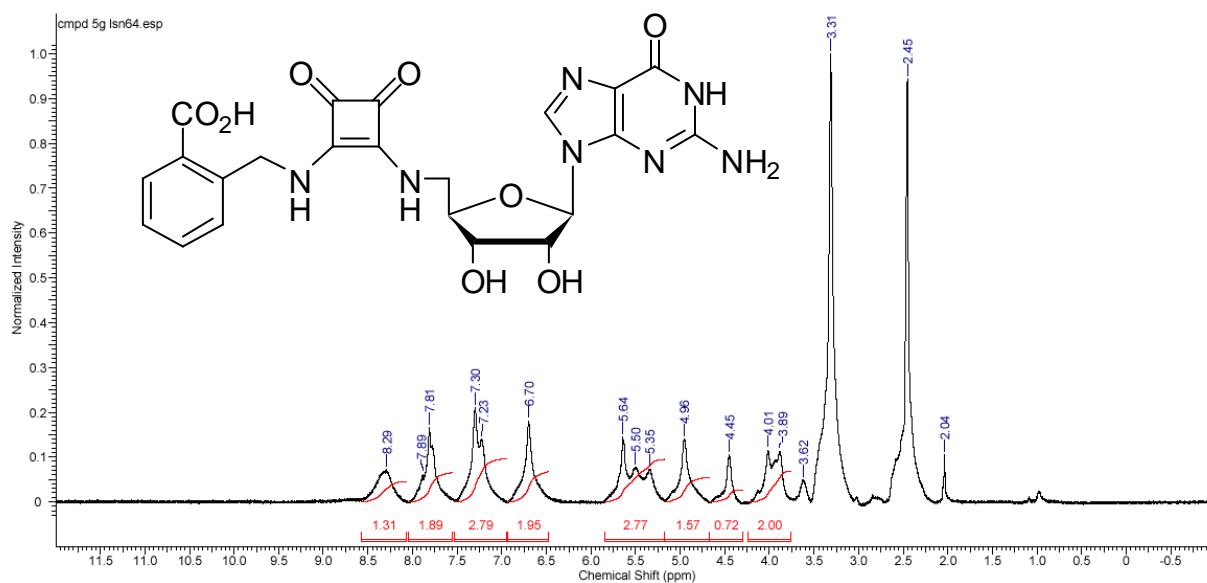
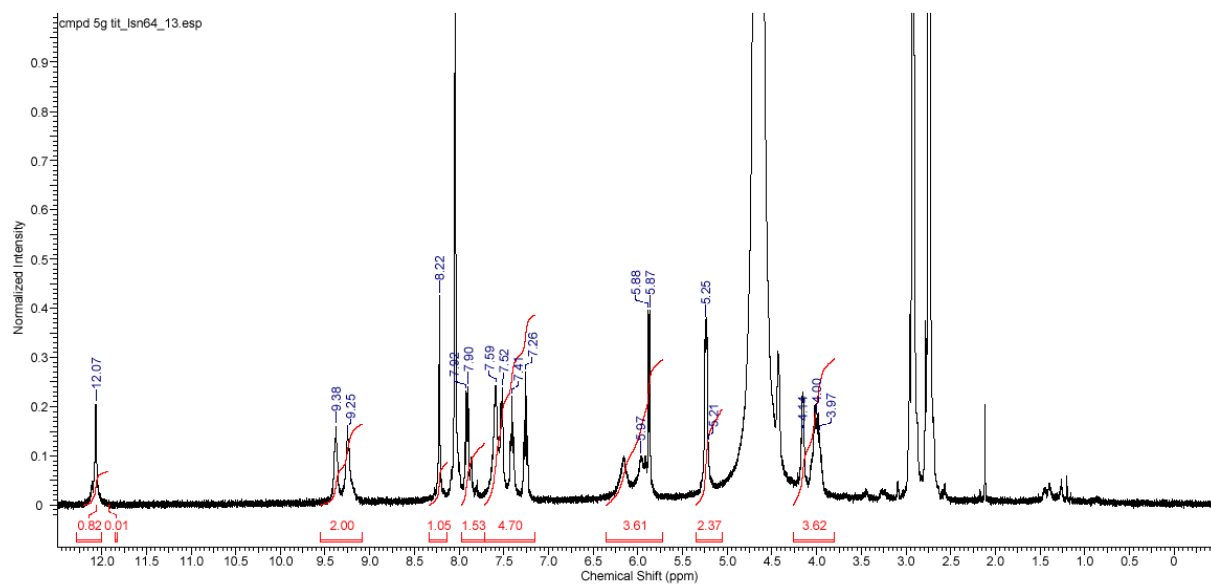
$^1\text{H-NMR}$  spectrum (400 MHz,  $d_6$ -DMSO) – **6g** $^1\text{H-NMR}$  spectrum (400 MHz,  $d_6$ -DMSO) – **7**

$^1\text{H-NMR}$  spectrum (400 MHz,  $d_6$ -DMSO) – **5a** $^1\text{H-NMR}$  spectrum (400 MHz,  $d_6$ -DMSO) – **5b**



<sup>1</sup>H-NMR spectrum (400 MHz, d6-DMSO) – **5c**<sup>1</sup>H-NMR spectrum (400 MHz, d6-DMSO) – **5d**

$^1\text{H-NMR}$  spectrum (400 MHz,  $d_6$ -DMSO) – **5e** $^1\text{H-NMR}$  spectrum (400 MHz,  $d_6$ -DMSO) – **5f**

$^1\text{H-NMR}$  spectrum (400 MHz,  $d_6$ -DMSO) – **5g** $^1\text{H-NMR}$  spectrum (400 MHz,  $d_7$ -DMF) – **5g**

$^1\text{H-NMR}$  spectra for titration of **5g** with  $\text{MgCl}_2$  (400 MHz,  $d_7\text{-DMF}$ )

