

## Supporting Information

### **Functionalized Polyhedral Oligosilsesquioxanes (POSS)based composites for Bone Tissue Engineering: synthesis, computational and biological studies**

Laura Legnani,<sup>a</sup> Daniela Iannazzo,<sup>b</sup> Alessandro Pistone,<sup>b</sup> Consuelo Celesti,<sup>b</sup> Salvatore Giofrè,<sup>c</sup> Roberto Romeo,<sup>c</sup> Angela Di Pietro,<sup>d</sup> Giuseppa Visalli,<sup>d</sup> Monica Fresta,<sup>a</sup> Paola Bottino,<sup>a</sup> Ignazio Blanco<sup>e</sup> and Maria Assunta Chiacchio\*<sup>a</sup>

<sup>a</sup> Dipartimento di Scienze del Farmaco, Università di Catania, Viale A. Doria 6, 95125 Catania, Italy.

<sup>b</sup> Dipartimento di Ingegneria, Università di Messina, Contrada Di Dio, 98166 Messina, Italy.

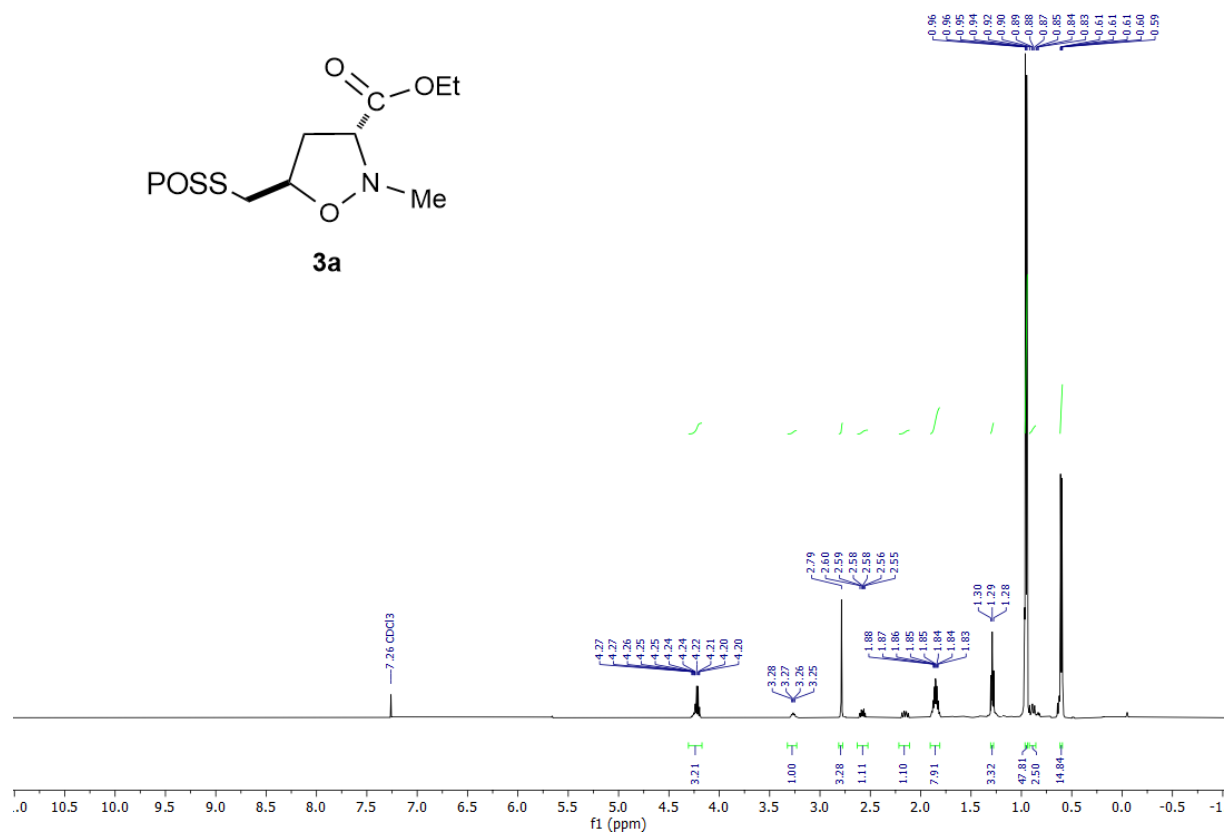
<sup>c</sup> Dipartimento di Scienze chimiche, biologiche, farmaceutiche ed ambientali, Università di Messina, Via S.S. Annunziata, 98168 Messina, Italy.

<sup>d</sup> Dipartimento di Scienze biomediche, odontoiatriche e delle immagini morfologiche e funzionali, via Consolare Valeria 1, 98100, Messina, Italy

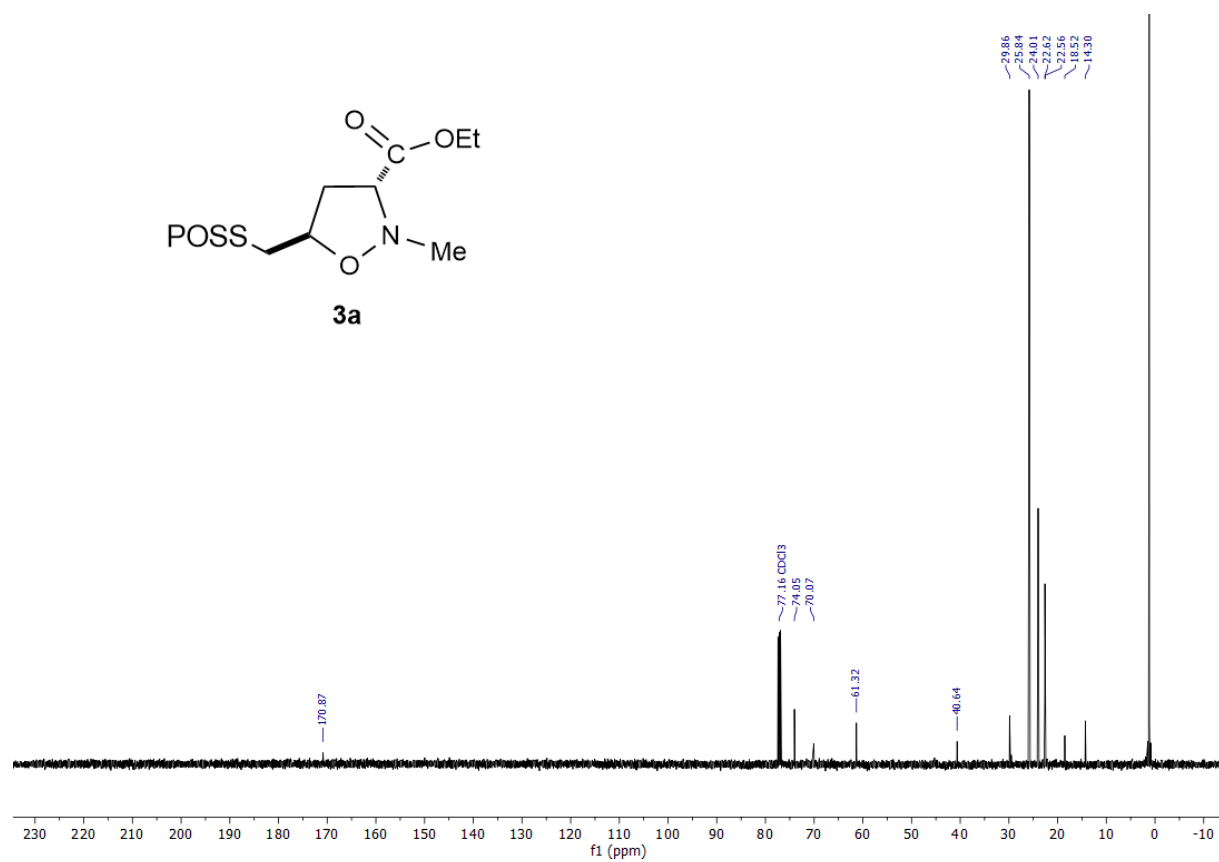
<sup>e</sup> Dipartimento di Ingegneria Civile e Architettura, Università di Catania, Viale A. Doria 6, 95125 Catania, Italy.

## Table of Contents

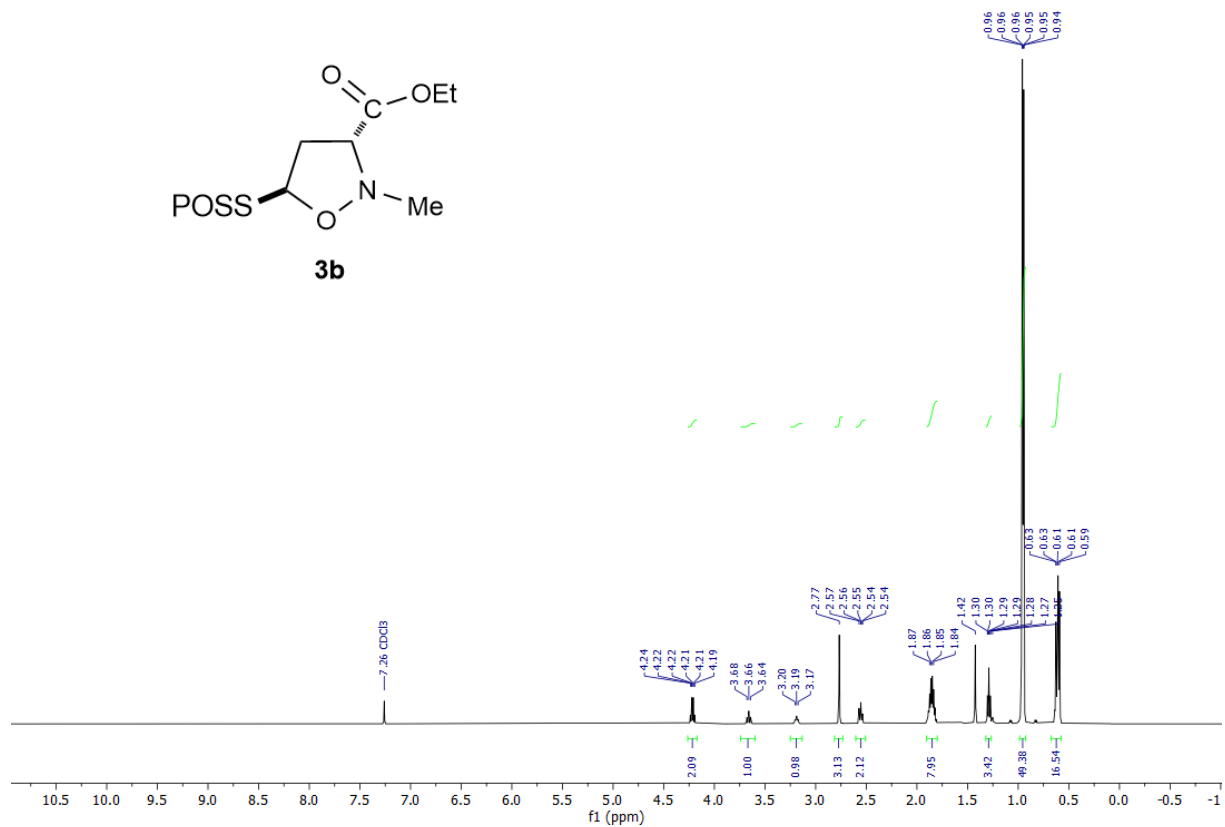
$^1\text{H}$ NMR and $^{13}\text{C}$ NMR of compounds <b>3a,b</b> and <b>4a,b</b> and <b>5b</b> .....	S3-S7
$^{29}\text{Si}$ NMR of compounds <b>3a</b> .....	S8
Transition states for the reaction of <b>2a</b> with <b>1</b> leading to stereoisomers <b>5a</b> and <b>6a</b> .....	S8
$^{29}\text{Si}$ NMR of compound <b>CS-POSS 7</b> .....	S9
Storage modulus ( $G'$ ) and loss modulus ( $G''$ ) of CS and CS-POSS <b>7</b> hydrogels.....	S9
Cell cultured with CS-POSS <b>7</b> hydrogel .....	S10



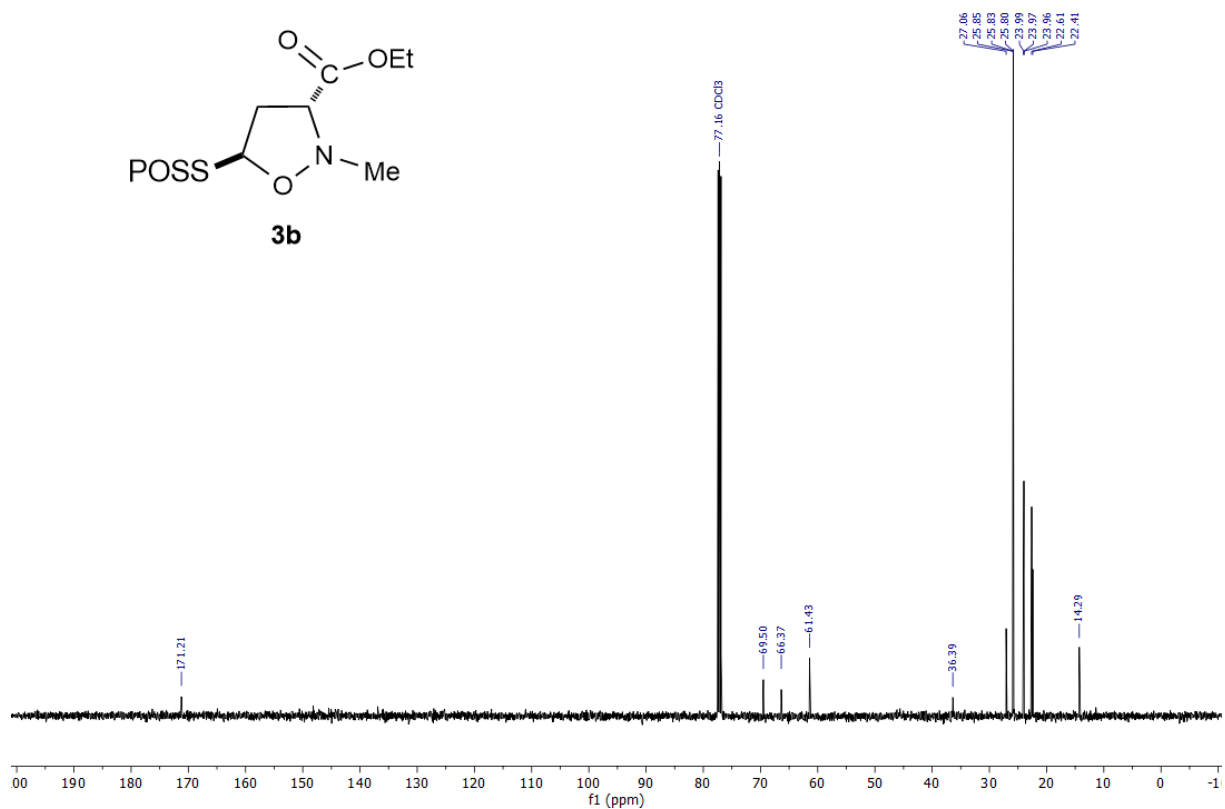
**Fig. S1** <sup>1</sup>H NMR spectrum of **3a** in CDCl<sub>3</sub>, recorded at 25°C and 500 MHz.



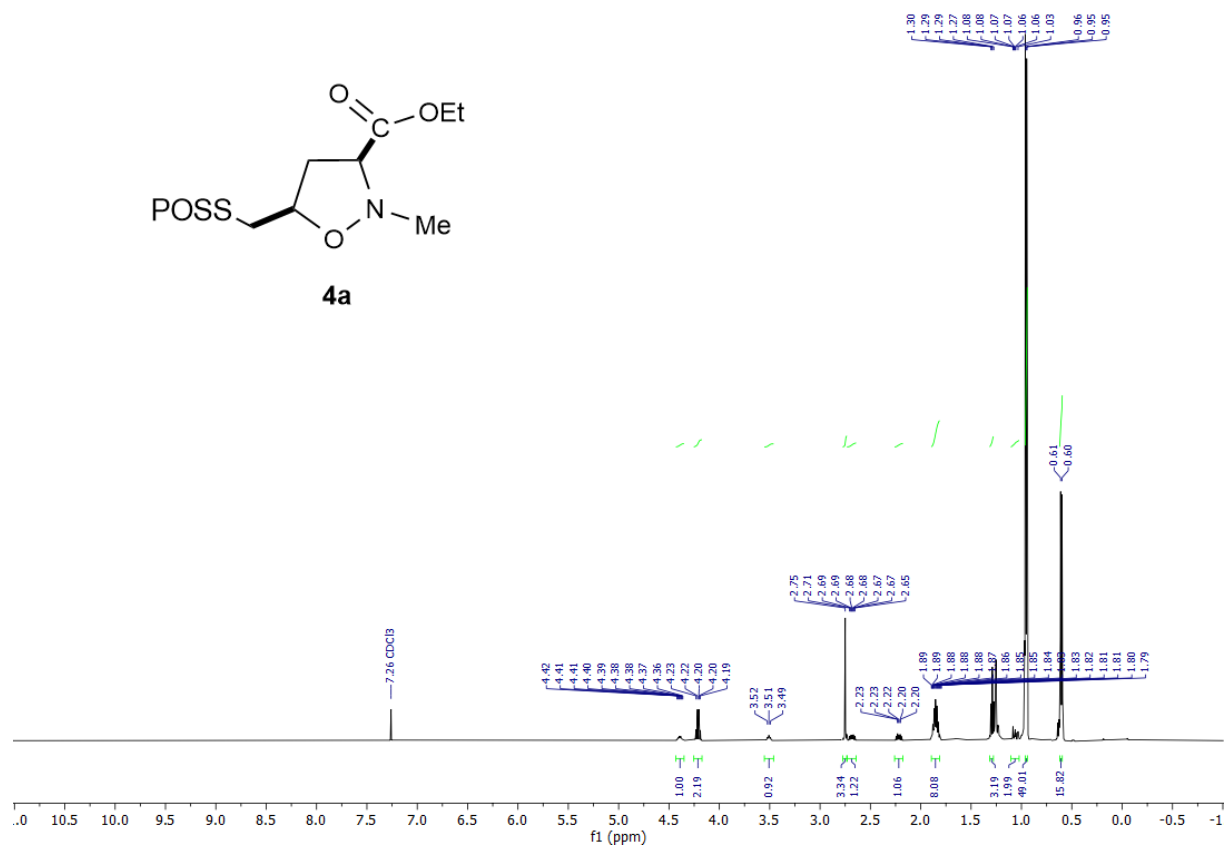
**Fig. S2** <sup>13</sup>C NMR spectrum of **3a** in CDCl<sub>3</sub>, recorded at 25°C and 126 MHz.



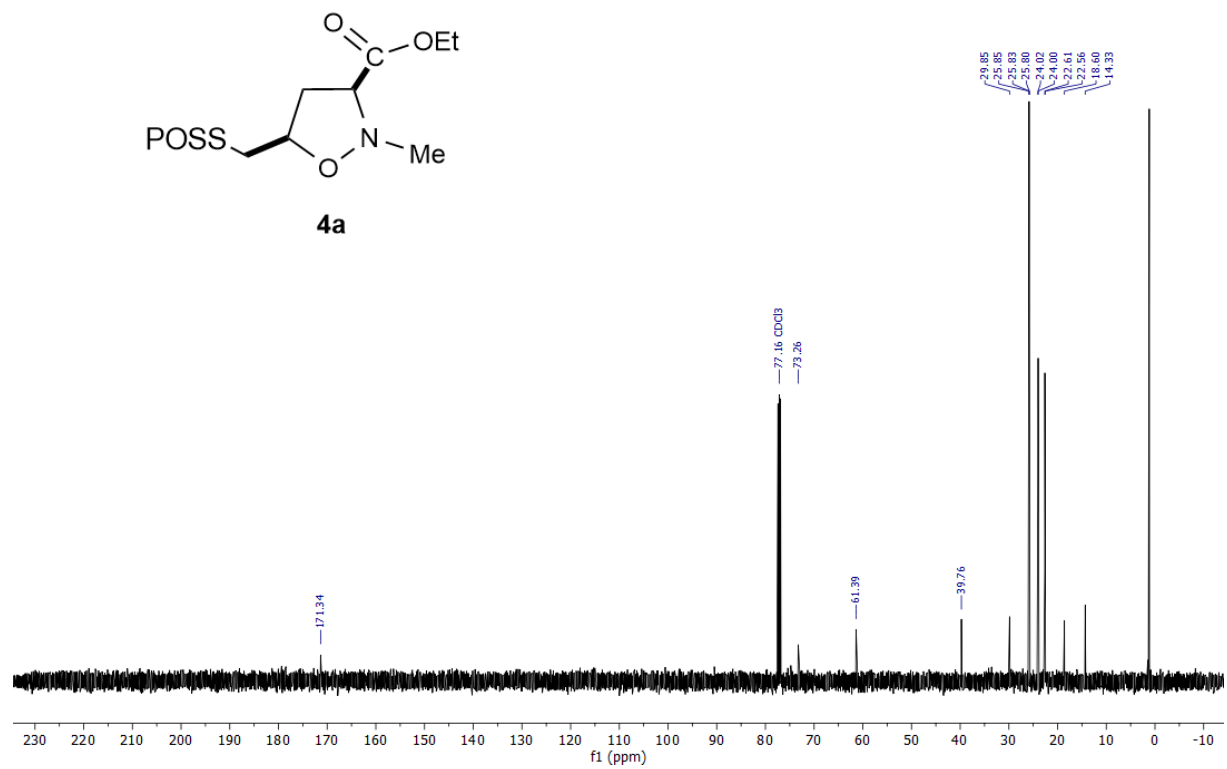
**Fig. S3** <sup>1</sup>H NMR spectrum of **3b** in CDCl<sub>3</sub>, recorded at 25°C and 500 MHz.



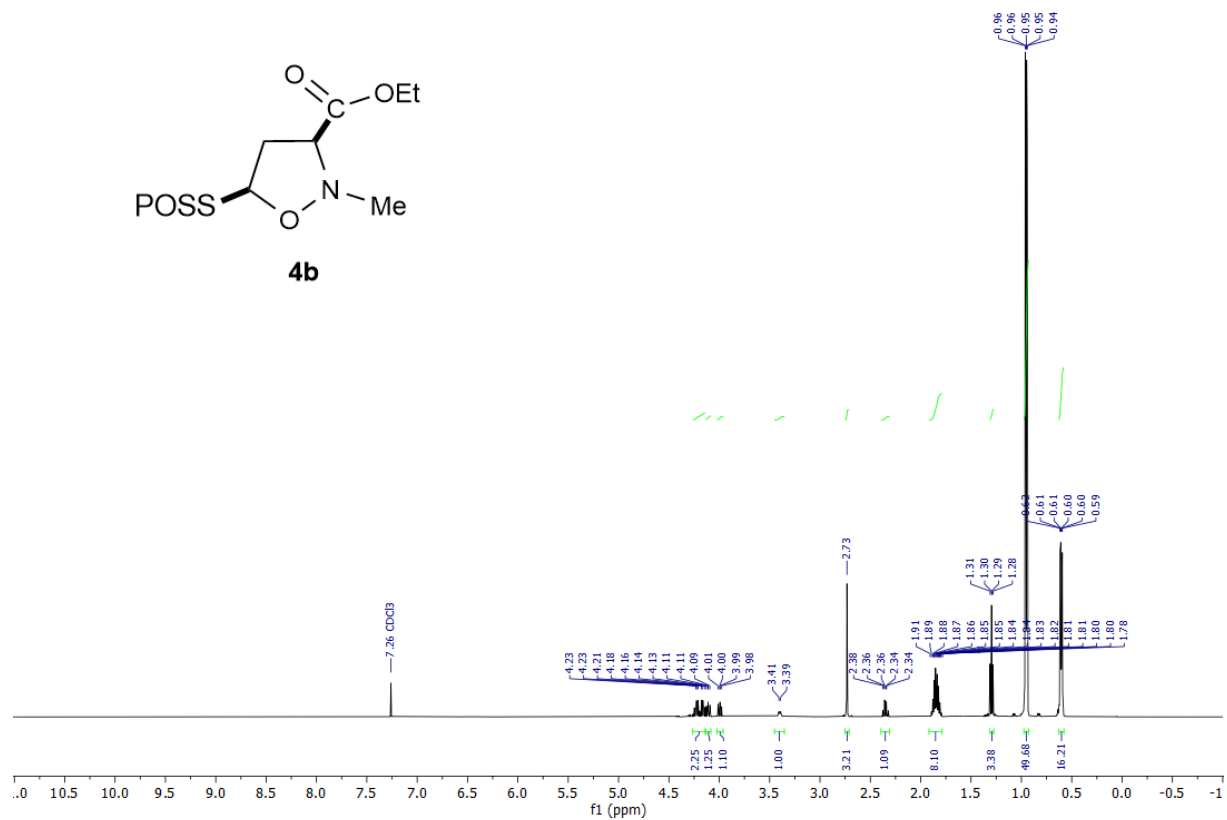
**Fig. S4** <sup>13</sup>C NMR spectrum of **3b** in CDCl<sub>3</sub>, recorded at 25°C and 126 MHz.



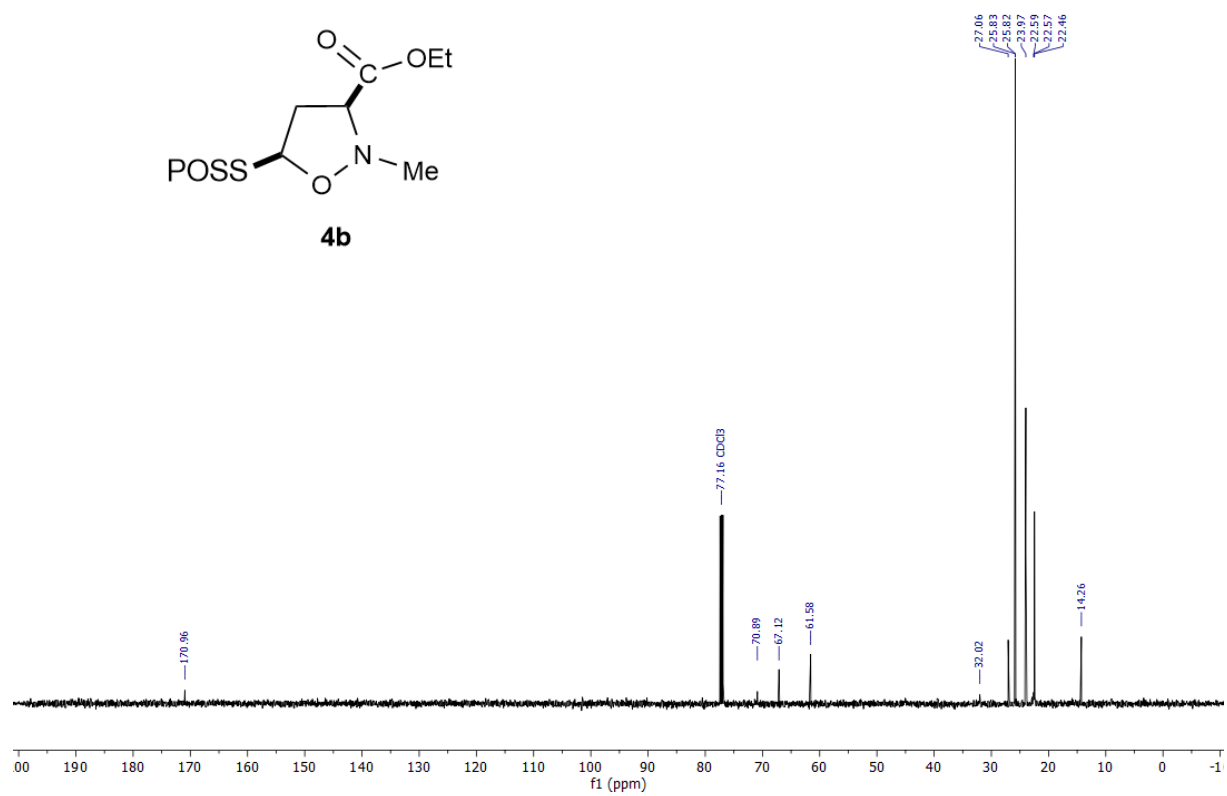
**Fig. S5** <sup>1</sup>H NMR spectrum of **4a** in CDCl<sub>3</sub>, recorded at 25°C and 500 MHz.



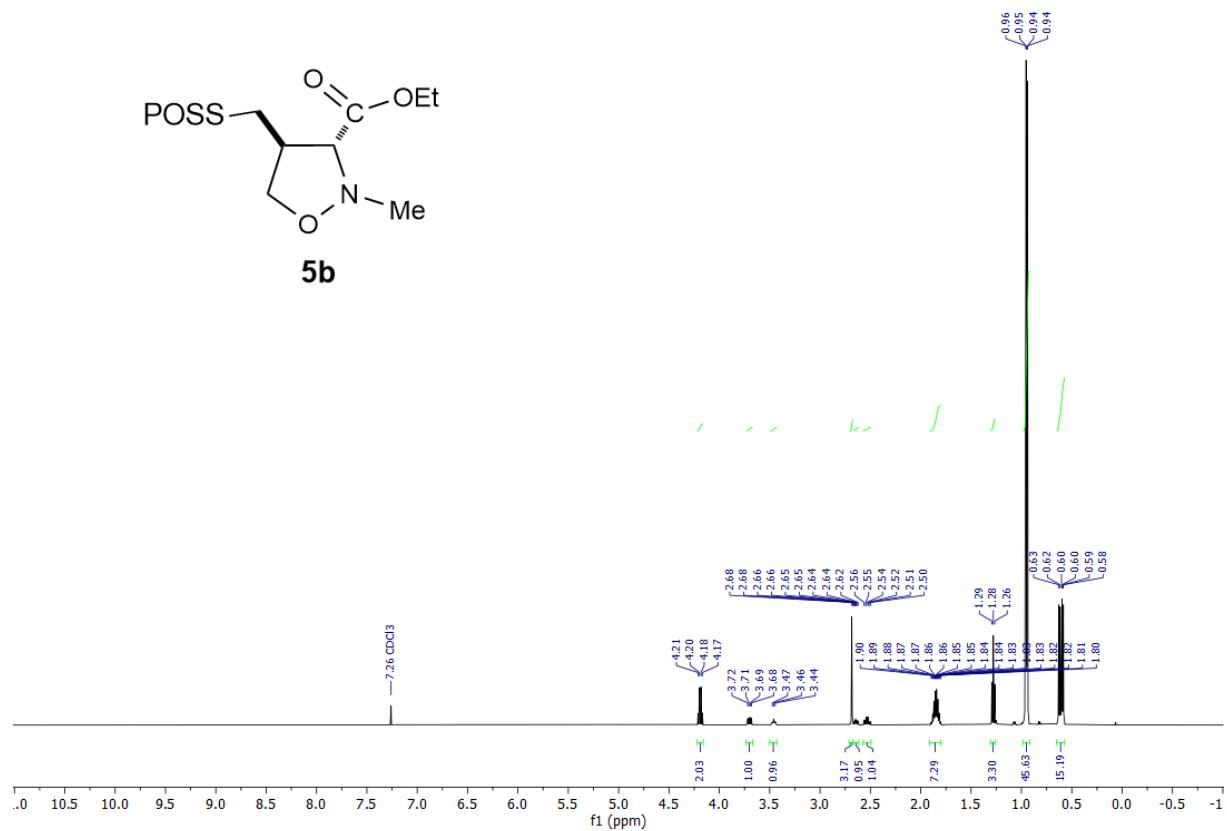
**Fig. S6** <sup>13</sup>C NMR spectrum of **4a** in CDCl<sub>3</sub>, recorded at 25°C and 126 MHz.



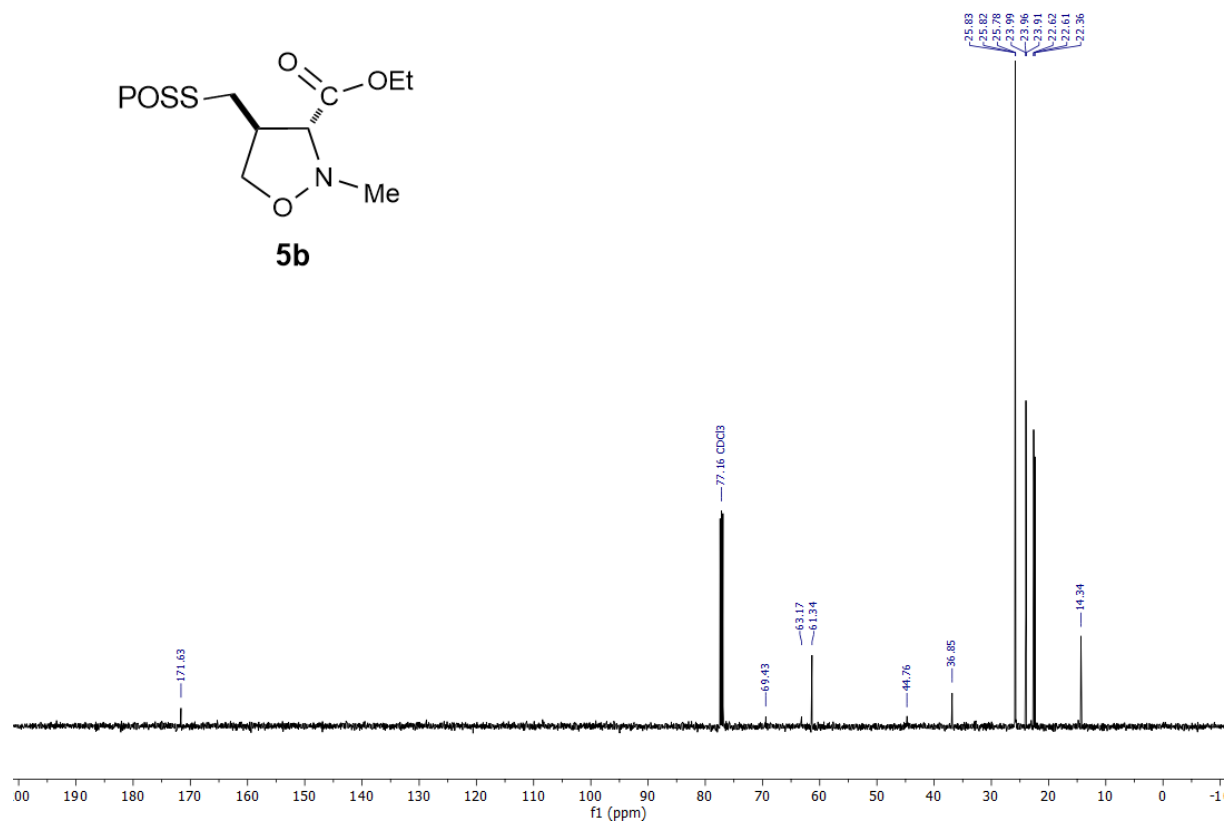
**Fig. S7** <sup>1</sup>H NMR spectrum of **4b** in CDCl<sub>3</sub>, recorded at 25°C and 500 MHz.



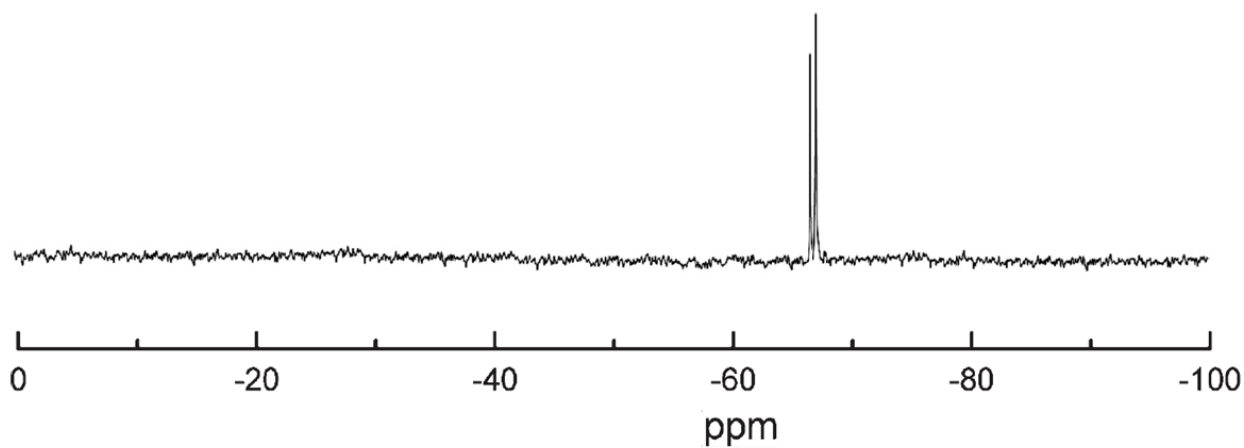
**Fig. S8** <sup>13</sup>C NMR spectrum of **4b** in CDCl<sub>3</sub>, recorded at 25°C and 126 MHz.



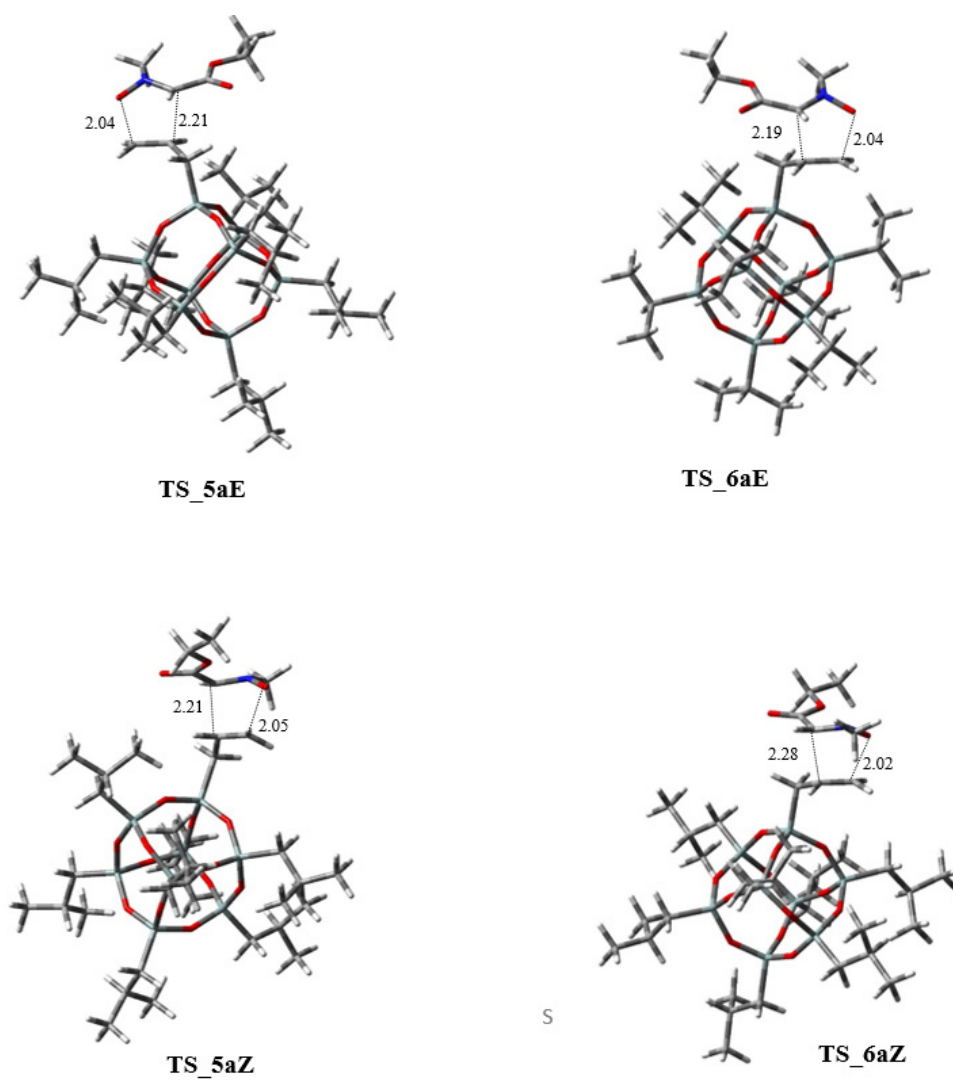
**Fig. S9** <sup>1</sup>H NMR spectrum of **5b** in CDCl<sub>3</sub>, recorded at 25°C and 500 MHz.



**Fig. S10** <sup>13</sup>C NMR spectrum of **5b** in CDCl<sub>3</sub>, recorded at 25°C and 126 MHz.

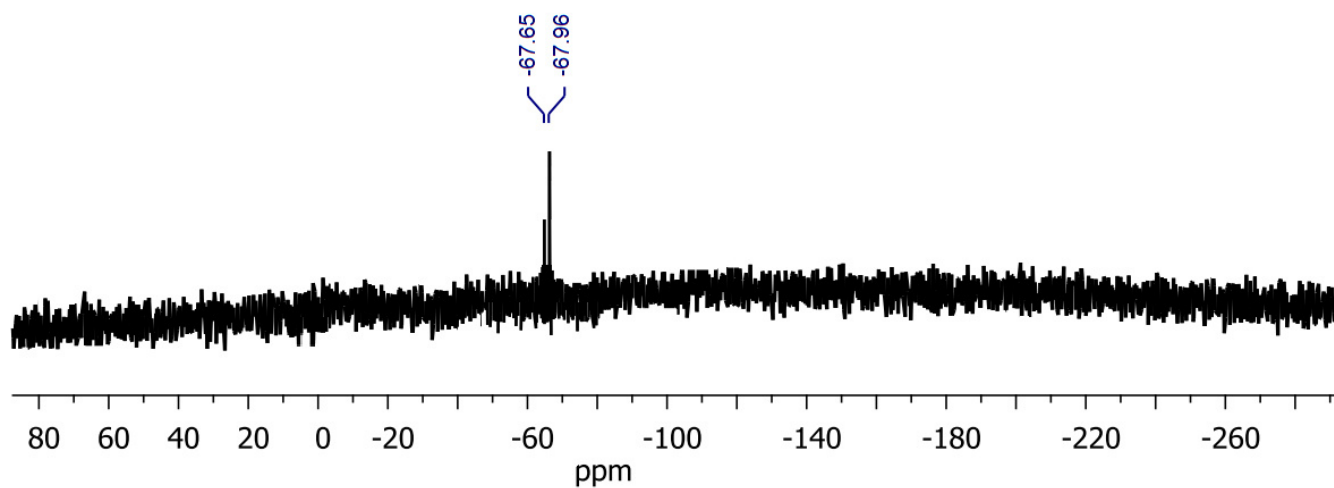


**Fig. S11**  $^{29}\text{Si}$  NMR of compound **3a** in  $\text{CDCl}_3$ , recorded at  $25^\circ\text{C}$  and 99.32 MHz.

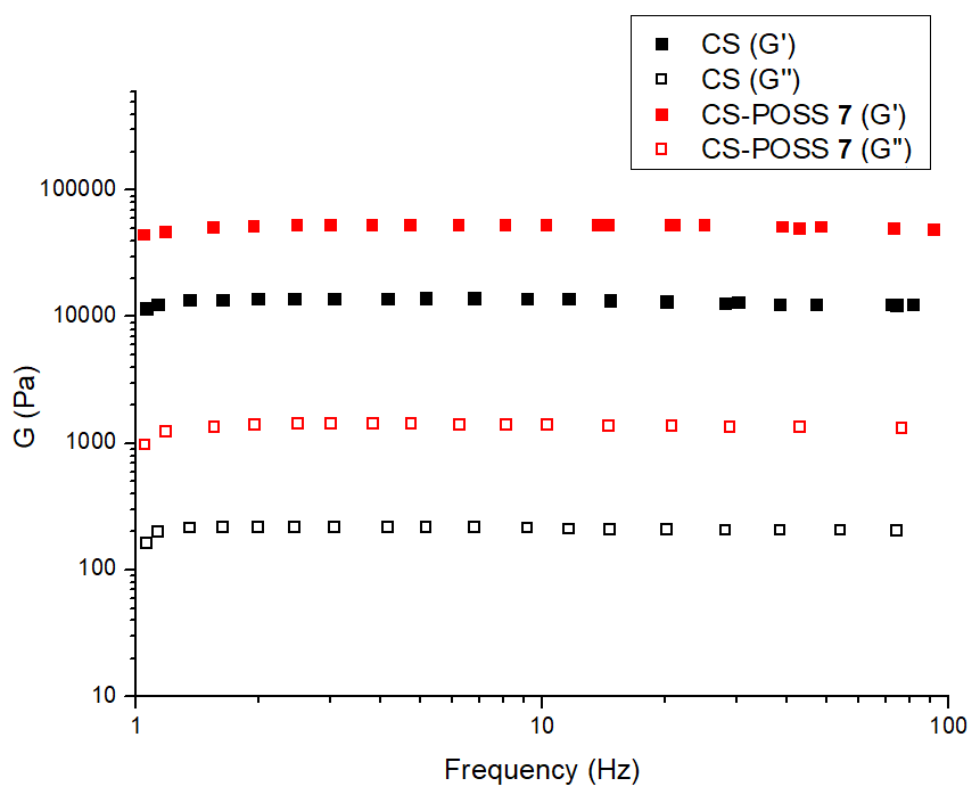


**Fig. S12** Transition states for the reaction of **2a** with **1** leading to stereoisomers **5a** and **6a**. Displacement vectors for TS imaginary frequencies are shown as grey arrows and the values of the forming bond lengths are reported in angstroms.

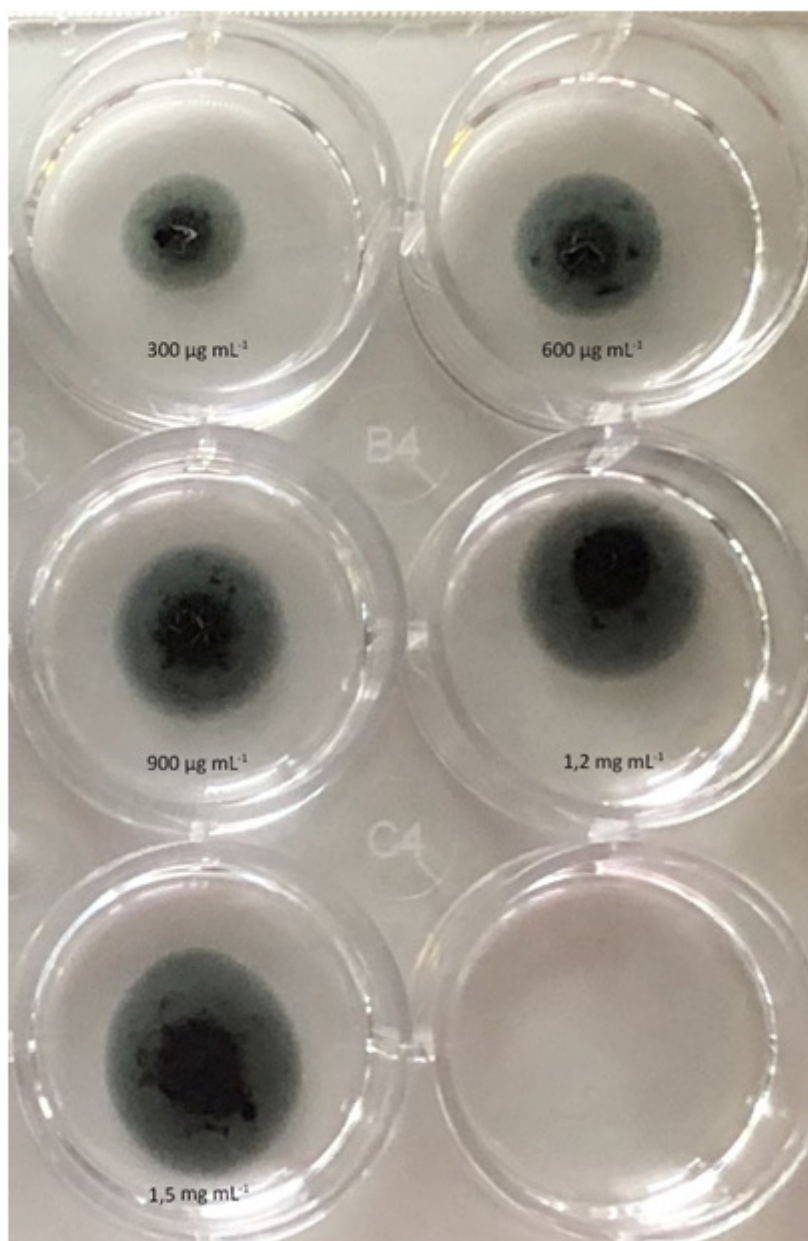




**Fig. S13**  $^{29}\text{Si}$  NMR of compound CS-POSS 7 in  $\text{CDCl}_3$ , recorded at  $25^\circ\text{C}$  and 99.32 MHz.



**Fig. S14** Storage modulus ( $G'$ ) and loss modulus ( $G''$ ) of CS and CS-POSS 7 hydrogels.



**Fig. S15** Cell cultured with CS-POSS 7 hydrogel at different concentrations and control.