

## Supporting information

### Synthesis, spectral characteristics and molecular docking studies of *N*-(2,2,2-trichloro-1-thioureidoethyl)carboxamides

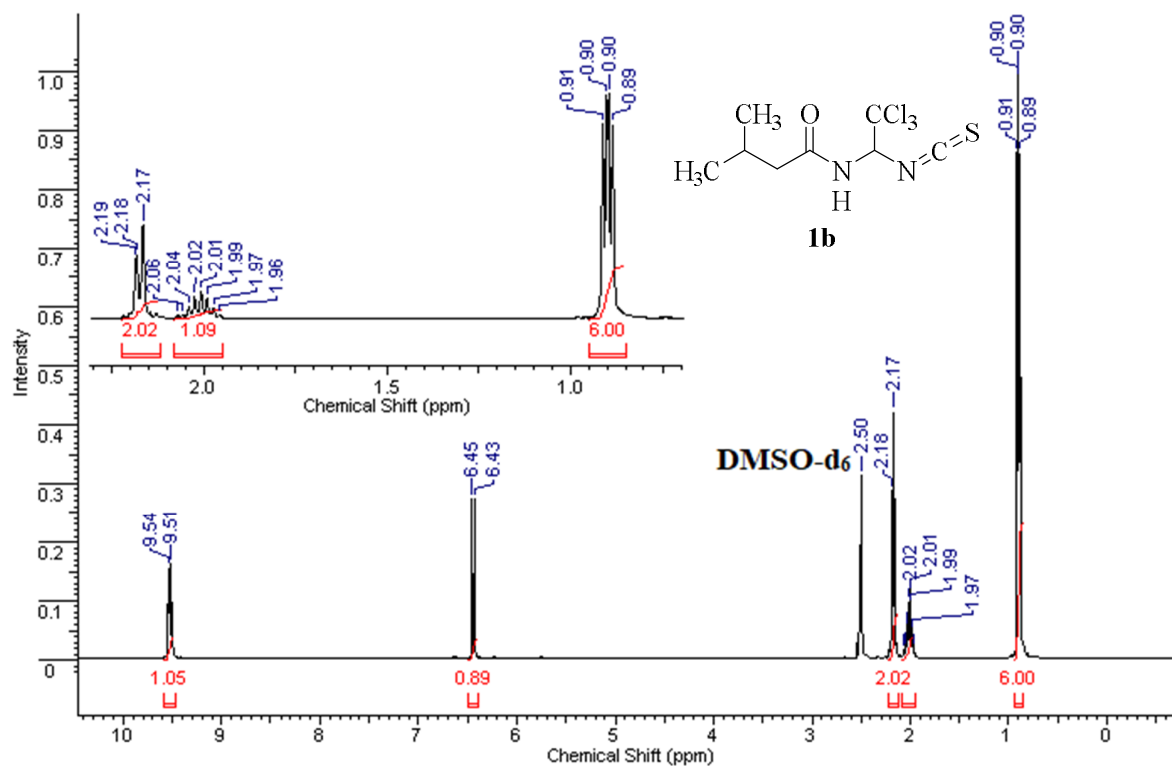
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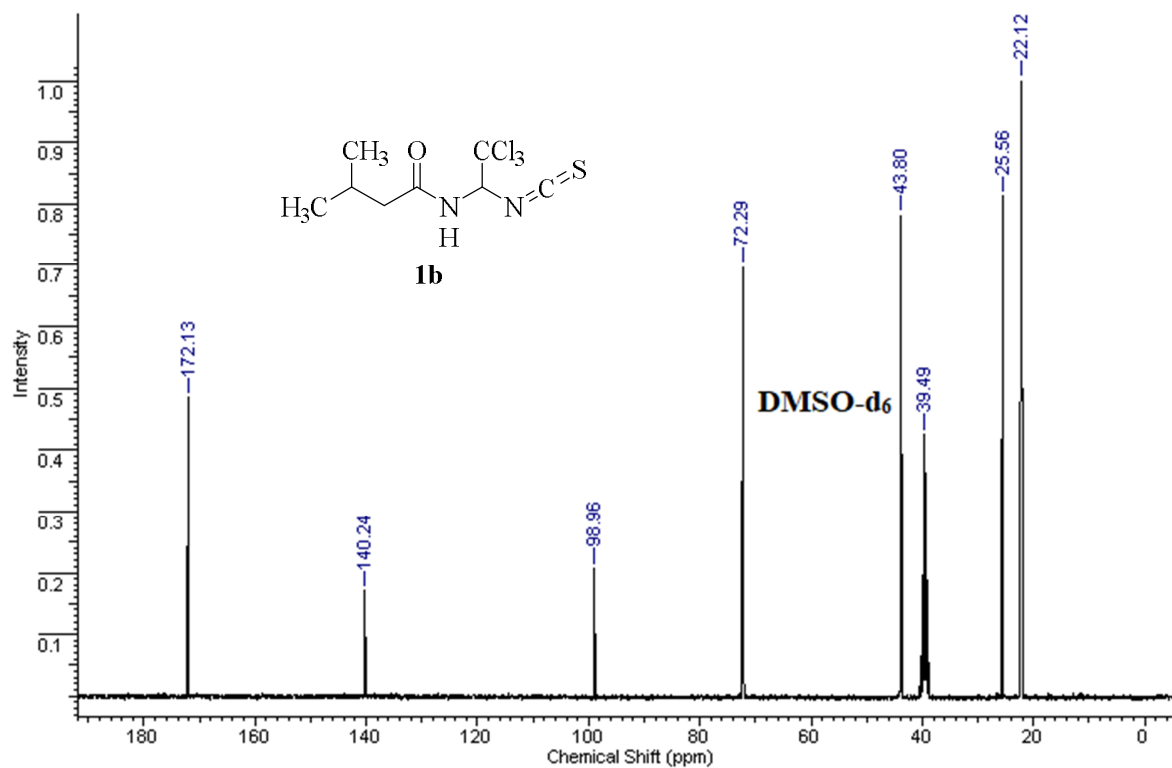
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### Table of Contents

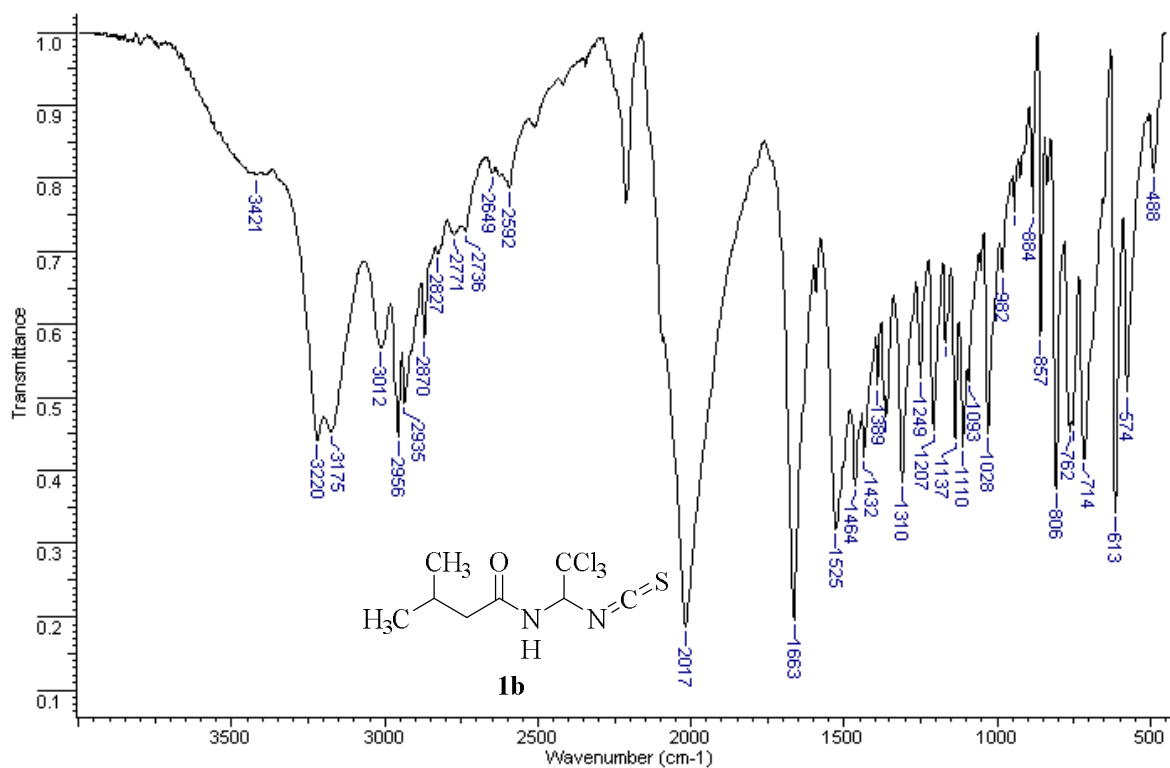
I.	<sup>1</sup> H, <sup>13</sup> C NMR and IR spectra of 3-methyl- <i>N</i> -(2,2,2-trichloro-1-isothiocyanoethyl)butanamide ( <b>1b</b> ).....	S2
II.	<sup>1</sup> H, <sup>13</sup> C NMR and IR spectra of 2-chloro- <i>N</i> -(2,2,2-trichloro-1-isothiocyanoethyl)benzamide ( <b>1j</b> ).....	S4
III.	<sup>1</sup> H, <sup>13</sup> C NMR and IR spectra of 3-methyl- <i>N</i> -(2,2,2-trichloro-1-thioureidoethyl)butanamide ( <b>5b</b> ).....	S6
IV.	<sup>1</sup> H, <sup>13</sup> C NMR and IR spectra of 2-chloro- <i>N</i> -(2,2,2-trichloro-1-thioureidoethyl)acetamide ( <b>5c</b> ).....	S8
V.	<sup>1</sup> H, <sup>13</sup> C NMR and IR spectra of <i>N</i> -(2,2,2-trichloro-1-thioureidoethyl)acrylamide ( <b>5d</b> ).....	S10
VI.	<sup>1</sup> H, <sup>13</sup> C NMR and IR spectra of 2-methyl- <i>N</i> -(2,2,2-trichloro-1-thioureidoethyl)benzamide ( <b>5g</b> ).....	S12
VII.	<sup>1</sup> H, <sup>13</sup> C NMR and IR spectra of 2-chloro- <i>N</i> -(2,2,2-trichloro-1-thioureidoethyl)benzamide ( <b>5i</b> ).....	S14
VIII.	<sup>1</sup> H, <sup>13</sup> C NMR and IR spectra of 2-bromo- <i>N</i> -(2,2,2-trichloro-1-thioureidoethyl)benzamide ( <b>5j</b> ).....	S16



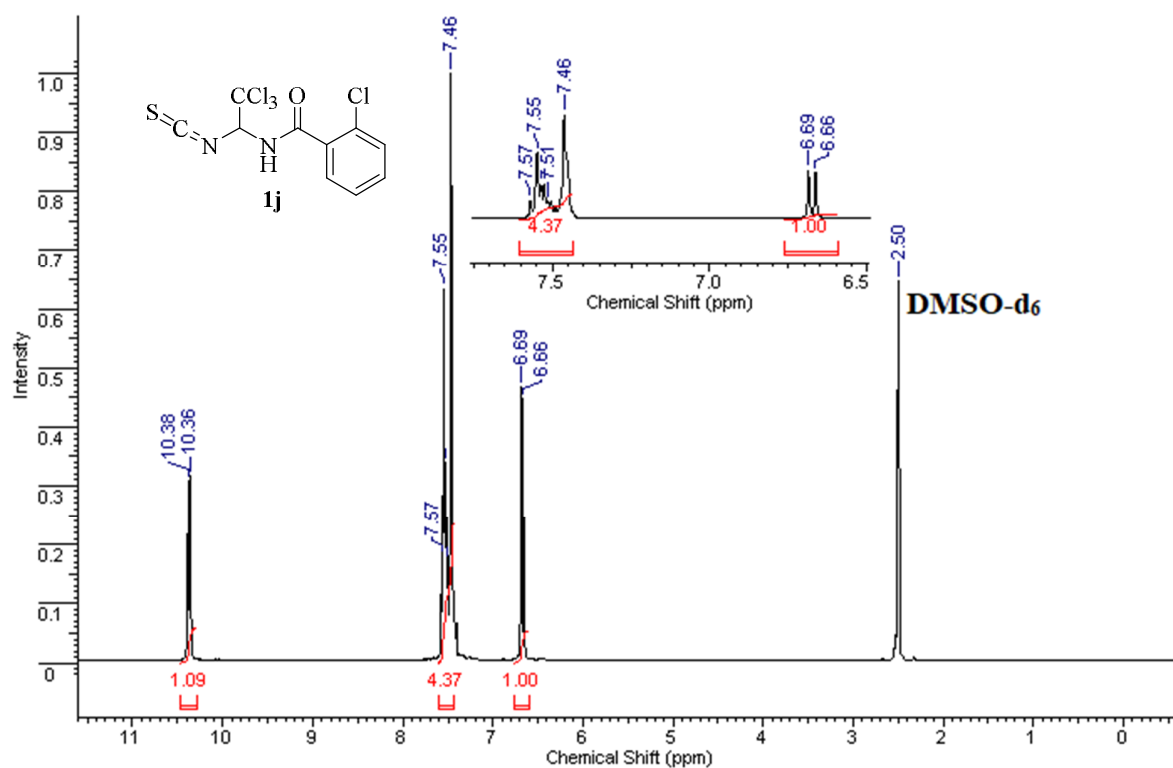
**Figure S1.**  $^1\text{H}$  NMR (DMSO- $d_6$ ) spectra of 3-methyl-*N*-(2,2,2-trichloro-1-isothiocyantoethyl)butanamide (**1b**).



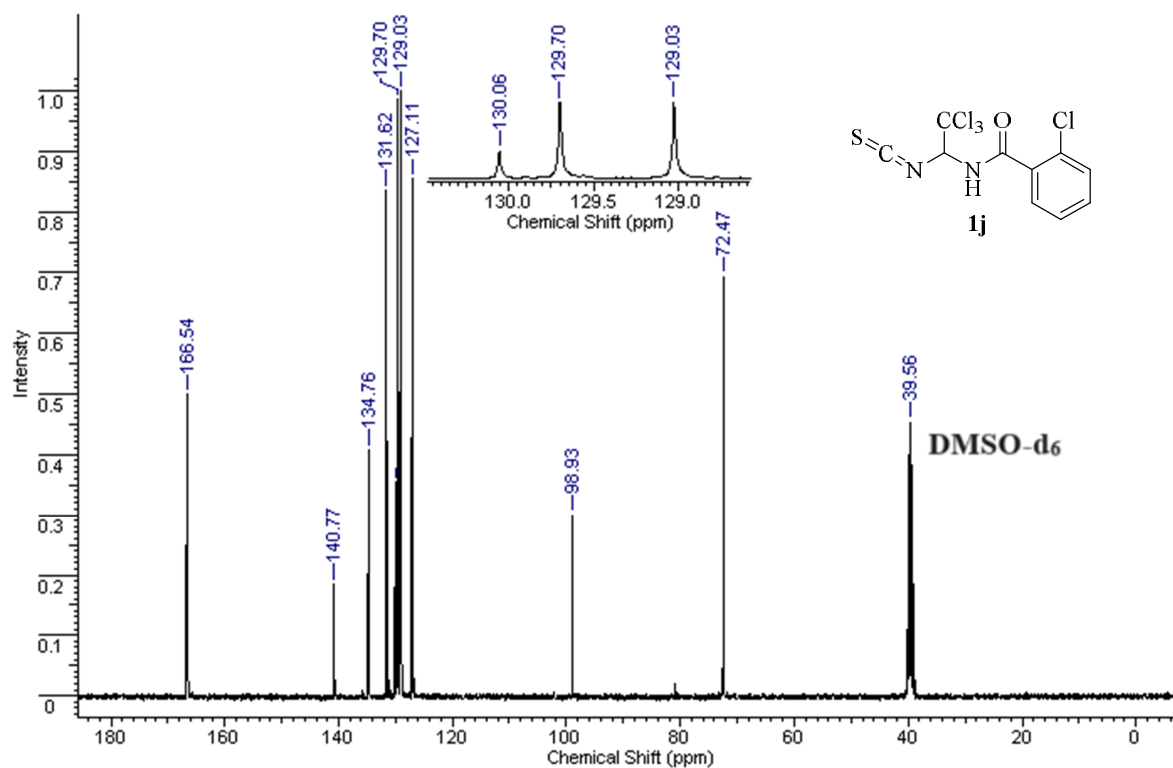
**Figure S2.**  $^{13}\text{C}$  NMR (DMSO- $d_6$ ) spectra of 3-methyl-*N*-(2,2,2-trichloro-1-isothiocyantoethyl)butanamide (**1b**).



**Figure S3.** IR (KBr) spectra of 3-methyl-*N*-(2,2,2-trichloro-1-isothiocyanatoethyl)butanamide (**1b**).

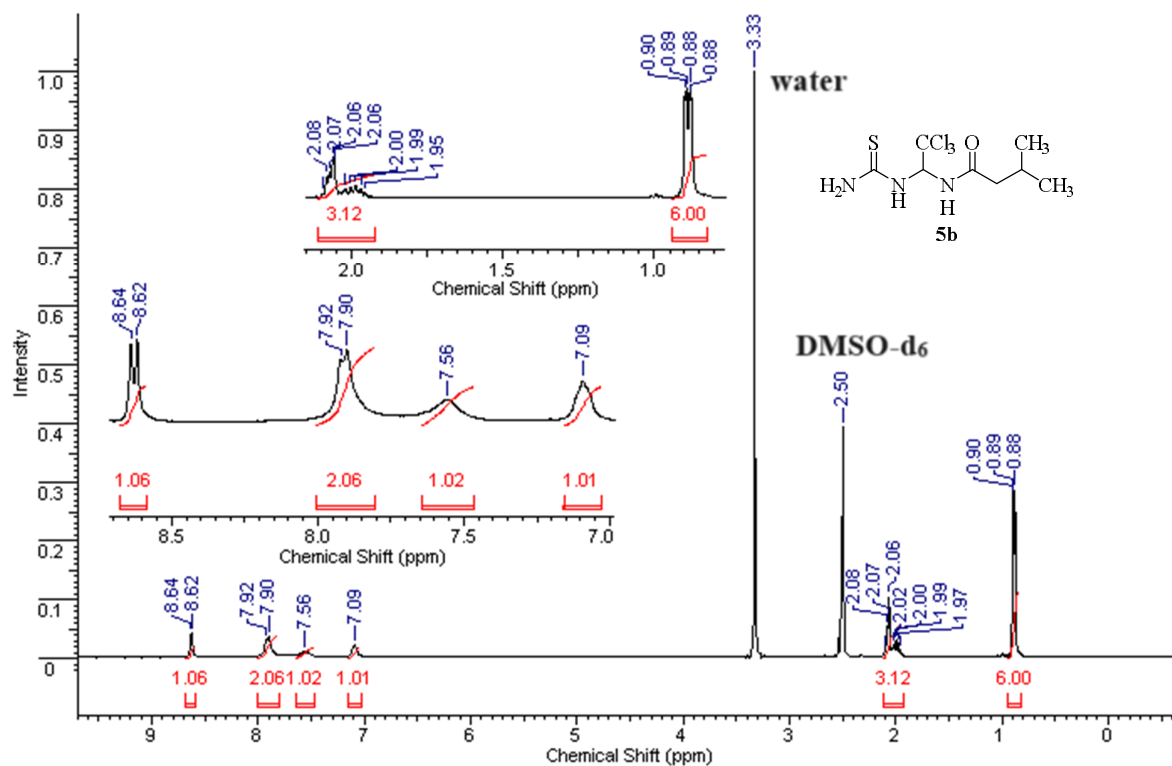


**Figure S4.** <sup>1</sup>H NMR (DMSO-d<sub>6</sub>) spectra of 2-chloro-*N*-(2,2,2-trichloro-1-isothiocyantoethyl)benzamide (**1j**).

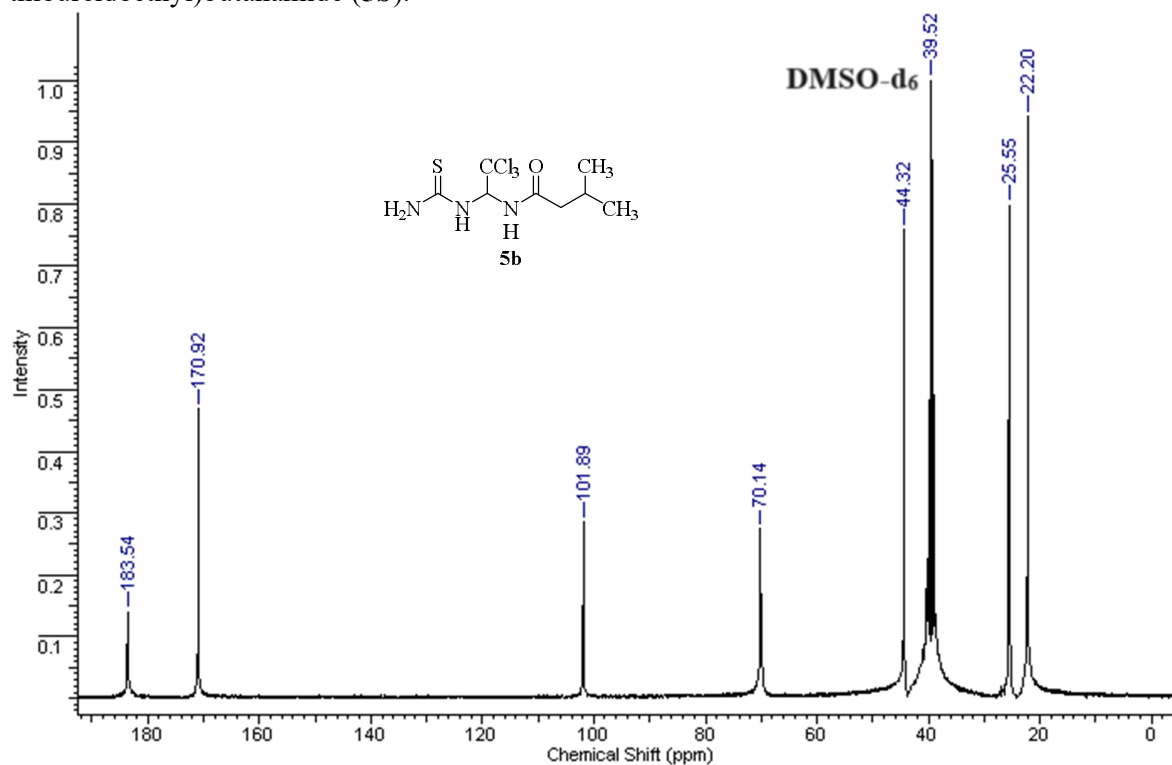


**Figure S5.** <sup>13</sup>C NMR (DMSO-d<sub>6</sub>) spectra of 2-chloro-*N*-(2,2,2-trichloro-1-isothiocyantoethyl)benzamide (**1j**).

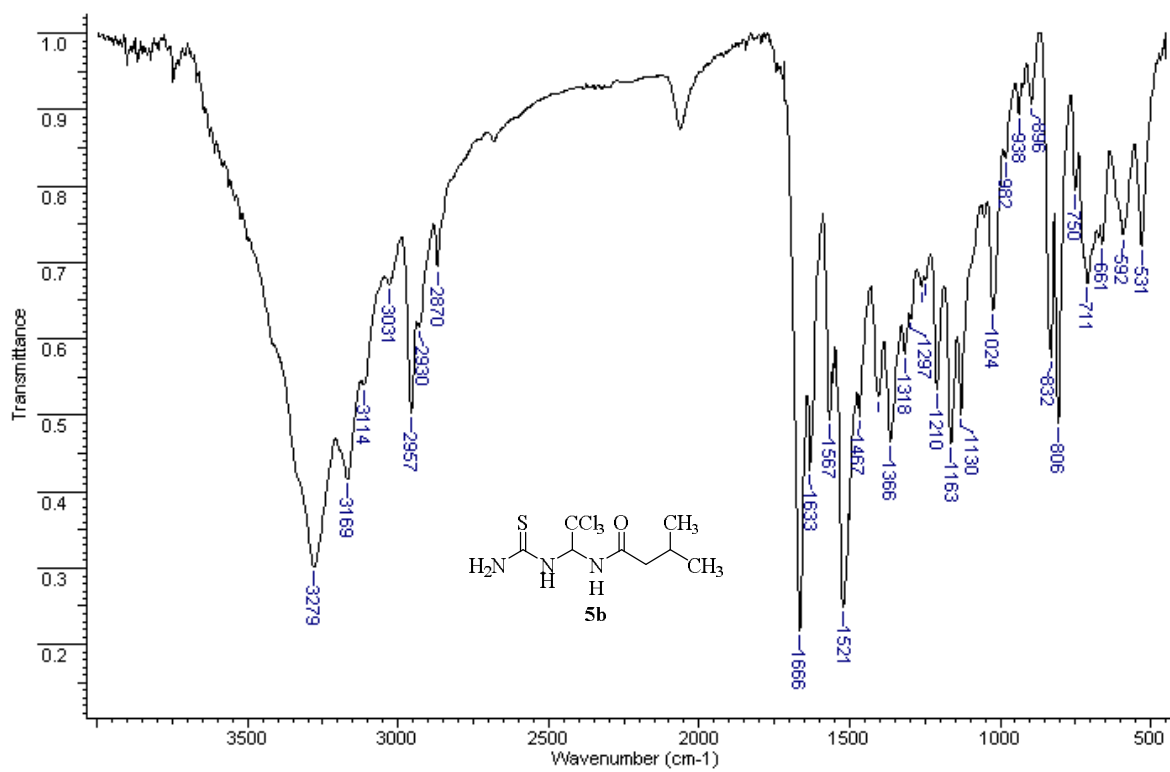




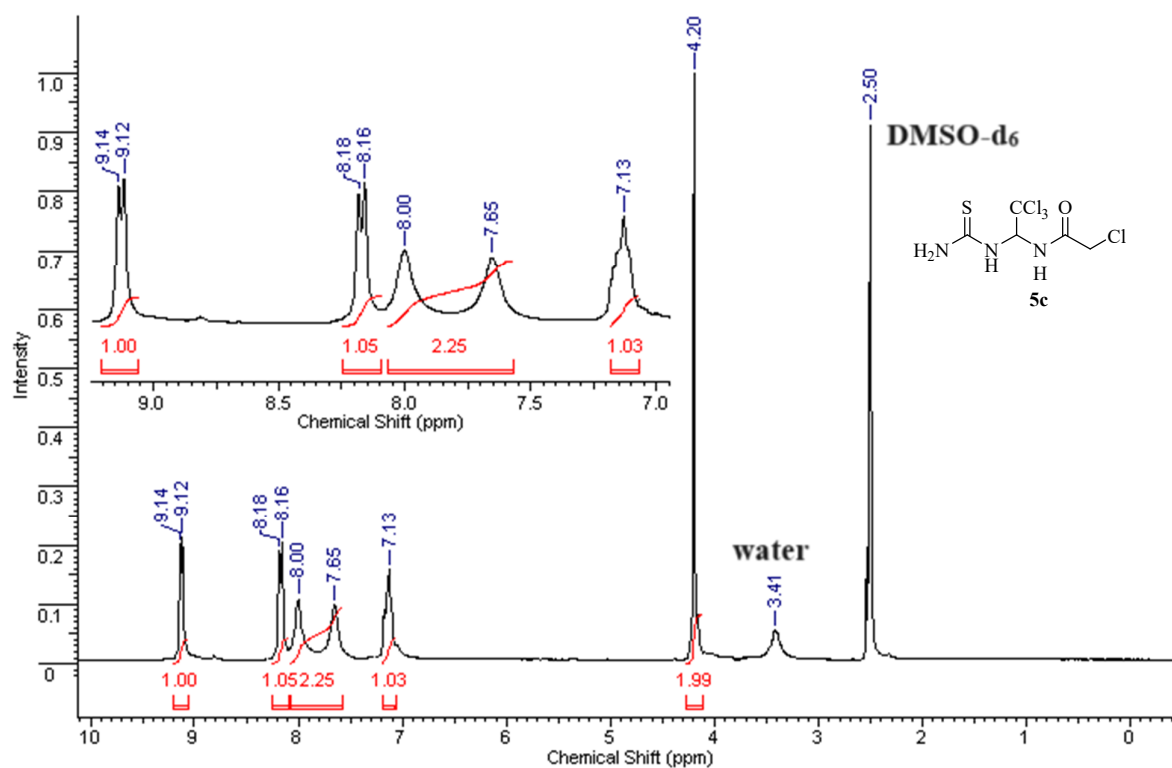
**Figure S7.**  $^1\text{H}$  NMR ( $\text{DMSO-d}_6$ ) spectra of 3-methyl-*N*-(2,2,2-trichloro-1-thioureidoethyl)butanamide (**5b**).



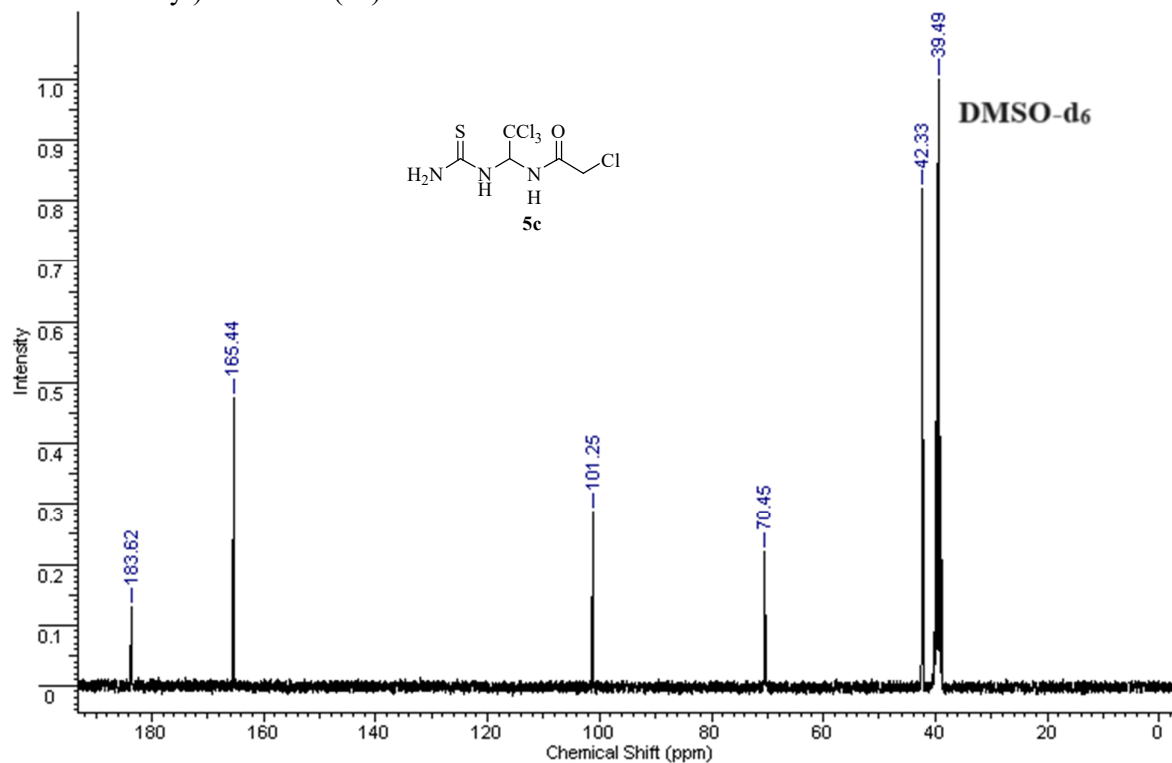
**Figure S8.**  $^{13}\text{C}$  NMR ( $\text{DMSO-d}_6$ ) spectra of 3-methyl-*N*-(2,2,2-trichloro-1-thioureidoethyl)butanamide (**5b**).



**Figure S9.** IR (KBr) spectra of 3-methyl-N-(2,2,2-trichloro-1-thioureidoethyl)butanamide (**5b**).



**Figure S10.**  $^1\text{H}$  NMR (DMSO- $d_6$ ) spectra of 2-chloro-*N*-(2,2,2-trichloro-1-thioureidoethyl)acetamide (**5c**).



**Figure S11.**  $^{13}\text{C}$  NMR (DMSO- $d_6$ ) spectra of 2-chloro-*N*-(2,2,2-trichloro-1-thioureidoethyl)acetamide (**5c**).

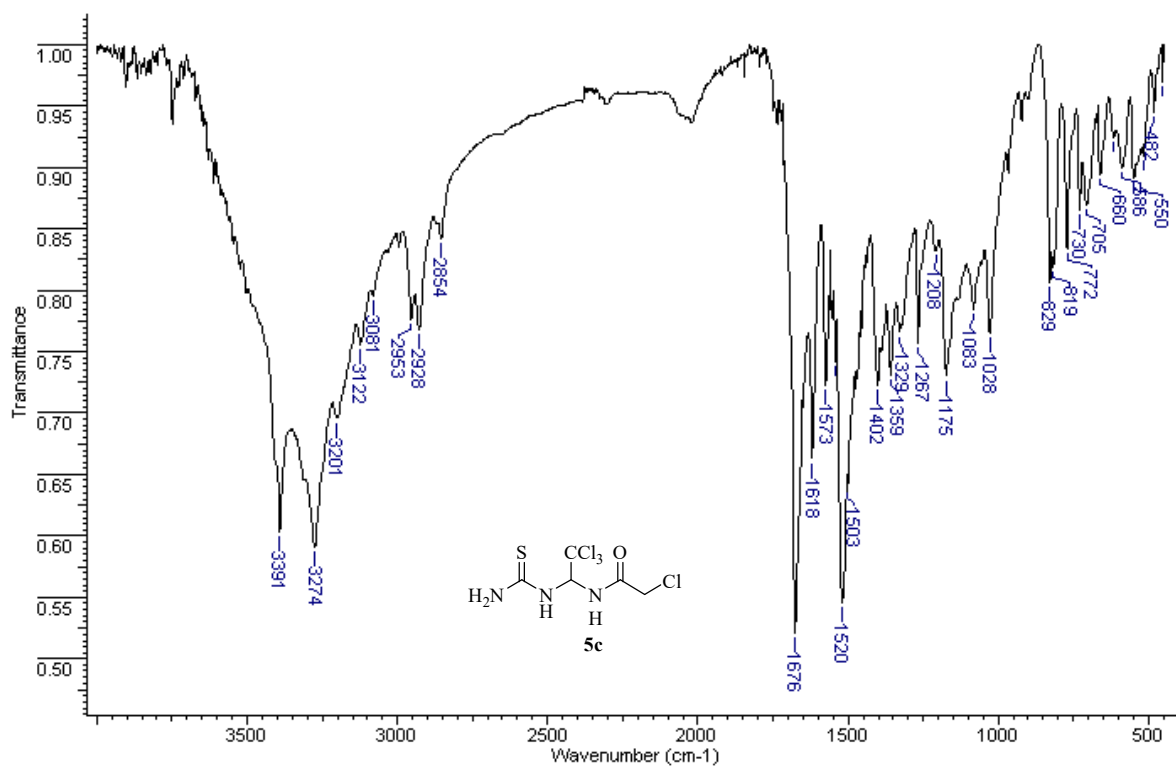
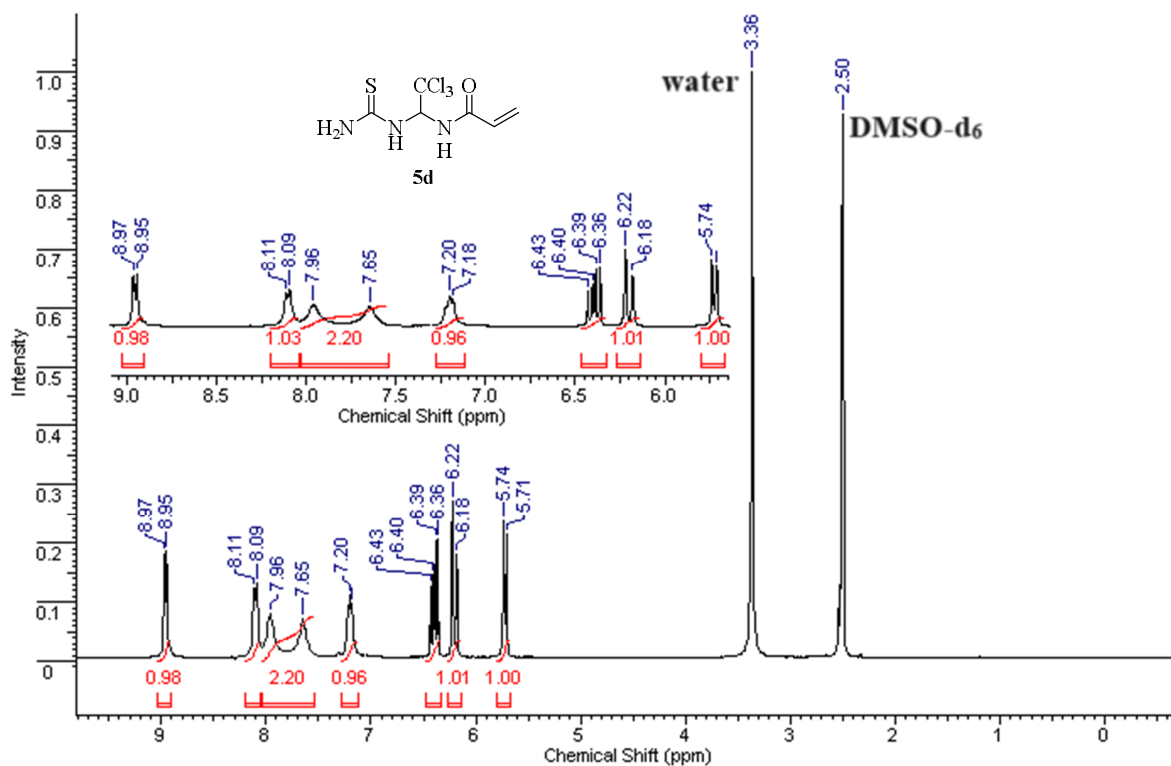
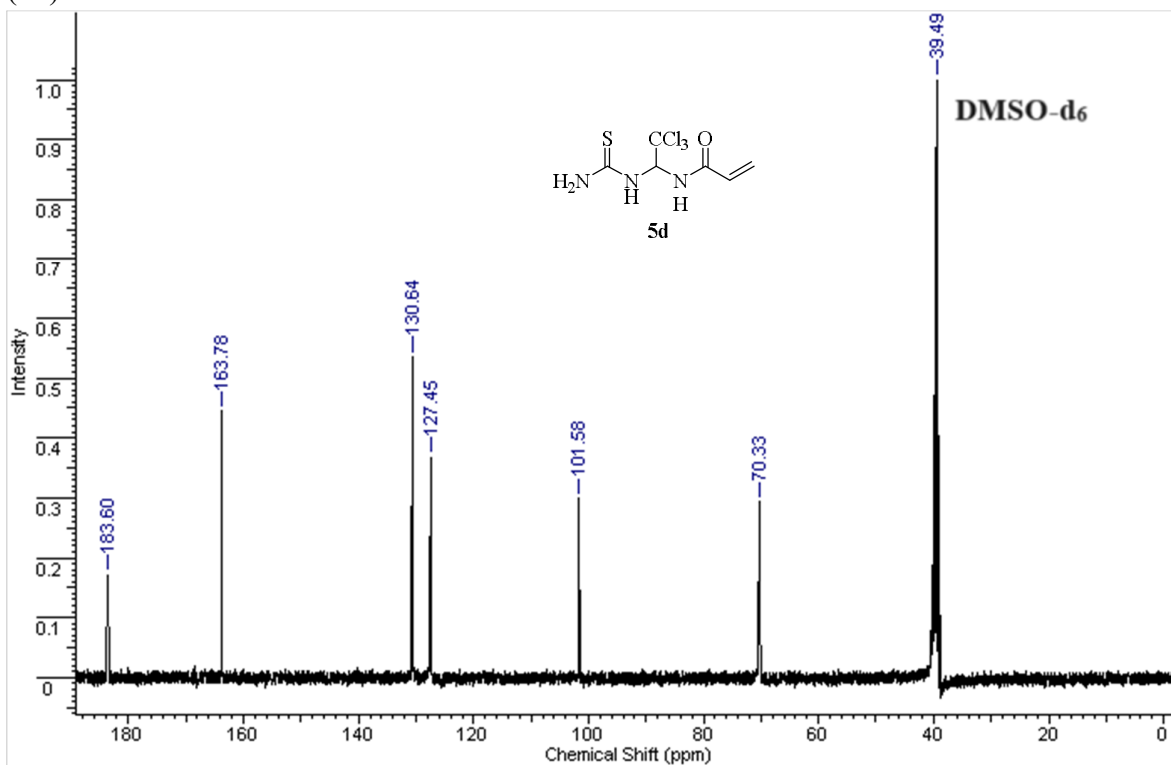


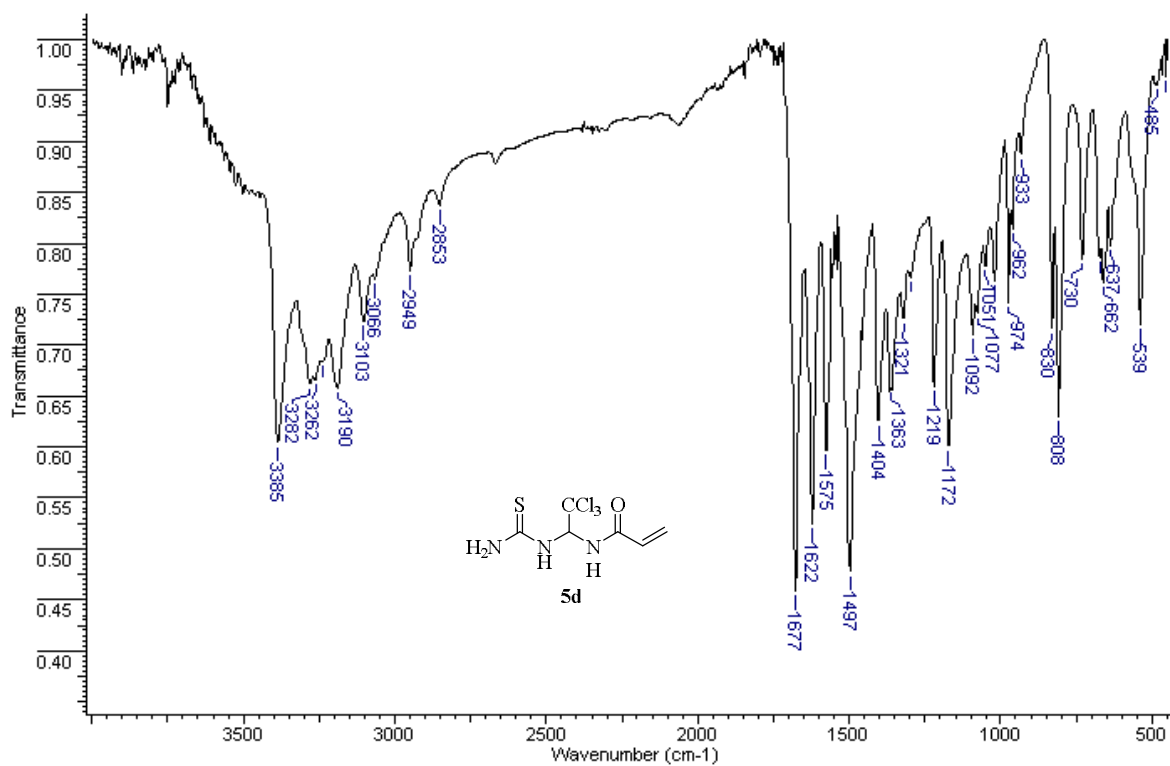
Figure S12. IR (KBr) spectra of 2-chloro-N-(2,2,2-trichloro-1-thioureidoethyl)acetamide (5c).



**Figure S13.**  $^1\text{H}$  NMR (DMSO- $d_6$ ) spectra of *N*-(2,2,2-trichloro-1-thioureidoethyl)acrylamide (**5d**).



**Figure S14.**  $^{13}\text{C}$  NMR (DMSO- $d_6$ ) spectra of *N*-(2,2,2-trichloro-1-thioureidoethyl)acrylamide (**5d**).



**Figure S15.** IR (KBr) spectra of *N*-(2,2,2-trichloro-1-thioureidoethyl)acrylamide (**5d**).

**Figure S16.**  $^1\text{H}$  NMR (DMSO- $d_6$ ) spectra of 2-methyl-*N*-(2,2,2-trichloro-1-thioureidoethyl)benzamide (**5g**).

**Figure S17.**  $^{13}\text{C}$  NMR (DMSO- $d_6$ ) spectra of 2-methyl-*N*-(2,2,2-trichloro-1-thioureidoethyl)benzamide (**5g**).