

## Supplementary Information

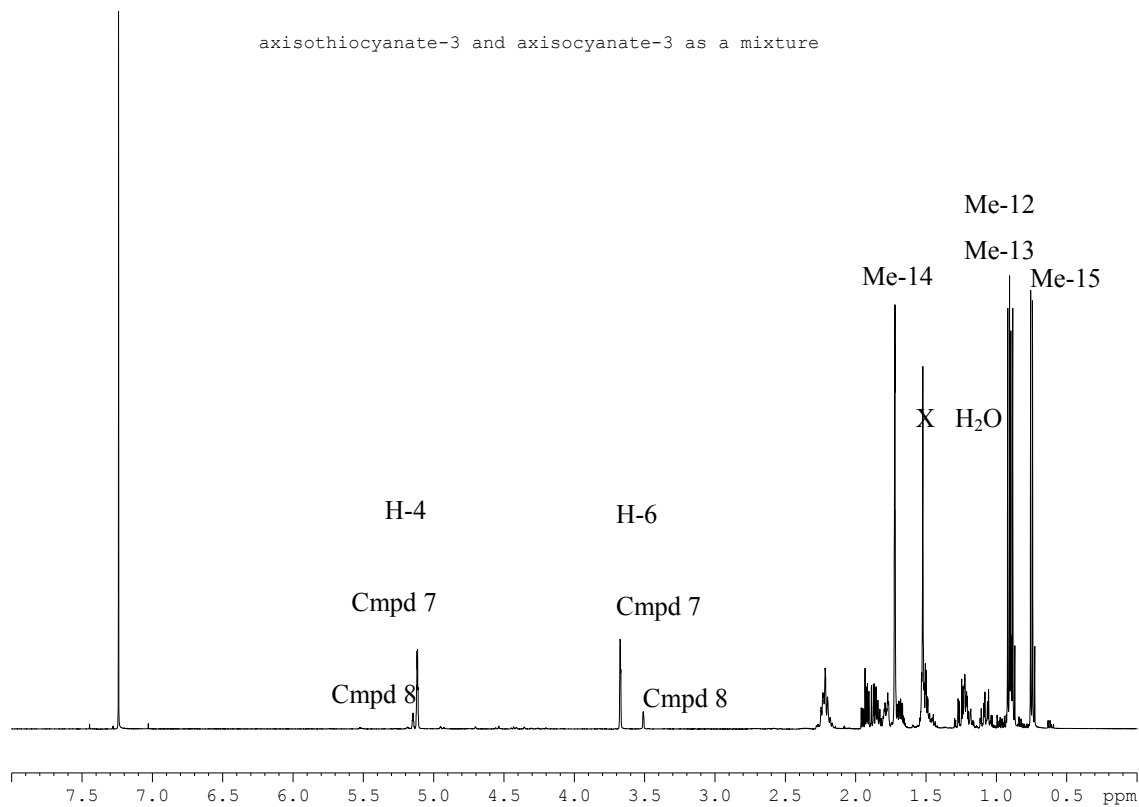
**Isocyanates in marine sponges: Axisocyanate-3, a new sesquiterpene from *Acanthella cavernosa***

Pinus Jumaryatno, Karen Rands-Trevor, Joanne T. Blanchfield, and Mary J. Garson\*

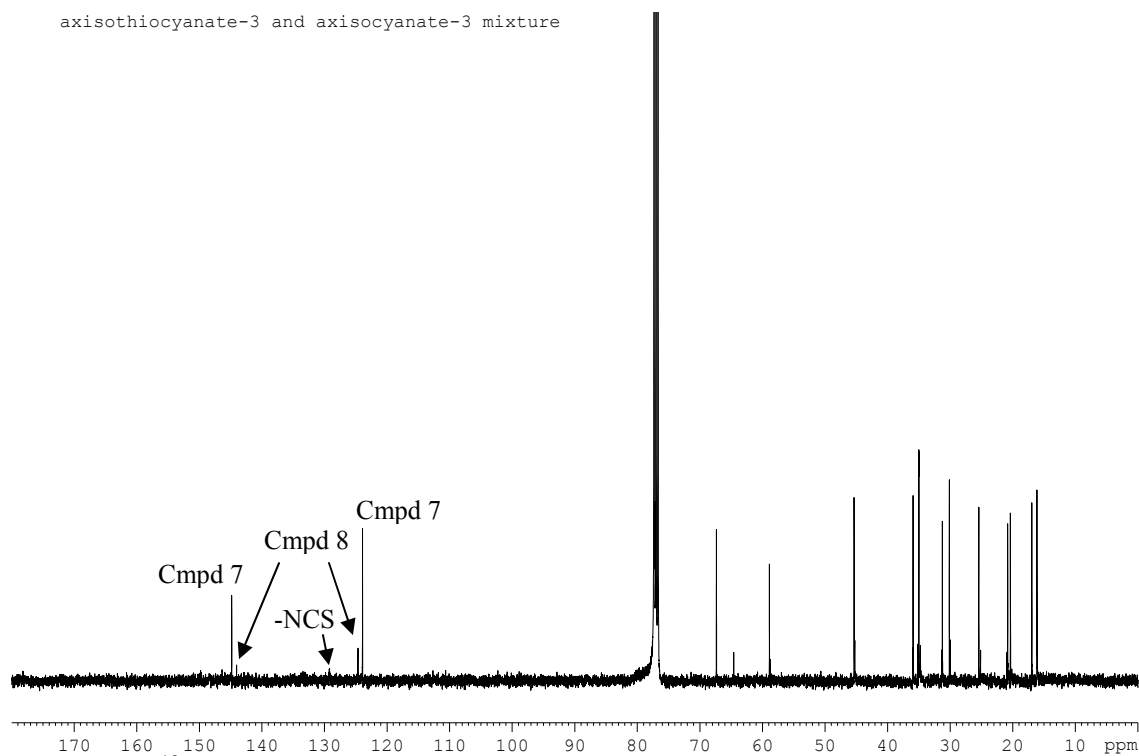
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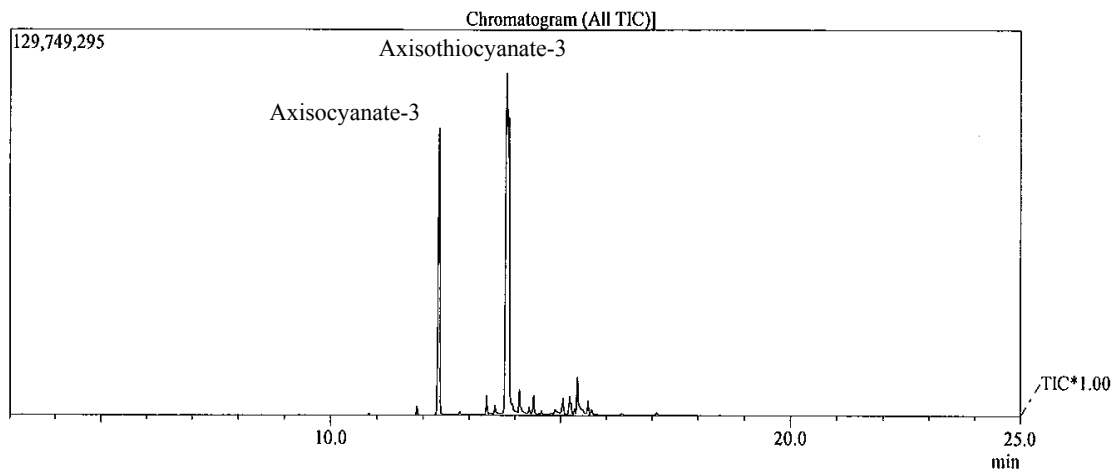
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**Figure S1.** <sup>1</sup>H NMR spectrum of axisothiocyanate-3 **7** and axisocyanate-3 **8** as a mixture



**Figure S2.** <sup>13</sup>C NMR spectrum of axisothiocyanate-3 **7** and axisocyanate-3 **8** as a mixture



(b) Mass spectrum of the axisocyanate-3 compound

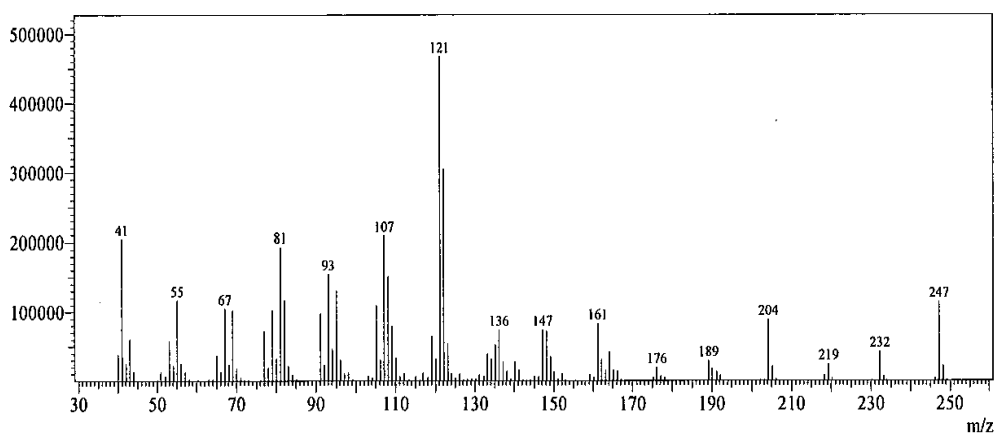
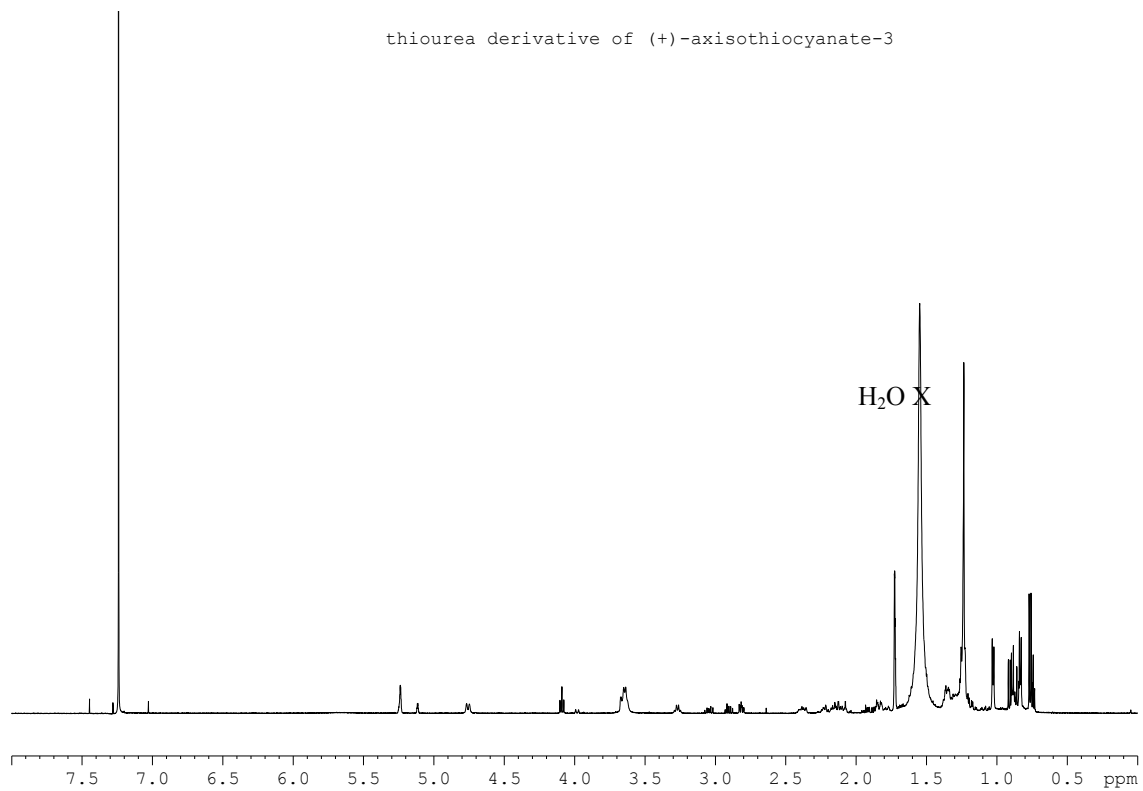
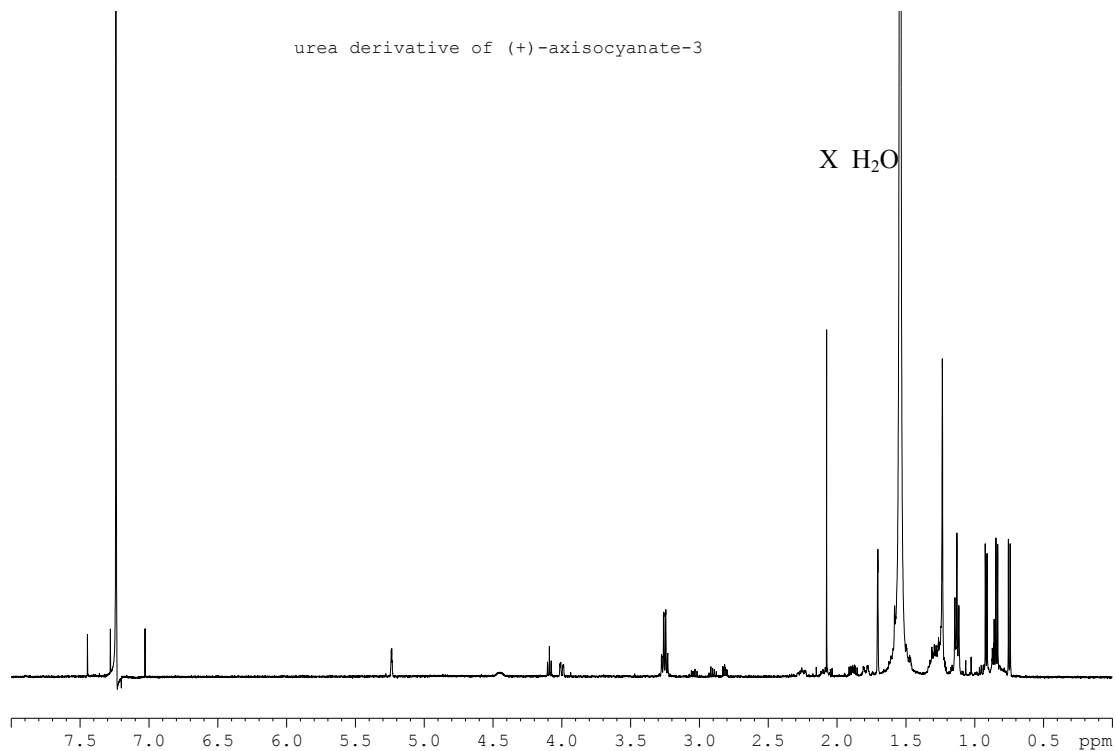


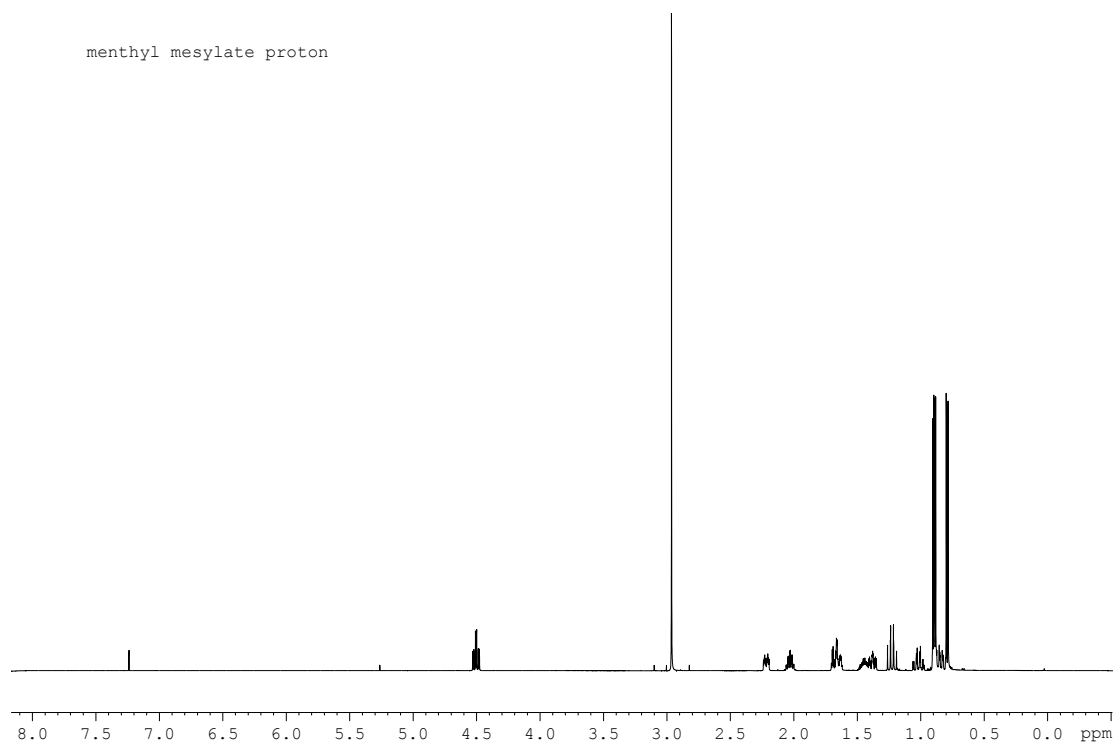
Figure S3. (a) GC-MS trace of axisothiocyante-3 **7** and axisocyanate-3 **8** as a mixture



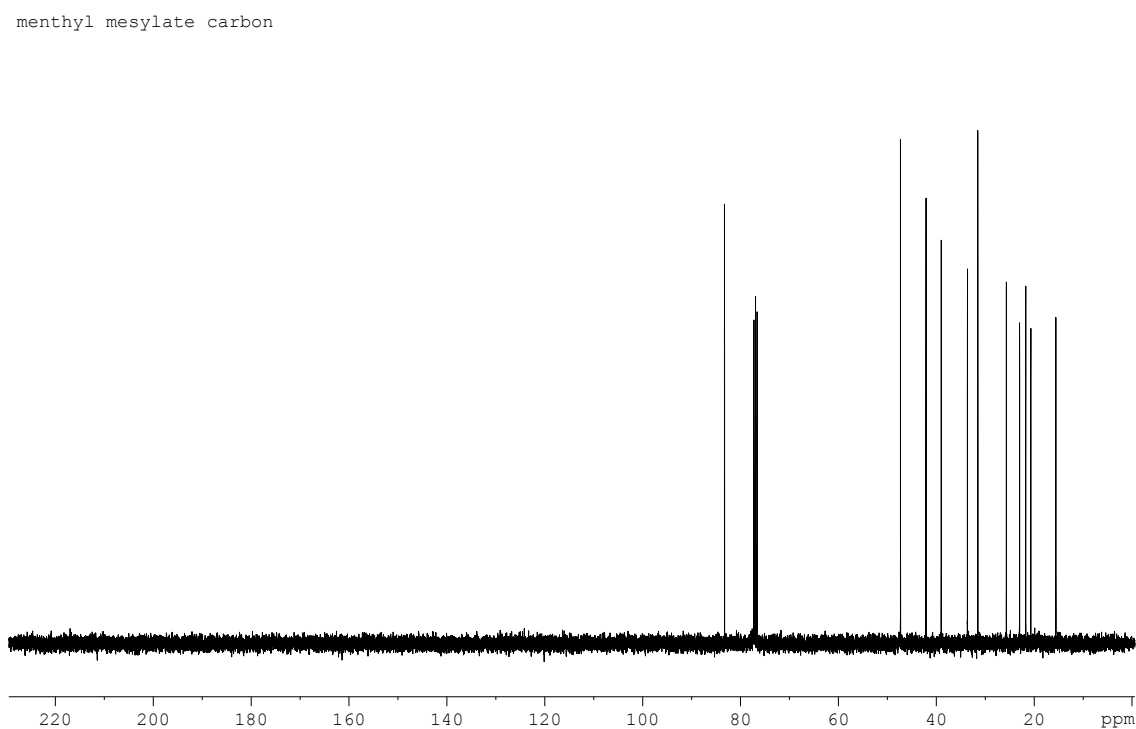
**Figure S4.** <sup>1</sup>H NMR spectrum of diethylthiourea derivative **9** of (+)-axisothiocyante-3



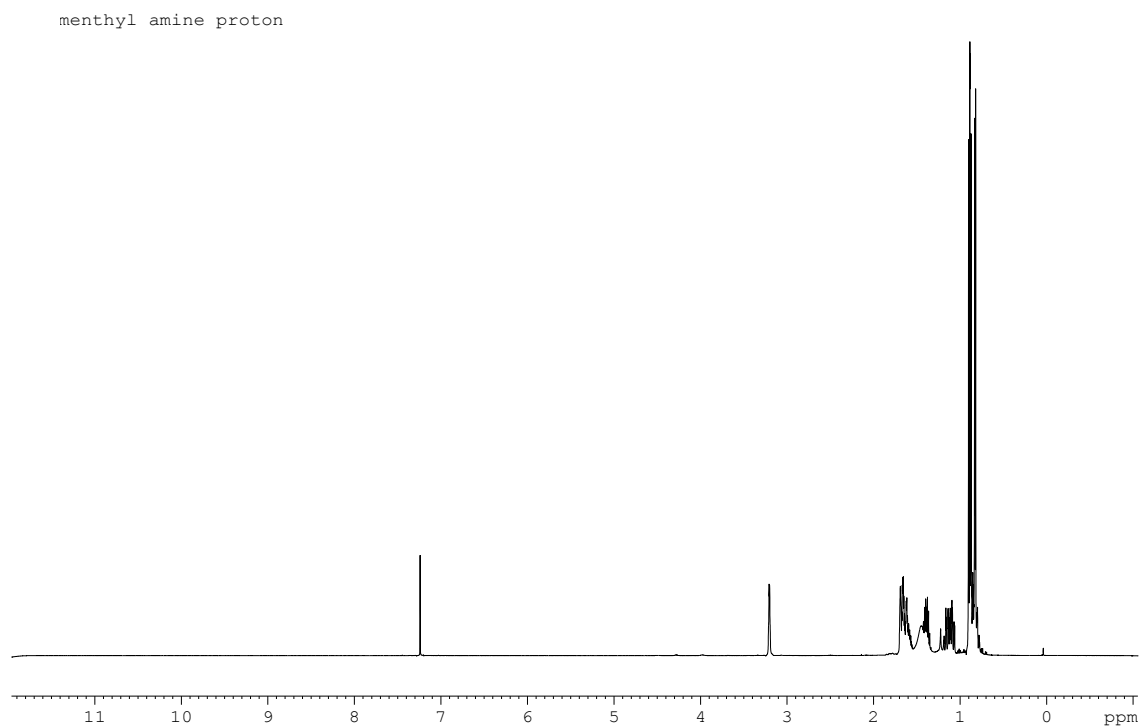
**Figure S5.** <sup>1</sup>H NMR spectrum of diethylurea derivative **10** of (+)-axisocyante-3



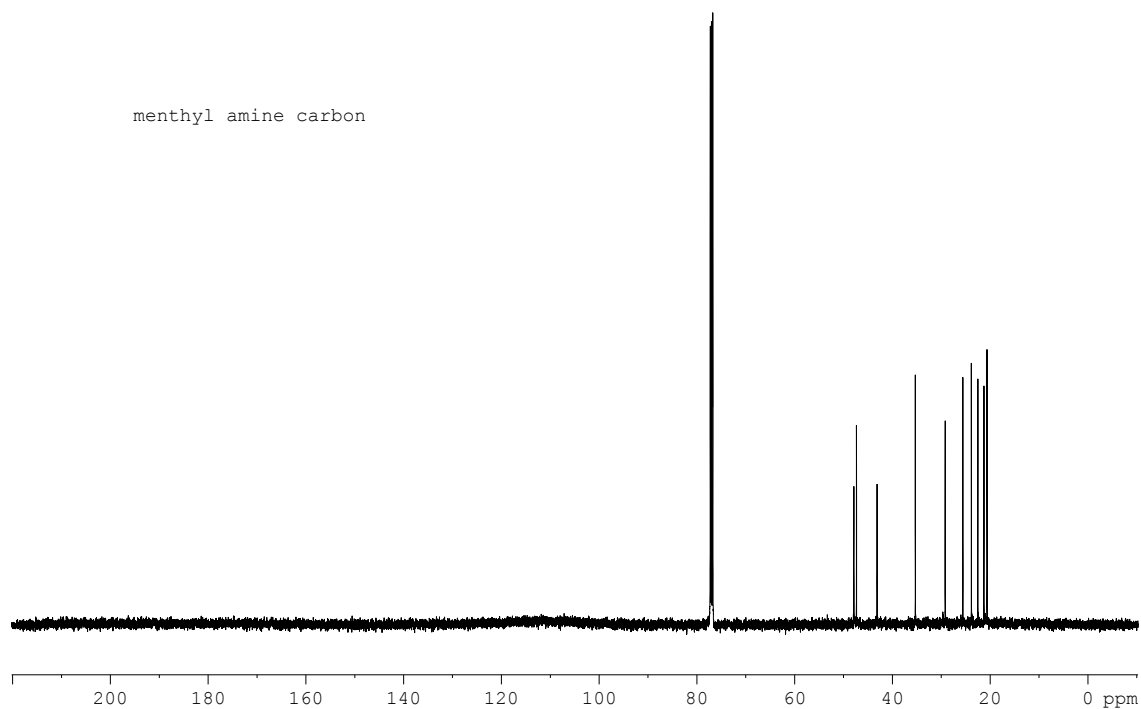
**Figure S6.**  $^1\text{H}$  NMR spectrum of menthyl mesylate **12**



**Figure S7.**  $^{13}\text{C}$  NMR spectrum of menthyl mesylate **12**

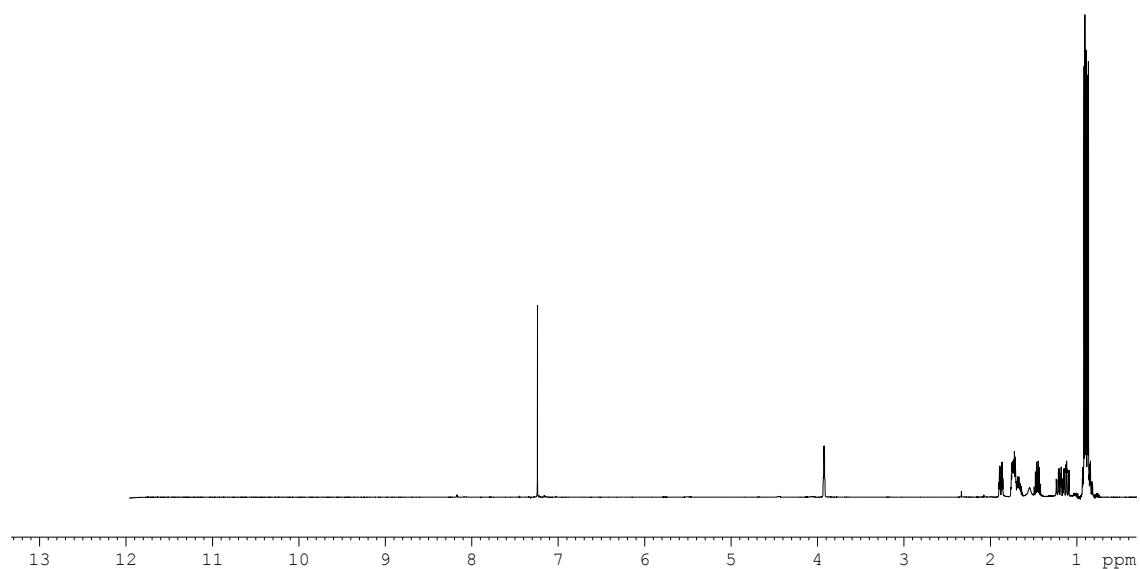


**Figure S8.**  $^1\text{H}$  NMR spectrum of menthyl amine **14**

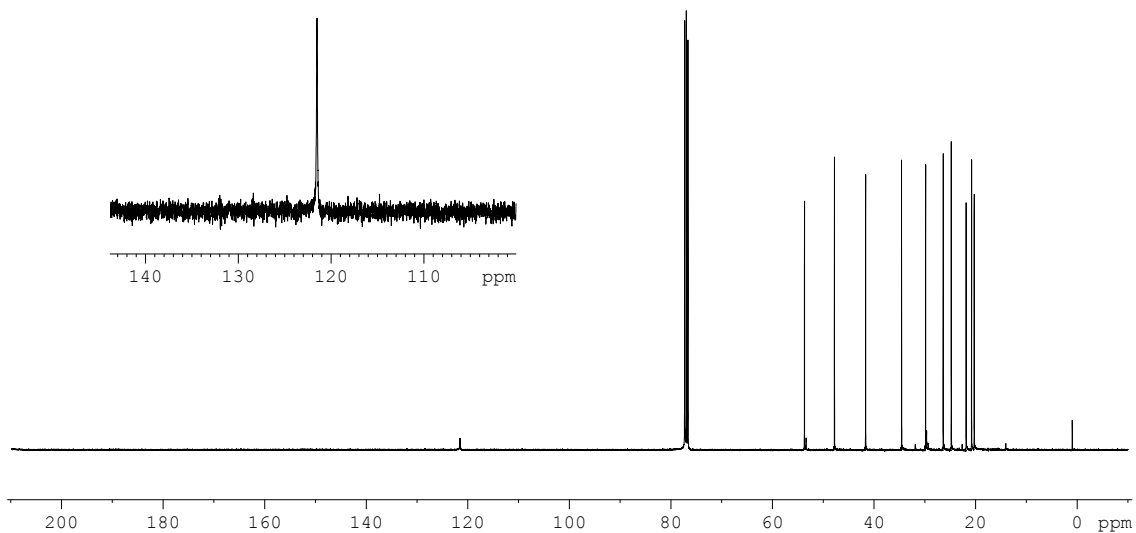


**Figure S9.**  $^{13}\text{C}$  NMR spectrum of menthyl amine **14**

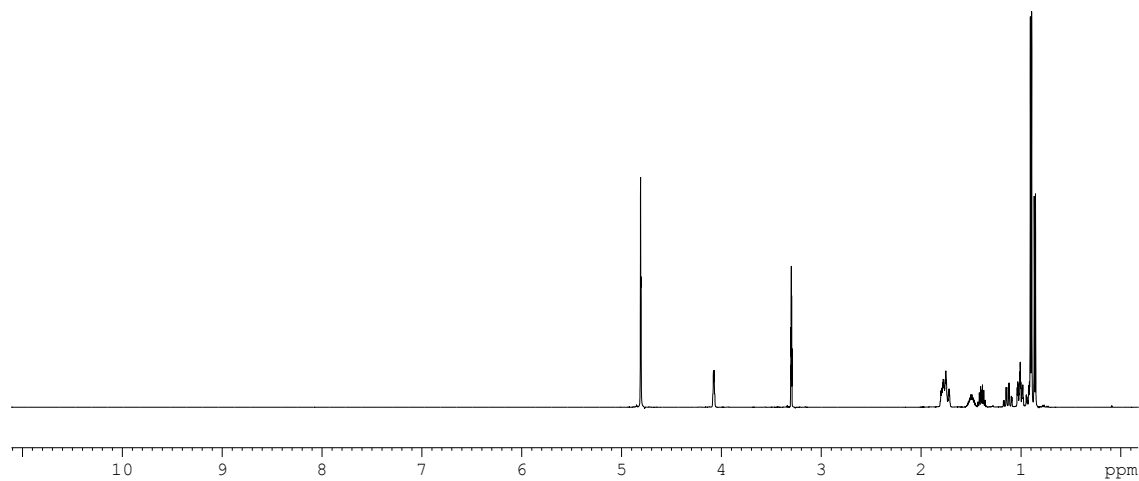
menthyl isocyanate proton

**Figure S10.**  $^1\text{H}$  NMR spectrum of menthyl isocyanate **15**

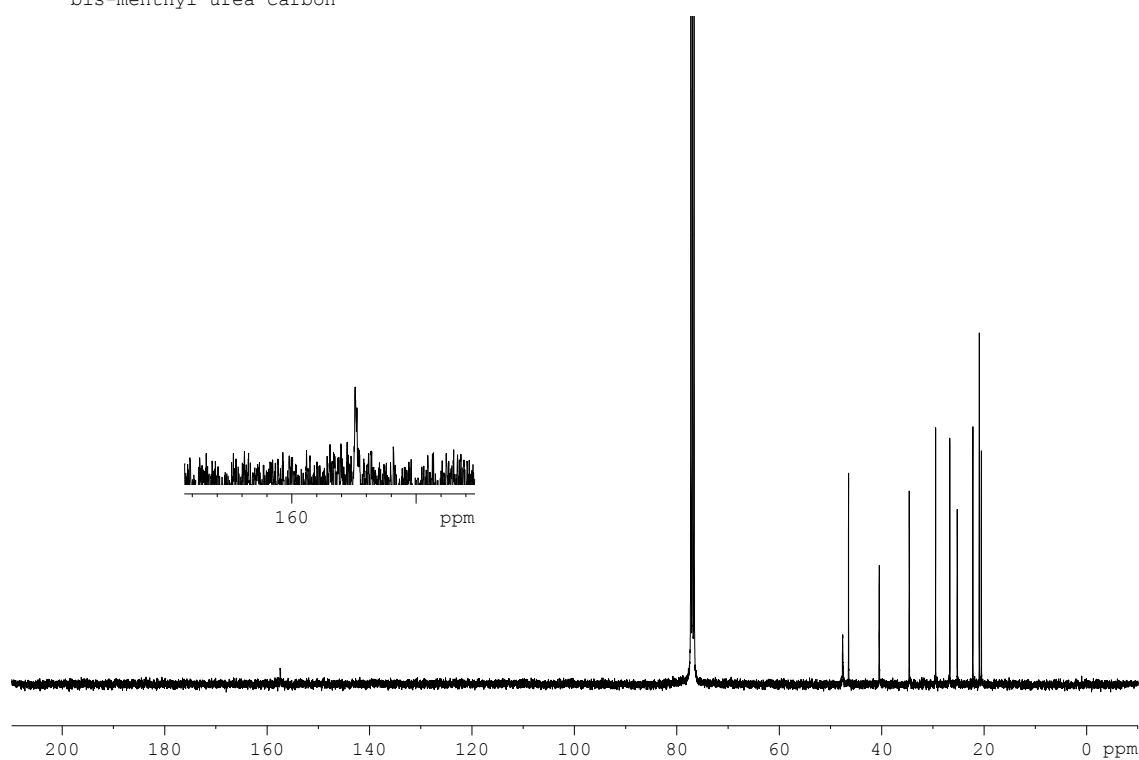
menthyl isocyanate carbon

**Figure S11.**  $^{13}\text{C}$  NMR spectrum of menthyl isocyanate **15**

bis-menthyl urea cd3od

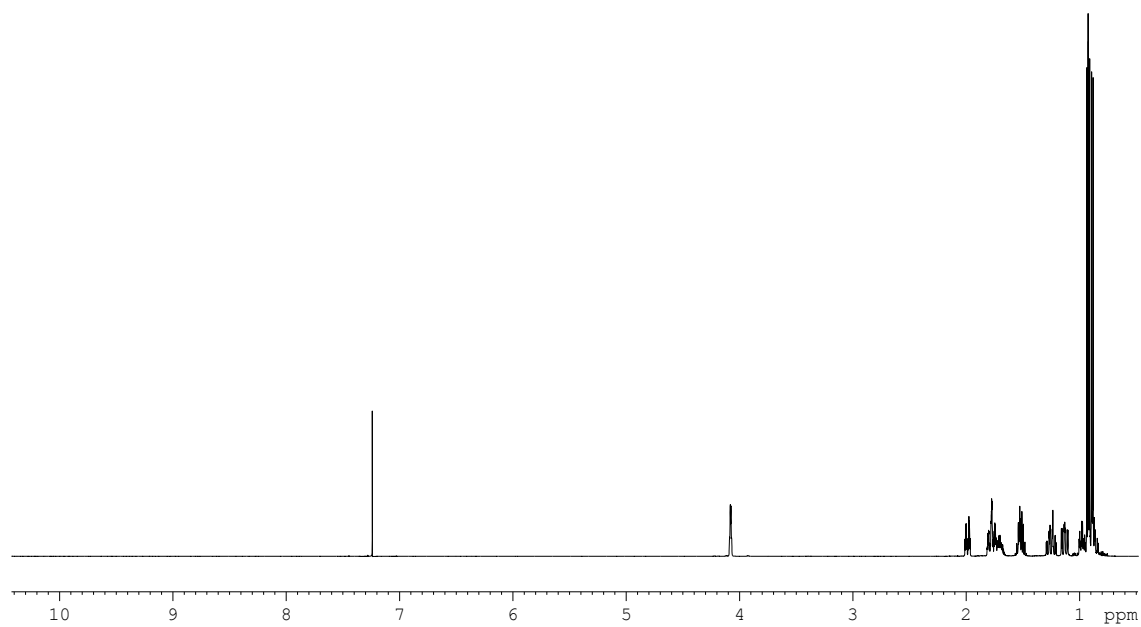
**Figure S12.**  $^1\text{H}$  NMR spectrum of *bis*-menthyl urea **16**

bis-menthyl urea carbon

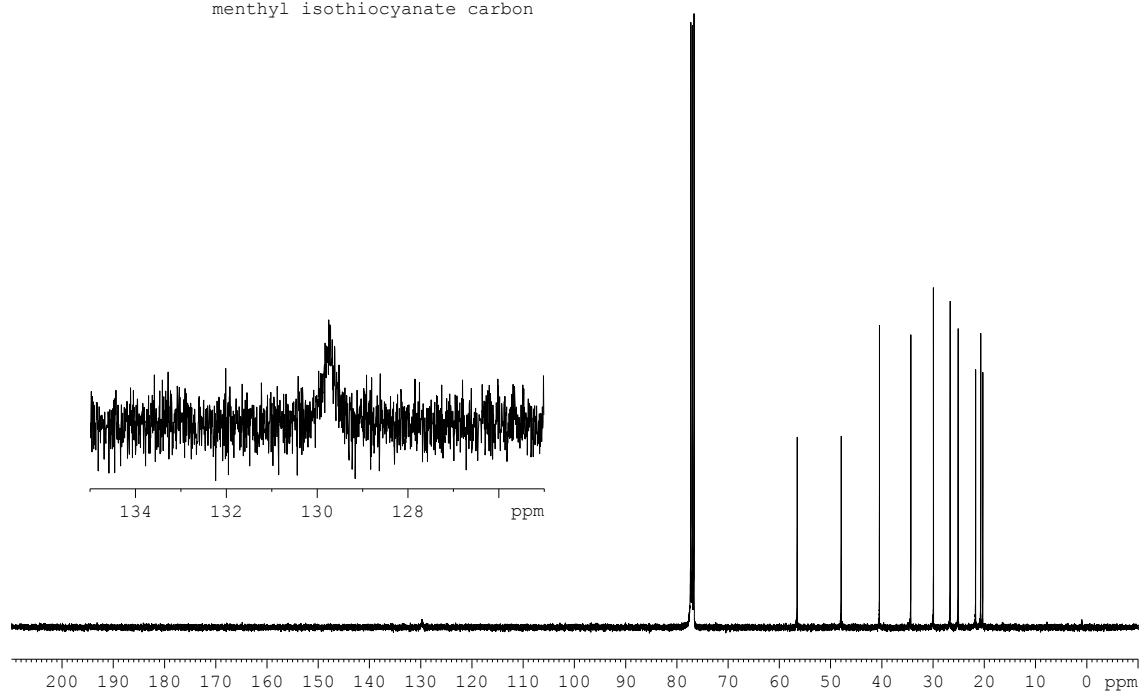
**Figure S13.**  $^{13}\text{C}$  NMR spectrum of *bis*-menthyl urea **16**



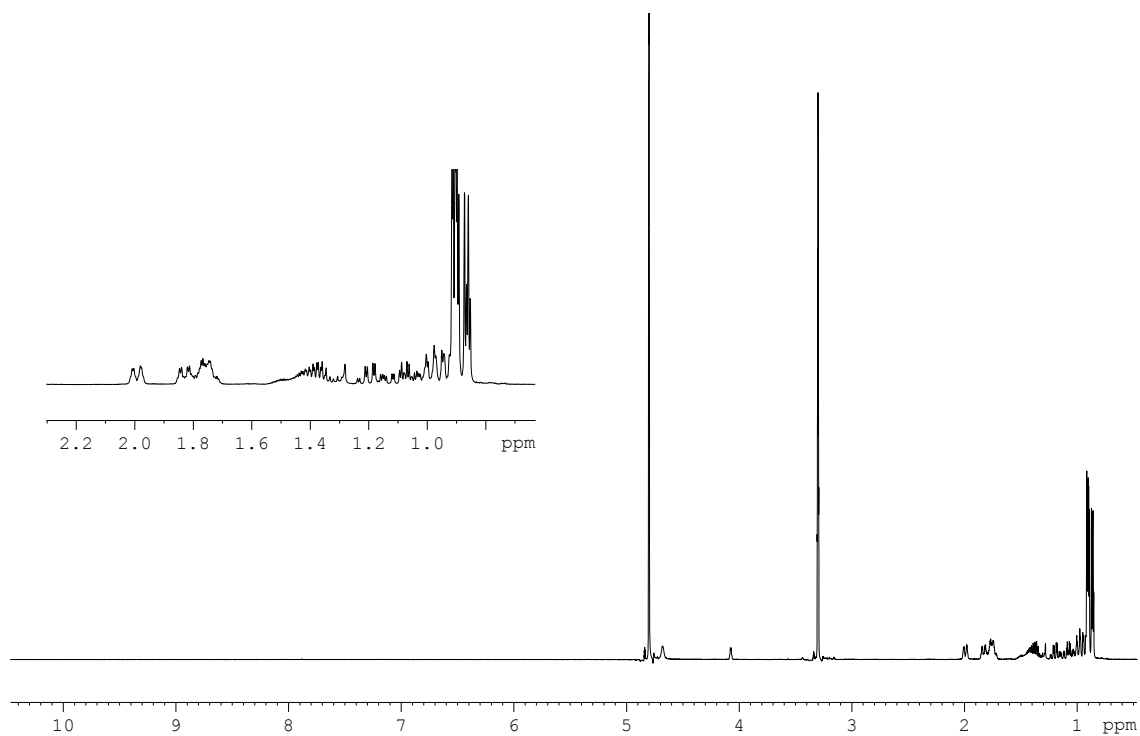
menthyl isothiocyanate proton

**Figure S14.**  $^1\text{H}$  NMR spectrum of menthyl isothiocyanate **21**

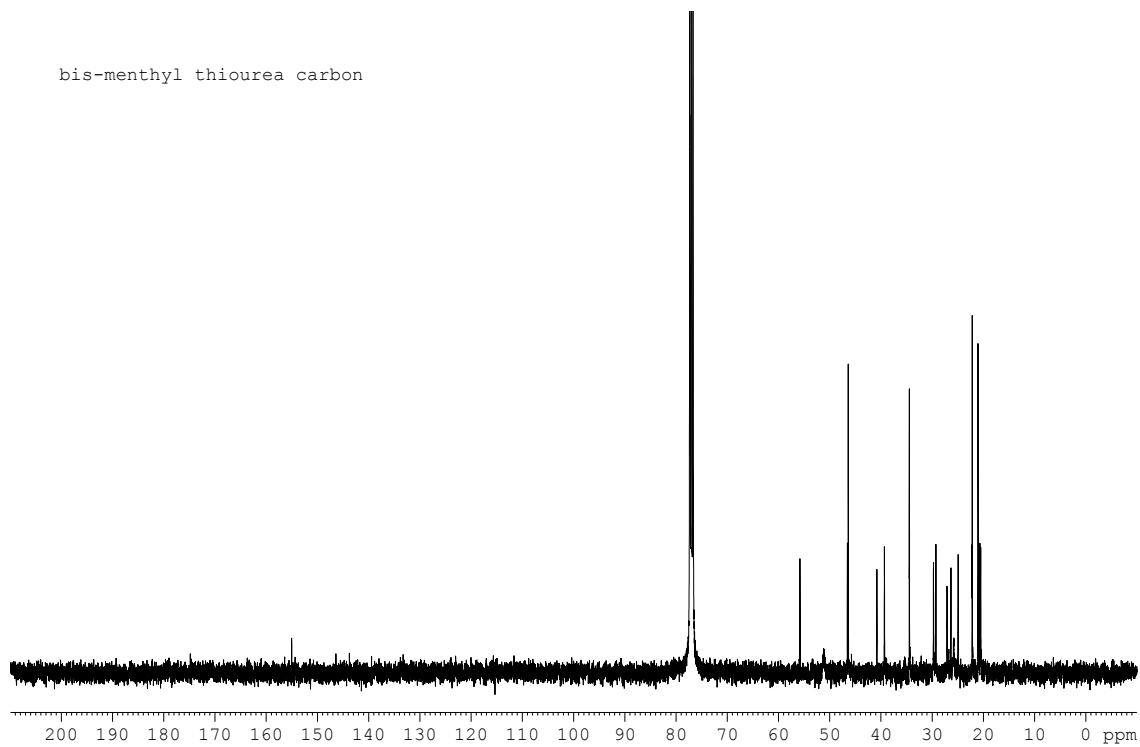
menthyl isothiocyanate carbon

**Figure S15.**  $^{13}\text{C}$  NMR spectrum of menthyl isothiocyanate **21**

bis-menthyl thiourea proton

**Figure S16.** <sup>1</sup>H NMR spectrum of *bis*-menthyl thiourea **22**

bis-menthyl thiourea carbon

**Figure S17.** <sup>13</sup>C NMR spectrum of *bis*-menthyl thiourea **22**