

Supplementary Information

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

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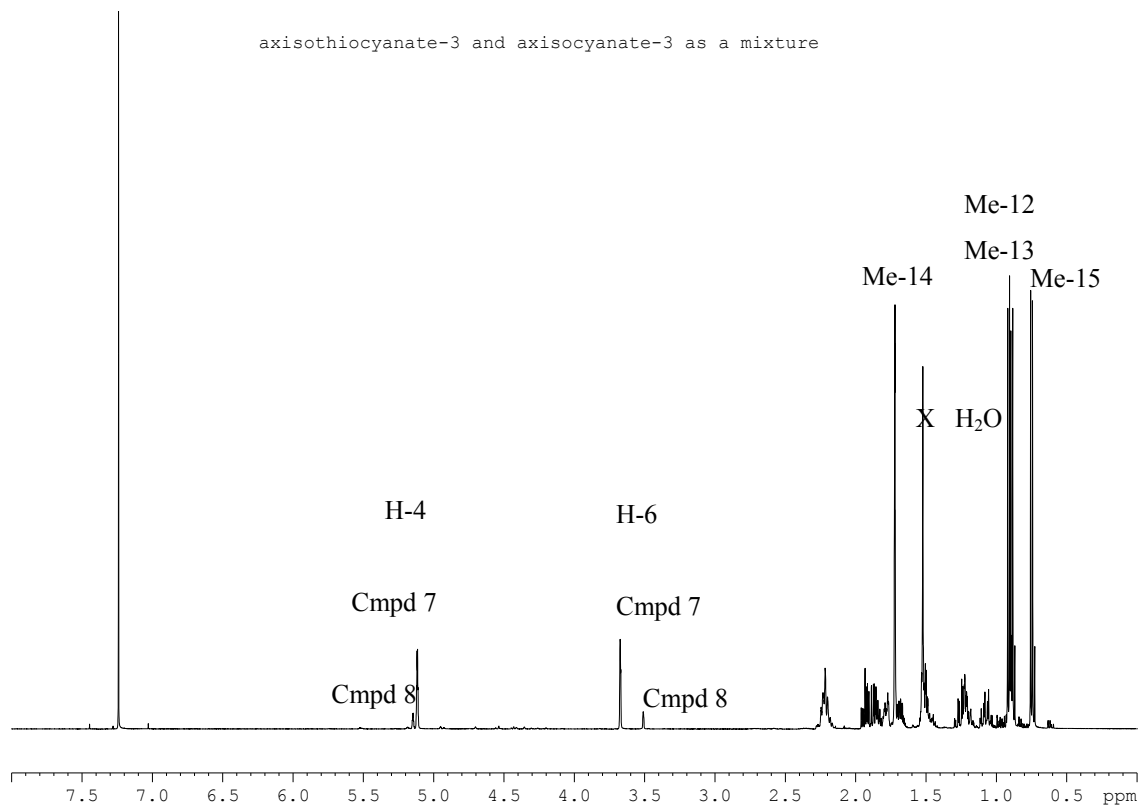


Figure S1. ¹H NMR spectrum of axisothiocyanate-3 **7** and axisocyanate-3 **8** as a mixture

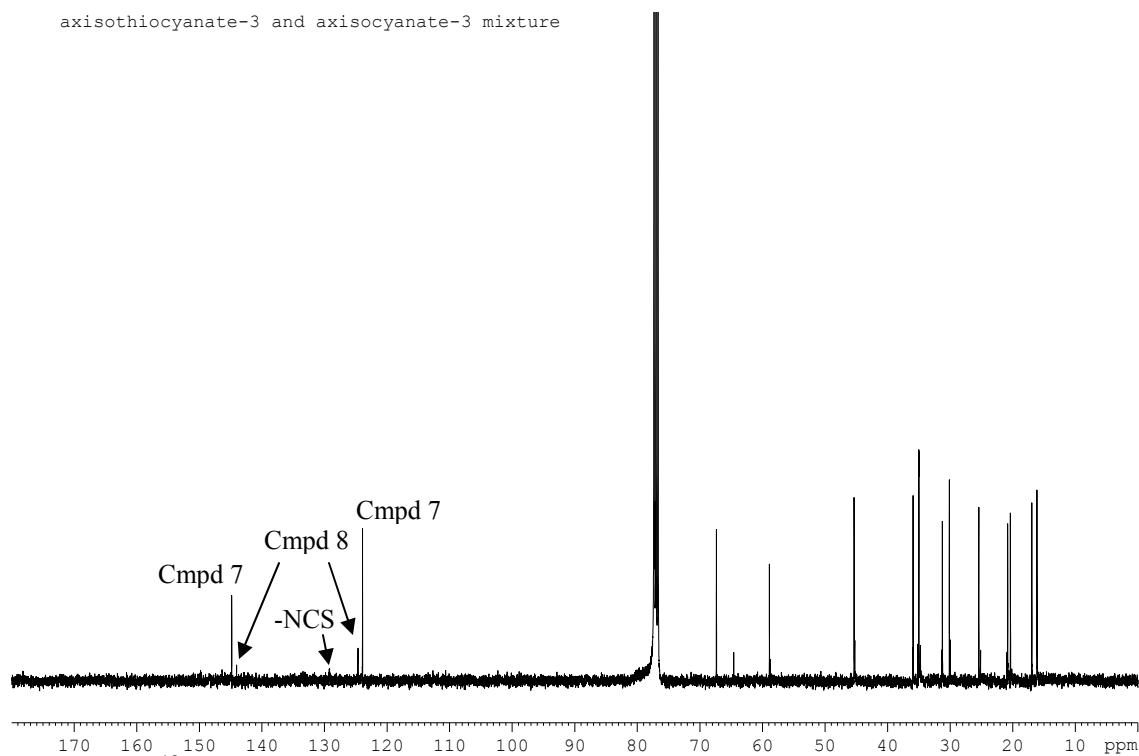
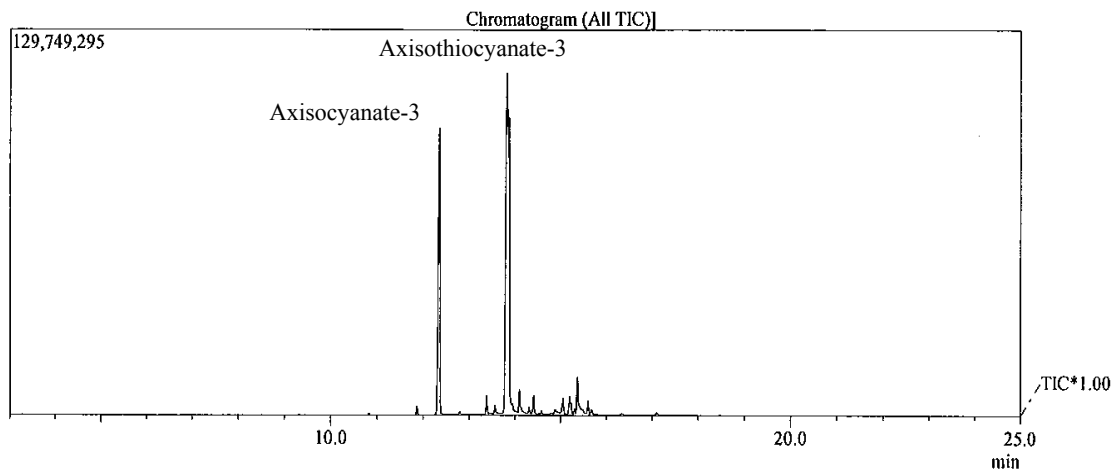


Figure S2. ¹³C NMR spectrum of axisothiocyanate-3 **7** and axisocyanate-3 **8** as a mixture



(b) Mass spectrum of the axisocyanate-3 compound

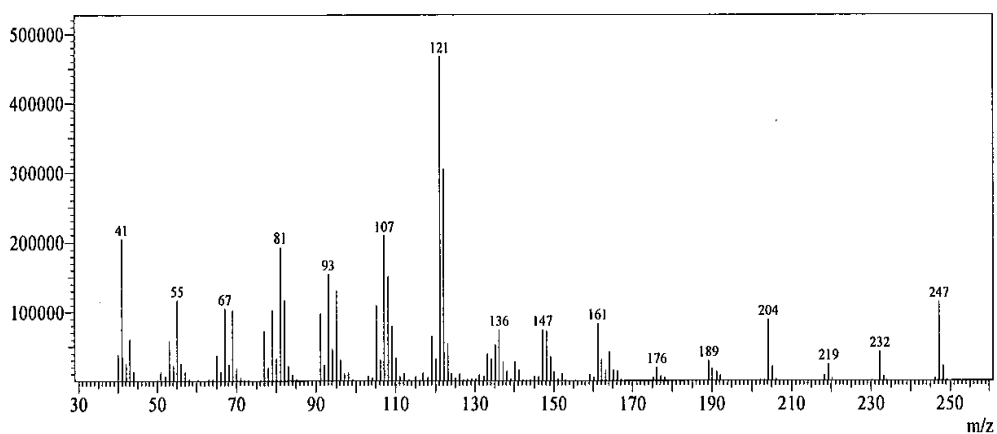


Figure S3. (a) GC-MS trace of axisothiocyante-3 **7** and axisocyanate-3 **8** as a mixture

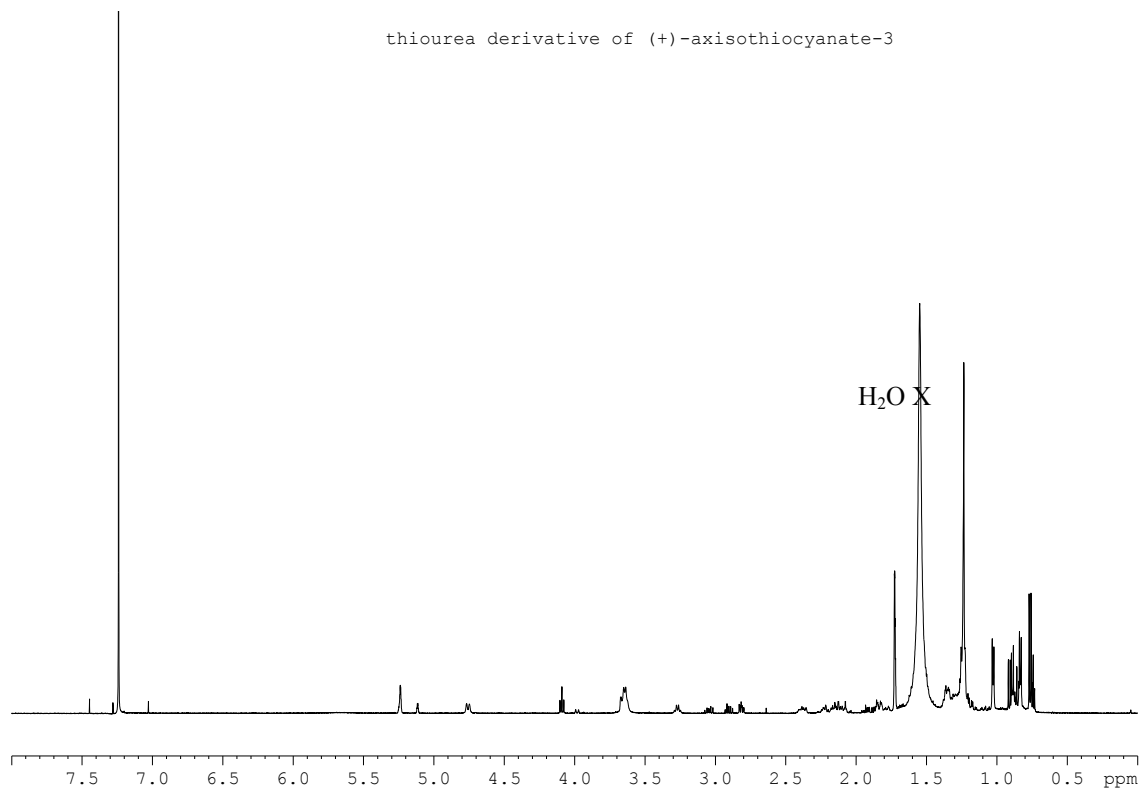


Figure S4. ¹H NMR spectrum of diethylthiourea derivative **9** of (+)-axisothiocyante-3

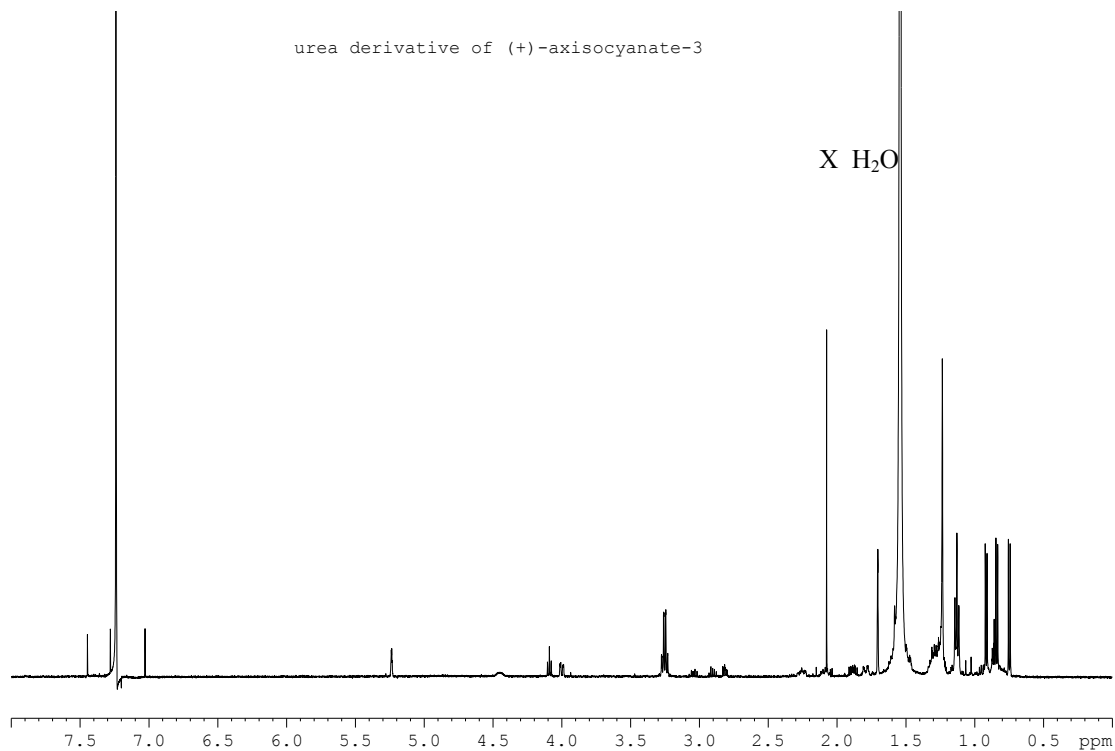


Figure S5. ¹H NMR spectrum of diethylurea derivative **10** of (+)-axisocyante-3

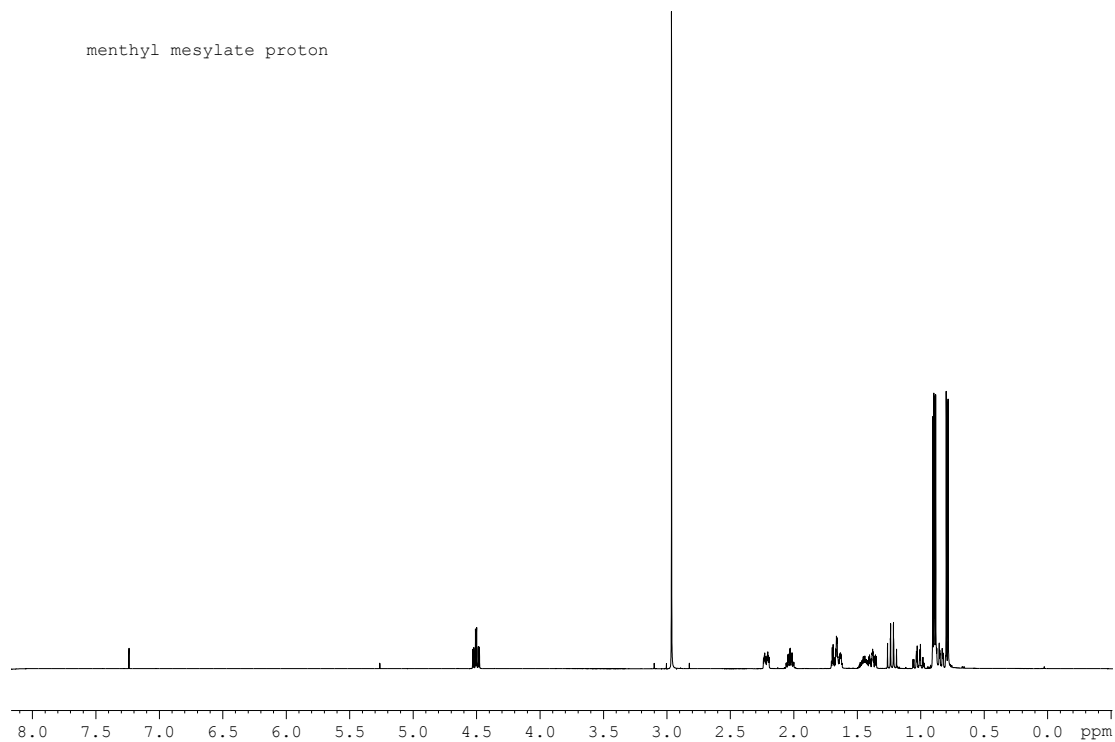


Figure S6. ^1H NMR spectrum of menthyl mesylate **12**

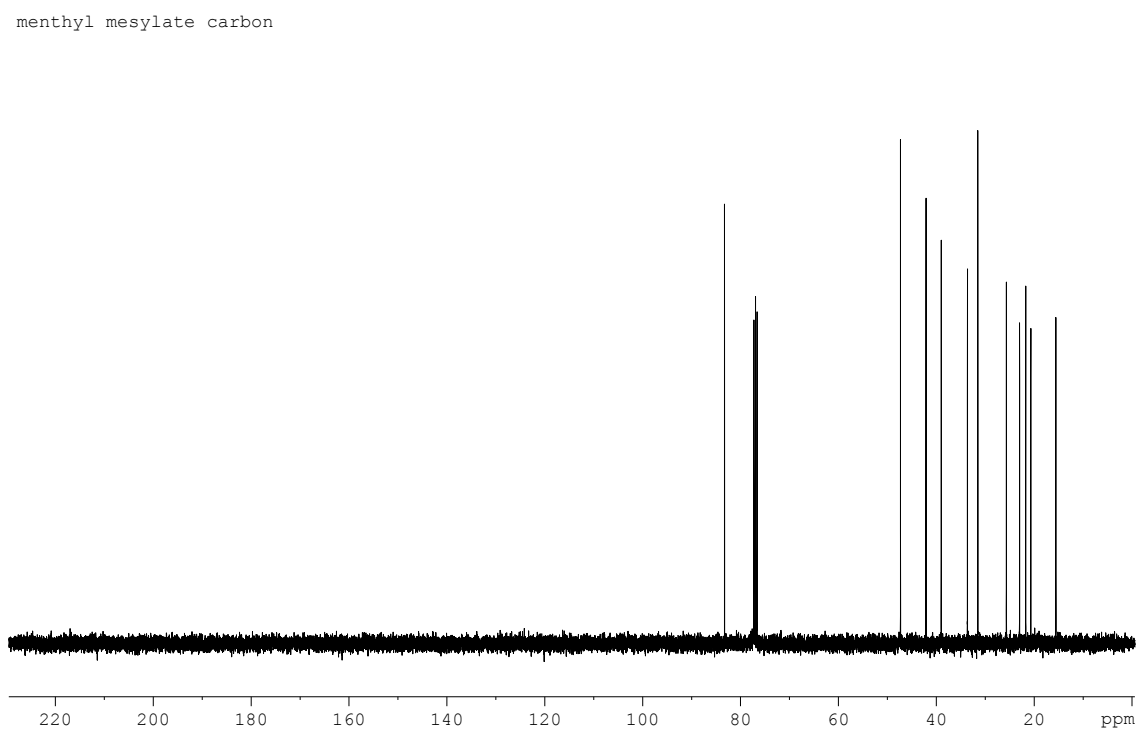


Figure S7. ^{13}C NMR spectrum of menthyl mesylate **12**

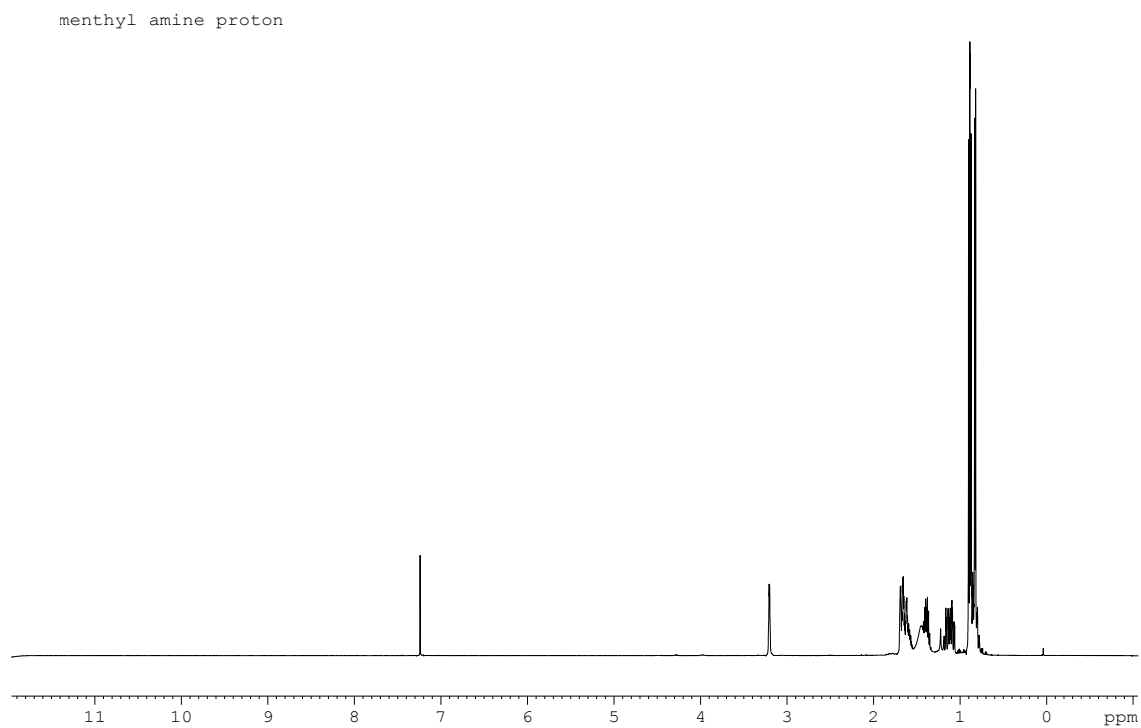


Figure S8. ¹H NMR spectrum of menthyl amine **14**

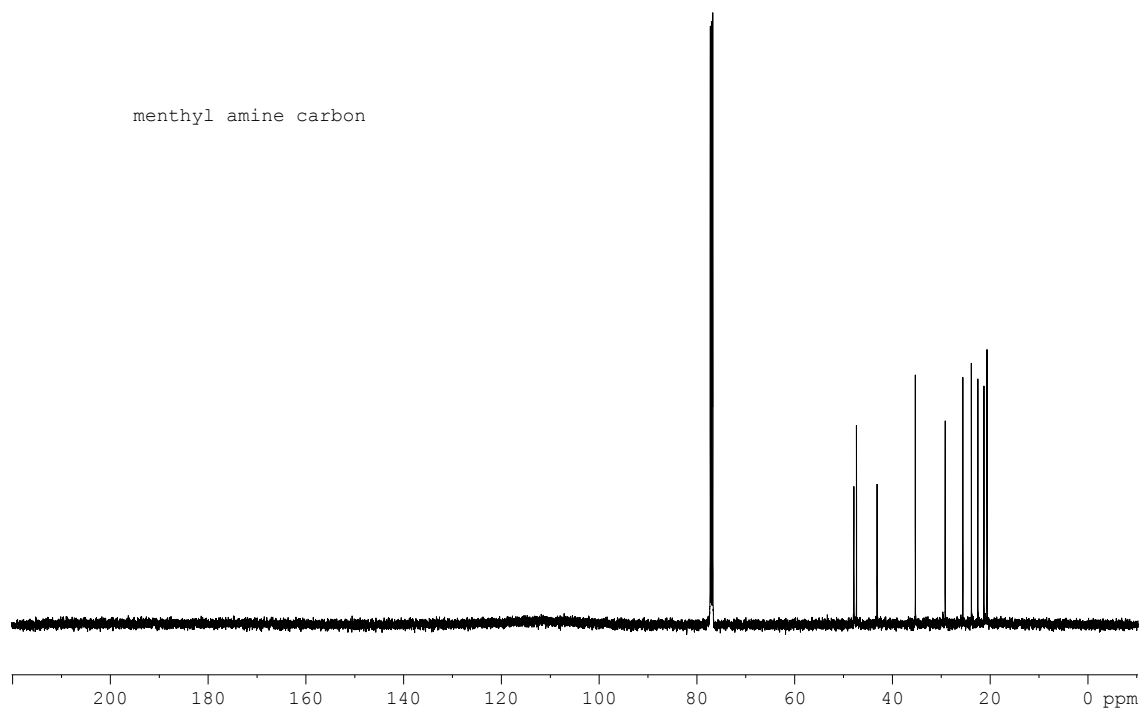
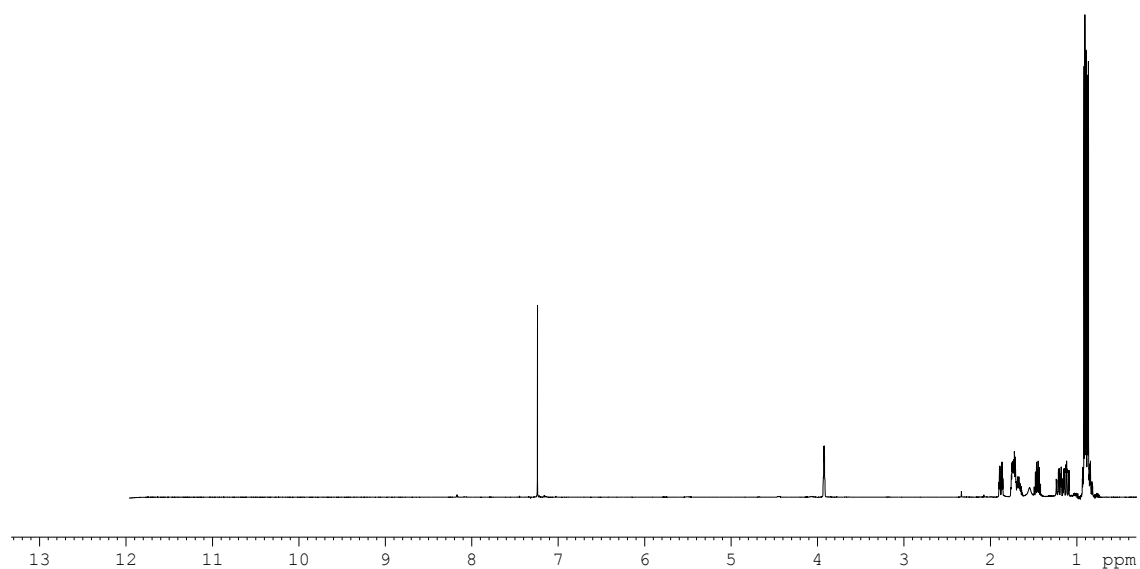
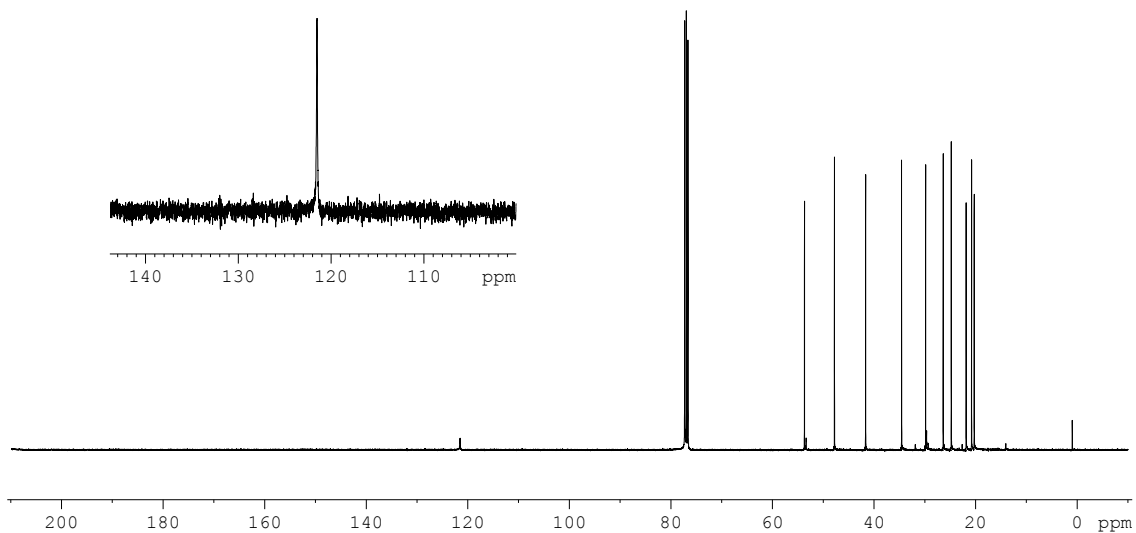


Figure S9. ¹³C NMR spectrum of menthyl amine **14**

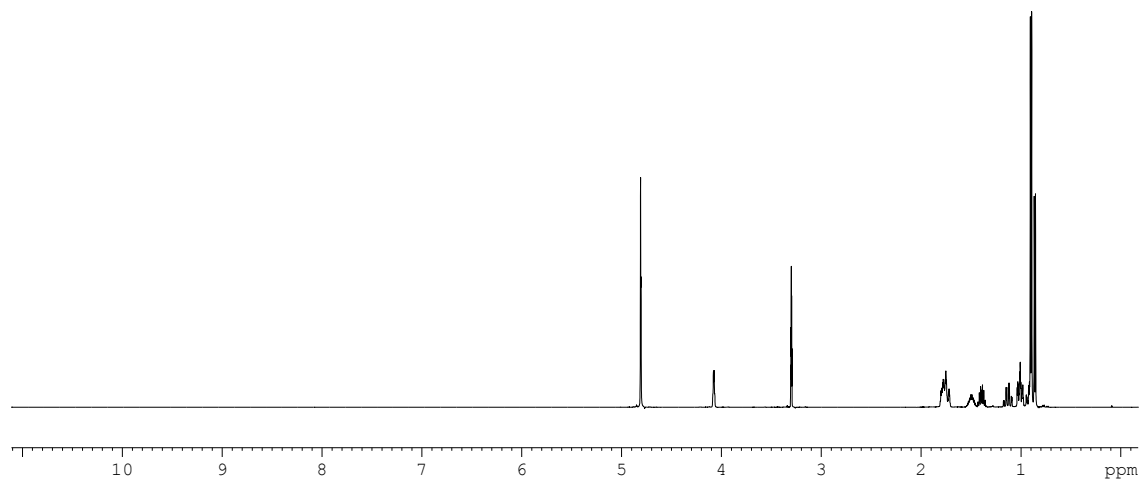
menthyl isocyanate proton

**Figure S10.** ^1H NMR spectrum of menthyl isocyanate **15**

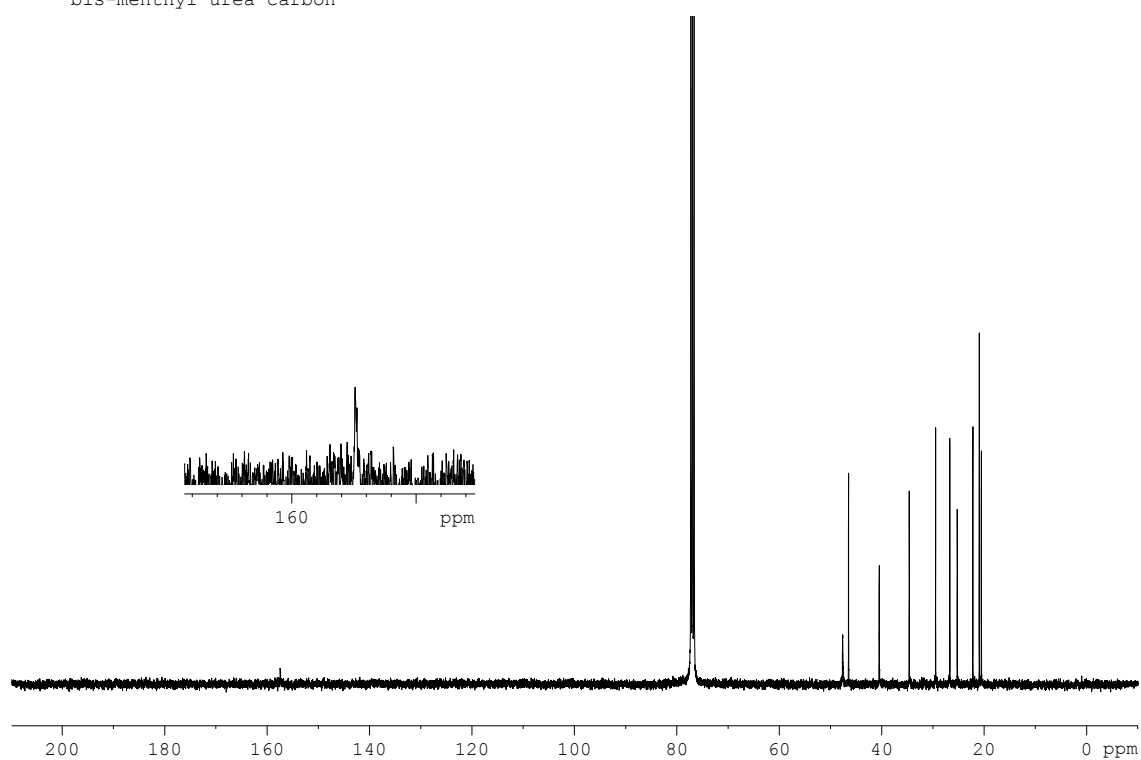
menthyl isocyanate carbon

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

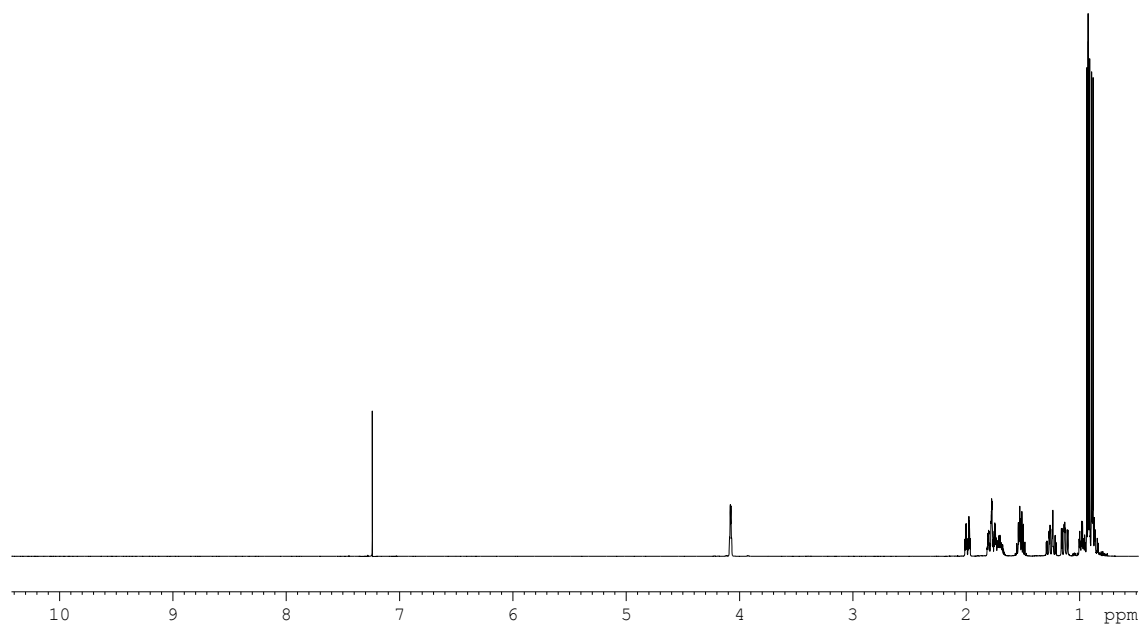
bis-menthyl urea cd3od

**Figure S12.** ^1H NMR spectrum of *bis*-menthyl urea **16**

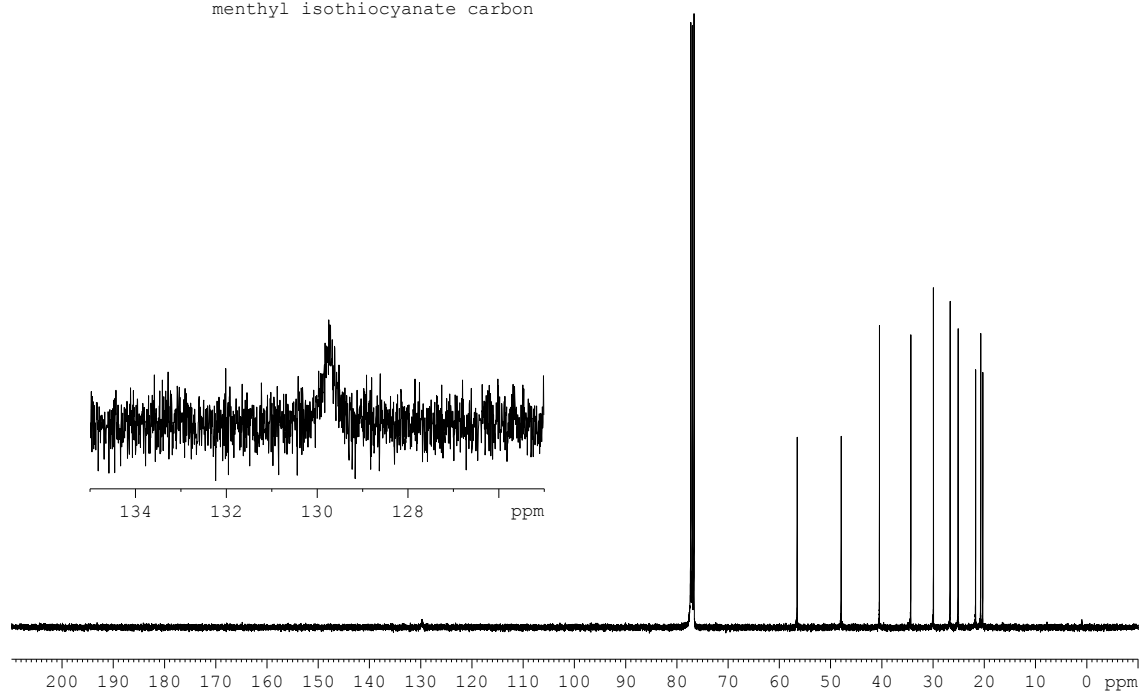
bis-menthyl urea carbon

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

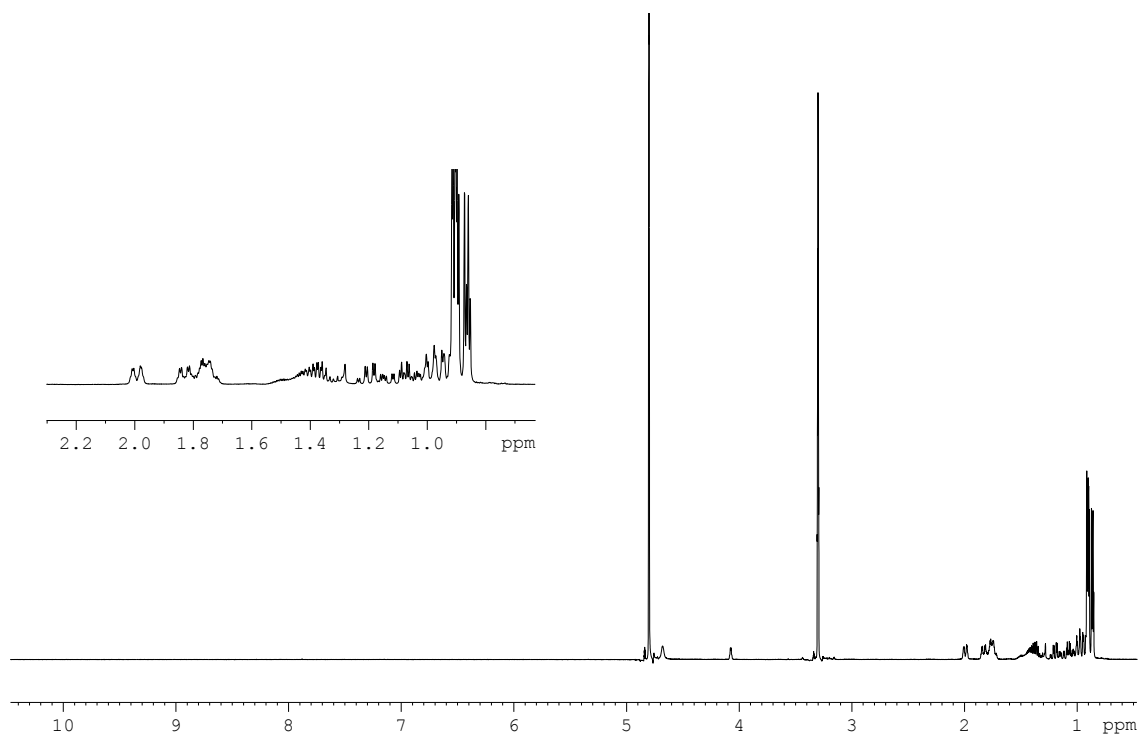
menthyl isothiocyanate proton

**Figure S14.** ¹H NMR spectrum of menthyl isothiocyanate **21**

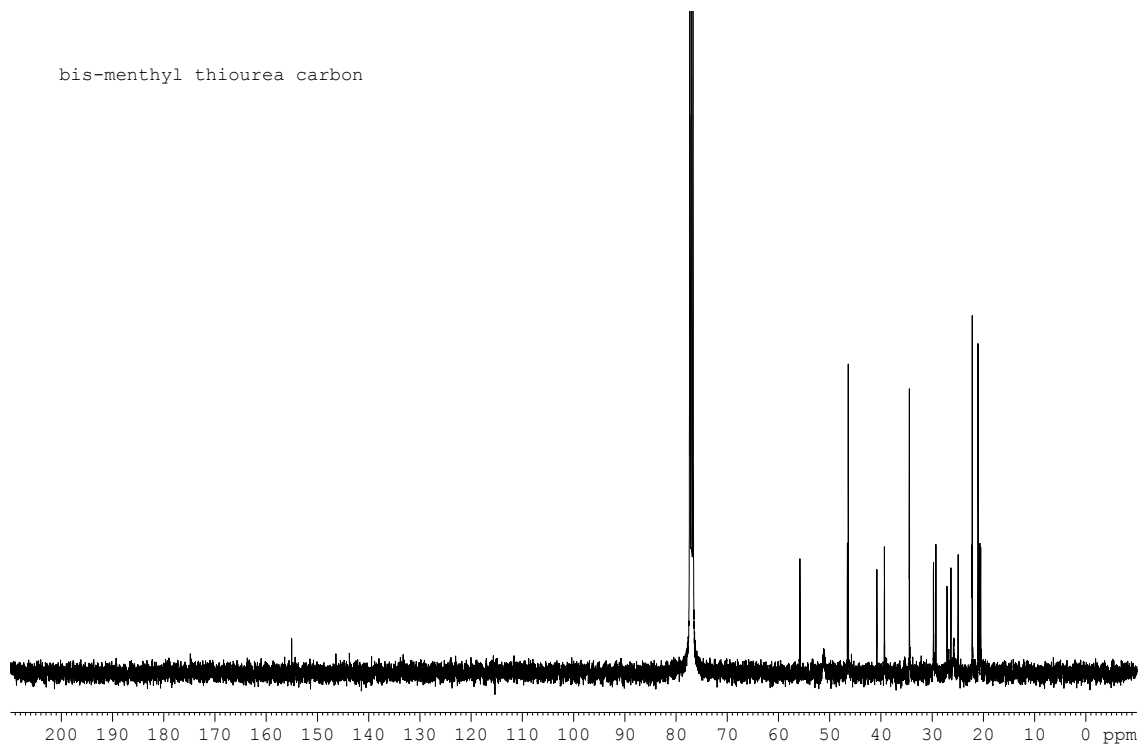
menthyl isothiocyanate carbon

**Figure S15.** ¹³C NMR spectrum of menthyl isothiocyanate **21**

bis-menthyl thiourea proton

**Figure S16.** ¹H NMR spectrum of *bis*-menthyl thiourea **22**

bis-menthyl thiourea carbon

**Figure S17.** ¹³C NMR spectrum of *bis*-menthyl thiourea **22**