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*

*a School of Molecular and Microbial Sciences, The University of Queensland, Brisbane QLD 4072, Australia

*b Department of Pharmacy, Islamic University of Indonesia, Yogyakarta 55584, Indonesia

E-mail: m.garson@uq.edu.au

Table of Contents

Figure S1  $^1$H NMR spectrum of axisothiocyanate-3 7 and axisocyanate-3 8 as a mixture  S2
Figure S2  $^{13}$C NMR spectrum of axisothiocyanate-3 7 and axisocyanate-3 8 as a mixture  S2
Figure S3  (a) GC-MS trace of axisothiocyanate-3 7 and axisocyanate-3 8 as a mixture; (b) Mass spectrum of the axisocyanate-3 component  S3
Figure S4  $^1$H NMR spectrum of diethylthiourea derivative 9 of (+)-axisothiocyanate-3  S4
Figure S5  $^1$H NMR spectrum of diethylurea derivative 10 of (+)-axisocyanate-3  S4
Figure S6  $^1$H NMR spectrum of menthyl mesylate 12  S5
Figure S7  $^{13}$C NMR spectrum of menthyl mesylate 12  S5
Figure S8  $^1$H NMR spectrum of menthyl amine 14  S6
Figure S9  $^{13}$C NMR spectrum of menthyl amine 14  S6
Figure S10  $^1$H NMR spectrum of menthyl isocyanate 15  S7
Figure S11  $^{13}$C NMR spectrum of menthyl isocyanate 15  S7
Figure S12  $^1$H NMR spectrum of bis-menthyl urea 16  S8
Figure S13  $^{13}$C NMR spectrum of bis-menthyl urea 16  S8
Figure S14  $^1$H NMR spectrum of menthyl isothiocyanate 21  S9
Figure S15  $^{13}$C NMR spectrum of menthyl isothiocyanate 21  S9
Figure S16  $^1$H NMR spectrum of bis-menthyl thiourea 22  S10
Figure S17  $^{13}$C NMR spectrum of bis-menthyl thiourea 22  S10
**Figure S1.** $^1$H NMR spectrum of axisothiocyanate-3 7 and axisocyanate-3 8 as a mixture

**Figure S2.** $^{13}$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 axisothiocyanate-3 7 and axisocyanate-3 8 as a mixture
Figure S4. $^1$H NMR spectrum of diethylthiourea derivative 9 of (+)-axisothiocyanate-3

Figure S5. $^1$H NMR spectrum of diethylurea derivative 10 of (+)-axisocyanate-3
Figure S6. $^1$H NMR spectrum of menthyl mesylate 12

Figure S7. $^{13}$C NMR spectrum of menthyl mesylate 12
Figure S8. $^1$H NMR spectrum of menthyl amine 14

Figure S9. $^{13}$C NMR spectrum of menthyl amine 14
Figure S10. $^1$H NMR spectrum of menthyl isocyanate 15

Figure S11. $^{13}$C NMR spectrum of menthyl isocyanate 15
**Figure S12.** $^1$H NMR spectrum of *bis*-menthyl urea 16

**Figure S13.** $^{13}$C NMR spectrum of *bis*-menthyl urea 16
Figure S14. $^1$H NMR spectrum of menthyl isothiocyanate 21

Figure S15. $^{13}$C NMR spectrum of menthyl isothiocyanate 21
**Figure S16.** $^1$H NMR spectrum of *bis*-menthyl thiourea 22

**Figure S17.** $^{13}$C NMR spectrum of *bis*-menthyl thiourea 22