

Supporting information

Identification and biosynthesis of tropone derivatives and sulfur volatiles produced by bacteria of the marine *Roseobacter* clade

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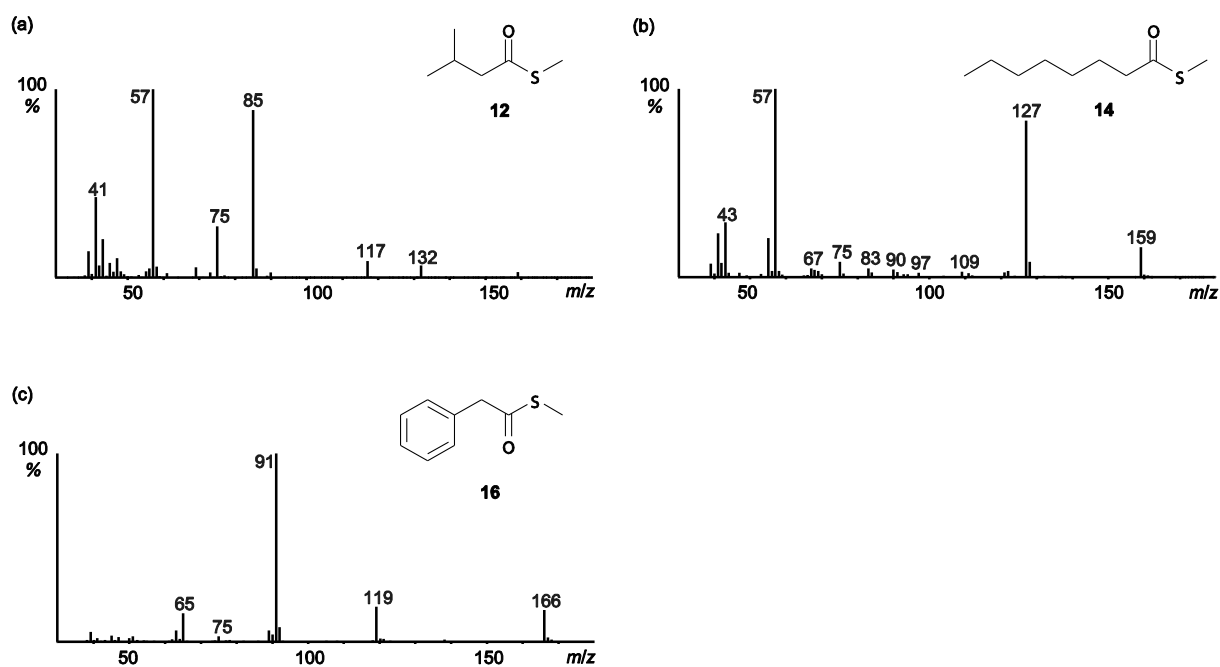


Fig. S1 Mass spectra of natural (a) *S*-methyl 3-methylbutanethioate (**12**), (b) *S*-methyl octanethioate (**14**), and (c) *S*-methyl 2-phenylethanethioate (**16**). The mass spectra of the synthetic material were identical.

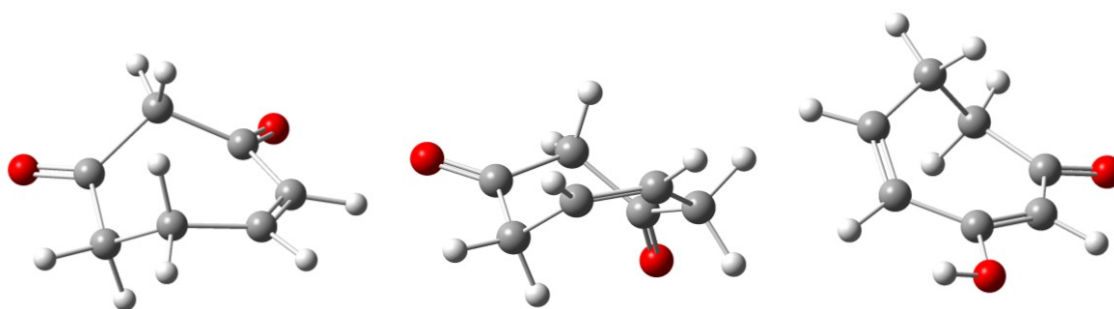


Fig. S2 Optimized gas phase structures of tautomers **42a-c** (M05-2X).

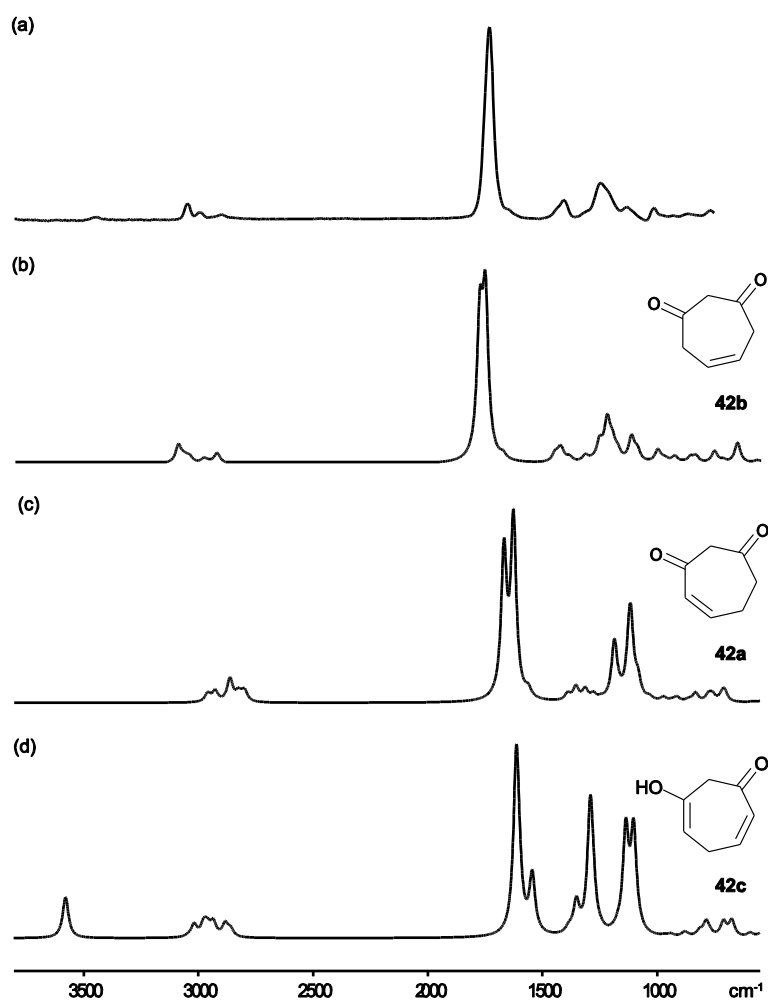


Fig. S3 Gas phase FT-IR spectrum of natural **42** (a) and calculated gas phase IR-spectra of the three most stable tautomers **42a** (c), **42b** (b), and **42c** (d). The experimental spectrum is most similar to tautomer **42b**.