Supporting Information

Lumiquinone A, an α-Aminomalonate-Derived Aminobenzoquinone from *Photorhabdus luminescens*

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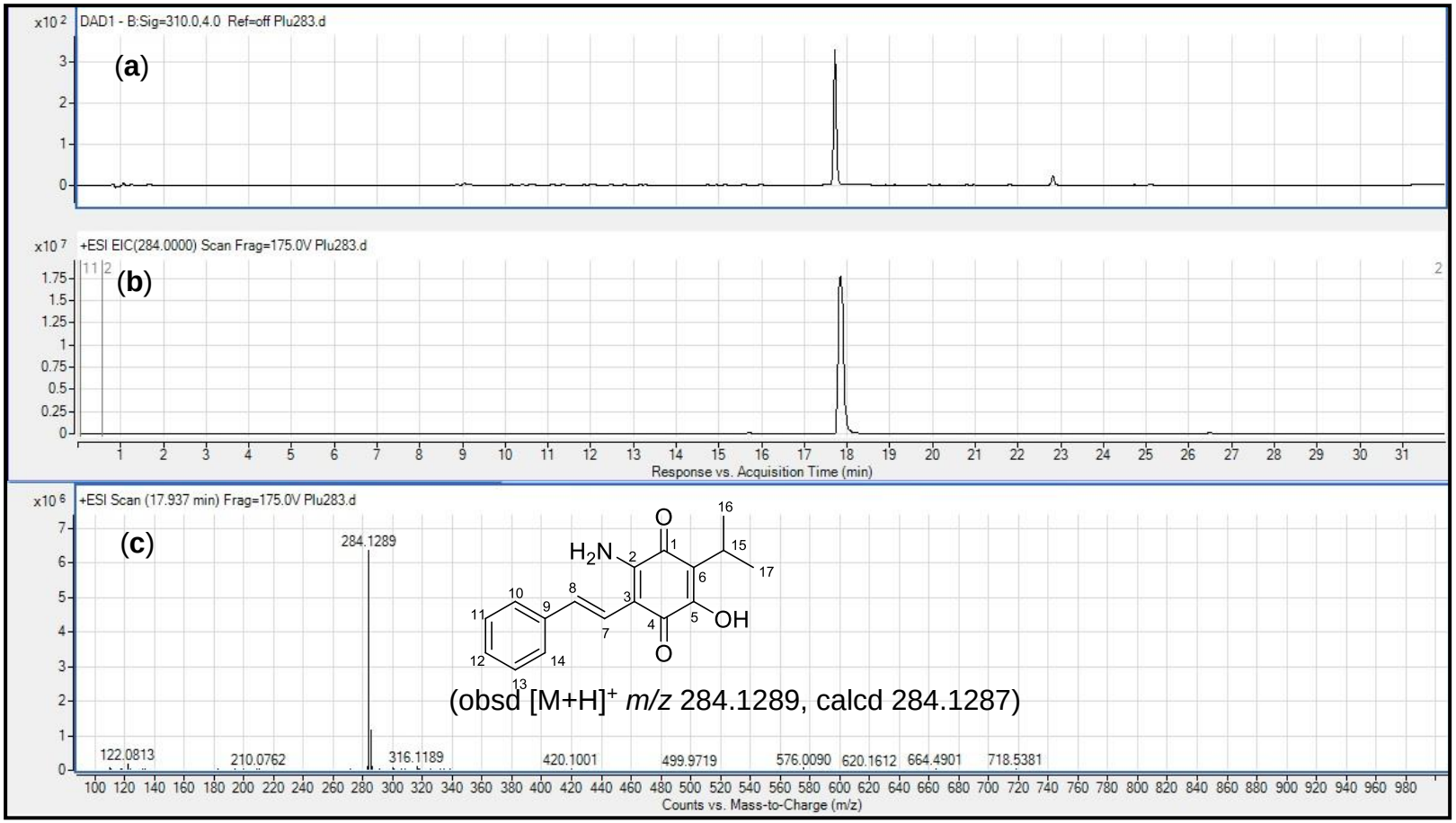


Figure S1. HR-ESI-Q-TOF-MS spectral data of compound **1** (**a**) HPLC chromatogram of **1** detected by UV 310 nm (**b**) Extracted ion chromatogram of *m/z* 284 for compound **1** (**c**) MS profiles of compound **1**

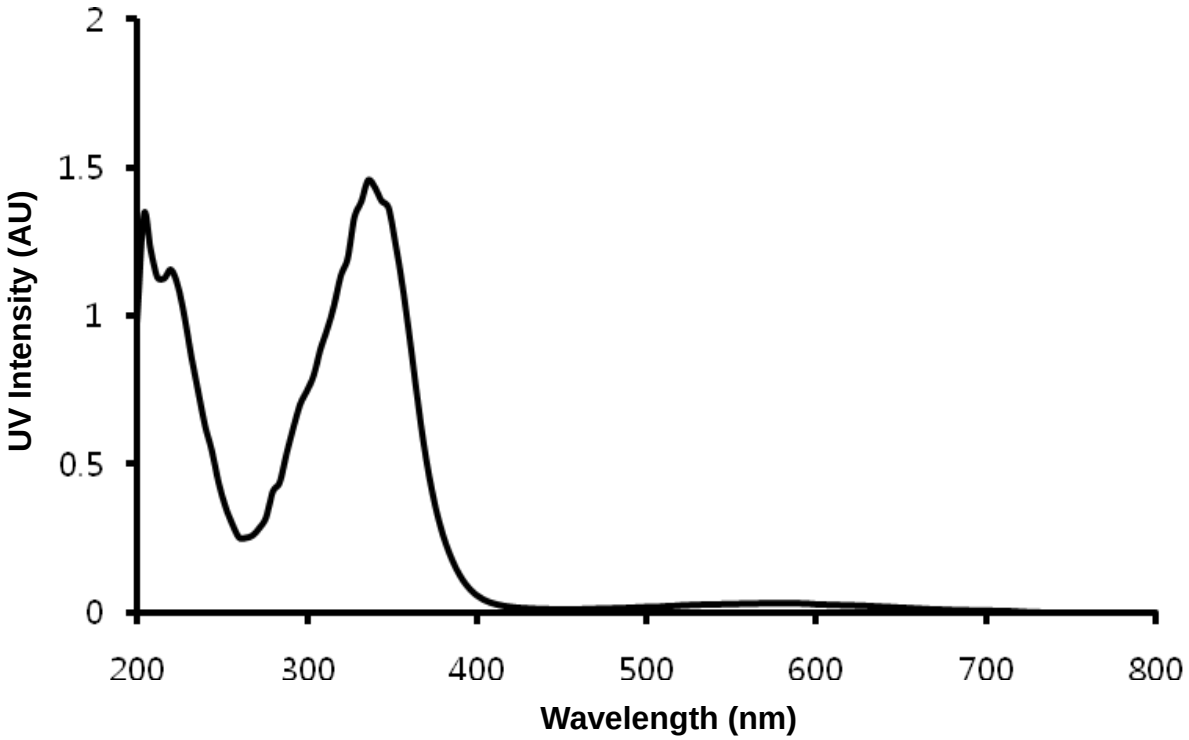


Figure S2. UV spectral data of compound **1** (1.5×10^4 M in methanol)

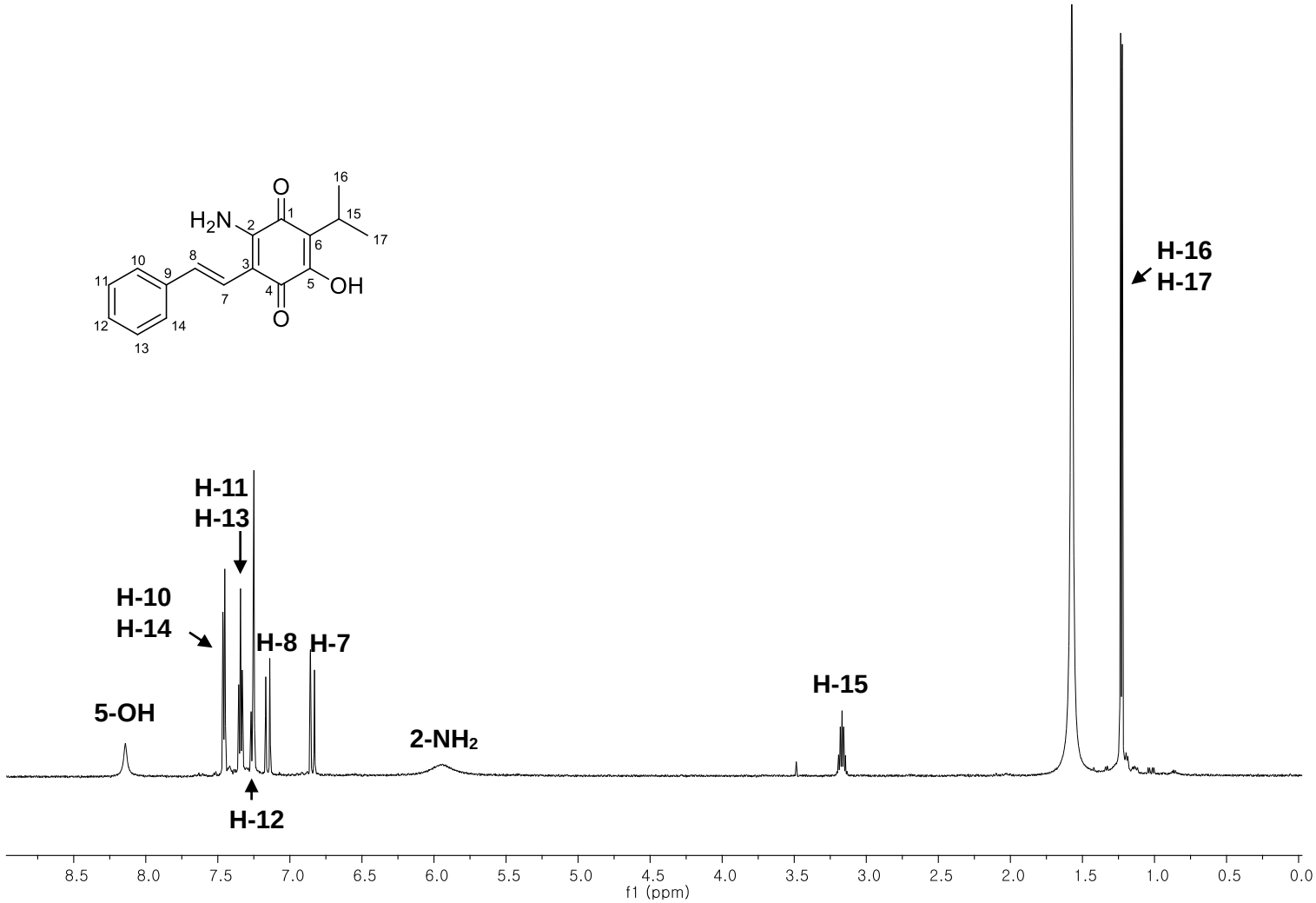


Figure S3. ^{1}H NMR spectral data of compound **1** in chloroform-d_1

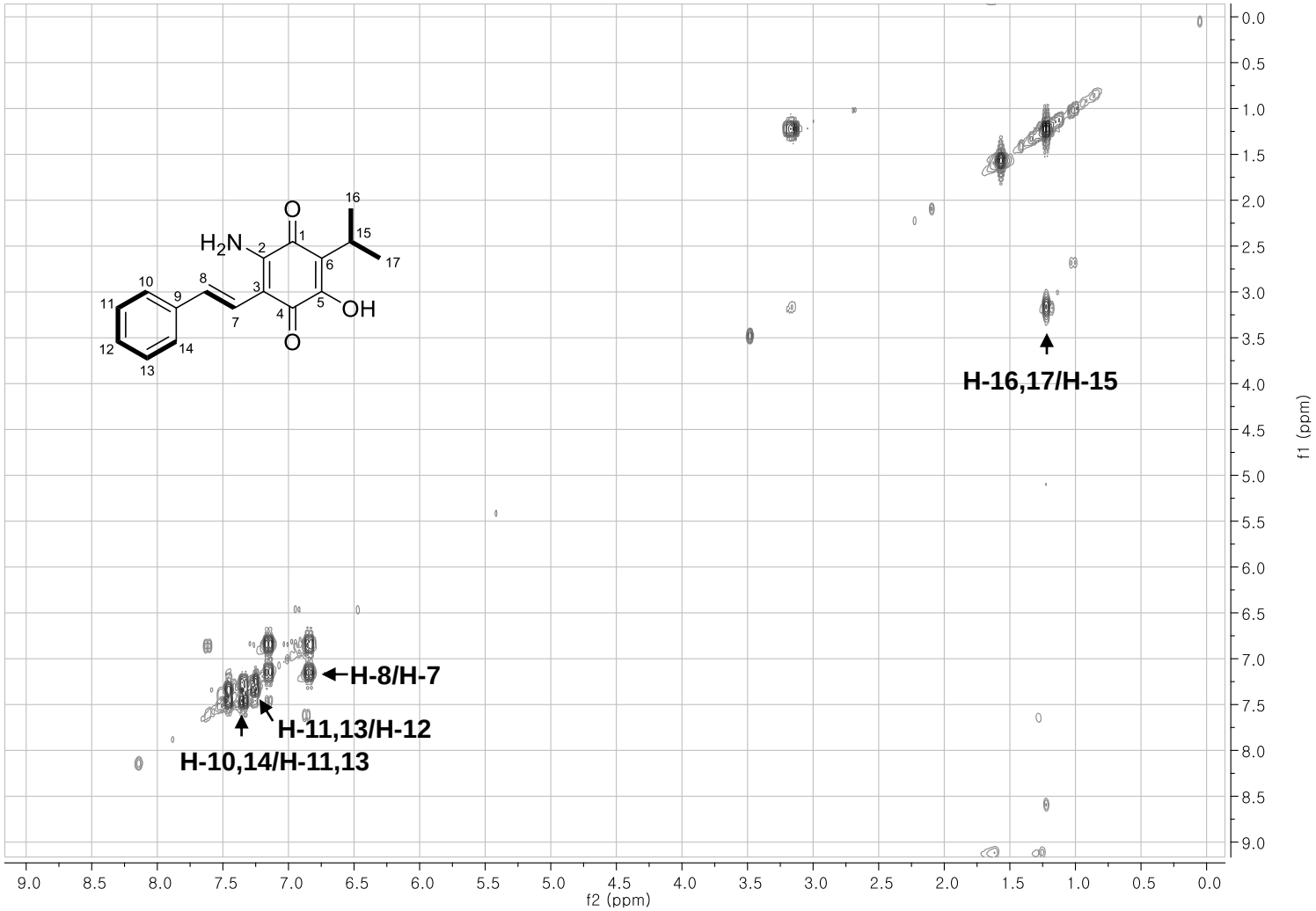


Figure S4. COSY NMR spectral data of compound **1** in chloroform-d_1

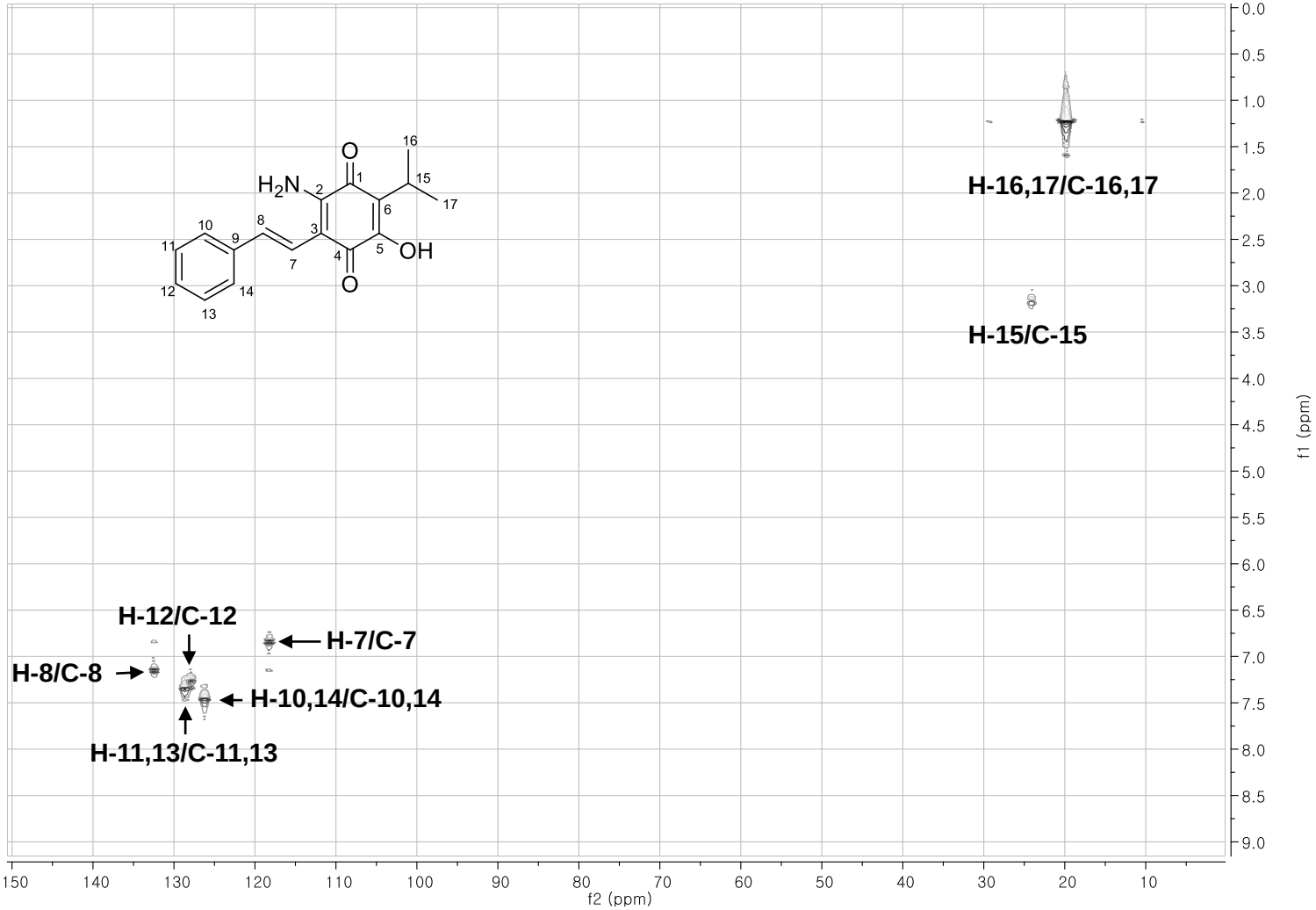


Figure S5. HSQC NMR spectral data of compound **1** in chloroform-d_1

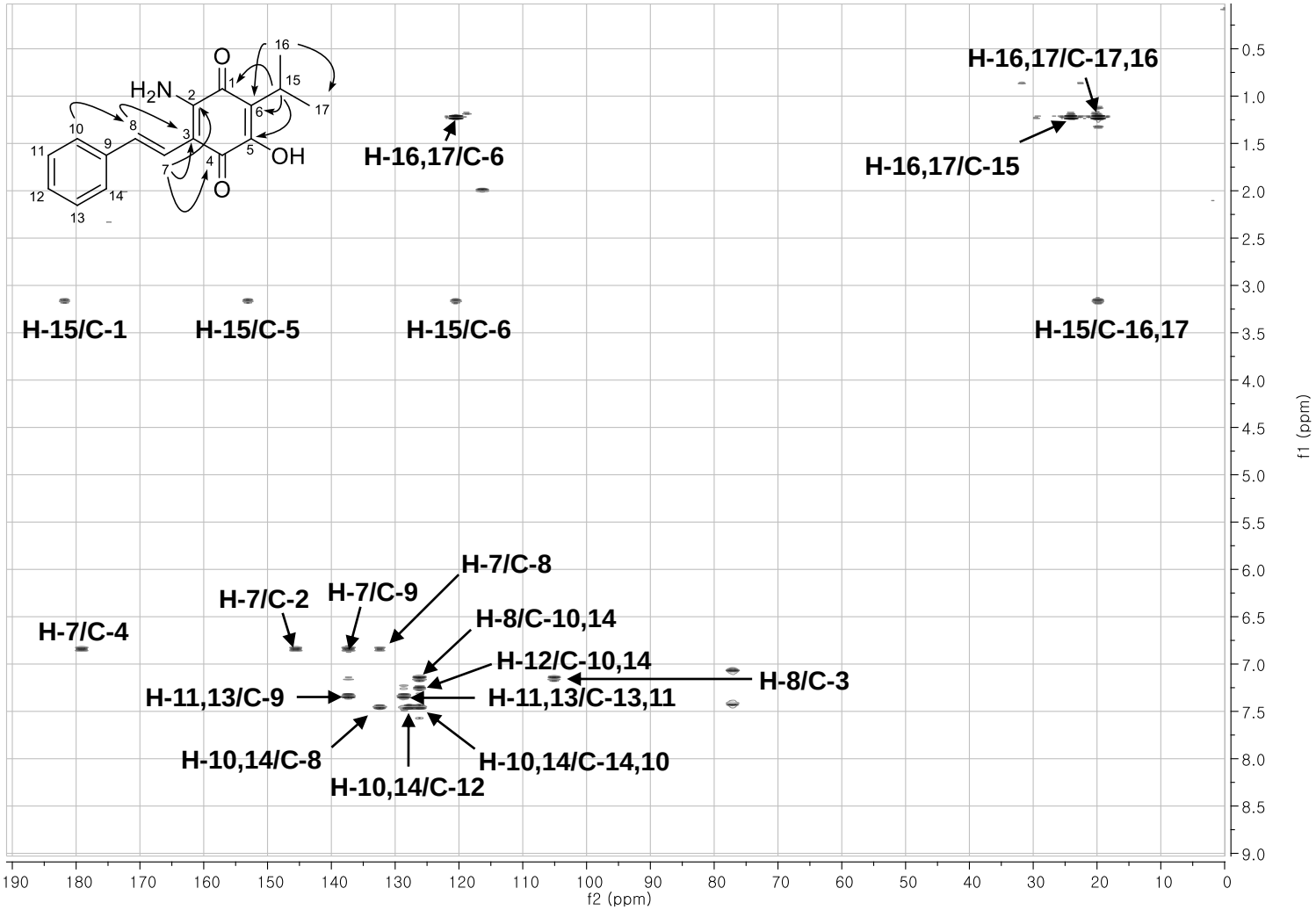


Figure S6. HMBC NMR spectral data of compound **1** in chloroform-d_1

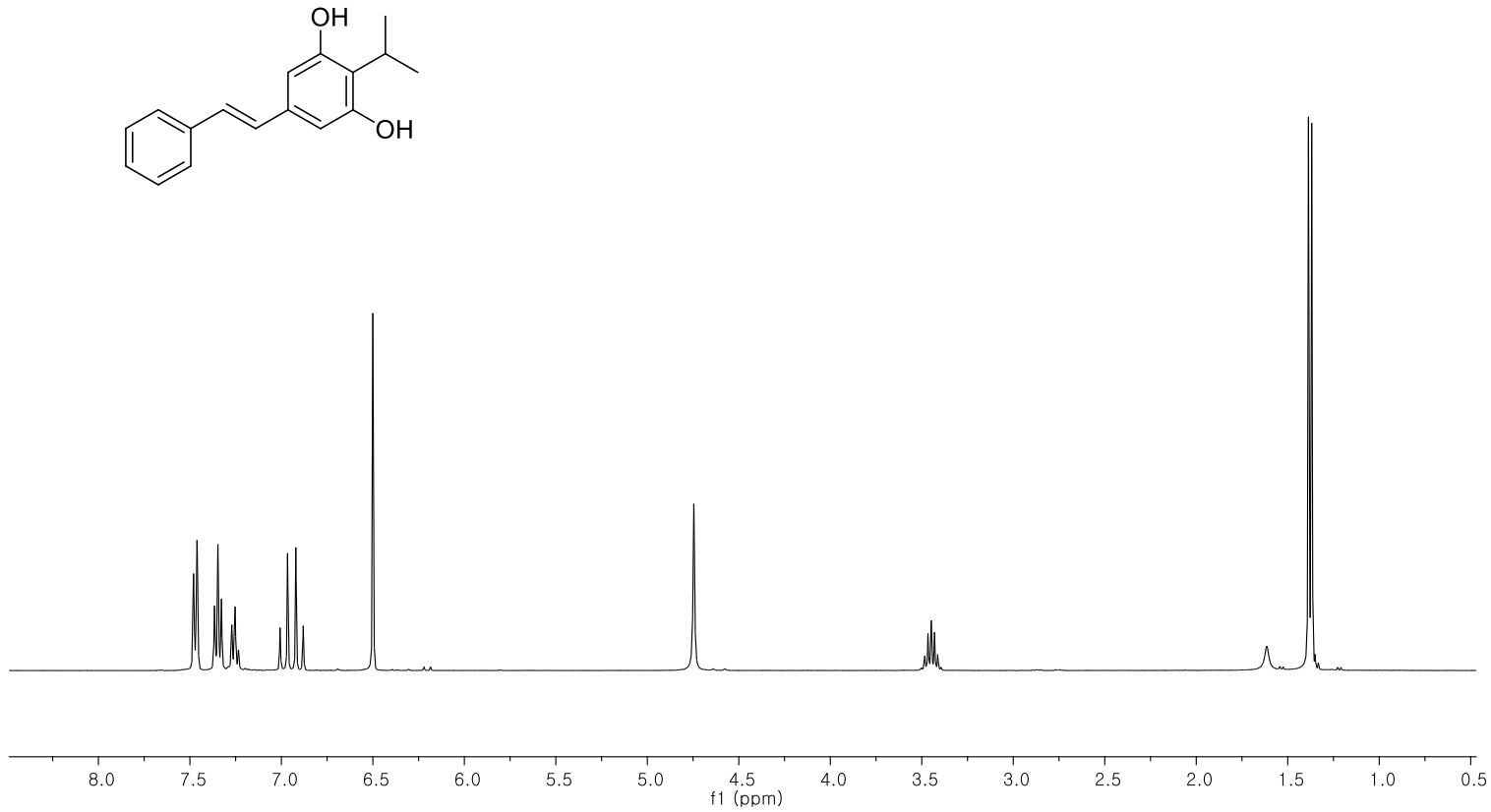
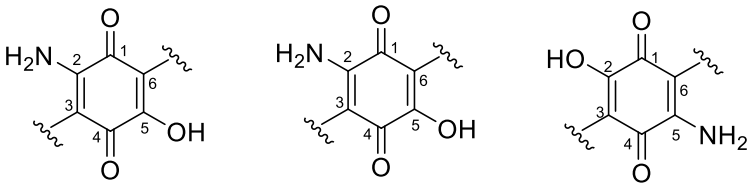


Figure S7. ^{1}H NMR spectral data of compound **2** in chloroform-d_1



Position	(a)	(b)	(c)
1	181.8	182.5	179.3
2	145.6	146.6	153.5
3	105.1	103.4	110.5
4	179.1	179.8	183.3
5	153.1	153.4	146.0
6	120.5	118.5	111.1

Figure S8. ^{13}C NMR chemical shift comparisons of heterosubstituted-1,4-benzoquinone core with those of literature values (a) carbon chemical shift of 2-amino-5-hydroxy-1,4-benzoquinone core of lumiquinone A (**1**) (b) carbon chemical shift of 2-amino-5-hydroxy-1,4-benzoquinone core described in the literature (c) carbon chemical shifts of 2-hydroxy-5-amino-1,4-benzoquinone core described in the literature (See reference 17)

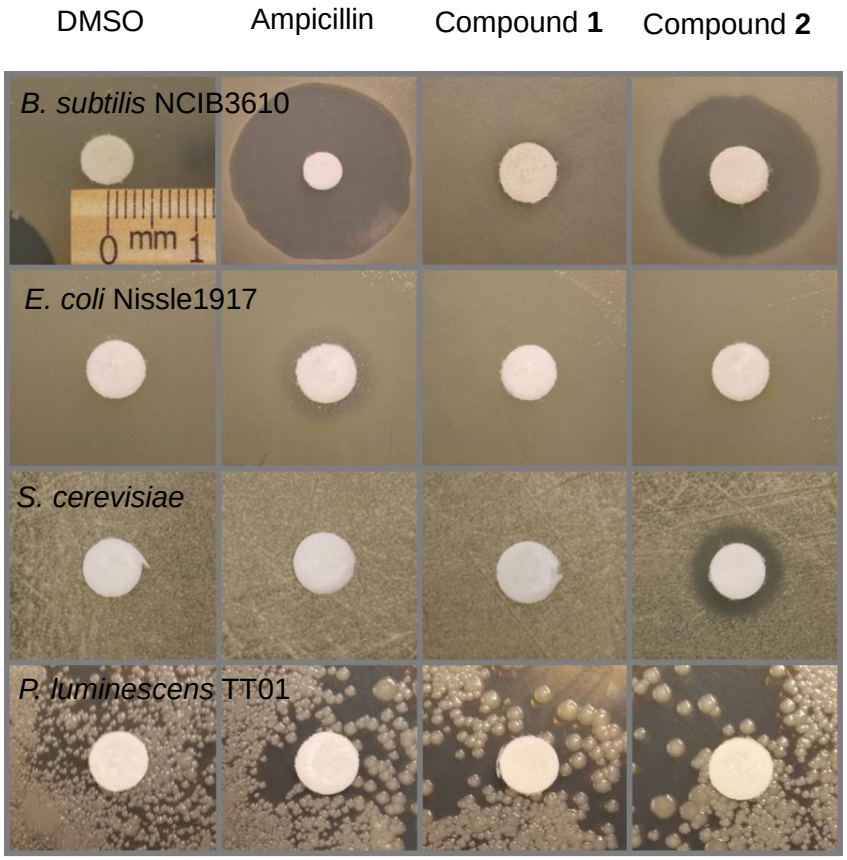


Figure S9. Paper disk test assay for antimicrobial activities of compounds **1** and **2**

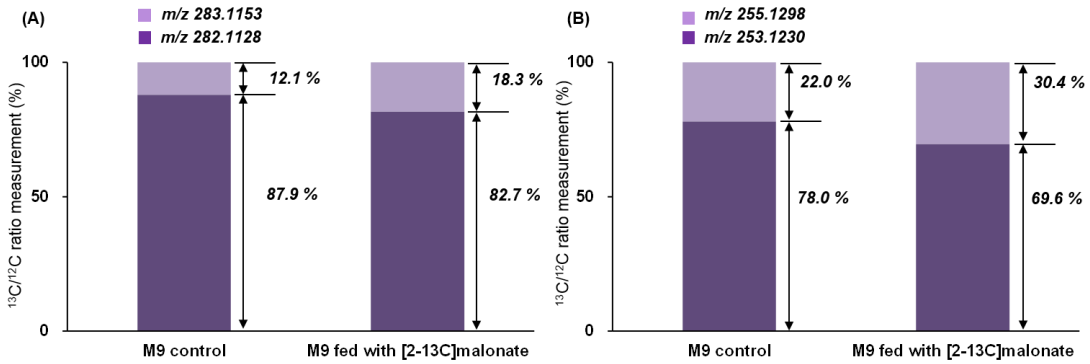


Figure 10. The incorporation of [2-^{13}C]malonate into compounds **1** (A) and **2** (B). The observed *m/z* 282.1128 and *m/z* 253.1230 peaks correspond to deprotonated molecular ions of **1** and **2** in the negative ion mode, respectively. The ^{13}C peak integration ratio measured by the [2-^{13}C]malonate feeding experiment showed a 6.2 percent increase for the singly labeled compound **1** (A) and a 8.4 percent increase for the doubly labeled compound **2** (B) when compared with non-labeled control. The percentage was determined by integration values of extracted peaks within 5 ppm mass error.

Feeding experiment with [2-^{13}C]malonate in *Photorhabdus luminescens* TT01

[2-^{13}C]malonate was purchased from Sigma-Aldrich. *Photorhabdus luminescens* TT01 was grown on 5 mL M9 minimal media supplemented with casamino acids (5 g/L) at 30 ℃ until OD_{600} was between 0.5-0.6. [2-^{13}C]malonate (100 mM final concentration) adjusted to pH 7.0 was then fed to the culture broth and cultivated at 30 ℃ in a shaking incubator (250 rpm). After 72 h, the whole culture broth was extracted with ethyl acetate (2 × 5 mL) and dried under reduced pressure. The crude extracts were analyzed by high-resolution ESI-Q-TOF-MS instrument (Column; Phenomenex kinetics C_{18} column, 250 × 4.6 mm, 5 μm, Flow rate; 0.3 mL/min, method; 60 min gradient elution from 10% aqueous acetonitrile to 100% acetonitrile).