SUPPORTING INFORMATION

ANTITUMORAL EFFECTS OF TWO NOVEL UNIQUE NATURALLY OCCURRING TERPENE QUINONES ISOLATED FROM THE MEDITERRANEAN ASCIDIAN *APLIDIUM CONICUM*

Anna Aiello Ernesto Fattorusso, Paolo Luciano, Antonio Macho, Marialuisa Menna, and
Eduardo Muñoz

Contents of SI:

1. ^1H NMR spectrum (CDCl_3) of thiaplidiaquinone A
2. ^{13}C NMR spectrum (CDCl_3) of thiaplidiaquinone A
3. ^{13}C NMR spectrum ($\text{DMSO-}d_6$) of thiaplidiaquinone A
4. Fully coupled ^{13}C NMR spectrum ($\text{DMSO-}d_6$) of thiaplidiaquinone A
5. Fully coupled ^{13}C NMR spectrum ($\text{DMSO-}d_6$) of thiaplidiaquinone A after addition of CD_3OD
6. Fully coupled ^{13}C NMR spectrum ($\text{DMSO-}d_6$) of thiaplidiaquinone A after addition of CD_3OD (δ 160-180)
7. COSY spectrum (CDCl_3) of thiaplidiaquinone A
8. HSQC spectrum (CDCl_3) of thiaplidiaquinone A
9. HMBC spectrum (CDCl_3) of thiaplidiaquinone A
10. HMBC spectrum ($\text{DMSO-}d_6$) of thiaplidiaquinone A
11. ESI mass spectrum of thiaplidiaquinone A
12. ^1H NMR spectrum (CDCl_3) of thiaplidiaquinone B
13. ^{13}C NMR spectrum (CDCl_3) of thiaplidiaquinone B
14. HPLC data of compounds **1** and **2** as criteria of purity.

^1H NMR spectrum (CDCl_3) of thiaplidiaquinone A

^{13}C NMR spectrum (CDCl_3) of thiaplidiaquinone A

^{13}C NMR spectrum (DMSO- d_6) of thiaplidiaquinone A

Fully coupled ^{13}C NMR spectrum (DMSO- d_6) of thiaplidiaquinone A

Fully coupled ^{13}C NMR spectrum (DMSO- d_6) of thiaplidiaquinone A after addition of CD_3OD

Fully coupled ^{13}C NMR spectrum (DMSO- d_6) of thiaplidiaquinone A after addition of CD_3OD (δ 160-180)

COSY spectrum (CDCl₃) of thiaplidiaquinone A

HSQC spectrum (CDCl₃) of thiaplidiaquinone A

HMBC spectrum (CDCl₃) of thiaplidiaquinone A

HMBC spectrum (DMSO- d_6) of thiaplidiaquinone A

ESI mass spectrum of thiaplidiaquinone A

^1H NMR spectrum (CDCl_3) of thiaplidiaquinone B

^{13}C NMR spectrum (CDCl_3) of thiaplidiaquinone B

Purity criteria for target compounds. The degree of purity of both compounds **1** and **2** was over 95% as indicated by the appearance of a single peak in two diverse HPLC eluent systems., using a SiO₂ column (Luna 5μm, 250 x 4.60 mm).

Retention times (t_R) are expressed in minutes.

Thiaplidiaquinone A:

Hexane/EtOAc 1:1, t_R 45.5

CHCl₃/EtOAc 6:4, t_R 17.7

Thiapliaquinone B:

Hexane/EtOAc 1:1, t_R 50.5

CHCl₃/EtOAc 6:4, t_R 19.3