J. Braz. Chem. Soc., Vol. 25, No. 10, S1-S3, 2014.
Printed in Brazil - ©2014 Sociedade Brasileira de Química
0103 - 5053 $6.00+0.00

Supplementary Information

Development and Validation of a Method for Simultaneous Determination of Bioactive Compounds of *Tanacetum parthenium* (L.) Schultz-Bip

Mirela F. Rabito,[a] Mariana B. Almeida,[b] Amanda L. Moreira,[a] Amadeu H. Iglesias,[c] Fernando de Paula,[c] Bruna P. da Silva,[a] Diógenes A. Cortez,[a] Suzana L. Nixdorf[b] and Izabel C. P. Ferreira*,[a]

[a]Departamento de Farmácia, Universidade Estadual de Maringá, Av. Colombo, 5790, 87020-900 Maringá-PR, Brazil

[b]Departamento de Química, Universidade Estadual de Londrina, Rod. Celso Garcia Cid, km 380, 86051-980 Londrina-PR, Brazil

[c]Laboratórios Aplicados Luiz Barssotti, Waters Technology do Brasil, Alameda Tocantins, 125, 06455-020 Barueri-SP, Brazil

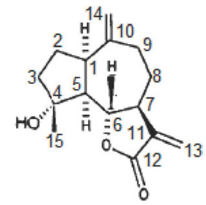

Figure S1. Chemical structure of the SL guaianolide (11,13-dehydrocompressanolide).

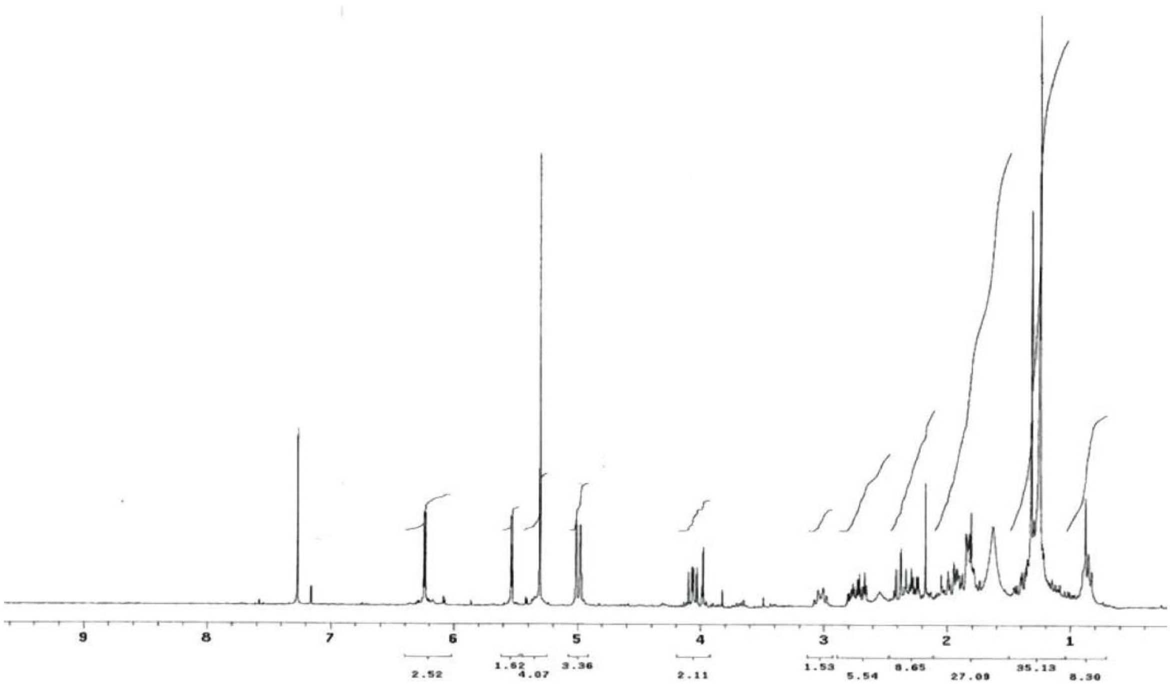

Figure S2. ^{1}H NMR spectrum ($CDCl_3$, 300 MHz) of the guaianolide.

*e-mail: icpferreira@uem.br

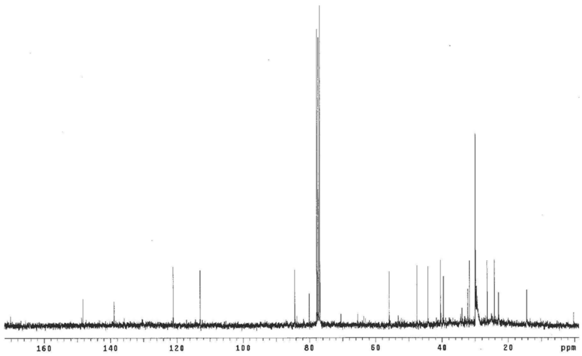

Figure S3. ^{13}C NMR spectrum (75.5 MHz, $CDCl_3$) of the guaianolide.

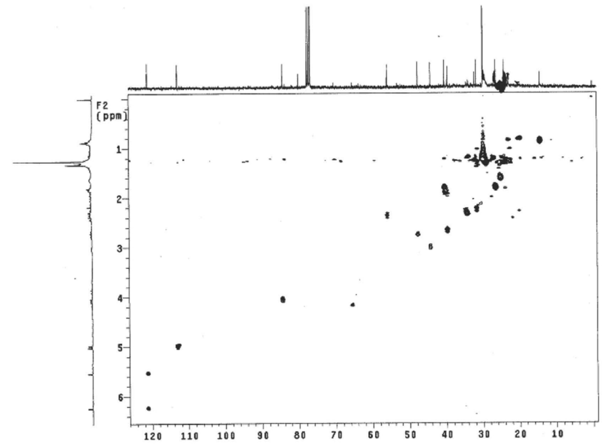

Figure S5. HMQC correlation spectrum ($CDCl_3$, 300 MHz) of the guaianolide.

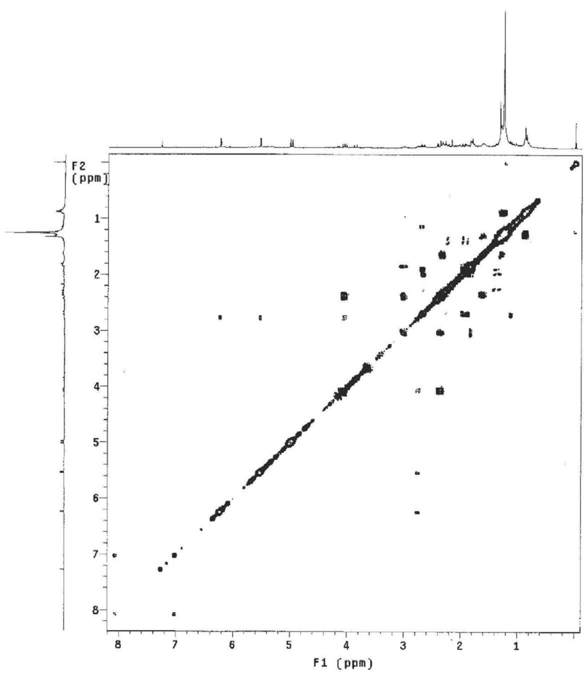

Figure S4. COSY spectrum ($CDCl_3$, 300 MHz) of the guaianolide.

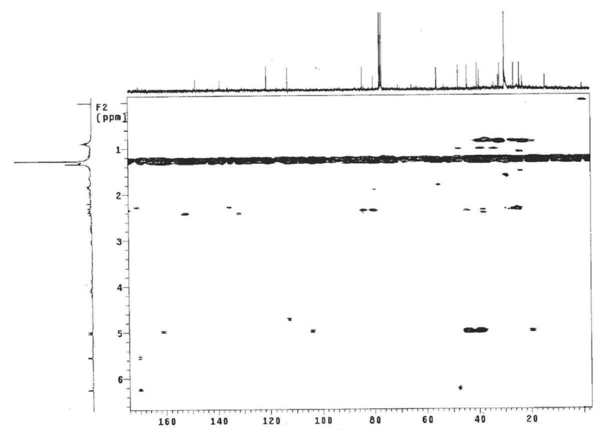

Figure S6. HMBC correlation spectrum ($CDCl_3$, 300 MHz) of the guaianolide.

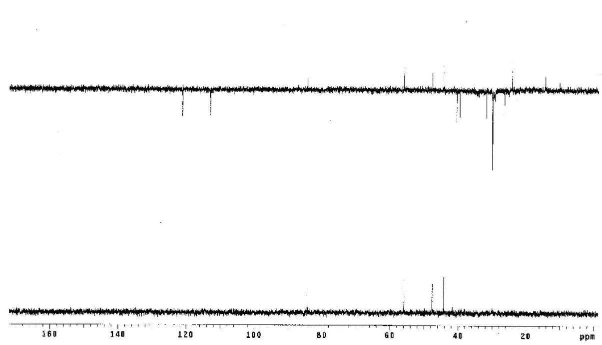

Figure S7. DEPT spectrum ($CDCl_3$, 75.5 MHz) of the guaianolide.

Table S1. ^{1}H NMR data ($CDCl_3$, 300 MHz) for the guaianolide compared to the same compound isolated from the cyclization of parthenolide from *Magnolia grandiflora* L. (Magnoliaceae)[1]

Proton	Literature (δ_H)	Isolated compound guaianolide (δ_H)
H-1	3.02 (ddd, 12.1, 8.7, 8.7)	3.01 (ddd,11.7, 9.0 and 9.0Hz)
H-2α	1.76-1.86	1.76-1.86 (m)
H-2β	1.76-1.86	1.76-1.86 (m)
H-3α	1.76-1.86	1.76-1.86 (m)
H-3β	1.89 (m)	1.86-1.89 (m)
H-4	–	–
H-5	2.37 (dd, 11.9, 11.9)	2.37 (dd, *J* 12.0 and 11.9)
H-6	4.05 (dd, 11.4, 11.3)	4.06 (dd, *J* 11.4 and 11.3)
H-7	2.76 (ddddd, 11.3, 8.6, 3.2, 3.2, 3)	2.69 (m, *J* 2.80)
H-8α	1.38 (m)	1.34-1.40 (m)
H-8β	2.25 (dddd, 13.2, 7.3, 3.7, 3.7)	2.23-2.30 (m)
H-9α	1.93	1.90-1.98 (m)
H-9β	2.68 (ddd,13, 3.8, 3.8)	2.66 (ddd, 12.9, 3.6, 3.6)
H-10	–	–
H-11	–	–
H-12	–	–
H-13α	6.23 (d, 3.6)	6.238 (d, *J* 3.6)
H-13β	5.52 (d, 3.1)	5.53 (d, *J* 3.3)
H-14α	5.00 (br,s)	5.012 (br s)
H-14β	4.97 (br, s)	4.976 (br s)
H-15	1.31 (s)	1.321 (s)
OH	–	2.337 (s)

δ_H: chemical shift (ppm); *J*: coupling constant (Hz).

Table S2. ^{13}C NMR data ($CDCl_3$, 75.5 MHz) of the guaianolide compared to the same compound isolated from the cyclization of parthenolide from *Magnolia grandiflora* L. (Magnoliaceae)[1]

Carbon	Literature (δ_H), DEPT	Literature (δ_H)	Isolated compound guaianolide, DEPT	Isolated compound guaianolide (δ_H)
C-1	CH	44.0 d	CH	44.15
C-2	CH_2	26.2 t	CH_2	26.37
C-3	CH_2	40.2 t	CH_2	40.38
C-4	C	79.7 s	C	79.90
C-5	CH	55.7 d	CH	55.90
C-6	CH	84.1 d	CH	84.32
C-7	CH	47.3 d	CH	47.57
C-8	CH_2	31.4 t	CH_2	31.65
C-9	CH_2	39.3 t	CH_2	39.5
C-10	C	148.0 s	C	148.25
C-11	C	138.7 s	C	138.92
C-12	C	169.7 s	C	170.11
C-13	CH_2	120.8 t	CH_2	121.03
C-14	CH_3	112.6 t	CH_2	112.90
C-15	CH_3	23.9 q	CH_3	24.1

δ_H: chemical shift (ppm); *J*: coupling constant (Hz).

References

1. Castañeda-Acosta, J.; Fischer, N. H.; Vargas, D.; *J. Nat. Prod.* **1993**, *56*, 90.