

**COMPLETE <sup>1</sup>H AND <sup>13</sup>C NMR STRUCTURAL ASSIGNMENTS FOR A GROUP OF FOUR GOYAZENSOLIDE-TYPE FURANOHELIANGOLIDES<sup>#</sup>**

**Ana Carolina Ferreira Soares, Aline Nazaré Silva, Priscilla Mendonça Matos, Eder Henrique da Silva e Vladimir Constantino Gomes Heleno\***

Núcleo de Pesquisas em Ciências Exatas e Tecnológicas, Universidade de Franca, Av. Dr. Armando de Salles Oliveira, 201, 14404-600 Franca – SP, Brasil

**Norberto Peporine Lopes e João Luis Callegari Lopes**

Departamento de Física e Química, Faculdade de Ciências Farmacêuticas de Ribeirão Preto, Universidade de São Paulo, Av. do Café, s/n, 14040-903 Ribeirão Preto – SP, Brasil

**Daiane Cristina Sass**

Departamento de Química, Faculdade de Filosofia, Ciências e Letras de Ribeirão Preto, Universidade de São Paulo, Av. Bandeirantes, 3900, 14040-901 Ribeirão Preto – SP, Brasil

**Table 1S.** 2D NMR data for lychnofolide (**1**). 500MHz, CDCl<sub>3</sub>

C	H	HMBC	COSY	HMQC
1	---	H2, H9 $\alpha$ , H9 $\beta$ , H14	---	---
2	2	H14	---	H2
3	---	H5, H2, H15	---	---
4	---	H15	---	---
5	5	H15	H15, H6	H5
6	6	H15, H8	H5, H15, H7	H6
7	7	H15, H9 $\alpha$ , H9 $\beta$ , H13a, H13b	H8, H6, H13a, H13b	H7
8	8	H9 $\alpha$ , H9 $\beta$ , H13a, H13b, H14	H9 $\alpha$ , H9 $\beta$ , H7	H8
9	9a	H8, H14	H9 $\beta$ , H8	H9 $\alpha$ , H9b
	9 $\beta$	---	H9 $\alpha$ , H8	---
10	---	H2, H8, H9 $\alpha$ , H9 $\beta$ , H14	---	---
11	---	H13a, H13b	---	---
12	---	H13a, H13b	---	---
13	13a	---	H7	H13a, H13b
	13b	---	H7	---
14	14	H9 $\alpha$	---	H14
15	15	H5	H5, H6	H15
1'	---	H3', H4', H5', H8	---	---
2'	---	H5', H4'	---	---
3'	3'	H4', H5'	H4', H5'	H3'
4'	4'	H3'	H3', H5'	H4'
5'	5'	H3', H4'	H3', H4'	H5'

\*e-mail: vheleno\_05@yahoo.com.br

<sup>#</sup>Artigo em homenagem ao Prof. Otto R. Gottlieb (31/8/1920-19/6/2011)

**Table 2S.** 2D NMR data for centratherin (2). 500MHz, CDCl<sub>3</sub>

C	H	HMBC	COSY	HMQC
1	---	H2, H9 $\alpha$ , H9 $\beta$ , H14	---	---
2	2	H9a	---	H2
3	---	H5, H2, H15	---	---
4	---	H5, H6, H15	---	---
5	5	H6, H7, H15	H15, H6	H5
6	6	H8	H5, H15, H7, H8	H6
7	7	H15, H9 $\alpha$ , H9 $\beta$ , H13a, H13b, H6, H8	H8, H6, H13a, H13b	H7
8	8	H6, H9 $\alpha$ , H9 $\beta$ , H13a, H13b, H14	H9 $\alpha$ , H9 $\beta$ , H7, H-6	H8
9	9 $\alpha$	H7, H8, H14	H9 $\beta$ , H8	H9 $\alpha$ , H9 $\beta$
	9 $\beta$	---	H9 $\alpha$ , H8	---
10	---	H2, H8, H9 $\alpha$ , H9 $\beta$ , H14	---	---
11	---	H6, H7, H8, H13a, H13b	---	---
12	---	H13a, H13b	---	---
13	13a	---	H7, H13b	H13a, H13b
	13b	---	H7, H13a	---
14	14	H9 $\alpha$ , H9 $\beta$	---	H14
15	15	H5	H5, H6	H15
1'	---	H3', H4', H5', H8	---	---
2'	---	H5', H4'	---	---
3'	3'	H4', H5'	H4', H5'	H3'
4'	4'	H3'	H3', H5'	H4'
5'	5'	H3', H4'	H3', H4'	H5'

**Table 3S.** 2D NMR data for goyazensolide (3). 500MHz, CDCl<sub>3</sub>

C	H	HMBC	COSY	HMQC
1	---	H2, H14, H9 $\alpha$ , H9 $\beta$	---	---
2	2	---	---	H2
3	---	H2, H5, H15	---	---
4	---	H15	---	---
5	5	H7, H15a, H15b	H6, H15	H5
6	6	H7, H8	H5, H7, H8, H15	H6
7	7	H5, H11, H9 $\alpha$ , H9 $\beta$ , H13	H6, H8, H13	H7
8	8	H14, H11, H9 $\alpha$ , H9 $\beta$	H6, H7, H9 $\alpha$ , H9 $\beta$	H8
9	9 $\alpha$	H8, H7, H14	H8, H9 $\beta$	H9
	9b		H8, H9 $\alpha$	
10	---	H8, H2, H14, H9 $\alpha$ , H9 $\beta$	---	---
11	---	H7, H13	---	---
12	---	H13	---	---
13	13a	H7	H7, H13b	H13
	13b		H7, H13a	
14	14	H2, H9 $\alpha$ , H9 $\beta$	---	H14
15	15a	H5, H6	H15b, H5, H6	H15
	15b		H15a, H5, H6	
1'	---	H4'	---	---
2'	---	H3', H4'	---	H3', H4'
3'	3'a	H4'	H3'b	H4'
	3'b		H3'a, H4'	H4'
4'	4'	H3'	H3'b	---

**Table 4S.** 2D NMR data for goyazensolide acetate (**4**). 500MHz, CDCl<sub>3</sub>

C	H	HMBC	COSY	HMQC
1	---	H2, H14, H9 $\alpha$ , H9 $\beta$	---	---
2	2	---	---	H2
3	---	H2, H5, H15	---	---
4	---	H15	---	---
5	5	H7, H15	H15, H6	H5
6	6	H7, H8	H5, H7, H8, H15	H6
7	7	H5, H11, H9 $\alpha$ , H9 $\beta$ , H13	H6, H8, H11	H7
8	8	H14, H11, H9 $\alpha$ , H9 $\beta$	H6, H7, H9 $\alpha$ , H9 $\beta$	H8
9	9 $\alpha$	H8, H7, H14	H8, H9 $\beta$	H9
	9 $\beta$		H8, H9 $\alpha$	
10	---	H8, H2, H14, H9 $\alpha$ , H9 $\beta$	---	---
11	---	H7, H13	---	H11
12	---	H11, H13	---	---
13	13a	H7, H11	H13b	H13
	13b		H13a	
14	14	H9 $\alpha$ , H9 $\beta$	---	H14
15	15a	H5	H5, H6	H15
	15b		H5, H6	
1'	---	H8, H3'a, H3'b, H4'	---	---
2'	---	H3'b, H4'	---	---
3'	3'a	H4'	H3'b, H4'	H3'
	3'b		H3'a, H4'	
4'	4'	H3'a, H3'b	H3'b, H3'a	H4'
1''	---	H2''	---	---
2''	2''	---	---	H2''