SUPPLEMENTARY MATERIAL

Icosandrin, a novel peltogynoid from the fruits of *Phytolacca icosandra* (Phytolaccaceae)

Elier Galarraga M.[a]* and Juan Manuel Amaro-Luis[b]

[a]*Departamento de Química. Edificio de Química y Procesos. Universidad Simón Bolívar (USB). Apartado 89000. Caracas-1080A. Venezuela;* [b]*Laboratorio de Productos Naturales. Departamento de Química. Facultad de Ciencias. Universidad de Los Andes (ULA). Mérida, Venezuela-5101*

(Tel.: +58 0212 9063983; e-mail: *eliergalarraga@usb.ve*)

Abstract

Besides the known compounds (±) 3,3-*bis*-demethylpinoresinol (**2**), americanol A (**3**), spergulagenic acid (**4**), *epi*-acetylaleuritolic acid (**5**), 6'-palmityl-α-spinateryl-D-glucoside (**6a**) and 6'-palmityl-Δ^7-stigmastenyl-D-glucoside (**6b**), a novel peltogynoid (**1**) named icosandrin, was obtained from the dried fruits of *Phytolacca icosandra*. This new compound was characterized by 1D-/2D-NMR, UV, IR, and HR-MS techniques as 11ξ-methoxy-6,7-methylenedioxy-[2]benzopyrano-[4,3-*b*][1]-benzopyran-4-one. Toxicity of **1** was assessed through the brine shrimp lethality assay. Lignan **2** is reported for first time in Phytolaccaceae family.

Keywords: Phytolaccaceae, *Phytolacca icosandra*, Peltogynoids, Lignans, BSLA.

*Corresponding autor. Email: eliergalarraga@usb.ve

Figure S1: ESI-MS (positive ion mode) spectrum of Icosandrin (**1**)

Figure S2: HR-EI-MS (70 eV) spectrum of Icosandrin (**1**)

Figure S3: ^{1}H-NMR spectrum of Icosandrin (**1**)

Figure S4: ^{13}C-NMR spectrum if Icosandrin (**1**)

Figure S5: ^{1}H-^{1}H COSY spectrum of Icosandrin (**1**)

Figure S6: HMQC spectrum of Icosandrin (**1**)

Figure S7: HMBC spectrum of Icosandrin (**1**)

Figure S8: ^{1}H NMR (400 MHz), ^{13}C NMR (150 MHz) and HMBC data of Icosandrin (**1**).

Figure S1: ESI-MS (positive ion mode) spectrum of Icosandrin (**1**)

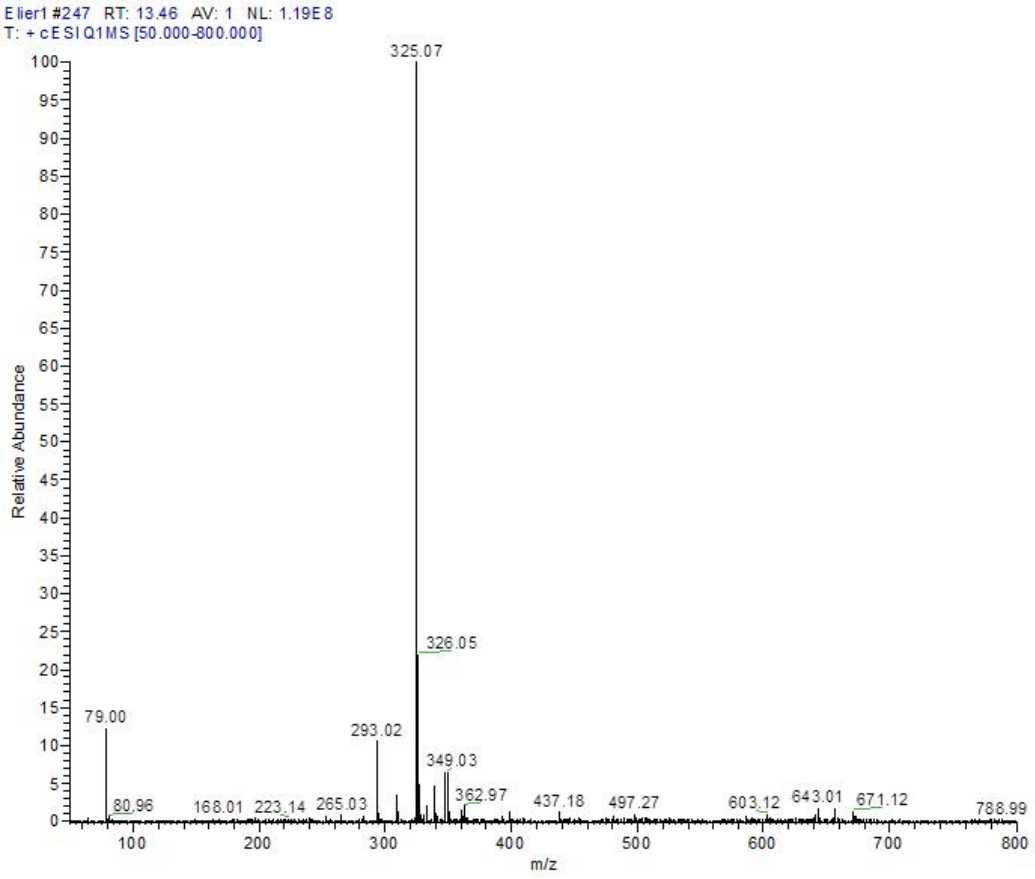

Figure S2: HR-EI-MS (70 eV) spectrum of Icosandrin (**1**)

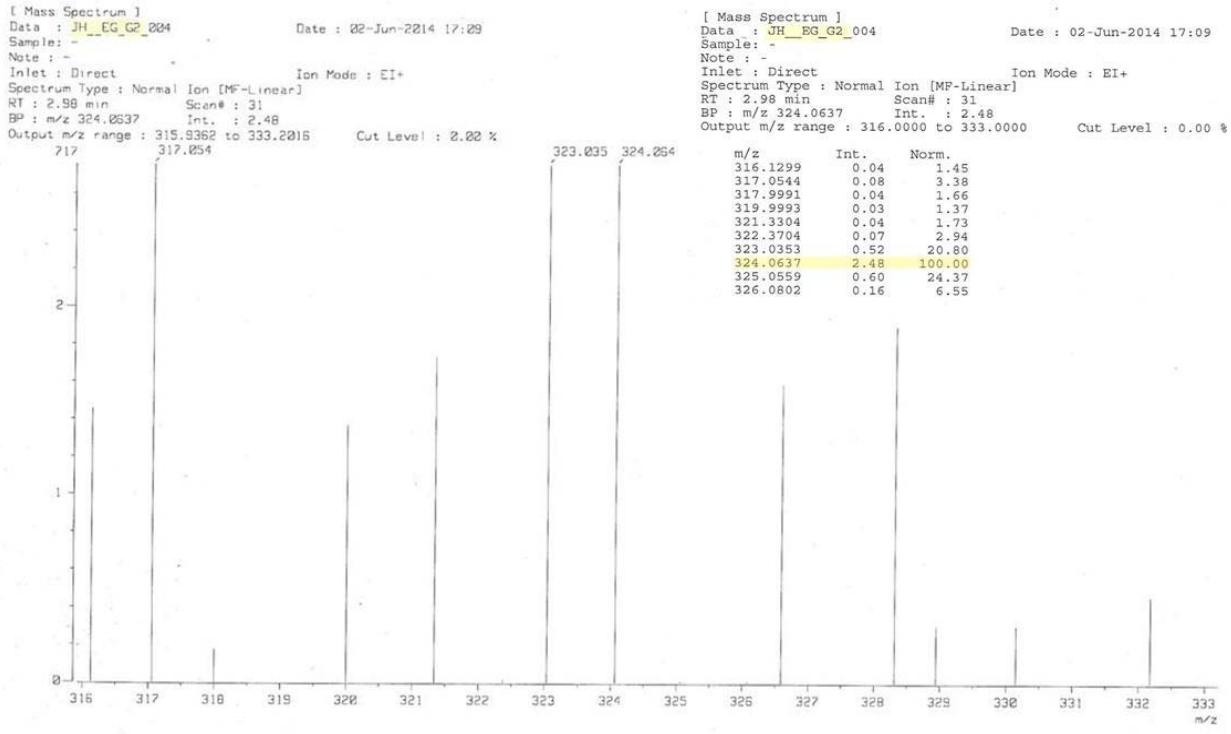

Figure S3: ^{1}H-NMR spectrum of Icosandrin (**1**)

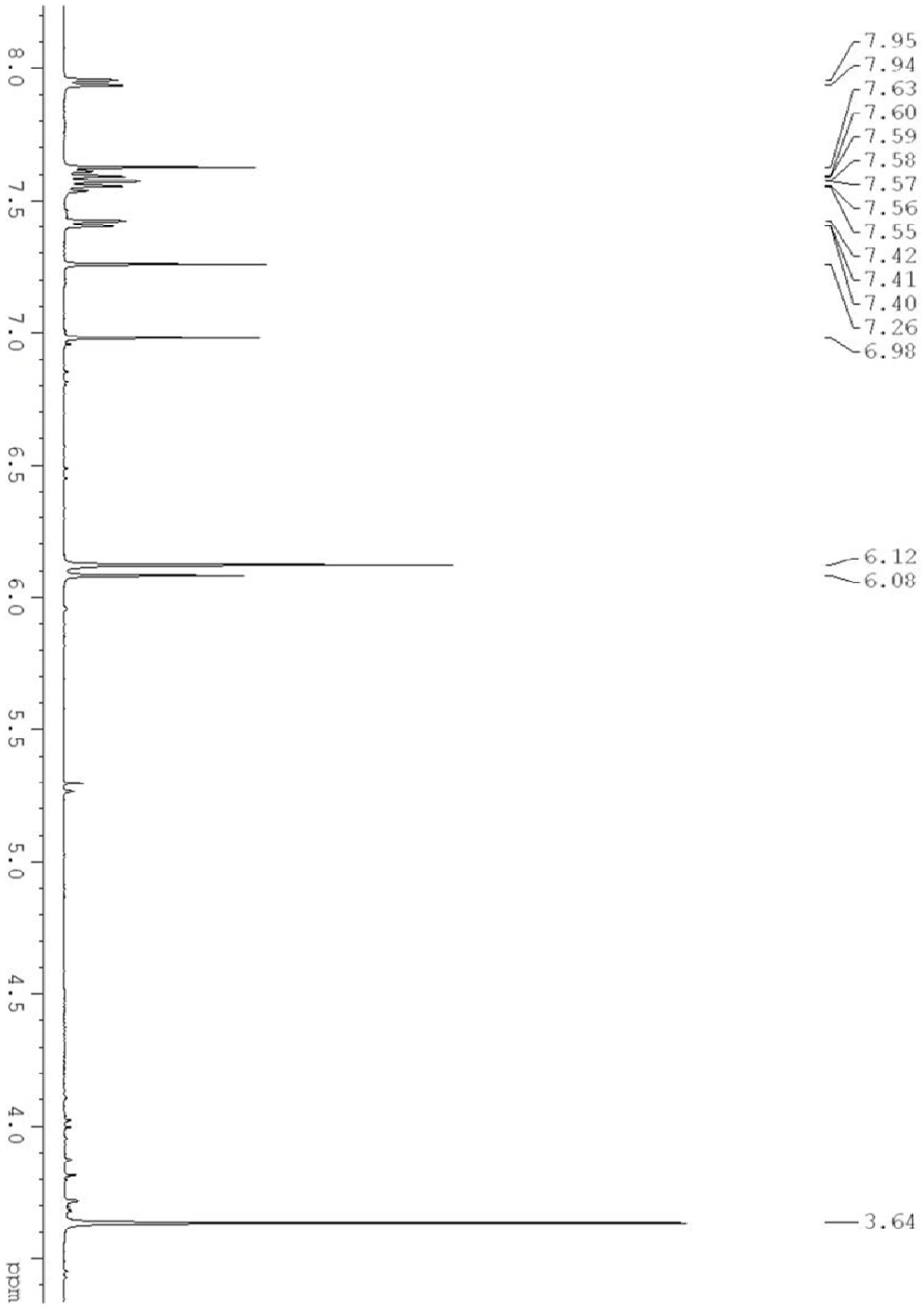

Figure S4: ^{13}C-NMR spectrum if Icosandrin (**1**)

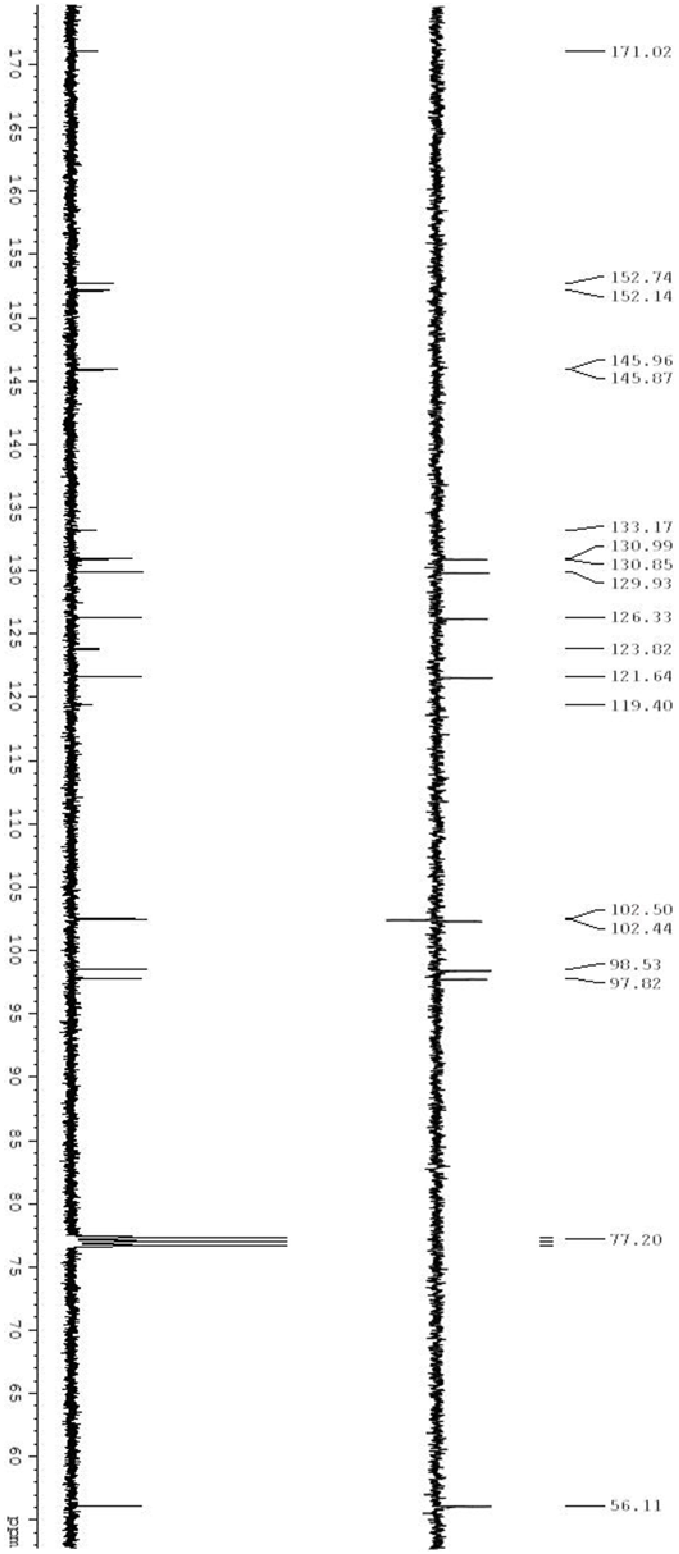

Figure S5: ^{1}H-^{1}H COSY spectrum of Icosandrin (**1**)

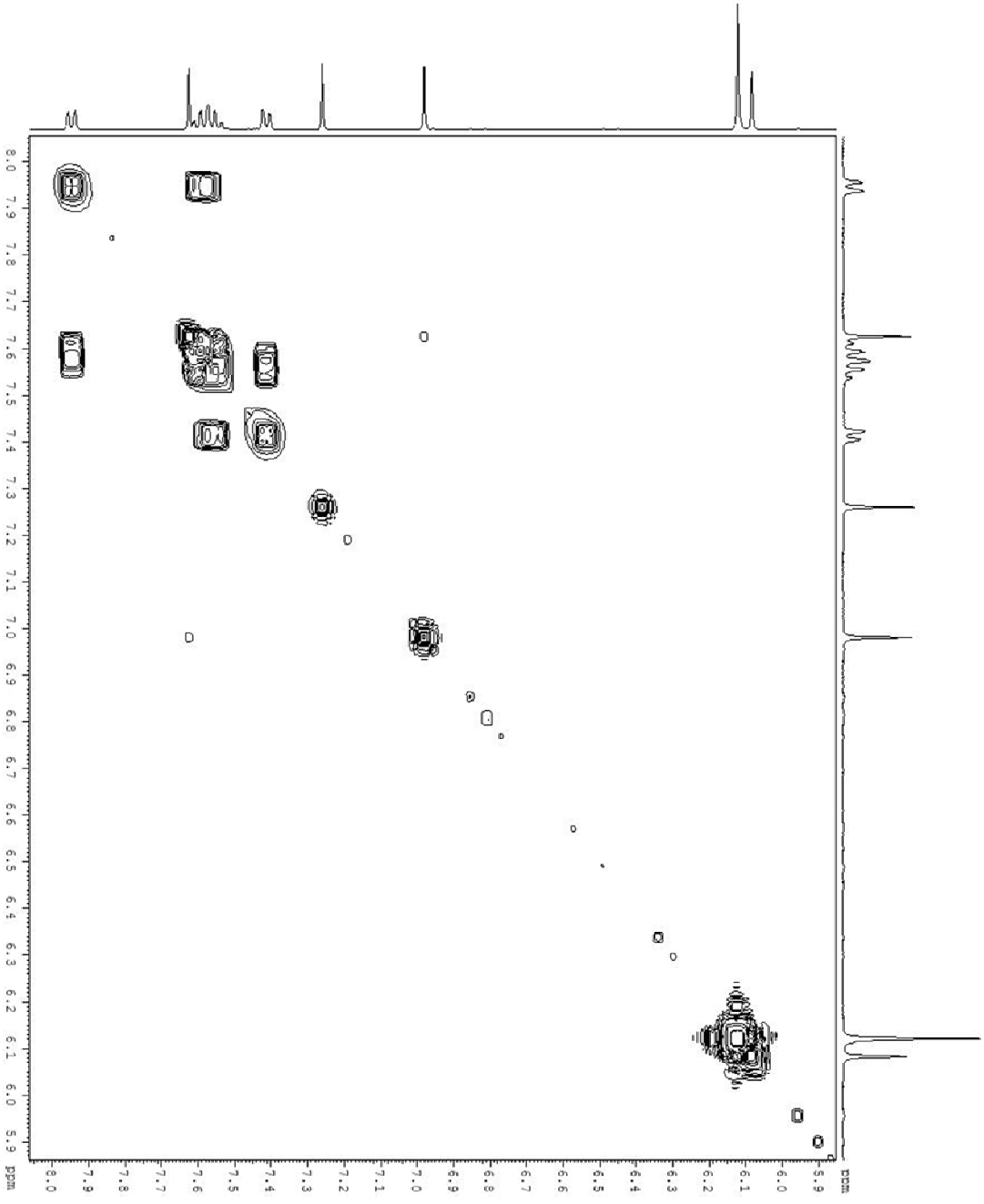

Figure S6: HMQC spectrum of Icosandrin (**1**)

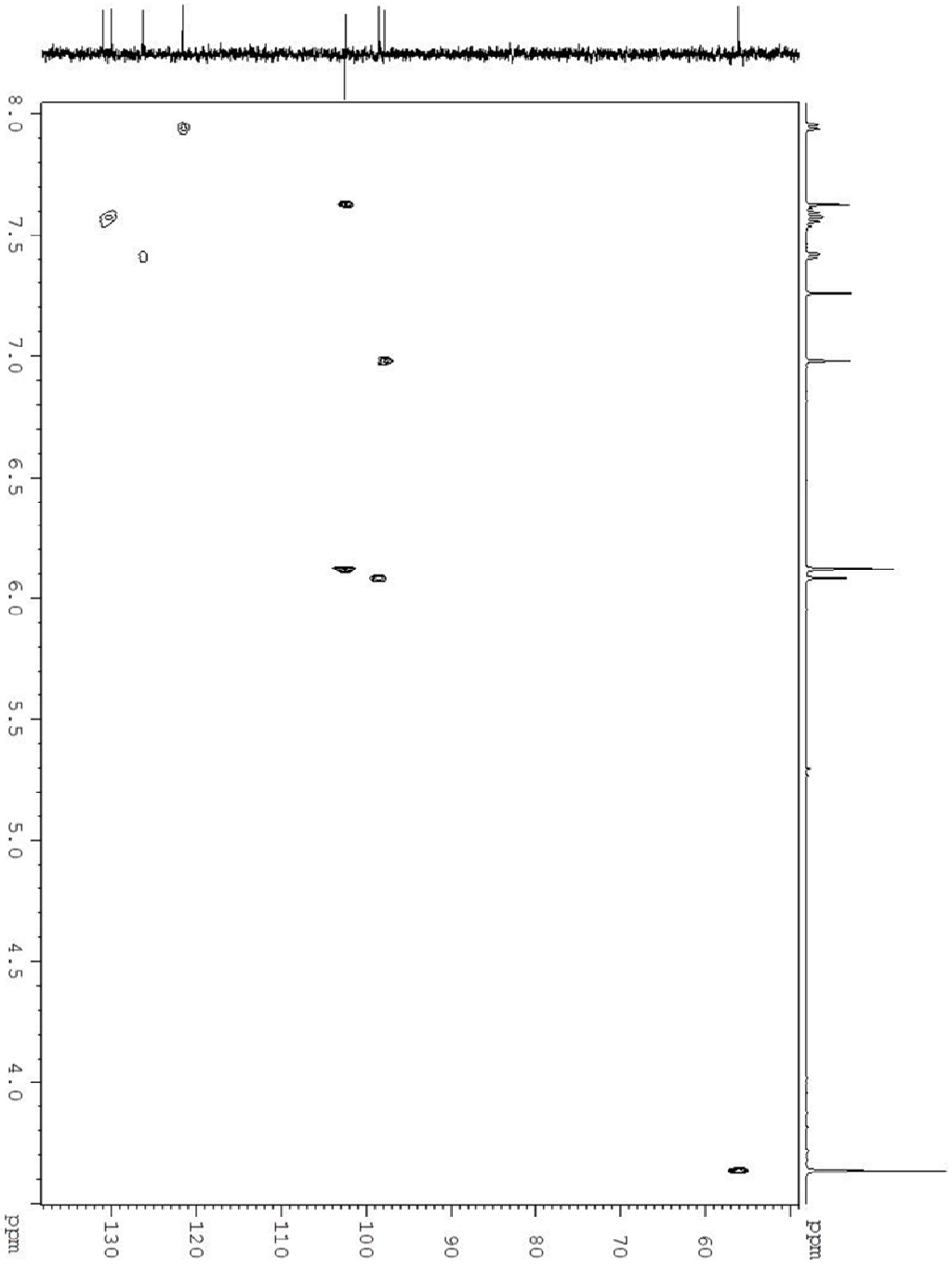

Figure S7: HMBC spectrum of Icosandrin (**1**)

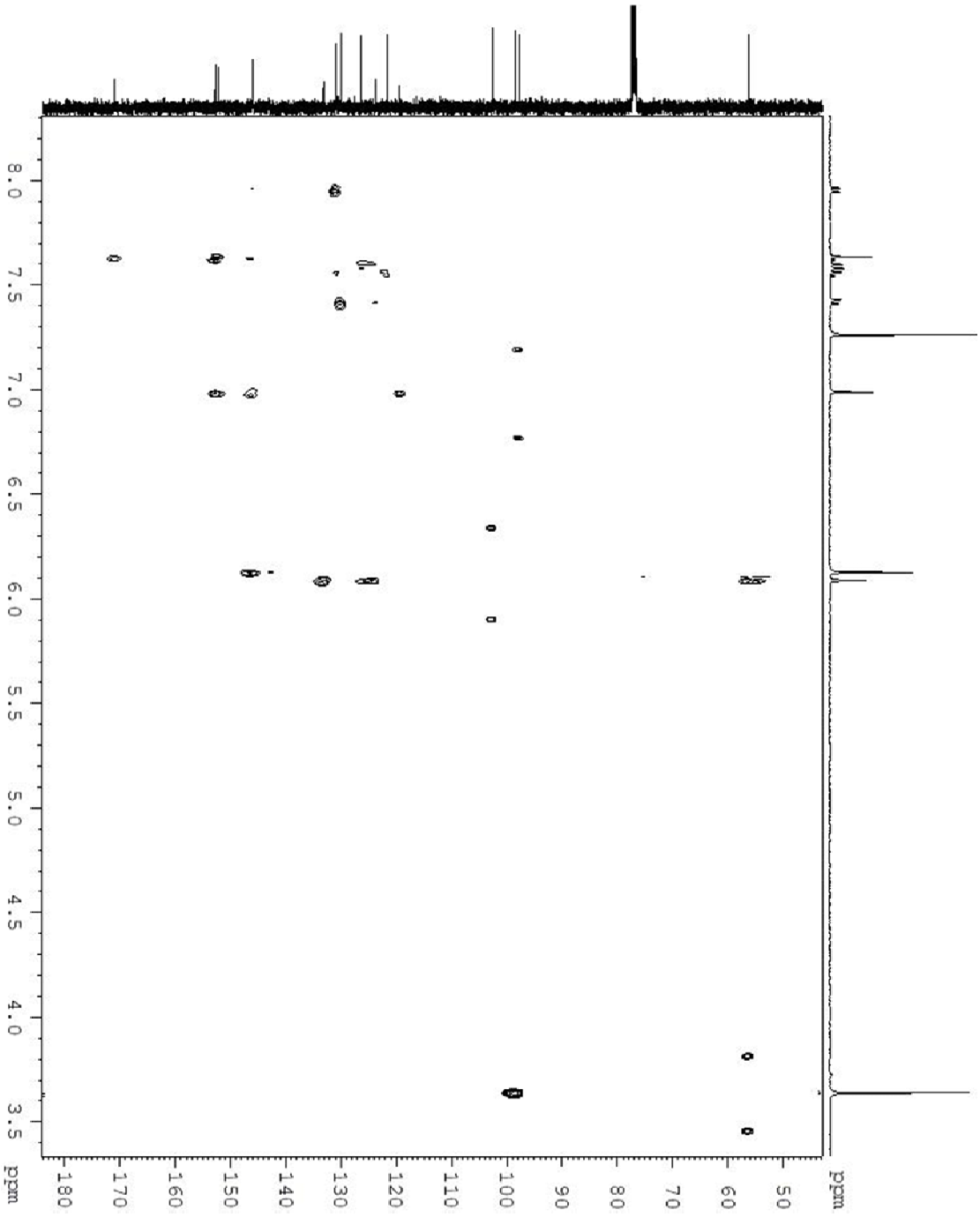

Figure S8: ^{1}H NMR (400 MHz), ^{13}C NMR (150 MHz) and HMBC data of (**1**).

	Icosandrin (**1**)		
No.	δ_C[a]	δ_H (*mult*, *J* in Hz)	HMBC
2	145.9 (s)		6'
3	133.7 (s)		11
4	171.0 (s)		5
5	102.4 (d)	7.63 (*s*)	4, 6, 7, 9
6	146.0 (s)		5, O-CH_2-O
7	152.7 (s)		5, 8, O-CH_2-O
8	97.8 (d)	6.98 (*s*)	6, 7, 10
9	152.1 (s)		5
10	119.4 (s)		8
11	98.5 (d)	6.08 (*s*)	3, 1', 3', -OCH_3
1'	123.8 (s)		11, 3'
2'	130.9 (s)		6'
3'	126.3 (d)	7.41 (*dd*, *J*=1.2, 7.2)	11, 1' 5'
4'	131.0 (d)	7.59 (*td*, *J*= 1.3, 7.5)	6'
5'	129.9 (d)	7.56 (*td*, *J*= 1.3, 7.5)	1', 3'
6'	121.6 (d)	7.94 (*dd*, *J*= 1.2, 7.2)	2, 2', 4'
-O-CH_2-O-	102.5 (t)	6.12 (*s*)	6, 7
-OCH_3	56.1 (q)	3.64 (*s*)	11

[a]Multiplicity determined by DEPT experiments (s= quaternary, d= methine, t = methylene, q= methyl).