Quim. Nova, Vol. 49, 2026

Material Suplementar

LAPACHOL COMO MODELO PARA O ENSINO DE RMN: MODIFICAÇÃO ESTRUTURAL E CARACTERIZAÇÃO

Matheus Vieira Castro[a], Cristiane Costa Lima[a], Arlan de Assis Gonsalves[b] e Cleônia Roberta Melo Araújo[a,*]

[a]Programa de Pós-Graduação Ciências da Saúde e Biológicas, Universidade Federal do Vale do São Francisco, 56304-917 Petrolina – PE, Brasil

[b]Programa de Pós-Graduação Ciências dos Materiais, Universidade Federal do Vale do São Francisco, 56304-917 Petrolina – PE, Brasil

Recebido: 08/05/2026; aceito: 27/07/2026; publicado online: 06/08/2026

*e-mail: cleonia.araujo@univasf.edu.br

ORCID:
Matheus Vieira Castro: https://orcid.org/0000-0001-7649-1174
Cleônia Roberta Melo Araújo: https://orcid.org/0000-0003-0422-5541

Dados de caracterização

*Lapachol (**1**)*

Sólido amarelo; rendimento médio de 1,2% (m/m); ponto de fusão: 161-162 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8,12 (dd, $^{3}J_1$ 7,6 Hz; $^{4}J_2$ 1,2 Hz, 1H), 8,07 (dd, $^{3}J_1$ 7,6 Hz; $^{4}J_2$ 1,2 Hz, 1H), 7,75 (td, $^{3}J_1$ 7,6 Hz; $^{4}J_2$ 1,2 Hz, 1H), 7,68 (td, $^{3}J_1$ 7,6 Hz; $^{4}J_2$ 1,2 Hz, 1H), 7,34 (s, 1H), 5,21 (m, 1H), 3,31 (d, *J* 7,4 Hz, 2H), 1,80 (sl, 3H), 1,69 (sl, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184,7 (C1), 123,6 (C2), 152,8 (C3), 181,8 (C4), 129,6 (C6), 126,9 (C7), 135,0 (C8), 133,0 (C9), 126,2 (C10), 22,8 (C11), 119,8 (C12), 134,0 (C13), 18,1 (C14↔C15), 25,9 (C14↔C15).

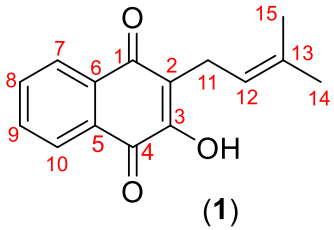
*β-Lapachona (**2**)*

Sólido laranja; rendimento de 94%; ponto de fusão: 164-165 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7,89 (dt, $^{3}J_1$ 7,6 Hz, $^{4}J_2$ 1,2 Hz, 1H), 7,75 (m, 1H), 7,74 (m, 1H), 7,59 (m, 1H), 2,38 (t, ^{3}J 6,6 Hz, 2H), 1,81 (t, ^{3}J 6,6 Hz, 2H), 1,41 (s, 6H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 177,6 (C1), 178,8 (C2), 129,7 (C3), 131,9 (C4), 160,4 (C5), 112,3 (C6), 123,5 (C7), 134,8 (C8), 130,6 (C9), 127,6 (C10), 78,8 (C11), 30,6 (C12), 15,7 (C13), 26,1 (C14), 26,1 (C15).

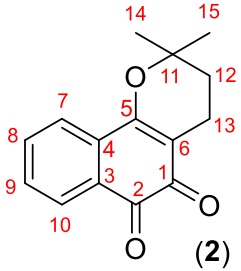
*Ácido 3-sulfônico-β-lapachona (**3**)*

Sólido vermelho; rendimento de 80%; ponto de fusão: 168-160 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7,91 (d, $^{3}J_1$ 7,4 Hz, 1H), 7,76 (m, 2H), 7,61 (m, 1H), 2,85 (m, 2H), 2,50 (m, 1H), 1,77 (s, 3H), 1,43 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 177,6 (C1), 179,1 (C2), 130,0 (C3), 131,9 (C4), 159,8 (C5), 112,8 (C6), 123,8 (C7), 135,0 (C8), 130,8 (C9), 127,8 (C10), 82,0 (C11), 59,5 (C12), 20,5 (C13), 21,1 (C14↔C15), 28,7 (C14↔C15).

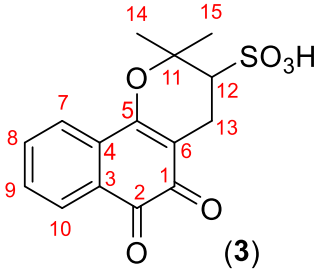
Tabela 1S. Deslocamentos químicos de ^{1}H e ^{13}C do lapachol (**1**), β-lapachona (**2**) e ácido 3-sulfônico-β-lapachona (**3**)



(**1**)



(**2**)



(**3**)

	^{1}H RMN (400 MHz)			^{13}C RMN (100 MHz)		
	Lapachol	β-lapachona	Ácido 3-sulfônico-β-lapachona	Lapachol	β-lapachona	Ácido 3-sulfônico-β-lapachona
1	–	–	–	184,7	177,6	177,6
2	–	–	–	123,6	178,8	179,1
3	–	–	–	152,8	129,7	130,0
4	–	–	–	181,8	131,9	131,9
5	–	–	–	-	160,4	159,8
6	–	–	–	129,6	112,3	112,8
7	8,12 (dd, $^{3}J_1$ = 7,6 Hz; $^{4}J_2$ = 1,2 Hz, 1H)	7,74 (m, 1H)	7,76 (m, 1H)	126,9	123,5	123,8
8	7,75 (td, $^{3}J_1$ = 7,6; $^{4}J_2$ = 1,2 Hz, 1H)	7,75 (m, 1H)	7,76 (m, 1H)	135,0	134,8	135,0
9	7,68 (td, $^{3}J_1$ = 7,6; $^{4}J_2$ = 1,2 Hz, 1H)	7,59 (m, 1H)	7,61 (m, 1H)	133,0	130,6	130,8

10	8,07 (dd, $^{3}J_{1}$ = 7,6 Hz; $^{4}J_{2}$ = 1,2 Hz, 1H)	7,89 (d, $^{3}J_{1}$ = 7,6 Hz, 1H)	7,91 (d, $^{3}J_{1}$ = 7,4 Hz; 1H)	126,2	127,6	127,8
11	3,31 (d, J = 7,4 Hz, 2H)	–	–	22,8	78,8	82,0
12	5,21 (m, 1H)	1,81 (t, ^{3}J = 6,6 Hz, 2H)	2,85 (m, 1H)	119,8	30,6	59,5
13	–	2,38 (t, ^{3}J = 6,6 Hz, 2H)	2,50 (m, 1H) 2,85 (m, 1H)	134,0	15,7	20,5
14↔15	1,80 (sl, 3H)	1,41 (s, 3H)	1,43 (s, 3H)	18,1	26,1	21,1
14↔15	1,69 (sl, 3H)	1,41 (s, 3H)	1,77 (s, 3H)	25,9	26,1	28,7
OH	7,34 (s, 1H)	–	–	–	–	–

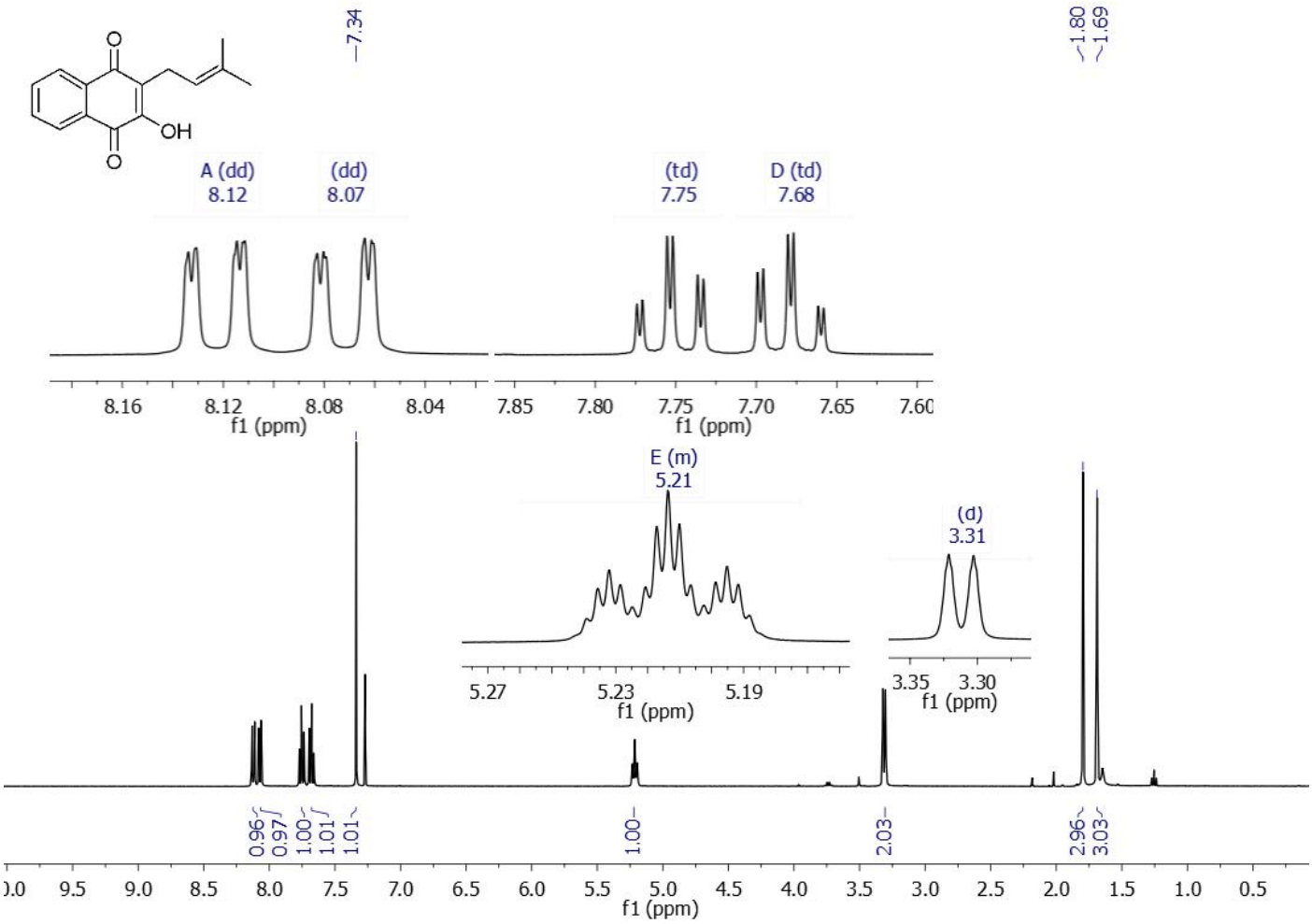


Figura 1S. *Espectro de RMN ^{1}H (400MHz, $CDCl_3$) do lapachol (**1**)*

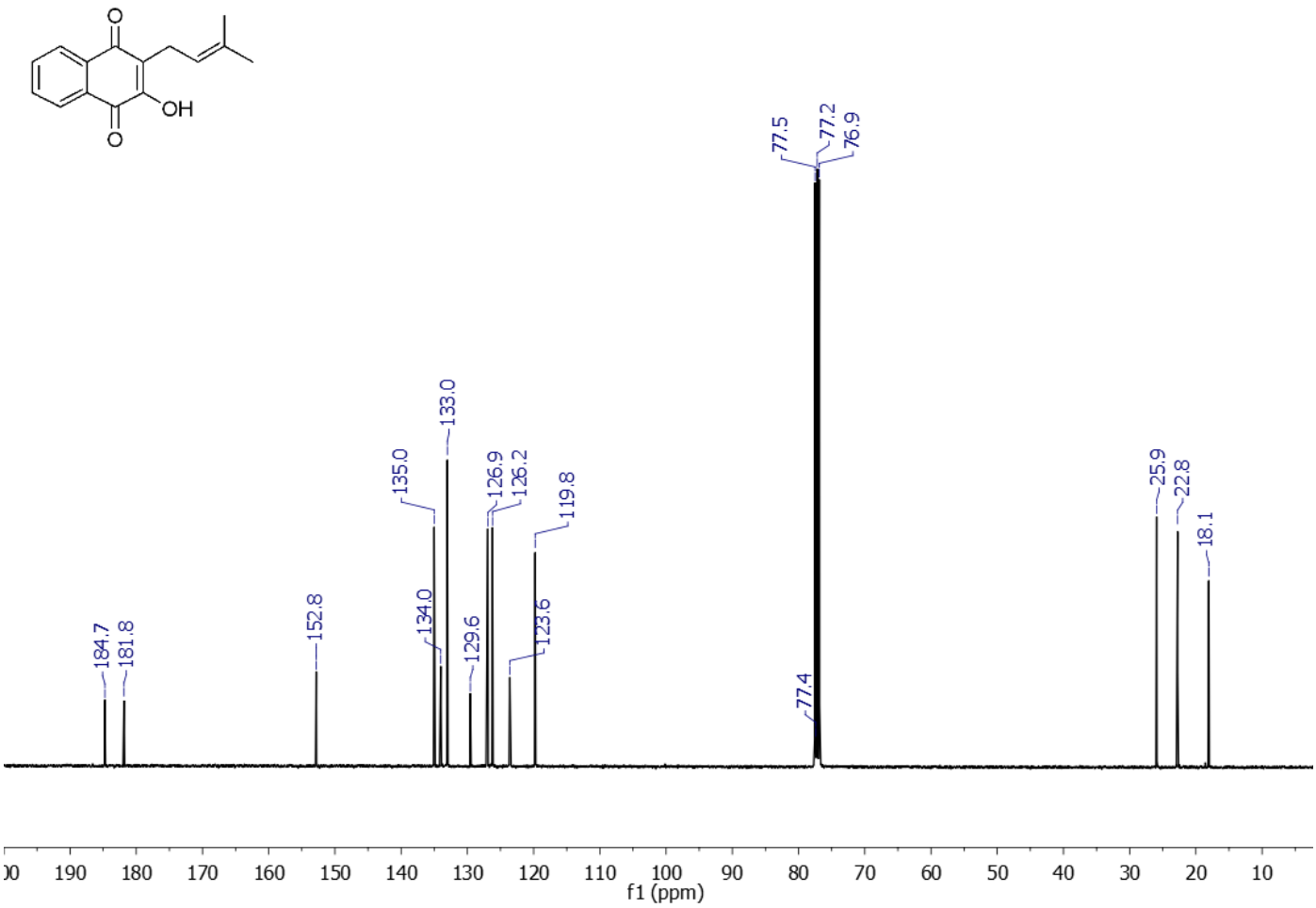


Figura 2S. *Espectro de RMN ^{13}C (100MHz, $CDCl_3$) do lapachol (**1**)*

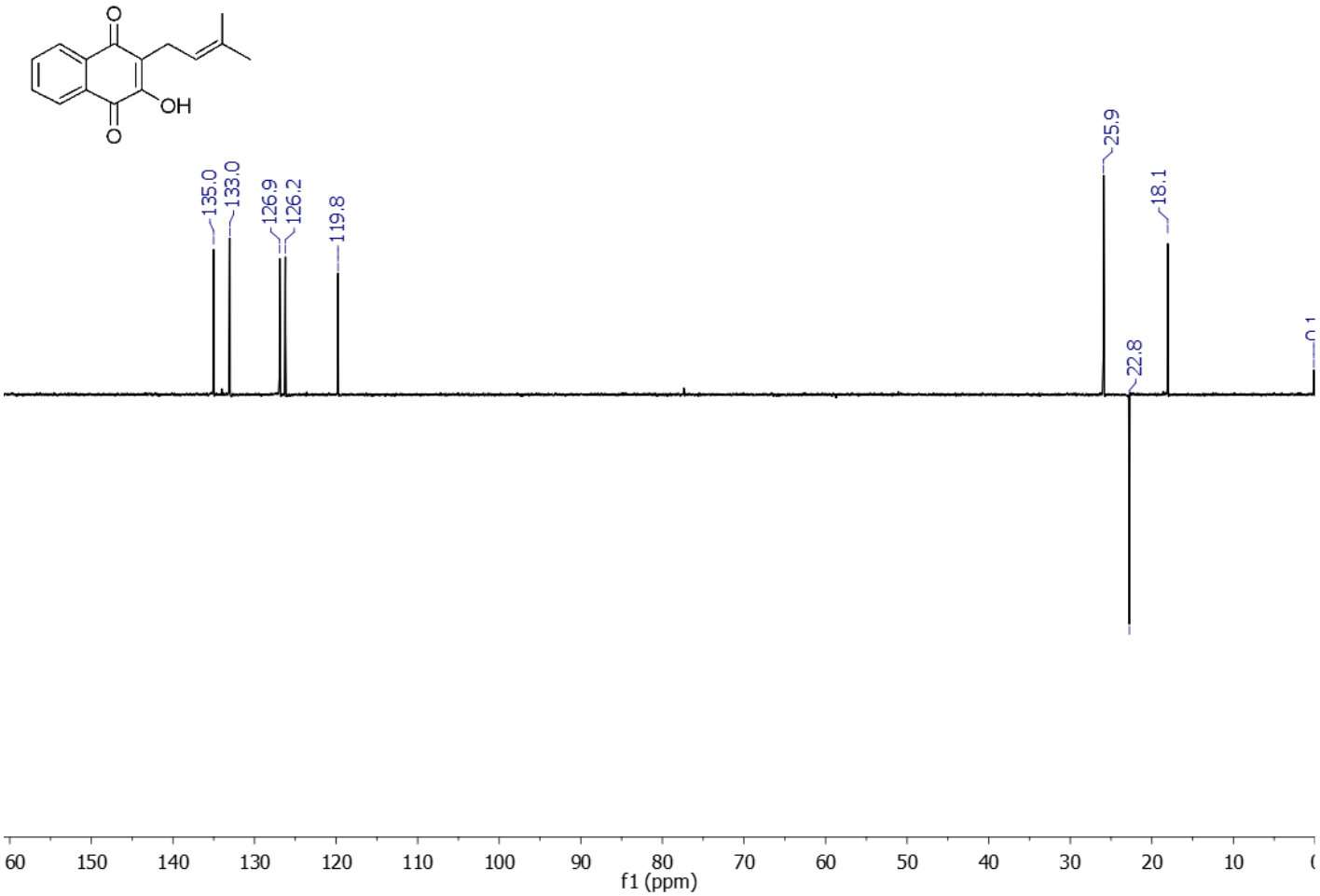


Figura 3S. *Espectro de RMN ^{13}C-DEPT 135° (100MHz, $CDCl_3$) do lapachol (**1**)*

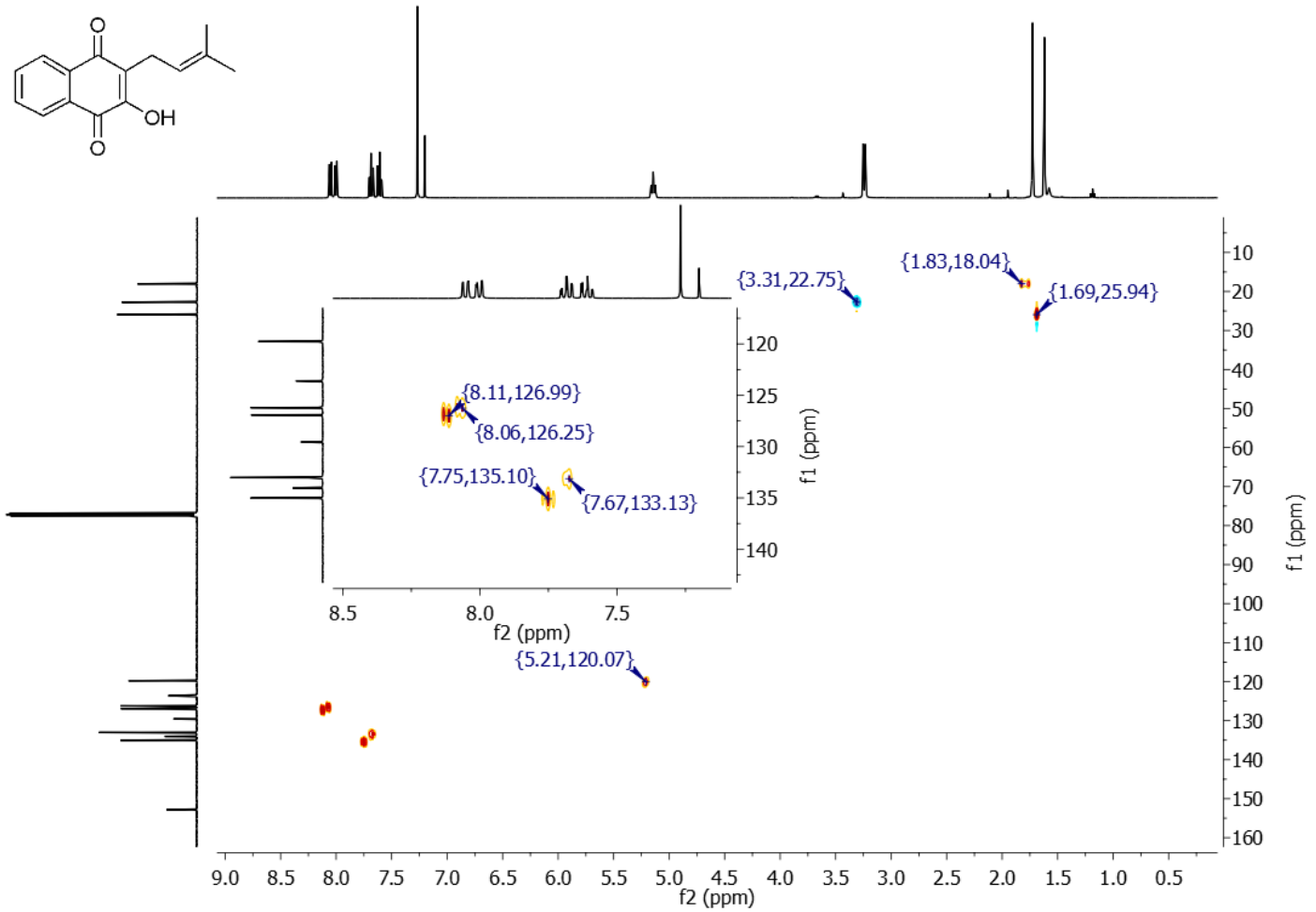


Figura 4S. *Espectro de RMN ^{1}H-^{13}C-HSQC (400-100 MHz, $CDCl_3$) do lapachol (**1**)*

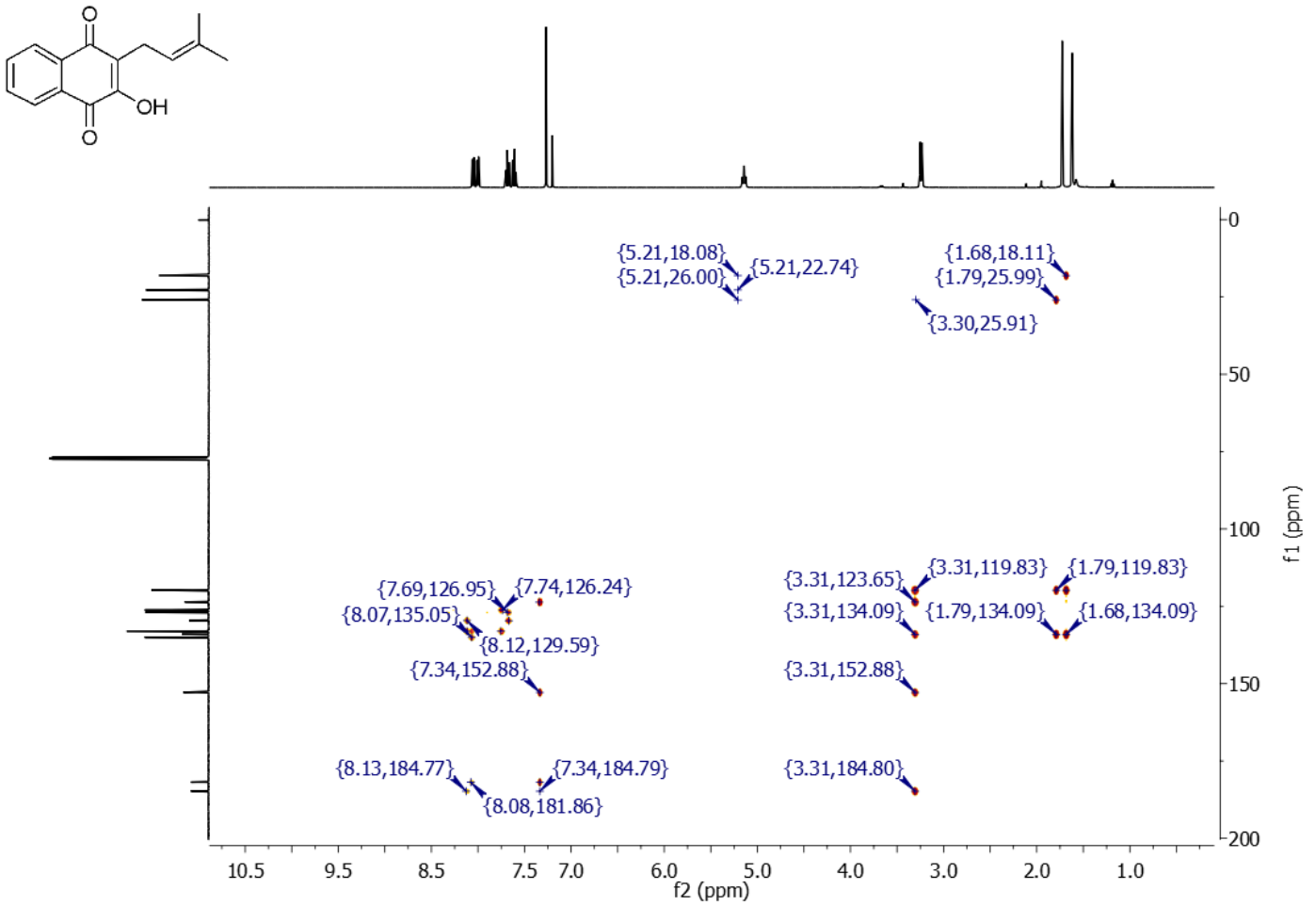


Figura 5S. *Espectro de RMN ^{1}H-^{13}C HMBC (400-100 MHz, $CDCl_3$) do lapachol (**1**)*

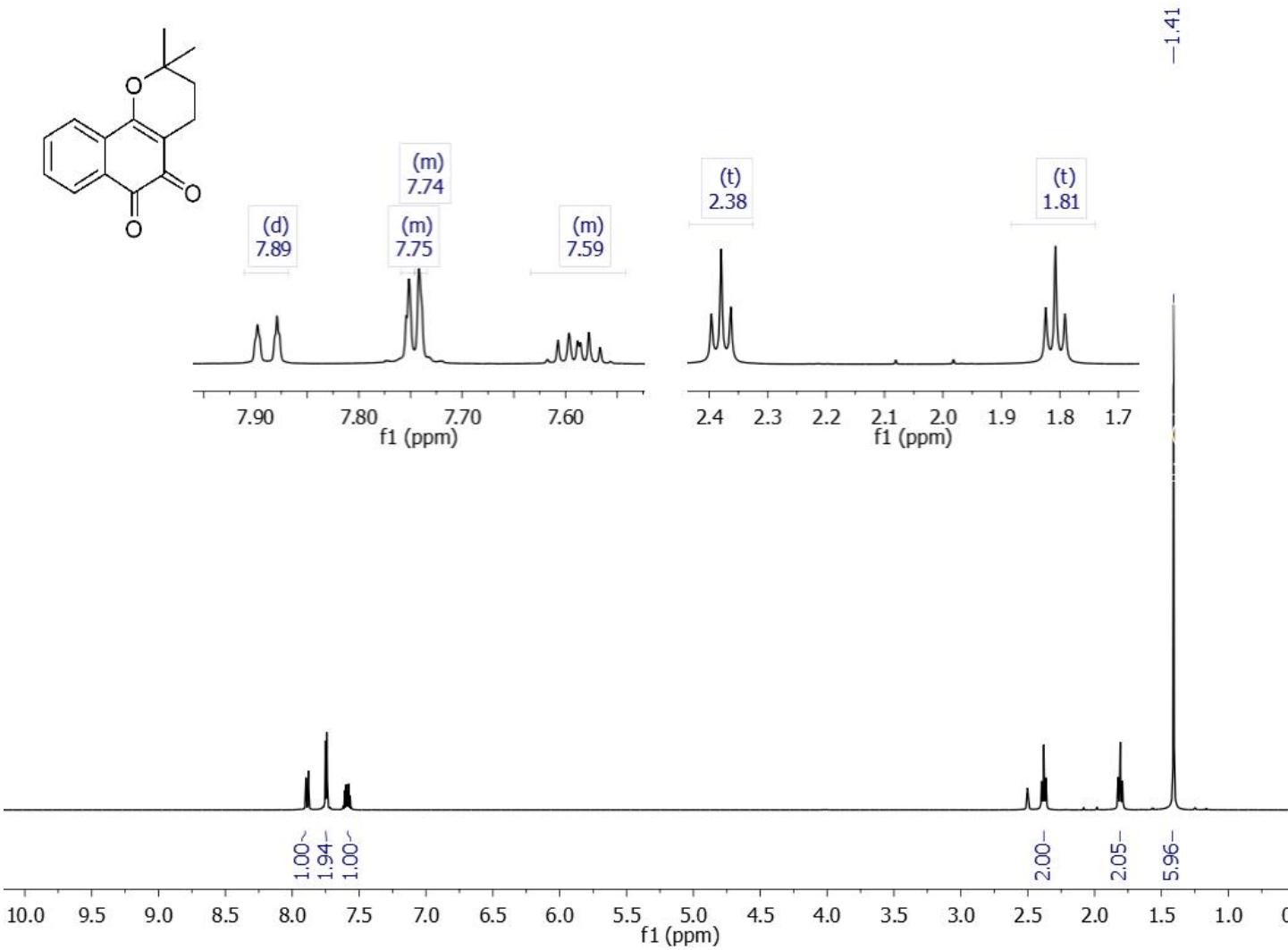


Figura 6S. *Espectro de RMN ^{1}H (400 MHz, DMSO-d_6) da β-lapachona (**2**)*

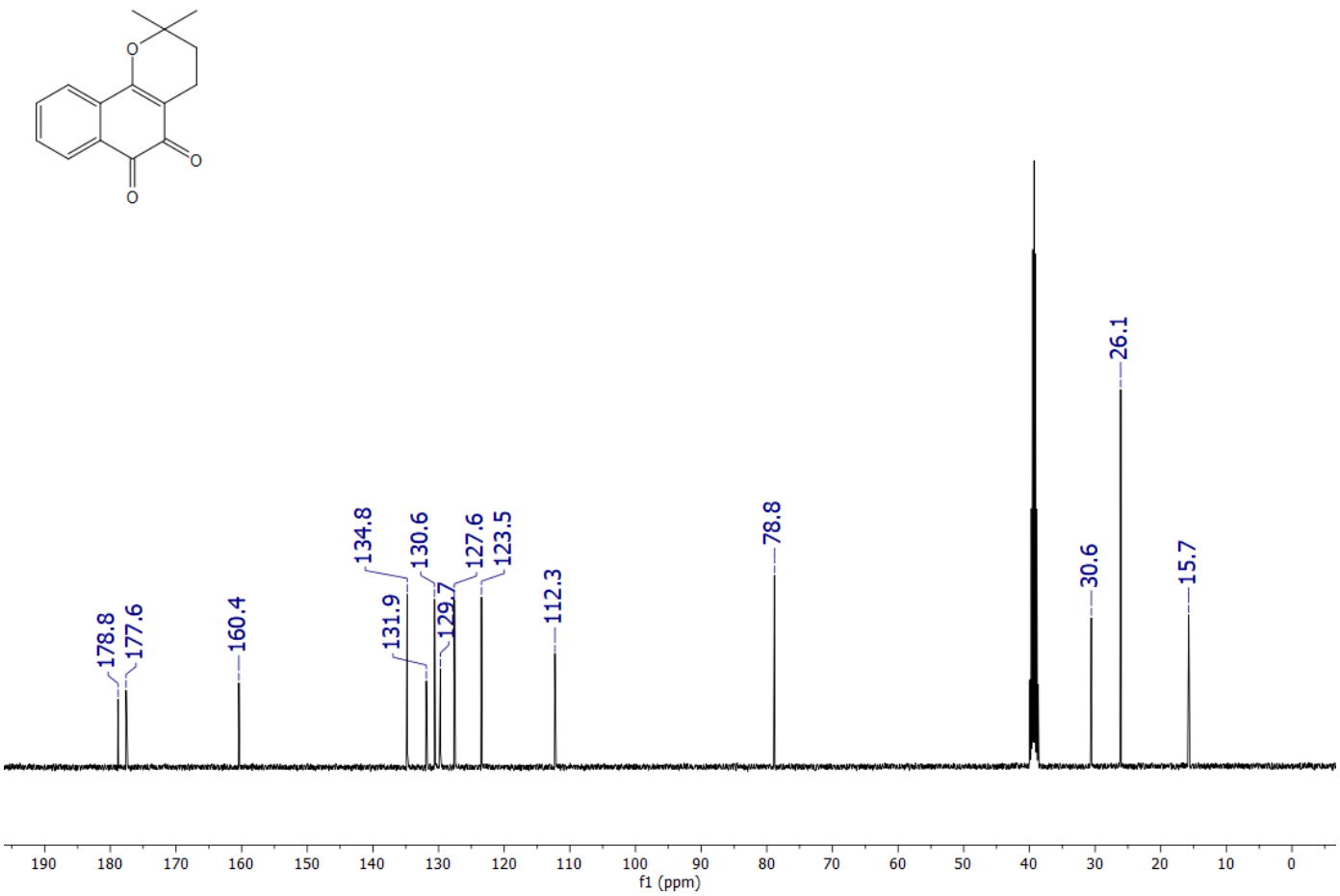


Figura 7S. *Espectro de RMN ^{13}C (100 MHz, DMSO-d_6) da β-lapachona (**2**)*

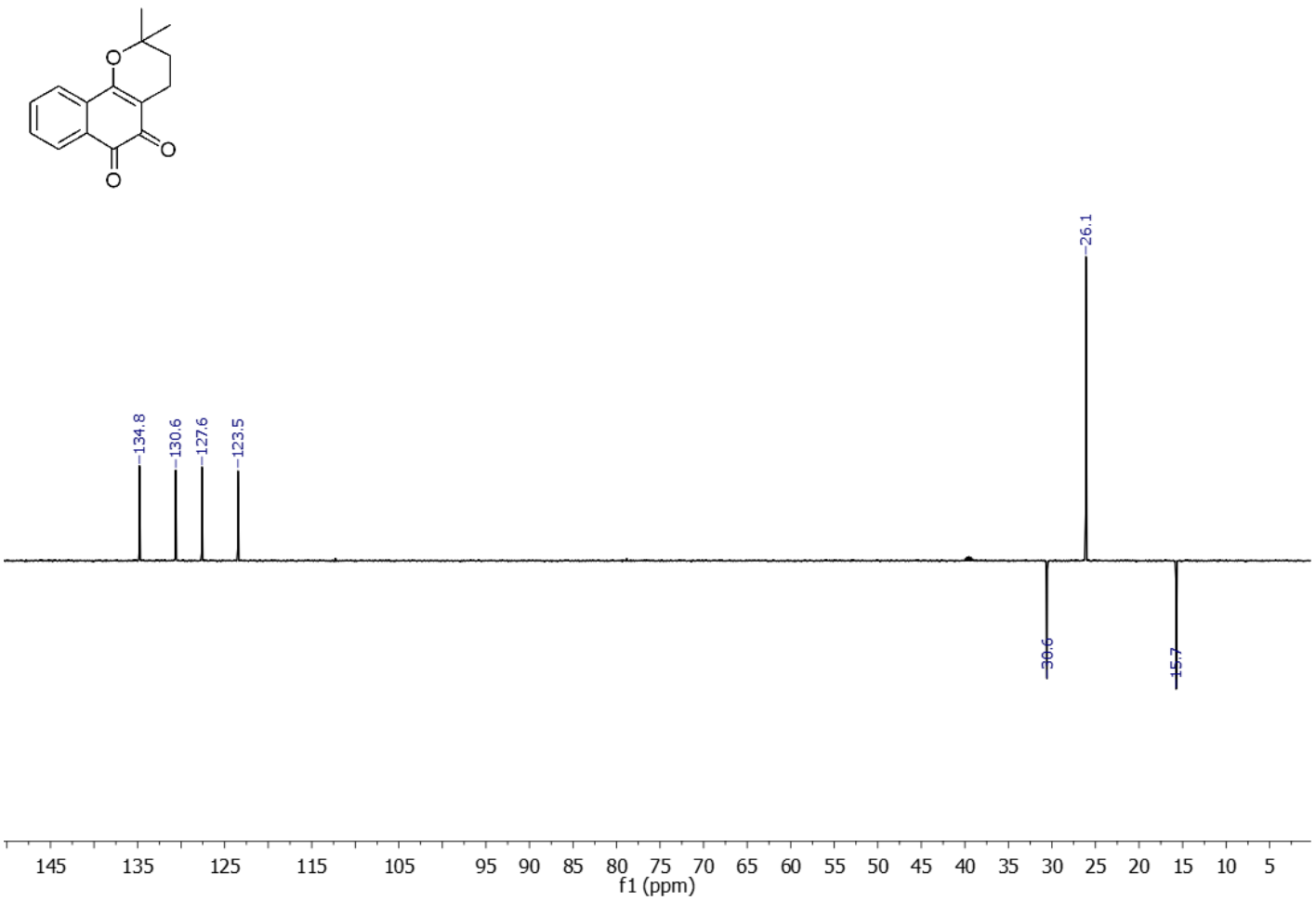


Figura 8S. *Espectro de RMN ^{13}C-DEPT 135° (100 MHz, DMSO-d_6) da β-lapachona (**2**)*

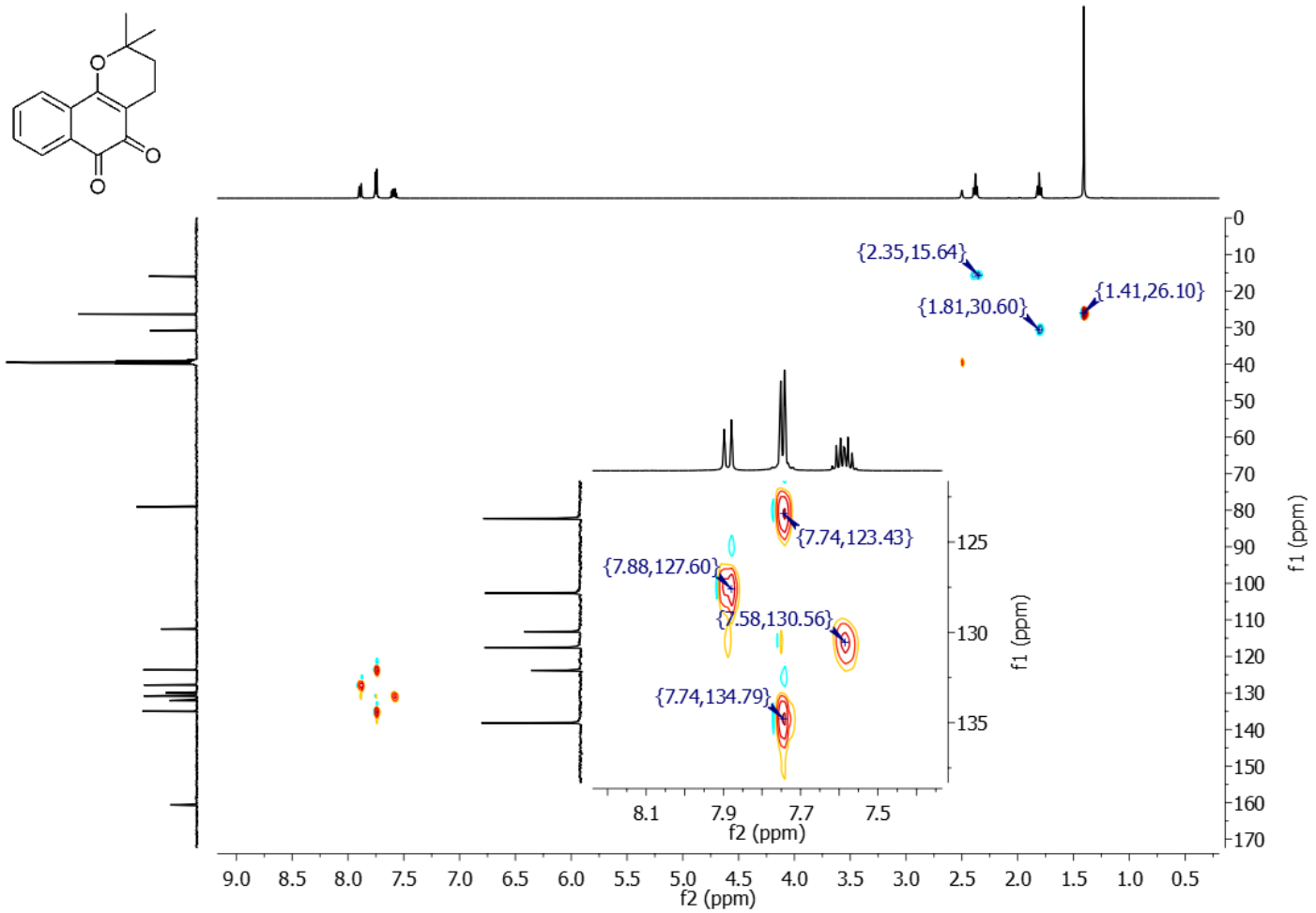


Figura 9S. *Espectro de RMN ^{1}H-^{13}C HSQC (400-100 MHz, DMSO-d_6) da β-lapachona (**2**)*

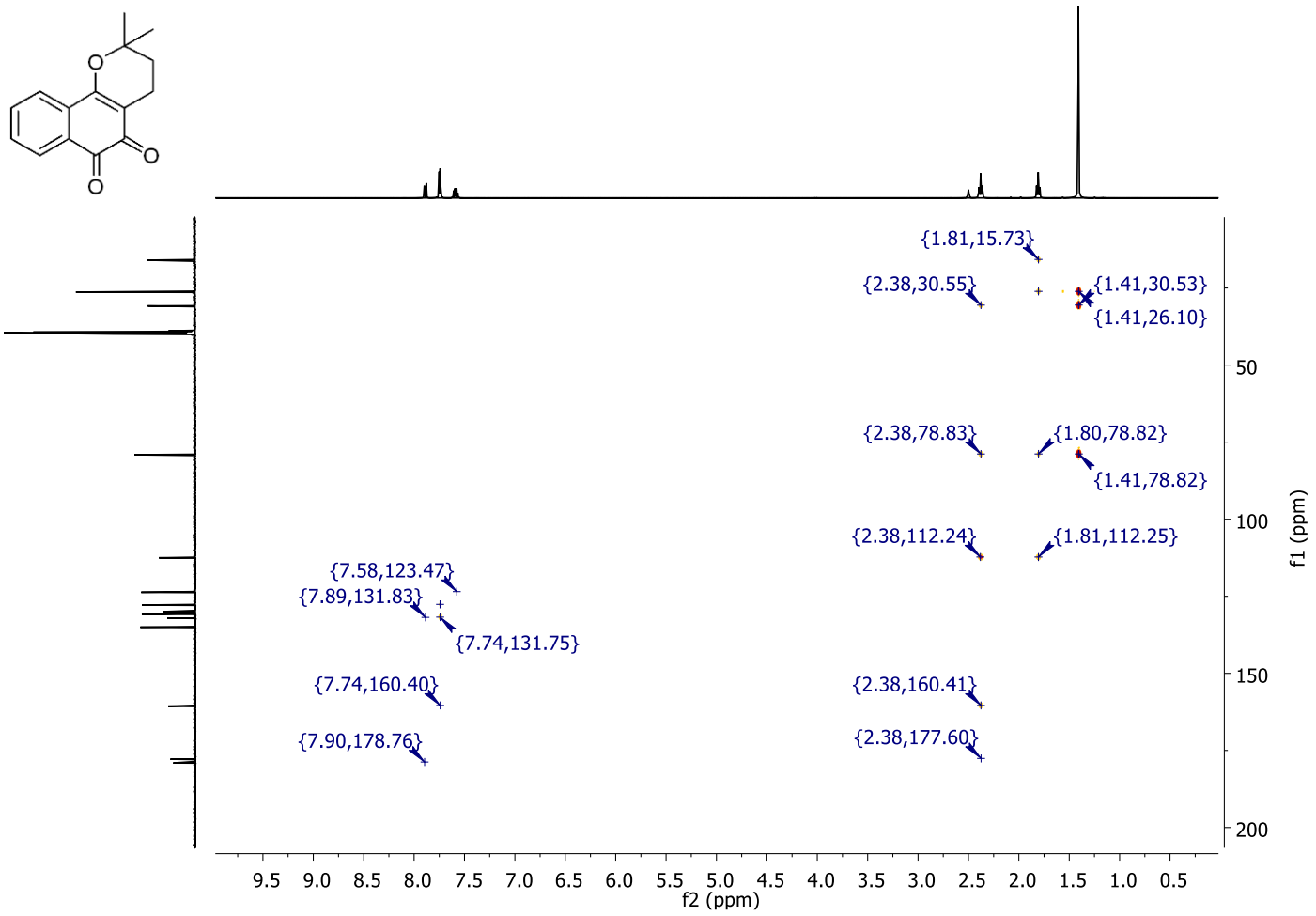


Figura 10S. *Espectro de RMN ^{1}H-^{13}C HMBC (400-100 MHz, DMSO-d_6) da β-lapachona (**2**)*

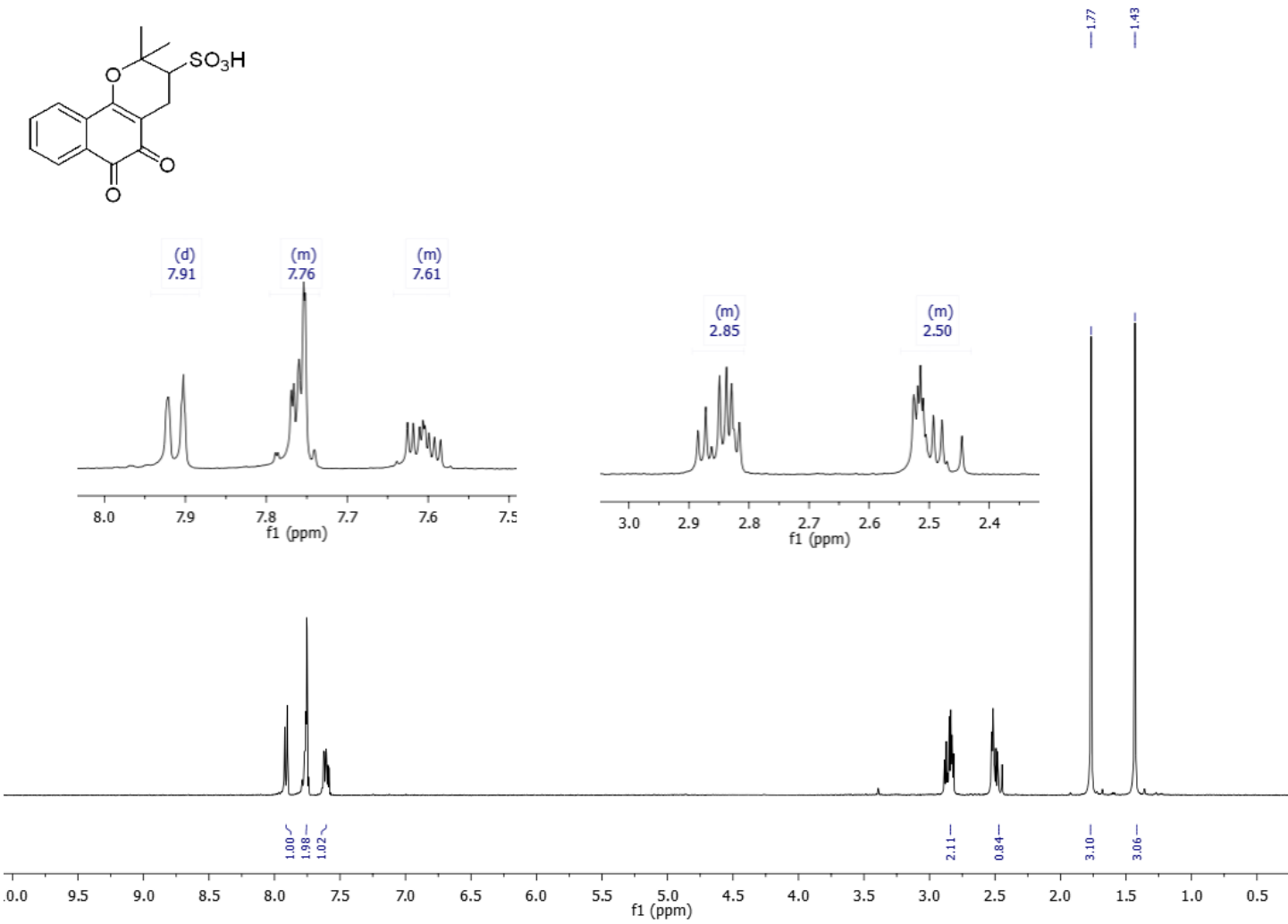


Figura 11S. *Espectro de RMN ^{1}H (400 MHz, DMSO-d_6) do ácido 3-sulfônico-β-lapachona* ***(3)***

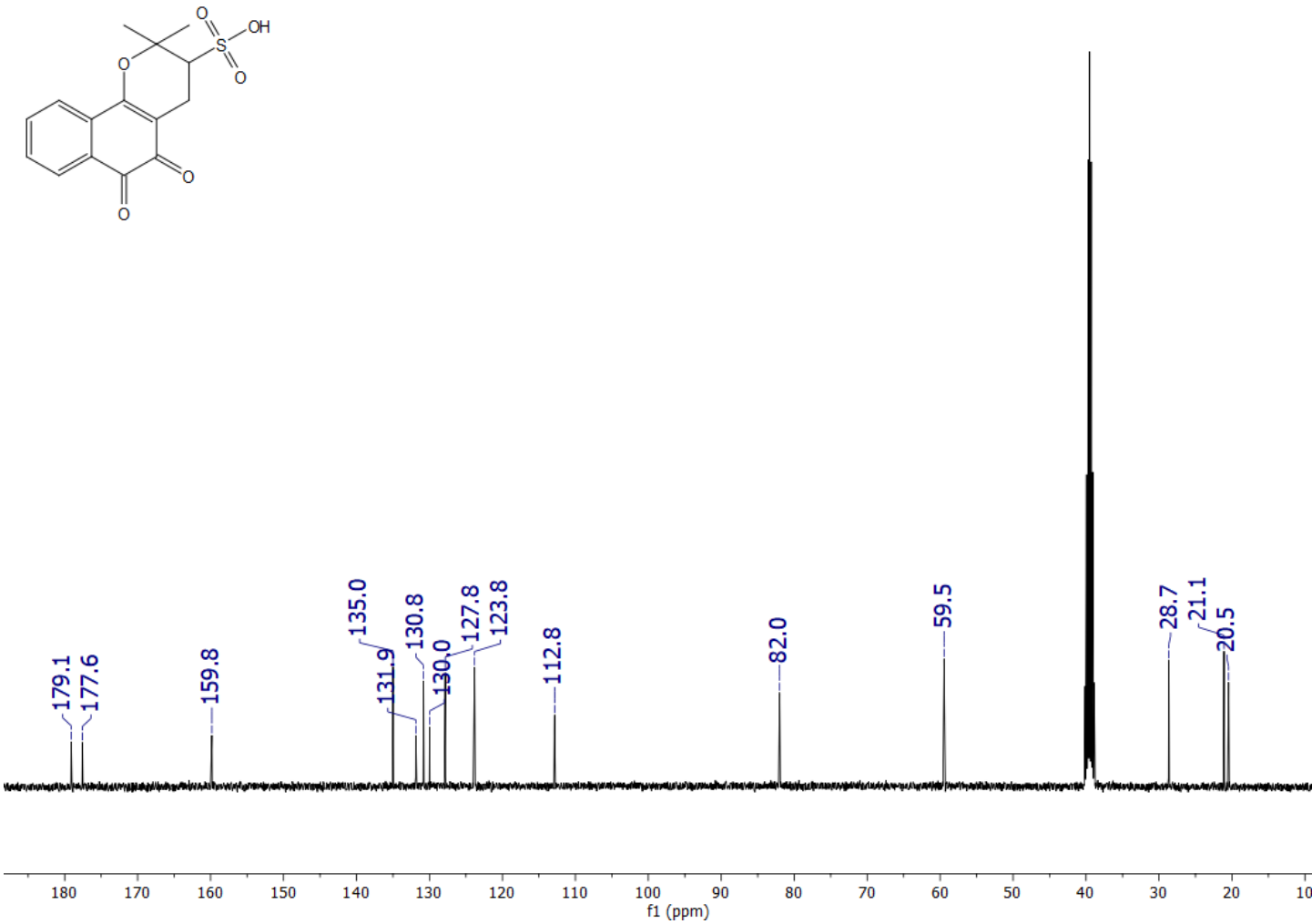


Figura 12S. *Espectro de RMN ^{13}C (100 MHz, DMSO-d_6) do ácido 3-sulfônico-β-lapachona (**3**)*

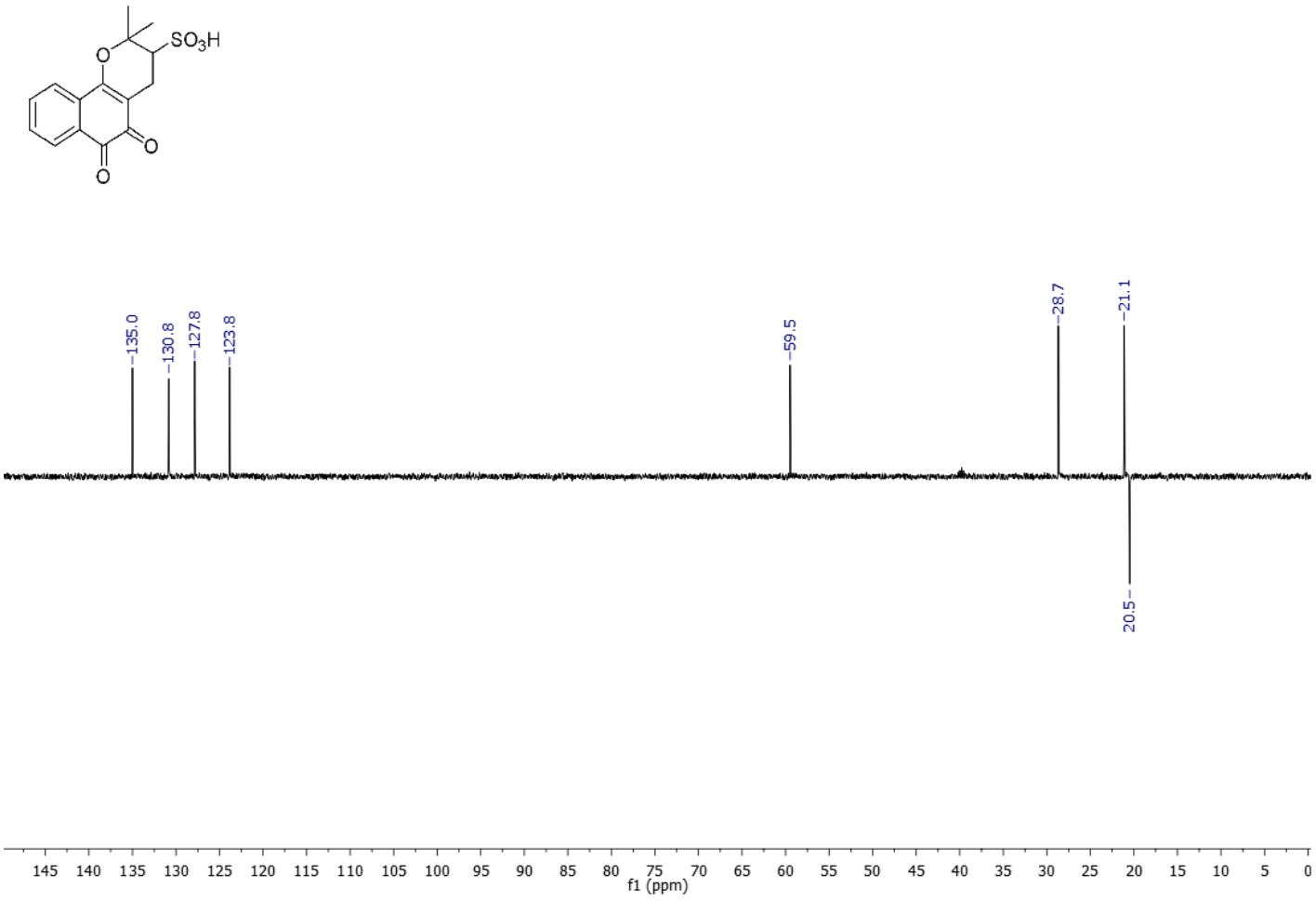


Figura 13S. *Espectro de RMN ^{13}C-DEPT 135° (100 MHz, DMSO-d_6) do ácido 3-sulfônico-β-lapachona* ***(3)***

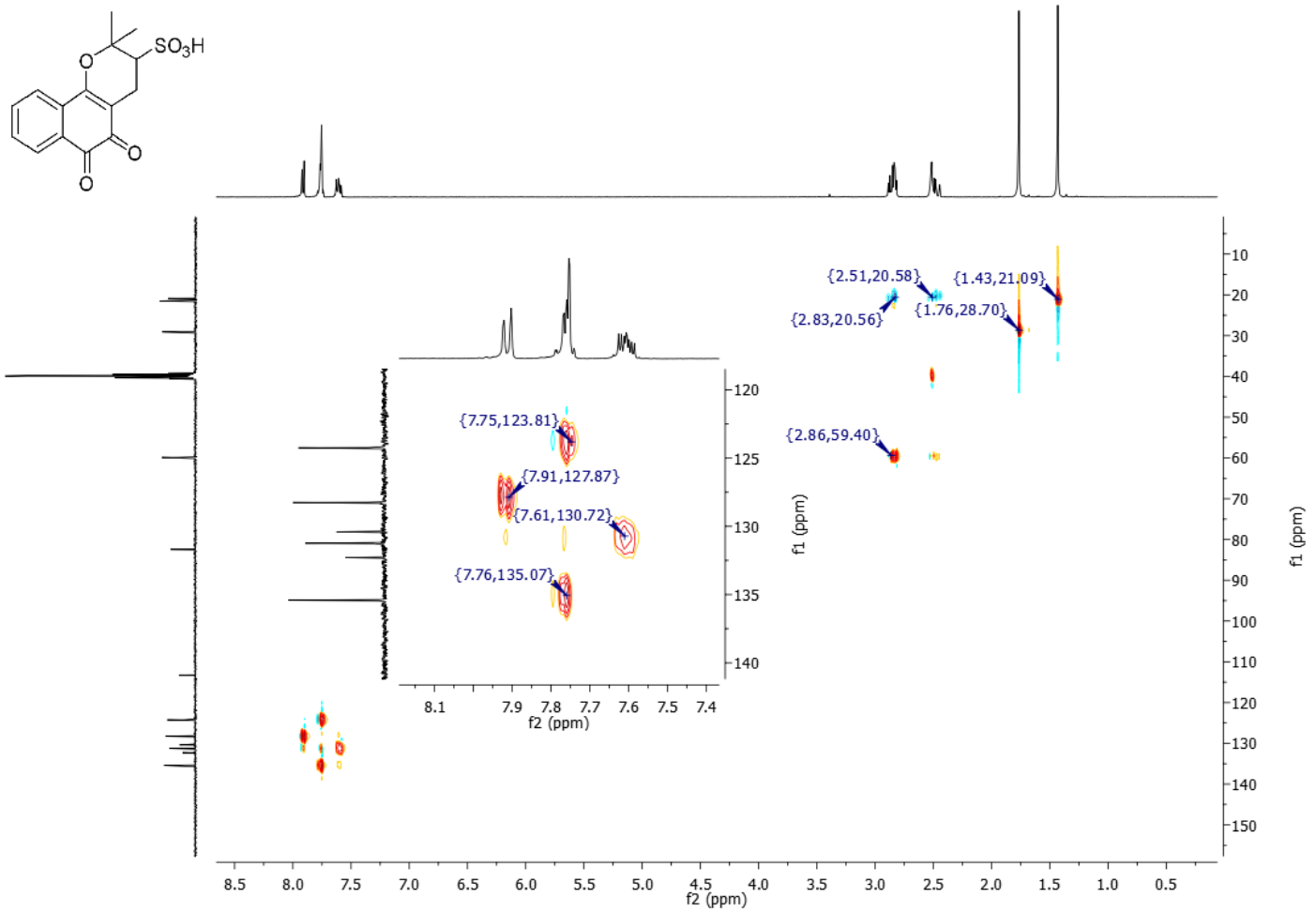


Figura 14S. *Espectro de RMN ^{1}H-^{13}C HSQC (400-100 MHz, DMSO-d_6) do ácido 3-sulfônico-β-lapachona (**3**)*

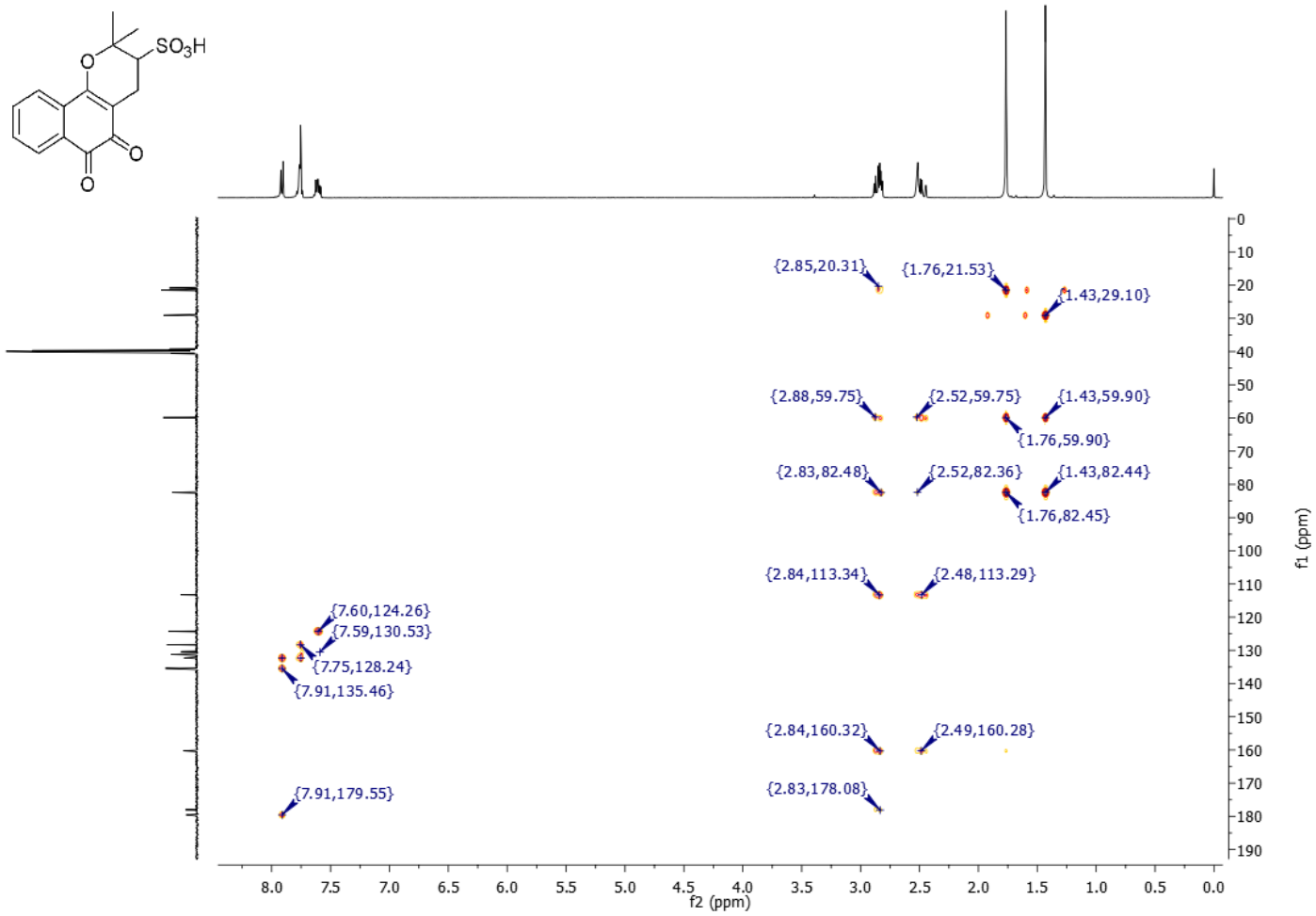


Figura 15S. *Espectro de RMN ^{1}H-^{13}C HMBC (400-100 MHz, DMSO-d_6) do ácido 3-sulfônico-β-lapachona (**3**)*