

Supporting Information

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A Quinone Derivative from an Endophytic Fungus *Phomopsis* sp. from *Morus cathayana*

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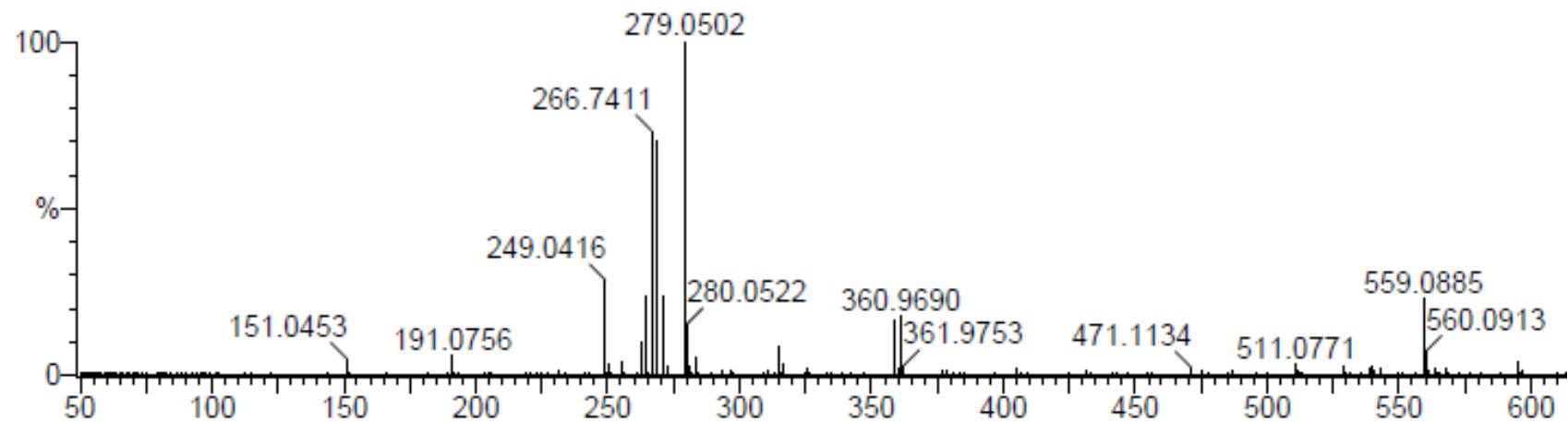
* Corresponding author: E- Mail:elvira@chem.itb.ac.id (E. Hermawati).

No.	δ_H , mult. (<i>J</i> in Hz)	δ_C	HMBC	No.	δ_H , mult. (<i>J</i> in Hz)	δ_C	HMBC
1	3.83, d (12.6) 4.85, d (12.6)	57.9	C-1a, C-2	6	7.11, d (2.0)	108.1	C-4, C-2a, C-7, C-5
1a	-	65.4	-	6a	-	133.5	-
2	-	194.2	-	7	-	190.7	-
2a	-	108.9	-	7a	-	65.6	-
3	-	164.8	-	8	3.84, d (12.6) 4.82, d (12.6)	58.5	C-7, C-7a
4	6.68, d (2.0)	106.9	C-2a, C-6, C-3, C-5	a)	11.64, v br s	-	c)
5	-	166.7	-	b)	3.90, s	56.1	C-5
				d)	2.97, v br s	-	c)

a) 3-OH; b) 5-OCH₃; c) no HMBC correlations were detected due to a very broad singlet of 3-OH signal.

d) 1-OH/-8-OH.

S1: Table of NMR data of compound **1** (epoxyquinophomopsin)



S2: HRESITOFMS spectrum of compound 1 (epoxyquinophomopsin)

Monoisotopic Mass, Even Electron Ions

51 formula(e) evaluated with 3 results within limits (up to 1 closest results for each mass)

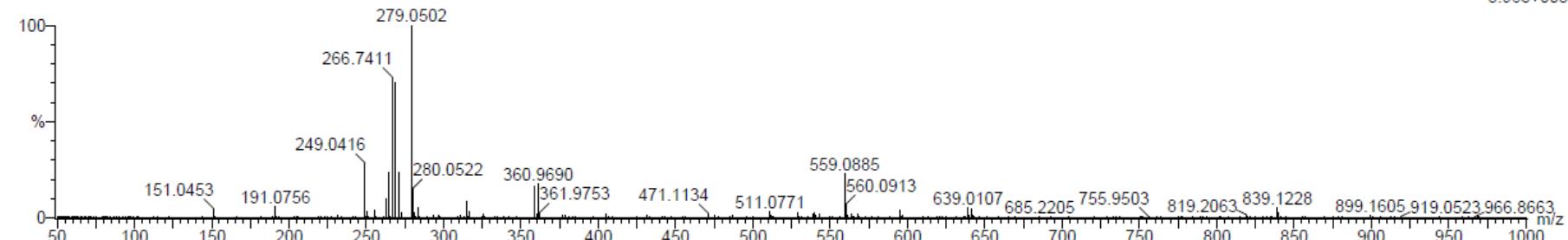
Elements Used:

C: 0-1000 H: 0-1000 O: 0-500

standar

elvira AB13_smp 279-0505_neg 4 (0.056) Cm (4)

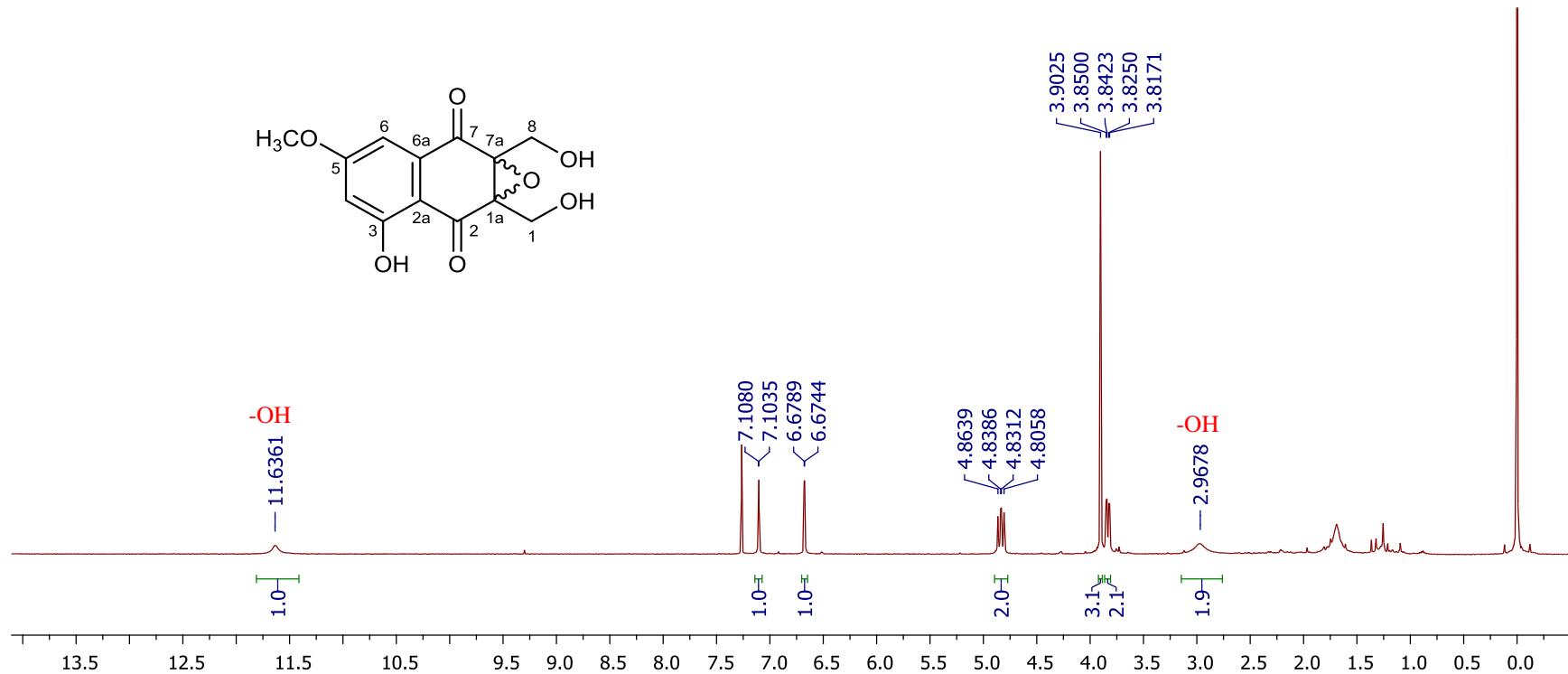
TOF MS ES-
3.96e+003



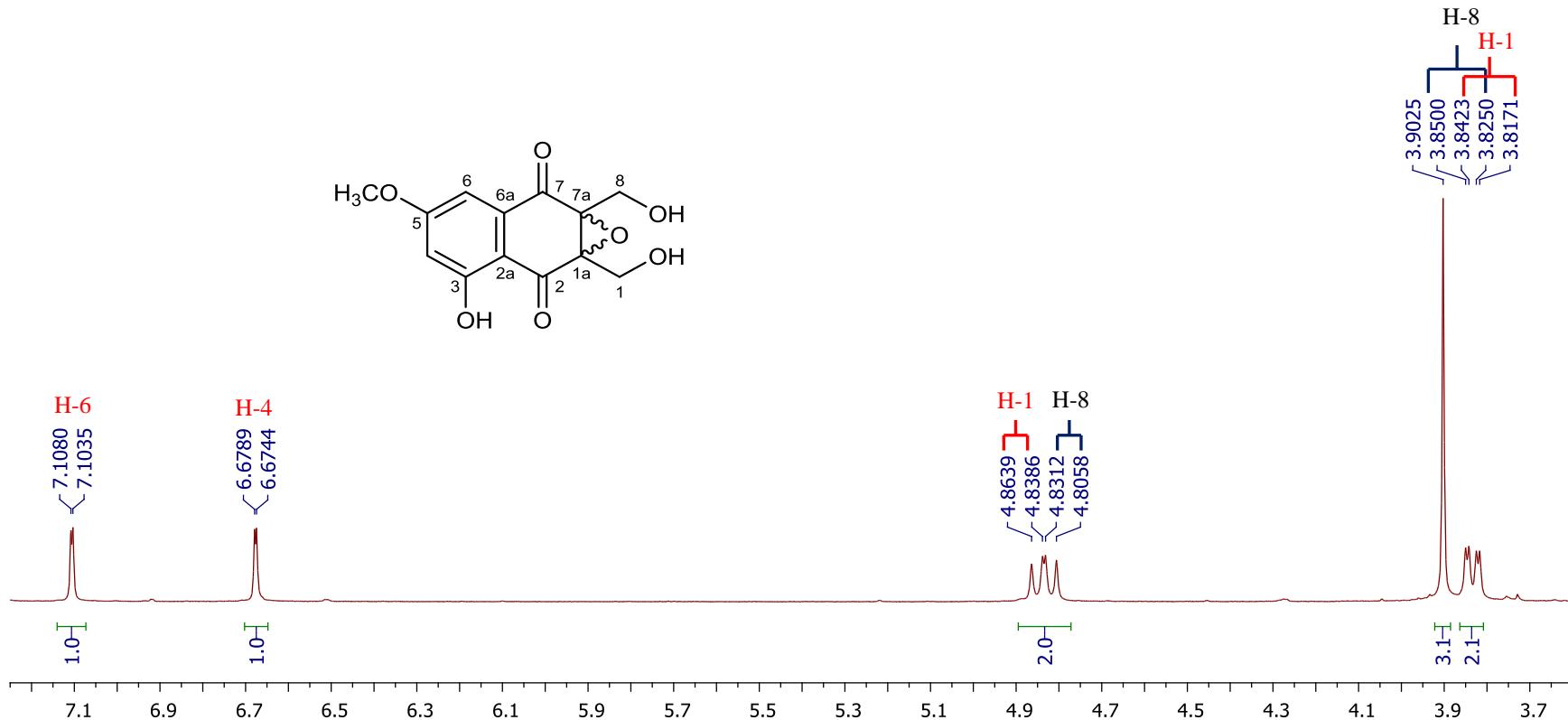
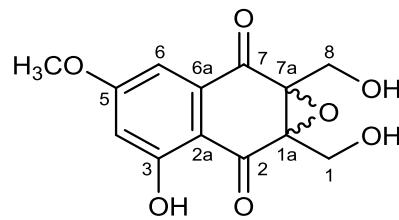
Minimum:
Maximum:

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
279.0502	279.0505	-0.3	-1.1	8.5	331.9	0.0	C13 H11 O7

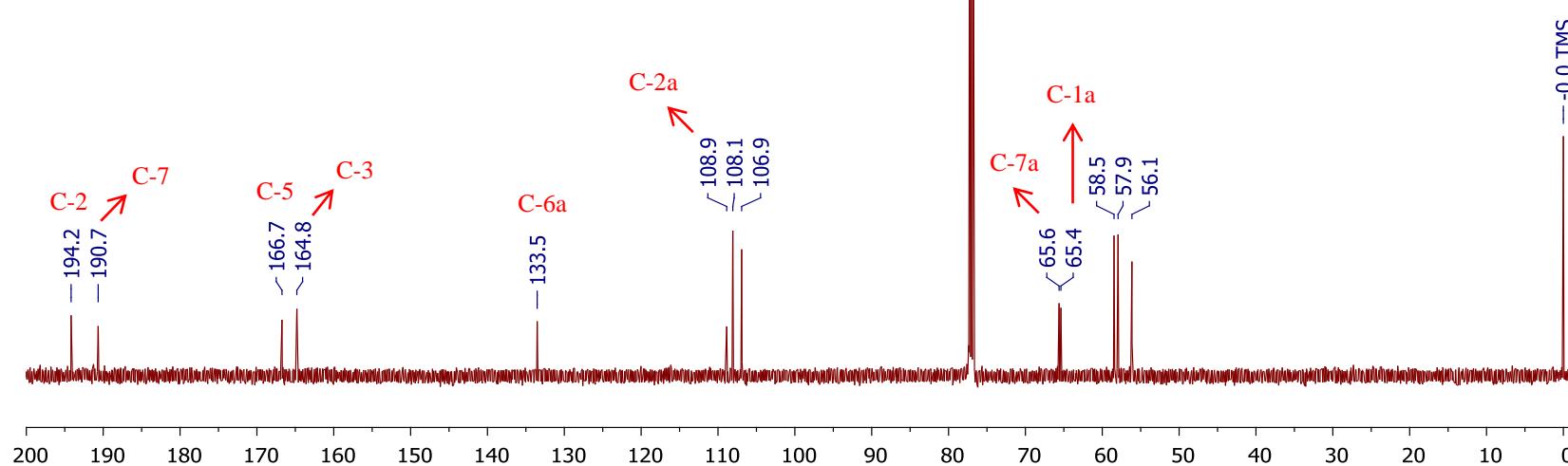
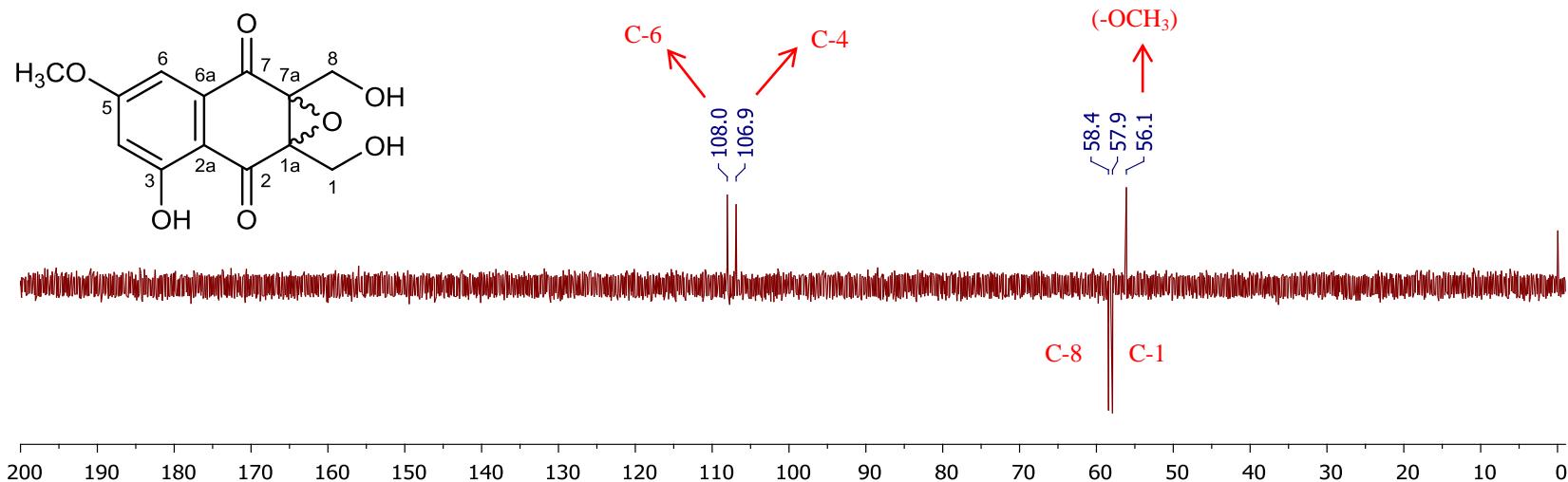
S3: Expansion of HRESITOFMS spectrum of compound **1** (epoxyquinophomopsin)



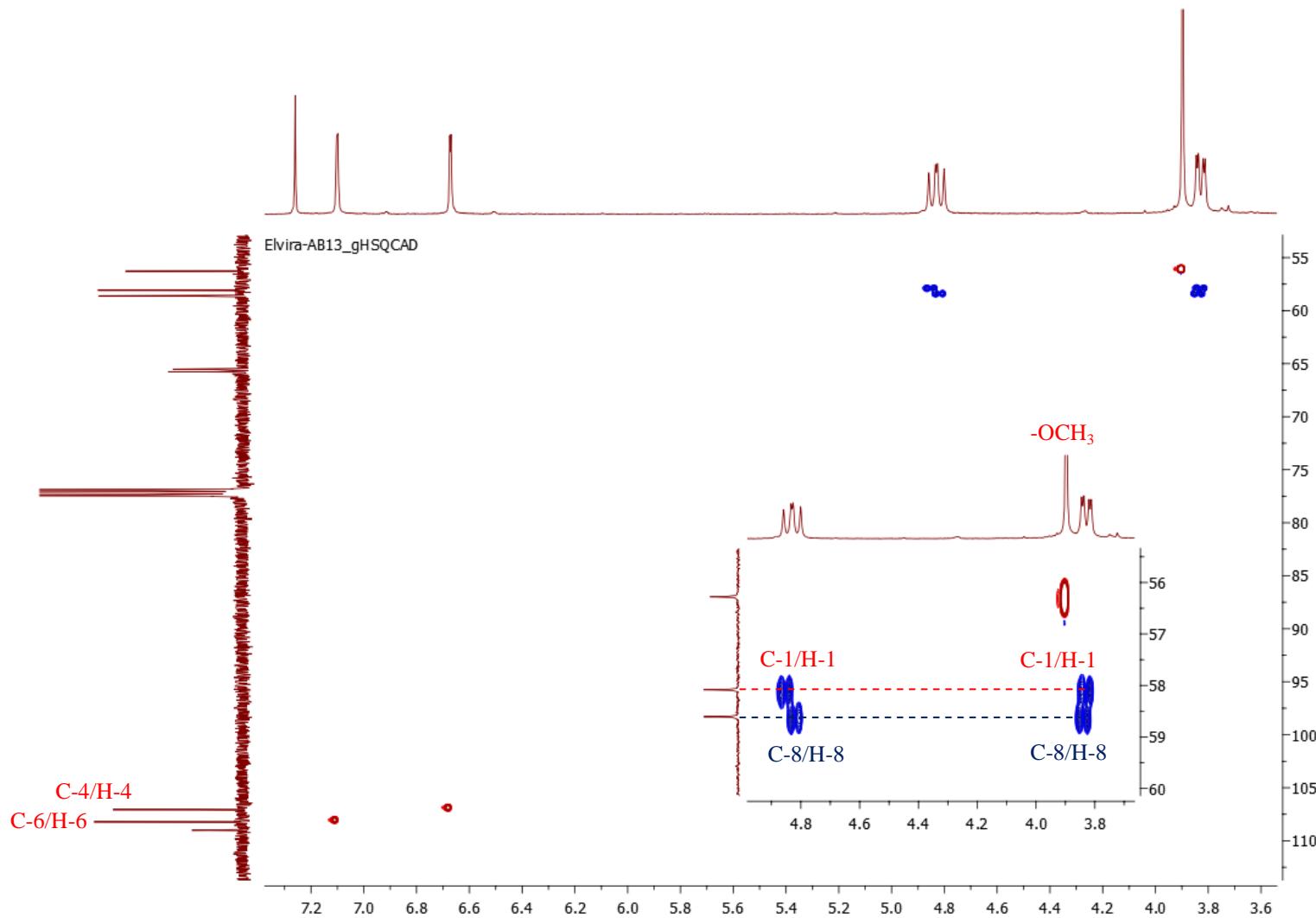
S4: ^1H -NMR (500 MHz, CDCl_3) spectrum of compound **1** (epoxyquinophomopsin)



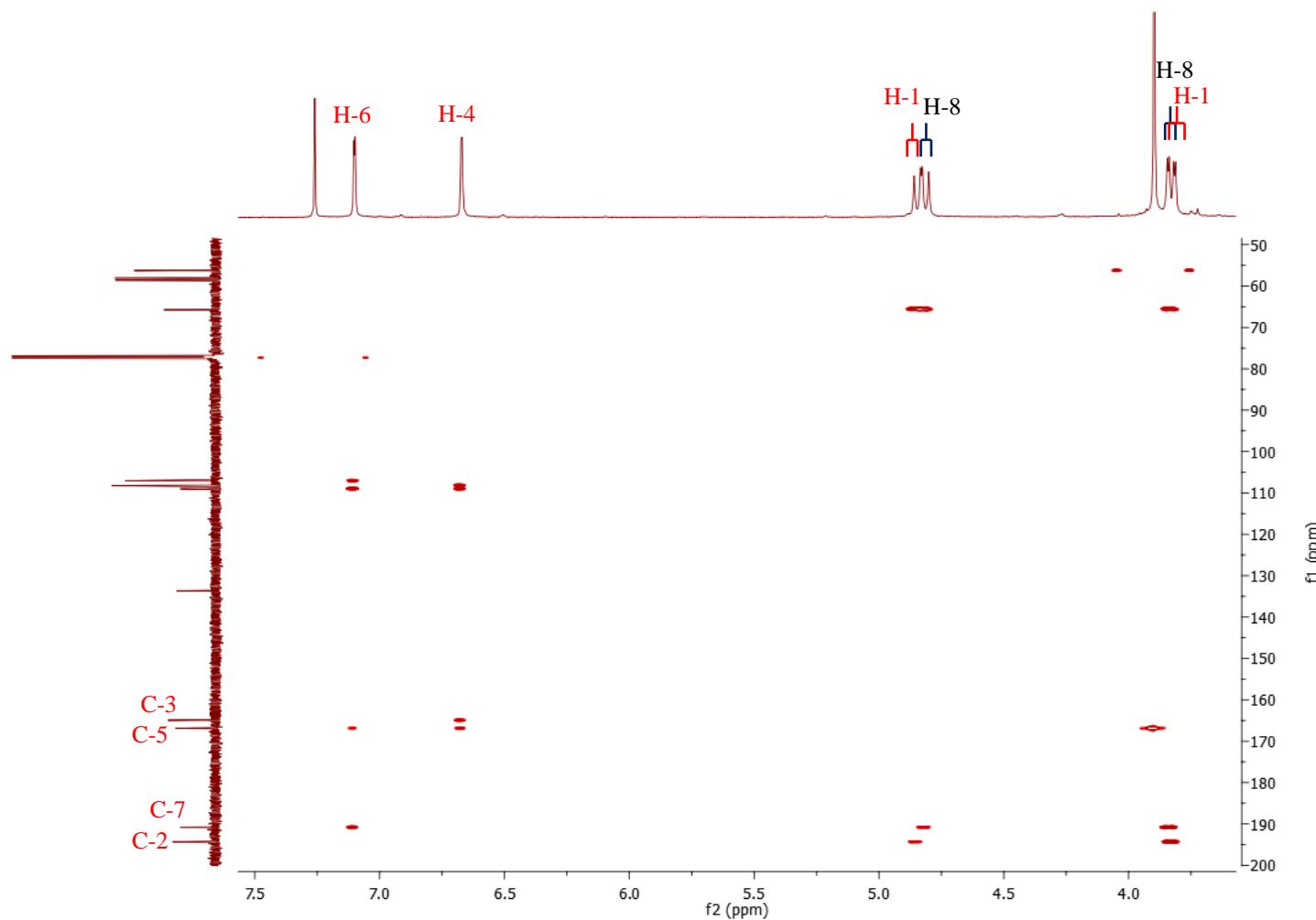
S5: ^1H -NMR spectrum of compound **1** (epoxyquinophomopsin) (From 3.60 to 7.25 ppm)



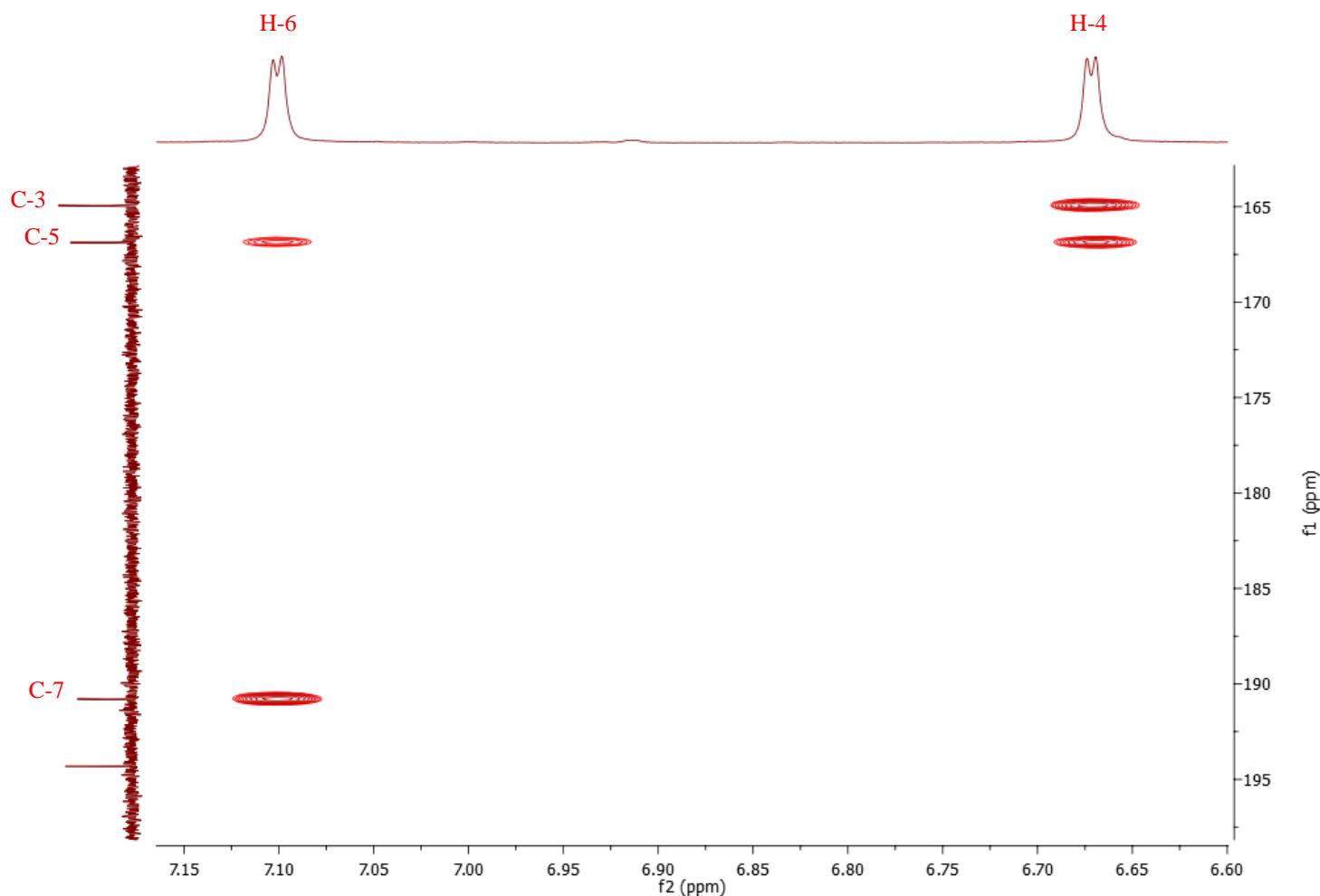
S6: ¹³C-NMR + DEPT (125 MHz, CDCl₃) spectrum of compound 1 (epoxyquinophomopsin)



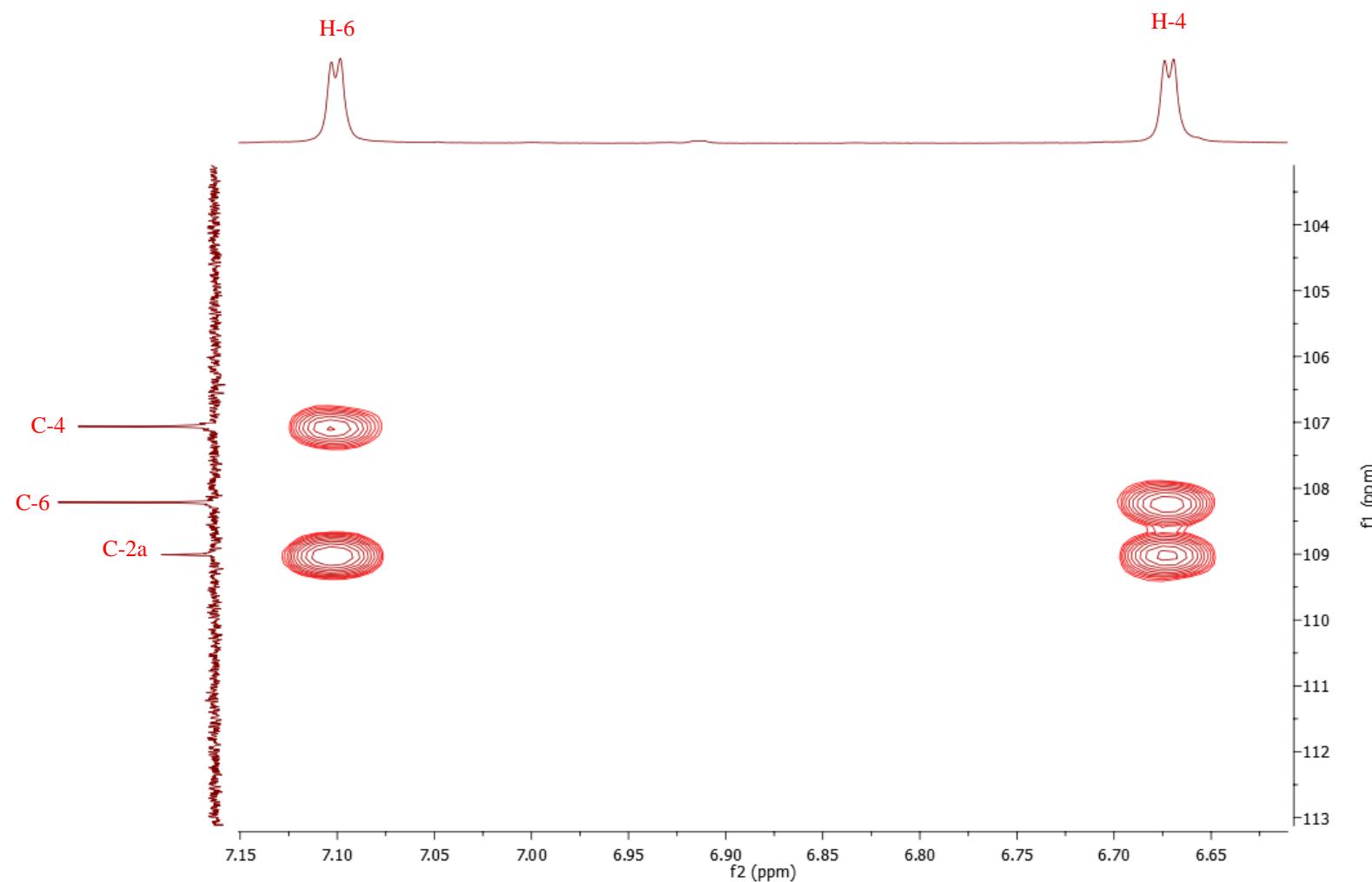
S7: HSQC (500 MHz) spectrum of compound **1** (epoxyquinophomopsin)



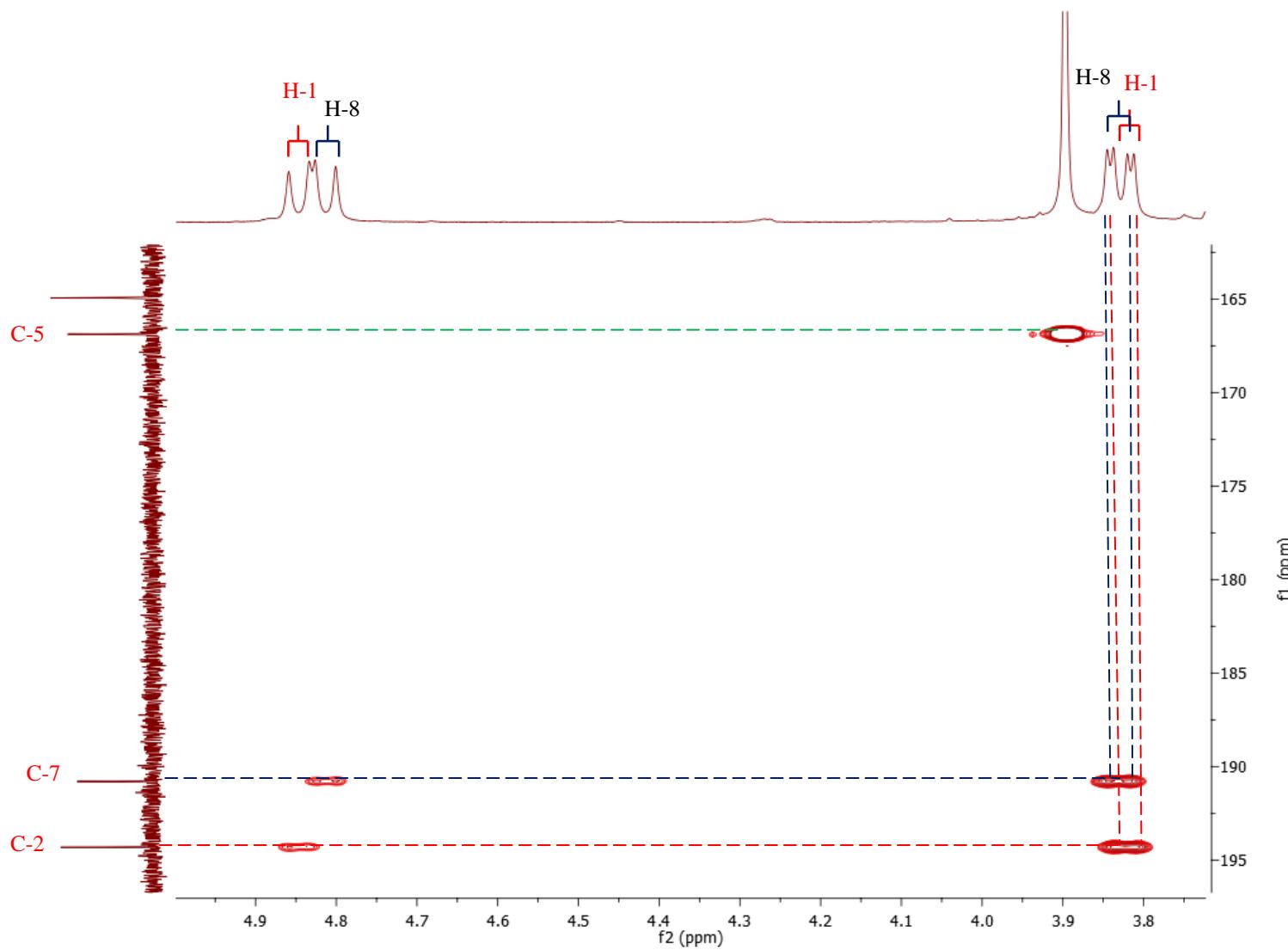
S8: HMBC (500 MHz) spectrum of compound 1 (epoxyquinophomopsin)



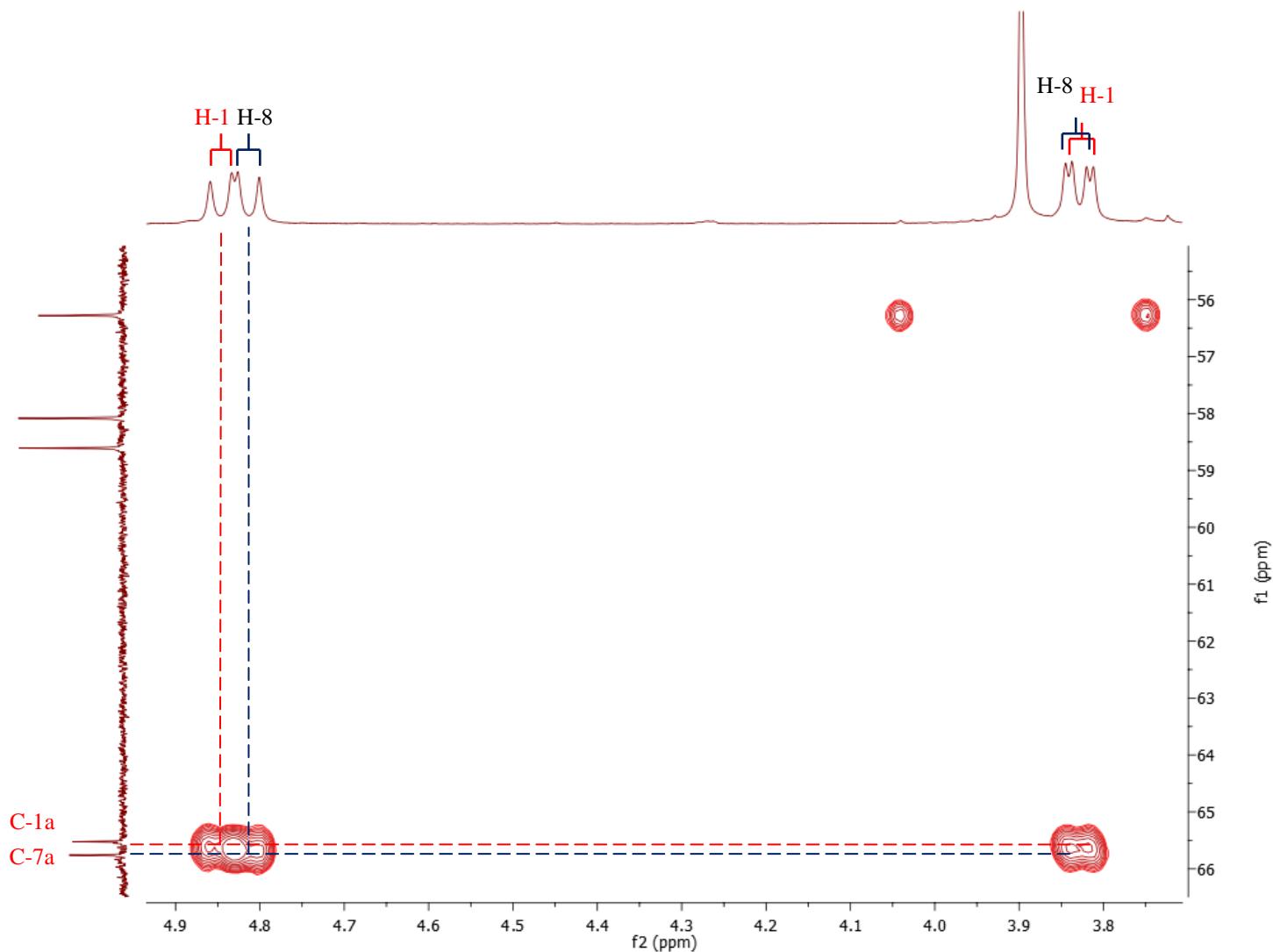
S9: Expansion of the HMBC spectrum of compound **1** (epoxyquinophomopsin)



S10: Expansion of the HMBC spectrum of compound **1** (epoxyquinophomopsin)



S11: Expansion of the HMBC spectrum of Compound 1 (epoxyquinophomopsin)



S12: Expansion of the **HMBC** spectrum of compound **1** (epoxyquinophomopsin)