

5,9,11-Trihydroxy-10-(2''-hydroxy-3''-methylbut-3''-en-1-yl)-2,2-dimethyl-3-(2'-methylbut-3'-en-2'-yl)-2H,12H-pyrano[2,3-a] xanthen-12-one from *Calophyllum pseudomole*

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Abstract: A new pyranocoumarin namely 5,9,11-trihydroxy-10-(2''-hydroxy-3''-methylbut-3''-en-1-yl)-2,2-dimethyl-3-(2'-methylbut-3'-en-2'-yl)-2H,12H-pyrano[2,3-a] xanthen-12-one (**1**) was isolated from the stem bark of *Calophyllum pseudomole*. The structure of compound **1** was elucidated based on their UV, IR, HRESIMS, 1D and 2D NMR spectral data.

Keywords: 5,9,11-Trihydroxy-10-(2''-hydroxy-3''-methylbut-3''-en-1-yl)-2,2-dimethyl-3-(2'-methylbut-3'-en-2'-yl)-2H,12H-pyrano[2,3-a] xanthen-12-one, *Calophyllum pseudomole*, Pyranoxanthone.

Monoisotopic Mass, Even Electron Ions

115 formula(e) evaluated with 4 results within limits (up to 25 closest results for each mass)

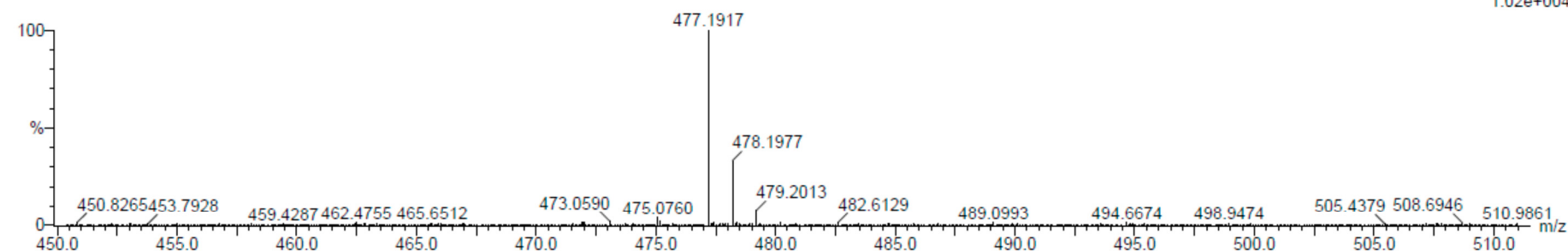
Elements Used:

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

standard

Ucok_Cal-2_477-1913_std_393-1338_neg 5 (0.074) Cm (5:6)

TOF MS ES-
1.02e+004



Minimum:

Maximum: 10.0 15.0 -1.5

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
477.1917	477.1913	0.4	0.8	14.5	369.5	0.1	C28 H29 O7

Figure S1. HRESIMS spectrum of 5,9,11-trihydroxy-10-(2''-hydroxy-3''-methylbut-3''-en-1-yl)-2,2-dimethyl-3-(2'-methylbut-3'-en-2'-yl)-2H,12H-pyrano[2,3-a] xanthen-12-one

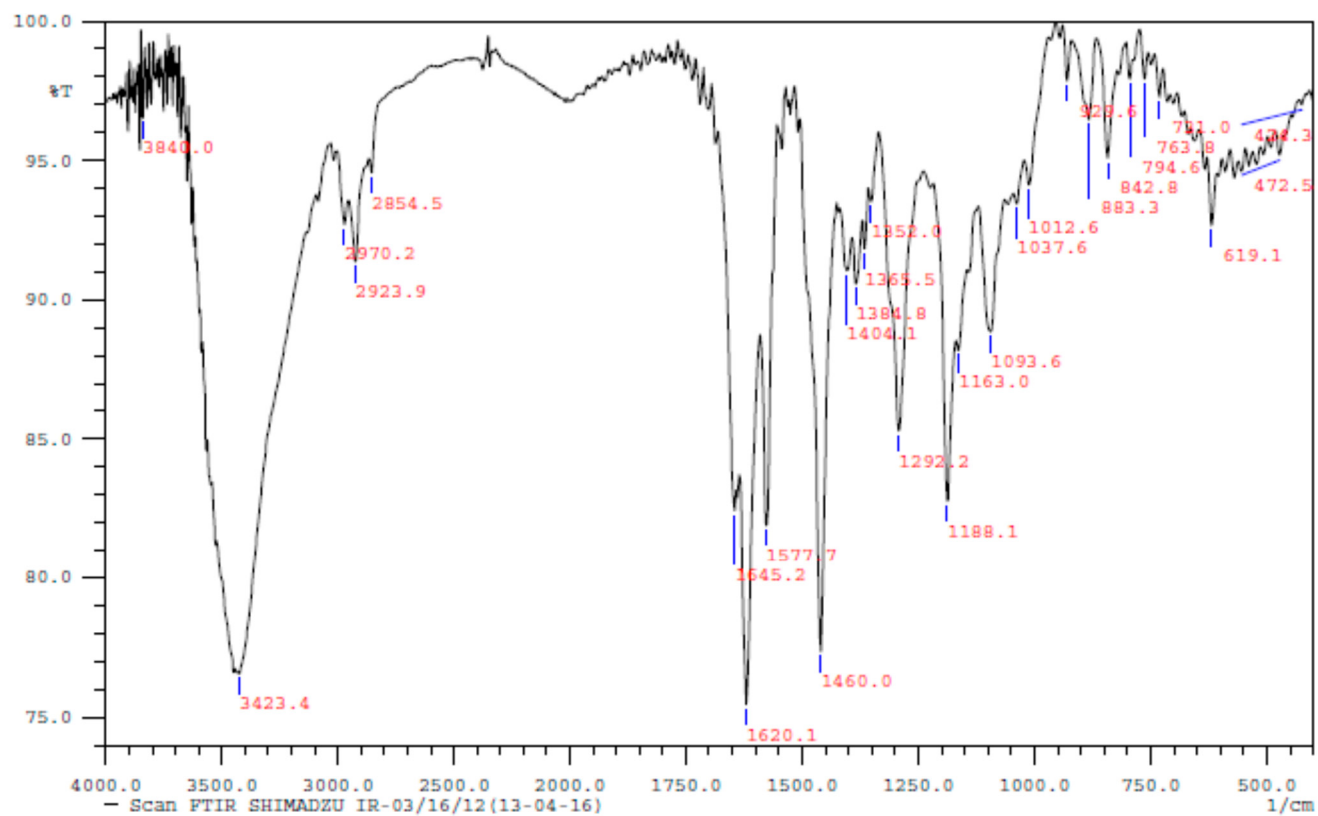


Figure S2. IR spectrum of 5,9,11-trihydroxy-10-(2''-hydroxy-3''-methylbut-3''-en-1-yl)-2,2-dimethyl-3-(2'-methylbut-3'-en-2'-yl)-2H,12H-pyrano[2,3-a] xanthen-12-one

CALT9-2-MULYADIT-23FEB2016
single_pulse

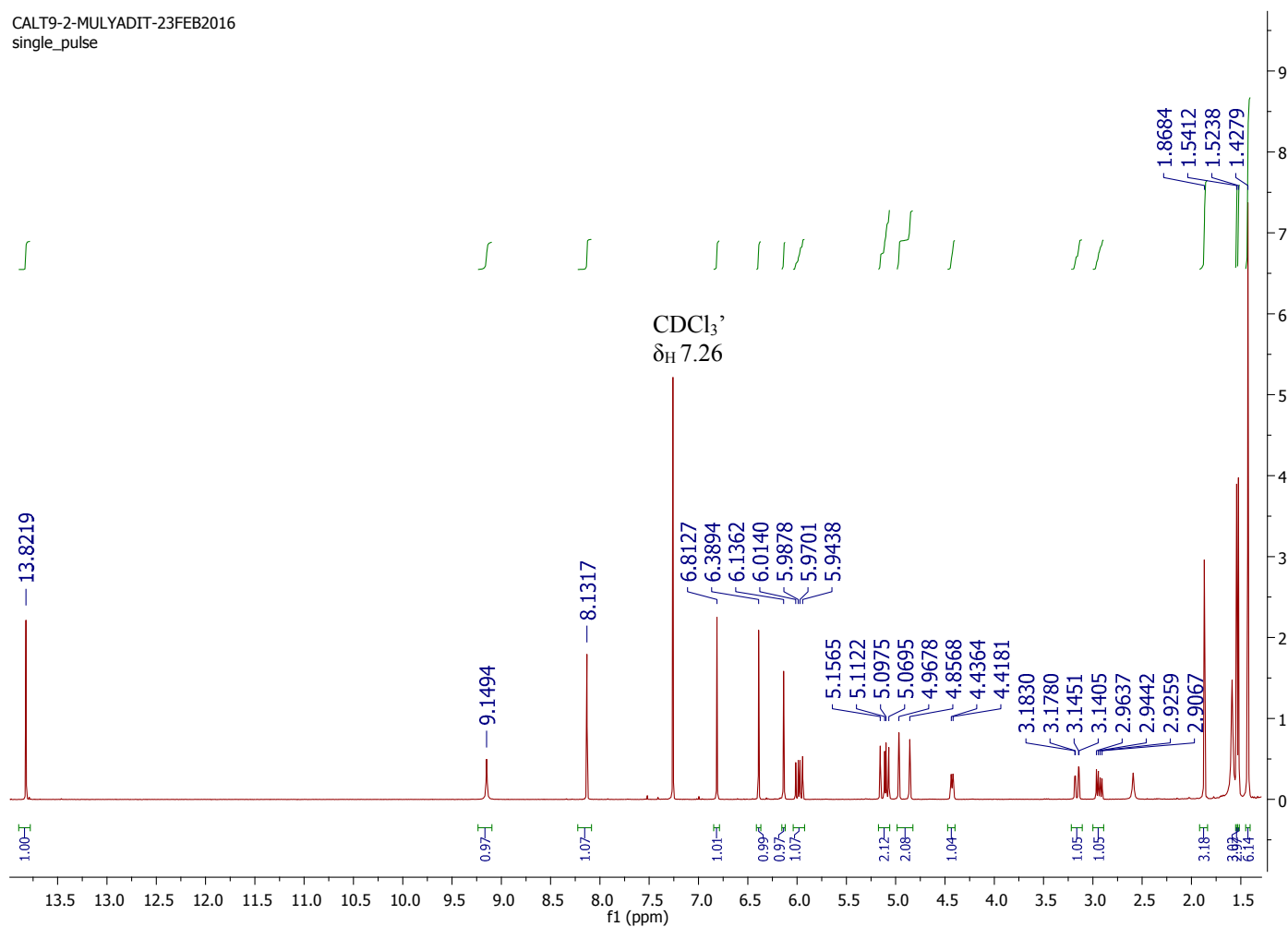


Figure S3. ^1H NMR spectrum of 5,9,11-trihydroxy-10-(2''-hydroxy-3''-methylbut-3''-en-1-yl)-2,2-dimethyl-3-(2'-methylbut-3'-en-2'-yl)-2H,12H-pyrano[2,3-a] xanthen-12-one

CALT9-2-MULYADIT-23FEB2016
APT Experiment

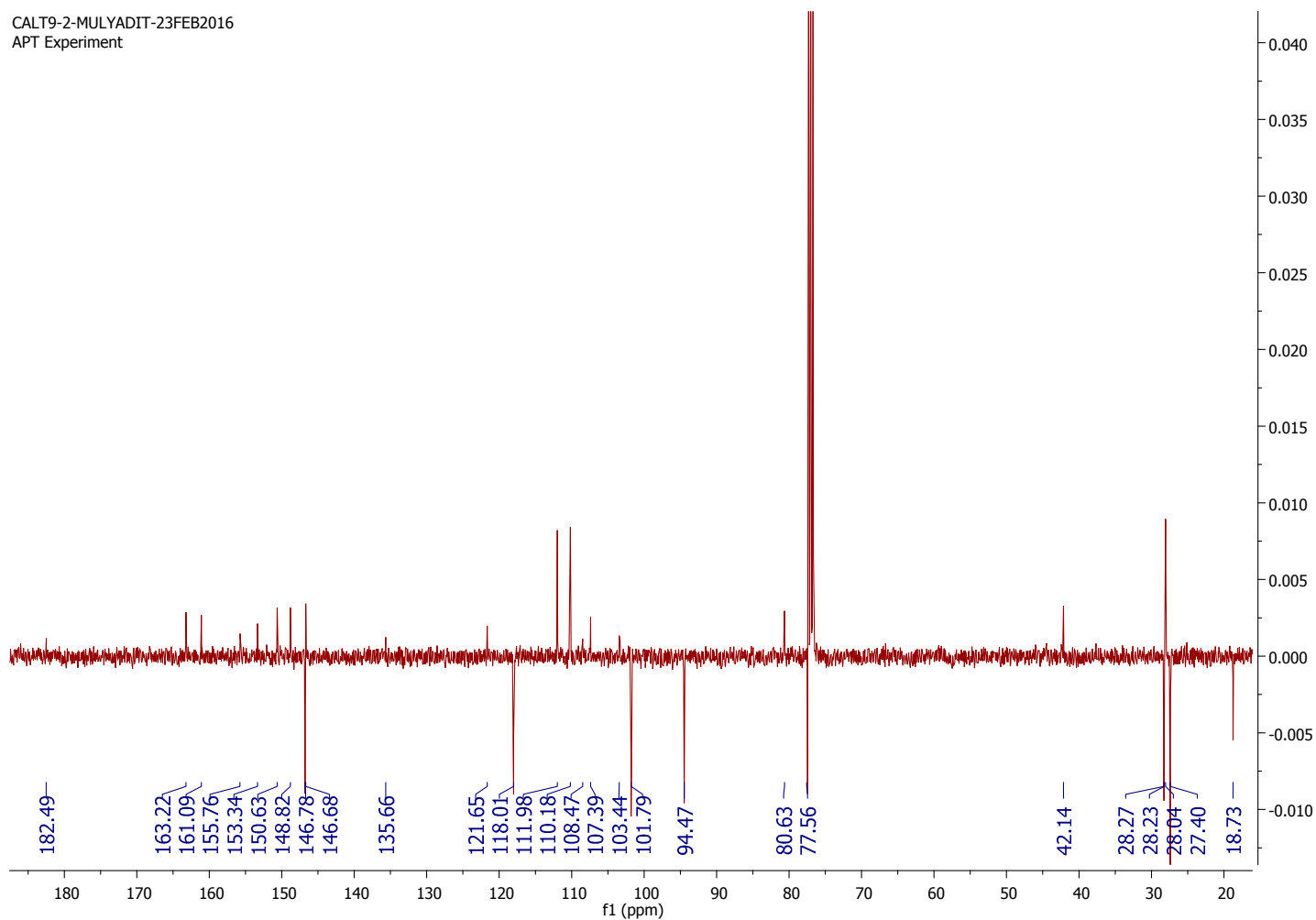


Figure S4. ^{13}C NMR (APT experiment) spectrum of 5,9,11-trihydroxy-10-(2''-hydroxy-3''-methylbut-3''-en-1-yl)-2,2-dimethyl-3-(2'-methylbut-3'-en-2'-yl)-2H,12H-pyrano[2,3-a] xanthen-12-one

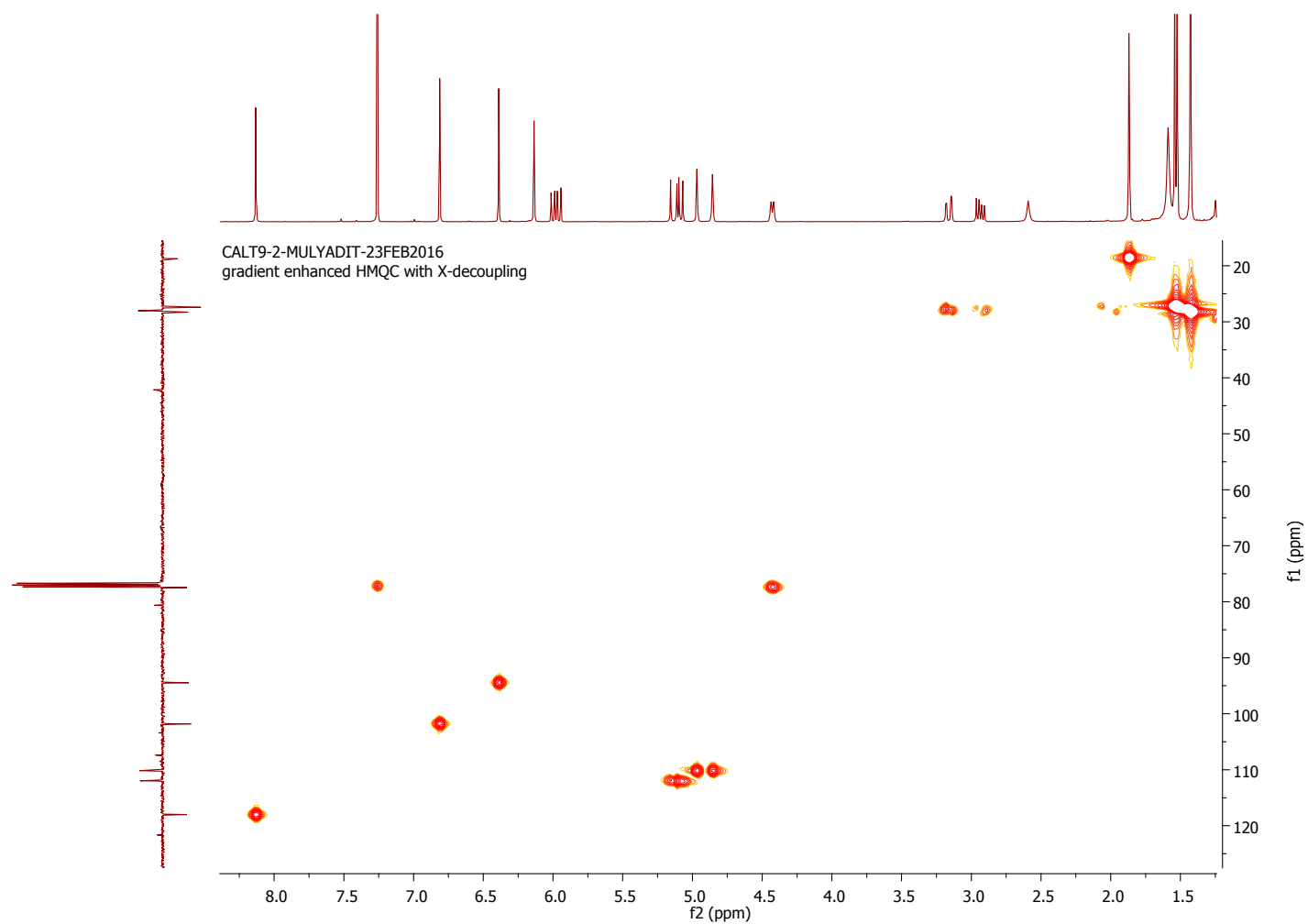


Figure S5. HMQC spectrum of 5,9,11-trihydroxy-10-(2''-hydroxy-3''-methylbut-3''-en-1-yl)-2,2-dimethyl-3-(2'-methylbut-3'-en-2'-yl)-2H,12H-pyrano[2,3-a] xanthen-12-one

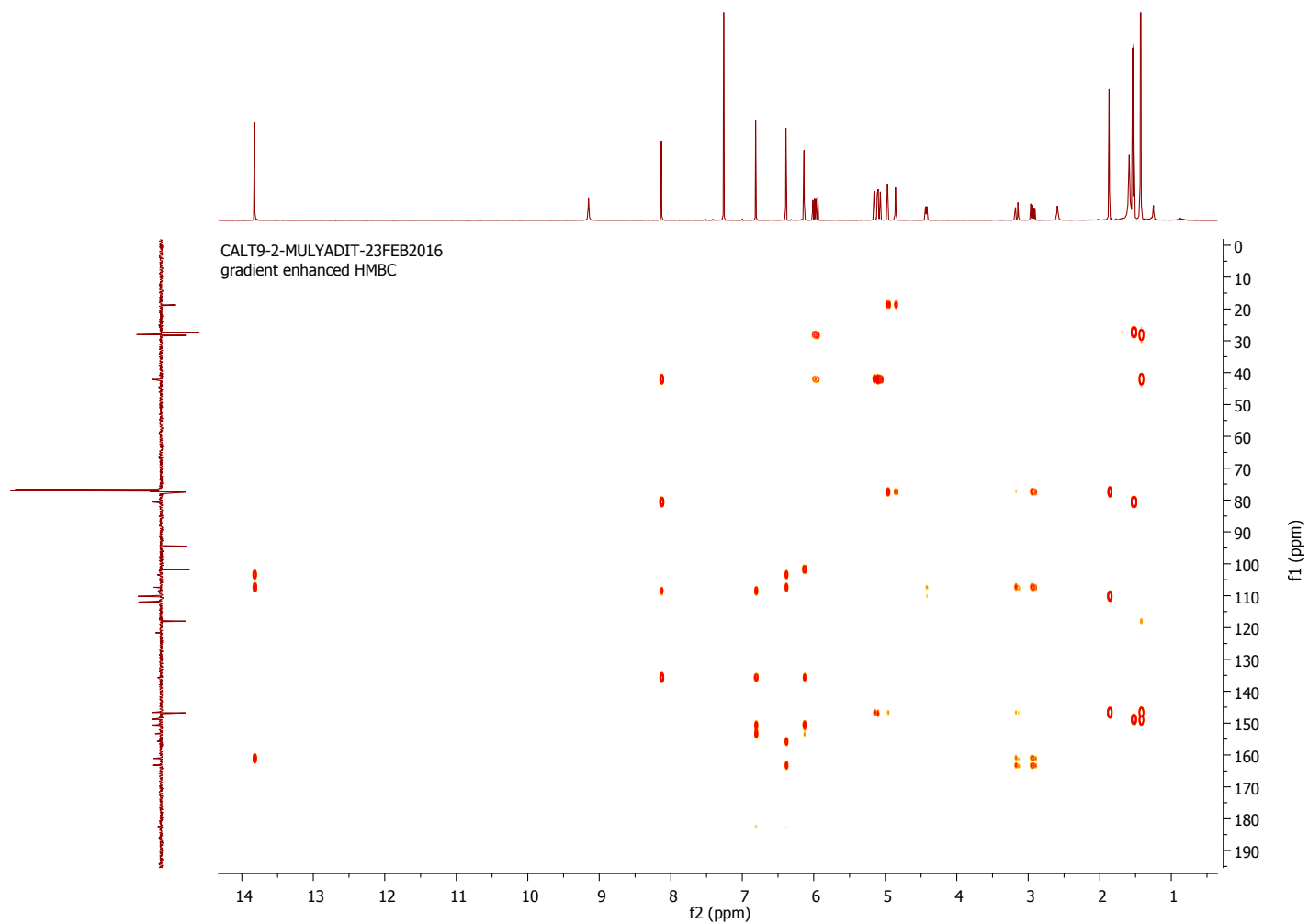


Figure S6. HMBC spectrum of 5,9,11-trihydroxy-10-(2''-hydroxy-3''-methylbut-3''-en-1-yl)-2,2-dimethyl-3-(2'-methylbut-3'-en-2'-yl)-2H,12H-pyrano[2,3-a] xanthen-12-one