

**5,9,11-Trihydroxy-2,2-dimethyl-3-(2-methylbut-3-en-2-yl)pyrano[2,3-a] xanthen-12(2H)-one from the stem bark of
Calophyllum tetrapterum Miq.**

Tjitjik Srie Tjahjandarie^{1,2*}, Ratih Dewi Saputri¹, Mulyadi Tanjung¹

¹Natural Products Chemistry Research Group, Organic Chemistry Division, Department of Chemistry, Faculty of Science and Technology, Universitas Airlangga, Surabaya 60115, Indonesia

²Airlangga Health Science Institute, Universitas Airlangga, Surabaya 60115, Indonesia

Abstract: A new pyranocoumarin namely 5,9,11-trihydroxy-2,2-dimethyl-3-(2-methylbut-3-en-2-yl)pyrano[2,3-a]xanthen-12(2H)-one (**1**) was isolated from the stem bark of *Calophyllum tetrapterum* Miq. The structure of compound **1** was determined by means of spectroscopic methods including UV, IR, HRESIMS, 1D and 2D NMR spectrometry experiments.

Keywords: *Calophyllum tetrapterum* Miq., Pyranoxanthone, 5,9,11-trihydroxy-2,2-dimethyl-3-(2-methylbut-3-en-2-yl) pyrano[2,3-a]xanthen-12(2H)-one.

*Corresponding author. E-mail: tjitjiktjahjandarie@fst.unair.ac.id; Tel.: +62-31-5936501; Fax: +62-31-5936502

CALT-F-MLT-17NOV2015
single_pulse

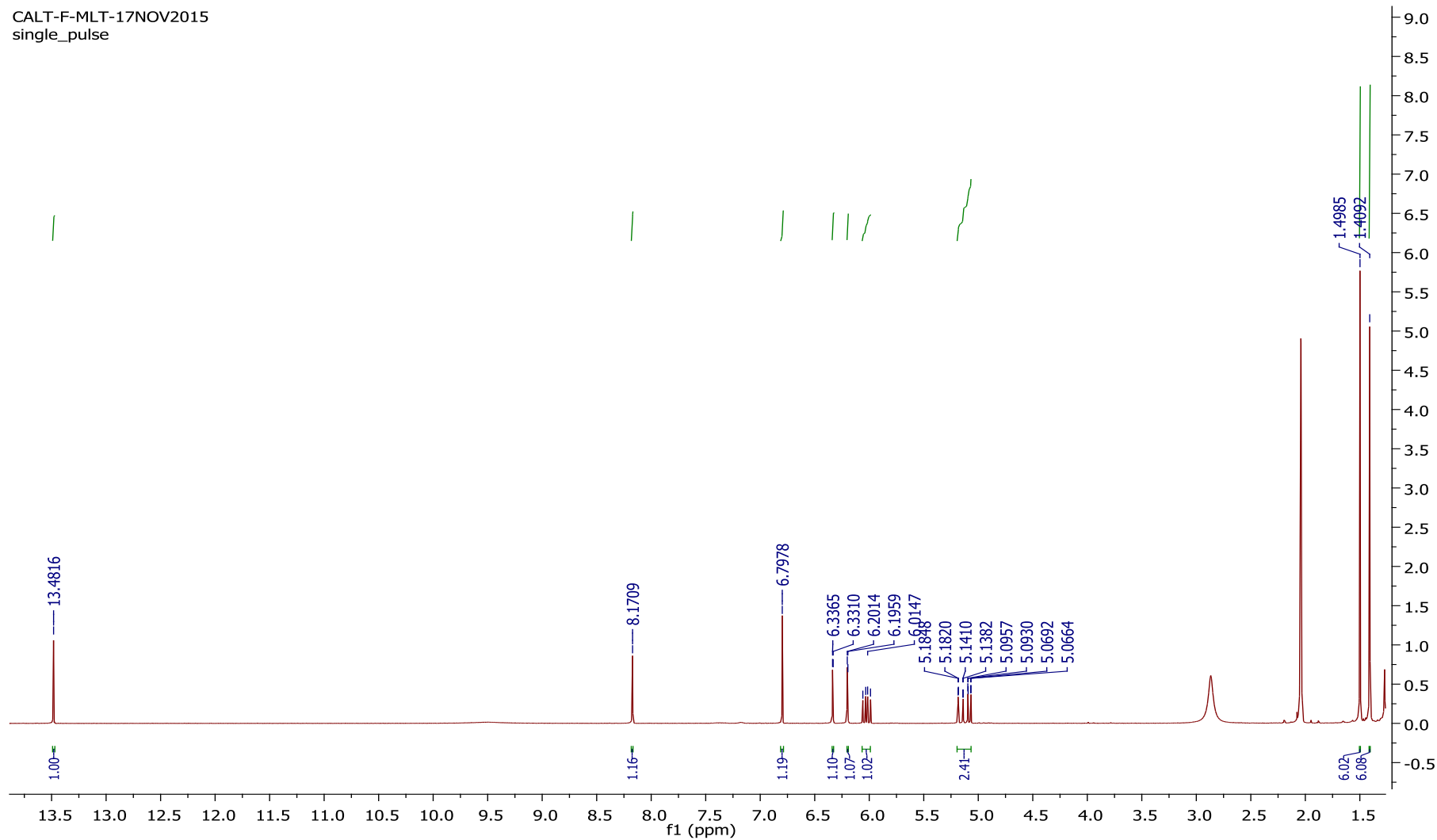


Figure S1. ^1H NMR spectra of 5,9,11-trihydroxy-2,2-dimethyl-3-(2-methylbut-3-en-2-yl)pyrano[2,3-a]xanthen-12(2H)-one

CALT-F-MLT-17NOV2015
single_pulse

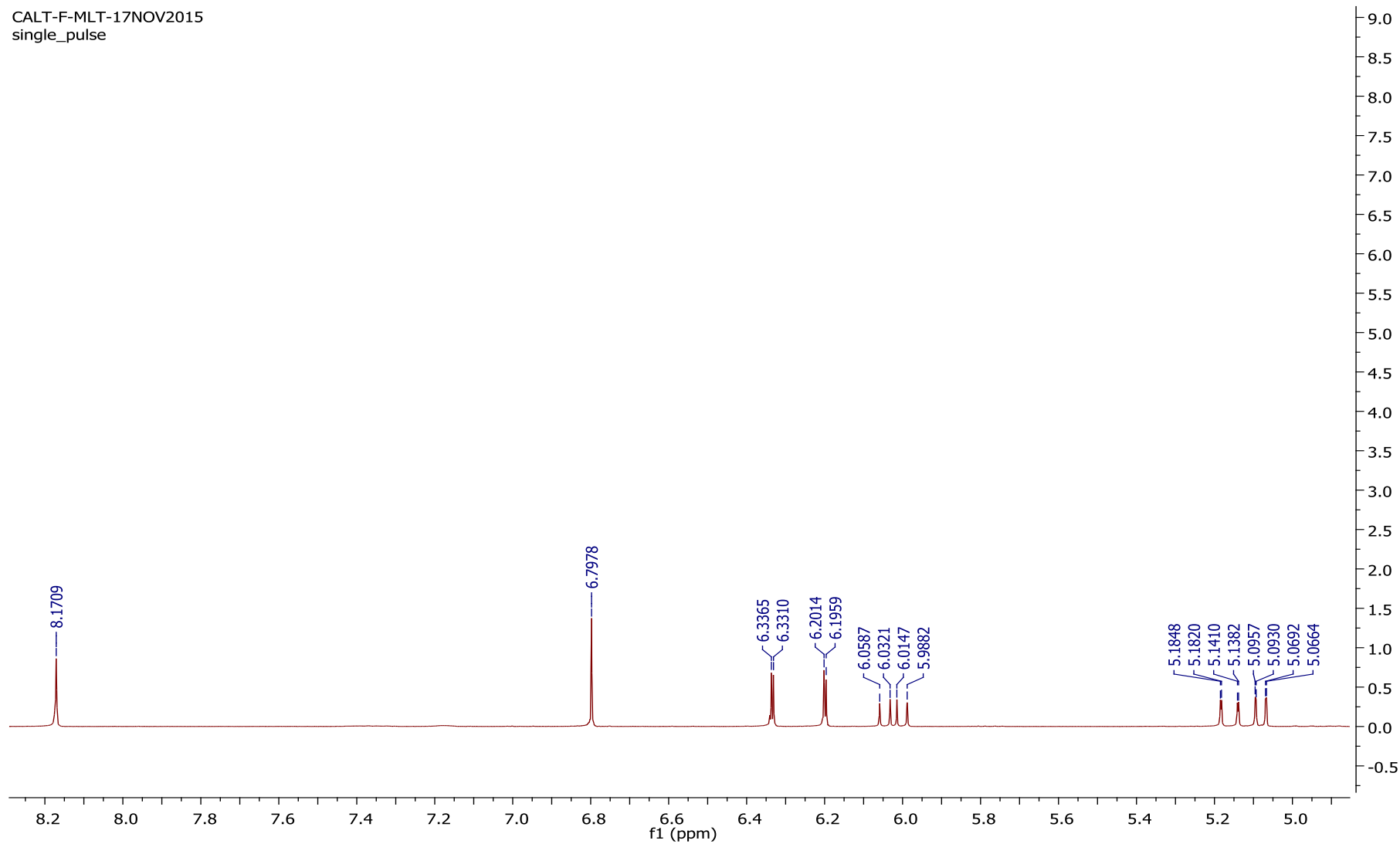


Figure S2. ¹H NMR spectra [δ H 5–7 ppm] of 5,9,11-trihydroxy-2,2-dimethyl-3-(2-methylbut-3-en-2-yl)pyrano[2,3-a]xanthen-12(2H)-one

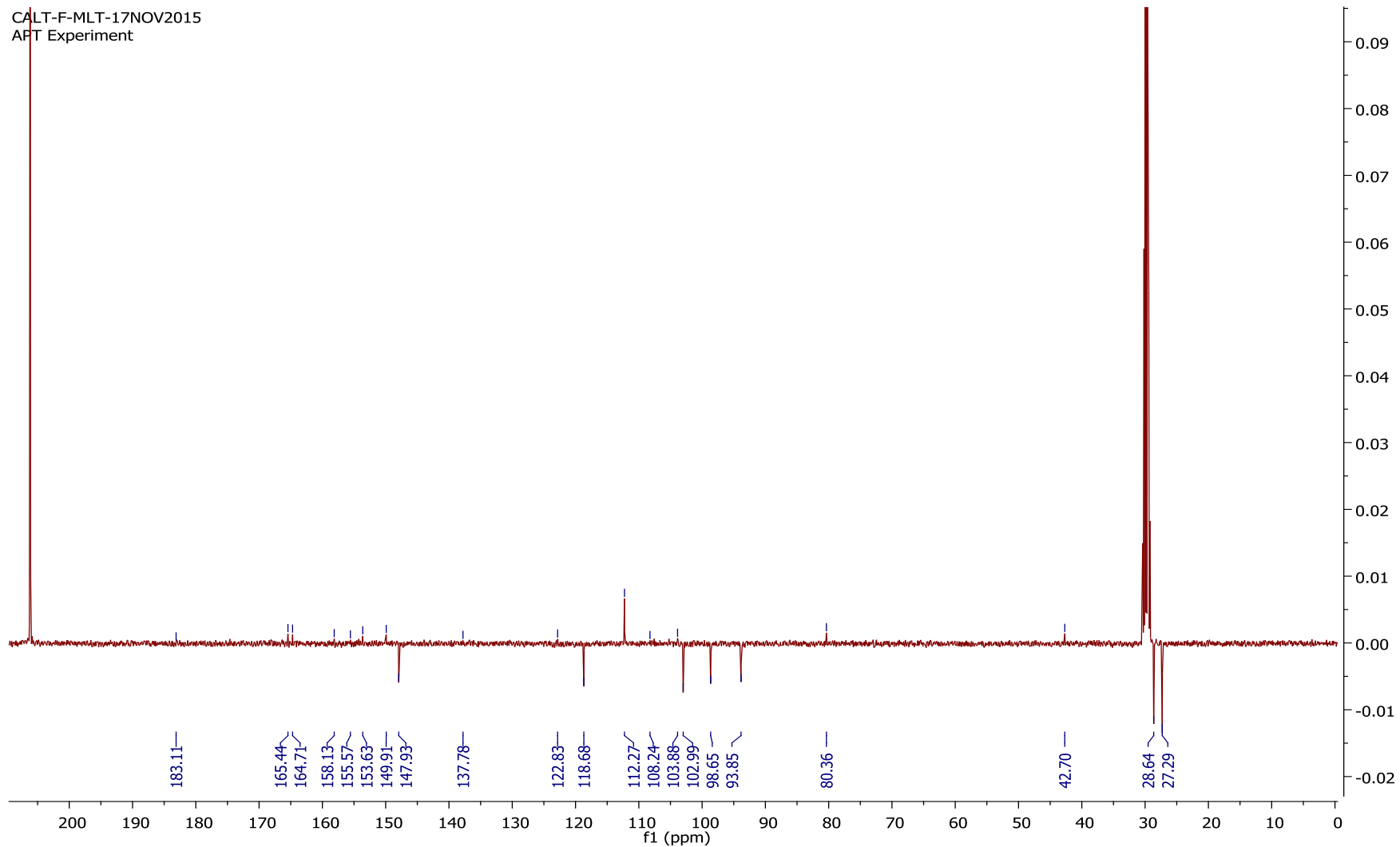


Figure S3. ^{13}C NMR spectra of 5,9,11-trihydroxy-2,2-dimethyl-3-(2-methylbut-3-en-2-yl)pyrano[2,3-a]xanthen-12(2H)-one

CALT-F-MLT-17NOV2015
APT Experiment

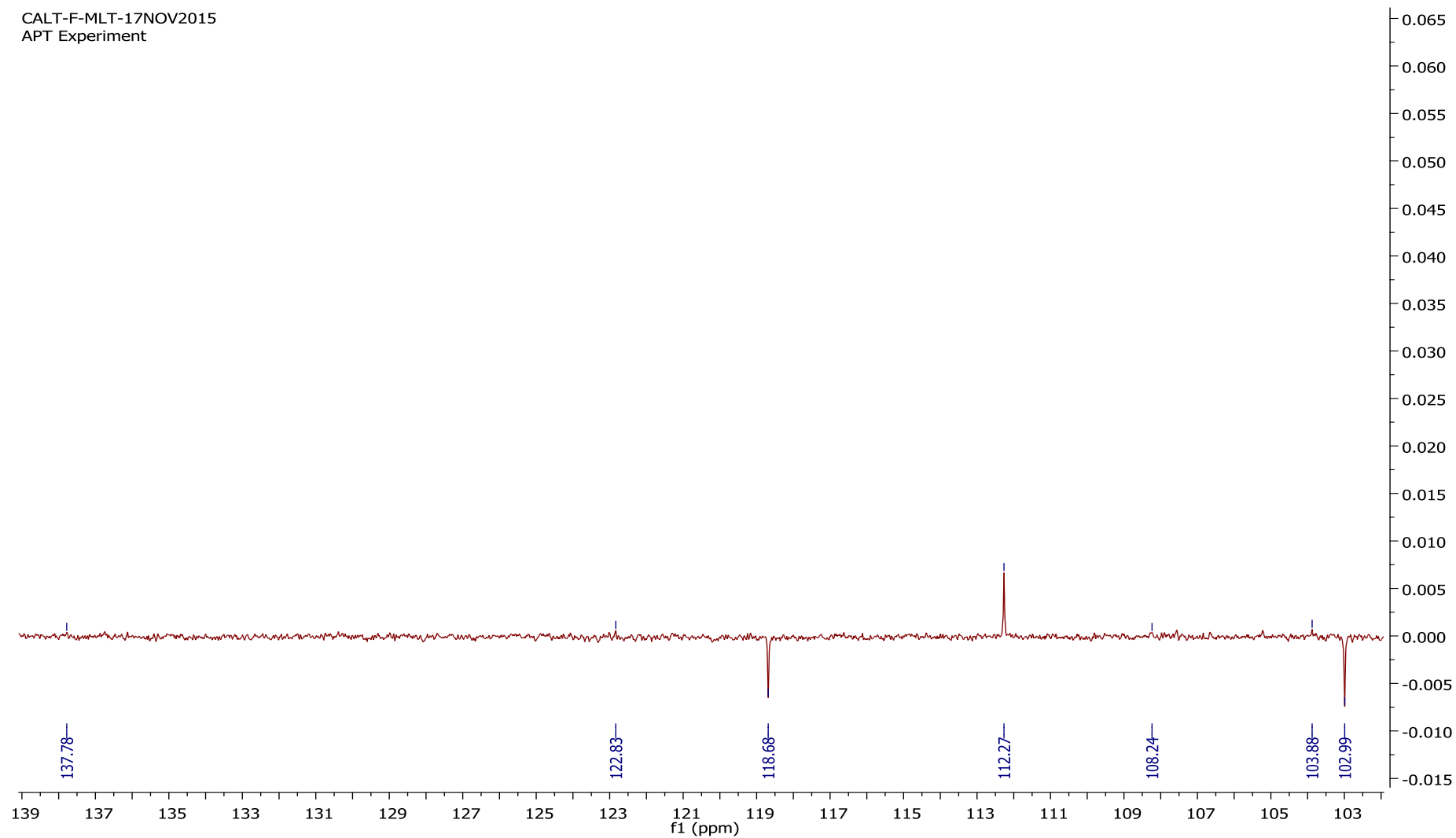


Figure S4. ¹³C NMR spectra [δ c 102–139 ppm] of 5,9,11-trihydroxy-2,2-dimethyl-3-(2-methylbut-3-en-2-yl)pyrano[2,3-a]xanthen-12(2H)-one

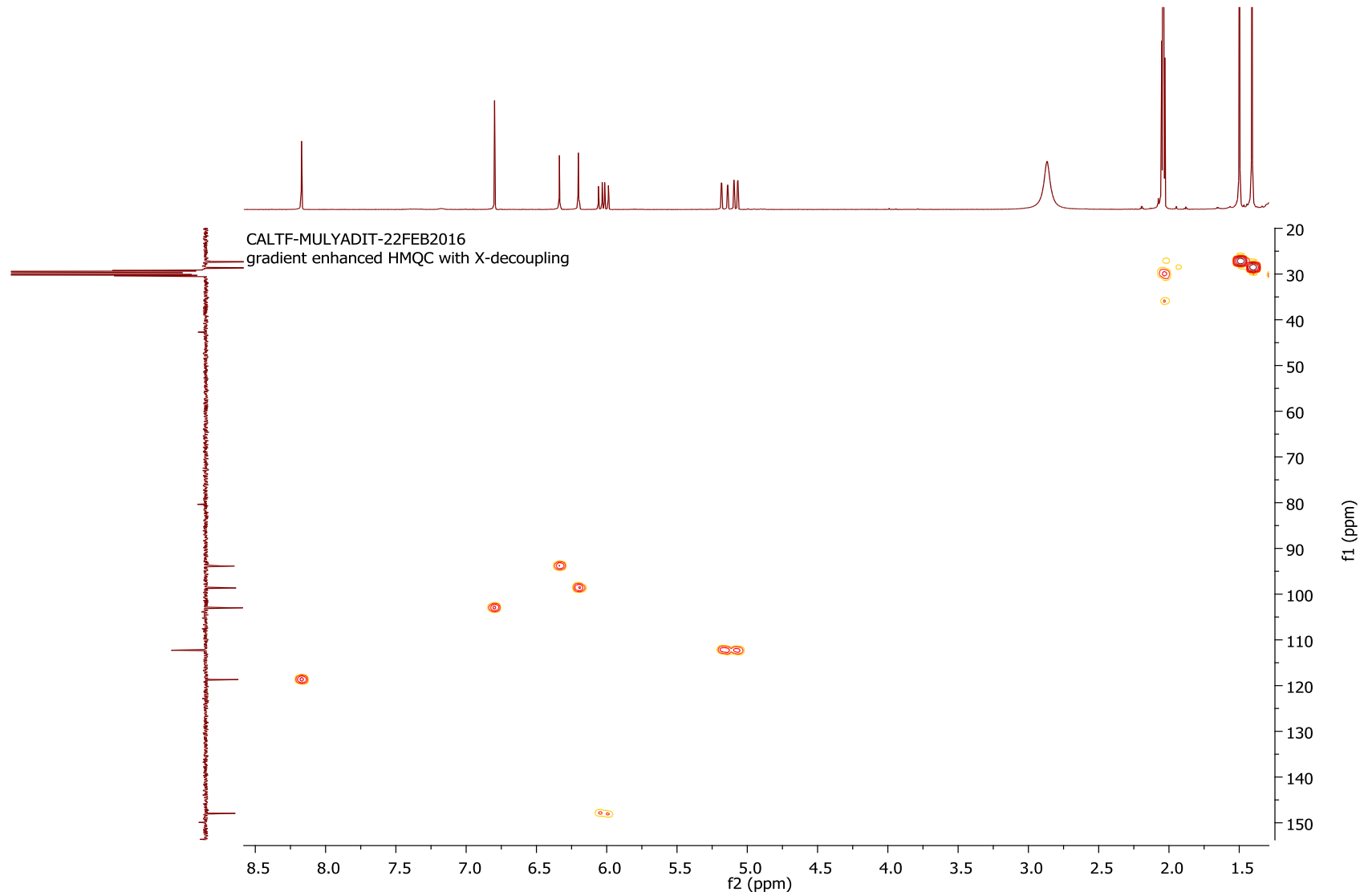


Figure S5. HMQC NMR spectra of 5,9,11-trihydroxy-2,2-dimethyl-3-(2-methylbut-3-en-2-yl)pyrano[2,3-a]xanthen-12(2H)-one

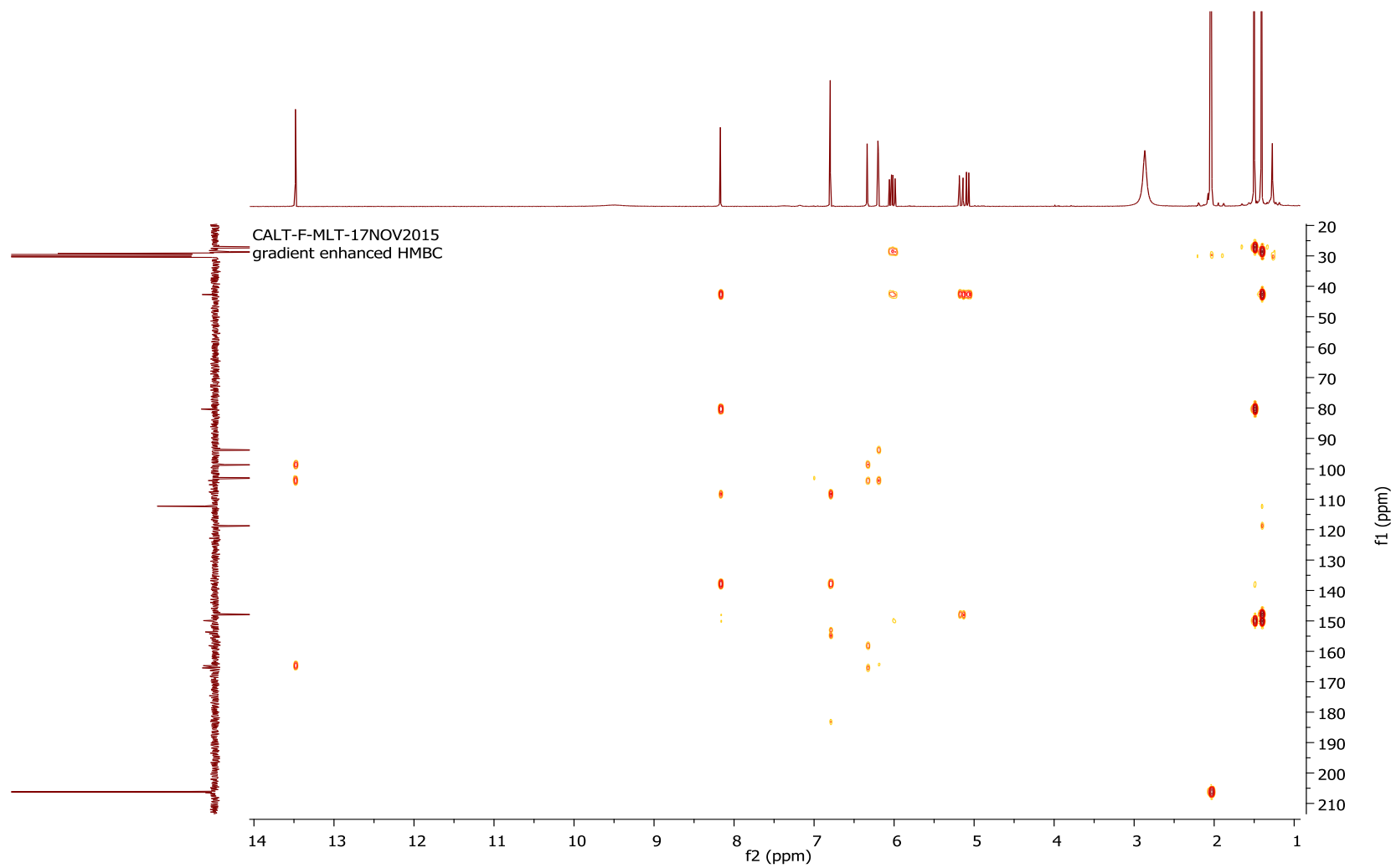


Figure S6. HMBC NMR spectra of 5,9,11-trihydroxy-2,2-dimethyl-3-(2-methylbut-3-en-2-yl)pyrano[2,3-a]xanthen-12(2H)-one

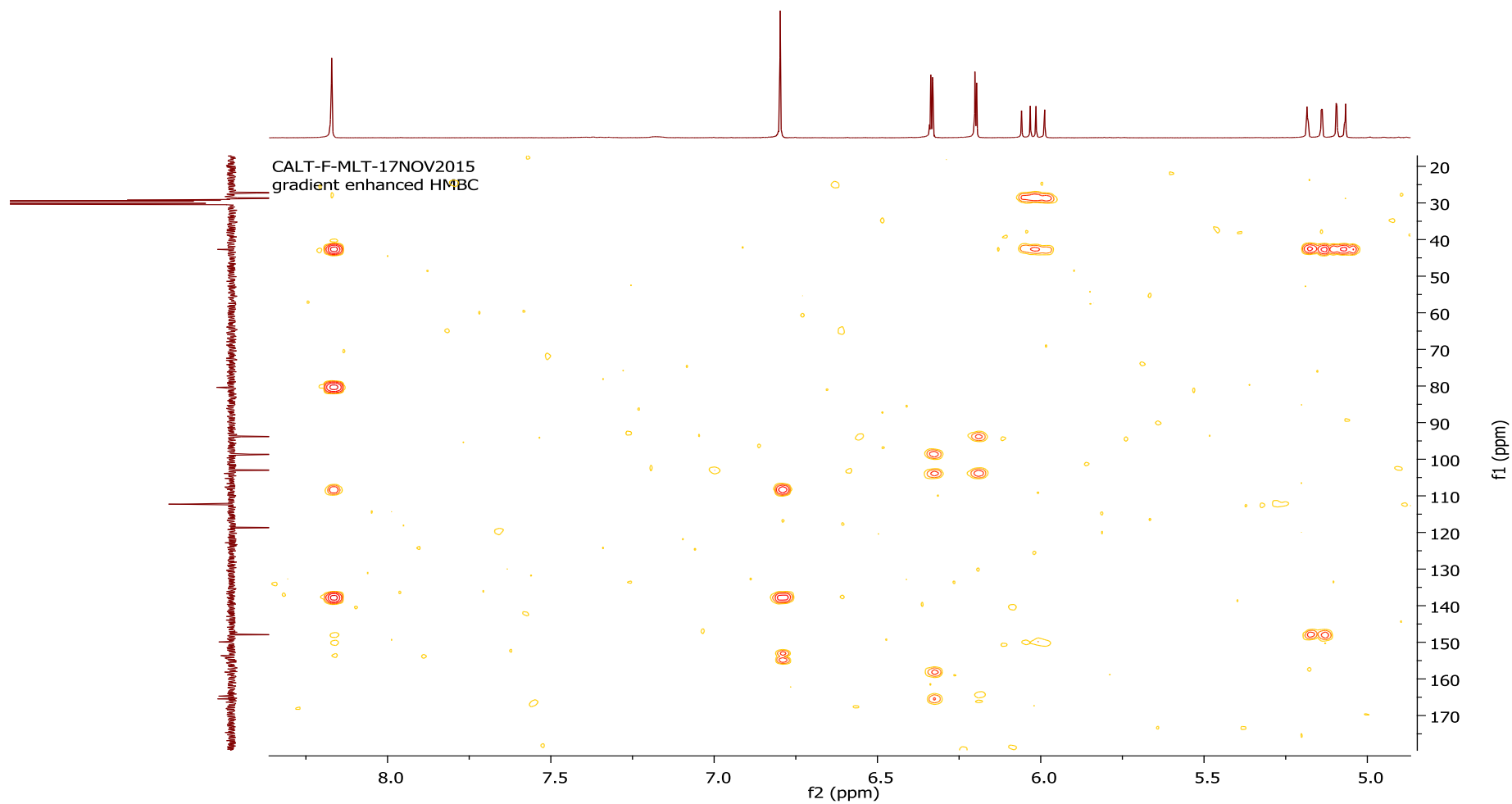


Figure S7. HMBC NMR spectra [δ_{H} 5–7 ppm] of 5,9,11-trihydroxy-2,2-dimethyl-3-(2-methylbut-3-en-2-yl)pyrano[2,3-a]xanthen-12(2H)-one

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

83 formula(e) evaluated with 3 results within limits (up to 25 closest results for each mass)

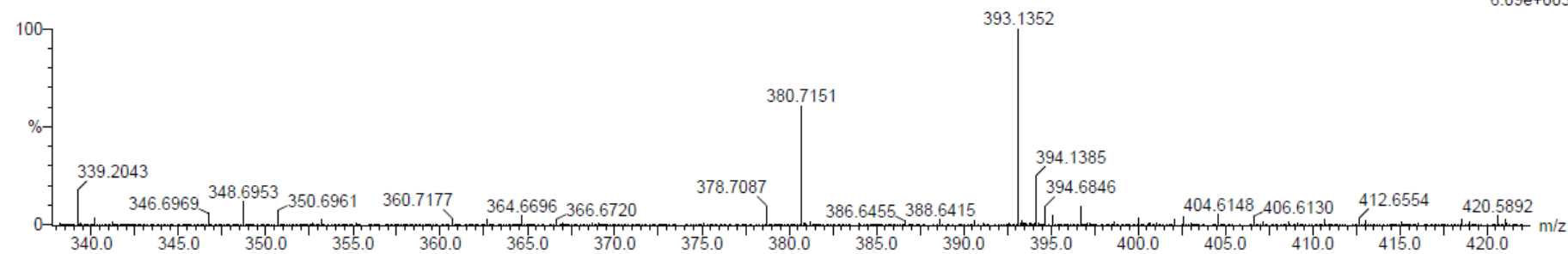
Elements Used:

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

standar

Ucok_CaltF_393-1338_neg 4 (0.055) Cm (4)

TOF MS ES-
6.09e+003



Minimum:

Maximum: 10.0 15.0 -1.5

Maximum: 10.0 15.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
393.1352	393.1338	1.4	3.6	13.5	293.7	0.0	C23 H21 O6

Figure S8. HRESIMS spectra of 5,9,11-trihydroxy-2,2-dimethyl-3-(2-methylbut-3-en-2-yl)pyrano[2,3-a]xanthen-12(2H)-one