4-Methoxy-3-(3-methylbut-2-en-1-yl)-7-[(3-methylbut-2-en-1-yl)oxy] quinolin-2(1H)-one from *Melicope moluccana* T.G. Hartley

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Abstract: 4-Methoxy-3-(3-methylbut-2-en-1-yl)-7-((3-methylbut-2-en-1-yl)oxy)quinolin-2(1H)-one (**1**) was isolated from the leaves of *Melicope moluccana* T.G. Hartley. The chemical structure of **1** was elucidated using mainly UV, IR, HRESIMS, 1D and 2D NMR spectroscopy.

Keywords:4-Methoxy-3-(3-methylbut-2-en-1-yl)-7-[(3-methylbut-2-en-1-yl)oxy]quinolin-2(1H)-one, 2-quinolone alkaloid, *Melicope moluccana*

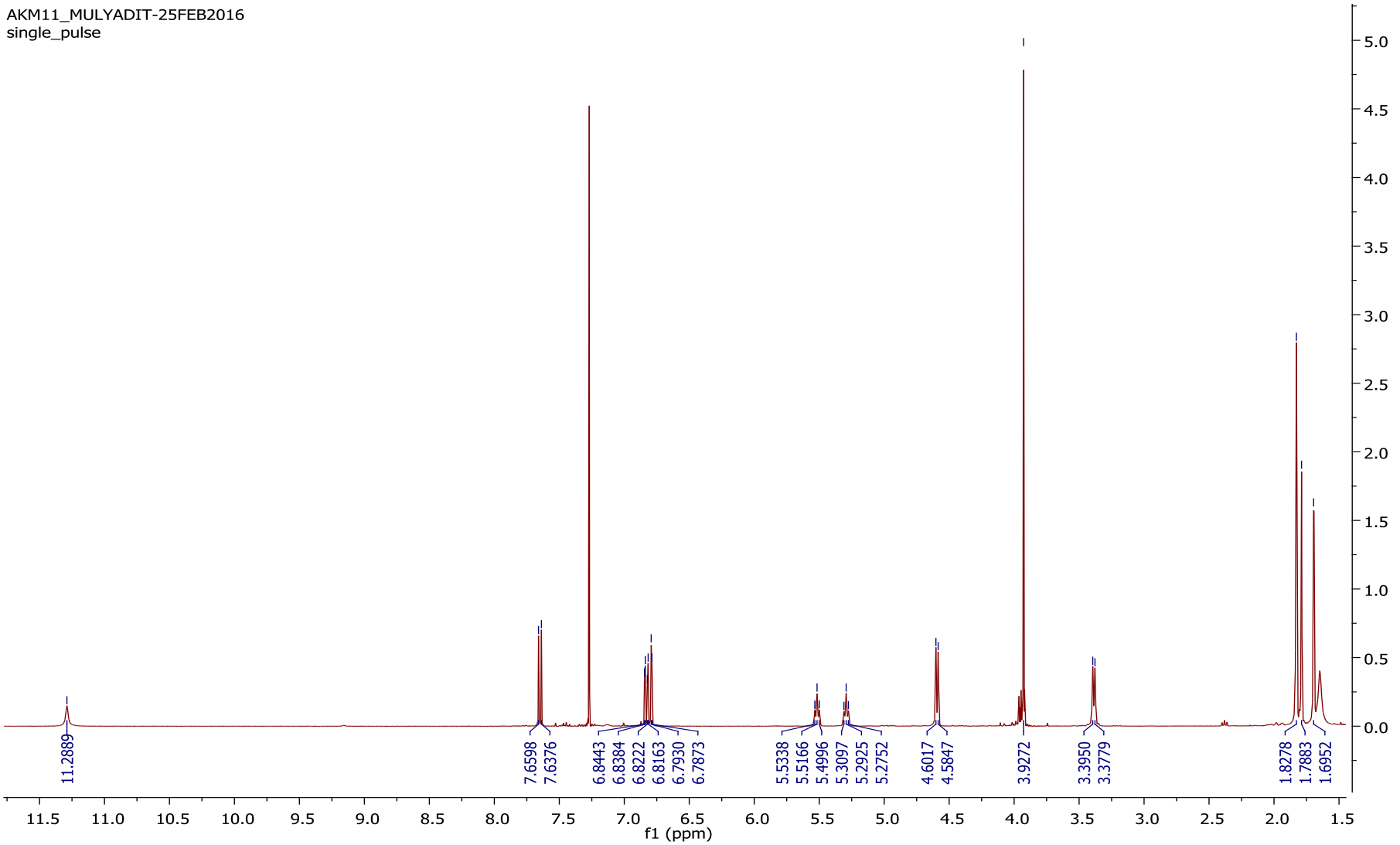


Figure S1. [1]H NMR spectra of 4-methoxy-3-(3-methylbut-2-en-1-yl)-7-[(3-methylbut-2-en-1-yl)oxy]quinolin-2(1H)-one

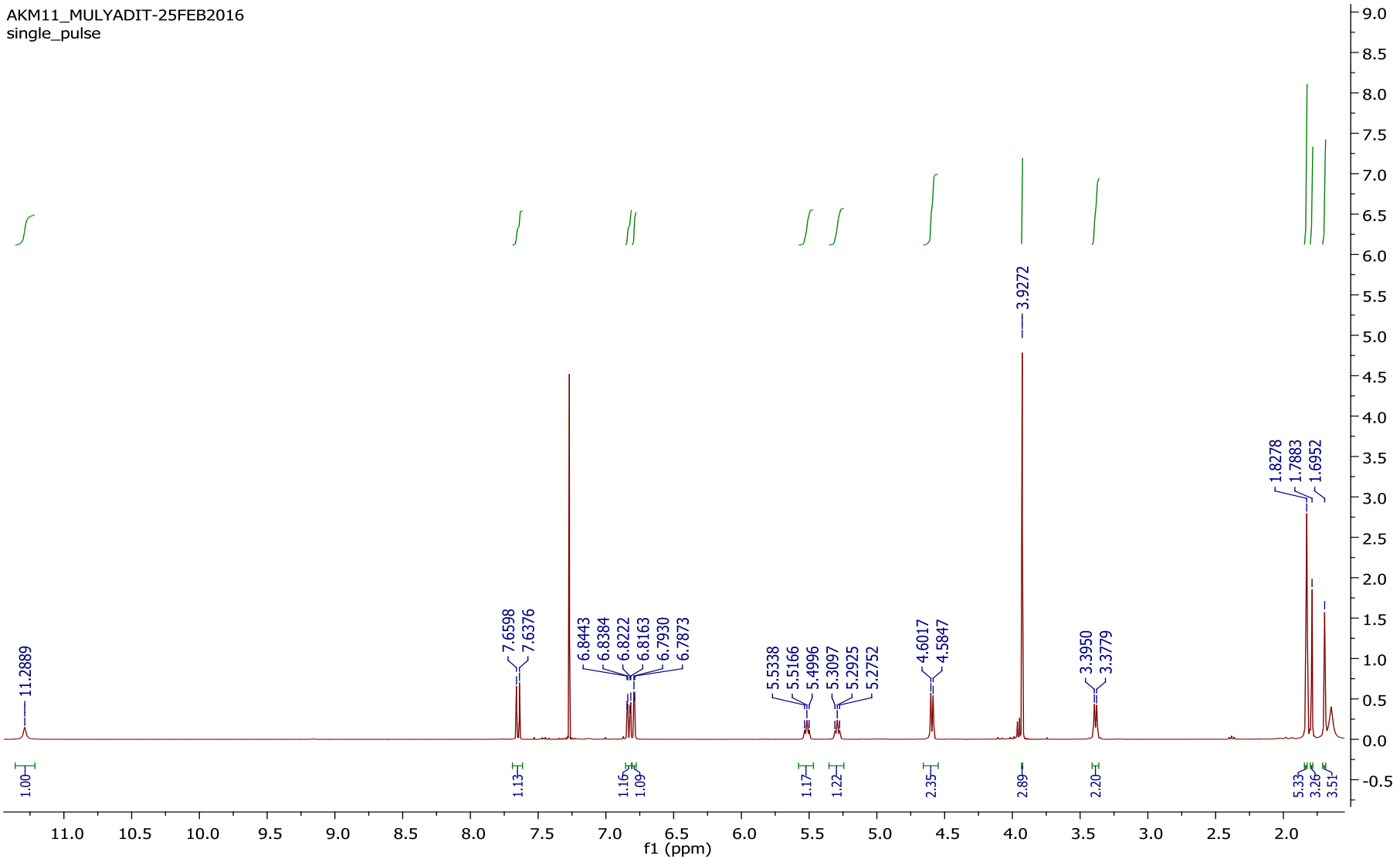


Figure S2. ^{1}H NMR spectra of 4-methoxy-3-(3-methylbut-2-en-1-yl)-7-[(3-methylbut-2-en-1-yl)oxy]quinolin-2(1H)-one

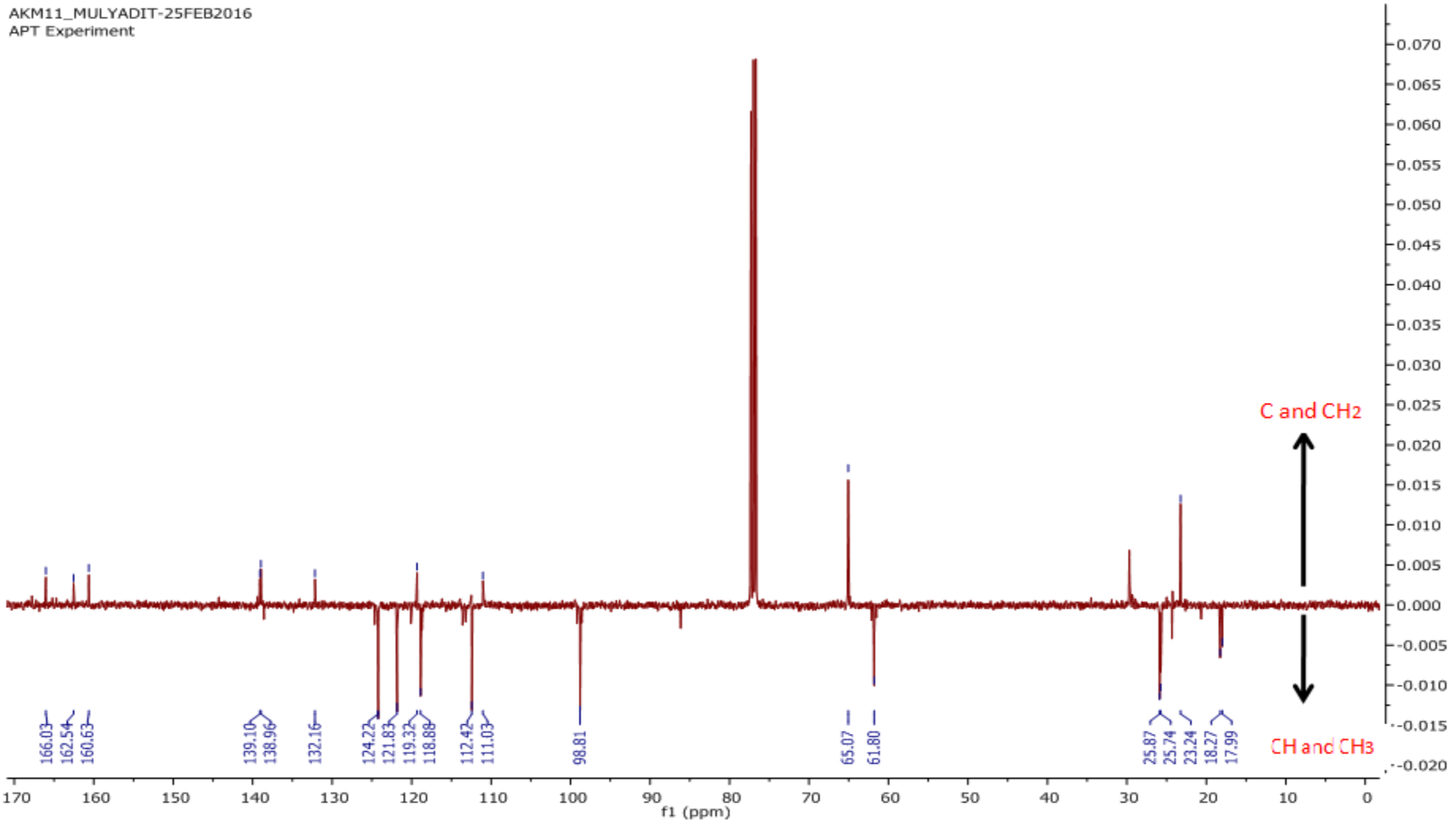


Figure S3. ^{13}C NMR spectra of 4-methoxy-3-(3-methylbut-2-en-1-yl)-7-[(3-methylbut-2-en-1-yl)oxy]quinolin-2(1H)-one

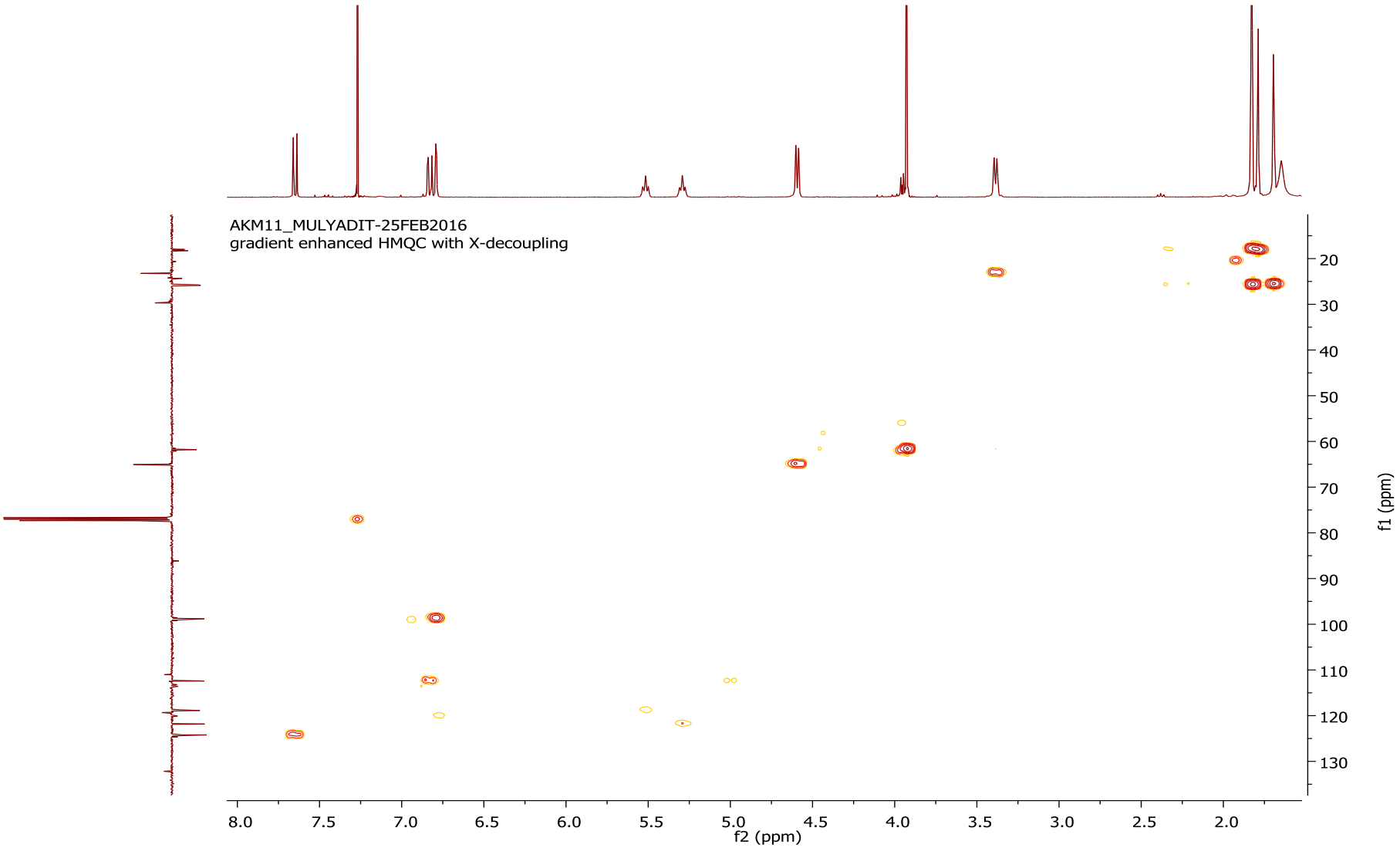


Figure S4. HMQC spectra of 4-methoxy-3-(3-methylbut-2-en-1-yl)-7-[(3-methylbut-2-en-1-yl)oxy]quinolin-2(1H)-one

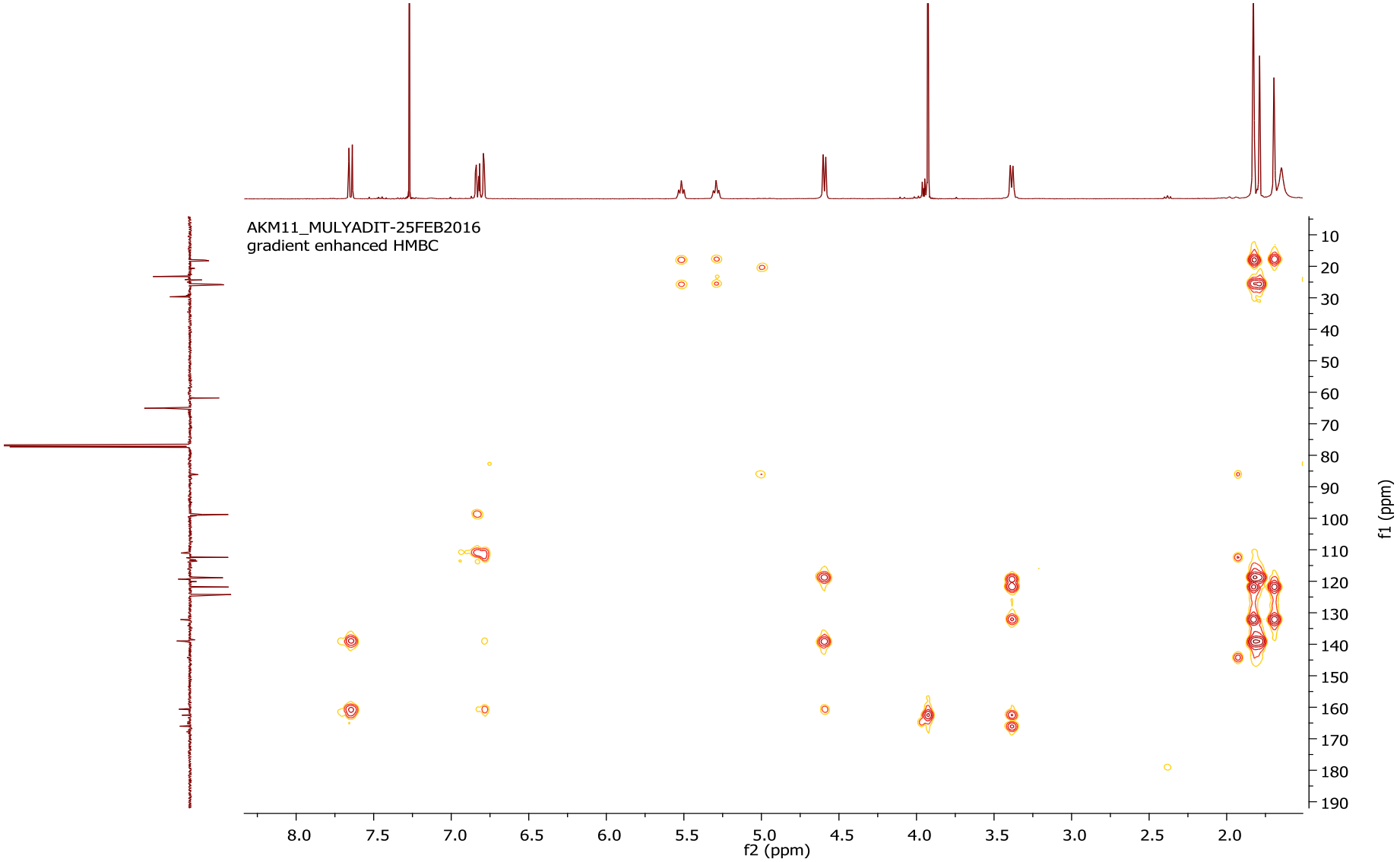
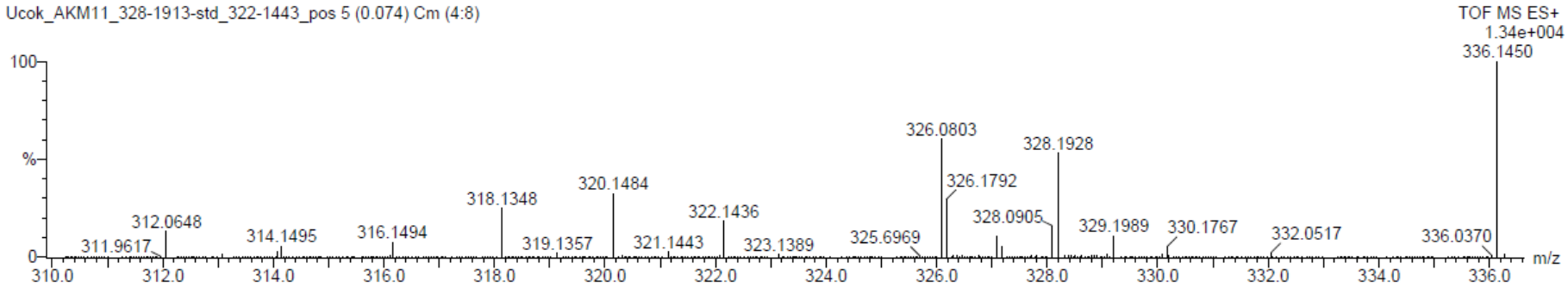


Figure S5. HMBC spectra of 4-methoxy-3-(3-methylbut-2-en-1-yl)-7-[(3-methylbut-2-en-1-yl)oxy]quinolin-2(1H)-one

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
734 formula(e) evaluated with 15 results within limits (up to 5 closest results for each mass)
Elements Used:
C: 0-1000 H: 0-1000 N: 0-500 O: 0-500
standar
Ucok_AKM11_328-1913-std_322-1443_pos 5 (0.074) Cm (4:8)



Minimum:				-1.5			
Maximum:		10.0	15.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
328.1928	328.1931	-0.3	-0.9	6.5	536.3	4.5	C6 H18 N17
	328.1918	1.0	3.0	1.5	537.2	5.5	C5 H22 N13 O4
	328.1913	1.5	4.6	8.5	532.3	0.6	C20 H26 N O3

Figure S6. HRESIMS spectra of 4-methoxy-3-(3-methylbut-2-en-1-yl)-7-[(3-methylbut-2-en-1-yl)oxy]quinolin-2(1H)-one

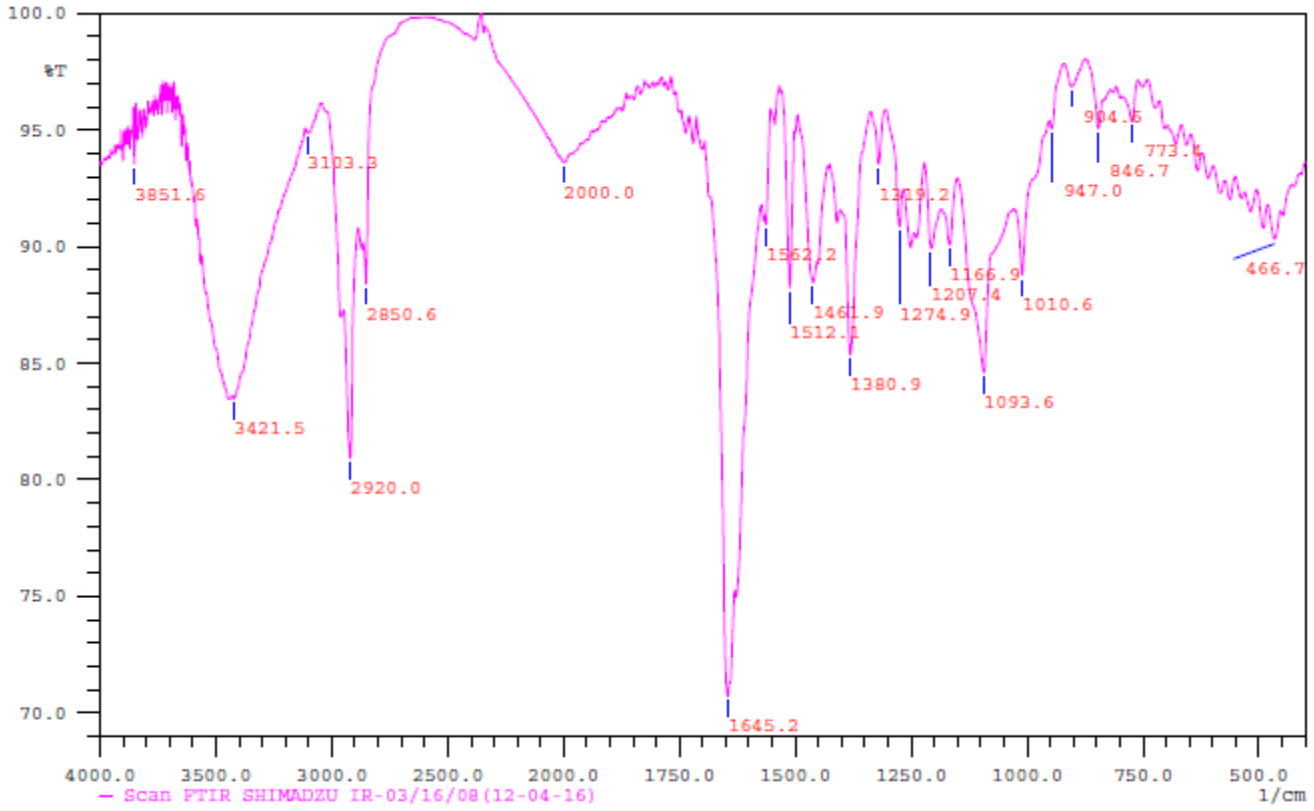


Figure S7. IR spectra of 4-methoxy-3-(3-methylbut-2-en-1-yl)-7-[(3-methylbut-2-en-1-yl)oxy]quinolin-2(1H)-one