

Supporting Information

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Phytotoxic and Antimicrobial Metabolites from *Paraphaeosphaeria* sp. QTYC11 Isolated from the Gut of *Pantala flavescens* Larvae

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Table of Contents	Page
S1: HRESI-MS Spectrum of Compound 1	2
S2: ¹ H NMR spectrum (600 MHz) of the compound in Acetone- <i>d</i> ₆	3
S3: ¹³ C NMR spectrum (150 MHz) of compound in Acetone- <i>d</i> ₆ .	4
S4: DEPT 135 spectrum (600 MHz) of compound in Acetone- <i>d</i> ₆ .	5
S5: ¹ H- ¹ H COSY spectrum (600 MHz) of compound in Acetone- <i>d</i> ₆ .	6
S6: HMQC spectrum (600 MHz) of compound in Acetone- <i>d</i> ₆	7
S7: HMBC spectrum (600 MHz) of compound in Acetone- <i>d</i> ₆ .	8

Mass Spectrum SmartFormula Report

Analysis Info

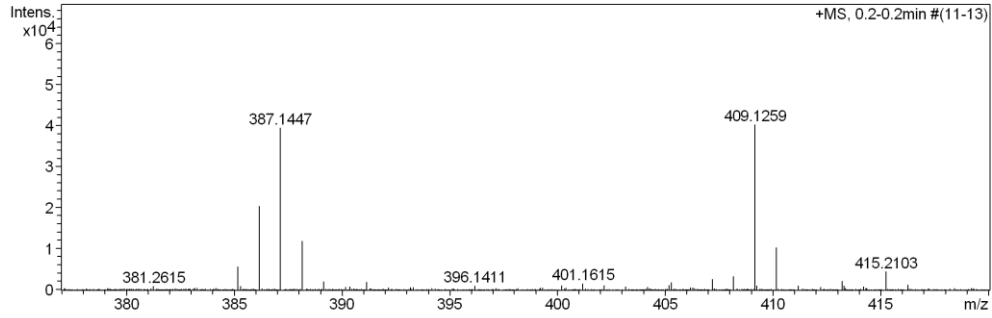
Analysis Name D:\Data\MS\data\201509\Q11-C28_pos_10_01_354.d
Method LC_Direct Infusion_pos_100-1000mz.m
Sample Name Q11-C28_pos
Comment

Acquisition Date 9/8/2015 1:16:04 AM

Operator SCSIO
Instrument / Ser# maXis 29

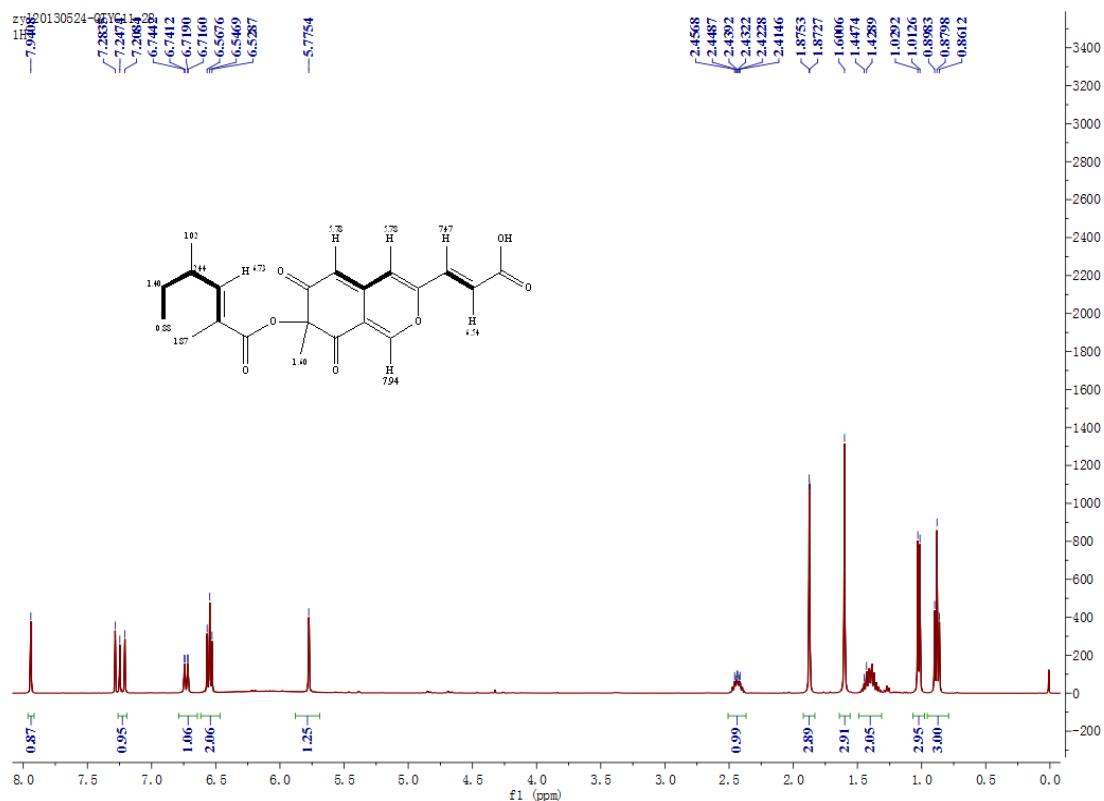
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Waste



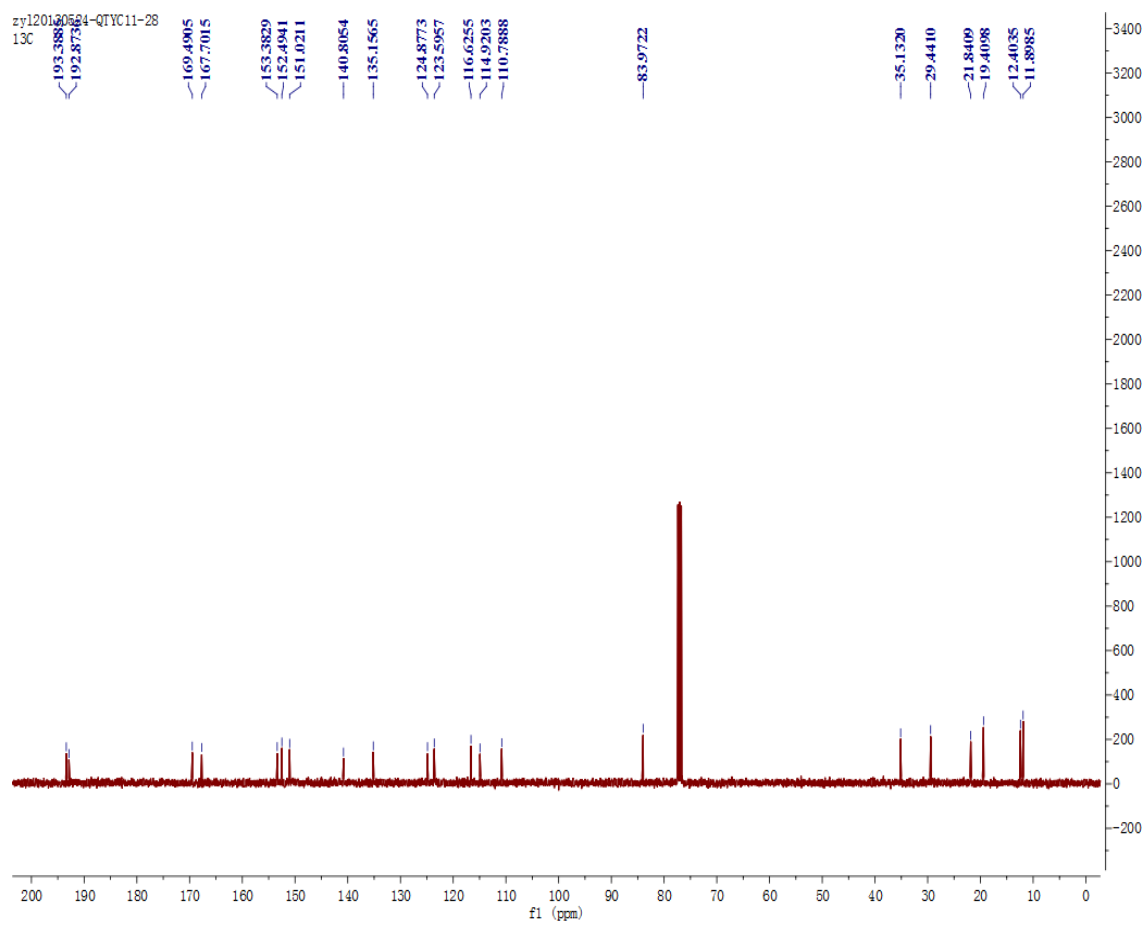
Meas. m/z	#	Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e ⁻ Conf	N-Rule
387.1447	1	C 21 H 23 O 7	56.77	387.1438	-2.2	-0.9	41.9	10.5	even	ok
409.1259	1	C 21 H 22 Na O 7	100.00	409.1258	-0.3	-0.1	27.5	10.5	even	ok

S1: HRESI-MS Spectrum of Compound 1

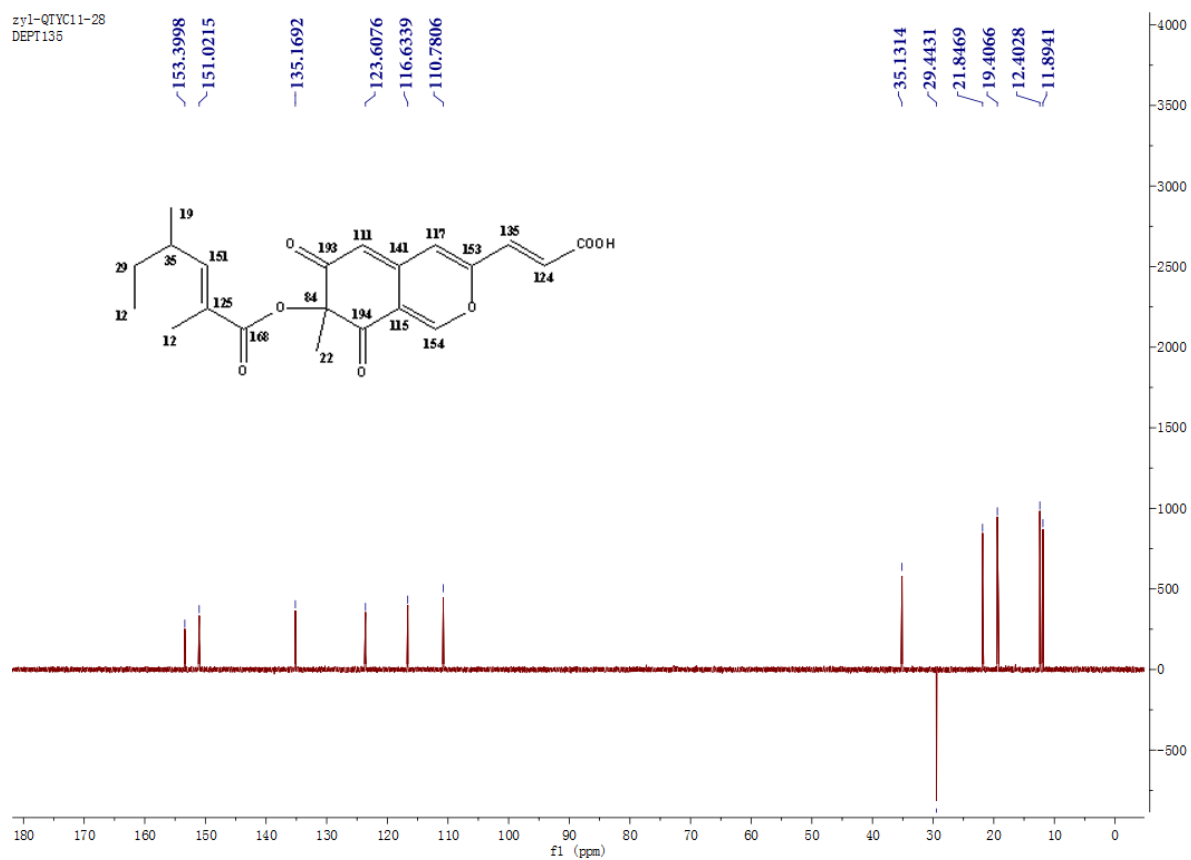


S2: ^1H NMR spectrum (600 MHz) of the compound in Acetone- d_6 .

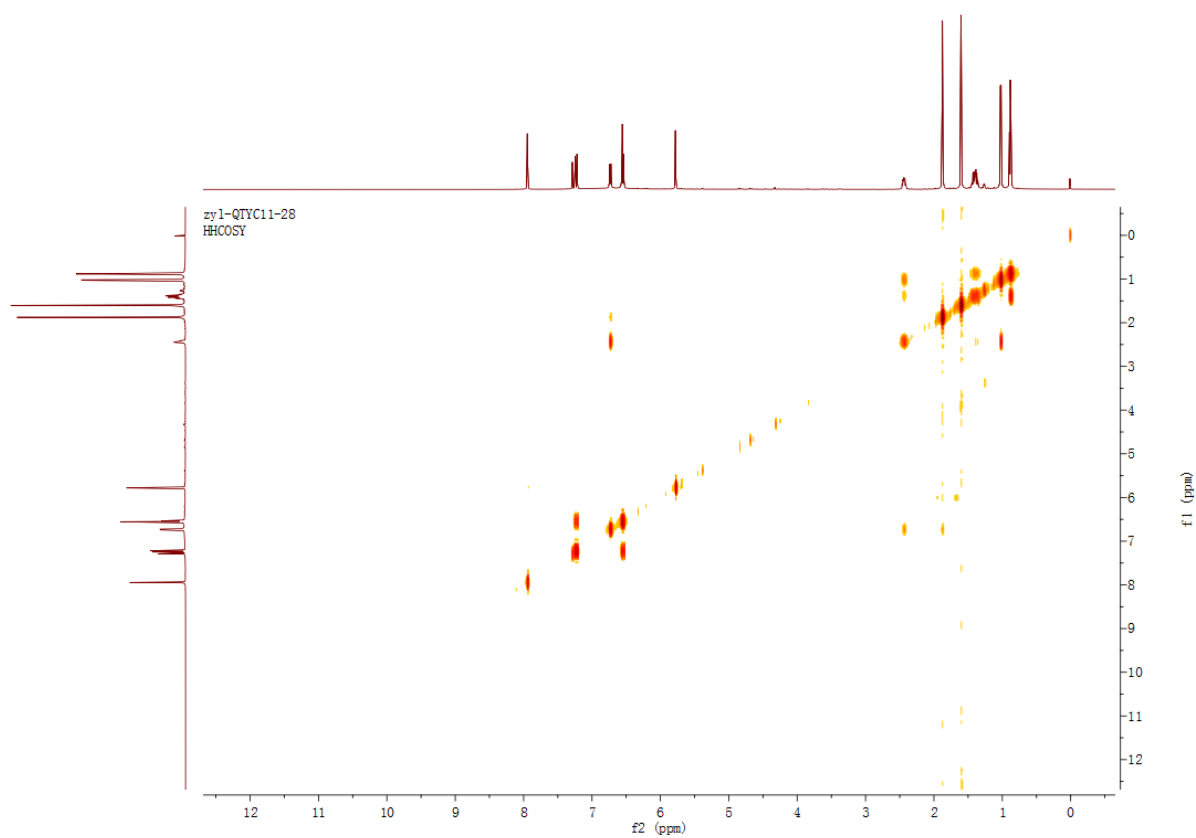
Lunatoic acid C (1): Yellow color needles; HR-ESI-MS: m/z 409 $[\text{M}+\text{H}]^+$, calculated for $\text{C}_{21}\text{H}_{22}\text{O}_7$, 386.1366, 795 $[\text{M}+\text{Na}]^+$; ^1H NMR (Acetone- d_6) δ : 0.88 (3H, t, H-6'), 1.02 (3H, d, H-8'), 1.40 (2H, m, H-5'), 1.60 (3H, s, H-14), 1.87 (3H, s, H-7'), 2.44 (1H, m, H-4'), 5.78 (1H, s, H-7), 6.54 (1H, d, H-12), 6.55 (1H, s, H-9), 6.73 (1H, d, H-3'), 7.23 (1H, d, H-11), 7.94 (1H, s, H-2). ^{13}C NMR (CHCl_3 - d) δ : 193.4 (C-4), 192.9 (C-6), 169.5 (C-13), 167.7 (C-1'), 153.4 (C-2), 152.5 (C-10), 151.0 (C-3'), 140.8 (C-8), 135.2 (C-11), 124.9 (C-2'), 123.6 (C-12), 116.6 (C-9), 114.9 (C-3), 110.8 (C-7), 84.0 (C-5), 35.1 (C-4'), 29.5 (C-5'), 21.8 (C-14), 19.4 (C-8'), 12.4 (C-7'), 11.9 (C-6').



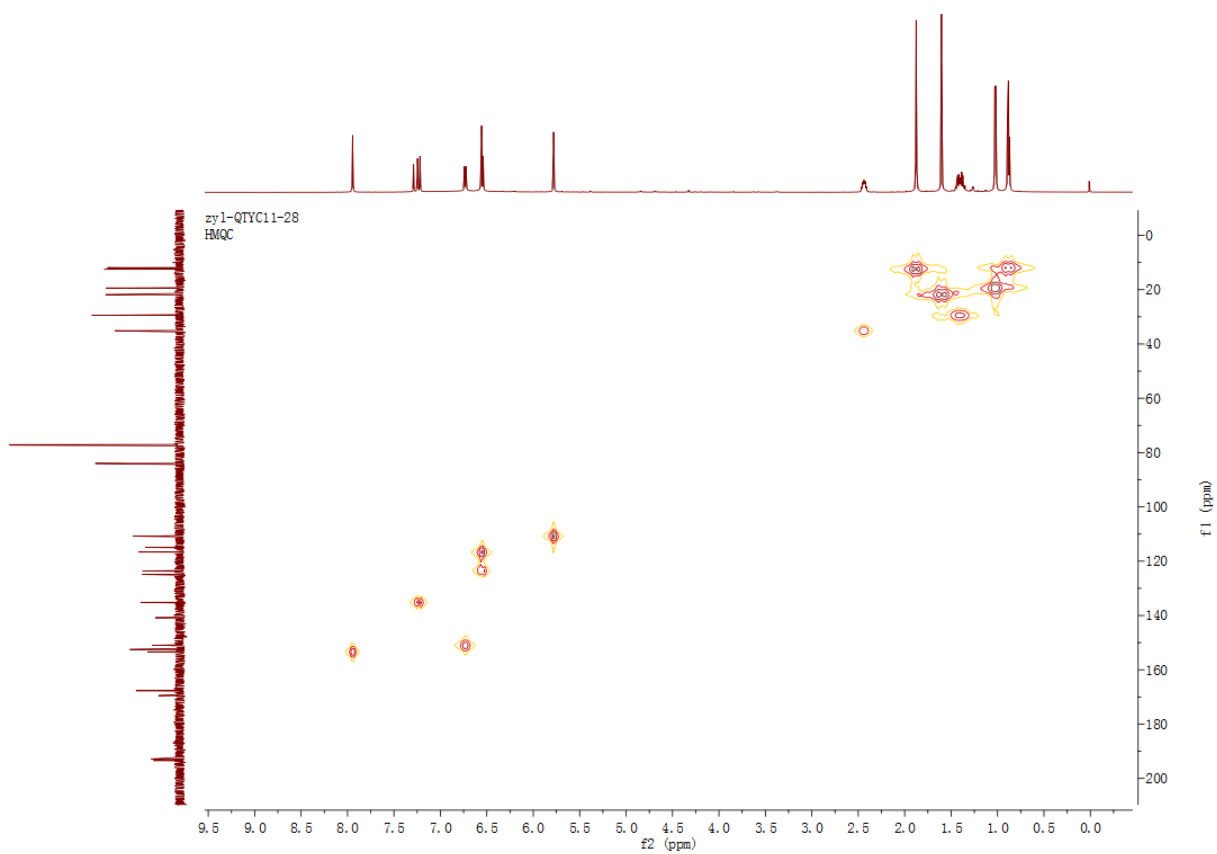
S3: ^{13}C NMR spectrum (150 MHz) of compound in Acetone- d_6



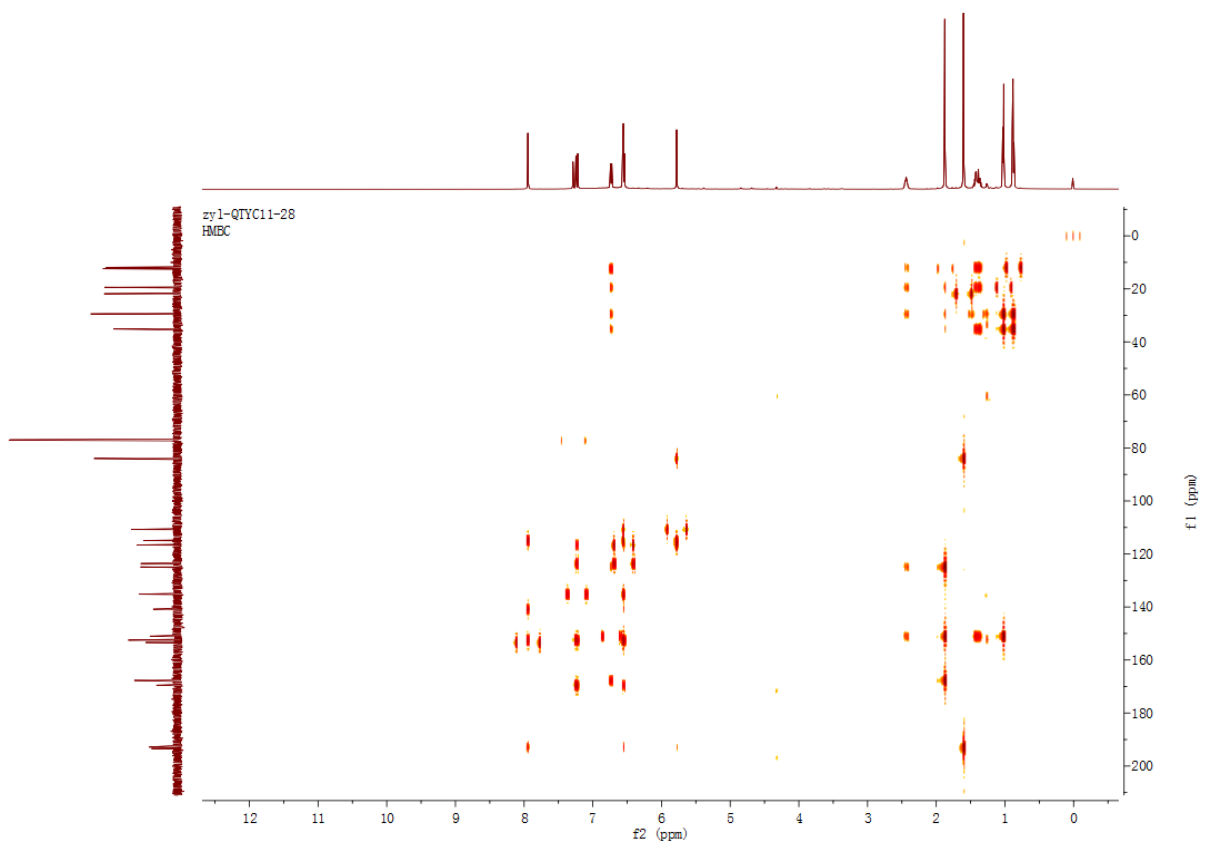
S4: DEPT 135 spectrum (600 MHz) of compound in Acetone- d_6



S5: ^1H - ^1H COSY spectrum (600 MHz) of compound in Acetone- d_6



S6: HMQC spectrum (600 MHz) of compound in Acetone- d_6



S7: HMBC spectrum (600 MHz) of compound in Acetone-*d*₆.