

Supporting Information

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A New Siderophore from Sponge Associated *Pseudomonas fluorescens* 4.9.3

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Table of Contents	Page
S1: HR-MS (Q-TOF) Spectrum of Compound 1 (+ mode)	2
S2: ¹ H-NMR (DMSO-d ₆ at 400 MHz) Spectrum of Compound 1	3
S3: ¹³ C-NMR (DMSO-d ₆ at 100 MHz) Spectrum of Compound 1	4
S4: Exchangeable H-NMR (DMSO-d ₆ at 400 MHz) Spectrum of Compound 1	5
S5: HRESI-MS Spectrum of Compound 2 (+ mode)	6
S6: HRESI-MS Spectrum of Compound 2 (- mode)	7
S7: ¹ H-NMR (DMSO-d ₆ at 400 MHz) Spectrum of Compound 2	8

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Qualitative Compound Report

Data File	FC1.d	Sample Name	FC1
Sample Type	Sample	Position	P1-E2
Instrument Name	Instrument 1	User Name	
Acq Method	10 MIN - MEOH-TFA WATER GRD - POS MS MOD.m	Acquired Time	2/25/2015 11:34:44 AM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

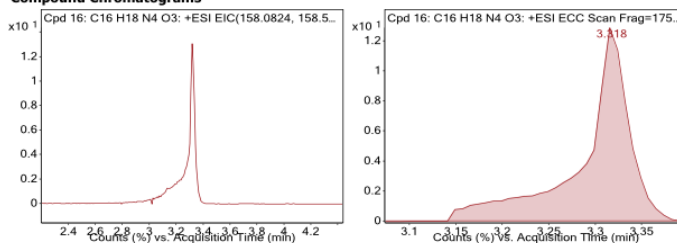
Sample Group	Info.
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125.2)

Compound Table

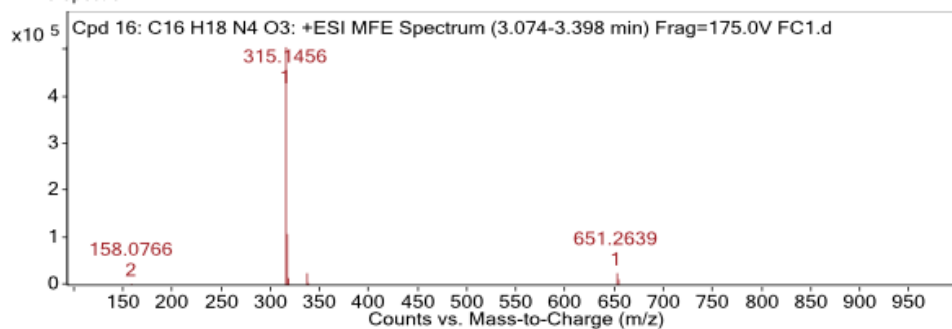
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 16: C16 H18 N4 O3	3.318	314.1384	C16 H18 N4 O3	C16 H18 N4 O3	-1.7	C16 H18 N4 O3

Compound Label	m/z	RT	Algorithm	Mass
Cpd 16: C16 H18 N4 O3	315.1456	3.318	Find by Molecular Feature	314.1384

Compound Chromatograms

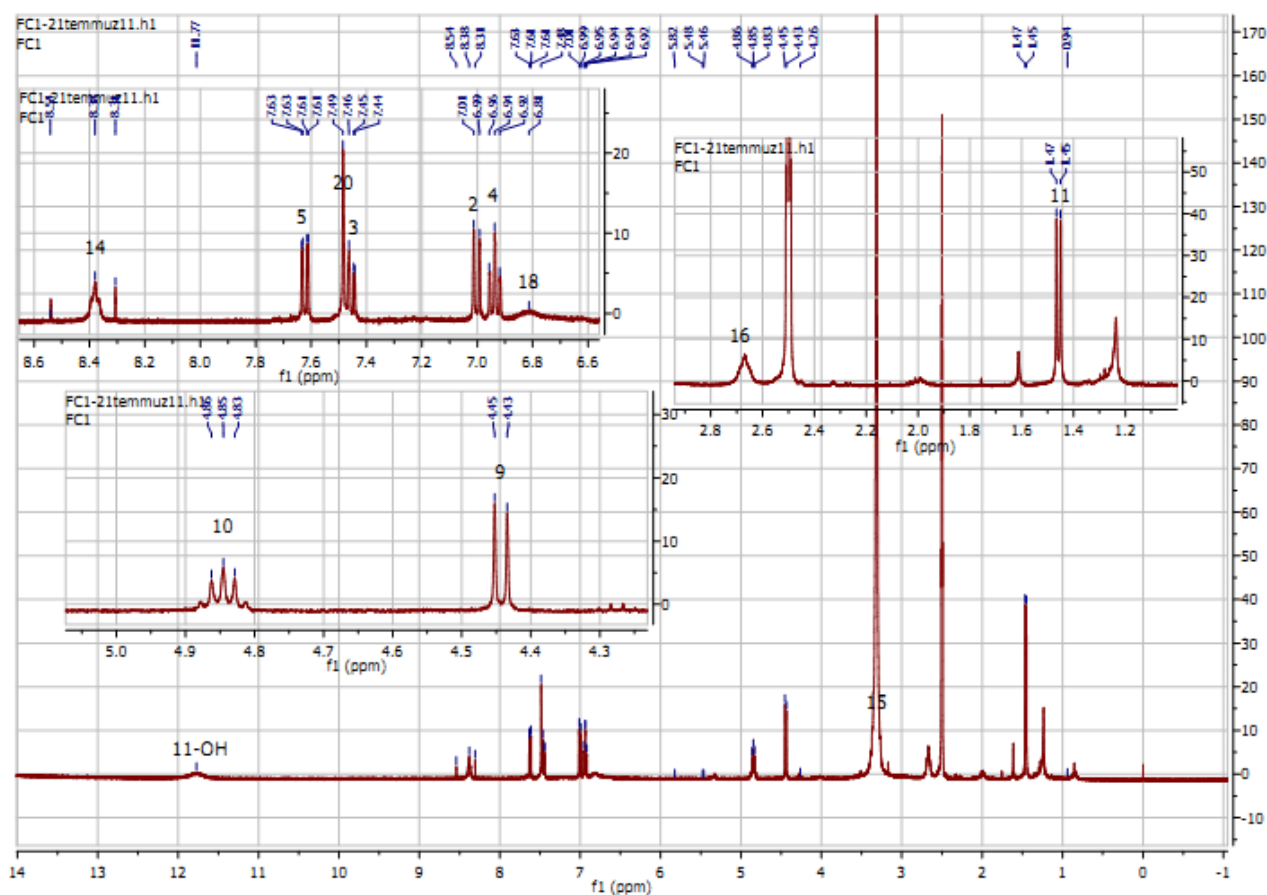


MFE MS Spectrum



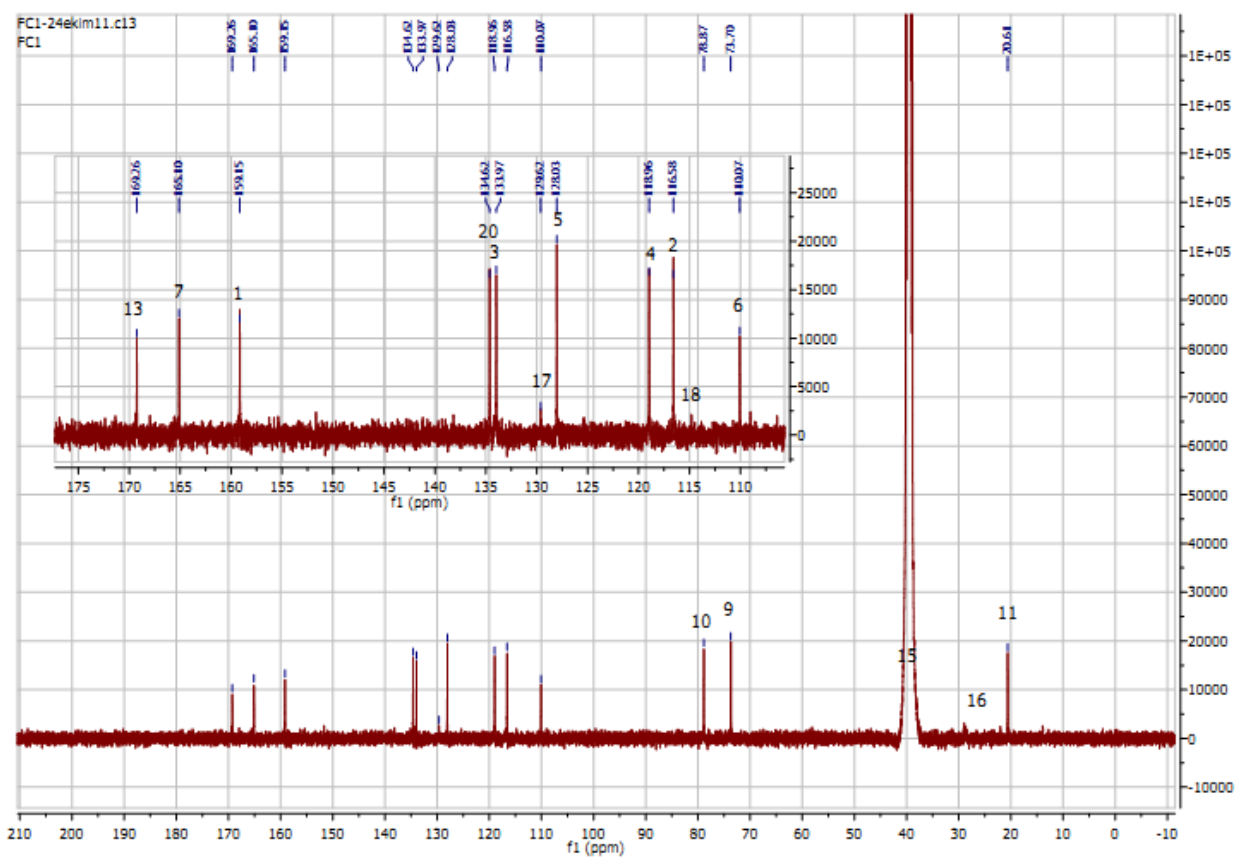
MFE MS Zoomed Spectrum

S1: HR-MS (Q-TOF) Spectrum of Compound 1 (+ mode)

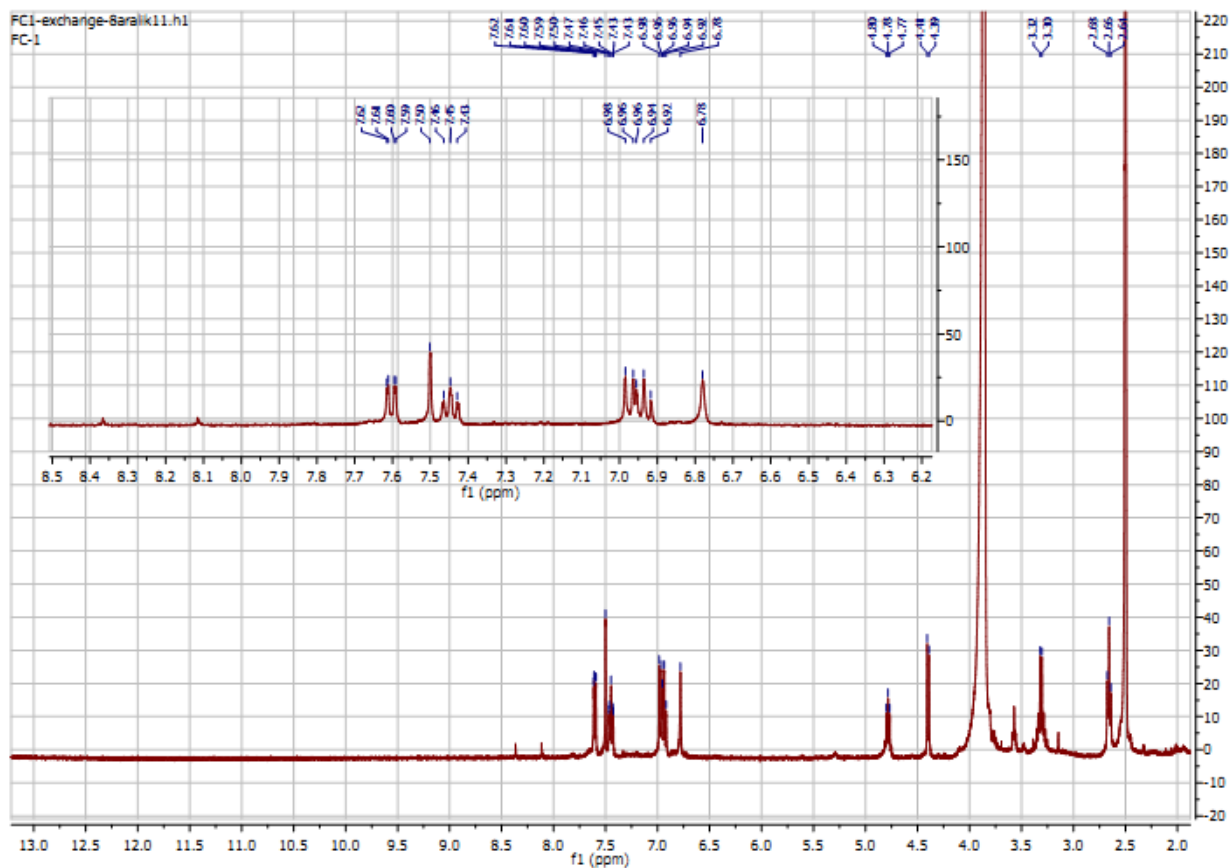


S2: $^1\text{H-NMR}$ (DMSO-d_6 at 400 MHz) Spectrum of Compound 1

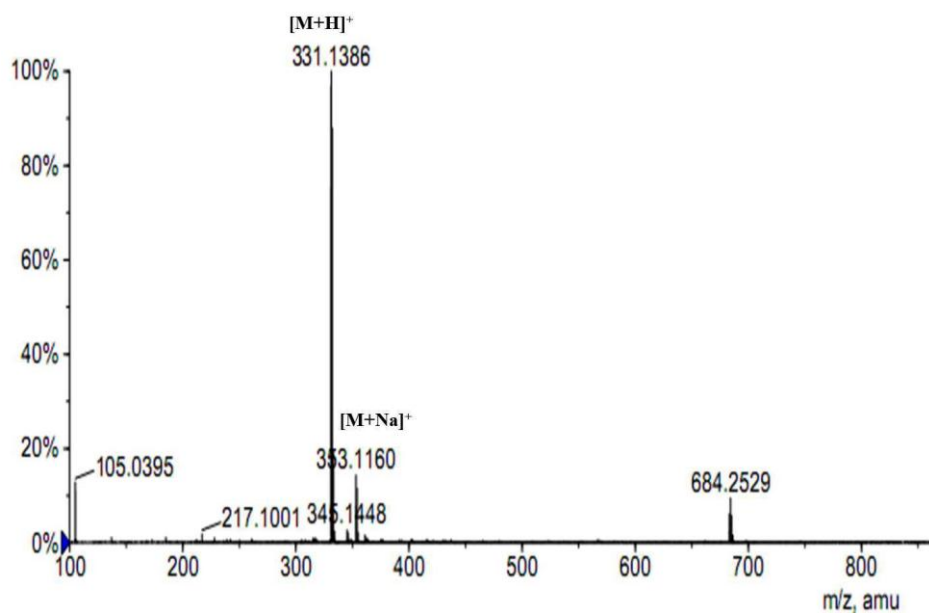
Chemical Formula	Exact MS (amu)	Observed m/z	Calculated m/z	Error (amu)
$\text{C}_{16}\text{H}_{18}\text{N}_4\text{O}_3$	314.1378	315.1456 $[\text{M}+\text{H}]^+$	315.1457	0.0001



S3: ^{13}C -NMR (DMSO- d_6 at 100 MHz) Spectrum of Compound 1

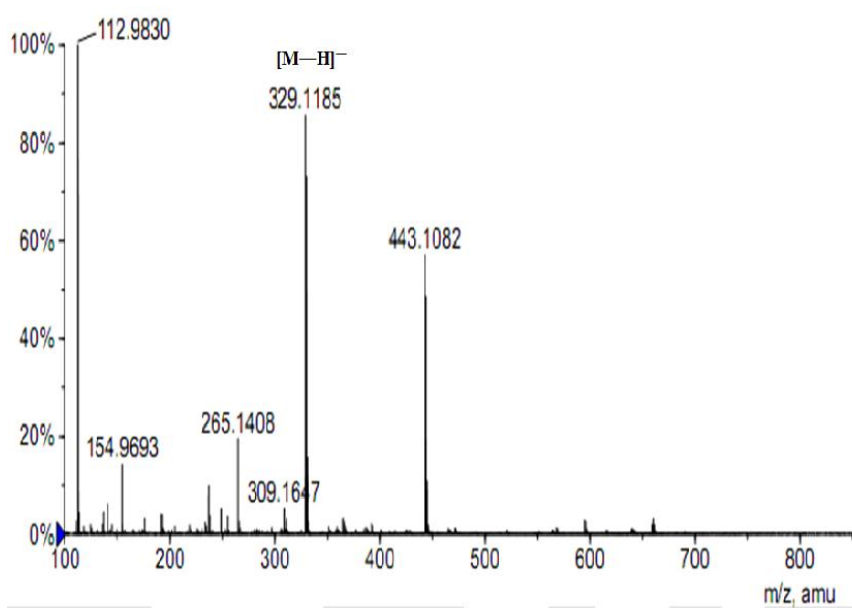


S4: Exchangeable $^1\text{H-NMR}$ (DMSO-d_6 at 400 MHz) Spectrum of Compound 1



Chemical Formula	Exact MS (amu)	Observed m/z	Calculated m/z	Error (amu)
C ₁₆ H ₁₈ N ₄ O ₄	330.1328	331.1386 [M+H] ⁺	331.1407	0.0019
		353.1160 [M+Na] ⁺	353.1225	0.0065

S5: HRESI-MS Spectrum of Compound **2** (+ mode)



Chemical Formula	Exact MS (amu)	Observed m/z	Calculated m/z	Error (amu)
C ₁₆ H ₁₈ N ₄ O ₄	330.1328	329.1185 [M-H] ⁻	329.1249	0.0065

S6: Expansion of HRESI-MS Spectrum of Compound **2** (- mode)

