

*Supplementary Information*

# Inhibition of the Quorum Sensing System, Elastase Production and Biofilm Formation in *Pseudomonas aeruginosa* by Psammaplin A and Bisaprasin

Emmanuel T. Oluwabusola <sup>1,\*</sup>, Nursheena Parveen Katermeran <sup>2</sup>, Wee Han Poh <sup>3</sup>, Teo Min Ben Goh <sup>2</sup>, Lik Tong Tan <sup>2</sup>, Oluwatofunmilayo Diyaolu <sup>4</sup> Jioji Tabudravu <sup>5</sup>, Rainer Ebel <sup>4</sup>, Scott A. Rice <sup>3,6,7</sup> and Marcel Jaspars <sup>4,\*</sup>

<sup>1</sup> DDT College of Medicine, Department of Pharmacy, P.O. Box 70587, Gaborone, Botswana.

<sup>2</sup> Natural Sciences and Science Education, National Institute of Education, Nanyang Technological University, 1 Nanyang Walk, Singapore 637616, Singapore; nursheena92@gmail.com (N.P.K.); bengoh93@yahoo.com.sg (T.M.B.G.); liktong.tan@nie.edu.sg (L.T.T.)

<sup>3</sup> Singapore Centre for Environmental Life Sciences Engineering, Singapore 637551, Singapore; whpoh@ntu.edu.sg (W.H.P.); rscott@ntu.edu.sg (S.A.R.)

<sup>4</sup> Marine Biodiscovery Centre, Department of Chemistry, University of Aberdeen, Aberdeen AB24 3UE, Scotland, UK; r01oad17@abdn.ac.uk (O.D.); r.ebel@abdn.ac.uk (R.E.)

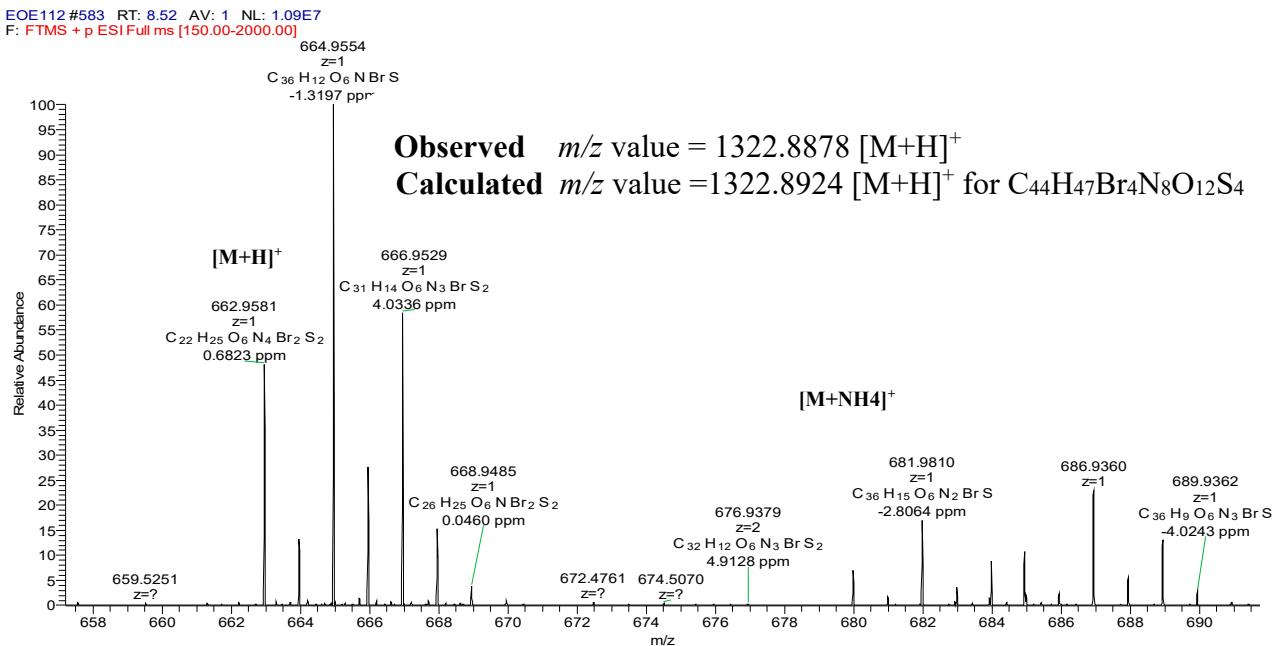
<sup>5</sup> School of Forensic and Applied Sciences, Faculty of Science and Technology, University of Central Lancashire, Preston PR1 2HE, England, UK; jtabudravu@uclan.ac.uk

<sup>6</sup> The School of Biological Sciences, Nanyang Technological University, Singapore 639798, Singapore

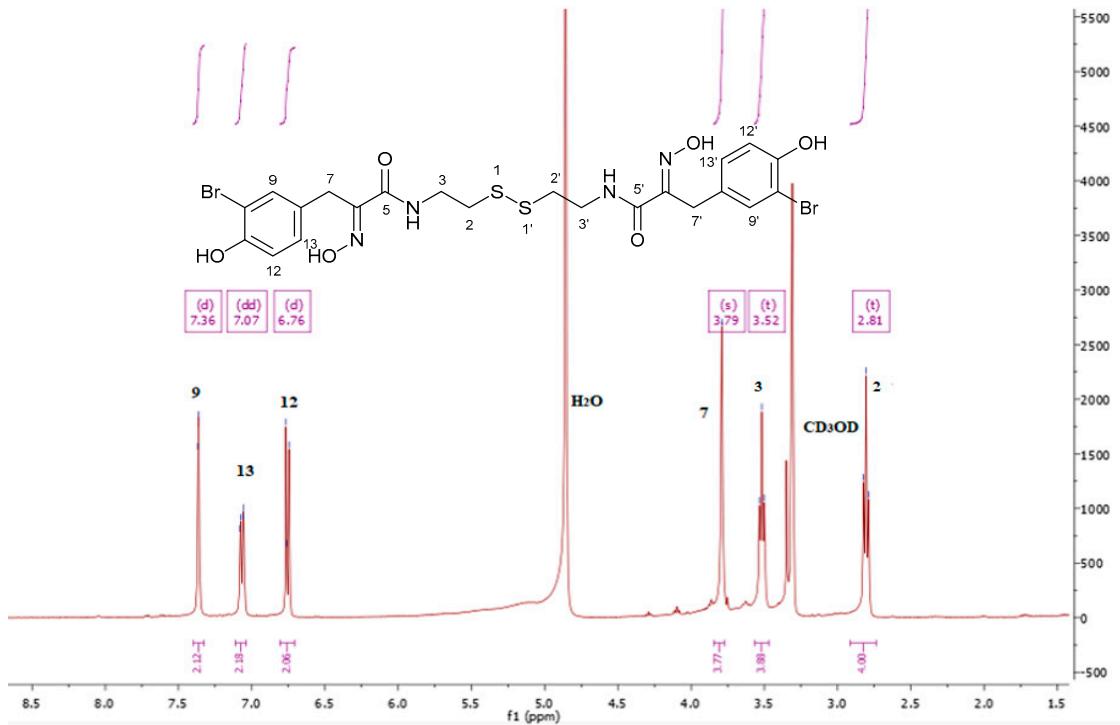
<sup>7</sup> The iThree Institute, The University of Technology Sydney, Sydney, NSW 2007, Australia

\* Correspondence: emmanuel.oluw@ddtcollegeofmedicine.com (E.T.O.); m.jaspars@abdn.ac.uk (M.J.); Tel.: +26-775-298-641 (E.T.O.); +44-(0)12-2427-2895 (M.J.)

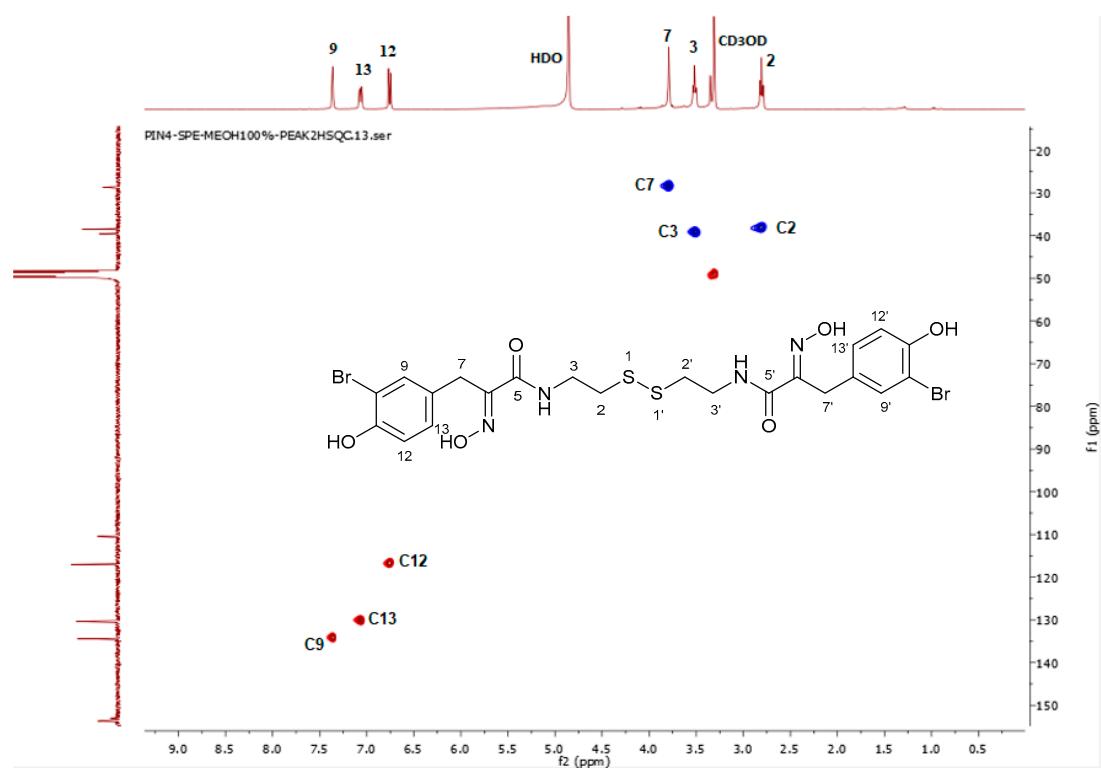
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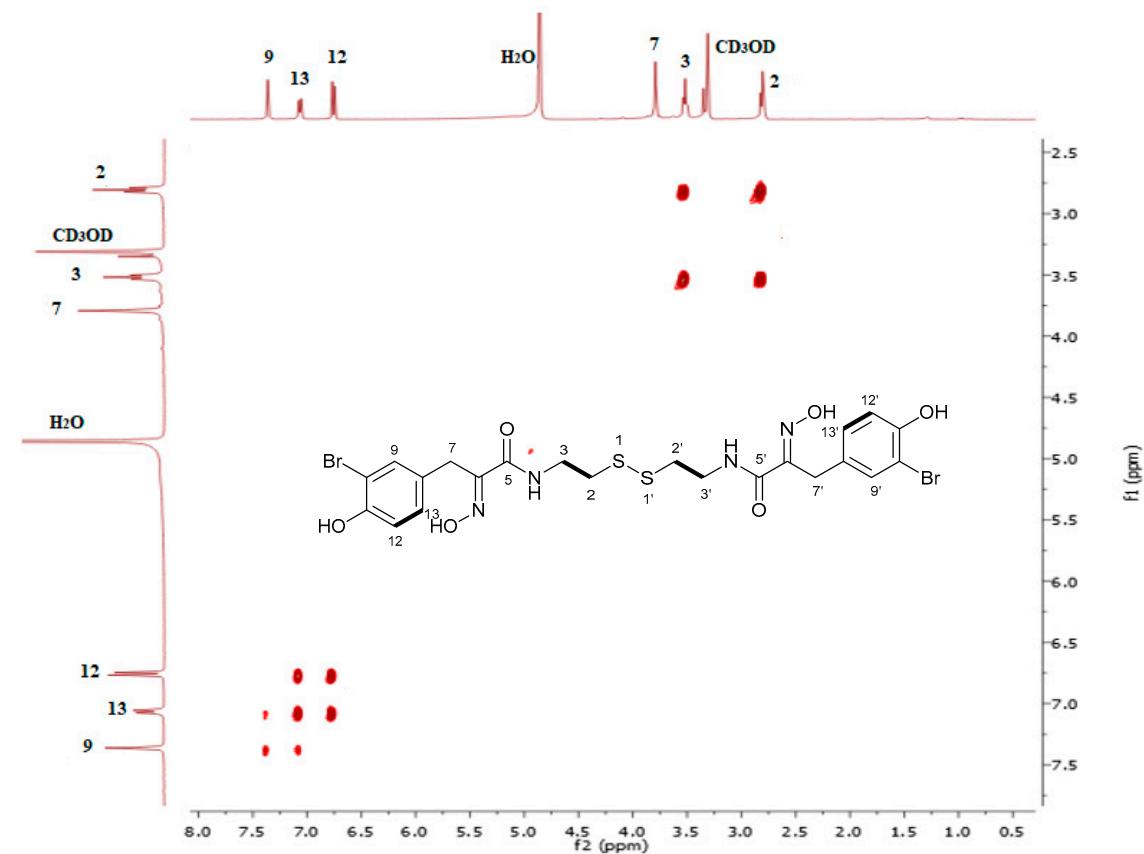
**Figure S1.** Orbitrap-(+)-HRMS of **1**



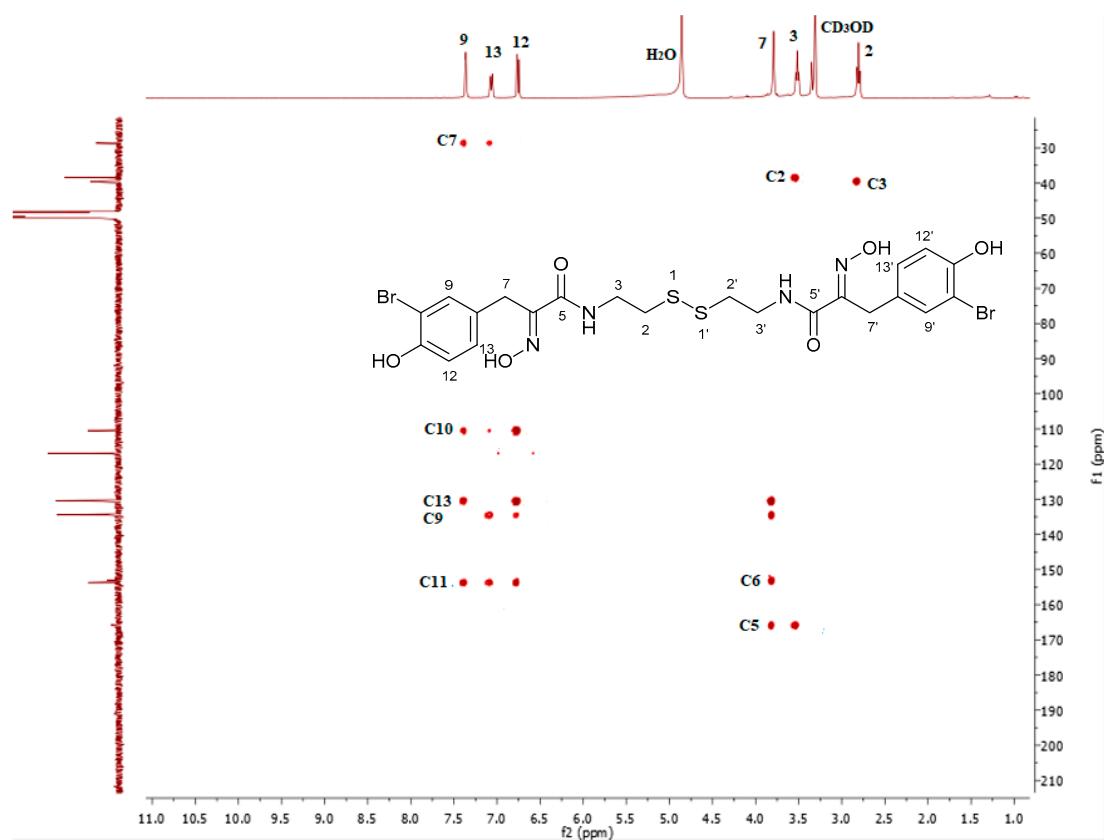
**Figure S2.**  $^1H$  NMR spectrum of **1** at 600MHz in  $CD_3OD$



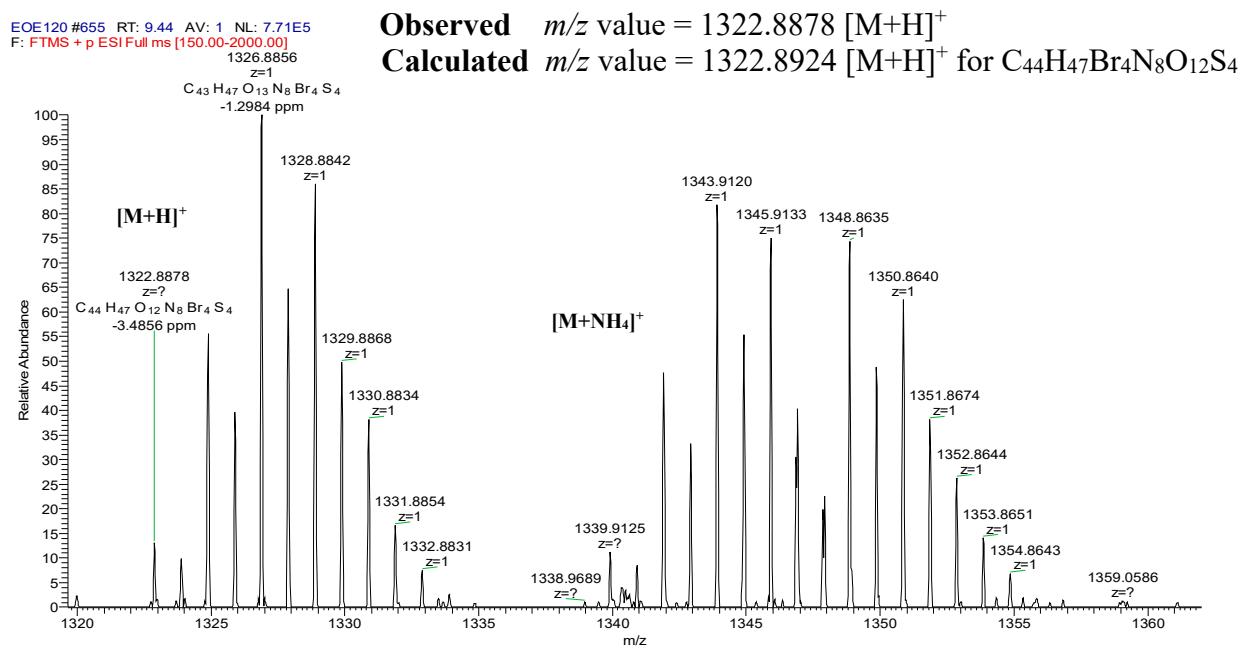
**Figure S3.** HSQC NMR spectrum of **1** at 600MHz in CD<sub>3</sub>OD



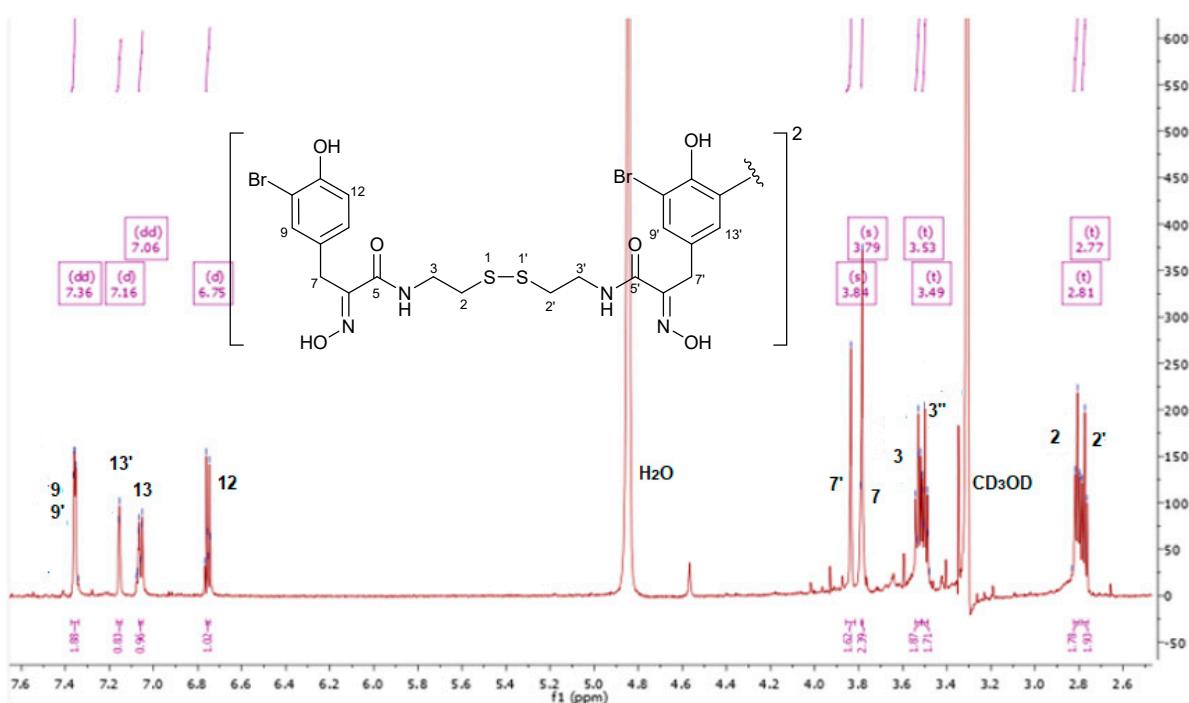
**Figure S4.** COSY NMR spectrum of **1** at 600MHz in CD<sub>3</sub>OD



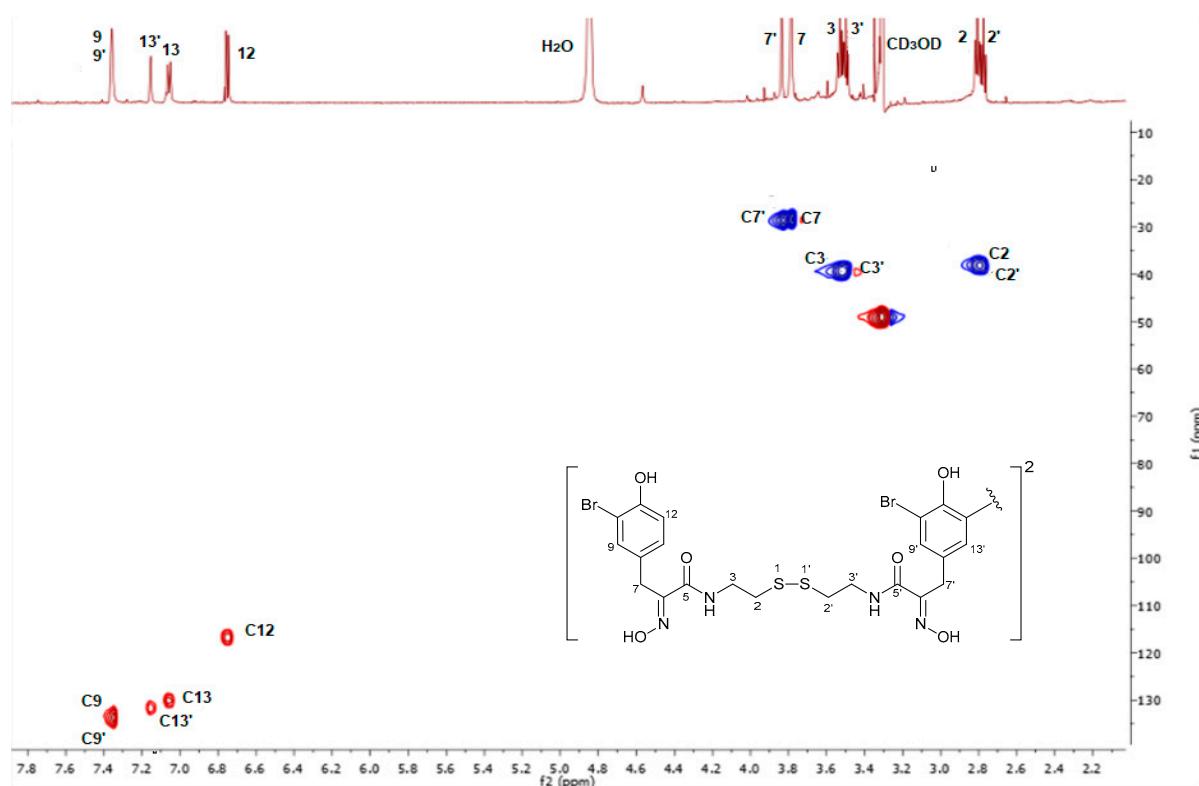
**Figure S5.** HMBC NMR spectrum of **1** at 600MHz in  $\text{CD}_3\text{OD}$



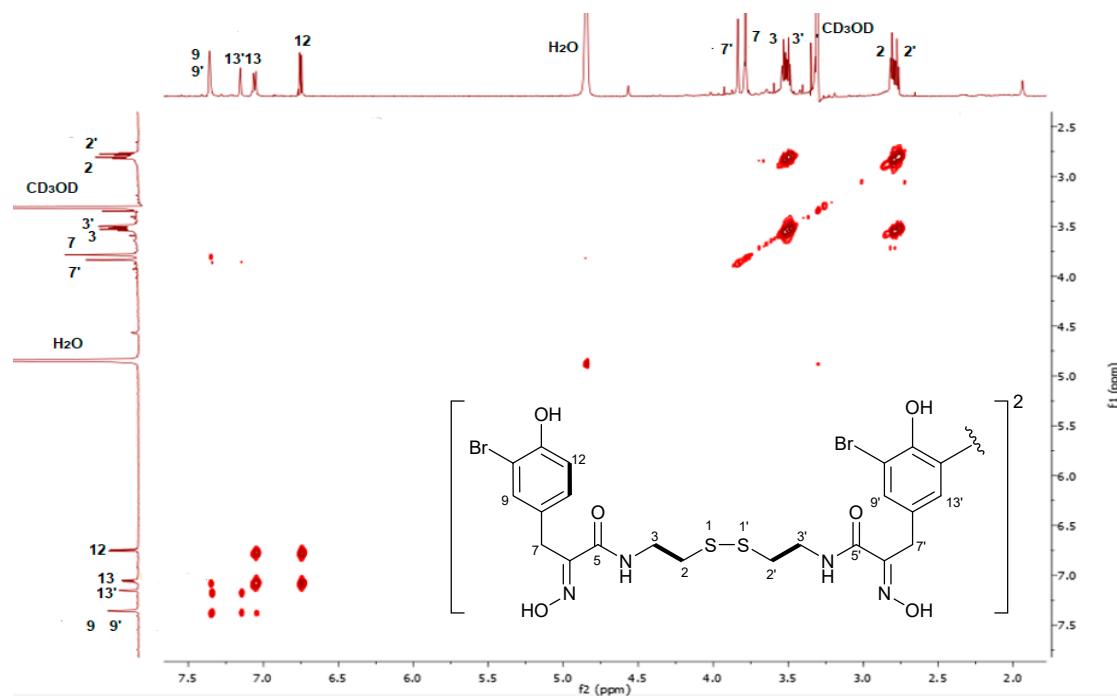
**Figure S6.** Orbitrap-(+)-HRMS of **2**



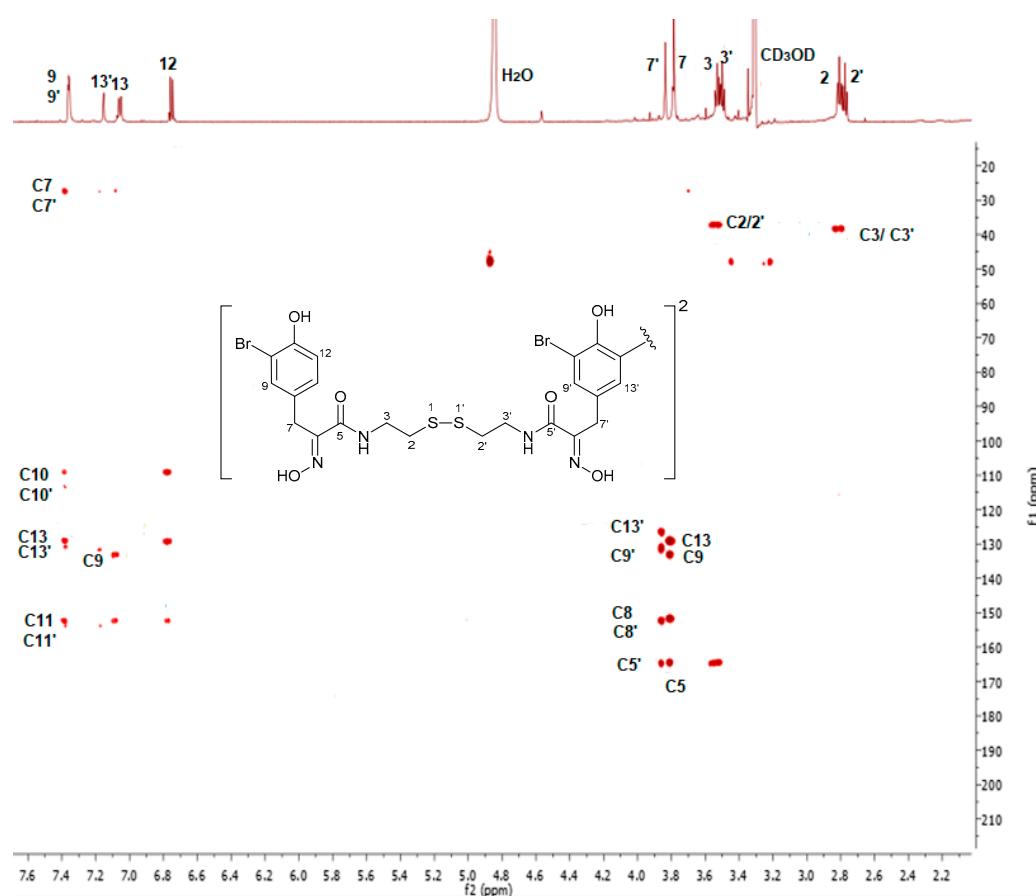
**Figure S7.**  $^1\text{H}$  NMR spectrum of **2** at 600MHz in  $\text{CD}_3\text{OD}$



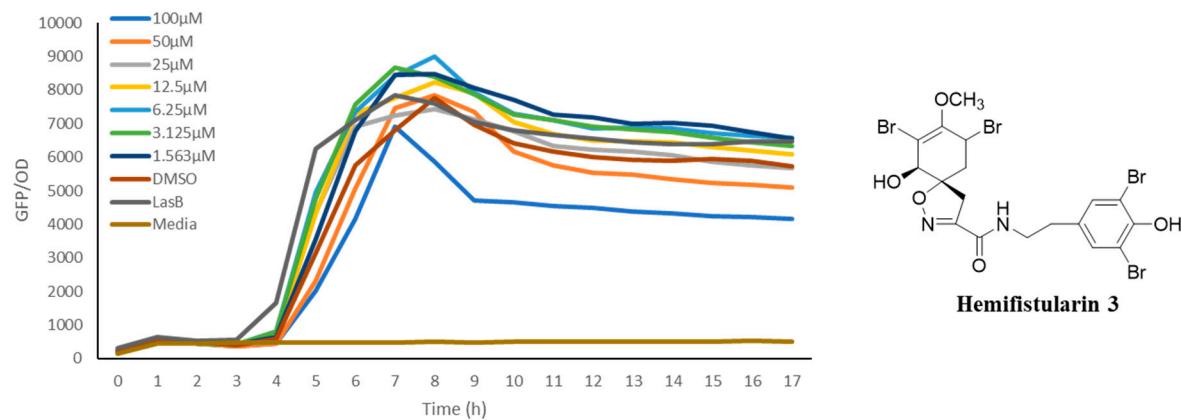
**Figure S8.** HSQC NMR spectrum of **2** at 600MHz in  $\text{CD}_3\text{OD}$



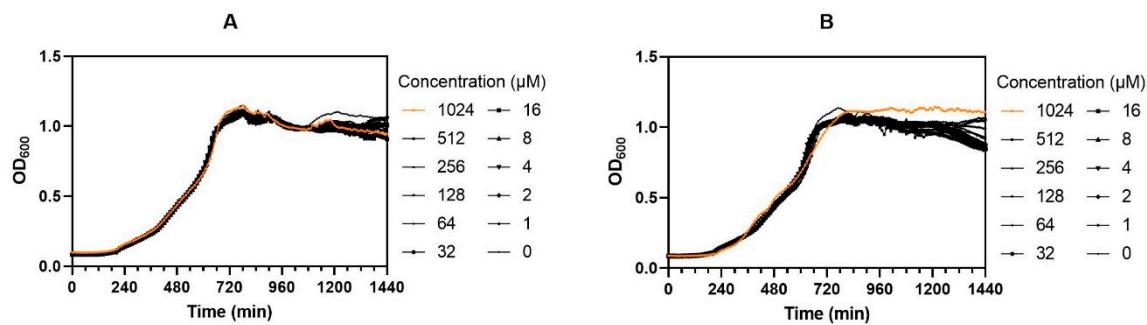
**Figure S9.** COSY NMR spectrum of **2** at 600MHz in CD<sub>3</sub>OD



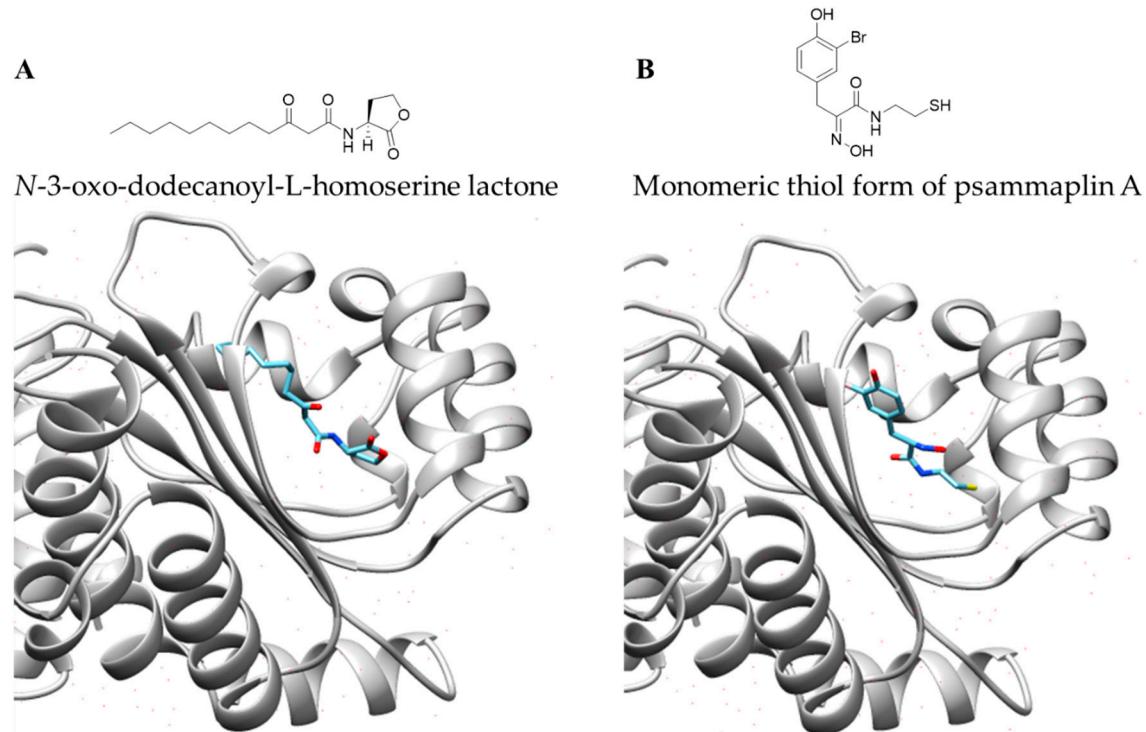
**Figure S10.** HMBC NMR spectrum of **2** at 600MHz in CD<sub>3</sub>OD



**Figure S11.** Hemifistularin 3 incubated with *P. aeruginosa* PAO1 *lasB-gfp*(ASV) strain at various concentrations



**Figure S12.** The growth curve (OD600) of *P. aeruginosa* WT incubated with psammaphlin A (1) (A) and bisaprasin (2) (B) at concentrations ranging from 1.0  $\mu$ M to 1024.0  $\mu$ M



**Figure S13.** Molecular docking of the LasR-ligand binding domain (PBD ID: 2UV0) with the native autoinducer, *N*-3-oxo-dodecanoyl-L-homoserine lactone (**A**) and the monomeric thiol form of psammaplin A (**B**)

**Table S1** NMR data for Psammaplin A (**1**)

Position	$\delta_C$ , Type	$\delta_H$ , mult. ( <i>J</i> in Hz)	HMBC (H→C)
2, 2'	38.4, CH <sub>2</sub>	2.81, t (6.0)	3/3'
3, 3'	39.5, CH <sub>2</sub>	3.52, t (6.0)	2/2', 5/5'
5, 5'	165.8, C		
6, 6'	152.1, C		
7, 7'	28.6, CH <sub>2</sub>	3.79, s	5/5', 6/6', 9/9' 13/13'
8, 8'	130.6, C		
9, 9'	134.3, CH	7.36, d 2.0)	7/7', 10/10', 11/11', 13/13'
10, 10'	110.4, C		
11, 11'	153.7, C		
12, 12'	116.8, CH	6.76, d (8.4 )	9/9', 10/10', 11/11', 13/13'
13, 13'	130.6, CH	7.07, dd (8.4,2.0)	7/7', 9/9', 10/10', 11/11'
NMR solvents used for <b>1</b> was CD <sub>3</sub> OD at 600 MHz.			

**Table S2** NMR data for Bisaprasin (**2**)

Position	$\delta_{\text{C}}$ , Type	$\delta_{\text{H}}$ , mult.( $J$ in Hz)	HMBC (H → C)
2, 2'	38.4, CH <sub>2</sub>	3.52, t (6.0)	3/3'
3, 3'	39.5, CH <sub>2</sub>	3.58, t (6.0)	2/2', 5/5'
5, 5'	165.8, C		
6, 6'	153.8, C		
7, 7'	28.6, CH <sub>2</sub>	3.79, s	5/5', 6/6', 9/9' 13/13'
8, 8'	130.6, C		
9, 9'	134.3, CH	7.36, d (1.6)	7/7', 10/10', 11/11', 13/13'
10, 10'	110.4, C		
11,11'	155.7, C		
12, 12'	116.8, CH	6.75, d (8.0)	9/9', 10/10', 11/11', 13/13'
13, 13'	130.6, CH	7.07, dd (8.0,1.6)	7/7', 9/9', 10/10', 11/11'
2'',2'''	38.7, CH <sub>2</sub>	2.77, t (6.0)	3''/3'''
3'',3'''	39.8, CH <sub>2</sub>	3.49, t (6.0)	2''/2''', 5''/5'''
5'', 5'''	166.1, C		
6'', 6'''	153.5, C		
7'', 7'''	28.6, CH <sub>2</sub>	3.88 s	5''/5''', 6''/6''', 9''/9''', 13''/13'''
8'', 8'''	128.3, C		
9'', 9'''	133.4, CH	7.36, d (1.6)	7''/7''', 10''/10''', 11''/11''', 13''/13'''
10'', 10'''	111.4, C		
11'',11'''	153.1, C		
12'', 12'''	112.7, C		
13'', 13'''	130.5, CH	7.16, d (1.6)	7''/7''', 9''/9''', 10''/10''', 11''/11'''
NMR solvents used for <b>2</b> was CD <sub>3</sub> OD at 600 MHz.			

**Table S3.** *Pseudomonas aeruginosa* strains used in the study

Name and Genotype	Description <sup>a</sup>	Reference
PAO1	Wild type; ATCC <i>Pseudomonas aeruginosa</i>	[1]
PAO1-gfp	GFP-tagged wild-type <i>Pseudomonas aeruginosa</i>	[2]
PAO1 lasB-gfp	Gmr; PAO1 containing <i>lasB-gfp</i> (ASV) reporter fusion	[1]
PAO1 rhlA-gfp	Gmr; PAO1, <i>rhlA-gfp</i> (ASV) reporter fusion	[3]
PAO1 ΔlasI ΔrhlI	Gmr; PAO1 <i>lasI</i> and <i>rhlI</i> mutant	[4]

<sup>a</sup> Description of the strains' antibiotic resistance: Gmr, gentamicin resistance.

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