Isolation and characterization of a Serratia rubidaea from a shallow water hydrothermal vent

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Supplementary Information

Table S1. NMR experiments data used in the structural elucidation of the putative prodigiosin. Q – quaternary; T – terciary, S – secondary; P – primary.

	^{1}H δ	^{1}H Integration	^{13}C Jmod δ	^{1}H-^{13}C HMBC	^{1}H-^{1}H COSY	^{1}H-^{1}H NOESY
1	12.59	1H	-	-	3, 4, 5	5
2	-	-	122.2 (Q)	2, 4	-	-
3	6.94	1H	117.0 (T)	3, 4, 5	1, 4	4, 4’
4	6.37	1H	111.9 (T)	2, 3, 5	1, 3, 5	3, 5
5	7.25	1H	127.0 (T)	2, 3, 4	1, 4	1, 4
1’	12.70	2H	-	2’, 3’, 4’, 5’,8’	4’, 8’, 11’’	1, 11’’
2’	-	-	120.9 (Q)	1’, 4’	-	-
3’	-	-	165.9 (Q)	1’, 7’, 4’’	-	-
4’	6.10	1H	92.9 (S)	2’, 5’	1’	3, 7’
5’	-	-	147.5 (Q)	4’, 8’ 11’’	-	-
7’	4.03	3H	58.9 (OCH_3)	3’	-	4’
8’	6.70	1H	128.3 (T)	2’’, 4’’	1’, 11’’	4’’
3’’	-	-	146.9 (Q)	8’, 11’’	-	-
4’’	6.97	1H	116.0 (T)	3’, 8’	8’	8’
6’’	2.43-2.34	4H	33.7 (S)	12’’	7’’	7’’
7’’	1.70-1.52	4H	29.9 (S)	8’’	9’’, 10’’	6’’, 9’’
8’’	1.33	7 H	22.4 (S)	-	7’’, 10’’	7’’
9’’	1.22	15H	29.6 (S)	7’’	7’’, 10’’	-
10’’	0.93	6H	14.2 (P)	9’’	8’’	8’’
11’’	2.57	3H	12.7 (P)	8’, 2’’	1’, 8’	1’