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Table S1: NMR data (data set C) of oroidin (COCON input file).

No.	an^a	H^b	$\delta(^{13}C)$	$Atype^c$	COSY (6)^d	$^1H,^{13}C$-HMBC (23)^e	1,1-ADEQ. (8)^f	$^1H,^{15}N$-HMBC (8)^g
1	7	1	---	–NH–	---	2, 3, 4	---	---
2	6	0	128	=C<	---	---	---	---
3	6	1	113	=CH–	---	2, 5	2, 4	1
4	6	0	98	=C<	---	---	---	---
5	6	0	105	=C<	---	---	---	---
6	6	0	159	=C<	---	---	---	---
7	7	1	---	–NH–	8	6, 8	---	---
8	6	2	40	>CH2	7, 9	6, 9, 10	9	7
9	6	1	127	=CH–	8, 10	8, 10, 11	8, 10	7
10	6	1	116	=CH–	9	8, 9, 11, 12	9, 11	15
11	6	0	125	=C<	---	---	---	---
12	6	1	111	=CH–	---	10, 11, 14	11	13, 15
13	7	1	---	=N–	---	---	---	---
14	6	0	148	=C<	---	---	---	---
15	7	1	---	–NH–	---	11, 12, 14	---	---
16	7	2	---	–NH2	---	---	---	13, 15
17	8	0	---	=O	---	---	---	---
18	35	0	---	–Br	---	---	---	---
19	35	0	---	–Br	---	---	---	---

[a] *an* stands for atomic number.

[b] *H* stands for the number of protons attached to the atom.

[c] *Atype* stands for atom type which represents the hybridisation state of the atom.

[d] The $^1H,^1H$-COSY correlations are given for both sides of the diagonal. The number given in parenthesis is the total number of correlations.

[e] The $^1H,^{13}C$-HMBC correlations are given from protons to carbons (H# → C#). The number given in parenthesis is the total number of correlations. The correlations for data set A are: H-3 → C-2, C-5; H-7 → C-6; H-8 → C-6, C-9, C-10; H-9 → C-11; H-12 → C-11, C-14. The correlations for data B are as shown in Table S1 without: H-1 → C-2; H-9 → C-8; H-15 → C-11, C-12, C-14. The correlations for data set D are as shown in Table S1 plus: H-1 → C-5; H-3 → C-4, C-6.

[f] The 1,1-ADEQUATE correlations are theoretical data. The number in parenthesis is the total number of correlations.

[g] The HMBC correlations are given from protons to nitrogens. The number in parenthesis is the total number of correlations.
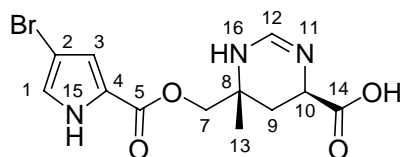
2

Table S2: NMR data of manzacidin (COCON input file).

No.	*an*[a]	*H*[b]	δ(^{13}C)	*Atype*[c]	COSY (6)[d]	^{1}H,^{13}C-HMBC (18)[e]	1,1-ADEQ. (9)[f]	^{1}H,^{15}N-HMBC (10)[g]
1	6	1	124	=CH–	15	2, 3, 4	2	15
2	6	0	96	=C<	---	---	---	---
3	6	1	117	=CH–	---	1, 4	2, 4	15
4	6	0	122	=C<	---	---	---	---
5	6	0	159	=C<	---	---	---	---
6	8	0	---	–O–	---	---	---	---
7	6	2	68	>CH2	---	5, 8, 9, 13	8	16
8	6	0	52	>C<	---	---	---	---
9	6	2	29	>CH2	10	8, 10, 13	8, 10	11, 16
10	6	1	48	–CH<	9	14	9, 14	11
11	7	0	---	=N–	---	---	---	---
12	6	1	151	=CH–	16	8, 10	---	11, 16
13	6	3	23	–CH3	---	7, 8, 9	8	16
14	6	0	170	=C<	---	---	---	---
15	7	1	---	–NH–	1	---	---	---
16	7	1	---	–NH–	12	---	---	11
17	35	0	---	–Br	---	---	---	---
18	8	1	---	–OH	---	---	---	---
19	8	0	---	=O	---	---	---	---
20	8	0	---	=O	---	---	---	---

[a] *an* stands for atomic number.

[b] *H* stands for the number of protons attached to the atom.

[c] *Atype* stands for atom type which represents the hybridisation state of the atom.

[d] The ^{1}H,^{1}H-COSY correlations are given for both sides of the diagonal. The number given in parenthesis is the total number of correlations.

[e] The ^{1}H,^{13}C-HMBC correlations are given from protons to carbons (H# → C#). The number given in parenthesis is the total number of correlations.

[f] The 1,1-ADEQUATE correlations are theoretical data. The number in parenthesis is the total number of correlations.

[g] The ^{1}H,^{15}N-HMBC correlations are theoretical data. The number in parenthesis is the total number of correlations.