Cremenolide, a new 10-member lactone from *Trichoderma cremeum* with plant growth promotion activity

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Appendix A. Supplementary data

Figure S1. ¹H NMR spectrum (δ, CDCl₃) of **1**.

Figure S2. ¹³C NMR spectrum (δ, CDCl₃) of **1**.

Figure S3. ¹³C DEPT135 NMR spectrum (δ, CDCl₃) of **1**

Figure S4. ¹H-¹H COSY spectrum (δ, CDCl₃) of **1**.

Figure S5. ¹H-¹³C HSQC spectrum (δ, CDCl₃) of **1**.

Figure S6. ¹H-¹³C HMBC spectrum (δ, CDCl₃) of **1**.

Figure S7. ¹H-¹H TOCSY spectrum (δ, CDCl₃) of **1**.

Figure S8. ¹H-¹H NOESY spectrum (δ, CDCl₃) of **1**.

Figure S9. Mass spectrum (HRMS) of compound **1**.

Figure S10. MS/MS of compound **1**.

Figure S11. Determinant TOCSY (A) and NOESY (B) correlations detected for cremenolide (**1**).

Table S1 ¹H and ¹³C NMR spectral data of cremenolide (in CDCl₃).

Figure S1. ^1H NMR spectrum (δ, CDCl_3) of **1**.

Figure S2. ^{13}C NMR spectrum (δ, CDCl_3) of **1**.

Figure S3. ^{13}C DEPT135 NMR spectrum (δ, CDCl_3) of **1**.

Figure S4. ^1H - ^1H COSY spectrum (δ, CDCl_3) of **1**.

Figure S5. ^1H - ^{13}C HSQC spectrum (δ , CDCl_3) of **1**.

Figure S6. ^1H - ^{13}C HMBC spectrum (δ , CDCl_3) of **1**.

Figure S7. ^1H - ^1H TOCSY spectrum (δ, CDCl_3) of **1**.

Figure S8. ^1H - ^1H NOESY spectrum (δ , CDCl_3) of **1**.

Figure S9. Mass spectrum (HRMS) of **1**. (**A** – Full spectrum; **B** – Enlarged spectrum from 250 to 380 m/z)

B

Figure S10. MS/MS of compound **1**.

Figure S11. Determinant TOCSY (A) and NOESY (B) correlations detected for cremenolide (**1**).

Table S1 ^1H and ^{13}C NMR spectral data of cremenolide (in CDCl_3).

Cremenolide (1).			
position	δ_{C} mult.	δ_{H} (J in Hz)	HMBC*
1	174.99 qC		9, 2a,2b, 3a,3b
2	32.61 CH_2	2.46 ^a 2.13 m	3a, 3b, 4
3	23.86 CH_2	2.44 ^a 1.64m	2a, 4, 5
4	77.17 CH	4.74 dt	2a, 2b, 3a, 3b, 5, 2''
5	70.49 CH	4.5 s	3a,3b, 4, 6, 7
6	78.50 CH	4.96 m	7, 8, 9, 10
7	130.50 CH	5.62 ^a	8, 2', 6, 5
8	128.56 CH	5.63 br s	2', 7, 6, 5, 9
9	71.63 CH	5.06 m	10, 8
10	16.64 CH_3	1.3 d	9, 6
1'	165.38 qC		6, 2', 3', 4'
2'	122.01 CH	5.82 dd (1.56, 5.09)	3', 4'
3'	145.88 CH	6.9 dd (1.55, 7.05)	2', 4'
4'	17.96 CH_3	1.86 dd (7.05, 7.4)	2', 3'2''
1''	169.98 qC		4, 2''
2''	21.15 CH_3	2.06 s	4, 1''

*All correlations represent 2 or 3 bond couplings. ^a overlapping NMR signals.
Abbreviation, s: singlet, d: doublet, t: triplet, dd: doublet of doublets.