Supporting Information

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A New Antibacterial Diterpene with a Fused 6-5-6-6 Ring System, Trichodermanin I, Isolated from the Soil-Derived Fungus *Trichoderma atroviride* YD-13

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Elemental Composition -								-		>	×	
<u>F</u> ile <u>E</u> dit	jile <u>E</u> dit <u>V</u> iew <u>P</u> rocess <u>H</u> elp											
• • • • • • • • • • • • • • • • • • •												
Single Mass Analysis Tolerance = 20.0 PPM / DBE: min = 0.5, max = 20.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3 Monoisotopic Mass, Even Electron Ions 12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)												
Elements Used:												
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	н	0	
307.2634	307.2637	-0.3	-1.0	3.5	C20 H35 O2	30.6	n/a	n/a	20	35	2	
100 307.2634												
30	7.000	307.10	0	30	07.200	307.300	307	.400	307.5	00		m/z
For Help, pres	is F1											1

Figure S1: HRESIMS spectrum of 1



Figure S3: Enlarged ¹H-NMR (500 MHz, CDCl₃) spectrum of 1



Figure S5: Enlarged ¹³C-NMR and DEPT (125 MHz, CDCl₃) spectra of 1

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Figure S6: HSQC spectrum of 1

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Figure S7: Enlarged HSQC spectrum of 1



Figure S8: Enlarged HSQC spectrum of 1



Figure S9: HMBC spectrum of 1



Figure S10: Enlarged HMBC spectrum of 1



Figure S11: Enlarged HMBC spectrum of 1



Figure S12: ¹H-¹H COSY spectrum of 1

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Figure S13: Enlarged ¹H-¹H COSY spectrum of 1



Figure S14: Enlarged ¹H-¹H COSY spectrum of 1



Figure S15: NOESY spectrum of 1

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Figure S16: Enlarged NOESY spectrum of 1



Figure S17: Enlarged NOESY spectrum of 1

Substances search for drawn structure 0 1 References -📱 Reactions 👻 📜 Suppliers 👻 Save -Filtering: Similarity: 3 Selected - X Number of Components: 1 X Clear All Filters Structure Match As Drawn (0) 381 Results Sort: Relevance - View: Partial -Substructure (0) 1 3 98 ••• 2 92 ••• 92 ••• к И Similarity (198K) 1355394-77-2 95221-82-2 л К 2933872-44-5 л И **Chemscape Analysis** Visually explore structure similarity with a powerful new tool. Absolute stereoche istry shown, Rotation (+) Absolute Absolute stereochemistry sho wn, Rotation (+) Learn more about Chemscape. C₂₀H₃₄O₂ C22H38O2 C₁₉H₃₂O₃ (2aS,3S,5aR,6R,8S,9S,10aS,10bR)-Dodeca hydro-3,6,10a,11,11-pentamethyl-3H-5a, 5α-Androstane-3β,17β-diol, 4,4,17-trimethyl-Create Chemscape Analysis 9-me... Filter Behavior A o 5 7 ▲ 53K **) 0** 5 1 0 1 8,824 0 Exclude References Reactions References Reference Reactions Search Within Results 92 ••• 92 ••• 92 ••• 4 5 6 Similarity к И х К R 87013-77-2 1818243-49-0 1818243-48-9 95-98 (1) **90-94** (18) 85-89 (362) 80-84 (1,791) 75-79 (6,366) stry s stry :

Figure S18: Scifinder search results of 1

	HO, 9 10 7 8 19 7 H 15 6 5 18 3 13 2 1 17 1 17 1 17 1 17		$\begin{array}{c} 20 \\ 7 \\ 6 \\ 19 \\ 19 \\ 19 \\ 19 \\ 19 \\ 19 \\ 19 $		20 7 8 19 4 	¹⁰ H	⁹ 10 7 8 12 11 H OH 6		
Pos			$\begin{array}{c}1 & 5 & 178 \\ 2 & 17 \\ 2 & 17 \\ 2 & 17 \end{array}$		HO ¹¹ 23	13 17 [5]	OH 4 17 [8]		
	$\delta_{\rm H} \left(J \text{ in Hz} \right)$	$\delta_{\rm C}$, type	$\delta_{\rm H} \left(J \text{ in Hz} \right)$	$\delta_{\rm C}$, type	$\delta_{\rm H} \left(J \text{ in Hz} \right)$	$\delta_{\rm C}$, type	$\delta_{\rm H} \left(J \text{ in Hz} \right)$	$\delta_{\rm C}$, type	
1a	2.14, m	26.2, CH ₂	2.09, m	25.7, CH ₂	4.18, dd	72.7, CH	2.54, ddd	36.5, CH ₂	
1b	1.63, m		1.61, m				1.68, m		
2a	2.04, m	28.7, CH ₂	2.00, dddd	28.8, CH ₂	2.61, ddd	42.3, CH ₂	4.30, ddd	74.2, CH	
2b	1.47, m		1.46, m		1.43, ddd				
3	2.17, m	27.2, CH	2.11, m	26.6, CH	2.01, ddq	27.1, CH	1.98, qd	37.9, CH	
4		38.5, C		38.8, C		39.3, C		40.8, C	
5		38.7, C		38.7, C		39.6, C		39.0, C	
6	1.59, m	40.8, CH	1.48, m	41.1, CH	1.42, m	52.8, CH	1.62, m	41.8, CH	
7a	2.05, m	35.0, CH ₂	1.67, dd	43.0, CH ₂	1.74, dd	41.6, CH ₂	1.71, dd	42.5, CH ₂	
7b	1.15, dd		1.49, m		1.64, dd		1.56, dd		
8		43.9, C		39.2, C		39.8, C		39.7, C	
9a	3.57, d	79.6, CH	1.41, d	43.9, CH ₂	1.43, m	43.9, CH ₂	1.02, m	43.9, CH ₂	
9b			1.01, d		1.02, m		1.43, m		
10a	2.25, ddd	33.2, CH ₂	1.78, m	21.6, CH ₂	1.79, m	22.2, CH ₂	1.60, m	21.6, CH ₂	
10b	1.39, dd		1.56, m		1.58, m		1.81, m		
11	1.86, ddd	43.9, CH	1.87, ddd	44.4, CH	1.81, ddd	44.6, CH	1.85, m	44.4, CH	
12	1.74, d	46.2, CH	1.27, d	52.0, CH	1.28, d	52.2, CH	1.30, d	51.9, CH	
13a	1.71, dt	26.7, CH ₂	1.68, m	26.4, CH ₂	1.74, ddd	26.8, CH ₂	1.18, ddd	26.4, CH ₂	
13b	1.26, ddd		1.21, ddd		1.24, ddd		1.68, m		
14a	1.59, m	41.0, CH ₂	1.57, ddd	40.8, CH ₂	1.62, ddd	41.4, CH ₂	1.62, m	41.1, CH ₂	
14b	1.46, m		1.44, m		1.45, m		1.46, ddd		
15		73.8, C		73.9, C		73.8, C		73.8, C	
16	1.20, s	21.2, CH ₃	1.17, s	20.5, CH ₃	1.18, s	21.3, CH ₃	1.18, s	20.4, CH ₃	
17	1.04, d	23.2, CH ₃	1.02, d	22.9, CH ₃	1.07, d	23.1, CH ₃	1.19, s	20.4, CH ₃	
18	1.06, s	24.8, CH ₃	1.05, s	24.6, CH ₃	0.98, s	26.6, CH ₃	0.95, s	25.3, CH ₃	
19	0.99, s	25.5, CH ₃	0.94, s	25.6, CH ₃	1.13, s	25.6, CH ₃	0.96, s	25.4, CH ₃	
20	0.97, s	19.6, CH ₃	1.05, s	19.9, CH ₃	0.91, d	20.5, CH ₃	1.13, s	20.3, CH ₃	

 Table S1: ¹H and ¹³C NMR data of compounds 1-4