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Novel peptaibiotics identified from *Trichoderma* clade *Viride*

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Abstract

This study focuses on the peptaibiome produced by different species of *Trichoderma* belonging to clade *Viride*: *T. koningii* SZMC 28387 (CBS 979.70), *T. cf. strigosellum* SZMC 28007 (TUCIM 4886/IQ 191), *T. cf. dorotheopsis* SZMC 28390 (TUCIM 416/TUB F-597), *T. cf. strigosellum* SZMC 28391 (TUCIM 423/DAOM 230018), *T. atroviride* SZMC 28748 (IMI 206040), *T. hamatum* SZMC 28747 (TUCIM 2730) and *T. cf. dorotheopsis* SZMC 28005 (TUCIM 4882/IQ 11). We were able to identify new compounds with similarity to already known groups of peptaibiotics, as well as completely newly discovered compounds using high-performance liquid chromatography (HPLC) -mass spectrometry (MS). From the 367 peptaibiotics identified, 216 are peptaibols and 111 are lipopeptaibols. Out of all peptaibols, 55 are previously known, while 161 are newly discovered. The new peptaibol subgroups Strigosellin A, B and Dorotheopsin A, B are introduced. Furthermore, besides 38 previously known lipopeptaibols, 73 new lipopeptaibol sequences, named Lipostrigosellins and Lipohamatins are also reported. In addition, 41 peptaibol-like compounds with unusual C-terminus were also found. Out of the 7 strains examined, 5 produced both peptaibols and lipopeptaibols, while 2 only peptaibols. The well-known compound, Trikonigin KA V (TRK-V) also produced by *T. koningii* SZMC 28387 (CBS 979.70), was studied for its folding dynamics using accelerated molecular dynamics simulations (aMD) for understanding the plausible three-dimensional structures adopted by these peptaibols of clade *Viride*. We observed a propensity to form kinked, right-handed helical structures when simulated in an aqueous environment.

Keywords *Trichoderma*, Clade *Viride*, Peptaibol, Lipopeptaibol, Peptaibiome, HPLC–MS, Accelerated MD simulations

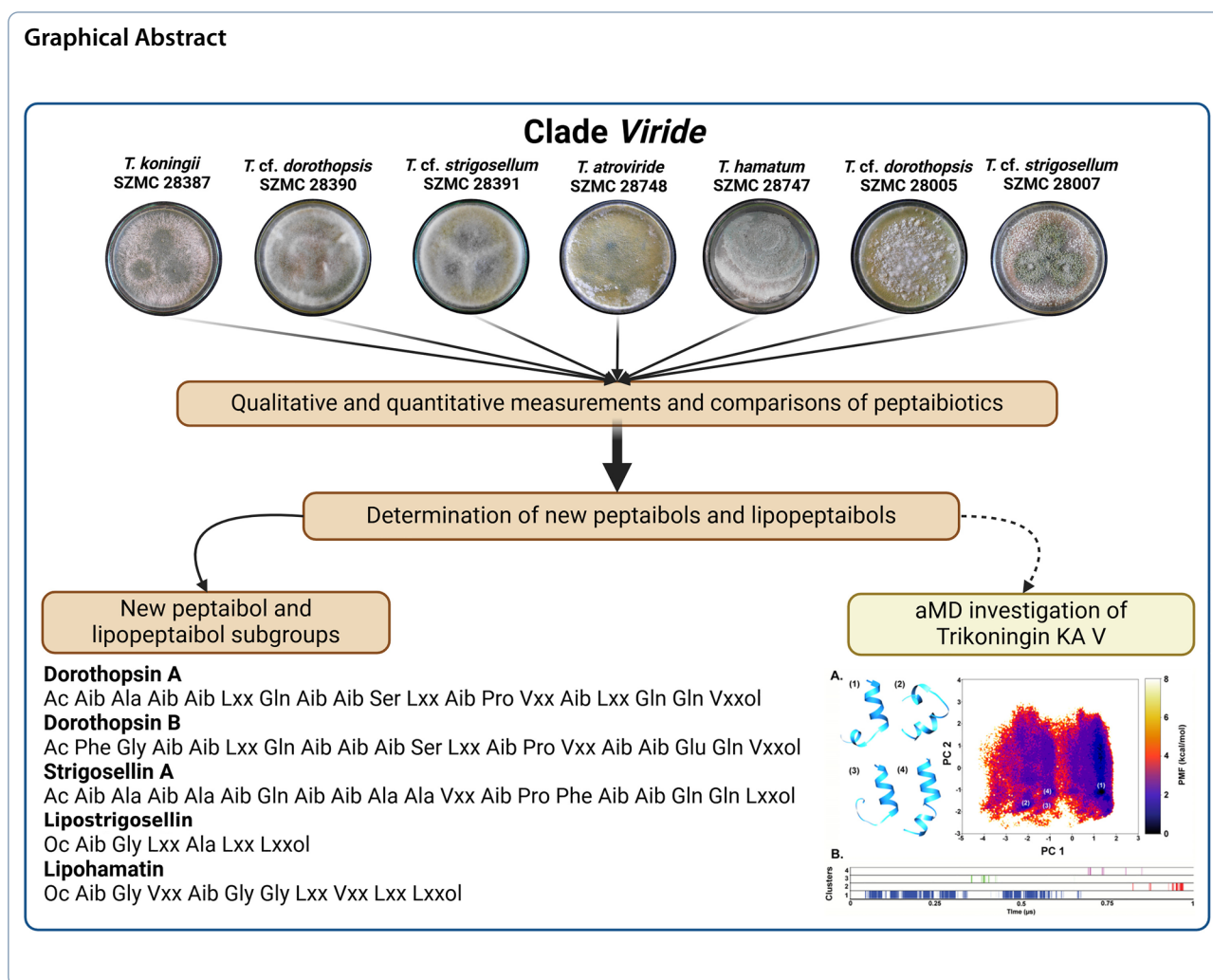
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Graphical Abstract



1 Introduction

Clade *Viride* stands as one of the most extensive and varied group within the genus *Trichoderma*. Members of this clade exhibit a broad range of habitats and are found across diverse geographic regions [1]. They play significant roles in various sectors including industry, agriculture, and medicine [2]. One notable example is *T. viride*, which effectively combats decay in Obeche wood (*Triplochiton scleroxylon*) caused by *Gloeophyllum* sp. and *G. sepiarium* through mycoparasitism and nutrient competition [3]. Certain species within this clade, such as *T. asperellum* and *T. atroviride*, were thought to be problematic for commercial mushroom cultivation, but eventually, they were not found to cause green mould infection of mushrooms even though they appeared in mushroom growing substrates [4]. *Trichoderma* green mould affects both *Agaricus bisporus* and *Pleurotus ostreatus*, two of the most important mushroom crops, leading to inquiries into the particular strains implicated

and their preference for substrates. Green mould agents were described as *T. aggressivum*, *T. pleuroti* and *T. pleuroticola* belonging to clade *Harzianum* of the genus *Trichoderma*, while no green mould infections could be attributed to *T. asperellum* and *T. atroviride* [4–7]. Morphological characteristics of clade *Viride* representatives are consistent slow growth rate, globose to subglobose and strongly warted conidia, often solitary conidiophores and hooked phialides [8]. However, these morphological characteristics are not sufficient for exact species-level identification due to the overlap of morphology of *Trichoderma* species, and therefore, they need to be combined with molecular characterization. The mainly used one being integration of phenetic and phylogenetic characters, which is emphasized for species recognition, with a focus on concordance between both approaches, the translation elongation factor 1 α (*tef1 α*), internal transcribed spacer 1 and 2 (ITS1 and 2) regions, as well as, sequence analysis of fragments RNA polymerase II gene

(*rpb2*) genes with subsequent phylogenetic analysis. These altogether are essential for characterizing new species and understanding the genetic diversity within the clade [9].

Genus *Trichoderma* is recognized for generating secondary metabolites, including polyketides, alkaloids, terpenoids, non-ribosomally biosynthesized peptides, and mixed biogenesis metabolites [10]. Currently, extensive research on this genus is underway due to the production of bioactive peptaibiotics. Besides *Trichoderma* species, members of other closely related genera like *Emerizellopsis* and *Gliocladium* are also significant producers of peptaibiotics [11]. The analytical exploration of peptaibiotics is referred to as peptaibiotics [12]. Peptaibiotics is described as the entirety of fungal peptides which contain the amino acid residue α -aminoisobutyric acid (Aib) [12, 13]. These acyclic peptides are synthesized by non-ribosomal peptide synthetase (NRPS) enzymes [14].

In this study, peptaibols and lipopeptaibols were identified out of the 5 groups of peptaibiotics, which were categorized based on their length and chemical structures [12]. Peptaibols constitute a class of linear antibiotic peptides characterized by their length, usually ranging from five to twenty amino acids. Notable features of peptaibols include a high occurrence of non-proteinogenic C-alpha tetrasubstituted amino acids [15], such as the relatively uncommon isovaline (Iva) or the achiral Aib. Typically, the N-terminal amino acid of peptaibols is acylated, while the C-terminus consists of a β -amino alcohol. Among the most prevalent types of β -amino alcohols at the C-terminus are isoleucinol, phenylalaninol, valinol, and leucinol (Leuol). These compounds represent the most extensive category within peptaibiotics and several peptaibols are already known to be produced by members of clade *Viride* [16]. Lipopeptaibols represent naturally occurring short peptides possessing antimicrobial properties [17]. They are distinguished by a lipophilic acyl chain at the N-terminus, a significant presence of turn/helix forming Aib, and a 1,2-amino alcohol at the C-terminus. These peptides typically consist of 6 to 11 amino acid residues and feature fatty acyl moieties ranging from 8 to

15 carbon atoms, which is shorter compared to the non-lipidated peptaibols that typically contain 11 to 20 amino acid residues [17, 18]. Due to the presence of a lipophilic N-terminal group, these peptides are known as lipopeptaibols. They have been extracted from several fungal cultures including *T. koningii* (trikoningsins) and *T. viride* (trichodecenins) from clade *Viride*, as well as *T. longibrachiatum* (trichogins), *T. polysporum* (trichopolysins), *Tolypocladium geodes* (antibiotics LP 237), and *Mycogone rosea* (helioferins) [17, 18]. It is then imperative that more unknown structures of peptaibiotics should be studied and analyzed to continue the growth of the scientific knowledge and industrial application of this unique and promising group of secondary metabolites.

2 Materials and methods

2.1 Fungal strains, media, culture conditions

Trichoderma strains were selected from the TU Collection of Industrially Important Microorganisms (TUCIM), Vienna, Austria and deposited at Szeged Microbiology Collection (SZMC) (Table 1). The selected strains were cultivated on yeast-glucose agar medium enriched with malt extract (3 g/L yeast extract, 10 g/L glucose, 20 g/L agar, and 50 mL of 20% liquid malt extract solution). To increase peptaibol production, the strains were cultivated on malt extract agar (MEA) medium containing 150 mL (20%) malt extract solution, 3 g/L soybean peptone, and 15 g/L agar. Incubation was carried out for 7 days at 25 °C, and mycelial growth was subsequently observed.

2.2 Extraction of peptaibols

Following the incubation period, peptaibols were extracted from the *Trichoderma* cultures using a solution composed of chloroform and methanol in a 2/1 (v/v) ratio. The resulting mixture was subjected to evaporation using an IKA RV 10 rotatory evaporator (IKA Works, USA) until complete dryness. The resultant dry mass was reconstituted in 1 mL of methanol and thoroughly mixed. Subsequently, the samples underwent centrifugation for 15 min (Heraeus Fresco 17, Thermo

Table 1 *Trichoderma* strains selected for this study. The re-identification was based on the sequence analysis of the *tef1a* region

SZMC code	TUCIM code	Other code	Species	Reference	Re-identified species
28387	201	CBS 979.70	<i>T. sp.</i>	[19]	<i>T. koningii</i>
28390	416	TUB F-597	<i>T. taiwanense</i>	[20]	<i>T. cf. dorotheopsis</i>
28391	423	DAOM 230018	<i>T. strigosellum</i>	[21]	<i>T. cf. strigosellum</i>
28748	1680	IMI 206040	<i>T. atroviride</i>	[22]	<i>T. atroviride</i>
28747	2730	—	<i>T. fertile</i>	—	<i>T. hamatum</i>
28005	4882	IQ 11	<i>T. koningiopsis</i>	[23]	<i>T. cf. dorotheopsis</i>
28007	4886	IQ 191	<i>T. cf. strigosellum</i>	[23]	<i>T. cf. strigosellum</i>

Scientific, CA, USA) to eliminate insoluble particles, and the clarified samples were stored at -20°C for further analysis.

2.3 Species reidentification

To cultivate mycelia of the *Trichoderma* strains, liquid medium was prepared in Eppendorf tubes on yeast-glucose agar medium enriched with malt extract mentioned above. The tubes were incubated for 2 days at 25°C . After incubation, approximately 100 mg of fungal tissue was introduced into sterile Eppendorf tubes. Glass beads with particle sizes of 0.4–0.6 mm and 0.9–0.15 mm were added to the tubes, and liquid nitrogen was employed for cell disruption. The tubes were placed in a cell disruptor for 4 min, and this process was repeated three times.

Following the initial procedures, DNA extraction was carried out using the E.Z.N.A.[®] Fungal DNA Mini Kit in accordance with the manufacturer's instructions. Subsequent to DNA purification, the *tefla* region was amplified through polymerase chain reaction (PCR). The PCR master mixture for each sample (1 μL) consisted of 2 μL of Dream Taq buffer, 2 μL of dNTP mix, 4–4 μL of 1 μM *tefla* primers (forward: 5'-CATCGAGAAGTTCGAGAA GG-3' and reverse: 5'-AACTTGCAAGCAATGTGG-3'), 7 μL of water, and 0.1 μL of Dream Taq DNA polymerase. The PCR cycle was conducted using the MJ Mini[™] Personal Thermal Cycler (BIO-RAD) following these steps: an initial step at 94°C for 5 min; cycling steps at 94°C for 30 s (denaturation), 57°C for 30 s (annealing), and 72°C for 30 s (elongation), repeated for 40 cycles; and a final elongation step at 72°C for 4 min. Agarose gel electrophoresis was performed to check the success of the reaction on 1% agarose gel (35 mL TAE buffer, 0.35 g agarose, 2 μL ethidium bromide). Two μL of DNA samples were applied with 2 μL of bromophenol blue. The run time for gel electrophoresis was 30 min at 90 V. The DNA fragments were sent for sequence analysis to an external service (Eurofins Scientific). Sequences were analyzed by using Finch TV 1.4.0 (Geospiza Inc.) and NCBI Nucleotide BLAST softwares (<https://blast.ncbi.nlm.nih.gov/Blast.cgi>).

Multiple sequence alignment of partial *tefla* sequences (provided in the supplementary file) was made by PAGAN v1.53 [24] with default settings. The final dataset consisted of two partitions for the intron and exon regions. For both partitions, the best fitting model was TrN+G4, determined by using ModelTest-NG v0.1.7 [25], based on the Bayesian Information Criterion (BIC). Maximum likelihood analysis with the selected models was carried out by RAXML-NG v1.2.2 [26], with 1000 bootstrap replicates.

2.4 Analytical procedures for peptaibols

The analysis of crude peptaibol extracts was conducted using high-performance liquid chromatography-mass spectrometry (HPLC–MS) based on a method previously described by Marik et al. [27]. For the analysis, an Orbitrap (QExactive Plus, Thermo Scientific, CA, USA) MS was used with a heated electrospray ion source (HESI) in positive mode coupled with an Dionex Ultimate 3000 (Thermo Scientific, CA, USA) HPLC containing a quaternary pump, a vacuum degasser, an autosampler, and a column heater. The instruments were controlled by the Xcalibur 4.2 Software (Thermo Scientific, CA, USA). The separation was achieved using a Purospher Star RP-15 HPLC column (100×2.1 , 2 μm), while the solvent A consisted of $\text{H}_2\text{O}/\text{MeOH}/\text{MeCN}$ (8/1/1, v/v) with 5 mM ammonium acetate and 0.1% (v/v) acetic acid and solvent B comprised of acetonitrile/methanol (1/1, v/v) with 5 mM ammonium acetate and 0.1% (v/v) acetic acid. The flow rate was set to 0.2 mL/min, and the gradient program for Solvent B was as follows: 0 min—65%, 2 min—65%, 42 min—80%, 54 min—90%, 55 min—95%, 58 min—95%, 58.5—65% and 62.5—65%. The column temperature was maintained at 30°C , and the injection volume was 3 μL . The HESI parameters were as follows: spray voltage – 4.5 kV, sheath gas flow rate – 30 arbitrary units, aux gas flow rate – 12 arbitrary units, capillary temperature – 300°C , aux gas heater – 300°C . The acquisition mode was Full-MS-ddMS². Full-MS parameters were: resolution – 70,000 at m/z 200, AGC target – $3\text{e}6$, maximum injection time – 100 ms, scan range – 200–2000 m/z . The ddMS² parameters: fixed first scan at m/z 80, resolution 17500 at m/z 200, AGC target – $1\text{e}6$, maximum injection time – 50 ms, isolation window – 1 m/z , collision energy – 25 NCE. Loop count was set to 5.

2.5 Determination and nomenclature of peptaibol sequences

Peptaibols typically undergo fragmentation between Aib–Pro residues already in the ion source resulting in the generation of b- and y-ions. The identification of a specific peptaibol compound relies on its retention times (R_t) and on the mass of its b- and y-fragment ions as well as the mass of the hydrogen adduct of the primary mass of the compound $[\text{M}+\text{H}]^+$ (b-ion + y-ion). During full scan measurements, the mass of the protonated molecular ion coexists with other adduct ions such as the primary mass and sodium adduct $[\text{M}+\text{Na}]^+$, the primary mass and 2 hydrogen adducts $[\text{M}+2\text{H}]^{2+}$, the primary mass and 2 sodium adducts $[\text{M}+2\text{Na}]^{2+}$, and the primary mass and hydrogen and sodium adducts $[\text{M}+\text{H}+\text{Na}]^{2+}$. In the longer peptaibols (16–19 residues), the fragmentation typically occurred between the centrally located

Aib–Pro residues, leading to the formation of b_{11-12} and y_{5-7} ions. The analysis of MS² results from b- and y-ion fragments provided insights into the complete sequences of the compounds (Supplementary Fig. 1).

Lipopeptaibols were identified based on the MS² fragmentation of $[M+H]^+$. The whole sequence could be observed on the MS² spectra.

To assess the novelty of the obtained sequences, an initial comparison was made using the ‘Comprehensive Peptaibiotics Database’ [28]. This database is not available online since 2017, however, Prof. Rainer Schuhmacher kindly provided the offline version of the Peptaibiotics Database including the peptaibiotics records till 2017. Consequently, to gather more information and conduct a comprehensive comparison, an additional online literature search was conducted using PubMed (<https://pubmed.ncbi.nlm.nih.gov/>) with the keywords ‘peptaibol’ or ‘lipopeptaibol’.

The quantity of peptaibols were defined based on the integration of the peaks under the major y-ions originated from the decomposition of the Aib–Pro bond in the ion source on the extracted ion chromatograms (EIC) of the full scan MS measurement. Adding the separately integrated peaks resulted in the total peptaibol production of the strain, out of which, percentages were calculated for each compound. The quantity of lipopeptaibols was defined based on the integration of the peaks under the $[M+H]^+$ on the EIC of the full scan MS measurement. Percentages of each compound were calculated as mentioned above.

The known peptaibols and lipopeptaibols were named using the closest identified compounds attached to a Roman numeral based on their elution order. The completely novel sequences were named after the producer species attached to a Roman numeral based on their elution order.

2.6 aMD simulations to reveal folding dynamics of Trikonigin KA V (TRK-V)

Trikonigin KA V was selected because the isotype of Vxx and Lxx residues of this compound was determined by Goulard et al. [29]. For non-standard amino acid residues, Aib and Leuol, the partial charges and force fields were calculated using a previously developed method reported by Tyagi et al. [30]. The unfolded peptide topology was prepared using the ‘tleap’ module of AmberTools20 using the Amberff19SB force field and solvated in TIP3P water solvent model [31]. The peptide solvation added 2324 water residues with the periodic box size of 45.96×44.35×46.88 Å and volume of 95587 Å³. The system preparation, minimization and equilibration steps were carried out as described in Tyagi et al. [32]. To calculate boost parameters, total number of atoms in the

system (Natoms=19467), number of residues (Nres=20) and coefficients a1, a2 (4.5) and b1, b2 (0.20) were utilized. The aMD simulation was run for 1000 ns or 1 μs in total. The resulting trajectory files were prepared by the removal of water molecules. Dihedral angles were calculated for every residue from each frame of the simulation and the distribution was reweighted using Maclaurin series expansion.

3 Results and discussion

3.1 Reidentification of the investigated *Trichoderma* strains

The examined isolates were assigned to species based on sequence analysis of partial *tef1α* sequences (provided in the supplementary file). Figure 1 shows the phylogenetic relation between the strains investigated in this article and the type strains of closely related species. *T. koningii* SZMC 28387 and *T. atroviride* SZMC 28748 showed 100% identity with their type strains. Strain SZMC 28747 originally was identified as *T. fertile*, however, it showed 100% identity with the type strains of *T. hamatum*. *T. cf. strigosellum* SZMC 28391 and SZMC 28007 could not be identified to species level, therefore, *cf. strigosellum* was introduced. *T. taiwanense* SZMC 28390 and *T. cf. dorotheopsis* SZMC 28005 did not match with their type strains either, but were similar to *T. dorotheopsis* type strain and were named as *T. cf. dorotheopsis* SZMC 28390 and *T. cf. dorotheopsis* SZMC 28005.

3.2 Peptaibiome of the investigated *Trichoderma* strains

Out of the 7 strains investigated, (Table 1), 5 produced both peptaibols and lipopeptaibols (*T. cf. strigosellum* SZMC 28391 and SZMC 28007, *T. koningii* SZMC 28387, *T. hamatum* SZMC 28747, and *T. cf. dorotheopsis* SZMC 28005), while *T. cf. dorotheopsis* SZMC 28390 and *T. atroviride* SZMC 28748 did not produce any lipopeptaibols, their peptaibiome consisted of exclusively SF1 peptaibols (Table 2, Supplementary Fig. 1). The two *T. cf. strigosellum* strains produced ~40/60% ratio of peptaibols/lipopeptaibols *T. koningii* SZMC 28387 and *T. cf. dorotheopsis* SZMC 28005 produced one third ratio of peptaibols of the peptaibiome, while *T. hamatum* SZMC 28747 produced only one fourth of peptaibols of the peptaibiome (Table 2). Based on their length, lipopeptaibols could be categorised into the short (6–7-residue long), medium (10–11-residue long) or long (15-residue long) groups. The most amount of short lipopeptaibols was produced by *T. cf. strigosellum* SZMC 28007 with 61.35% of the peptaibiome, while the greatest number of long lipopeptaibols were produced by *T. hamatum* SZMC 28747 with 40.36% of the peptaibiome. The amount of

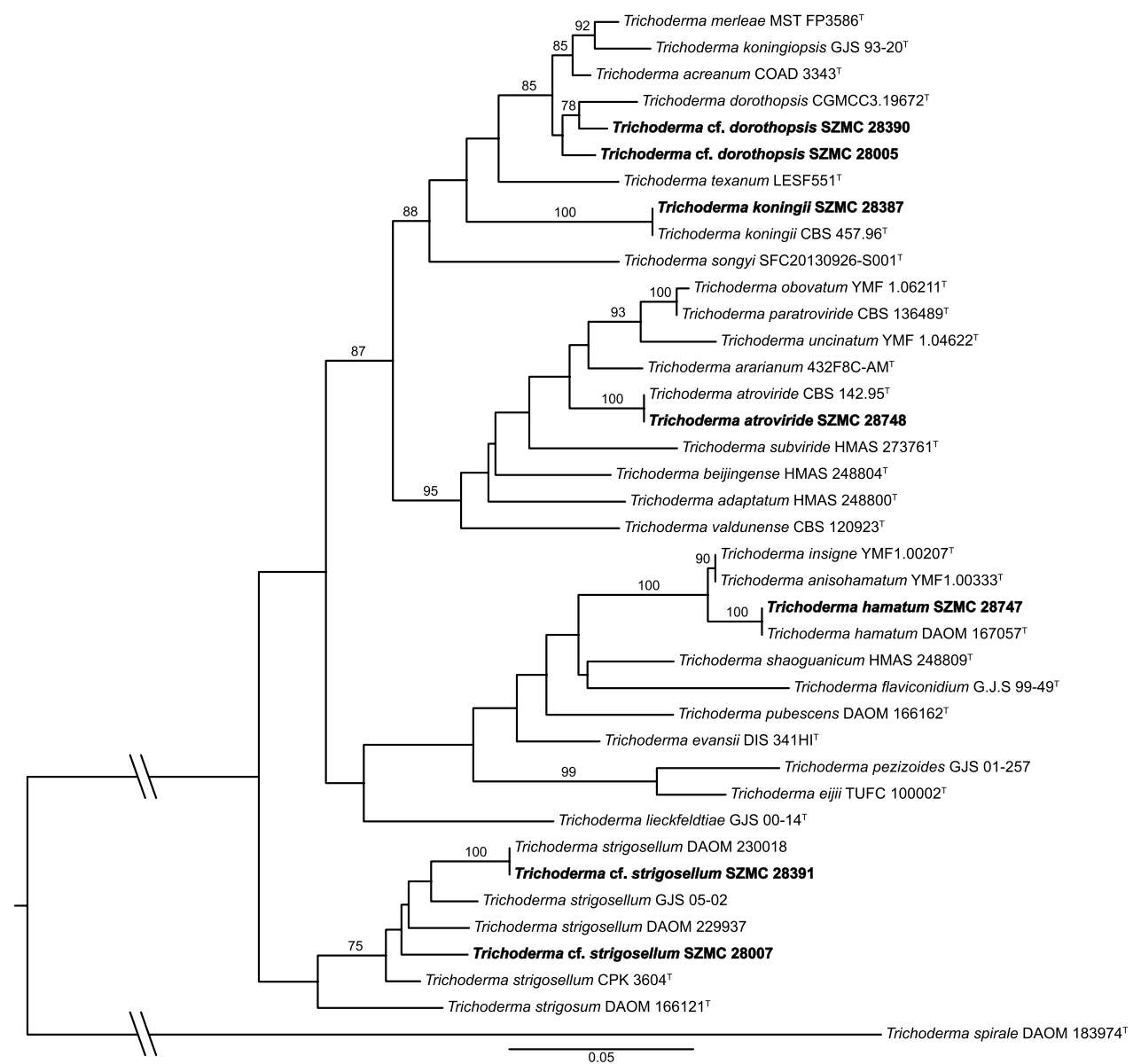


Fig. 1 Phylogenetic tree of the examined strains from clade *Viride* based on their partial *tef1a* sequences

Table 2 Ratio of peptaibiotics (peptaibiome) produced by the members of clade *Viride* investigated in this study

Species	SZMC	Peptaibols	Short lipopeptaibols	Medium lipopeptaibols	Long lipopeptaibols
<i>T. cf. strigosellum</i>	28391	39.25%	60.25%	—	—
<i>T. cf. strigosellum</i>	28007	39.35%	61.35%	—	—
<i>T. koningii</i>	28387	32.08%	2.78%	65.14%	—
<i>T. cf. dorotheopsis</i>	28390	100.00%	—	—	—
<i>T. atroviride</i>	28748	100.00%	—	—	—
<i>T. hamatum</i>	28747	23.62%	3.71%	32.36%	40.36%
<i>T. cf. dorotheopsis</i>	28005	33.25%	—	53.15%	13.60%

medium lipopeptaibols was ranging from 30 to 65% of the total production (Table 2).

3.3 Peptaibol profiles of the investigated *Trichoderma* strains

Tables 3 and 4 were obtained from the chromatographic and MS analysis of the investigated *Trichoderma* strains and show the subfamily 1 (SF-1) peptaibols of the investigated *Trichoderma* strains. The diagnostic fragment ions resulted by MS² fragmentation are collected in Supplementary Table 1.

3.3.1 Identification of new Strigaibol sequences and the new groups of Strigosellins from *T. cf. strigosellum*

Investigation of the peptaibol profile of *T. cf. strigosellum* SZMC 28391 revealed twenty-one 19-residue peptaibols belonging to the SF-1 peptaibol family (Tables 3 and 4). Apart from the known Strigaibol sequences, 14 proved to be new. Their closest positional isomers are Strigaibol sequences described by Park et al. [33]. MS and chromatographical analysis of *T. cf. strigosellum* SZMC 28007 revealed the production of 14 peptaibols novel to science and were named as Strigosellin A as well as further 6 sequences named as Strigosellin B peptaibols. These peptaibols showed a great similarity to the sequences of Trichokonin TKO-V, Trichokonin V, Tricholongin B and Tricholongin LBI sequences [34–37].

Strain *T. cf. strigosellum* SZMC 28391 produced two peptaibols in higher quantities, which were Strigaibol XII and XIV (36.15% and 27.59% of the total peptaibol production, respectively). Four more sequences were produced above 4%, Strigaibol V, VI, X and XX (5.14%, 6.44%, 4.34% and 7.2%, respectively). Strain *T. cf. strigosellum* SZMC 28007 produced Strigosellin A IX covering 14.55% of the total peptaibol production, while Strigosellins A XII, XIII, and XIV were also produced in relatively higher quantities (10.73%, 13.01% and 10.95%, respectively). Strigosellins A II, V, VI, and VIII, were also produced in significant quantities between 2.78 and 7.41%, while Strigosellins A I, III, IV, VII, X, and XI were produced at 0.48–1.78% of the total peptaibol production. Strigosellins B I, II and V were produced also in significant quantities (5.38%, 8.2% and 6.51%, respectively), while Strigosellin B I, B III, B IV and B VI were below 2.44%.

3.3.2 New Trikoningin KA-like peptaibol compounds from *T. koningii*

T. koningii SZMC 28387 produced thirty-eight new sequences, while nineteen were positionally isomeric with the previously described Trikoningin KA V from *T. koningii* described by Goulard et al. [29], and

Trikoningin KA-like compounds Ia, IVa, IVb, Va, VIa and XI from *T. gamsii* SZMC 1656 described by Marik et al. [38] (Tables 3 and 4).

T. koningii SZMC 28387 also produced two peptaibols, Trikoningin KA-like XLIII and XLV (25.83% and 28.48%, respectively) in high quantities, while apart from Trikoningin KA-like XL, XLVI and XLVIII (4.65%, 6.25% and 6.74%, respectively), the rest of the peptaibols were produced for less than 3% and mostly below 1%.

3.3.3 Identification of the new group of Dorothopsins from *T. cf. dorothopsis*

Strain *T. cf. dorothopsis* SZMC 28390 produced thirteen 19-residue peptaibols also belonging to the SF-1 peptaibol family. All the thirteen compounds were completely new (Tables 3, 4) and their closest positional isomers are Trichostrigocins TSG-A and TSG-B described by Degenkolb et al. [37]. These new compounds were named as Dorothopsins A-a I–XIII (Table 3). However, 18-residue peptaibols, Dorothopsins A-b I–VIII and Dorothopsins A-d I–III, as well as, the 17-residue Dorothopsin A-c I and Dorothopsin A-f I–II sequences, furthermore, a 16-residue Dorothopsin A-e I sequence were also produced by this strain (Table 3). All Dorothopsin A sequences are also new additions to literature (Table 4). Strain *T. cf. dorothopsis* SZMC 28390 produced Dorothopsin A-a VII covering more than half of the total peptaibol production (54.05%). After that, Dorothopsins A-a VIII and A-d I, were produced the second highest with 10.48% and 8.35%, respectively. Among the Dorothopsin A-a sequences, a few peptaibols were 1.5%–4.5%, but the rest and all Dorothopsin A-b, -c, -d, -e and -f sequences were below 1.5% apart from Dorothopsin A-d I with 8.35%.

T. cf. dorothopsis SZMC 28005 produced thirty-four new sequences, which were the most unique among the already known SF1 peptaibols and named as Dorothopsin B. They had the most varied sequences, sometimes with differences in 6 positions from the already known Tricholongin LBI sequence described by Degenkolb et al. [37]. The most interesting characteristic of these sequences is the substitution of the acetylated Aib1 (Ac-Aib1) and Phe3 known from Tricholongin sequences to the acetylated Phe1 (Ac-Phe1) and Aib3. Furthermore, Phe1 was also substituted with Trp1 in several Dorothopsin B sequences. The most produced sequence by *T. cf. dorothopsis* SZMC 28005 was Dorothopsin B XXVI with a relatively low quantity of 10.15%, which was followed by Dorothopsins B VII, XIII, XV, XXV, XXXI, and XXXIV (5.05%, 9.71%, 7.95%, 6.16%, 4.01% and 4.53%, respectively). All the other sequences were produced below 4%.

Table 3 SF1 peptaibols produced by *Trichoderma* strains from clade *Viride*

Peptaibol	[M+H] ⁺	b ₁₃	y ₇	RT (min)	Area (%) peptaibome	Area (%) total peptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19	
T. cf. strigosellum SZMC 28391																											
Strigai- bol-like I	1893.12	1152.66	740.46	24.66	0.38%	0.96%	Ac	Alb	Ser	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Vxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Lxxol	
Strigai- bol-like II	1907.14	1166.68	740.46	24.66	0.33%	0.85%	Ac	Vxx	Ser	Alb	Alb	Lxx	Gln	Alb	Ala	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Lxxol	
Strigai- bol-like III	1893.13	1166.68	726.45	24.9	0.03%	0.08%	Ac	Vxx	Ser	Alb	Alb	Lxx	Gln	Alb	Ala	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Ala	Gln	Gln	Lxxol	
Strigai- bol-like IV	1907.14	1180.69	726.45	25.53	0.10%	0.24%	Ac	Vxx	Ser	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Vxxol	
Strigai- bol-like V	1907.14	1166.68	740.46	26.67	2.02%	5.14%	Ac	Alb	Ser	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Lxxol	
Strigai- bol-like VI	1907.14	1166.68	740.46	27.53	2.53%	6.44%	Ac	Vxx	Ser	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Vxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Lxxol	
Strigai- bol-like VII	1893.13	1166.68	726.45	27.75	0.09%	0.23%	Ac	Vxx	Ser	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Vxx	Alb	Pro	Vxx	Alb	Ala	Gln	Gln	Lxxol	
Strigai- bol-like VIII	1877.13	1150.68	726.45	28.2	0.14%	0.35%	Ac	Alb	Ala	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Vxxol	
Strigai- bol-like IX	1891.14	1150.68	740.46	28.4	0.27%	0.68%	Ac	Alb	Ala	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Lxxol	
Strigai- bol-like X	1877.13	1136.67	740.46	29.66	1.70%	4.34%	Ac	Alb	Ala	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Vxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Lxxol	
Strigai- bol-like XI	1907.14	1166.68	740.46	29.66	0.22%	0.57%	Ac	Alb	Ser	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Lxxol	
Strigai- bol-like XII	1921.15	1180.69	740.46	29.66	14.19%	36.15%	Ac	Vxx	Ser	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Lxxol	
Strigai- bol-like XIII	1907.14	1166.68	740.46	30.52	1.01%	2.58%	Ac	Vxx	Ser	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Vxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Lxxol	
Strigai- bol-like XIV	1891.14	1150.68	740.46	32.31	10.83%	27.59%	Ac	Alb	Ala	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Lxxol	
Strigai- bol-like XV	1905.16	1164.7	740.46	32.31	0.83%	2.11%	Ac	Vxx	Ser	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Lxxol	

Table 3 (continued)

Peptaibol	[M+H] ⁺	b ₁₃	y ₇	RT (min)	Area (%) peptaibome	Area (%) total peptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19	
Strigai-bol-like XVI	1921.15	1180.69	740.46	32.31	0.01%	0.02%	Ac	Vxx	Ser	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Lxxol	
Strigai-bol-like XVII	1877.13	1136.67	740.46	33.98	0.34%	0.85%	Ac	Alb	Ala	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Vxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Lxxol	
Strigai-bol-like XVIII	1875.15	1134.69	740.46	34.86	0.41%	1.06%	Ac	Alb	Ala	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ala	Lxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Lxxol	
Strigai-bol-like XIX	1905.16	1164.7	740.46	34.86	0.63%	1.61%	Ac	Alb	Alb	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Lxxol	
Strigai-bol-like XX	1891.14	1150.68	740.46	36.1	2.83%	7.20%	Ac	Alb	Ala	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Lxxol	
Strigai-bol-like XXI	1919.17	1178.71	740.46	37.55	0.37%	0.94%	Ac	Alb	Vxx	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Lxxol	
T. koningii SZMC 28387																											
Trikon-ingin KA-like I	1863.12	1108.64	754.48	31.31	0.02%	0.06%	Ac	Alb	Gly	Ala	Alb	Vxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Vxx	Gln	Gln	Lxxol	
Trikon-ingin KA-like II	1864.10	1108.64	755.46	31.88	0.02%	0.06%	Ac	Alb	Gly	Ala	Alb	Vxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Vxx	Glu	Gln	Lxxol	
Trikon-ingin KA-like III	1878.11	1122.65	755.46	31.88	0.01%	0.02%	Ac	Alb	Gly	Ala	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Vxx	Glu	Gln	Lxxol	
Trikon-ingin KA-like IV	1877.13	1108.64	768.49	32.89	0.09%	0.29%	Ac	Alb	Gly	Gly	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Lxx	Gln	Gln	Lxxol	
Trikon-ingin KA-like V	1907.28	1138.79	768.49	32.89	0.22%	0.70%	Ac	Alb	Gly	Ser	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Lxx	Gln	Gln	Lxxol	
Trikon-ingin KA-like VI	1878.12	1108.64	769.48	33.42	0.09%	0.28%	Ac	Alb	Gly	Ala	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Lxx	Glu	Gln	Lxxol	
Trikon-ingin KA-like VII	1908.27	1138.79	769.48	33.42	0.15%	0.48%	Ac	Alb	Gly	Ser	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Lxx	Glu	Gln	Lxxol	
Trikon-ingin KA-like VIII	1847.12	1092.64	754.48	34.01	0.01%	0.02%	Ac	Alb	Gly	Gly	Alb	Lxx	Gln	Alb	Alb	Alb	Ala	Lxx	Alb	Pro	Vxx	Alb	Vxx	Gln	Gln	Lxxol	

Table 3 (continued)

Peptabool	[M+H] ⁺	b ₁₃	y ₇	RT (min)	Area (%) total peptabiome	Area (%) peptabool	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19
Trikon- ingin KA- like IX	1863.12	1108.64	754.48	34.01	0.05%	0.16%	Ac	Aib	Gly	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol
Trikon- ingin KA- like X	1877.13	1122.65	754.48	34.01	0.03%	0.08%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol
Trikon- ingin KA- like XI	1877.13	1108.64	768.49	34.76	0.13%	0.40%	Ac	Aib	Gly	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol
Trikon- ingin KA- like XII	1907.14	1138.65	768.49	34.76	0.19%	0.60%	Ac	Aib	Gly	Ser	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol
Trikon- ingin KA- like XIII	1863.12	1108.64	754.48	34.97	0.01%	0.02%	Ac	Aib	Gly	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol
Trikon- ingin KA- like XIV	1877.13	1122.65	754.48	34.97	0.00%	0.01%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol
Trikon- ingin KA- like XV	1878.12	1108.64	769.48	35.36	0.17%	0.52%	Ac	Aib	Gly	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Lxxol
Trikon- ingin KA- like XVI	1908.27	1138.79	769.48	35.36	0.16%	0.50%	Ac	Aib	Gly	Ser	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Lxxol
Trikon- ingin KA-like XVII	1878.11	1122.65	755.46	35.5	0.01%	0.02%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Glu	Gln	Lxxol
Trikon- ingin KA-like XVIII	1877.13	1108.64	768.49	35.88	0.05%	0.17%	Ac	Aib	Gly	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol
Trikon- ingin KA- like XIX	1891.14	1122.65	768.49	35.88	0.13%	0.41%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol
Trikon- ingin KA- like XX	1878.12	1108.64	769.48	36.34	0.69%	2.15%	Ac	Aib	Gly	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Lxxol
Trikon- ingin KA- like XXI	1892.13	1122.65	769.48	36.34	0.05%	0.17%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Lxxol

Table 3 (continued)

Peptaibol	[M+H] ⁺	b ₁₃	y ₇	RT (min)	Area (%) peptaibome	Area (%) total peptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19
Trikon- ingin KA-like XXII	1861.13	1092.64	768.49	37.36	0.03%	0.09%	Ac	Aib	Gly	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol
Trikon- ingin KA-like XXIII	1877.13	1108.64	768.49	37.36	0.20%	0.63%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Ala	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol
Trikon- ingin KA-like XXIV	1847.12	1092.64	754.48	37.46	0.04%	0.13%	Ac	Aib	Gly	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol
Trikon- ingin KA-like XXV	1863.12	1108.64	754.48	37.46	0.22%	0.69%	Ac	Aib	Gly	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol
Trikon- ingin KA-like XXVI	1877.13	1122.65	754.48	37.46	0.40%	1.26%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol
Trikon- ingin KA-like XXVII	1862.12	1092.64	769.48	37.94	0.11%	0.35%	Ac	Aib	Gly	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Lxxol
Trikon- ingin KA-like XXVIII	1878.12	1108.64	769.48	37.94	0.28%	0.86%	Ac	Aib	Gly	Gly	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Lxxol
Trikon- ingin KA-like XXIX	1848.10	1092.64	755.46	38.08	0.05%	0.17%	Ac	Aib	Gly	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Vxx	Glu	Gln	Lxxol
Trikon- ingin KA-like XXX	1864.10	1108.64	755.46	38.08	0.10%	0.30%	Ac	Aib	Gly	Ala	Ala	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Glu	Gln	Lxxol
Trikon- ingin KA-like XXXI	1878.11	1122.65	755.46	38.08	0.42%	1.31%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Glu	Gln	Lxxol
Trikon- ingin KA-like XXXII	1847.12	1092.64	754.48	38.94	0.01%	0.03%	Ac	Ab	Gly	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol

Table 3 (continued)

Peptaibol	[M+H] ⁺	b ₁₃	y ₇	RT (min)	Area (%) total peptaibome	Area (%) peptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19
Trikon- ingin KA-like XXXIII	1861.14	1106.66	754.48	38.94	0.01%	0.04%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol
Trikon- ingin KA-like XXXIV	1877.13	1122.65	754.48	38.94	0.09%	0.28%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol
Trikon- ingin KA-like XXXV	1891.14	1122.65	768.49	39.41	0.97%	3.03%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol
Trikon- ingin KA-like XXXVI	1848.10	1092.64	755.46	39.46	0.00%	0.01%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Vxx	Glu	Gln	Lxxol
Trikon- ingin KA-like XXXVII	1862.12	1106.66	755.46	39.46	0.01%	0.03%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Vxx	Glu	Gln	Lxxol
Trikon- ingin KA-like XXXVIII	1878.11	1122.65	755.46	39.46	0.08%	0.23%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Glu	Gln	Lxxol
Trikon- ingin KA-like XXXIX	1892.13	1122.65	769.48	39.85	0.55%	1.71%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Lxxol
Trikon- ingin KA- like XL	1891.14	1122.65	768.49	40.59	1.49%	4.65%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol
Trikon- ingin KA- like XLI	1892.13	1122.65	769.48	40.9	0.64%	1.99%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Lxxol
Trikon- ingin KA- like XLII	1875.13	1106.64	768.49	41.88	0.32%	0.99%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol
Trikon- ingin KA-like XLIII	1891.14	1122.65	768.49	41.88	8.28%	25.83%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol

Table 3 (continued)

Peptabool	[M+H] ⁺	b ₁₃	y ₇	RT (min)	Area (%) total peptabiome	Area (%) peptabool	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19
Trikon- ingin KA-like XLIV	1876.12	1106.64	769.48	42.36	0.19%	0.59%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Lxxol
Trikon- ingin KA-like XLV	1892.13	1122.65	769.48	42.36	9.14%	28.48%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Lxxol
Trikon- ingin KA-like XLVI	1875.15	1106.66	768.49	43.33	2.01%	6.25%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol
Trikon- ingin KA-like XLVII	1905.16	1136.67	768.49	43.33	0.07%	0.20%	Ac	Aib	Ala	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol
Trikon- ingin KA-like XLVIII	1876.12	1106.64	769.48	43.83	2.16%	6.74%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Lxxol
Trikon- ingin KA-like XLIX	1906.15	1136.67	769.48	43.83	0.07%	0.21%	Ac	Aib	Ala	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Lxxol
Trikon- ingin KA- like L	1891.14	1122.65	768.49	46.05	0.07%	0.23%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol
Trikon- ingin KA- like LI	1905.16	1136.67	768.49	46.05	0.71%	2.22%	Ac	Aib	Ala	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol
Trikon- ingin KA- like LII	1892.13	1122.65	769.48	46.43	0.07%	0.20%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Lxxol
Trikon- ingin KA- like LIII	1906.15	1136.67	769.48	46.43	0.74%	2.31%	Ac	Aib	Ala	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Lxxol
Trikon- ingin KA- like LIV	1889.16	1120.67	768.49	47.39	0.10%	0.32%	Ac	Aib	Ala	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol
Trikon- ingin KA- like LV	1905.16	1136.67	768.49	47.39	0.01%	0.04%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Vxx	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol

Table 3 (continued)

Peptabool	[M + H] ⁺	b ₁₃	y ₇	RT (min)	Area (%) peptabiome	Area (%) total peptabool	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19	
Trikon- ingin KA- like LVI	1890.15	1120.67	769.48	47.77	0.12%	0.38%	Ac	Aib	Ala	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Lxxol	
	1906.15	1136.67	769.48	47.77	0.04%	0.13%	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Vxx	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Lxxol	
T. cf. dorothopsis SZMC 28390																											
Doro- thopsin A-a I	1821.05	1150.68	670.37	12.56	0.31%	0.31%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Ala	Alaol	
Doro- thopsin A-a II	1821.05	1150.68	670.37	13.59	1.33%	1.33%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Ala	Alaol	
Doro- thopsin A-a III	1891.14	1150.68	740.46	32.28	0.37%	0.37%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Vxxol	
Doro- thopsin A-a IV	1891.14	1150.68	740.46	33.3	1.64%	1.64%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Vxxol	
Doro- thopsin A-a V	1892.13	1150.68	741.45	33.76	0.72%	0.72%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Glu	Gln	Vxxol	
Doro- thopsin A-a VI	1905.16	1150.68	754.48	36.28	6.66%	6.66%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Vxxol	
Doro- thopsin A-a VII	1905.16	1150.68	754.48	37.53	54.05%	54.05%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Vxxol	
Doro- thopsin A-a VIII	1906.14	1150.68	755.46	37.98	10.48%	10.48%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Vxxol	
Doro- thopsin A-a IX	1906.22	1164.7	741.52	39.99	0.09%	0.09%	Ac	Vxx	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Glu	Gln	Vxxol	
Doro- thopsin A-a X	1919.18	1164.7	754.48	40.0	4.26%	4.26%	Ac	Vxx	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Vxxol	
Doro- thopsin A-a XI	1920.16	1164.7	755.46	40.4	0.10%	0.10%	Ac	Vxx	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Vxxol	
Doro- thopsin A-a XII	1919.17	1150.68	768.49	41.9	2.63%	2.63%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol	

Table 3 (continued)

Peptabiol	[M+H] ⁺	b ₁₃	Y ₇	RT (min)	Area (%) total peptabiome	Area (%) peptabiol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19
Doro-thopsin A-a XIII	1933.19	1164.7	768.49	42.26	0.27%	0.27%	Ac	Vxx	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxx	
Doro-thopsin A-b I	1736.00	1065.63	670.37	7.84	0.08%	0.08%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	-	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Ala	Alaol
Doro-thopsin A-b II	1736.00	1065.63	670.37	8.98	0.42%	0.42%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	-	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Ala	Alaol
Doro-thopsin A-b III	1806.09	1065.63	740.46	24.46	0.09%	0.09%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	-	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Vxxol
Doro-thopsin A-b IV	1807.08	1065.63	741.45	25.72	0.07%	0.07%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	-	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Glu	Gln	Vxxol
Doro-thopsin A-b V	1806.09	1065.63	740.46	29.68	0.36%	0.36%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	-	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Vxxol
Doro-thopsin A-b VI	1807.08	1065.63	741.45	30.61	0.03%	0.03%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	-	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Glu	Gln	Vxxol
Doro-thopsin A-b VII	1820.11	1065.63	754.48	29.29	2.51%	2.51%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	-	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Vxxol
Doro-thopsin A-b VIII	1821.09	1065.63	755.46	30.44	1.29%	1.29%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	-	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Glu	Gln	Vxxol
Doothop-sin A-c I	1606.96	1065.63	541.33	9.5	1.28%	1.28%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	-	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	-	Ala	Alaol
Doro-thopsin A-d I	1692.01	1150.68	541.33	16.09	8.35%	8.35%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	-	Ala	Alaol
Doro-thopsin A-d II	1692.01	1150.68	541.33	18.36	0.47%	0.47%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	-	Ala	Alaol
Doro-thopsin A-d III	1706.03	1164.7	541.33	18.36	0.28%	0.28%	Ac	Vxx	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	-	Ala	Alaol
Dorothop-sin A-e I	1478.91	1065.63	413.28	10.69	0.12%	0.12%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	-	Ser	Lxx	Aib	Pro	Vxx	Aib	-	-	Gly	Alaol
Doro-thopsin A-f I	1563.96	1150.68	413.28	18.29	0.29%	0.29%	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	-	-	Gly	Alaol

Table 3 (continued)

Peptaibol	[M + H] ⁺	b ₁₃	y ₇	RT (min)	Area (%) peptaibome	Area (%) total peptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19	
Doro- thopsin A-fII	1563.96	1150.68	413.28	19.49	1.46%	1.46%	Ac	Alb	Ala	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	-	-	Gly	Alaol	
T. atrovide SZMC 28748																											
Trichor- zianin TA-like I	1964.14	1108.64	855.5	20.26	0.09%	0.19%	Ac	Alb	Ala	Ala	Alb	Alb	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Lxx	Alb	Lxx	Gln	Gln	Trpol	
Trichor- zianin TA-like II	1950.13	1108.64	841.49	21.39	0.37%	0.75%	Ac	Alb	Ala	Ala	Alb	Alb	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Lxx	Gln	Gln	Trpol	
Trichor- zianin TA-like III	1964.14	1108.64	855.5	23.02	0.23%	0.48%	Ac	Alb	Gly	Ala	Alb	Vxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Lxx	Alb	Lxx	Gln	Gln	Trpol	
Trichor- zianin TA-like IV	1950.13	1108.64	841.49	24.2	0.88%	1.81%	Ac	Alb	Gly	Ala	Alb	Vxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Lxx	Gln	Gln	Trpol	
Trichor- zianin TA-like V	1964.14	1108.64	855.5	25.43	0.92%	1.89%	Ac	Alb	Ala	Ala	Alb	Alb	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Lxx	Alb	Lxx	Gln	Gln	Trpol	
Trichor- zianin TA-like VI	1964.14	1108.64	855.5	25.9	0.21%	0.42%	Ac	Alb	Ala	Ala	Alb	Alb	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Lxx	Alb	Lxx	Gln	Gln	Trpol	
Trichor- zianin TA-like VII	1950.13	1108.64	841.49	26.72	3.74%	7.68%	Ac	Alb	Ala	Ala	Alb	Alb	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Lxx	Gln	Gln	Trpol	
Trichor- zianin TA-like VIII	1941.12	1124.63	816.49	27.55	0.24%	0.49%	Ac	Alb	Ala	Ser	Alb	Alb	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Lxx	Alb	Lxx	Gln	Gln	Pheol	
Trichor- zianin TA-like IX	1950.13	1108.64	841.49	28.13	0.47%	0.96%	Ac	Alb	Ala	Ala	Alb	Vxx	Gln	Ala	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Lxx	Gln	Gln	Trpol	
Trichor- zianin TA-like X	1978.15	1122.65	855.5	28.62	1.35%	2.77%	Ac	Alb	Ala	Ala	Alb	Vxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Lxx	Alb	Lxx	Gln	Gln	Trpol	
Trichor- zianin TA-like XI	1964.14	1122.65	841.49	28.84	0.26%	0.54%	Ac	Alb	Ala	Ala	Alb	Vxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Lxx	Gln	Gln	Trpol	

Table 3 (continued)

Peptaibol	[M+H] ⁺	b ₁₃	y ₇	RT (min)	Area (%) total peptaibome	Area (%) peptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19
Trichor- zianin TA-like XII	1911.11	1094.62	816.49	28.98	0.10%	0.21%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Ala	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	Pheol
Trichor- zianin TA-like XIII	1978.15	1122.65	855.5	29.09	0.24%	0.49%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	Trpol
Trichor- zianin TA-like XIV	1927.11	1124.63	802.48	29.25	0.99%	2.03%	Ac	Aib	Ala	Ser	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Pheol
Trichor- zianin TA-like XV	1964.14	1122.65	841.49	29.94	4.37%	8.99%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Trpol
Trichor- zianin TA-like XVI	1955.14	1138.65	816.49	30.54	0.65%	1.33%	Ac	Aib	Ser	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	Pheol
Trichor- zianin TA-like XVII	1962.16	1106.66	855.5	31.09	0.09%	0.18%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	Trpol
Trichor- zianin TA-like XVIII	1897.10	1094.62	802.48	31.33	0.82%	1.68%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Ala	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Pheol
Trichor- zianin TA-like XIX	1948.15	1106.66	841.49	31.97	0.41%	0.83%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Trpol
Trichor- zianin TA-like XX	1941.13	1138.65	802.48	32.35	2.56%	5.26%	Ac	Aib	Ser	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Pheol
Trichor- zianin TA-like XXI	1925.13	1108.64	816.49	32.78	0.36%	0.75%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	Pheol
Trichor- zianin TA-like XXII	1925.13	1108.64	816.49	33.16	2.65%	5.44%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	Pheol

Table 3 (continued)

Peptabool	[M+H] ⁺	b ₁₃	y ₇	RT (min)	Area (%) total peptabiome	Area (%) peptabool	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19
Trichor- zianin TA-like XXIII	1911.12	1108.64	802.48	33.81	1.88%	3.86%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Pheol
Trichor- zianin TA-like XXIV	1925.13	1108.64	816.49	34.42	0.35%	0.72%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Ala	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	Pheol
Trichor- zianin TA-like XXV	1911.12	1108.64	802.48	35.02	7.42%	15.24%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Pheol
Trichor- zianin TA-like XXVI	1939.14	1122.65	816.49	35.97	0.57%	1.17%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	Pheol
Trichor- zianin TA-like XXVII	1939.14	1122.65	816.49	36.45	3.01%	6.19%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	Pheol
Trichor- zianin TA-like XXVIII	1925.13	1122.65	802.48	37.03	2.60%	5.34%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Pheol
Trichor- zianin TA-like XXIX	1925.13	1122.65	802.48	38.2	8.56%	17.59%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Pheol
Trichor- zianin TA-like XXX	1923.15	1106.66	816.49	38.7	0.41%	0.85%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	Pheol
Trichor- zianin TA-like XXXI	1909.14	1106.66	802.48	40.1	0.90%	1.84%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Pheol
Trichor- zianin TA-like XXXII	1939.14	1122.65	816.49	40.36	0.19%	0.39%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	Pheol
Trichor- zianin TA-like XXXIII	1925.13	1122.65	802.48	42.16	0.82%	1.68%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Pheol

Table 3 (continued)

Peptai- bol	[M + H] ⁺	b ₁₃	y ₇	RT (min)	Area (%) peptai- biome	Area (%) total peptai- bol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19
Peptai- bol-like I	1792.04	1108.64	683.4	4.57	0.04%	1.65%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	146	
Peptai- bol-like II	1791.05	1122.65	668.4	5.69	0.12%	4.47%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	145	
Peptai- bol-like III	1792.04	1108.64	683.4	6.81	0.01%	0.50%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	146	
Peptai- bol-like IV	1778.03	1108.64	669.39	6.9	0.04%	1.52%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	146	
Peptai- bol-like V	1777.04	1108.64	668.4	7.4	0.04%	1.64%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	145	
Peptai- bol-like VI	1792.04	1108.64	683.4	7.75	0.05%	1.86%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	146	
Peptai- bol-like VII	1778.03	1108.64	669.39	8.09	0.13%	4.72%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	146	
Peptai- bol-like VIII	1805.06	1122.65	682.41	8.28	0.00%	0.13%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	145	
Peptai- bol-like IX	1792.04	1122.65	669.39	9.12	0.02%	0.90%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	146	
Peptai- bol-like X	1806.05	1122.65	683.4	9.59	0.07%	2.48%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	146	
Peptai- bol-like XI	1792.04	1122.65	669.39	9.97	0.16%	6.04%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	146	
Peptai- bol-like XII	1791.05	1122.65	668.4	10.27	0.02%	0.86%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	145	
Peptai- bol-like XIII	1791.05	1108.64	682.41	10.64	0.01%	0.28%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	145	
Peptai- bol-like XIV	1777.04	1108.64	668.4	11.97	0.10%	3.57%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	145	
Peptai- bol-like XV	1791.05	1108.64	682.41	12.19	0.02%	0.80%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	145	

Table 3 (continued)

Peptaibol	[M+H] ⁺	b ₁₃	y ₇	RT (min)	Area (%) peptaibol	Area (%) total peptaibome	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19
Peptai- bol- <i>like</i> XVI	1791.05	1122.65	668.4	13.37	0.02%	0.57%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	145
Peptai- bol- <i>like</i> XVII	1791.05	1108.64	682.41	13.82	0.00%	0.14%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	145
Peptai- bol- <i>like</i> XVIII	1791.05	1122.65	668.4	14.45	0.13%	4.70%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	145
Peptai- bol- <i>like</i> XIX	1805.06	1122.65	682.41	14.73	0.04%	1.31%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	145
Peptai- bol- <i>like</i> XX	1806.05	1122.65	683.4	14.73	0.02%	0.74%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	160
Peptai- bol- <i>like</i> XXI	1791.05	1122.65	668.4	16.01	0.02%	0.65%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	145
Peptai- bol- <i>like</i> XXII	1791.05	1108.64	682.41	16.51	0.01%	0.22%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	145
Peptai- bol- <i>like</i> XXIII	1792.04	1108.64	683.4	16.93	0.09%	3.50%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	160
Peptai- bol- <i>like</i> XXIV	1792.04	1108.64	683.4	18.36	0.02%	0.70%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	160
Peptai- bol- <i>like</i> XXV	1806.05	1122.65	683.4	19.95	0.12%	4.54%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	160
Peptai- bol- <i>like</i> XXVI	1806.05	1122.65	683.4	21.55	0.02%	0.80%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	160
Peptai- bol- <i>like</i> XXVII	1982.12	1108.64	873.48	9.81	0.17%	6.31%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	222
Peptai- bol- <i>like</i> XXVIII	1996.14	1108.64	887.5	10.53	0.05%	1.76%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	222
Peptai- bol- <i>like</i> XXIX	1982.12	1108.64	873.48	11.6	0.07%	2.53%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	222

Table 3 (continued)

Peptaibol	[M+H] ⁺	b ₁₃	γ ₇	RT (min)	Area (%) peptaibiome	Area (%) total peptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19
Peptai- bol-like XXX	1982.12	1108.64	873.48	11.9	0.22%	8.09%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	222
Peptai- bol-like XXXI	1996.14	1108.64	887.5	12.00	0.03%	1.30%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	222
Peptai- bol-like XXXII	2010.15	1122.65	887.5	12.78	0.06%	2.14%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	222
Peptai- bol-like XXXIII	1996.13	1122.65	873.48	14.04	0.15%	5.73%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	222
Peptai- bol-like XXXIV	1996.14	1108.64	887.5	14.45	0.06%	2.38%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	222
Peptai- bol-like XXXV	1996.13	1122.65	873.48	15.49	0.04%	1.53%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	222
Peptai- bol-like XXXVI	1996.14	1108.64	887.5	16.57	0.05%	1.96%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	222
Peptai- bol-like XXXVII	1996.14	1108.64	887.5	17.62	0.03%	1.05%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	222
Peptai- bol-like XXXVIII	1982.12	1108.64	873.48	17.81	0.14%	5.35%	Ac	Aib	Ala	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	222
Peptai- bol-like XXXIX	2010.15	1122.65	887.5	19.43	0.06%	2.34%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	222
Peptai- bol-like XL	2010.15	1122.65	887.5	20.6	0.04%	1.55%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Lxx	Aib	Lxx	Gln	Gln	222
Peptai- bol-like XLI	1996.13	1122.65	873.48	20.69	0.18%	6.68%	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	222
<i>T. hamatum</i> SZMC 28747																										
Tricho- longin LB-like I	1925.14	1170.66	754.48	16.82	0.28%	1.17%	Ac	Aib	Gly	Phe	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol
Tricho- longin LB-like II	1835.08	1094.62	740.46	19.69	0.39%	1.66%	Ac	Aib	Gly	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Lxxol

Table 3 (continued)

Peptaibol	[M+H] ⁺	b ₁₃	y ₇	RT (min)	Area (%) peptaibome	Area (%) peptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19
Tricho- longin LB-like III	1897.10	1156.64	740.46	20.39	0.21%	0.91%	Ac	Ala	Gly	Phe	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Lxxol
Tricho- longin LB-like IV	1849.10	1094.62	754.48	22.32	0.36%	1.50%	Ac	Aib	Gly	Ala	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol
Tricho- longin LB-like V	1927.10	1186.64	740.46	22.83	0.31%	1.29%	Ac	Aib	Gly	Tyr	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Lxxol
Tricho- longin LB-like VI	1911.12	1156.64	754.48	22.94	0.31%	1.31%	Ac	Ala	Gly	Phe	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol
Tricho- longin LB-like VII	1941.12	1186.64	754.48	25.48	0.35%	1.47%	Ac	Aib	Gly	Tyr	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol
Tricho- longin LB-like VIII	1897.10	1156.64	740.46	26.14	0.59%	2.49%	Ac	Aib	Gly	Phe	Aib	Aib	Gln	Ala	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Lxxol
Tricho- longin LB-like IX	1897.10	1156.64	740.46	26.66	0.46%	1.93%	Ac	Aib	Gly	Phe	Ala	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Lxxol
Tricho- longin LB-like X	1911.12	1156.64	754.48	27.13	0.50%	2.10%	Ac	Aib	Gly	Phe	Aib	Ala	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol
Tricho- longin LB-like XI	1911.11	1170.65	740.46	27.43	0.34%	1.43%	Ac	Aib	Gly	Phe	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Lxxol
Tricho- longin LB-like XII	1911.12	1156.64	754.48	28.14	0.45%	1.90%	Ac	Aib	Gly	Phe	Aib	Aib	Gln	Aib	Ala	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol
Tricho- longin LB-like XIII	1911.11	1170.65	740.46	28.7	6.07%	25.68%	Ac	Aib	Gly	Phe	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Lxxol

Table 3 (continued)

Peptaiabol	[M+H] ⁺	b ₁₃	y ₇	RT (min)	Area (%) peptaibiome	Area (%) total peptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19	
Tricho- longin LB-like XIV	1911.12	1156.64	754.48	29.36	0.71%	3.01%	Ac	Aib	Gly	Phe	Ala	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol	
Tricho- longin LB-like XV	1911.11	1170.65	740.46	29.91	0.40%	1.70%	Ac	Aib	Gly	Phe	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Lxxol	
Tricho- longin LB-like XVI	1925.13	1170.65	754.48	31.37	6.87%	29.09%	Ac	Aib	Gly	Phe	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol	
Tricho- longin LB-like XVII	1925.13	1184.67	740.46	32.02	1.68%	7.13%	Ac	Aib	Ala	Phe	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Lxxol	
Tricho- longin LB-like XVIII	1925.13	1170.65	754.48	32.53	0.59%	2.51%	Ac	Aib	Gly	Phe	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol	
Tricho- longin LB-like XIX	1939.15	1184.67	754.48	34.64	2.37%	10.03%	Ac	Aib	Ala	Phe	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol	
Tricho- longin LB-like XX	1909.13	1168.67	740.46	34.74	0.09%	0.36%	Ac	Aib	Ala	Phe	Aib	Aib	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Lxxol	
Tricho- longin LB-like XXI	1923.15	1168.67	754.48	37.27	0.31%	1.33%	Ac	Aib	Ala	Phe	Aib	Aib	Gln	Aib	Aib	Aib	Ala	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol	
<i>T. cf. dorathopsis</i> SZMC 28005																											
Doro- thopsin B I	1897.10	1170.65	726.45	20.25	0.46%	1.38%	Ac	Phe	Gly	Aib	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Vxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol	
Doro- thopsin B II	1898.08	1170.65	727.43	20.39	0.61%	1.85%	Ac	Phe	Gly	Aib	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Vxx	Aib	Pro	Vxx	Aib	Aib	Glu	Gln	Vxxol	
Doro- thopsin B III	1911.12	1184.67	726.45	21.53	0.31%	0.92%	Ac	Phe	Gly	Aib	Aib	Lxx	Gln	Aib	Ala	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol	

Table 3 (continued)

Peptaibol	[M+H] ⁺	b ₁₃	γ ₇	RT (min)	Area (%) total peptaibome	Area (%) peptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19
Doro- thopsin B IV	1912.10	1184.67	727.43	21.68	0.49%	1.47%	Ac	Phe	Gly	Aib	Aib	Lxx	Gln	Aib	Ala	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Glu	Gln	Vxxol
Doro- thopsin B V	1911.12	1184.67	726.45	22.34	0.78%	2.35%	Ac	Phe	Gly	Aib	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol
Doro- thopsin B VI	1912.10	1184.67	727.43	22.51	1.29%	3.89%	Ac	Phe	Gly	Aib	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Glu	Gln	Vxxol
Doro- thopsin B VII	1964.14	1237.69	726.45	23.4	1.67%	5.03%	Ac	Trp	Gly	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol
Doro- thopsin B VIII	1965.12	1237.69	727.43	23.65	1.01%	3.03%	Ac	Trp	Gly	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Glu	Gln	Vxxol
Doro- thopsin B IX	1911.12	1184.67	726.45	23.81	0.34%	1.03%	Ac	Phe	Gly	Aib	Aib	Lxx	Gln	Aib	Ala	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol
Doro- thopsin B X	1912.10	1184.67	727.43	24.06	1.00%	2.99%	Ac	Phe	Gly	Aib	Aib	Lxx	Gln	Aib	Ala	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Glu	Gln	Vxxol
Doro- thopsin B XI	1911.12	1184.67	726.45	25.05	0.54%	1.62%	Ac	Phe	Gly	Aib	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol
Doro- thopsin B XII	1964.14	1237.69	726.45	25.05	0.24%	0.72%	Ac	Trp	Gly	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol
Doro- thopsin B XIII	1925.13	1198.68	726.45	25.99	3.23%	9.71%	Ac	Phe	Gly	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol
Doro- thopsin B XIV	1964.14	1237.69	726.45	25.99	0.74%	2.22%	Ac	Trp	Gly	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol
Doro- thopsin B XV	1926.11	1198.68	727.43	26.18	2.64%	7.95%	Ac	Phe	Gly	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Glu	Gln	Vxxol
Doro- thopsin B XVI	1965.12	1237.69	727.43	26.18	0.60%	1.82%	Ac	Trp	Gly	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Glu	Gln	Vxxol
Doro- thopsin B XVII	1911.12	1184.67	726.45	27.78	0.14%	0.41%	Ac	Phe	Gly	Aib	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol

Table 3 (continued)

Peptaibol	[M+H] ⁺	b ₁₃	γ ₇	RT (min)	Area (%) total peptaibome	Area (%) peptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19
Doro- thopsin B XVIII	1964.14	1237.69	726.45	27.78	0.23%	0.70%	Ac	Trp	Gly	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol
Doro- thopsin B XIX	1925.13	1198.68	726.45	27.78	1.27%	3.83%	Ac	Phe	Gly	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol
Doro- thopsin B XX	1978.16	1251.71	726.45	27.78	0.23%	0.69%	Ac	Trp	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol
Doro- thopsin B XXI	1912.10	1184.67	727.43	28.01	0.14%	0.43%	Ac	Phe	Gly	Aib	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Glu	Gln	Vxxol
Doro- thopsin B XXII	1965.12	1237.69	727.43	28.01	0.24%	0.72%	Ac	Trp	Gly	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Glu	Gln	Vxxol
Doro- thopsin B XXIII	1926.11	1198.68	727.43	28.01	1.31%	3.93%	Ac	Phe	Gly	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Glu	Gln	Vxxol
Doro- thopsin B XXIV	1979.14	1251.71	727.43	28.01	0.24%	0.71%	Ac	Trp	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Glu	Gln	Vxxol
Doro- thopsin B XXV	1925.13	1198.68	726.45	28.58	2.05%	6.16%	Ac	Phe	Gly	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol
Doro- thopsin B XXVI	1926.11	1198.68	727.43	28.73	3.38%	10.15%	Ac	Phe	Gly	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Glu	Gln	Vxxol
Doro- thopsin B XXVII	1939.15	1212.7	726.45	29.68	1.25%	3.75%	Ac	Phe	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol
Doro- thopsin B XXVIII	1940.13	1212.7	727.43	29.89	1.23%	3.71%	Ac	Phe	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Glu	Gln	Vxxol
Doro- thopsin B XXIX	1925.13	1198.68	726.45	30.57	0.79%	2.38%	Ac	Phe	Gly	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol
Doro- thopsin B XXX	1978.16	1251.71	726.45	30.57	0.16%	0.48%	Ac	Trp	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol
Doro- thopsin B XXXI	1926.11	1198.68	727.43	30.6	1.33%	4.01%	Ac	Phe	Gly	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Glu	Gln	Vxxol

Table 3 (continued)

Peptaibol	[M + H] ⁺	b ₁₃	γ ₇	RT (min)	Area (%) total peptaibome	Area (%) peptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19	
Doro- thopsin B XXXII	1979.14	1251.71	727.43	30.6	0.27%	0.80%	Ac	Trp	Ala	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Glu	Gln	Vxxol	
Doro- thopsin B XXXIII	1939.15	1212.7	726.45	32.41	0.93%	2.78%	Ac	Phe	Ala	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Vxxol	
Doro- thopsin B XXXIV	1940.13	1212.7	727.43	32.56	1.51%	4.53%	Ac	Phe	Ala	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Glu	Gln	Vxxol	
Doro- thopsin B XXXV	1939.15	1212.7	726.45	35.05	0.23%	0.69%	Ac	Phe	Ala	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Gln	Gln	Vxxol	
Doro- thopsin B XXXVI	1940.13	1212.7	727.43	35.18	0.38%	1.15%	Ac	Phe	Ala	Alb	Alb	Lxx	Gln	Alb	Alb	Alb	Ser	Lxx	Alb	Pro	Vxx	Alb	Alb	Glu	Gln	Vxxol	
T. cf. strigosellum SZMC 28007																											
Strigo- sellin A I	1870.06	1080.61	789.45	12.97	0.18%	0.48%	Ac	Alb	Ser	Alb	Ala	Alb	Gln	Alb	Alb	Ala	Ala	Vxx	Alb	Pro	Phe	Alb	Alb	Glu	Gln	Lxxol	
Strigo- sellin A II	1869.07	1080.61	788.46	13.58	2.87%	7.41%	Ac	Alb	Ser	Alb	Ala	Alb	Gln	Alb	Alb	Ala	Ala	Vxx	Alb	Pro	Phe	Alb	Alb	Gln	Gln	Lxxol	
Strigo- sellin A III	1869.07	1080.61	788.46	14.29	0.69%	1.78%	Ac	Alb	Ala	Alb	Ala	Alb	Gln	Alb	Alb	Ser	Ala	Vxx	Alb	Pro	Phe	Alb	Alb	Gln	Gln	Lxxol	
Strigo- sellin A IV	1884.07	1094.62	789.45	14.57	0.19%	0.49%	Ac	Alb	Ser	Alb	Ala	Alb	Gln	Alb	Alb	Ala	Ala	Lxx	Alb	Pro	Phe	Alb	Alb	Glu	Gln	Lxxol	
Strigo- sellin A V	1883.08	1094.62	788.46	15	1.96%	5.07%	Ac	Alb	Ser	Alb	Ala	Alb	Gln	Alb	Alb	Ala	Ala	Lxx	Alb	Pro	Phe	Alb	Alb	Gln	Gln	Lxxol	
Strigo- sellin A VI	1883.09	1080.61	802.48	15.83	2.16%	5.60%	Ac	Alb	Ser	Alb	Ala	Alb	Gln	Alb	Alb	Ala	Ala	Vxx	Alb	Pro	Phe	Vxx	Alb	Gln	Gln	Lxxol	
Strigo- sellin A VII	1854.07	1080.61	789.45	16.55	0.40%	1.03%	Ac	Alb	Ala	Alb	Ala	Alb	Gln	Alb	Alb	Ser	Ala	Vxx	Alb	Pro	Phe	Alb	Alb	Glu	Gln	Lxxol	
Strigo- sellin A VIII	1897.1	1094.62	802.48	17.25	1.07%	2.78%	Ac	Alb	Ser	Alb	Ala	Alb	Gln	Alb	Alb	Ala	Ala	Lxx	Alb	Pro	Phe	Vxx	Alb	Gln	Gln	Lxxol	
Strigo- sellin A IX	1853.08	1064.62	788.46	17.08	5.62%	14.55%	Ac	Alb	Ala	Alb	Ala	Alb	Gln	Alb	Alb	Ala	Ala	Vxx	Alb	Pro	Phe	Alb	Alb	Gln	Gln	Lxxol	

Table 3 (continued)

Peptaibol	[M+H] ⁺	b ₁₃	y ₇	RT (min)	Area (%) total peptaibome	Area (%) peptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19
Strigo-sellin A X	1884.07	1094.62	789.45	18.32	0.47%	1.21%	Ac	Aib	Ser	Aib	Ala	Aib	Gln	Aib	Aib	Ala	Ala	Lxx	Aib	Pro	Phe	Aib	Aib	Glu	Gln	Lxxol
Strigo-sellin A XI	1883.09	1080.61	802.48	18.32	0.21%	0.55%	Ac	Aib	Ser	Aib	Ala	Aib	Gln	Aib	Aib	Ala	Ala	Vxx	Aib	Pro	Phe	Vxx	Aib	Gln	Gln	Lxxol
Strigo-sellin A XII	1867.09	1078.63	788.46	18.79	4.15%	10.73%	Ac	Aib	Ala	Aib	Ala	Aib	Gln	Aib	Aib	Ala	Ala	Lxx	Aib	Pro	Phe	Aib	Aib	Gln	Gln	Lxxol
Strigo-sellin A XIII	1867.09	1064.61	802.48	19.75	5.03%	13.01%	Ac	Aib	Ala	Aib	Ala	Aib	Gln	Aib	Aib	Ala	Ala	Vxx	Aib	Pro	Phe	Vxx	Aib	Gln	Gln	Lxxol
Strigo-sellin A XIV	1881.11	1078.63	802.48	21.33	4.23%	10.95%	Ac	Aib	Ala	Aib	Ala	Aib	Gln	Aib	Aib	Ala	Ala	Lxx	Aib	Pro	Phe	Vxx	Aib	Gln	Gln	Lxxol
Strigo-sellin B I	1833.11	1078.63	754.48	22.13	2.08%	5.38%	Ac	Aib	Ala	Aib	Ala	Aib	Gln	Aib	Aib	Ala	Ala	Lxx	Aib	Pro	Lxx	Aib	Aib	Gln	Gln	Lxxol
Strigo-sellin B II	1833.1	1064.61	768.49	22.45	3.17%	8.20%	Ac	Aib	Ala	Aib	Ala	Aib	Gln	Aib	Aib	Ala	Ala	Vxx	Aib	Pro	Lxx	Aib	Vxx	Gln	Gln	Lxxol
Strigo-sellin B III	1819.09	1064.61	754.48	23.17	0.94%	2.44%	Ac	Aib	Ala	Aib	Ala	Aib	Gln	Aib	Aib	Ala	Ala	Vxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol
Strigo-sellin B IV	1833.11	1078.63	754.48	24.27	0.31%	0.80%	Ac	Aib	Ala	Aib	Ala	Aib	Gln	Aib	Aib	Ala	Ala	Lxx	Aib	Pro	Lxx	Aib	Aib	Gln	Gln	Lxxol
Strigo-sellin B V	1847.12	1078.63	768.49	24.92	2.51%	6.51%	Ac	Aib	Ala	Aib	Ala	Aib	Gln	Aib	Aib	Ala	Ala	Lxx	Aib	Pro	Lxx	Aib	Vxx	Gln	Gln	Lxxol
Strigo-sellin B VI	1833.11	1078.63	754.48	25.76	0.58%	1.51%	Ac	Aib	Ala	Aib	Ala	Aib	Gln	Aib	Aib	Ala	Ala	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol

Table 4 Similarities of SF1 peptaibols produced by *Trichoderma* strains from clade *Viride* to known peptaibols

Peptaibol	Compound identical or positionally isomeric with	Reference
<i>T. cf. strigosellum</i> SZMC 28391		
Strigaibol-like I	Strigaibol A	[33]
Strigaibol-like II	New: Strigaibol B: [Aib] ¹ → [Vxx] ¹ ; [Aib] ⁸ → [Ala] ⁸	[33]
Strigaibol-like III	New: Strigaibol B: [Aib] ¹ → [Vxx] ¹ ; [Aib] ⁸ → [Ala] ⁸ ; [Gln] ¹⁶ → [Ala] ¹⁶	→ Strigaibol-like II
Strigaibol-like IV	New: Strigaibol B: [Aib] ¹ → [Vxx] ¹ ; [Lxx] ¹⁹ → [Vxx] ¹⁹	[33]
Strigaibol-like V	Strigaibol B	[33]
Strigaibol-like VI	New: Strigaibol D: [Aib] ¹ → [Vxx] ¹ ; [Ala] ² → [Ser] ² (Positional isomer of Strigaibol-like XIII)	[33]
	New: Strigaibol C: [Aib] ¹ → [Vxx] ¹ ; [Lxx] ¹¹ → [Vxx] ¹¹	[33]
Strigaibol-like VII	New: Strigaibol D: [Aib] ¹ → [Vxx] ¹ ; [Ala] ² → [Ser] ² ; [Gln] ¹⁶ → [Ala] ¹⁶	[33]
	New: Strigaibol C: [Aib] ¹ → [Vxx] ¹ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Gln] ¹⁶ → [Ala] ¹⁶	[33]
Strigaibol-like VIII	New: Strigaibol E: [Lxx] ¹⁹ → [Vxx] ¹⁹	[33]
Strigaibol-like IX	Strigaibol E (Positional isomer of Strigaibol-like XIV, XX)	[33]
Strigaibol-like X	Strigaibol D	[33]
Strigaibol-like XI	Strigaibol C	[33]
Strigaibol-like XII	New: Strigaibol C: [Aib] ¹ → [Vxx] ¹	[33]
Strigaibol-like XIII	New: (Positional isomer of Strigaibol-like VI)	→ Strigaibol-like VI
Strigaibol-like XIV	(Positional isomer of Strigaibol-like IX, XX)	→ Strigaibol-like IX
Strigaibol-like XV	New: Strigaibol C: [Aib] ¹ → [Vxx] ¹ ; [Aib] ¹⁰ → [Vxx] ¹⁰	[33]
	New: Strigaibol G: [Aib] ¹ → [Vxx] ¹ ; [Ser] ¹⁰ → [Ala] ¹⁰	[33]
Strigaibol-like XVI	New: (Positional isomer of Strigaibol-like XII)	→ Strigaibol-like XII
Strigaibol-like XVII	Strigaibol F	→ Strigaibol-like X
Strigaibol-like XVIII	Strigaibol G	[33]
Strigaibol-like XIX	Strigaibol H	[33]
Strigaibol-like XX	(Positional isomer of Strigaibol-like IX, XIV)	→ Strigaibol-like IX
Strigaibol-like XXI	New: Strigaibol E, H: [Ala] ² → [Vxx] ²	[33]
<i>T. koningii</i> SZMC 28387		
Trikoningin KA-like I	Pept-Ia	[38]
Trikoningin KA-like II	New: Pept-Ia: [Gln] ¹⁷ → [Glu] ¹⁷	[38]
Trikoningin KA-like III	New: Pept-VIa: [Gln] ¹⁷ → [Glu] ¹⁷	[38]
Trikoningin KA-like IV	New: Trikoniging KA V: [Ala] ³ → [Gly] ³	[29]
Trikoningin KA-like V	New: Trikoniging KA V: [Ala] ³ → [Ser] ³ (Positional isomer of Trikoniging KA-like XII)	[29]
Trikoningin KA-like VI	New: Trikoniging KA V: [Gln] ¹⁷ → [Glu] ¹⁷ (Positional isomer of Trikoniging KA-like XXI, XXXIX, XLI, XLV, LII)	[29]
Trikoningin KA-like VII	New: Trikoniging KA V: [Ala] ³ → [Ser] ³ ; [Gln] ¹⁷ → [Glu] ¹⁷ (Positional isomer of Trikoniging KA-like XVI)	[29]
Trikoningin KA-like VIII	New: Pept-VIa: [Ala] ³ → [Gly] ³ ; [Ser] ¹⁰ → [Ala] ¹⁰	[38]
Trikoningin KA-like IX	Pept-IVa (Positional isomer of Trikoniging KA-like XIII, XXV)	[38]
Trikoningin KA-like X	Pept-VIa	[38]
Trikoningin KA-like XI	Pept-IVb (Positional isomer of Trikoniging KA-like XVIII)	[38]
Trikoningin KA-like XII	New: (Positional isomer of Trikoniging KA-like V)	→ Trikoniging KA-like V
Trikoningin KA-like XIII	(Positional isomer of Trikoniging KA-like XIII, XXV)	→ Trikoniging KA-like IX
Trikoningin KA-like XIV	Pept-Va	[38]
Trikoningin KA-like XV	New: Pept-IVb: [Gln] ¹⁷ → [Glu] ¹⁷ (Positional isomer of Trikoniging KA-like XX)	[38]
Trikoningin KA-like XVI	New: (Positional isomer of Trikoniging KA-like VII)	→ Trikoniging KA-like VII
Trikoningin KA-like XVII	New: Pept-Va: [Lxx] ¹⁶ → [Vxx] ¹⁶ ; [Gln] ¹⁷ → [Glu] ¹⁷	[38]
Trikoningin KA-like XVIII	(Positional isomer of Trikoniging KA-like XI)	→ Trikoniging KA-like XI
Trikoningin KA-like XIX	Trikoningin KA V (Positional isomer of Trikoniging KA-like XXXV, XL, XLIII, L)	[29]
Trikoningin KA-like XX	New: (Positional isomer of Trikoniging KA-like XV)	→ Trikoniging KA-like XV
Trikoningin KA-like XXI	New: (Positional isomer of Trikoniging KA-like VI, XXXIX, XLI, XLV, LII)	→ Trikoniging KA-like VI
Trikoningin KA-like XXII	New: Pept-IVb: [Ser] ¹⁰ → [Ala] ¹⁰	[38]

Table 4 (continued)

Peptaibol	Compound identical or positionally isomeric with	Reference
Trikoningin KA-like XXIII	New: Trikoningin KA V: [Aib] ⁸ → [Ala] ⁸	[29]
Trikoningin KA-like XXIV	New: Pept-IVa: [Ser] ¹⁰ → [Ala] ¹⁰ (Positional isomer of Trikoningin KA-like XXXII)	[38]
Trikoningin KA-like XXV	(Positional isomer of Trikoningin KA-like IX, XIII)	→ Trikoningin KA-like IX
Trikoningin KA-like XXVI	(Positional isomer of Trikoningin KA-like XIV, XXXIV)	→ Trikoningin KA-like XIV
Trikoningin KA-like XXVII	New: Pept-IVa: [Ser] ¹⁰ → [Ala] ¹⁰ ; [Gln] ¹⁷ → [Glu] ¹⁷	[38]
Trikoningin KA-like XXVIII	New: Trikoningin KA V: [Ala] ³ → [Gly] ³ ; [Gln] ¹⁷ → [Glu] ¹⁷	[29]
Trikoningin KA-like XXIX	New: Pept-IVa: [Ser] ¹⁰ → [Ala] ¹⁰ ; [Gln] ¹⁷ → [Glu] ¹⁷	[38]
Trikoningin KA-like XXX	New: Pept-Va: [Aib] ⁴ → [Ala] ⁴ ; [Gln] ¹⁷ → [Glu] ¹⁷	[38]
Trikoningin KA-like XXXI	New: Pept-Va: [Gln] ¹⁷ → [Glu] ¹⁷	[38]
Trikoningin KA-like XXXII	New: (Positional isomer of Pept-XXIV)	→ Trikoningin KA-like XXIV
Trikoningin KA-like XXXIII	New: Pept-Va: [Ser] ¹⁰ → [Ala] ¹⁰	[38]
Trikoningin KA-like XXXIV	(Positional isomer of Pept-XIV, Pept-XXVI)	→ Trikoningin KA-like XIV
Trikoningin KA-like XXXV	(Positional isomer of Pept-XIX, Pept-XL, Pept-XLIII, Pept-L)	→ Trikoningin KA-like XIX
Trikoningin KA-like XXXVI	New: Pept-Va: [Aib] ⁹ → [Ala] ⁹ ; [Ser] ¹⁰ → [Ala] ¹⁰ ; [Gln] ¹⁷ → [Glu] ¹⁷	[38]
Trikoningin KA-like XXXVII	New: Pept-Va: [Ser] ¹⁰ → [Ala] ¹⁰ ; [Gln] ¹⁷ → [Glu] ¹⁷	[38]
Trikoningin KA-like XXXVIII	New: Pept-Va: [Gln] ¹⁷ → [Glu] ¹⁷	[38]
Trikoningin KA-like XXXIX	New: (Positional isomer of Trikoningin KA-like VI, XXI, XLI, XLV, LII)	→ Trikoningin KA-like VI
Trikoningin KA-like XL	(Positional isomer of Trikoningin KA-like XIX, XXXV, XLIII, L)	→ Trikoningin KA-like XIX
Trikoningin KA-like XLI	New: (Positional isomer of Trikoningin KA-like VI, XXI, XXXIX, XLV, LII)	→ Trikoningin KA-like VI
Trikoningin KA-like XLII	Pept-XVI (Positional isomer of Trikoningin KA-like XLVI)	[38]
Trikoningin KA-like XLIII	(Positional isomer of Trikoningin KA-like XIX, XXXV, XL, L)	→ Trikoningin KA-like XIX
Trikoningin KA-like XLIV	New: Trikoningin KA V: [Ser] ¹⁰ → [Ala] ¹⁰ ; [Gln] ¹⁷ → [Glu] ¹⁷ (Positional isomer of Trikoningin KA-like XLVIII)	[29]
Trikoningin KA-like XLV	New: (Positional isomer of Trikoningin KA-like VI, XXI, XXXIX, XLI, LII)	→ Trikoningin KA-like VI
Trikoningin KA-like XLVI	(Positional isomer of Trikoningin KA-like XLII)	→ Trikoningin KA-like XLII
Trikoningin KA-like XLVII	Pept-XI	[38]
Trikoningin KA-like XLVIII	New: (Positional isomer of Trikoningin KA-like XLIV)	→ Trikoningin KA-like XLIV
Trikoningin KA-like XLIX	New: Trikoningin KA V: [Gly] ² → [Ala] ² ; [Gln] ¹⁷ → [Glu] ¹⁷ (Positional isomer of Trikoningin KA-like LIII)	[29]
Trikoningin KA-like L	(Positional isomer of Trikoningin KA-like XIX, XXXV, XL, XLIII)	→ Trikoningin KA-like XIX
Trikoningin KA-like LI	Pept-XI	[38]
Trikoningin KA-like LII	New: (Positional isomer of Trikoningin KA-like VI, XXI, XXXIX, XLI, XLV)	→ Trikoningin KA-like VI
Trikoningin KA-like LIII	New: Trikoningin KA V: [Gly] ² → [Ala] ² ; [Gln] ¹⁷ → [Glu] ¹⁷ (Positional isomer of Trikoningin KA-like XLIX)	→ Trikoningin KA-like XLIX
Trikoningin KA-like LIV	New: Trikoningin KA V: [Gly] ² → [Ala] ² ; [Ser] ¹⁰ → [Ala] ¹⁰	[29]
Trikoningin KA-like LV	New: Trikoningin KA V: [Aib] ⁷ → [Vxx] ⁷	[29]
Trikoningin KA-like LVI	New: Pept-XI: [Ser] ¹⁰ → [Ala] ¹⁰ ; [Gln] ¹⁷ → [Glu] ¹⁷	[38]
Trikoningin KA-like LVII	New: Trikoningin KA V: [Aib] ⁹ → [Vxx] ⁹ ; [Gln] ¹⁷ → [Glu] ¹⁷	[29]
<i>T. cf. dorotheopsis</i> SZMC 28390		
Dorothopsin A-a I	New: Trichostrigocin TSG-A, TSG-B: [Vxx] ¹⁶ → [Lxx] ¹⁶ ; [Gln] ¹⁷ → [Glu] ¹⁷ ; [Gln] ¹⁸ → [Ala] ¹⁸ ; [Lxxol] ¹⁹ → [Alaol] ¹⁹ (Positional isomer of Dorothopsin A-a II)	[37]
Dorothopsin A-a II	New: (Positional isomer of Dorothopsin A-a I)	→ Dorothopsin A-a I
Dorothopsin A-a III	New: Trichostrigocin TSG-A, TSG-B: [Lxxol] ¹⁹ → [Vxxol] ¹⁹ (Positional isomer of Dorothopsin A-a IV)	[37]
Dorothopsin A-a IV	New: (Positional isomer of Dorothopsin A-a III)	→ Dorothopsin A-a III
Dorothopsin A-a V	New: Trichostrigocin TSG-A, TSG-B: [Gln] ¹⁷ → [Glu] ¹⁷ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹	[37]
Dorothopsin A-a VI	New: Trichostrigocin TSG-A, TSG-B: [Vxx] ¹⁶ → [Lxx] ¹⁶ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹ (Positional isomer of Dorothopsin A-a VII)	[37]
Dorothopsin A-a VII	New: (Positional isomer of Dorothopsin A-a VI)	→ Dorothopsin A-a VI
Dorothopsin A-a VIII	New: Trichostrigocin TSG-A, TSG-B: [Gln] ¹⁷ → [Glu] ¹⁷ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹	[37]

Table 4 (continued)

Peptaibol	Compound identical or positionally isomeric with	Reference
Dorothopsin A-a IX	New: Trichostrogocin TSG-A, TSG-B: [Aib] ¹ → [Vxx] ¹ ; [Gln] ¹⁷ → [Glu] ¹⁷ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹	[37]
Dorothopsin A-a X	New: Trichostrogocin TSG-A, TSG-B: [Aib] ¹ → [Vxx] ¹ ; [Vxx] ¹⁶ → [Lxx] ¹⁶ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹	[37]
Dorothopsin A-a XI	New: Trichostrogocin TSG-A, TSG-B: [Aib] ¹ → [Vxx] ¹ ; [Vxx] ¹⁶ → [Lxx] ¹⁶ ; [Gln] ¹⁷ → [Glu] ¹⁷ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹	[37]
Dorothopsin A-a XII	New: Trichostrogocin TSG-A, TSG-B: [Vxx] ¹⁶ → [Lxx] ¹⁶	[37]
Dorothopsin A-a XIII	New: Trichostrogocin TSG-A, TSG-B: [Aib] ¹ → [Vxx] ¹ ; [Vxx] ¹⁶ → [Lxx] ¹⁶	[37]
Dorothopsin A-b I	New: Trichostrogocin TSG-A, TSG-B: [Aib] ⁹ ; [Vxx] ¹⁶ → [Lxx] ¹⁵ ; [Gln] ¹⁷ → [Glu] ¹⁶ ; [Gln] ¹⁸ → [Ala] ¹⁷ ; [Lxxol] ¹⁹ → [Alaol] ¹⁸ (Positional isomer of Dorothopsin A-b II)	[37]
Dorothopsin A-b II	New: (Positional isomer of Dorothopsin A-b I)	→ Dorothopsin A-b I
Dorothopsin A-b III	New: Trichostrogocin TSG-A, TSG-B: [Aib] ⁹ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁸ (Positional isomer of Dorothopsin A-b V)	[37]
Dorothopsin A-b IV	New: Trichostrogocin TSG-A, TSG-B: [Aib] ⁹ ; [Gln] ¹⁷ → [Glu] ¹⁶ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁸ (Positional isomer of Dorothopsin A-b VI)	[37]
Dorothopsin A-b V	New: (Positional isomer of Dorothopsin A-b III)	→ Dorothopsin A-b III
Dorothopsin A-b VI	New: (Positional isomer of Dorothopsin A-b IV)	→ Dorothopsin A-b IV
Dorothopsin A-b VII	New: Trichostrogocin TSG-A, TSG-B: [Aib] ⁹ ; [Vxx] ¹⁶ → [Lxx] ¹⁵ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁸	[37]
Dorothopsin A-b VIII	New: Trichostrogocin TSG-A, TSG-B: [Aib] ⁹ ; [Vxx] ¹⁶ → [Lxx] ¹⁵ ; [Gln] ¹⁷ → [Glu] ¹⁶ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁸	[37]
Dorothopsin A-c I	New: Trichostrogocin TSG-A, TSG-B: [Aib] ⁹ ; [Vxx] ¹⁶ → [Lxx] ¹⁵ ; [Gln] ¹⁷ ; [Gln] ¹⁸ → [Ala] ¹⁶ ; [Lxxol] ¹⁹ → [Alaol] ¹⁷	[37]
Dorothopsin A-d I	New: Trichostrogocin TSG-A, TSG-B: [Vxx] ¹⁶ → [Lxx] ¹⁶ ; [Gln] ¹⁷ ; [Gln] ¹⁸ → [Ala] ¹⁷ ; [Lxxol] ¹⁹ → [Alaol] ¹⁸ (Positional isomer of Dorothopsin A-d II)	[37]
Dorothopsin A-d II	New: (Positional isomer of Dorothopsin A-d I)	→ Dorothopsin A-d I
Dorothopsin A-d III	New: Trichostrogocin TSG-A, TSG-B: [Aib] ¹ → [Vxx] ¹ ; [Vxx] ¹⁶ → [Lxx] ¹⁶ ; [Gln] ¹⁷ ; [Gln] ¹⁸ → [Ala] ¹⁷ ; [Lxxol] ¹⁹ → [Alaol] ¹⁸	[37]
Dorothopsin A-e I	New: Trichostrogocin TSG-A, TSG-B: [Aib] ⁹ ; [Vxx] ¹⁶ ; [Gln] ¹⁷ ; [Gln] ¹⁸ → [Gly] ¹⁵ ; [Lxxol] ¹⁹ → [Alaol] ¹⁶	[37]
Dorothopsin A-f I	New: Trichostrogocin TSG-A, TSG-B: [Vxx] ¹⁶ ; [Gln] ¹⁷ ; [Gln] ¹⁸ → [Gly] ¹⁶ ; [Lxxol] ¹⁹ → [Alaol] ¹⁷ (Positional isomer of Dorothopsin A-f II)	[37]
Dorothopsin A-f II	New: (Positional isomer of Dorothopsin A-f I)	→ Dorothopsin A-f I
<i>T. atroviride</i> SZMC 28748		
Trichorzianin TA-like I	Trichorzianin TA IIa (Positional isomer of Trichorzianin TA-like V and VI)	[41]
Trichorzianin TA-like II	Trichorzianin TA IIIb; IIIc (Positional isomer of Trichorzianin TA-like VII)	[41]
Trichorzianin TA-like III	New: Trichorzianin TA IIIa: [Ala] ² → [Gly] ²	[41]
Trichorzianin TA-like IV	New: Trichorzianin TA IVb: [Ala] ² → [Gly] ²	[41]
Trichorzianin TA-like V	(Positional isomer of Trichorzianin TA-like I and VI)	→ Trichorzianin TA-like I
Trichorzianin TA-like VI	(Positional isomer of Trichorzianin TA-like I and V)	→ Trichorzianin TA-like I
Trichorzianin TA-like VII	(Positional isomer of Trichorzianin TA-like II)	→ Trichorzianin TA-like I
Trichorzianin TA-like VIII	New: Trichorzianin TA Vb: [Ala] ³ → [Ser] ³	[41]
Trichorzianin TA-like IX	Trichorzianin TA IVb (Positional isomer of Trichorzianin TA-like XI and XV)	[41]
Trichorzianin TA-like X	Trichorzianin TA IIIa (Positional isomer of Trichorzianin TA-like XIII)	[41]
Trichorzianin TA-like XI	(Positional isomer of Trichorzianin TA-like IX and XV)	→ Trichorzianin TA-like IX
Trichorzianin TA-like XII	New: Trichorzianin TA Vb: [Aib] ⁸ → [Ala] ⁸	[41]
Trichorzianin TA-like XIII	(Positional isomer of Trichorzianin TA-like X)	→ Trichorzianin TA-like X
Trichorzianin TA-like XIV	New: Trichorzianin TA VIb: [Ala] ³ → [Ser] ³	[41]
Trichorzianin TA-like XV	(Positional isomer of Trichorzianin TA-like IX and XI)	→ Trichorzianin TA-like IX
Trichorzianin TA-like XVI	New: Trichorzianin TA VIa: [Ala] ² → [Ser] ²	[41]
Trichorzianin TA-like XVII	New: Trichorzianin TA IIIa: [Ser] ¹⁰ → [Ala] ¹⁰	[41]
Trichorzianin TA-like XVIII	New: Trichorzianin TA VIb: [Aib] ⁸ → [Ala] ⁸	[41]
Trichorzianin TA-like XIX	New: Trichorzianin TA IVb: [Ser] ¹⁰ → [Ala] ¹⁰	[41]

Table 4 (continued)

Peptaibol	Compound identical or positionally isomeric with	Reference
Trichorzianin TA-like XX	New: Trichorzianin TA VII: [Ala] ² → [Ser] ²	[41]
Trichorzianin TA-like XXI	Trichorzianin TA Vb (Positional isomer of Trichorzianin TA-like XXII)	[41]
Trichorzianin TA-like XXII	(Positional isomer of Trichorzianin TA-like XXI)	→ Trichorzianin TA-like XXI
Trichorzianin TA-like XXIII	Trichorzianin TA VIb (Positional isomer of Trichorzianin TA-like XXV)	[41]
Trichorzianin TA-like XXIV	New: Trichorzianin TA VIa: [Aib] ⁷ → [Ala] ⁷	[41]
Trichorzianin TA-like XXV	(Positional isomer of Trichorzianin TA-like XXIII)	→ Trichorzianin TA-like XXIII
Trichorzianin TA-like XXVI	Trichorzianin TA VIa (Positional isomer of Trichorzianin TA-like XXVII and XXXII)	[41]
Trichorzianin TA-like XXVII	(Positional isomer of Trichorzianin TA-like XXVI and XXXII)	→ Trichorzianin TA-like XXVI
Trichorzianin TA-like XXVIII	Trichorzianin TA VII (Positional isomer of Trichorzianin TA-like XXIX)	[41]
Trichorzianin TA-like XXIX	(Positional isomer of Trichorzianin TA-like XXVIII)	→ Trichorzianin TA-like XXVIII
Trichorzianin TA-like XXX	New: Trichorzianin TA VIa: [Ser] ¹⁰ → [Ala] ¹⁰	[41]
Trichorzianin TA-like XXXI	New: Trichorzianin TA VII: [Ser] ¹⁰ → [Ala] ¹⁰	[41]
Trichorzianin TA-like XXXII	(Positional isomer of Trichorzianin TA-like XXVI and XXVII)	→ Trichorzianin TA-like XXVI
Trichorzianin TA-like XXXIII	Trichorzianin TA VII	[41]
Peptaibol-like compounds I-XLI	New: incomplete at C-terminus	Discussed in text
<i>T. hamatum</i> SZMC 28747		
Tricholongin LB-like I	Tricholongin LBII and Tricholongin LBIV (Positional isomer of Tricholongin LB-like XVI and XVIII)	[37]
Tricholongin LB-like II	New: Tricholongin LBI: [Phe] ³ → [Ala] ³	[37]
Tricholongin LB-like III	New: Tricholongin LBI: [Aib] ¹ → [Ala] ¹	[37]
Tricholongin LB-like IV	New: Tricholongin LBII and Tricholongin LBIV: [Phe] ³ → [Ala] ³	[37]
Tricholongin LB-like V	New: Tricholongin LBI: [Phe] ³ → [Tyr] ³	[37]
Tricholongin LB-like VI	New: Tricholongin LBII and Tricholongin LBIV: [Aib] ¹ → [Ala] ¹	[37]
Tricholongin LB-like VII	New: Tricholongin LBII and Tricholongin LBIV: [Phe] ³ → [Tyr] ³	[37]
Tricholongin LB-like VIII	New: Tricholongin LBI: [Aib] ⁷ → [Ala] ⁷	[37]
Tricholongin LB-like IX	New: Tricholongin LBI: [Aib] ⁴ → [Ala] ⁴	[37]
Tricholongin LB-like X	New: Tricholongin LBII and Tricholongin LBIV: [Aib] ⁵ → [Ala] ⁵	[37]
Tricholongin LB-like XI	Tricholongin LBI (Positional isomer of Tricholongin LB-like XIII and XV)	[37]
Tricholongin LB-like XII	New: Tricholongin LBII and Tricholongin LBIV: [Aib] ⁸ → [Ala] ⁸	[37]
Tricholongin LB-like XIII	(Positional isomer of Tricholongin LB-like XI and XV)	→ Tricholongin LB-like XI
Tricholongin LB-like XIV	New: Tricholongin LBII and Tricholongin LBIV: [Aib] ⁴ → [Ala] ⁴	[37]
Tricholongin LB-like XV	(Positional isomer of Tricholongin LB-like XI and XIII)	→ Tricholongin LB-like XI
Tricholongin LB-like XVI	(Positional isomer of Tricholongin LB-like I and XVIII)	→ Tricholongin LB-like I
Tricholongin LB-like XVII	New: Tricholongin LBI: [Gly] ² → [Ala] ²	[37]
Tricholongin LB-like XVIII	(Positional isomer of Tricholongin LB-like I and XVI)	→ Tricholongin LB-like I
Tricholongin LB-like XIX	New: Tricholongin LBII and Tricholongin LBIV: [Gly] ² → [Ala] ²	[37]
Tricholongin LB-like XX	New: Tricholongin LBI: [Gly] ² → [Ala] ² ; [Ser] ¹⁰ → [Ala] ¹⁰	[37]
	New: Tricholongin LBIII: [Gly] ² → [Ala] ² ; [Vxx] ¹⁶ → [Aib] ¹⁶	[37]
Tricholongin LB-like XXI	New: Tricholongin LBIII: [Gly] ² → [Ala] ²	[37]
<i>T. cf. dorotheopsis</i> SZMC 28005		
Dorotheopsin B I	New: Tricholongin LBI: [Aib] ¹ ↔ [Phe] ³ ; [Aib] ⁵ → [Vxx] ⁵ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹	[37]
Dorotheopsin B II	New: Tricholongin LBI: [Aib] ¹ ↔ [Phe] ³ ; [Aib] ⁵ → [Vxx] ⁵ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Gln] ¹⁷ → [Glu] ¹⁷ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹	[37]
Dorotheopsin B III	New: Tricholongin LBI: [Aib] ¹ ↔ [Phe] ³ ; [Aib] ⁵ → [Lxx] ⁵ ; [Aib] ⁸ → [Ala] ⁸ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹ (Positional isomer of Dorotheopsin B IX)	[37]
Dorotheopsin B IV	New: Tricholongin LBI: [Aib] ¹ ↔ [Phe] ³ ; [Aib] ⁵ → [Lxx] ⁵ ; [Gln] ¹⁷ → [Glu] ¹⁷ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹ (Positional isomer of Dorotheopsin B X)	[37]

Table 4 (continued)

Peptaibol	Compound identical or positionally isomeric with	Reference
Dorothopsin B V	New: Tricholongin LBI: [Aib] ¹ ↔ [Phe] ³ ; [Aib] ⁵ → [Vxx] ⁵ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹ (Positional isomer of Dorothopsin B XI and Dorothopsin B XVII)	[37]
Dorothopsin B VI	New: Tricholongin LBI: [Aib] ¹ ↔ [Phe] ³ ; [Aib] ⁵ → [Vxx] ⁵ ; [Gln] ¹⁷ → [Glu] ¹⁷ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹ (Positional isomer of Dorothopsin B XXI)	[37]
Dorothopsin B VII	New: Tricholongin LBI: [Aib] ¹ → [Trp] ¹ ; [Phe] ³ → [Aib] ³ ; [Aib] ⁵ → [Lxx] ⁵ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹ (Positional isomer of Dorothopsin B XII, Dorothopsin B XIV and Dorothopsin B XVIII)	[37]
Dorothopsin B VIII	New: Tricholongin LBI: [Aib] ¹ → [Trp] ¹ ; [Phe] ³ → [Aib] ³ ; [Aib] ⁵ → [Lxx] ⁵ ; [Gln] ¹⁷ → [Glu] ¹⁷ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹ (Positional isomer of Dorothopsin B XVI and Dorothopsin B XXII)	[37]
Dorothopsin B IX	New: (Positional isomer of Dorothopsin B III)	→ Dorothopsin B III
Dorothopsin B X	New: (Positional isomer of Dorothopsin B IV)	→ Dorothopsin B IV
Dorothopsin B XI	New: (Positional isomer of Dorothopsin B V and Dorothopsin B XVII)	→ Dorothopsin B V
Dorothopsin B XII	New: (Positional isomer of Dorothopsin B VII, Dorothopsin B XIV and Dorothopsin B XVIII)	→ Dorothopsin B VII
Dorothopsin B XIII	New: Tricholongin LBI: [Aib] ¹ ↔ [Phe] ³ ; [Aib] ⁵ → [Lxx] ⁵ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹ (Positional isomer of Dorothopsin B XIX; Dorothopsin B XXV and Dorothopsin B XXIX)	[37]
Dorothopsin B XIV	New: (Positional isomer of Dorothopsin B VII, Dorothopsin B XII and Dorothopsin B XVIII)	→ Dorothopsin B VII
Dorothopsin B XV	New: Tricholongin LBI: [Aib] ¹ ↔ [Phe] ³ ; [Aib] ⁵ → [Lxx] ⁵ ; [Gln] ¹⁷ → [Glu] ¹⁷ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹ (Positional isomer of Dorothopsin B XXIII; Dorothopsin B XXVI and Dorothopsin B XXXI)	[37]
Dorothopsin B XVI	New: (Positional isomer of Dorothopsin B VIII and Dorothopsin B XXII)	→ Dorothopsin B VIII
Dorothopsin B XVII	New: (Positional isomer of Dorothopsin B V and Dorothopsin B XI)	→ Dorothopsin B V
Dorothopsin B XVIII	New: (Positional isomer of Dorothopsin B VII, Dorothopsin B XII and Dorothopsin B XIV)	→ Dorothopsin B VII
Dorothopsin B XIX	New: (Positional isomer of Dorothopsin B XIII; Dorothopsin B XXV and Dorothopsin B XXIX)	→ Dorothopsin B XIII
Dorothopsin B XX	New: Tricholongin LBI: [Aib] ¹ → [Trp] ¹ ; [Gly] ² → [Ala] ² ; [Phe] ³ → [Aib] ³ ; [Aib] ⁵ → [Lxx] ⁵ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹ (Positional isomer of Dorothopsin B XXX)	[37]
Dorothopsin B XXI	New: (Positional isomer of Dorothopsin B VI)	→ Dorothopsin B VI
Dorothopsin B XXII	New: (Positional isomer of Dorothopsin B VIII and Dorothopsin B XVI)	→ Dorothopsin B VIII
Dorothopsin B XXIII	New: (Positional isomer of Dorothopsin B XV; Dorothopsin B XXVI and Dorothopsin B XXXI)	→ Dorothopsin B XV
Dorothopsin B XXIV	New: Tricholongin LBI: [Aib] ¹ → [Trp] ¹ ; [Gly] ² → [Ala] ² ; [Phe] ³ → [Aib] ³ ; [Aib] ⁵ → [Lxx] ⁵ ; [Gln] ¹⁷ → [Glu] ¹⁷ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹ (Positional isomer of Dorothopsin B XXXII)	[37]
Dorothopsin B XXV	New: (Positional isomer of Dorothopsin B XIII; Dorothopsin B XIX and Dorothopsin B XXIX)	→ Dorothopsin B XIII
Dorothopsin B XXVI	New: (Positional isomer of Dorothopsin B XV; Dorothopsin B XXIII and Dorothopsin B XXXI)	→ Dorothopsin B XV
Dorothopsin B XXVII	New: Tricholongin LBI: [Aib] ¹ ↔ [Phe] ³ ; [Gly] ² → [Ala] ² ; [Aib] ⁵ → [Lxx] ⁵ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹ (Positional isomer of Dorothopsin B XXXIII and Dorothopsin B XXXV)	[37]
Dorothopsin B XXVIII	New: Tricholongin LBI: [Aib] ¹ ↔ [Phe] ³ ; [Gly] ² → [Ala] ² ; [Aib] ⁵ → [Lxx] ⁵ ; [Gln] ¹⁷ → [Glu] ¹⁷ ; [Lxxol] ¹⁹ → [Vxxol] ¹⁹ (Positional isomer of Dorothopsin B XXXIV and Dorothopsin B XXXVI)	[37]
Dorothopsin B XXIX	New: (Positional isomer of Dorothopsin B XIII; Dorothopsin B XIX and Dorothopsin B XXV)	→ Dorothopsin B XIII
Dorothopsin B XXX	New: (Positional isomer of Dorothopsin B XX)	→ Dorothopsin B XX
Dorothopsin B XXXI	New: (Positional isomer of Dorothopsin B XV; Dorothopsin B XXIII and Dorothopsin B XXVI)	→ Dorothopsin B XV
Dorothopsin B XXXII	New: (Positional isomer of Dorothopsin B XXIV)	→ Dorothopsin B XXIV
Dorothopsin B XXXIII	New: (Positional isomer of Dorothopsin B XXVII and Dorothopsin B XXXV)	→ Dorothopsin B XXXIII
Dorothopsin B XXXIV	New: (Positional isomer of Dorothopsin B XXVIII and Dorothopsin B XXXVI)	→ Dorothopsin B XXXIV
Dorothopsin B XXXV	New: (Positional isomer of Dorothopsin B XXVII and Dorothopsin B XXXIII)	→ Dorothopsin B XXXIII
Dorothopsin B XXXVI	New: (Positional isomer of Dorothopsin B XXVIII and Dorothopsin B XXXIV)	→ Dorothopsin B XXXIV

Table 4 (continued)

Peptaibol	Compound identical or positionally isomeric with	Reference
Strigosellin A I	New: Trichokonin TKO-V: [Ala] ² → [Ser] ² ; [Vxx] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Vxx] ¹⁴ → [Phe] ¹⁴ ; [Gln] ¹⁷ → [Glu] ¹⁷ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[34]
	New: Trichokonin V: [Ala] ² → [Ser] ² ; [Val] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Vxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴ ; [Gln] ¹⁷ → [Glu] ¹⁷ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[35]
	New: Tricholongin Bl: [Gly] ² → [Ser] ² ; [Phe] ³ → [Aib] ³ ; [Aib] ⁴ → [Ala] ⁴ ; [Aib] ⁹ → [Ala] ⁹ ; [Ser] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Vxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴ ; [Gln] ¹⁷ → [Glu] ¹⁷	[36]
	New: Tricholongin LBl: [Gly] ² → [Ser] ² ; [Phe] ³ → [Aib] ³ ; [Aib] ⁴ → [Ala] ⁴ ; [Aib] ⁹ → [Ala] ⁹ ; [Ser] ¹⁰ → [Ala] ¹⁰ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Vxx] ¹⁴ → [Phe] ¹⁴ ; [Gln] ¹⁷ → [Glu] ¹⁷	[37]
Strigosellin A II	New: Trichokonin TKO-V: [Ala] ² → [Ser] ² ; [Vxx] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Vxx] ¹⁴ → [Phe] ¹⁴ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[34]
	New: Trichokonin V: [Ala] ² → [Ser] ² ; [Val] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Vxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[35]
	New: Tricholongin Bl: [Gly] ² → [Ser] ² ; [Phe] ³ → [Aib] ³ ; [Aib] ⁴ → [Ala] ⁴ ; [Aib] ⁹ → [Ala] ⁹ ; [Ser] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Vxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴	[36]
	New: Tricholongin LBl: [Gly] ² → [Ser] ² ; [Phe] ³ → [Aib] ³ ; [Aib] ⁴ → [Ala] ⁴ ; [Aib] ⁹ → [Ala] ⁹ ; [Ser] ¹⁰ → [Ala] ¹⁰ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Vxx] ¹⁴ → [Phe] ¹⁴	[37]
Strigosellin A III	New: Trichokonin TKO-V: [Vxx] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ser] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Vxx] ¹⁴ → [Phe] ¹⁴ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[34]
	New: Trichokonin V: [Val] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ser] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Vxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[35]
Strigosellin A IV	New: Trichokonin TKO-V: [Ala] ² → [Ser] ² ; [Vxx] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Vxx] ¹⁴ → [Phe] ¹⁴ ; [Gln] ¹⁷ → [Glu] ¹⁷ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹ (Positional isomer of Strigosellin A X)	[34]
	New: Trichokonin V: [Ala] ² → [Ser] ² ; [Val] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Vxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴ ; [Gln] ¹⁷ → [Glu] ¹⁷ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[35]
	New: Tricholongin Bl: [Gly] ² → [Ser] ² ; [Phe] ³ → [Aib] ³ ; [Aib] ⁴ → [Ala] ⁴ ; [Aib] ⁹ → [Ala] ⁹ ; [Ser] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Lxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴ ; [Gln] ¹⁷ → [Glu] ¹⁷	[36]
	New: Tricholongin LBl: [Gly] ² → [Ser] ² ; [Phe] ³ → [Aib] ³ ; [Aib] ⁴ → [Ala] ⁴ ; [Aib] ⁹ → [Ala] ⁹ ; [Ser] ¹⁰ → [Ala] ¹⁰ ; [Vxx] ¹⁴ → [Phe] ¹⁴ ; [Gln] ¹⁷ → [Glu] ¹⁷	[37]
Strigosellin A V	New: Trichokonin TKO-V: [Ala] ² → [Ser] ² ; [Vxx] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Vxx] ¹⁴ → [Phe] ¹⁴ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[34]
	New: Trichokonin V: [Ala] ² → [Ser] ² ; [Val] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Lxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[35]
	New: Tricholongin Bl: [Gly] ² → [Ser] ² ; [Phe] ³ → [Aib] ³ ; [Aib] ⁴ → [Ala] ⁴ ; [Aib] ⁹ → [Ala] ⁹ ; [Ser] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Lxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴	[36]
	New: Tricholongin LBl: [Gly] ² → [Ser] ² ; [Phe] ³ → [Aib] ³ ; [Aib] ⁴ → [Ala] ⁴ ; [Aib] ⁹ → [Ala] ⁹ ; [Ser] ¹⁰ → [Ala] ¹⁰ ; [Vxx] ¹⁴ → [Phe] ¹⁴	[37]
Strigosellin A VI	New: Trichokonin TKO-V: [Ala] ² → [Ser] ² ; [Vxx] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Vxx] ¹⁴ → [Phe] ¹⁴ ; [Aib] ¹⁵ → [Vxx] ¹⁵ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹ (Positional isomer of Strigosellin A XI)	[34]
	New: Trichokonin V: [Ala] ² → [Ser] ² ; [Val] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Vxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴ ; [Aib] ¹⁵ → [Vxx] ¹⁵ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[35]
	New: Tricholongin Bl: [Gly] ² → [Ser] ² ; [Phe] ³ → [Aib] ³ ; [Aib] ⁴ → [Ala] ⁴ ; [Aib] ⁹ → [Ala] ⁹ ; [Ser] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Lxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴ ; [Aib] ¹⁵ → [Vxx] ¹⁵	[36]
	New: Tricholongin LBl: [Gly] ² → [Ser] ² ; [Phe] ³ → [Aib] ³ ; [Aib] ⁴ → [Ala] ⁴ ; [Aib] ⁹ → [Ala] ⁹ ; [Ser] ¹⁰ → [Ala] ¹⁰ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Vxx] ¹⁴ → [Phe] ¹⁴ ; [Aib] ¹⁵ → [Vxx] ¹⁵	[37]
Strigosellin A VII	New: Trichokonin TKO-V: [Vxx] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ser] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Vxx] ¹⁴ → [Phe] ¹⁴ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[34]
	New: Trichokonin V: [Val] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ser] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Vxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴ ; [Gln] ¹⁷ → [Glu] ¹⁷ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[35]

Table 4 (continued)

Peptaibol	Compound identical or positionally isomeric with	Reference
Strigosellin A VIII	New: Trichokonin TKO-V: [Ala] ² → [Ser] ² ; [Vxx] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Vxx] ¹⁴ → [Phe] ¹⁴ ; [Aib] ¹⁵ → [Vxx] ¹⁵ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[34]
	New: Trichokonin V: [Ala] ² → [Ser] ² ; [Val] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Lxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴ ; [Aib] ¹⁵ → [Vxx] ¹⁵ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[35]
	New: Tricholongin BI: [Gly] ² → [Ser] ² ; [Phe] ³ → [Aib] ³ ; [Aib] ⁴ → [Ala] ⁴ ; [Aib] ⁹ → [Ala] ⁹ ; [Ser] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Lxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴ ; [Aib] ¹⁵ → [Vxx] ¹⁵	[36]
	New: Tricholongin LBI: [Gly] ² → [Ser] ² ; [Phe] ³ → [Aib] ³ ; [Aib] ⁴ → [Ala] ⁴ ; [Aib] ⁹ → [Ala] ⁹ ; [Ser] ¹⁰ → [Ala] ¹⁰ ; [Vxx] ¹⁴ → [Phe] ¹⁴ ; [Aib] ¹⁵ → [Vxx] ¹⁵	[37]
Strigosellin A IX	New: Trichokonin TKO-V: [Vxx] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Vxx] ¹⁴ → [Phe] ¹⁴ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[34]
	New: Trichokonin V: [Val] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Vxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[35]
Strigosellin A X	New: (Positional isomer of Strigosellin A IV)	→ Strigosellin A IV
Strigosellin A XI	New: (Positional isomer of Strigosellin A VI)	→ Strigosellin A VI
Strigosellin A XII	New: Trichokonin TKO-V: [Vxx] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Vxx] ¹⁴ → [Phe] ¹⁴ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[34]
	New: Trichokonin V: [Val] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Lxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[35]
Strigosellin A XIII	New: Trichokonin TKO-V: [Vxx] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Vxx] ¹⁴ → [Phe] ¹⁴ ; [Aib] ¹⁵ → [Vxx] ¹⁵ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[34]
	New: Trichokonin V: [Val] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Vxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴ ; [Aib] ¹⁵ → [Vxx] ¹⁵ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[35]
Strigosellin A XIV	New: Trichokonin TKO-V: [Vxx] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Vxx] ¹⁴ → [Phe] ¹⁴ ; [Aib] ¹⁵ → [Vxx] ¹⁵ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[34]
	New: Trichokonin V: [Val] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Lxx] ¹¹ ; [Val] ¹⁴ → [Phe] ¹⁴ ; [Aib] ¹⁵ → [Vxx] ¹⁵ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[35]
Strigosellin B I	New: Trichokonin TKO-V: [Vxx] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Vxx] ¹⁴ → [Lxx] ¹⁴ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹ (Positional isomer of Strigosellin B IV and Strigosellin B VI)	[34]
	New: Trichokonin V: [Val] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Lxx] ¹¹ ; [Val] ¹⁴ → [Lxx] ¹⁴ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[35]
Strigosellin B II	New: Trichokonin TKO-V: [Vxx] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Vxx] ¹⁴ → [Lxx] ¹⁴ ; [Aib] ¹⁶ → [Vxx] ¹⁶ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[34]
	New: Trichokonin V: [Val] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Vxx] ¹¹ ; [Val] ¹⁴ → [Lxx] ¹⁴ ; [Aib] ¹⁶ → [Vxx] ¹⁶ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[35]
Strigosellin B III	New: Trichokonin TKO-V: [Vxx] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Aib] ¹⁶ → [Vxx] ¹⁶ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[34]
	New: Trichokonin V: [Val] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Vxx] ¹¹ ; [Val] ¹⁴ → [Lxx] ¹⁴ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[35]
Strigosellin B IV	New: (Positional isomer of Strigosellin B I and Strigosellin B VI)	→ Strigosellin B I
Strigosellin B V	New: Trichokonin TKO-V: [Vxx] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Vxx] ¹⁴ → [Lxx] ¹⁴ ; [Aib] ¹⁶ → [Vxx] ¹⁶ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[34]
	New: Trichokonin V: [Val] ⁸ → [Aib] ⁸ ; [Aib] ⁹ → [Ala] ⁹ ; [Gly] ¹⁰ → [Ala] ¹⁰ ; [Leu] ¹¹ → [Lxx] ¹¹ ; [Val] ¹⁴ → [Lxx] ¹⁴ ; [Aib] ¹⁶ → [Vxx] ¹⁶ ; [Pheol] ¹⁹ → [Lxxol] ¹⁹	[35]
Strigosellin B VI	New: (Positional isomer of Strigosellin B I and Strigosellin B IV)	→ Strigosellin B I

3.3.4 Identification of new Trichorzianin TA sequences and peptaibol-like compounds from *T. atroviride*

T. atroviride SZMC 28748 produced thirty-three peptaibol compounds, as well as forty-one incomplete peptaibol sequences named as Peptaibol-like compounds in Tables 3 and 4. The thirty-three peptaibol sequences

were positionally isomeric with the Trichorzianin TA sequences [41], out of which, thirteen proved to be new. The Peptaibol-like sequences were also identical with the thirty-three trichorzianin TA sequences [41], but unusual at their C-terminus, where the last part of the sequences is shown with the remaining mass difference,

Table 5 The ¹most produced sequences, ²consensus sequences and ³amino acid varieties of the peptaibols produced by each strain

Name of compound	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19
¹ Strigabiol-like XII	Ac	Vxx	Ser	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Lxxol
² Strigabiol-like	Ac	Aib	Ser	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Lxxol
³ Strigabiol-like	Ac	Vxx/Aib	Aib/Vxx/Ala/Ser	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ala/Ser	Vxx/Lxx	Aib	Pro	Vxx	Aib	Ala/Aib	Gln	Gln	Vxxol/Lxxol
¹ Trikonigin KA-like XLV	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Lxxol
² Trikonigin KA-like	Ac	Aib	Gly	Ala	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	<u>Gln</u>	Gln	Lxxol
³ Trikonigin KA-like	Ac	Aib	Ala/Gly	Gly/Ser/Ala	Aib	Vxx/Lxx	Gln	Vxx/Aib	Ala/Aib	Vxx/Ala/Aib	Ala/Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx/Lxx	Gln/Glu	Gln	Lxxol
¹ Dorotheopsin A-a VII	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Vxxol
² Dorotheopsin A	Ac	Aib	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Vxxol
³ Dorotheopsin A	Ac	Aib/Vxx	Ala	Aib	Aib	Lxx	Gln	Aib	Aib	Aib/-	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx/Lxx/-	Gln/Glu/-	Gly/Ala/Gln	Alaol/Vxxol/Lxxol
¹ Trichorzianin TA-like XXIX	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Lxx	Gln	Gln	Phcol
² Trichorzianin TA-like	Ac	Aib	Ala	Ala	Aib	Vxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	<u>Lxx</u>	Aib	Lxx	Gln	Gln	Phcol
³ Trichorzianin TA-like	Ac	Aib	Gly/Ala/Ser	Ala/Ser	Aib	Aib/Vxx	Gln	Ala/Aib	Ala/Aib	Aib	Ala/Ser	Lxx	Aib	Pro	Vxx/Lxx	Aib	Lxx	Gln	Gln	Phcol/Tpcol
¹ Tricholongin LB-like XVI	Ac	Aib	Gly	Phe	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Vxx	Gln	Gln	Lxxol
² Tricholongin LB-like	Ac	Aib	Gly	Phe	Aib	Aib	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	<u>Aib/Vxx</u>	Gln	Gln	Lxxol
³ Tricholongin LB-like	Ac	Ala/Aib	Gly/Ala	Phe/Tyr	Ala/Aib	Ala/Aib	Gln	Ala/Aib	Aib	Aib	Ala/Ser	Lxx	Aib	Pro	Vxx	Aib	Aib/Vxx	Gln	Gln	Lxxol
¹ Dorotheopsin B XXVI	Ac	Phe	Gly	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	Gln	Gln	Vxxol
² Dorotheopsin B	Ac	Phe	Gly	Aib	Aib	Lxx	Gln	Aib	Aib	Aib	Ser	Lxx	Aib	Pro	Vxx	Aib	Aib	<u>Gln</u>	Gln	Vxxol
³ Dorotheopsin B	Ac	Phe/Tip	Gly/Ala	Aib	Aib	Vxx/Lxx	Gln	Aib	Ala/Aib	Aib	Ser	Vxx/Lxx	Aib	Pro	Vxx	Aib	Aib	Glu/Gln	Gln	Vxxol
¹ Strigosellin A VII	Ac	Aib	Ala	Aib	Ala	Aib	Gln	Aib	Aib	Ala	Ala	Vxx	Aib	Pro	Phe	Aib	Aib	Gln	Gln	Lxxol
² Strigosellin A	Ac	Aib	Ala	Aib	Ala	Aib	Gln	Aib	Aib	Ala	Ala	Vxx	Aib	Pro	Phe	Aib	Aib	Gln	Gln	Lxxol
³ Strigosellin A	Ac	Aib	Ala/Ser	Aib	Ala	Aib	Gln	Aib	Aib	Ala/Ser	Ala	Vxx/Lxx	Aib	Pro	Phe/Lxx	Aib/Vxx	Aib/Vxx	Glu/Gln	Gln	Lxxol

Amino acids in consensus sequences differing from the most produced compound are underlined. Darker color denotes the most produced sequences of the strain, lighter color denotes the consensus sequences denoting from the most abundant amino acid at each position

which were Δm = 145, 146, 160, or 222 D, furthermore, all MS² spectra contain the water loss [y₆–H₂O]⁺ fragment ions (Supplementary Fig. 2), which usually occurs when the C-terminus is an aminoalcohol. The sequences contain only two variable positions, R5 contains Aib/Vxx, while R14 Vxx/Lxx. All other residues are the same in the sequences, compared to each other. These sequences were produced in a relatively low concentration (all below 0.25%), therefore, they were not investigated further.

The two most produced peptaibols of *T. atroviride* SZMC 28748 were Trichorzianin TA-like XXV and XXIX with 15.24% and 17.59% of the total peptaibol production. They were followed by Trichorzianin TA-like VII, XV, XX, XXII, XXVII and XXVIII peptaibols with 7.68%, 8.99%, 5.26%, 5.44%, 6.19% and 5.34%, respectively. The rest of the peptaibols produced by this strain were around or below 1–2%. All the 41 Peptaibol-like compounds produced by *T. atroviride* SZMC 28748 were below 0.25% of the total peptaibiome.

3.3.5 Identification of new Tricholongin sequences from *T. hamatum*

The chromatographic and MS analysis of the *T. hamatum* SZMC 28747 extract revealed the production of twenty-one 19-residue-peptaibols belonging to the SF-1 peptaibol family (Tables 3 and 4). Among them, 6 peptaibols were new to science and the other sequences were identical to already determined sequences of Tricholongins LB I, II, III, and IV [37]. The newly identified sequences also shared similarities with the sequences of Tricholongins LB I, II, III, and IV. The known peptaibols are produced by *T. cf.*

strigosum BBA 69577 and *T. cf. pubescens* BBA 66989 strains [37].

Tricholongin LB-like XIII and XVI sequences produced by *T. hamatum* SZMC 28747 covered 25.68% and 29.09% of the total peptaibol production, which were followed by Tricholongin LB-like XVII and XIX sequences (7.13% and 10.03%, respectively). All other sequences were produced mostly around 1%.

3.3.6 Module skipping hypothesis

The microheterogeneity of non-ribosomal peptides like peptaibols arises from the ability of NRPSs to incorporate various amino acids [42]. Usually, *Trichoderma* species produce 1 to 4 main peptaibol compounds in high quantities, while the rest of the peptaibol variants are in much lower quantities, which can be the result of the modular synthesis and the misassembly of the peptaibol compounds by NRPS and the lack of repair mechanisms compared to ribosomal synthesis. This may be the reason for the wide range of new peptaibols that can be identified even from already known peptaibol subgroups. This hypothesis needs a thorough genetic data support based on the number of NRPS genes that can be found in the available *Trichoderma* full genomes.

Based on the results of this study, we hypothesize that the 16, 17 and 18-residue peptaibols produced by *T. cf. dorotheopsis* SZMC 28390 also occurred through a ‘module skipping’ event, which means that the NRPS enzyme skipped a module during the synthesis [27, 39].

Two skipping mechanisms were proposed in the literature: direct intermediate transfer between nonadjacent modules caused by a “loss of function mutation” [40], or nonfunctional thiolation or condensation domains of the NRPSs during biosynthesis [39]. Module skipping is usually seen in the case of 10-, 13-, 18-, and 19-residue peptaibols. Similar results were found in the case of SF-1 peptaibols produced by *T. flagellatum*, *T. sinense* and *T. parareesei*, which produced 19-residue peptaibols among the 20-residue peptaibols, but the investigation of the genome of the producer strains revealed no extra 19-module NRPS synthetases, only the gene of a 20-module enzyme was present [27]. Based on this hypothesis, the positions at which module skipping most probably occurred are shown in Table 4 with a minus sign. Our prediction is based on comparing the sequences of 16-residue (Dorothopsin A-e), 17-residue (Dorothopsin A-c) and 18-residue (Dorothopsins A-b and A-d) peptaibols to the sequences of 19-residue peptaibols (Dorothopsin A-a) (Tables 3 and 5).

3.4 Comparative analysis of peptaibols produced by species of clade *Viride*

The microheterogeneity within the sequences occurs in the positions where one amino acid is substituted by another one. The strictest positions were found to be in the middle of the sequences usually appearing as the Gln6-Aib7-Aib8-Aib9-Ser10-Lxx11-Aib12-Pro13-Vxx14 motif. This motif was different only in Strigosellin A sequences, where it was substituted with Gln6-Aib7-Aib8-Ala9-Ala10-Vxx11-Aib12-Pro-13-Phe14/Lxx14 produced by *T. cf. strigosellum* SZMC 28007. R1 usually contained an acetylated Aib except for a few *T. cf. strigosellum* SZMC 28391 and *T. cf. dorothopsis* SZMC 28390 sequences, where it was often substituted with Vxx. Acetylated Vxx is not present in SF-1 peptaibols, only in 11–16-residue peptaibols [10, 34, 37, 39]. Mostly, AcAib can be found in SF-1 peptaibols, however, several compounds produced by these strains contained another amino acid residue at the N-terminus (Table 3). Dorothopsin B sequences produced by *T. cf. dorothopsis* SZMC 28005 always contained Phe1 or Trp1. Boletusin 1, Chrysospermins and Peptaivirins, a group of another 19 residue-peptaibols identified from *Boletus* spp., *Apiocrea chrysosperma* and *Trichoderma* spp. (KGT142), respectively, also contained AcPhe at their N-termini [43–45]. Phe occurred strictly in R1, R3, R14 and R19 positions in *T. cf. dorothopsis* SZMC 28005, *T. hamatum* SZMC 28747, *T. cf. strigosellum* SZMC 28007 and *T. atroviride* SZMC 28748, respectively, while the other strains investigated did not contain Phe at all. The difference in Strigosellin A and B sequences relies in Phe14 and Lxx14 from *T. cf. strigosellum* SZMC 28007. Interestingly, both types

are produced almost equally by this strain. Regularly, Phe is close to one of the termini of the sequences in all peptaibols, however, Phe is in the middle of the sequences in Strigosellin A peptaibols. This strain shows production of both Strigosellin A (Phe14) and B (Lxx14) sequences, as if the production of the regular Lxx14 containing peptaibols were replaced to the rare Phe14 sequences. AcPhe1 was often substituted with AcTrp1 in Dorothopsin sequences, also observed in the literature for 15–16-residue peptaibols (Ampullosporins and Zervamicins) produced by *Sepedonium ampullosporum* (HKI-0053) and *Emericellopsis salmosynnemata*, respectively [46, 47]. Sequences of *T. hamatum* SZMC 28747 contained Ala1 instead of Aib1 in case of only 2 sequences. Only three 20-residue sequences (Trichoareocin 1a, Trichokonin IIb and Atroviridin D) with AcAla were identified from *T. aureoviride*, *T. koningii* Oudemans and an unidentified *Trichoderma* sp., respectively [35, 48, 49], out of which, the first two species belong to clade *Viride*, while the latter one was later reidentified as *T. arundinaceum* belonging to clade *Brevicompectum* [50]. Gly2 was substituted to Ala or Ser in several sequences of all strains investigated, while R3 contained mostly Ala or Aib. However, in the sequences of *T. hamatum* SZMC 28747, Phe or Tyr was always identified at the R3 position. Tyr has never been identified from peptaibols at this position, only from lipopeptaibols and other peptaibiotics, such as LP237 F5 and Trichoatrokontins, respectively [18, 51, 52], as well as from all-Aib-replaced peptides by *Amycolatopsis azurea*, used for bioconversion of AS 1387392 [53]. R4 was strictly Aib in all sequences except for a few sequences produced by *T. hamatum* SZMC 28747. At R5, mostly Vxx and Lxx were identified, except for *T. hamatum* SZMC 28747 and *T. cf. strigosellum* SZMC 28007 sequences, which mostly contained Aib5. This position was followed by the R6-R7-R8-R9-R10-R11 and R12-R13-R14 motifs discussed above. The module skipping occurred at R9 position in all Dorothopsin A-b, -c and -e sequences. R15 contained mostly Aib like in R4, except for a few sequences produced by *T. cf. strigosellum* SZMC 28007, where it was substituted to Vxx in several sequences. R16 contained either Ala, Aib, Vxx or Lxx which determined the mass of the γ_7 ion fragments. Gln16 was often substituted with Glu which, apart from the mass of the γ_7 ion fragments, defines the acidity of the peptaibols as Gln is neutral and Glu shows acidic characteristics. Dorothopsin A sequences also showed the 2nd module skipping at this position. One Dorothopsin A sequence (Dorothopsin A-e I from Table 3) showed in total 3 module skipplings at R9, R16 and R17. R18 mostly contained Gln except for Dorothopsin A compounds, where it was often substituted with Gly or Ala. The aminoalcohol was mostly Vxxol or Lxxol, except

for Dorotheopsin A and Tricholongin LB-like sequences, which often contained Alaninol (Alaol) or phenylalaninol (Pheol)/tryptophanol (Trpol) at the C-terminus, respectively. Pheol is often identified as the C-terminus of peptaibols. The first naming of peptaibols by Pandey et al. [54] as ‘peptaibophols’ was also based on the inclusion of Pheol, which was defined as peptide antibiotics containing the marker amino acid Aib and a C-terminal Pheol residue [54, 55]. After this, additional 2-alcohols such as valanol (Valol) in TXT-A40 and Leuol in Hypelcin from *Hypocrea peltata* (current name: *T. peltatum*) were detected as C-terminal constituents, the above definition of ‘peptaibophols’ needed to be revised and updated. Nevertheless, Trpol is rare at the C-terminus of peptaibols. It was only identified from Boletusin 1, Chrysospermis, Peptaivirin A, as well as Trichorzianin TA and PA sequences [41, 43–45, 56, 57].

In a few cases, the consensus sequence (which is a created sequence based on the most abundant amino acid present at each position) was different from the most produced sequence of the strain. These residues are underlined in Table 5. Trikonigin KA-like peptaibols mostly contained Gln at R17 while the most produced Trikonigin KA-like XLV had Glu at this position. Exactly this could be observed among Dorotheopsin B sequences where Dorotheopsin B XXVI contained Glu instead of Gln. Similarly, Trichorzianin TA-like peptaibols at R14 contained Lxx instead of Vxx in the most produced Trichorzianin TA-like XXIX. Tricholongin LB-like sequences equally produced Aib and Vxx containing sequences at R16, however, the most produced Tricholongin LB-like XVI had Vxx at this position.

3.5 Lipopeptaibol production of the investigated *Trichoderma* strains

Strain *T. cf. dorotheopsis* SZMC 28390 and *T. atroviride* SZMC 28748 did not produce any lipopeptaibols (Table 1), their peptaibiomes consist of exclusively SF1 peptaibols. In Tables 6 and 7 the sequences are ordered based on their similarities to each other, the producer strains are shown in the 2nd column. The diagnostic fragment ions resulted by MS² fragmentation are collected in Supplementary Table 2.

3.5.1 Identification of the new group of Lipostrigosellins from *T. cf. strigosellum*

T. cf. strigosellum SZMC 28391 produced a total of 12 lipopeptaibols, out of which, four were 6-residue long, while eight were 7-residue long (Table 6). Seven sequences were new, while five were positionally isomeric with already identified Lipostrigocin LSG sequences [37] (Table 7). All the 6-residue lipopeptaibols

were new to science and named as Lipostrigosellin I–IV. They are different from 7-residue lipopeptaibols in skipping of Aib/Vxx4. Other *Trichoderma* species were not found to produce 6-residue lipopeptaibols. Only Halovir A–E sequences from *Scytalidium* sp. CNL240 [58] and Lipohexin from *Moeszia lindtneri* HKI-0054 [59] were identified as 6-residue lipopeptaibols. Strain *T. cf. strigosellum* SZMC 28391 also produced a unique compound in a relatively high amount, the amino acid composition of which could not be revealed. The mass differences (Δm) on the MS² spectra are shown in Table 6, which is a repetition of 72 and 127 mass differences. Strain *T. cf. strigosellum* SZMC 28007 produced nine already known and seven new 7-residue sequences which were named as Lipostrigaibols I–XVI. The sequences always started with an OcGly only known from Lipostrigaibols [33]. It is followed by an Ala2, which is again unique, because this position is usually taken by Gly2. R3 and 4 were highly variable, Ala/Aib/Vxx/Lxx and Ala/Aib/Vxx were at these positions. R5 was strictly Ala and R6–7 contained either Vxx-Lxxol, or Lxx-Lxxol, which are usual in the lipopeptaibols (Table 7).

Strain *T. cf. strigosellum* SZMC 28391 produced two lipopeptaibols in higher quantities, which were Lipostrigocin LSG-like VIIIb and VI, with 37.08% and 31.96% of the total lipopeptaibol production, respectively (Table 6). The “unidentified compound” mentioned above was also produced in a relatively higher amount, 17.45%, compared to the rest of the lipopeptaibols, which were all below 4% (Table 6). The 7-residue lipopeptaibols were more produced than the 6-residue lipopeptaibols, the latter all being below 2.17%. Three lipopeptaibols were produced in high quantities by *T. cf. strigosellum* SZMC 28007, Lipostrigaibols XV, XIII and XVI (23.7%, 22.15% and 20.8%, respectively) followed by Lipostrigaibols XIV and XII with 9.97% and 8.77%, respectively. The rest of the sequences were all produced below 5.22%.

3.5.2 New Lipostrigocin LSG-like sequences peptaibol compounds from *T. koningii*

T. koningii SZMC 28387 produced a total of 25 lipopeptaibols, out of which seven were 7-residue long while eighteen were 11-residue long (Table 6). Twelve sequences were new, while thirteen were positionally isomeric with already identified Lipostrigocin LSG sequences [37].

T. koningii SZMC 28387 produced more 11-residue than 7-residue lipopeptaibols, out of which Lipostrigocin LSG-like XIV was the most produced (37.46%). Lipostrigocin LSG-like XV, XVI and XX were also produced in a relatively high amount, at 9.6%, 11.01% and

Table 6 Lipopeptaibols produced by *Trichoderma* strains from clade *Viride* The area percentages are calculated based on the total lipopeptaibol production of each strain

Lipopeptaibols	Producer species	[M + H] ⁺	RT (min)	Area (%) total peptaibome	Area (%) lipopeptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15
Lipostrigosellin I	<i>T. cf. strigosellum</i> *	669.48	6.57	1.16%	1.91%	Oc	Aib	Gly	Lxx	Gly	Lxx	Lxxol									
Lipostrigosellin II	<i>T. cf. strigosellum</i> *	669.48	7.23	0.17%	0.28%	Oc	Aib	Gly	Lxx	Gly	Lxx	Lxxol									
Lipostrigosellin III	<i>T. cf. strigosellum</i> *	683.5	9.3	1.32%	2.17%	Oc	Aib	Gly	Lxx	Ala	Lxx	Lxxol									
Lipostrigosellin IV	<i>T. cf. strigosellum</i> *	683.5	10.54	0.17%	0.28%	Oc	Aib	Gly	Lxx	Ala	Lxx	Lxxol									
Lipostrigocin LSG-like I	<i>T. cf. strigosellum</i> *	740.52	10.96	0.14%	0.23%	Oc	Ala	Gly	Lxx	Aib	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like II	<i>T. cf. strigosellum</i> *	740.52	12.15	0.18%	0.30%	Oc	Ala	Gly	Lxx	Aib	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like IIIa	<i>T. hamatum</i>	740.52	14.34	0.83%	1.08%	Oc	Aib	Gly	Vxx	Aib	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like IIIb	<i>T. koningii</i>	740.52	13.16	0.87%	1.28%	Oc	Aib	Gly	Vxx	Aib	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like IIIb	<i>T. cf. strigosellum</i> *	740.52	13.2	0.83%	1.37%	Oc	Aib	Gly	Lxx	Aib	Gly	Vxx	Lxxol								
Lipostrigocin LSG-like IVa	<i>T. hamatum</i>	740.52	15.83	0.06%	0.08%	Oc	Aib	Gly	Vxx	Aib	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like V	<i>T. hamatum</i>	754.54	16.32	0.28%	0.37%	Oc	Vxx	Gly	Vxx	Aib	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like VI	<i>T. koningii</i>	754.54	15.06	0.82%	1.21%	Oc	Vxx	Gly	Vxx	Aib	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like VI	<i>T. hamatum</i>	754.54	16.82	0.27%	0.35%	Oc	Aib	Gly	Lxx	Aib	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like VI	<i>T. koningii</i>	754.54	16.47	0.41%	0.61%	Oc	Aib	Gly	Lxx	Aib	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like VII	<i>T. cf. strigosellum</i> *	754.54	16.51	19.42%	31.96%	Oc	Aib	Gly	Lxx	Aib	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like VII	<i>T. hamatum</i>	754.54	17.84	1.31%	1.71%	Oc	Aib	Gly	Lxx	Aib	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like VII	<i>T. koningii</i>	754.54	18.24	0.07%	3.05%	Oc	Aib	Gly	Lxx	Aib	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like VIIa	<i>T. cf. strigosellum</i> *	754.54	18.28	1.85%	3.70%	Oc	Aib	Gly	Lxx	Aib	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like VIIa	<i>T. hamatum</i>	768.55	20.56	0.90%	1.18%	Oc	Vxx	Gly	Lxx	Aib	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like VIIa	<i>T. koningii</i>	768.56	19.06	0.42%	0.62%	Oc	Vxx	Gly	Lxx	Aib	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like VIIb	<i>T. cf. strigosellum</i> *	768.56	19.81	22.53%	37.08%	Oc	Aib	Gly	Lxx	Vxx	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like IXa	<i>T. hamatum</i>	768.55	22.51	0.07%	0.09%	Oc	Vxx	Gly	Lxx	Aib	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like IXa	<i>T. koningii</i>	768.56	20.94	0.08%	0.12%	Oc	Vxx	Gly	Lxx	Aib	Gly	Lxx	Lxxol								
Lipostrigocin LSG-like IXb	<i>T. cf. strigosellum</i> *	768.56	22.05	2.12%	3.49%	Oc	Aib	Gly	Lxx	Vxx	Gly	Lxx	Lxxol								
Lipostrigaibol-like I	<i>T. cf. strigosellum</i> *	726.51	8.14	0.05%	0.08%	Oc	Gly	Ala	Ala	Vxx	Ala	Lxx	Lxxol								
Lipostrigaibol-like II	<i>T. cf. strigosellum</i> *	726.51	8.68	0.21%	0.35%	Oc	Gly	Ala	Vxx	Ala	Ala	Lxx	Lxxol								
Lipostrigaibol-like III	<i>T. cf. strigosellum</i> *	726.51	9.46	0.15%	0.25%	Oc	Gly	Ala	Aib	Aib	Ala	Lxx	Lxxol								

Table 6 (continued)

Lipopeptaibols	Producer species	[M + H] ⁺	RT (min)	Area (%) peptaibolome	Area (%) lipopeptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15
Lipostrigaibol-like IV	<i>T. cf. strigosellum</i> [#]	726.51	9.93	0.07%	0.11%	Oc	Gly	Ala	Alb	Alb	Ala	Lxx	Lxxol								
Lipostrigaibol-like V	<i>T. cf. strigosellum</i> [#]	726.51	10.47	0.14%	0.22%	Oc	Gly	Ala	Vxx	Alb	Ala	Vxx	Lxxol								
Lipostrigaibol-like VI	<i>T. cf. strigosellum</i> [#]	740.52	12.13	0.91%	1.49%	Oc	Gly	Ala	Lxx	Alb	Ala	Vxx	Lxxol								
Lipostrigaibol-like VII	<i>T. cf. strigosellum</i> [#]	740.52	12.82	0.76%	1.24%	Oc	Gly	Ala	Lxx	Alb	Ala	Vxx	Lxxol								
Lipostrigaibol-like VIII	<i>T. cf. strigosellum</i> [#]	740.52	13.32	3.20%	5.22%	Oc	Gly	Ala	Lxx	Alb	Ala	Vxx	Lxxol								
Lipostrigaibol-like IX	<i>T. cf. strigosellum</i> [#]	740.52	13.85	2.36%	3.85%	Oc	Gly	Ala	Vxx	Alb	Ala	Lxx	Lxxol								
Lipostrigaibol-like X	<i>T. cf. strigosellum</i> [#]	754.54	13.99	0.30%	0.49%	Oc	Gly	Ala	Vxx	Vxx	Ala	Lxx	Lxxol								
Lipostrigaibol-like XI	<i>T. cf. strigosellum</i> [#]	754.54	14.41	0.81%	1.31%	Oc	Gly	Ala	Vxx	Vxx	Ala	Lxx	Lxxol								
Lipostrigaibol-like XII	<i>T. cf. strigosellum</i> [#]	754.54	15.52	5.38%	8.77%	Oc	Gly	Ala	Vxx	Vxx	Ala	Lxx	Lxxol								
Lipostrigaibol-like XIII	<i>T. cf. strigosellum</i> [#]	754.54	16.29	13.59%	22.15%	Oc	Gly	Ala	Lxx	Alb	Ala	Lxx	Lxxol								
Lipostrigaibol-like XIV	<i>T. cf. strigosellum</i> [#]	754.54	17.25	6.12%	9.97%	Oc	Gly	Ala	Lxx	Alb	Ala	Lxx	Lxxol								
Lipostrigaibol-like XV	<i>T. cf. strigosellum</i> [#]	768.56	19.28	14.54%	23.70%	Oc	Gly	Ala	Lxx	Vxx	Ala	Lxx	Lxxol								
Lipostrigaibol-like XVI	<i>T. cf. strigosellum</i> [#]	768.56	20.75	12.76%	20.80%	Oc	Gly	Ala	Lxx	Vxx	Ala	Lxx	Lxxol								
Lipohamatin I	<i>T. hamatum</i>	1009.7	12.27	0.08%	0.11%	Oc	Alb	Gly	Lxx	Alb	Gly	Gly	Vxx	Vxx	Lxx	Lxxol					
Lipohamatin II	<i>T. hamatum</i>	1009.7	15.39	0.23%	0.30%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Lxx	Vxx	Lxx	Lxxol					
Lipohamatin III	<i>T. hamatum</i>	1023.71	17.63	0.19%	0.25%	Oc	Alb	Gly	Lxx	Alb	Gly	Gly	Vxx	Lxx	Lxx	Lxxol					
Lipohamatin IV	<i>T. hamatum</i>	1023.71	18.06	0.15%	0.19%	Oc	Alb	Gly	Lxx	Alb	Gly	Gly	Lxx	Vxx	Lxx	Lxxol					
Lipostrigocin LSG-like X	<i>T. koningii</i>	1024.67	13.59	0.17%	0.25%	Oc	Ala	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XI	<i>T. koningii</i>	1024.67	14.19	0.11%	0.16%	Oc	Alb	Gly	Vxx	Ala	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XII	<i>T. koningii</i>	1024.67	17.31	0.31%	0.45%	Oc	Ala	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XIII	<i>T. koningii</i>	1024.67	18.5	0.89%	1.31%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Vxx	Lxxol				
Lipostrigocin LSG-like XIV	<i>T. koningii</i>	1038.69	22.61	25.44%	37.46%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol				

Table 6 (continued)

Lipoheptaibols	Producer species	[M + H] ⁺	RT (min)	Area (%) total peptaibolome	Area (%) lipoheptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15
Lipostrigocin LSG-like XV	<i>T. koningii</i>	1052.71	23.71	6.52%	9.60%	Oc	Alb	Gly	Lxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XVI	<i>T. koningii</i>	1052.71	24.56	7.48%	11.01%	Oc	Vxx	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XVII	<i>T. koningii</i>	1038.69	25.16	4.17%	6.13%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XVIII	<i>T. koningii</i>	1052.71	25.91	0.87%	1.29%	Oc	Alb	Gly	Lxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XIX	<i>T. koningii</i>	1066.72	26.25	2.79%	4.11%	Oc	Vxx	Gly	Lxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XX	<i>T. koningii</i>	1052.71	27.17	7.72%	11.37%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Lxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XXI	<i>T. koningii</i>	1066.72	28.46	2.59%	3.81%	Oc	Vxx	Gly	Lxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XXII	<i>T. koningii</i>	1052.71	29.52	0.77%	1.14%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Lxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XXIII	<i>T. koningii</i>	1066.72	29.3	3.40%	5.01%	Oc	Vxx	Gly	Vxx	Alb	Gly	Gly	Lxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XXIV	<i>T. koningii</i>	1066.72	30.54	0.39%	0.57%	Oc	Alb	Gly	Lxx	Alb	Gly	Gly	Lxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XXV	<i>T. koningii</i>	1080.74	31.17	1.10%	1.61%	Oc	Vxx	Gly	Lxx	Alb	Gly	Gly	Lxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XXVI	<i>T. koningii</i>	1066.72	31.66	0.35%	0.51%	Oc	Vxx	Gly	Vxx	Alb	Gly	Gly	Lxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XXVII	<i>T. koningii</i>	1080.74	33.24	0.08%	0.11%	Oc	Vxx	Gly	Lxx	Alb	Gly	Gly	Lxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XXVIII	<i>T. hamatum</i>	1024.67	18.83	0.14%	0.19%	Oc	Ala	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XXIX	<i>T. hamatum</i>	1024.67	20.06	0.41%	0.54%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Vxx	Lxxol				
Lipostrigocin LSG-like XXX	<i>T. hamatum</i>	1038.69	21.08	0.68%	0.89%	Oc	Alb	Gly	Lxx	Alb	Gly	Gly	Vxx	Alb	Gly	Vxx	Lxxol				
Lipostrigocin LSG-like XXXI	<i>T. hamatum</i>	1038.69	23.88	0.70%	0.91%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Lxx	Alb	Gly	Vxx	Lxxol				
Lipostrigocin LSG-like XXXII	<i>T. hamatum</i>	1038.69	24.38	2.36%	3.08%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XXXIII	<i>T. cf. dorotheopsis</i>	1038.69	24.29	16.29%	24.40%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XXXIV	<i>T. hamatum</i>	1052.71	24.63	0.40%	0.52%	Oc	Ala	Gly	Lxx	Alb	Gly	Gly	Lxx	Alb	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XXXV	<i>T. hamatum</i>	1052.71	25.46	4.80%	6.28%	Oc	Alb	Gly	Lxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol				

Table 6 (continued)

Lipopeptaibols	Producer species	[M + H] ⁺	RT (min)	Area (%) peptaibome	Area (%) total lipopeptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15
Lipostrigocin LSG-like XXXV	<i>T. hamatum</i>	1052.71	26.37	0.94%	1.23%	Oc	Vxx	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Lxx	Lxxol				
	<i>T. cf. dorothopsis</i>	1052.71	26.33	10.57%	15.84%	Oc	Vxx	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XXXVI	<i>T. hamatum</i>	1052.71	27.79	0.62%	0.81%	Oc	Aib	Gly	Lxx	Aib	Gly	Gly	Vxx	Aib	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XXXVII	<i>T. hamatum</i>	1052.71	29.05	2.86%	3.75%	Oc	Aib	Gly	Vxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XXXVIII	<i>T. hamatum</i>	1066.72	28.14	1.76%	2.31%	Oc	Vxx	Gly	Lxx	Aib	Gly	Gly	Vxx	Aib	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XXXIX	<i>T. hamatum</i>	1066.72	30.34	8.48%	11.10%	Oc	Aib	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XL	<i>T. hamatum</i>	1066.72	31.05	1.20%	1.58%	Oc	Aib	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XLI	<i>T. hamatum</i>	1066.72	32.41	1.29%	1.70%	Oc	Aib	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XLII	<i>T. hamatum</i>	1080.74	33.03	4.62%	6.05%	Oc	Vxx	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XLIII	<i>T. hamatum</i>	1080.74	35.08	0.37%	0.48%	Oc	Vxx	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XLIV	<i>T. hamatum</i>	1094.75	36.48	0.07%	0.09%	Oc	Vxx	Ala	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XLV	<i>T. cf. dorothopsis</i>	1038.69	21.9	1.29%	1.94%	Oc	Vxx	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Vxx	Lxxol				
Lipostrigocin LSG-like XLVI	<i>T. cf. dorothopsis</i>	1038.69	26.89	14.59%	21.86%	Oc	Aib	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Lxx	Lxxol				
Lipostrigocin LSG-like XLVII	<i>T. cf. dorothopsis</i>	1052.71	28.95	10.40%	15.58%	Oc	Vxx	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Lxx	Lxxol				
Trichogin GB IX-like I	<i>T. hamatum</i>	1322.85	31.89	0.01%	0.01%	Oc	Ala	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Vxxol
Trichogin GB IX-like II	<i>T. hamatum</i>	1336.86	32.76	0.07%	0.09%	Oc	Ala	Gly	Lxx	Aib	Gly	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Lxx	Lxxol
Trichogin GB IX-like III	<i>T. hamatum</i>	1322.85	33.42	0.09%	0.12%	Oc	Ala	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Lxx	Lxxol
Trichogin GB IX-like IV	<i>T. hamatum</i>	1336.86	33.79	0.17%	0.22%	Oc	Aib	Gly	Lxx	Aib	Gly	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Vxx	Lxxol
Trichogin GB IX-like V	<i>T. hamatum</i>	1322.85	34.63	0.12%	0.16%	Oc	Aib	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Vxx	Lxxol
Trichogin GB IX-like VI	<i>T. hamatum</i>	1336.86	35.39	0.26%	0.34%	Oc	Aib	Gly	Vxx	Aib	Gly	Gly	Lxx	Aib	Gly	Gly	Vxx	Aib	Gly	Vxx	Lxxol
Trichogin GB IX- like VII	<i>T. hamatum</i>	1350.87	35.39	0.26%	0.34%	Oc	Aib	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Gly	Vxx	Aib	Gly	Vxx	Lxxol

Table 6 (continued)

Lipoheptaibols	Producer species	[M + H] ⁺	RT (min)	Area (%) peptaibolome	Area (%) lipoheptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15
Trichogin GB IX-like VIII	<i>T. hamatum</i>	1322.85	36.18	0.01%	0.02%	Oc	Ala	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol
Trichogin GB IX-like IX	<i>T. hamatum</i>	1350.87	37.03	0.56%	0.73%	Oc	Alb	Gly	Lxx	Alb	Gly	Gly	Vxx	Alb	Gly	Gly	Lxx	Alb	Gly	Vxx	Lxxol
Trichogin GB IX-like X	<i>T. hamatum</i>	1336.86	37.84	0.52%	0.68%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Gly	Lxx	Alb	Gly	Vxx	Lxxol
Trichogin GB IX-like XI	<i>T. hamatum</i>	1350.87	38.7	2.93%	3.84%	Oc	Alb	Gly	Lxx	Alb	Gly	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol
Trichogin GB IX-like XII	<i>T. hamatum</i>	1364.89	39.19	0.60%	0.79%	Oc	Alb	Gly	Lxx	Alb	Gly	Gly	Lxx	Alb	Gly	Gly	Lxx	Alb	Gly	Vxx	Lxxol
Trichogin GB IX-like XIII	<i>T. hamatum</i>	1336.86	39.57	2.22%	2.90%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol
Trichogin GB IX-like XIV	<i>T. cf. dorotheopsis</i>	1336.86	39.51	3.54%	5.30%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol
	<i>T. hamatum</i>	1364.89	40.05	2.58%	3.38%	Oc	Alb	Gly	Lxx	Alb	Gly	Gly	Lxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol
Trichogin GB IX-like XV	<i>T. hamatum</i>	1350.87	40.18	2.31%	3.02%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Lxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol
Trichogin GB IX-like XVI	<i>T. hamatum</i>	1364.89	40.9	1.18%	1.55%	Oc	Vxx	Gly	Lxx	Alb	Gly	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol
Trichogin GB IX-like XVII	<i>T. cf. dorotheopsis</i>	1350.87	41.14		3.57%	Oc	Vxx	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol
Trichogin GB IX-like XVIII	<i>T. hamatum</i>	1350.87	41.22	1.24%	1.62%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Lxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol
Trichogin GB IX-like XIX	<i>T. hamatum</i>	1364.89	41.97	1.17%	1.54%	Oc	Vxx	Gly	Vxx	Alb	Gly	Gly	Lxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol
Trichogin GB IX-like XX	<i>T. hamatum</i>	1336.86	42.16	0.21%	0.28%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol
Trichogin GB IX-like XXI	<i>T. cf. dorotheopsis</i>	1336.86	42.17	4.45%	6.67%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol
	<i>T. hamatum</i>	1378.9	42.3	0.97%	1.28%	Oc	Vxx	Gly	Lxx	Alb	Gly	Gly	Lxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol
Trichogin GB IX-like XXII	<i>T. hamatum</i>	1350.87	42.65	0.22%	0.29%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Lxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol
Trichogin GB IX-like XXIII	<i>T. hamatum</i>	1364.89	42.68	4.08%	5.34%	Oc	Alb	Gly	Lxx	Alb	Gly	Gly	Vxx	Alb	Gly	Gly	Lxx	Alb	Gly	Lxx	Lxxol
Trichogin GB IX-like XXIV	<i>T. hamatum</i>	1350.87	43.72	3.54%	4.63%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Gly	Lxx	Alb	Gly	Lxx	Lxxol
Trichogin GB IX-like XXV	<i>T. cf. dorotheopsis</i>	1350.87	43.86	3.23%	4.83%	Oc	Vxx	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Gly	Vxx	Alb	Gly	Lxx	Lxxol
Trichogin GB IX-like XXVI	<i>T. hamatum</i>	1364.89	44.91	3.20%	4.19%	Oc	Alb	Gly	Vxx	Alb	Gly	Gly	Lxx	Alb	Gly	Gly	Lxx	Alb	Gly	Lxx	Lxxol
	<i>T. hamatum</i>	1378.9	44.53	5.09%	6.67%	Oc	Alb	Gly	Lxx	Alb	Gly	Gly	Lxx	Alb	Gly	Gly	Lxx	Alb	Gly	Lxx	Lxxol

Table 6 (continued)

Lipopeptaibols	Producer species	[M + H] ⁺	RT (min)	Area (%) total peptaibome	Area (%) lipopeptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15
Trichogin GB IX- like XXVII	<i>T. hamatum</i>	1364.89	45.42	1.39%	1.82%	Oc	Vxx	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol
Trichogin GB IX- like XXVIII	<i>T. hamatum</i>	1350.87	45.96	0.55%	0.72%	Oc	Aib	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol
Trichogin GB IX- like XXIX	<i>T. hamatum</i>	1378.9	46.36	2.03%	2.66%	Oc	Vxx	Gly	Vxx	Aib	Gly	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol
Trichogin GB IX- like XXX	<i>T. hamatum</i>	1392.92	46.57	1.80%	2.36%	Oc	Vxx	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol
Trichogin GB IX- like XXXI	<i>T. hamatum</i>	1364.89	46.83	0.56%	0.73%	Oc	Aib	Gly	Vxx	Aib	Gly	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol
Trichogin GB IX- like XXXII	<i>T. hamatum</i>	1392.92	48.09	0.29%	0.38%	Oc	Vxx	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol
Trichogin GB IX- like XXXIII	<i>T. hamatum</i>	1406.93	49.27	0.03%	0.04%	Oc	Vxx	Gly	Lxx	Aib	Gly	Gly	Lxx	Vxx	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol
Trichogin GB IX- like XXXIV	<i>T. hamatum</i>	1406.93	52.9	0.01%	0.01%	Oc	Lxx	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol
Trichogin GB IX- like XXXV	<i>T. hamatum</i>	1406.93	55.85	0.00%	0.01%	Oc	Vxx	Gly	Lxx	Aib	Ala	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol
Unidentified compound (val- ues given Δm)	<i>T. cf. strigosellum</i> *	814.51	10.24	10.60%	17.45%	200.1	72.0	127.1	72.0	127.1	72.0	127.1	170								

Amino acid exchanges in new compounds shown in Table 6 are set in italic. Lipopeptaibols produced by *T. cf. dorotheopsis* are from strain SZMC 28005 in this table

* Produced by *T. cf. strigosellum* SZMC 28391

produced by *T. cf. strigosellum* SZMC 28007

Table 7 Similarities to known compounds of lipopeptaibols produced by *Trichoderma* strains from clade *Viride*

Lipopeptaibol	Compound identical or positionally isomeric with	Reference
Lipostrigosellin I	New: Lipostrigocin LSG A3: [Aib] ⁴ → (Positional isomer of Lipostrigosellin II)	[37]
Lipostrigosellin II	New: (Positional isomer of Lipostrigosellin I)	→ Lipostrigosellin I
Lipostrigosellin III	New: Lipostrigocin LSG A1: [Aib] ⁴ → (Positional isomer of Lipostrigosellin IV)	[37]
Lipostrigosellin IV	New: Lipostrigocin LSG A1: [Aib] ⁴ → (Positional isomer of Lipostrigosellin III)	→ Lipostrigosellin III
Lipopeptaibol	Compound identical or positionally isomeric with	Reference
Lipostrigocin LSG-like I	Lipostrigocin LSG A1 (Positional isomer of Lipostrigocin LSG-like II)	[37]
Lipostrigocin LSG-like II	(Positional isomer of Lipostrigocin LSG-like I)	→ Lipostrigocin LSG-like I
Lipostrigocin LSG-like IIIa	New: Lipostrigocin LSG A3: [Lxx] ³ → [Vxx] ³ (Positional isomer of Lipostrigocin LSG-like IVa)	[37]
Lipostrigocin LSG-like IIIb	Lipostrigocin LSG A2	[37]
Lipostrigocin LSG-like Iva	New: (Positional isomer of Lipostrigocin LSG-like IIIa)	→ Lipostrigocin LSG-like IIIa
Lipostrigocin LSG-like IVb	New: Lipostrigocin LSG A3: [Lxx] ³ → [Phe] ³	[37]
Lipostrigocin LSG-like V	New: Lipostrigocin LSG A6: [Lxx] ³ → [Vxx] ³	[37]
Lipostrigocin LSG-like VI	Lipostrigocin LSG A3	[37]
Lipostrigocin LSG-like VII	Lipostrigocin LSG A4	[37]
Lipostrigocin LSG-like VIIIa	Lipostrigocin LSG A5	[37]
Lipostrigocin LSG-like VIIIb	New: Lipostrigocin LSG A4: [Aib] ⁴ → [Vxx] ⁴ (Positional isomer of Lipostrigocin LSG-like IXb)	[37]
Lipostrigocin LSG-like IXa	Lipostrigocin LSG A6	[37]
Lipostrigocin LSG-like IXb	New: (Positional isomer of Lipostrigocin LSG-like VIIIb)	→ Lipostrigocin LSG-like VIIIb
Lipostrigaibol-like I	New: Lipostrigaibol A: [Ala] ³ ↔ [Vxx] ⁴	[33]
Lipostrigaibol-like II	Lipostrigaibol A	[33]
Lipostrigaibol-like III	New: Lipostrigaibol B: [Vxx] ³ → [Aib] ³ (Positional isomer of Lipostrigaibol-like IV)	[33]
Lipostrigaibol-like IV	New: (Positional isomer of Lipostrigaibol-like III)	→ Lipostrigaibol-like III
Lipostrigaibol-like V	New: Lipostrigaibol A: [Lxx] ⁶ → [Vxx] ⁶	[33]
Lipostrigaibol-like VI	New: Lipostrigaibol A: [Vxx] ³ → [Lxx] ³ ; [Lxx] ⁶ → [Vxx] ⁶ (Positional isomer of Lipostrigaibol-like VII and VIII)	[33]
Lipostrigaibol-like VII	New: (Positional isomer of Lipostrigaibol-like VI and VIII)	[33]
Lipostrigaibol-like VIII	New: (Positional isomer of Lipostrigaibol-like VI and VII)	→ Lipostrigaibol-like VI
Lipostrigaibol-like IX	Lipostrigaibol B	[33]
Lipostrigaibol-like X	Lipostrigaibol C (Positional isomer of Lipostrigaibol-like XI and XII)	[33]
Lipostrigaibol-like XI	(Positional isomer of Lipostrigaibol-like X and XII)	→ Lipostrigaibol-like X
Lipostrigaibol-like XII	(Positional isomer of Lipostrigaibol-like X and XI)	→ Lipostrigaibol-like X
Lipostrigaibol-like XIII	Lipostrigaibol D (Positional isomer of Lipostrigaibol-like XIV)	[33]
Lipostrigaibol-like XIV	(Positional isomer of Lipostrigaibol-like XIII)	→ Lipostrigaibol-like XIII
Lipostrigaibol-like XV	Lipostrigaibol E (Positional isomer of Lipostrigaibol-like XVI)	[33]
Lipostrigaibol-like XVI	(Positional isomer of Lipostrigaibol-like XV)	→ Lipostrigaibol-like XV
Lipohamatin I	New: Linopubescin LPB B: [Vxx] ⁵ → [Gly] ⁵ ; [Lxx] ⁶ → [Gly] ⁶ ; [Aib] ⁷ → [Vxx] ⁷ ; [Gly] ⁸ → [Vxx] ⁸	[37]
	New: Linopubescin LPB C: [Vxx] ⁵ → [Gly] ⁵ ; [Lxx] ⁶ → [Gly] ⁶ ; [Aib] ⁷ → [Vxx] ⁷ ; [Aib] ⁹ → [Lxx] ⁹	[37]
Lipohamatin II	New: Linopubescin LPB A: [Vxx] ⁵ → [Gly] ⁵ ; [Lxx] ⁶ → [Gly] ⁶ ; [Aib] ⁷ → [Lxx] ⁷ ; [Gly] ⁸ → [Vxx] ⁸	[37]
Lipohamatin III	New: Linopubescin LPB B: [Vxx] ⁵ → [Gly] ⁵ ; [Lxx] ⁶ → [Gly] ⁶ ; [Aib] ⁷ → [Vxx] ⁷ ; [Gly] ⁸ → [Lxx] ⁸	[37]
Lipohamatin IV	New: Linopubescin LPB B: [Vxx] ⁵ → [Gly] ⁵ ; [Lxx] ⁶ → [Gly] ⁶ ; [Aib] ⁷ → [Lxx] ⁷ ; [Gly] ⁸ → [Vxx] ⁸	[37]
	New: Linopubescin LPB C: [Vxx] ⁵ → [Gly] ⁵ ; [Lxx] ⁶ → [Gly] ⁶ ; [Aib] ⁷ → [Lxx] ⁷ ; [Aib] ⁹ → [Lxx] ⁹	[37]
Lipostrigocin LSG-like X	New: Trikonigin KB I: [Aib] ¹ → [Ala] ¹ (Positional isomer of Lipostrigocin LSG-like XII)	[61]
Lipostrigocin LSG-like XI	New: Trikonigin KB I: [Aib] ⁴ → [Ala] ⁴	[61]
Lipostrigocin LSG-like XII	New: (Positional isomer of Lipostrigocin LSG-like X)	→ Lipostrigocin LSG-like X
Lipostrigocin LSG-like XIII	New: Trikonigin KB I: [Ile] ¹⁰ → [Vxx] ¹⁰	[61]
Lipostrigocin LSG-like XIV	Lipostrigocin LSG B3 (Positional isomer of Lipostrigocin LSG-like XVII)	[37]
Lipostrigocin LSG-like XV	Lipostrigocin LSG B04	[37]
Lipostrigocin LSG-like XVI	Lipostrigocin LSG B11	[37]

Table 7 (continued)

Lipopeptaibol	Compound identical or positionally isomeric with	Reference
Lipostrigocin LSG-like XVII	(Positional isomer of Lipostrigocin LSG-like XIV)	→ Lipostrigocin LSG-like XIV
Lipostrigocin LSG-like XVIII	Lipostrigocin LSG B06	[37]
Lipostrigocin LSG-like XIX	New: Lipostrigocin LSG B08: [Lxx] ⁷ → [Vxx] ⁷ (Positional isomer of Lipostrigocin LSG-like XXI)	[37]
Lipostrigocin LSG-like XX	Lipostrigocin LSG B03 (v2) (Positional isomer of Lipostrigocin LSG-like XXII)	[37]
Lipostrigocin LSG-like XXI	New: (Positional isomer of Lipostrigocin LSG-like XIX)	→ Lipostrigocin LSG-like XIX
Lipostrigocin LSG-like XXII	(Positional isomer of Lipostrigocin LSG-like XX)	→ Lipostrigocin LSG-like XX
Lipostrigocin LSG-like XXIII	New: Lipostrigocin LSG B08: [Lxx] ³ → [Vxx] ³	[37]
Lipostrigocin LSG-like XXIV	New: Lipostrigocin LSG B08: [Vxx] ¹ → [Aib] ¹	[37]
Lipostrigocin LSG-like XXV	Lipostrigocin LSG B08 (Positional isomer of Lipostrigocin LSG-like XXVII)	[37]
Lipostrigocin LSG-like XXVI	New: Lipostrigocin LSG B03 (v2): [Aib] ¹ → [Vxx] ¹	[37]
Lipostrigocin LSG-like XXVII	(Positional isomer of Lipostrigocin LSG-like XXV)	→ Lipostrigocin LSG-like XXV
Lipostrigocin LSG-like XXVIII	New: Lipostrigocin LSG B3: [Aib] ¹ → [Ala] ¹	[37]
Lipostrigocin LSG-like XXIX	New: Lipostrigocin LSG B3: [Lxx] ¹⁰ → [Vxx] ¹⁰	[37]
Lipostrigocin LSG-like XXX	New: Lipostrigocin LSG B4 and B5: [Lxx] ¹⁰ → [Vxx] ¹⁰	[37]
Lipostrigocin LSG-like XXXI	New: Lipostrigocin LSG B03 v2, B6 and B09: [Lxx] ¹⁰ → [Vxx] ¹⁰	[37]
Lipostrigocin LSG-like XXXII	New: Trichogin GA IV: [Aib] ¹ → [Ala] ¹	[37]
Lipostrigocin LSG-like XXXIV	Lipostrigocin LSG B04	[37]
Lipostrigocin LSG-like XXXV	Lipostrigocin LSG B11	[37]
Lipostrigocin LSG-like XXXVI	Lipostrigocin LSG B05	[37]
Lipostrigocin LSG-like XXXVII	Lipostrigocin LSG B06	[37]
Lipostrigocin LSG-like XXXVIII	Lipostrigocin LSG B07	[37]
Lipostrigocin LSG-like XXXIX	Trichogin GA IV (Positional isomer of Lipostrigocin LSG-like XL and XLI)	[37]
Lipostrigocin LSG-like XL	(Positional isomer of Lipostrigocin LSG-like XXXIX and XLI)	→ Lipostrigocin LSG-like XXXIX
Lipostrigocin LSG-like XLI	(Positional isomer of Lipostrigocin LSG-like XXXIX and XL)	→ Lipostrigocin LSG-like XXXIX
Lipostrigocin LSG-like XLII	Lipostrigocin LSG B08	[37]
Lipostrigocin LSG-like XLIII	Lipostrigocin LSG B10	[37]
Lipostrigocin LSG-like XLIV	New: Lipostrigocin LSG B10: [Gly] ² → [Ala] ²	[37]
Lipostrigocin LSG-like XLV	Lipostrigocin LSG B11 (Positional isomer of Lipostrigocin LSG-like XLVII)	[37]
Lipostrigocin LSG-like XLVI	Lipostrigocin LSG B3	[37]
Lipostrigocin LSG-like XLVII	(Positional isomer of Lipostrigocin LSG-like XLV)	→ Lipostrigocin LSG-like XLV
Trichogin GB IX-like I	New: Trichogin GB IX: [Aib] ¹ → [Ala] ¹ ; [Lxx] ³ → [Vxx] ³ ; [Lxx] ⁷ → [Vxx] ⁷ ; [Lxxol] ¹⁵ → [Vxxol] ¹⁵	[60]
Trichogin GB IX-like II	New: Trichogin GB IX: [Aib] ¹ → [Ala] ¹ ; [Lxx] ⁷ → [Vxx] ⁷ ; [Lxx] ¹¹ → [Vxx] ¹¹	[60]
Trichogin GB IX-like III	New: Trichogin GB IX: [Aib] ¹ → [Ala] ¹ ; [Lxx] ³ → [Vxx] ³ ; [Lxx] ⁷ → [Vxx] ⁷ ; [Lxx] ¹¹ → [Vxx] ¹¹ (Positional isomer of Trichogin GB IX-like VIII)	[60]
Trichogin GB IX-like IV	New: Trichogin GB IX: [Lxx] ⁷ → [Vxx] ⁷ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Lxx] ¹⁴ → [Vxx] ¹⁴	[60]
Trichogin GB IX-like V	New: Trichogin GB IX: [Lxx] ³ → [Vxx] ³ ; [Lxx] ⁷ → [Vxx] ⁷ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Lxx] ¹⁴ → [Vxx] ¹⁴	[60]
Trichogin GB IX-like VI	New: Trichogin GB IX: [Lxx] ³ → [Vxx] ³ ; [Lxx] ¹¹ → [Vxx] ¹¹ ; [Lxx] ¹⁴ → [Vxx] ¹⁴	[60]
Trichogin GB IX-like VII	New: Trichogin GB IX: [Lxx] ¹¹ → [Vxx] ¹¹ ; [Lxx] ¹⁴ → [Vxx] ¹⁴	[60]
Trichogin GB IX-like VIII	New: (Positional isomer of Trichogin GB IX-like III)	→ Trichogin GB IX-like III
Trichogin GB IX-like IX	New: Trichogin GB IX: [Lxx] ⁷ → [Vxx] ⁷ ; [Lxx] ¹⁴ → [Vxx] ¹⁴	[60]

Table 7 (continued)

Lipopeptaibol	Compound identical or positionally isomeric with	Reference
Trichogin GB IX-like X	New: Trichogin GB IX: [Lxx] ³ → [Vxx] ³ ; [Lxx] ⁷ → [Vxx] ⁷ ; [Lxx] ¹⁴ → [Vxx] ¹⁴	[60]
Trichogin GB IX-like XI	New: Trichogin GB IX: [Lxx] ⁷ → [Vxx] ⁷ ; [Lxx] ¹¹ → [Vxx] ¹¹	[60]
Trichogin GB IX-like XII	New: Trichogin GB IX: [Lxx] ¹⁴ → [Vxx] ¹⁴	[60]
Trichogin GB IX-like XIII	New: Trichogin GB IX: [Lxx] ³ → [Vxx] ³ ; [Lxx] ⁷ → [Vxx] ⁷ ; [Lxx] ¹¹ → [Vxx] ¹¹ (Positional isomer of Trichogin GB IX-like XX)	[60]
Trichogin GB IX-like XIV	New: Trichogin GB IX: [Lxx] ¹¹ → [Vxx] ¹¹	[60]
Trichogin GB IX-like XVI	New: Trichogin GB IX: [Aib] ¹ → [Vxx] ¹ ; [Lxx] ⁷ → [Vxx] ⁷ ; [Lxx] ¹¹ → [Vxx] ¹¹	[60]
Trichogin GB IX-like XVII	New: (Positional isomer of Trichogin GB IX-like XXIV)	→ Trichogin GB IX-like XXIV
Trichogin GB IX-like XVIII	New: (Positional isomer of Trichogin GB IX-like XV and XII)	→ Trichogin GB IX-like XV
Trichogin GB IX-like XIX	New: Trichogin GB IX: [Aib] ¹ → [Vxx] ¹ ; [Lxx] ³ → [Vxx] ³ ; [Lxx] ¹¹ → [Vxx] ¹¹	[60]
Trichogin GB IX-like XX	New: (Positional isomer of Trichogin GB IX-like XIII)	→ Trichogin GB IX-like XIII
Trichogin GB IX-like XXI	New: Trichogin GB IX: [Aib] ¹ → [Vxx] ¹ ; [Lxx] ¹¹ → [Vxx] ¹¹	[60]
Trichogin GB IX-like XXII	New: (Positional isomer of Trichogin GB IX-like XV and XVIII)	→ Trichogin GB IX-like XV
Trichogin GB IX-like XXIII	New: Trichogin GB IX: [Lxx] ⁷ → [Vxx] ⁷	[60]
Trichogin GB IX-like XXIV	New: (Positional isomer of Trichogin GB IX-like XVII)	→ Trichogin GB IX-like XVII
Trichogin GB IX-like XXV	New: Trichogin GB IX: [Lxx] ³ → [Vxx] ³ (Positional isomer of Trichogin GB IX-like XXXI)	[60]
Trichogin GB IX-like XXVI	Trichogin GB IX	[60]
Trichogin GB IX-like XXVII	New: Trichogin GB IX: [Aib] ¹ → [Vxx] ¹ ; [Lxx] ³ → [Vxx] ³ ; [Lxx] ⁷ → [Vxx] ⁷	[60]
Trichogin GB IX-like XXVIII	New: (Positional isomer of Trichogin GB IX-like XXIII)	→ Trichogin GB IX-like XXIII
Trichogin GB IX-like XXIX	New: Trichogin GB IX: [Aib] ¹ → [Vxx] ¹ ; [Lxx] ³ → [Vxx] ³	[60]
Trichogin GB IX-like XXX	New: Trichogin GB IX: [Aib] ¹ → [Vxx] ¹ (Positional isomer of Trichogin GB IX-like XXXII)	[60]
Trichogin GB IX-like XXXI	New: (Positional isomer of Trichogin GB IX-like XXV)	→ Trichogin GB IX-like XXV
Trichogin GB IX-like XXXII	New: (Positional isomer of Trichogin GB IX-like XXX)	→ Trichogin GB IX-like XXX
Trichogin GB IX-like XXXIII	New: Trichogin GB IX: [Aib] ¹ → [Vxx] ¹ ; [Aib] ⁸ → [Vxx] ⁸	[60]
Trichogin GB IX-like XXXIV	New: Trichogin GB IX: [Aib] ¹ → [Lxx] ¹	[60]
Trichogin GB IX-like XXXV	New: Trichogin GB IX: [Aib] ¹ → [Vxx] ¹ ; [Gly] ⁵ → [Ala] ⁵	[60]

11.37%, respectively. The 7-residue lipopeptaibols were produced below 1.28%.

3.5.3 Identification of the new group of Lipohamatinins from *T. hamatum*

T. hamatum SZMC 28747 produced sixty-two 7-, 10-, 11- and 15-residue lipopeptaibols, out of which 16 compounds were known, while 47 were newly identified, out of which all the 10-residue lipopeptaibols were completely new to science and were named as Lipohamatin I-IV. They were similar to Linopubescin LPB A, B and C [37]. The 7-, and 11- residue sequences showed similarity to the Lipostrigocin LSG sequences, while the 15-residue compounds to Trichogin GB IX [37, 60], which was the only 15-residue lipopeptaibol reported.

T. hamatum SZMC 28747 produced the most diverse lipopeptaibol profile. The lipopeptaibol most produced by this strain was Lipostrigocin LSG-like XXXIX with 11.1%. Trichogin GB IX-like XXVI was the most produced 15-residue lipopeptaibol by this strain (6.67%). All 7- and 10-residue lipopeptaibols were produced below 1.71%.

3.5.4 New Lipostrigocin LSG-like peptaibol sequences from *T. cf. dorotheopsis*

Strain *T. cf. dorotheopsis* SZMC 28005 produced only nine lipopeptaibols, out of which five were 11-residue, four were 15-residue sequences. Similarly to the lipopeptaibols of *T. hamatum* SZMC 28747, the 11-residue sequences were positionally isomeric with Lipostrigocin LSG B3 and B11 sequences, while all the 15-residue sequences were new but similar to Trichogin GB IX [37, 60]. Two sequences, Lipostrigocin LSG-like XXXII and XXXV were also produced by *T. hamatum* SZMC 28747 (Table 6).

Strain SZMC 28005 produced four 11-residue lipopeptaibols in high quantities, which were Lipostrigocin LSG-like XXXII, XLVI, XXXV and XLVII (24.4%, 21.86%, 15.84% and 15.58%, respectively), as well as a further 11-residue compound, Lipostrigocin LSG-like XLV at 1.94%. All the other 15-residue sequences were produced between 3.57% and 6.67% of the total lipopeptaibol production.

Table 8 The ¹most produced sequences, ²consensus sequences and ³amino acid varieties of lipopeptaibols produced by each strain (Lipostrigocin LSG like lipopeptaibols from *T. cf. strigosellum* were produced by SZMC 28391, while Lipostrigaibols were from *T. cf. strigosellum* SZMC 28007)

Species	Name of lipopeptaibol	R	R1	R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15
6-residue lipopeptaibols																	
<i>T. cf. strigosellum</i>	¹ Lipostrigocin LSG-like III	Oc	Aib	Gly	Lxx	Ala	Lxx	Lxxol									
	² Lipostrigocin LSG-like	Oc	Aib	Gly	Lxx	<u>Gly/Ala</u>	Lxx	Lxxol									
	³ Lipostrigocin LSG-like	Oc	Aib	Gly	Lxx	Gly/Ala	Lxx	Lxxol									
7-residue lipopeptaibols																	
<i>T. cf. strigosellum</i>	¹ Lipostrigocin LSG-like XIb	Oc	Aib	Gly	Lxx	Vxx	Gly	Lxx	Lxxol								
	² Lipostrigocin LSG-like	Oc	Aib	Gly	Lxx	<u>Aib</u>	Gly	Lxx	Lxxol								
	³ Lipostrigocin LSG-like	Oc	Ala/Aib	Gly	Lxx/Phe	Aib/Vxx	Gly	Vxx/Lxx	Lxxol								
<i>T. cf. strigosellum</i>	¹ Lipostrigaibol-like	Oc	Gly	Ala	Lxx	Vxx	Ala	Lxx	Lxxol								
	² Lipostrigaibol-like	Oc	Gly	Ala	Lxx	<u>Aib</u>	Ala	Lxx	Lxxol								
	³ Lipostrigaibol-like	Oc	Gly	Ala	Ala/Aib/ Vxx/Lxx	Ala/Aib/ Vxx	Ala	Vxx/Lxx	Lxxol								
<i>T. koningii</i>	¹ Lipostrigocin LSG-like VIIa	Oc	Aib	Gly	Vxx	Aib	Gly	Lxx	Lxxol								
	² Lipostrigocin LSG-like	Oc	Aib	Gly	<u>Lxx</u>	Aib	Gly	Lxx	Lxxol								
	³ Lipostrigocin LSG-like	Oc	Aib/Vxx	Gly	Vxx/Lxx	Aib	Gly	Lxx	Lxxol								
<i>T. hamatum</i>	¹ Lipostrigocin LSG-like XI	Oc	Aib	Gly	Lxx	Aib	Gly	Lxx	Lxxol								
	² Lipostrigocin LSG-like	Oc	Aib	Gly	Lxx	Aib	Gly	Lxx	Lxxol								
	³ Lipostrigocin LSG-like	Oc	Aib/Vxx	Gly	Vxx/Lxx	Aib	Gly	Lxx	Lxxol								
10-residue lipopeptaibols																	
<i>T. hamatum</i>	¹ Lipohamatin II	Oc	Aib	Gly	Vxx	Aib	Gly	Gly	Lxx	Vxx	Lxx	Lxxol					
	² Lipohamatin	Oc	Aib	Gly	<u>Lxx</u>	Aib	Gly	Gly	<u>Vxx/ Lxx</u>	Vxx	Lxx	Lxxol					
	³ Lipohamatin	Oc	Aib	Gly	Vxx/Lxx	Aib	Gly	Gly	Vxx/ Lxx	Vxx/ Lxx	Lxx	Lxxol					
11-residue lipopeptaibols																	
<i>T. koningii</i>	¹ Lipostrigocin LSG-like XVIII	Oc	Aib	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Lxx	Lxxol				
	² Lipostrigocin LSG-like	Oc	Aib	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Lxx	Lxxol				
	³ Lipostrigocin LSG-like	Oc	Ala/Aib/ Vxx	Gly	Vxx/Lxx	Ala/Aib	Gly	Gly	Vxx/ Lxx	Aib	Gly	Vxx/Lxx	Lxxol				
<i>T. hamatum</i>	¹ Lipostrigocin LSG-like XX	Oc	Aib	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol				
	² Lipostrigocin LSG-like	Oc	Aib	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol				
	³ Lipostrigocin LSG-like	Oc	Ala/Aib/ Vxx	Gly/ Ala	Vxx/Lxx	Aib	Gly	Gly	Vxx/ Lxx	Aib	Gly	Lxx	Lxxol				
<i>T. cf. dorotheopsis</i>	¹ Lipostrigocin LSG-like XXXII	Oc	Aib	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Lxx	Lxxol				
	² Lipostrigocin LSG-like	Oc	<u>Vxx</u>	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Lxx	Lxxol				
	³ Lipostrigocin LSG-like	Oc	Aib/Vxx	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Vxx/Lxx	Lxxol				
15-residue lipopeptaibols																	
<i>T. hamatum</i>	¹ Trichogin GB IX-like XXVI	Oc	Aib	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Gly	Lxx	Aib	Gly	Lxx	Lxxol
	² Trichogin GB IX-like	Oc	Aib	Gly	<u>Vxx</u>	Aib	Gly	Gly	Lxx	Aib	Gly	Gly	<u>Vxx</u>	Aib	Gly	Lxx	Lxxol
	³ Trichogin GB IX-like	Oc	Ala/Aib/ Vxx	Gly	Vxx/Lxx	Aib	Gly	Gly	Vxx/ Lxx	Aib/ Vxx	Gly	Gly	Vxx/ Lxx	Aib	Gly	Vxx/ Lxx	Lxxol
<i>T. cf. dorotheopsis</i>	¹ Trichogin GB IX-like XX	Oc	Aib	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Lxx	Lxxol
	² Trichogin GB IX-like	Oc	<u>Aib/Vxx</u>	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Lxx	Lxxol
	³ Trichogin GB IX-like	Oc	Aib/Vxx	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Gly	Vxx	Aib	Gly	Lxx	Lxxol

Amino acids in consensus sequences differing from the most produced compound are underlined. Darker color denotes the most produced sequences of the strain, lighter color denotes the consensus sequences showing the most abundant amino acid at each position

3.6 Comparative analysis of lipopeptaibols produced by species of clade *Viride*

The microheterogeneity within the lipopeptaibols were different from the SF1 peptaibols (Table 8). The repetitive motif Vxx/Lxx-Aib-Gly appeared in all sequences between R3-R5 in 7- and 10-residue lipopeptaibols, except for *T. cf. strigosellum* SZMC 28007 lipopeptaibols, where Gly5 was substituted with Ala5. In 11-residue lipopeptaibols, the R3-R5 Vxx/Lxx-Aib-Gly motif continued with a Gly with the repetition of the Vxx/Lxx-Aib-Gly

motif between R7-9. In 15-residue lipopeptaibols, the Vxx/Lxx-Aib-Gly motif appeared from R3-R5, R7-9, and R11-13. Between these motifs, Gly was at positions R6 and R10. This phenomenon can also be the result of module skipping based on the sequence similarities, that the “original” lipopeptaibols are the longer ones [27, 39], however, it needs further research and proof.

The 6-residue lipopeptaibols contained only one variable position at R4 which could be Gly/Ala (Table 8). Gly and Ala were present at this position equally. The same Gly/Ala variability is also present in 7-residue lipopeptaibols at R5, with Gly in Lipostrigocin LSG-like sequences and Ala in the Lipostrigaibol sequences. R1 could be Oc/Aib/OcVxx, while R6 was Vxx/Lxx. Lipostrigocin LSG-like IVb produced by *T. cf. strigosellum* SZMC 28391 is unique, because it has Phe at R3 instead of Lxx (Tables 6, 7 and 8). Only LP237 F7 and LP237 F8 lipopeptaibols from *Tolypocladium geodes* contain Phe3 in their sequences, however, they are 11-residue long [18, 51]. The microheterogeneity of 7-residue Lipostrigaibols appeared at R4, R5 and R6, which is discussed above. In the 10-residue Lipohamatin, Vxx/Lxx variability could be detected at R3, R7 and R8. The 11-residue Lipostrigocin LSG-like sequences showed microheterogeneity at R1, R3, R4, R7 and R10 (Table 8). R1 was OcAla/OcAib/OcVxx, R4 Ala/Aib, while R3, R7 and R10 were Vxx/Lxx. The microheterogeneity of the 15-residue Trichogin GA IX like lipopeptaibols was similar to the 11-residue lipopeptaibols, however, R4 was only Aib and R11 and R14 were also Vxx/Lxx (Table 8). Trichogin GB IX-like I was unique among these sequences, it contained Vxxol instead of Lxxol at its C terminus (Tables 6 and 7).

The consensus sequence was different from the most produced sequence of the two *T. cf. strigosellum* strains at R4, which are underlined in Table 8. At R3, Lipostrigocin LSG-like peptaibols containing mostly Lxx differed from the most produced Vxx containing Lipostrigocin LSG-like VIIa. This could also be observed among Lipohamatin where Lipohamatin II contained Vxx instead of the most abundant Lxx at R3. Lipohamatin also differed from the most produced Lipohamatin II at their R7, they contained equally Vxx and Lxx (Table 8). Lipostrigocin LSG-like peptaibols produced by *T. cf. strigosellum* SZMC 28391 contained Aib4, while the most produced Lipostrigocin LSG-like XIIb contained Vxx4 (Table 8). Lipostrigaibols produced by *T. cf. strigosellum* SZMC 28007 contained Aib4, while the most produced Lipostrigaibol-like XIIbV contained Vxx4 (Table 8). Similarly, Lipostrigocin LSG-like lipopeptaibols produced by *T. koningii* SZMC 28387 contained Lxx3, while the most produced Lipostrigocin LSG-like VIIa Vxx3 (Table 8). The most produced Lipohamatin II contained Vxx3 instead of the most abundant Lxx3 and Lxx7, while R7 was equally Vxx or Aib (Table 8). The most produced Trichogin GA IX like XXVI contained Lxx3 and Lxx11 instead of the most abundant Vxx3 and Vxx11 in lipopeptaibols produced by *T. hamatum* SZMC 28747. OcAib-1 was detected in Trichogin GB IX-like XX, while OcAib and OcVxx was equally present in Trichogin GB IX-like sequences produced by *T. cf. dorotheopsis* SZMC 28005.

3.7 Quantitative analysis of the whole peptaibiome produced by the members of clade *Viride*

Tables 3 and 6 also contain the integrated area of each peak belonging to each compound produced by the strains investigated. The values are based on the integrated area under each peak. In the previous sections, the peptaibols and lipopeptaibols were quantified based on the percentages of the total peptaibol and lipopeptaibol production separately, however, it is also important to quantify the entire peptaibiome altogether. *T. cf. dorotheopsis* SZMC 28390 produced exclusively peptaibols, which quantity was discussed above, while *T. atroviride* SZMC 28748 also produced peptaibol-like sequences apart from peptaibols, but no lipopeptaibols. Within the strains investigated in clade *Viride*, one peptaibol subgroup was produced by each strain, on the other hand, a few lipopeptaibols were the same produced by different strains, which are shown in Table 6. Strains *T. koningii* SZMC 28387, *T. cf. strigosellum* SZMC 28007 and *T. hamatum* SZMC 28747 all produced the 7-residue Lipostrigocins LSG VI and VII, while only *T. koningii* SZMC 28387 and *T. hamatum* SZMC 28747 produced Lipostrigocins LSG IIIa, IVa, V, VIIIa and IXa. *T. cf. strigosellum* SZMC 28007 produced similar lipopeptaibols only differing in 1 amino acid exchange from the 'a' type variants, which are Lipostrigocins LSG IIIb, IVb, VIIIb and IXb (Table 6). Strains *T. hamatum* SZMC 28747 and *T. cf. dorotheopsis* SZMC 28005 produced the same 11-residue Lipostrigocin LSG-like XXXII and XXXV, and the 15-residue Trichogin GB IX-like XIII and XX lipopeptaibols.

T. koningii SZMC 28387 produced only two peptaibol compounds in higher abundances, Trikonigins KA-like XLV and XLIII (9.14% and 8.28%, respectively). More lipopeptaibols were produced in higher quantities, Lipostrigocin LSG-like XIV (25.44%) is the most produced, followed by Lipostrigocin LSG-like XX (7.72%), Lipostrigocin LSG-like XVI (7.48%) and Lipostrigocin LSG-like XV (6.52%). The rest of the peptaibiome for *T. koningii* ranges from 0.002% to 4.17%. Strigaibol-like XII from *T. cf. strigosellum* SZMC 28391 appeared as the most produced peptaibol (14.19%), followed by Strigaibol-like XIV (10.83%). The most produced lipopeptaibol by this strain is Lipostrigocin LSG-like VIIIb (22.53%), followed by Lipostrigocin LSG-like VI (19.42%). The "unidentified compound" was also produced at higher quantity (10.6%). The rest of the peptaibiome ranges from 0.03 to 2.53%. Among *T. atroviride* SZMC 28748 peptaibols, the most produced compound is Trichorzianin TA-like XXIX (8.56%) followed by Trichorzianin TA-like XXV (7.42%). The rest of the peptaibiome ranged from 0.03 to 4.37%. The peptaibol-like compounds were produced in much less quantities ranging from 0.003 to 0.22%. *T. hamatum* SZMC 28747 produced Tricholongin

LB-like XVI (6.87%) as the most produced peptaibol, which was followed by Tricholongin LB-like XIII (6.07%). This strain also produced several lipopeptaibols in high amounts, the most produced being Lipostrigocin LSG-like XXXIX (8.48%) followed by Lipostrigocin LSG-like XXXIV (4.8%) and Lipostrigocin LSG-like XLII (4.62%). Other lipopeptaibols, Lipostrigocin LSG-like XXXVII, Trichogin GB IX-like XI, Trichogin GB IX-like XXIII, Trichogin GB IX-like XXIII, Trichogin GB IX-like XXV and Trichogin GB IX-like XXVI were also produced in high quantities ranging from 2.87% to 4.08%. This was the only investigated strain, which produced these many compounds in high amounts. The most produced peptaibol of *T. cf. dorotheopsis* SZMC 28005 is Dorotheopsin B XXVI (3.38%) and Dorotheopsin B XIII (3.23%), which is much less than the most produced lipopeptaibols, Lipostrigocin LSG-like XXXII (16.29%), Lipostrigocin LSG-like XLVI (14.59%), Lipostrigocin LSG-like XXXV (10.57%) and Lipostrigocin LSG-like XLVII (10.4%). *T. cf. strigosellum* SZMC 28007 produced less peptaibols than lipopeptaibols similarly to *T. cf. dorotheopsis* SZMC 28005. Strigosellin A IX (5.62%) was the most produced peptaibol followed by Strigosellin A XIII (5.03%), Strigosellin A XIV (4.23%) and Strigosellin A XII (4.15%). The most produced lipopeptaibols are Lipostrigaibol-like XV (14.54%), Lipostrigaibol-like XIII (13.59%) and Lipostrigaibol-like XVI (12.76%). The rest of the peptaibiome ranges from 0.05% to 6.12%.

3.8 Structural investigation of a representative peptaibol of clade *Viride*, Trikonigin KA V produced by *T. koningii*

Strain *T. koningii* SZMC 28387 produced Trikonigin KA-like peptaibols out of which Trikonigin KA-like XIX and its positional isomers (Trikonigin KA-like XXXV, XL, XLIII and L) from Tables 3 and 4 show the same sequences as Trikonigin KA (TRK-V) identified by Goulard et al. [29]. They also determined the isomers of Lxx and Vxx, and since TRK-V is a good representation of peptaibols produced by members of clade *Viride*, this sequence was selected for aMD simulations. Auvin-Guette et al. [61] firstly reported the structure of TRK-V to be “right-handed helical form” using circular dichroism spectroscopy and was found to be membrane active and displayed antibiotic activity against *Staphylococcus aureus*. We previously reported the classical MD simulations-based results of TRK-V [38]. Using the newly optimized aMD parameters, the previously reported TRK-V molecule was elucidated again to obtain the complete canonical ensemble and compare with short classical MD conducted earlier. TRK-V was previously identified as a peptaibol produced by *T. koningiopsis* along with two other 11-residue sequences, Trikonigins KB I and

KB II [62]. Another study by our group identified novel peptaibols which were named as “Koningiopsins” with TRK-V as the closest sequence [38]. TRK-V, positionally isomeric with sequences Pept-Vb, -Vib, and -VII of *T. gamsii*, is a 19-residue peptaibol with seven Aib residues in its sequence. Aib is an achiral residue, which has been shown to promote helix formation and can exist in both right- and left-handed helix regions on the Ramachandran plot. To determine the propensities of each residue for a given secondary structure type, their relative free energies were calculated which clearly describe an energetically favourable conformation (Fig. 2). The spread of dihedral angle scatter during the simulation indicates that the system underwent through all the conformations. The darkest regions indicate energetically preferable conformations.

Our previous results of Ramachandran plots of TRK-V [38] showed overall secondary structural propensity towards a left-handed helical conformation. However, upon comparing the reweighted phi-psi populations in Fig. 2 with the same plots from Fig. 1 from Marik et al. [38] (100 ns long classical MD), it becomes clear that most residues like Aib1-Ile5, Ser10, Leu11, Pro13, and Gln17-Gln18 lie in the same free energy minima. However, many others flanking the central region like Gln6-Aib9, Aib12, and Val14-Ile16 show shifts from the predominant left-handed helical regions to the right-handed helical region. It is understandable for all Aib residues as the probability of occurring in both left-handed and right-handed helical quadrants is the same due to its achiral nature. A significant shift was observed in the free energy minima of Gln6 and Val14 residues from the left-handed to the right-handed helical region.

Figure 3A describes the reweighted free-energy landscape of TRK-V as obtained from the first two principal components of dihedral PCA of 1 μ s long aMD simulation. It is clear that the largest cluster lies at the energy minimum and the corresponding representative structure presumes a helical shape with the C-terminus showing a hinge-like bend. The loss of helical fold before the C-terminus is responsible for this hinge-like motion and is a characteristic of the Aib-Pro bond found in all long peptaibols. The next two largest clusters 2 and 3 correspond to highly bent and C-terminus loss-of-helix conformations, respectively, which probably indicates intermediate states. The 4th cluster with the smallest population lies at a separate region on the free-energy landscape and corresponds to the highly helical, slightly bent conformation. This structure is most likely to be observed using experimental methods like X-ray crystallography along with the curved backbone conformations. The 1st cluster appears to populate a separate region on the FEL map which can be accessed under 2 kcal mol⁻¹.

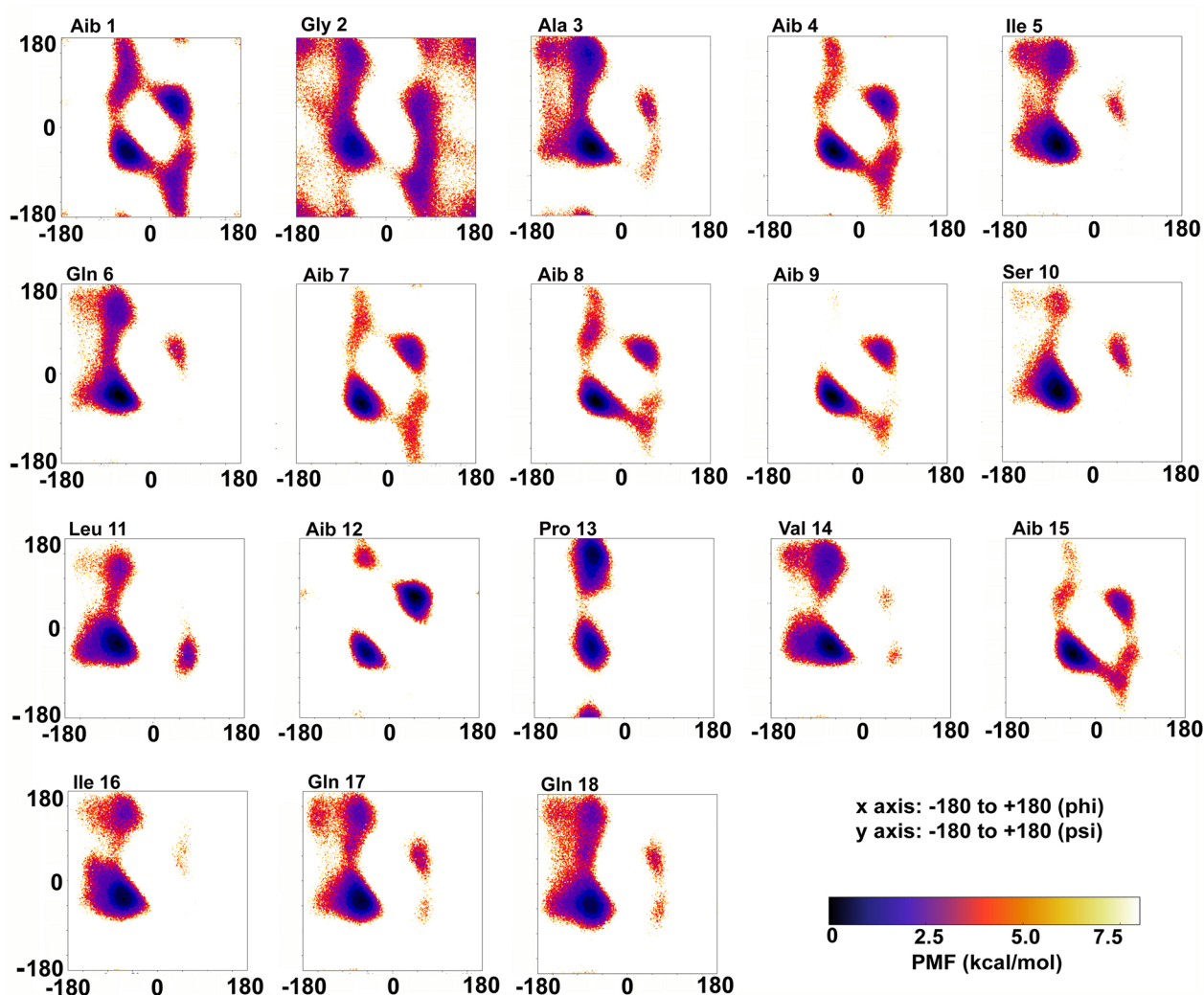


Fig. 2 The reweighted phi-psi torsional distribution for each residue of TRK-V. Most residues show an energy minimum in the right-handed α -helical region

Its representative structure can be explained by the presence of a helix-destabilizing residue Ile16 at the C-terminus [63]. Their occurrence along the course of the simulation can be visualized in Fig. 3B. Interestingly, Ile residues at the 5th and 16th positions also show a strong right-handed α -helical propensity (Fig. 2). Li and Deber [64] measured the helical propensity of amino acid residues in membrane and reported that β -branched Ile and Val can act as ‘helix-promoters’ in membrane environment but as ‘helix-destabilizers’ in aqueous environment. The effect of seemingly similar residues Leu/Ile/Val substitution on peptaibol sequences must be studied in detail. There is evidence in case of other antimicrobial peptides where a single substitution could affect interaction with lipid membranes and resulting bioactivity. For example, Aurein 2.2 and 2.3 vary only at a single position between Leu/Ile and show different bioactivities against

bacterial species [65]. Studies on derivatives of another peptide, δ -lysin, showed that peptides rich in Ile may bind bilayer membranes more efficiently than Leu-rich peptides [66]. Deber and Stone [67] published a systematic study of the effect of Leu/Ile substitution on membrane-active peptides and found that peptides with all Leu/Ile placed on one side (lipophilic side) in contrast to the less hydrophobic face on the other side, showed that the Ile-rich peptide had a higher capability to insert in the membrane than the Leu-rich peptide. Similarly, Ile-rich peptides were found to be more protected from the action of proteinases than Leu peptides in the presence of lipid bilayers. Recently, Nakatani et al. [68] also reported the construction of derivatives of Trichorovin-XII with varying Ile content where all of them folded into α -helix like β -bend spiral. However, the compound found to be the most bioactive contained the highest number of Ile in

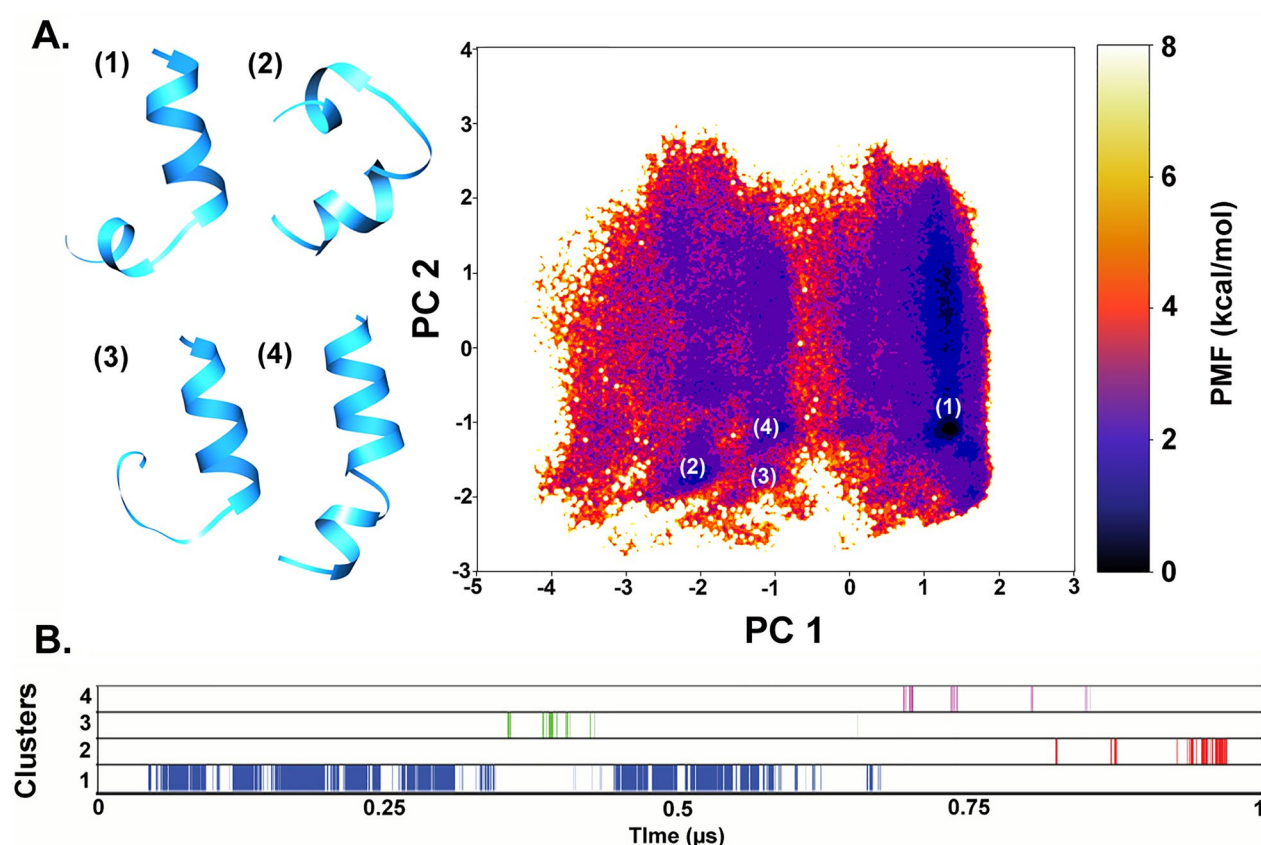


Fig. 3 **A** Reweighted FEL of the first two principal components calculated from dihedral angles, phi-psi, for better clustering based on internal motions. The representative structures of TRK-V corresponding to various energy minima have also been provided, **B** Diagrammatic representation of cluster distribution along the simulation trajectory

its sequence. Ile analogs also showed greater ion channel activity compared to Leu analogs.

3.9 Predicted bioactivity of peptaibiotics produced by the members of *Trichoderma* clade *Viride*

A detailed investigation of the bioactivity and function of the reported peptaibols is required to evaluate their application potential in agriculture or as therapeutics. However, their potential bioactivity can be predicted based on their sequences and the already available knowledge. First of all, the longer peptaibols (19-residues) are supposed to show higher bioactivity against bilayer membranes than their shorter counterparts. It is known that the 20-residue Alamethicin folds into a strict α -helix at the N-terminus and a 3_{10} -helix at the C-terminus, and the resulting length of the folded peptide exactly spans the transmembrane width to form ion-channels. On the other hand, the 15-residue Ampullosporin A rather shows a detergent-like activity in membranes and is less active [69]. Adam et al. [70] reported on the conclusive effect of Aib-foldamers (peptaibol) length and C-terminal lipophilicity on ionophoric and antibacterial activity. The

longer foldamers with a hydrophobic C-terminus were found to be more active, suggesting that the length of the peptides is an important criterion that may affect their activity. The 20-residue Paracelsins investigated in our previous work [27] folded into strict α -helices very similarly to Alamethicin, and thus, can be expected to have a similar mechanism of action.

Another major marker is the amount of Aib residues in the sequence which imparts a helical structure but not in a highly strict conformation. It can fluctuate between α -helical and 3_{10} -helical conformations, thereby, expanding the length of the folded peptide to span the transmembrane region and also provide space to fit in bulky neighbouring side chains [71]. In the newly reported subgroups of Strigosellins and Dorotheopsins, a total of 8 Aib residues could be found in the sequences. All peptaibol subgroups, except for Strigosellins, have 3 consecutive Aib residues from R7-R9. The presence of three consecutive helix-shape promoting Aib residues [72, 73] provides a strong helical character to the structure which seems to be crucial for most membrane-active peptides. Therefore,

the presence of helix-promoting residues is also one of the main crucial features.

Lastly, the presence and position of helix-breaking residues like Gly and Pro can give us crucial clues towards helical stability. Peptide curvature or “kink” may also be a crucial feature in determining the biological activity. Cheng and Chang [74] discussed the implication of the more stable kinked form of Alamethicin than the energetically less stable linear form in voltage-gating. They proposed that linearization of the Alamethicin helices from the kinked structure upon increasing electric potential beyond a threshold may be the first event in voltage-gating mechanism. The kinks are introduced by helix-breaker residues like Pro and Gly in peptaibols. Kaduk et al. [75] showed that the substitution of Gly11 and Pro14 in Alamethicin did not affect channel formation but reduced conductance levels and significantly reduced lifetimes. Duclohier [76] in his review noted that without any applied voltage to the membrane system, Alamethicin with a higher kink angle than Trichotoxin will have a greater embedment of the N-terminus in the hydrocarbon core while the C-terminus lies flat at the bilayer interface. This greater embedment of the N-terminus, in turn, explains the higher voltage dependence of Alamethicin. Similarly, Trikonigin KA-V with a helical N-terminus, 19-residue length and a slight kink at the Aib-Pro bond also seems to be ideal for transmembrane orientation and ion channel formation. In this study, all sequences have an Aib-Pro bond which is expected to introduce this influential ‘kink’ to the folded structure. Moreover, a high bioactivity is expected from lipopeptaibols due to the presence of the fatty acid chain which is prone to strongly interact with the lipid bilayer [77]. Due to their shorter length they may not form transmembrane ion channels, but may have a different mechanism of action than peptaibols.

4 Conclusions

The peptaibiotic production of *Trichoderma* clade *Viride* revealed known and new subgroups of peptaibiotics. The new subgroups of peptaibols are Strigosellins A and B with 14 and 6, Dorothopsins A-a, -b, -c, -d, -e and -f with 13, 8, 1, 3, 1 and 2, as well as, Dorothopsin B compounds with 36 completely new sequences, respectively. The already known and certain new compounds belong to the Trikonigin KA, Trichorzianin TA and Tricholongin LB subgroups with 51, 33 and 21 identified sequences, respectively. New lipopeptaibol subgroups are Lipostrigosellins and Lipohamatinins with 4, and 4 completely new sequences. The other identified new and already known lipopeptaibols belong to the Lipostrigocin LSG and Trichogin GB subgroups with a total of 103 sequences. The peptaibol subgroups produced by the

examined species were completely different from each other, while a few lipopeptaibols were produced by more than one species within the clade. We selected the TRK-V sequence for structure elucidation as a good representation of peptaibols produced by *T. koningii* SZMC 28387 which also has been elucidated before. Enhanced sampling of MD simulations allowed to observe that TRK-V takes a right-handed helical shape with a strong helix-disrupting effect of Ile residues when simulated in an aqueous environment. Previous research indicates towards a better membrane interactive potential of Ile-containing peptides in a hydrophobic environment. The results provide an idea about the three-dimensional structural folding of all Trikonigin-like peptaibols mentioned in this work.

Supplementary Information

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Additional file 1.

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Data availability

All data generated or analysed during this study are included in this published article.

Declarations

Competing interests

The authors declare that there are no conflicts of interest associated with this work.

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