Data in Brief 6 (2016) 359–367

Contents lists available at ScienceDirect

Data in Brief

journal homepage: www.elsevier.com/locate/dib

Data article

Comparison of bactericidal and cytotoxic activities of trichogin analogs

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ARTICLE INFO

Article history:
Received 25 September 2015
Received in revised form
30 November 2015
Accepted 4 December 2015
Available online 17 December 2015

Keywords:
Peptaibols
Trichogin
Antibaterial activity
Cytotoxicity

ABSTRACT

Peptaibiotics are a group of membrane active peptides of fungal origin. They typically contain α-aminoisobutyric acid (Aib; 1-letter code, U) and other non-coded residues (Toniolo and Brückner, 2009; Neumann et al., 2015; Benedett et al., 1982) [1–3] stabilizing their helical structure. Peptaibols are peptaibiotics carrying a 1, 2-aminoalcohol at the C-terminus. When a fatty acid chain (of 8–10 carbon atoms) is present at their N-terminus, they are called lipopeptaibols (Toniolo et al., 2001; Degenkolb et al., 2003) [4,5]. We found (Tavano et al., 2015) [6] that the lipopeptaibol trichogin displays no antibacterial effects up to 64 μM, against both Gram$^-$ and Gram$^+$ bacteria, but kills tumor and healthy human cells via a mechanism requiring both the C-terminal primary alcohol group and the N-terminal n-octanoyl moiety, with EC50s around 4–5 μM. However, the substitution of single Gly residues with Lys strongly improves anti-Gram$^+$ activity (Tavano et al., 2015; De Zotti, Biondi, Park et al., 2012; De Zotti, Biondi, Peggion et al., 2012) [6–8]. To further characterize the activity of trichogin analogs as antibiotics and cytotoxic agents, we here manipulated the peptide helix amphipathicity by means of two different substitutions: (i) Aib to Leu (De Zotti et al., 2012) [7] or (ii) multiple Gly to Lys changes (Tavano et al., 2015; De Zotti, Biondi, Park et al., 2012; De Zotti, Biondi, Peggion, Formaggio et al., 2012; De Zotti, Biondi, Peggion, De Poli et al., 2012) [6–9]. The antibacterial activity against four commensal or opportunistic bacterial species and the cytotoxicity against a panel of 9 healthy and tumor-derived

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http://dx.doi.org/10.1016/j.dib.2015.12.006

eukaryotic cell types (including erythrocytes) are reported as MIC and EC50 (MTS - [3-(4, 5-dimethylthiazol-2-yl)-5-(3-carboxymethoxyphenyl)-2-(4-sulfophenyl)]-2H-tetrazolium- reduction and LDH - lactate dehydrogenase - release assay).

Specifications Table

Subject area	*Chemistry, Biology*
More specific subject area	*Peptaibols*
Type of data	*Table, text file, graph, figures*
How data was acquired	*HPLC, mass spectrometry, FACS, spectrofluorimetry*
Data format	*Analyzed*
Experimental factors	*Different kind of bacterial or eukaryotic cells were treated with different concentrations of peptides for* 24 h
Experimental features	*After incubation with peptides, cell viability* (*MTS assay*), *type of death* (*Annexin-propidium iodide assay*) *or fluorescence associated to the cells* (*FACS analysis*) *were assessed*
Data source location	*University of Padova, Italy*
Data accessibility	*The data are supplied with this article*

Value of the data

- The need to find new antibacterial agents able to overcome antibiotic resistance and, at the same time, the expectation of having new effective antitumor drugs may benefit from the accurate quantification of the antimicrobial and cytotoxic efficacy and selectivity of peptaibols.
- We here report quantitative data from which it is possible to compare the antibiotic activity and the cytocidal efficacy of several analogs of trichogin GA IV.
- The data reported here may be useful since they provide a base for possible further design and refinement of either anti-microbial or anti-tumor activity of trichogin-derived peptides.

1. Data

1.1. Antibacterial activity of trichogin and its analogs

As previously observed [7], analogs L1 and L1,8 (Table 2; throughout text, the 1-letter code for amino acids was used) showed a moderately improved anti *Staphylococcus aureus* (*S. aureus*) activity (MIC after 24 from $>64\,\mu M$ to $32\,\mu M$), whilst L4, known to have a destabilized helix [7], showed no such increase. Introduction of one, two or three K residues in the sequence (Table 1) induced a strong MIC (24 h) decrease against the Gram$^+$ bacteria tested (2–5 μM) and the Gram$^-$ *Escherichia coli* (*E. coli*) (8–16 μM) (Table 2). Anti-Gram$^-$ *Pseudomonas aeruginosa* (*P. aeruginosa*) activity was also improved in di- or tri-K containing analogs (MIC, 12–16 μM). To further improve the antibacterial activity of the K-containing analogs we introduced an additional U residue at position 6, to stabilize the helix (K5U6, K2K5K9U6). In addition, we replaced U at position 1 with L (L1K2, L1K9) as this substitution was shown to improve the activity of