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Data Article

NMR and computational data of two novel antimicrobial peptides

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ABSTRACT

Here we report details on the design and conformational analysis of two novel peptides showing antimicrobial properties, as reported in the research article, “New antimicrobial peptides against foodborne pathogens: from in silico design to experimental evidence” G. Palmieri, M. Balestrieri, Y.T.R. Proroga, L. Falcigno, A. Facchiano, A. Riccio, F. Capuano, R. Marrone, G. Campanile, A. Anastasio (2016) [1]. NMR data, such as chemical shifts in two different solvents as well as aCH protons deviations from random coil values and NOE patterns, are shown together with the statistics of structural calculations. Strategy and particulars of molecular design are presented.

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Specifications Table

Subject area	*Chemistry*
More specific subject area	*Structural analysis*
Type of data	*Tables, graphs*
How data was acquired	*NMR (Varian Inova 600, equipped with a cryoprobe, and Varian Inova 400)*
Data format	*Analyzed*
Experimental factors	*Peptide solutions in DMSO-d_6 and in TFE-d_3/H_2O 50:50 (v/v)*
Experimental features	*Molecular modeling and peptide design. Acquisition and analysis of 1D and 2D NMR spectra of antimicrobial peptides to obtain NMR parameters, essentially NOE effects, used for molecular structures calculations by computational programs.*
Data source location	*Dept. of Pharmacy, University Federico II of Naples, Naples, Italy and Institute of Food Science National Research Council (CNR-ISA), Avellino, Italy*
Data accessibility	*Data is with this article*

Value of the data

- These data details the molecular design and NMR characterization of two novel antimicrobial peptides.
- NMR parameters, such as chemical shifts, in two different media can be useful for comparison with other peptides showing antimicrobial activities.
- The structural features emerging from in silico analysis and peptide molecular models can used to guide the design of analogs with enhanced biological activities.
- This data may provide insights for development of MTP-derived antimicrobials for food safety.

Data

Data reported in the following are distinguished in three sub-sections: NMR analysis; computational methods; peptide design. In the first we report the proton chemical shifts of MTP1 and MTP2 peptides in DMSO and TFE/H_2O 1:1 (Tables 1–4), together with the diagrams of the most relevant NOE effects (Figs. 1 and 2) and the deviations of the αCH protons from random coil values (Figs. 3 and 4). Next, we show the structural statistics of the molecular model calculations for MTP1 and MTP2 (Tables 5 and 6). Finally, the computed parameters from the computational tools used in the peptide designing.

1. Experimental design, materials and methods

1.1. NMR analysis

Two-dimensional (2D) experiments, such as total correlation spectroscopy (TOCSY) [2], nuclear Overhauser effect spectroscopy (NOESY) [3], and double quantum-filtered correlated spectroscopy (DQFCOSY) [4] were recorded by the phase sensitive States–Haberkorn method [5] on MTP1 and MTP2. TOCSY experiments were acquired with a 70 ms mixing time, while NOESY experiments were acquired with 150 and 300 ms mixing times; the water resonance was suppressed by using gradients [6].

Proton sequential assignments of the amino acid spin systems, obtained following the standard method proposed by Wuthrich [7], are reported in Tables 1–4.