A Novel Brominated Alkaloid Securidine A isolated from the marine bryozoan Securiflustra securifrons

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STUDY BACKGROUND
Marine bryozoans are producing a significant number of bioactive secondary metabolites including macrolides, alkaloids, sterols and heteroatom-containing compounds that possess antitumor, antibacterial and muscle relaxant activities.

In the present study, we isolated and elucidated the structure of the brominated tyrosine derivative Securidine A from the coldwater marine bryozoan Securiflustra securifrons, and its bioactivities were also investigated by selected bioassays. Previously, nine compounds were isolated from S. securifrons and no biological activities were reported.

RESULTS

METHODOLOGY
• S. securifrons was collected in the North Sea (71,0759° N, 24,4355° E)
• The frozen marine bryozoan was extracted and pre-fractionated by flash chromatography
• The elemental composition of Securidine A was calculated using UHPLC-HR-MS and followed by dereplication
• Purification was carried out on two different columns, Waters Xterra RP18 (10×300 mm, 10 µm) and Waters Phenyl-hexyl Prep (10×250 mm, 5 µm) in Prep-HPLC
• The structure of Securidine A was elucidated based on 1D and 2D NMR experiments

WORKSCHEME

Extraction

Prefractionation

Screening of bioactivity

High Resolution Mass Spectrometry (HR-MS) analysis

Dereplication (Novel/or Known compound)

Isolation by Prep-HPLC

Structure elucidation by Nuclear Magnetic Resonance (NMR)

Bioactivity profiles

Anticancer
Antibacterial
Antidiabetes
Inhibition of Biofilm growth

Figure 1: Ion chromatogram of active flash fractions (4 to 6) of Securiflustra showed the target compound with mass 357.0862 m/z.

Dereplication: (Figure 1)
The active fractions (4 to 6) were analyzed by UHPLC-HR-MS. The isotopic pattern indicated that the eluted compound was a mono-brominated compound and its elemental composition was C_{21}H_{24}BrN_{4}O_{2}. The target compound was dereplicated based on data base search, which was suggested that the compound was new.

Isolation: (Figure 2)
Preparative HPLC was used to isolate Securidine A. The mass of Securidine A (357.0926 m/z) was used as a collection trigger. The active fractions of S. securifrons were loaded onto a Waters - Xterra RP18 and Phenyl - hexyl Prep HPLC columns.

The purified compound was used for structure elucidation and to investigate its biological activities.

Structure Elucidation: (Figure 3)
The structure of the isolated compound was determined through interpretation of data from 1D and 2D (HMBC, ME-HSQC, H2BC, COSY and ROESY) NMR experiments. We have named the new compound ‘Securidine A’. 2D correlations of Securidine A is seen in the figure below.

Figure 2: Base peak intensity chromatogram showed the successful isolation of the target compound.

Figure 3: The key HMBC, ME-HSQC, H2BC, COSY and ROESY correlations of Securidine A

Summary:
The new brominated tyrosine derivative Securidine A was isolated from the aqueous extract of the marine bryozoan Securiflustra securifrons. The structure was determined by interpretation of data from 1D and 2D NMR experiments and mass spectrometry analysis. Securidine A did not show any biological activities in the applied bioassays. Further bioactivity profiling is required in order to identify any potential biological activities of the molecule.

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References: