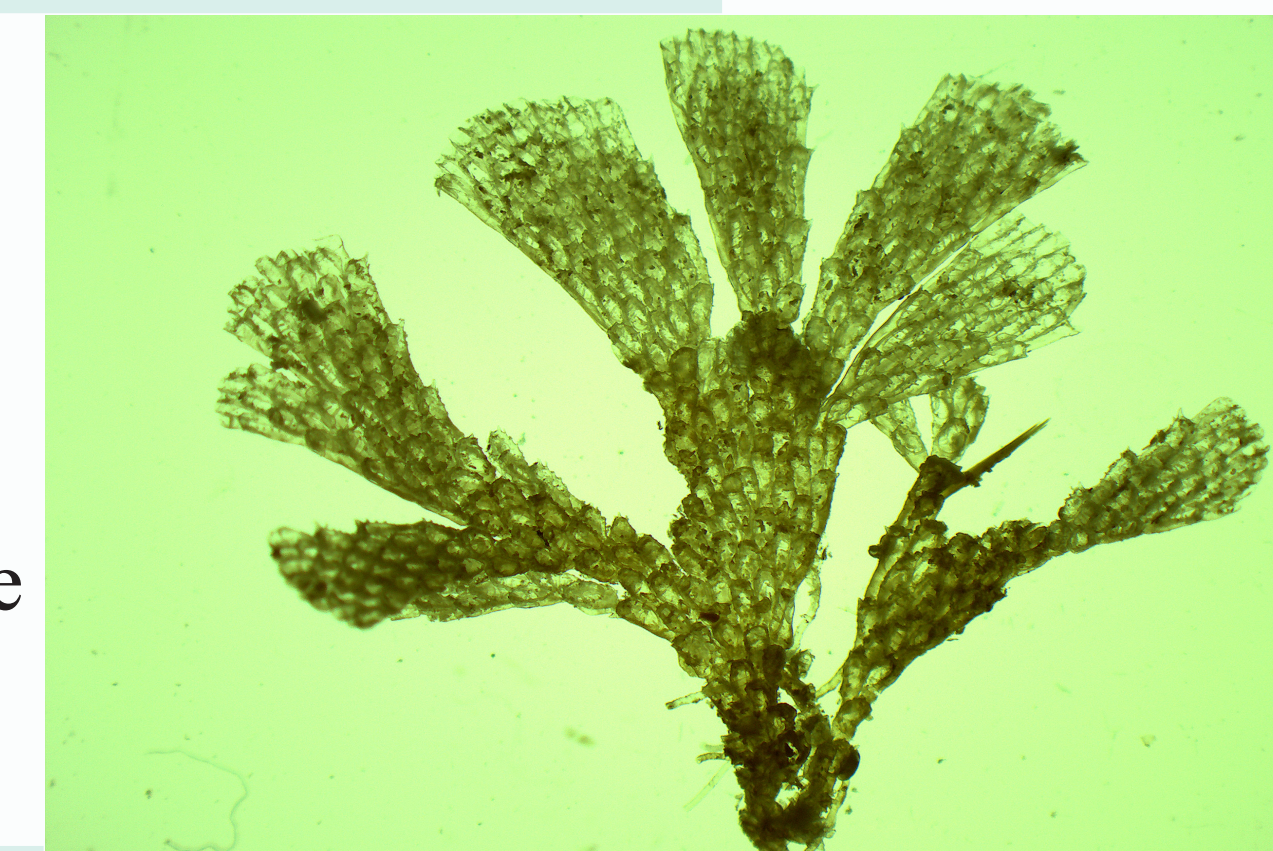


DENDROBEANIAMINE A, A NEW ALKALOID FROM THE ARCTIC
MARINE BRYOZOAN *DENDROBEANIA MURRAYANA*Priyanka Michael¹, Espen Hansen¹, Johan Isaksson², Jeanette H. Andersen¹ and Kine Ø.Hansen¹¹MARBIO, UiT–The Arctic University of Norway, Breivika, Tromsø N-9037, Norway;²Department of Chemistry, UiT–The Arctic University of Norway, Breivika, Tromsø N-9037, Norway.

*raja.p.siranjeevi@uit.no

/STUDY BACKGROUND:

Bryozoans are filter feeding, sessile and colony forming aquatic invertebrates which are producing structurally diverse bioactive secondary metabolites including the flustramine, the eusynstyelamides, the bryostatins and the securamines [1-2]. As part our ongoing search for new secondary metabolites from Arctic invertebrates [3], we are reporting a new secondary metabolite from the Arctic marine bryozoan *Dendrobeatia murrayana* (Figure 1).

Figure 1: An image of *D.murrayana*/CHEMICAL ANALYSIS OF ORGANIC CRUDE EXTRACT OF ARCTIC BRYOZOAN *D. MURRAYANA*:

The animal material was collected from the North Sea, freeze dried and extracted into organic extract. An aliquot of organic crude extract was analyzed by ultra performance liquid chromatography and high resolution of mass spectrometry (UPLC-HR-MS) with positive electrospray ionization (ESI⁺). Vcti gv'eqo r qwpf "3"y cu'ugrgev "dcugf "qp"j g"dcug" r gcn'l'p'v'puk' "ej gtqo cvqi tco u"qh'F0 wtc{cpc and other related bryozoans. An unique and prominent peak was observed in *D.murrayana* at the retention time (R_t) of 5.7 min with *m/z* 369.2863 (Figure 2). it was not found in other related bryozoans.

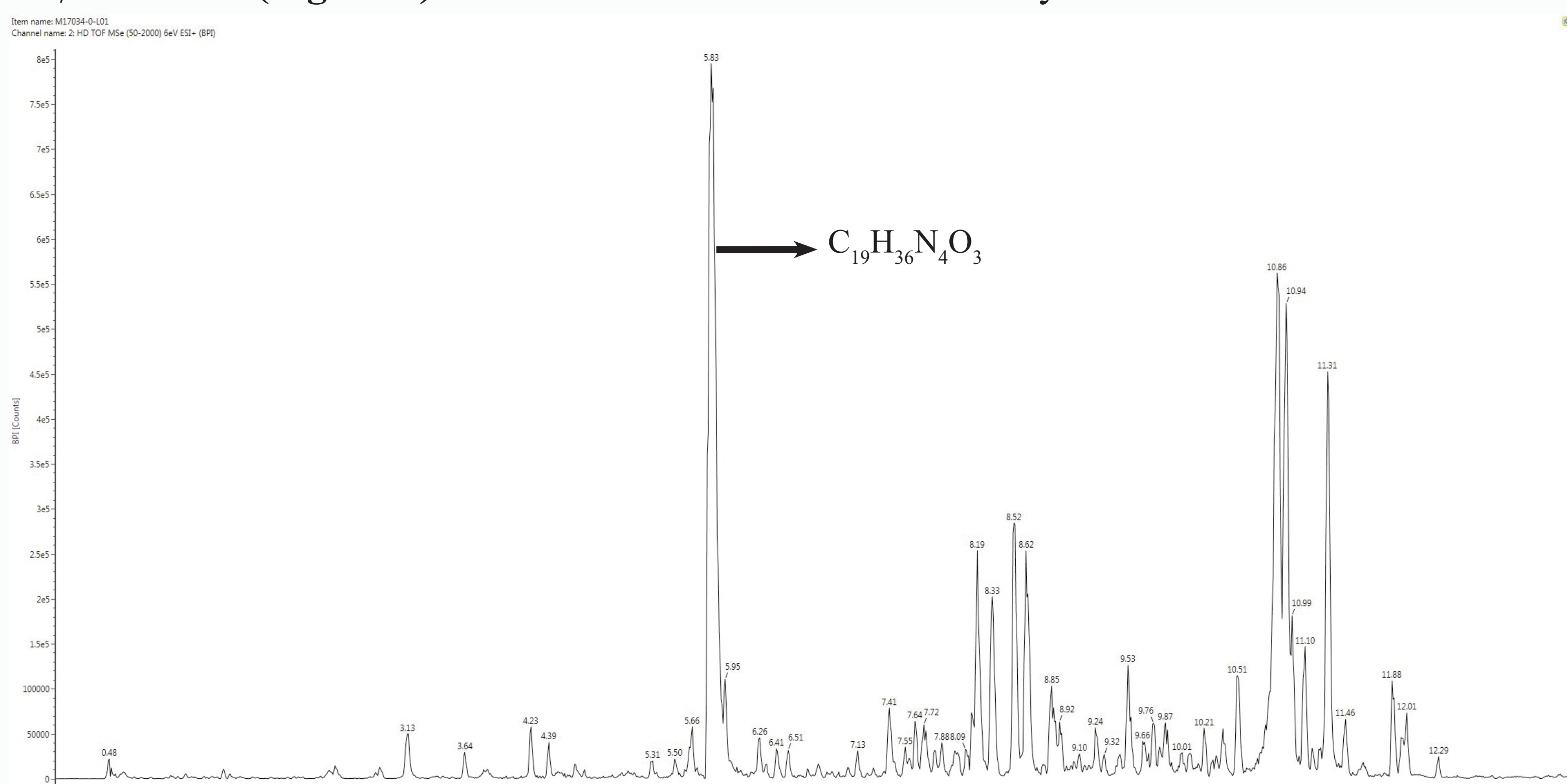


Figure 2: Positive electrospray base peak intensity (ESI⁺ BPI) chromatogram from the analysis of the organic crude extract of *D. murrayana*. The target peak was selected (marked with black arrow) based on the intensity and compound 1 eluted at the retention time (R_t) of 5.7 min.

/DEREPLICATION:

The mass spectrum qh'eqo r qwpf "1"kp'f'k'cv'gf "j cv'eqo r qwpf 1" had a protonated ion [M+H]⁺ with *m/z* 369.2861 (Figure 3) and the elemental composition was calculated as C₁₉H₃₆N₄O₃ (*m/z* 369.2865). The elemental composition of compound 1 was not found in relevant databases (Dictionary of Marine Natural Products and ChemSpider).

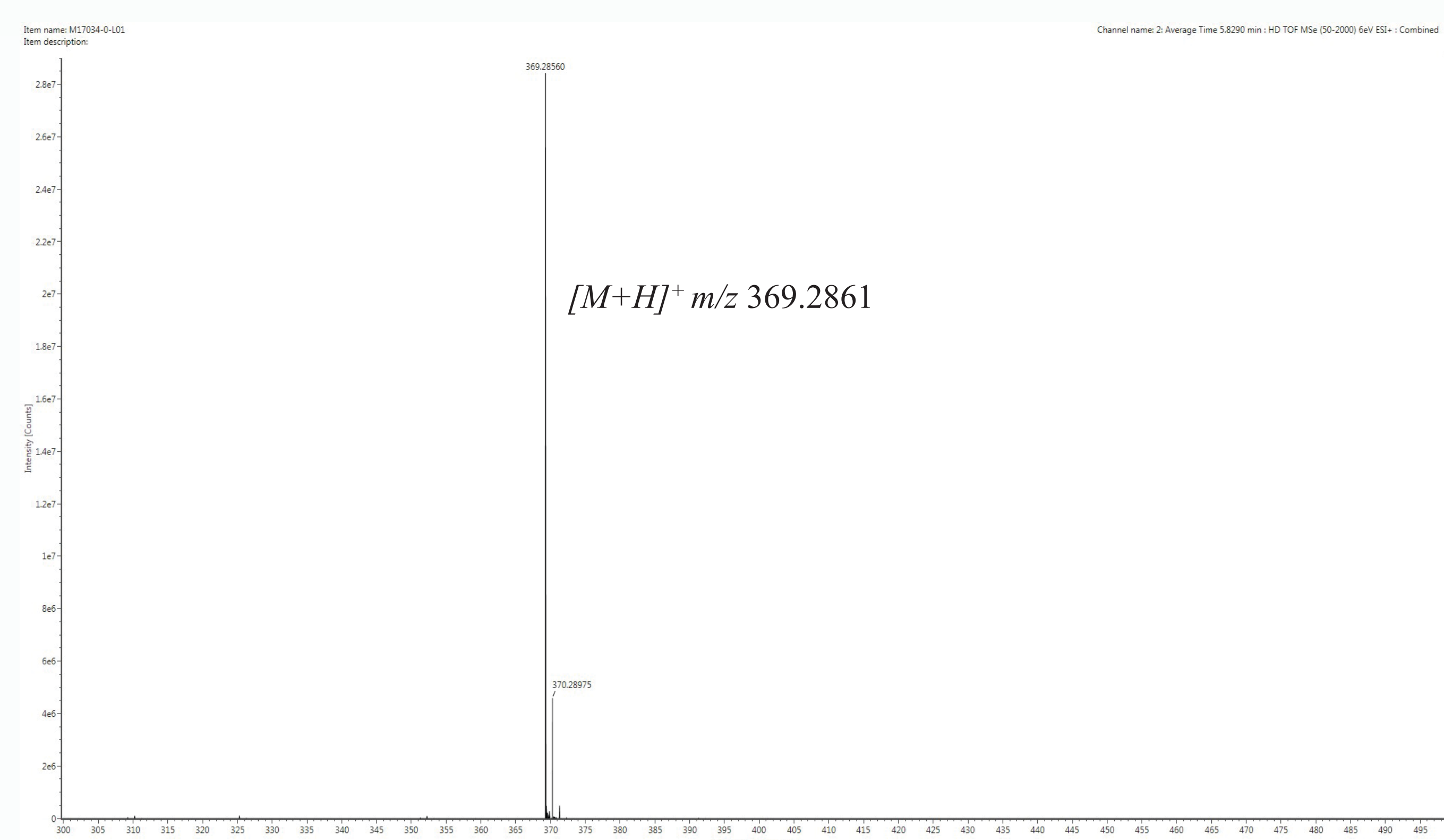


Figure 3: The mass spectrum of target compound 1 from HR-MS data, obtained in positive electrospray ionization (ESI⁺) mode.

/ISOLATION OF COMPOUND 1 BY USING PREP HPLC-MS:

Mass guided prep HPLC was used for the isolation of compound 1. Aliquots of organic crude extract were injected repeatedly onto a prep C₁₈ HPLC column for first round of isolation. The mass of the compound *m/z* 369.28 was used as collection trigger. Fluorophenyl prep HPLC column was used for second round of purification (Figure 4). The yield of pure compound was 2.5 mg out of 0.75 g of organic crude extract.

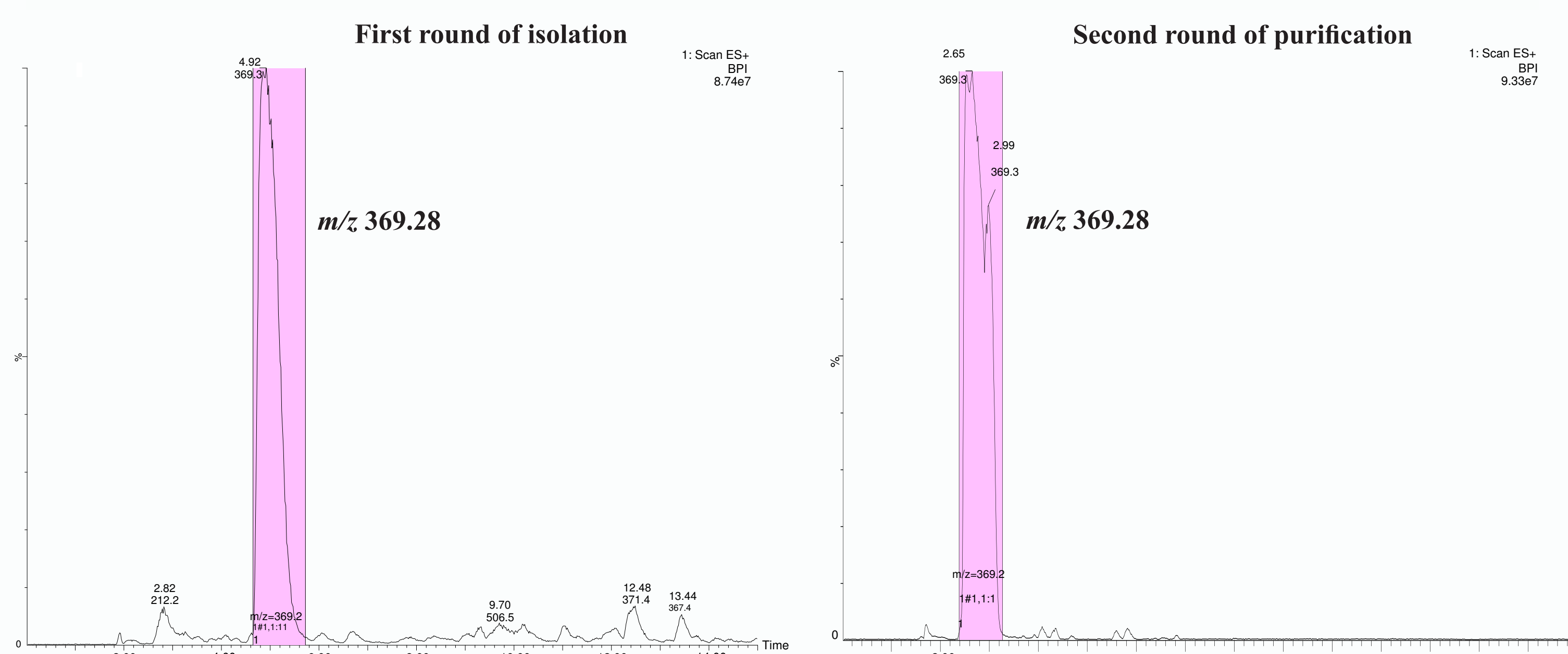


Figure 4: BPI chromatograms showed the stepwise purification of compound 1 (marked in pink colour) by using prep C₁₈ HPLC column (left) and fluorophenyl HPLC column (right).

/STRUCTURE ELUCIDATION OF COMPOUND 1 BY USING 1D & 2D NMR:

The chemical structure of compound 1 was determined by various ¹H, and ¹³C and NMR experiments including HSQC+HMBC, H2BC, DQCOSY, TOCSY, NOSEY, 15N HSQC and 15N HMBC. The structure of compound 1 was new and named "Dendrobeatiamine A". The chemical structure can be seen in Figure 5.

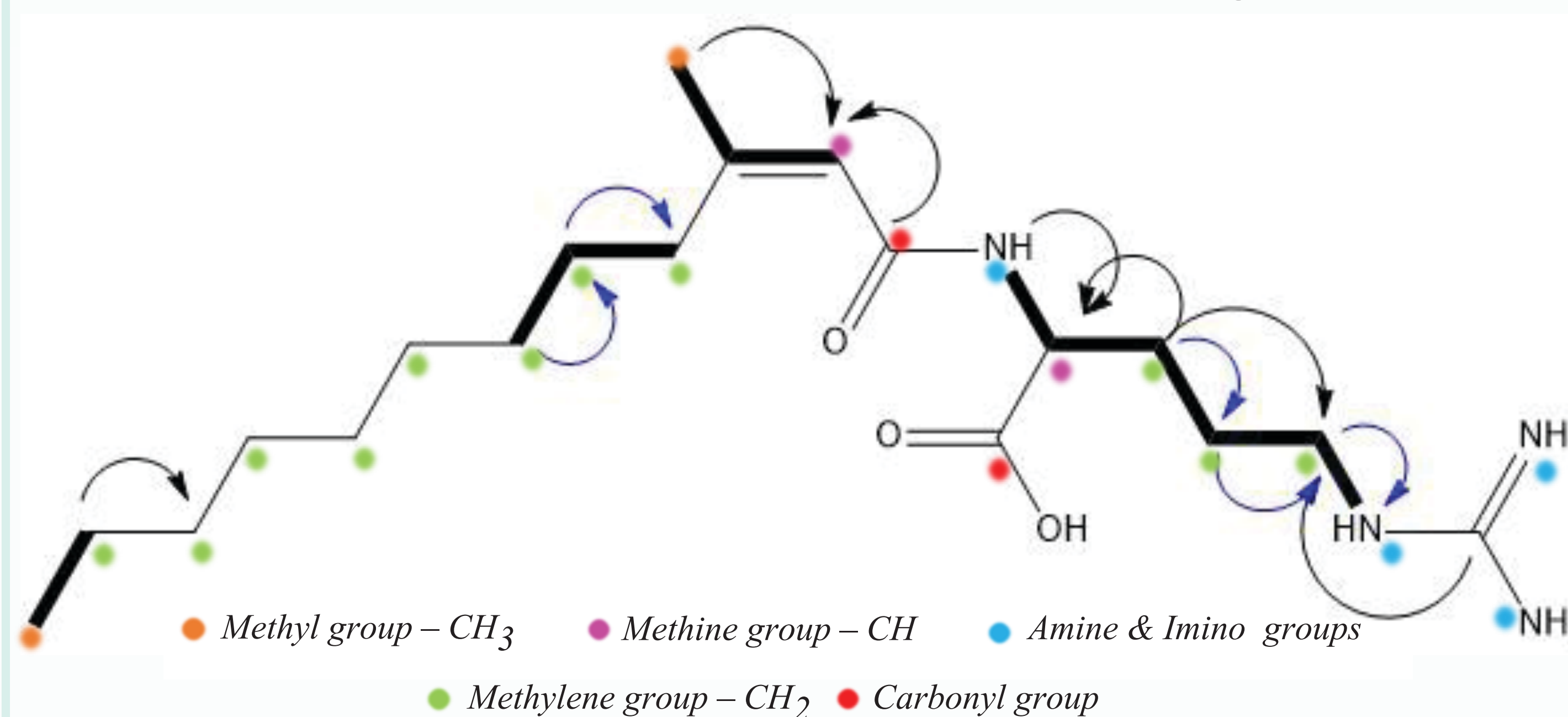


Figure 5: The chemical structure of the new compound *Dendrobeatiamine A*. Highlighted are key COSY (bold), HMBC (black arrows) and H2BC (blue arrows) correlations.

/BIOACTIVITY PROFILING OF COMPOUND 1:

Dendrobeatiamine A was evaluated for potential biological activities based on cellular and biochemical bioassays, but the compound did not show any significant cytotoxic anti-inflammatory, antimicrobial and antioxidant activities.

/SUMMARY:

Chemistry guided purification of the organic extract of the Arctic marine bryozoan *Dendrobeatia murrayana* yielded one new compound, Dendrobeatiamine A, and it was present in abundant amounts in the organic extract. Dendrobeatiamine A is a fusion of long chain aliphatic fatty acid and the cationic amino acid residue arginine. The bioactivity and natural function of this compound thus remain to be elucidated.

/ACKNOWLEDGEMENT:

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/REFERENCES:

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