Supplementary Material

Amaryllidaceae alkaloids of belladine-type from *Narcissus pseudonarcissus* cv. Carlton as new selective inhibitors of butyrylcholinesterase

Abdullah Al Mammun[1], Jana Maříková[2], Daniela Hulcová[1,3], Jiří Janoušek[1,3], Marcela Šafratová[1,3], Lucie Nováková[4], Tomáš Kučera[5], Martina Hrabinová[6,7], Jiří Kuneš[2], Jan Korábečný[6,7,*], Lucie Cahlíková[1,*]

[1] ADINACO Research Group, Department of Pharmaceutical Botany, Faculty of Pharmacy, Charles University, Heyrovského 1203, 500 05 Hradec Králové, Czech Republic; almamuna@faf.cuni.cz (AAM)
[2] Department of Organic and Bioorganic Chemistry, Faculty of Pharmacy, Charles University, Heyrovského 1203, 500 05 Hradec Králové, Czech Republic; marikoj2@faf.cuni.cz (JM); kunes@faf.cuni.cz (JK)
[3] Department of Pharmacognosy, Faculty of Pharmacy, Charles University, Heyrovského 1203, 500 05 Hradec Králové, Czech Republic; hulcovd@faf.cuni.cz (DH); safratom@faf.cuni.cz (MS); janousj2@faf.cuni.cz (JJ)
[4] Department of Analytical Chemistry, Faculty of Pharmacy, Charles University, Heyrovského 1203, 500 05 Hradec Králové, Czech Republic; novakoval@faf.cuni.cz (LN)
[5] Department of Military Medical Service Organisation and Management, Faculty of Military Health Sciences, University of Defence, Třebešská 1575, 500 05 Hradec Králové, Czech Republic; kucera-t@email.cz (TK)
[6] Department of Toxicoloxy and Military Pharmacy, Faculty of Military Health Sciences, University of Defence, Třebešská 1575, 500 05 Hradec Králové, Czech Republic; hrabinova@pmfhk.cz (MH)
[7] Biomedical Research Centre, University Hospital Hradec Kralove, Sokolska 581, 500 05 Hradec Kralove, Czech Republic

* Correspondence: cahlikova@faf.cuni.cz; Tel.: + 420 495 067 311; ORCID: 0000-0002-1555-8870 (LC); jan.korabecny@fnhk.cz; Tel.: + 420 495 833 447; ORCID: 0000-0001-6977-7596 (JKO)

Table of contents

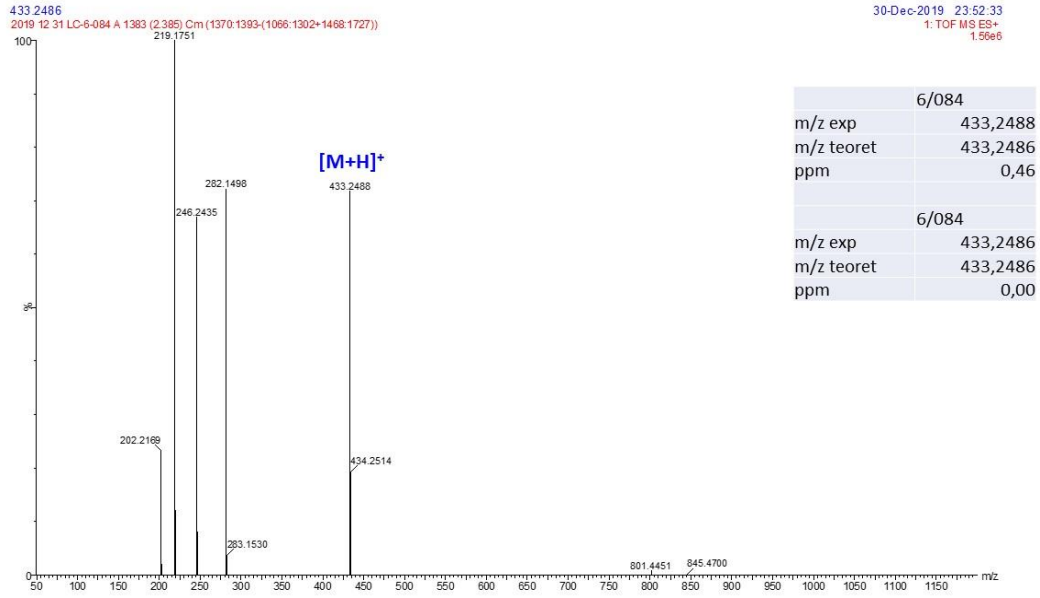


Figure S1-1. ESI-HRMS spectrum of carltonine A (**13**).

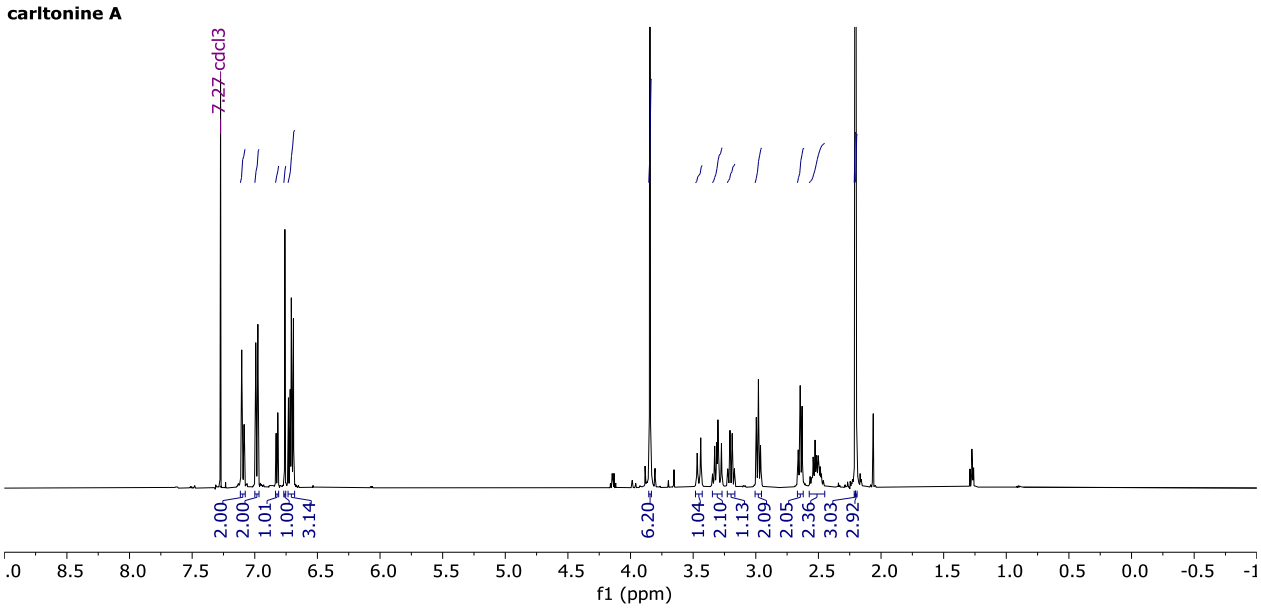


Figure S1-2. ^{1}H NMR spectrum of carltonine A (**13**) in $CDCl_3$.

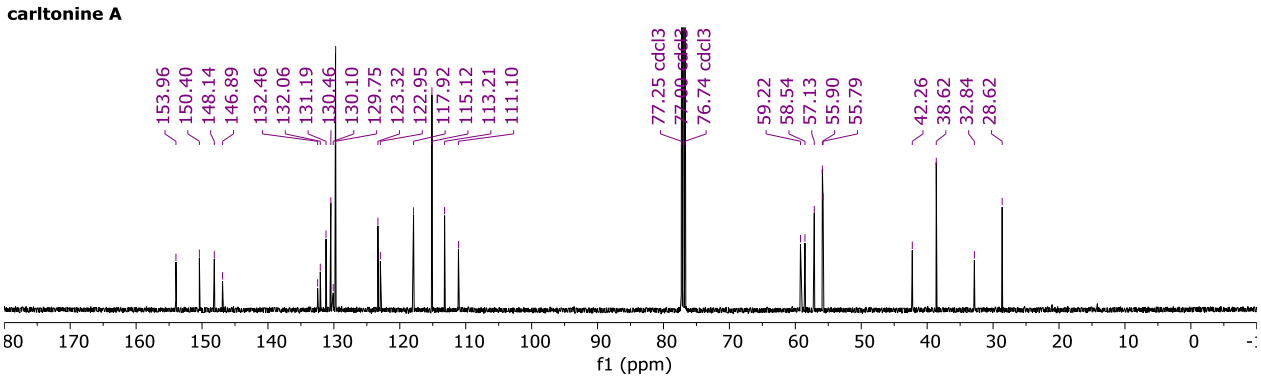


Figure S1-3. ^{13}C NMR spectrum of carltonine A (**13**) in $CDCl_3$.

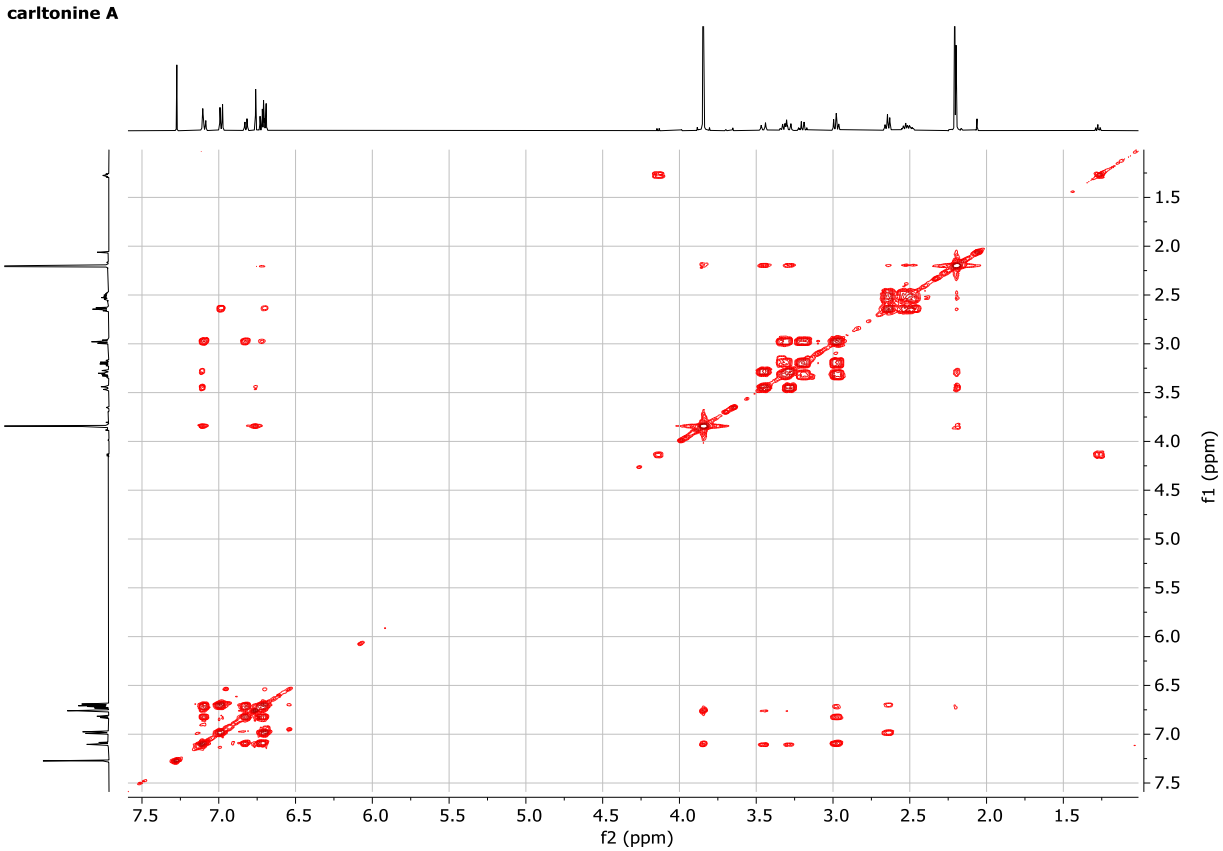


Figure S1-4. gCOSY spectrum of carltonine A (**13**) in $CDCl_3$.

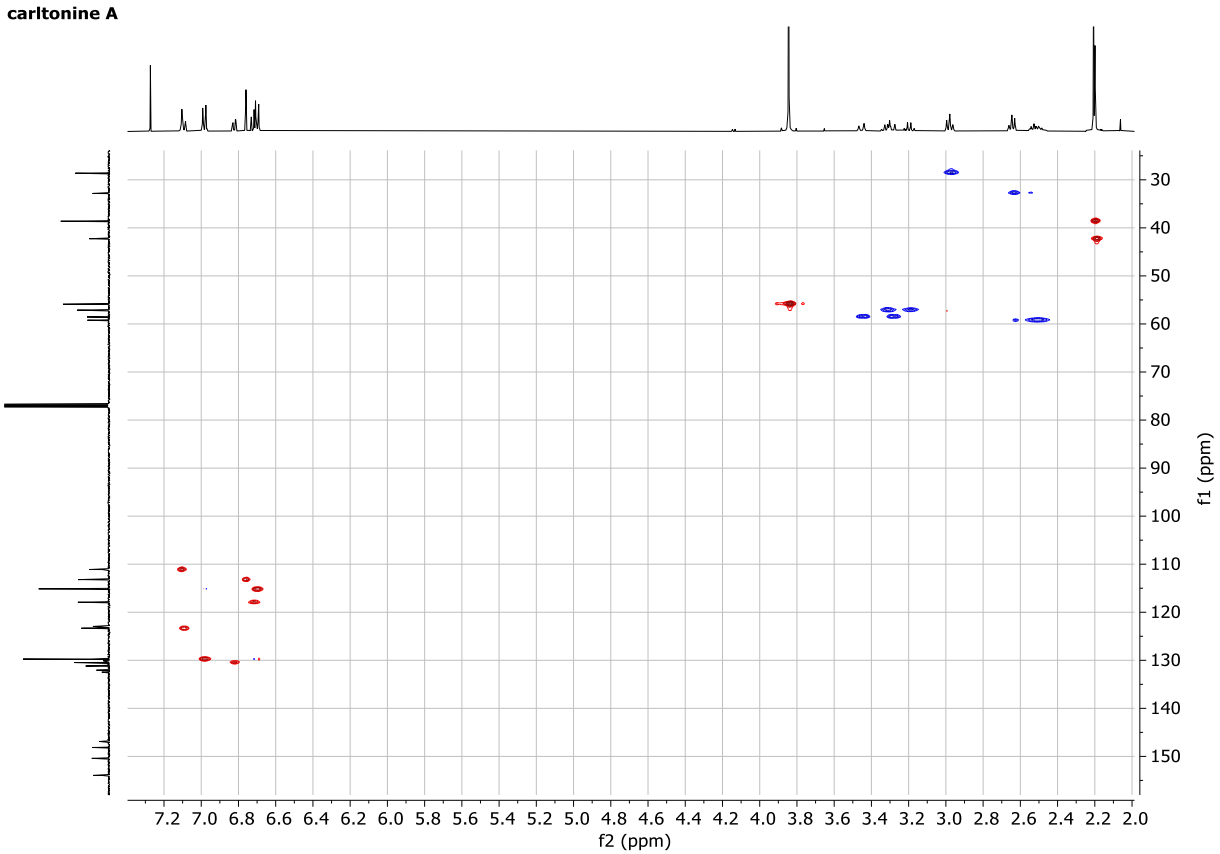


Figure S1-5. gHSQC spectrum of carltonine A (**13**) in $CDCl_3$.

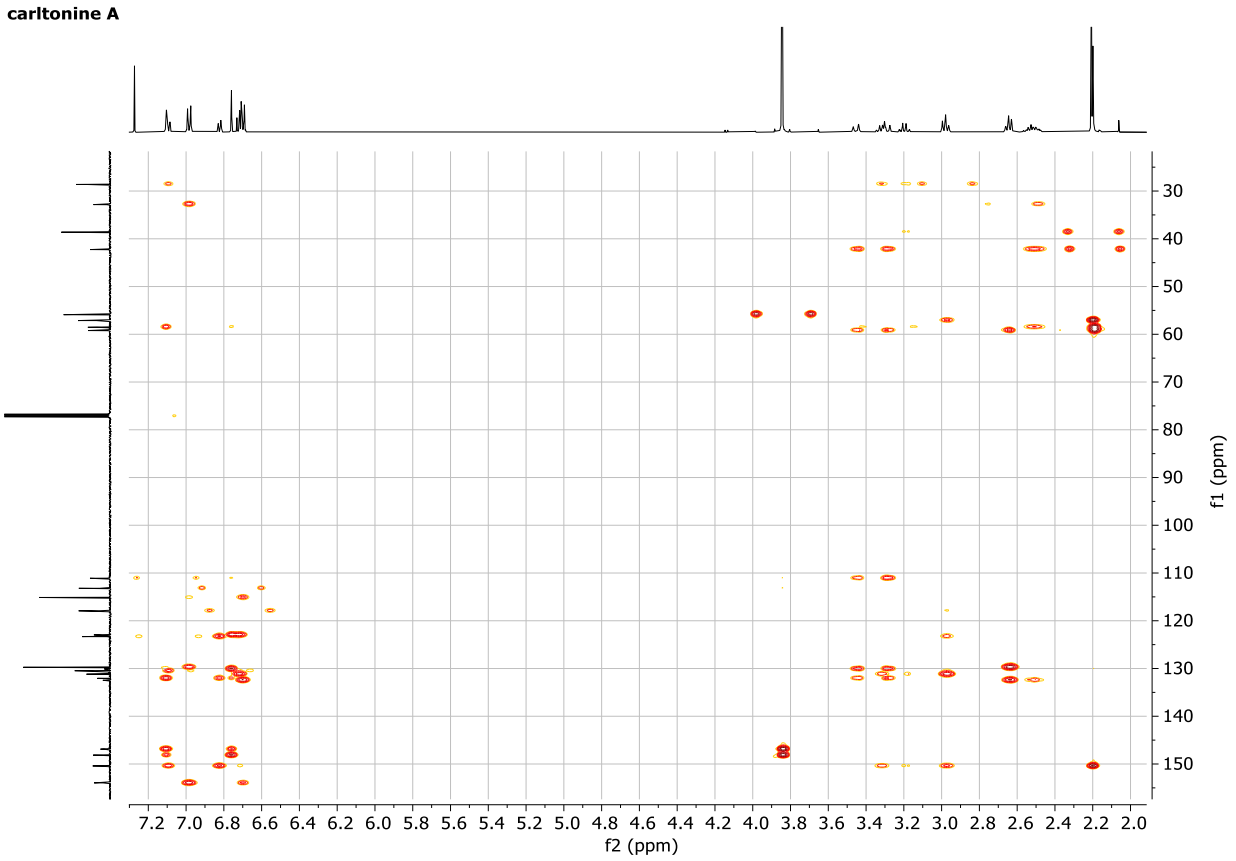


Figure S1-6. gHMBCAD spectrum of carltonine A (13) in $CDCl_3$.

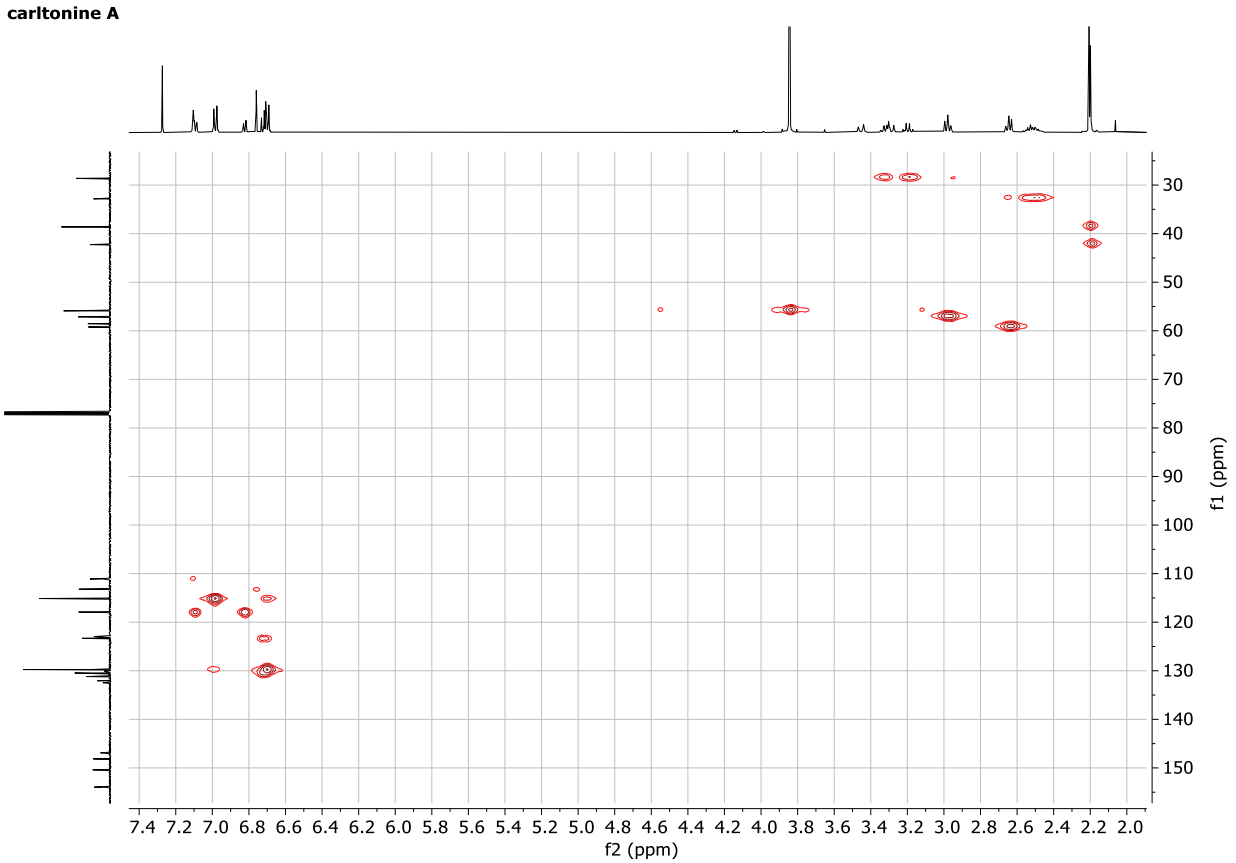
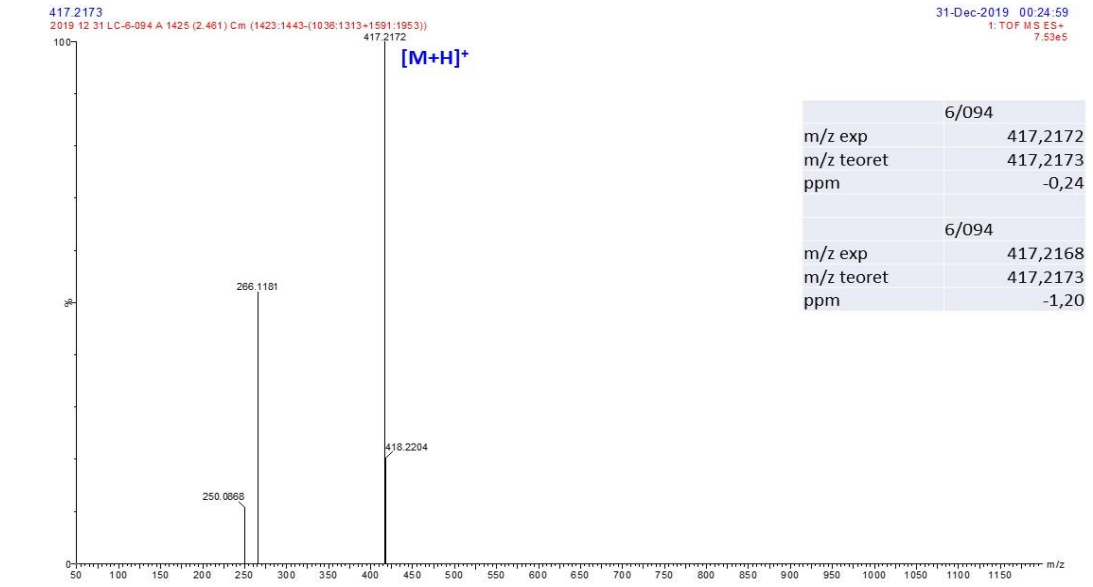


Figure S1-7. gH2BC spectrum of carltonine A (**13**) in $CDCl_3$.



	6/094
m/z exp	417,2172
m/z teoret	417,2173
ppm	-0,24

	6/094
m/z exp	417,2168
m/z teoret	417,2173
ppm	-1,20

Figure S2-1. ESI-HRMS spectrum of carltonine B (**14**).

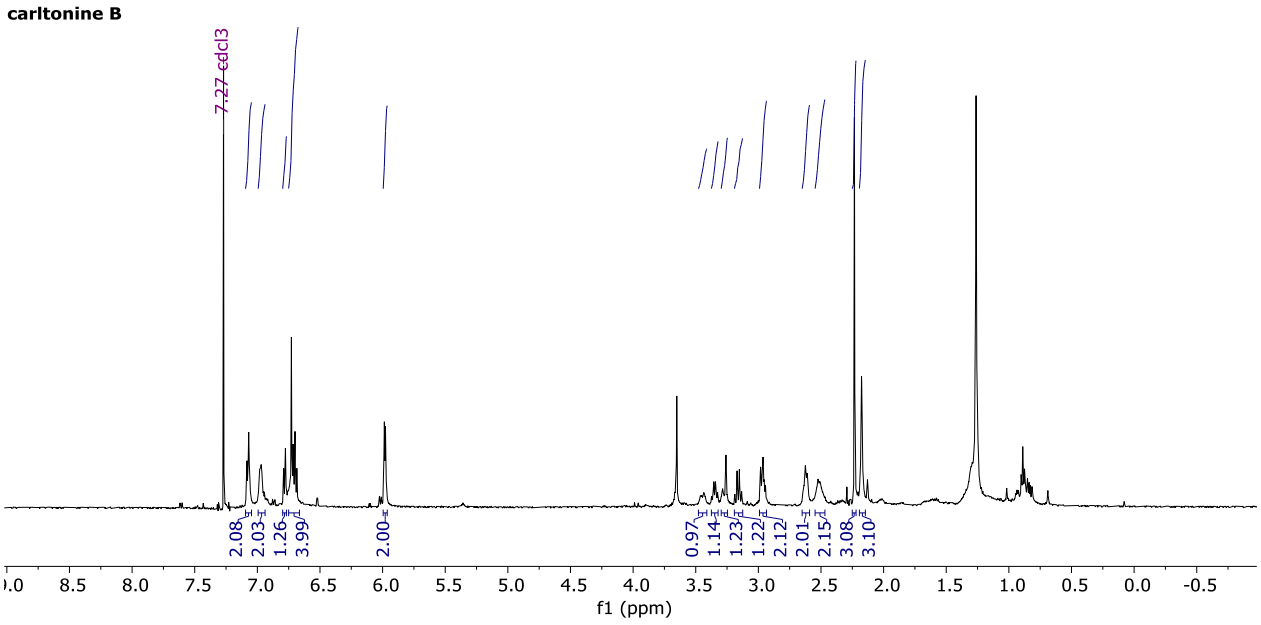


Figure S2-2. ^{1}H NMR spectrum of carltonine B (**14**) in $CDCl_3$.

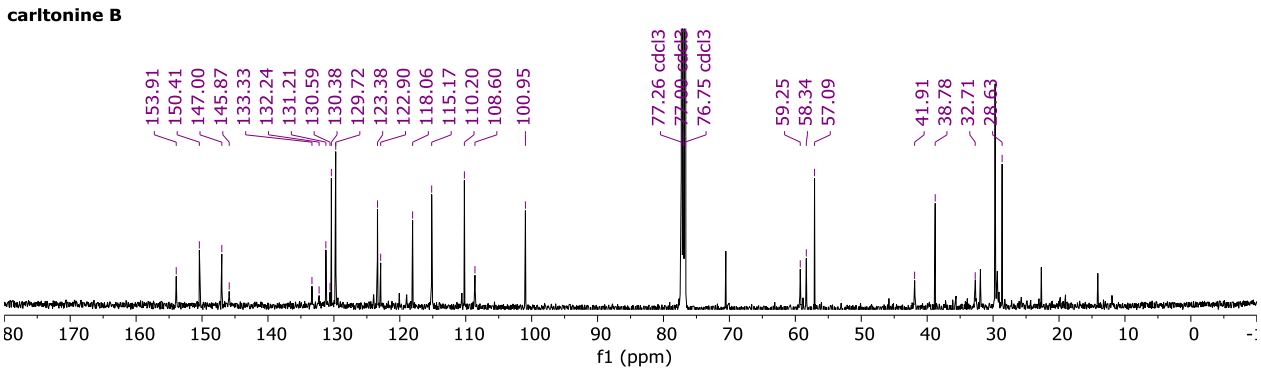


Figure S2-3. ^{13}C NMR spectrum of carltonine B (**14**) in $CDCl_3$.

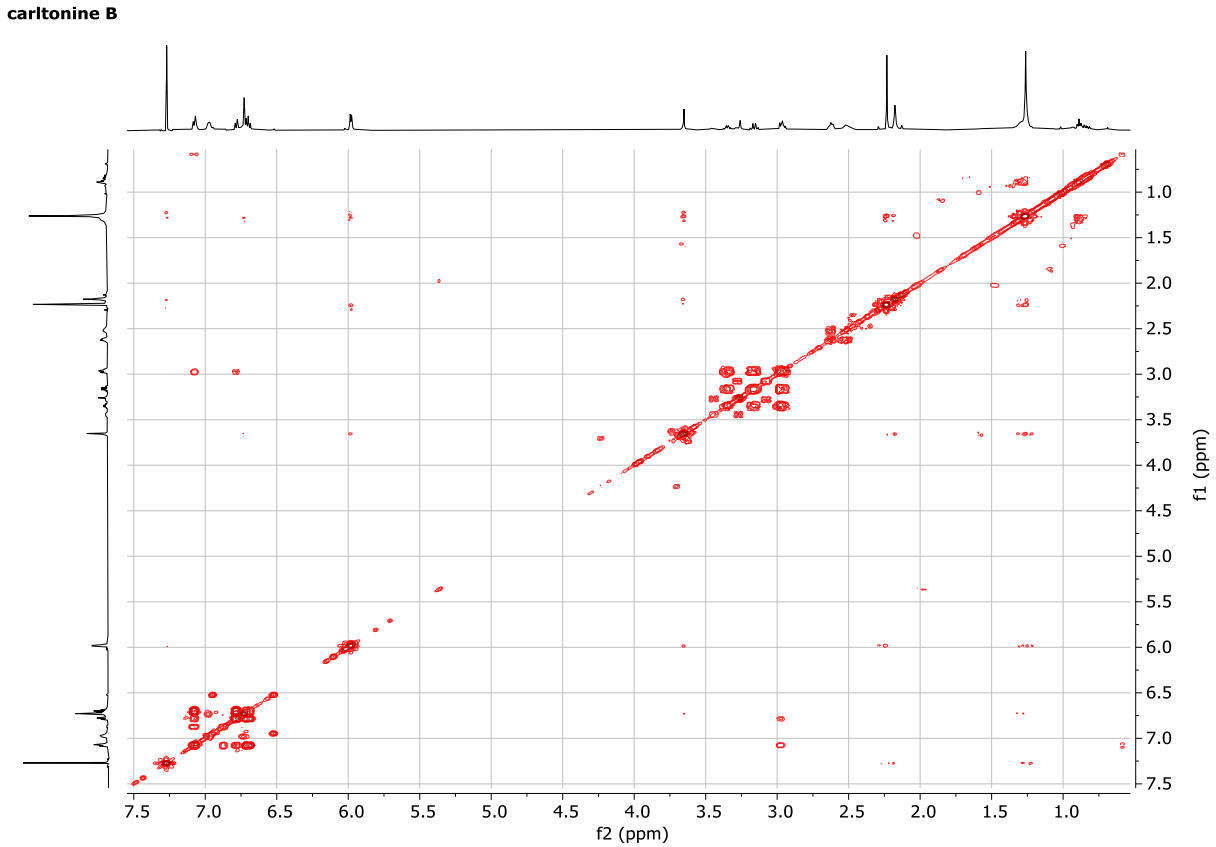


Figure S2-4. gCOSY spectrum of carltonine B (**14**) in $CDCl_3$.

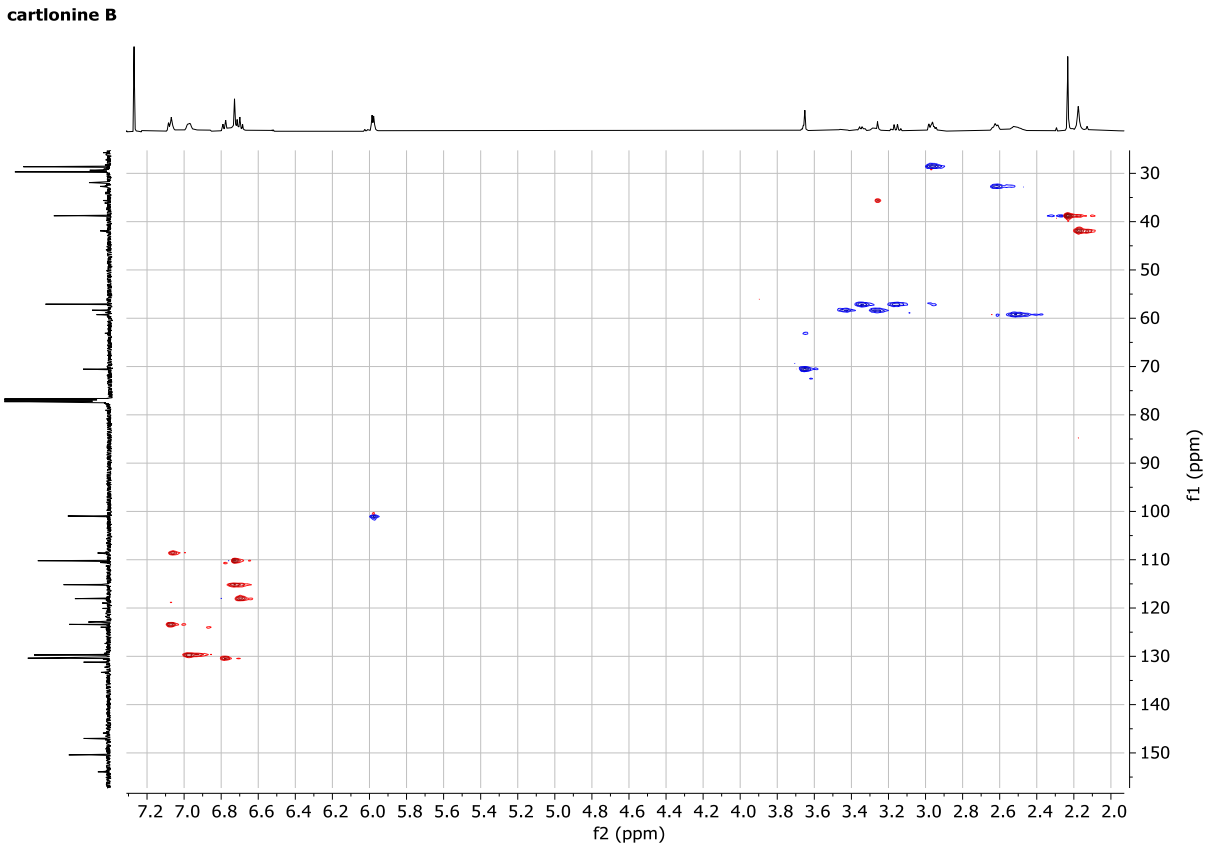


Figure S2-5. gHSQC spectrum of carltonine B (**14**) in $CDCl_3$.

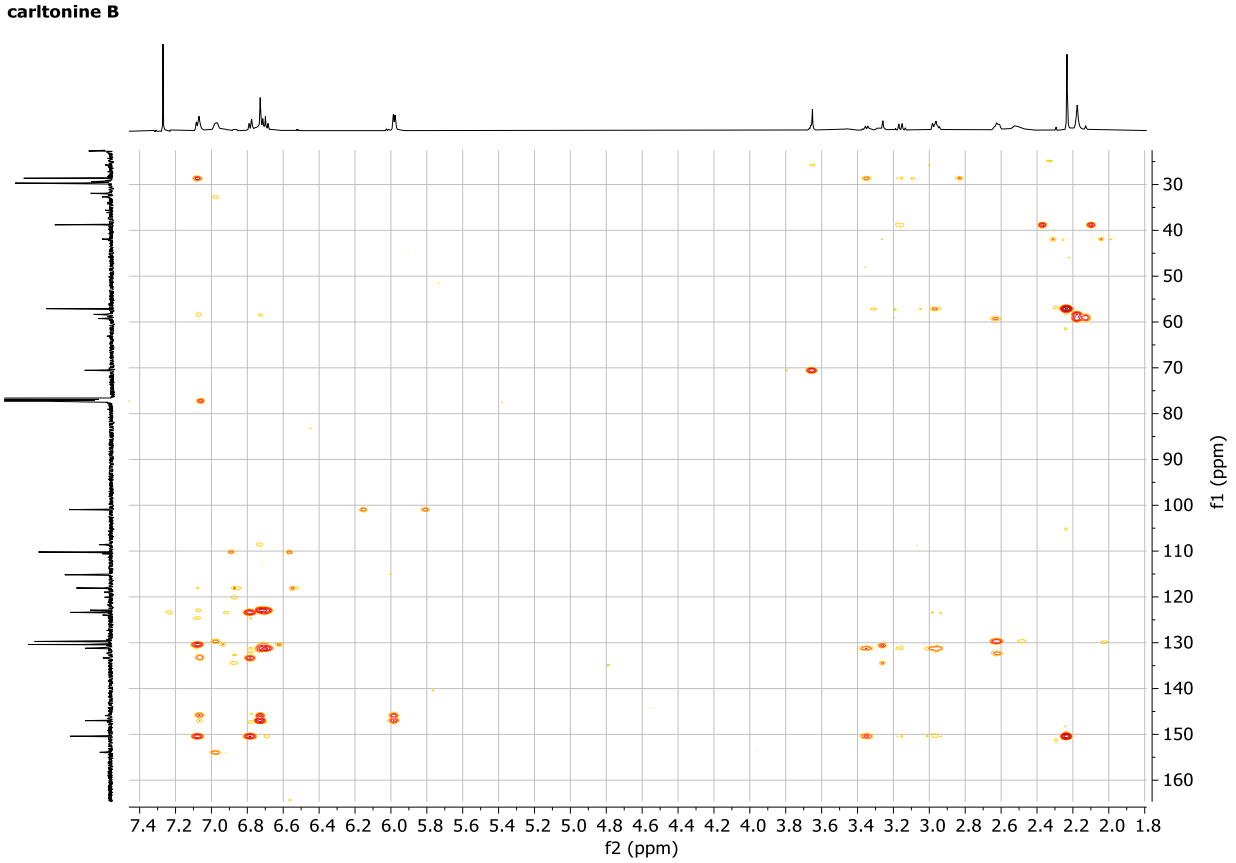


Figure S2-6. gHMBCAD spectrum of carltonine B (**14**) in $CDCl_3$.

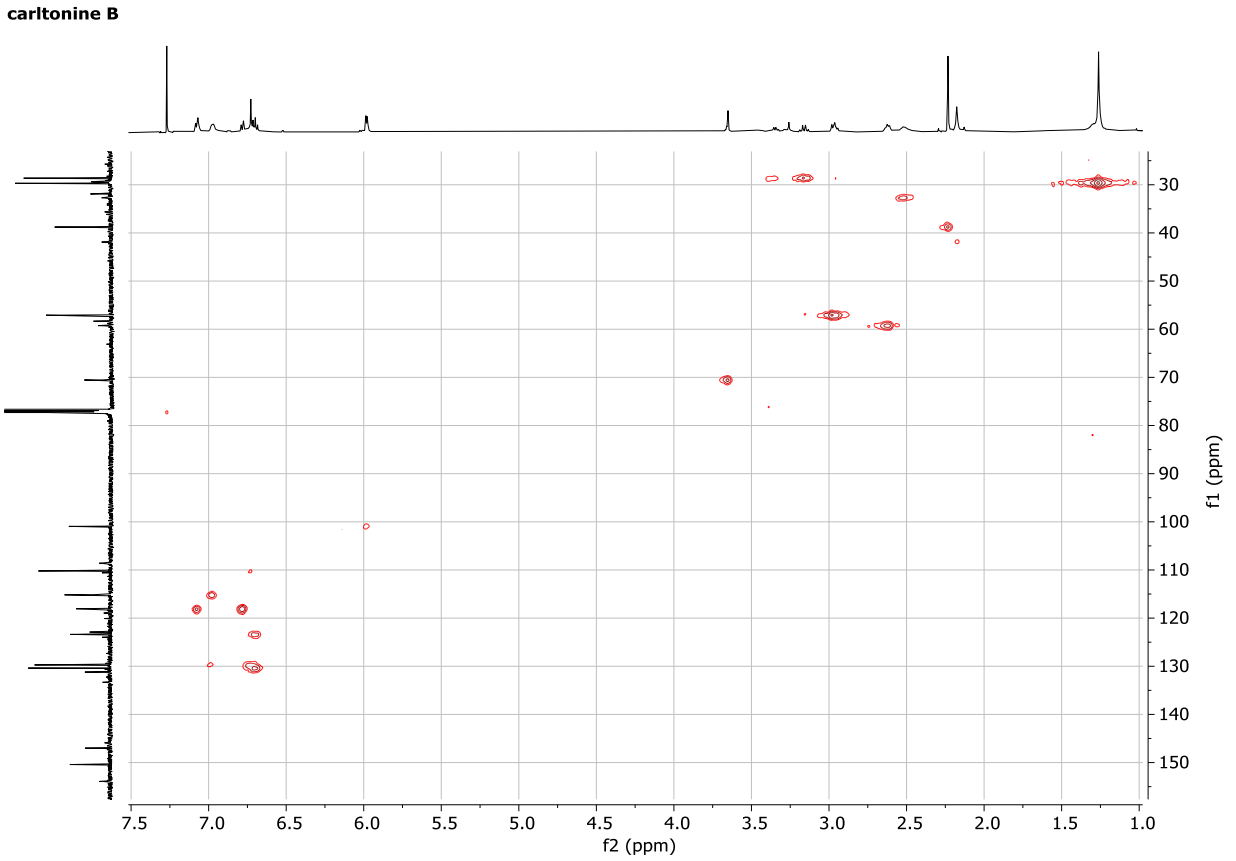


Figure S2-7. gH2BC spectrum of carltonine B (**14**) in $CDCl_3$.

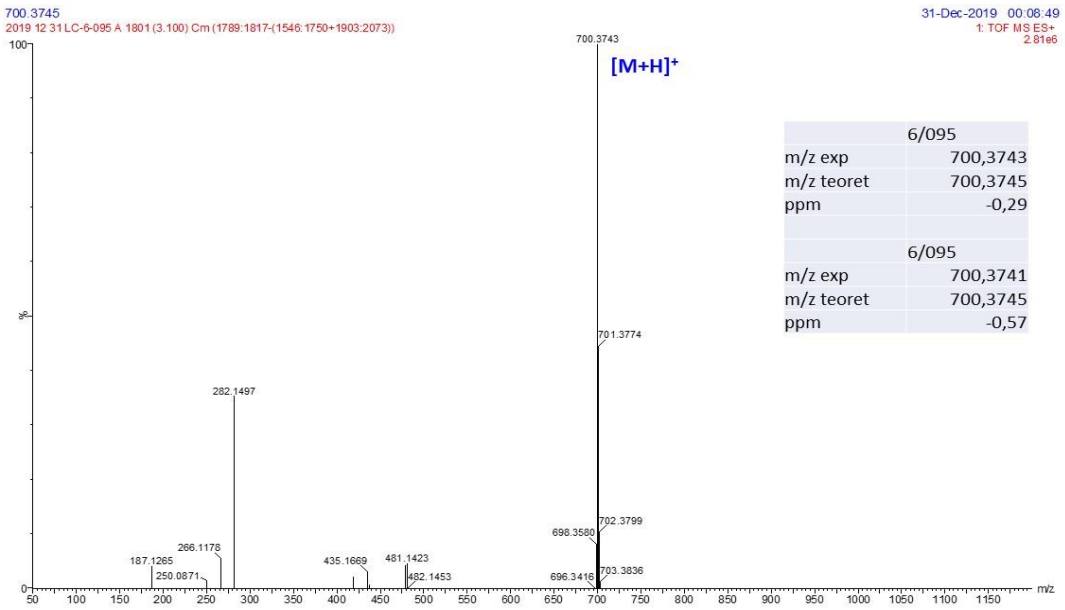


Figure S3-1. ESI-HRMS spectrum of carltonine C (15).

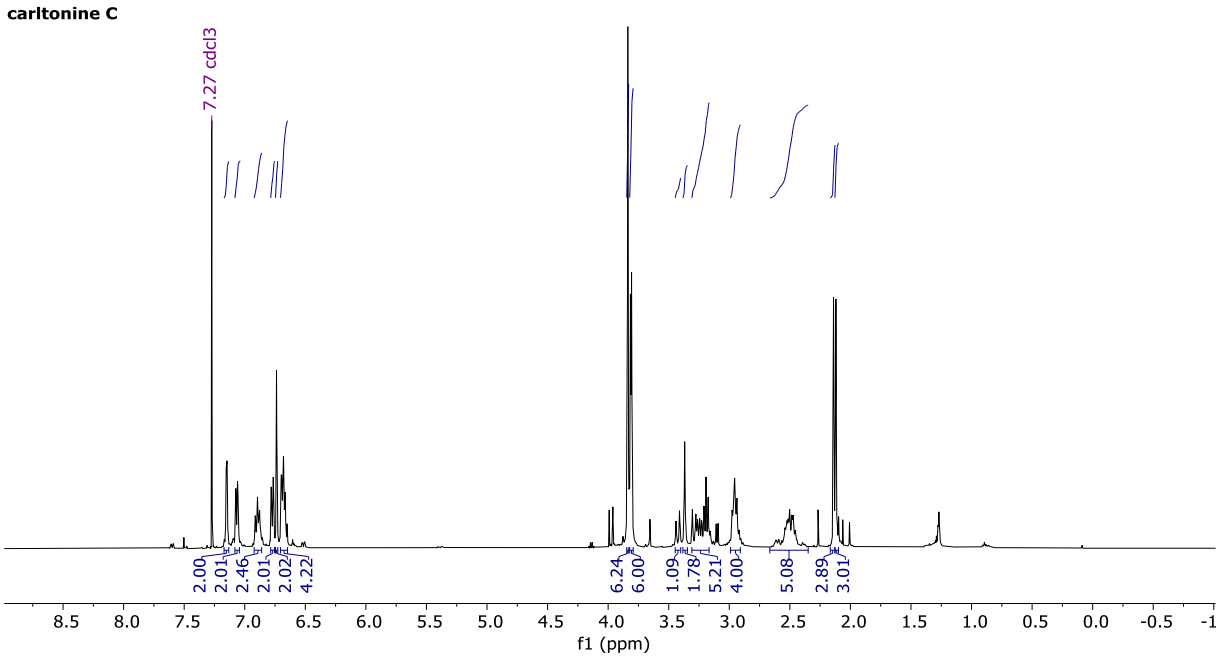


Figure S3-2. ^{1}H NMR spectrum of carltonine C (**15**) in $CDCl_3$.

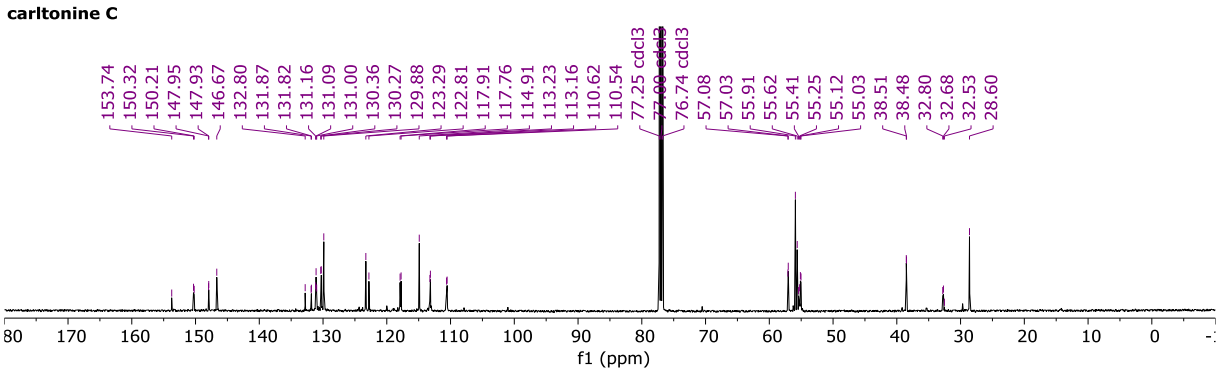


Figure S3-3. ^{13}C NMR spectrum of carltonine C (**15**) in $CDCl_3$.

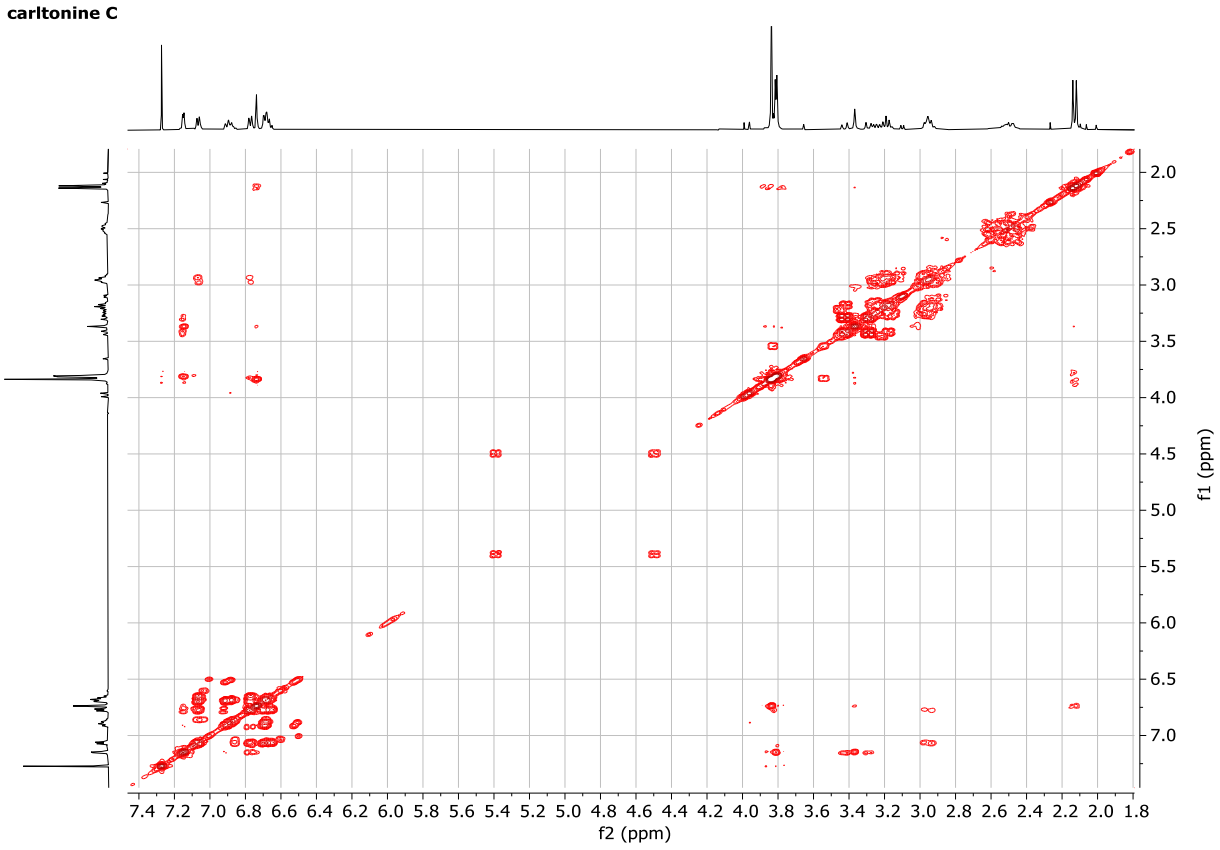


Figure S3-4. gCOSY spectrum of carltonine C (**15**) in $CDCl_3$.

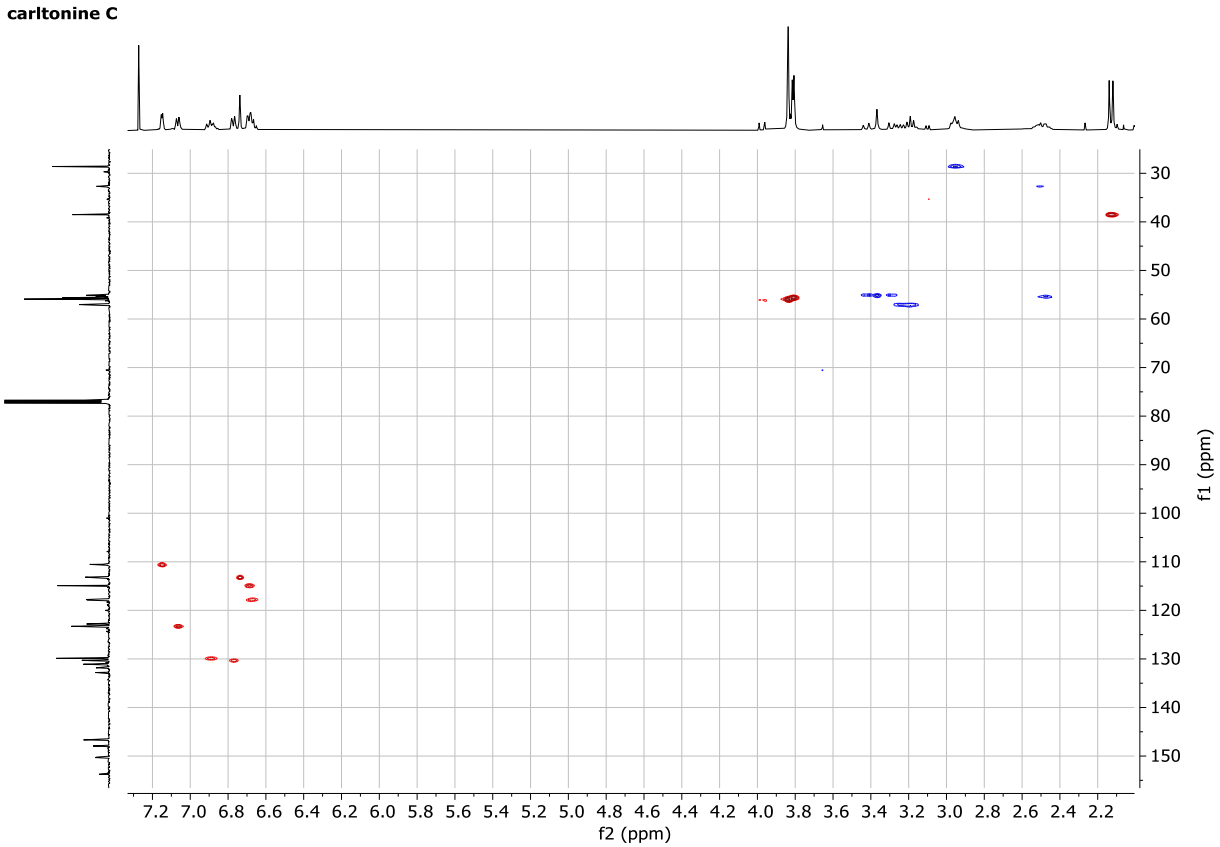


Figure S3-5. gHSQC spectrum of carltonine C (**15**) in $CDCl_3$.

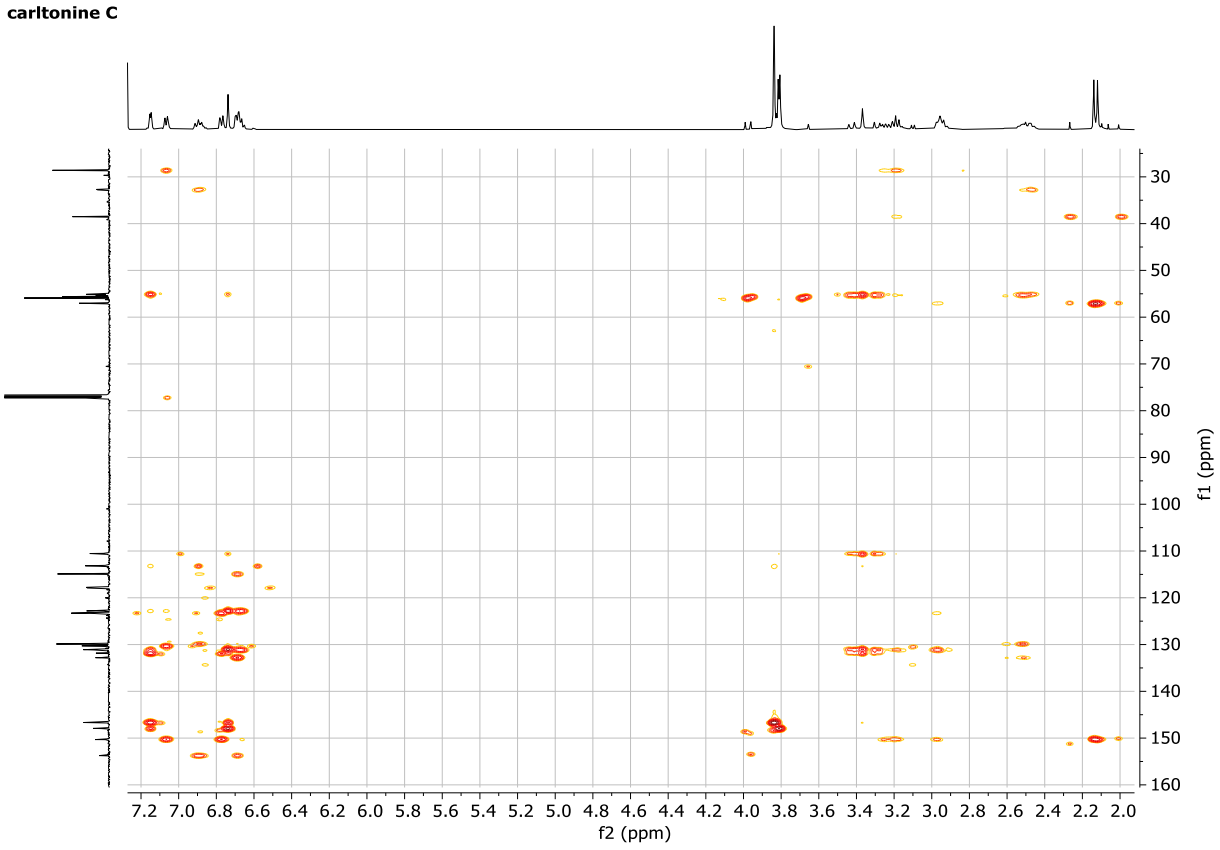


Figure S3-6. gHMBCAD spectrum of carltonine C (**15**) in $CDCl_3$.

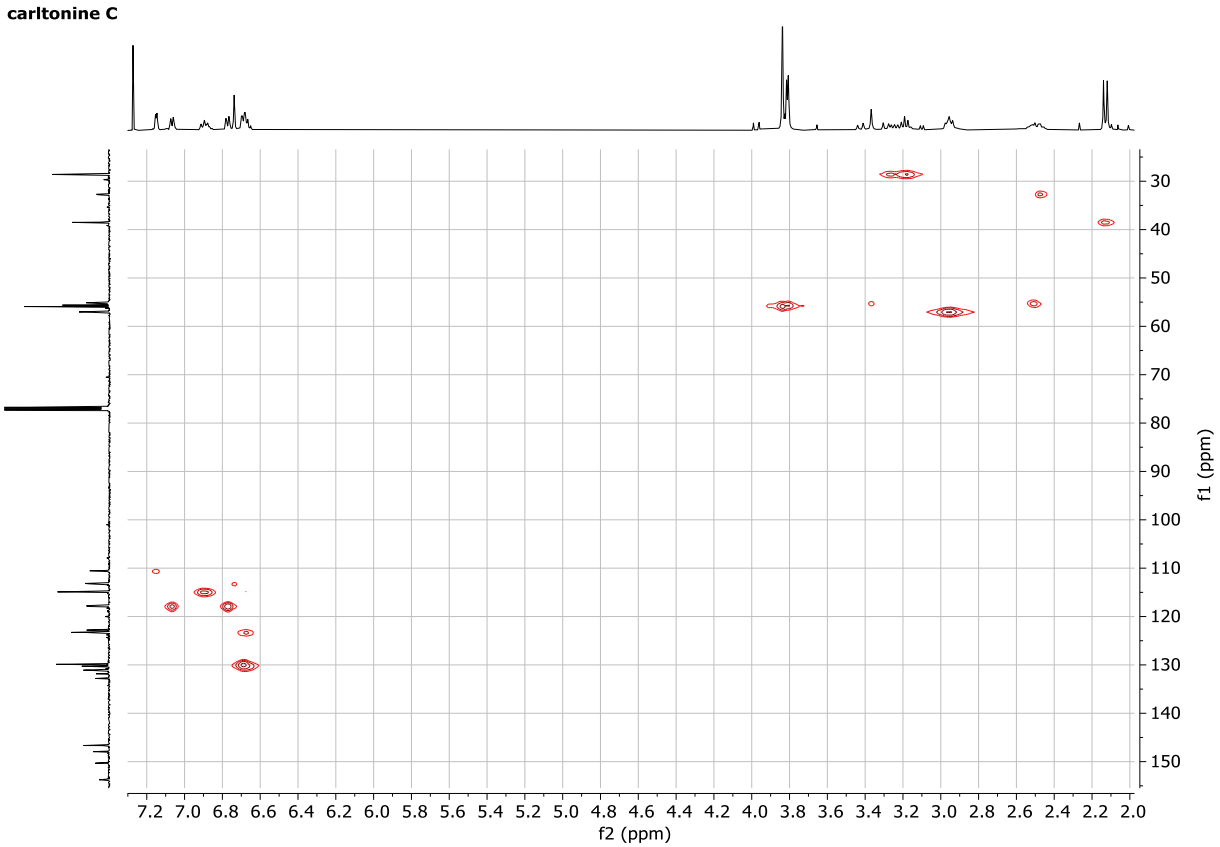


Figure S3-7. gH2BC spectrum of carltonine C (**15**) in $CDCl_3$.

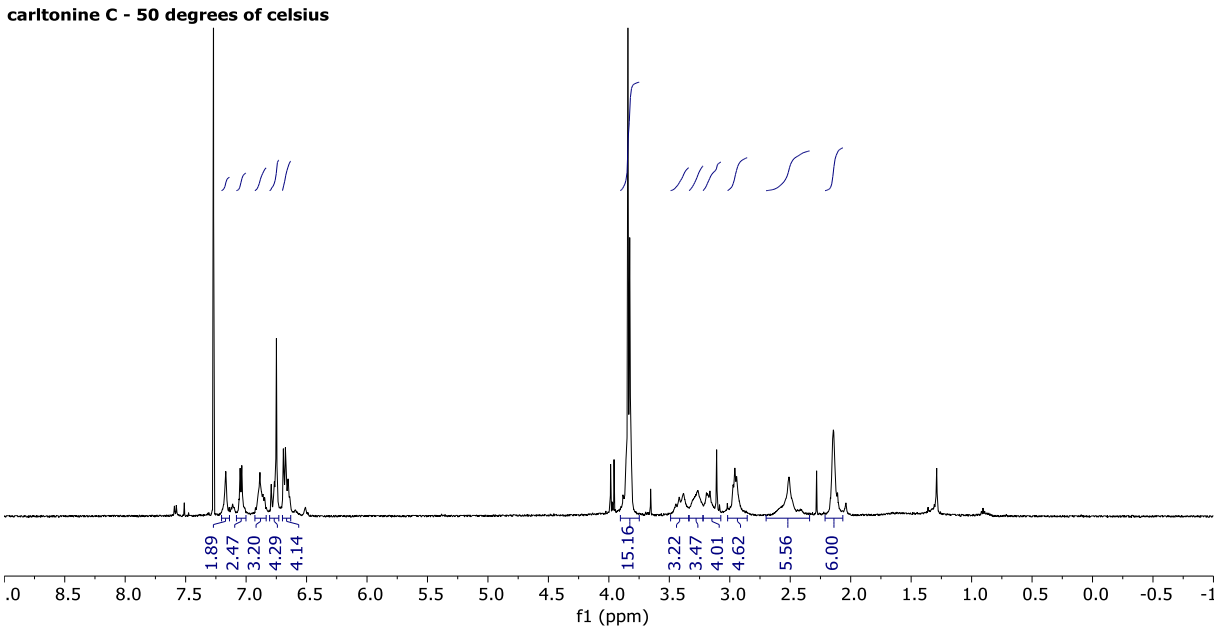


Figure S3-8. ^1H NMR spectrum of carltonine C (**15**) in $CDCl_3$ at 50 °C.

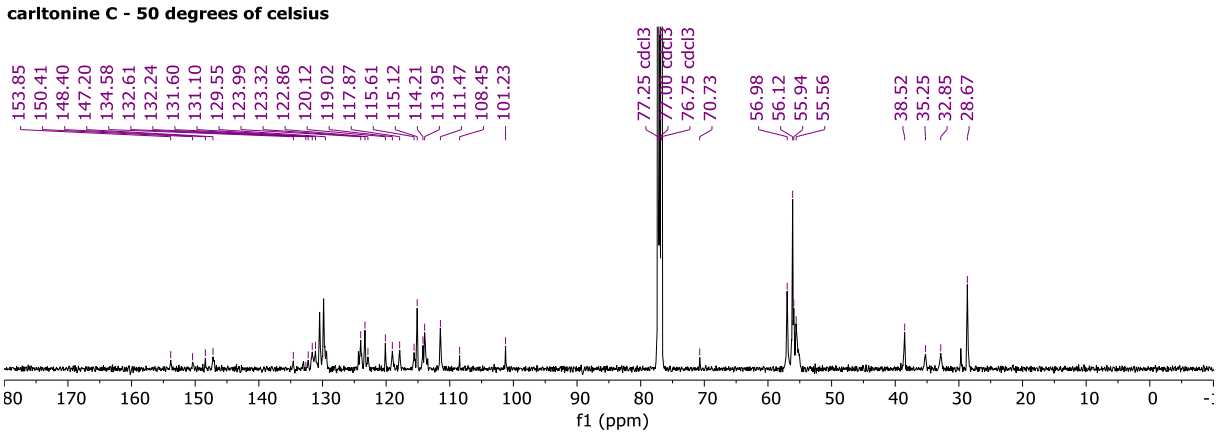


Figure S3-9. ^{13}C NMR spectrum of carltonine C (**15**) in $CDCl_3$ at 50 °C.

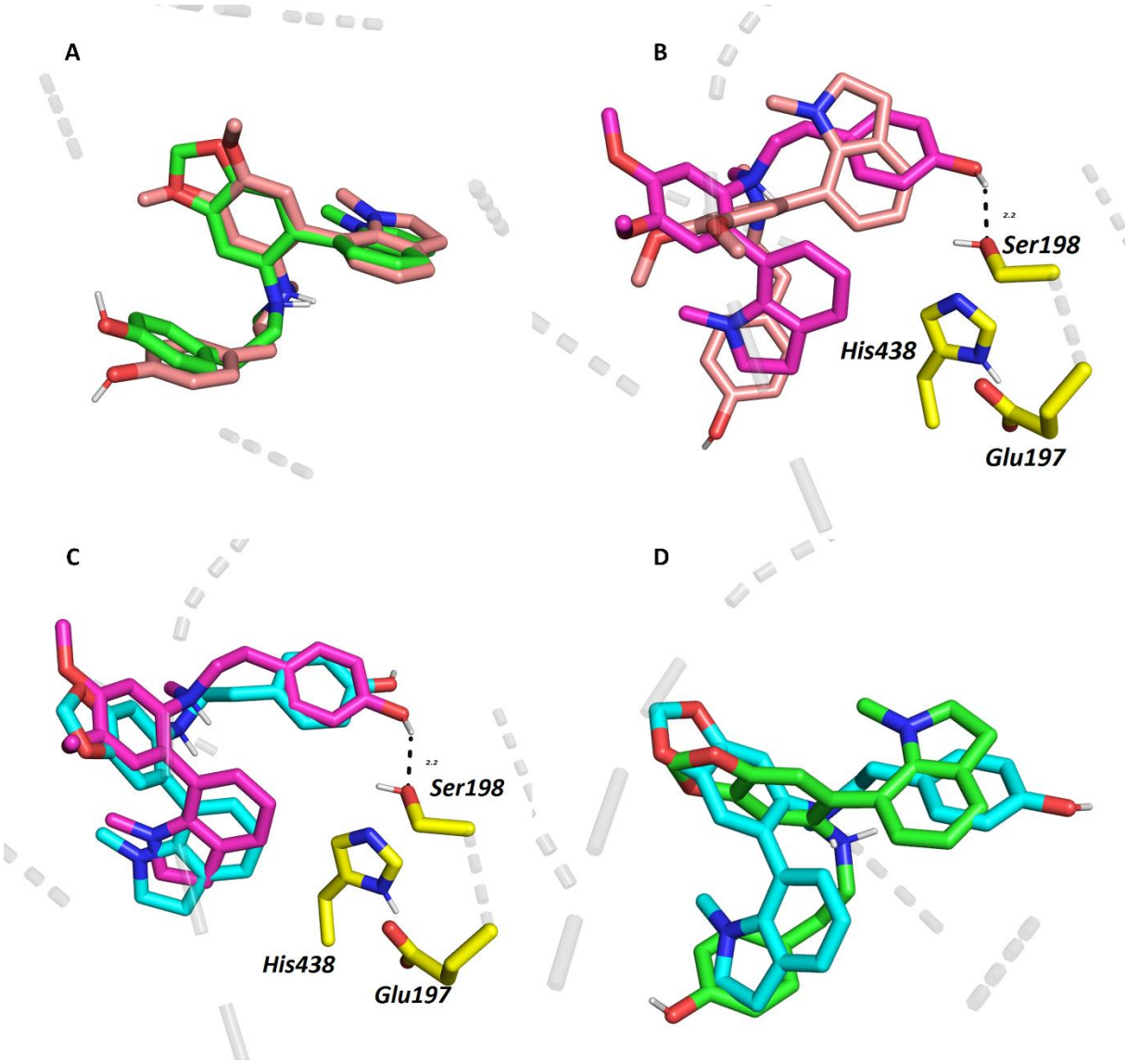


Figure S4. Overlapped *pseudo*-enantiomers in the *h*BuChE active site and their topology difference: (*R*)-**13**-(*R*)-**14** (A), (*S*)-**13**-(*R*)-**13** (B), (*S*)-**13**-(*S*)-**14** (C), and (S)-**14**-(*R*)-**14** (D). (*R*)-**13**, (*S*)-**13**, (*R*)-**14**, and (*S*)-**14** are shown in salmon, purple, green, and light blue, respectively. Catalytic triad residues are portrayed in yellow.