

Analysis of the Mycosporine-Like Amino Acid (MAA) Pattern of the Salt Marsh Red Alga *Bostrychia scorpioides*

Maria Orfanoudaki^a, Anja Hartmann^{a,*}, Julia Mayr, Félix L. Figueroa^b, Julia Vega^b, John West^c, Ricardo Bermejo^d, Christine Maggs, and Markus Ganzera^a

^a Institute of Pharmacy, Pharmacognosy, University of Innsbruck, Innrain 80-82, Innsbruck 6020, Austria; orfmaria@gmail.com (M.O.); anja.hartmann@uibk.ac.at (A.H.); julia_mayr1@gmx.at (J. M.); markus.ganzera@uibk.ac.at (M.G.)

^bUniversity of Malaga, Institute of Blue Biotechnology and Development (IBYDA), Experimental Centre Grice-Hutchinson, Lomas de San Julian, 29004-Malaga, Spain; felix_lopez@uma.es (F.L.F.); julia_vega@uma.es (J.V.)

^c School of BioSciences, University of Melbourne, Parkville, 3010 Victoria, Australia; jwest@unimelb.edu.au (J. W.)

^d Earth and Ocean Sciences, School of Natural Sciences and Ryan Institute, National University of Ireland, Galway, H91 TK33, Ireland; ricardo.bermejo@uca.es (R. B.)

^e Christine Maggs, School of Biological Sciences and Queen's University Marine Laboratory Portaferry, Queen's University Belfast, Northern Ireland, BT22 1PF, UK

*Correspondence: anja.hartmann@uibk.ac.at (A.H.); Tel.: +43 512 507-58430

Contents

Table S1. Overview of the investigated <i>B. scorpioides</i> samples, their collection sites and dates.	4
Figure S1. ^1H NMR spectrum of bostrychine A in D_2O at 400 MHz	5
Figure S2. COSY spectrum of bostrychine A in D_2O at 400 MHz.....	5
Figure S3. HSQC spectrum of bostrychine A in D_2O at 400 MHz.....	6
Figure S4. HMBC spectrum of bostrychine A in D_2O at 400 MHz.....	6
Figure S5. ^{13}C NMR spectrum of bostrychine A in D_2O at 100 MHz	7
Figure S6. NOESY spectrum of bostrychine A in D_2O at 400 MHz	7
Figure S7. UV spectrum of bostrychine A.....	8
Figure S8. ^1H NMR spectrum of bostrychine B in D_2O at 600 MHz	8
Figure S9. COSY spectrum of bostrychine B in D_2O at 600 MHz.....	9
Figure S10. HSQC spectrum of bostrychine B in D_2O at 600 MHz.....	9
Figure S11. HMBC spectrum of bostrychine B in D_2O at 600 MHz.....	10
Figure S12. ^{13}C NMR spectrum of bostrychine B in D_2O at 150 MHz	10
Figure S13.UV spectrum of bostrychine B	11
Figure S14. ^1H NMR spectrum of bostrychine C in D_2O at 600 MHz	11
Figure S15. COSY spectrum of bostrychine C in D_2O at 600 MHz.....	12
Figure S16. HSQC spectrum of bostrychine C in D_2O at 600 MHz.....	12
Figure S17. HMBC spectrum of bostrychine C in D_2O at 600 MHz.....	13
Figure S18. ^{13}C NMR spectrum of bostrychine C in D_2O at 150 MHz	13
Figure S19.UV spectrum of bostrychine C	14
Figure S20. ^1H NMR spectrum of bostrychine D in D_2O at 600 MHz	14
Figure S21. COSY spectrum of bostrychine D in D_2O at 600 MHz.....	15
Figure S22. HSQC spectrum of bostrychine D in D_2O at 600 MHz.....	15
Figure S23. HMBC spectrum of bostrychine D in D_2O at 600 MHz.....	16
Figure S24. ^{13}C NMR spectrum of bostrychine D in D_2O at 150 MHz	16
Figure S25.UV spectrum of bostrychine D	17
Figure S26. ^1H NMR spectrum of bostrychine E in D_2O at 600 MHz.....	17
Figure S27. COSY spectrum of bostrychine E in D_2O at 600 MHz	18
Figure S28. ^{13}C NMR spectrum of bostrychine E in D_2O at 150 MHz	18
Figure S29. HSQC spectrum of bostrychine E in D_2O at 600 MHz	19
Figure S30. HMBC spectrum of bostrychine E in D_2O at 600 MHz	19

Figure S31. NOESY spectrum of bostrychine E in D ₂ O at 600 MHz	20
Figure S32.UV spectrum of bostrychine E	20
Figure S33. ¹ H NMR spectrum of bostrychine F in D ₂ O at 600 MHz.....	21
Figure S34. COSY spectrum of bostrychine F in D ₂ O at 600 MHz	21
Figure S35. HSQC spectrum of bostrychine F in D ₂ O at 600 MHz	22
Figure S36. HMBC spectrum of bostrychine F in D ₂ O at 600 MHz	22
Figure S37 ¹³ C NMR spectrum of bostrychine F in D ₂ O at 150 MHz.....	23
Figure S38. NOESY spectrum of bostrychine F in D ₂ O at 600 MHz.....	23
Figure S39.UV spectrum of bostrychine F	24

Table S1. Overview of the investigated *B. scorpioides* samples, their collection sites and dates.

Sample	Collection Place	Collection Date	Origin	Longitude	Latitude
1	Plouescat, France	10/06/2019	Field	-4.222010	48.648812
2	Sene, France	31/05/2019	Field	-2.743194	47.623058
3	Hillion, France	03/6/2019	Field	-2.676122	48.514435
4	Saint Colombier, France	31/05/2019	Field	-2.734889	47.552583
5	Saint Armel, Chenal de Saint Leonard, France	31/05/2019	Field	-2.713022	47.589354
6	Promenade des Rosvelec, Vannes, France	30/05/2019	Field	-2.748475	47.6209582
7	Saint Armel, Passage A lile de Tascon, France	31/05/2019	Field	-2.726754	47.569157
8	Kerbourbon, Vannes, France	30/05/2019	Field	-2.754591	47.6344224
9	Plouescat, France	14/06/2018	Field	-4.222010	48.648812
10	Mi ño, Galicia, Spain	October 2019	Field	- 8.206211	43.352718
11	Puente Lavaera, San Fernando, Cádiz, Spain	14/07/2019	Field	6.191112	36.4575345
12	Salt marsh of Palmones, Spain	12/07/2019	Field	-5.439694	36.173694
13	Burnham-on-Crouch, Essex, United Kingdom	01/09/2019	Field	0.843817	51.623467
14	Finavarra Demesne, Co. Clare, Ireland	03/09/2015	Culture	-9.091785	53.147615
15	Lettermore, Ireland	October 2019	Field	- 9.711216	53.2983547
16	Tolka, Ireland	October 2019	Field	- 6.157918	53.37177582
17	Argideen-Timoleague, Ireland	October 2019	Field	- 8.764898	51.641662

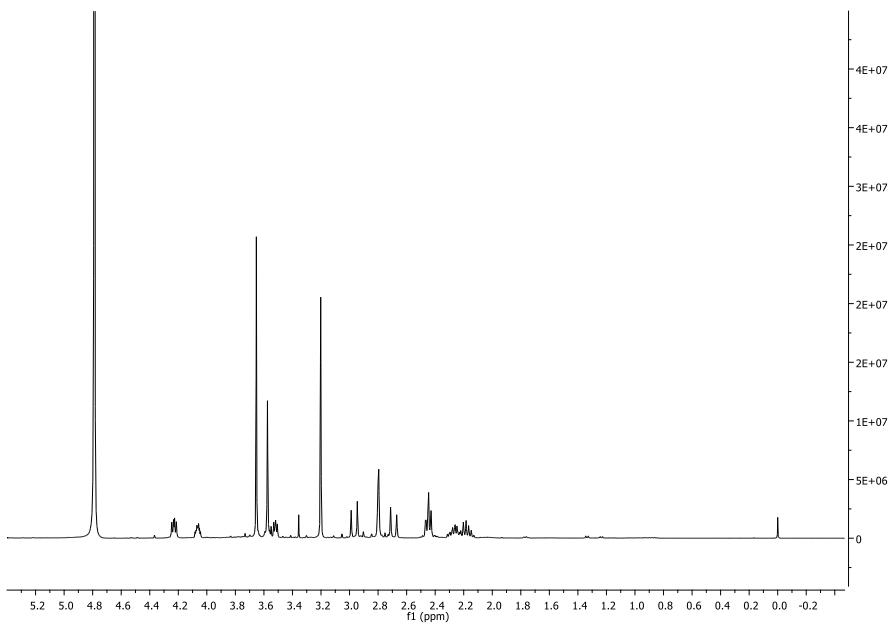


Figure S1. ¹H NMR spectrum of bostrychine A in D_2O at 400 MHz

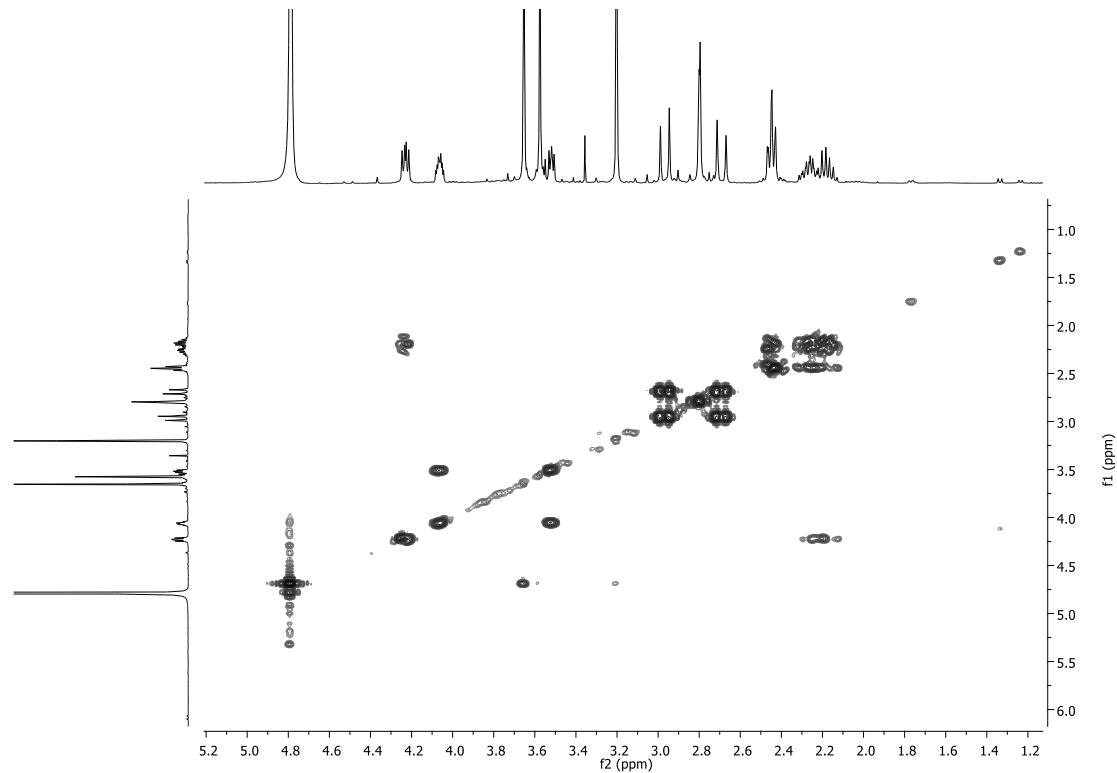


Figure S2. COSY spectrum of bostrychine A in D_2O at 400 MHz

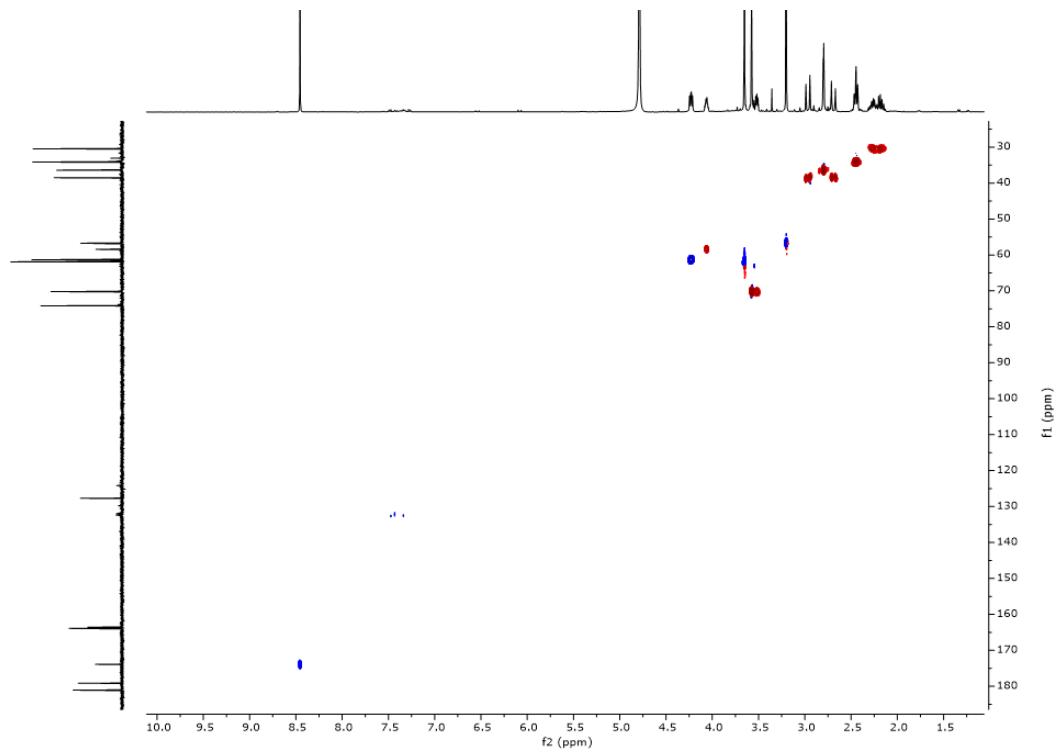


Figure S3. HSQC spectrum of bostrychine A in D_2O at 400 MHz

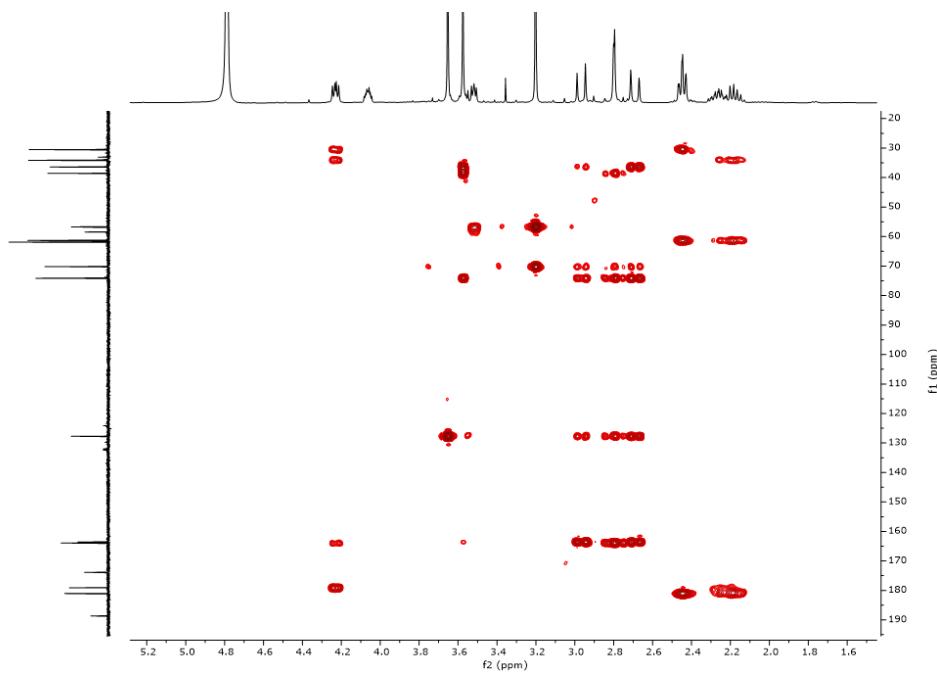


Figure S4. HMBC spectrum of bostrychine A in D_2O at 400 MHz

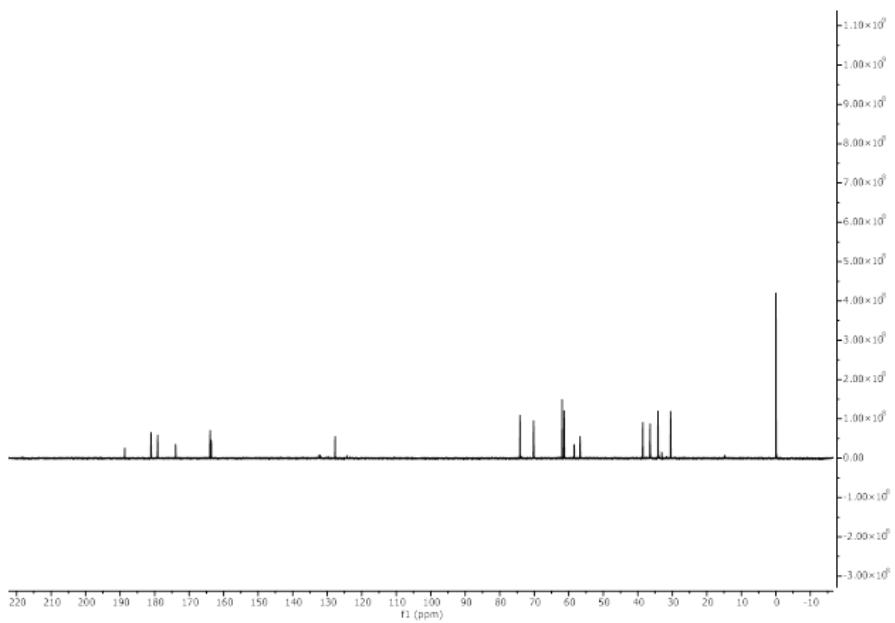


Figure S5. ^{13}C NMR spectrum of bostrychine A in D_2O at 100 MHz

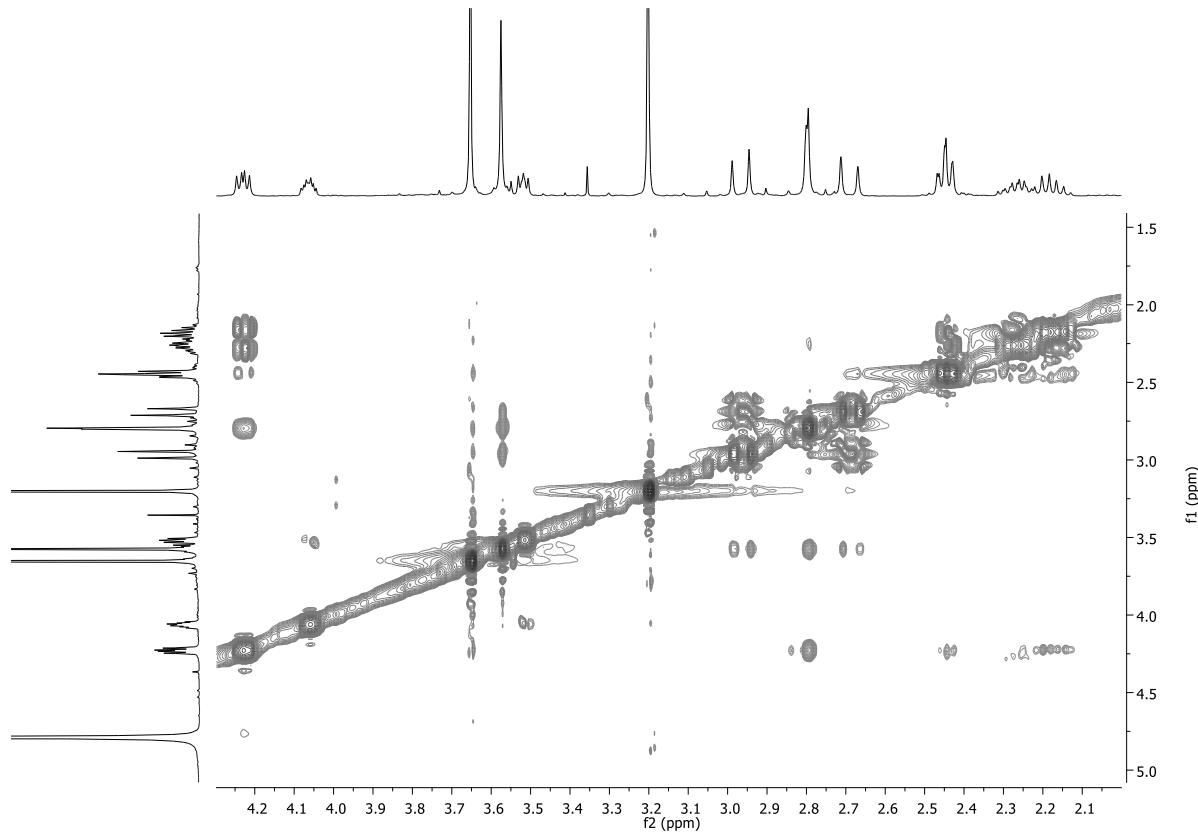


Figure S6. NOESY spectrum of bostrychine A in D_2O at 400 MHz

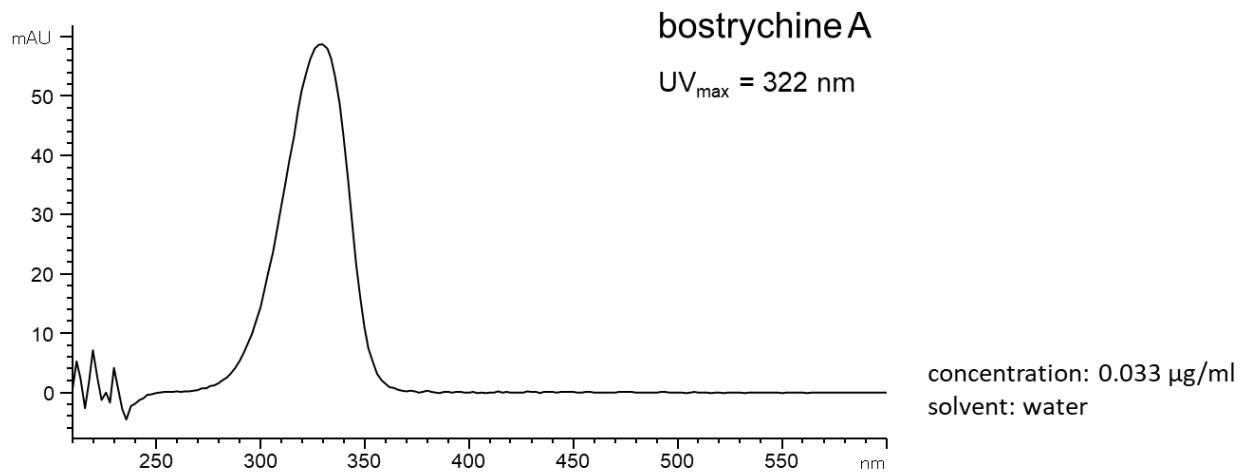


Figure S7. UV spectrum of bostrychine A

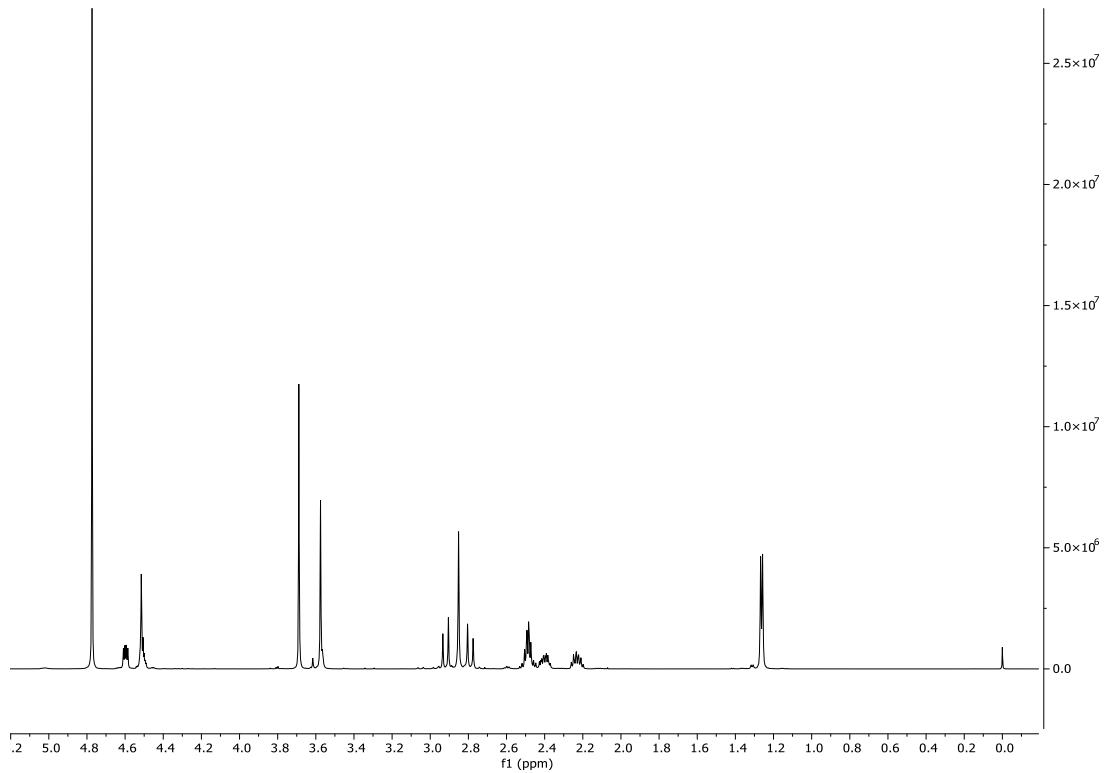


Figure S8. ^1H NMR spectrum of bostrychine B in D_2O at 600 MHz

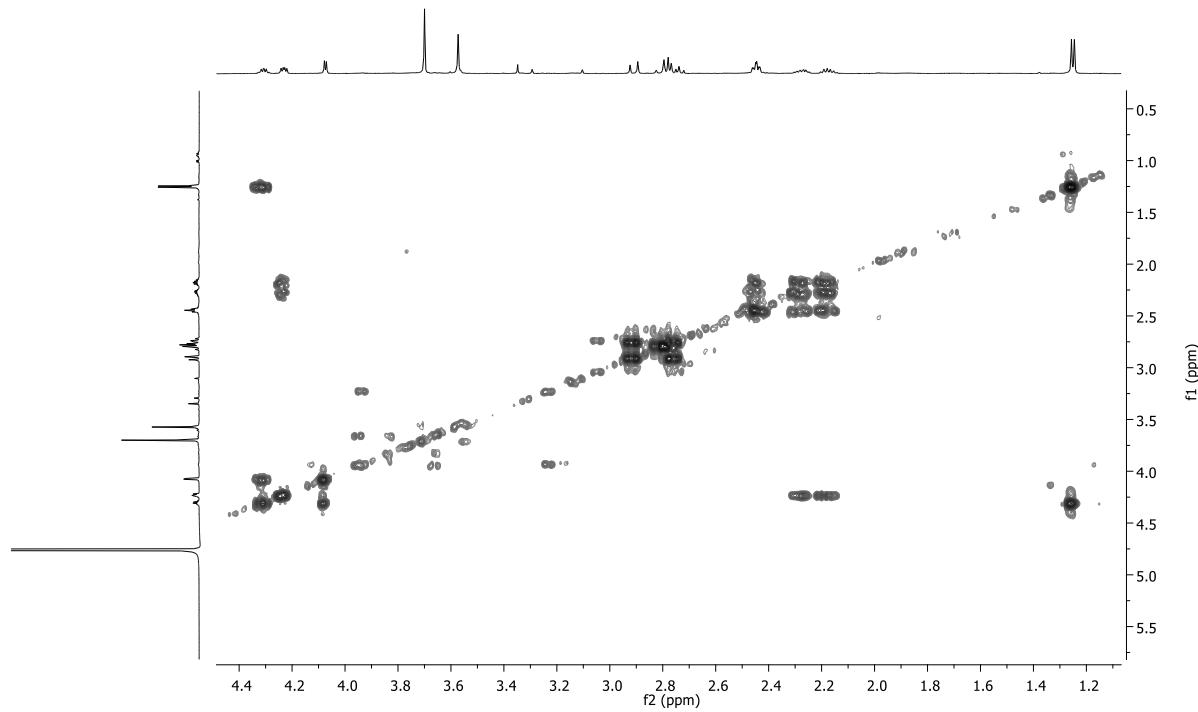


Figure S9. COSY spectrum of bostrychine B in D_2O at 600 MHz

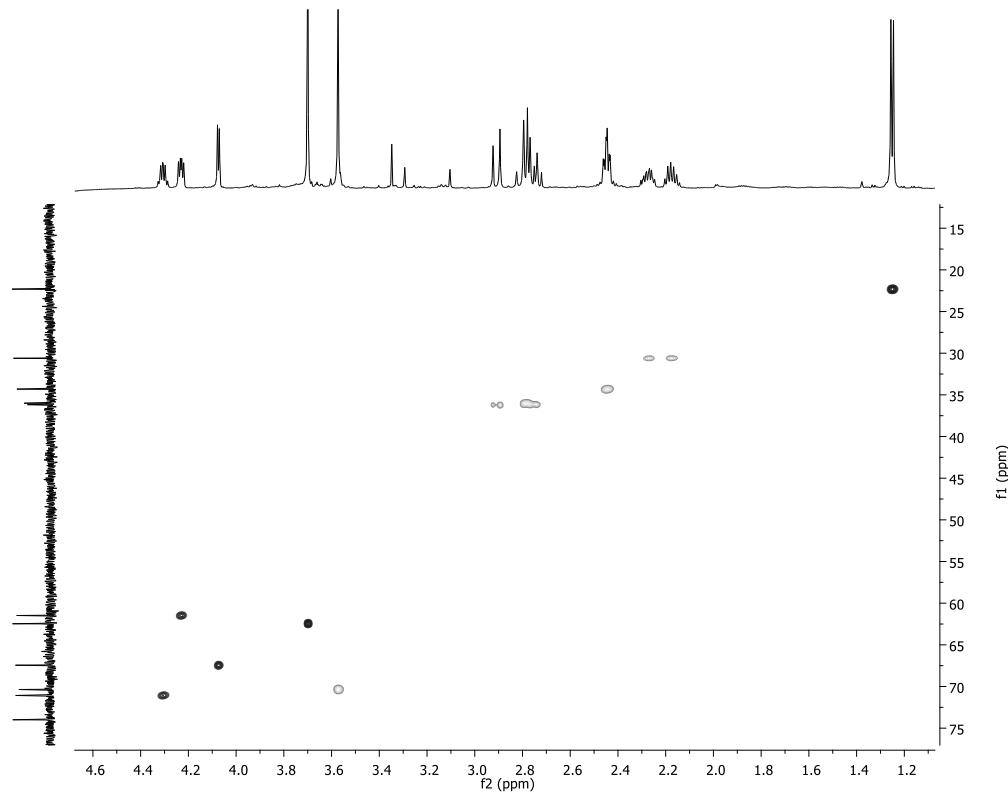


Figure S10. HSQC spectrum of bostrychine B in D_2O at 600 MHz

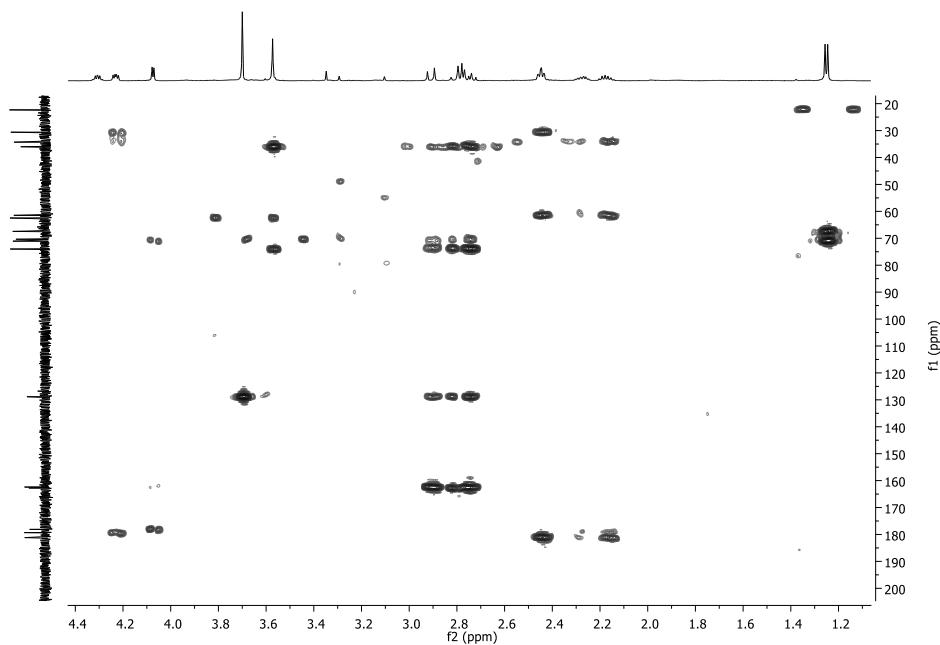


Figure S11. HMBC spectrum of bostrychine B in D₂O at 600 MHz

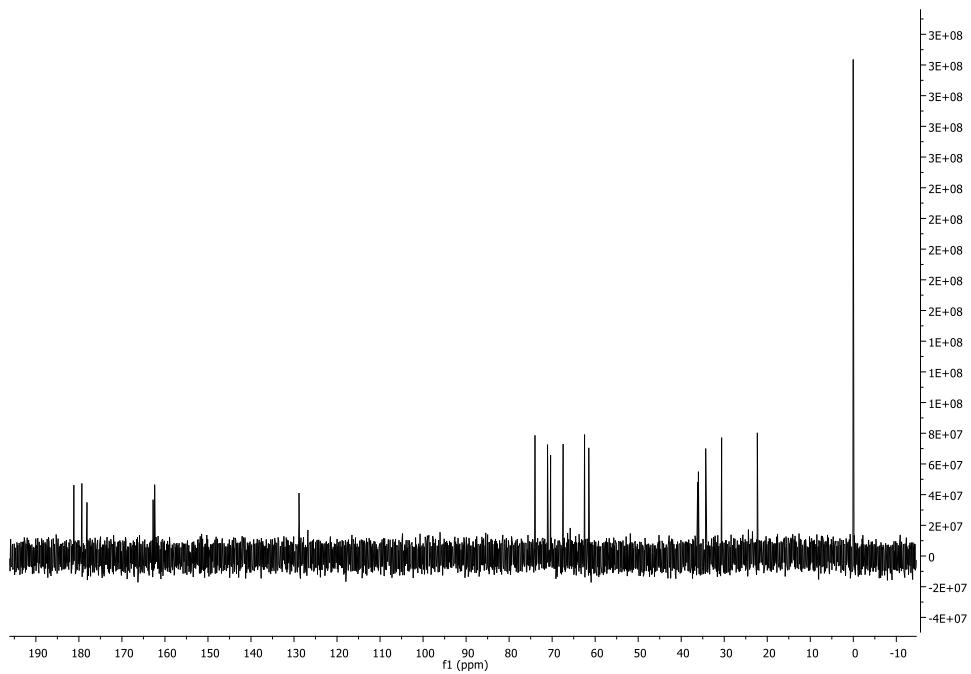


Figure S12. ¹³C NMR spectrum of bostrychine B in D₂O at 150 MHz

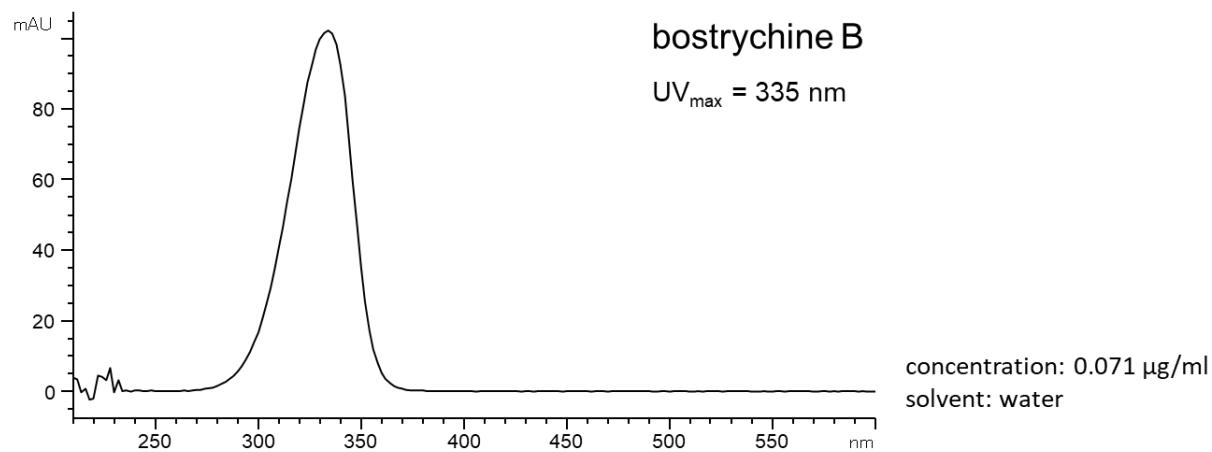


Figure S13.UV spectrum of bostrychine B

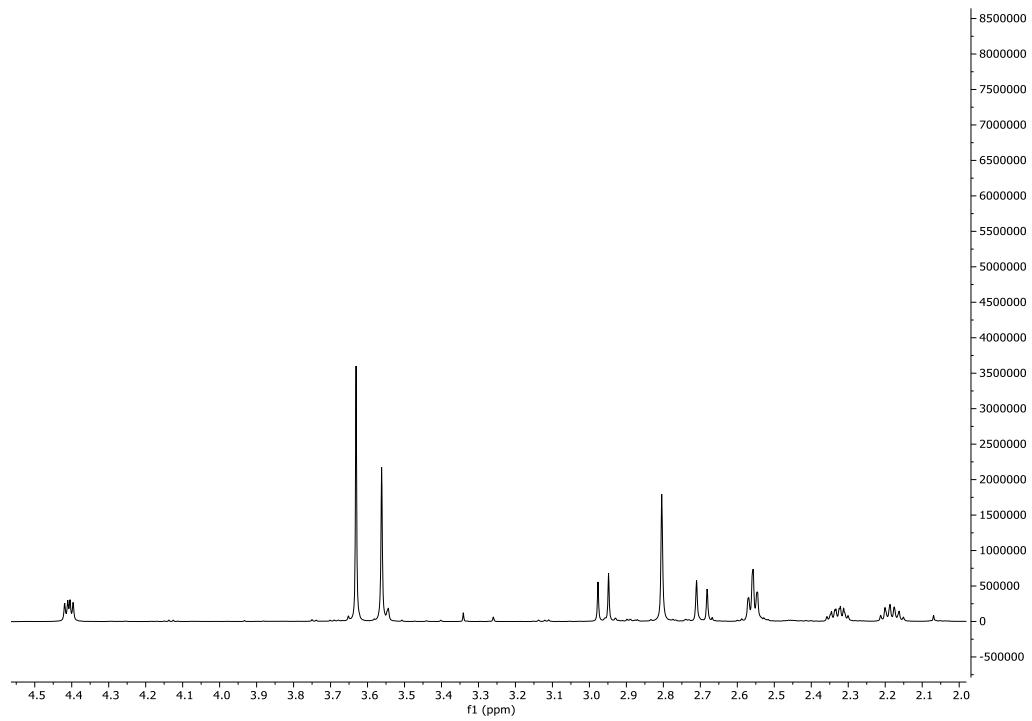


Figure S14. ^1H NMR spectrum of bostrychine C in D_2O at 600 MHz

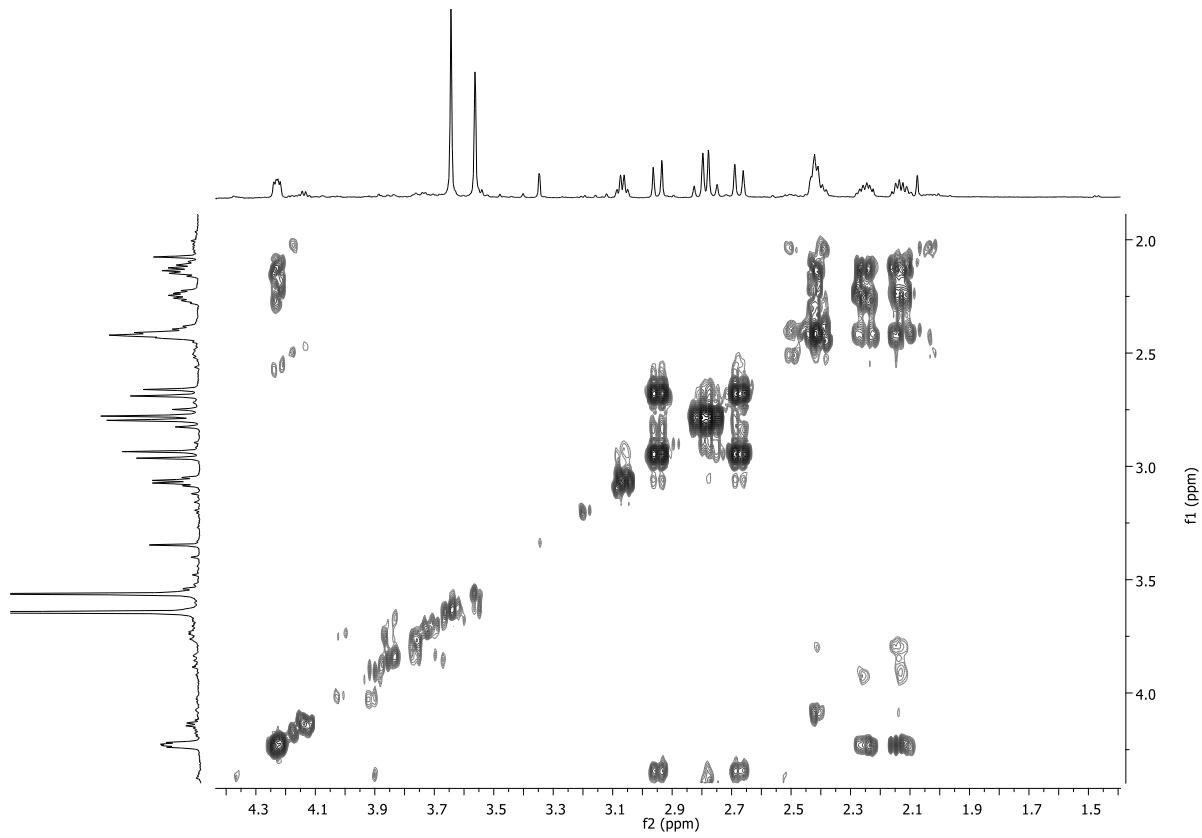


Figure S15. COSY spectrum of bostrychine C in D_2O at 600 MHz

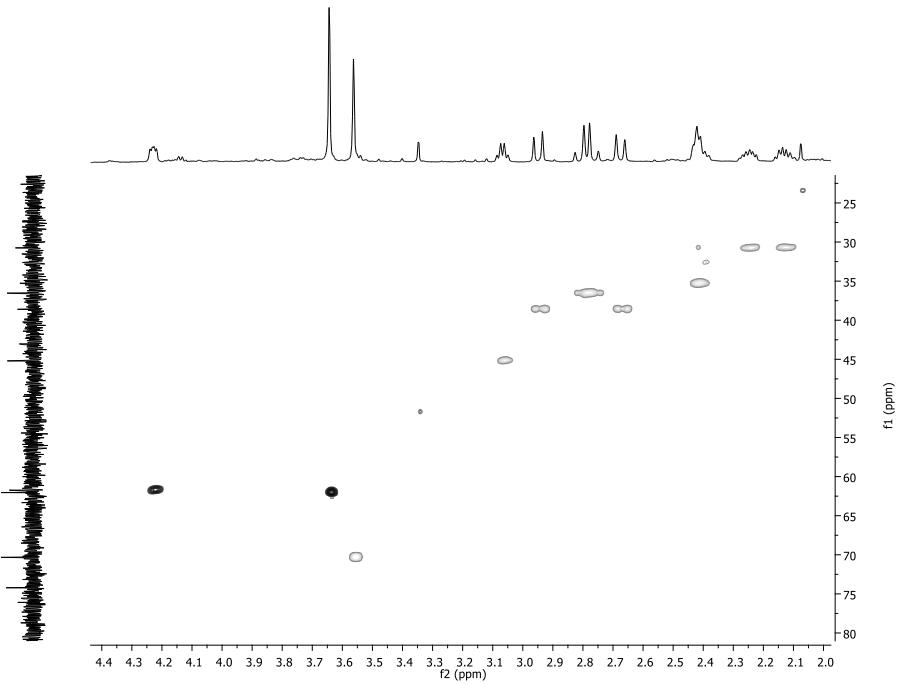


Figure S16. HSQC spectrum of bostrychine C in D_2O at 600 MHz

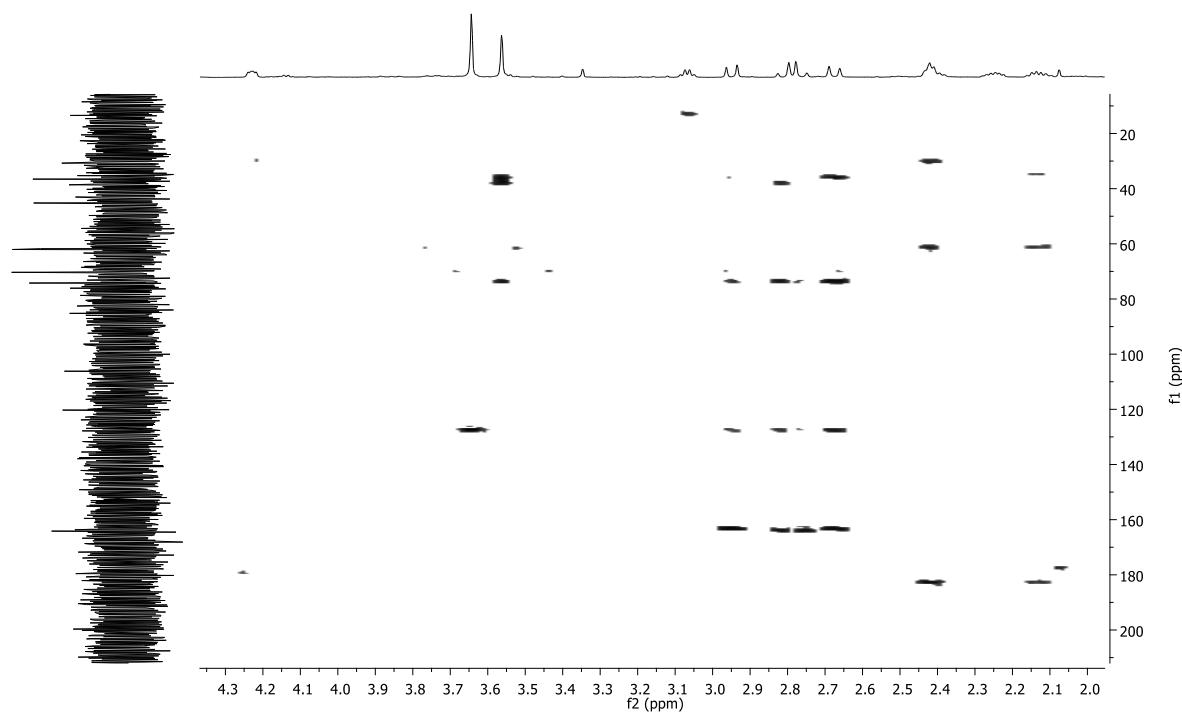


Figure S17. HMBC spectrum of bostrychine C in D₂O at 600 MHz

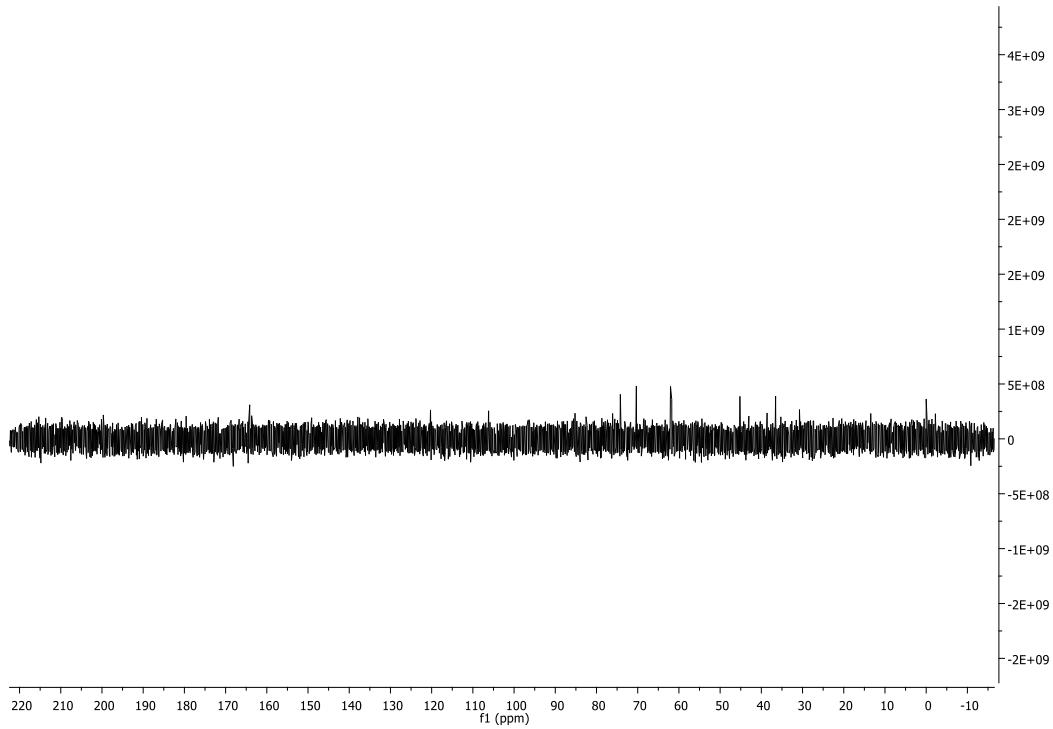


Figure S18. ¹³C NMR spectrum of bostrychine C in D₂O at 150 MHz

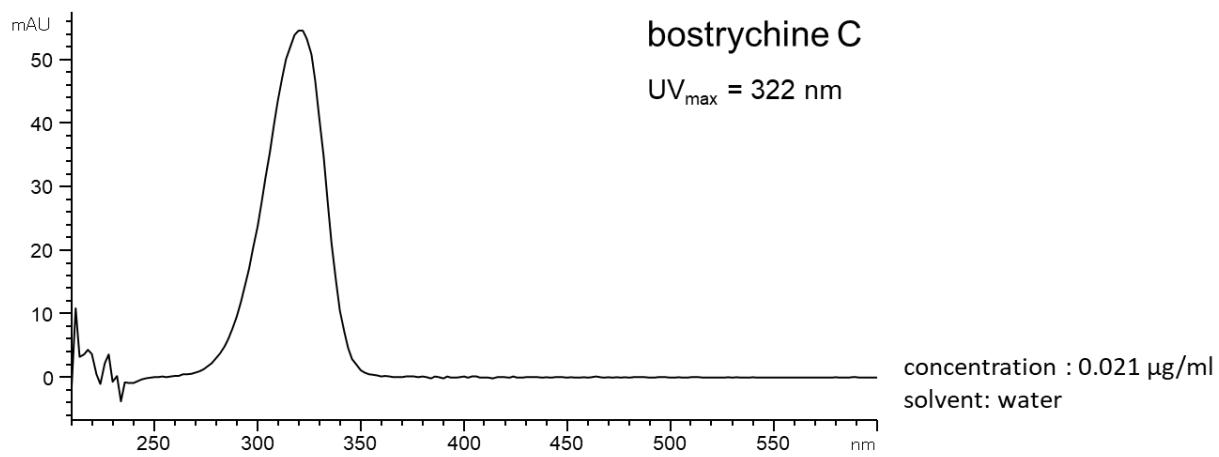


Figure S19.UV spectrum of bostrychine C

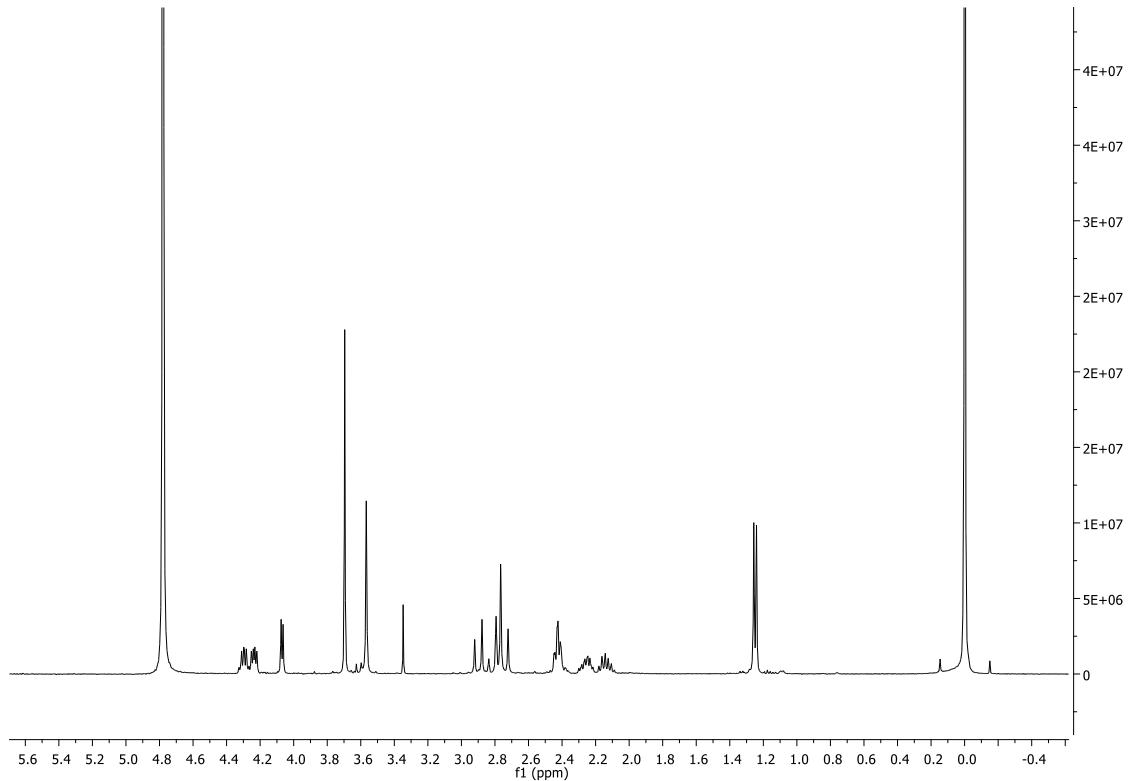


Figure S20.¹H NMR spectrum of bostrychine D in D₂O at 600 MHz

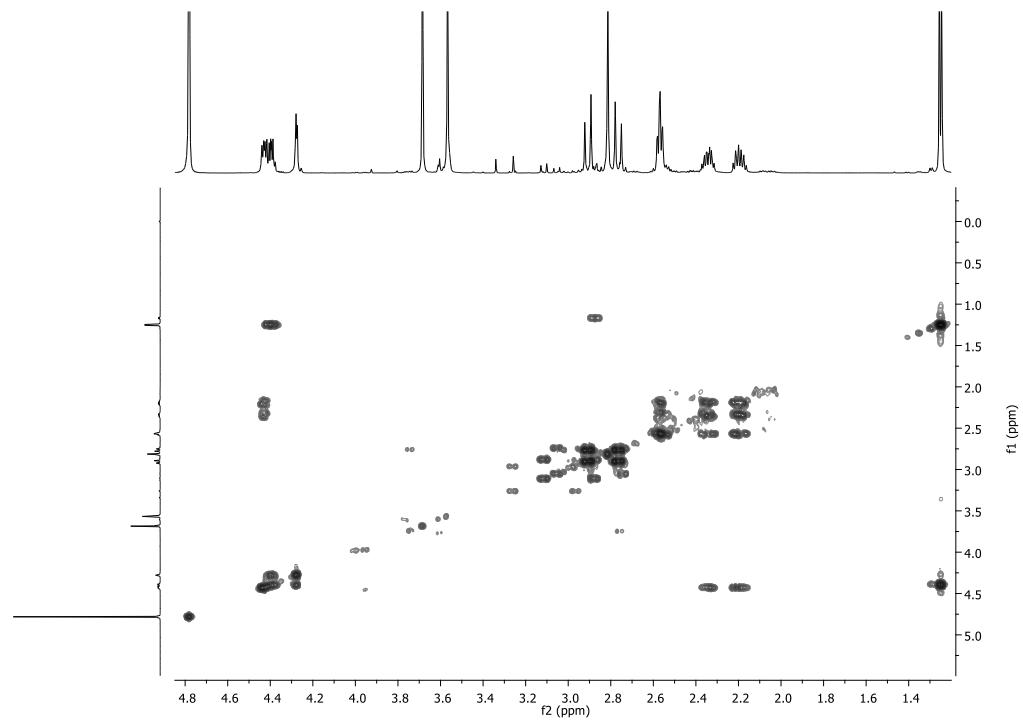


Figure S21. COSY spectrum of bostrychine D in D_2O at 600 MHz

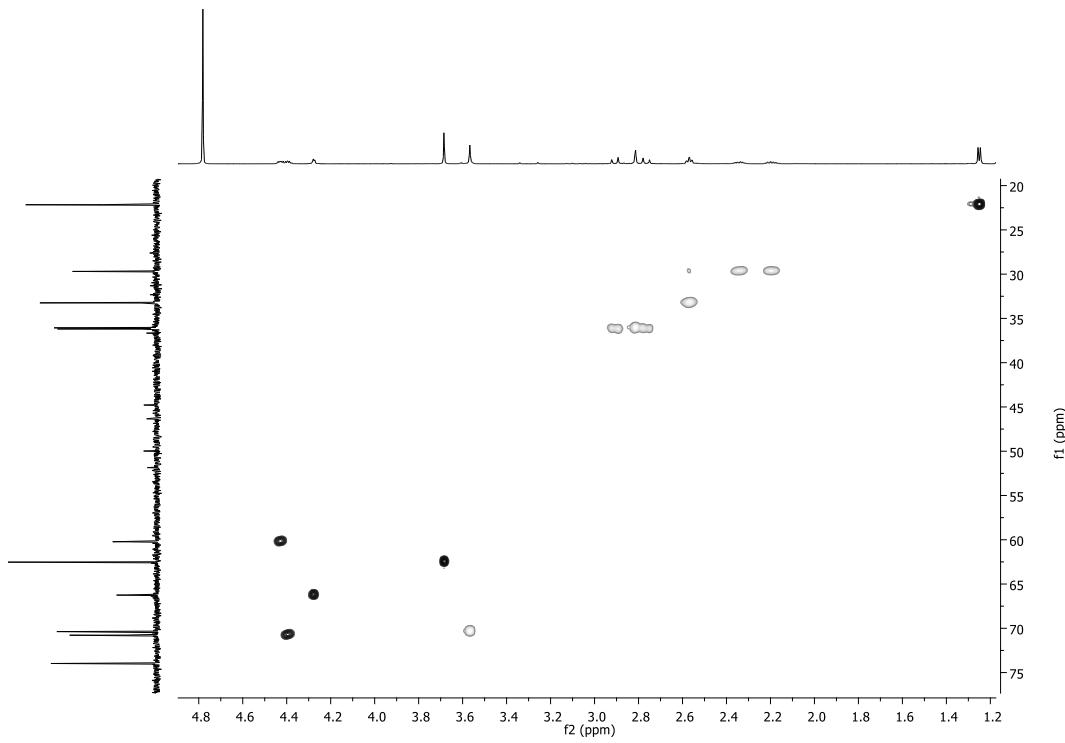


Figure S22. HSQC spectrum of bostrychine D in D_2O at 600 MHz

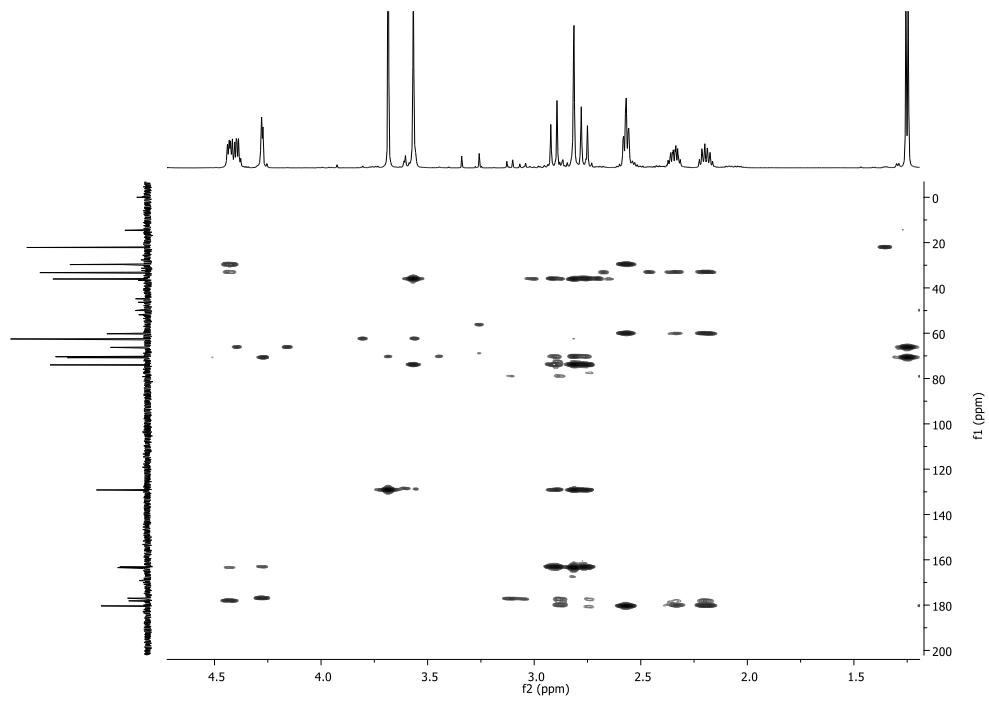


Figure S23. HMBC spectrum of bostrychine D in D₂O at 600 MHz

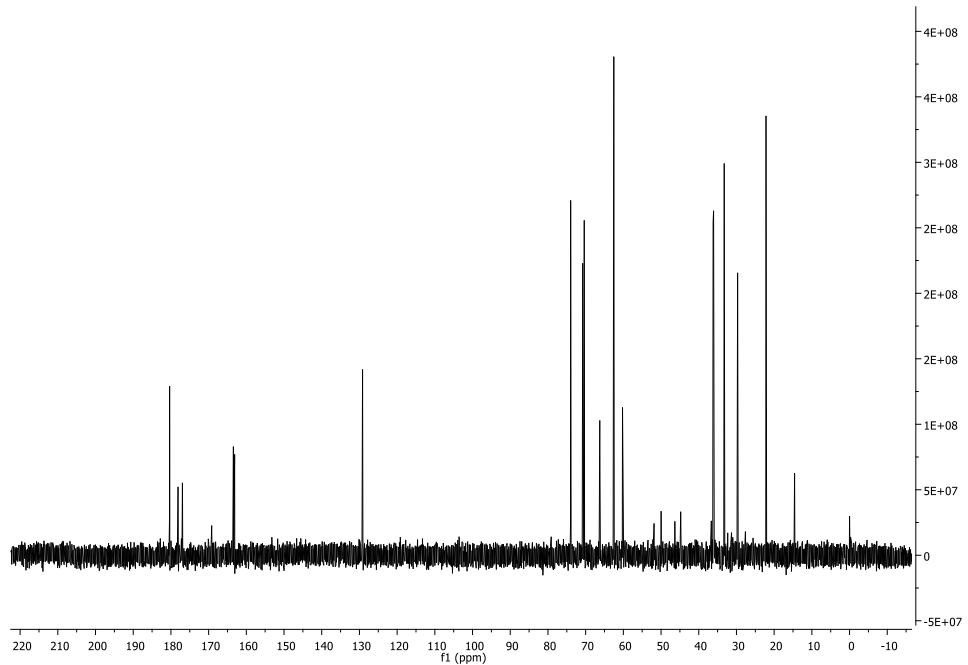


Figure S24. ¹³C NMR spectrum of bostrychine D in D₂O at 150 MHz

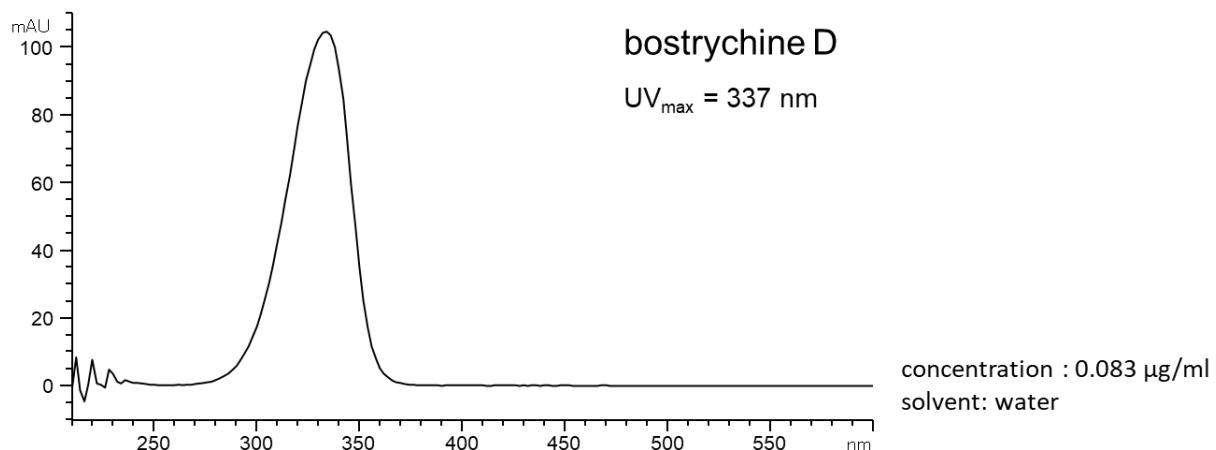


Figure S25.UV spectrum of bostrychine D

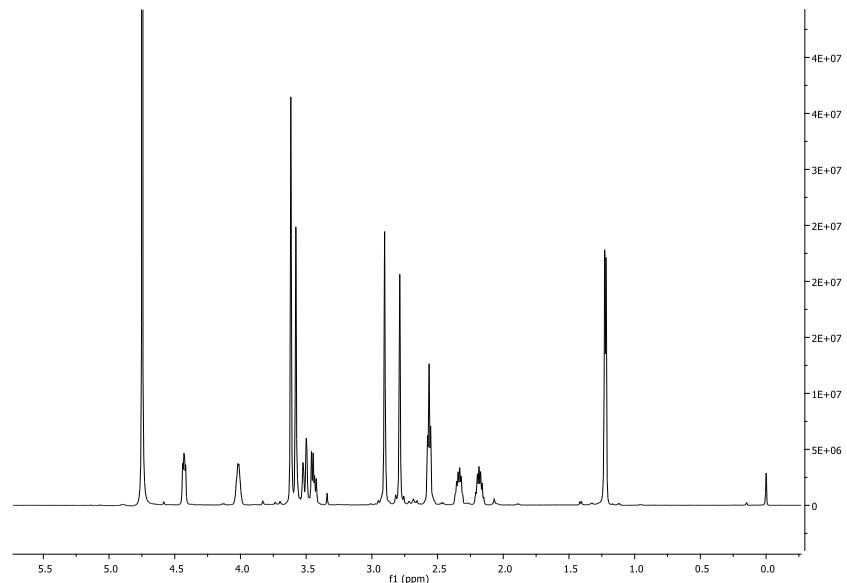


Figure S26.¹H NMR spectrum of bostrychine E in D₂O at 600 MHz

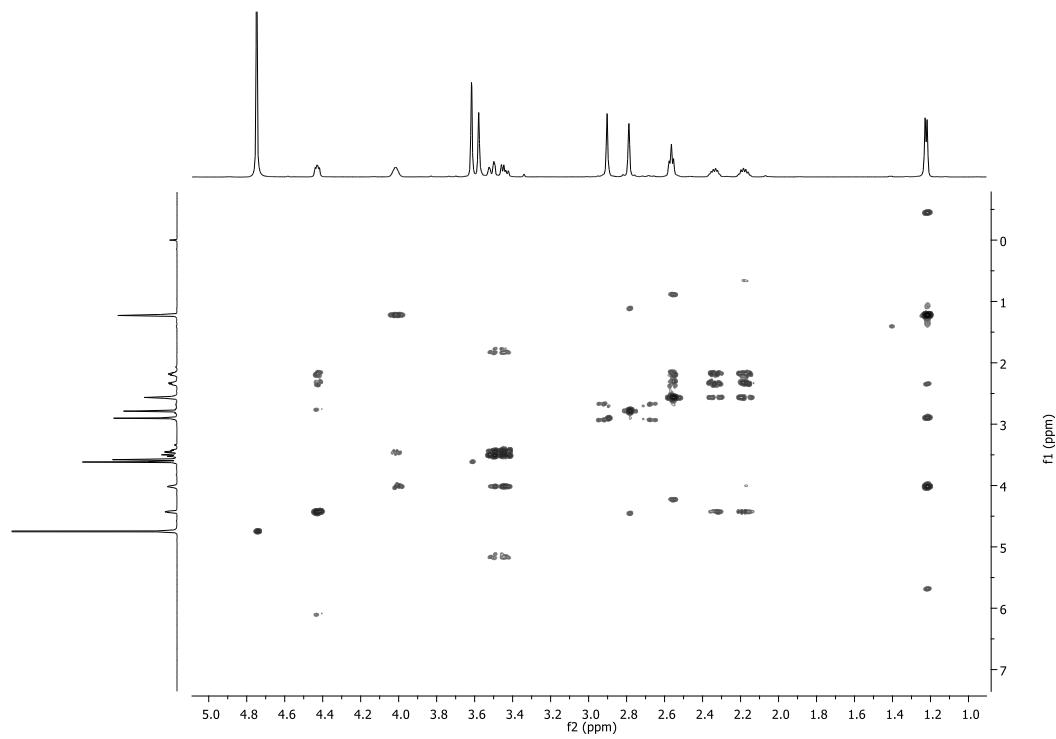


Figure S27. COSY spectrum of bostrychine E in D_2O at 600 MHz

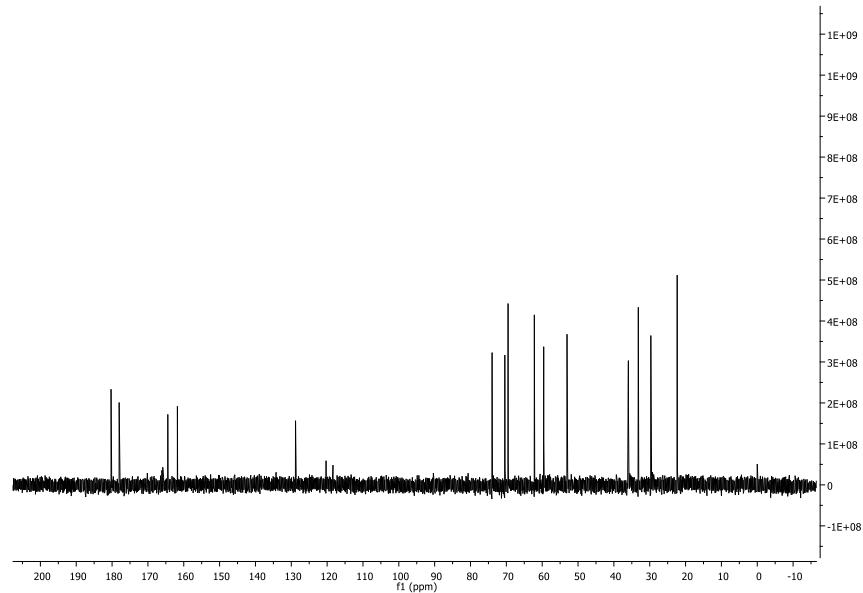


Figure S28. ^{13}C NMR spectrum of bostrychine E in D_2O at 150 MHz

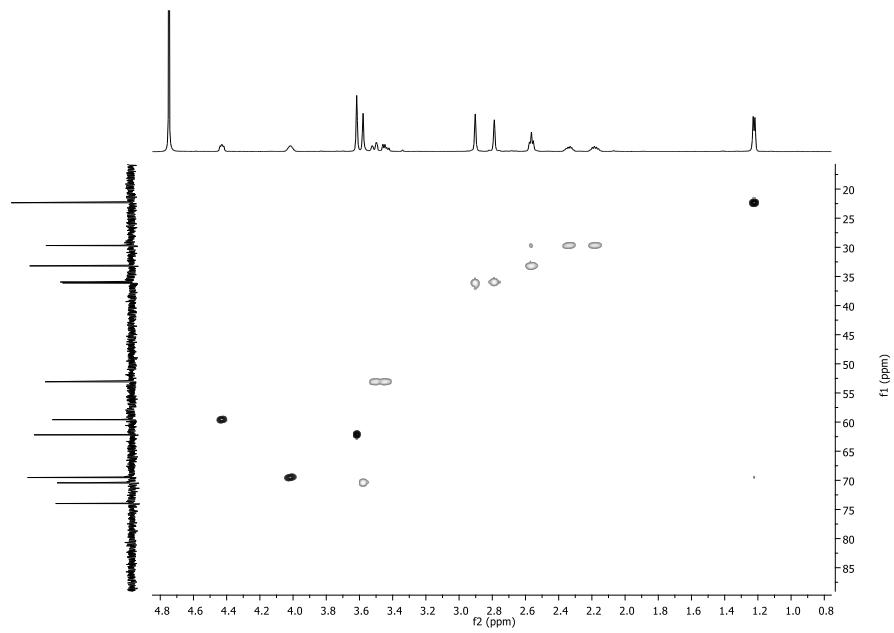


Figure S29. HSQC spectrum of bostrychine E in D₂O at 600 MHz

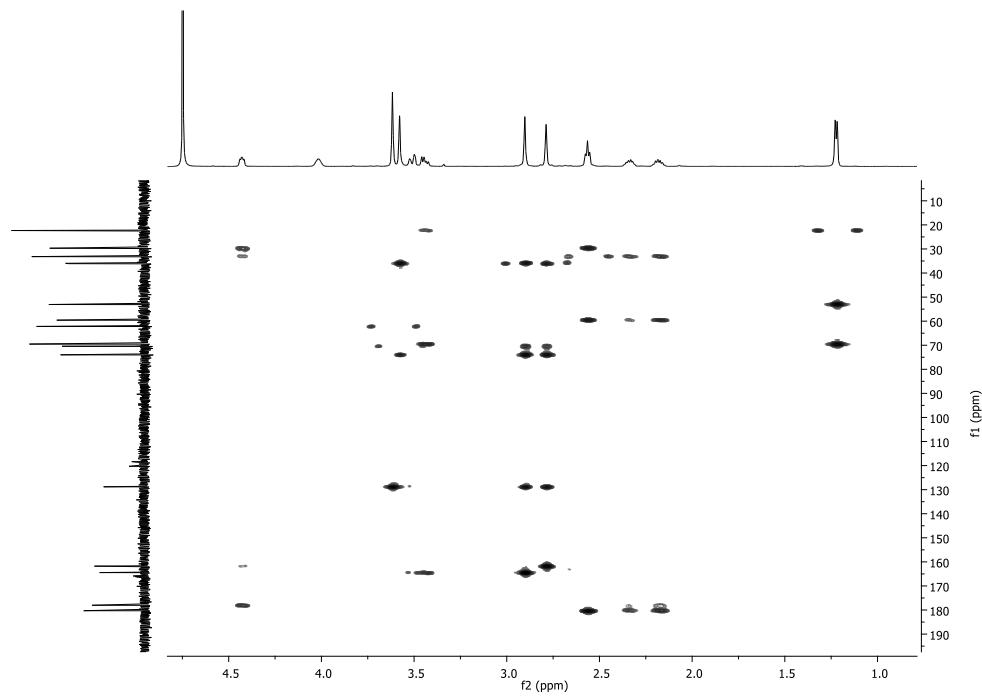


Figure S30. HMBC spectrum of bostrychine E in D₂O at 600 MHz

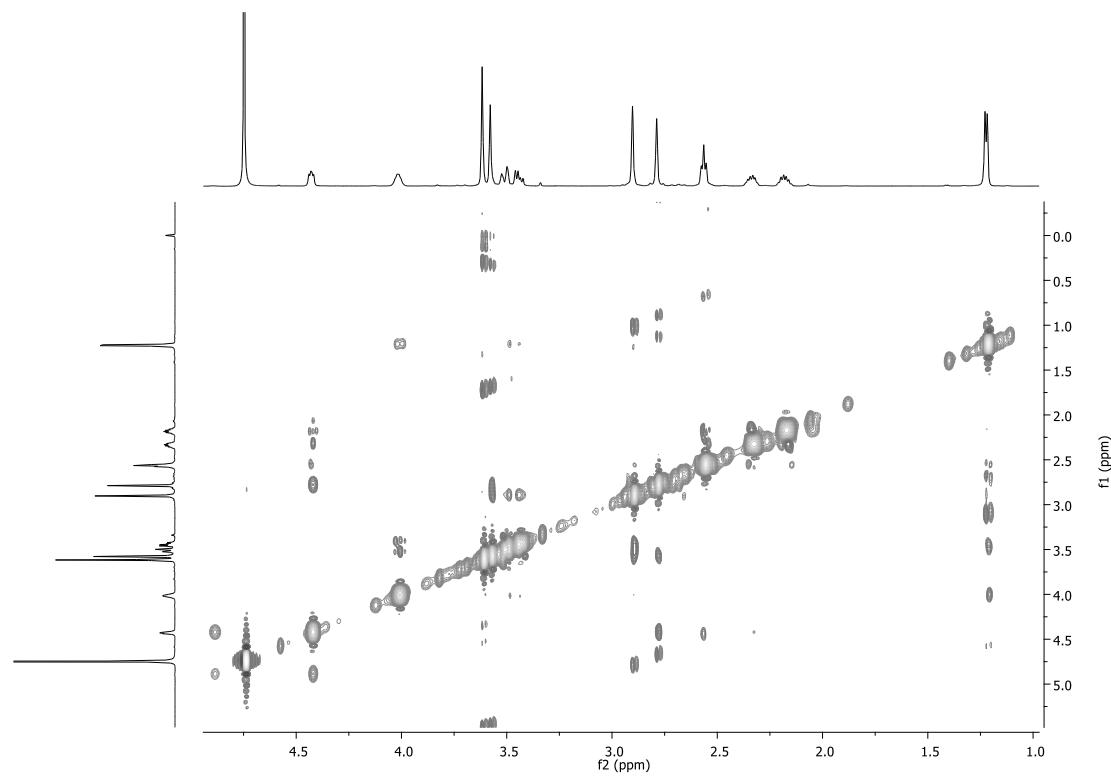


Figure S31. NOESY spectrum of bostrychine E in D_2O at 600 MHz

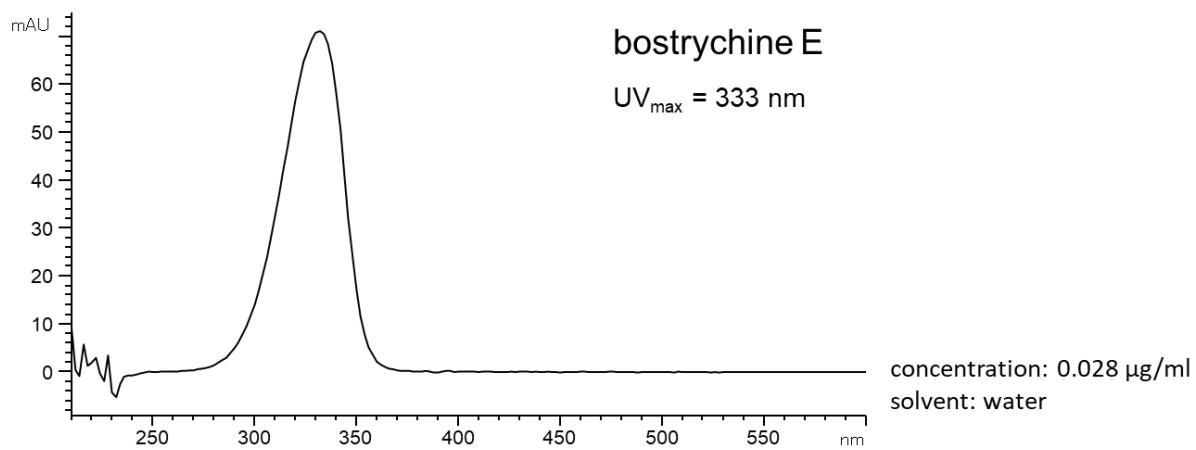


Figure S32.UV spectrum of bostrychine E

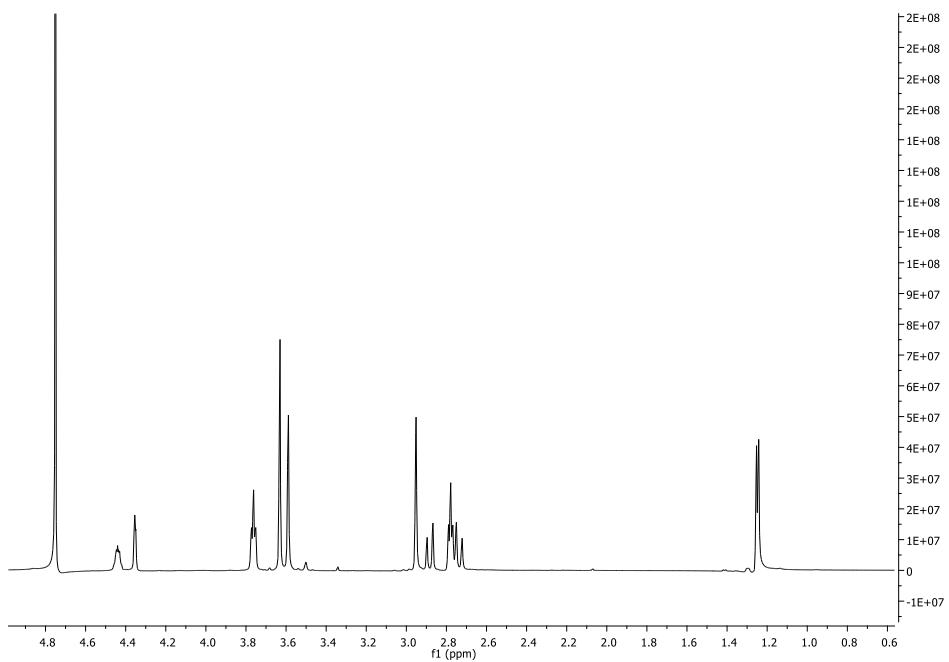


Figure S33. ¹H NMR spectrum of bostrychine F in D₂O at 600 MHz

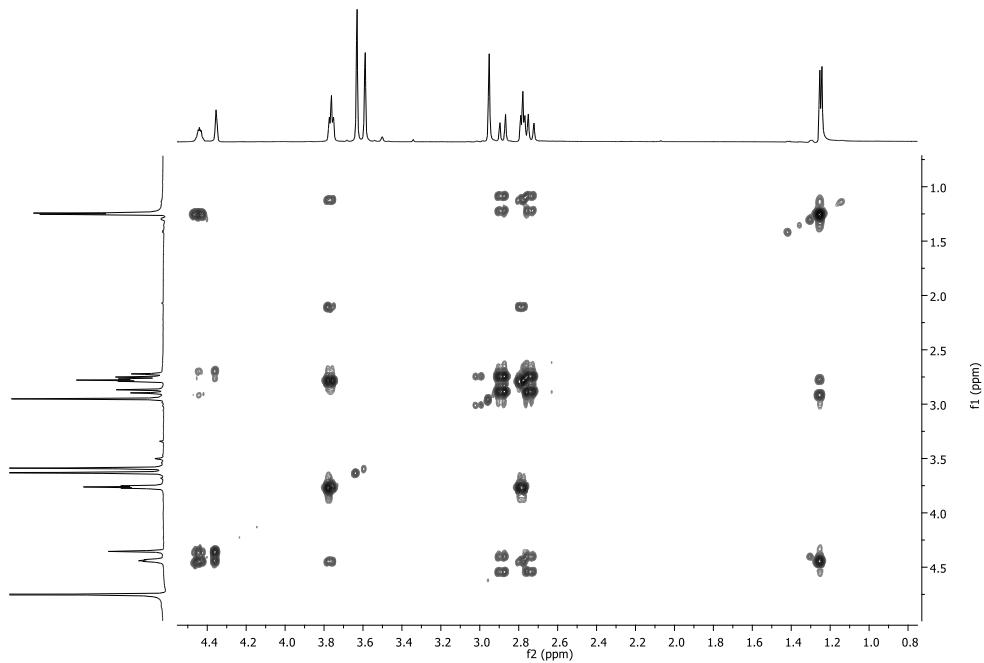


Figure S34. COSY spectrum of bostrychine F in D₂O at 600 MHz

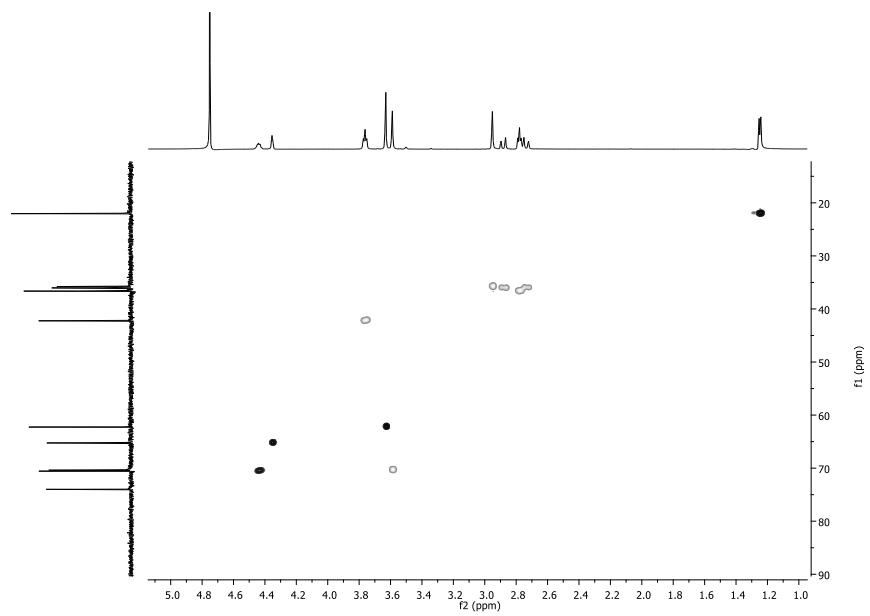


Figure S35. HSQC spectrum of bostrychine F in D₂O at 600 MHz

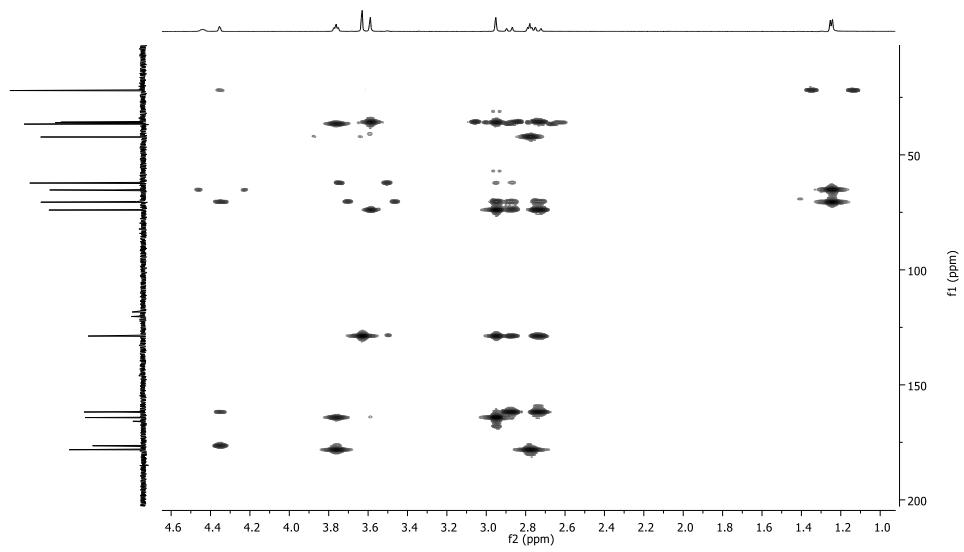


Figure S36. HMBC spectrum of bostrychine F in D₂O at 600 MHz

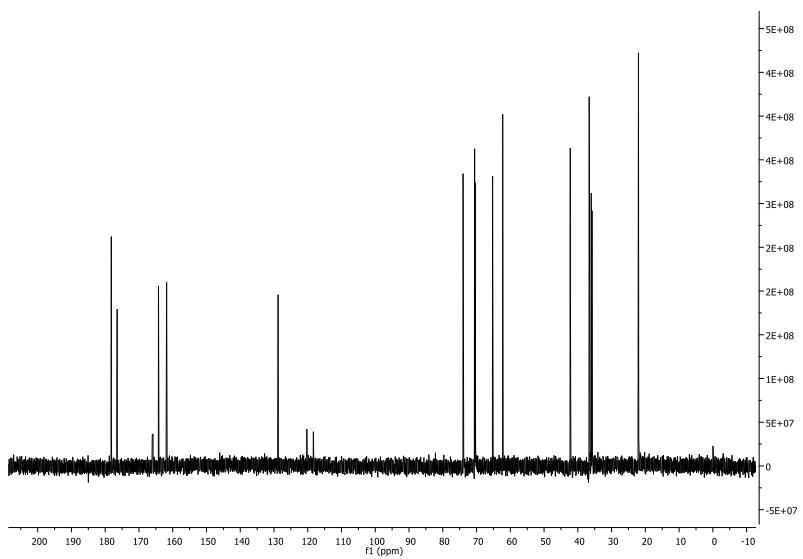


Figure S37 ^{13}C NMR spectrum of bostrychine F in D_2O at 150 MHz

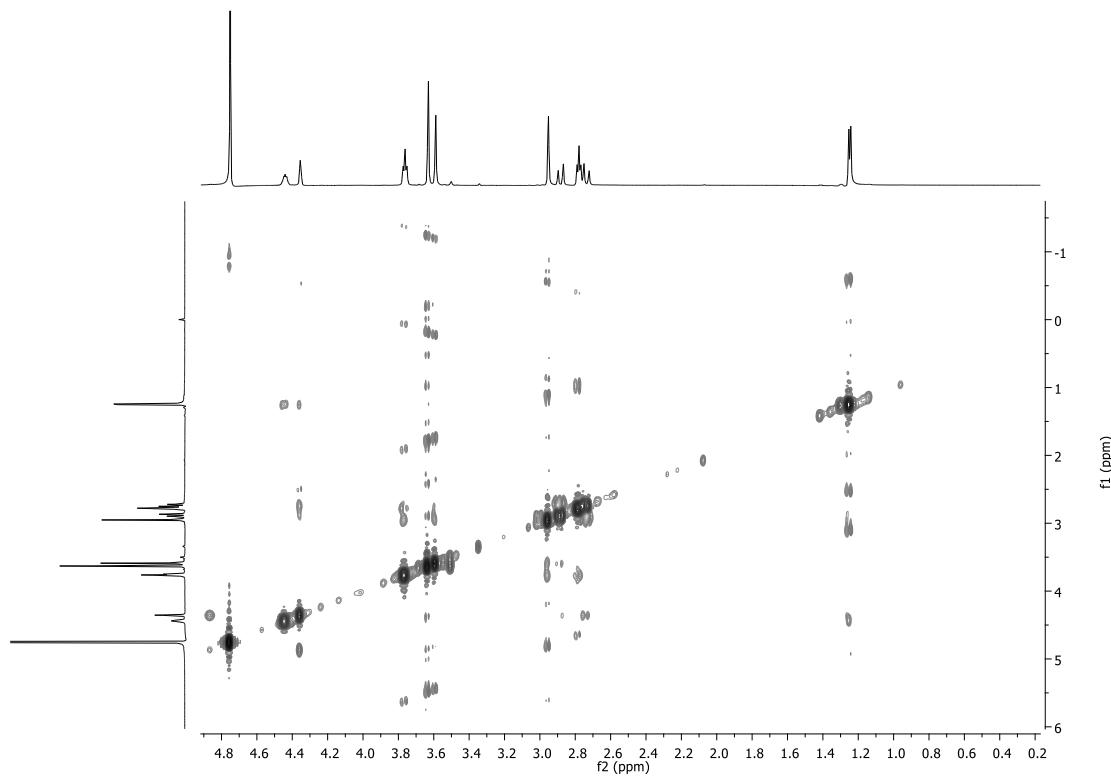


Figure S38. NOESY spectrum of bostrychine F in D_2O at 600 MHz

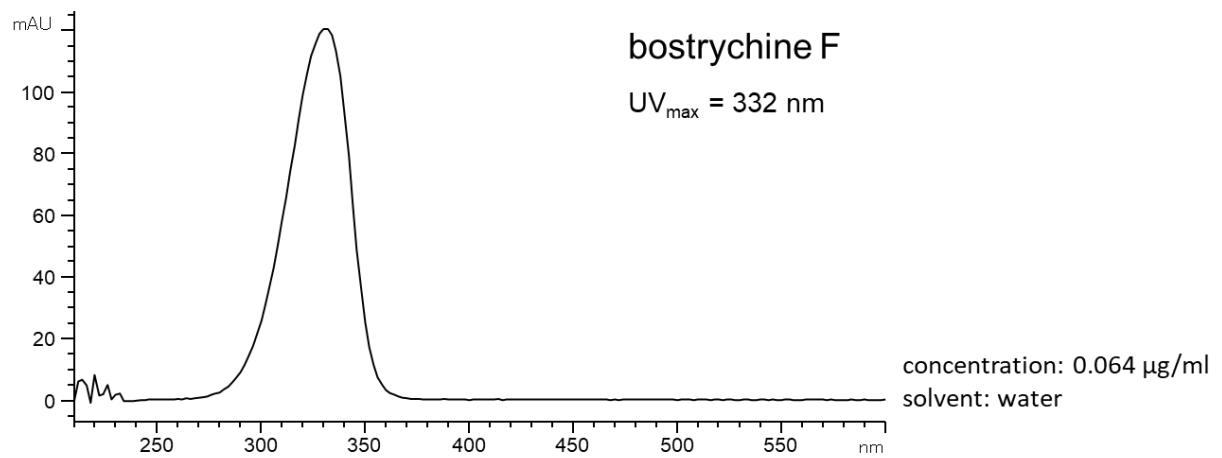


Figure S39.UV spectrum of bostrychine F