Supplementary Material

In Vitro and in Vivo Assessment of the Efficacy of Bromoageliferin, an Alkaloid Isolated from the Sponge *Agelas dilatata,* against *Pseudomonas aeruginosa*

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† Same contribution to this work

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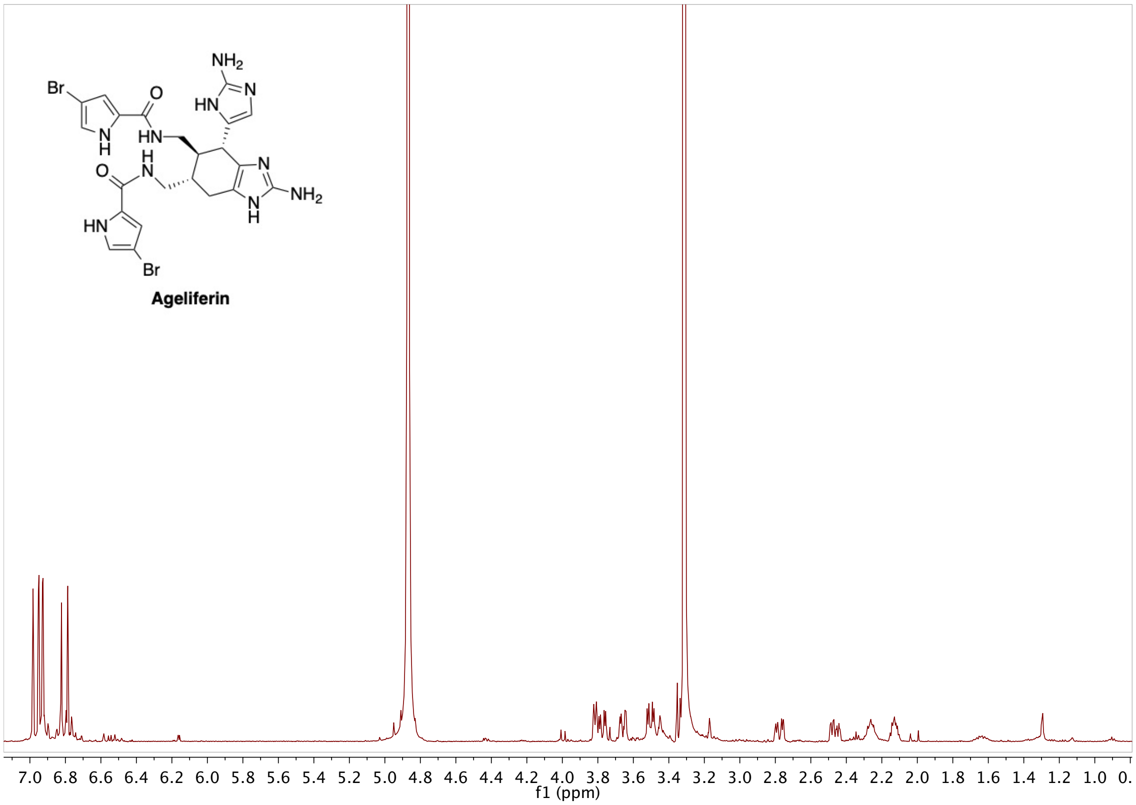


Figure S1. ^{1}H NMR spectrum of **1** (500 MHz, CD_3OD).

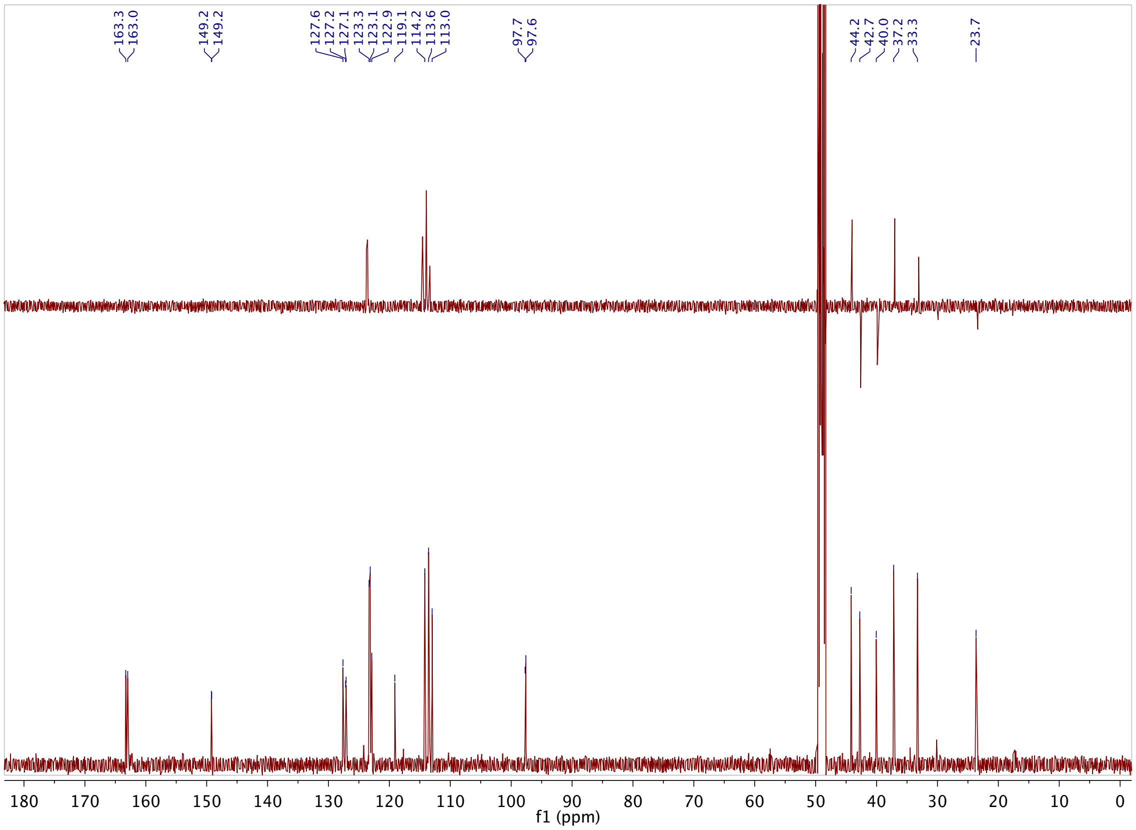
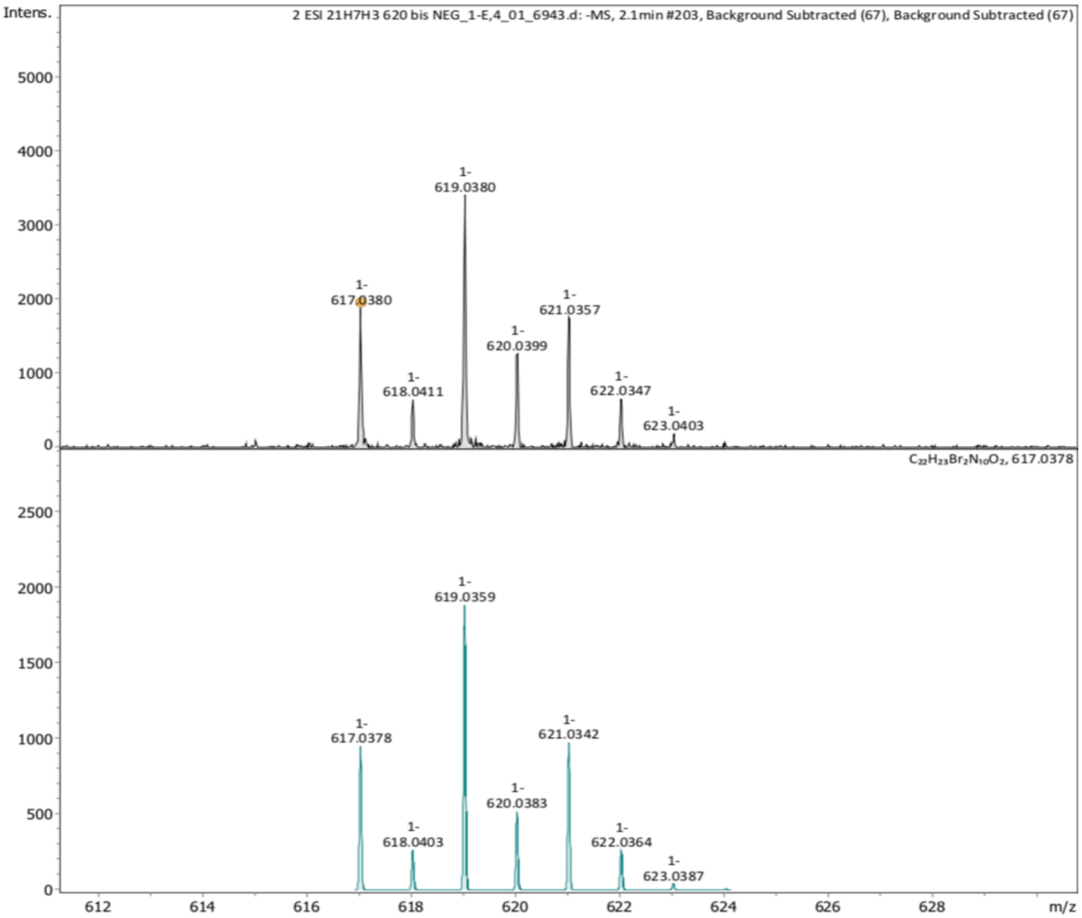


Figure S2. ^{13}C NMR and DEPT-135 spectra of **1** (125 MHz, CD_3OD).



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
617.0380	1	C22H23Br2N10O2	100.00	617.0378	-0.2	-0.4	51.0	19.0	even	ok
	2	C23H29Br2N3O7	86.31	617.0378	-0.2	-0.4	55.8	13.5	odd	ok

Figure S3. (-)-HRESIMS of **1**.

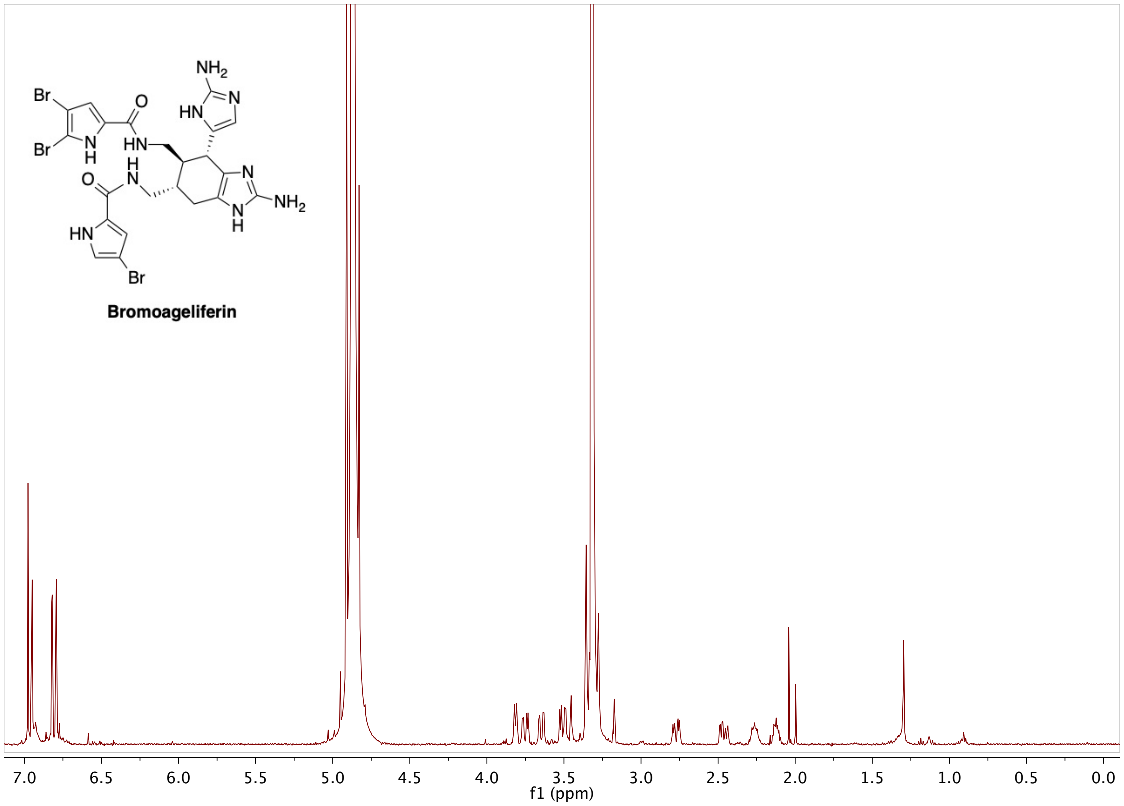


Figure S4. ^{1}H NMR spectrum of **2** (500 MHz, CD_3OD).

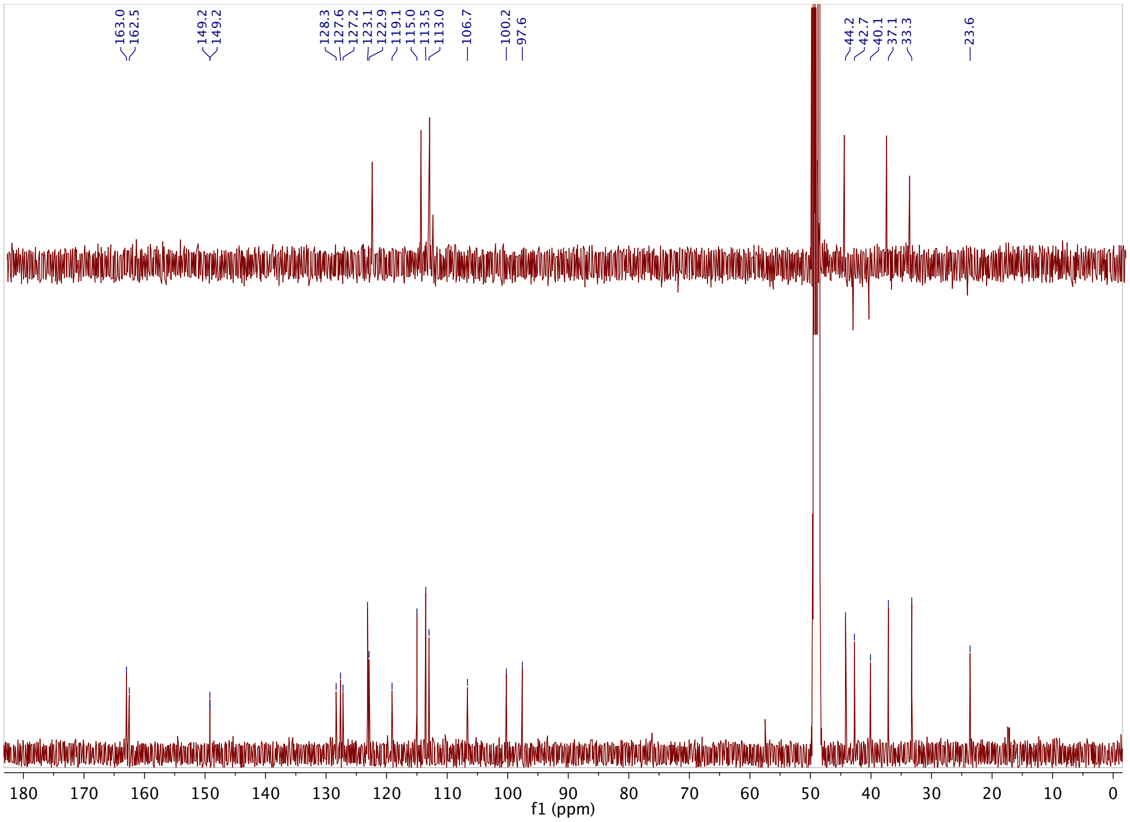
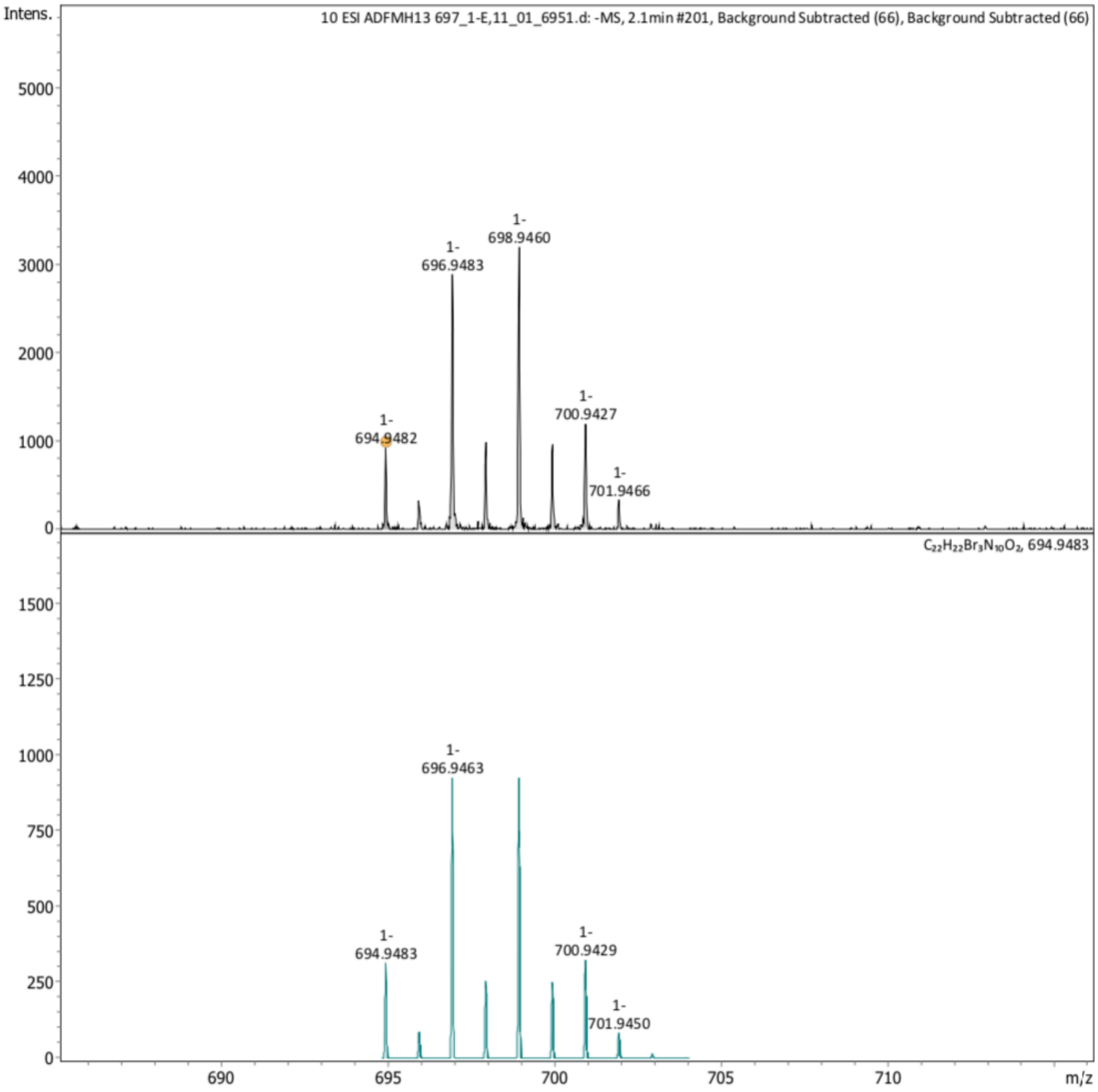


Figure S5. ^{13}C NMR and DEPT-135 spectra of **2** (125 MHz, CD_3OD).



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
694.9482	1	C23H28Br3N3O7	100.00	694.9483	0.1	0.2	41.7	15.5	odd	ok
	2	C22H22Br3N10O2	86.11	694.9483	0.1	0.2	42.9	21.0	even	ok

Figure S6. (-)-HRESIMS of **2**.

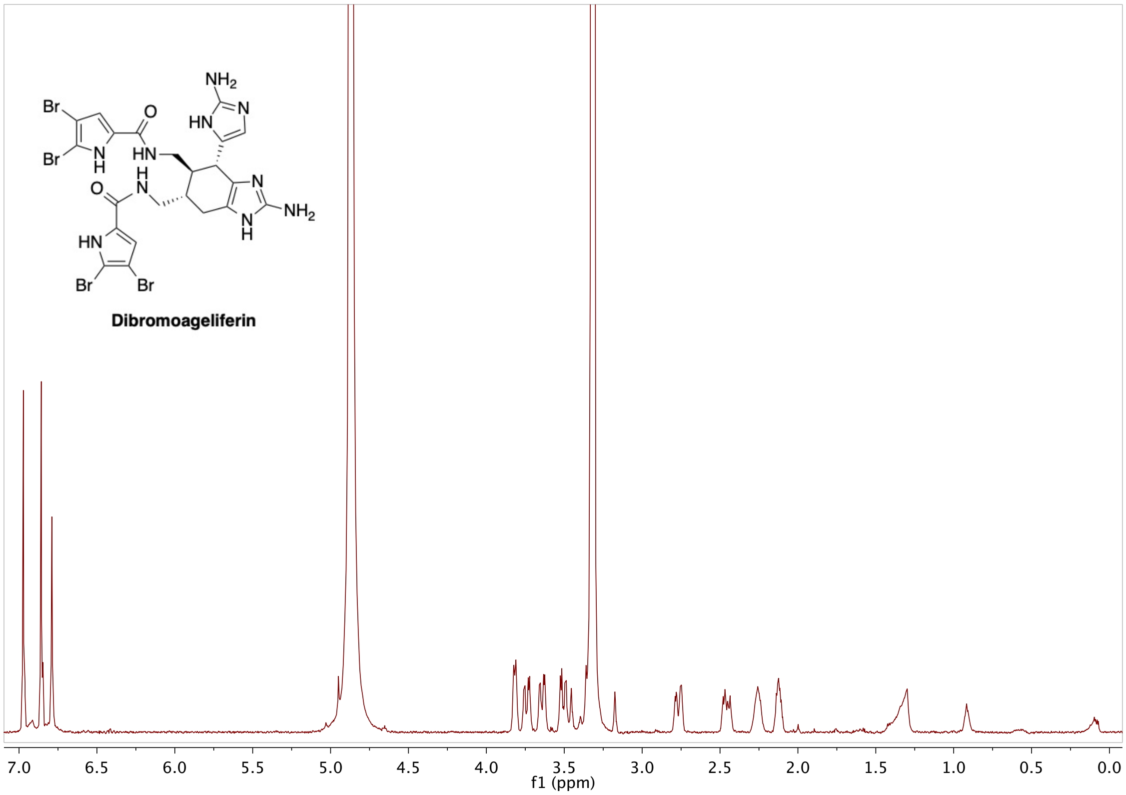


Figure S7. ^{1}H NMR spectrum of **3** (500 MHz, CD$_3$OD).

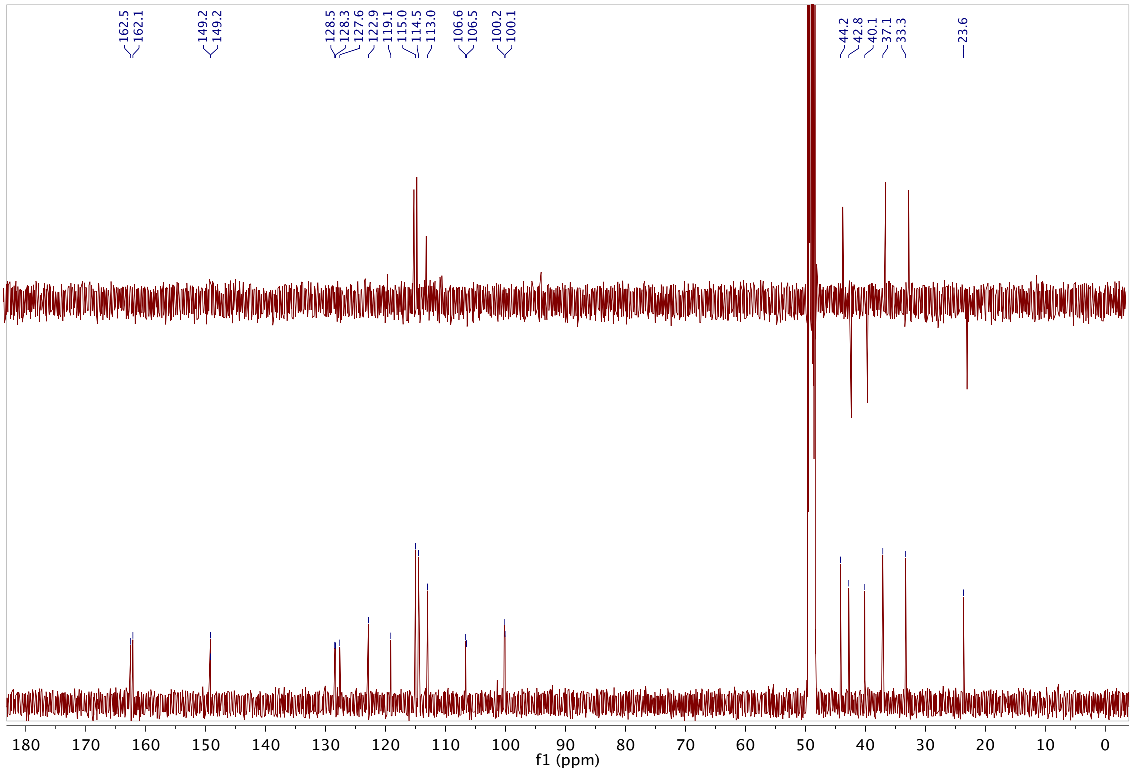
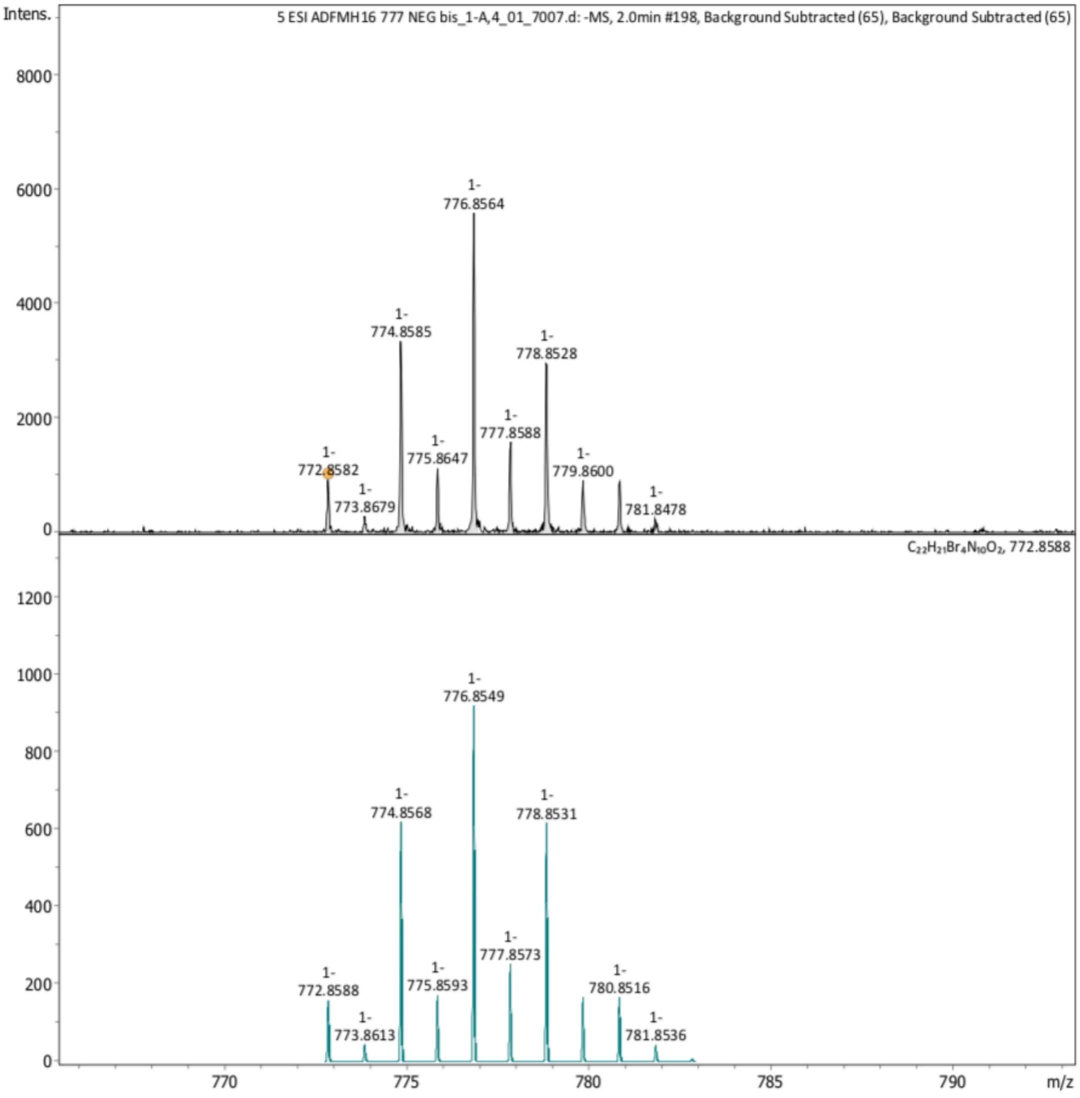


Figure S8. ^{13}C NMR and DEPT-135 spectra of **3** (125 MHz, CD$_3$OD).



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
772.8582	1	C20H19Br4N13O	94.77	772.8575	-0.7	-1.0	52.5	23.5	odd	ok
	2	C18H17Br4N16	39.54	772.8561	-2.1	-2.7	52.6	24.0	even	ok
	3	C22H21Br4N10O2	100.00	772.8588	0.6	0.8	52.8	23.0	even	ok
	4	C24H23Br4N7O3	42.17	772.8601	2.0	2.5	53.6	22.5	odd	ok
	5	C23H27Br4N3O7	95.59	772.8588	0.6	0.8	54.2	17.5	odd	ok

Figure S9. (-)-HRESIMS of **3**.

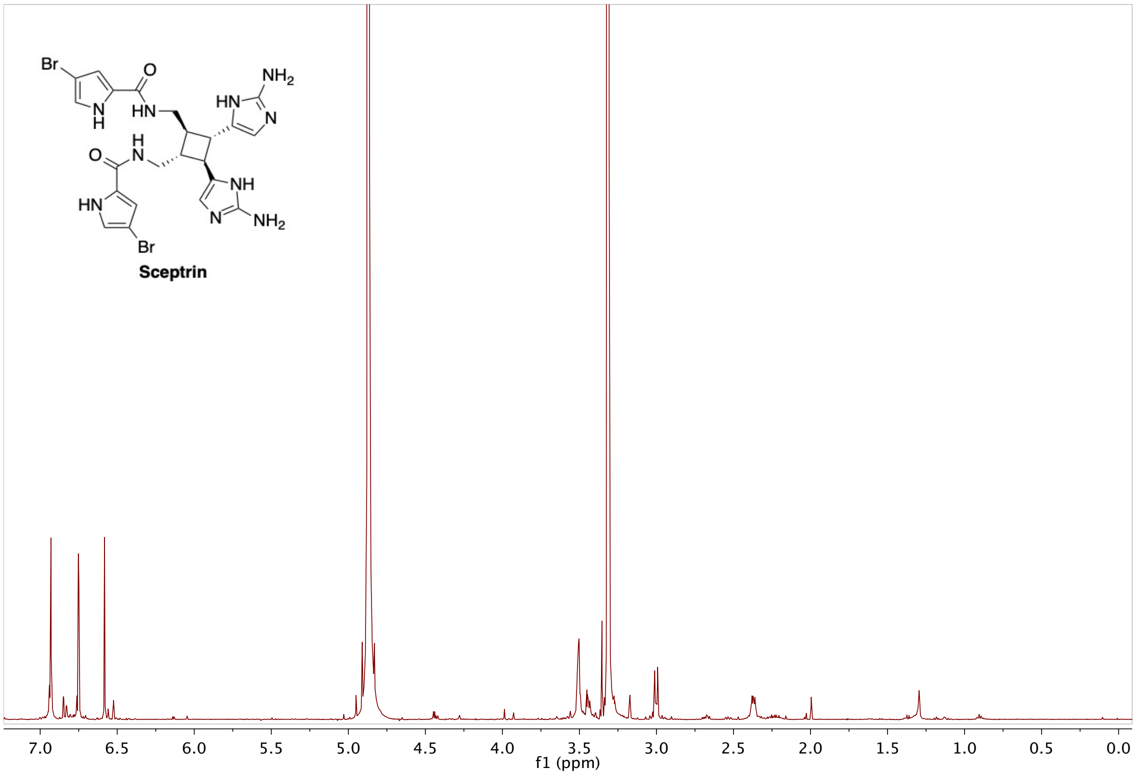


Figure S10. ^{1}H NMR spectrum of **4** (500 MHz, CD$_3$OD).

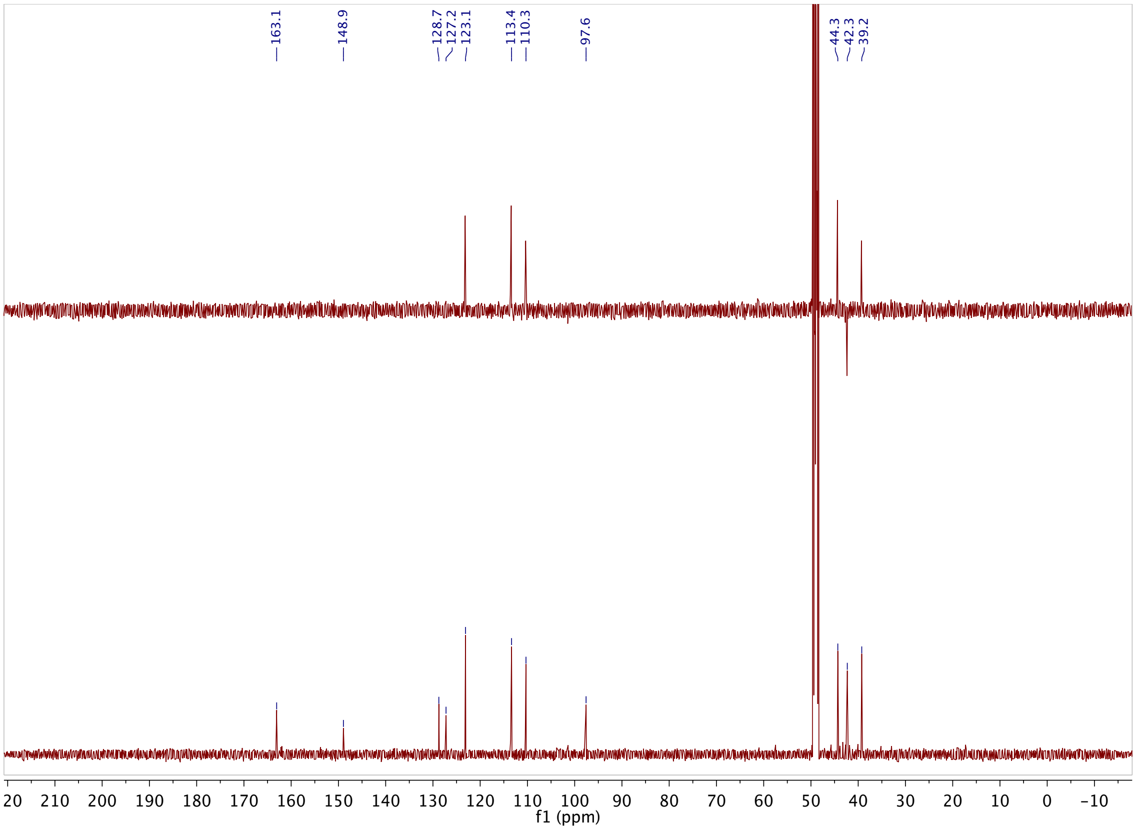
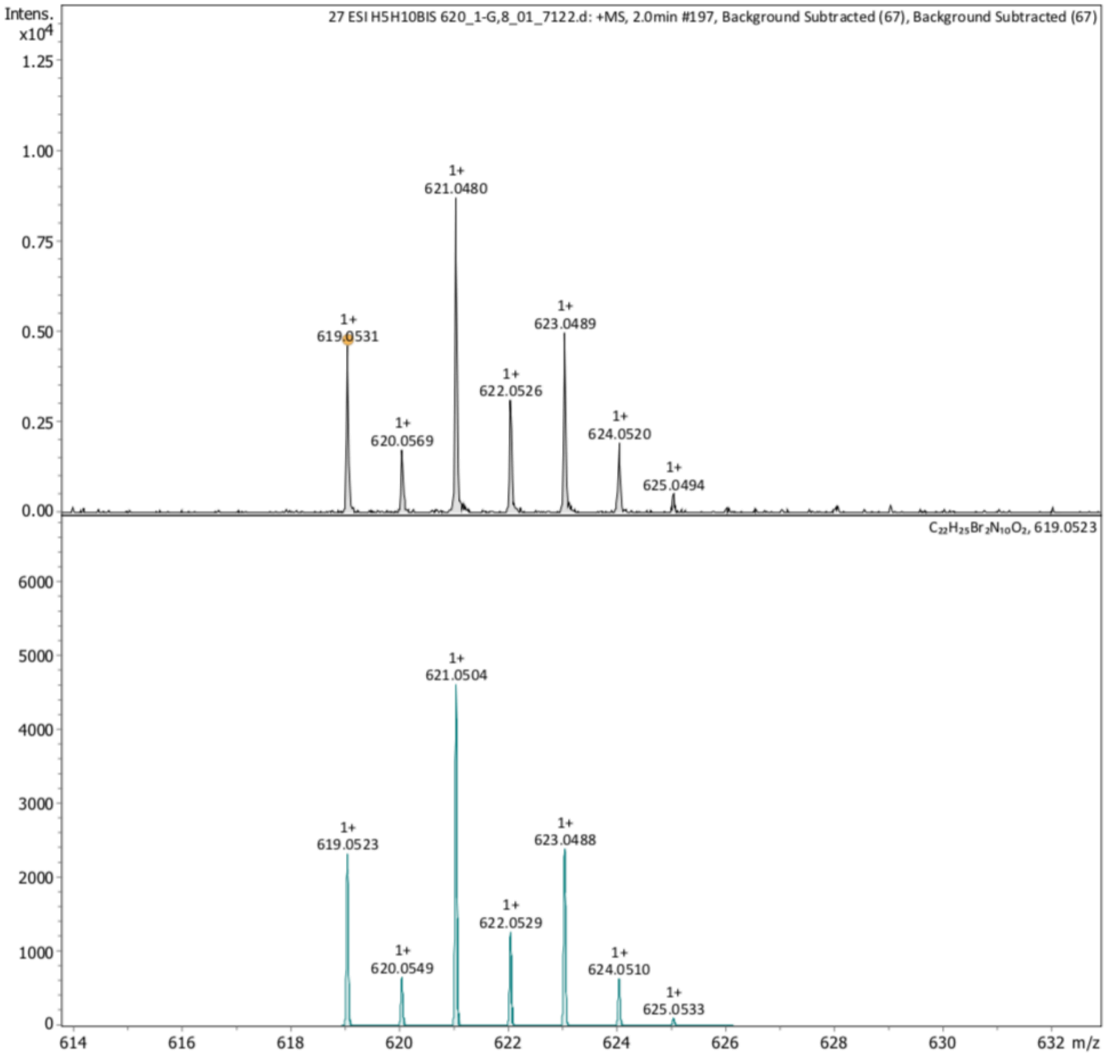


Figure S11. ^{13}C NMR and DEPT-135 spectra of **4** (125 MHz, CD$_3$OD).



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
619.0531	1	C26H29Br2N4O4	50.48	619.0550	1.9	3.1	47.1	18.0	even	ok
	2	C24H27Br2N7O3	100.00	619.0537	0.6	0.9	52.0	18.5	odd	ok
	3	C25H33Br2O8	89.48	619.0537	0.6	0.9	55.4	13.0	even	ok
	4	C22H25Br2N10O2	77.93	619.0523	-0.8	-1.2	56.9	19.0	even	ok
	5	C23H31Br2N3O7	69.50	619.0523	-0.8	-1.2	60.4	13.5	odd	ok

Figure S12. (+)-HRESIMS of **4**.

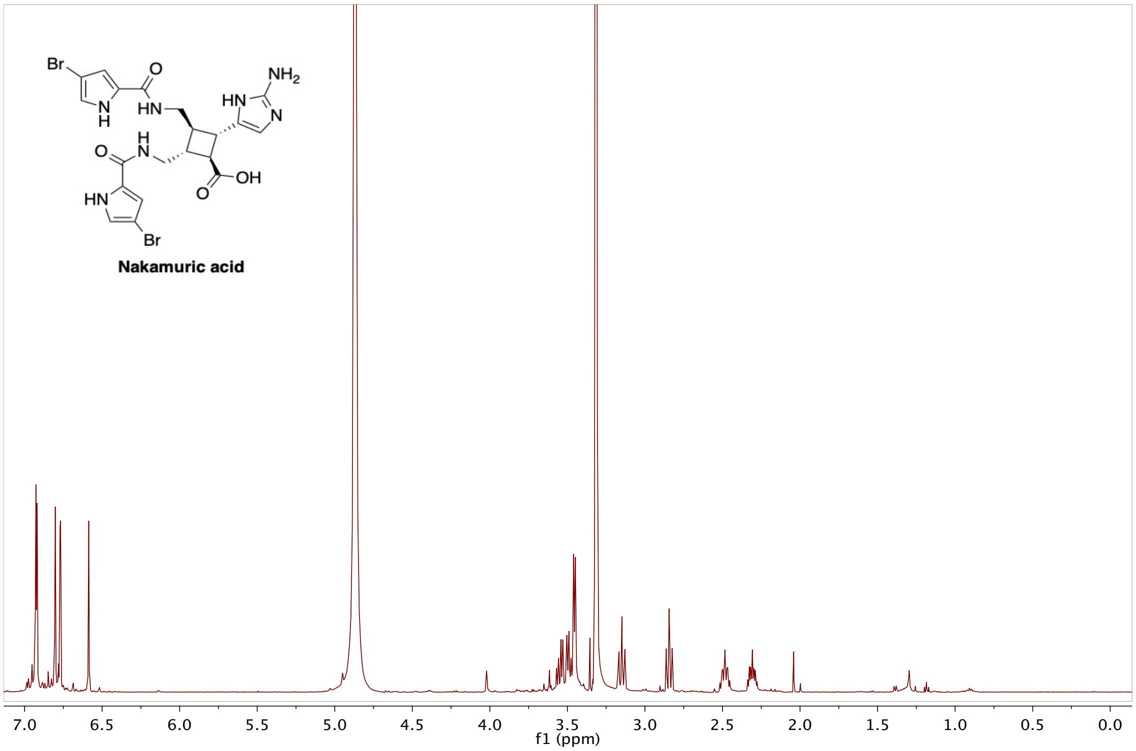


Figure S13. ^{1}H NMR spectrum of **5** (500 MHz, CD_3OD).

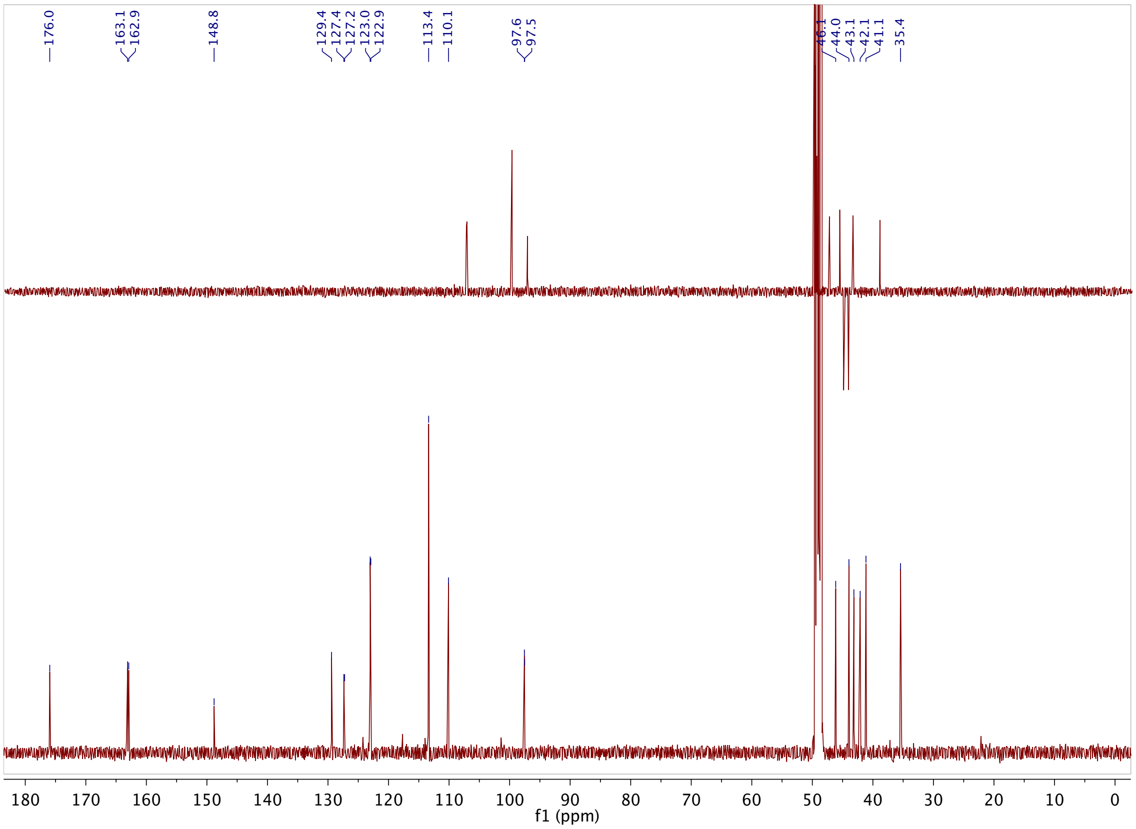
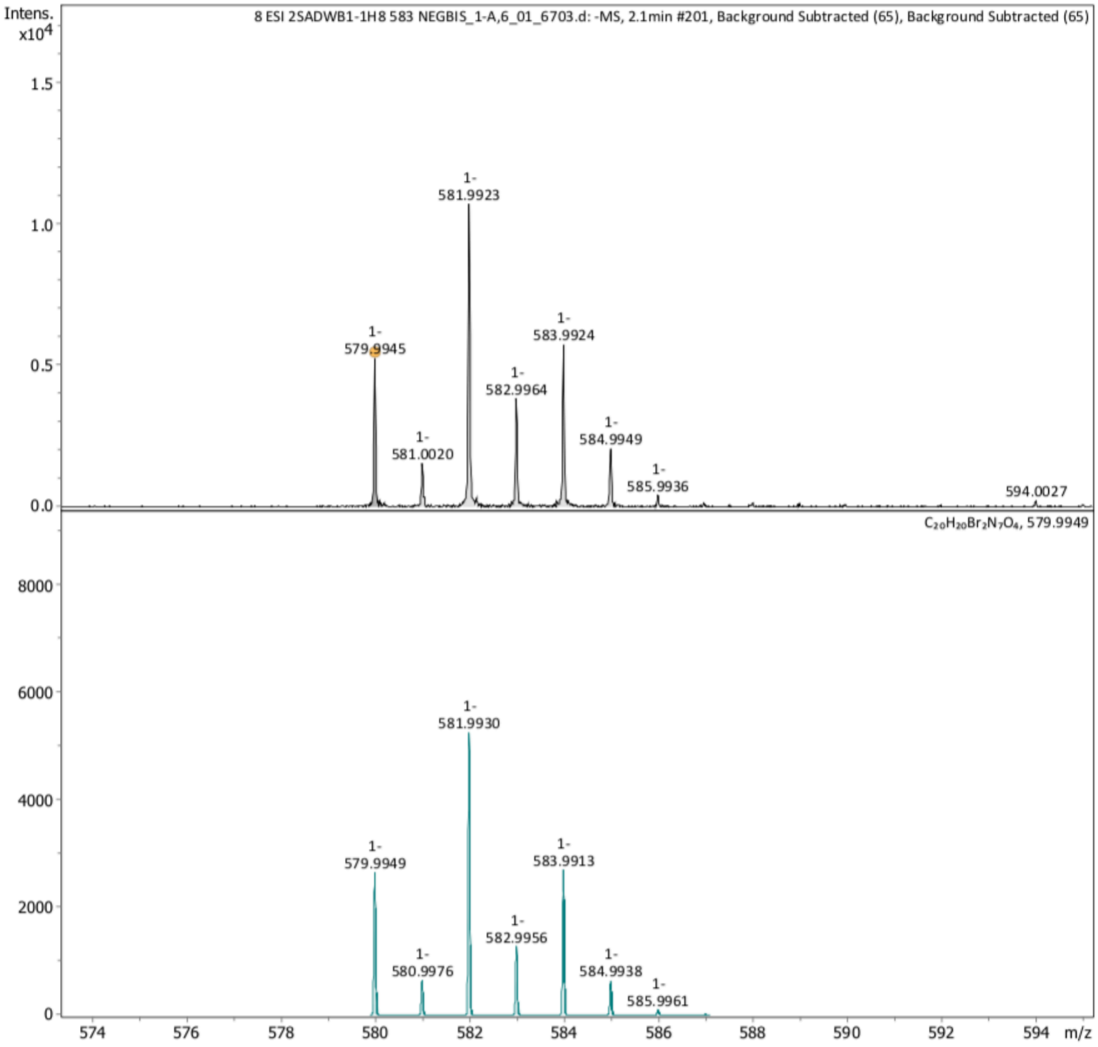


Figure S14. ^{13}C NMR and DEPT-135 spectra of **5** (125 MHz, CD_3OD).



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
579.9945	1	C20H20Br2N7O4	100.00	579.9949	0.4	0.6	52.2	17.0	even	ok
	2	C21H26Br2O9	86.64	579.9949	0.4	0.6	56.6	11.5	odd	ok
	3	C18H18Br2N10O3	61.72	579.9936	-1.0	-1.7	57.4	17.5	odd	ok
	4	C19H24Br2N3O8	53.34	579.9936	-1.0	-1.7	61.8	12.0	even	ok

Figure S15. (-)-HRESIMS of **5**.

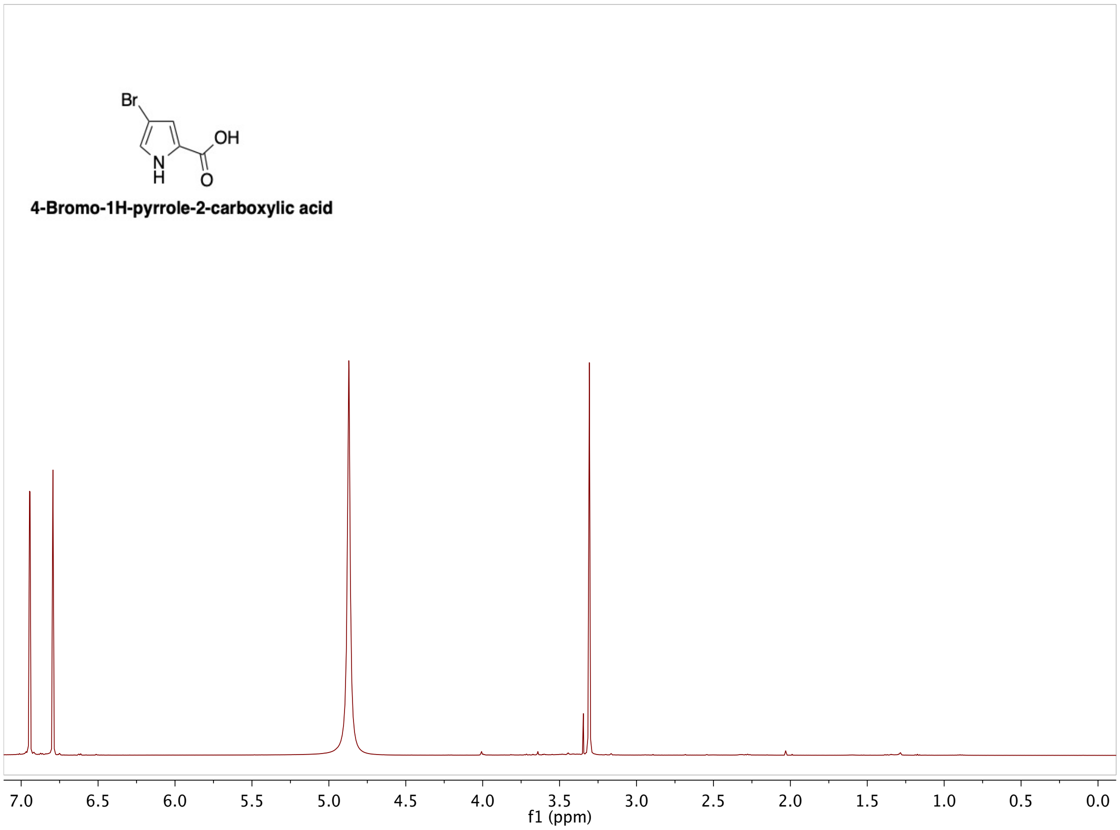


Figure S16. ^{1}H NMR spectrum of **6** (500 MHz, CD_3OD).

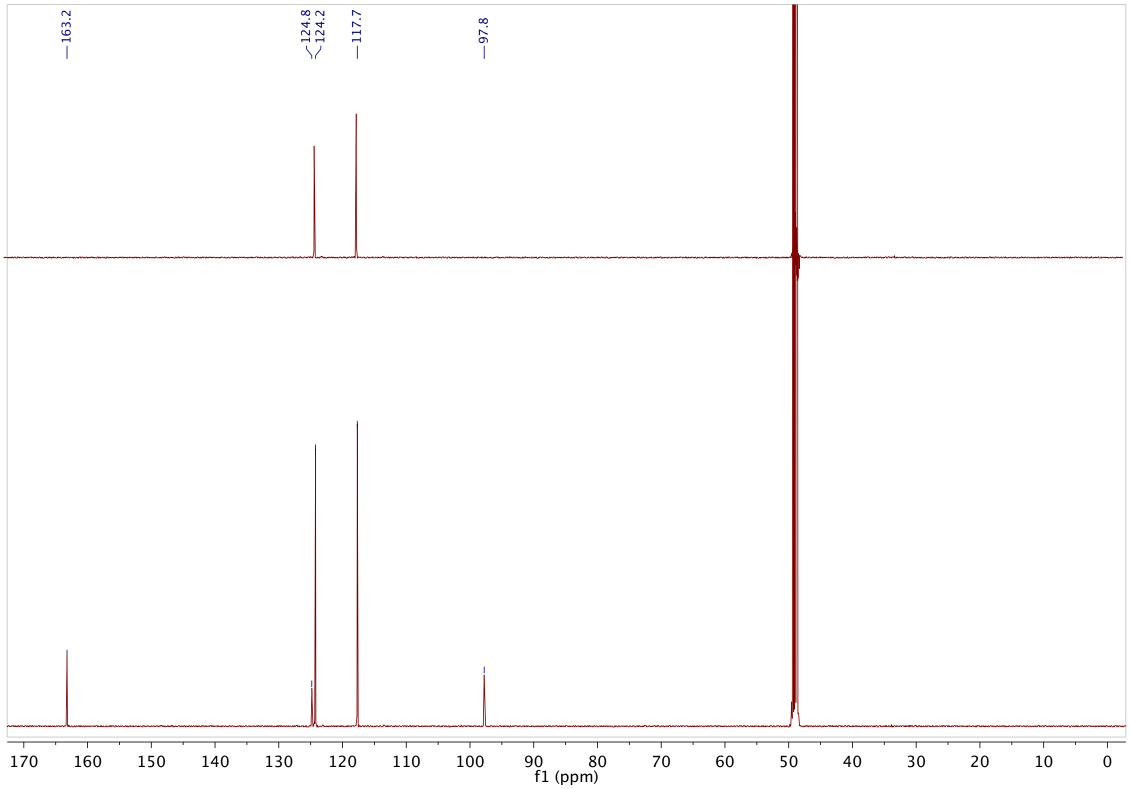
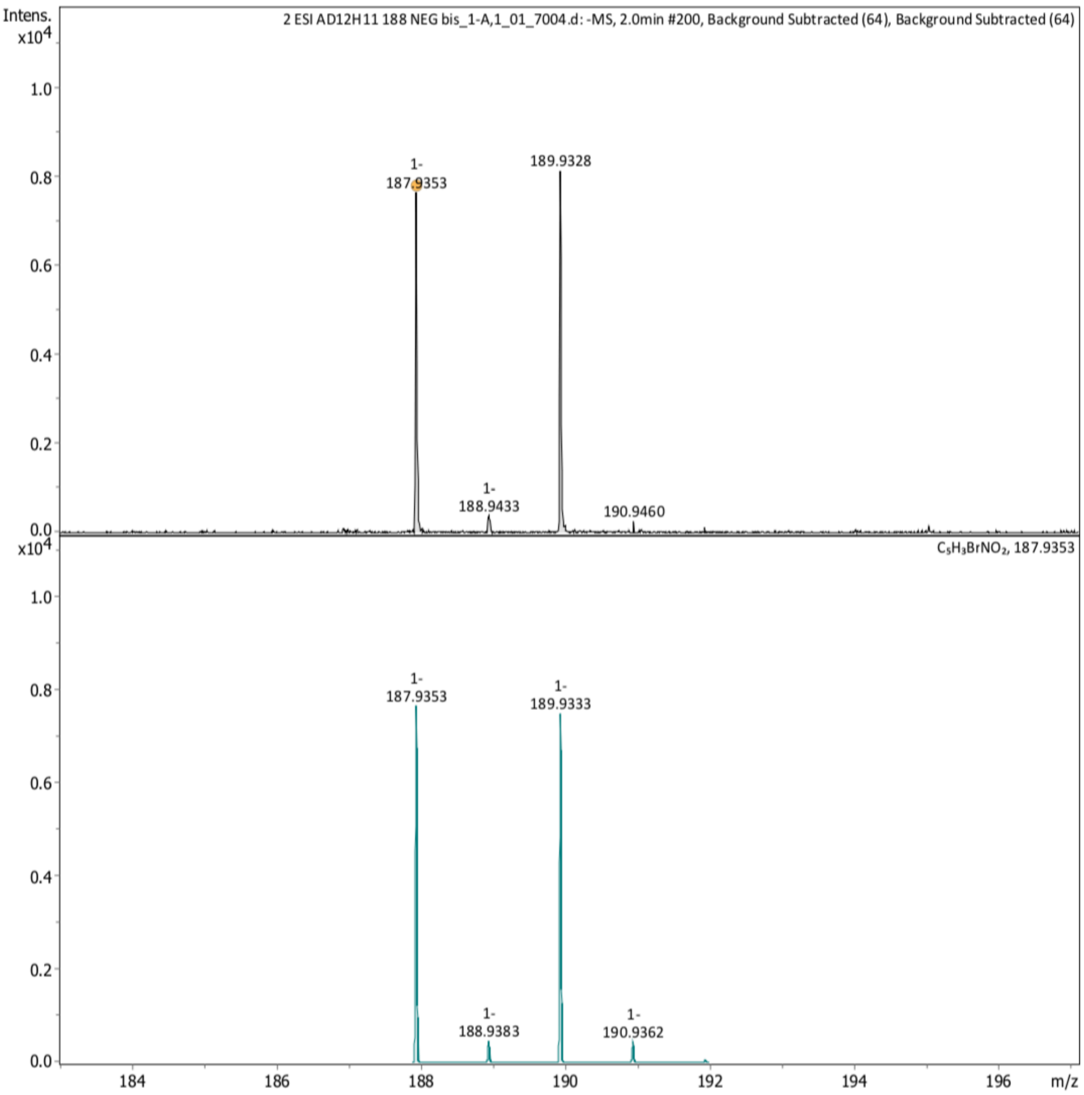


Figure S17. ^{13}C NMR and DEPT-135 spectra of compound **6** (125 MHz, CD_3OD).



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e^- Conf	N-Rule
187.9353	1	C5H3BrNO2	100.00	187.9353	-0.0	-0.3	34.9	6.0	even	ok

Figure S18. (-)-HRESIMS of **6**.

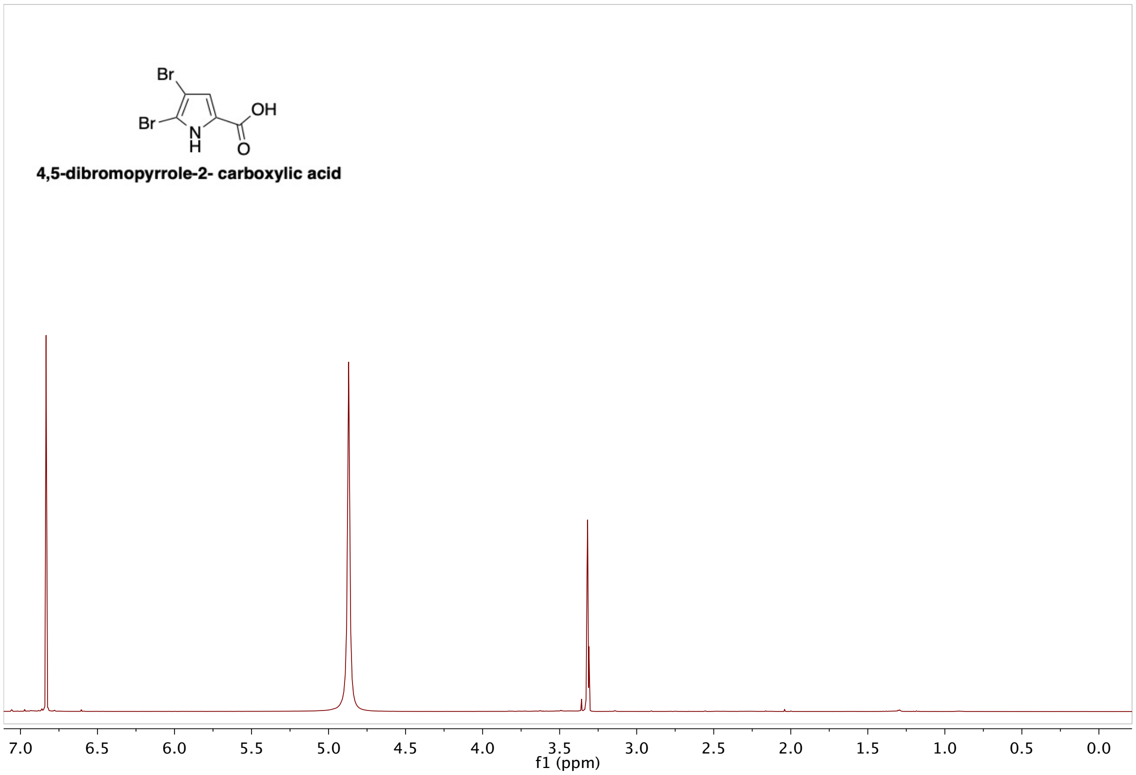


Figure S19. ^{1}H NMR spectrum of **7** (500 MHz, CD_3OD).

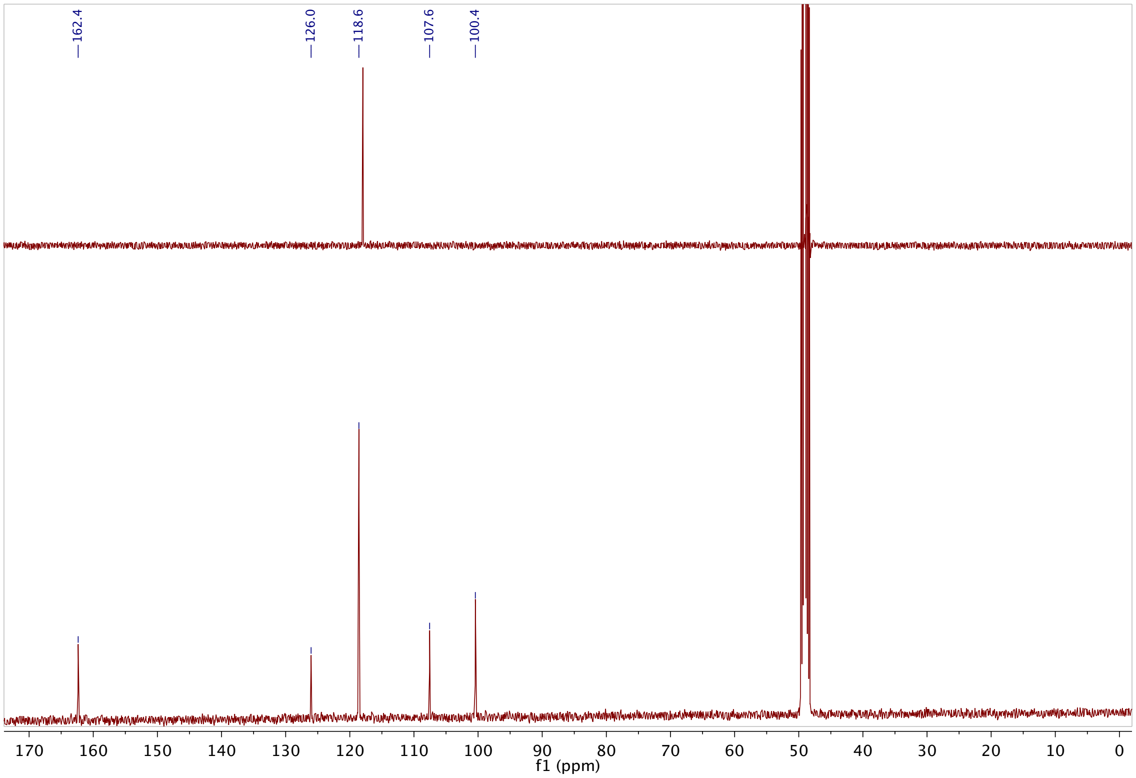
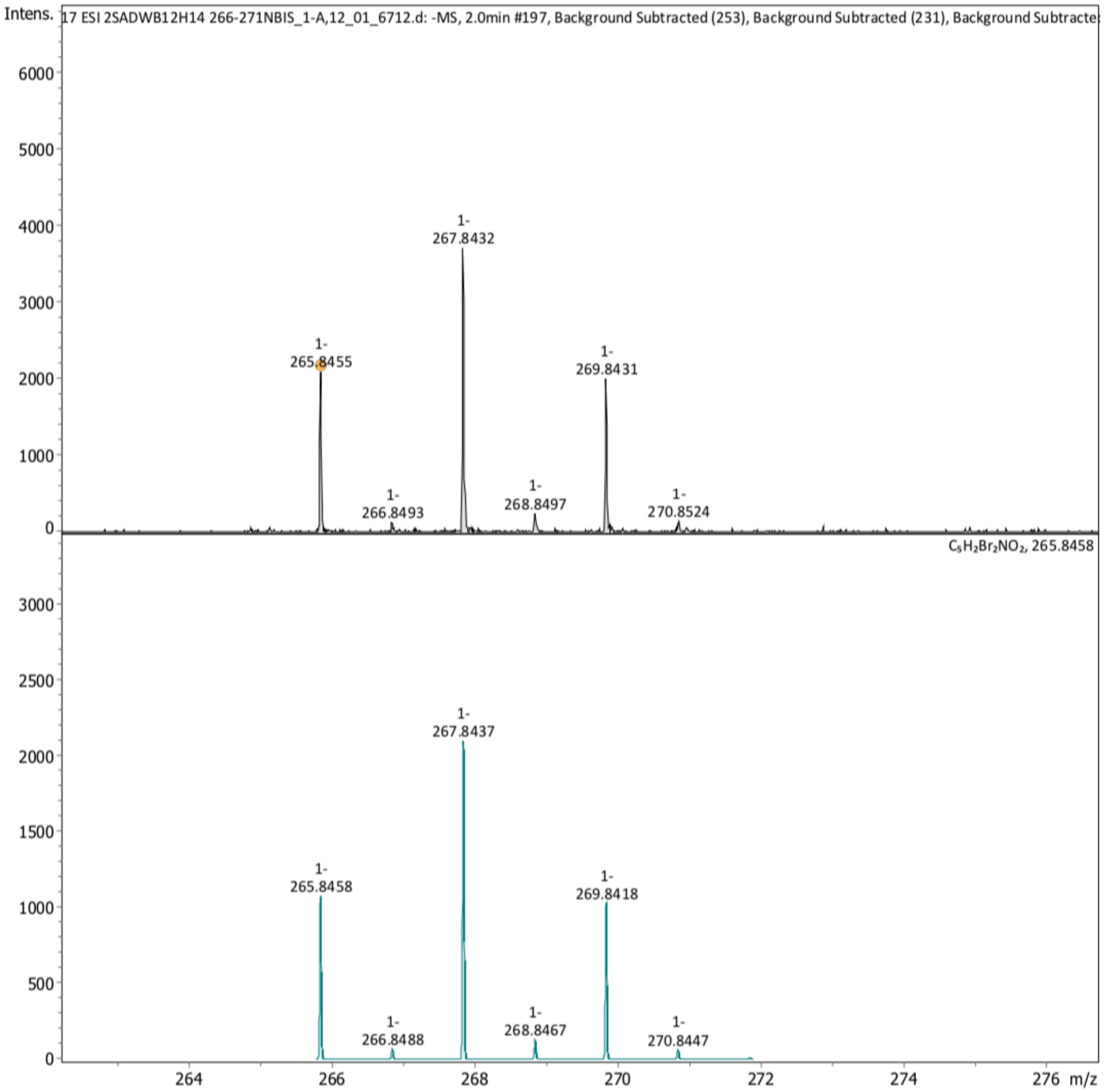


Figure S20. ^{13}C NMR and DEPT-135 spectra of **7** (125 MHz, CD_3OD).



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e$^-$ Conf	N-Rule
265.8455	1	C5H2Br2NO2	100.00	265.8458	0.2	0.9	28.7	8.0	even	ok

Figure S21. (-)-HRESIMS of **7**.

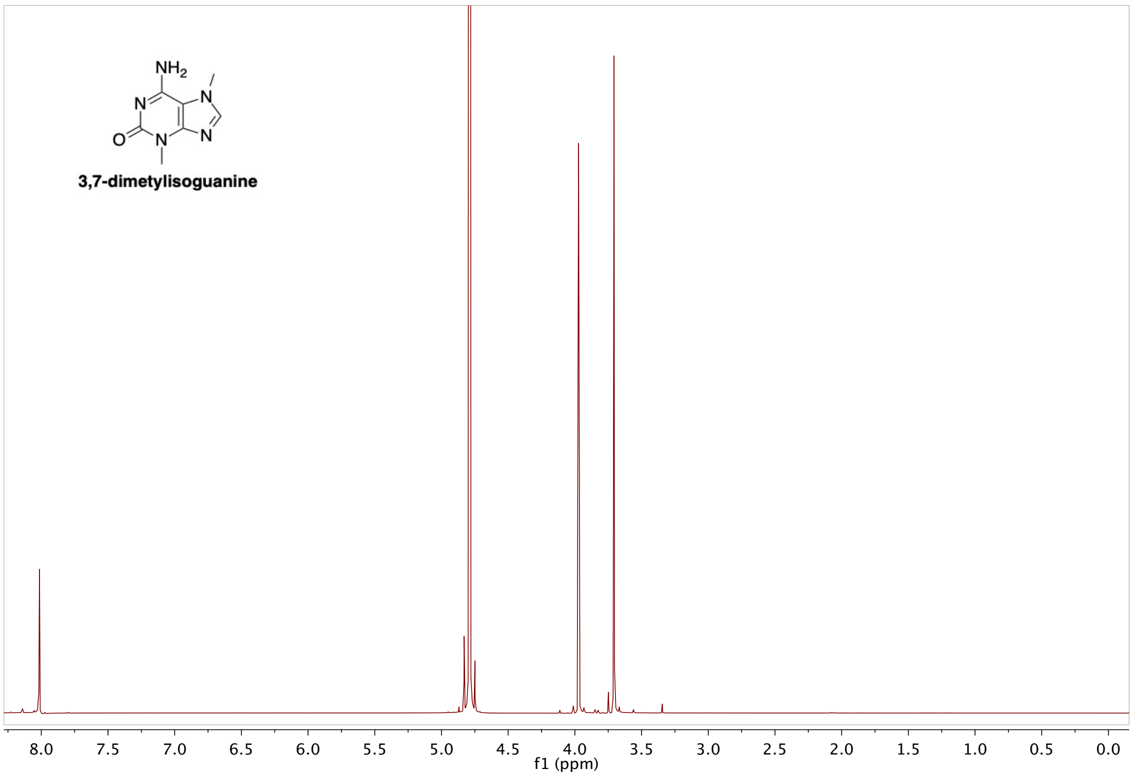


Figure S22. ^{1}H NMR spectrum of **8** (500 MHz, D_2O).

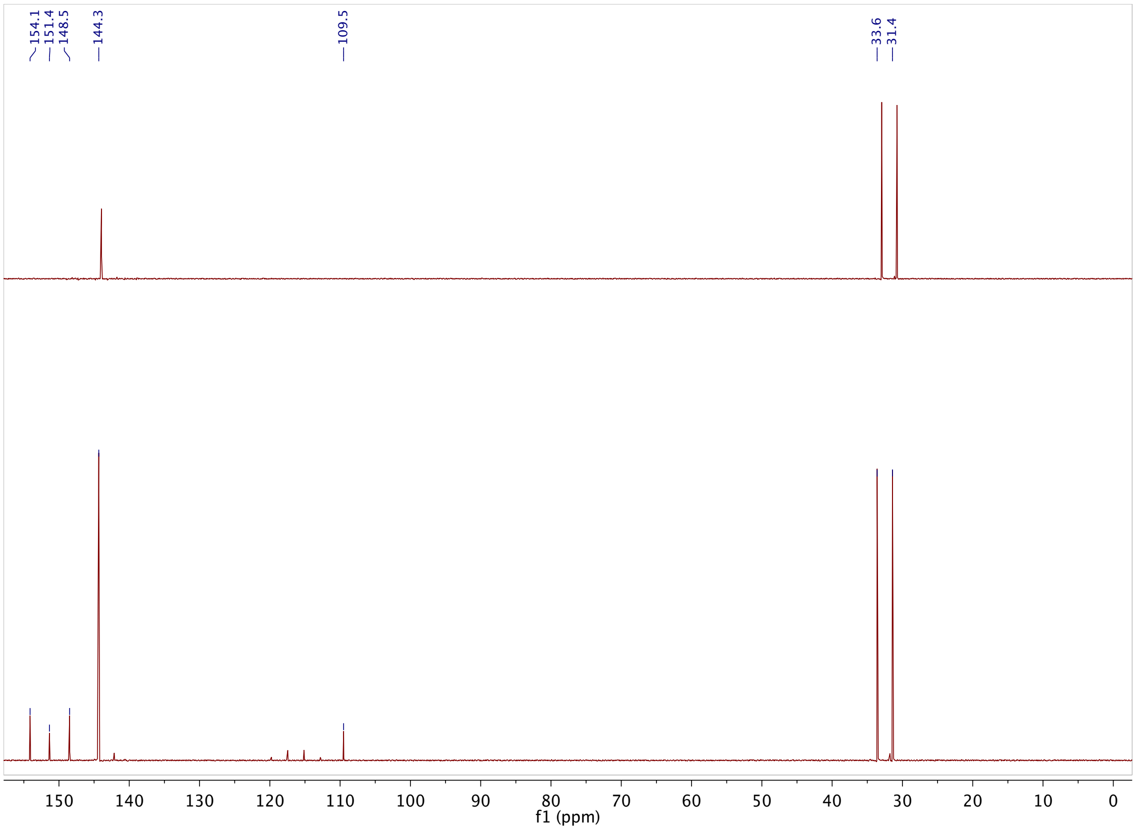
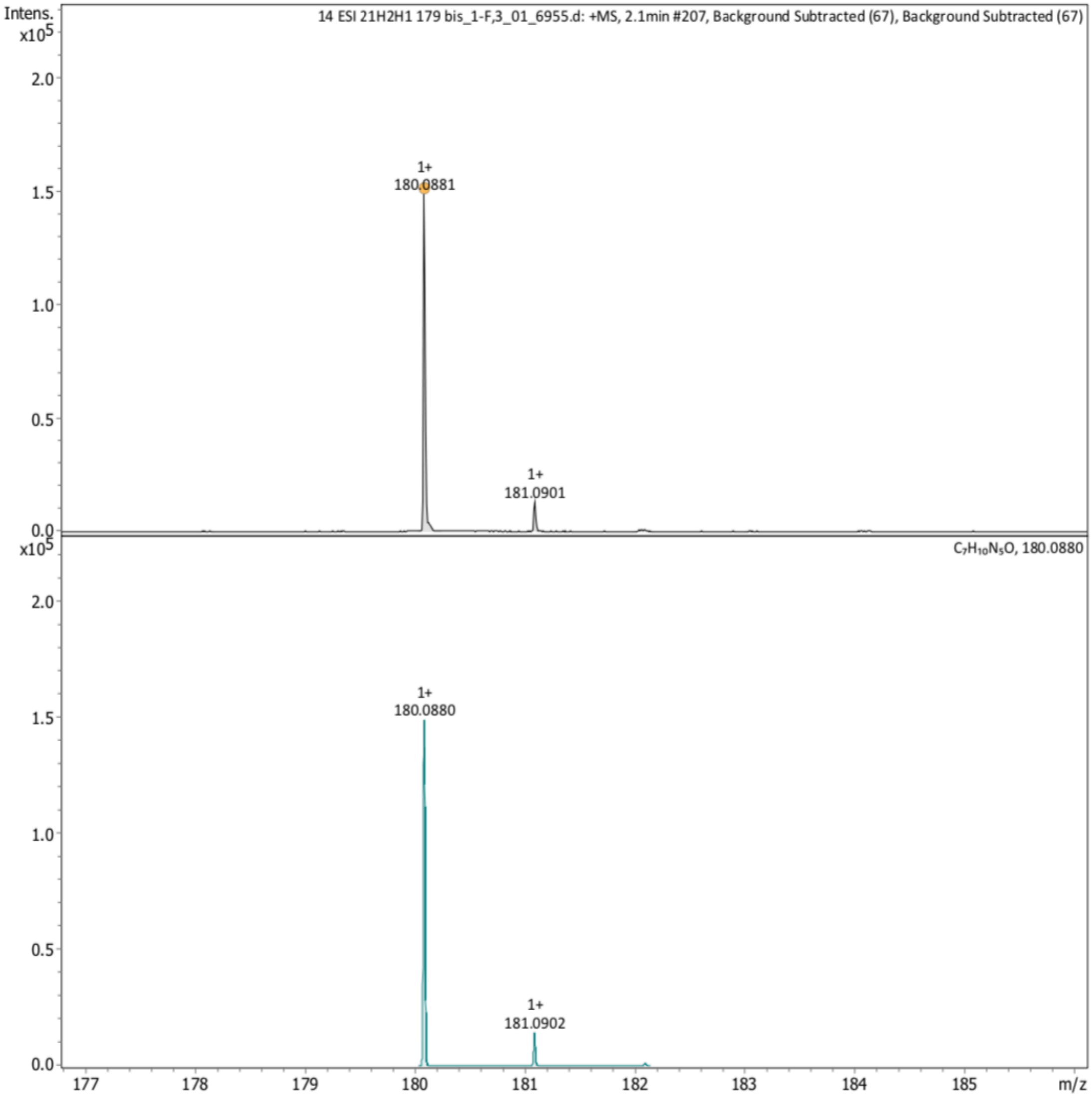


Figure S23. ^{13}C NMR and DEPT-135 spectra of **8** (125 MHz, D_2O).



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e^- Conf	N-Rule
180.0881	1	C7H10N5O	100.00	180.0880	-0.1	-0.7	6.1	6.0	even	ok

Figure S24. (+)-HRESIMS of **8**.