Supporting Information

Antimicrobial Benzyltetrahydroisoquinoline-Derived Alkaloids from the Leaves of *Doryphora aromatica*

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Table S1. Stable conformers of (*R*)-nomimantharine trifluoroacetate (**2**)

Spectroscopic data of phaeantharine trifluoroacetate (**1**)

*Phaeantharine trifluoroacetate (**1**):* bright yellow solid; UV (MeOH) λ_{max} (log ε) 199 nm (1.43), 229 nm (2.24), 256 nm (4.08), 316 nm (0.85); ^{1}H NMR (800 MHz, DMSO-d_6) and ^{13}C NMR data (200 MHz, DMSO-d_6), Tables 1 and 2; (+)-HRESIMS *m/z* 316.143891 [M − $2CF_3COO^-$]$^{2+}$ (calcd for $C_{39}H_{40}N_2O_6^{2+}$, 316.143770), *m/z* 631.2813 [M − $2CF_3COO^-$ − H]$^+$ (calcd for $C_{39}H_{39}N_2O_6^+$, 631.2802).

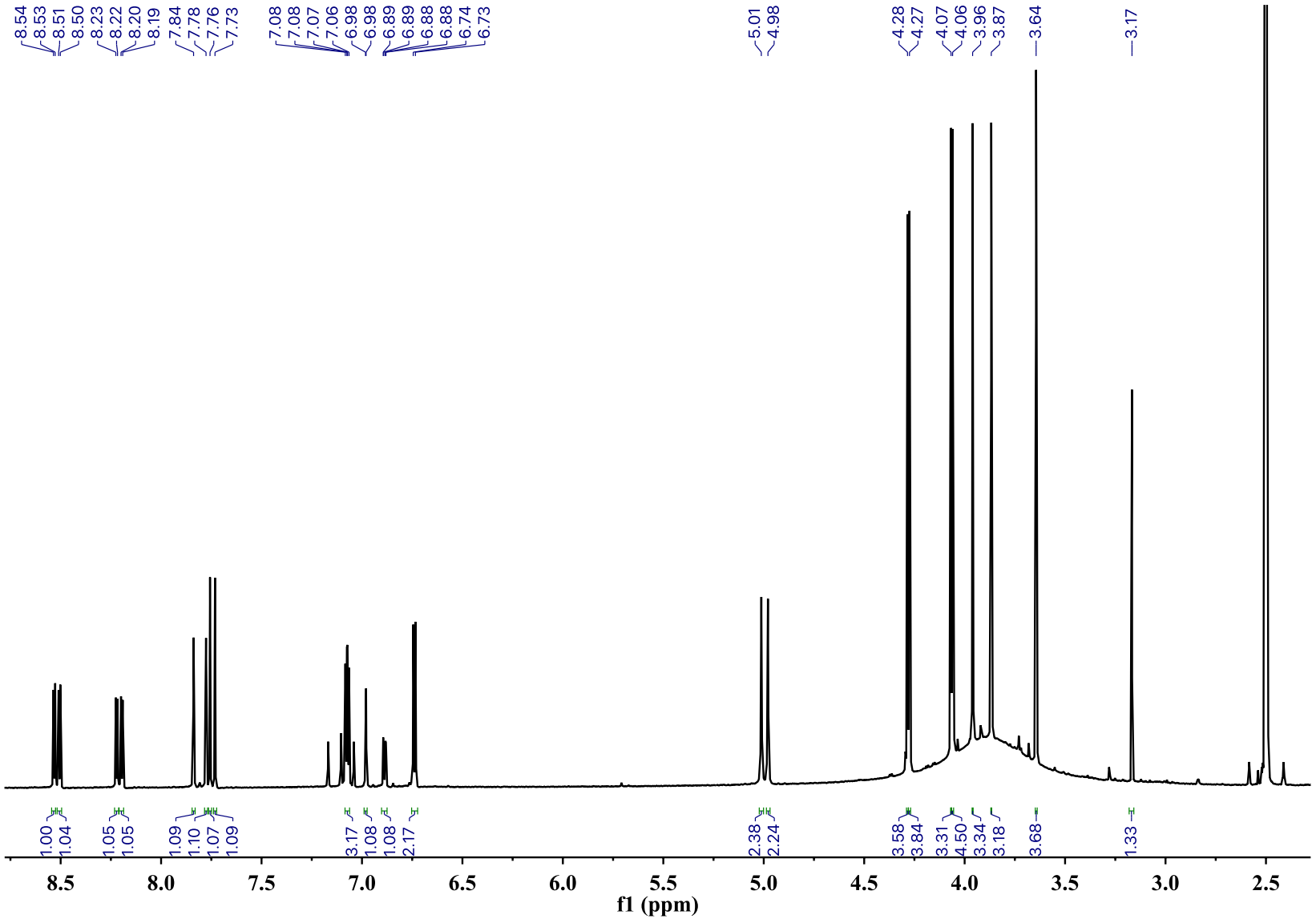


Figure S1. ^{1}H NMR spectrum of phaeantharine trifluoroacetate (**1**)

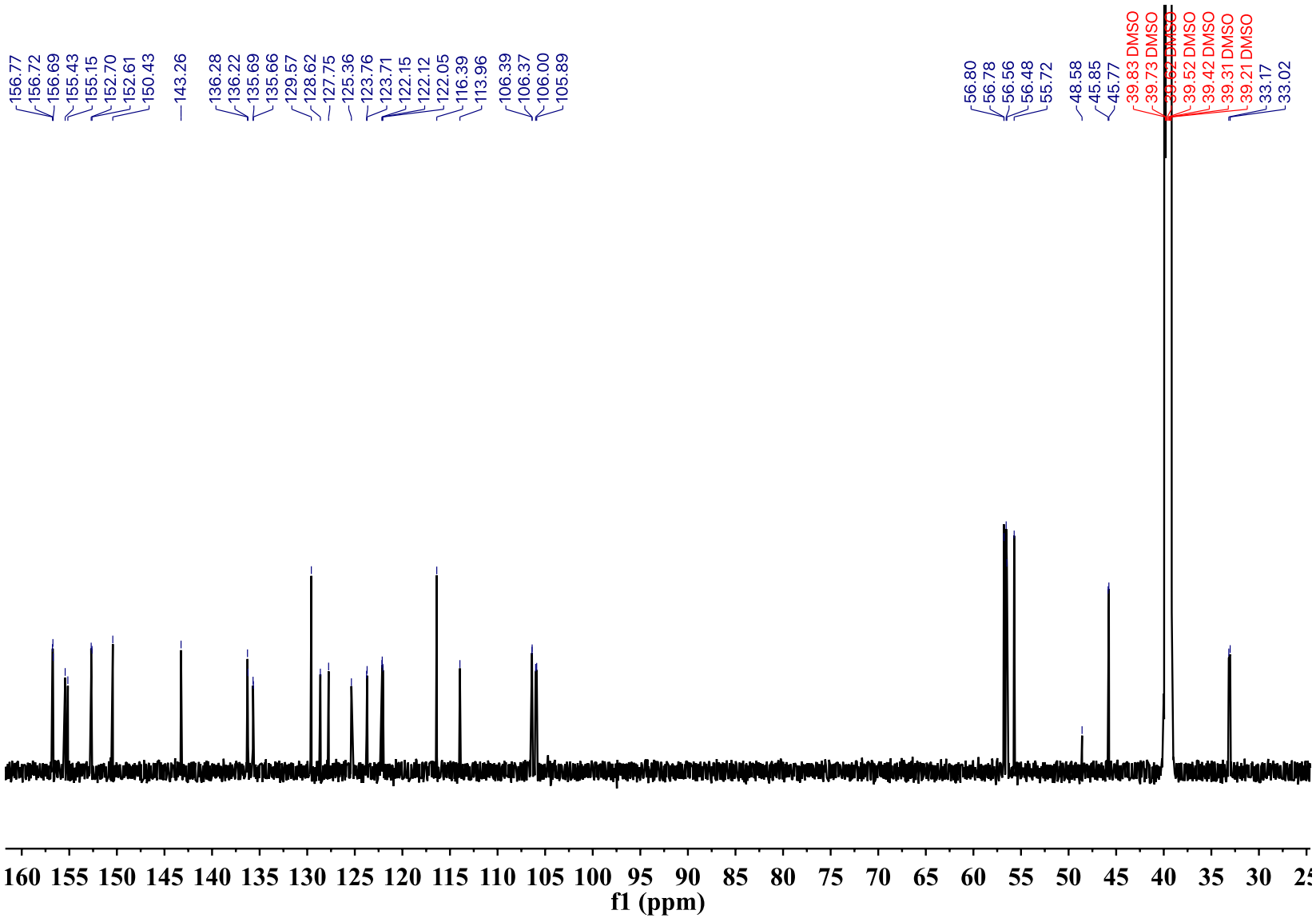


Figure S2. ^{13}C NMR spectrum of phaeantharine trifluoroacetate (**1**)

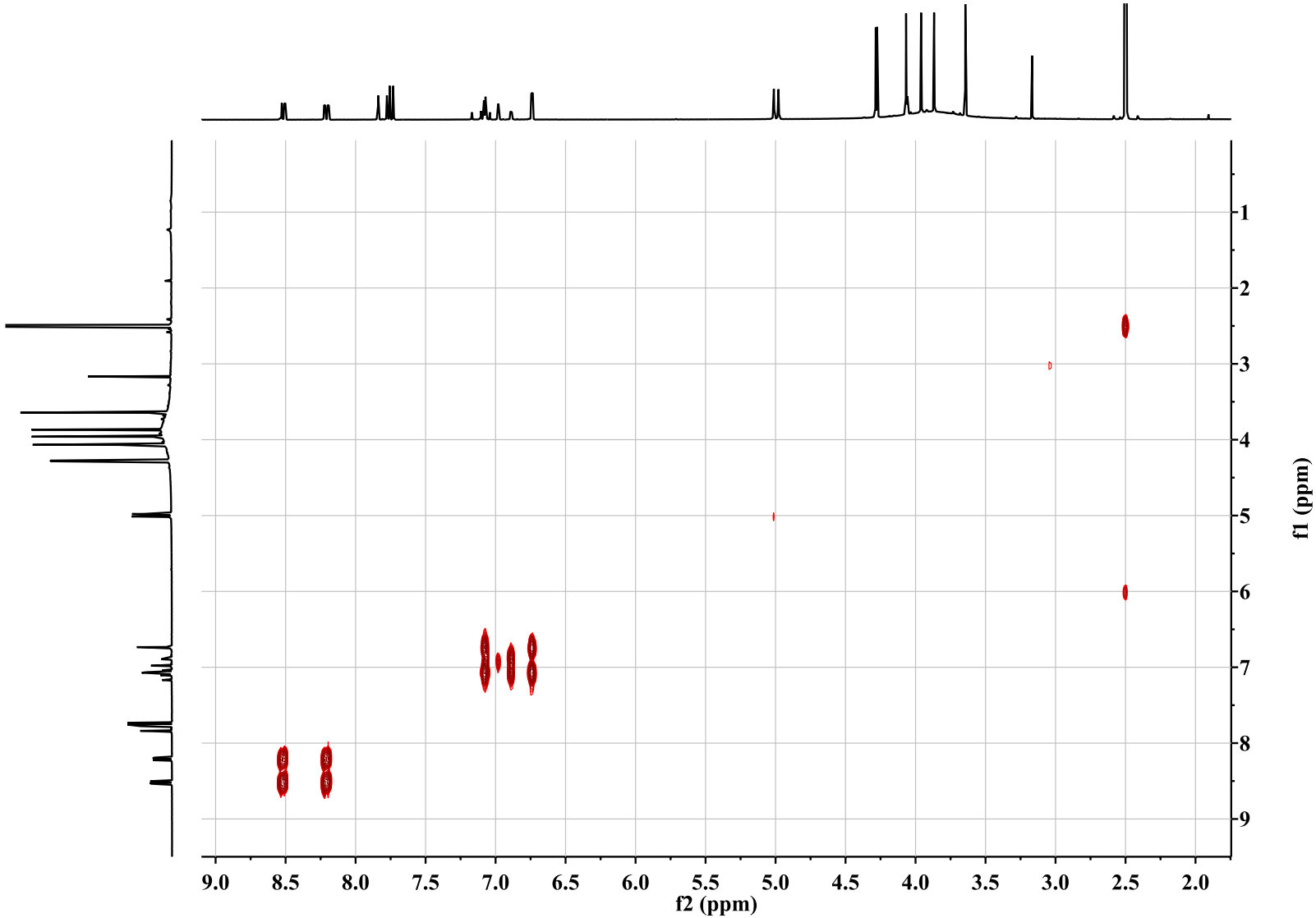


Figure S3. COSY NMR spectrum of phaeantharine trifluoroacetate (**1**)

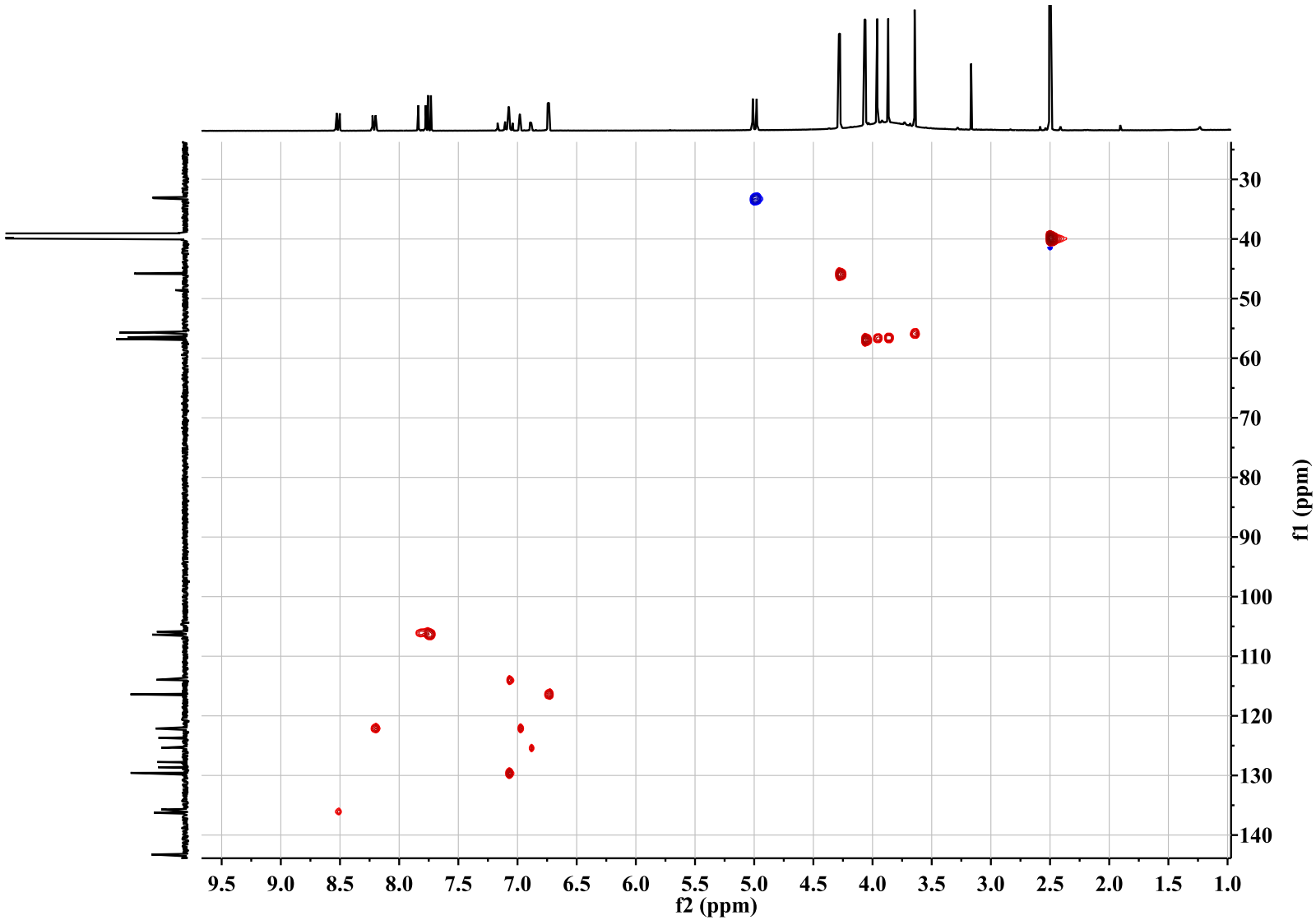


Figure S4. HSQC NMR spectrum of phaeantharine trifluoroacetate (**1**)

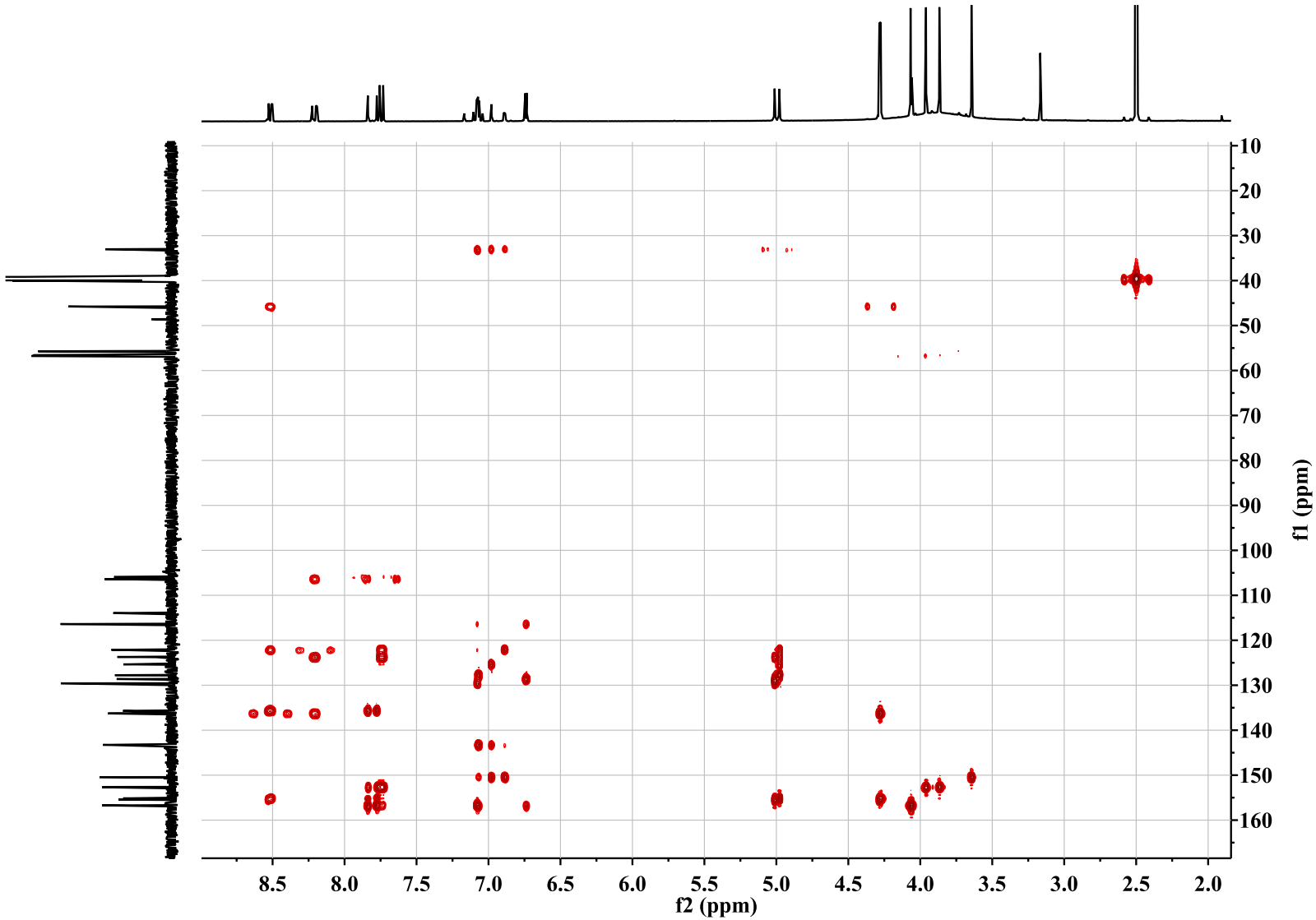
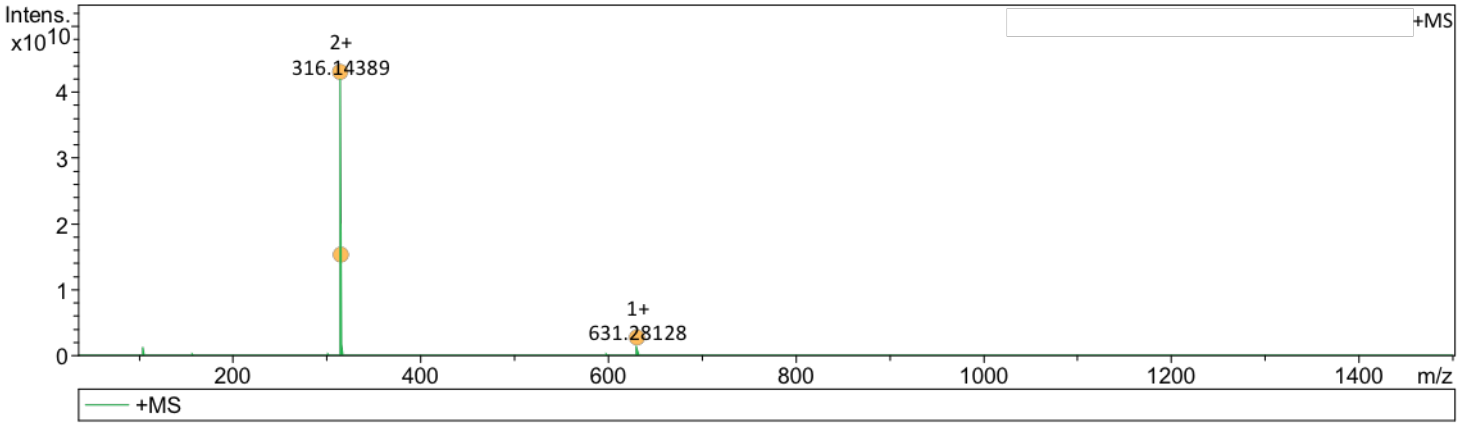


Figure S5. HMBC NMR spectrum of phaeantharine trifluoroacetate (**1**)



Means. m/z	Ion formula	calc. m/z	err [ppm]	rdb	e⁻Conf	N-Rule
316.143891	$C_{39}H_{40}N_2O_6$	316.143770	-0.4	22.0	even	ok
631.281278	$C_{39}H_{39}N_2O_6$	631.280263	-1.6	22.0	even	ok

Figure S6. HRMS spectrum of trifluoroacetate phaeantharine (**1**)

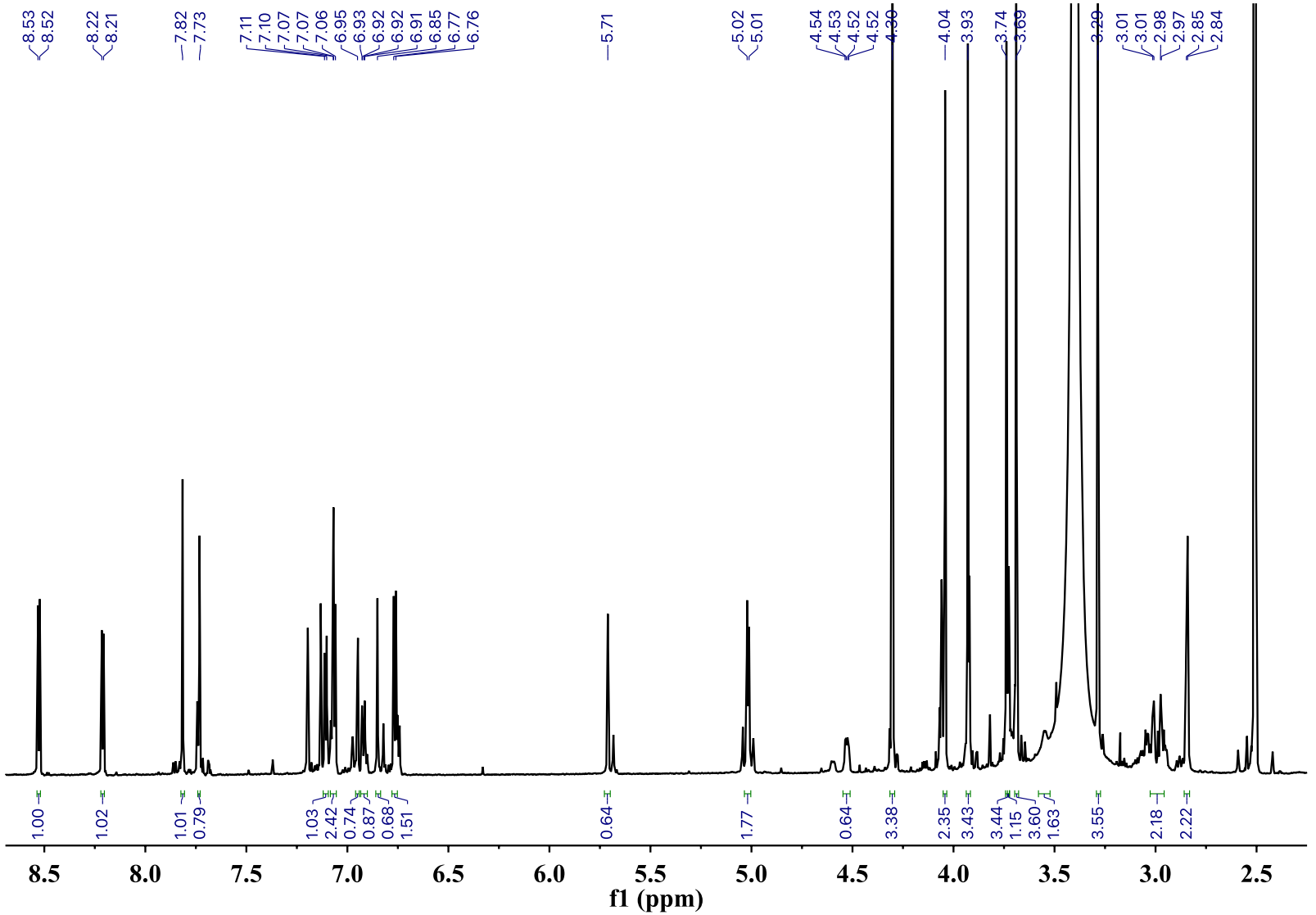


Figure S7. ^{1}H NMR spectrum of (*R*)-nomimantharine trifluoroacetate (**2**)

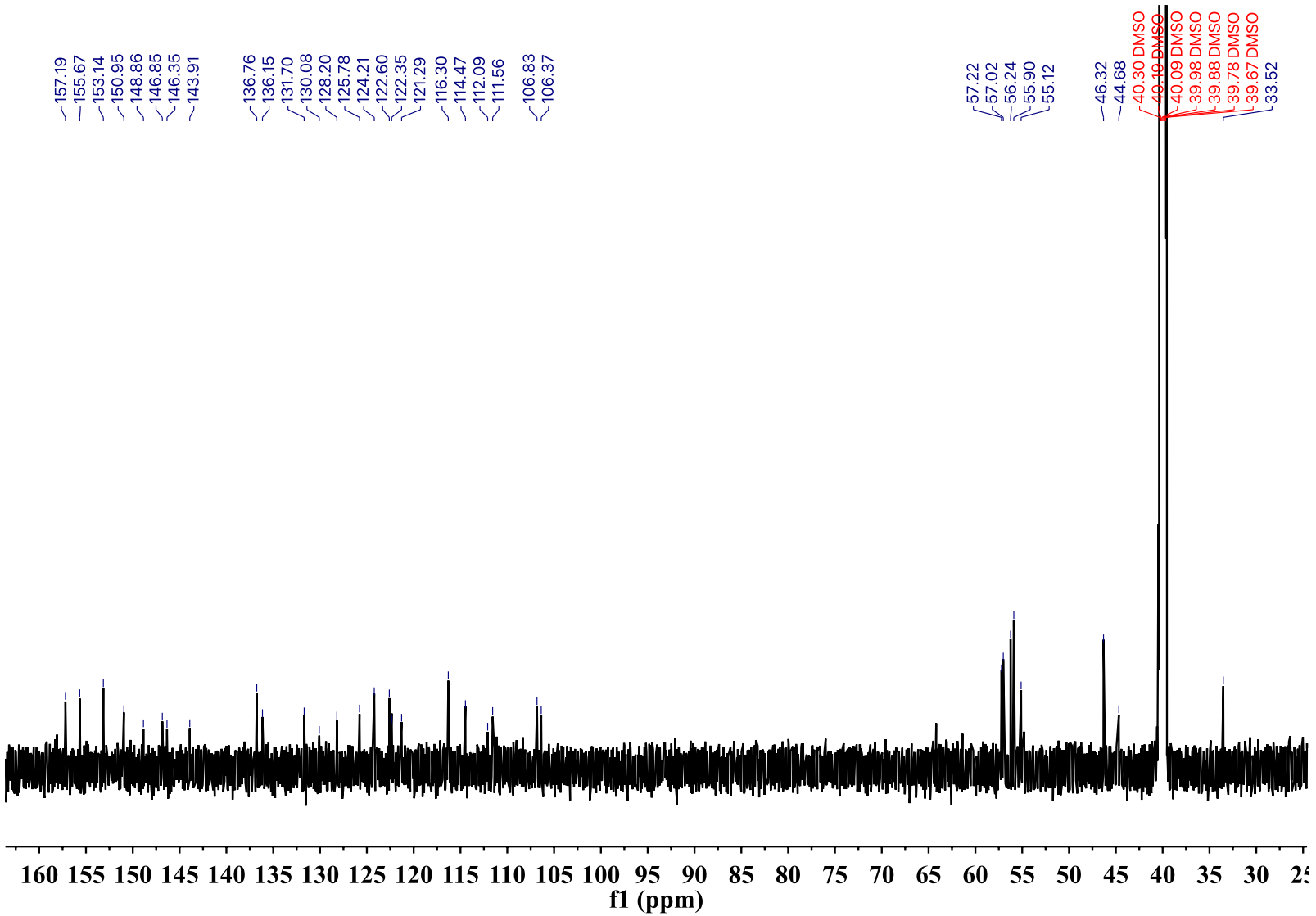


Figure S8. ^{13}C NMR spectrum of (*R*)-nomimantharine trifluoroacetate (**2**)

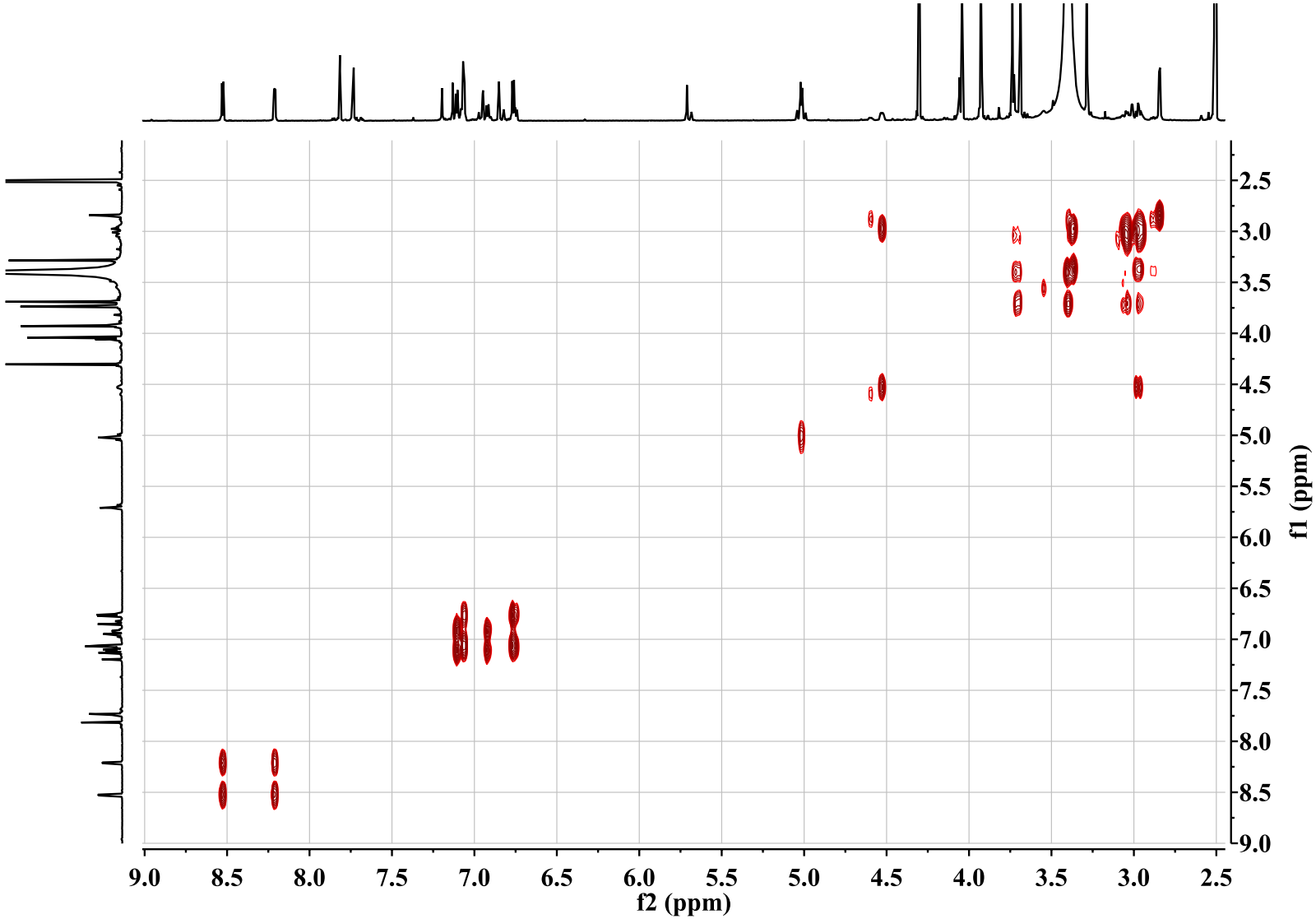


Figure S9. COSY NMR spectrum of (*R*)-nomimantharine trifluoroacetate (**2**)

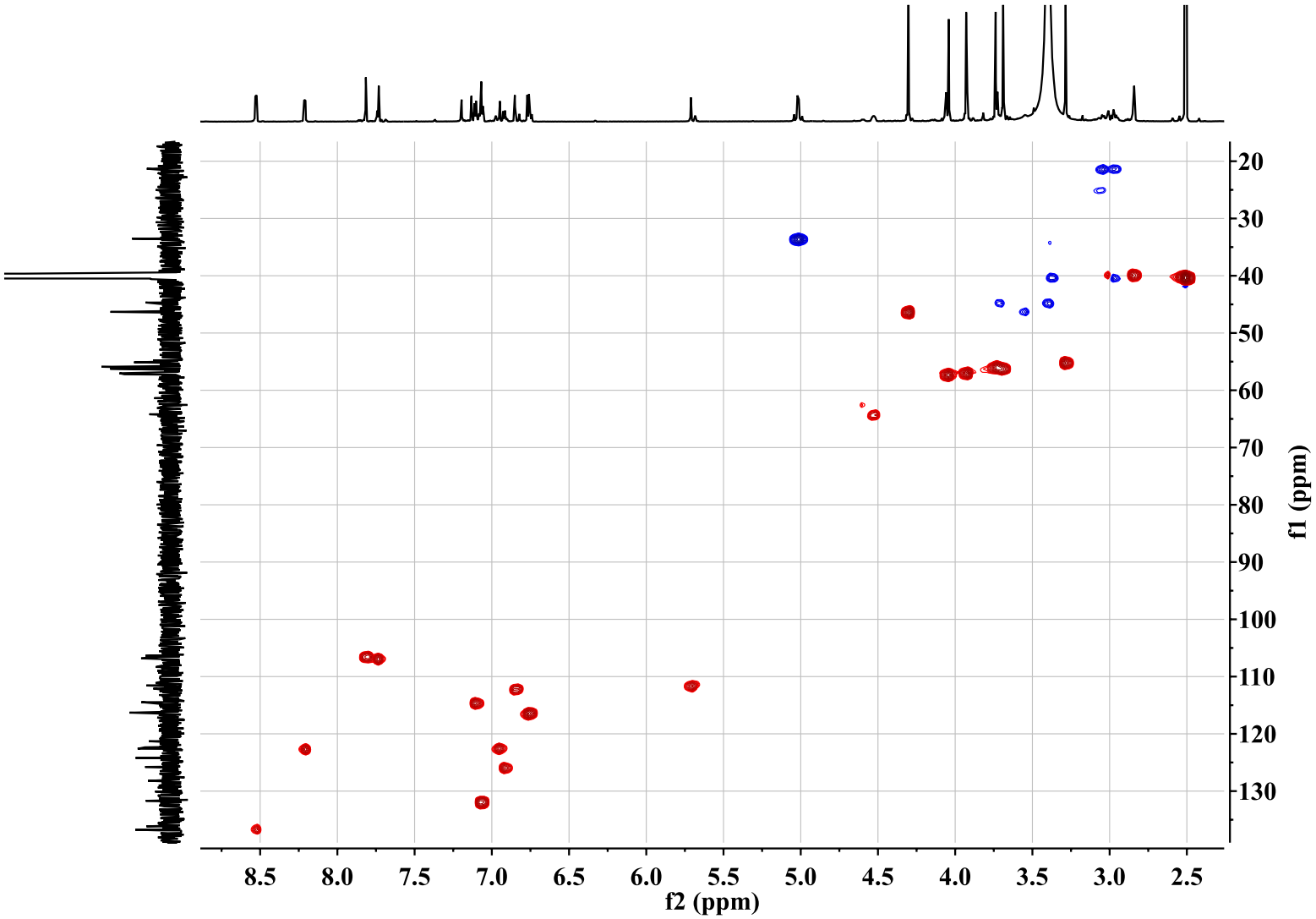


Figure S10. HSQC NMR spectrum of (*R*)-nomimantharine trifluoroacetate (**2**)

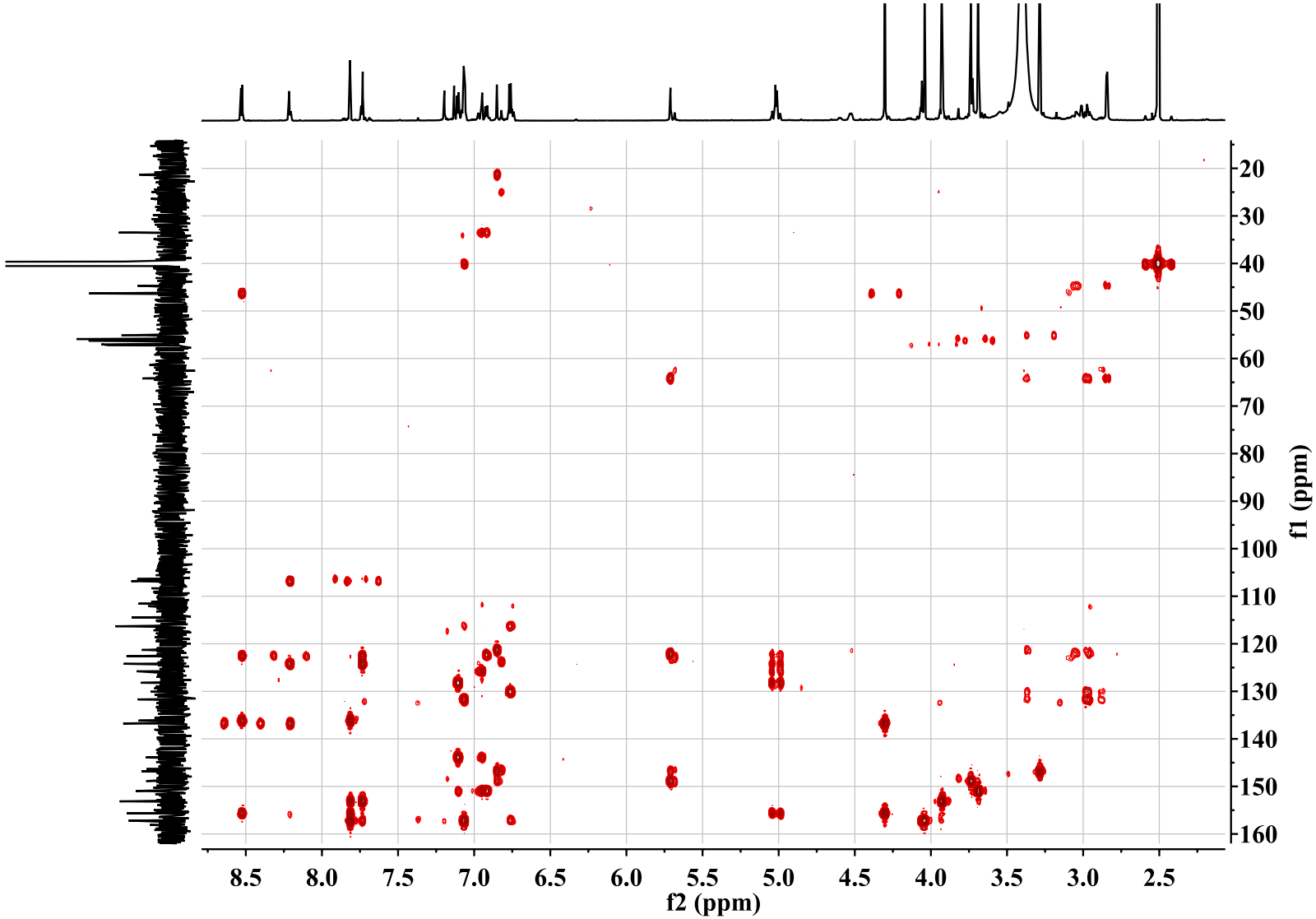
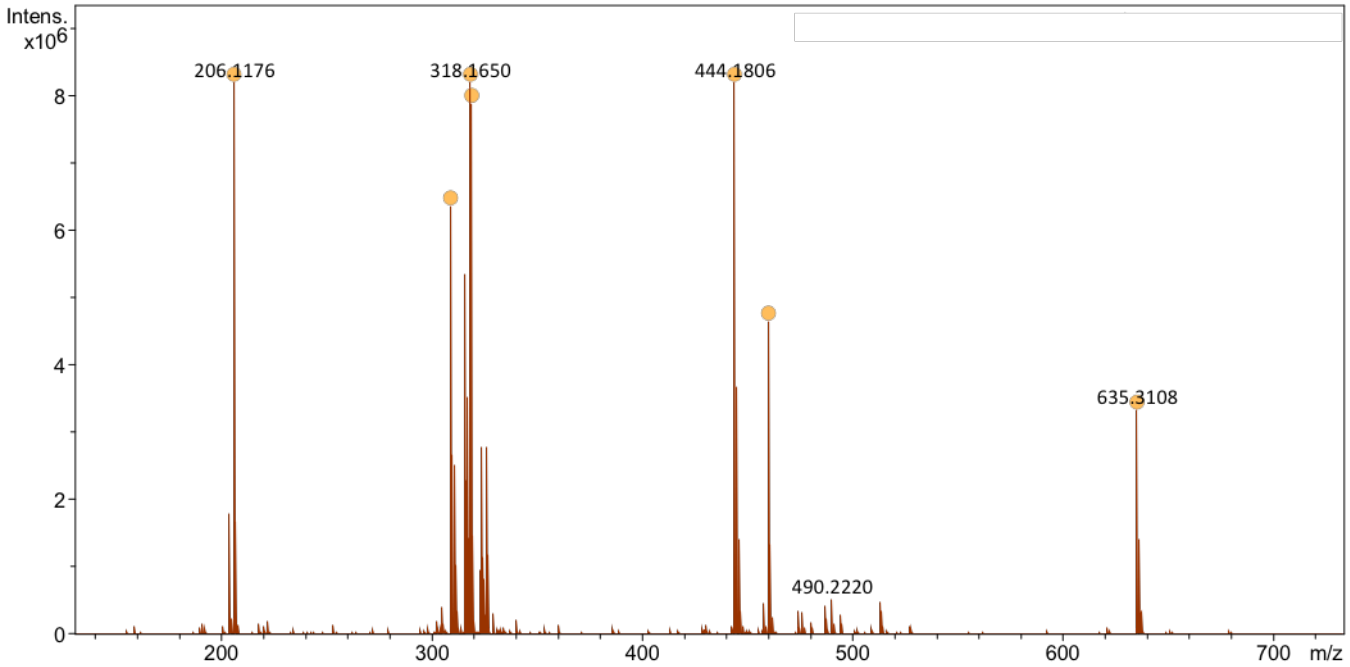


Figure S11. HMBC NMR spectrum of (*R*)-nomimantharine trifluoroacetate (**2**)



Means. m/z	Ion formula	calc. m/z	err [ppm]	rdb	e⁻Conf	N-Rule
635.3108	$C_{39}H_{43}N_2O_6$	635.3116	1.2	19.5	even	ok

Figure S12. HRMS spectrum of (*R*)-nomimantharine trifluoroacetate (**2**)

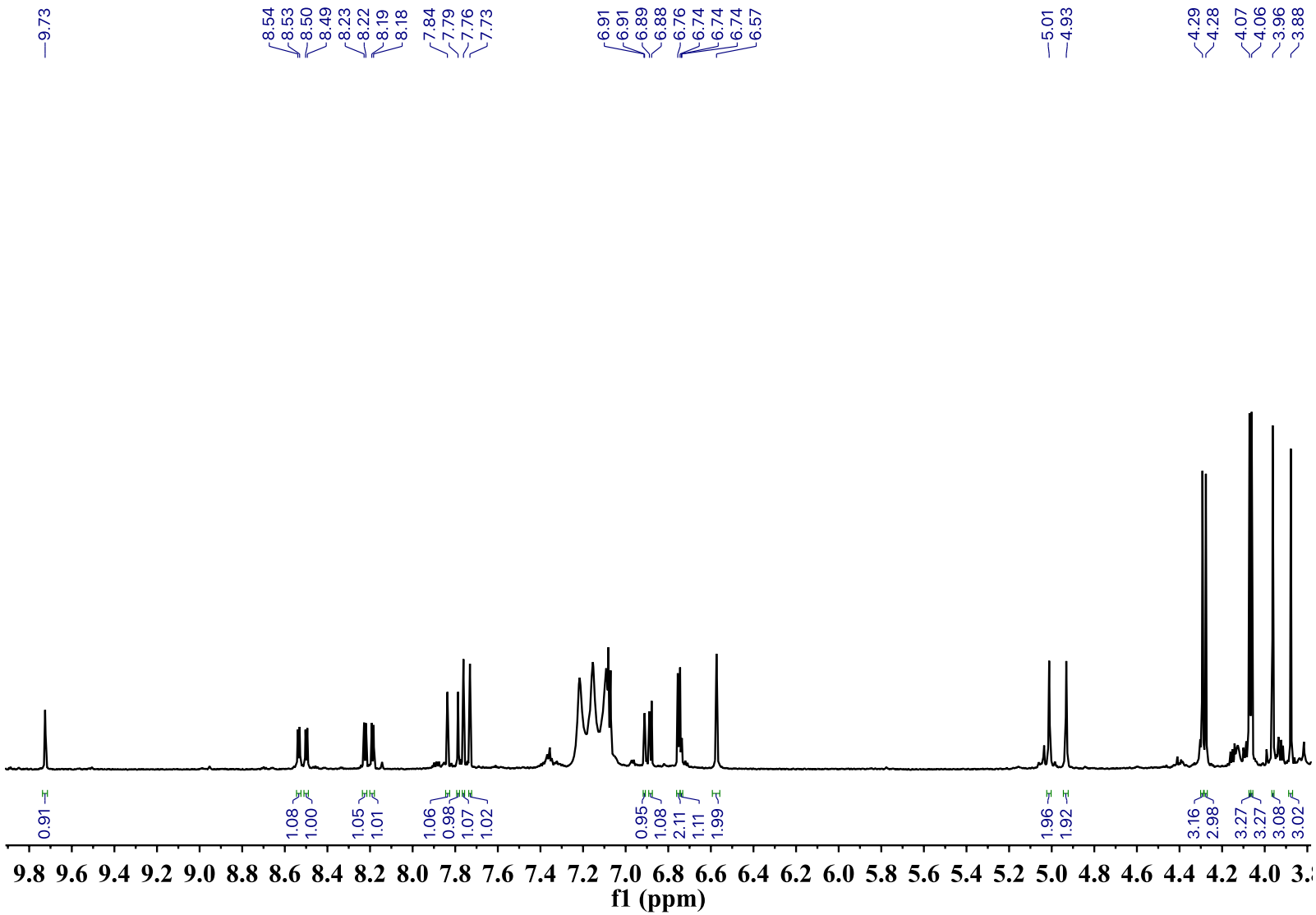


Figure S13. ^{1}H NMR spectrum of 12-de-*O*-methyphaeantharine trifluoroacetate (**3**)

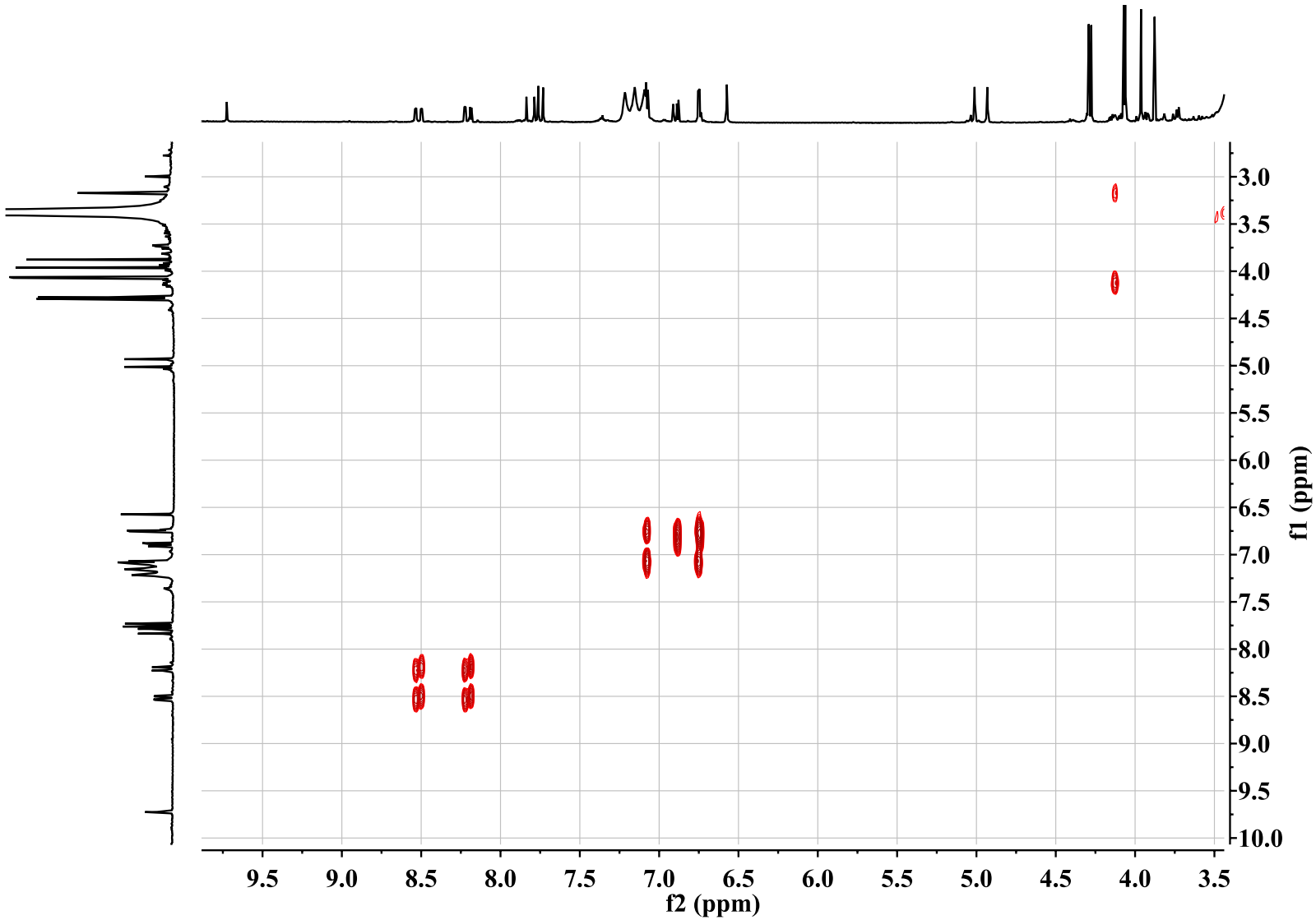


Figure S14. COSY NMR spectrum of 12-de-*O*-methyphaeantharine trifluoroacetate (**3**)

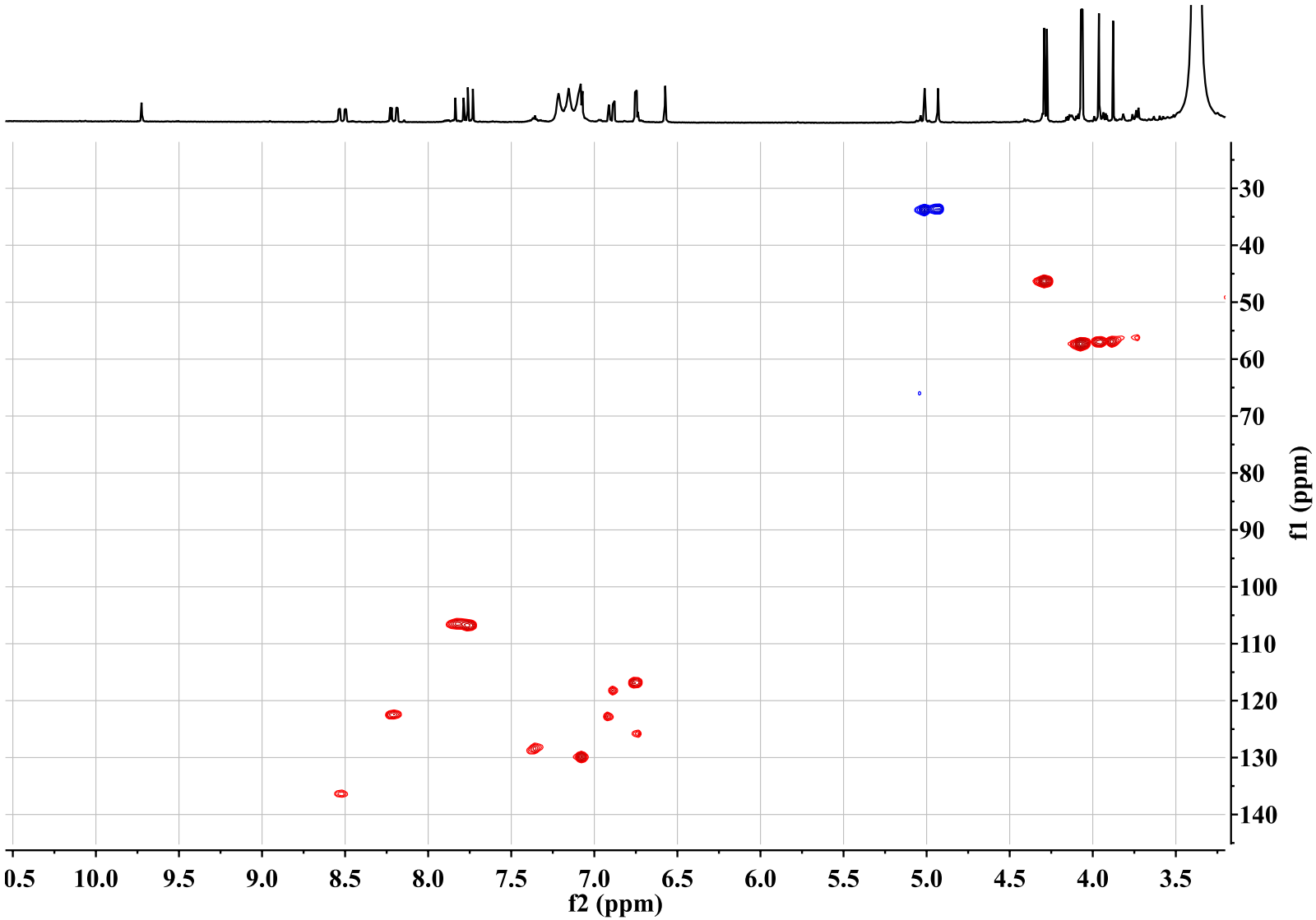


Figure S15. HSQC NMR spectrum of 12-de-*O*-methyphaeantharine trifluoroacetate (**3**)

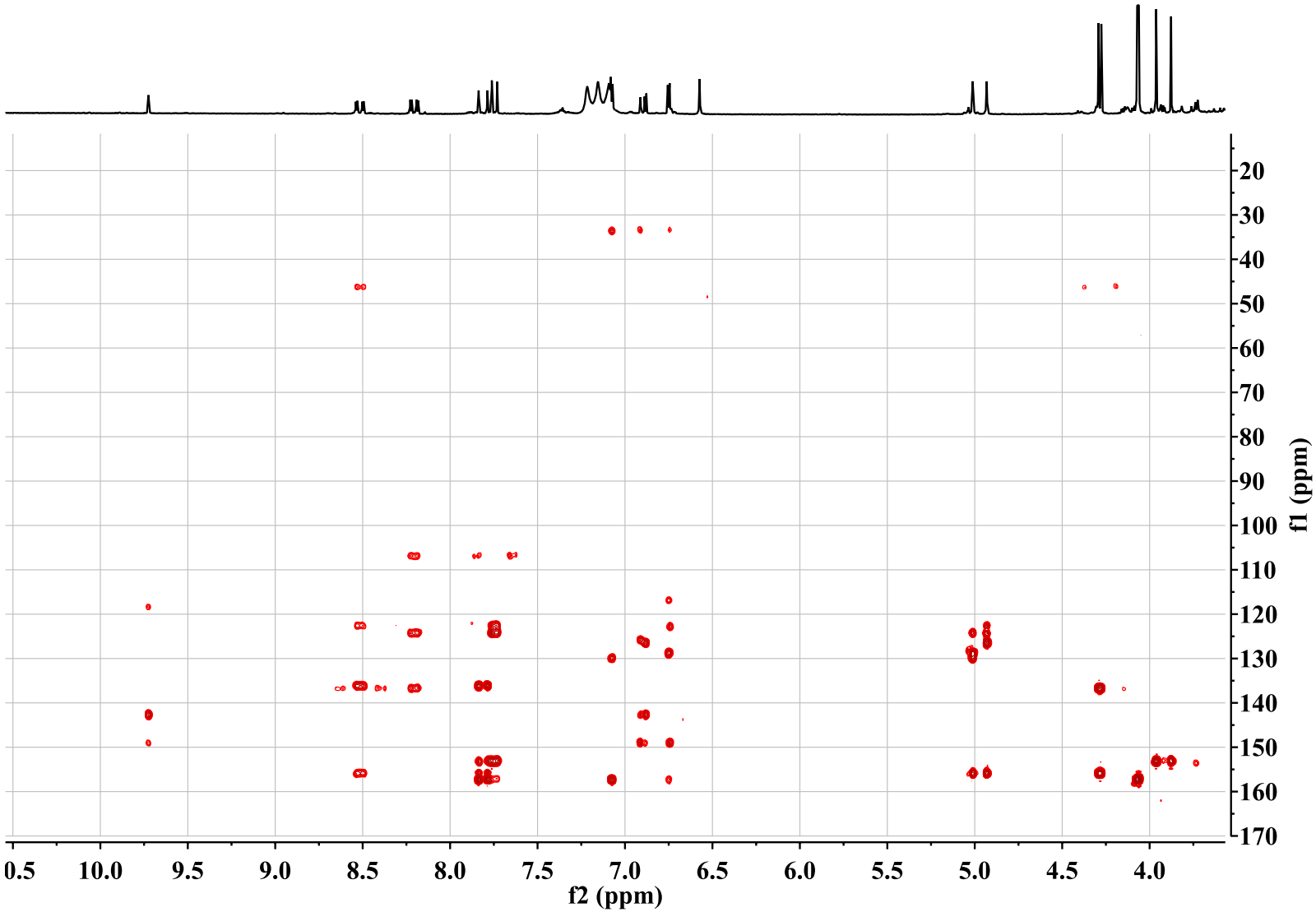
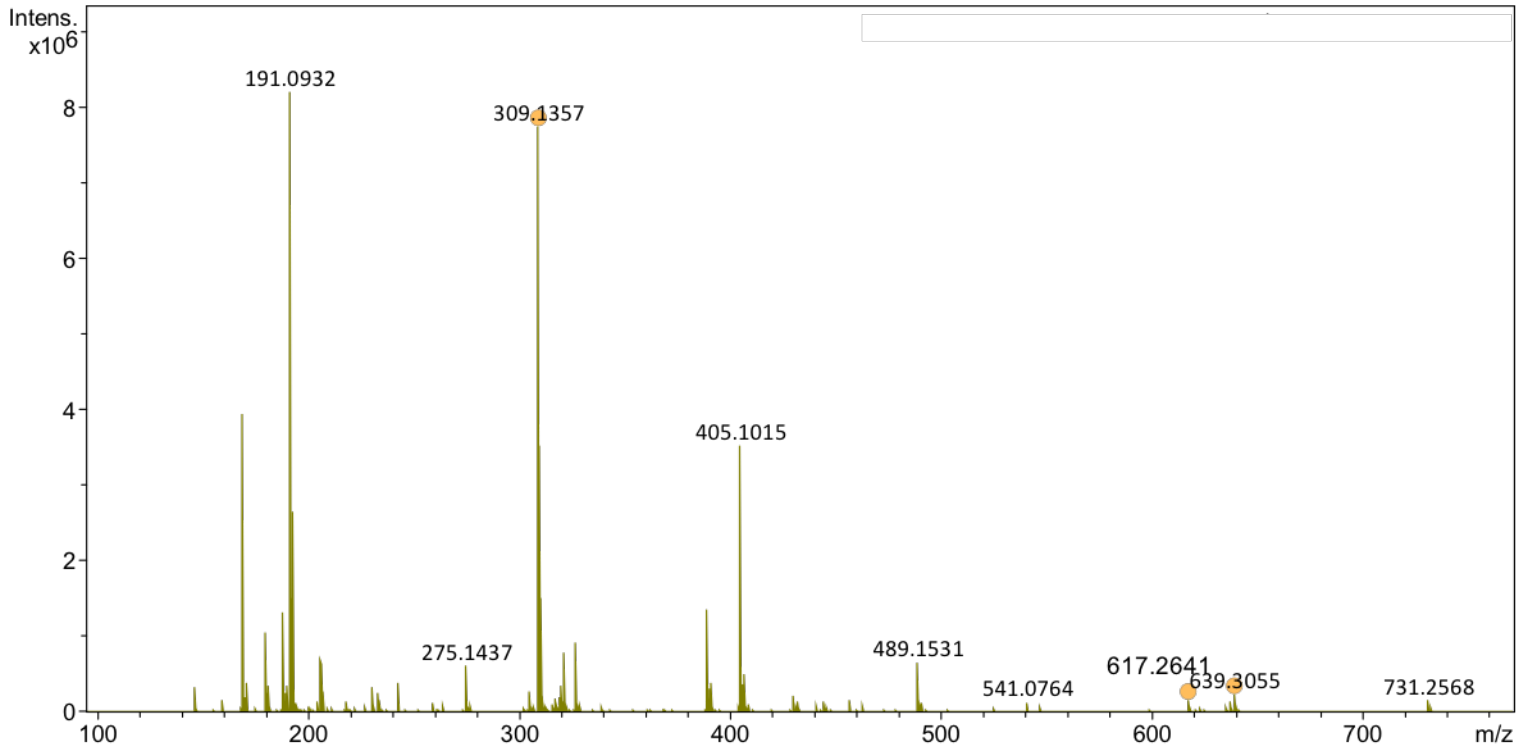


Figure S16. HMBC NMR spectrum of 12-de-*O*-methyphaeantharine trifluoroacetate (**3**)



Means. m/z	Ion formula	calc. m/z	err [ppm]	rdb	e⁻Conf	N-Rule
309.1357	$C_{38}H_{38}N_2O_6$	309.1359	0.6	21.0	even	ok
617.2641	$C_{38}H_{37}N_2O_6$	617.2646	-1.6	21.5	even	ok

Figure S17. HRMS spectrum of 12-de-*O*-methyphaeantharine trifluoroacetate (**3**)

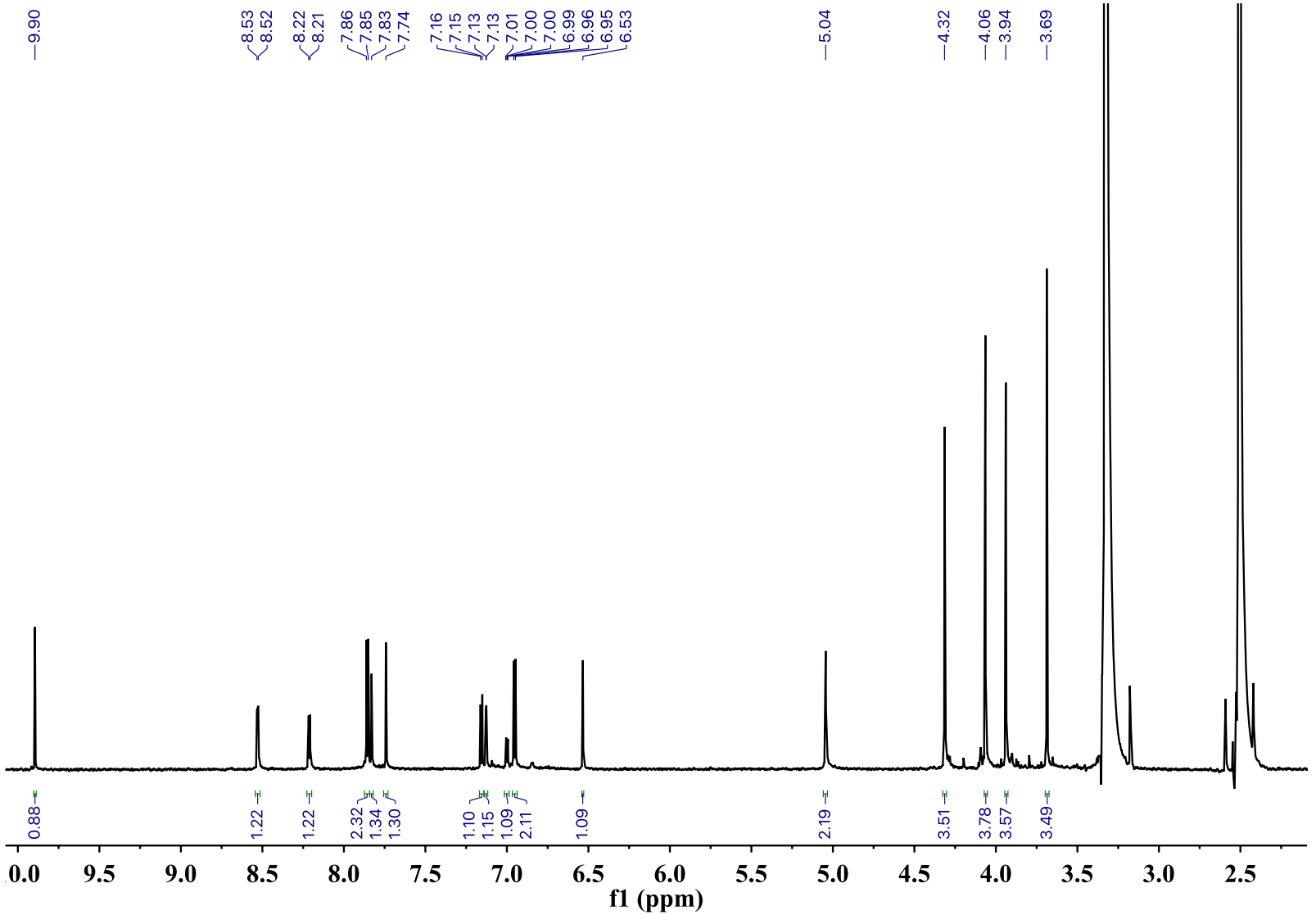


Figure S18. ^{1}H NMR spectrum of nominanthranal trifluoroacetate (**4**)

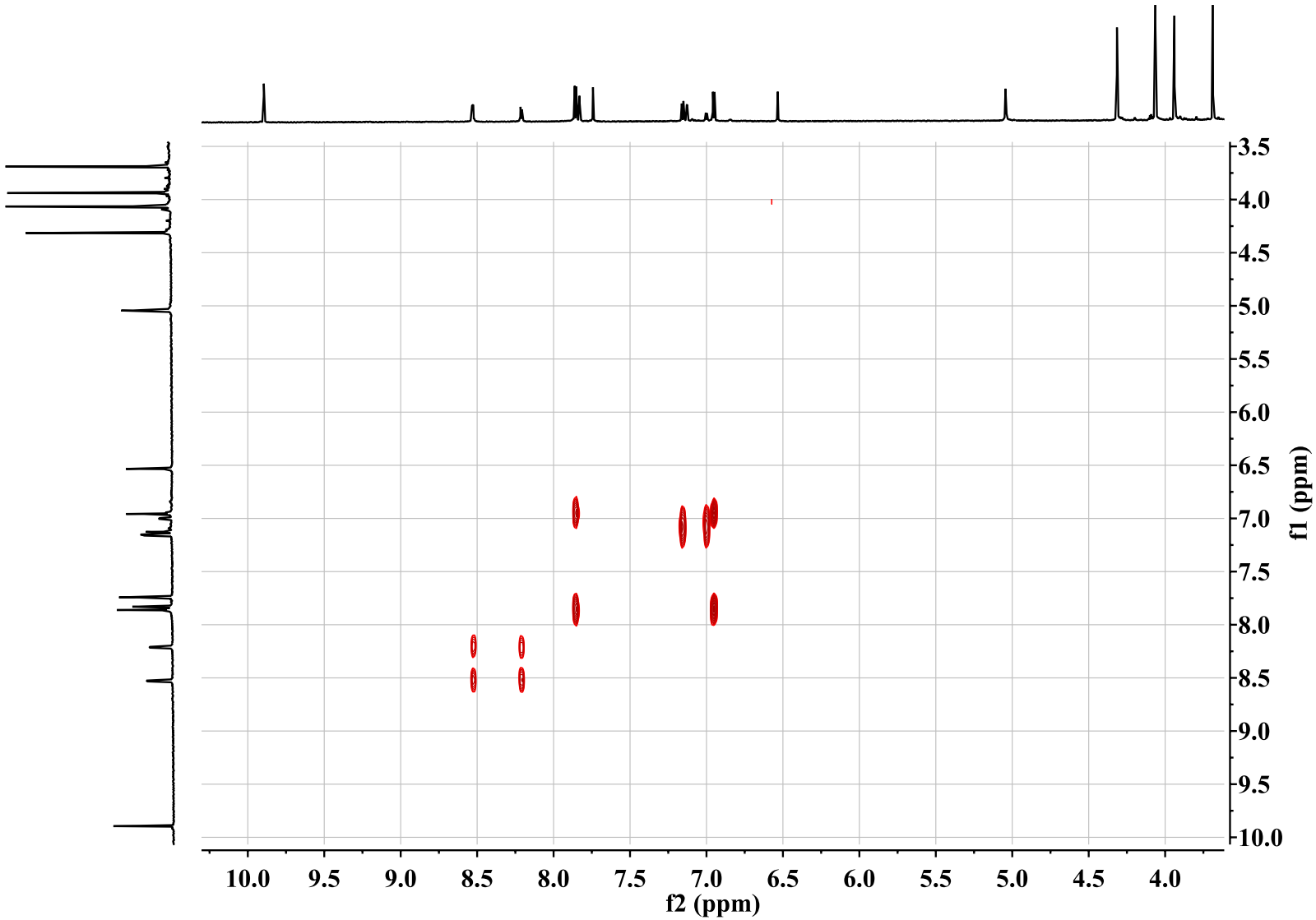


Figure S19. COSY NMR spectrum of nominanthranal trifluoroacetate (**4**)

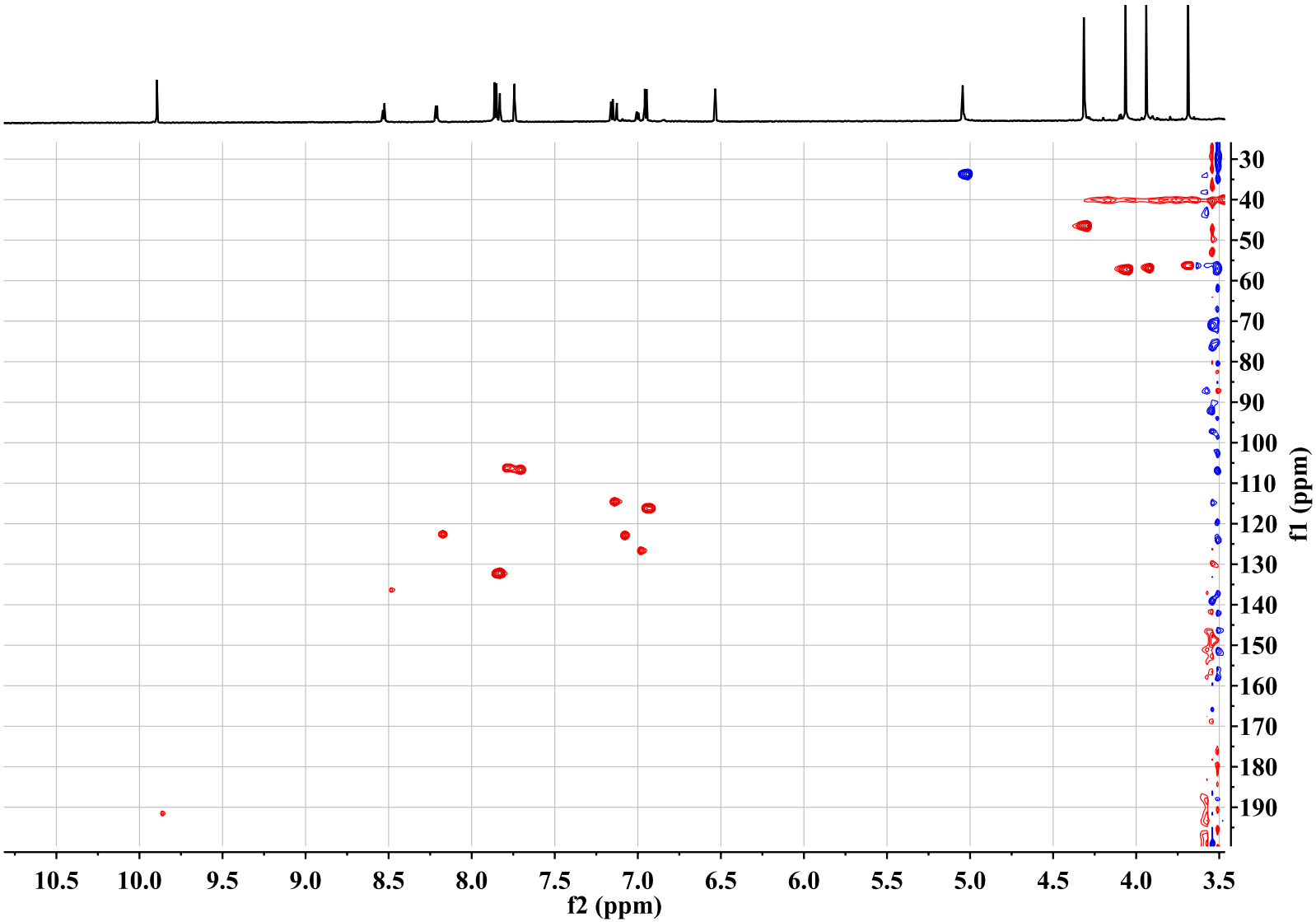


Figure S19. HSQC NMR spectrum of nominanthranal trifluoroacetate (**4**)

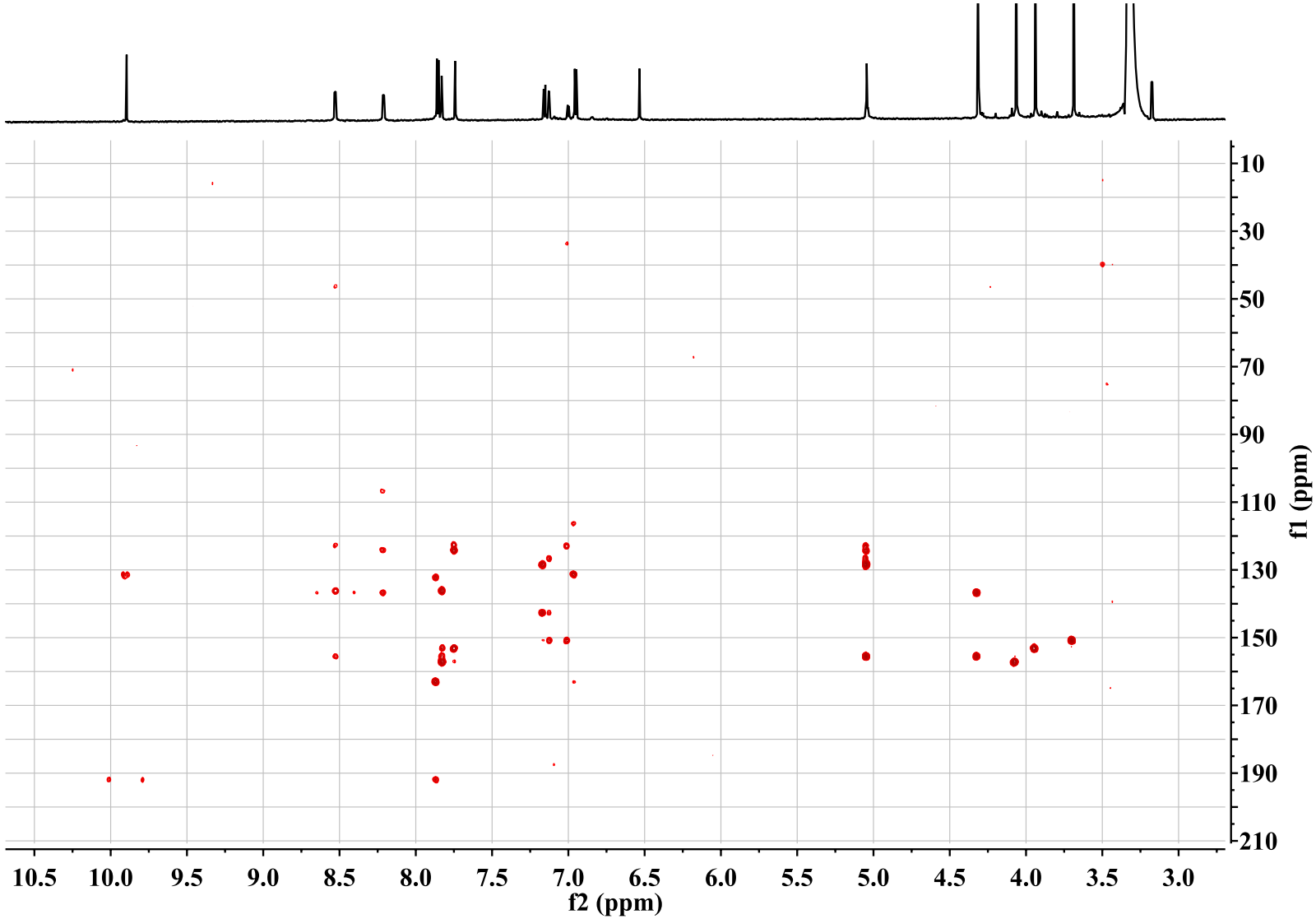
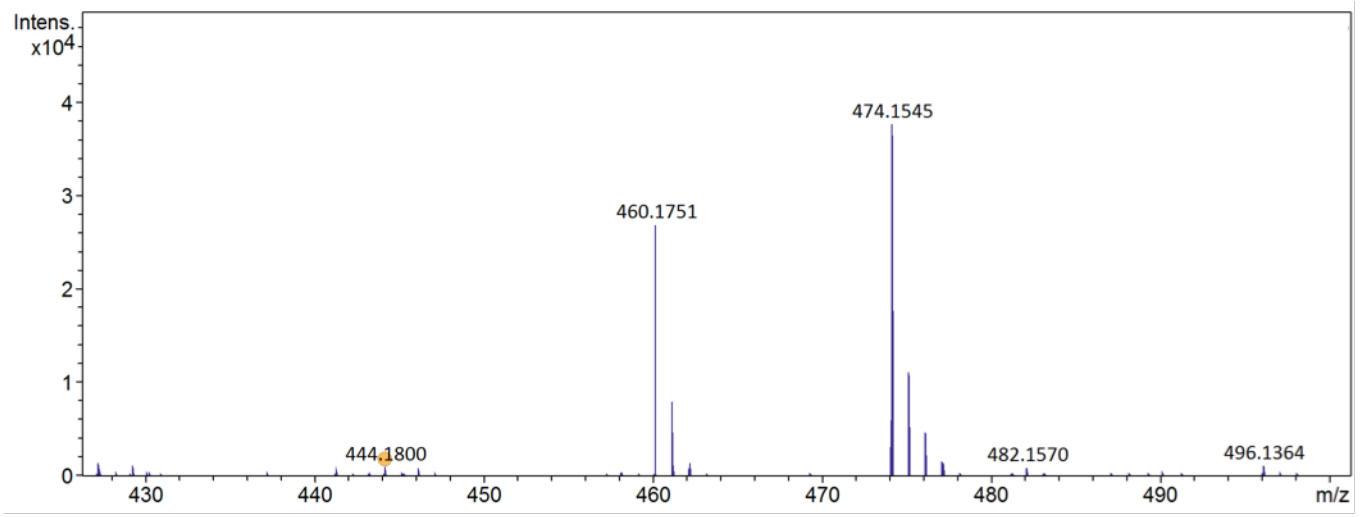


Figure S20. HMBC NMR spectrum of nominanthranal trifluoroacetate (**4**)



Means. m/z	Ion formula	calc. m/z	err [ppm]	rdb	e⁻Conf	N-Rule
444.1800	$C_{27}H_{26}NO_5$	444.1805	1.2	15.5	even	ok

Figure S21. HRMS spectrum of nominanthranal trifluoroacetate (**4**)

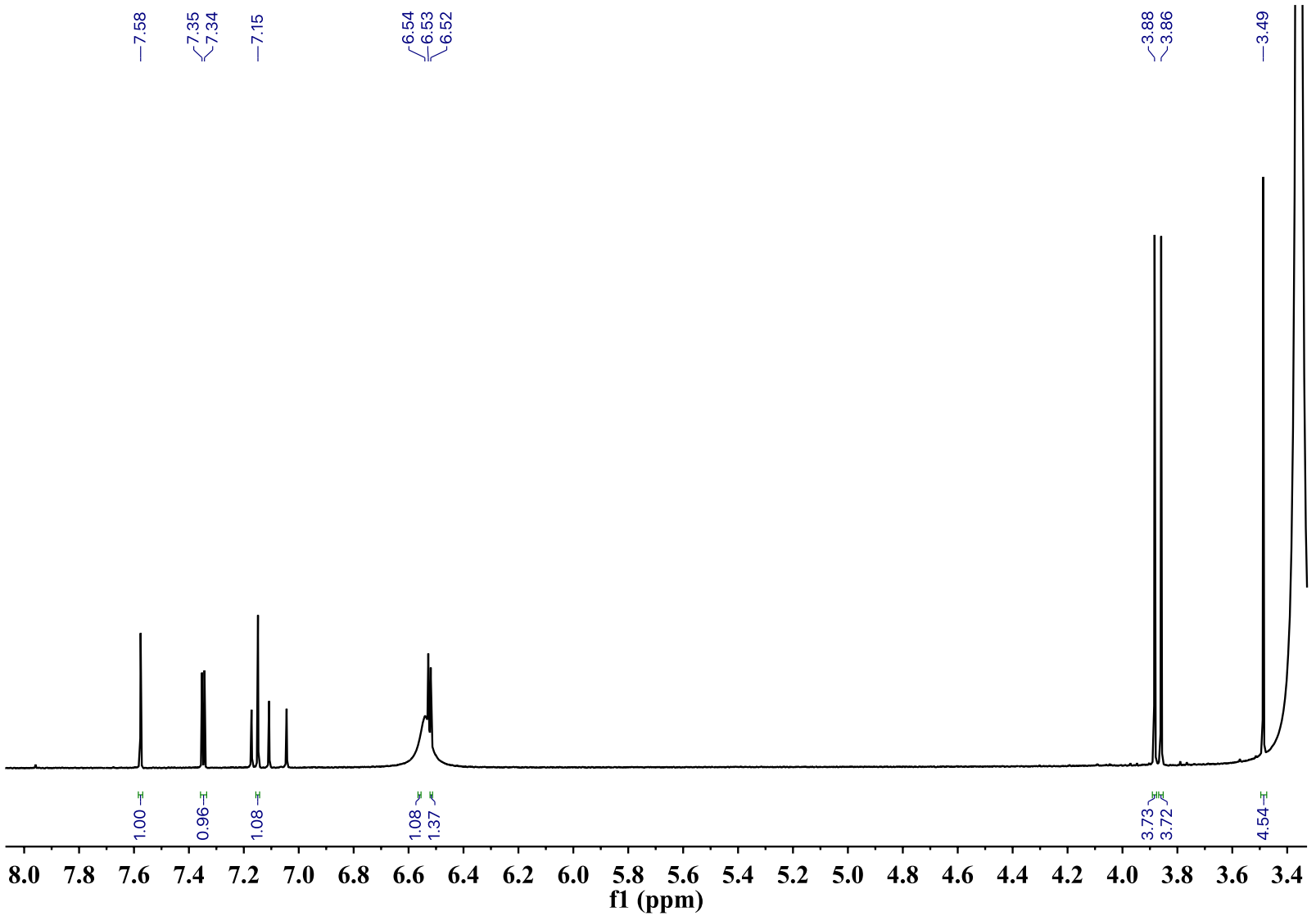


Figure S22. ^{1}H NMR spectrum of 1-hydroxy-6,7-dimethoxy-2-methylisoquinoline trifluoroacetate (**5**)

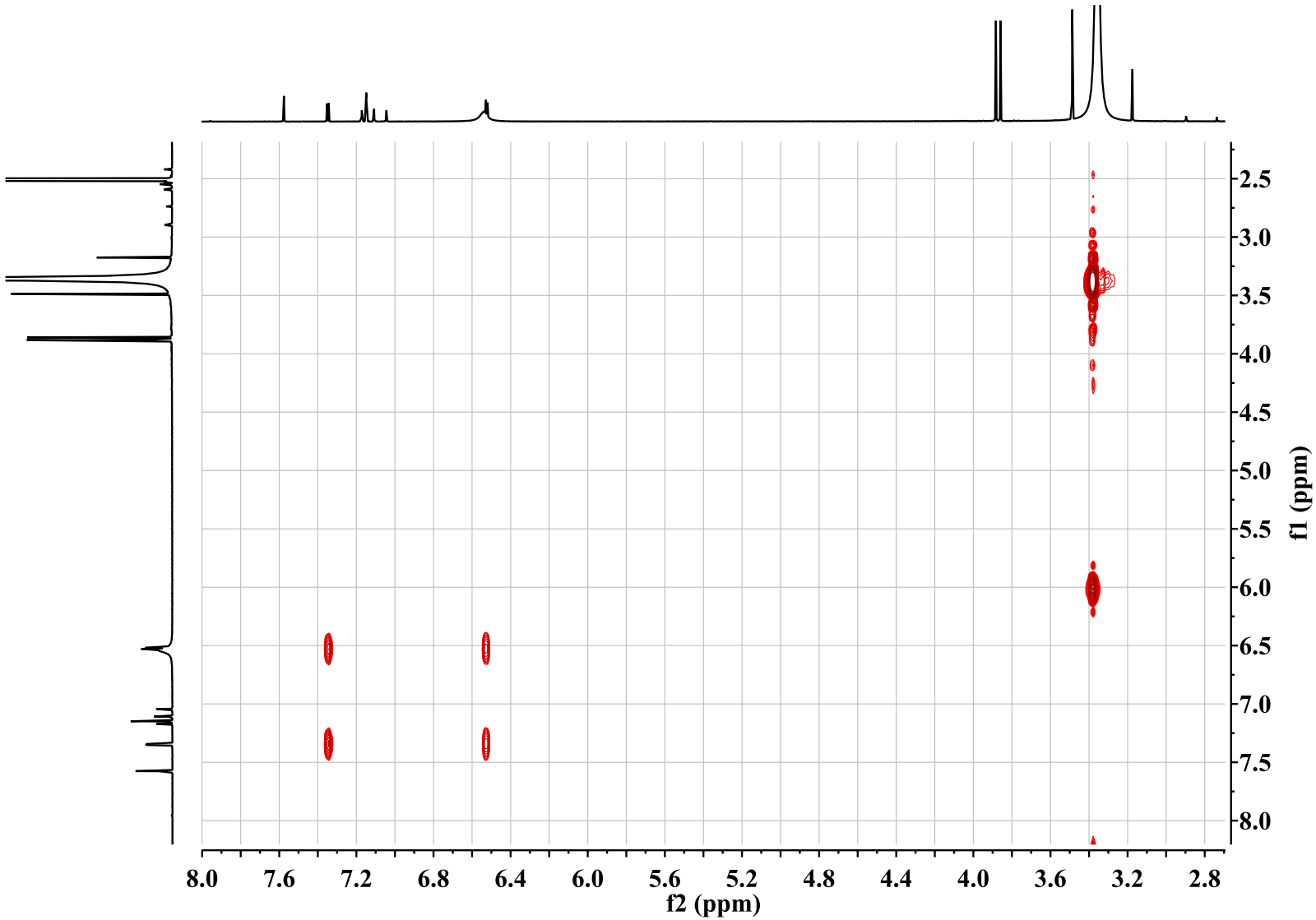


Figure S23. COSY NMR spectrum of 1-hydroxy-6,7-dimethoxy-2-methylisoquinoline trifluoroacetate (**5**)

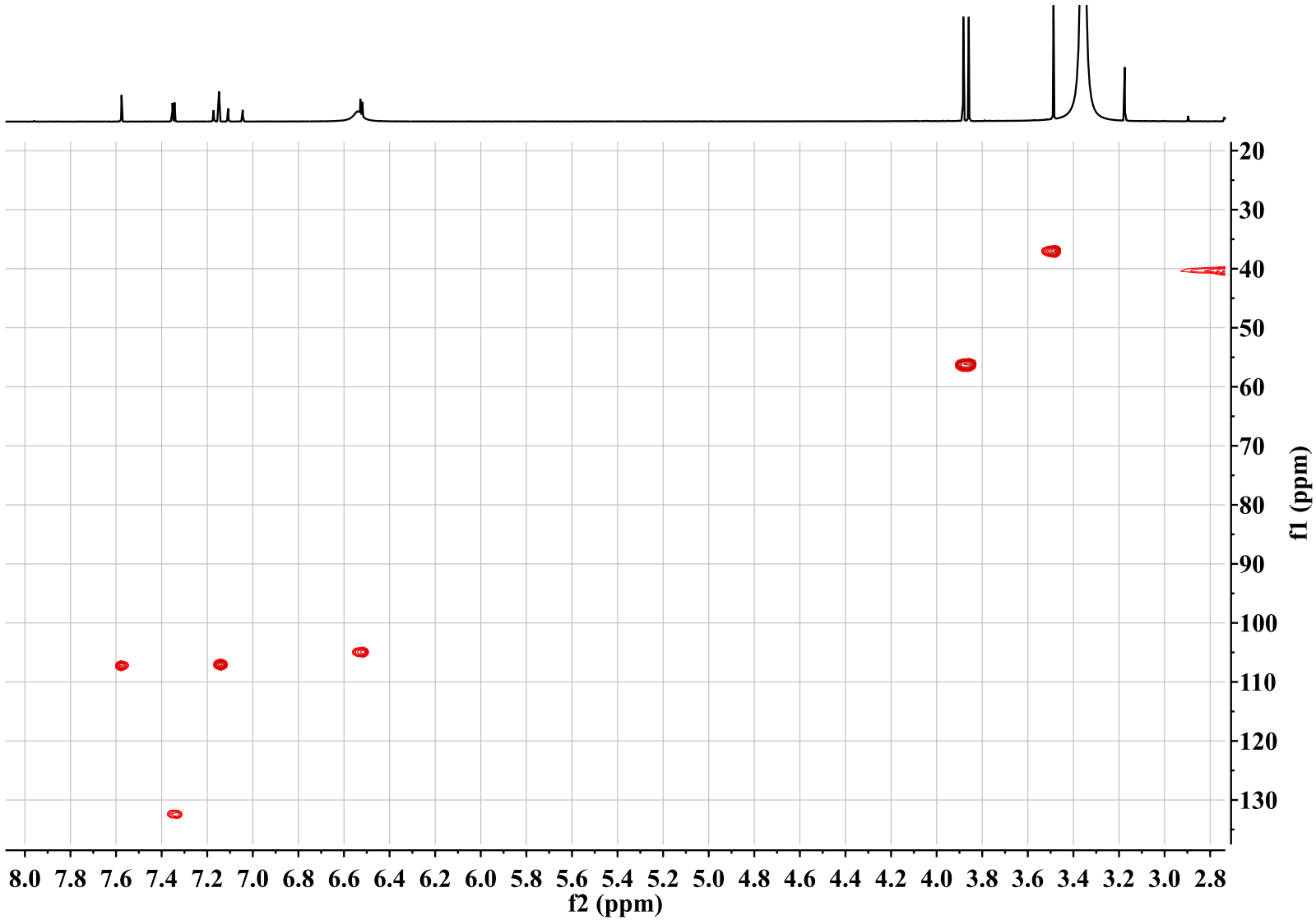


Figure S24. HSQC NMR spectrum of 1-hydroxy-6,7-dimethoxy-2-methylisoquinoline trifluoroacetate (**5**)

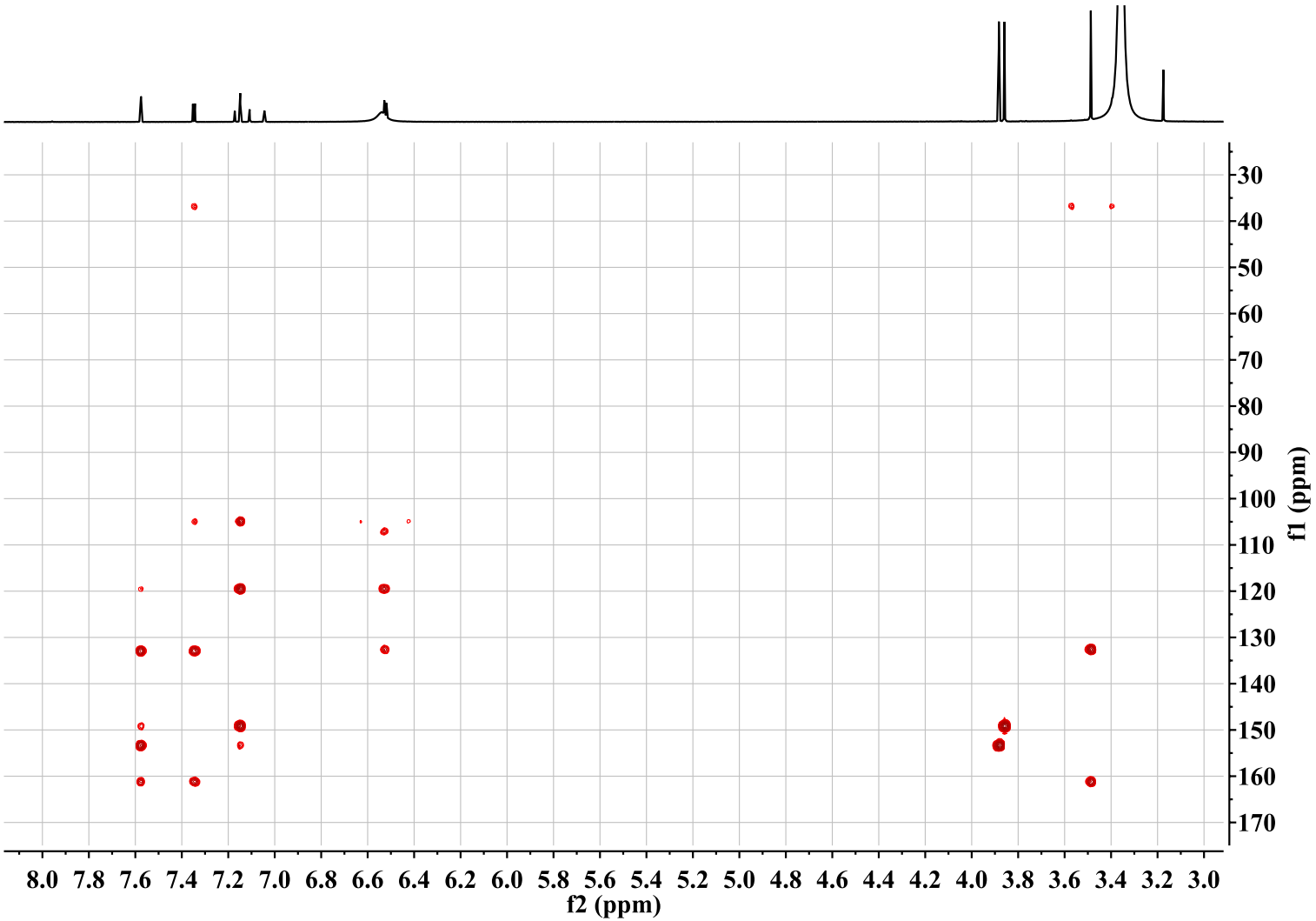
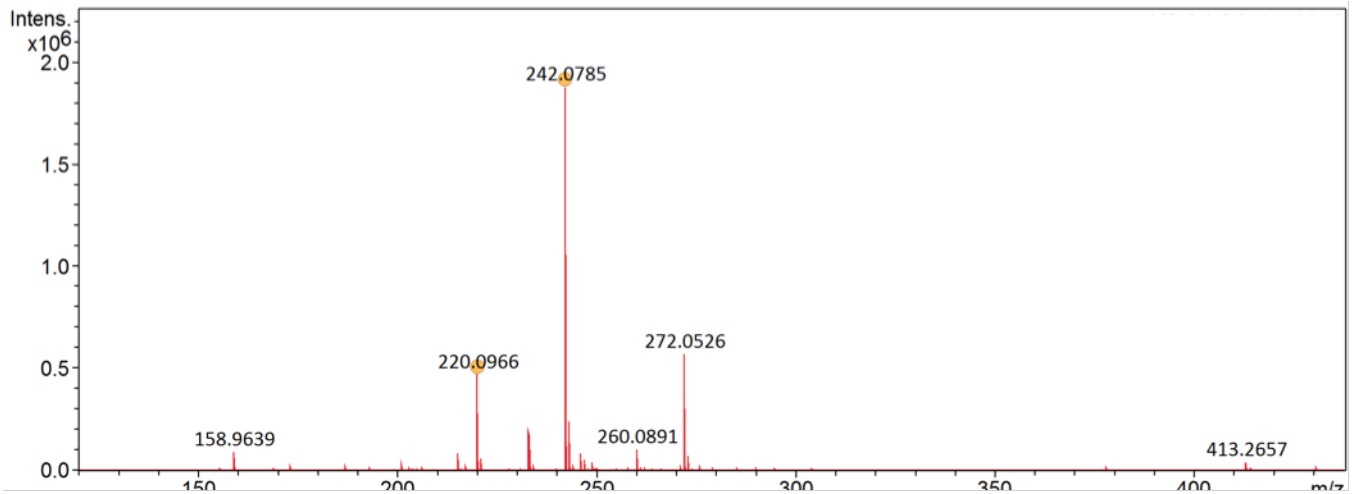


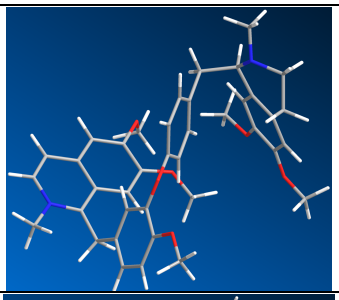
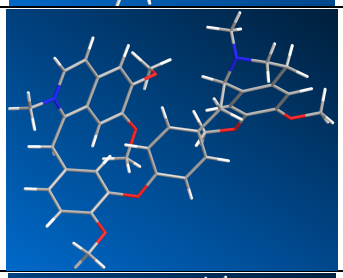
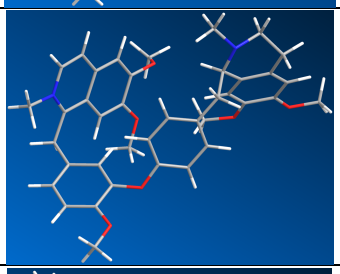
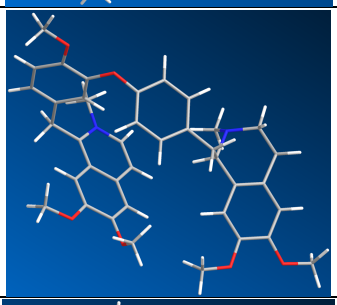
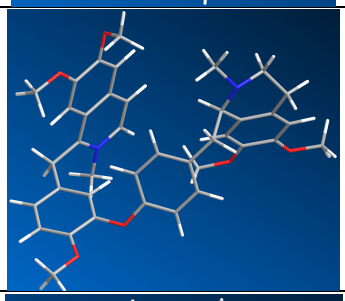
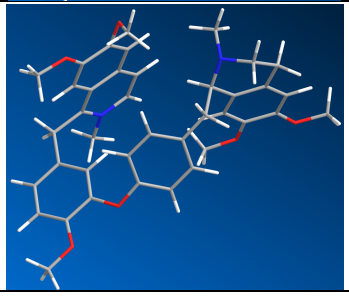
Figure S25. HMBC NMR spectrum of 1-hydroxy-6,7-dimethoxy-2-methylisoquinoline trifluoroacetate (**5**)



Means. m/z	Ion formula	calc. m/z	err [ppm]	rdb	e⁻Conf	N-Rule
220.0966	$C_{12}H_{14}NO_3$	220.0968	1.0	6.5	even	ok
242.0785	$C_{12}H_{13}NNaO_3$	242.0788	1.1	6.5	even	ok

Figure S26. HRMS spectrum of 1-hydroxy-6,7-dimethoxy-2-methylisoquinoline trifluoroacetate (**5**)

Table S1. Stable conformers of (*R*)-nomimantharine trifluoroacetate (**2**)

Conformer	Conformation	Energy (kcal/mol)	Percent (%)
2-1		-1300666.800	67.3
2-2		-1300665.662	9.8
2-3		-1300665.576	8.5
2-4		-1300665.506	7.5
2-5		-1300665.079	3.7
2-6		-1300664.989	3.2