

Steroidal Alkaloids from the Marine Sponge *Corticium niger* that Inhibit Growth of Human Colon Carcinoma Cells

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Supporting Information

S1 Plakinamine N (1) ¹H NMR (600 MHz, CD₃OD)

S2 Plakinamine N (1) ¹³C NMR (150 MHz, CD₃OD)

S3 Plakinamine N (1) gCOSY (CD₃OD)

S4 Plakinamine N (1) gHSQC (CD₃OD)

S5 Plakinamine N (1) gHMBC (CD₃OD)

S6 Plakinamine N (1) ROESY (CD₃OD)

S7 Plakinamine N (1) HRESIMS (+)

S8 Plakinamine O (2) ¹H NMR (600 MHz, CD₃OD)

S9 Plakinamine O (2) ¹³C NMR (150 MHz, CD₃OD)

S10 Plakinamine O (2) gCOSY (CD₃OD)

S11 Plakinamine O (2) gHSQC (CD₃OD)

S12 Plakinamine O (2) gHMBC (CD₃OD)

S13 Plakinamine O (2) ROESY (CD₃OD)

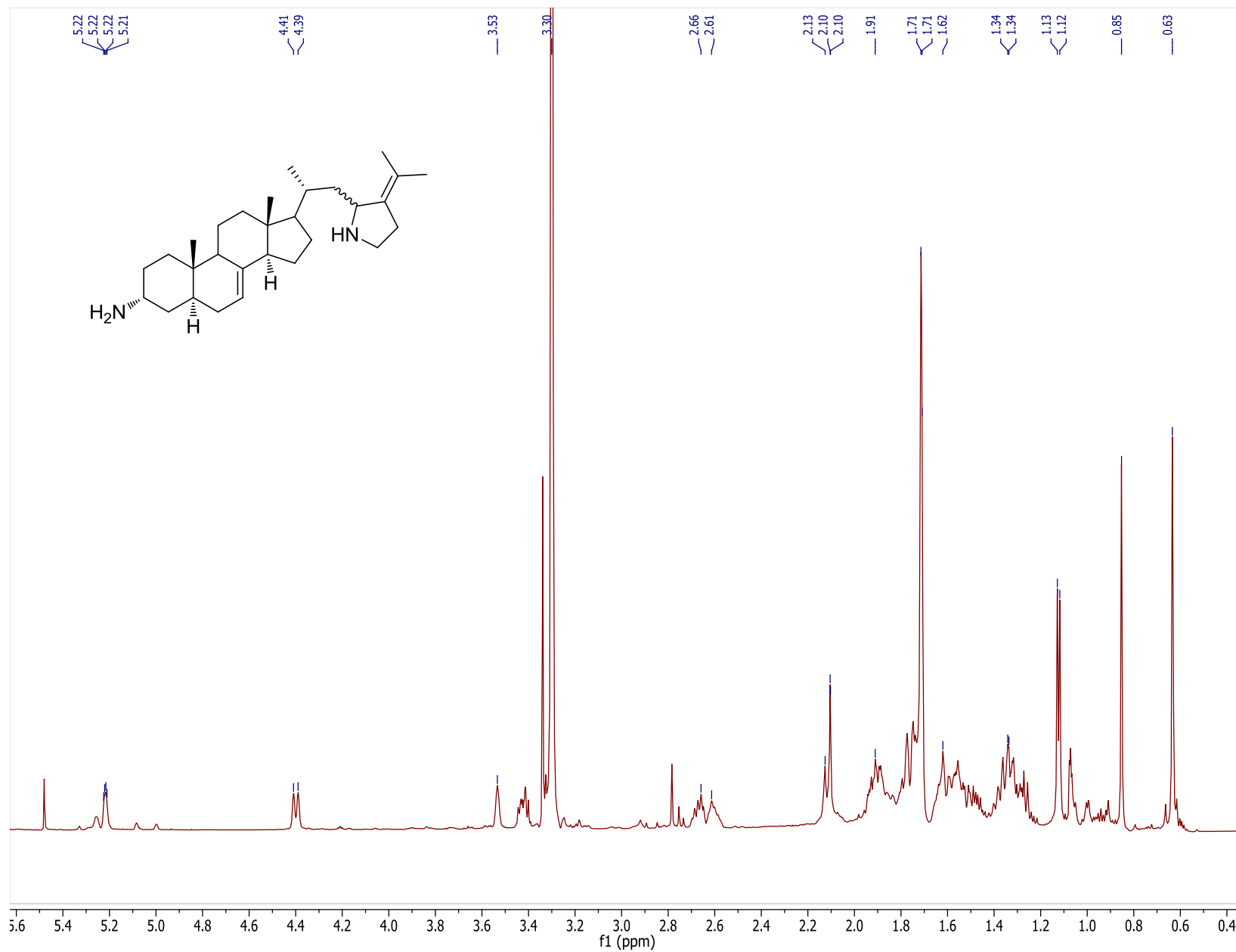
S14 Plakinamine O (2) HRESIMS (+)

S15 Plakinamine N (1) NCI-60 mean bar graphs

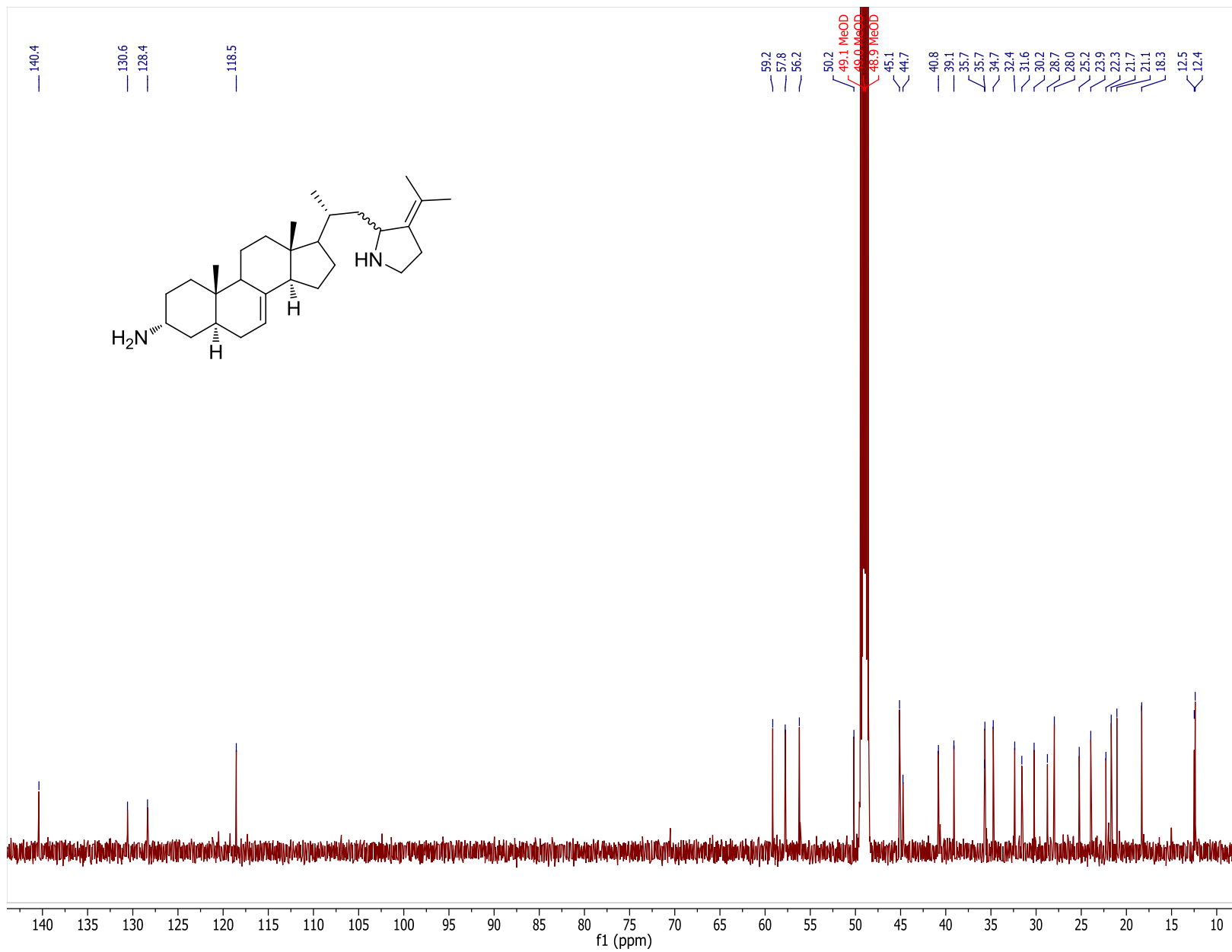
S16 Plakinamine O (2) NCI-60 mean bar graphs

S17 Plakinamine J (4) NCI-60 mean bar graphs

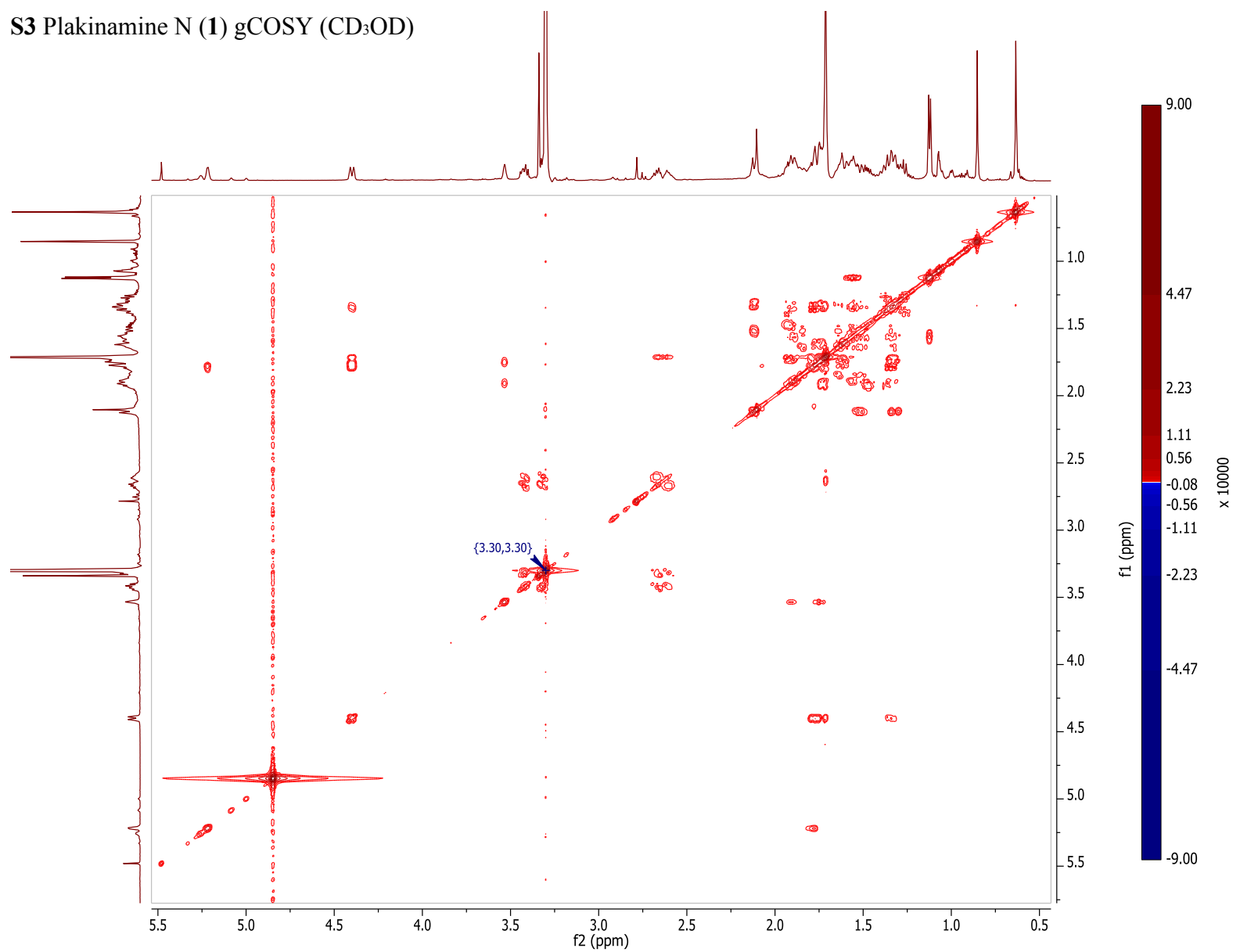
S1 Plakinamine N (1) ¹H NMR (600 MHz, CD₃OD)



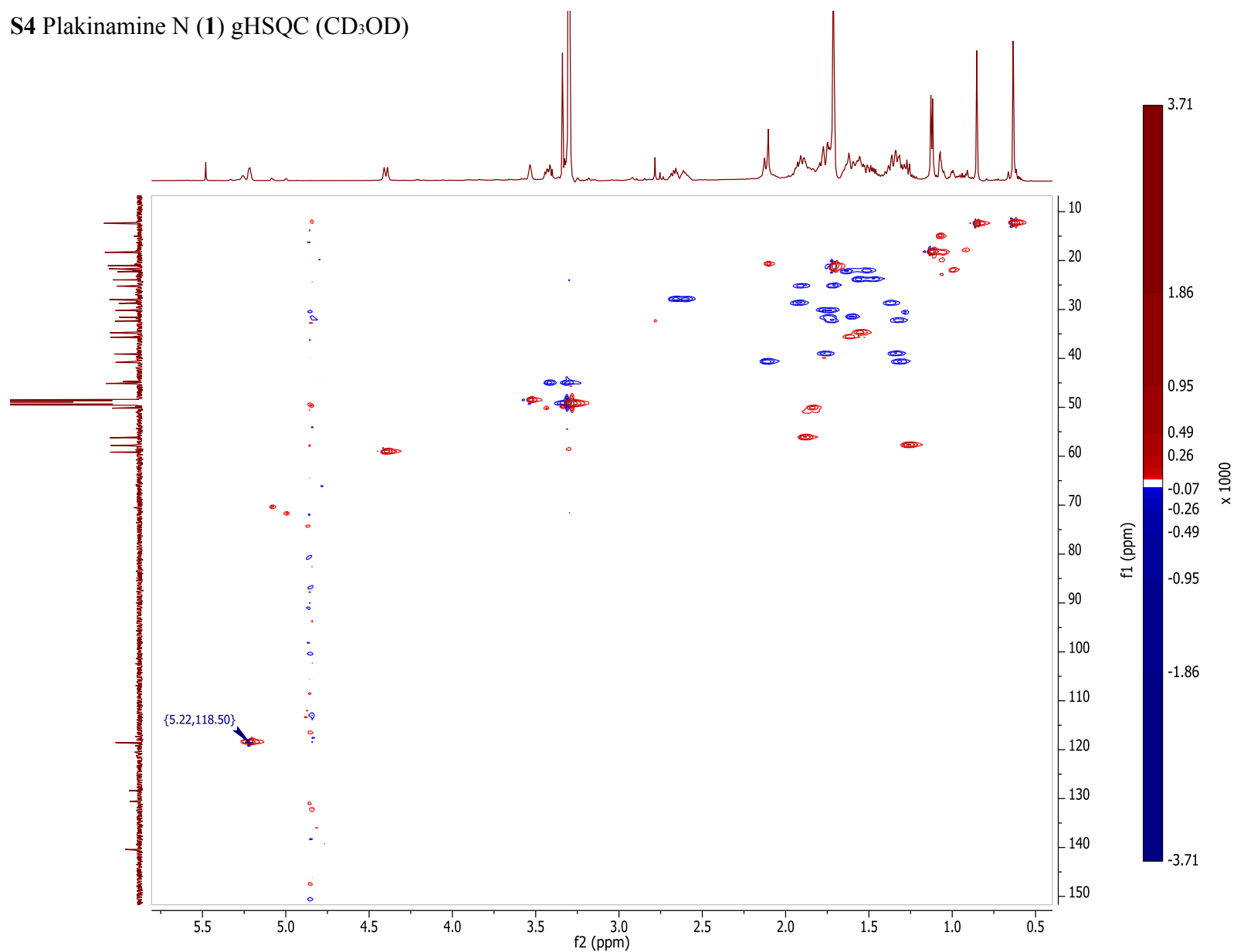
S2 Plakinamine N (1) ¹³C NMR (150MHz, CD₃OD)



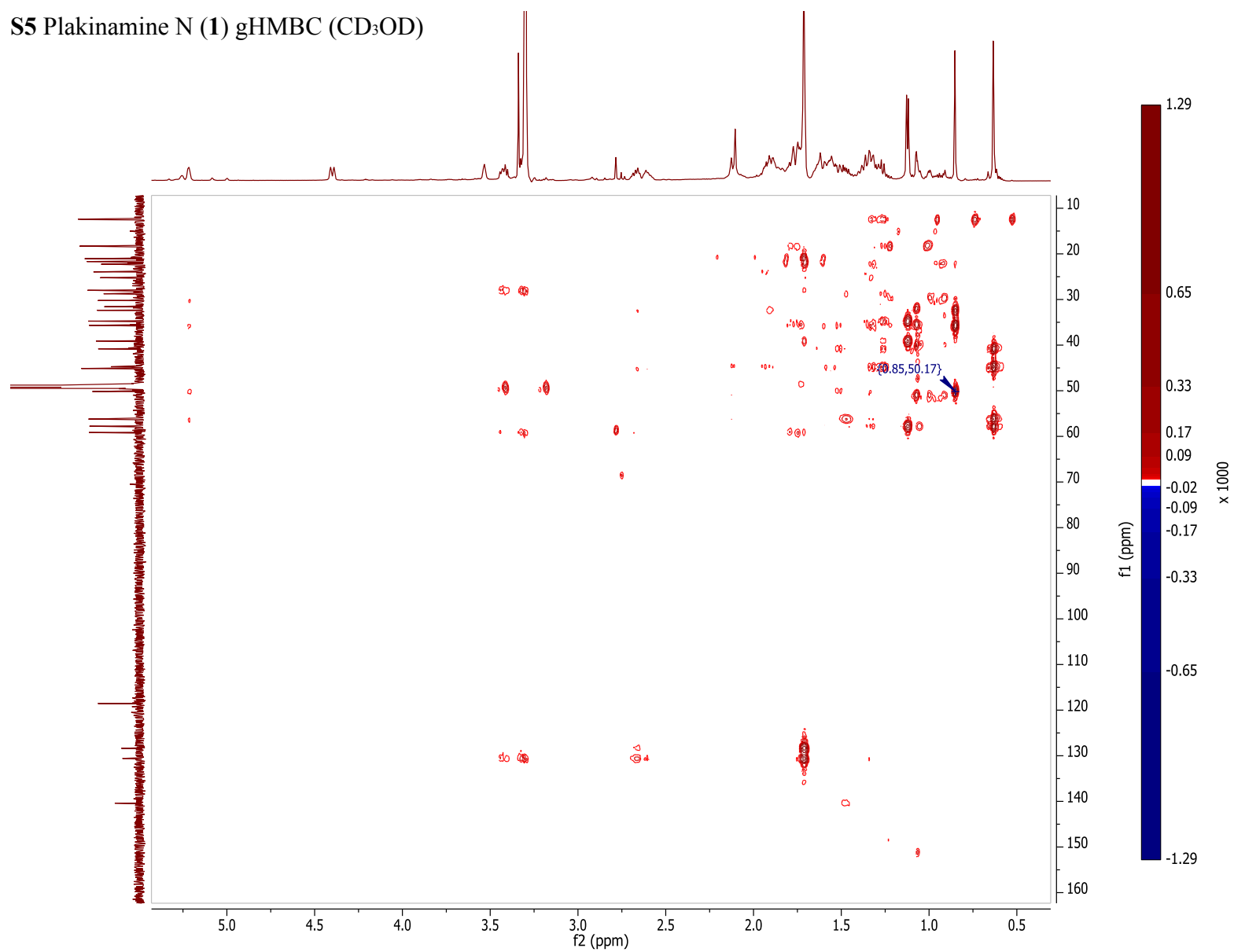
S3 Plakinamine N (1) gCOSY (CD₃OD)



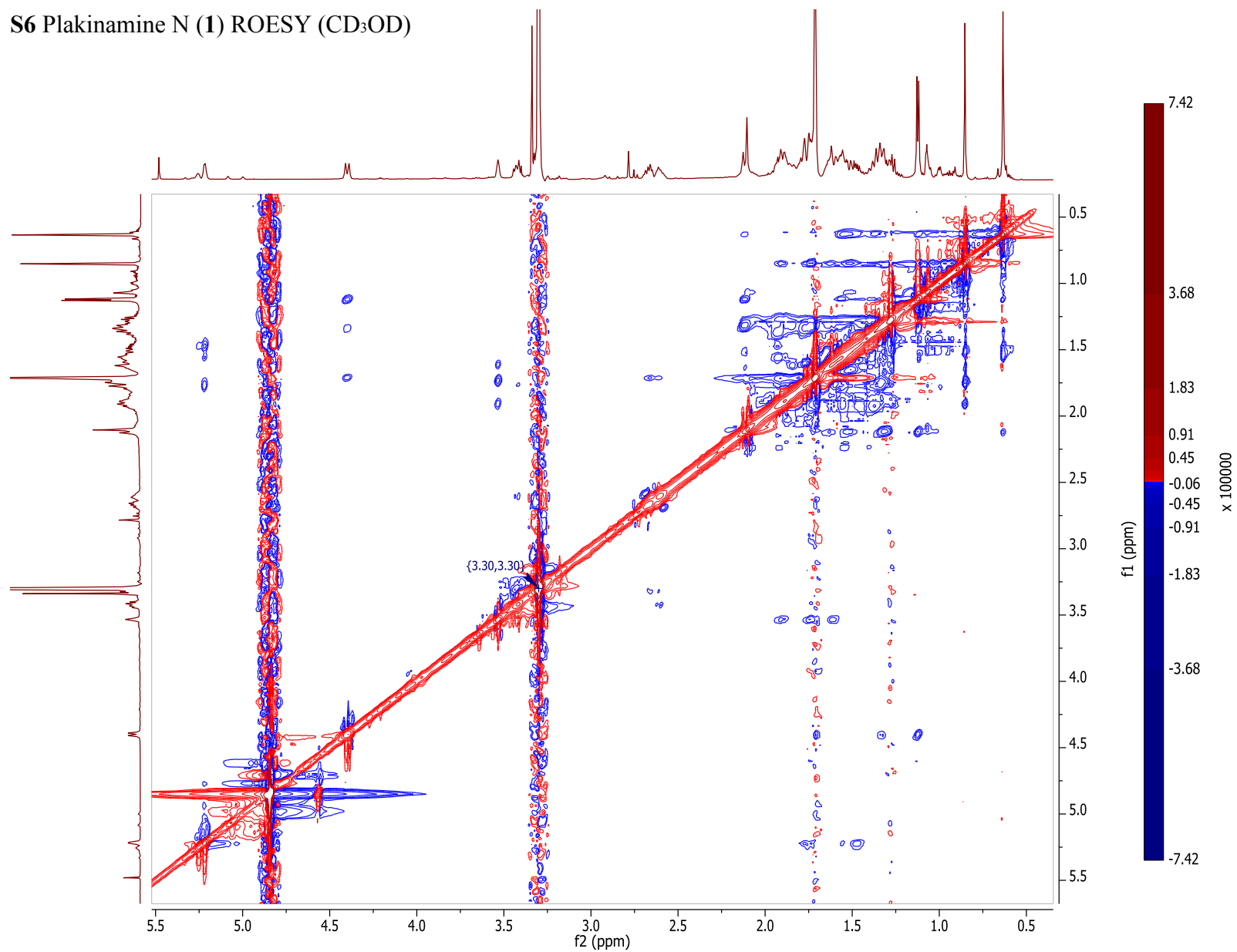
S4 Plakinamine N (1) gHSQC (CD₃OD)



S5 Plakinamine N (1) gHMBC (CD₃OD)



S6 Plakinamine N (1) ROESY (CD₃OD)



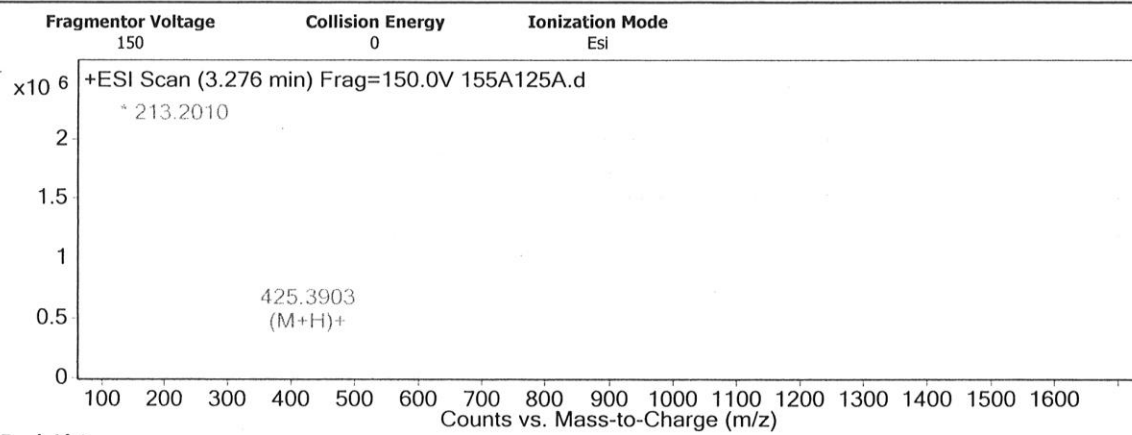
S7 Plakinamine N (1) HRESIMS (+)

MS Formula Results: + Scan (3.276 min) (155A125A.d)

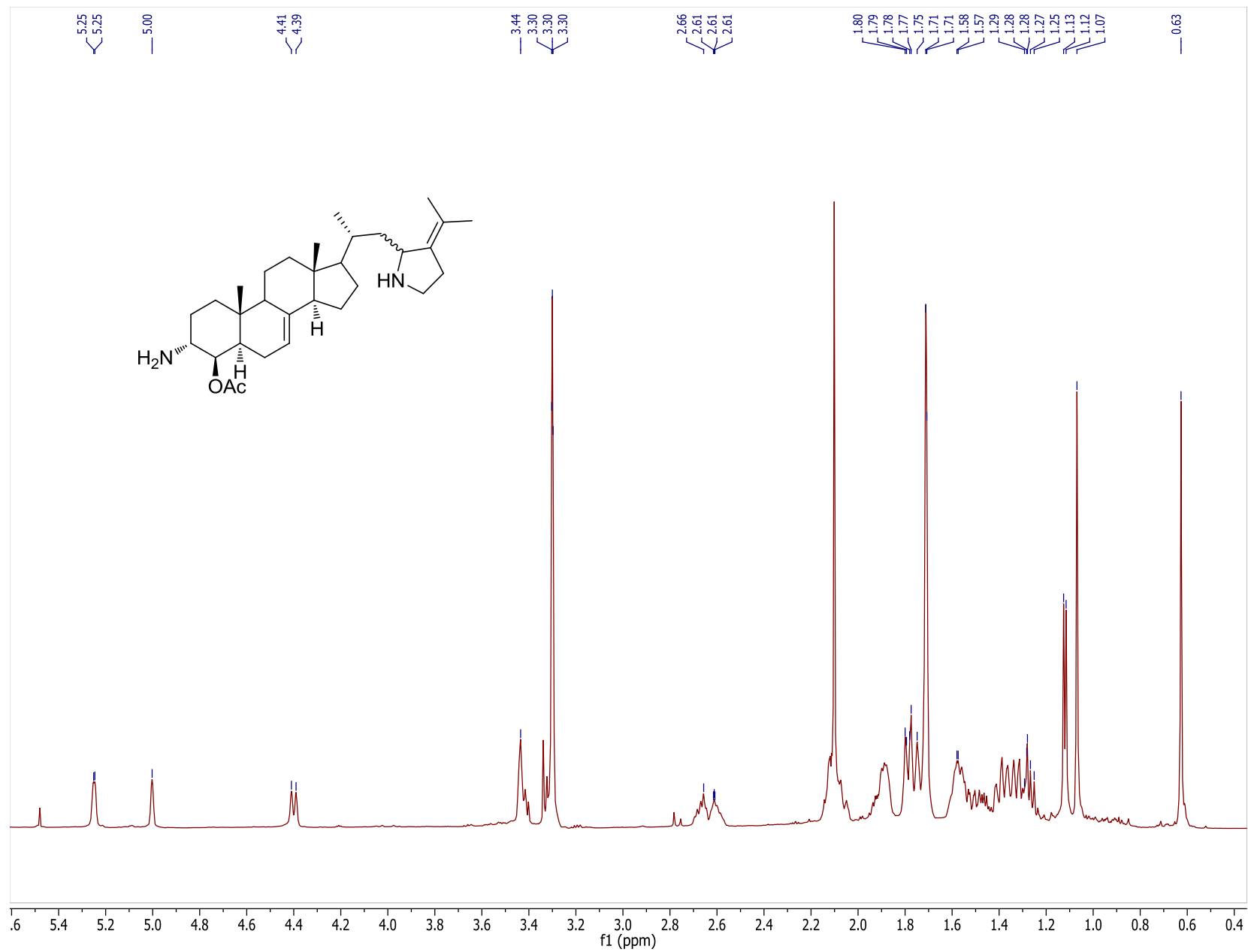
m/z	Ion	Formula	Abundance
425.3903	(M+H) ⁺	C ₂₉ H ₄₉ N ₂	362242.6

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
✓	C ₂₉ H ₄₈ N ₂	C ₂₉ H ₄₉ N ₂	94.16		425.389	-2.99	91.95	99.47	92.21
	C ₂₆ H ₅₂ N ₂ S	C ₂₆ H ₅₃ N ₂ S	82.57		425.3924	4.94	79.53	82.42	88.81

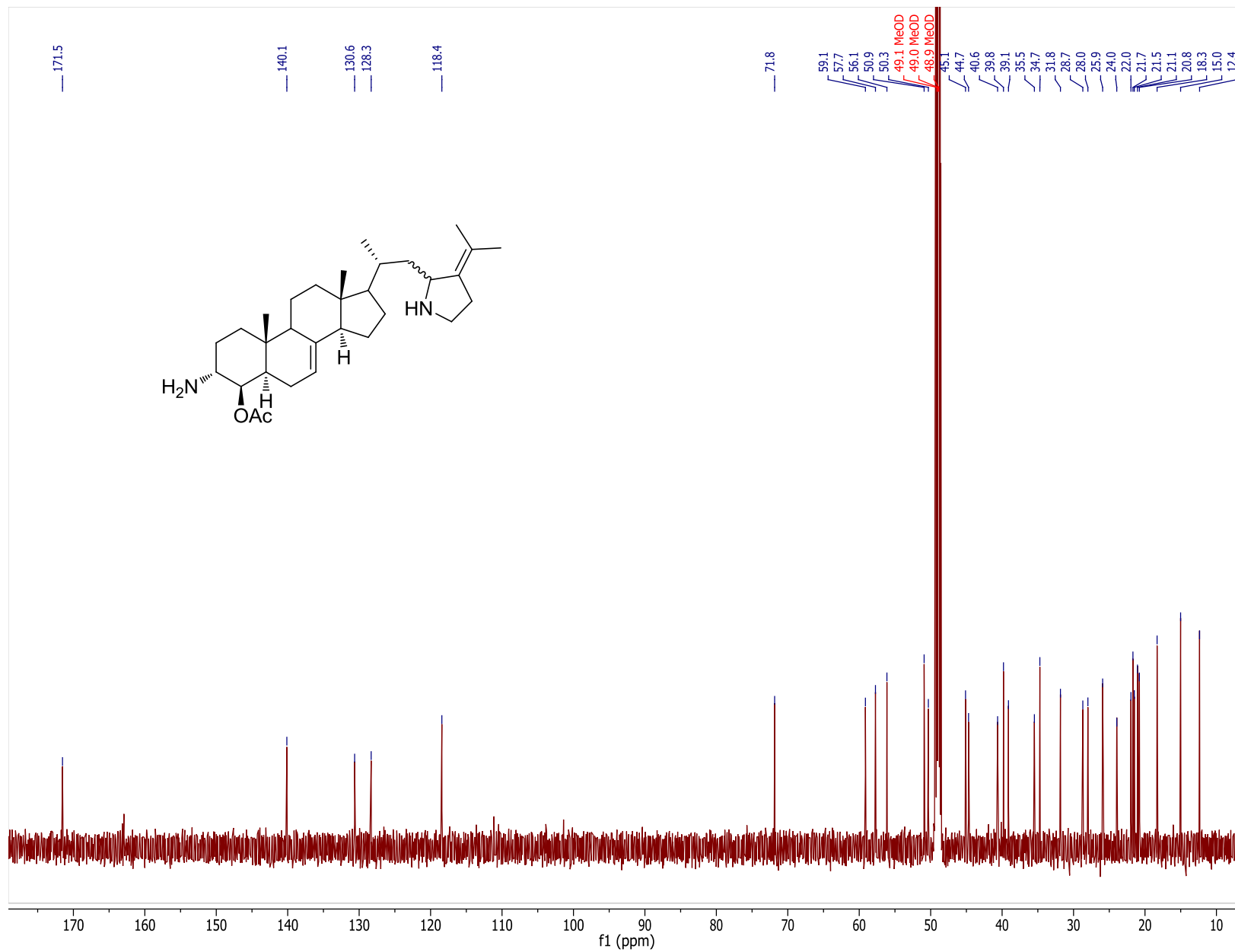
User Spectra



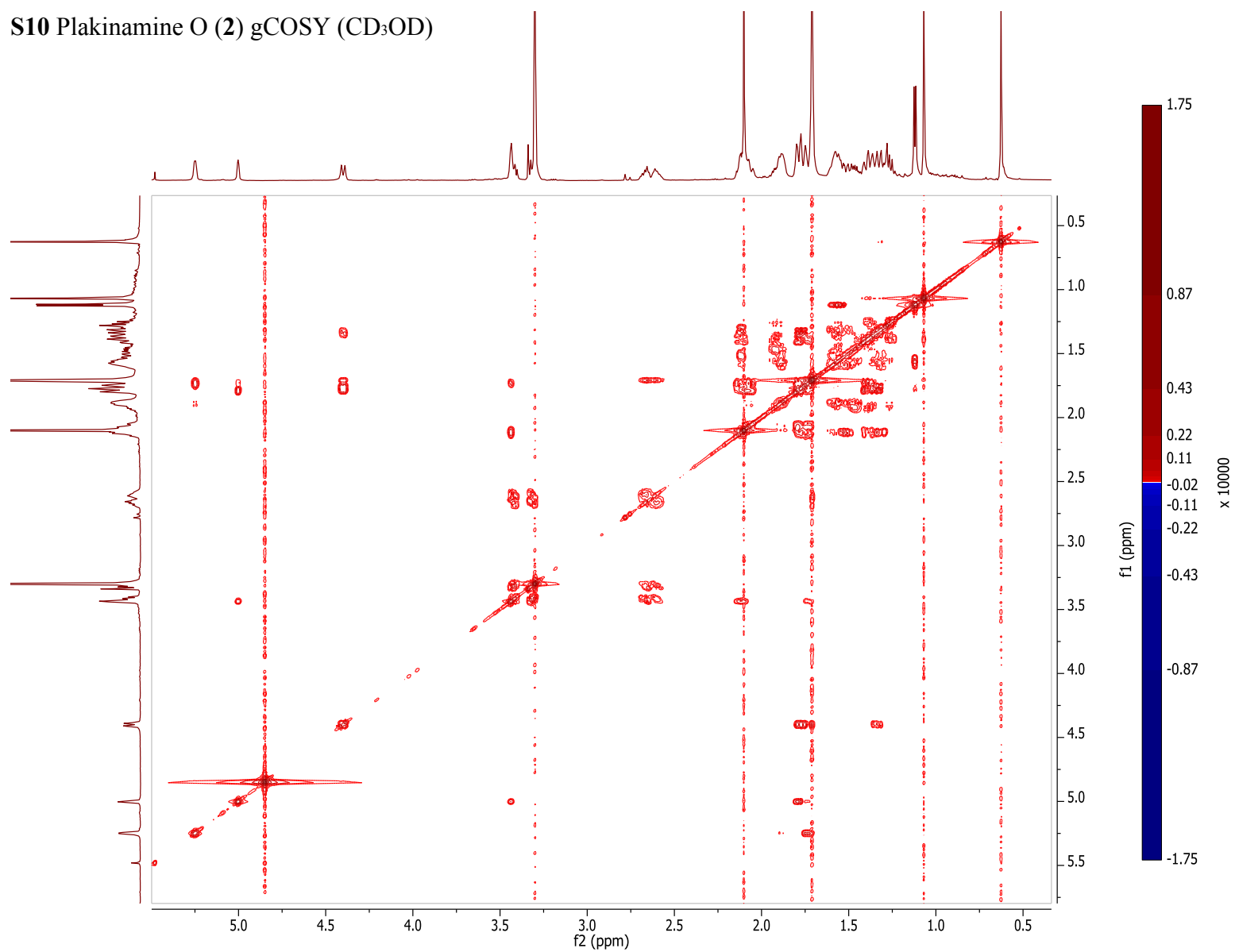
S8 Plakinamine O (2) ¹H NMR (600 MHz, CD₃OD)



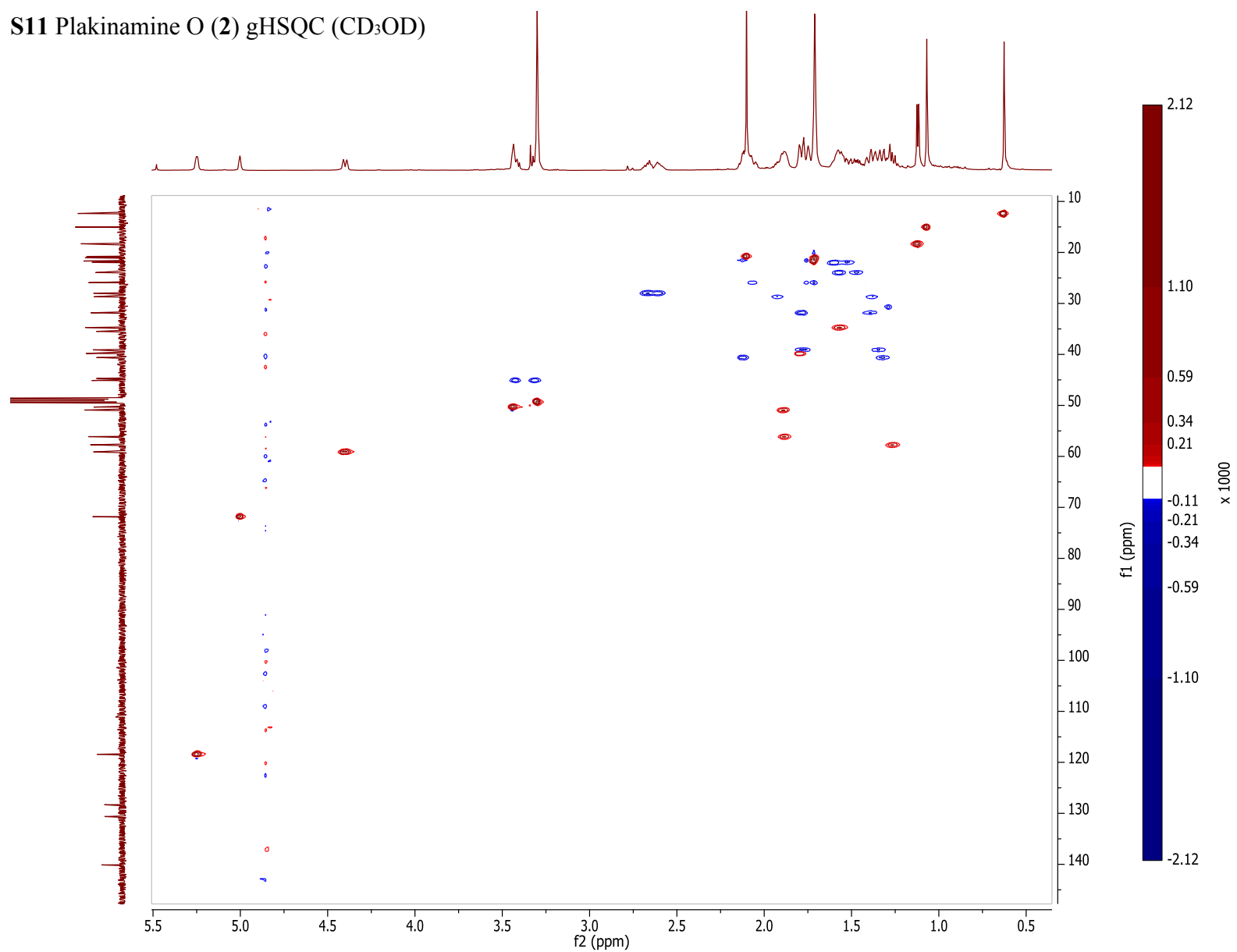
S9 Plakinamine O (2) ¹³C NMR (150 MHz, CD₃OD)



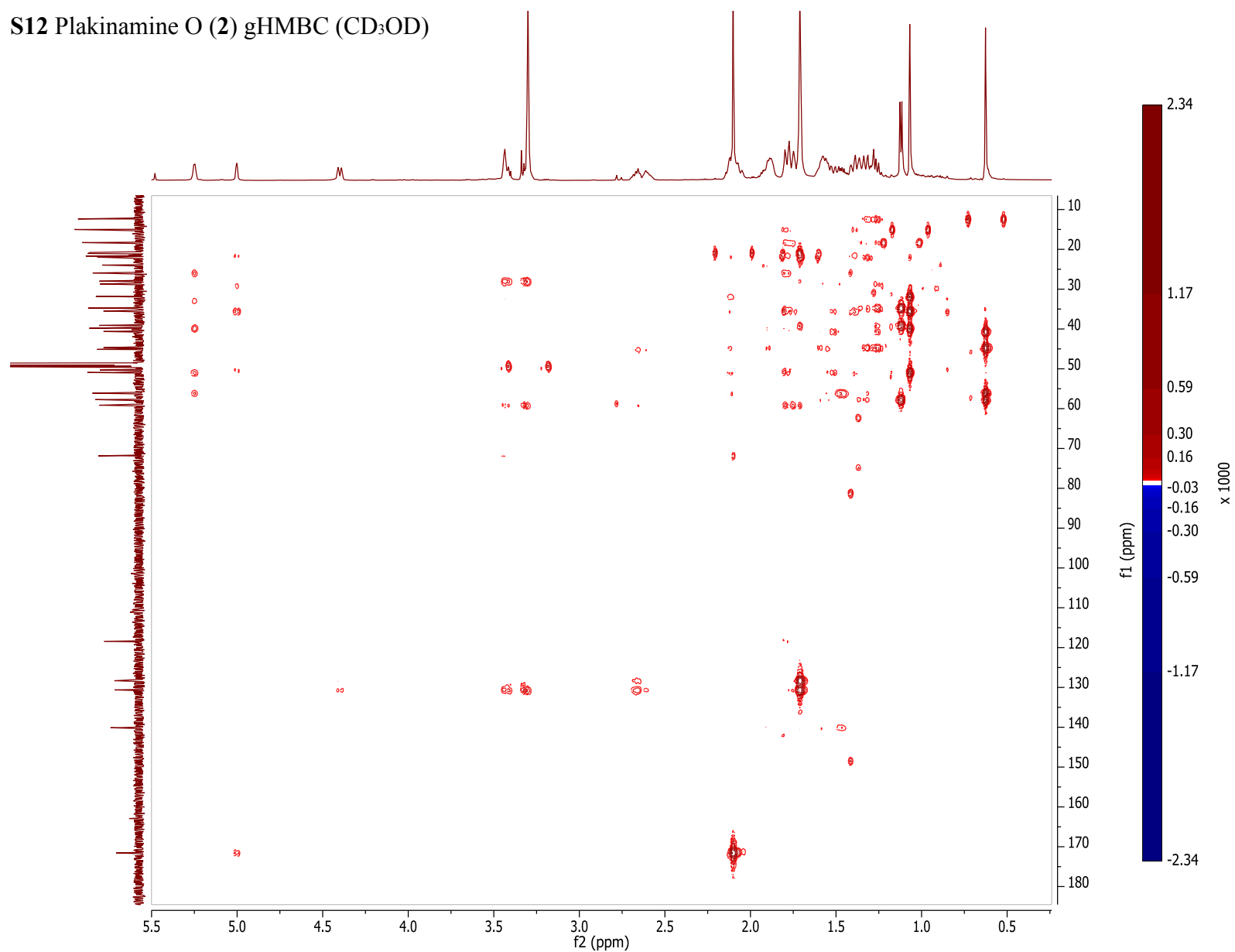
S10 Plakinamine O (2) gCOSY (CD₃OD)



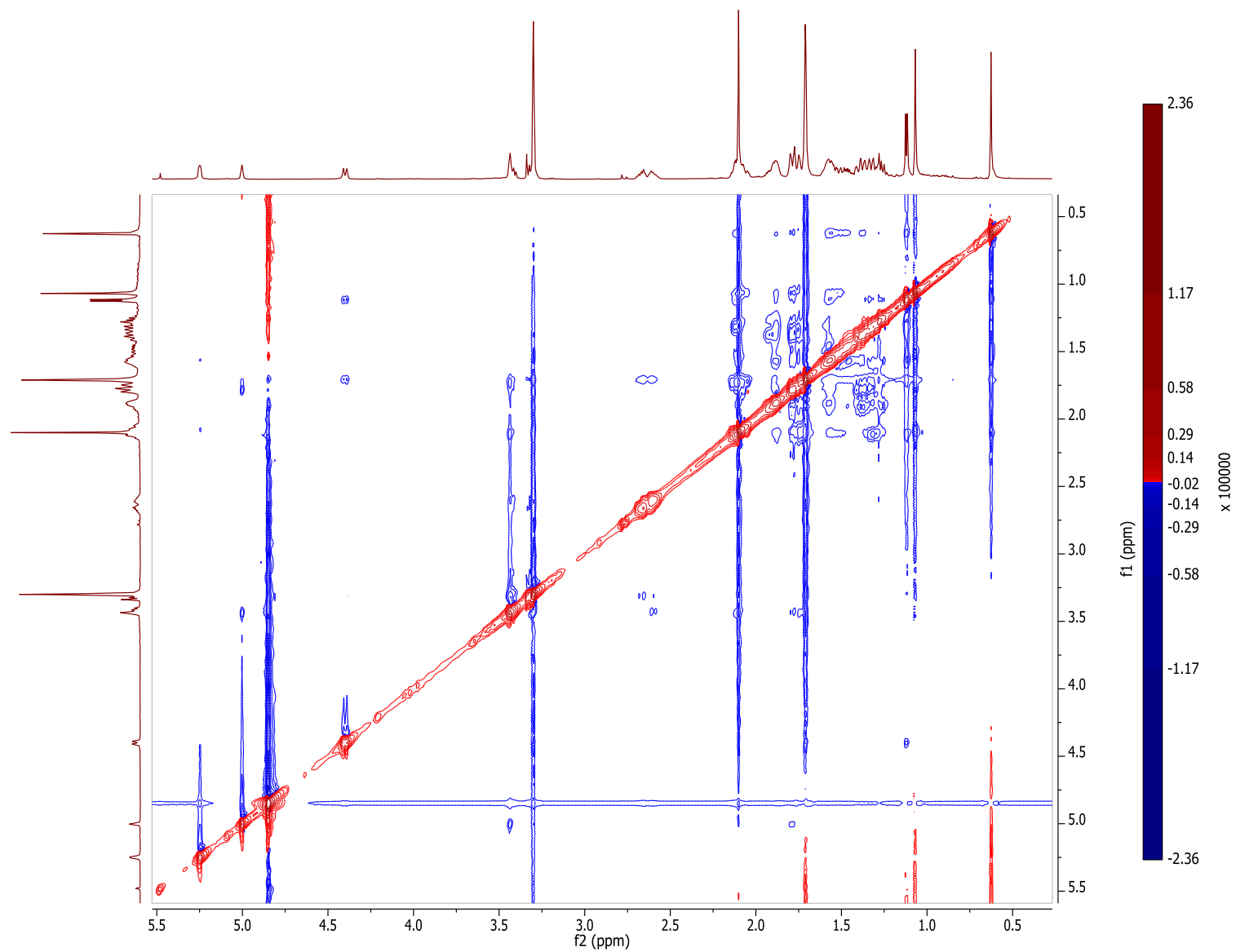
S11 Plakinamine O (2) gHSQC (CD₃OD)



S12 Plakinamine O (2) gHMBC (CD₃OD)



S13 Plakinamine O (2) ROESY (CD₃OD)



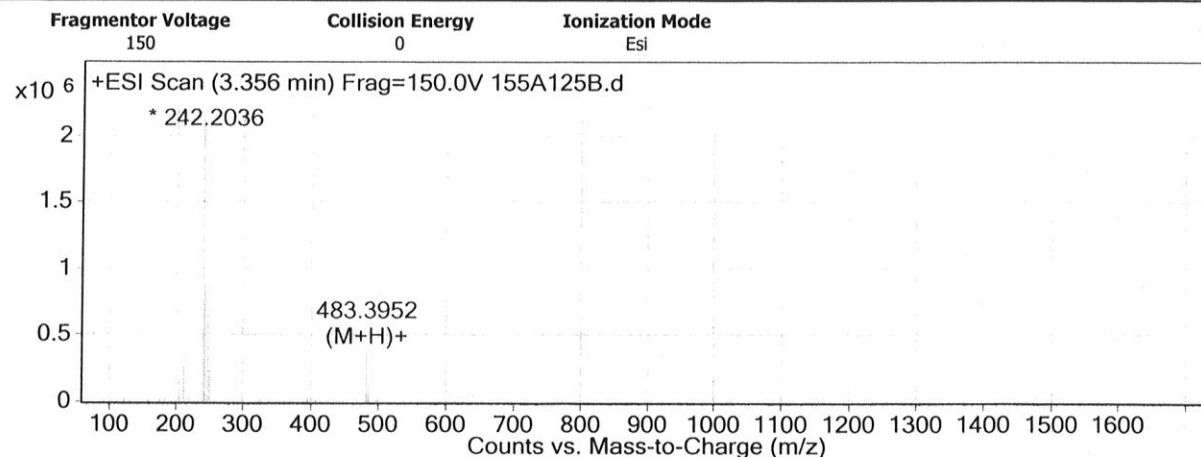
S14 Plakinamine O (2) HRESIMS (+)

MS Formula Results: + Scan (3.356 min) (155A125B.d)

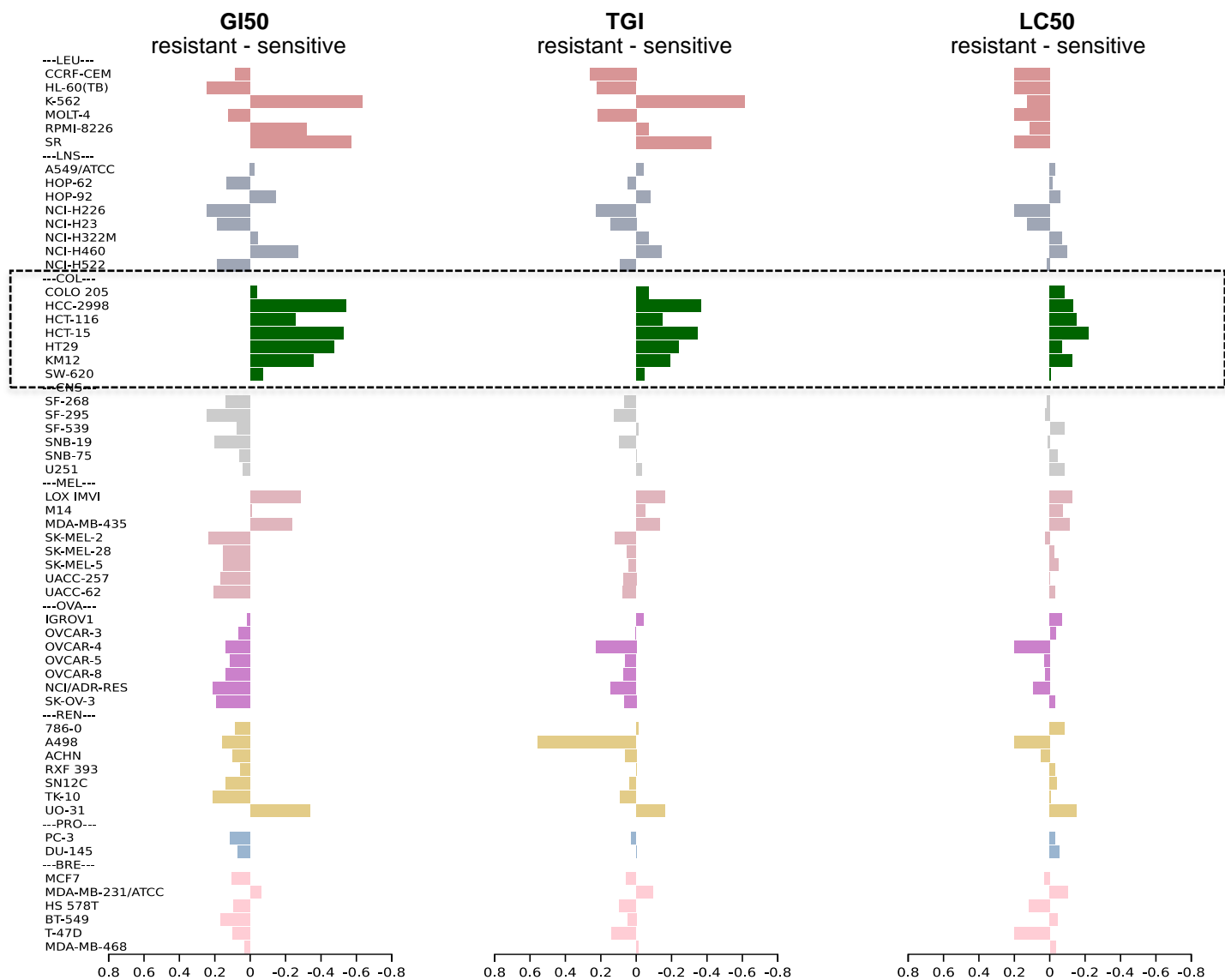
m/z	Ion	Formula	Abundance
483.3952	(M+H) ⁺	C ₃₁ H ₅₁ N ₂ O ₂	379393.1

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
<input checked="" type="checkbox"/>	C ₃₁ H ₅₀ N ₂ O ₂	C ₃₁ H ₅₁ N ₂ O ₂	98.22		483.3945	-1.35	98.09	97.46	99.37
<input type="checkbox"/>	C ₂₄ H ₅₀ N ₈ S	C ₂₄ H ₅₁ N ₈ S	93.05		483.3952	0.02	100	85.45	88.28
<input type="checkbox"/>	C ₂₇ H ₄₆ N ₈	C ₂₇ H ₄₇ N ₈	80.79		483.3918	-6.95	60.2	99.51	99.53
<input type="checkbox"/>	C ₂₈ H ₅₄ N ₂ O ₂ S	C ₂₈ H ₅₅ N ₂ O ₂ S	80.53		483.3979	5.62	71.73	85.03	92.72

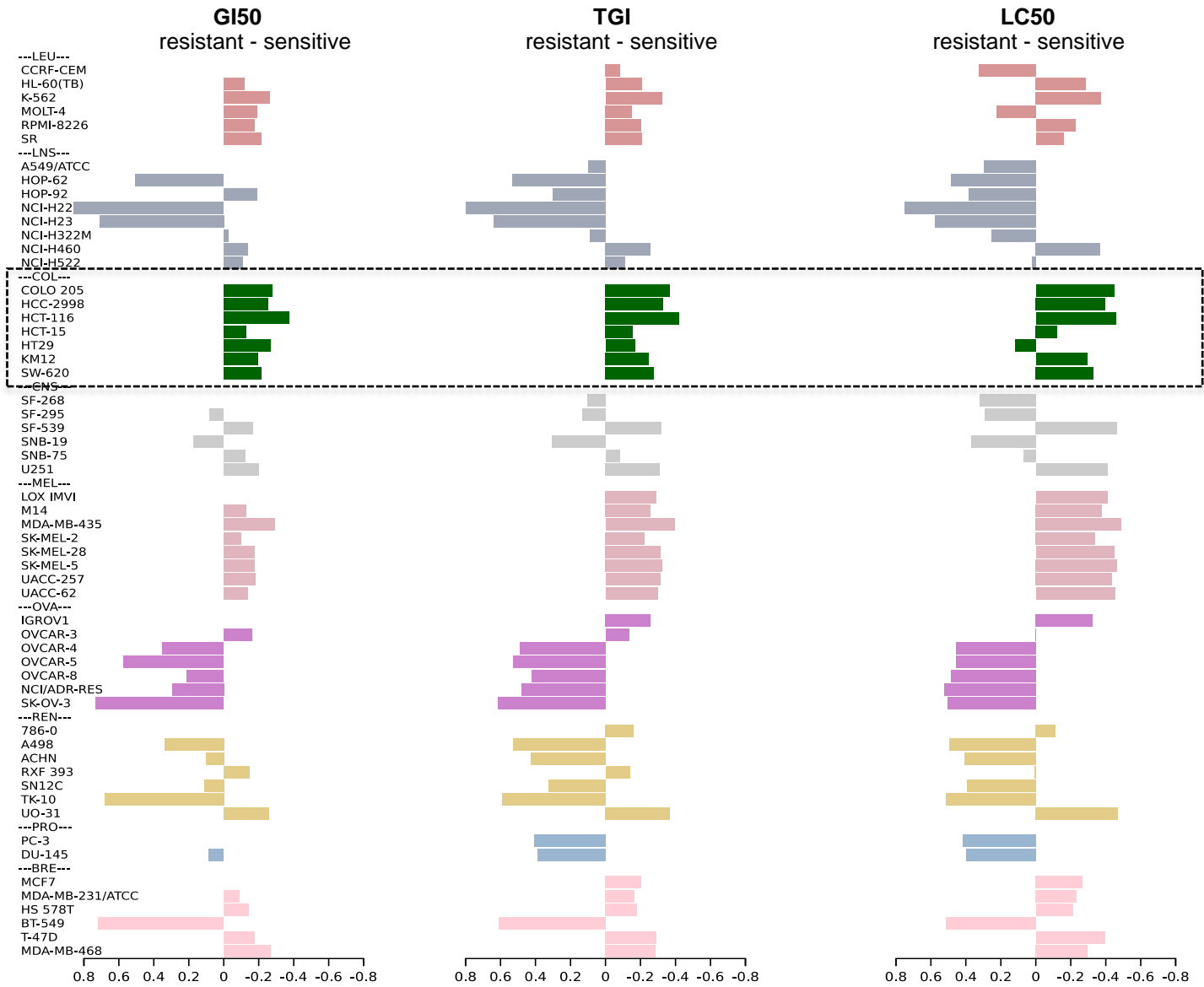
User Spectra



S15 Plakinamine N (1), NSC 775605: NCI-60 mean bar graphs



S16 Plakinamine O (2), NSC 775606: NCI-60 mean bar graphs



S17 Plakinamine J (4), NSC 775603: NCI-60 mean bar graphs

