Supporting information

An Aminopyrimidone and Aminoimidazoles Alkaloids from the Rodrigues Calcareous Marine Sponge *Ernsta naturalis*

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Supporting information

In situ Ernsta naturalis Photo

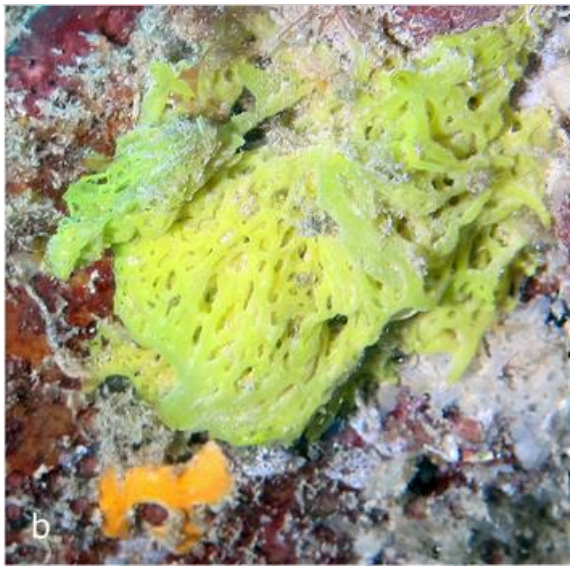

Figure S1: HRESIMS spectrum for ernstine A (1)

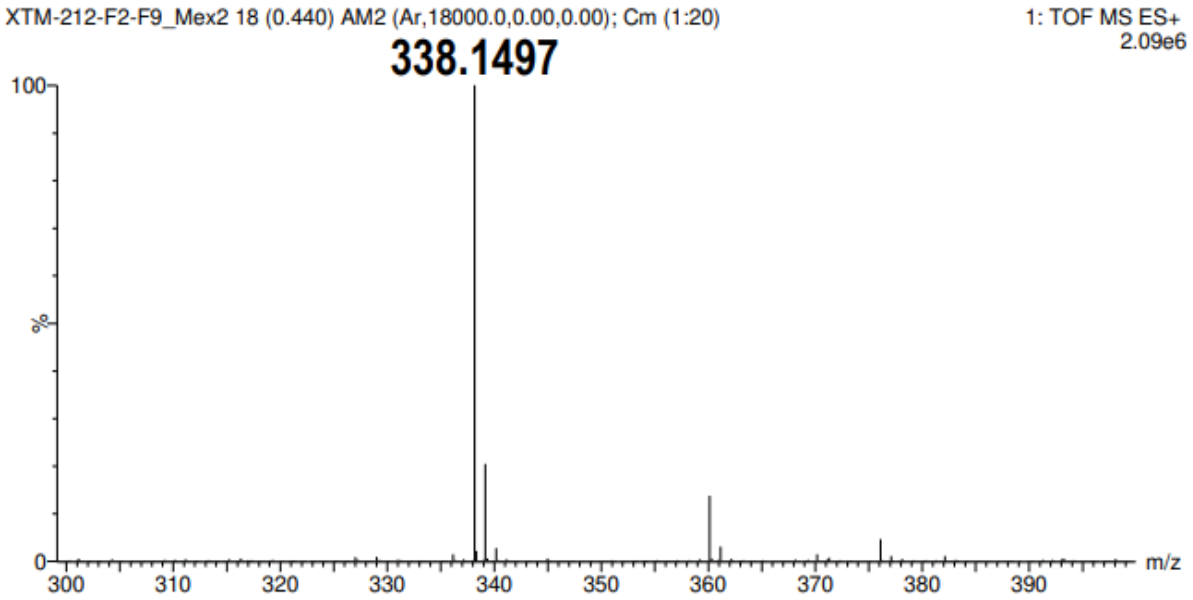

Figure S2: ^{1}H NMR (600 MHz, CD_3OD) spectrum for ernstine A (1)

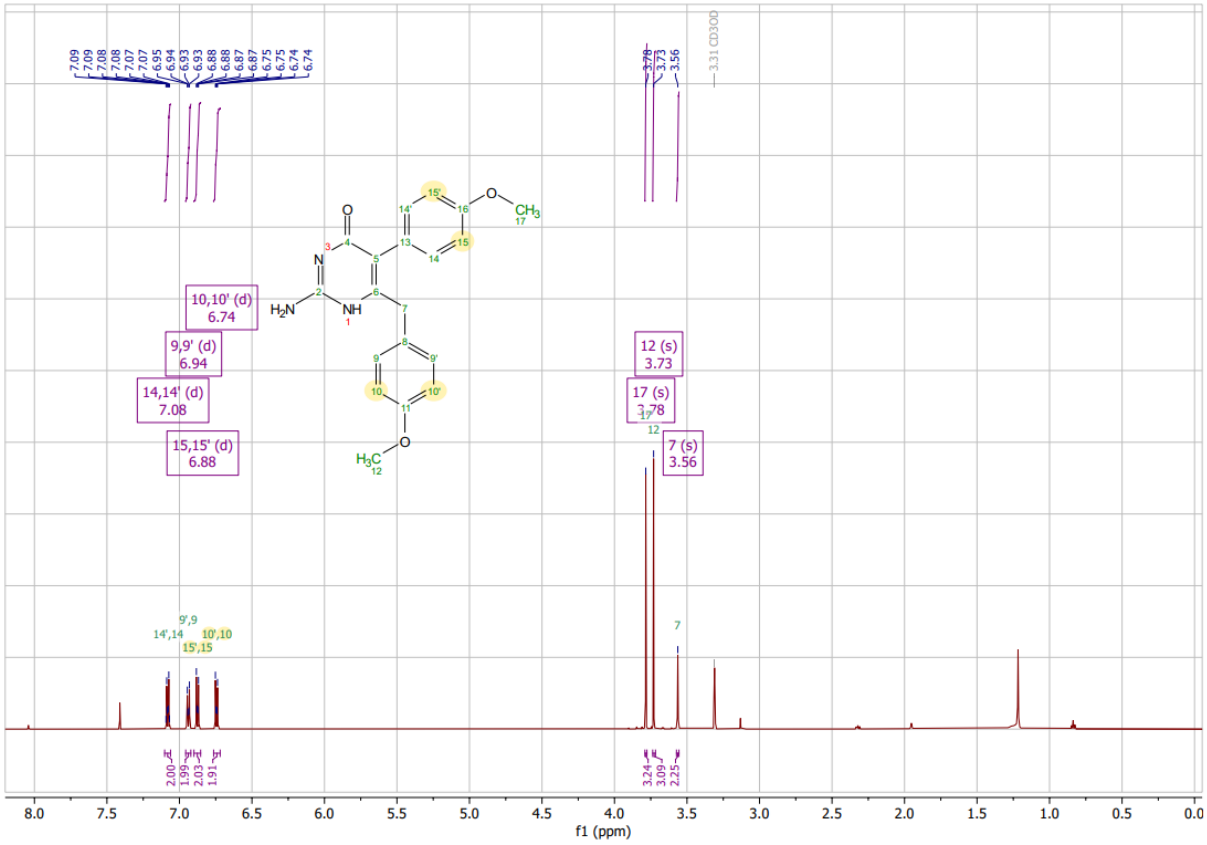

Figure S3: ^{1}H-^{1}H COSY NMR (600 MHz) spectrum for ernstine A (1)

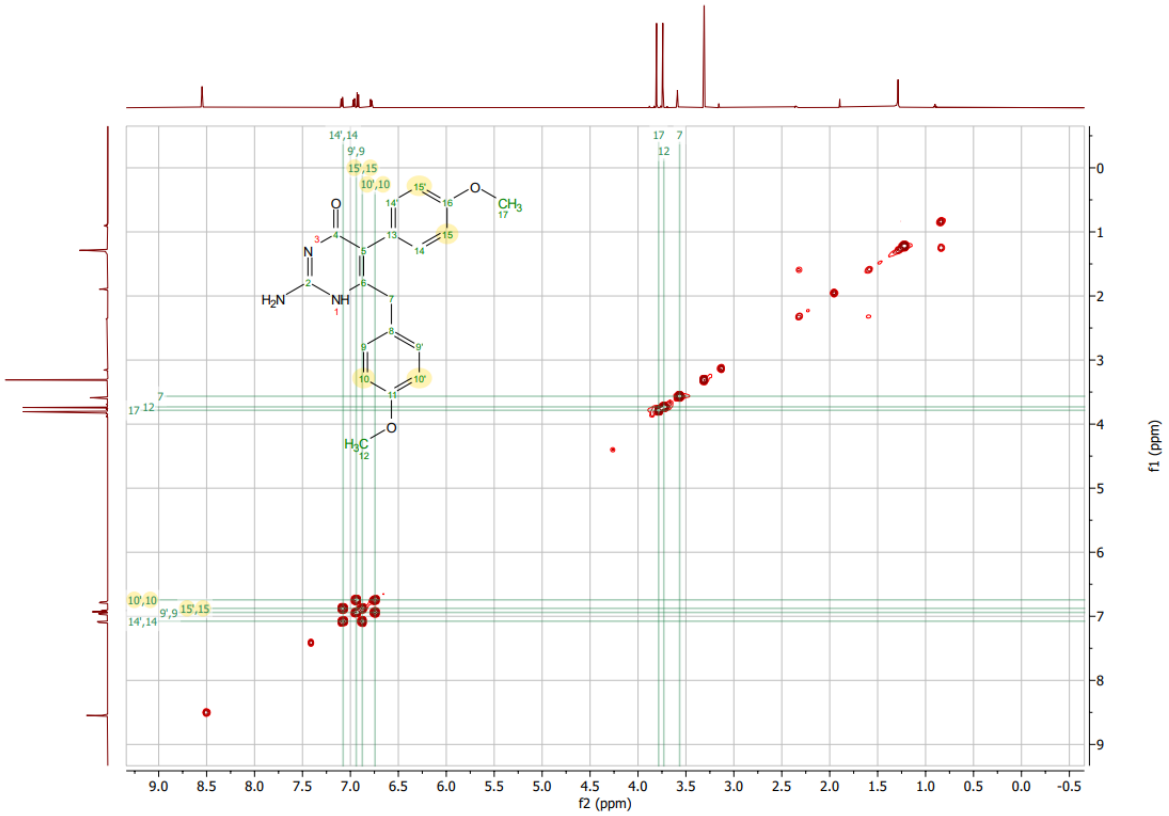

Figure S4: ^{1}H-^{13}C HSQC NMR (600 MHz) spectrum for ernstine A (1)

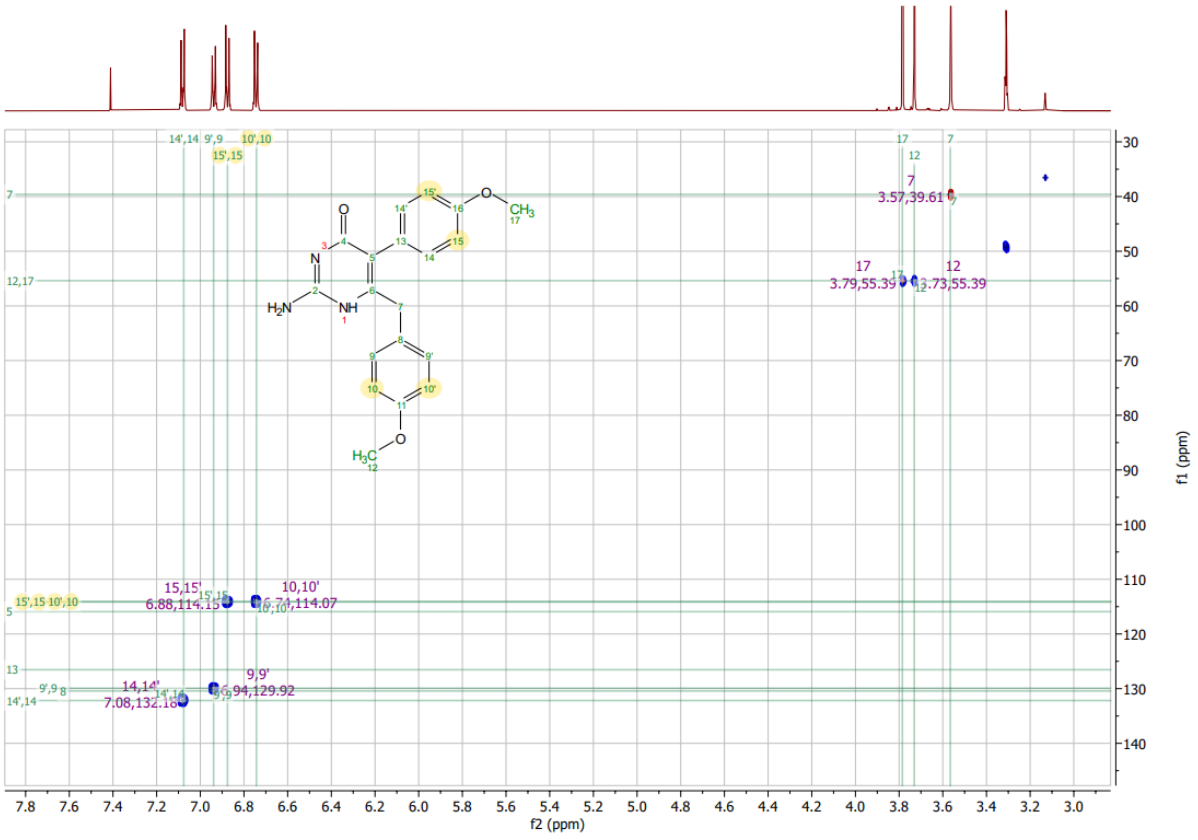

Figure S5: ^{1}H-^{13}C HMBC NMR (600 MHz) spectrum for ernstine A (1)

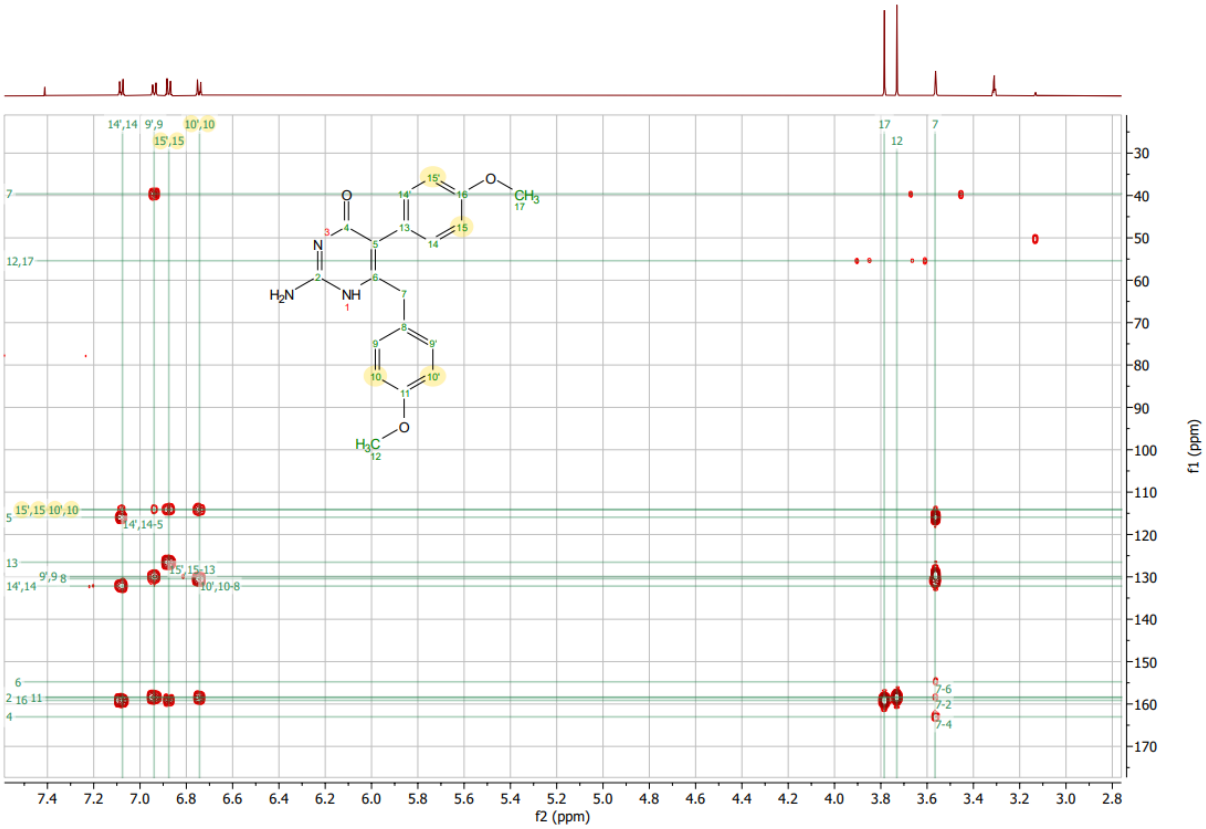

Figure S6: ^{1}H-^{1}H NOESY NMR (600 MHz) spectrum for ernstine A (1)

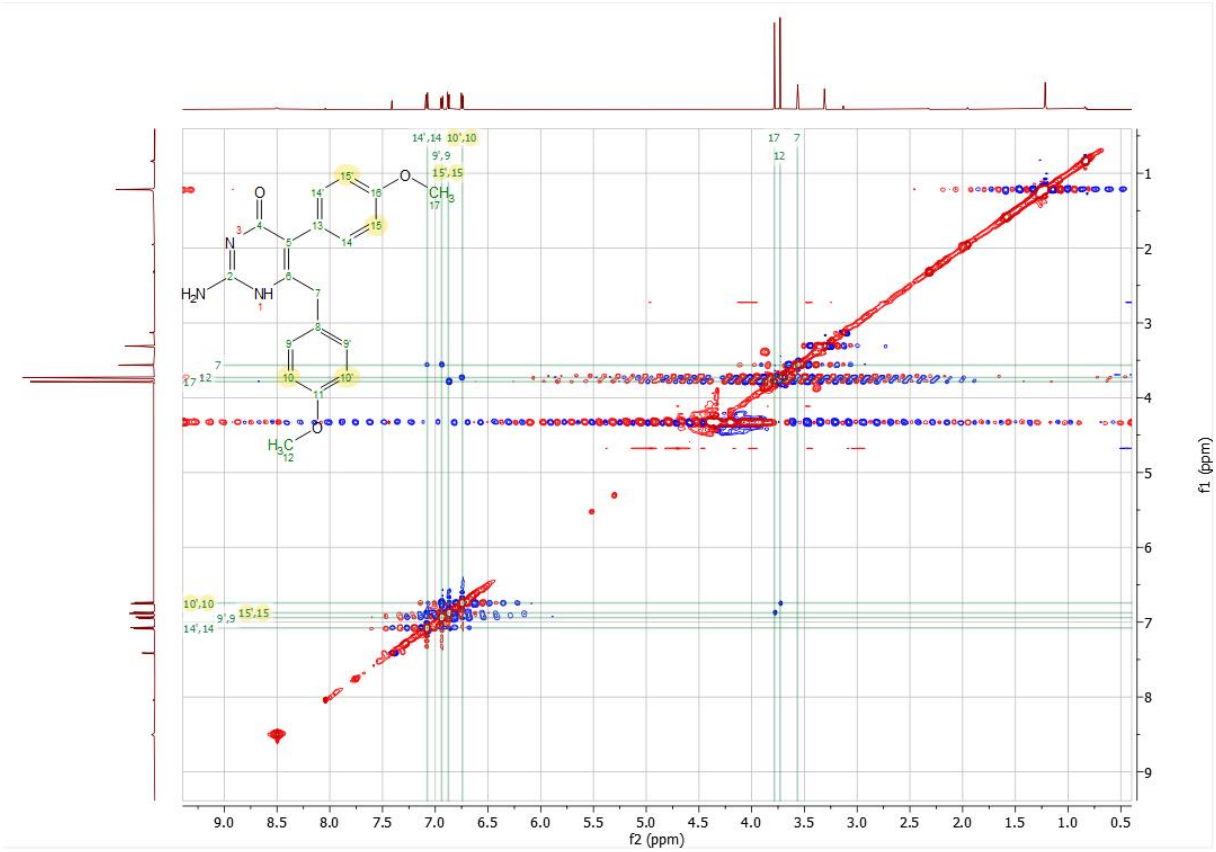

Figure S7: HRESIMS spectrum for phorbatopsin D (2)

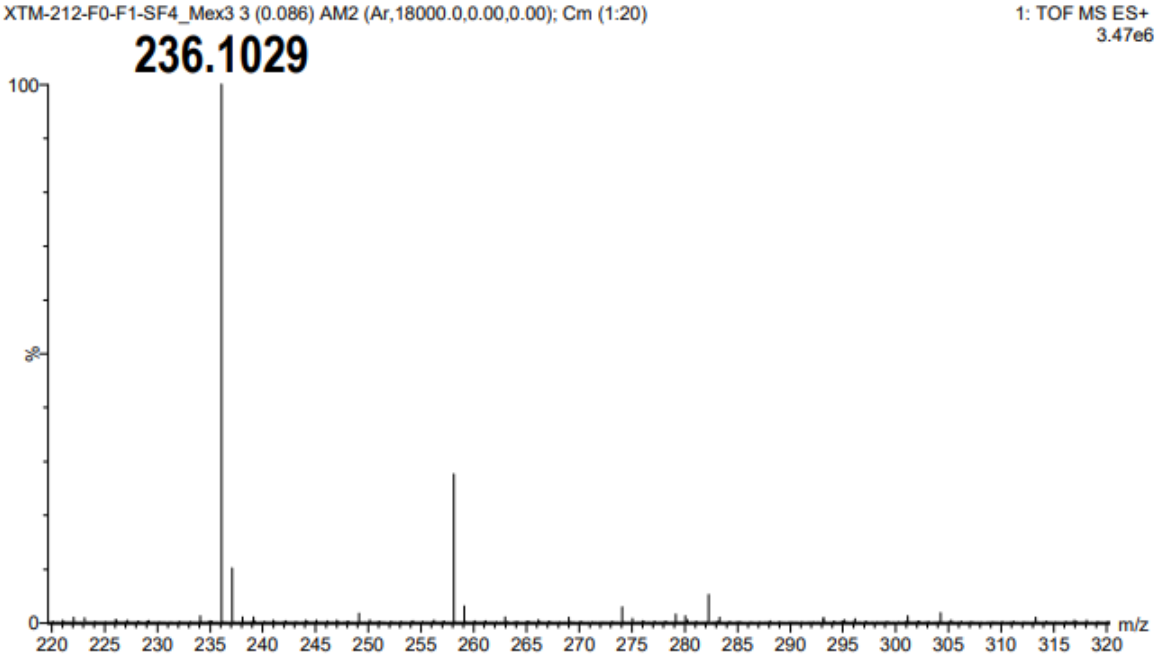

Figure S8: ^{1}H NMR (600 MHz, CD_3OD) spectrum for phorbatopsin D (2)

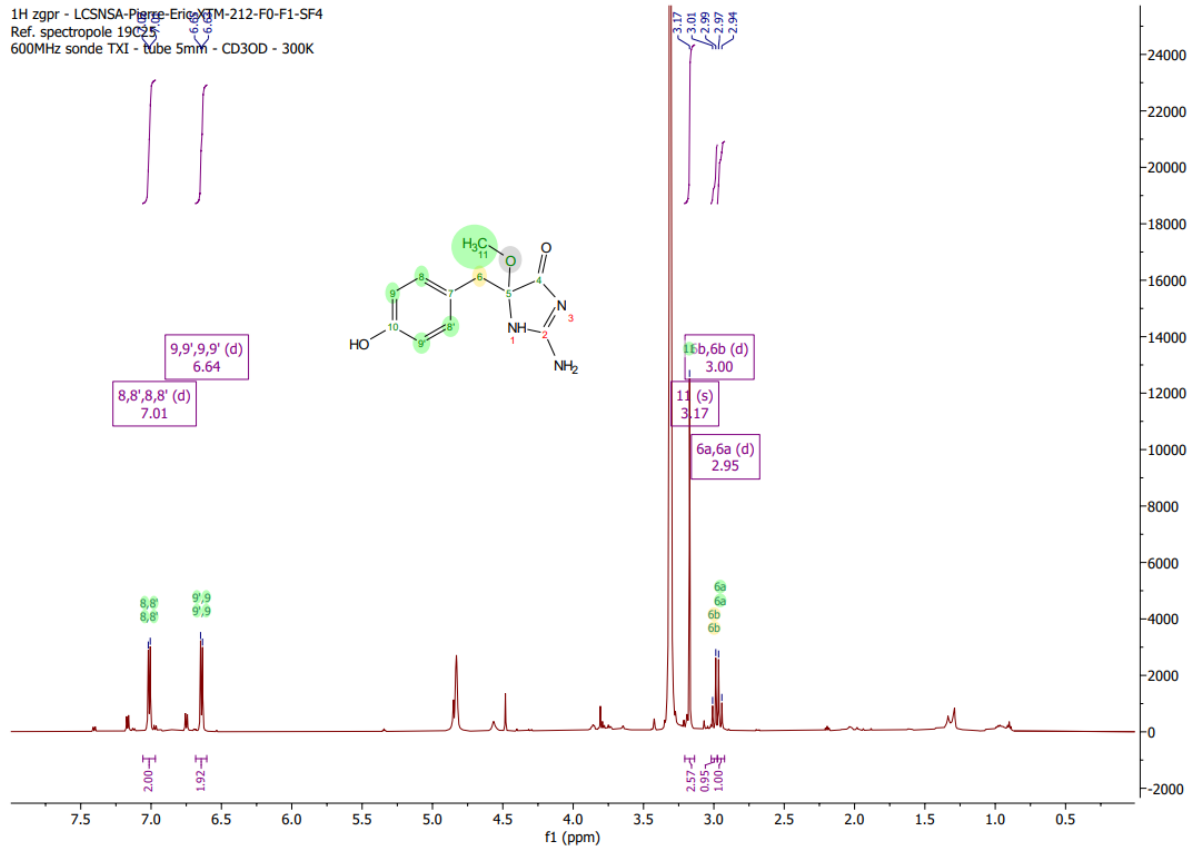

Figure S9: ^{13}C NMR (125 MHz, CD_3OD) spectrum for phorbatopsin D (2)

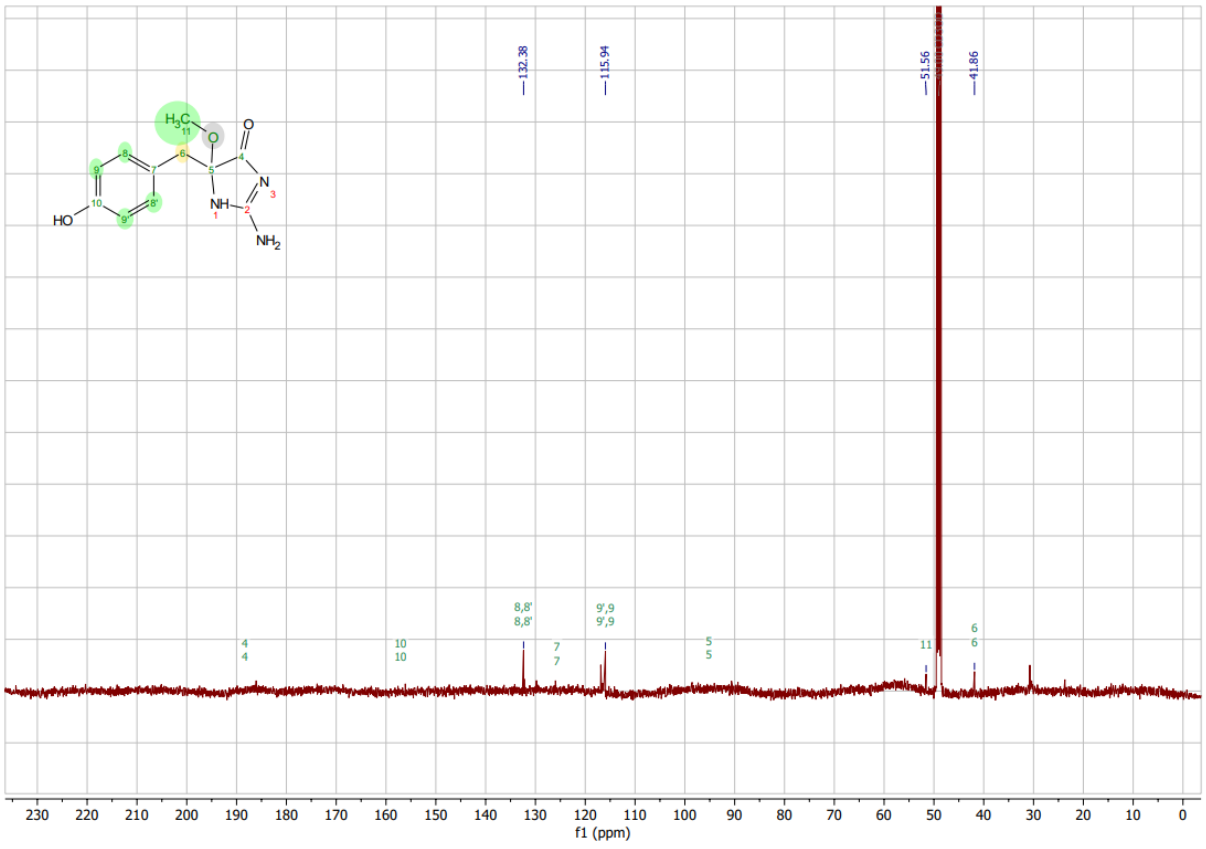

Figure S10: ^{1}H-^{13}C HSQC NMR (600 MHz) spectrum for phorbatopsin D (2)

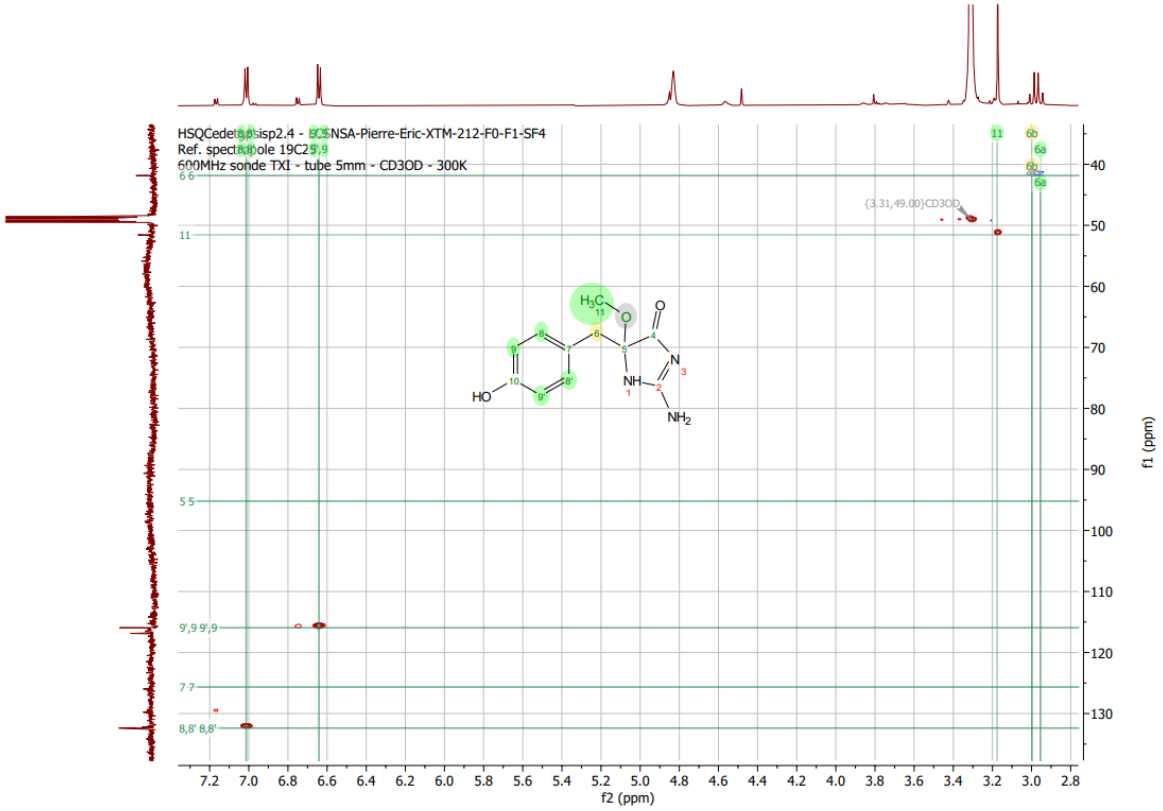

Figure S11: ^{1}H-^{13}C HMBC NMR (600 MHz) spectrum for phorbatopsin D (2)

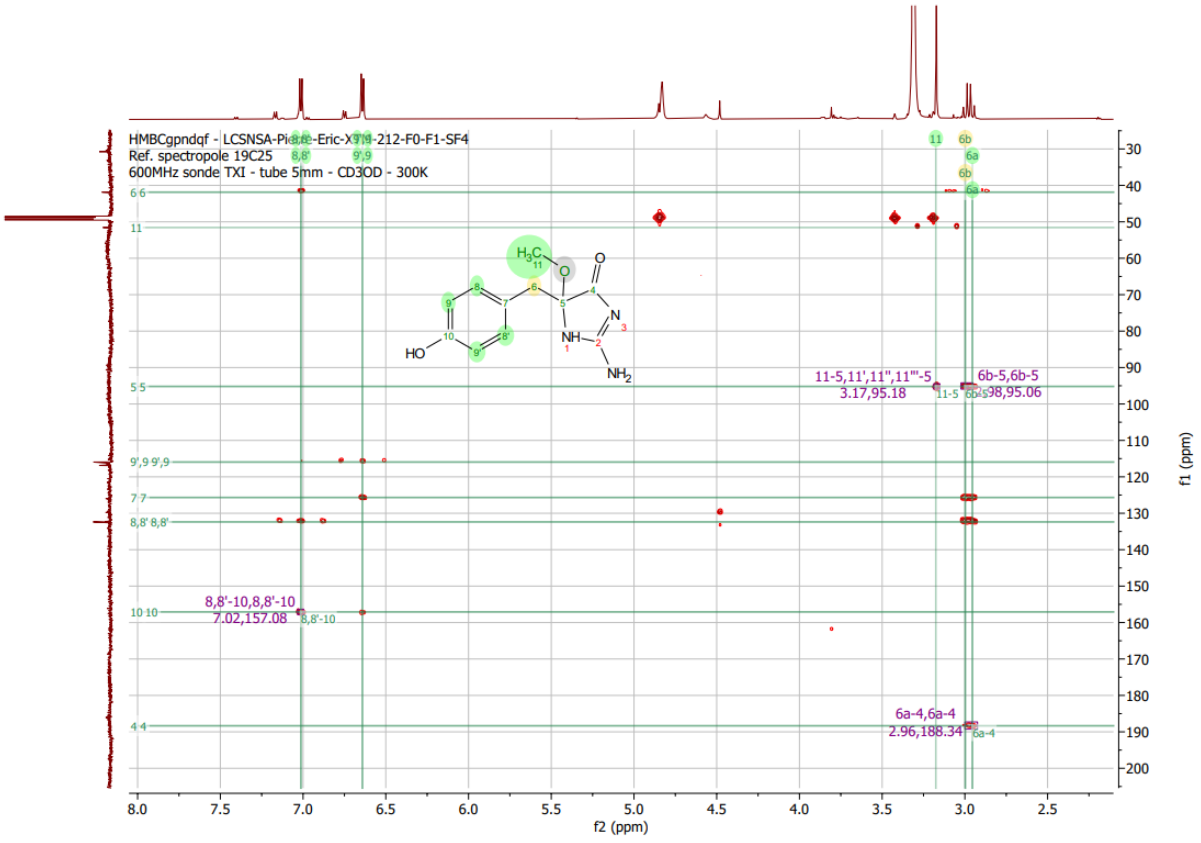

Figure S12: HRESIMS spectrum for phorbatopsin E (3)

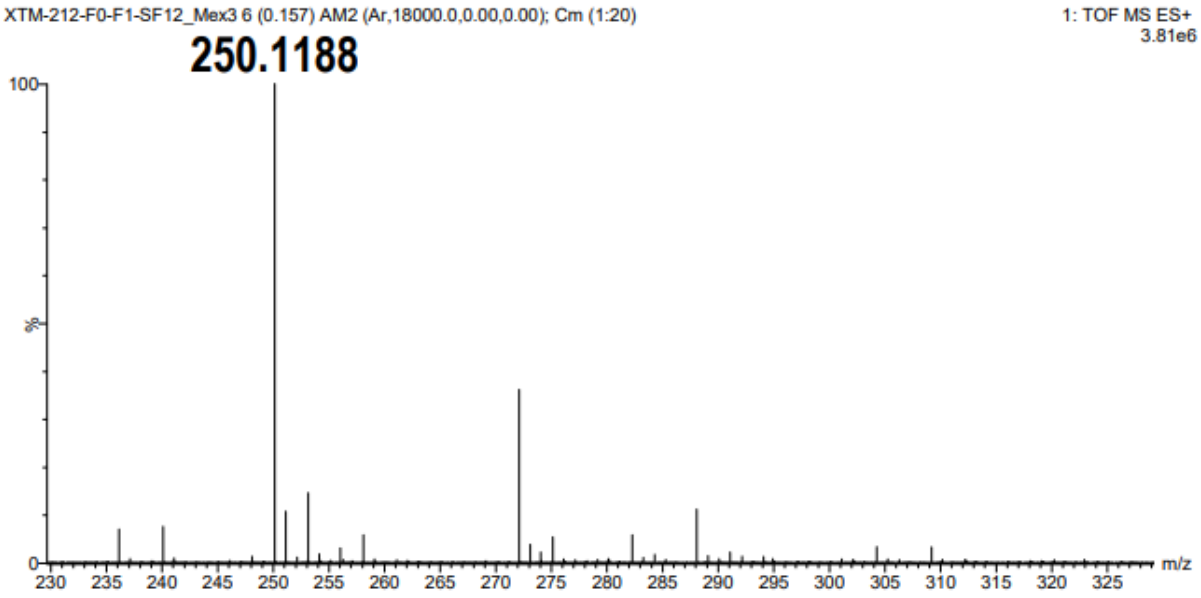

Figure S13: ^{1}H NMR (600 MHz, CD_3OD) spectrum for phorbatopsin E (3)

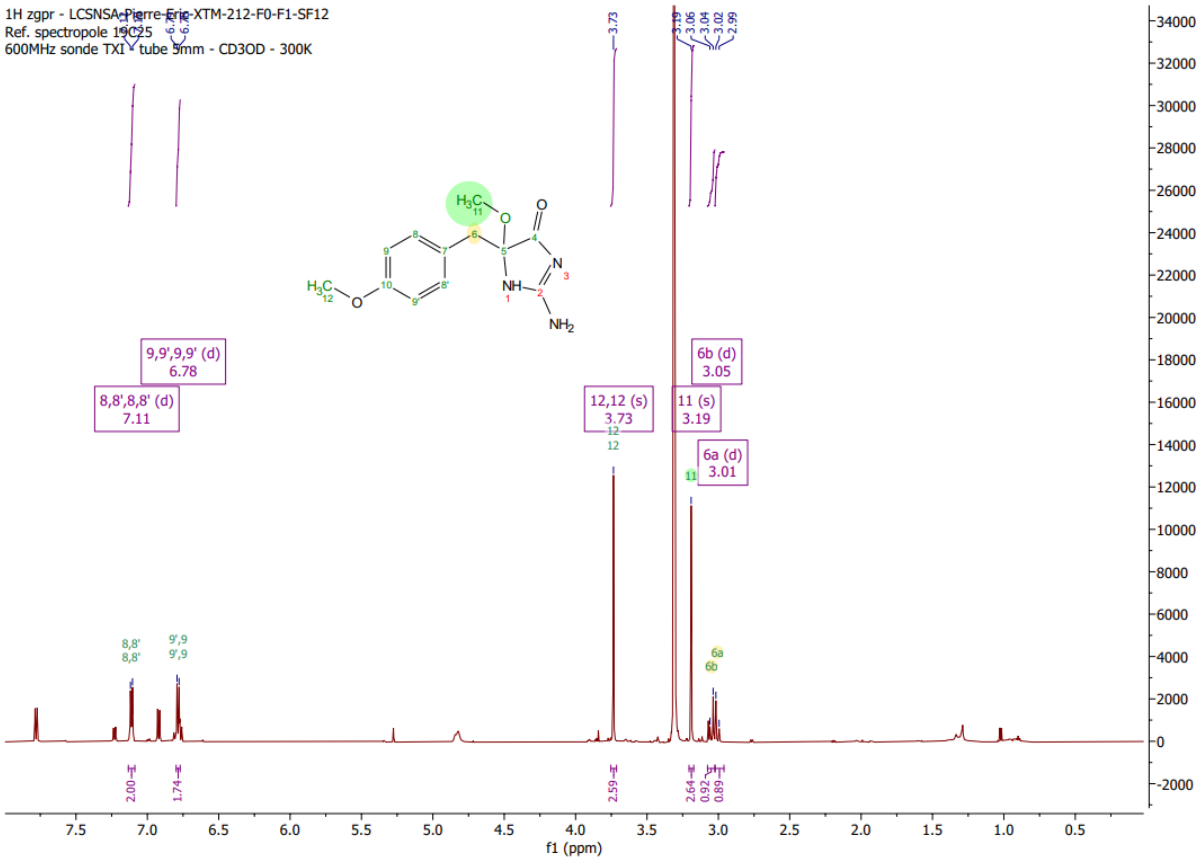

Figure S14: ^{1}H-^{13}C HSQC NMR (600 MHz) spectrum for phorbatopsin E (3)

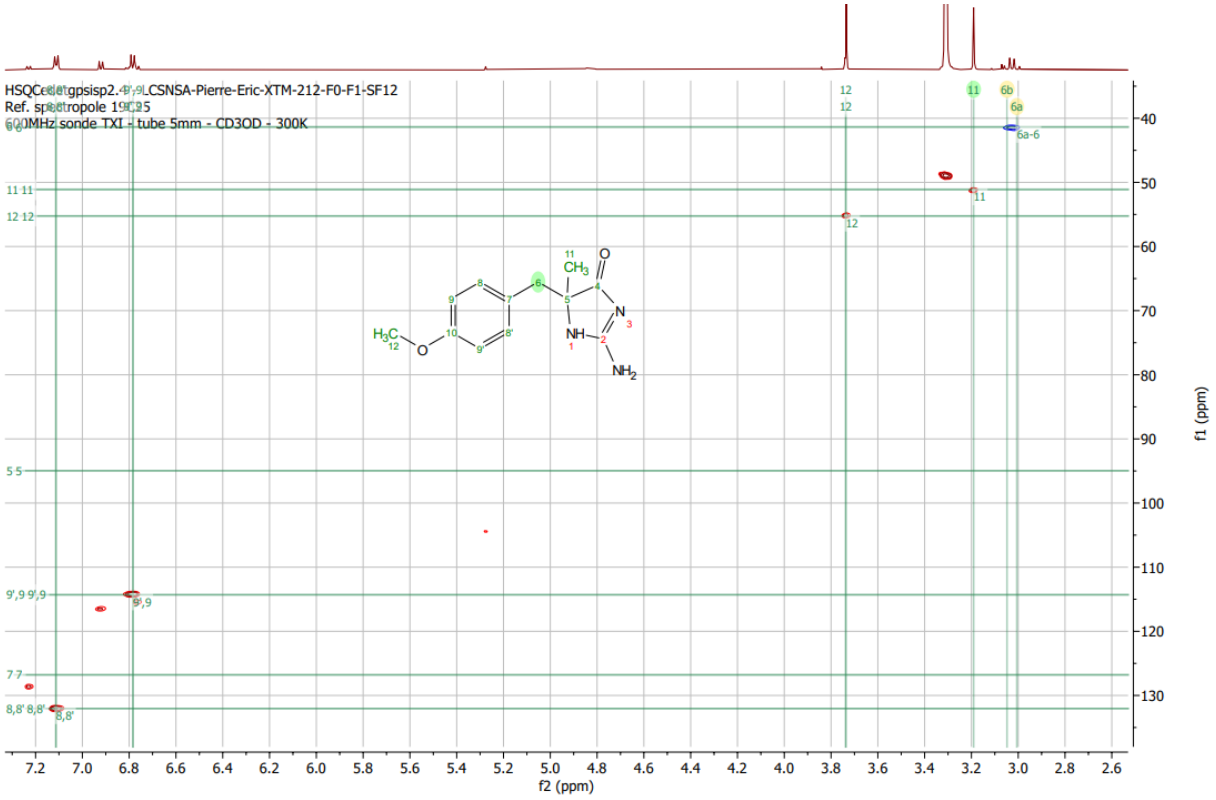

Figure S15: ^{1}H-^{13}C HMBC NMR (600 MHz) spectrum for phorbatopsin E (3)

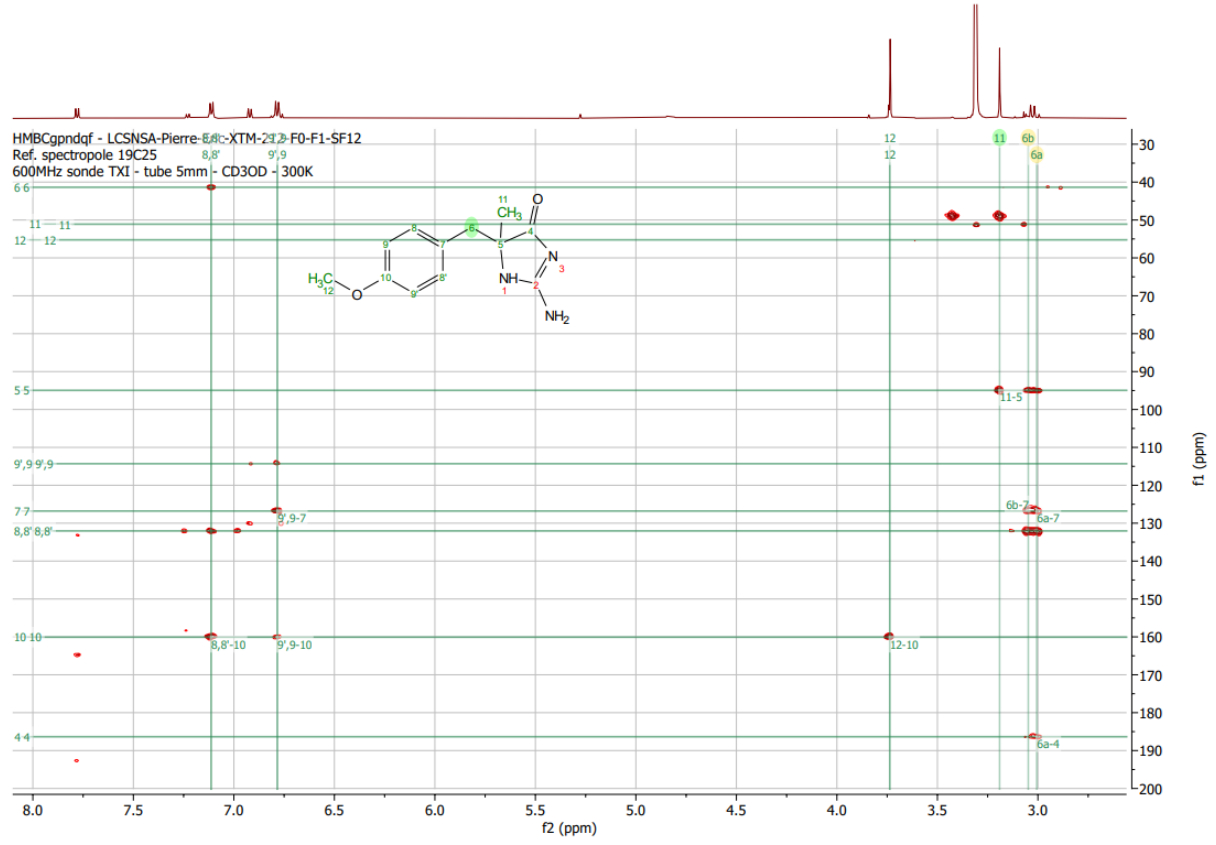

Figure S16: ^{1}H-^{1}H NOESY NMR (600 MHz) spectrum for phorbatopsin E (3)

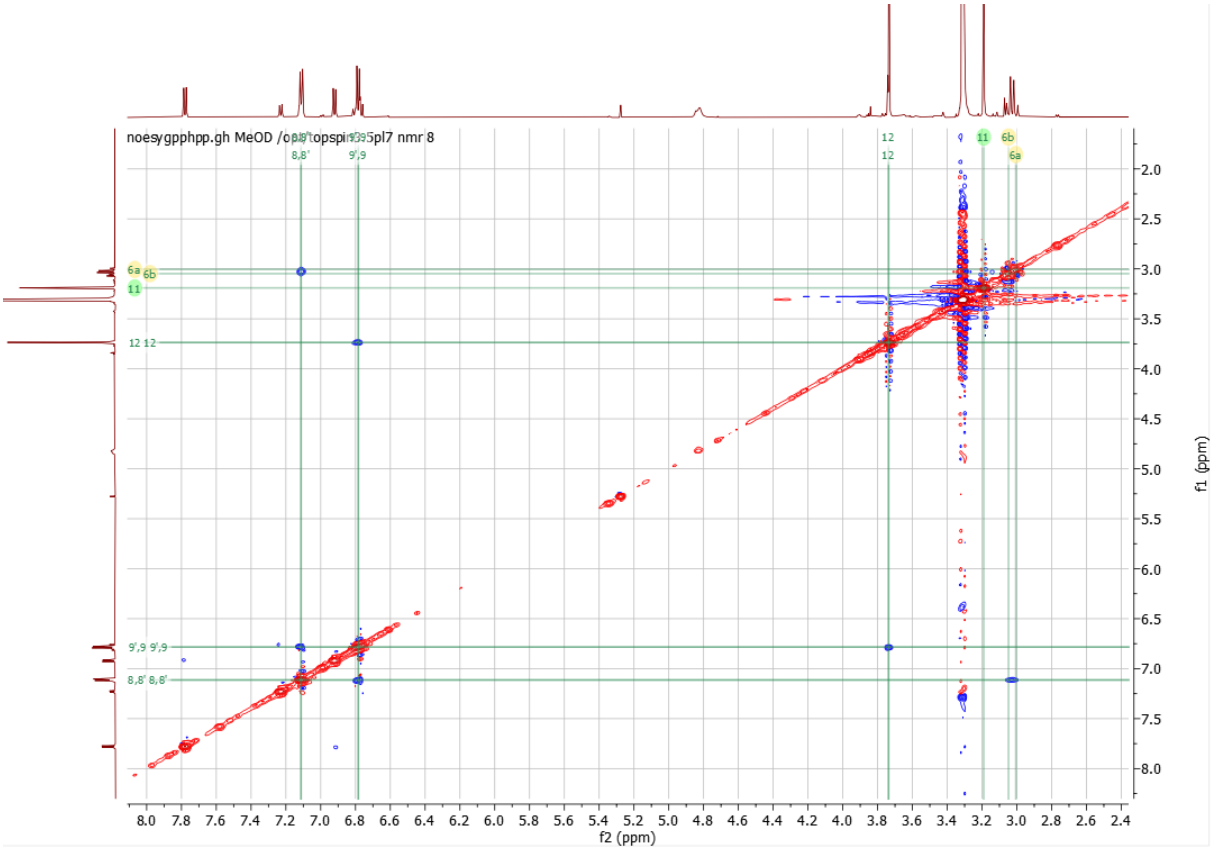

Figure S17: HRESIMS spectrum for calcaridine C (4)

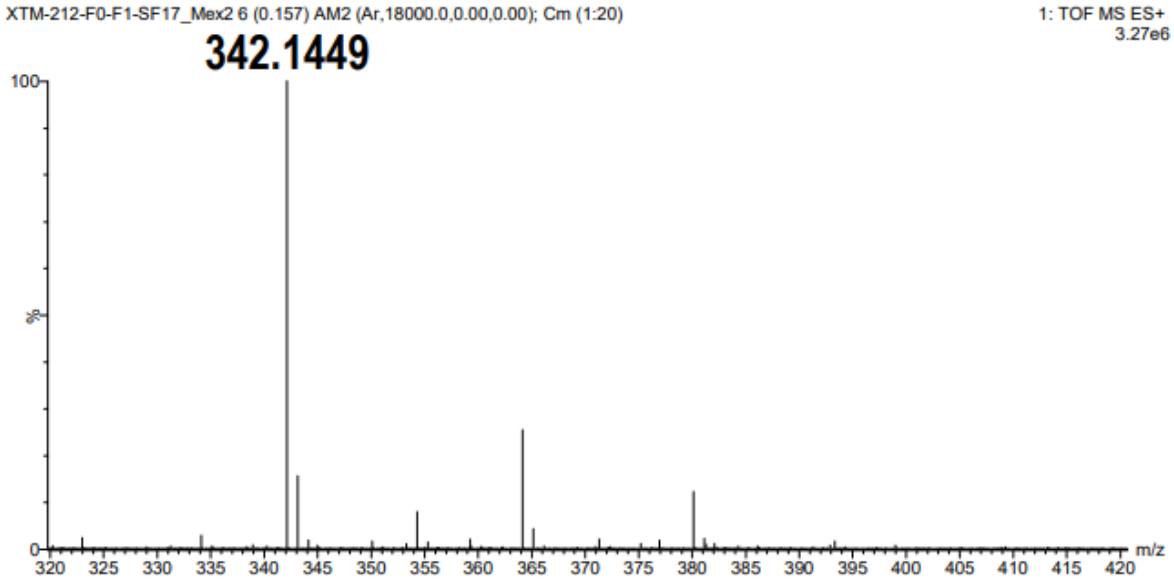

Figure S18: ^{1}H NMR (600 MHz, CD_3OD) spectrum for calcaridine C (4)

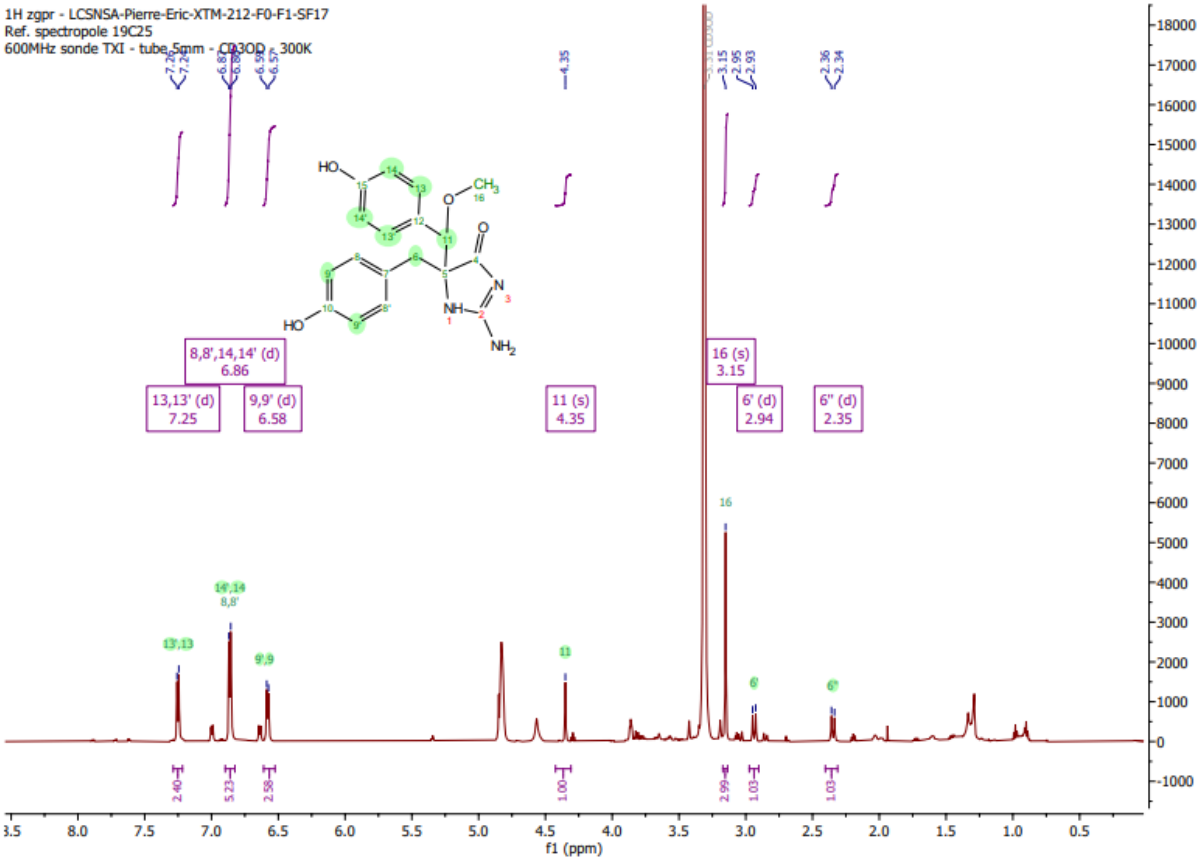

Figure S19: ^{13}C NMR (125 MHz, CD_3OD) spectrum for calcaridine C (4)

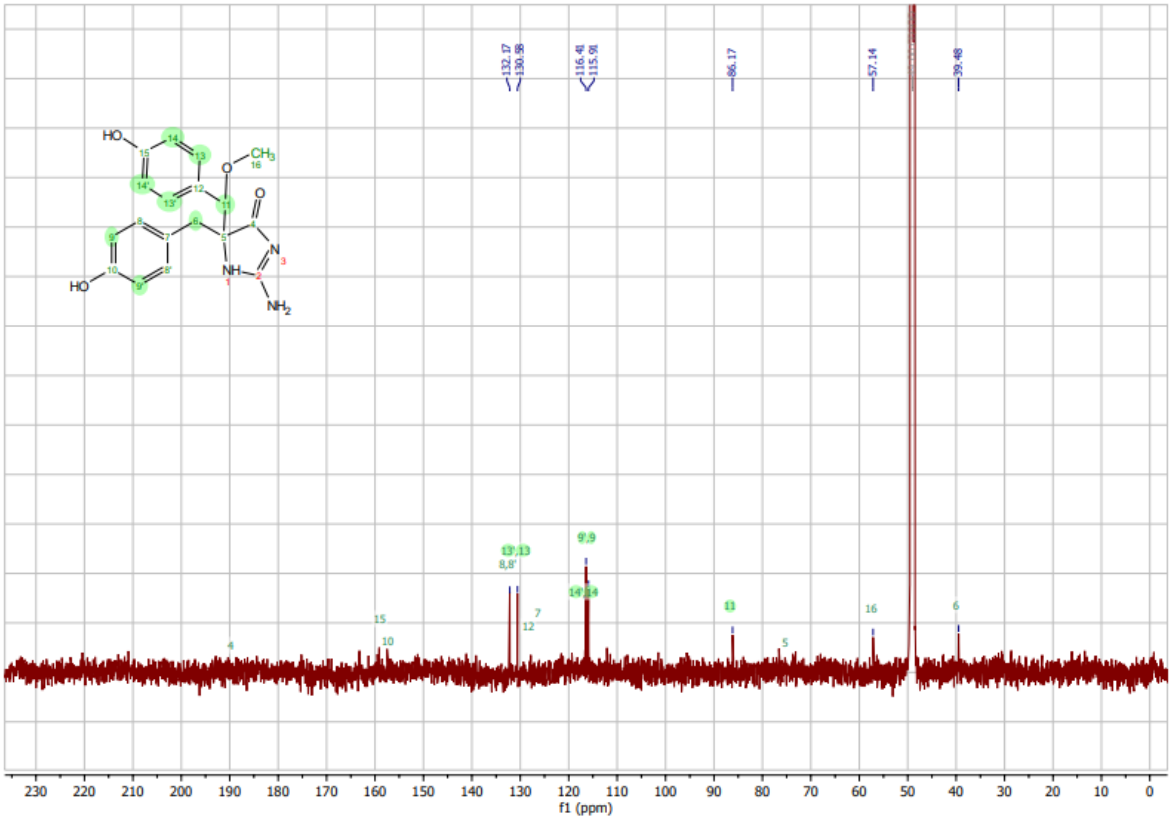

Figure S20: ^{1}H-^{1}H COSY NMR (600 MHz) spectrum for calcaridine C (4)

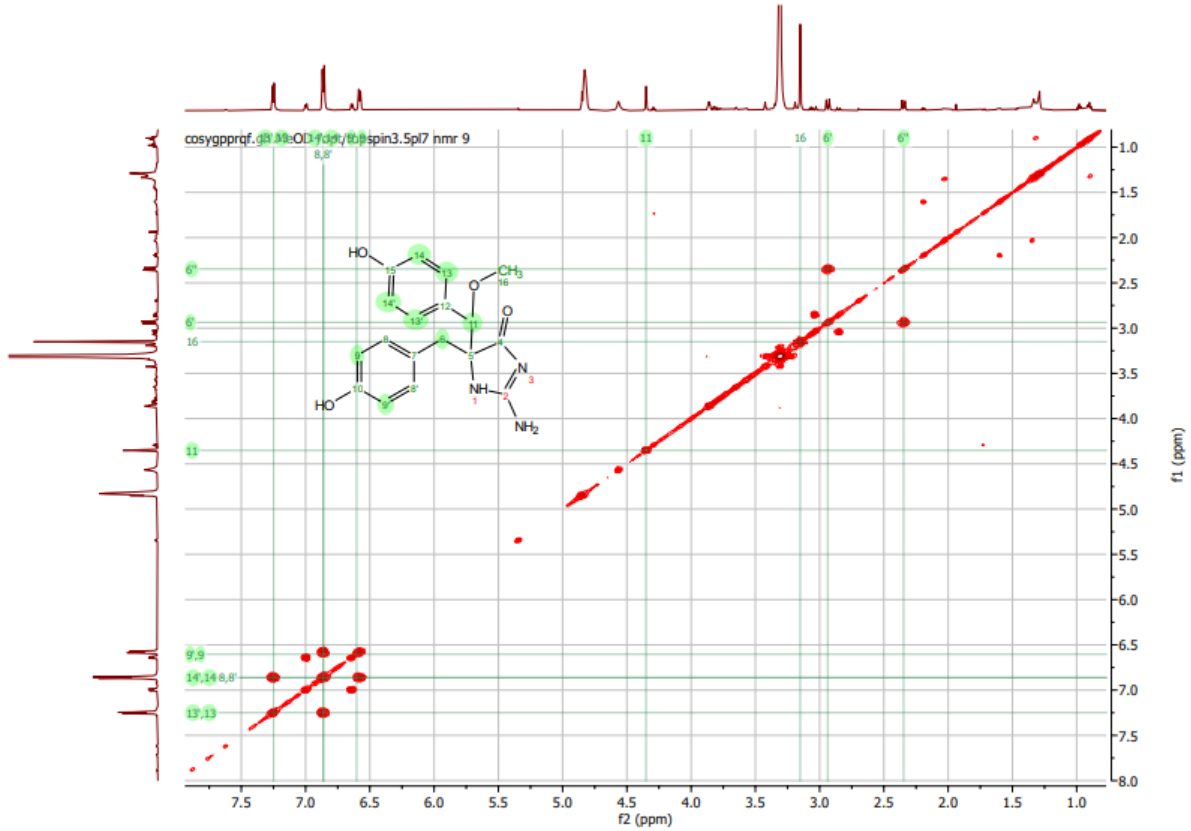

Figure S21: ^{1}H-^{13}C HSQC NMR (600 MHz) spectrum for calcaridine C (4)

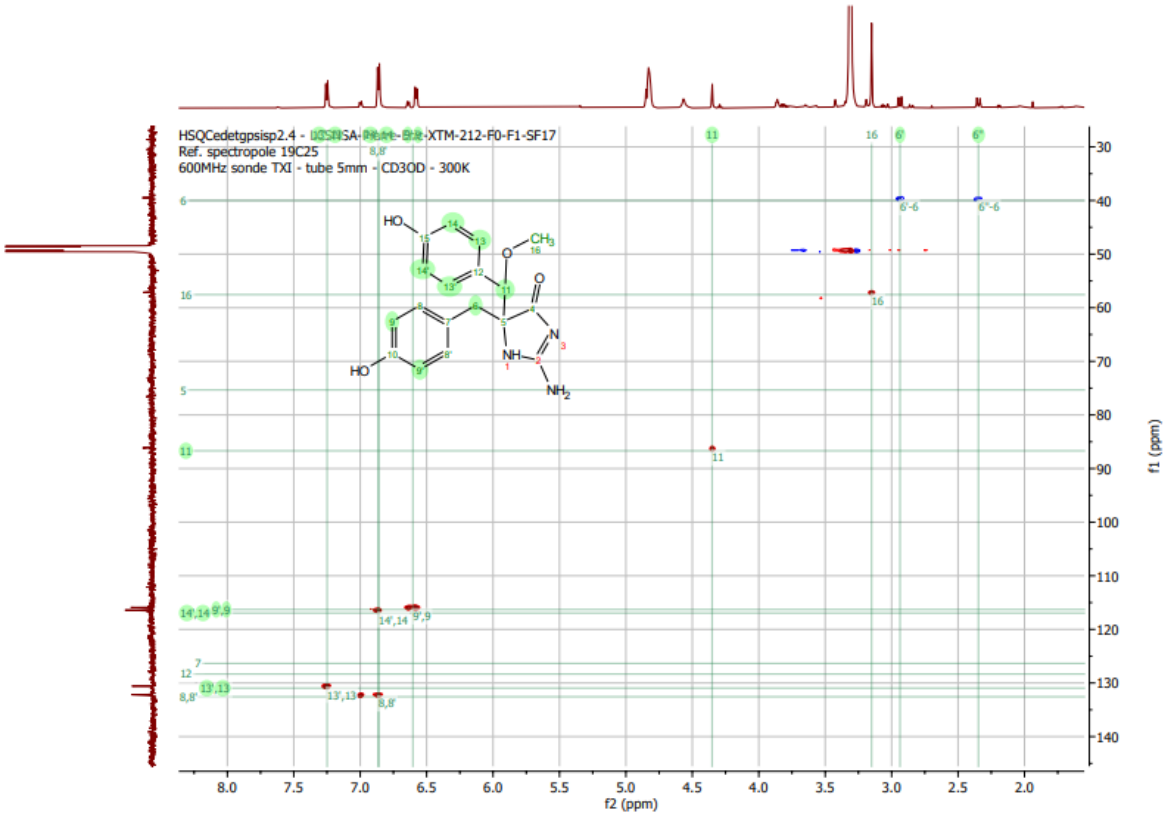

Figure S22: ^{1}H-^{13}C HMBC NMR (600 MHz) spectrum for calcaridine C (4)

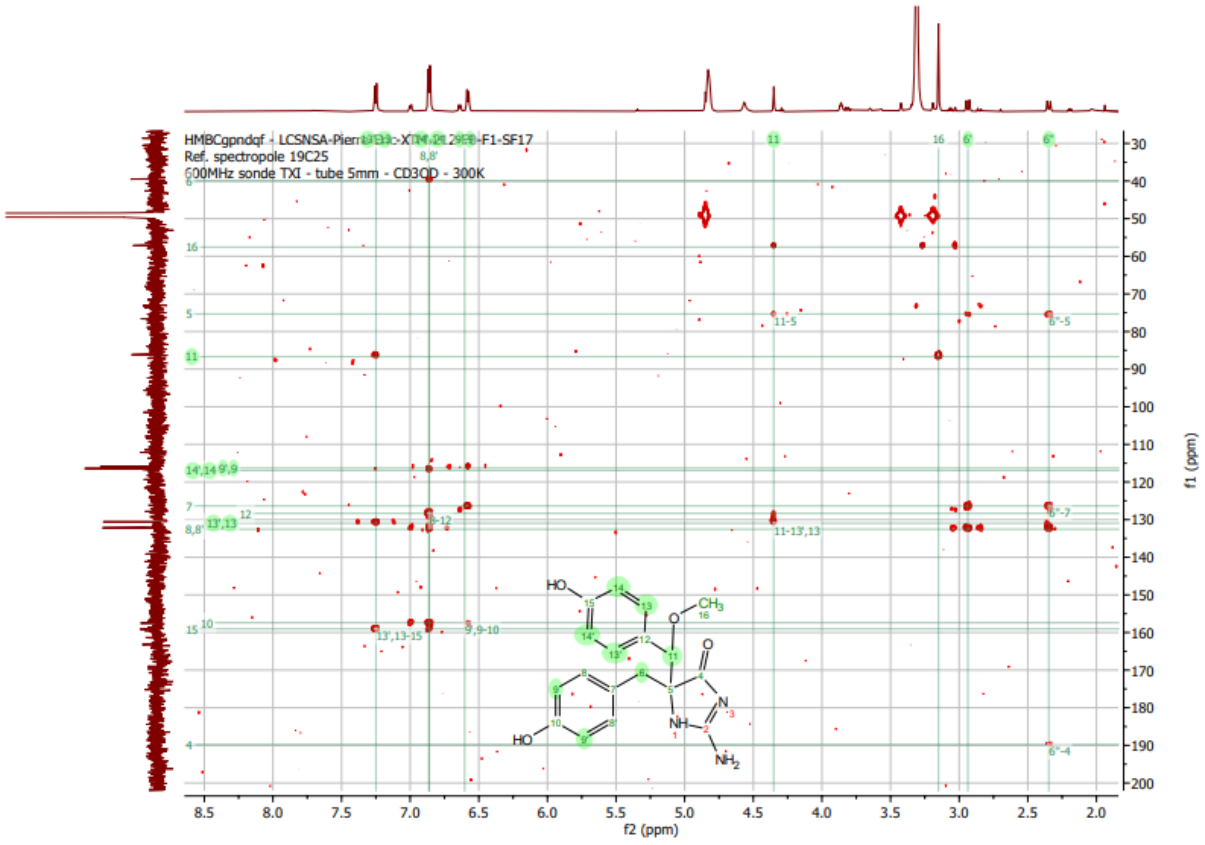

Figure S23: ^{1}H-^{1}H NOESY NMR (600 MHz) spectrum for calcaridine C (4)

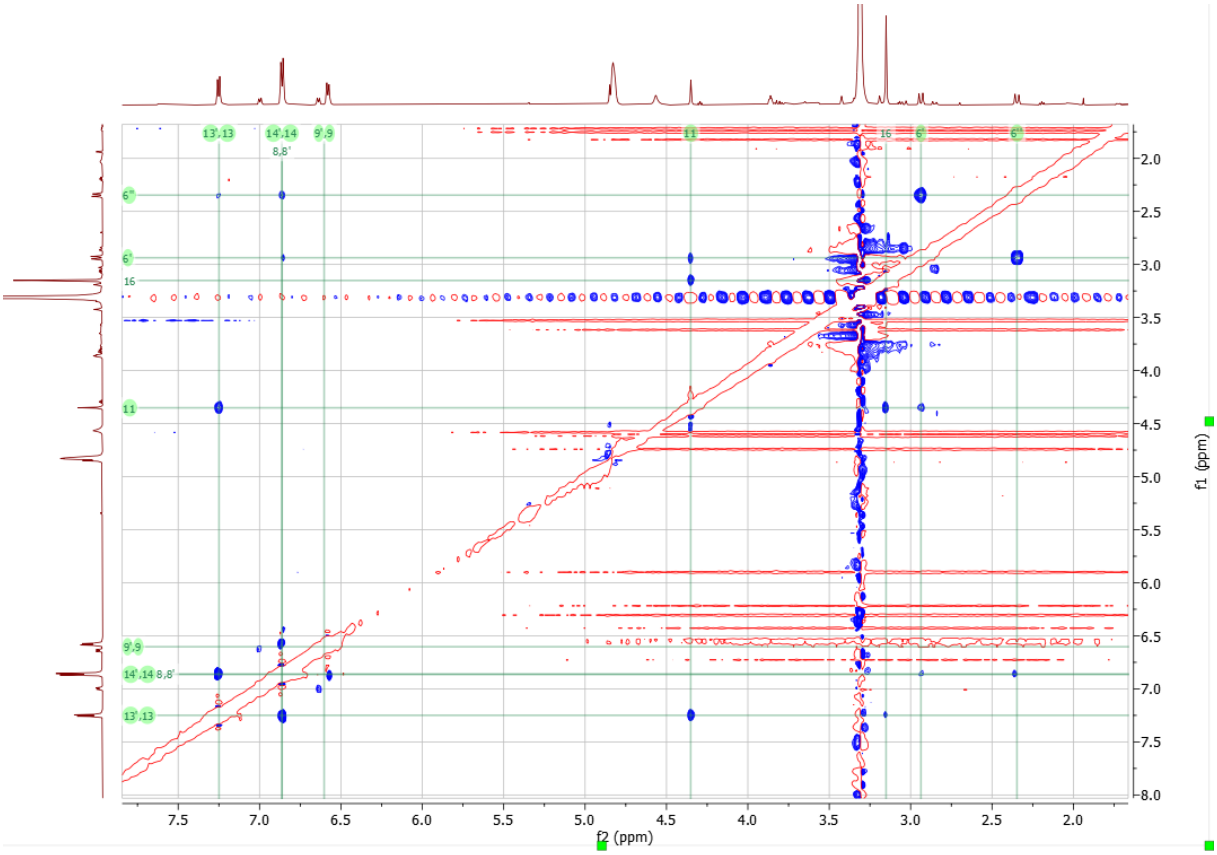

Figure S24: HRESIMS spectrum for naamine H (5)

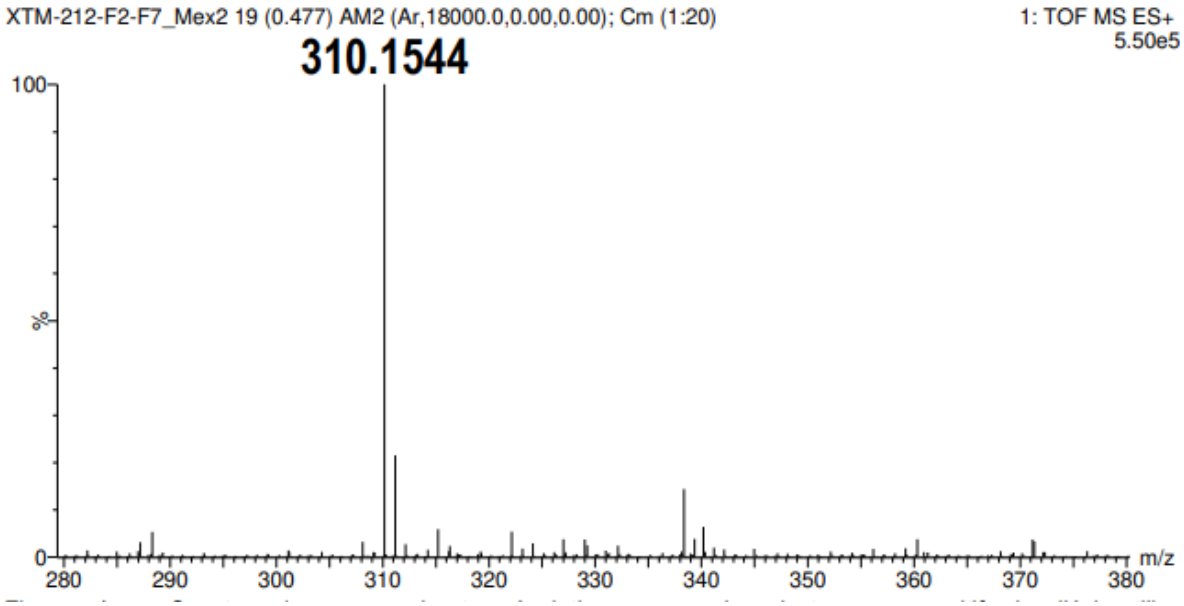

Figure S25: ^{1}H NMR (600 MHz, CD_3OD) spectrum for naamine H (5)

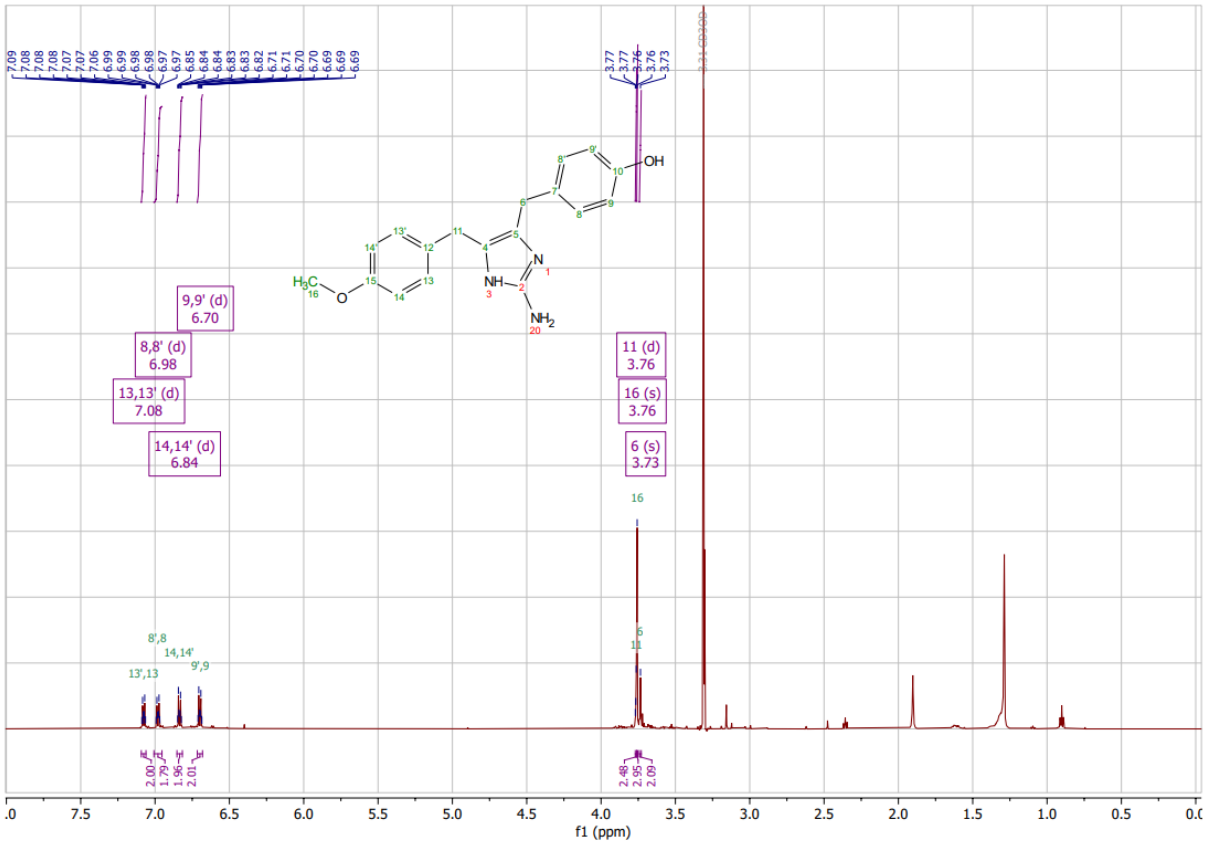

Figure S26: ^{1}H-^{13}C HSQC NMR (600 MHz) spectrum for naamine H (5)

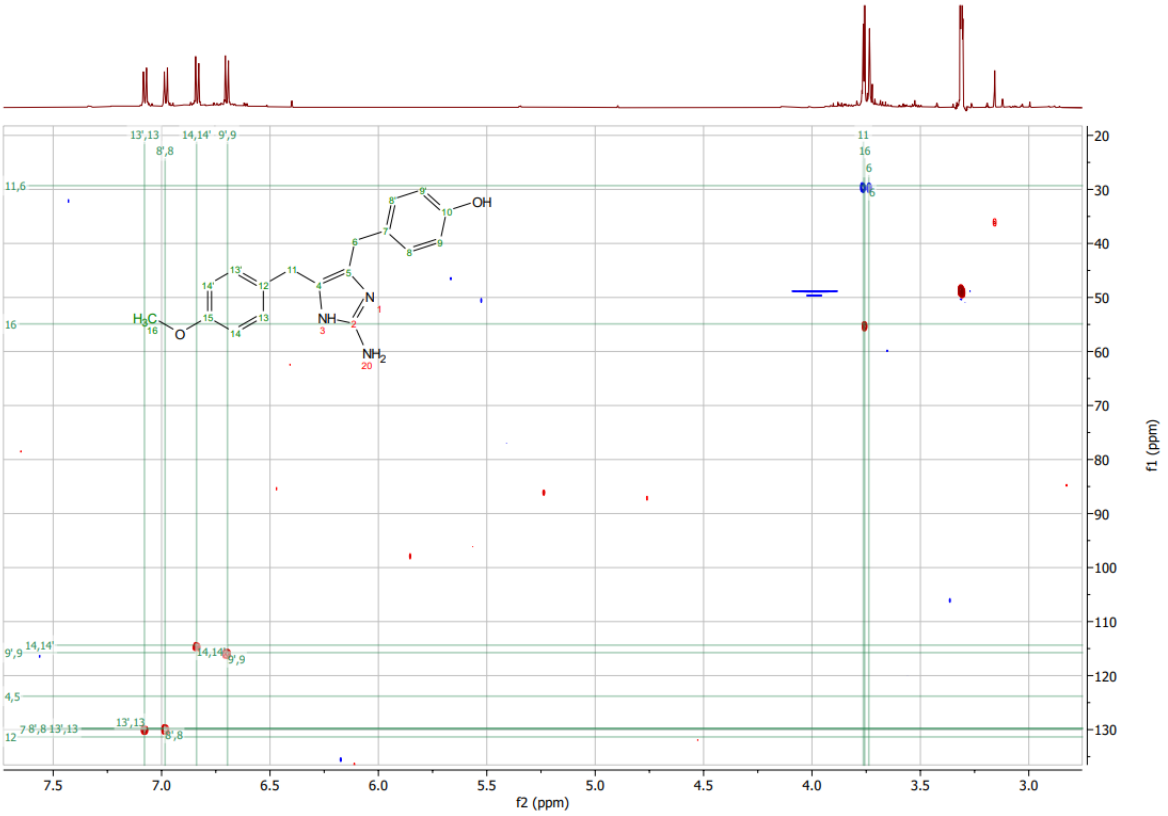

Figure S27: ^{1}H-^{13}C HMBC NMR (600 MHz) spectrum for naamine H (5)

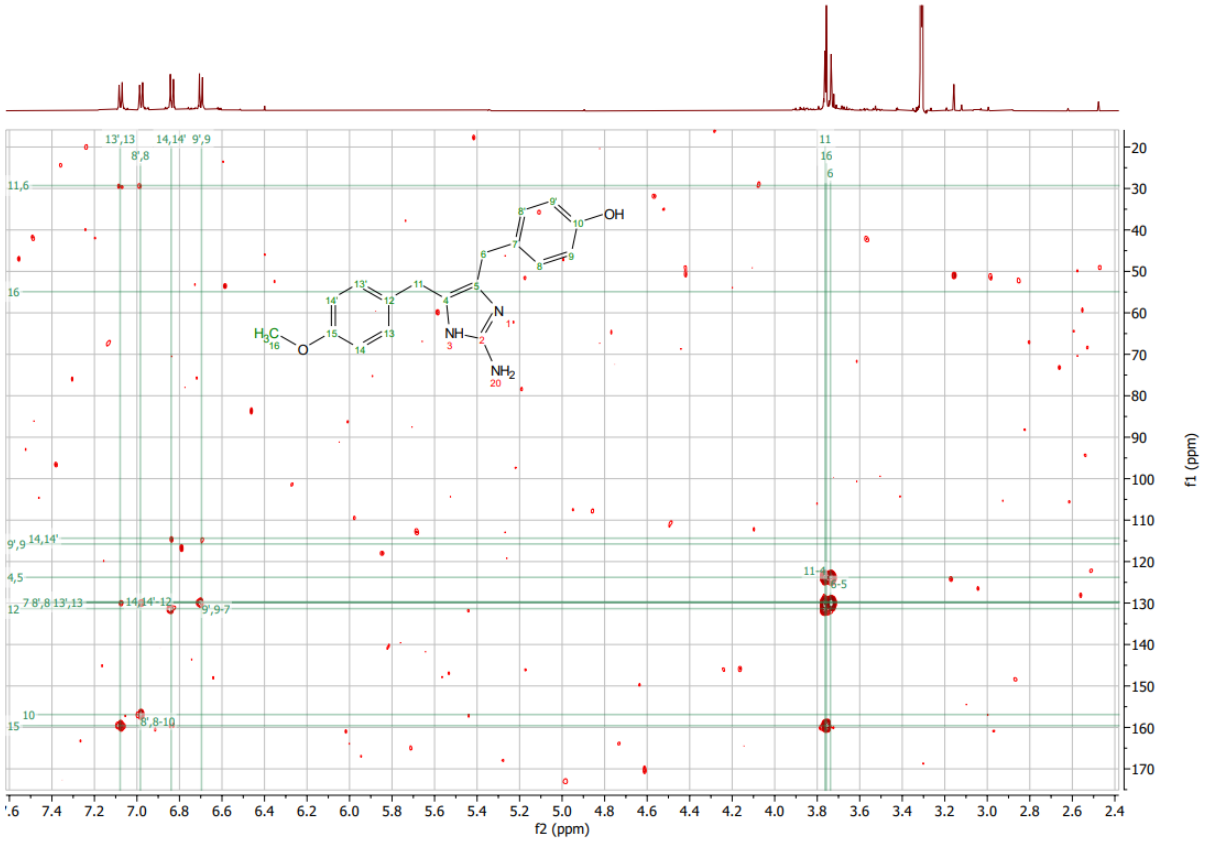

Figure S28: ^{1}H-^{1}H NOESY NMR (600 MHz) spectrum for naamine H (5)

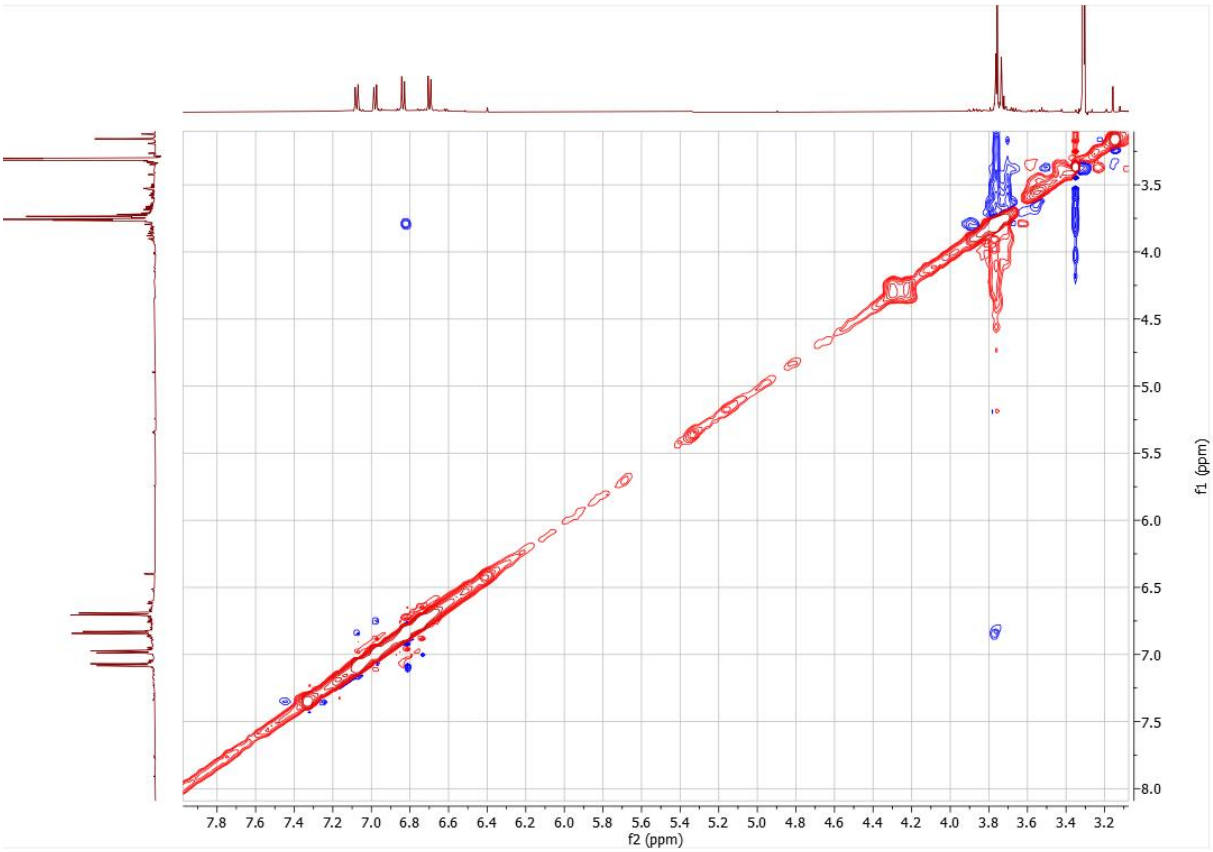

Figure S29: HRESIMS spectrum for naamidine J (6)

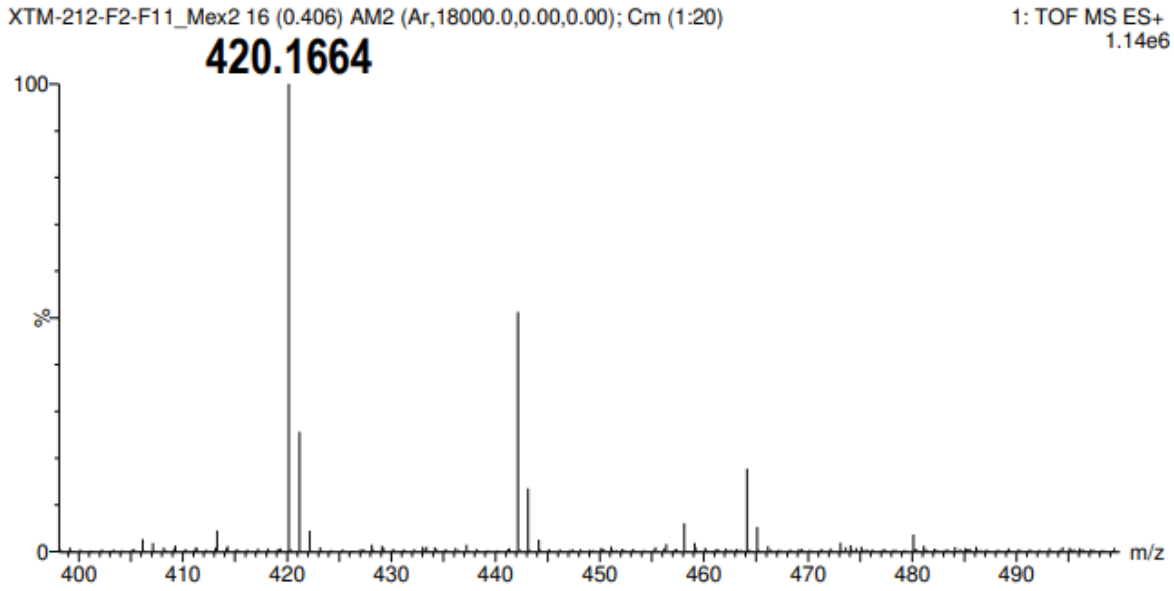

Figure S30: ^{1}H NMR (600 MHz, CD_3OD) spectrum for naamidine J (6)

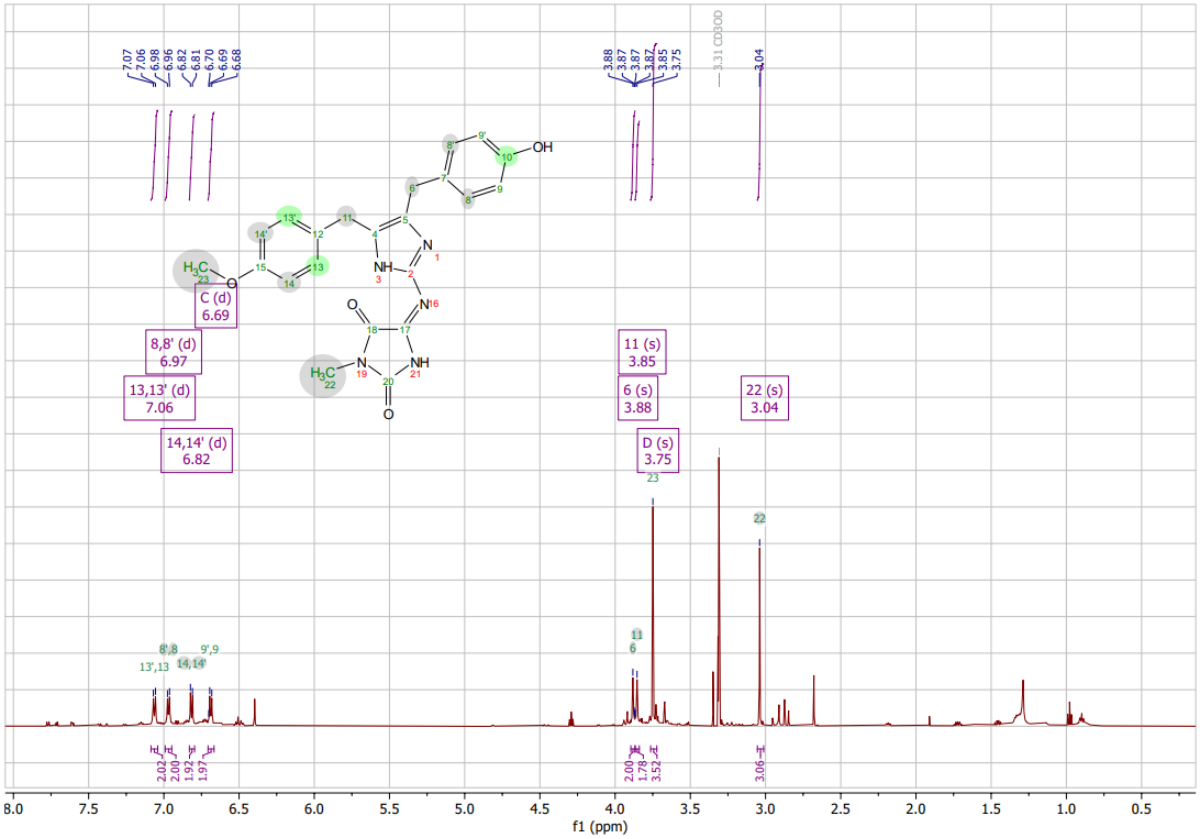

Figure S31: ^{13}C NMR (125 MHz, CD_3OD) spectrum for naamidine J (6)

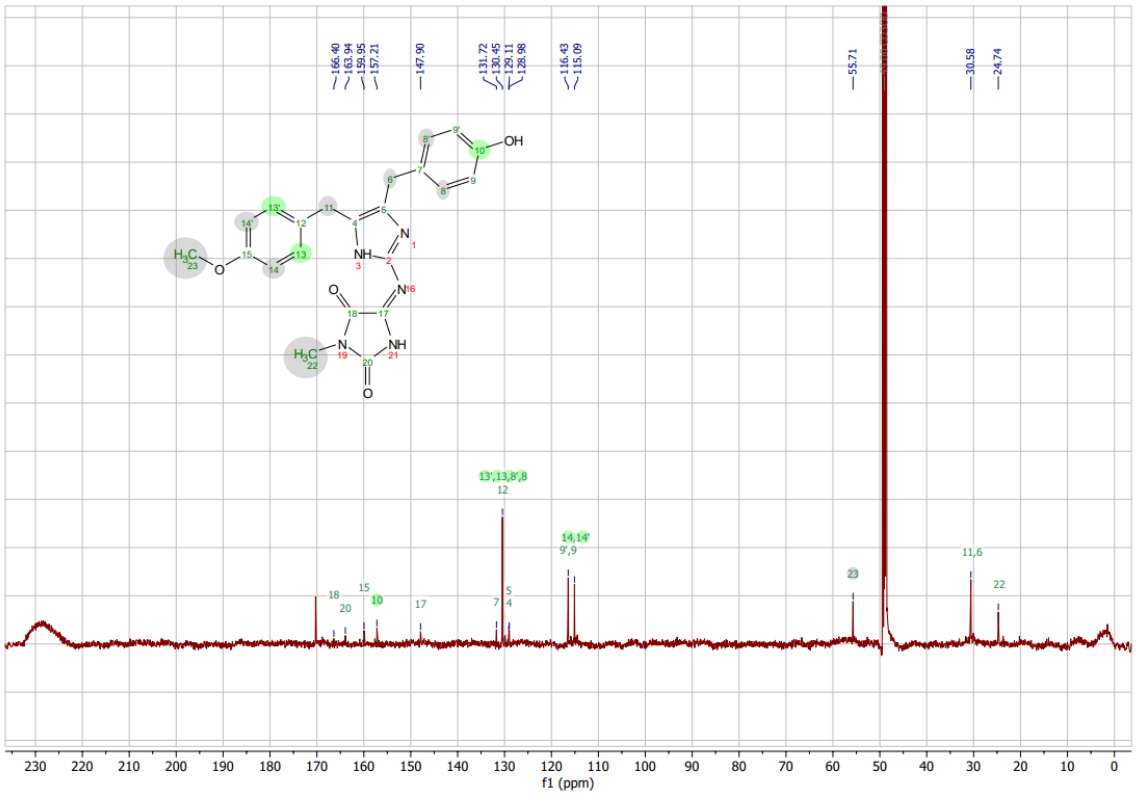

Figure S32: ^{1}H-^{1}H COSY NMR (600 MHz) spectrum for naamidine J (6)

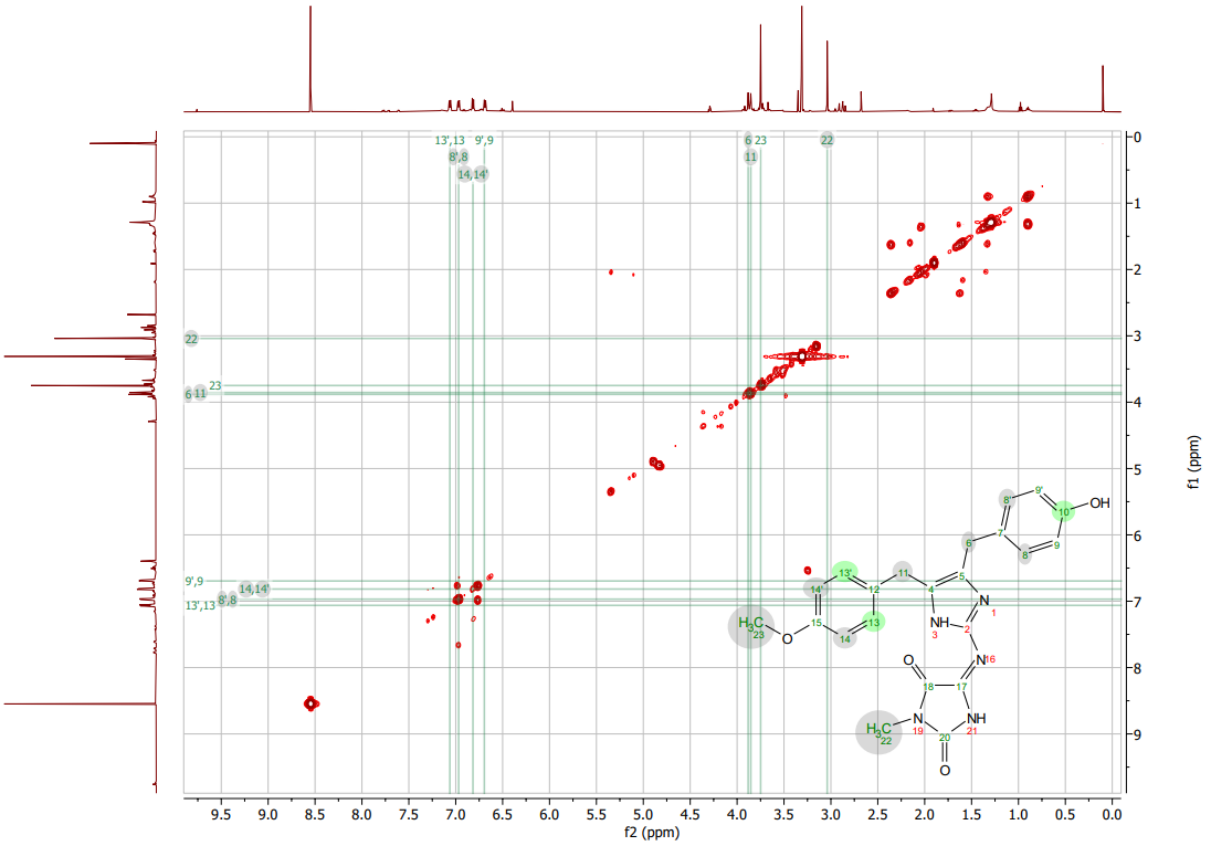

Figure S33: ^{1}H-^{13}C HSQC NMR (600 MHz) spectrum for naamidine J (6)

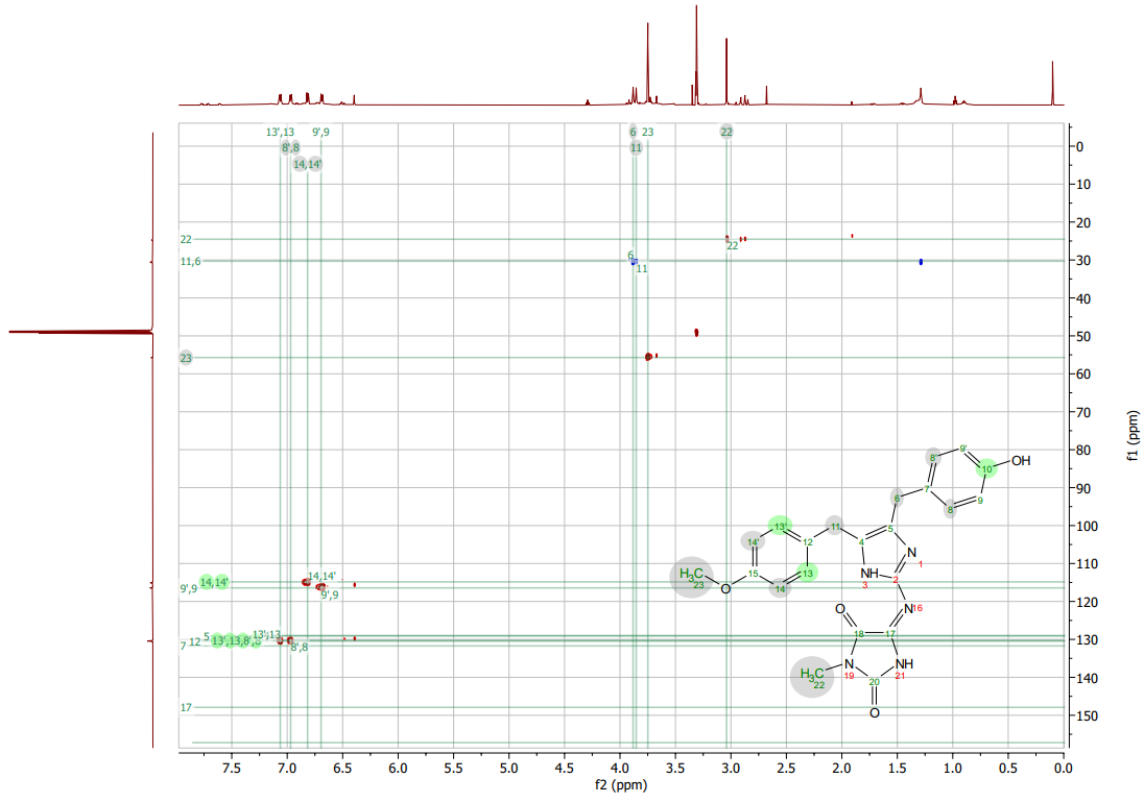

Figure S34: ^{1}H-^{13}C HMBC NMR (600 MHz) spectrum for naamidine J (6)

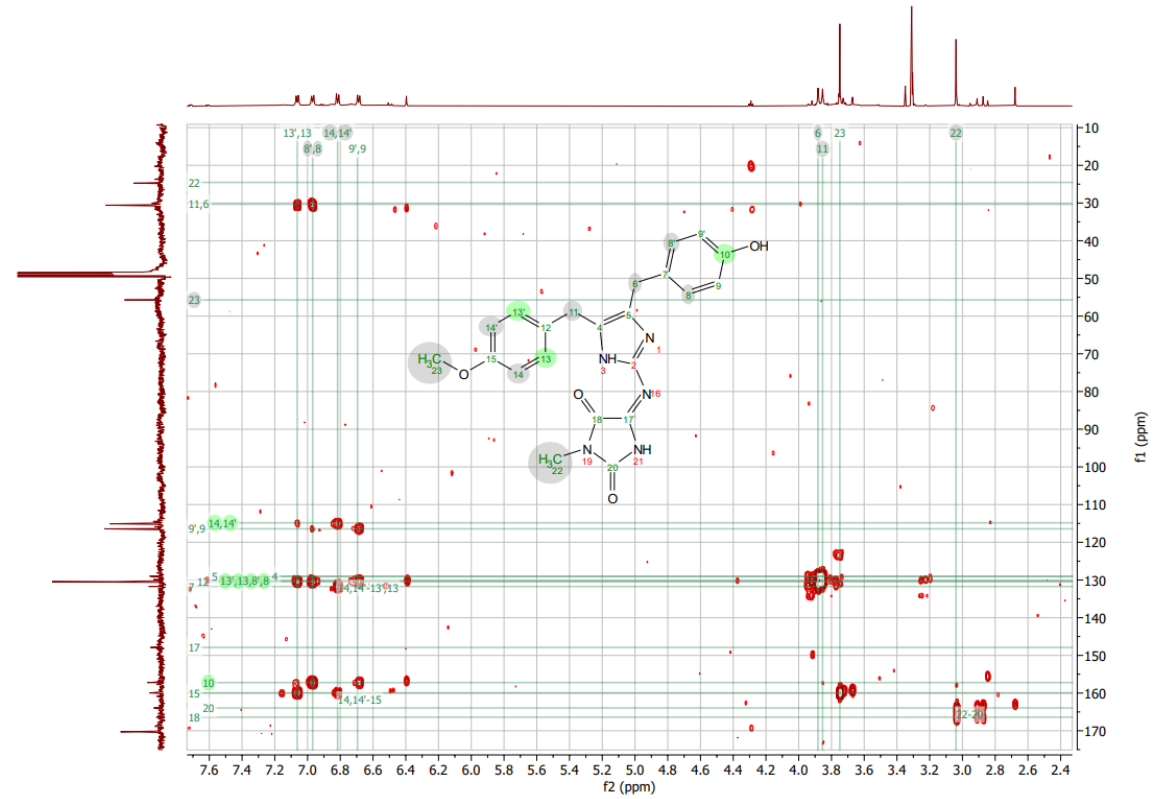

Figure S35: ^{1}H-^{1}H NOESY NMR (600 MHz) spectrum for naamidine J (6)

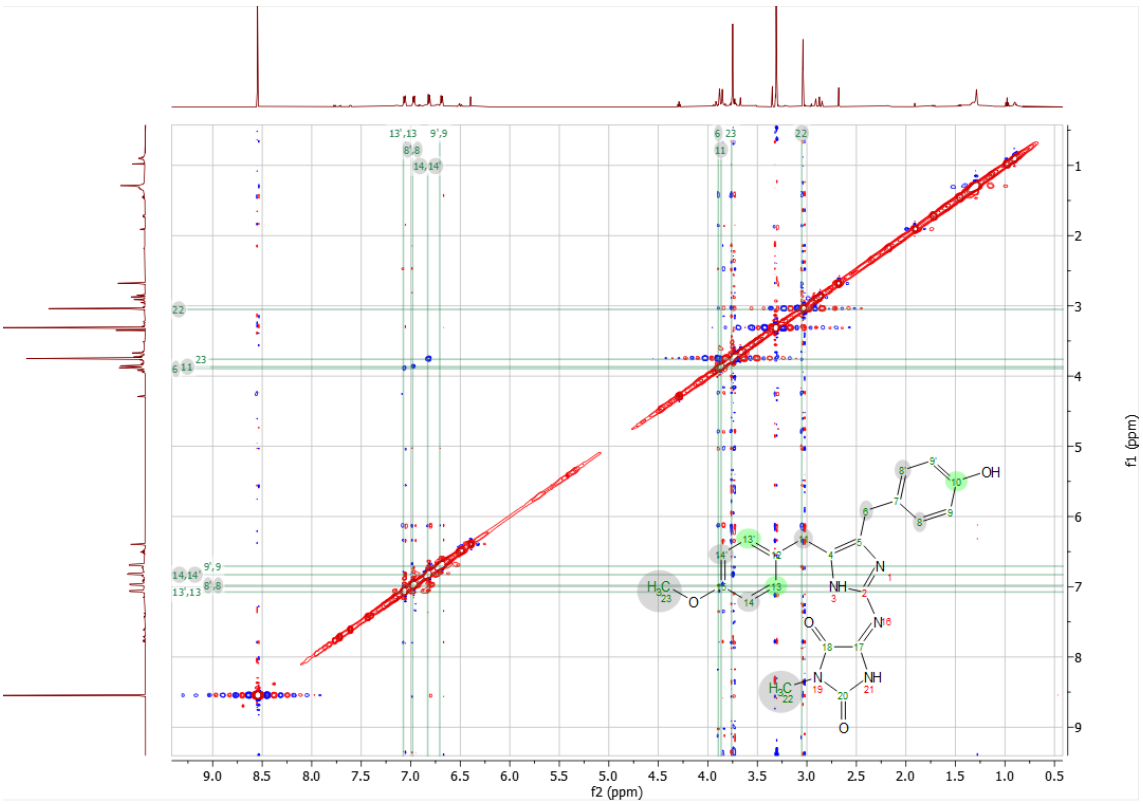

Figure S36: HRESIMS spectrum for naamine I (7)

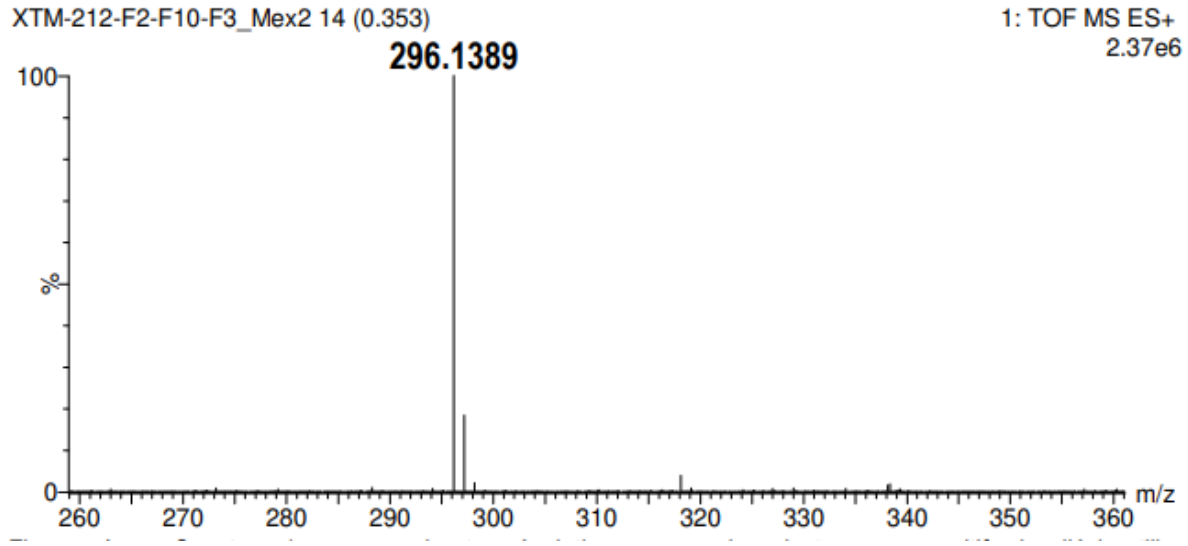

Figure S37: HRESIMS spectrum for naamidine K (8)

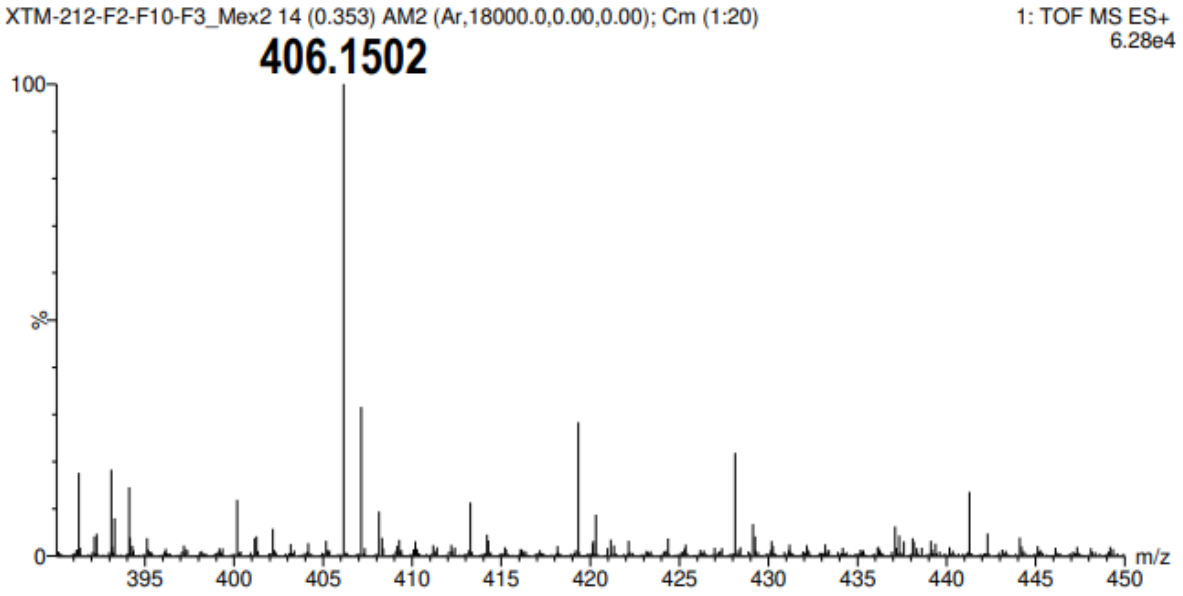

Figure S38: ^{1}H NMR (600 MHz, CD_3OD) spectrum for mixture of naamine I (7) and naamidine K (8)

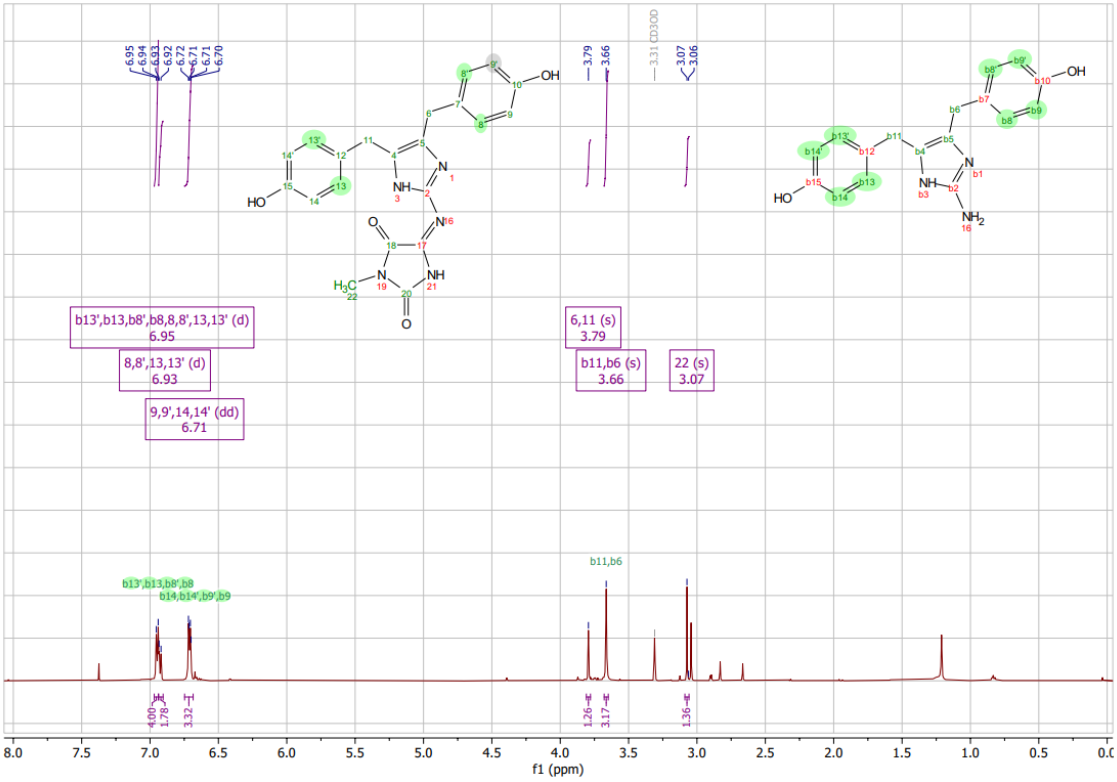

Figure S39: ^{1}H-^{13}C HSQC NMR (600 MHz) spectrum for mixture of naamine I (7) and naamidine K (8)

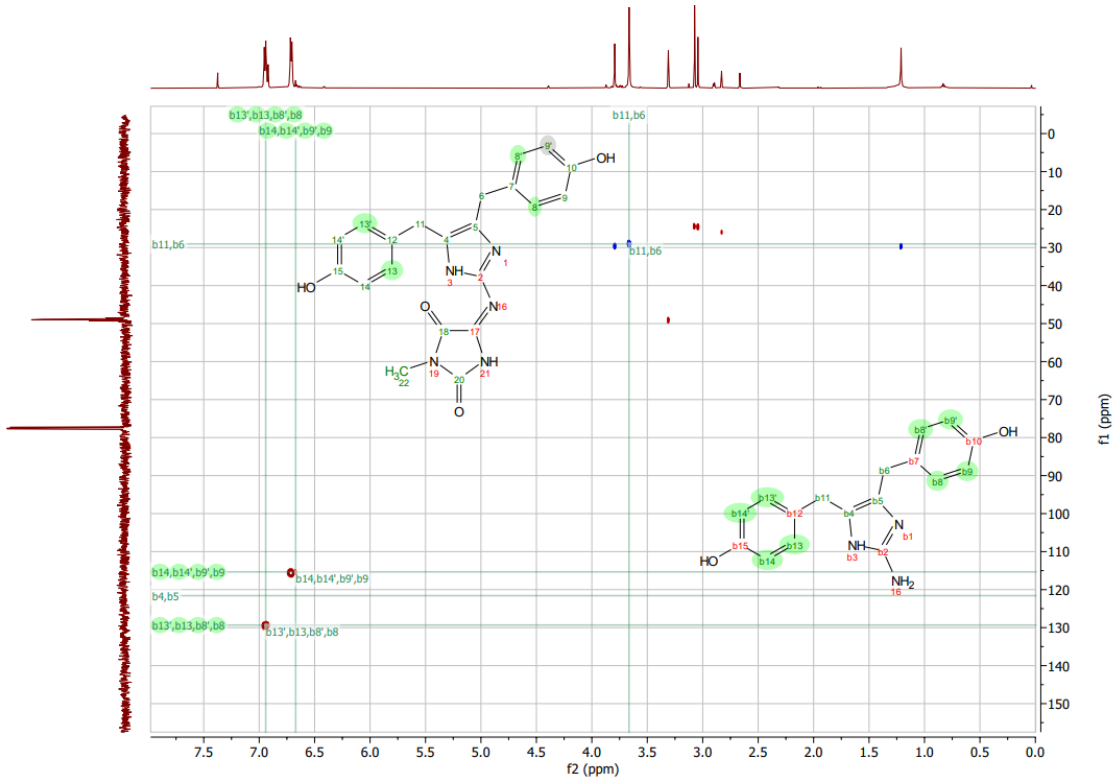

Figure S40: ^{1}H-^{13}C HMBC NMR (600 MHz) spectrum for mixture of naamine I (7) and naamidine K (8)

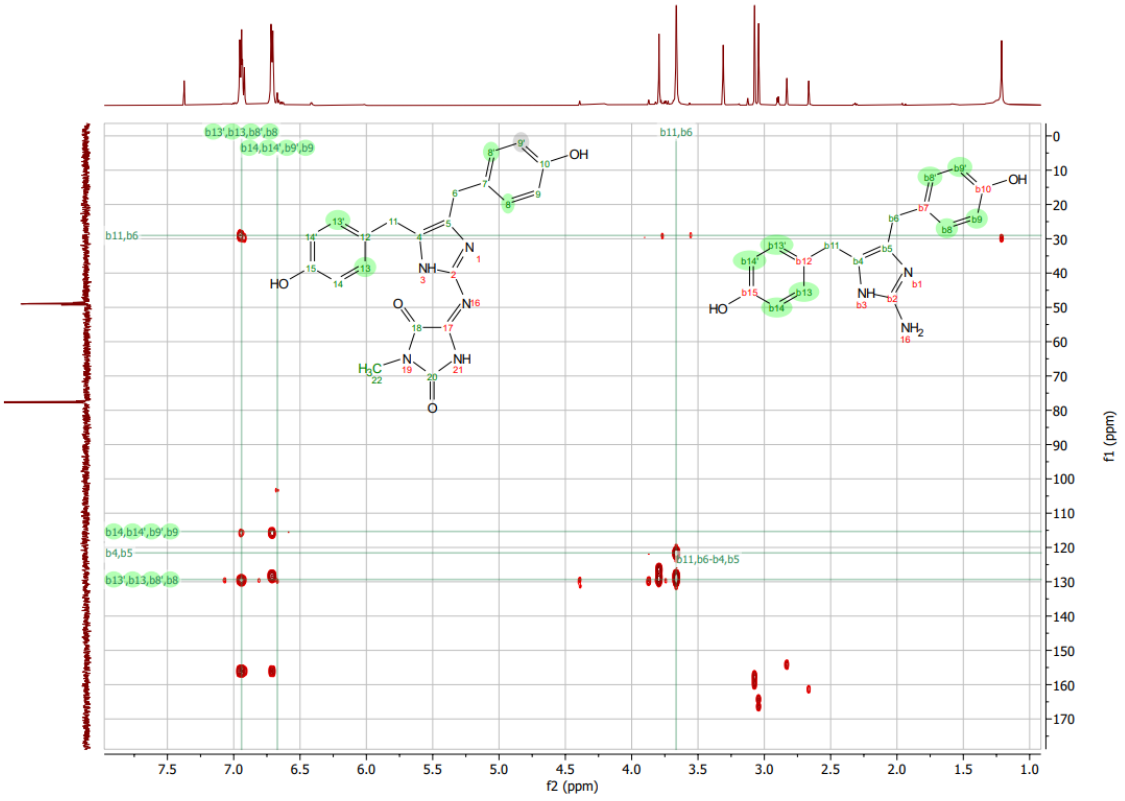

Figure S41: ^{1}H NMR (600 MHz, CD_3OD) spectrum for thymidine (9)

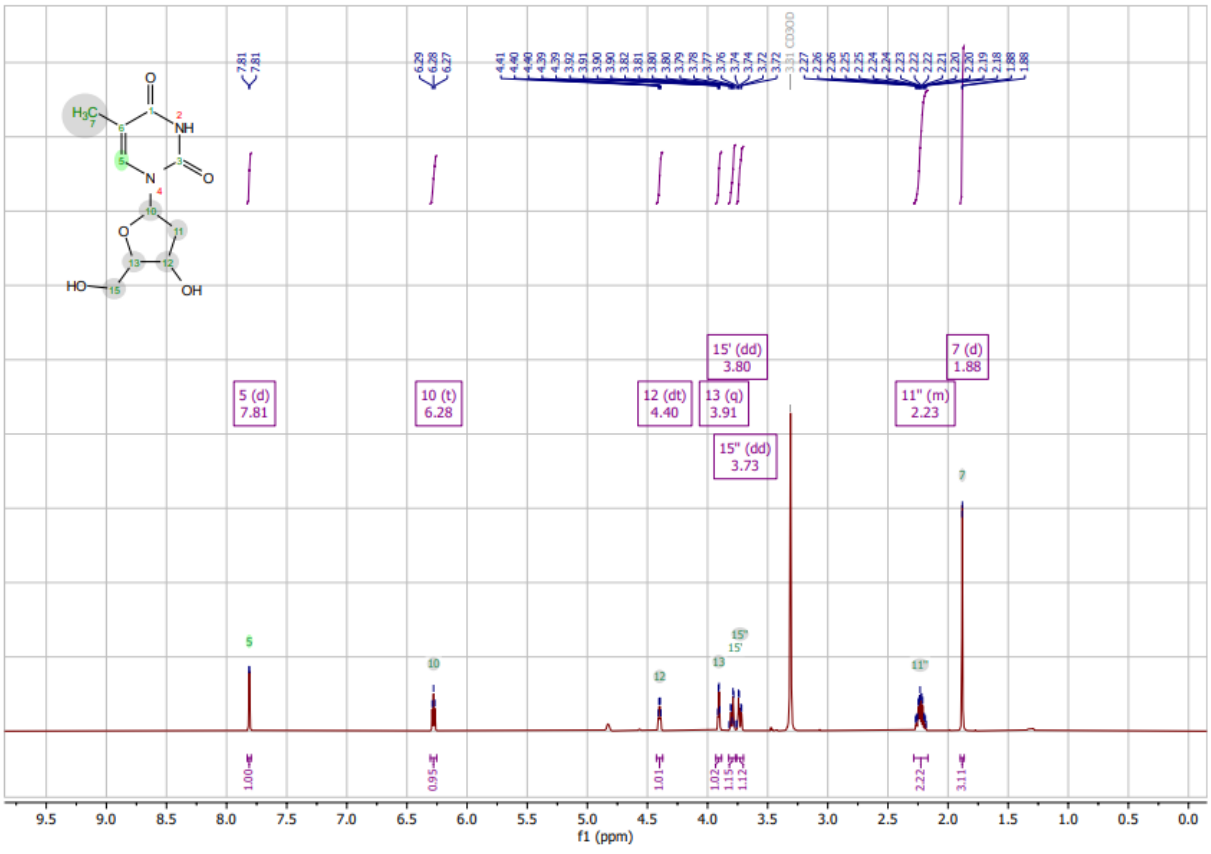

Figure S42: ^{13}C NMR (125 MHz, CD_3OD) spectrum for thymidine (9)

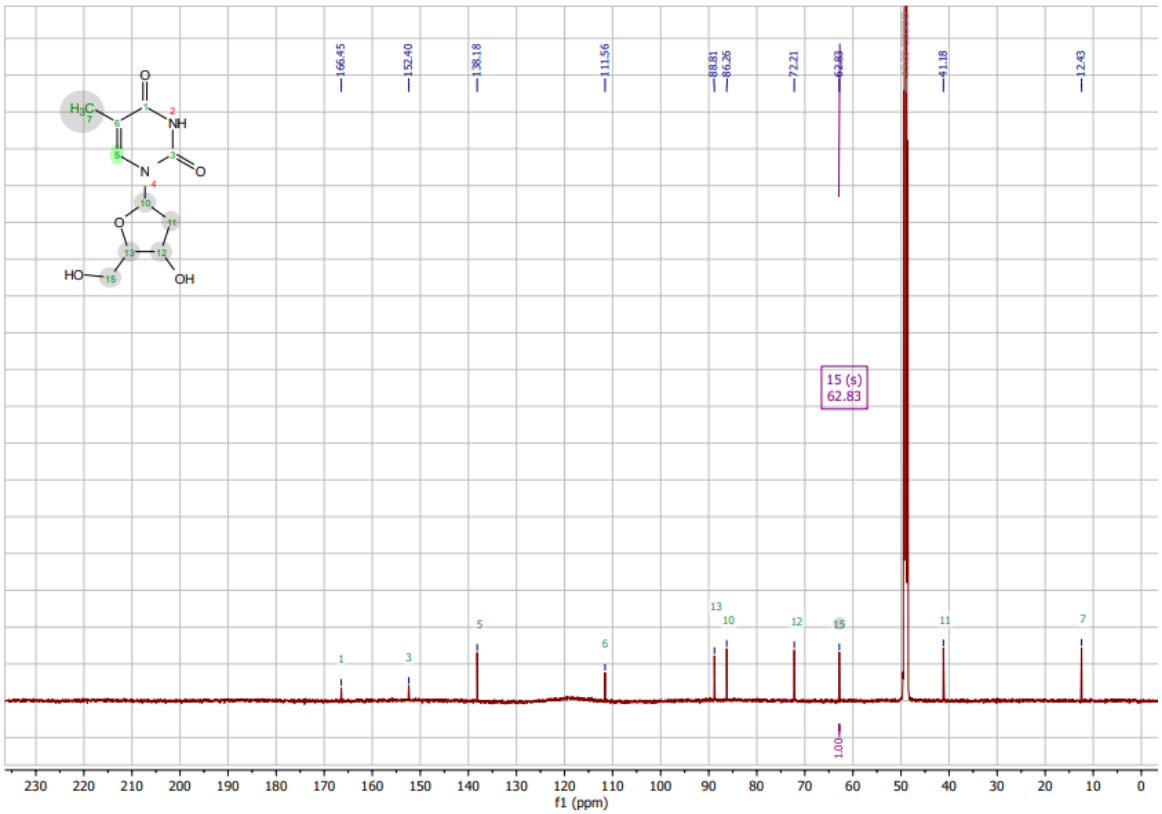

Figure S43: ^{1}H-^{1}H COSY NMR (600 MHz) spectrum for thymidine (9)

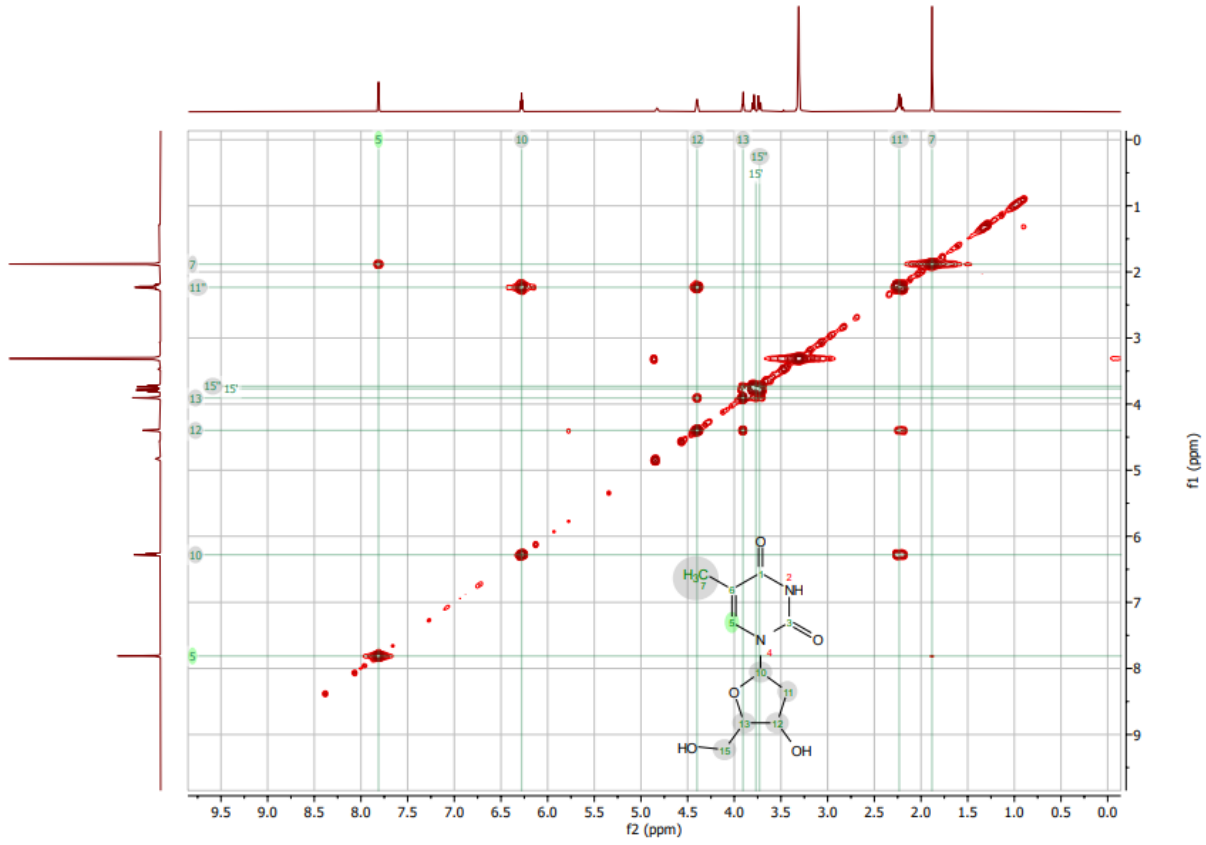

Figure S44: ^{1}H-^{13}C HSQC NMR (600 MHz) spectrum for thymidine (9)

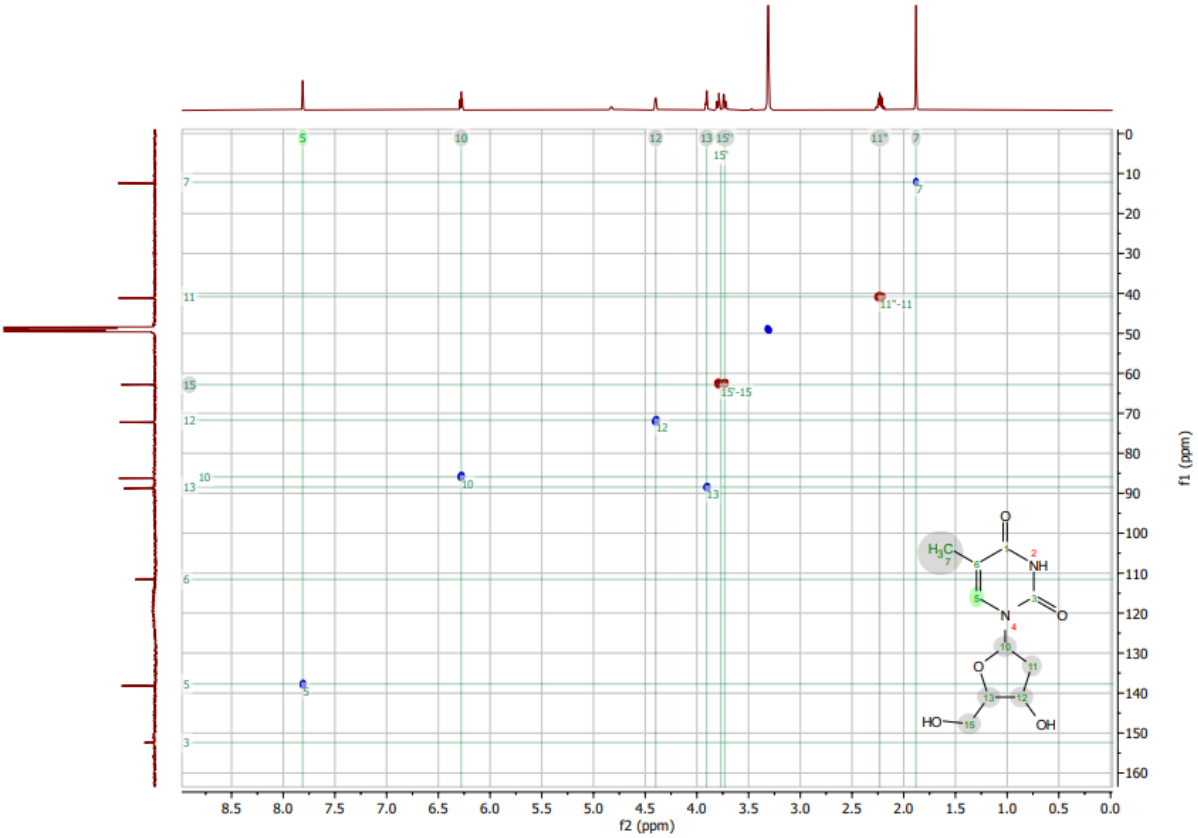

Figure S45: ^{1}H-^{13}C HMBC NMR (600 MHz) spectrum for thymidine (9)

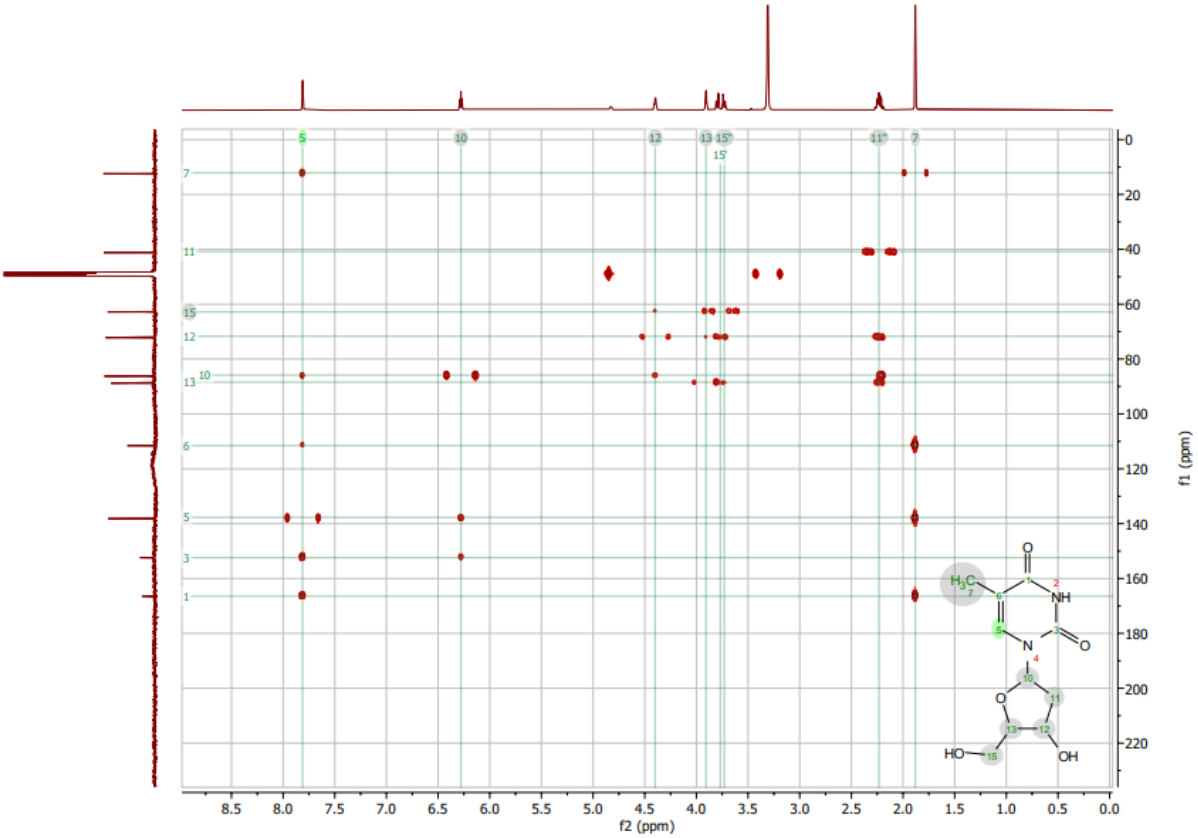

Figure S46: MS/MS spectra of the isolated compounds were deposited in the GNPS spectral libraries under following identifier

Compound	GNPS accession code
Phorbatopin E	CCMSLIB00009919260
Calcaridine C	CCMSLIB00009919261
Erstine A	CCMSLIB00009919262
Naamine H	CCMSLIB00009919263
Naamine I	CCMSLIB00009919264
Naamidine J	CCMSLIB00009919265
Naamidine K	CCMSLIB00009919266

Figure S47: MS/MS spectrum of ernstine A (1)

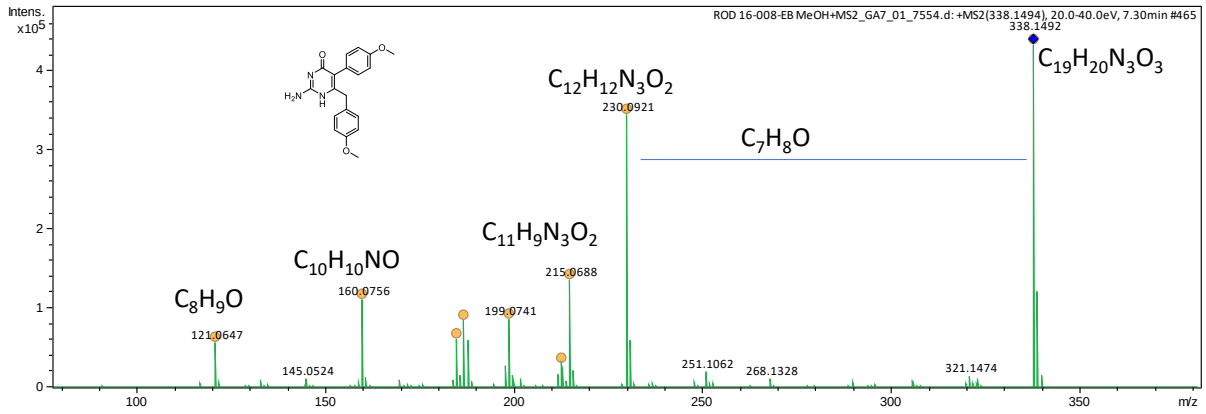

Figure S48: MS/MS spectrum of Phorbatopsin D (2)

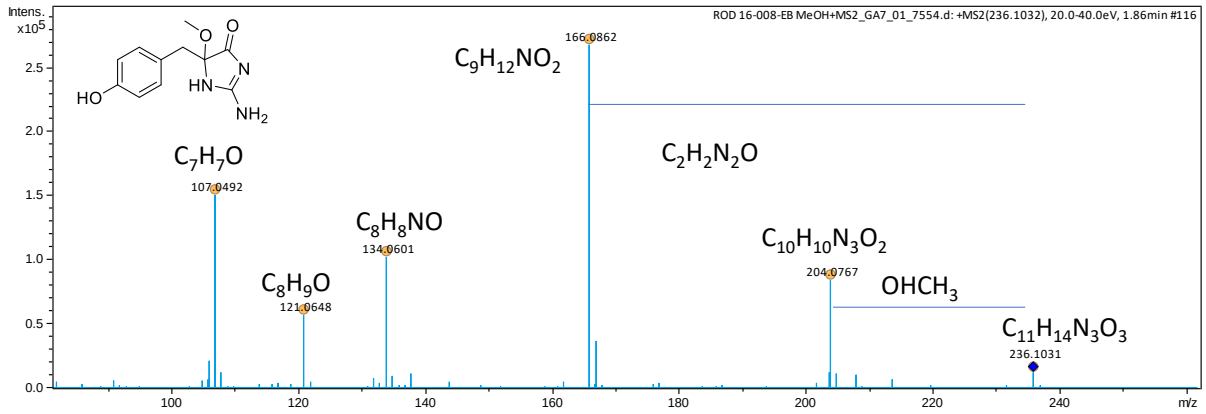

Figure S49: MS/MS spectrum of Phorbatopsin E(3)

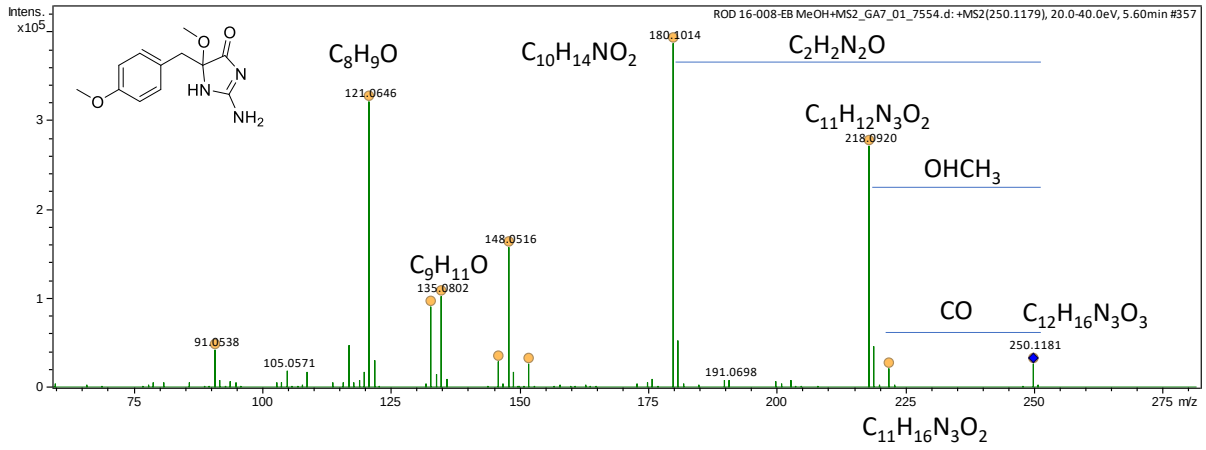

Figure S50: MS/MS spectrum of Naamine H (5)

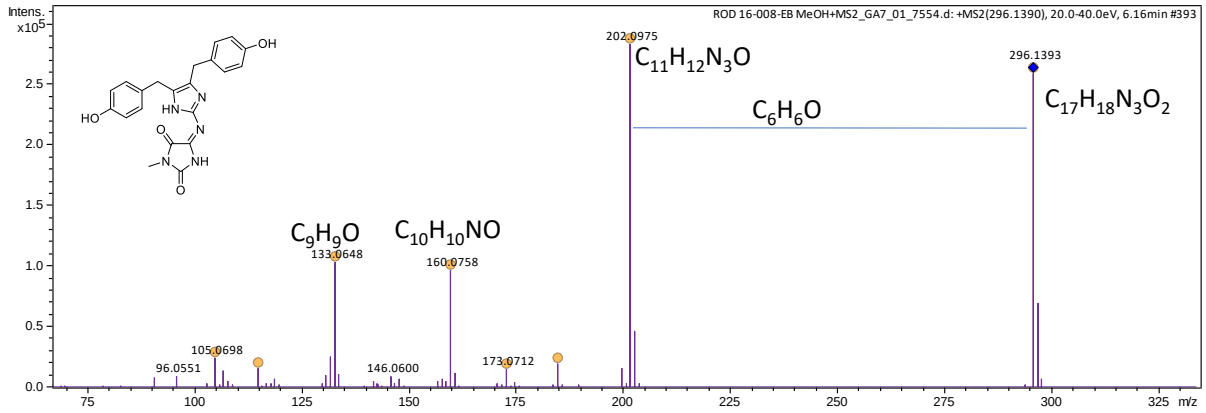

Figure S51: MS/MS spectrum of Naamine I (7)

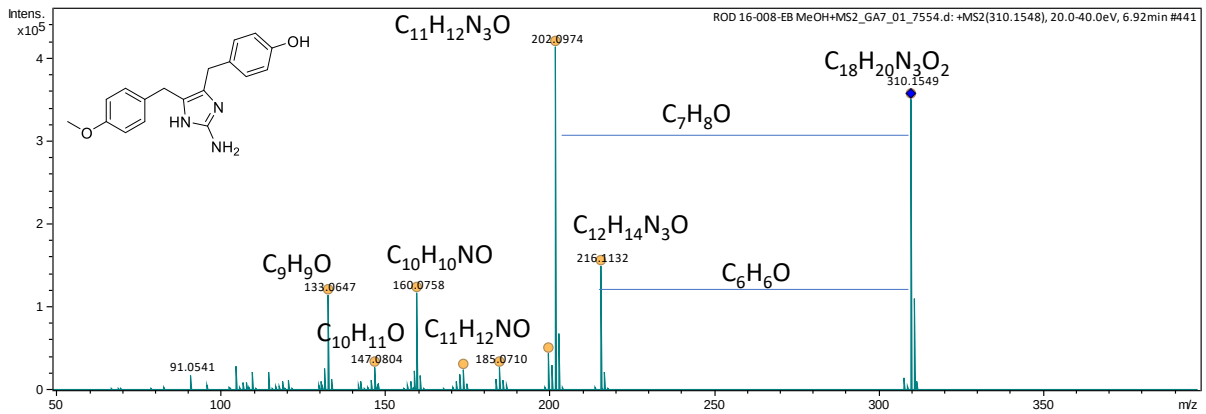

Figure S52: MS/MS spectrum of Naamidine J (6)

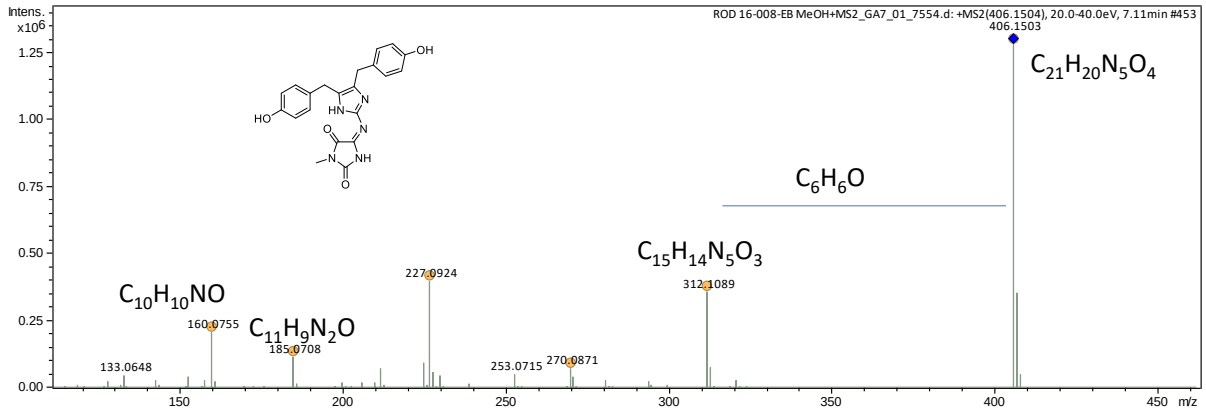

Figure S53: MS/MS spectrum of Naamidine K (8)

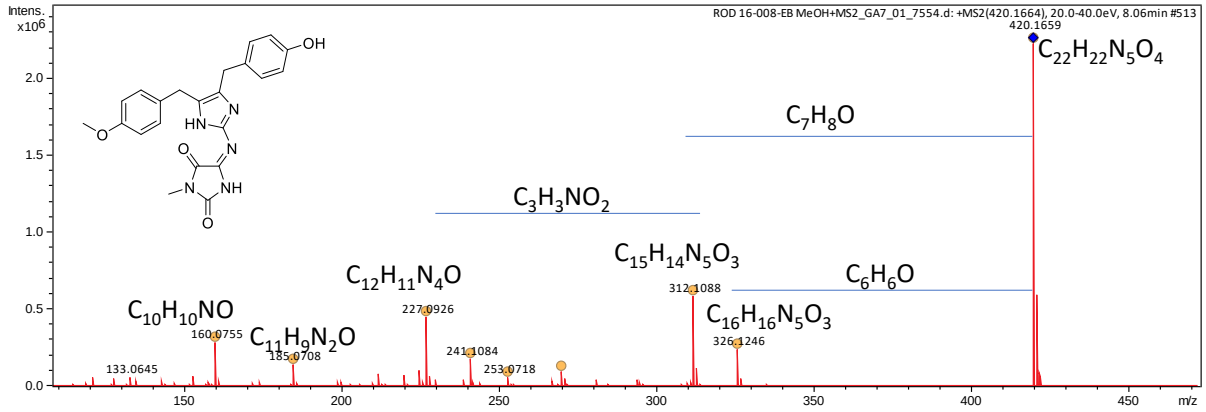

Figure S54: MS/MS spectrum of Calcaridine C (4)