

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

Pierre-Eric Campos<sup>1,2</sup>, Gaëtan Herbette<sup>3</sup>, Laetitia Fougère<sup>2</sup>, Patricia Clerc<sup>1</sup>, Florent Tintillier<sup>1</sup>, Nicole J. de Voogd<sup>4,5</sup>, Géraldine Le Goff<sup>6</sup>, Jamal Ouazzani<sup>6</sup> and Anne Gauvin-Bialecki<sup>1\*</sup>

<sup>1</sup> Laboratoire de chimie et de biotechnologie des produits naturels, Faculté des Sciences et Technologies, Université de La Réunion, 15 Avenue René Cassin, CS 92003, 97744 Saint-Denis Cedex 9, La Réunion, France

<sup>2</sup> Institut de Chimie Organique et Analytique, Université d'Orléans – CNRS - Pôle de chimie, rue de Chartres – UMR 6759, BP6759, 45067 Orléans Cedex 2, France

<sup>3</sup> Aix-Marseille Univ, CNRS, Centrale Marseille, FSCM, Spectropole, Campus de St Jérôme-Service 511, 13397 Marseille, France

<sup>4</sup> Naturalis Biodiversity Center, Darwinweg 2, 2333 CR Leiden, Netherlands

<sup>5</sup> Institute of Environmental Sciences, Leiden University, Einsteinweg 2, 2333 CC Leiden, Netherlands

<sup>6</sup> Institut de Chimie des Substances Naturelles, CNRS UPR 2301, Univ. Paris-Sud, Université Paris-Saclay, 1, av. de la Terrasse, 91198 Gif-sur-Yvette, France

\* Correspondence: anne.bialecki@univ-reunion.fr; Tel.: +262 262 93 81 97

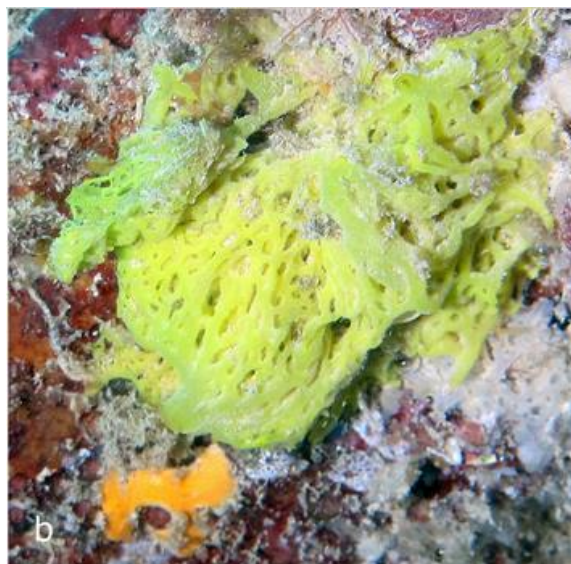
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## Supporting information

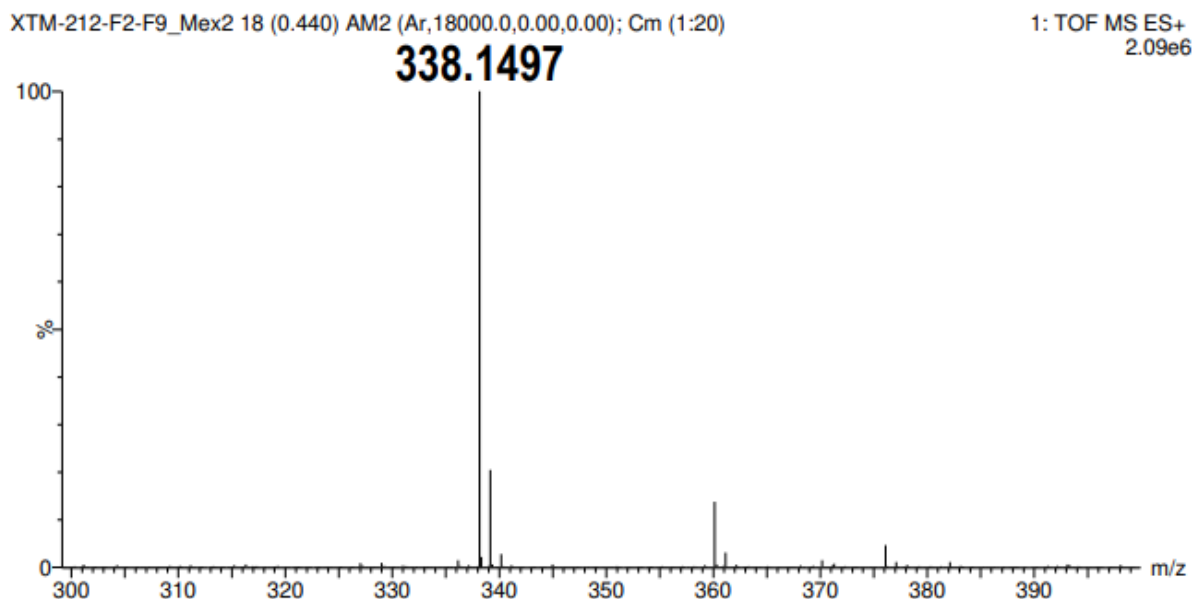
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*In situ* *Ernsta naturalis* Photo

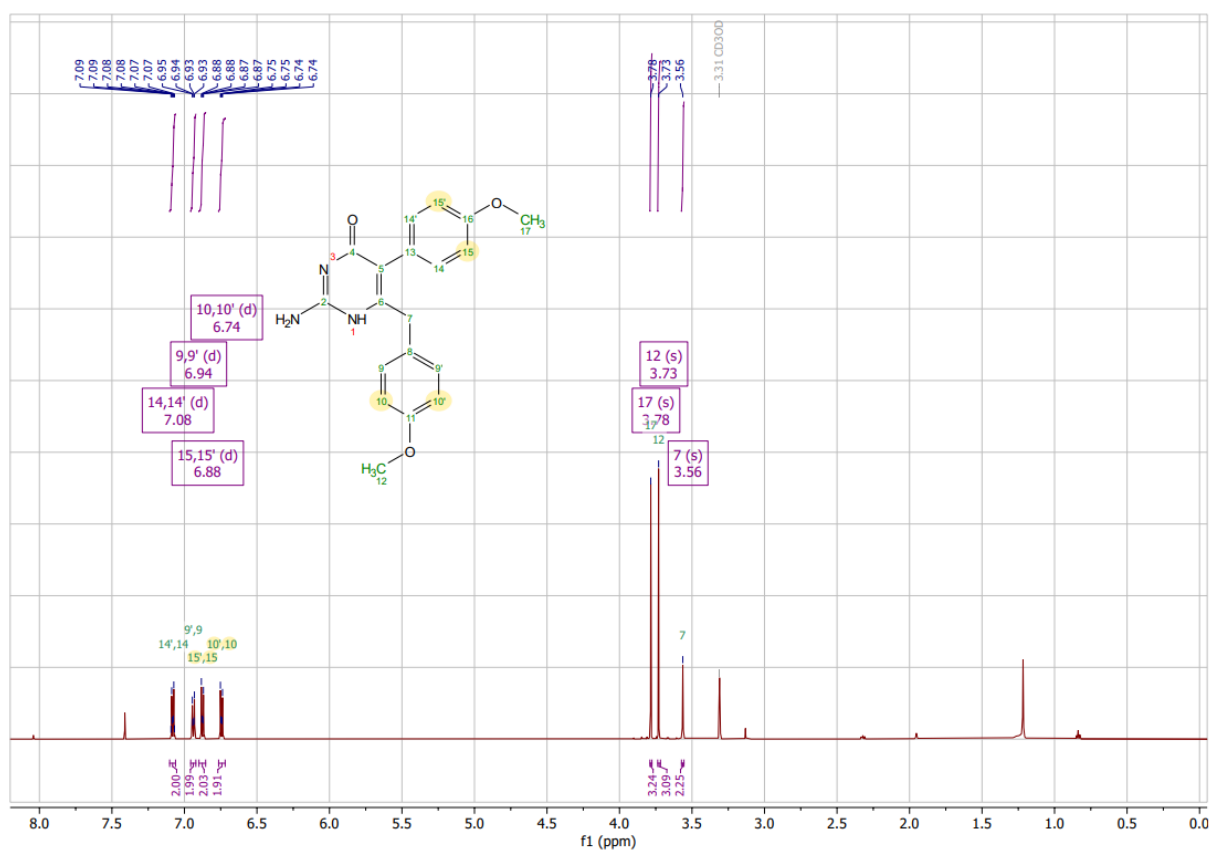


## Supporting information

**Figure S1:** HRESIMS spectrum for ernstine A (1)

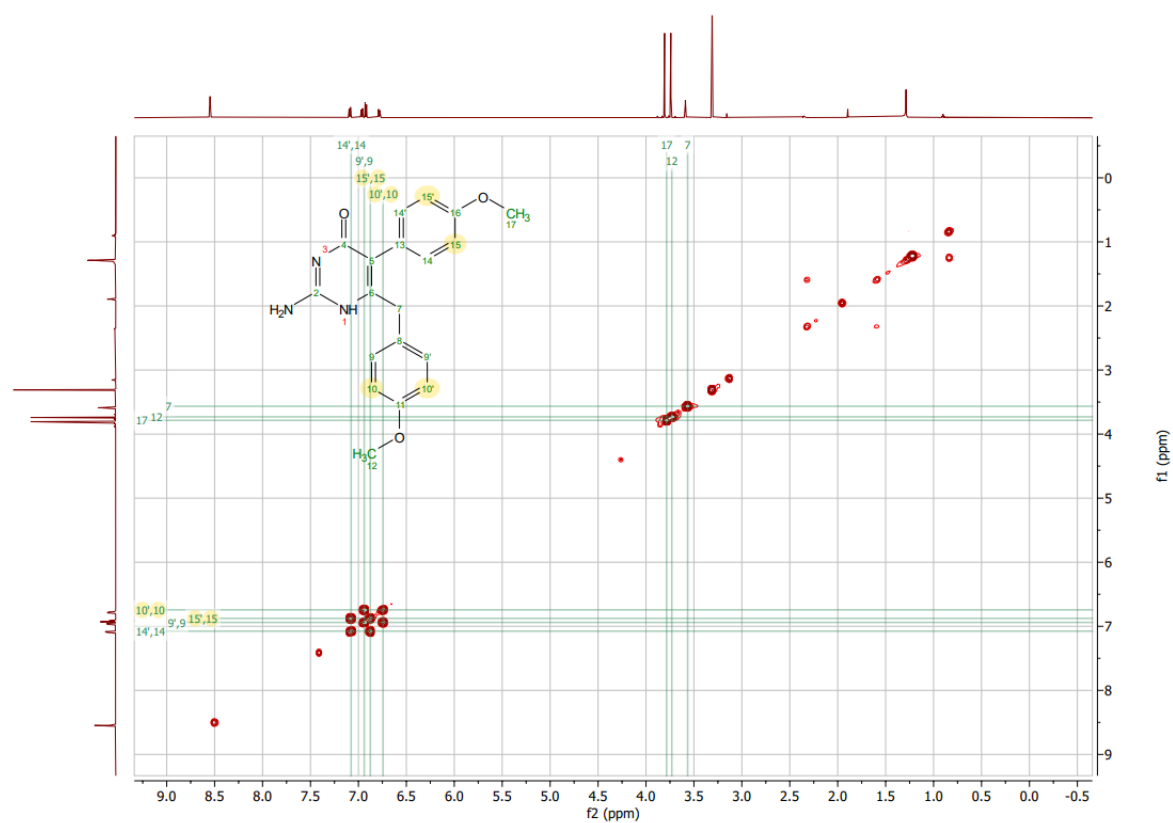


**Figure S2:**  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum for ernstine A (1)

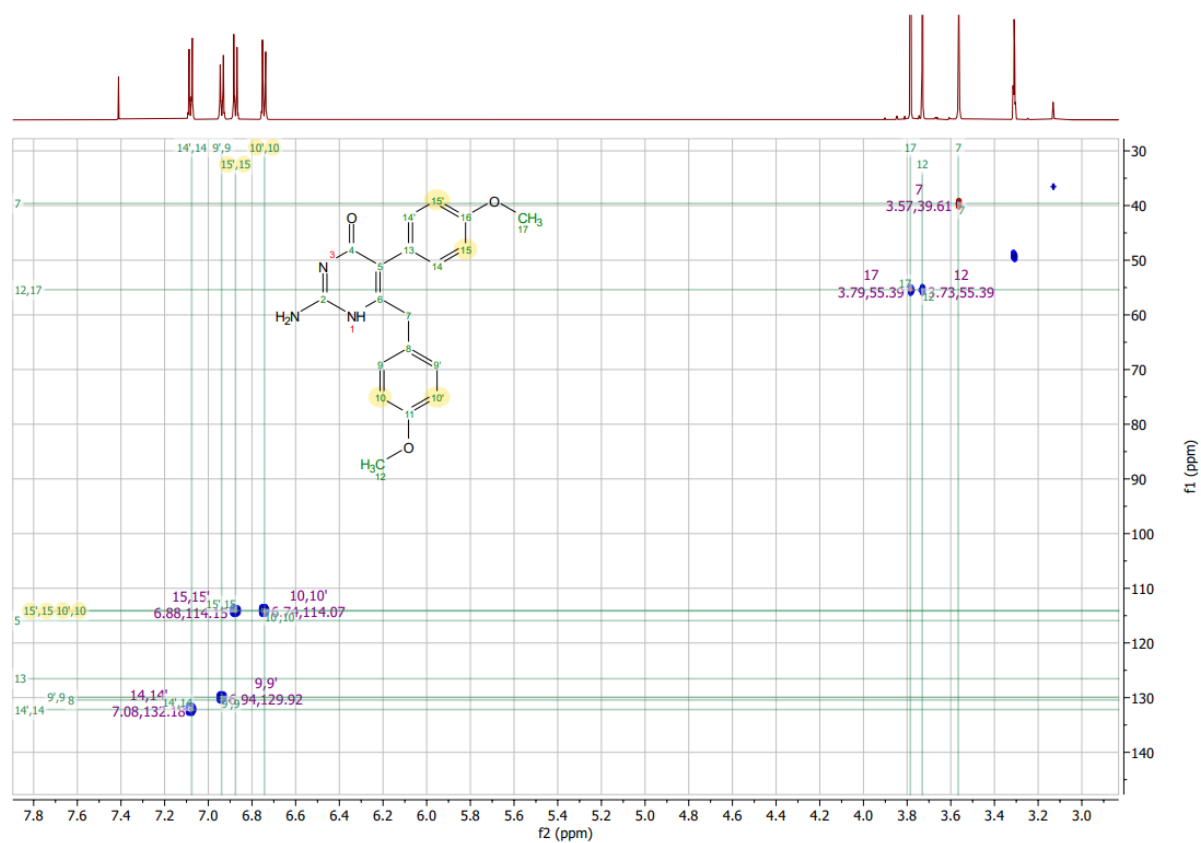


# Supporting information

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

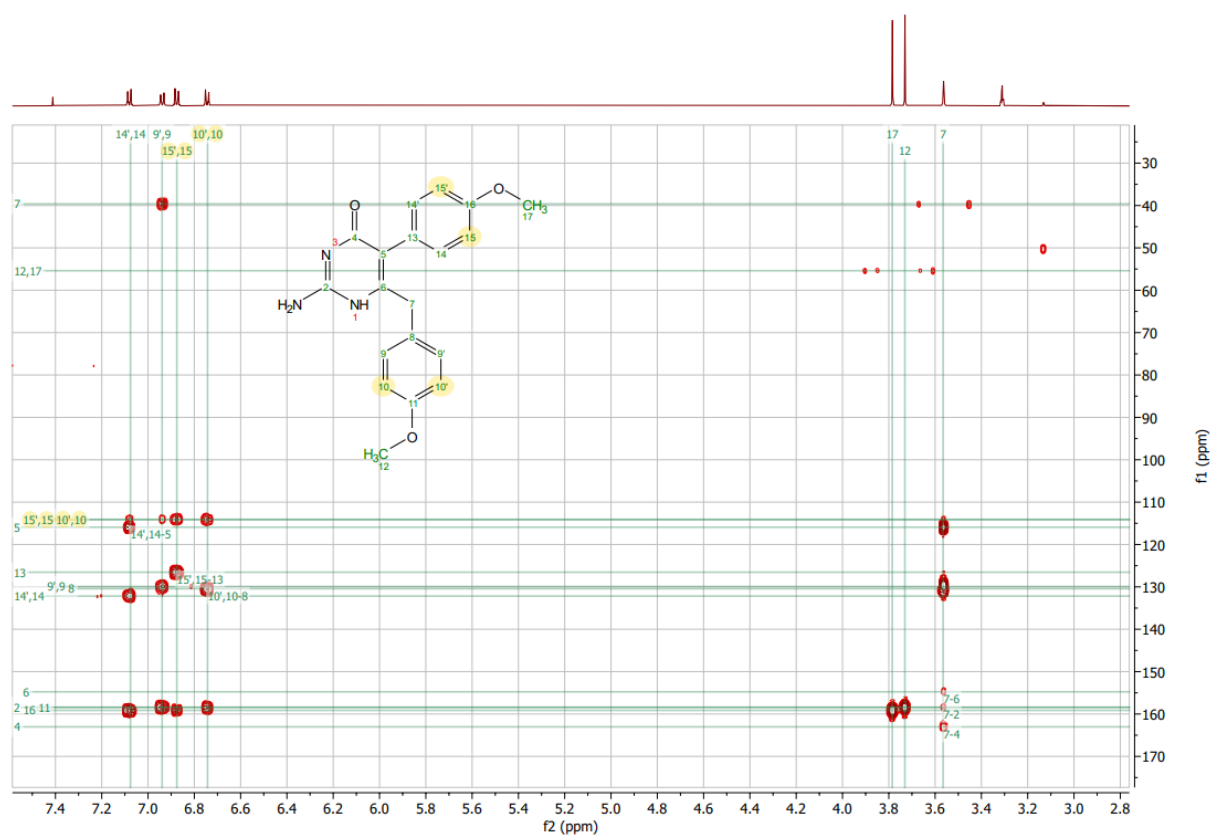


**Figure S4:**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (600 MHz) spectrum for ernstine A (1)



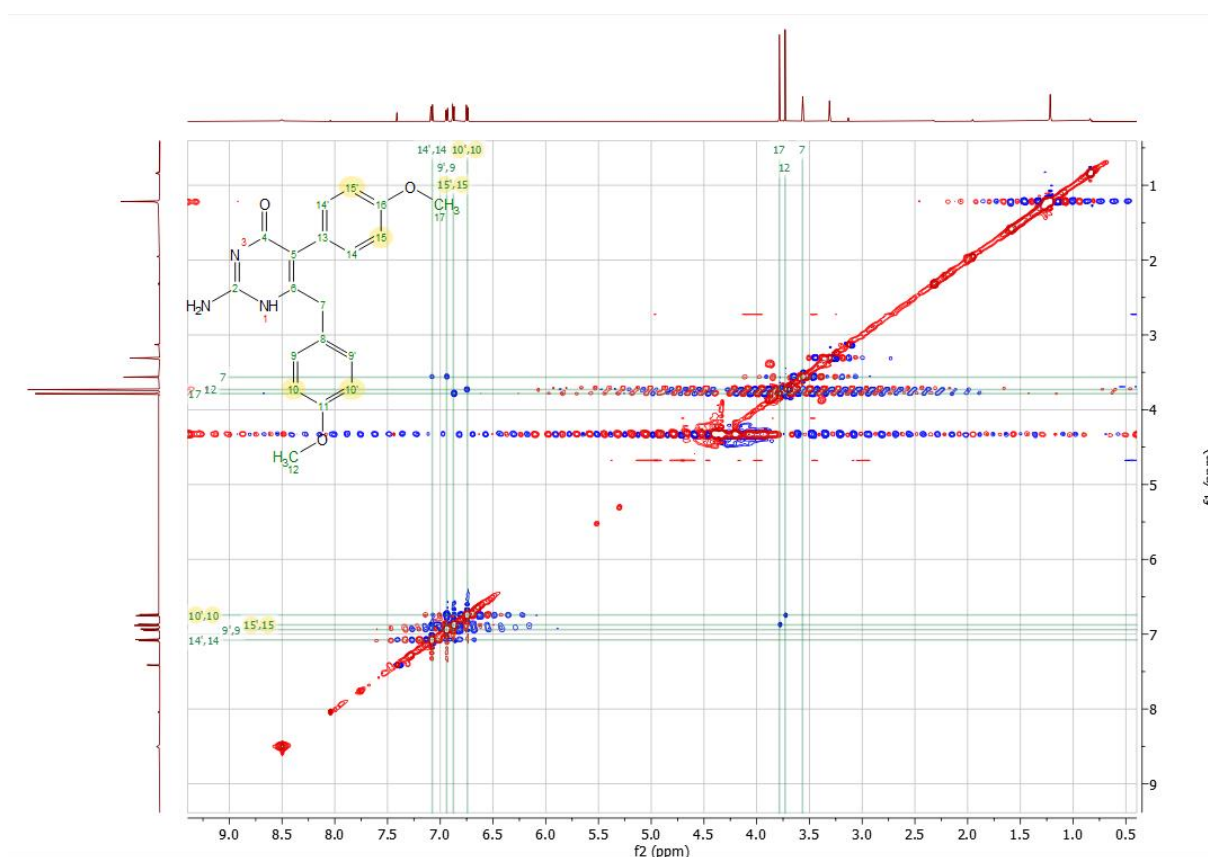
# Supporting information

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



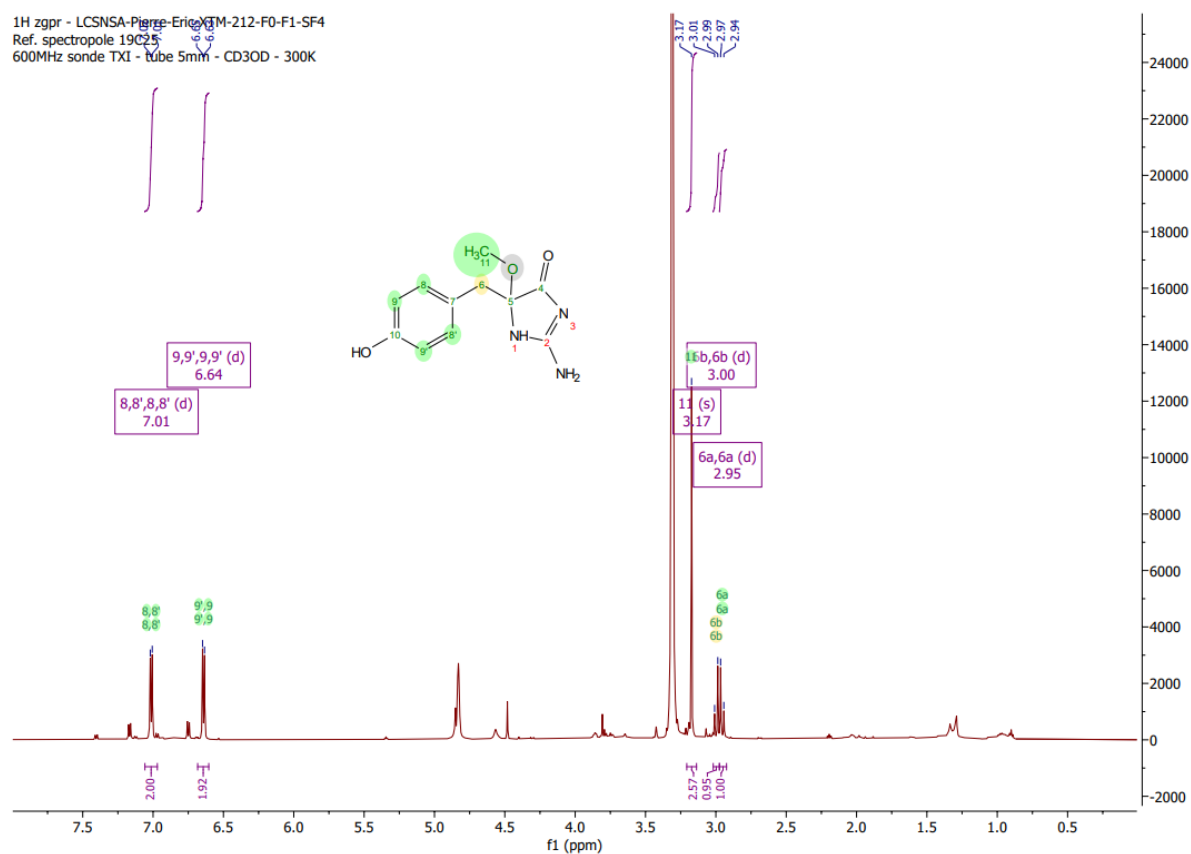
# Supporting information

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

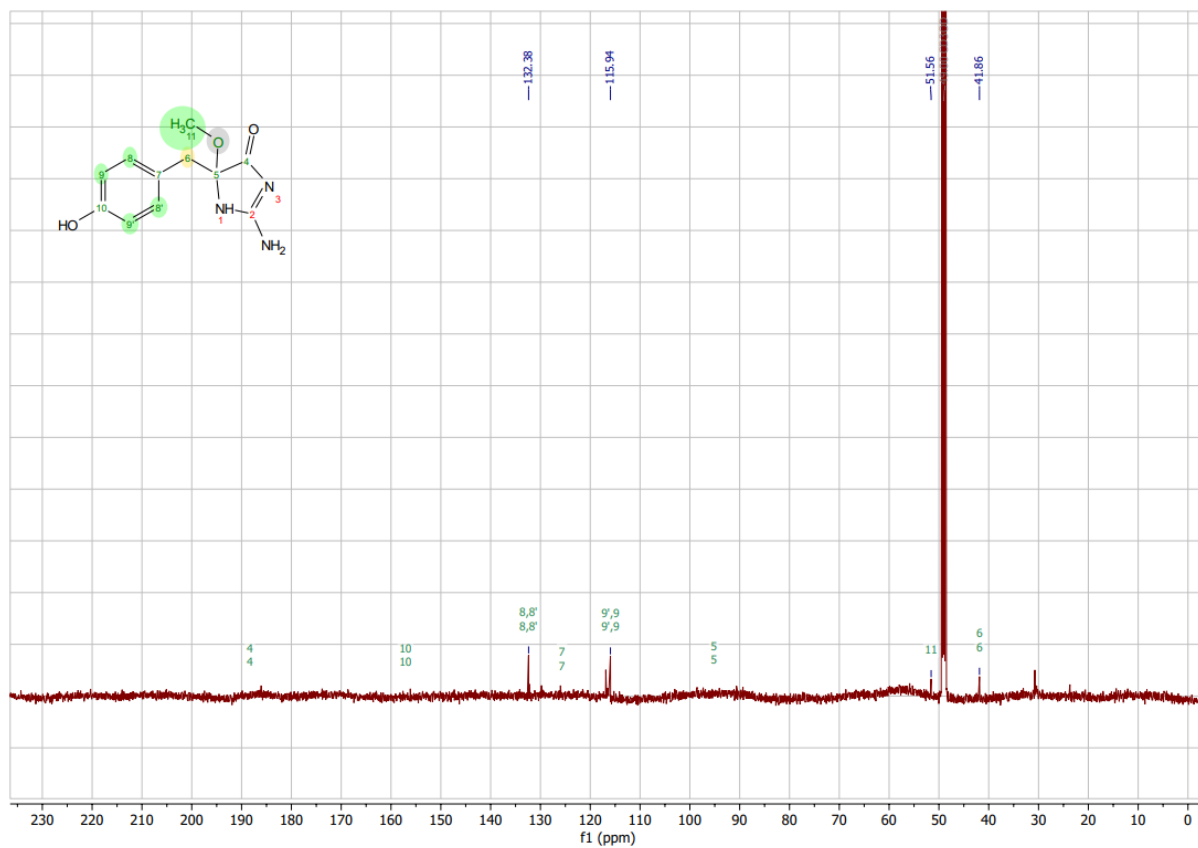


# Supporting information

**Figure S8:**  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum for phorbatopsin D (2)



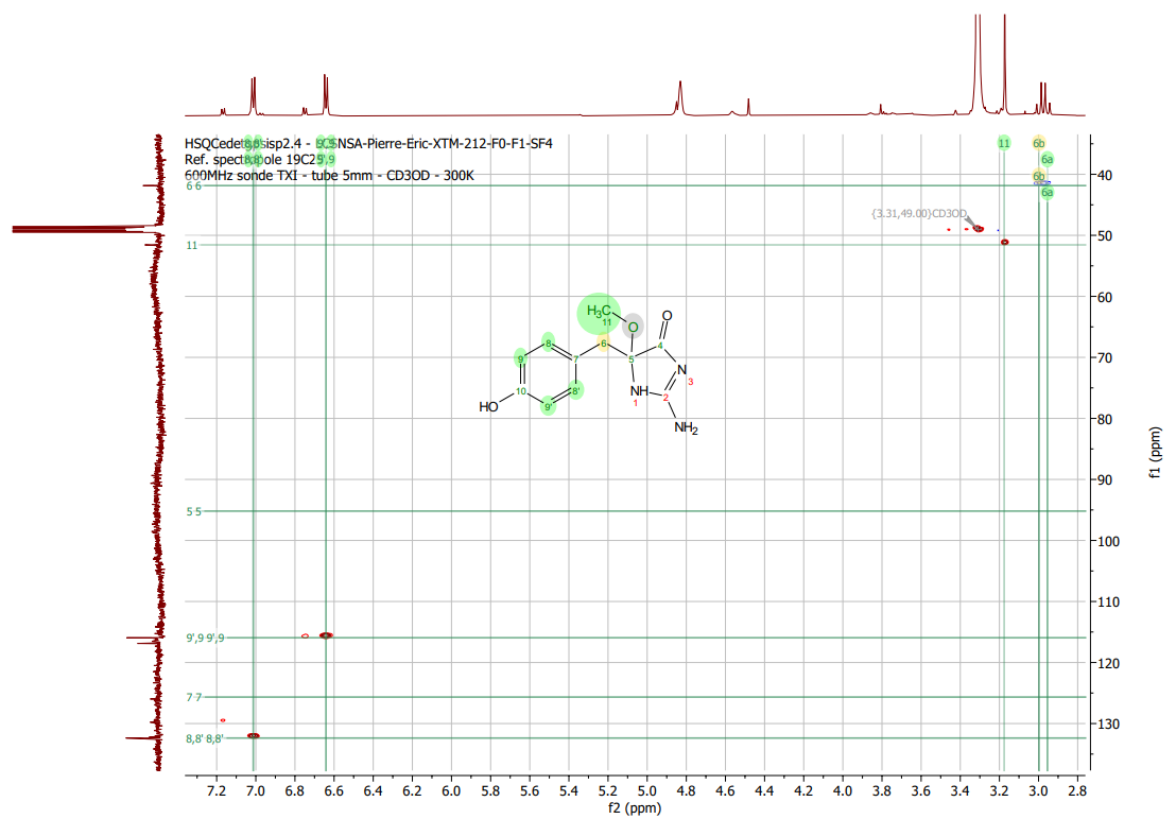
**Figure S9:**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{OD}$ ) spectrum for phorbatopsin D (2)



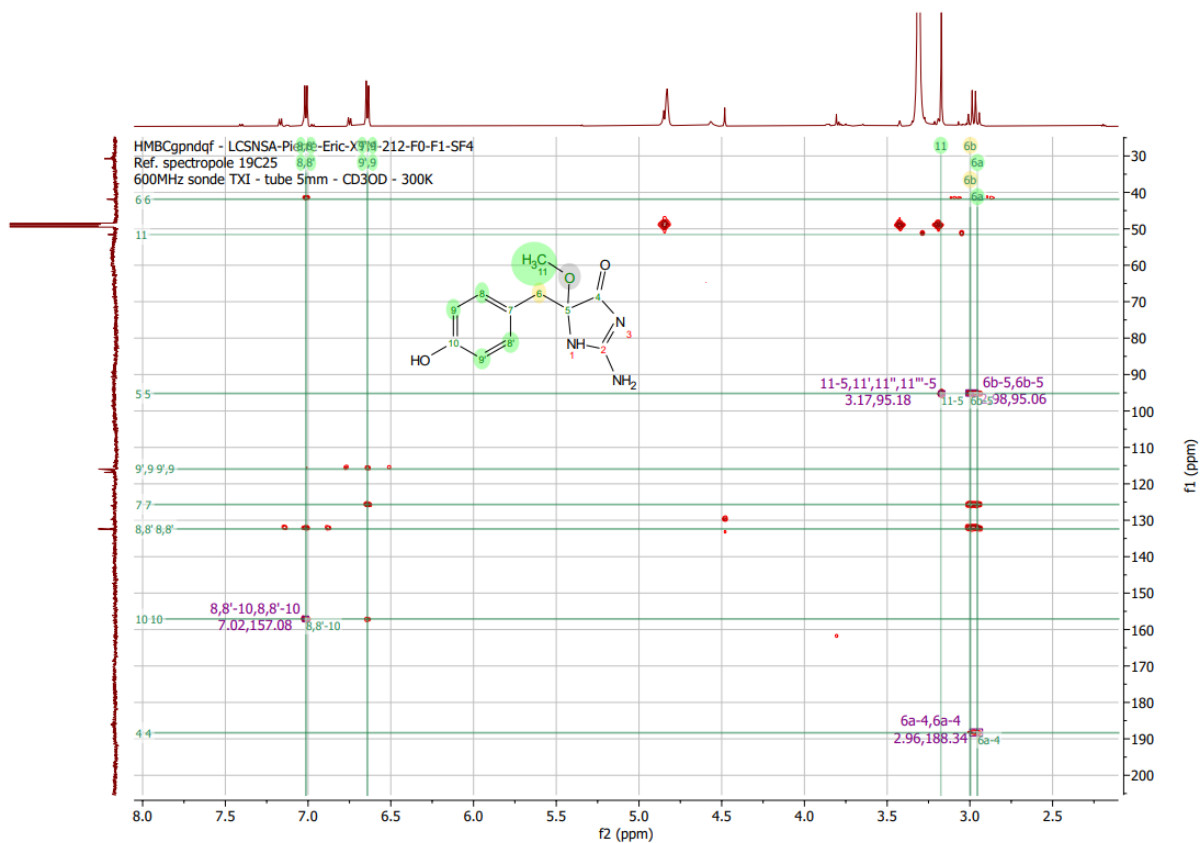


# Supporting information

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

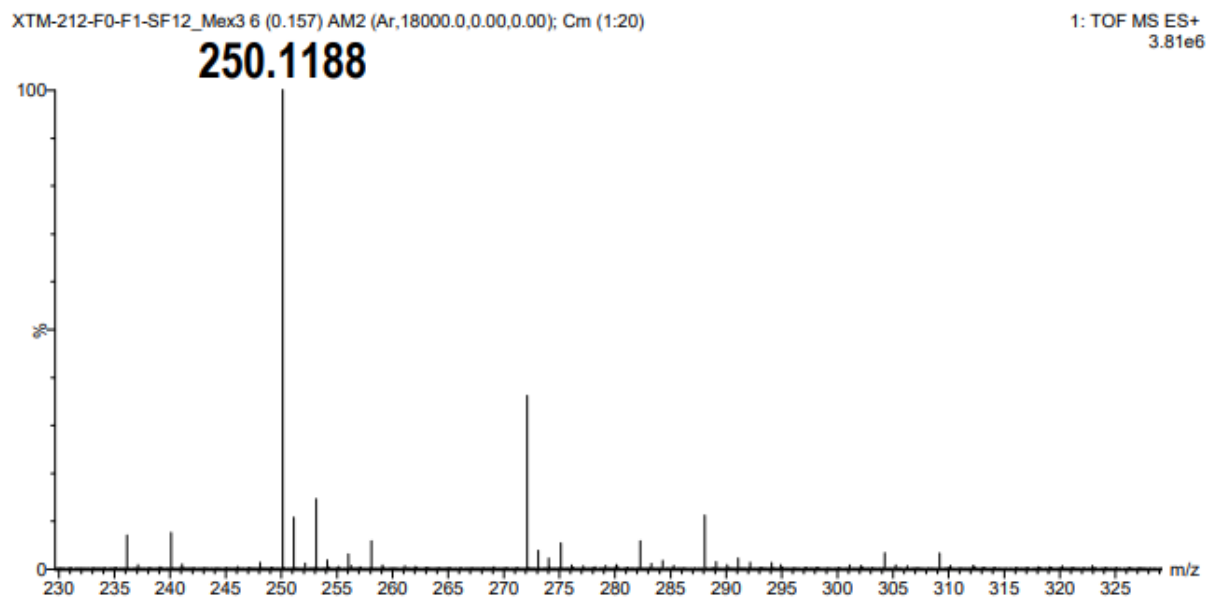


**Figure S11:**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (600 MHz) spectrum for phorbatopsin D (2)

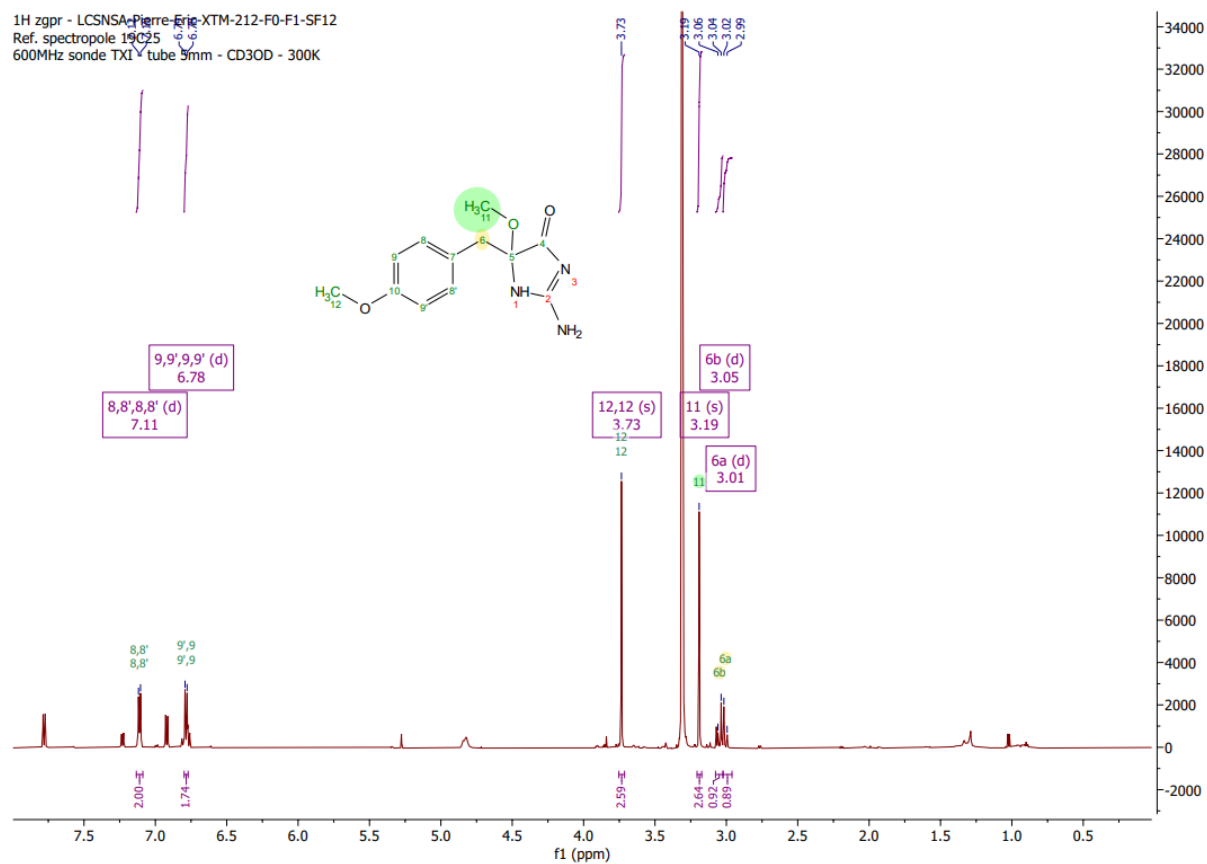


# Supporting information

**Figure S12:** HRESIMS spectrum for phorbatopsin E (3)

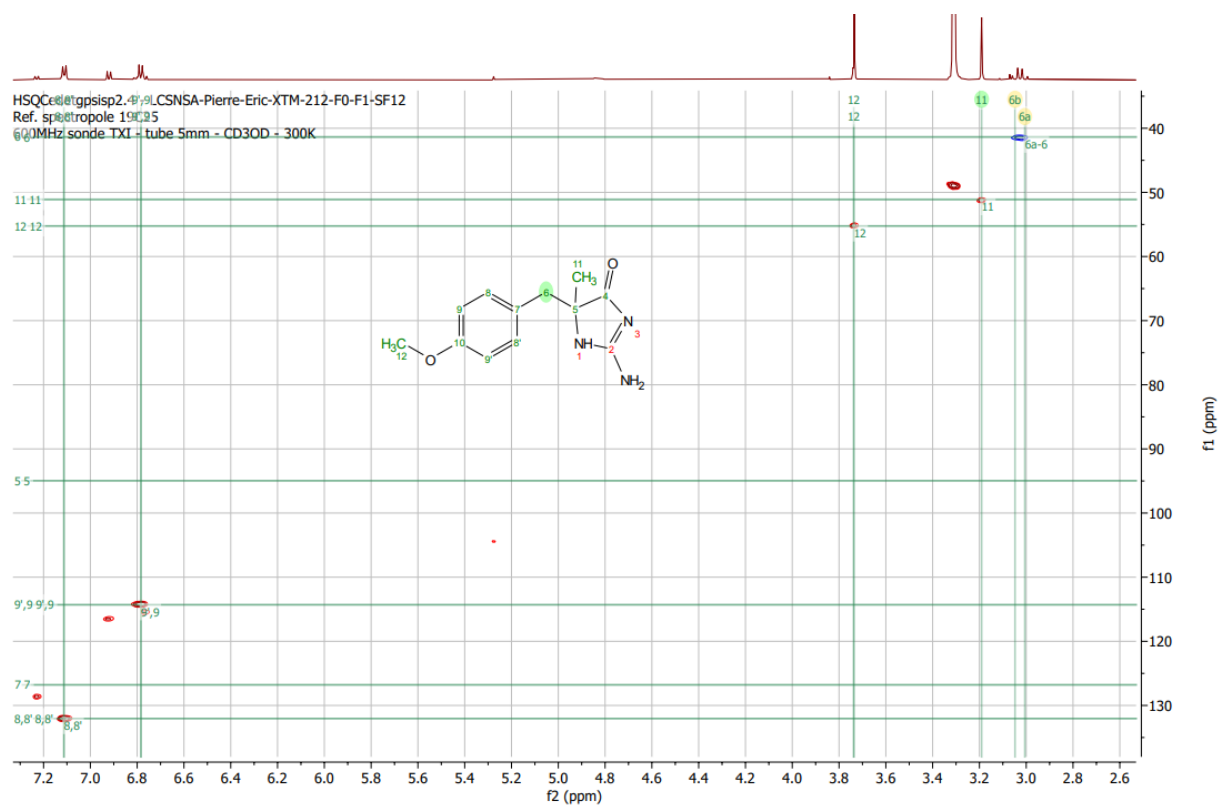


**Figure S13:**  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum for phorbatopsin E (3)

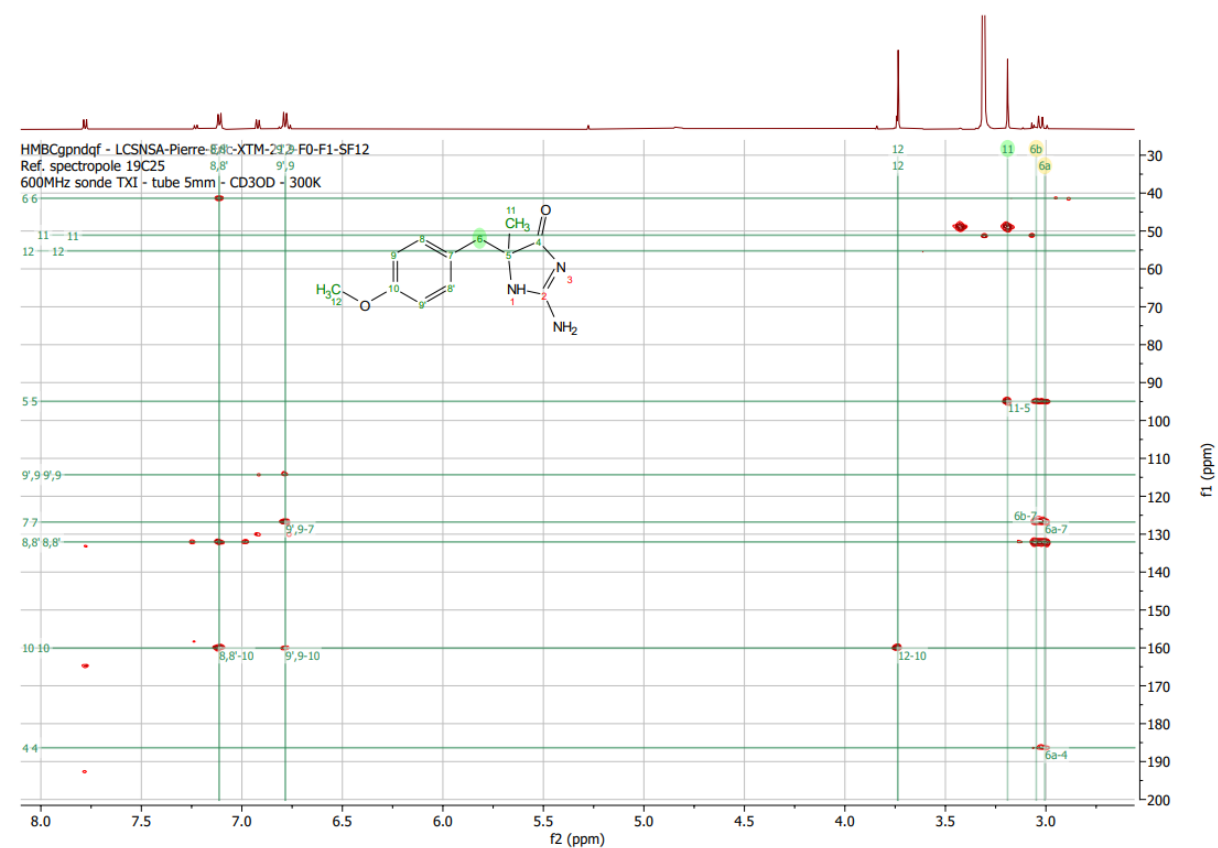


# Supporting information

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

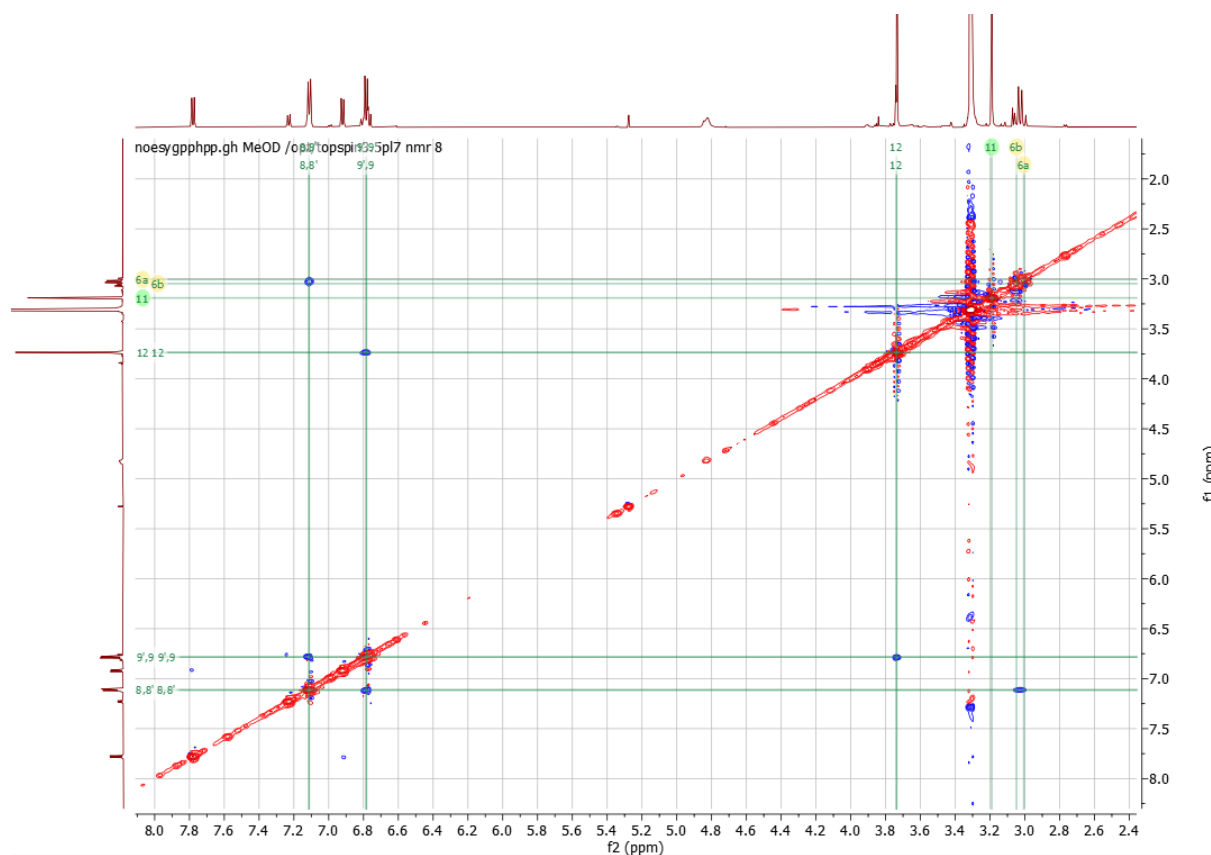


**Figure S15:**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (600 MHz) spectrum for phorbatopsin E (3)

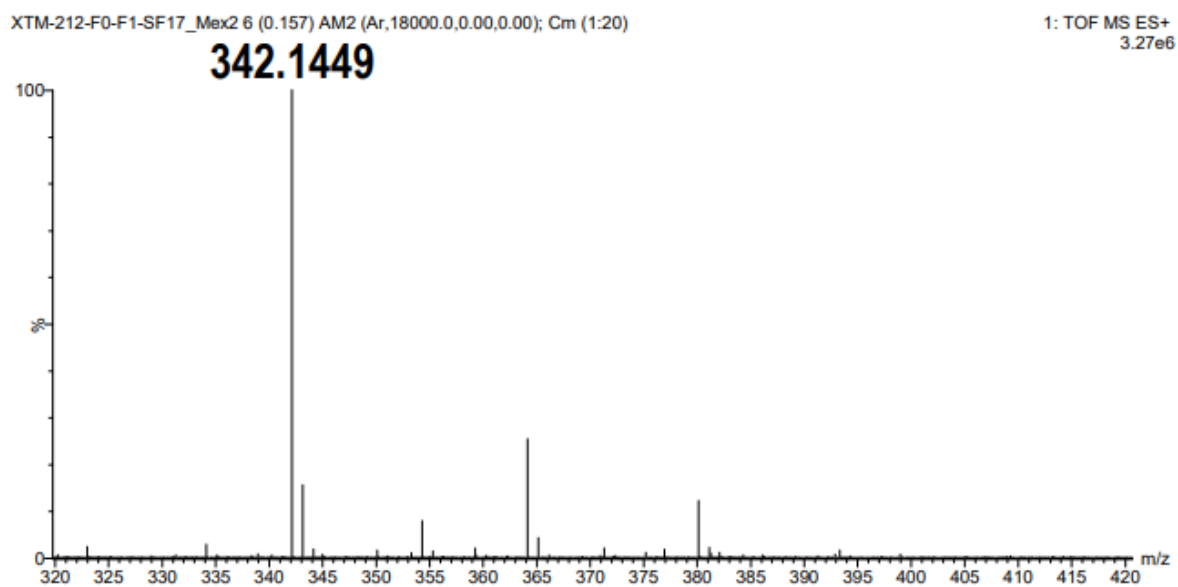


## Supporting information

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

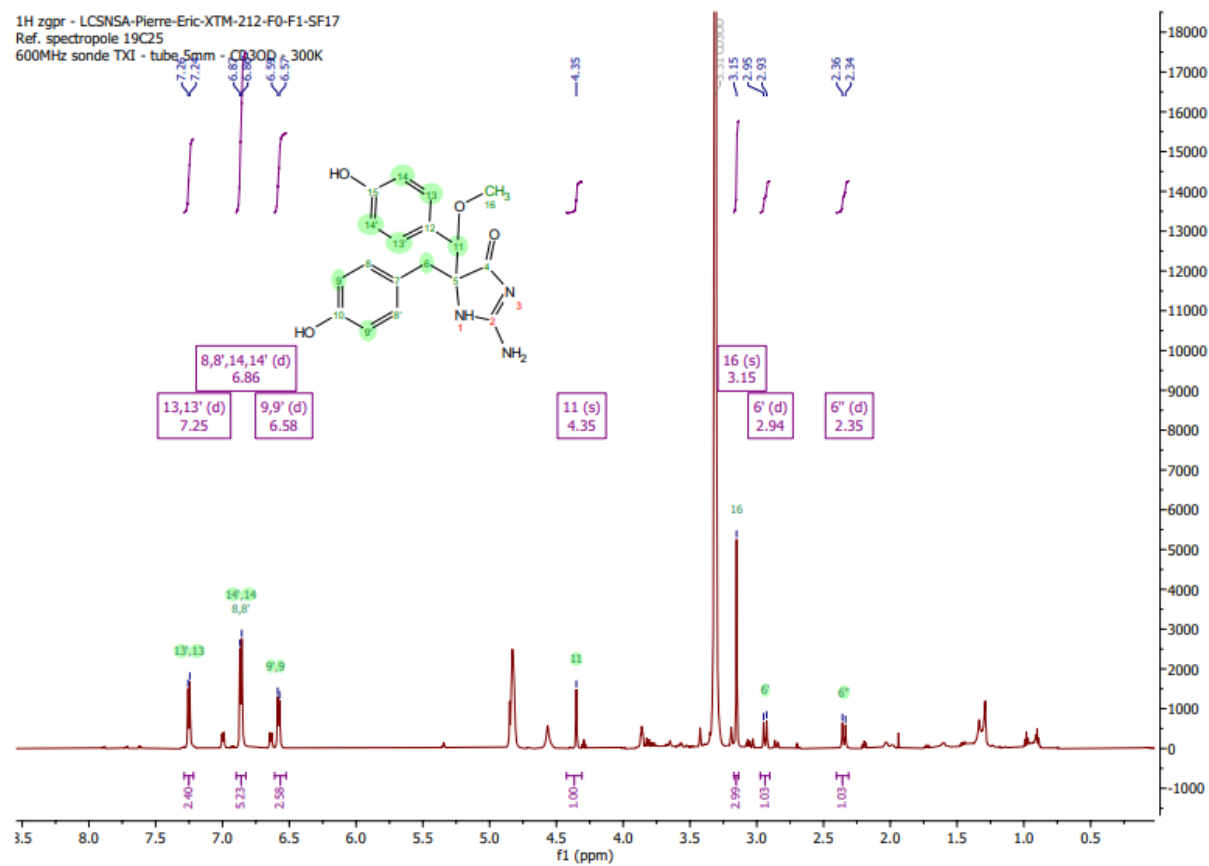


**Figure S17:** HRESIMS spectrum for calcaridine C (4)



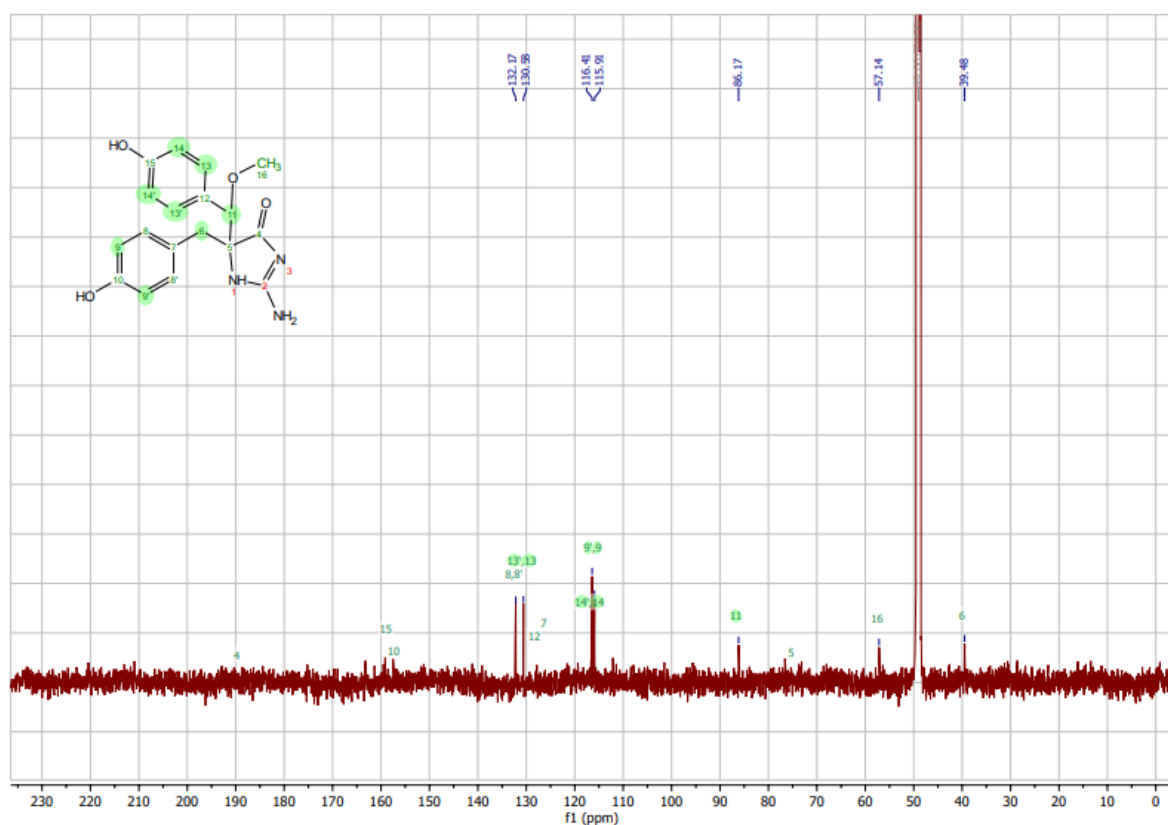
# Supporting information

**Figure S18:**  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum for calcaridine C (4)

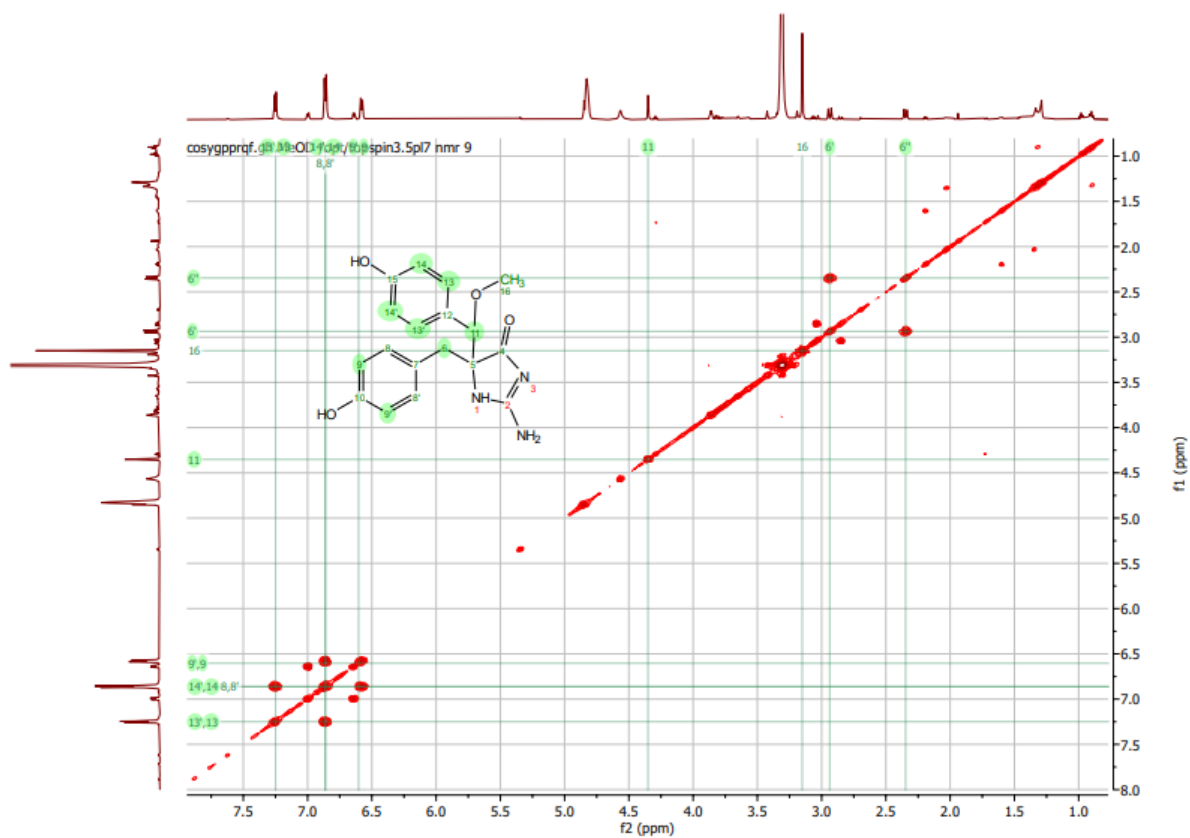


# Supporting information

**Figure S19:**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{OD}$ ) spectrum for calcaridine C (4)

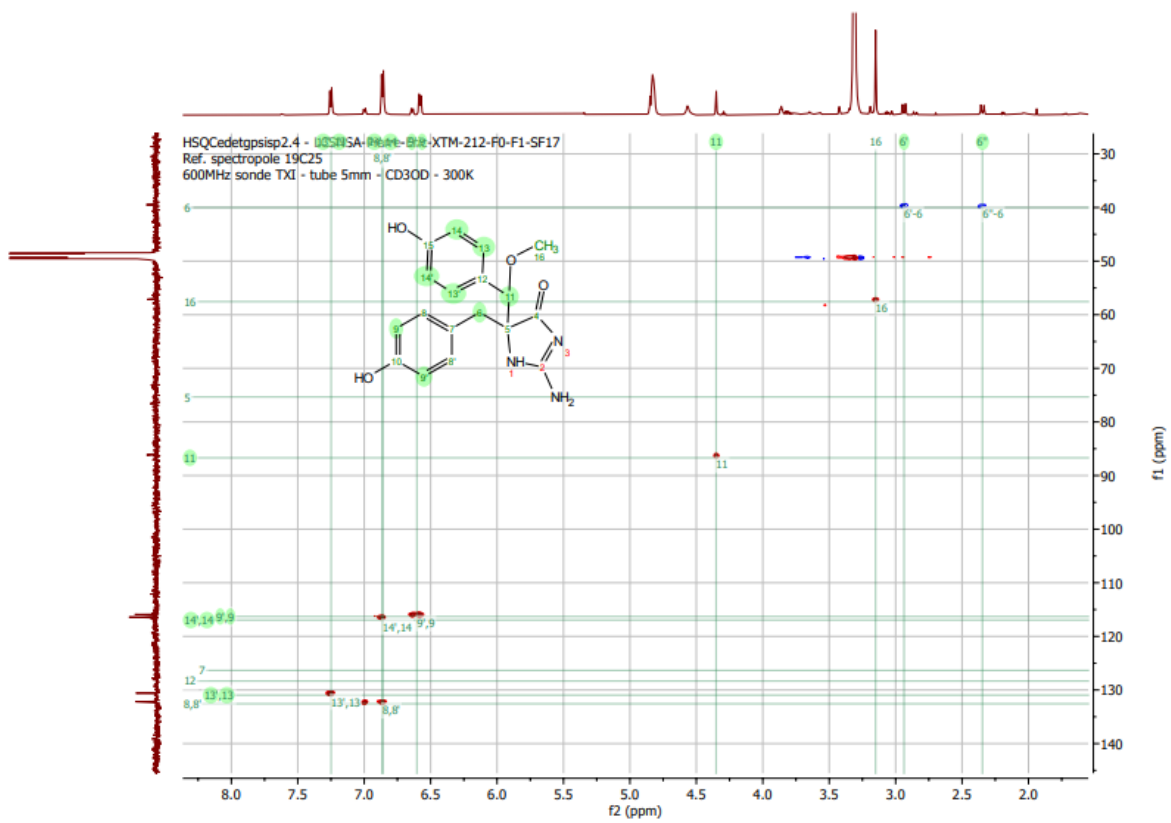


**Figure S20:**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (600 MHz) spectrum for calcaridine C (4)

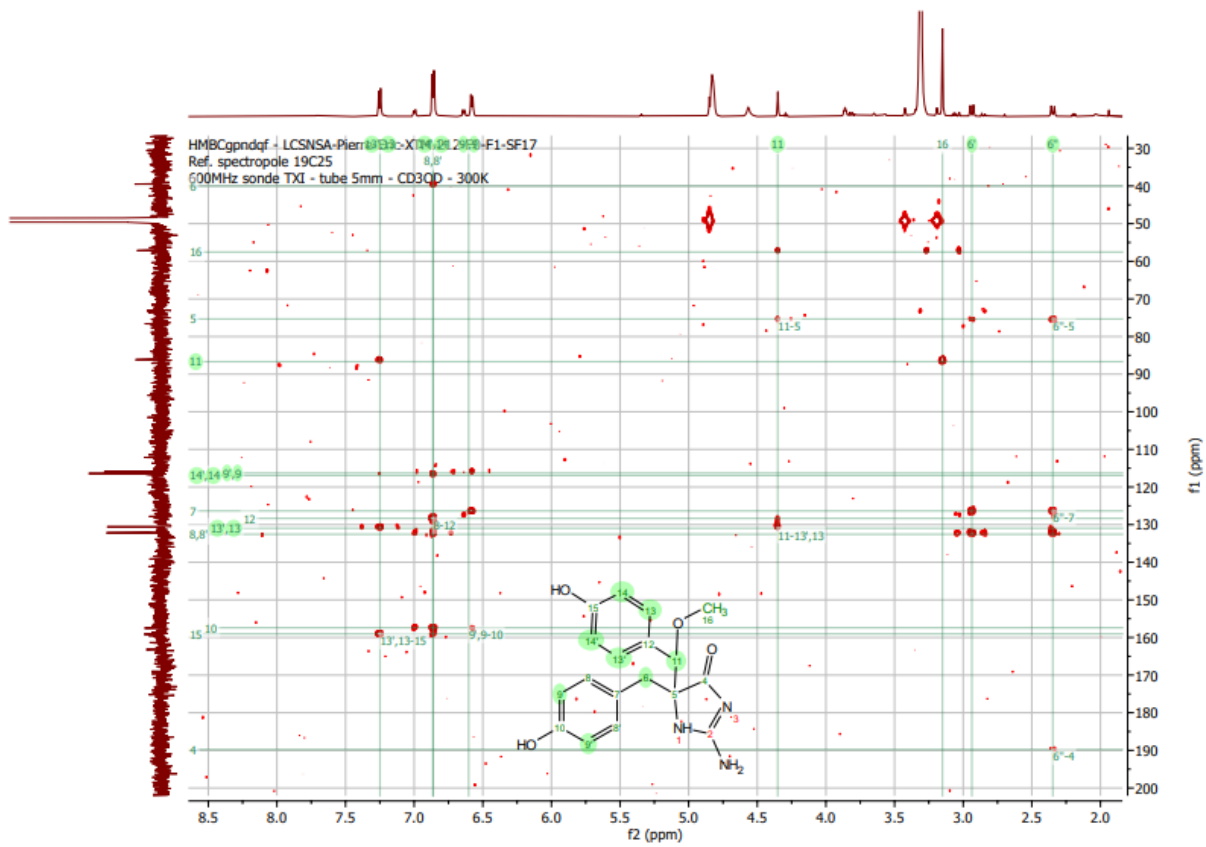


## Supporting information

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

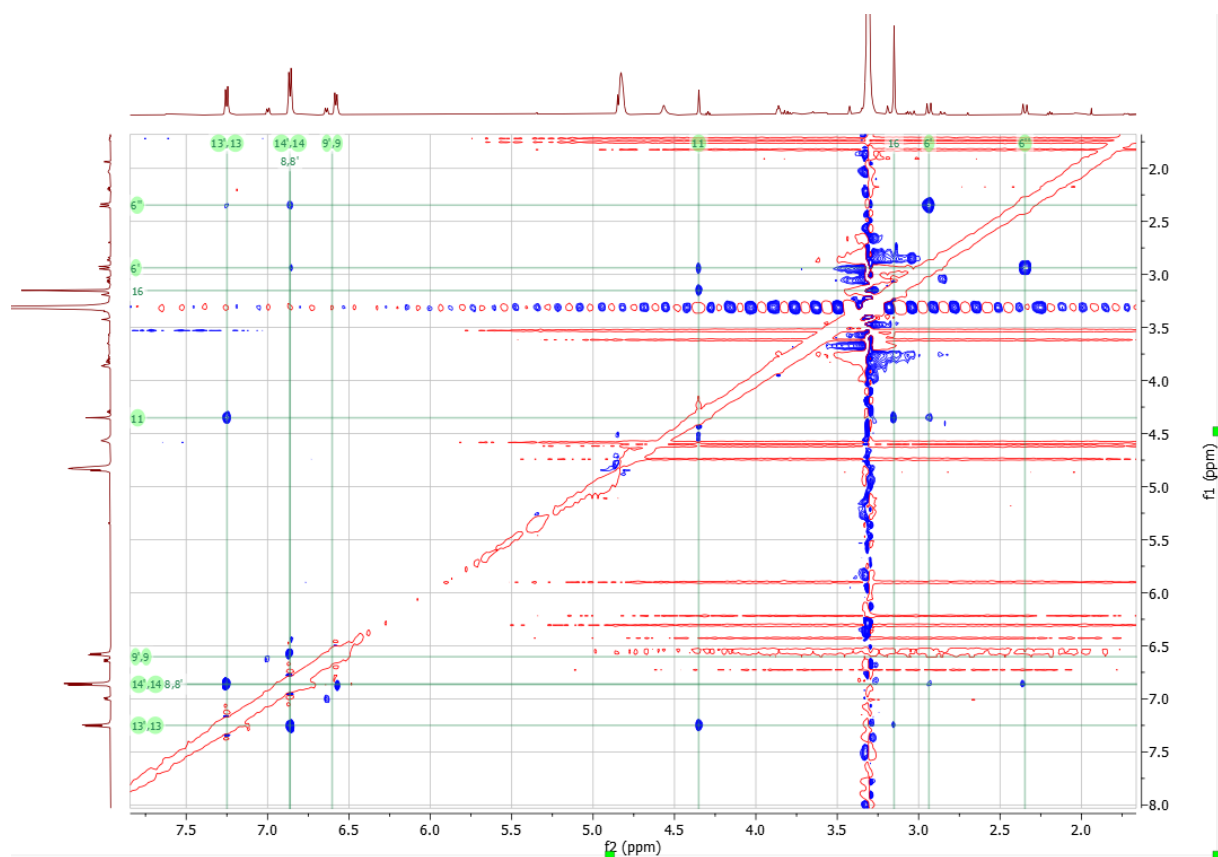


**Figure S22:**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (600 MHz) spectrum for calcaridine C (4)

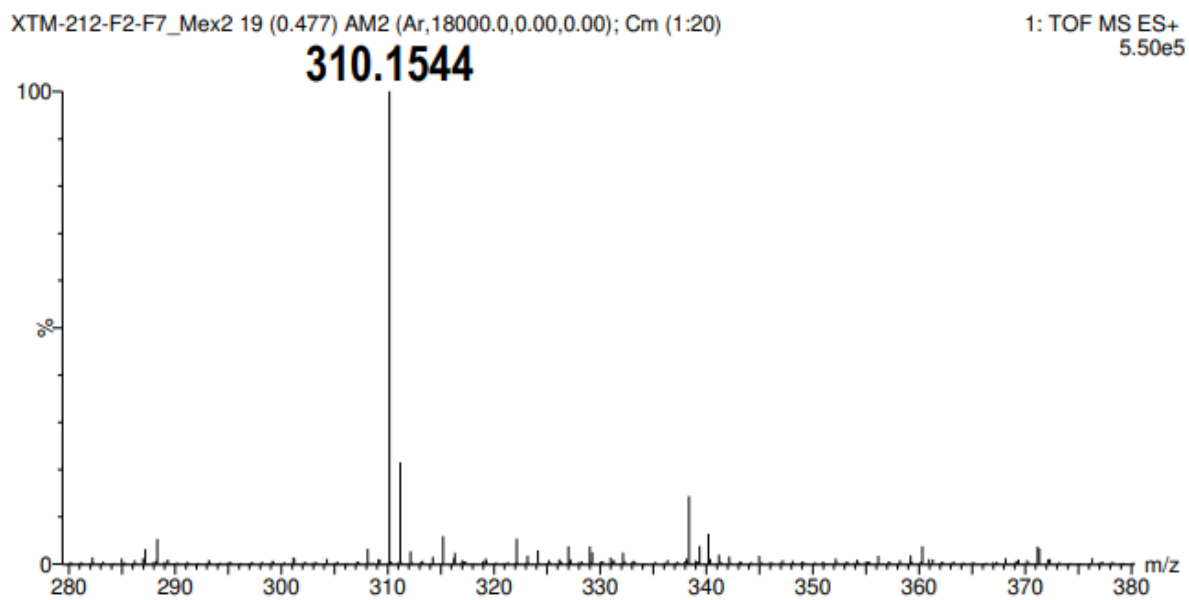


## Supporting information

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



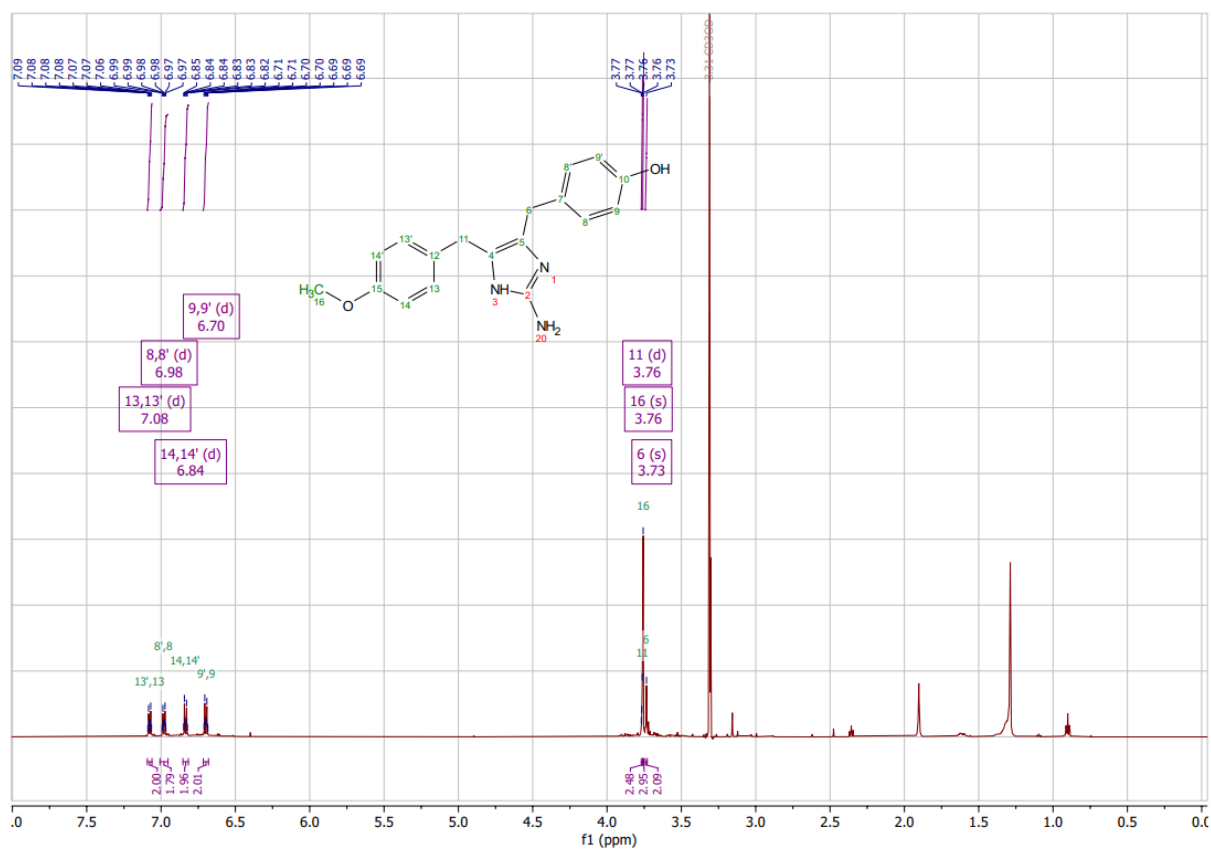
**Figure S24:** HRESIMS spectrum for naamine H (5)





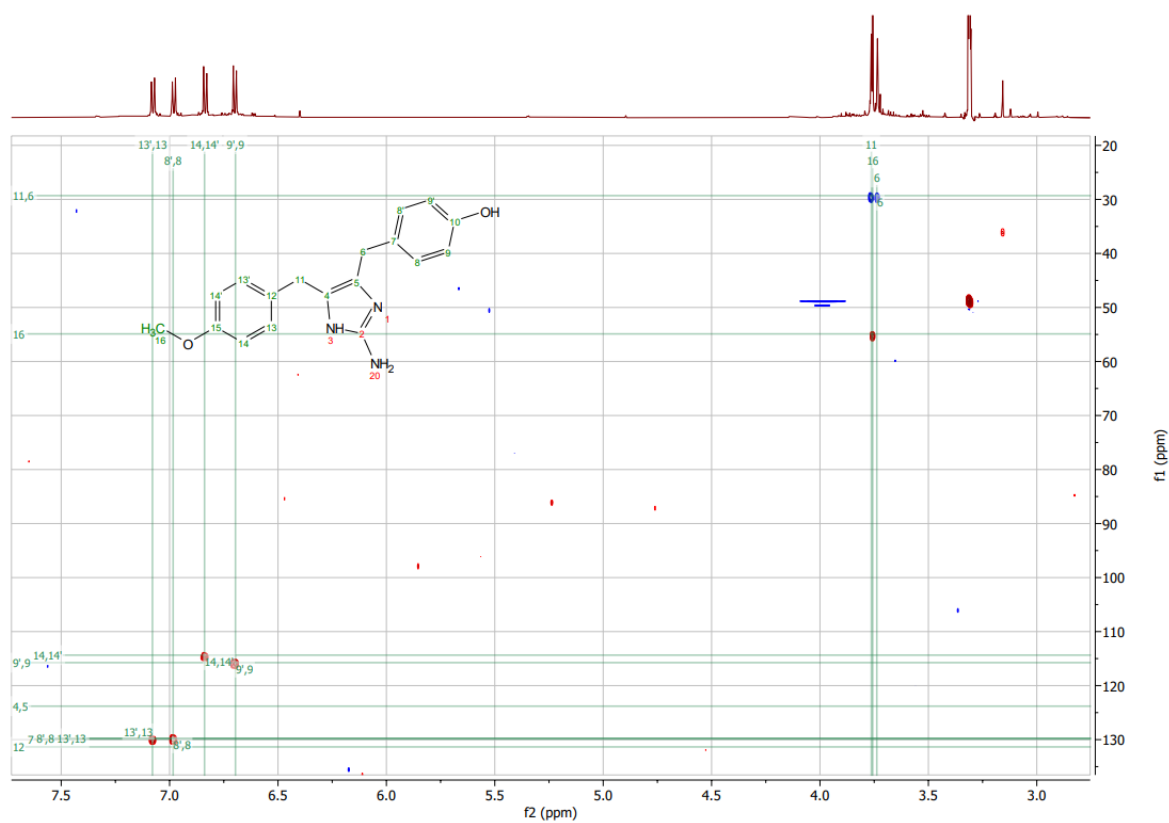
## Supporting information

Figure S25:  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum for naamine H (5)

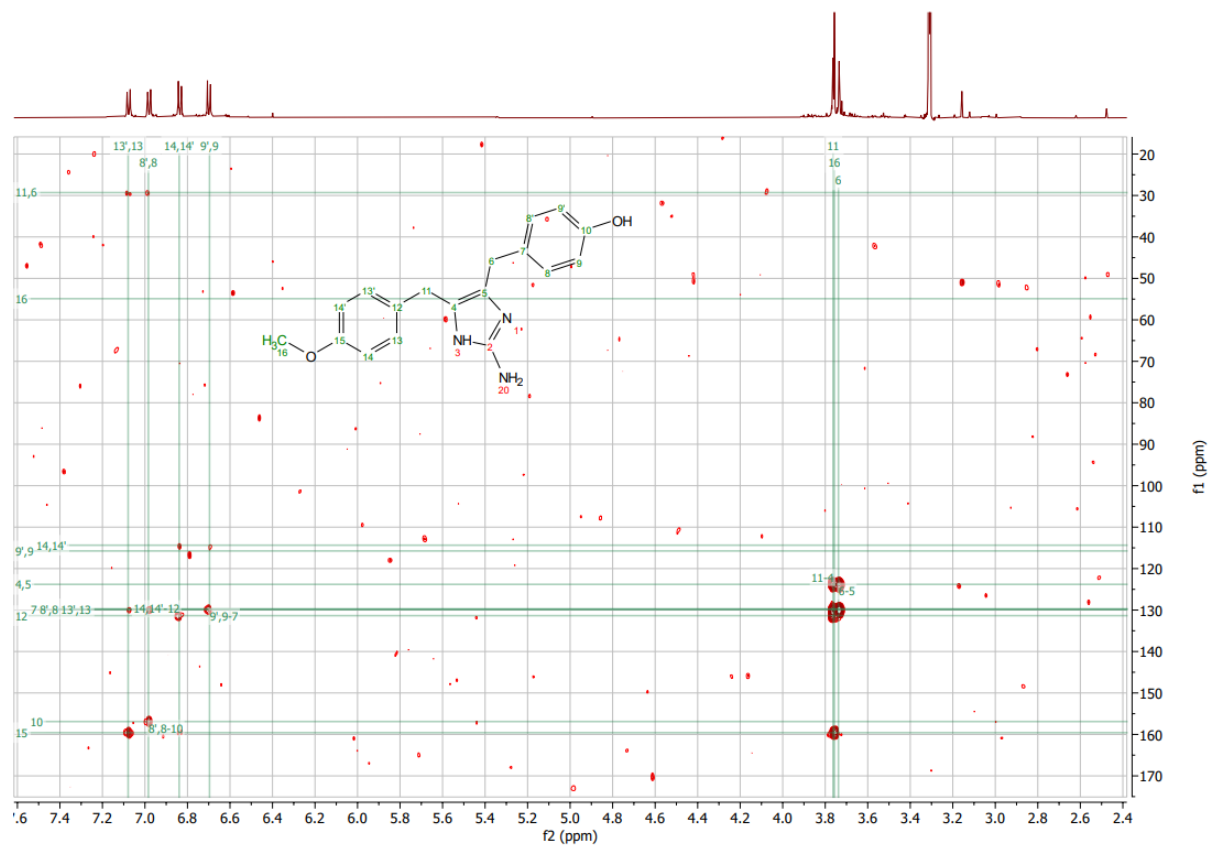


## Supporting information

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

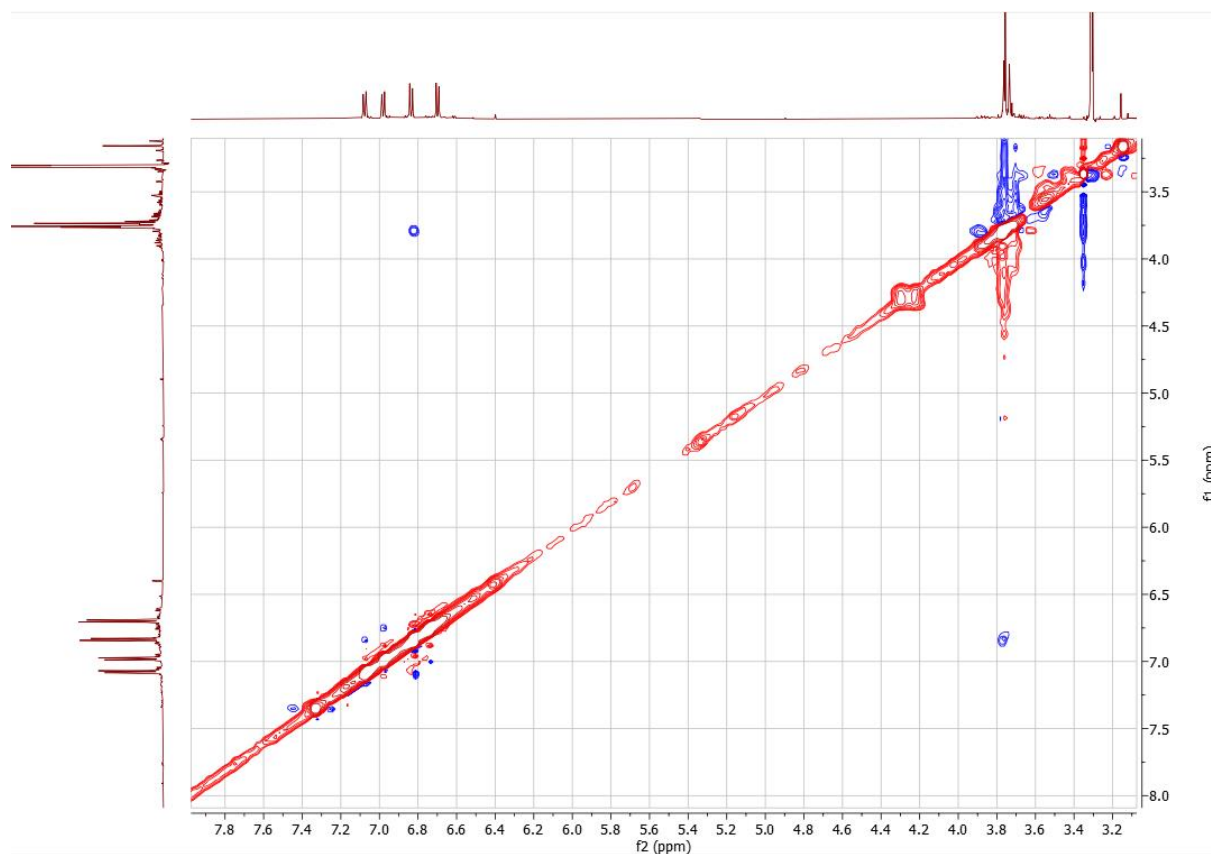


**Figure S27:**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR (600 MHz) spectrum for naamine H (5)



## Supporting information

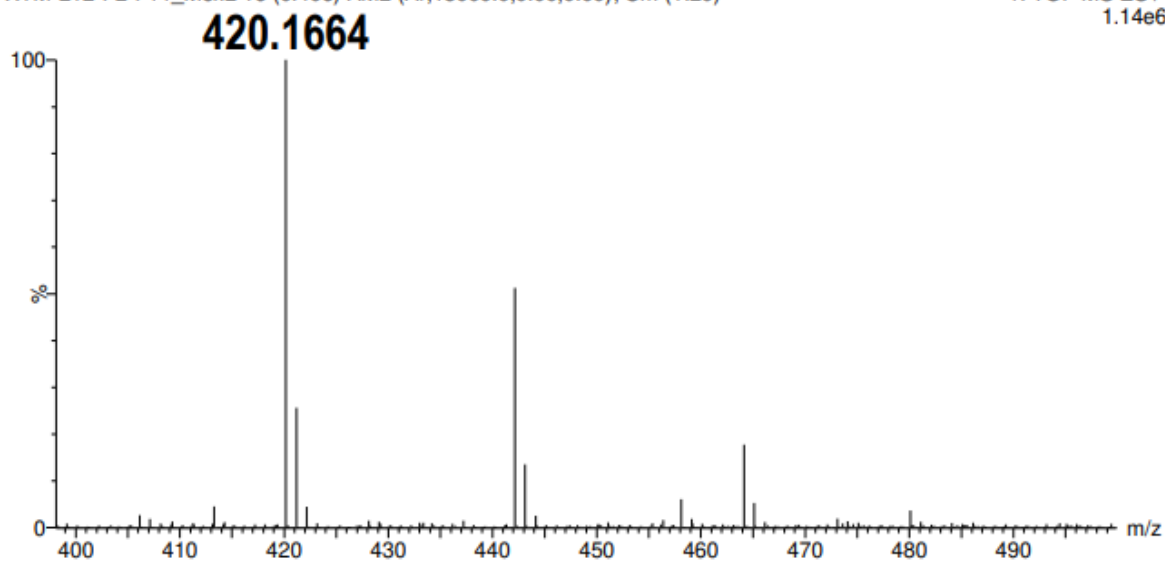
**Figure S28:**  $^1\text{H}$ - $^1\text{H}$  NOESY NMR (600 MHz) spectrum for naamine H (5)



**Figure S29:** HRESIMS spectrum for naamidine J (6)

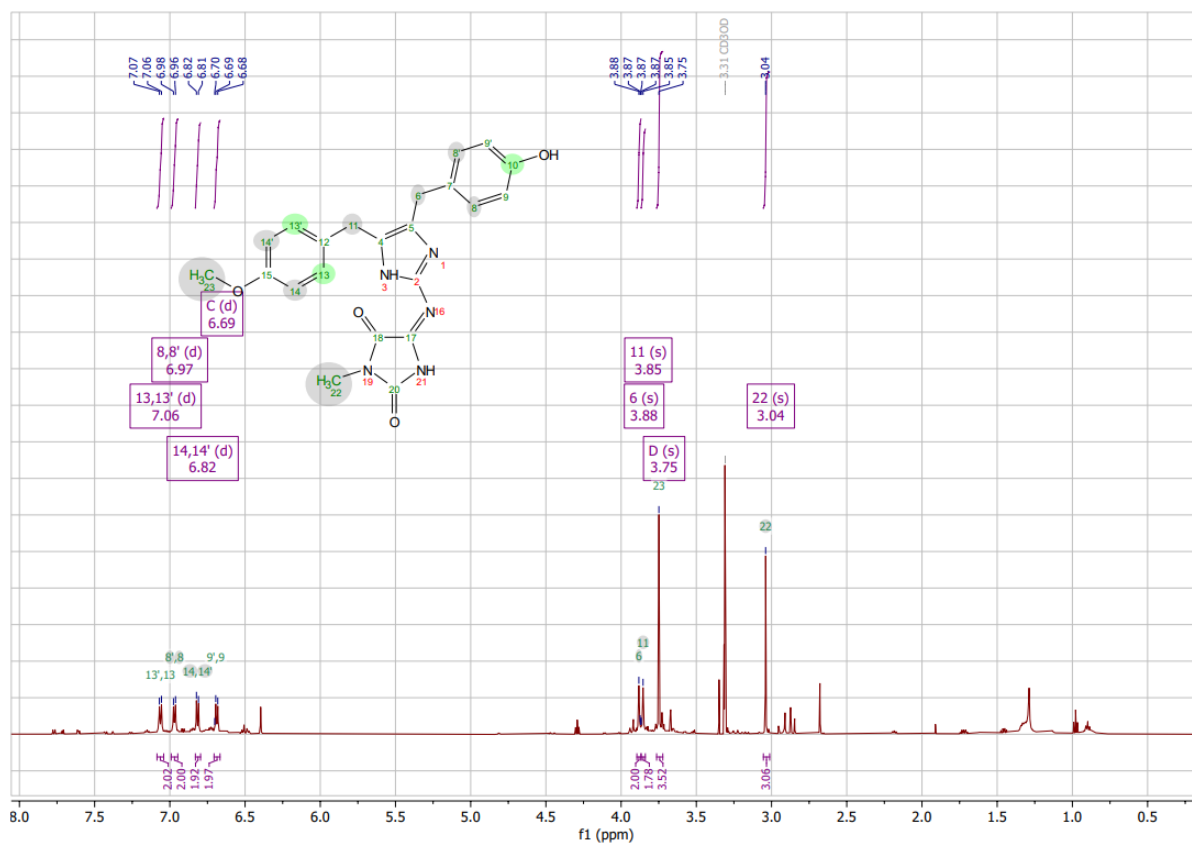
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1.14e6

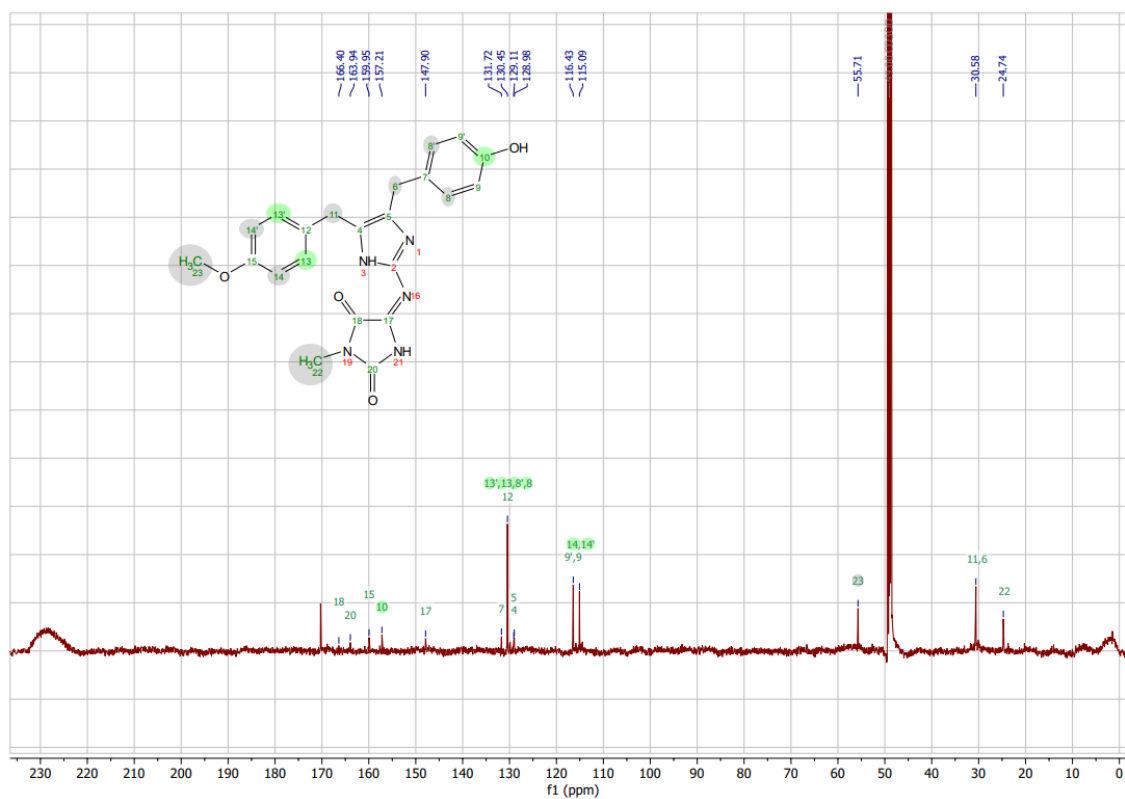


# Supporting information

**Figure S30:**  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum for naamidine J (6)

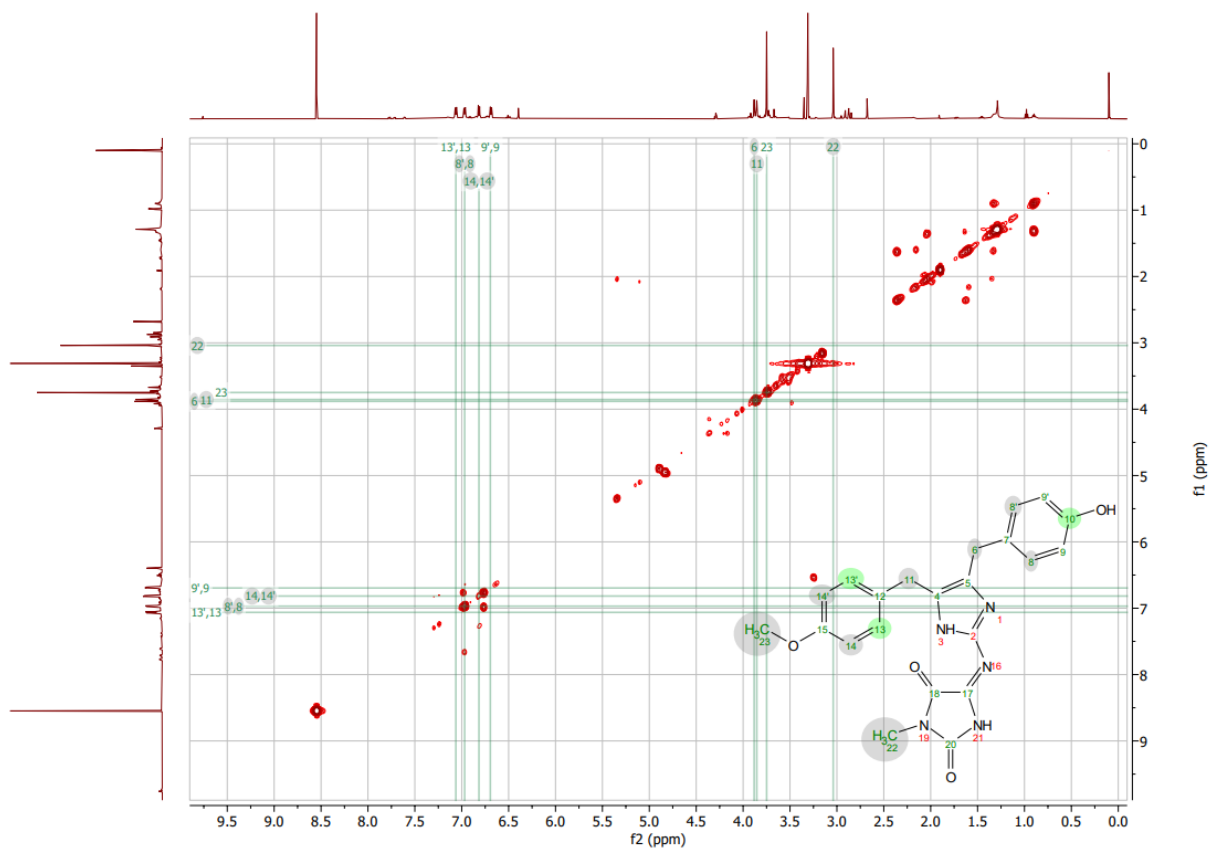


**Figure S31:**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{OD}$ ) spectrum for naamidine J (6)

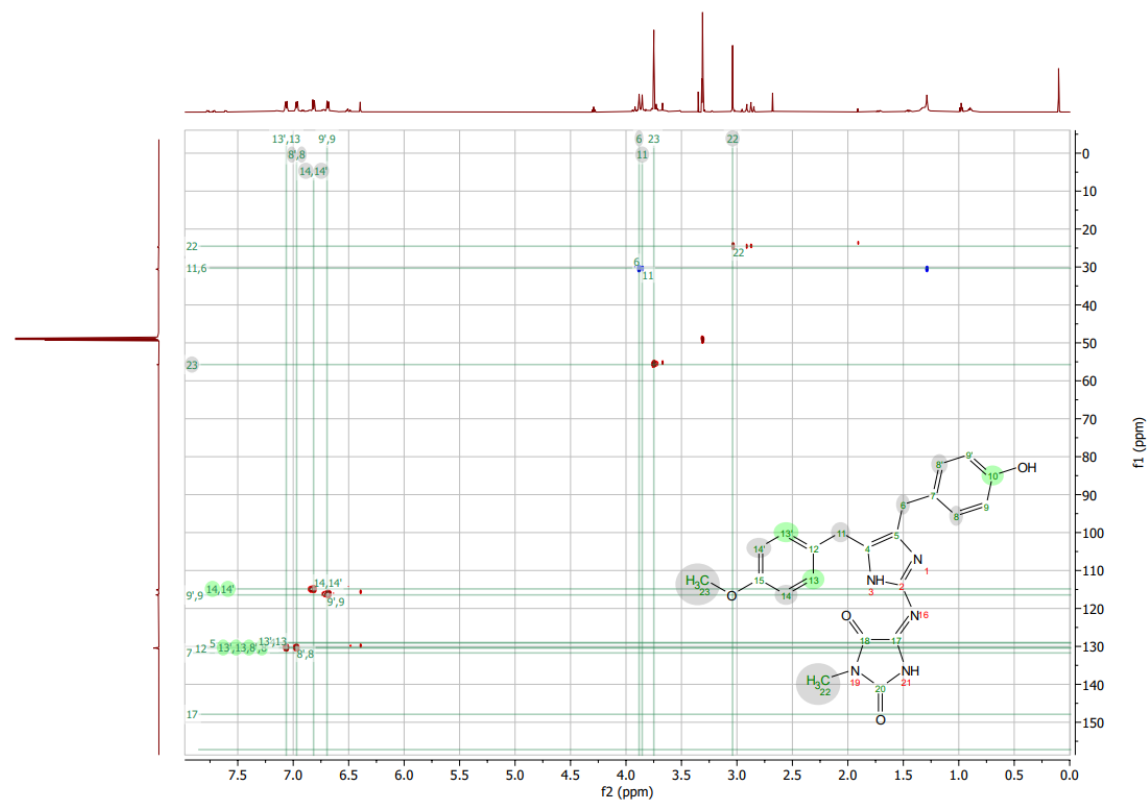


# Supporting information

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

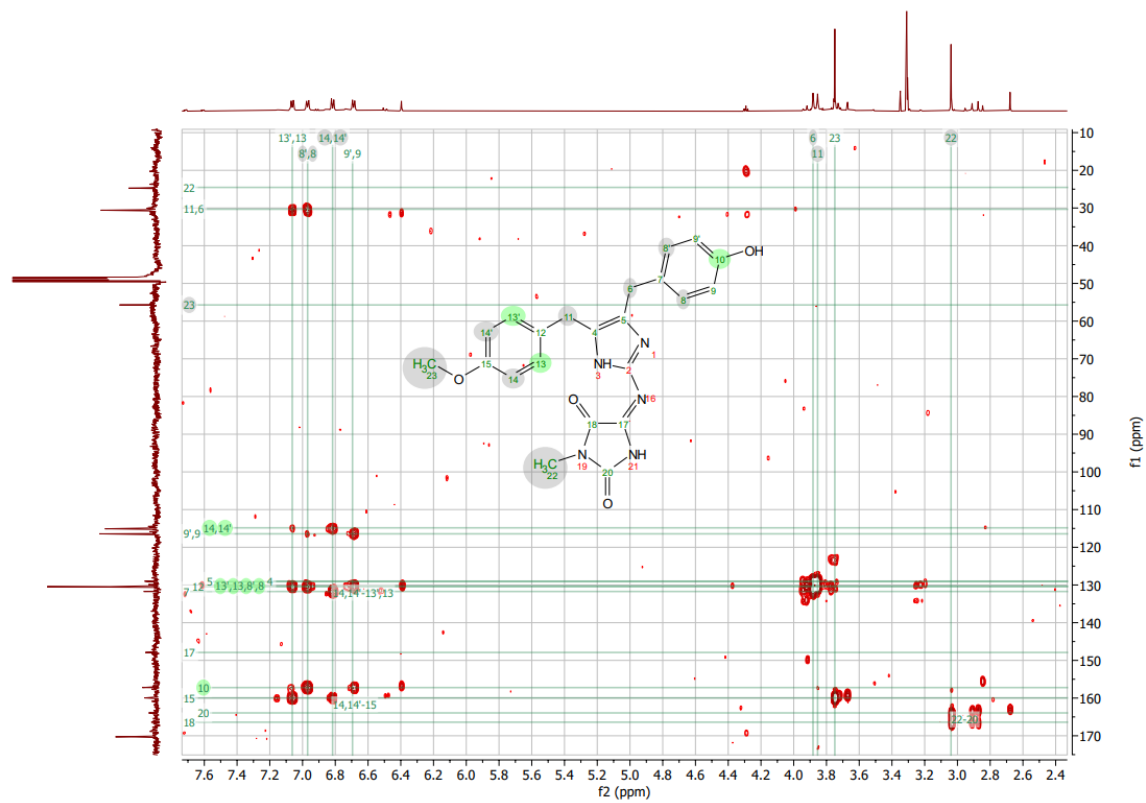


**Figure S33:**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (600 MHz) spectrum for naamidine J (6)

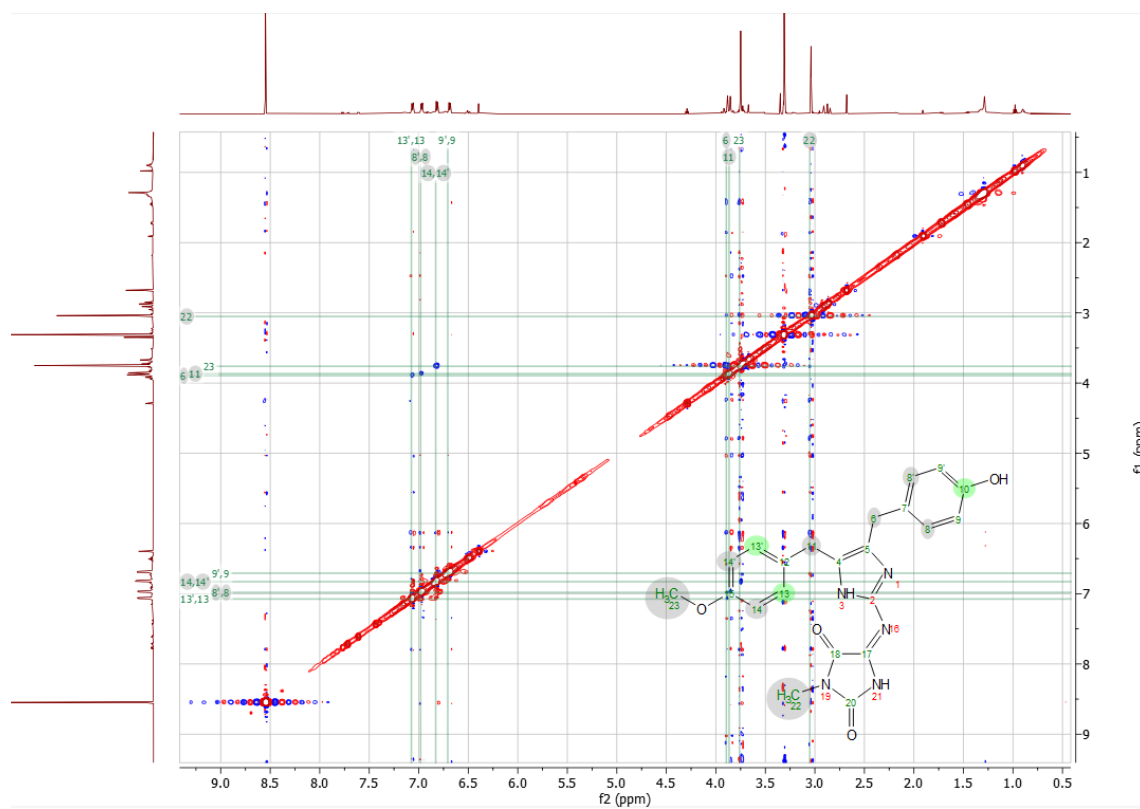


# Supporting information

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

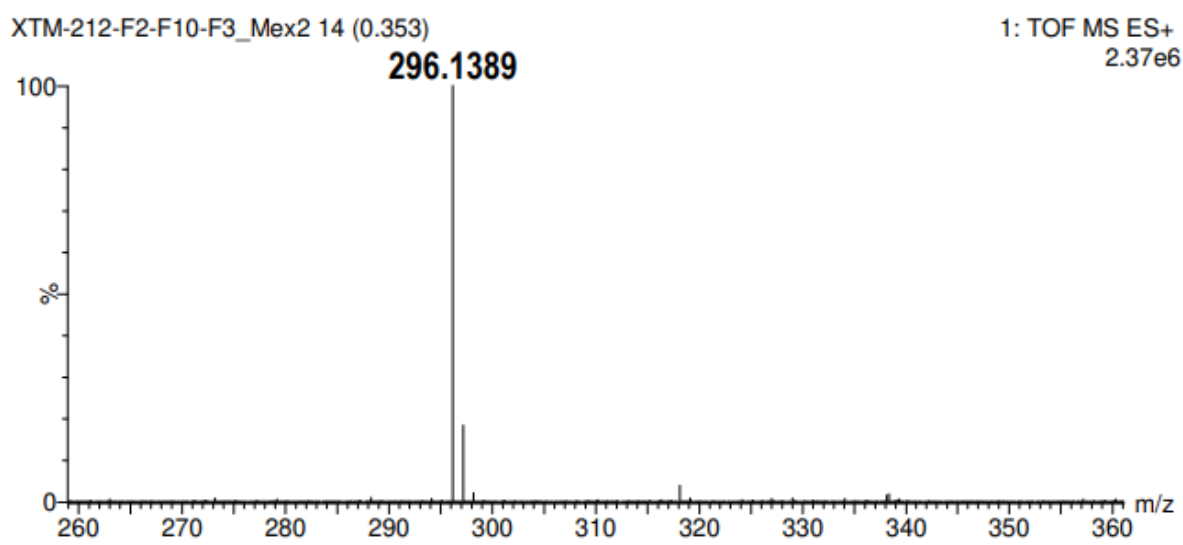


**Figure S35:**  $^1\text{H}$ - $^1\text{H}$  NOESY NMR (600 MHz) spectrum for naamidine J (6)

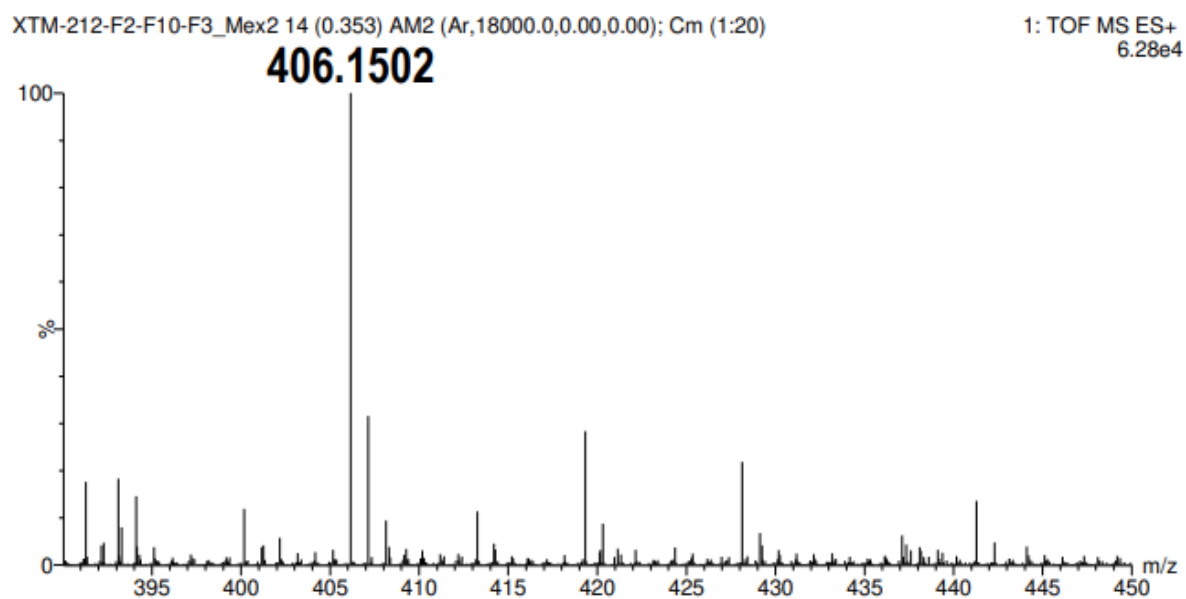


## Supporting information

**Figure S36:** HRESIMS spectrum for naamine I (7)

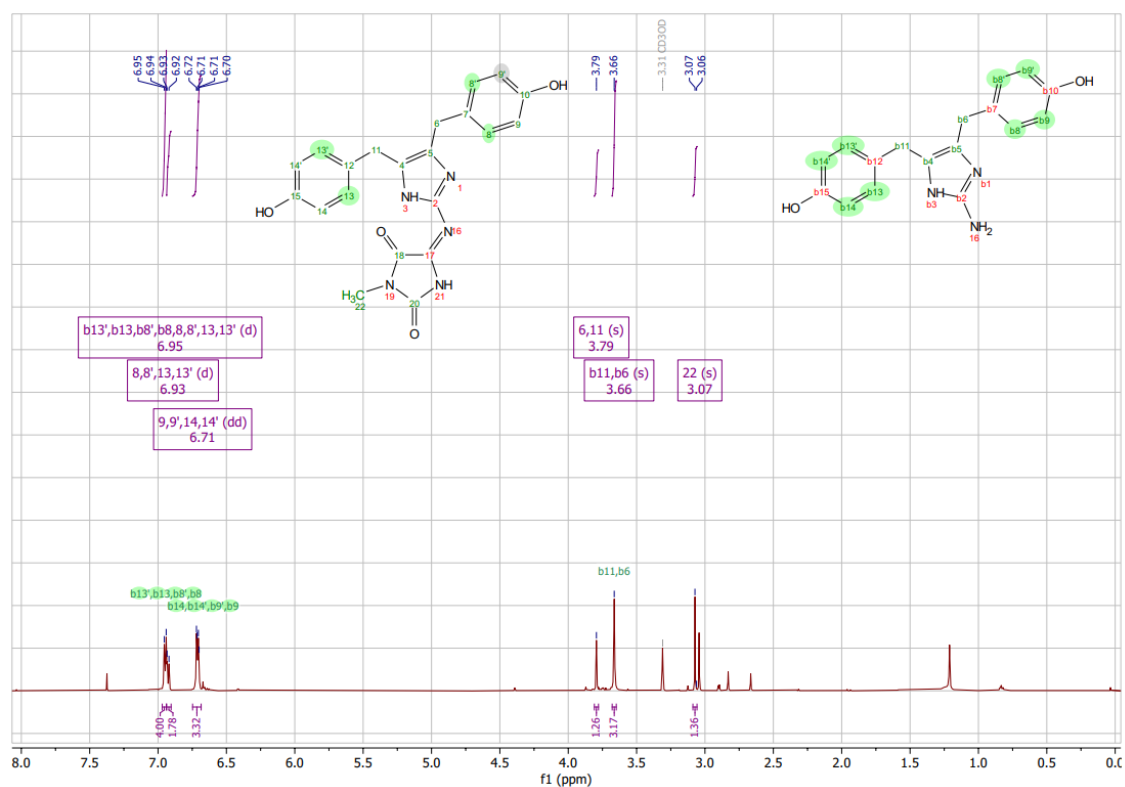


**Figure S37:** HRESIMS spectrum for naamidine K (8)

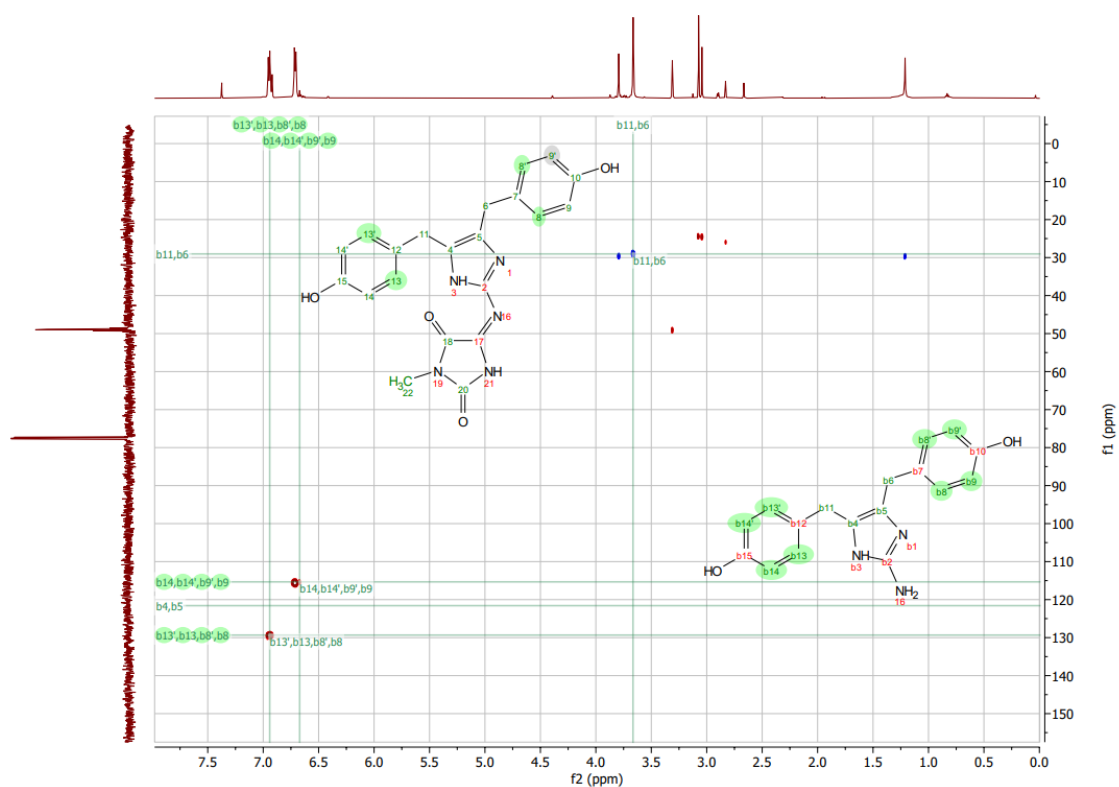


## Supporting information

**Figure S38:**  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum for mixture of naamine I (7) and naamidine K (8)



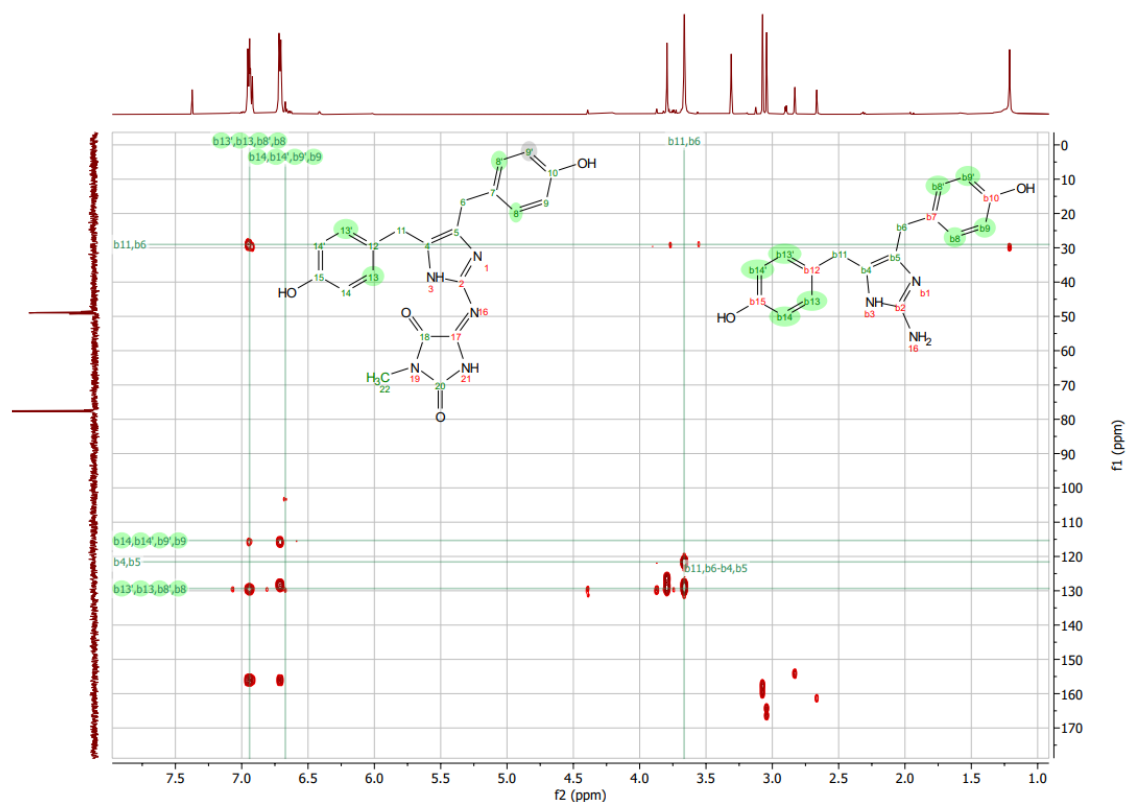
**Figure S39:**  $^1\text{H}$ - $^{13}\text{C}$  HSQC NMR (600 MHz) spectrum for mixture of naamine I (7) and naamidine K (8)



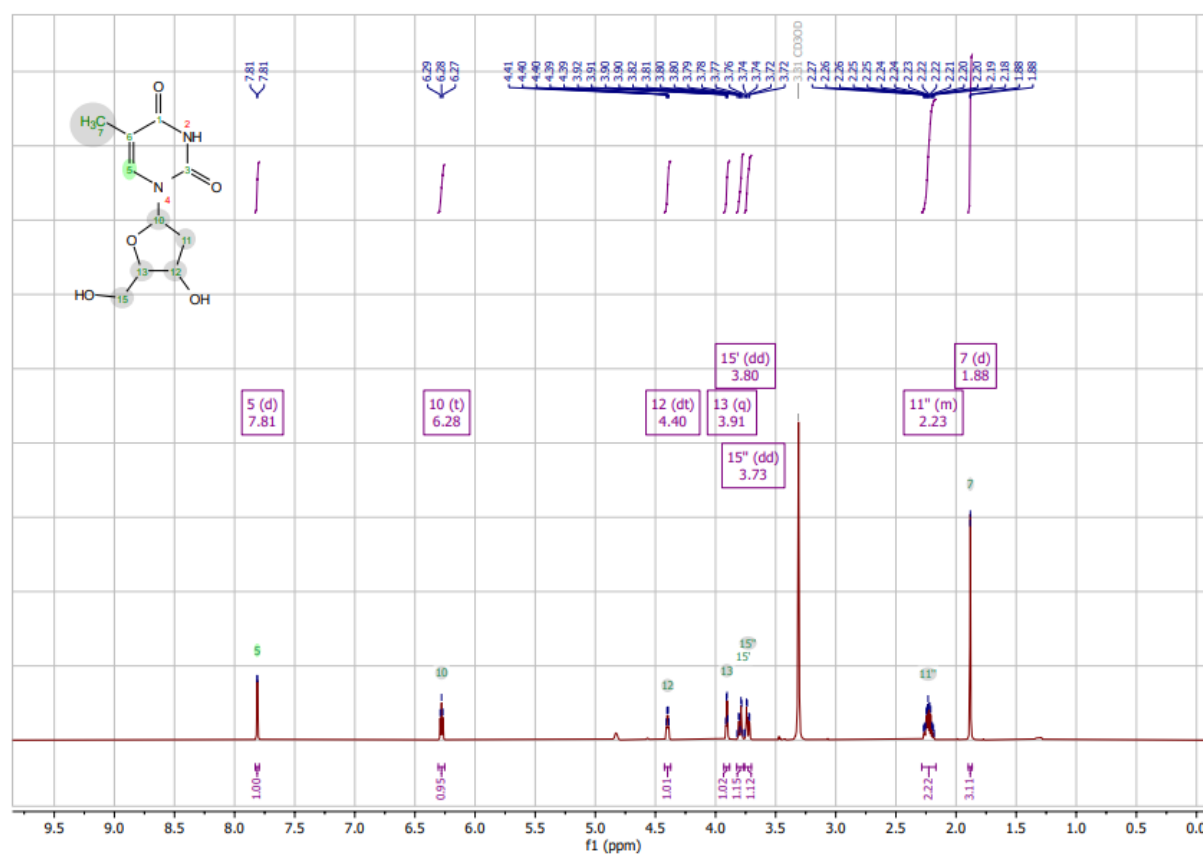


## Supporting information

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

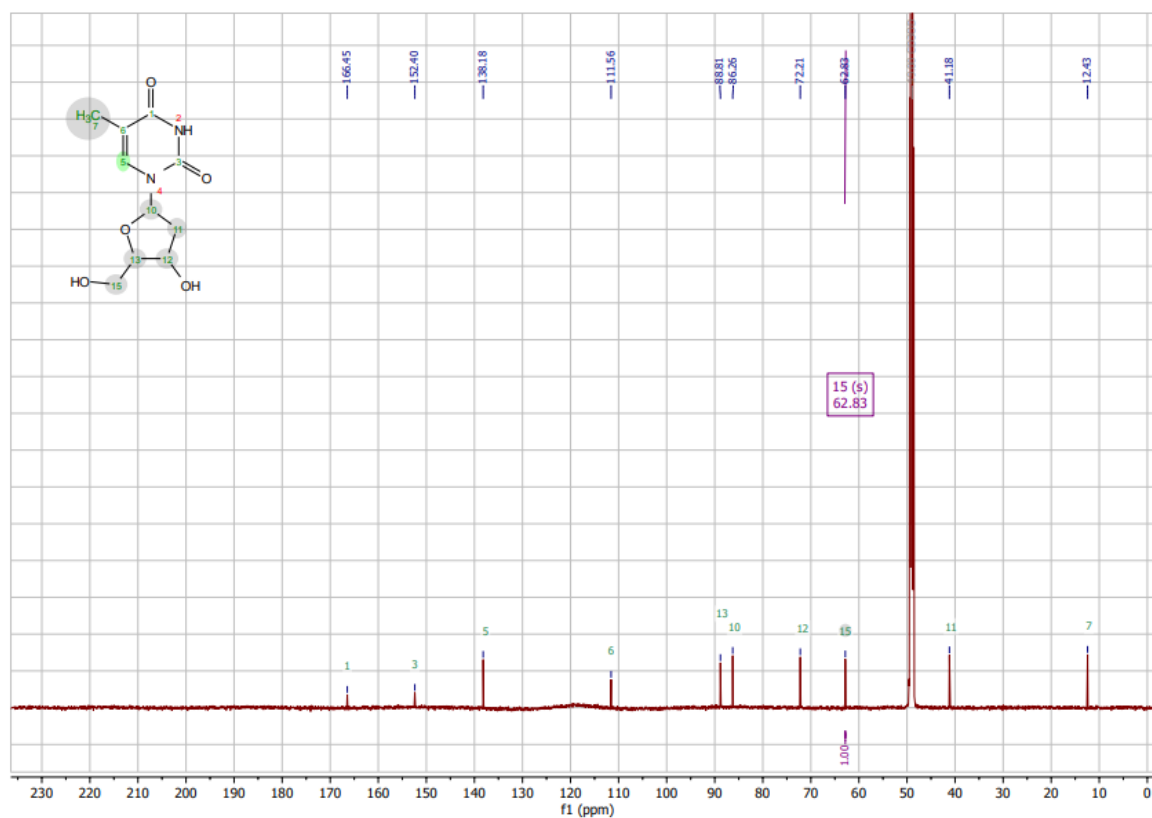


**Figure S41:**  $^1\text{H}$  NMR (600 MHz,  $\text{CD}_3\text{OD}$ ) spectrum for thymidine (9)

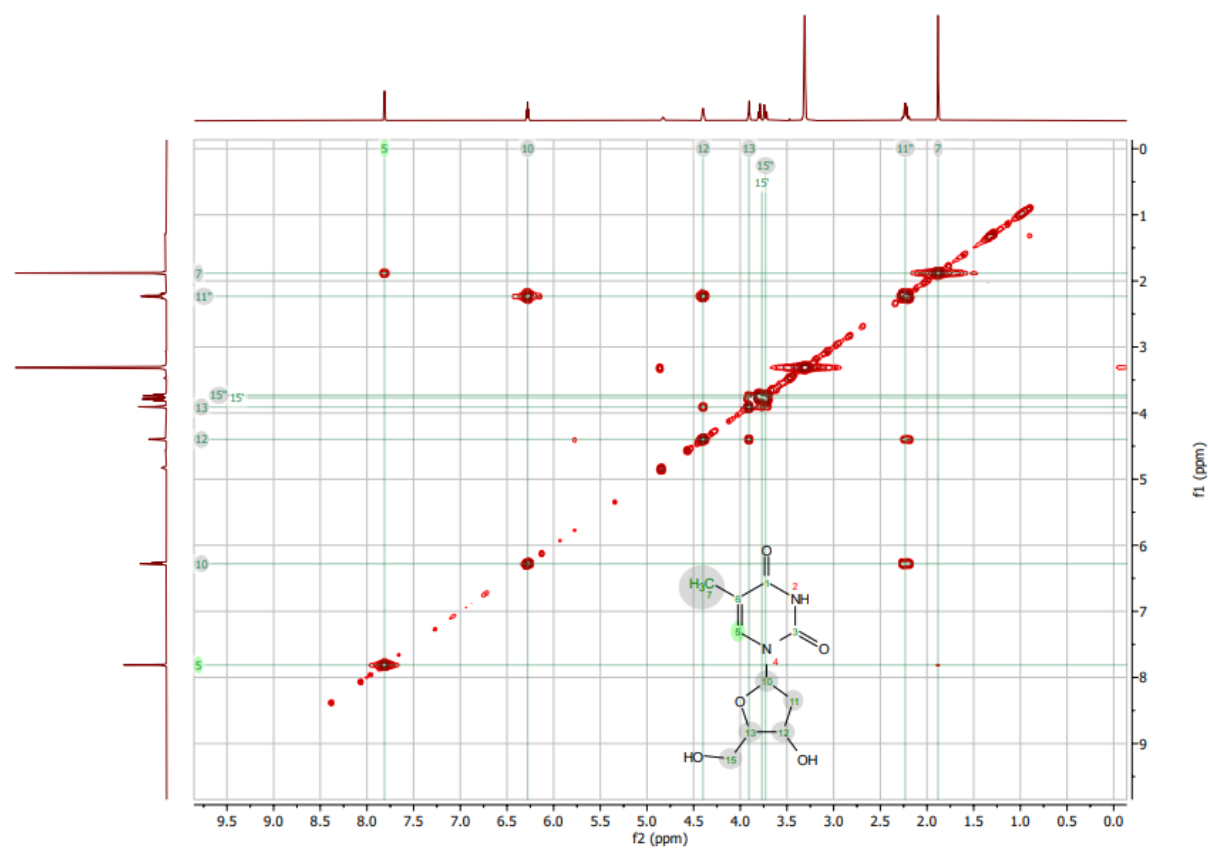


## Supporting information

**Figure S42:**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{OD}$ ) spectrum for thymidine (9)

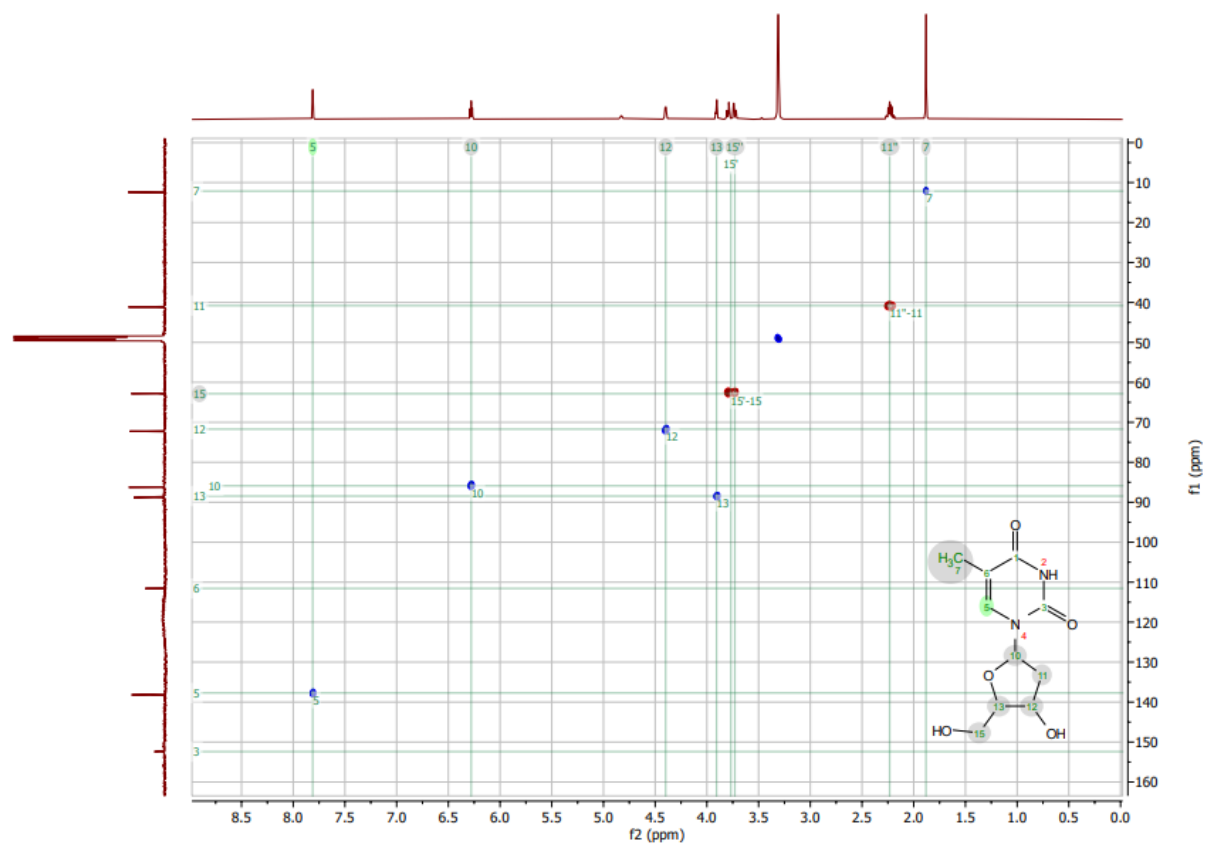


**Figure S43:**  $^1\text{H}$ - $^1\text{H}$  COSY NMR (600 MHz) spectrum for thymidine (9)

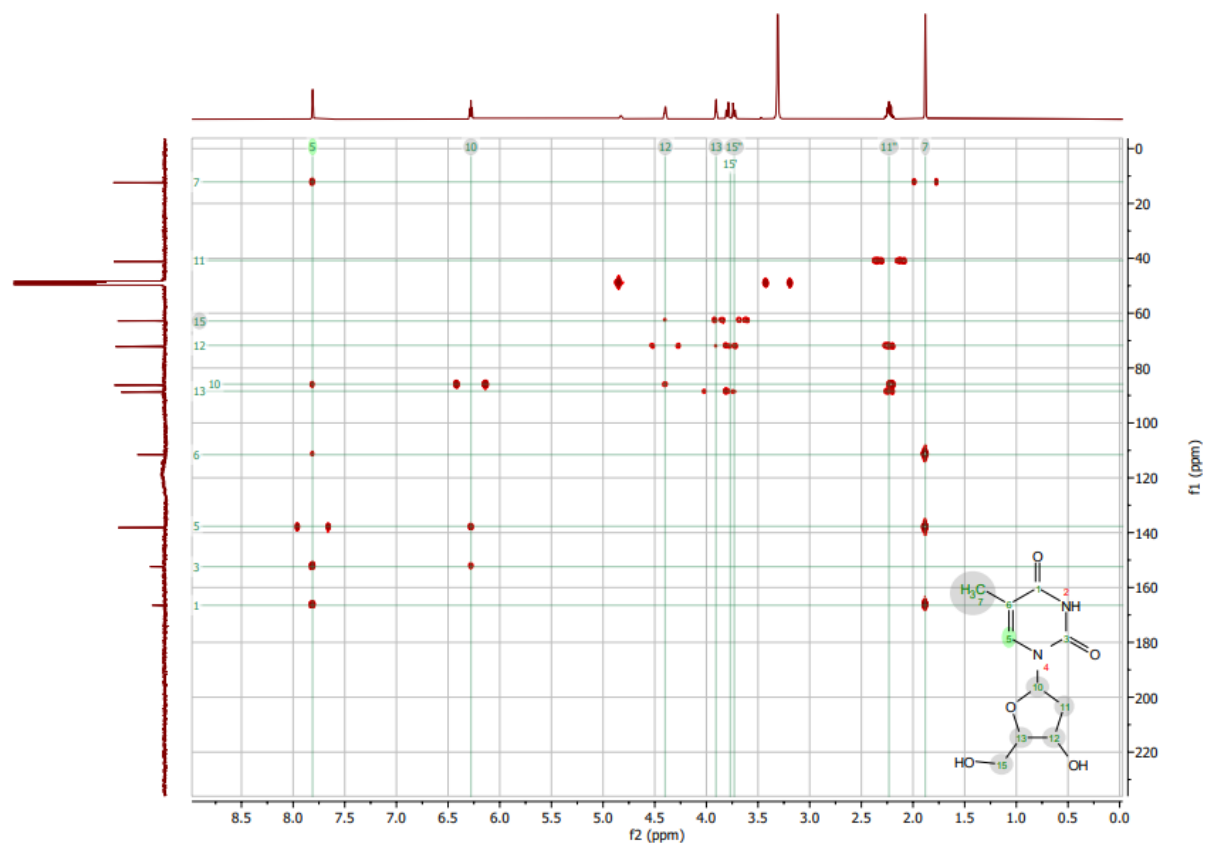


# Supporting information

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



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

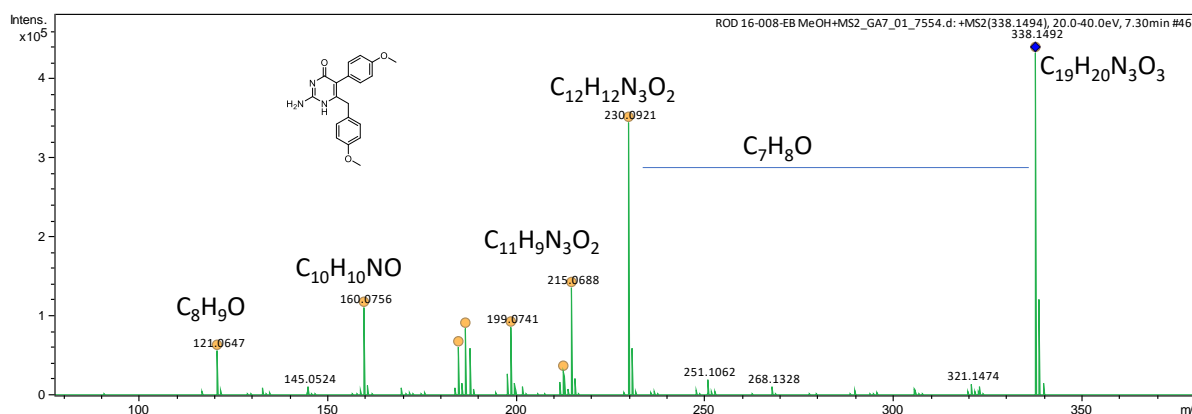


## Supporting information

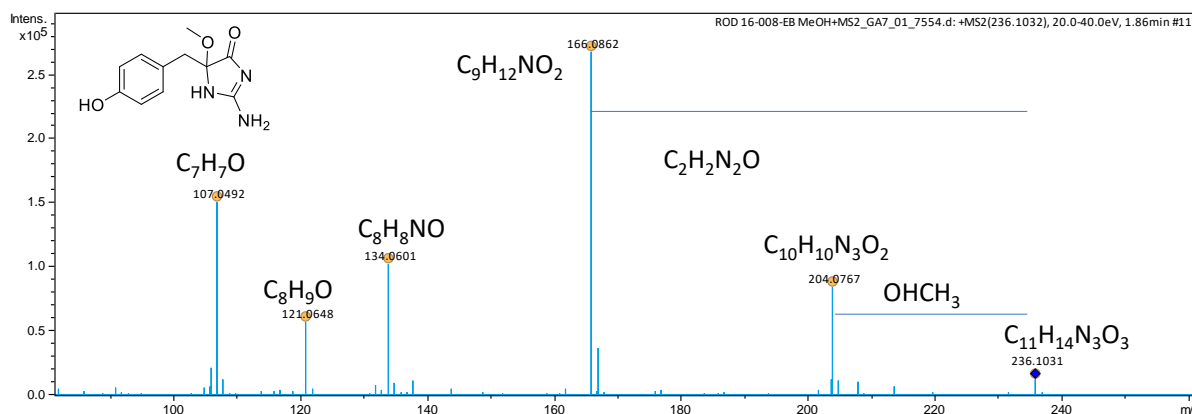
**Figure S46:** MS/MS spectra of the isolated compounds were deposited in the GNPS spectral libraries under following identifier

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)

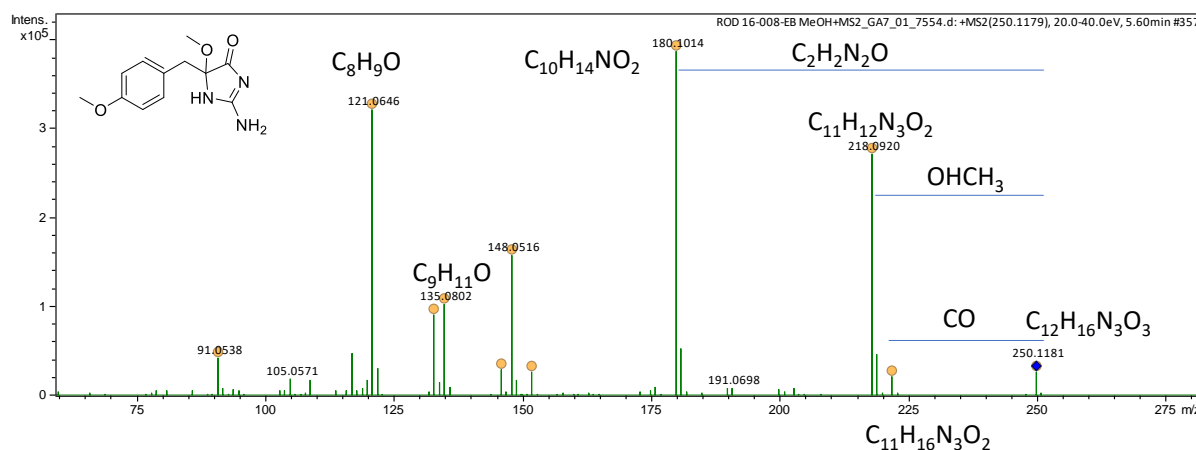


**Figure S48:** MS/MS spectrum of Phorbatopsin D (2)

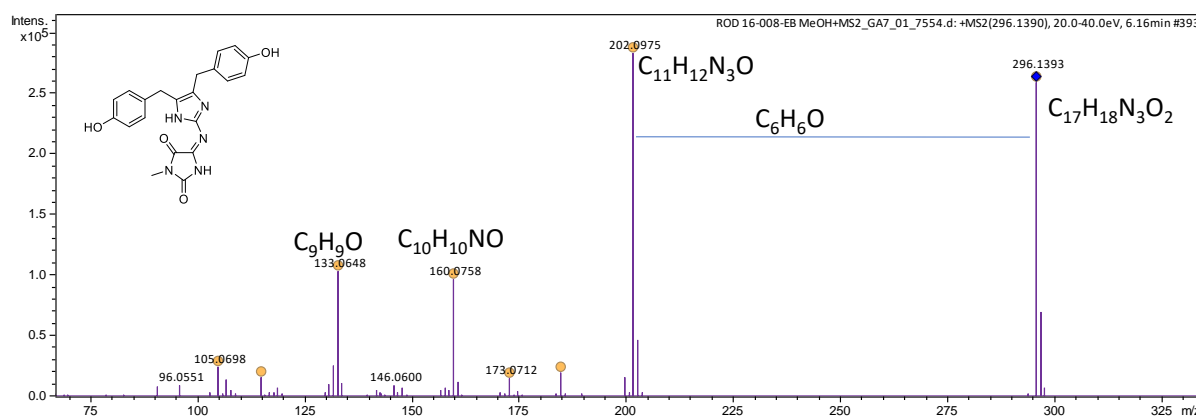


## Supporting information

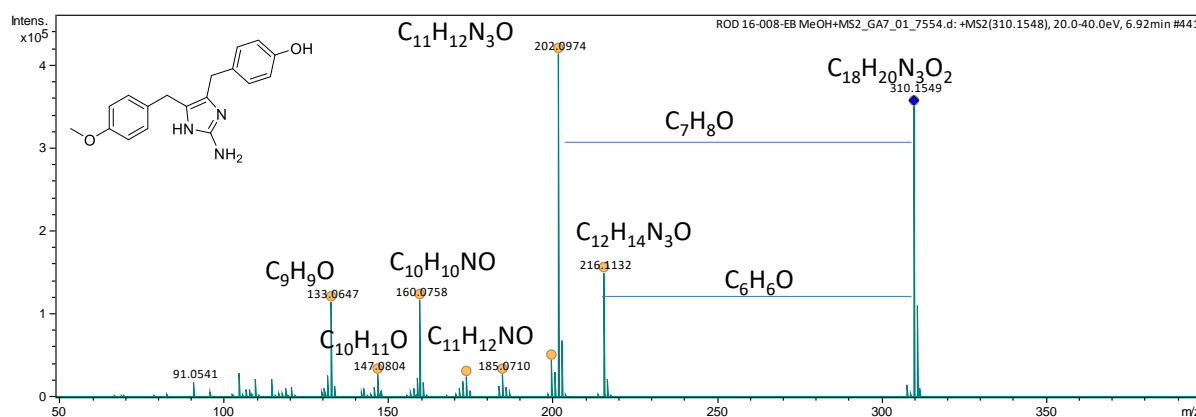
**Figure S49:** MS/MS spectrum of Phorbatopsin E(3)



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

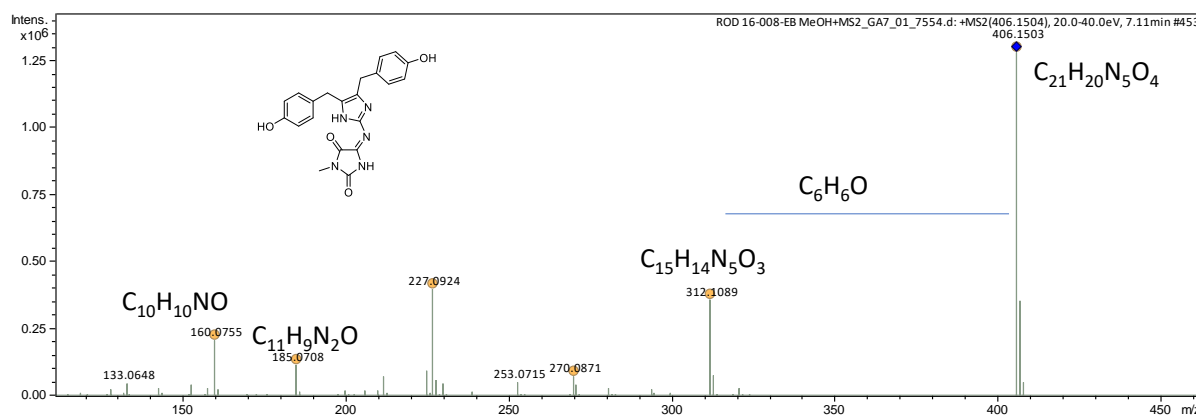


**Figure S51:** MS/MS spectrum of Naamine I (7)

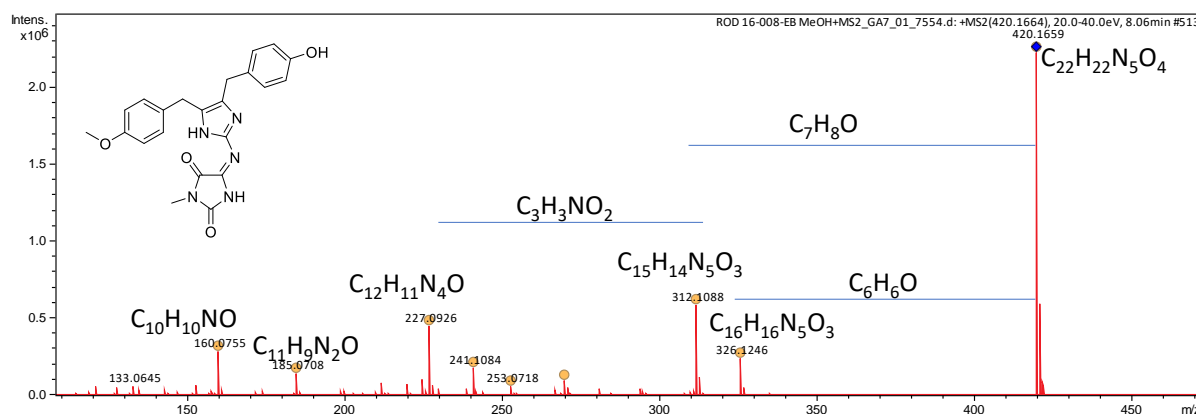


## Supporting information

**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)

