Supporting Information

GPCR Pharmacological Profiling of Aaptamine from the Philippine Sponge Stylissa sp. Extends its Therapeutic Potential for Noncommunicable Diseases

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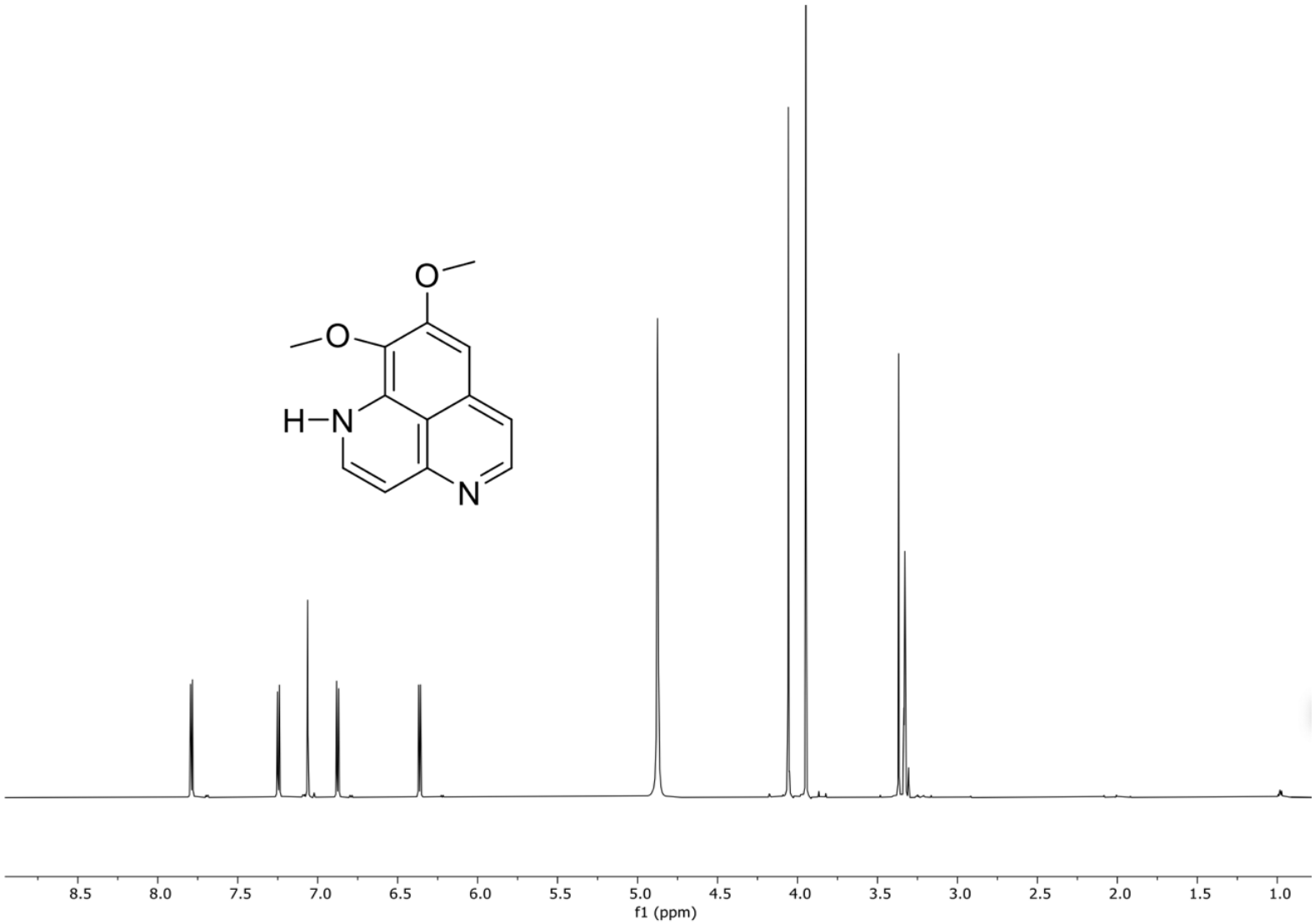

Figure S1. ^{1}H NMR (600 MHz, MeOH-d_4) spectrum of aaptamine.

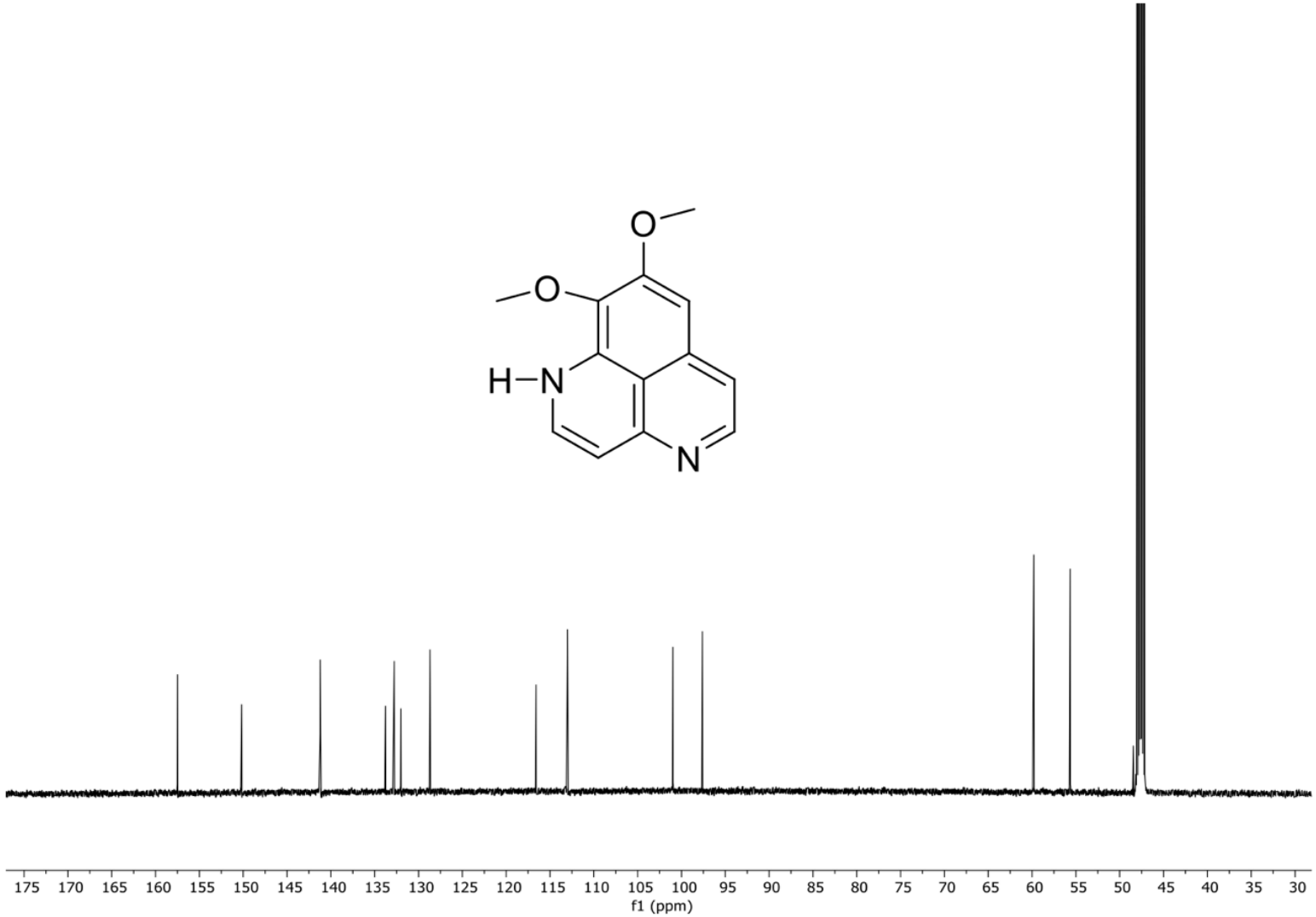

Figure S2. ^{13}C NMR (150 MHz, MeOH-d_4) spectrum of aaptamine.

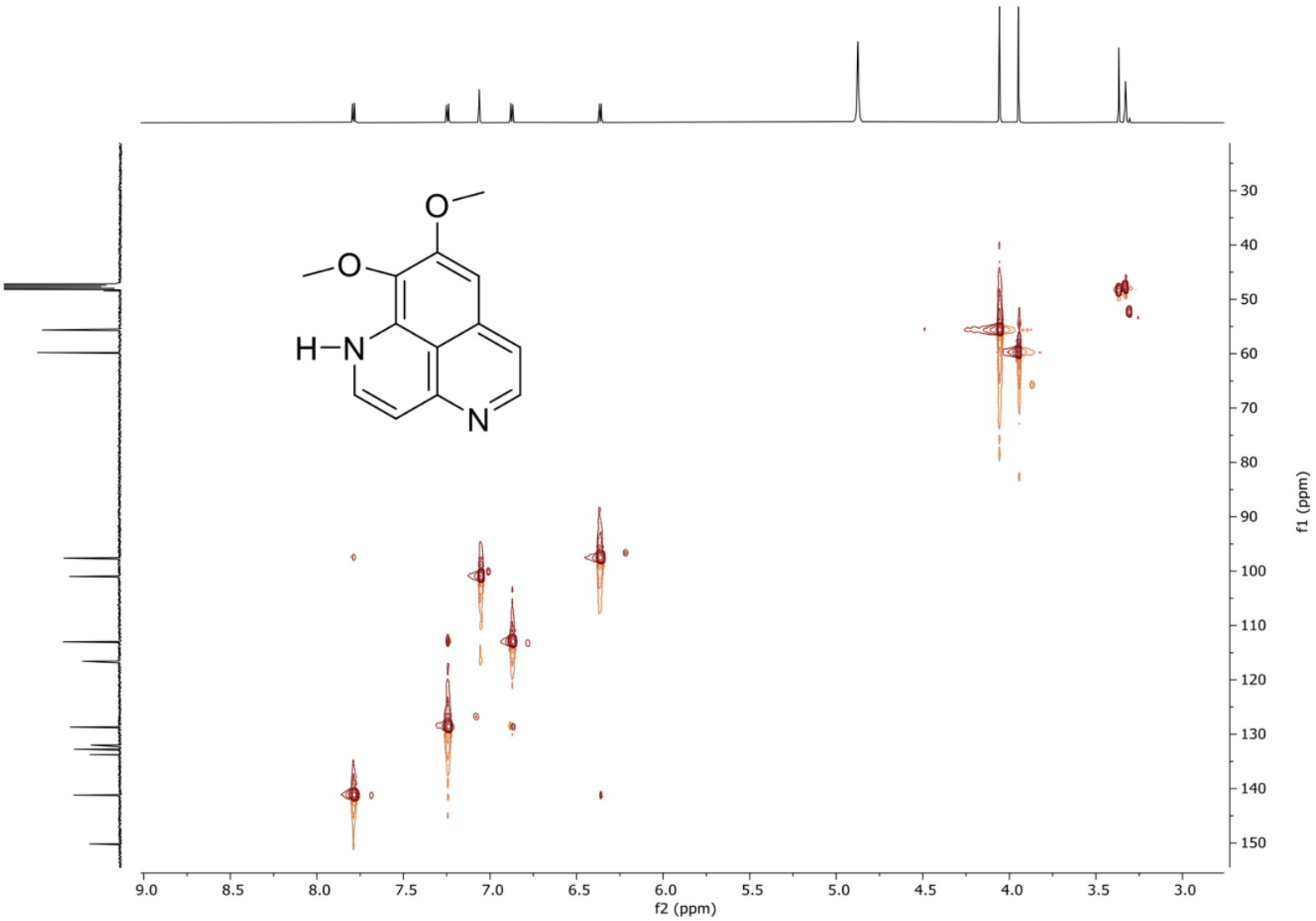

Figure S3. HSQC (600 MHz, MeOH-d_4) spectrum of aaptamine.

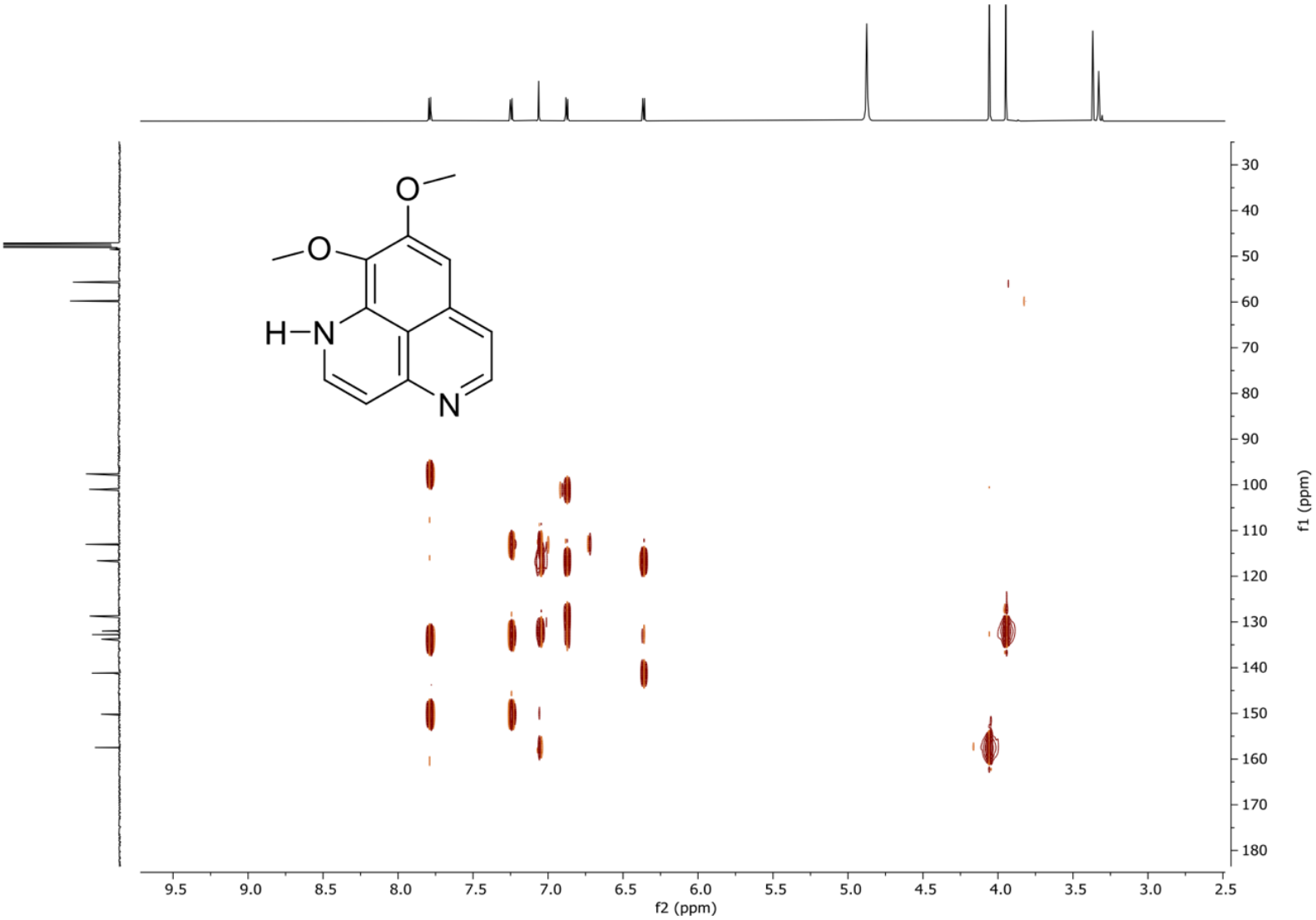

Figure S4. HMBC (600 MHz, MeOH-d_4) spectrum of aaptamine.

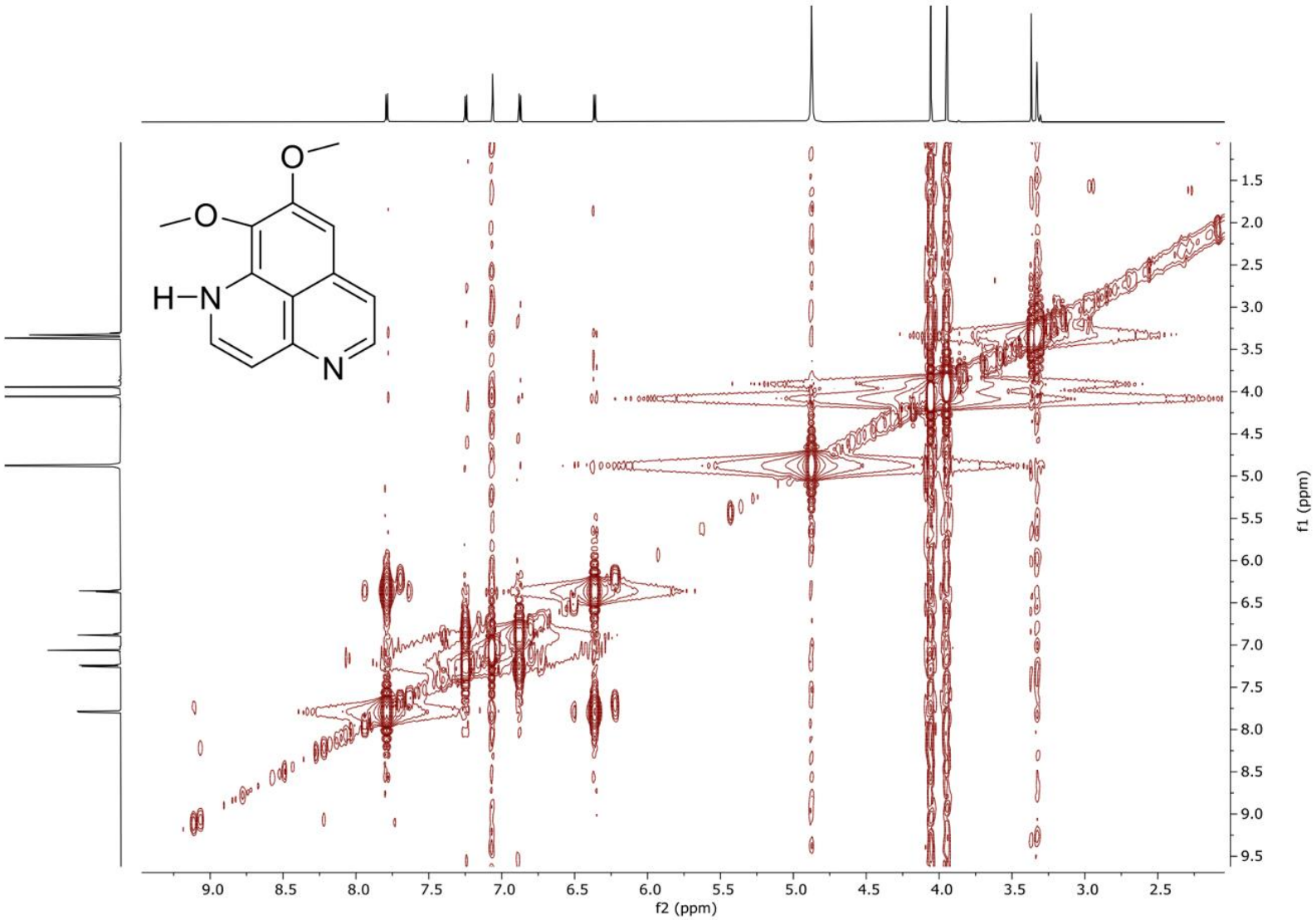

Figure S5. COSY (600 MHz, MeOH-d_4) spectrum of aaptamine.

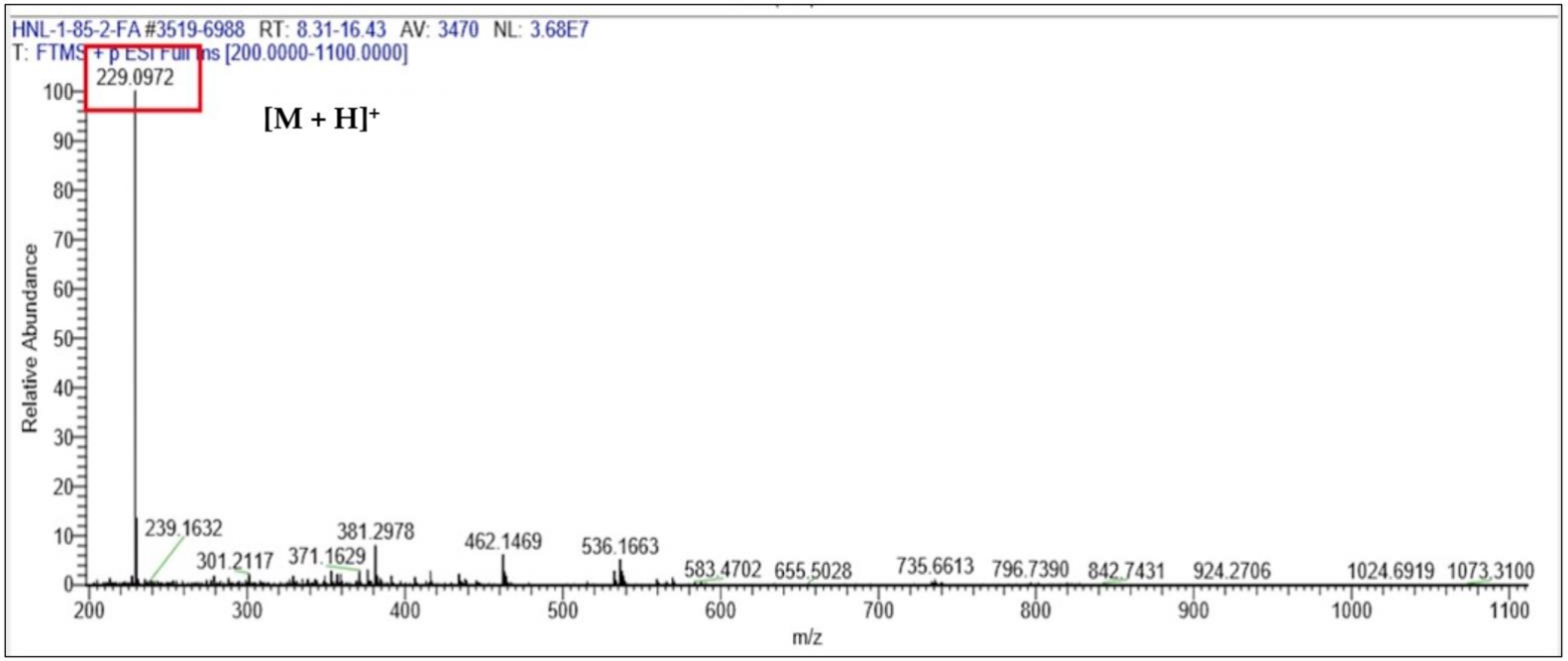

Figure S6. Mass spectrum obtained by High Resolution Electrospray Ionization Mass Spectrometry (HRESIMS).

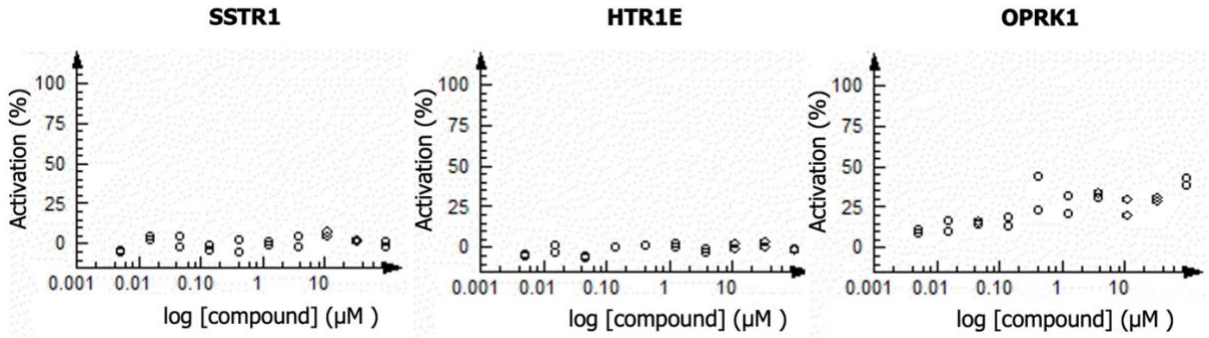

Figure S7. Positive Allosteric Modulators (PAMs) assay data. Dose-response curve of aaptamine against SSTR1, HTR1E, and OPRK1 observed in the secondary screening. The control agonist was added at EC_{20} to determine superactivation of the GPCR in the presence of the compound. The PAM mode showed that the hits identifed in the primary screen may be considered false positives. Somatostatin 28 (EC_{50} 4.0 x 10^{-3} μM), Serotonin/5-HT (EC_{50} 8.4 x 10^{-3} μM), and Dynorphin A (EC_{50} 3.4 x 10^{-2} μM) were the ligand used as positive control for SSTR1, HTR1E, and OPRK1, respectively. Data are presented as mean ± SD (n = 2).