

**Title:** A Novel Brominated Alkaloid Securidine A, Isolated from the Marine Bryozoan *Securiflustra securifrons*

**Supplementary materials:** 1D NOE, 13C-NMR, HMBC, ME-HSQC, H2BC, COSY and ROESY correlations of compound Securidine A (**1**)

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**Figure S1.** 1D NOE spectrum of securidine A (**1**)

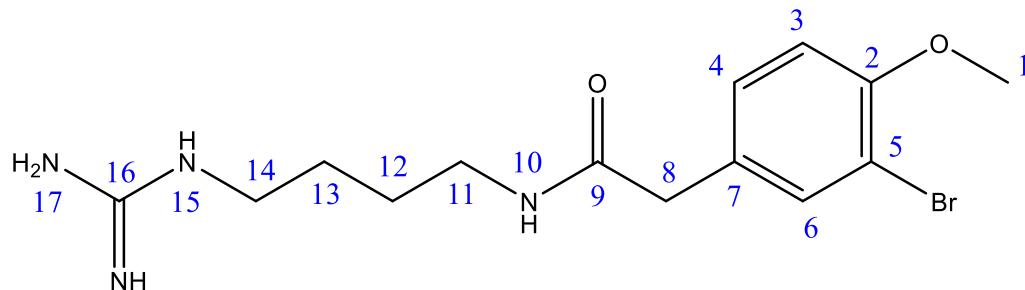
**Figure S2.** 13C-NMR spectrum of **1**.

**Figure S3.** Combined HSQC and HMBC spectra of **1**.

**Figure S4.** H2BC spectra of **1**

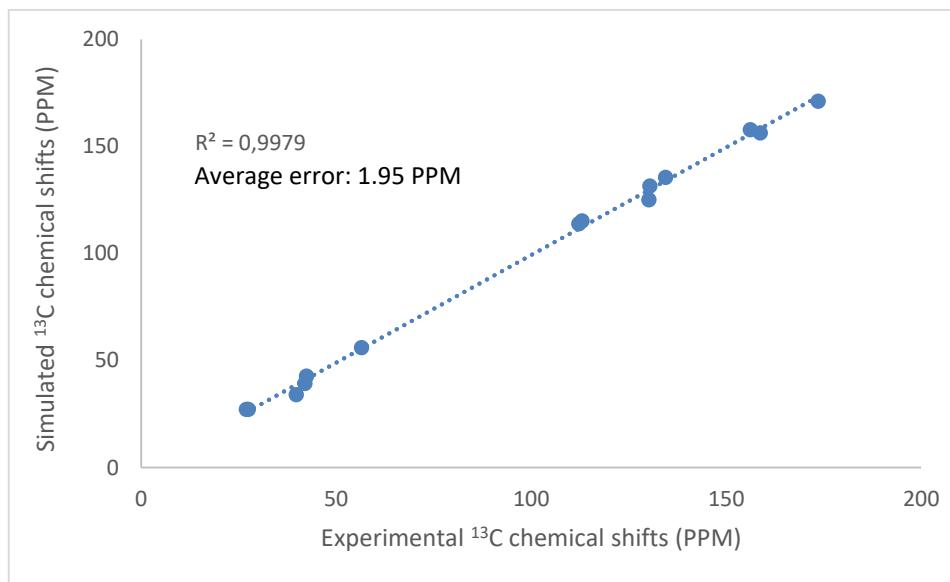
**Figure S5.** COSY Spectrum of **1**.

**Figure S6.** ROESY spectrum of **1**.



Chemical Formula: C<sub>14</sub>H<sub>21</sub>BrN<sub>4</sub>O<sub>2</sub>

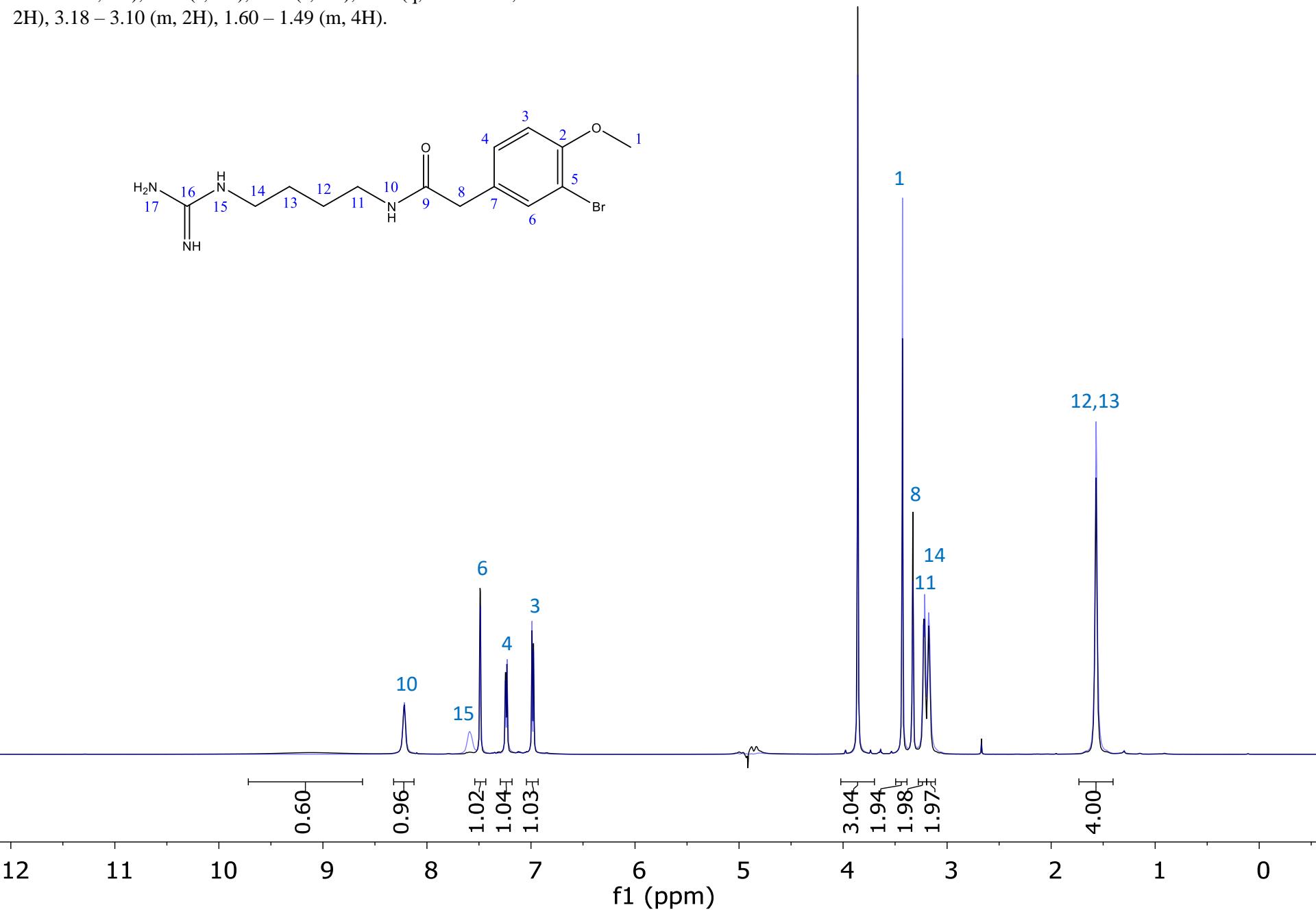
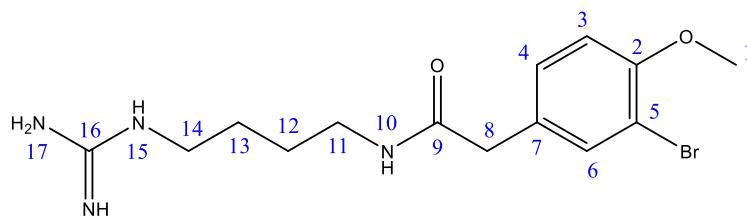
Exact Mass: 356,08



<sup>1</sup>H NMR (600 MHz, Methanol-*d*<sub>4</sub>) δ 8.20 (s, 1H), 7.57 (s, 1H), 7.47 (d, *J* = 2.3 Hz, 1H), 7.22 (dd, *J* = 8.6, 2.3 Hz, 1H), 6.96 (d, *J* = 8.8 Hz, 1H), 3.84 (s, 3H), 3.41 (s, 4H), 3.20 (q, *J* = 6.4 Hz, 2H), 3.18 – 3.10 (m, 2H), 1.60 – 1.49 (m, 4H).

### 1D NOE + ES

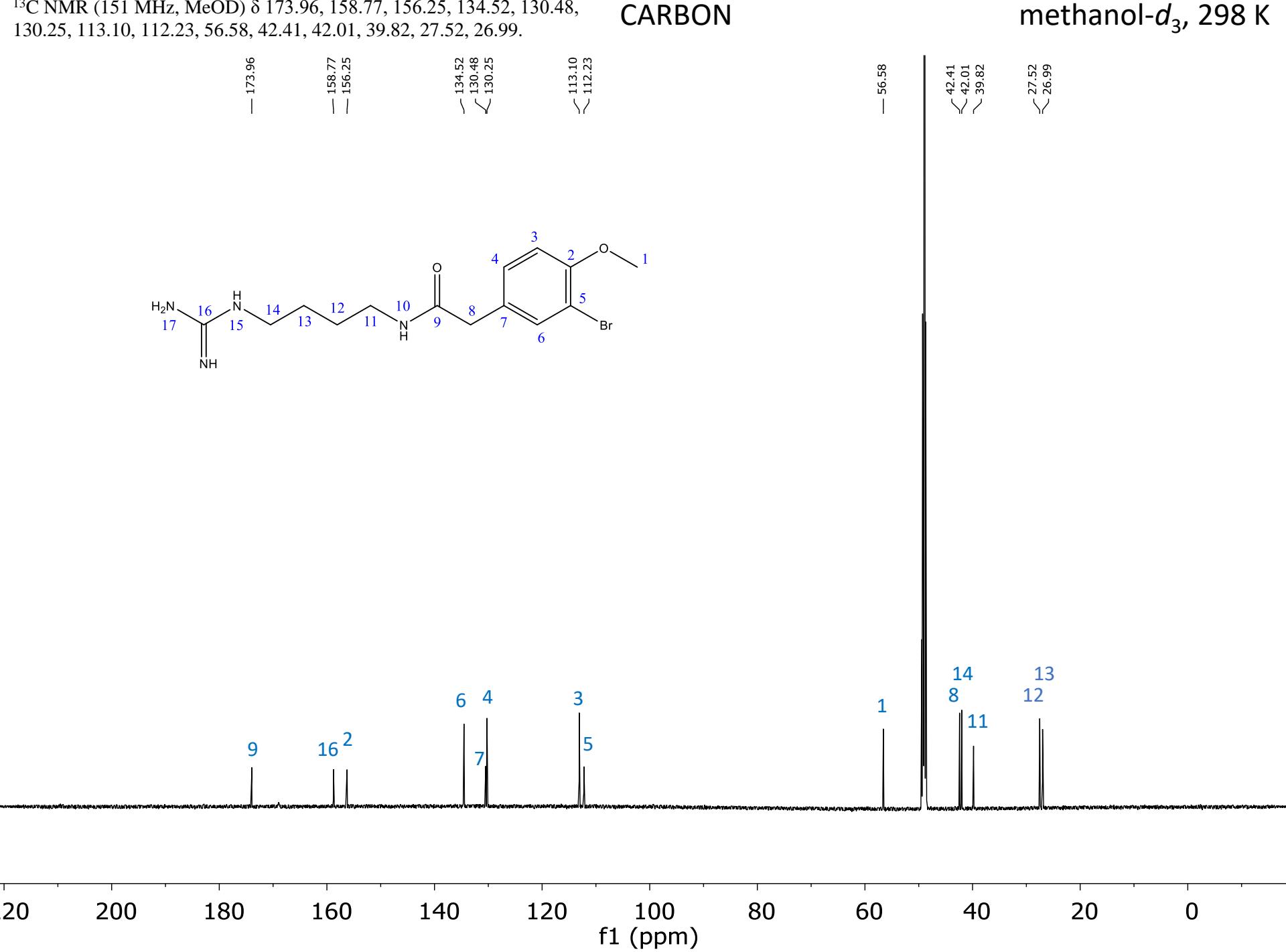
methanol-*d*<sub>3</sub>, 298 K

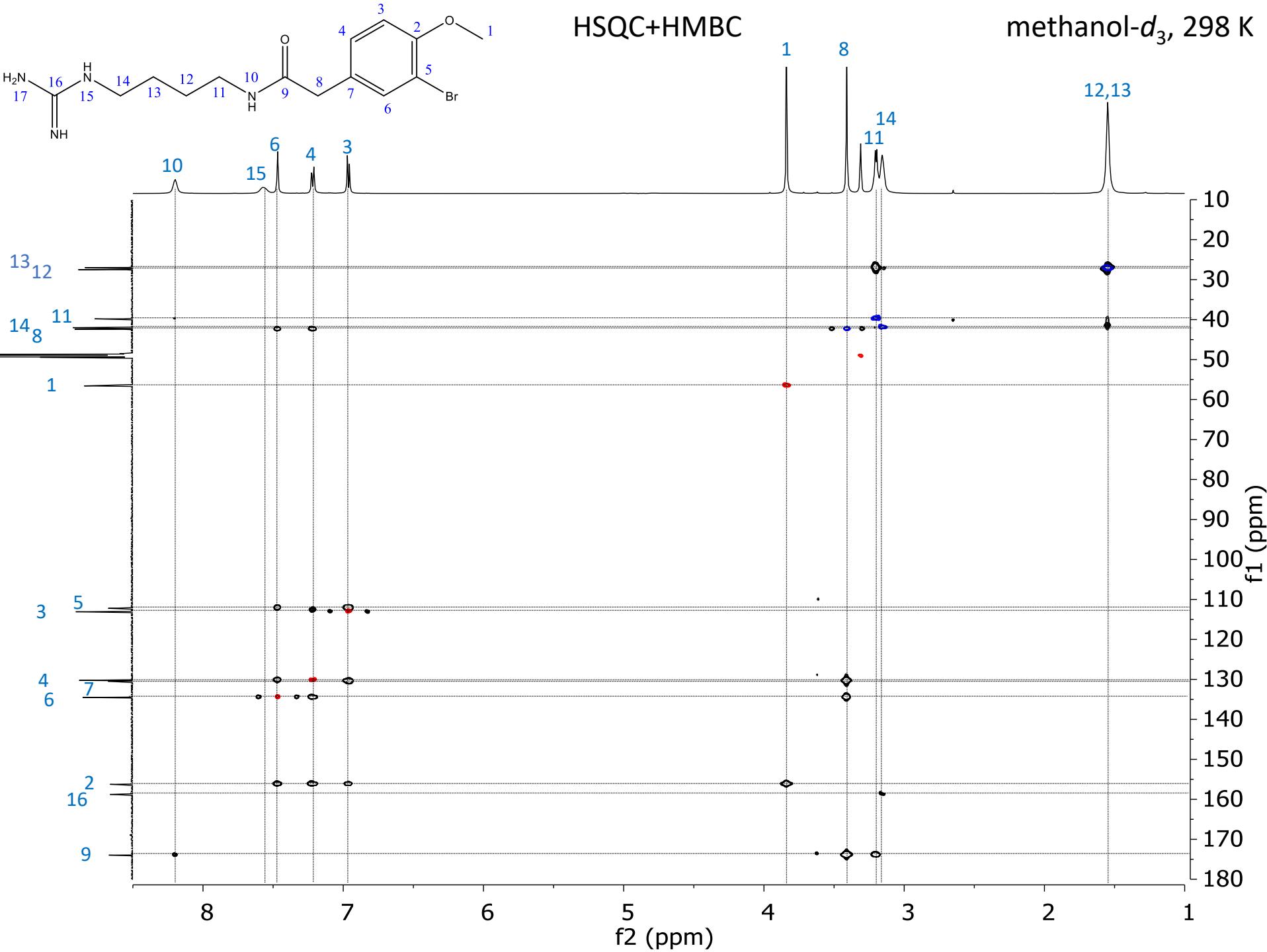


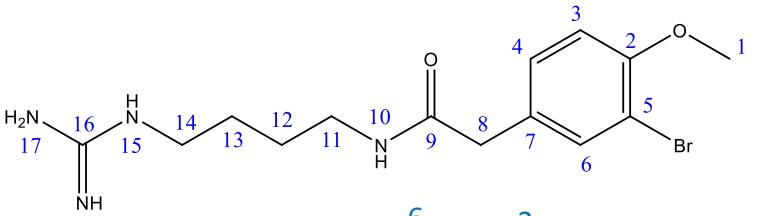
$^{13}\text{C}$  NMR (151 MHz, MeOD)  $\delta$  173.96, 158.77, 156.25, 134.52, 130.48, 130.25, 113.10, 112.23, 56.58, 42.41, 42.01, 39.82, 27.52, 26.99.

## CARBON

methanol- $d_3$ , 298 K

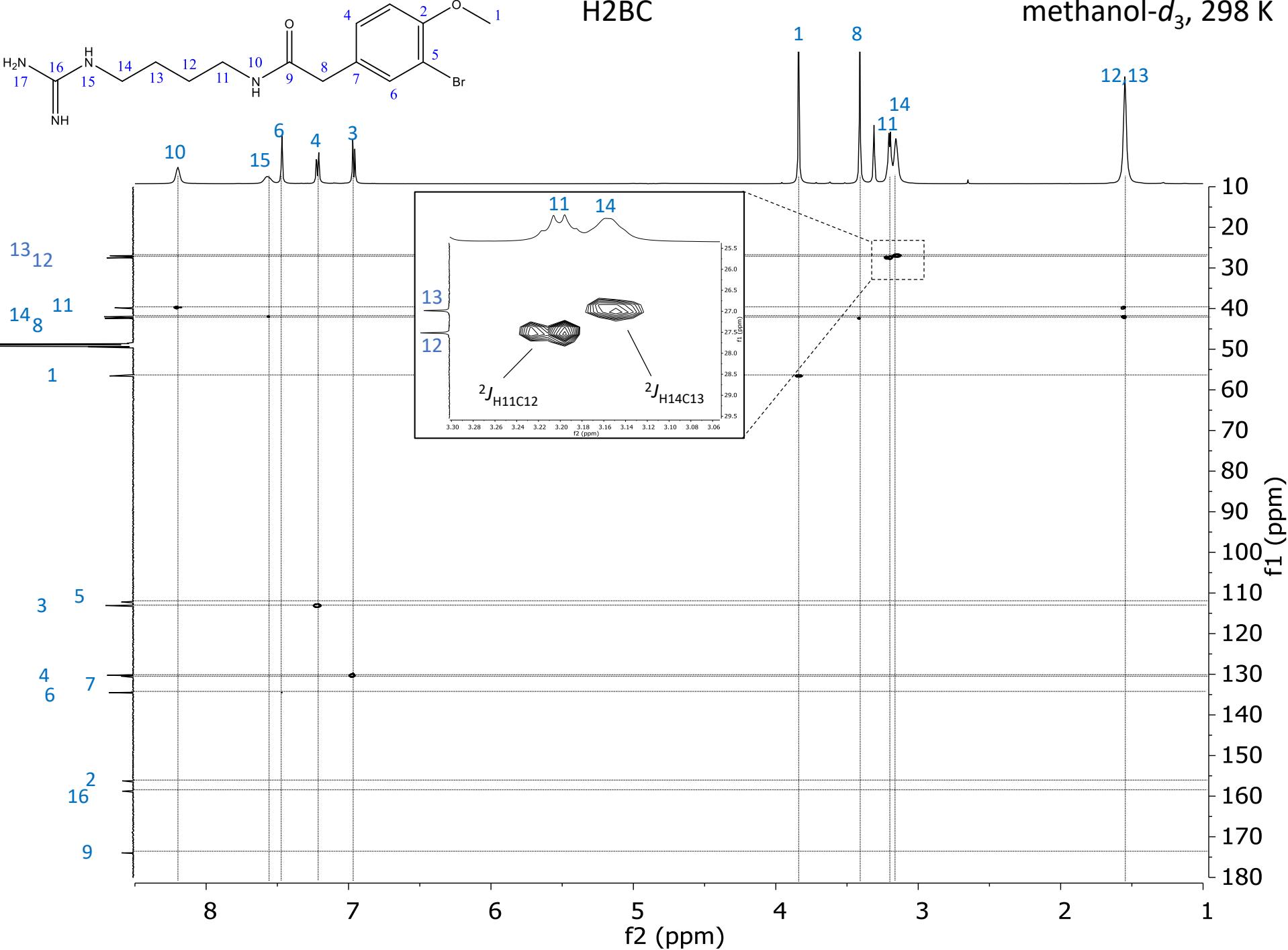


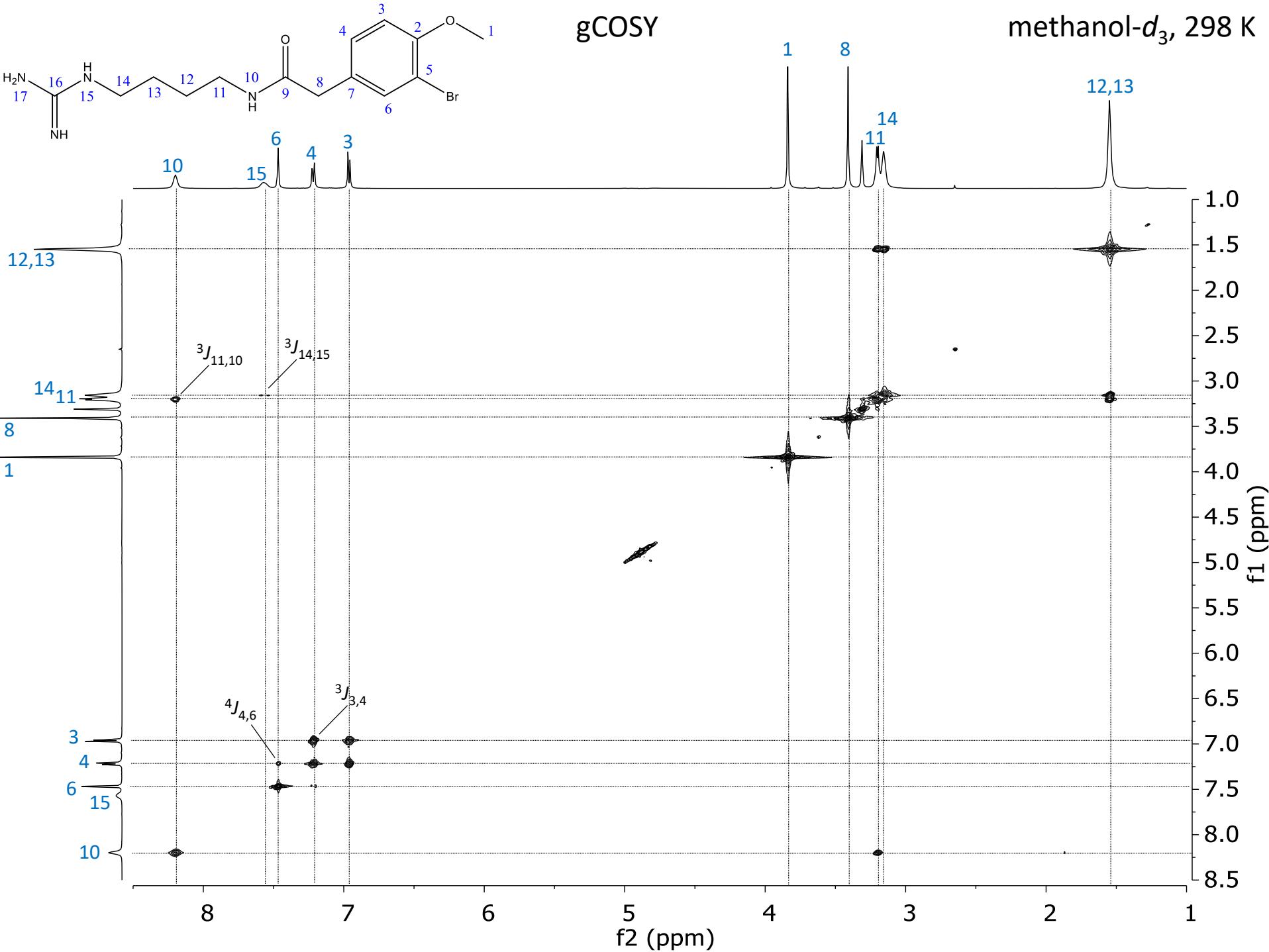


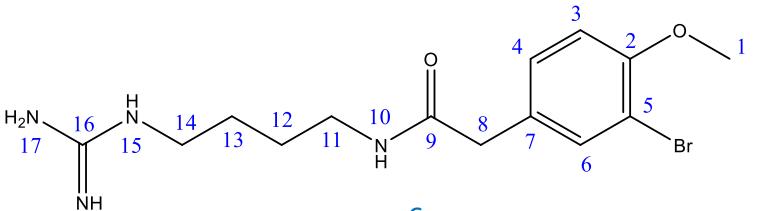


H2BC

## **methanol-*d*<sub>3</sub>, 298 K**







# ROESYAD 300ms

methanol-*d*<sub>3</sub>, 298 K

