APLYSFISTULARINE: A NOVEL DIBROMOTYROSINE DERIVATIVE ISOLATED FROM *Aplysina fistularis*[#]

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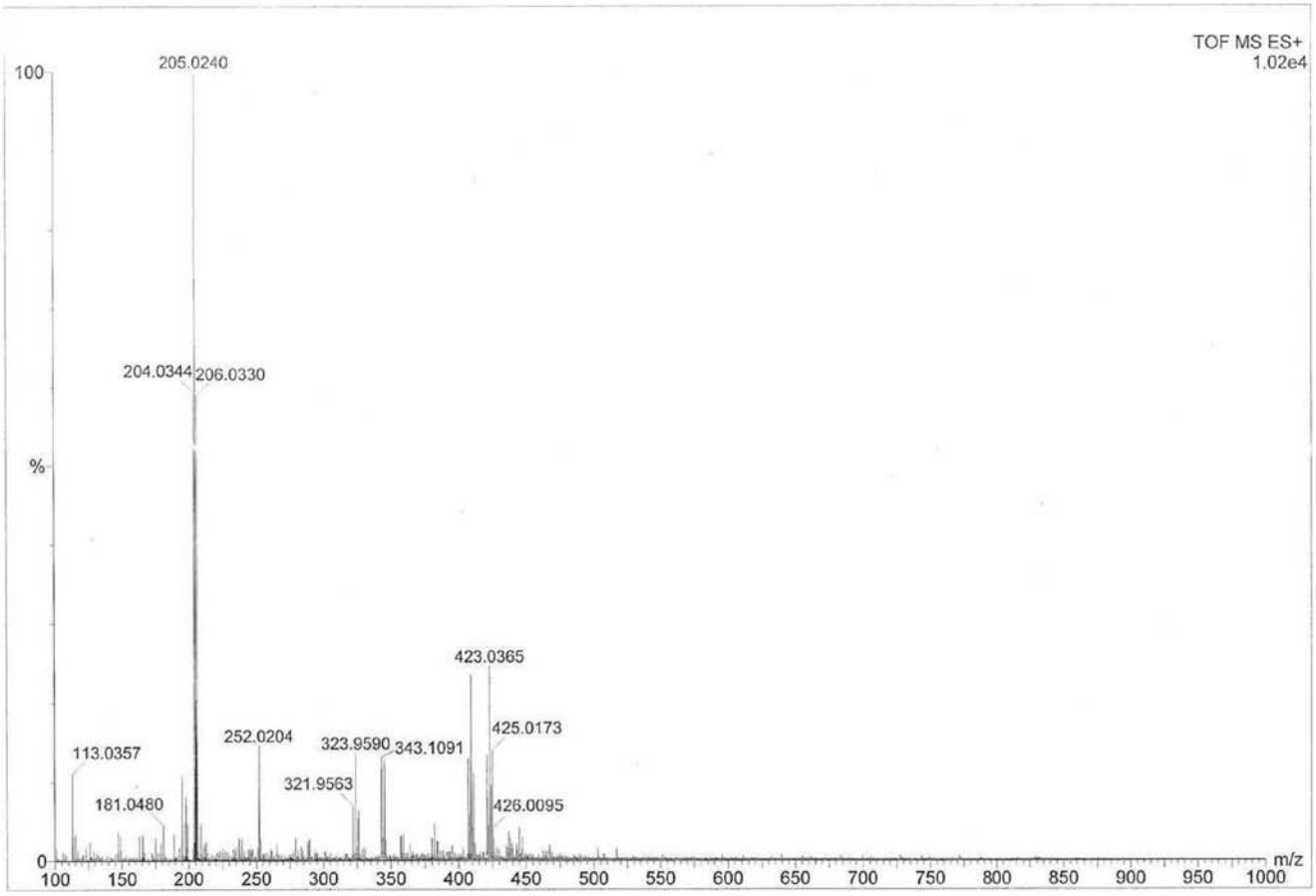

Figure 1S. *HRESIMS spectrum of compound* ***1***

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[#]Artigo em homenagem ao Prof. Otto R. Gottlieb (31/8/1920-19/6/2011)

The approximate Relative intensities of the ions (with a difference of two mass units), containing two bromine atoms (isotopes 79 and 81), are marked in **bold**.

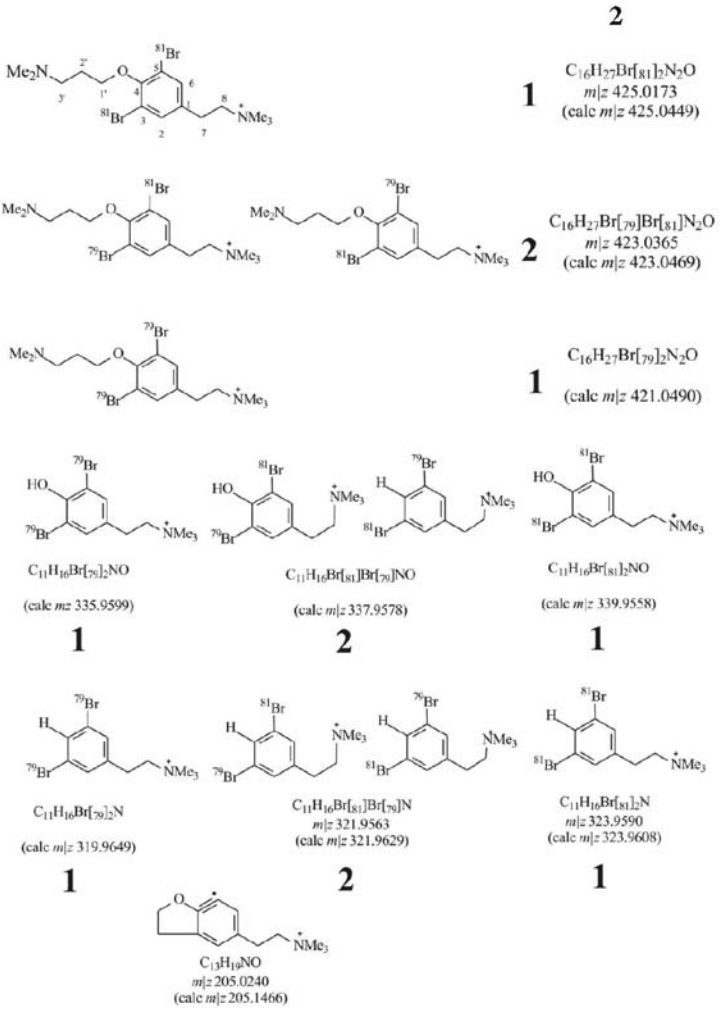

Figure 2S. *NMR proposed fragmentation for the molecule of compound* ***1***

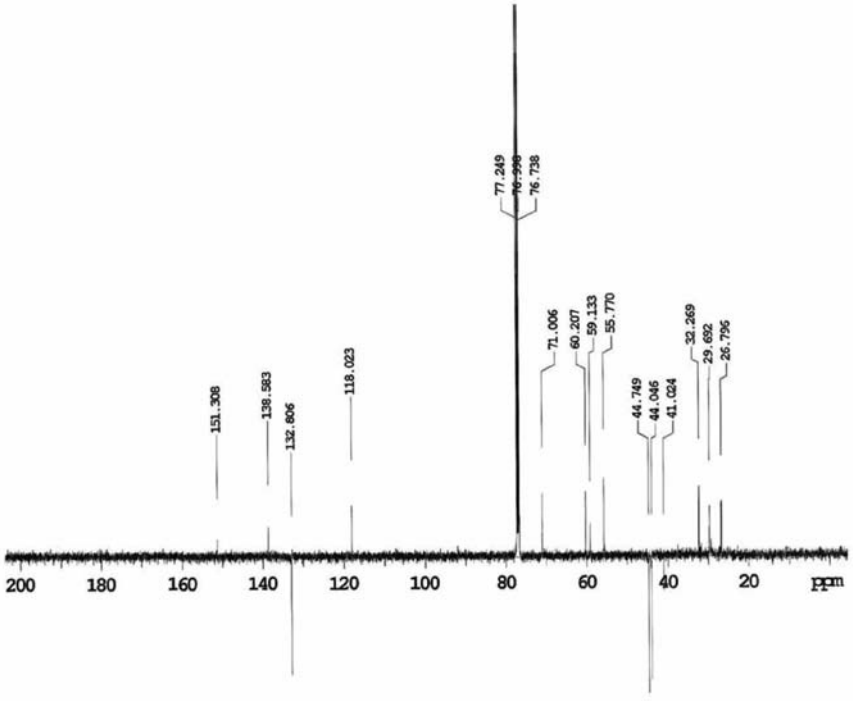

Figure 3S. *NMR* ^{13}*C-APT spectrum of compound* ***1*** *(*CD_3OD*, 125 MHz)*

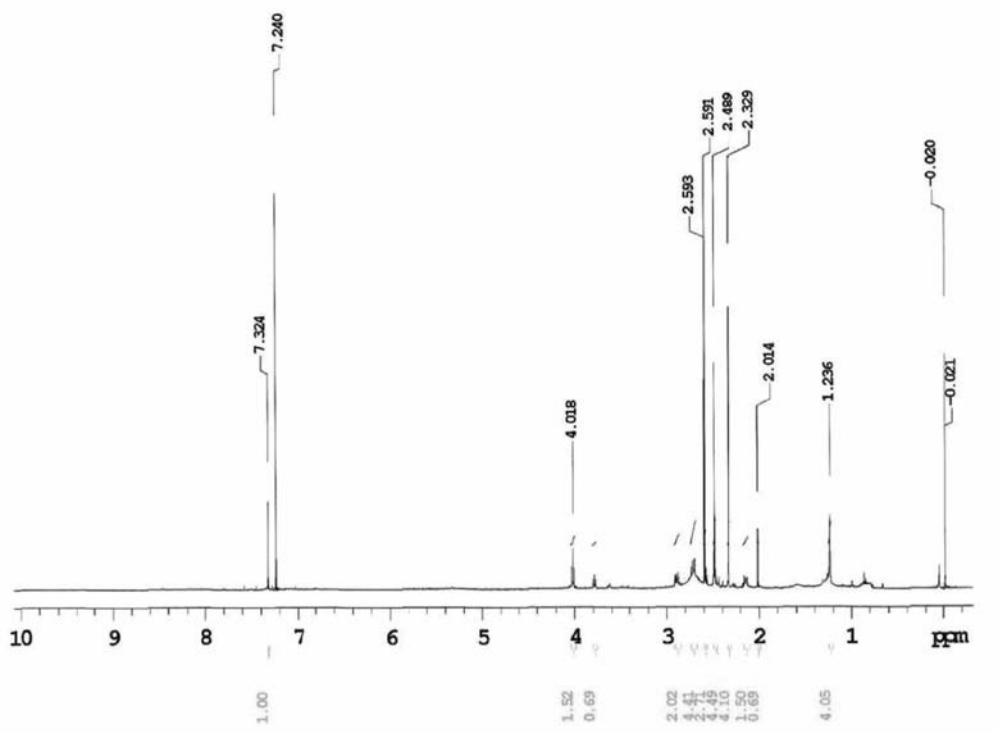

Figure 4S. *^{1}H NMR spectrum data of compound **1** (CD_3OD, 500 MHz)*

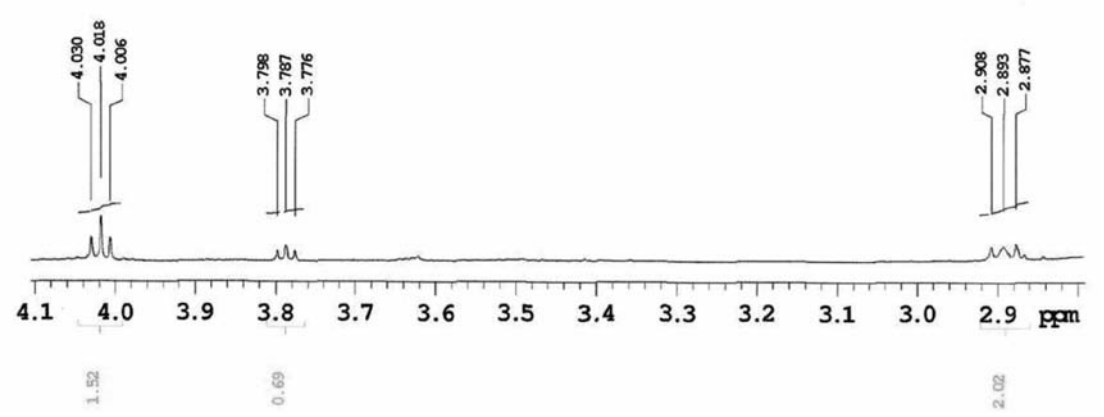

Figure 5S. *Expansion of ^{1}H NMR spectrum at the region of 4.1 – 2.9 of compound **1** (CD_3OD, 500 MHz)*

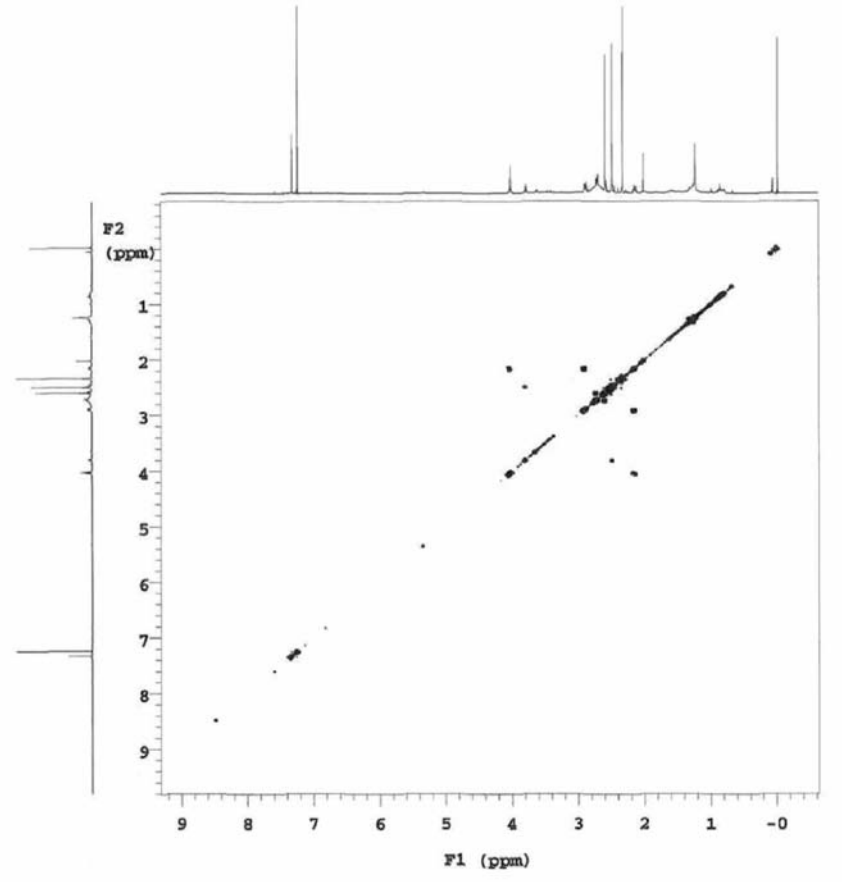

Figure 6S. *^{1}H x ^{1}H-COSY correlation spectrum of compound **1** (CD_3OD, 500 MHz)*

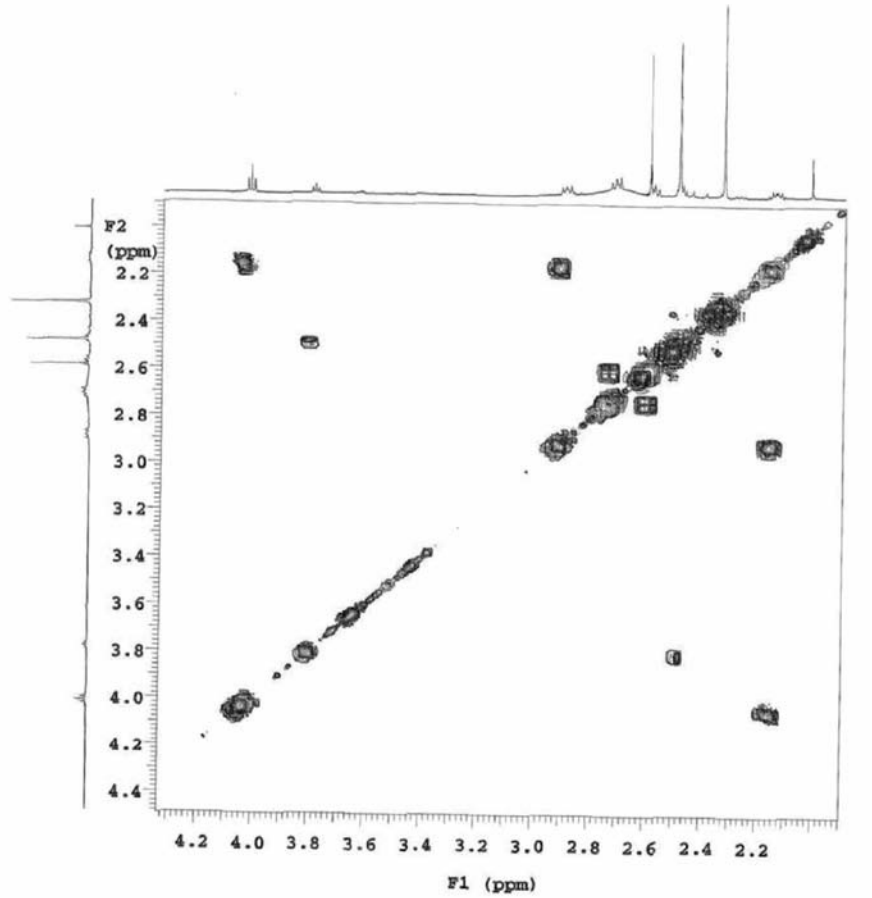

Figure 7S. *Expansion of ^{1}H x ^{1}H-COSY correlation spectrum of compound **1** (CD_3OD, 500 MHz)*

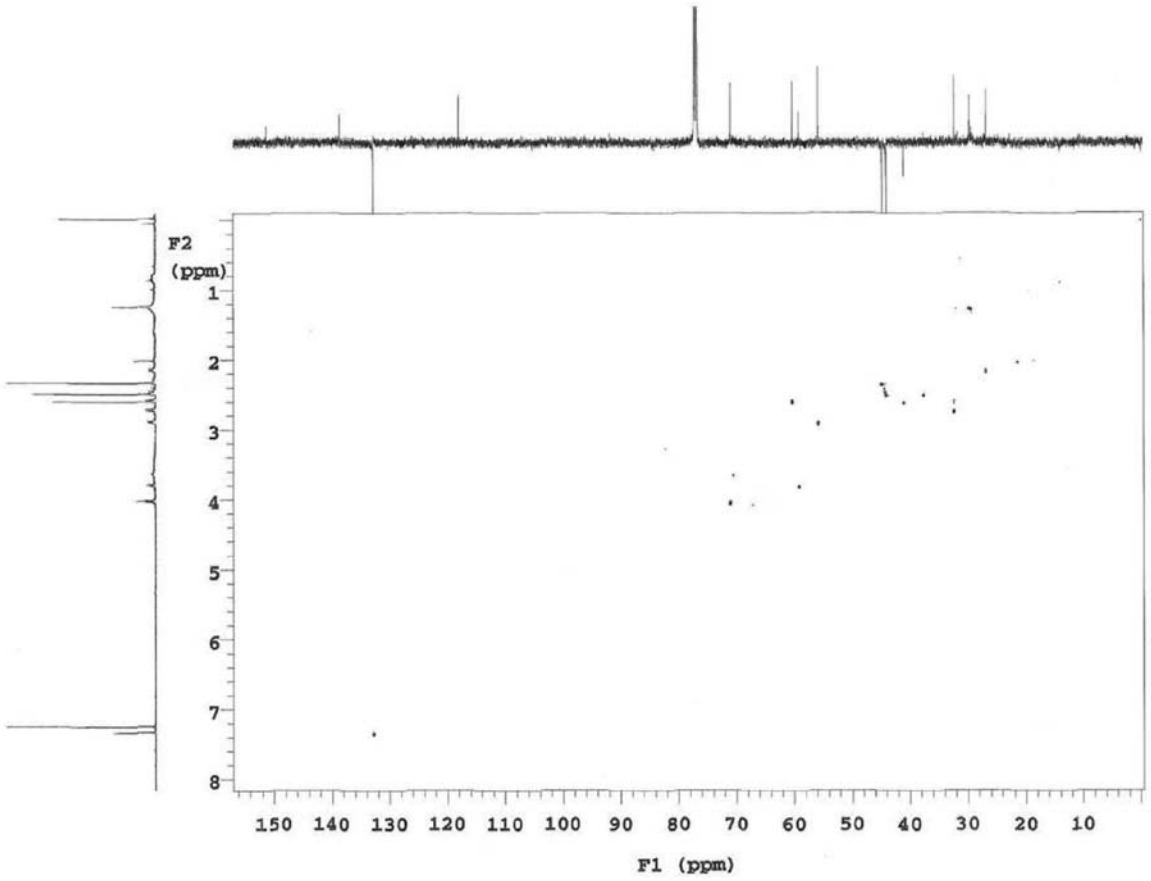

Figure 8S. *^{1}H x ^{13}C-HMQC correlation spectrum of compound **1** (CD_3OD, 500 and 125 MHz respectively)*

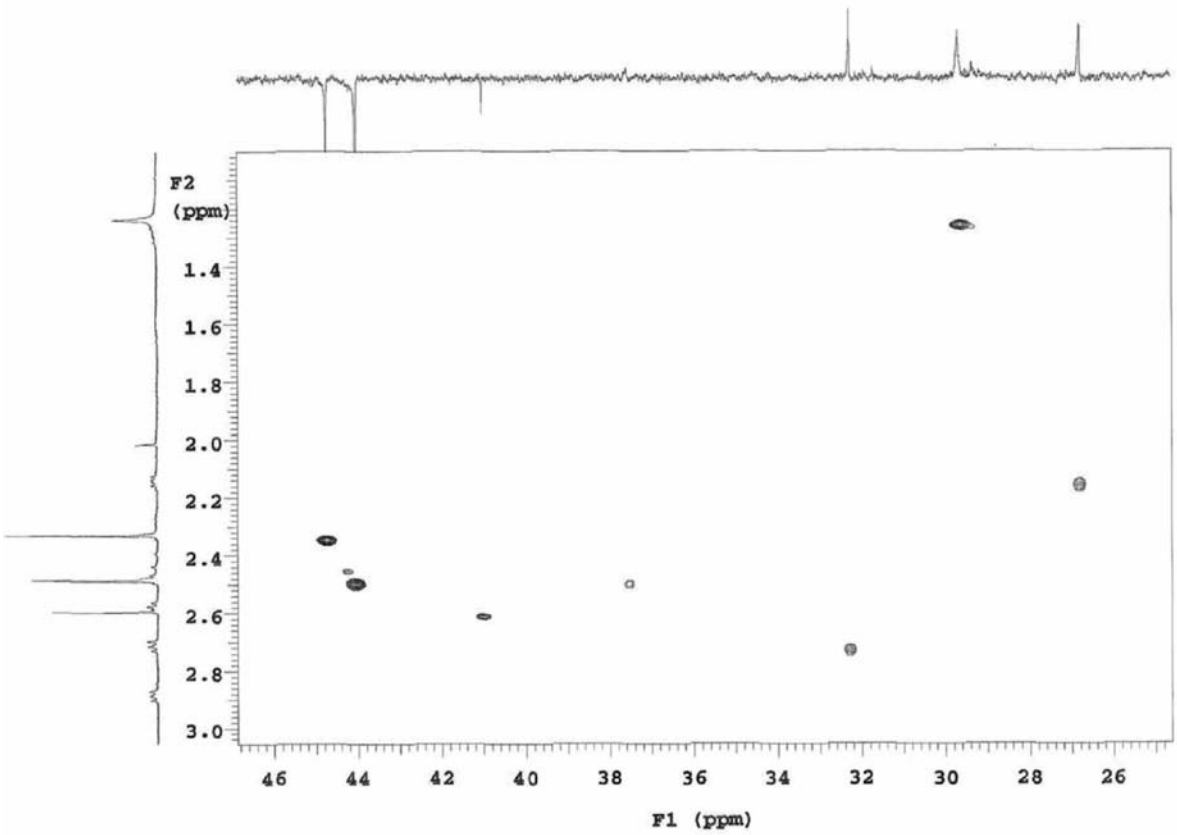

Figure 9S. *Expansion of ^{1}H x ^{13}C-HMQC correlation spectrum of compound **1** (CD_3OD, 500 and 125 MHz respectively)*

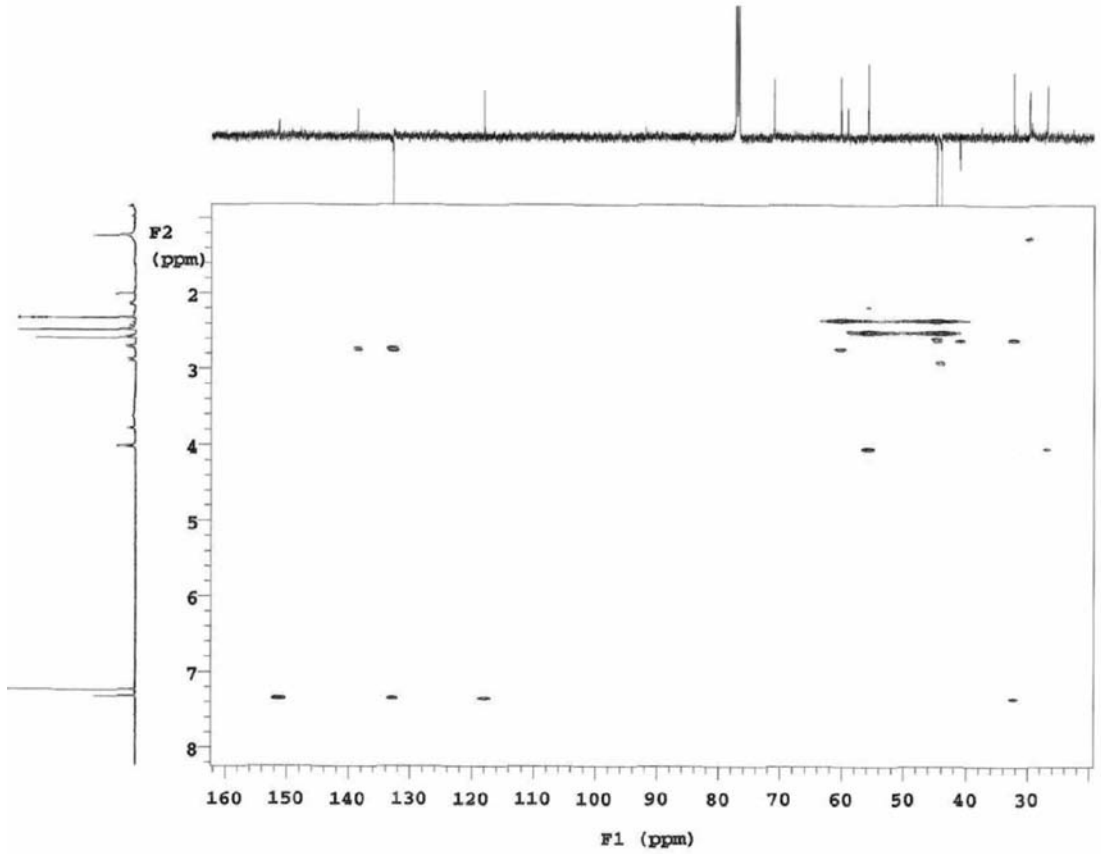

Figure 10S. *^{1}H x ^{13}C-HMBC correlation spectrum of compound **1** (CD_3OD, 500 and 125 MHz respectively)*

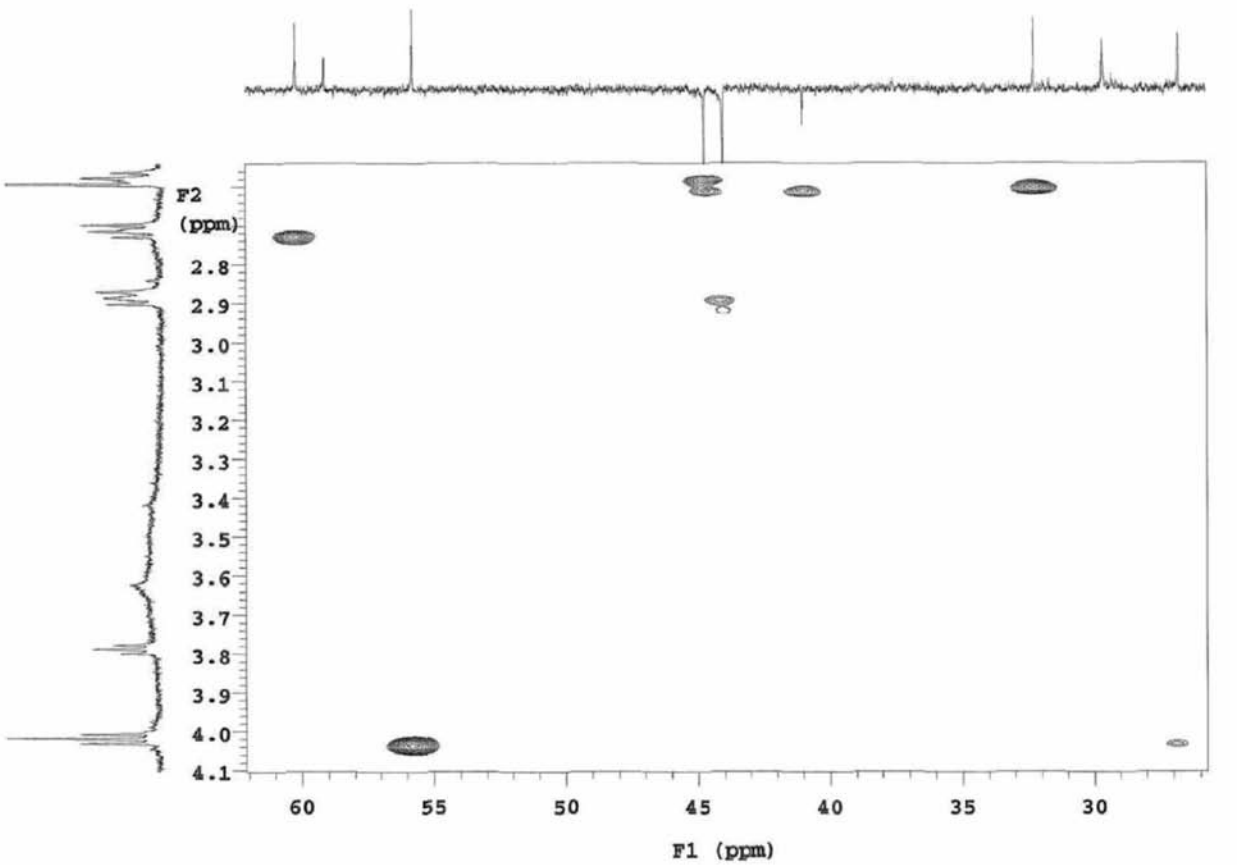

Figure 11S. *Expansion of ^{1}H x ^{13}C-HMBC correlation spectrum of compound **1** (CD_3OD, 500 and 125 MHz respectively)*

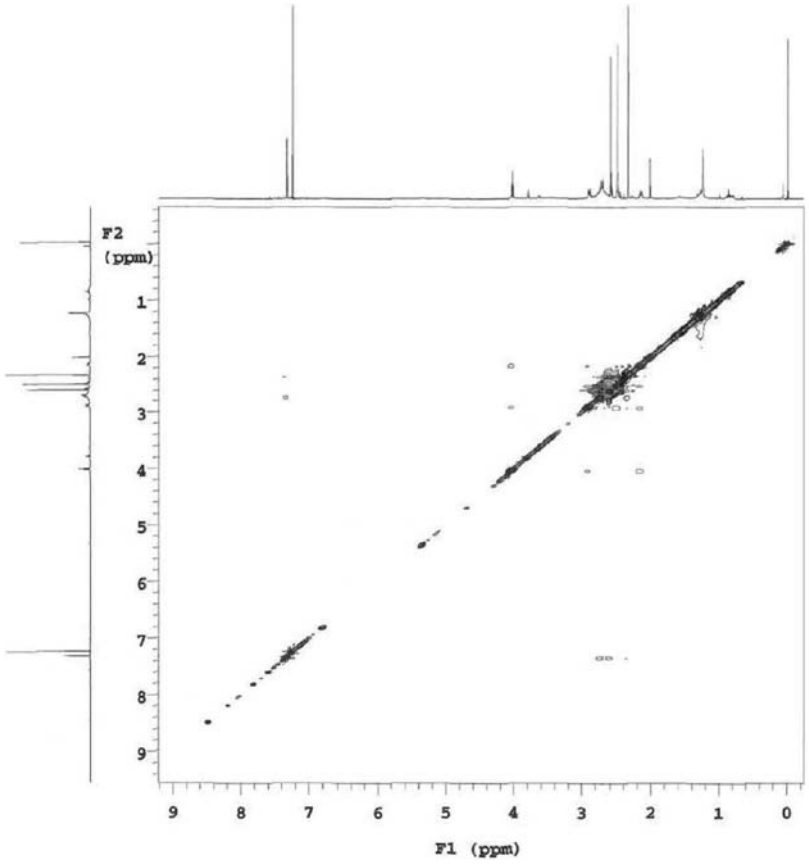

Figure 12S. *^{1}H x ^{1}H-NOESY spatial correlation spectrum of compound **1** (CD_3OD, 500 MHz)*

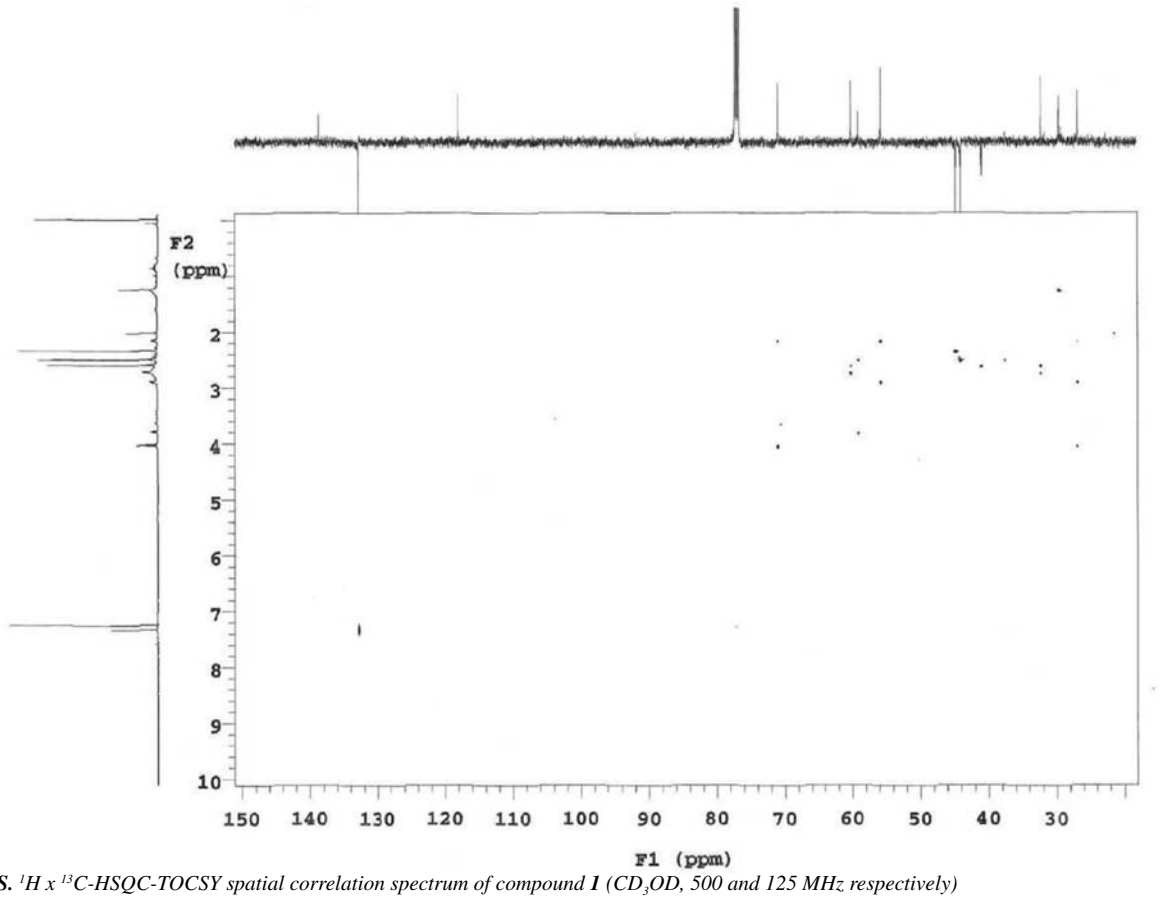

Figure 13S. *^{1}H x ^{13}C-HSQC-TOCSY spatial correlation spectrum of compound **1** (CD_3OD, 500 and 125 MHz respectively)*

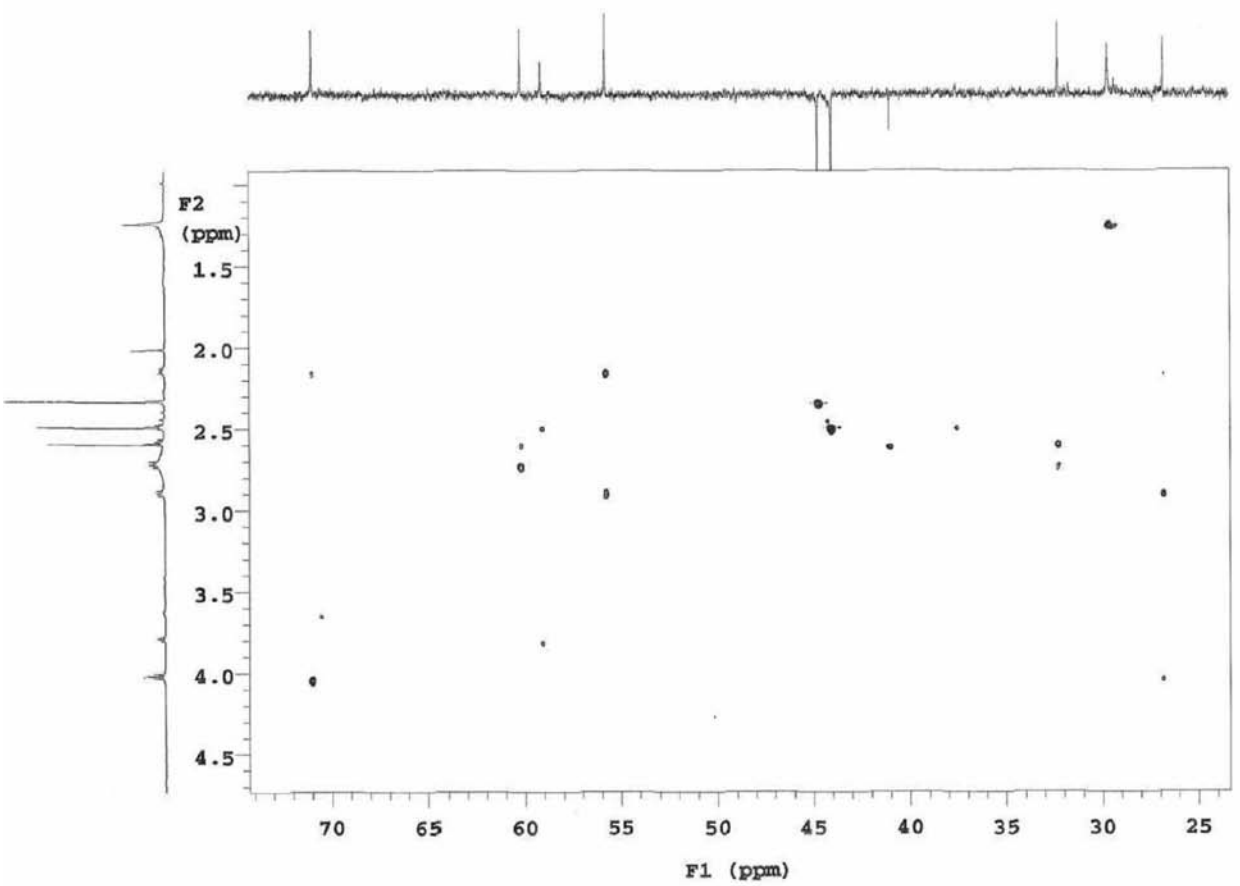

Figure 14S. *Expansion of ^{1}H x ^{13}C-HSQC-TOCSY spatial correlation spectrum of compound **1** (CD_3OD, 500 and 125 MHz respectively)*

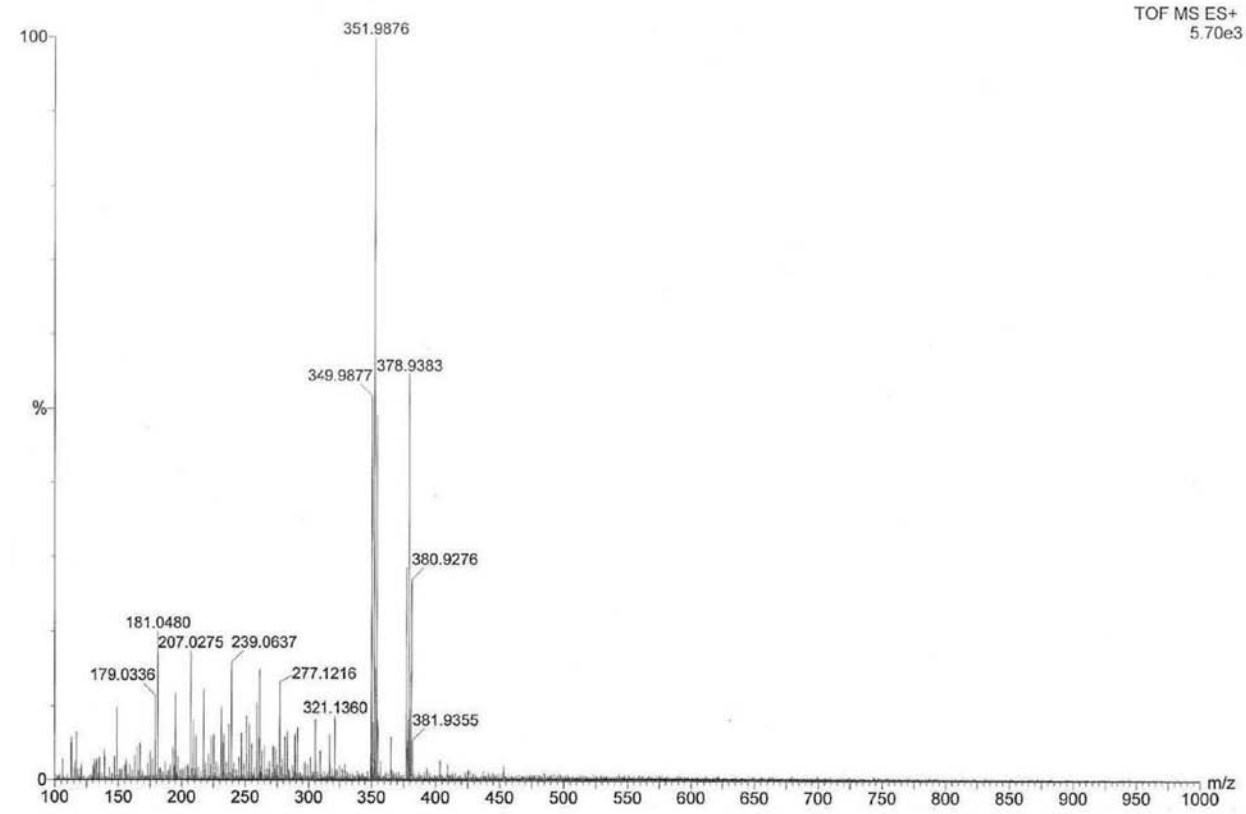

Figure 15S. *HRESIMS spectrum of compound **2***

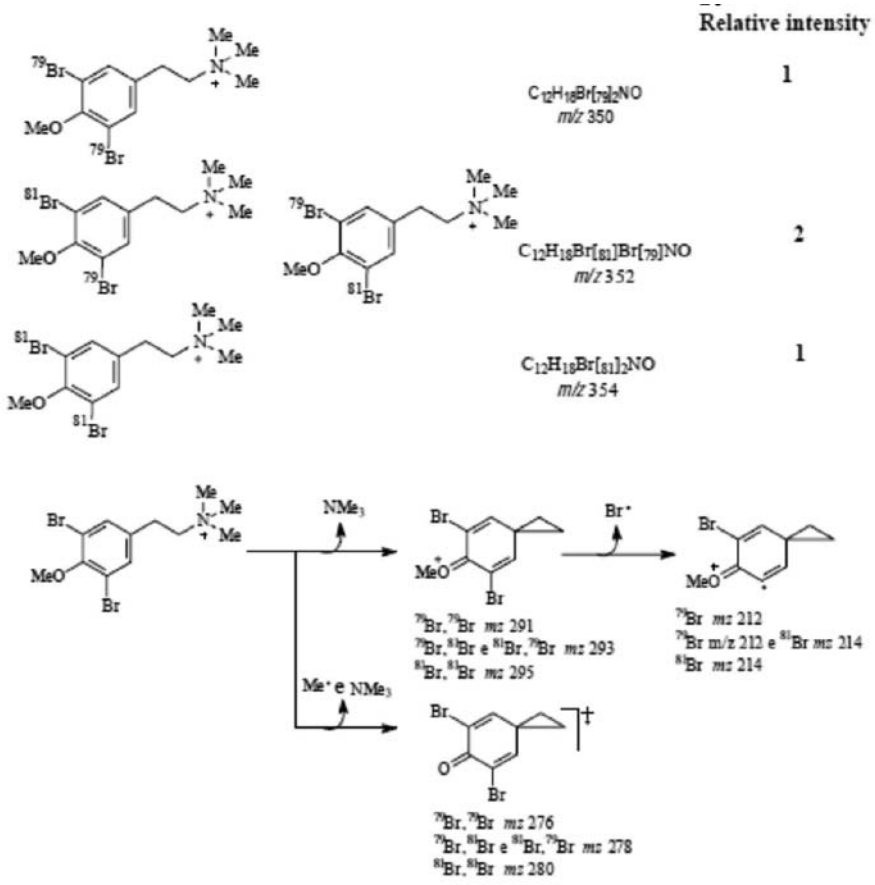

Figure 16S. *Proposed fragmentation for the molecule of compound* ***2***

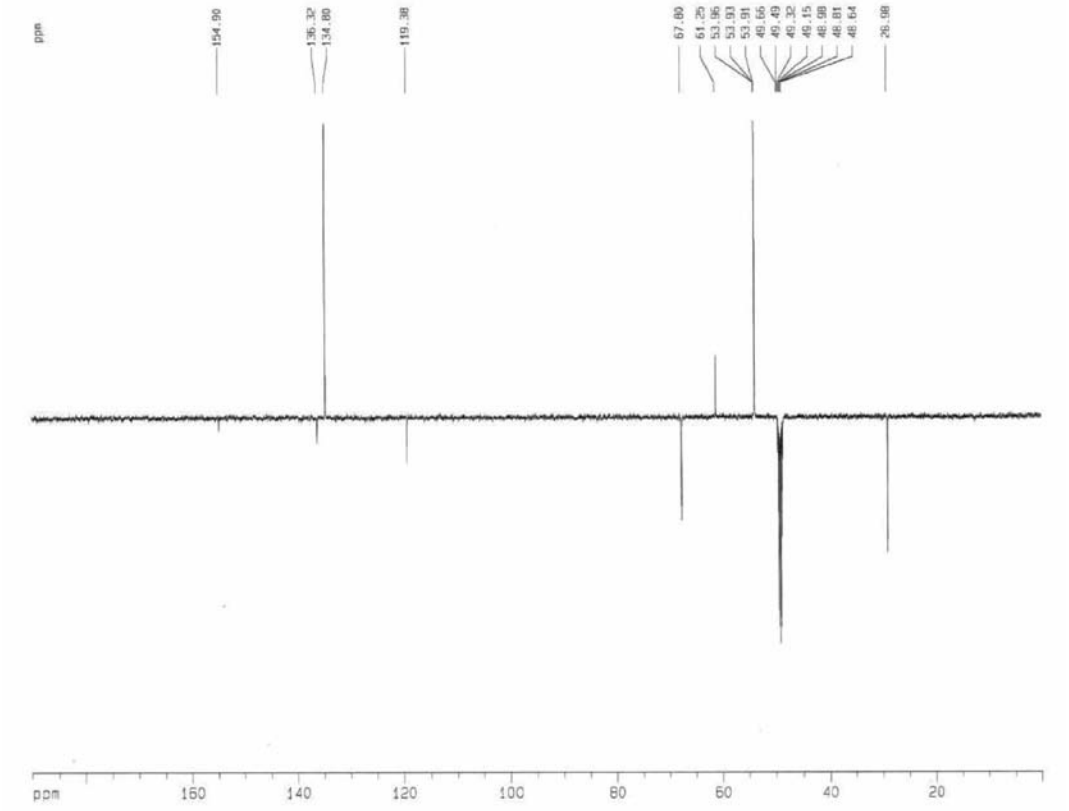

Figure 17S. *NMR* ^{13}*C-APT spectrum of compound* ***2*** *(*CD_3OD*, 125 MHz)*

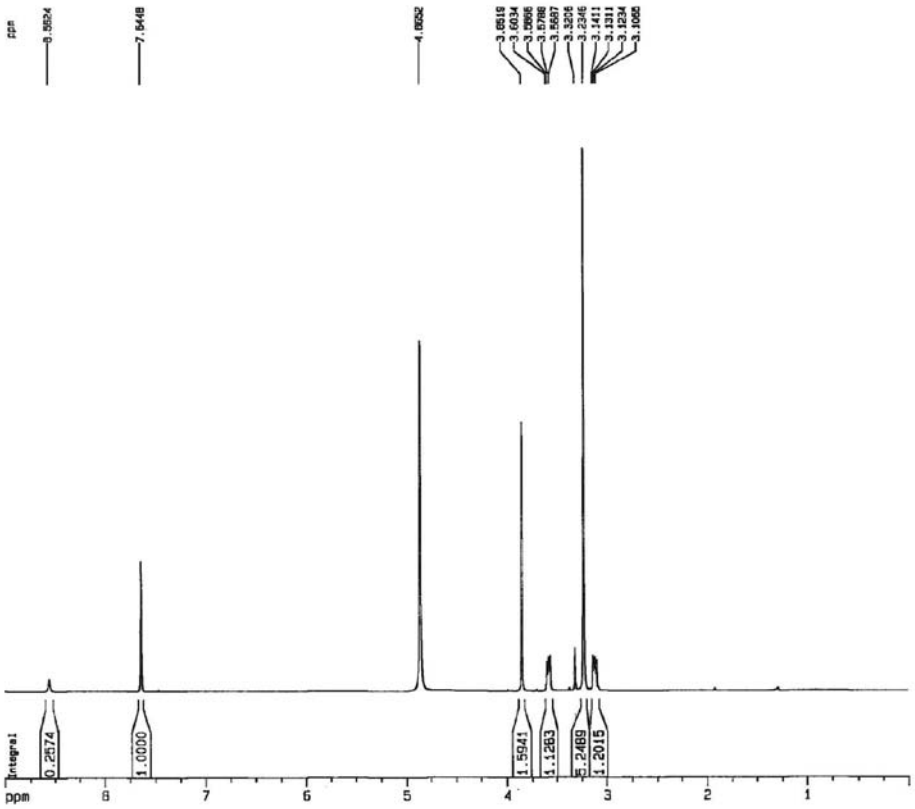

Figure 18S. *^{1}H NMR spectrum data of compound* ***2*** *(CD_3OD, 500 MHz)*

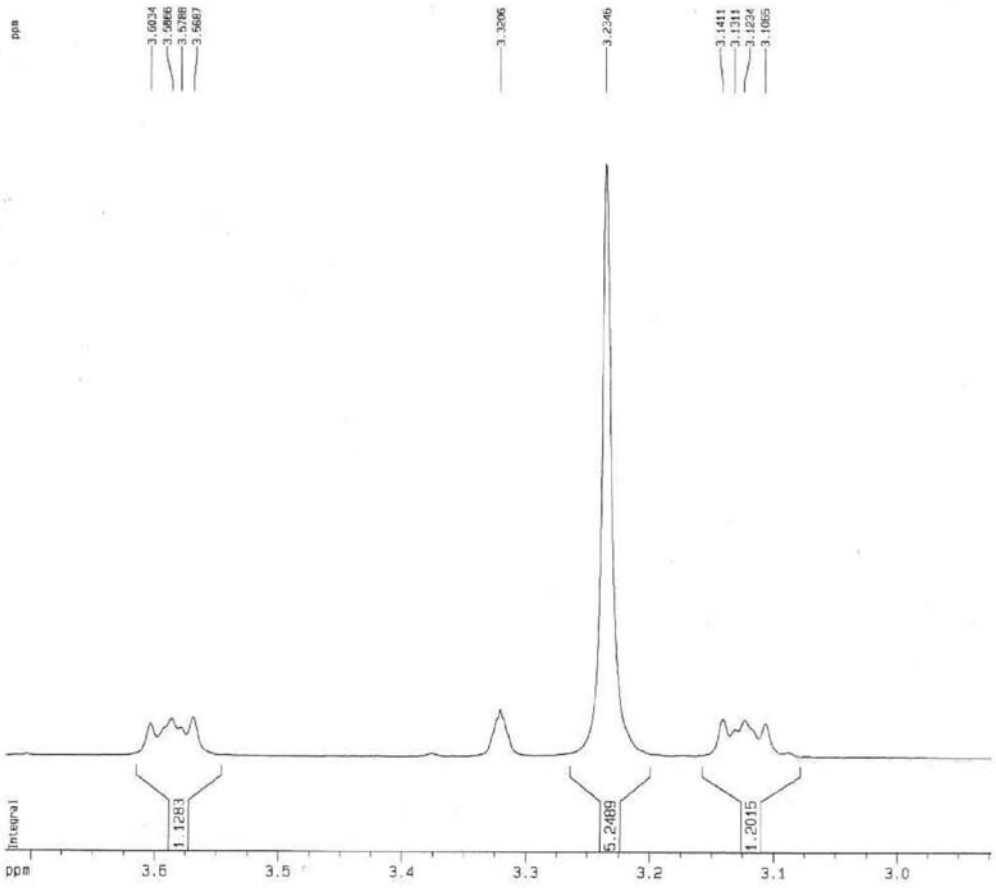

Figure 19S. *Expansion of ^{1}H NMR spectrum at the region of 3.0 – 3.6 of compound* ***2*** *(CD_3OD, 500 MHz)*

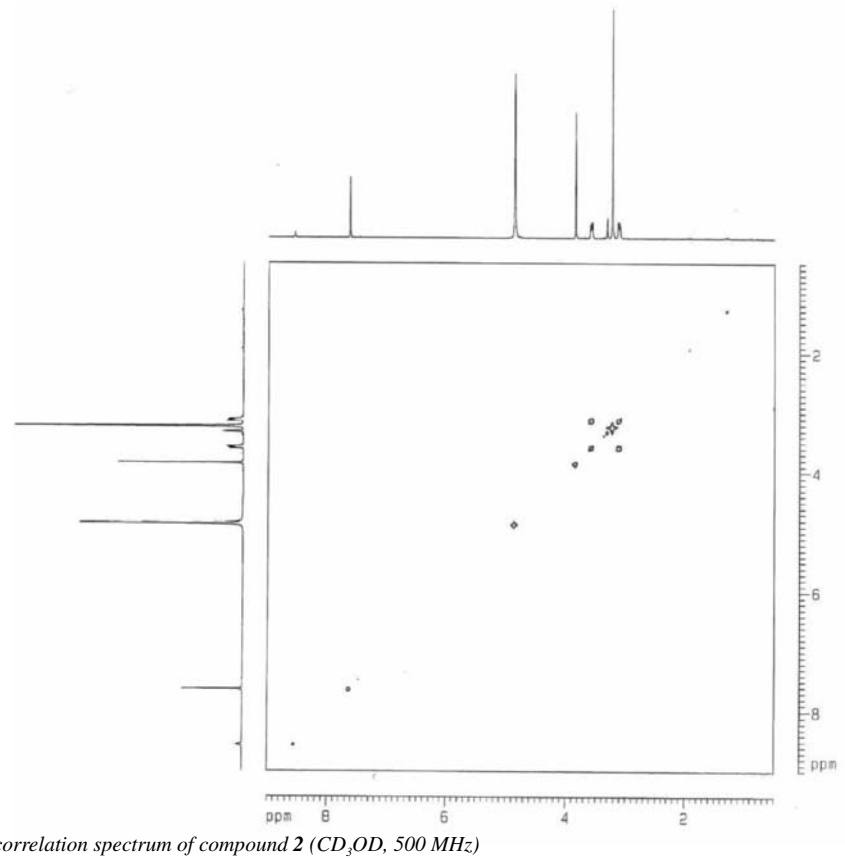

Figure 20S. *^{1}H x ^{1}H-COSY correlation spectrum of compound **2** (CD_3OD, 500 MHz)*

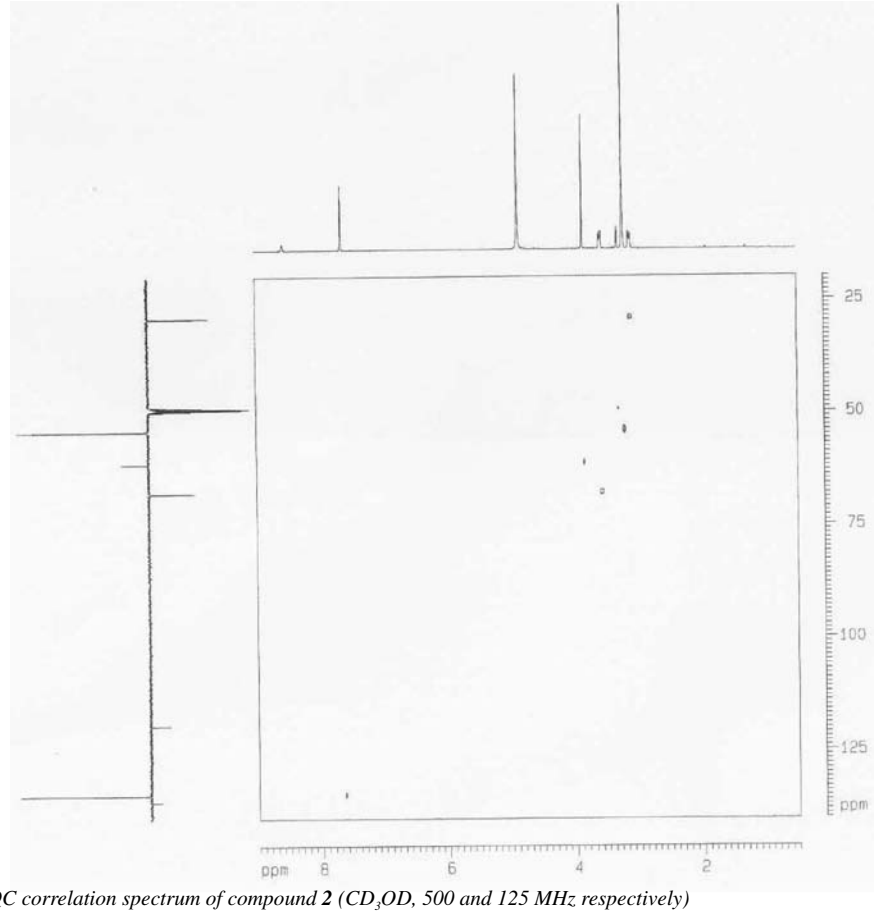

Figure 21S. *^{1}H x ^{13}C-HMQC correlation spectrum of compound **2** (CD_3OD, 500 and 125 MHz respectively)*

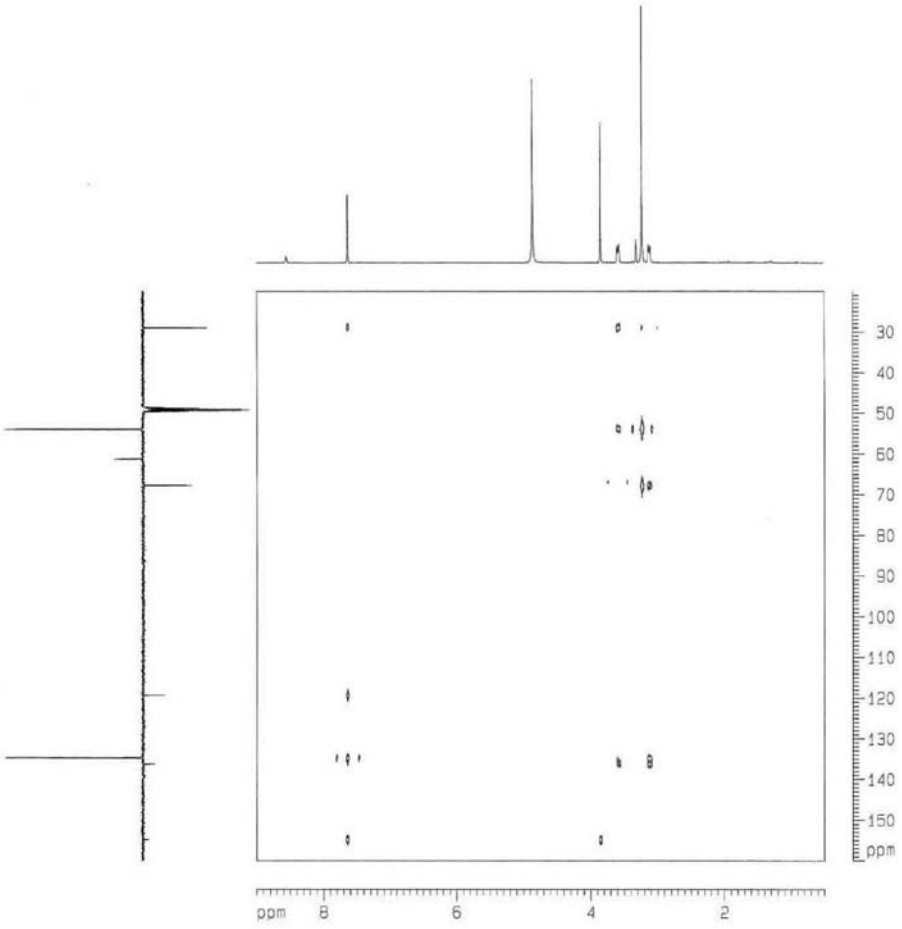

Figure 22S. *^{1}H x ^{13}C-HMBC correlation spectrum of compound **2** (CD_3OD, 500 and 125 MHz respectively)*

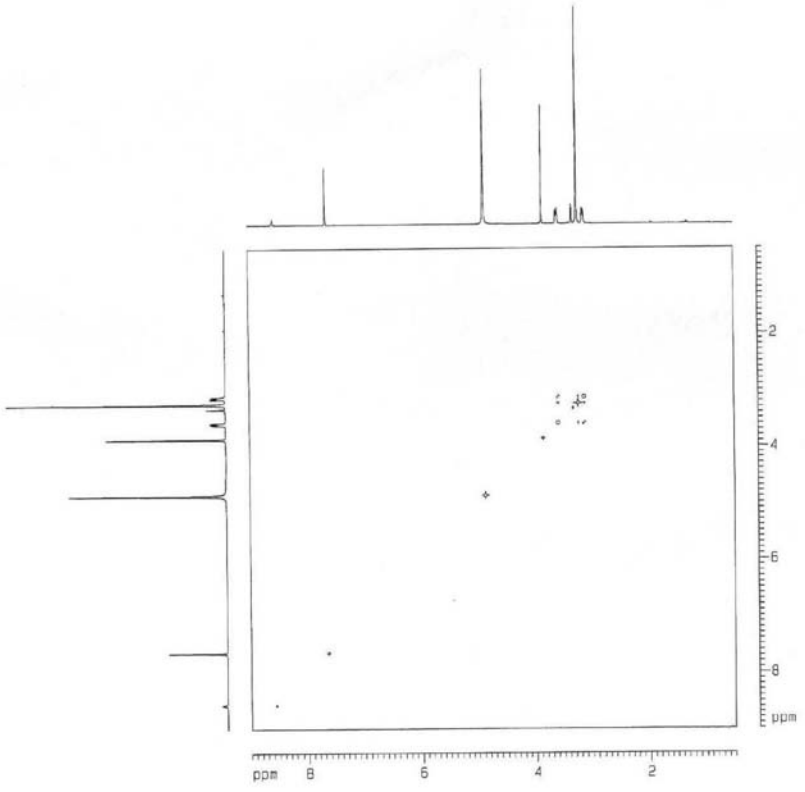

Figure 23S. *^{1}H x ^{1}H-NOESY spatial correlation spectrum of compound **2** (CD_3OD, 500 MHz)*