

## Silver (I) N-Heterocyclic carbene complexes: A winning and broad spectrum of antimicrobial properties

Filippo Prencipe, Anna Zanfardino, Michela Di Napoli, Filomena Rossi, Stefano D'Errico, Gennaro Piccialli, Giuseppe Felice Mangiatordi, Michele Saviano, Luisa Ronga, Mario Varcamonti, Diego Tesauro

Analytical data of the reported compounds [19]:

[AgCl(PhCH<sub>2</sub>imAcr)] (**2MC**). <sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 400 MHz, 298 K): δ 8.22 (br, 2H, acr), 7.86 (br, 2H, acr), 7.45 (br, 2H, acr), 7.31-7.21 (br, 2H, acr and 3H, Ph), 6.93 (br, 2H, Ph), 4.93 (br, 2H, CH<sub>2</sub>). <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 100.6 MHz, 298 K): δ 179.1 (im), 148.4 (acr), 139.5 (acr), 136.2 (Ph), 130.8 (acr), 129.3 (Ph), 128.7 (acr), 128.0 (Ph), 127.9 (Ph), 127.3 (acr), 125.6 (im), 122.9 (im), 121.8 (acr), 121.7 (acr), 54.1 (CH<sub>2</sub>). ESI<sup>+</sup>-MS, m/z: .442 [M-Cl]. Anal. Calcd (%) for C<sub>23</sub>H<sub>17</sub>N<sub>3</sub>ClAg: C, 57.70; H, 3.58; N, 8.78. Found: C, 57.55; H, 3.32; N, 8.66

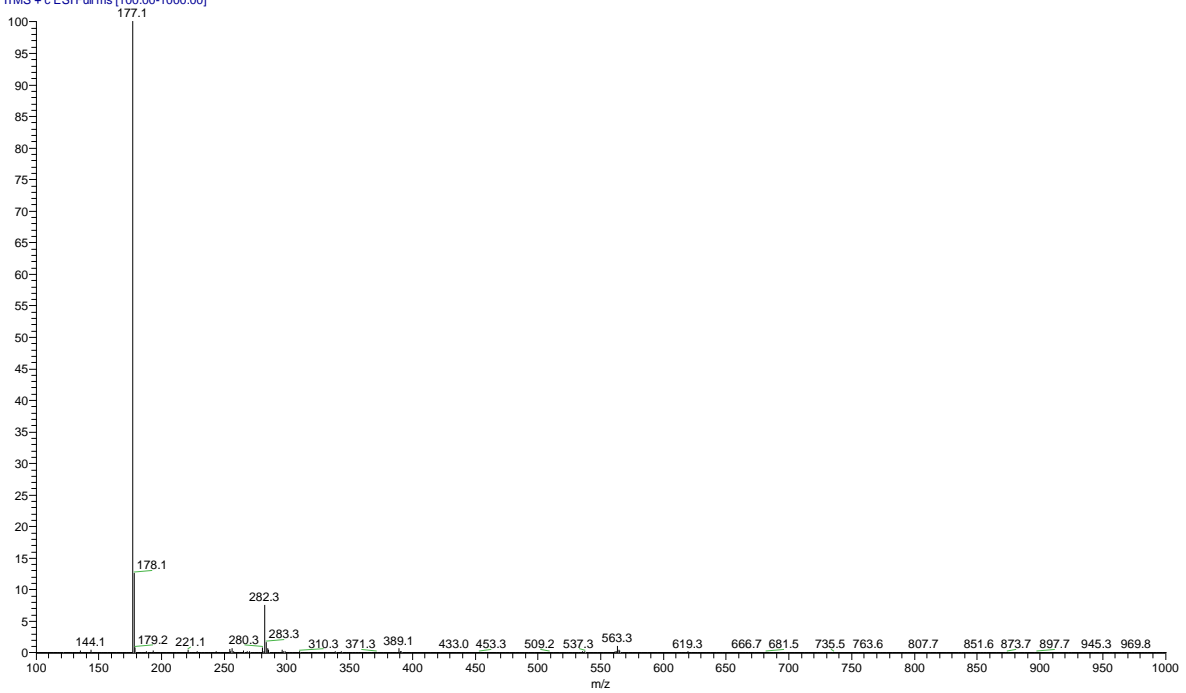
[AgCl(CH<sub>3</sub>imAcr)] (**3MC**). <sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 400 MHz, 298 K) δ 8.26 (d, 2H, acr), 7.90-7.82 (br, 4H, acr, im), 7.53 (br, 2H, acr), 7.33 (br, 2H, acr), 3.60 (br, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 100.6 MHz, 298 K): δ 174.0 (im), 148.4 (acr), 139.7 (acr), 130.8 (acr), 129.3 (acr), 127.8 (acr), 125.0 (im), 123.8 (im), 122.1 (acr), 121.8 (acr), 37.9 (CH<sub>3</sub>). ESI<sup>+</sup>-MS, m/z: .366 [M-Cl]. Anal. Calcd (%) for C<sub>17</sub>H<sub>13</sub>N<sub>3</sub>ClAg: C, 50.71; H, 3.25; N, 10.44. Found: C, 50.88; H, 2.88; N, 10.22

[Ag(PhCH<sub>2</sub>imAcr)<sub>2</sub>]BF<sub>4</sub>. (**2BC**). <sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 400 MHz, 298 K): δ 8.20 (d, 2H, acr), 7.85-7.81 (m, 2H, acr, 2H, im), 7.43 (m, 2H, acr) 7.31-7.27 (br, 1H, Ph), 7.20 (d, 2H, Ph), 7.16 (d, 2H, acr), 6.99 (d, 2H, Ph), 4.88 (s, 2H, CH<sub>2</sub>). <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 100.6 MHz, 298 K) δ 181.7 (im), 148.9 (acr), 139.9 (acr), 136.6 (Ph), 131.3 (acr), 129.9 (Ph), 129.2 (acr), 128.6 (Ph), 128.5 (Ph), 127.7 (acr), 126.2 (im), 123.4 (im), 122.2 (2C, acr), 54.6 (CH<sub>2</sub>). ESI<sup>+</sup>-MS, m/z: .777 [M<sup>+</sup>]. Anal. Calcd (%) C<sub>46</sub>H<sub>34</sub>N<sub>6</sub>BF<sub>4</sub>Ag: C, 63.84%; H, 3.96%; N, 9.71%. Found C, 63.92%; H, 3.97%; N, 9.78.

# Selected Mass Spectra:

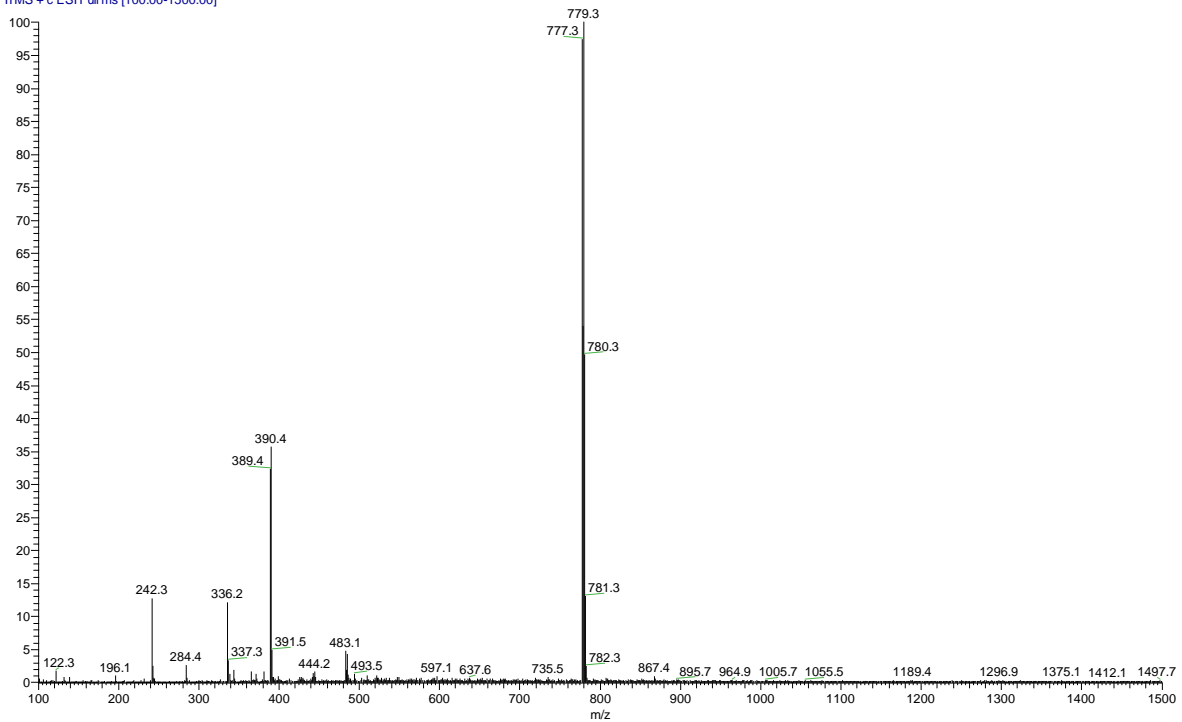
## 1MC

FP16\_16112020 #10-103 RT: 0.02-0.22 AV: 94 NL: 2.98E7  
T: ITMS + c ESI Full ms [100.00-1000.00]

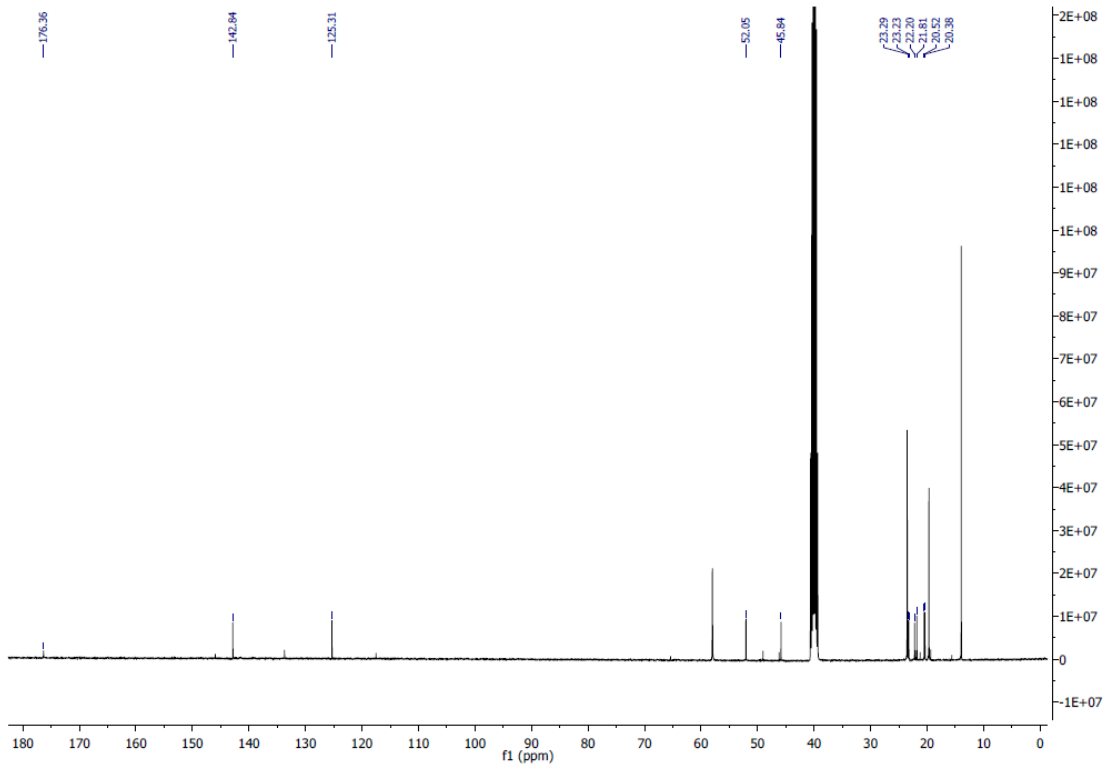
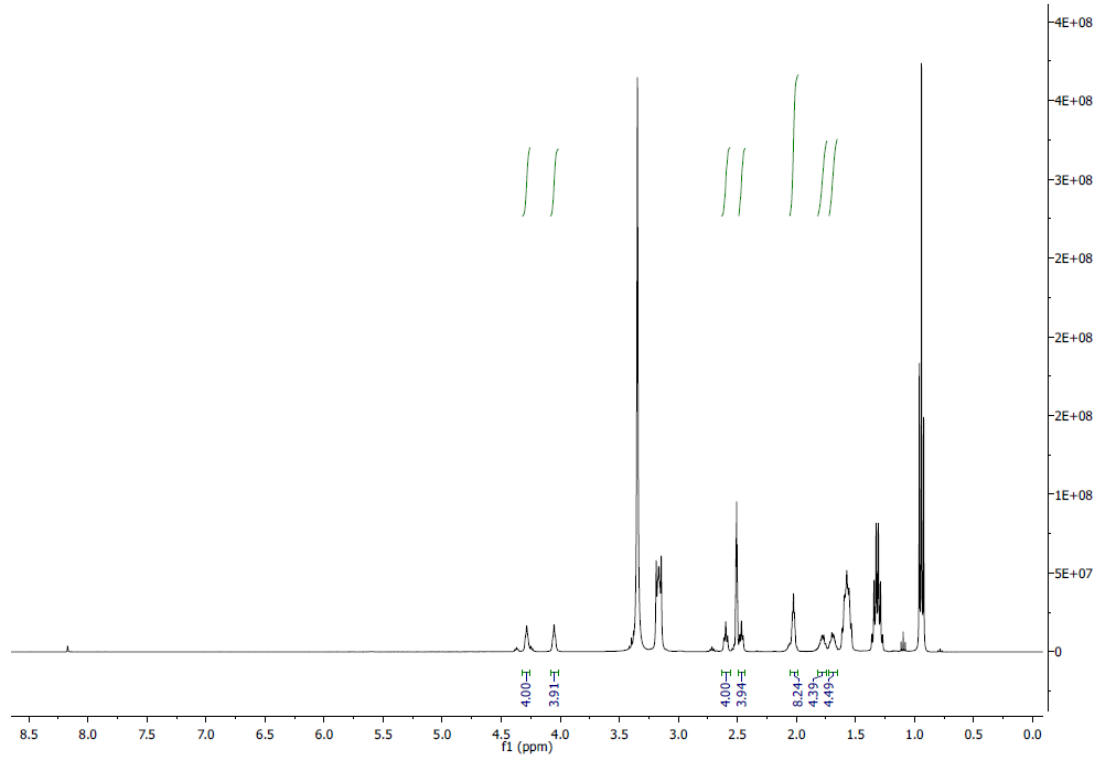


## 2BC

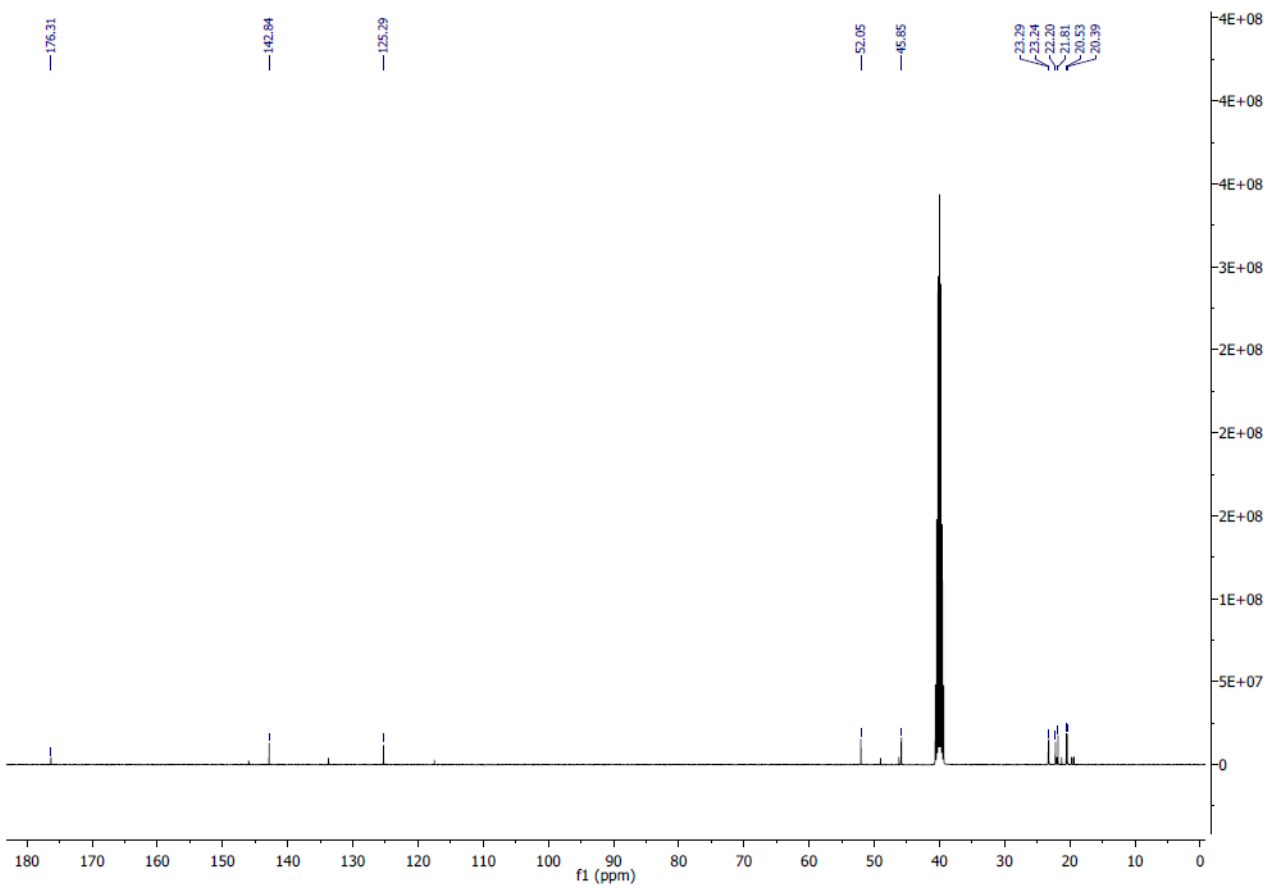
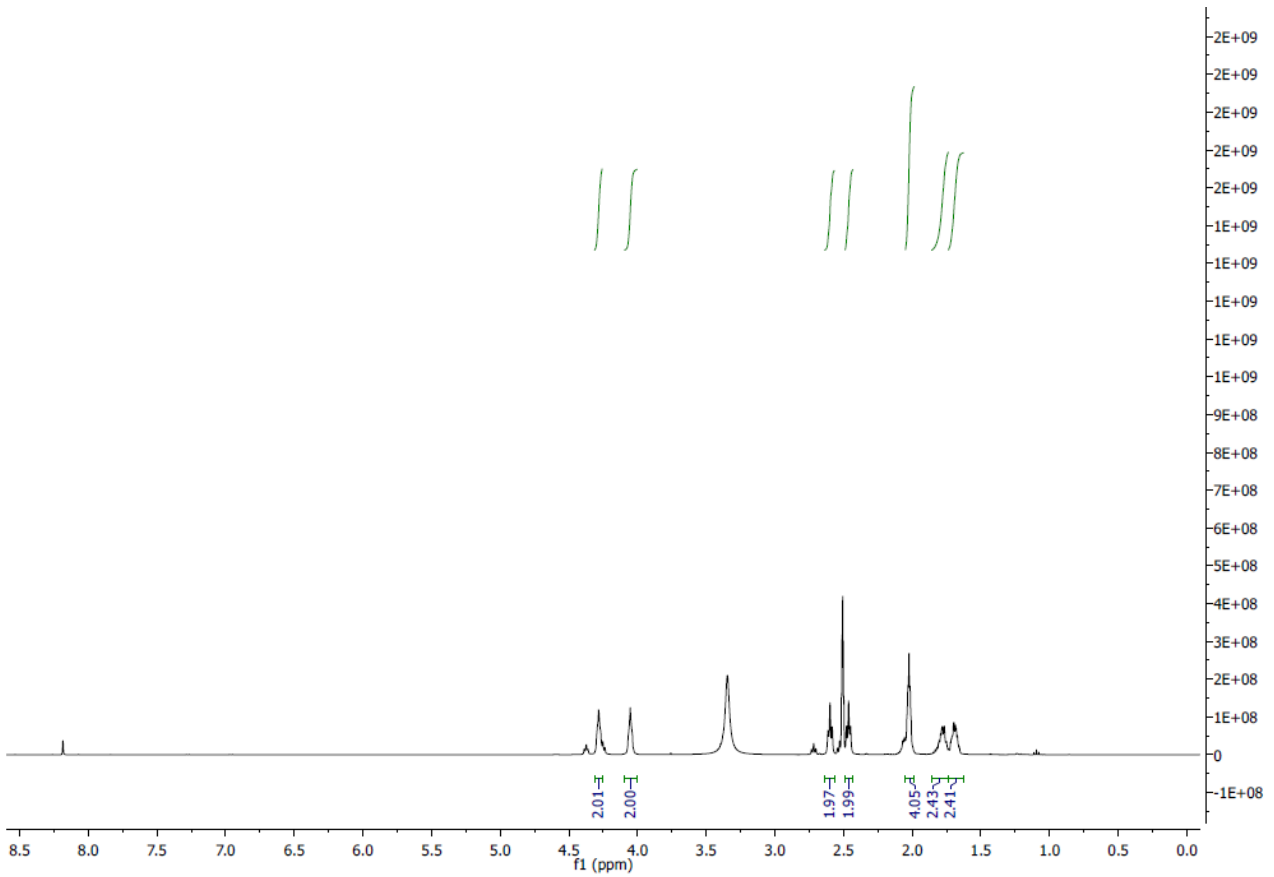
2bc\_19022021 #5-42 RT: 0.01-0.11 AV: 38 NL: 7.14E6  
T: ITMS + c ESI Full ms [100.00-1500.00]



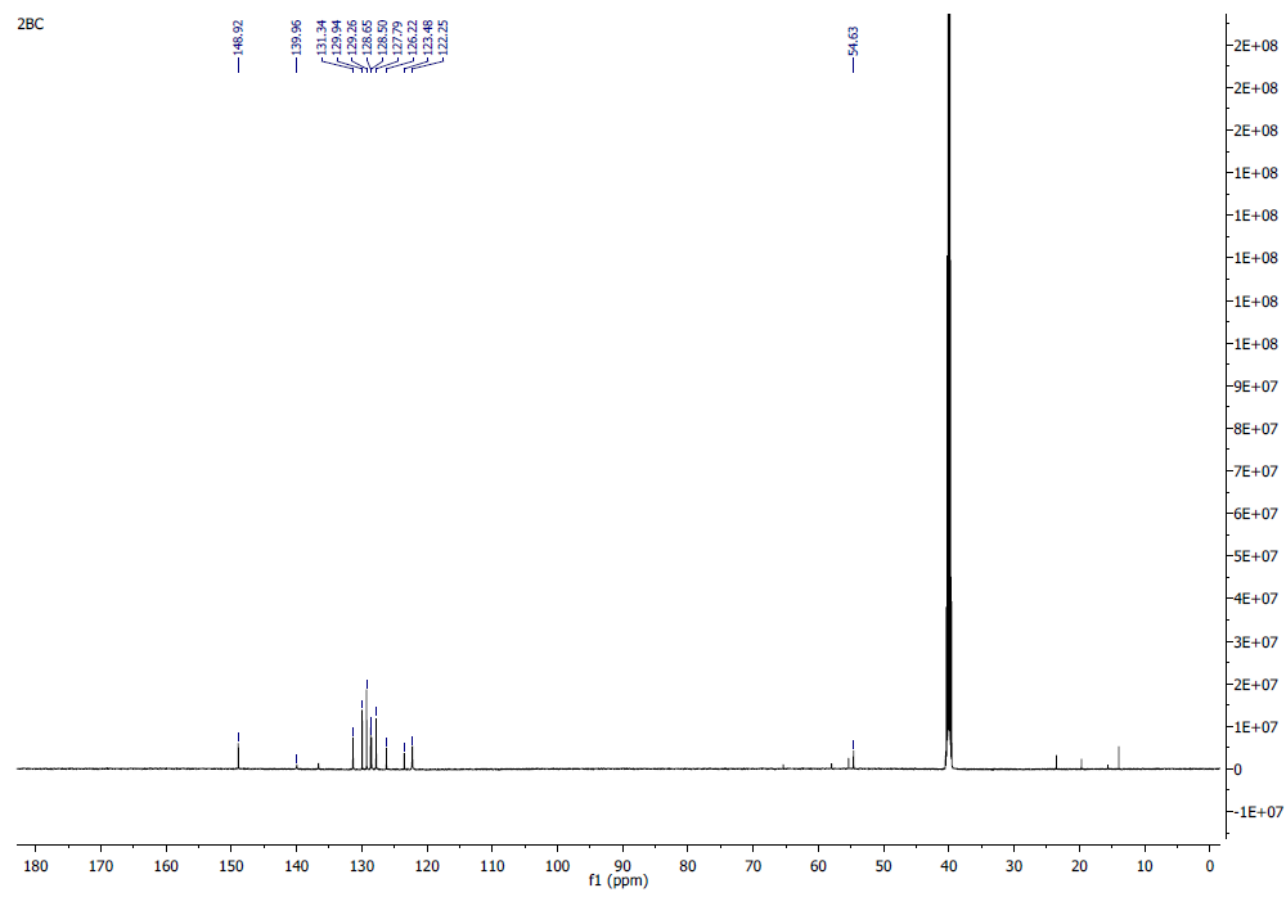
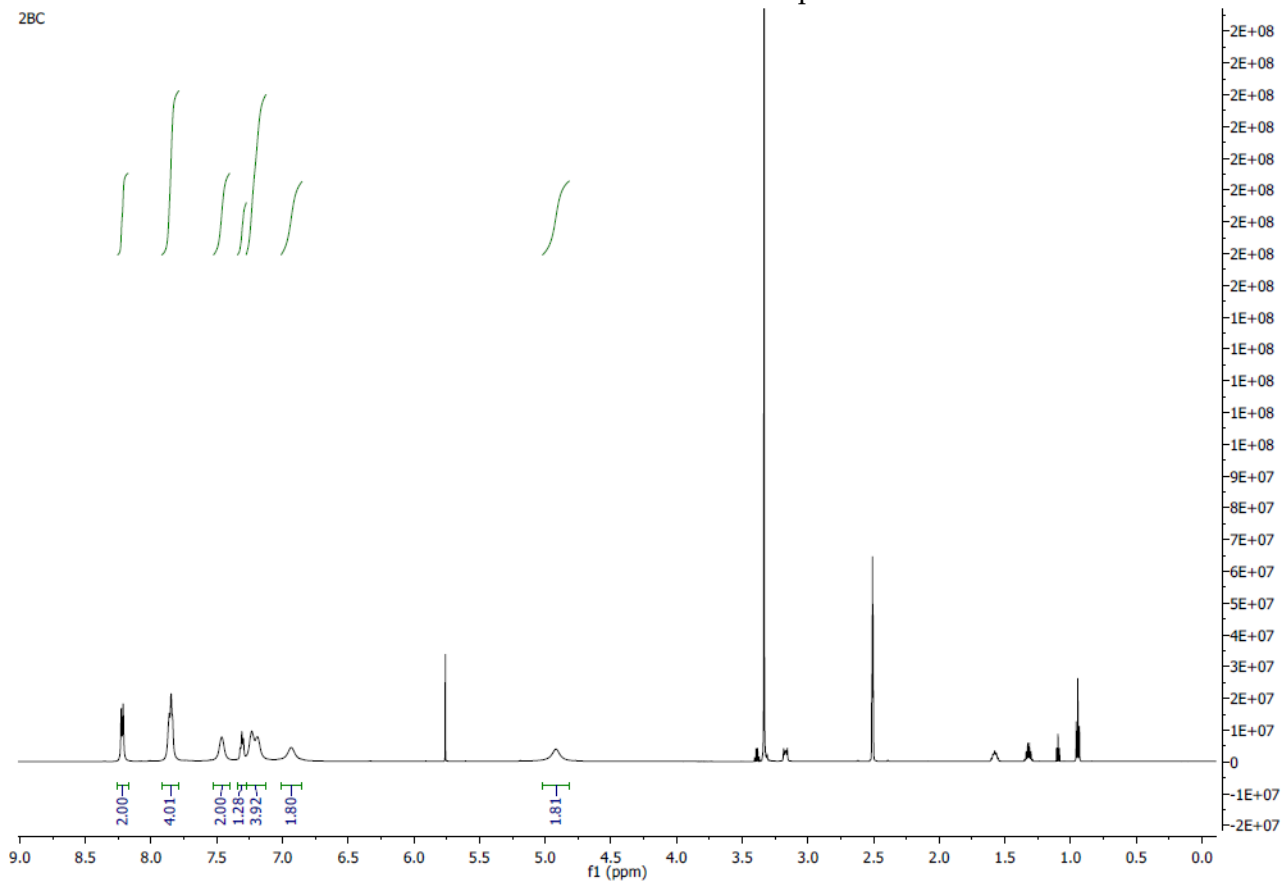
# <sup>1</sup>H NMR and <sup>13</sup>C NMR 1BC Spectra



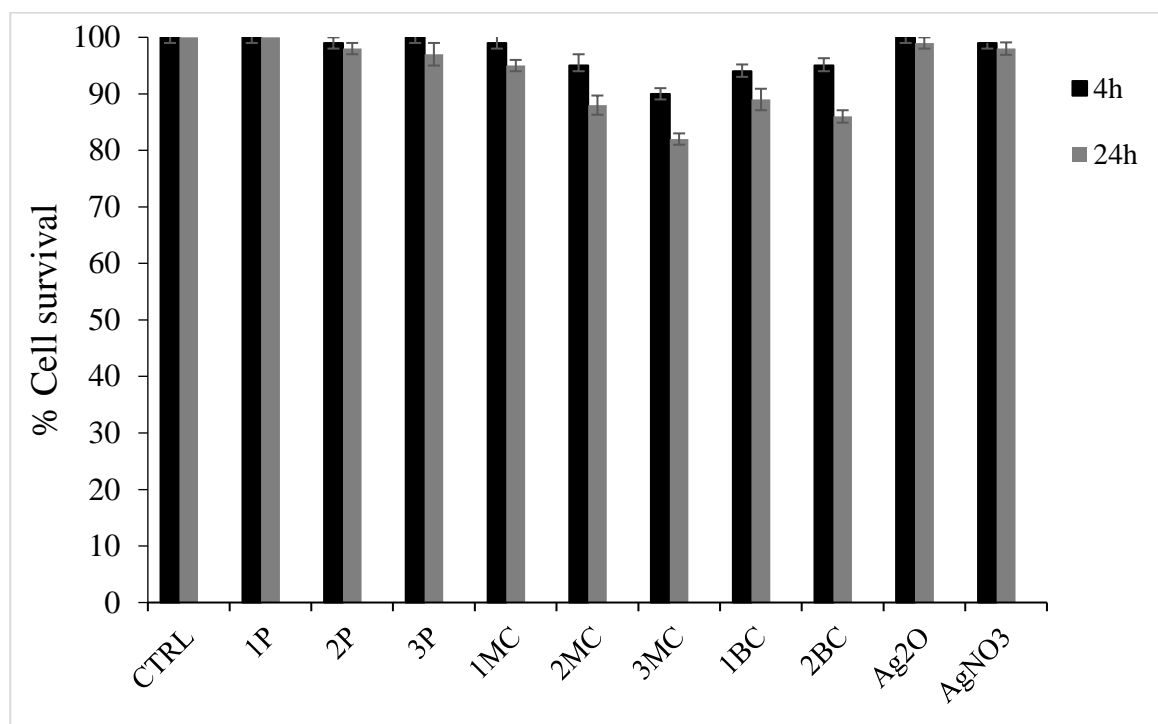
# <sup>1</sup>H NMR and <sup>13</sup>C NMR 1MC Spectra



# <sup>1</sup>H NMR and <sup>13</sup>C NMR 2BC Spectra



### Viability test on HEK 293 cells



**Figure S1:** Cytotoxic effects of compounds [ $1\mu\text{M}$ ] on HEK 293 cells (human embryonic kidney) by MTT assay. The mean values and SD of two independent experiments performed in triplicate are shown.