

Unexpected cytosine-AuCl₄⁻ interaction under ESI-MS conditions - formation of
cytosine-Au(I) complexes - **supplemental material**

It is well known that Cu(II) is very prone to be reduced under ESI conditions, producing Cu(I) containing ions (Henderson W and McIndoe JS. Mass Spectrometry of Inorganic, Coordination and Organometallic Compounds. John Wiley & Sons, Ltd 2005; p. 117). Figure 1s shows the full scan mass spectrum obtained for a solution containing cytosine and CuCl₂. As clearly seen in Figure 1s, cytosine, under ESI condition formed complexes with both Cu(II) and Cu(I) with comparable abundances. Therefore, cytosine cannot be regarded as especially prone to form complexes with Cu(I).

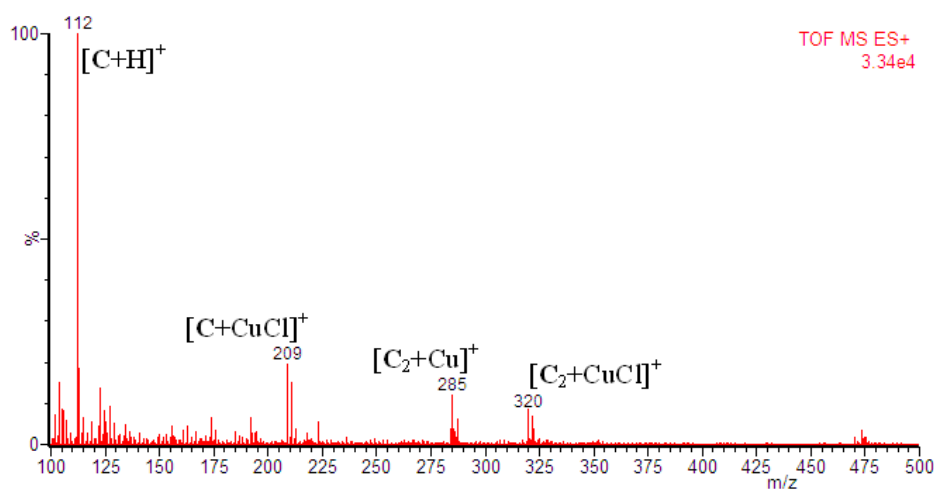


Figure 1s. Full scan mass spectrum obtained for solution containing cytosine and CuCl₂.

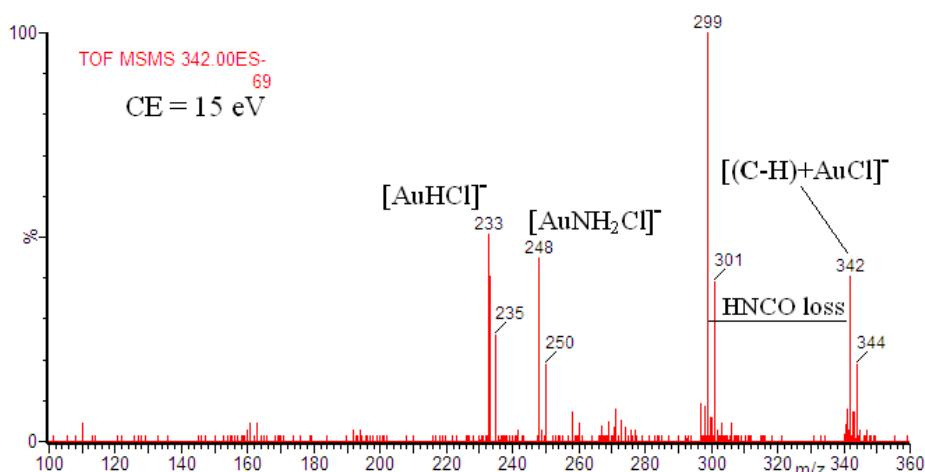


Figure 2s. The product ion spectrum of ion [(C-H)+AuCl]⁻. Analogically as for ion [C₂+Au]⁺, decomposition of cytosine ligand occurs (the loss of HNCO molecule). There are also signals of product ions [AuNH₂Cl]⁻ and [AuHCl]⁻ (amide/azanide and hydride, respectively), however their formation is difficult to rationalize.