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## Investigation on bimolecular complexes in natural extracts by parent ion and neutral loss MS/MS experiments

**Pietro Traldi**

Pediatric Research Institute Città della Speranza, Italy

Many of the mechanisms of action of drugs can be explained by the theory of lock and key. An active molecule to produce a pharmacological effect has to interact with the receptor site. However, in a highly complex biological system, such as a plant extract, hundreds of different molecules interact with each other leading to aggregation phenomena between different molecular systems. Then the formation of complexes between different molecules must be considered highly probable and the biological activity would have to be ascribed to molecular complexes rather than to a single molecule. A good example of this aspect is that related to tea, with complexes between caffeine and catechins, in particular epigallocatechin gallate (EGCg). The formation of these complexes has been studied in detail, showing that caffeine and EGCg in the solid state pile up to form complex stacks. By studying solutions <sup>1</sup>H-NMR investigations show clear differences among the caffeine signals in the spectrum of pure, synthetic compound and those present in tea extracts. In the present investigation, the capabilities of tandem mass spectrometry for the detection of these bimolecular complexes have been studied by ESI-QqQ instrumental approach. The presence of complexes in tea extracts has been tested either by precursor ion scans of the caffeine protonated molecule or by neutral loss scans aimed to find all the possible ionic species which loose neutral caffeine. By these approaches different molecular caffeine containing complexes have been evidenced.

### Biography

Pietro Traldi completed his Graduation in Physics in 1973 at Milan University. From 1974 to 2015, he was Research Executive at Italian Research Council, working mainly in the field of Mass Spectrometry. He has published more than 600 papers in international journals. He collaborates with the Pediatric Research Institute "Città della Speranza" in Padova and with Aboca Spa, Italy.

p.traldi@irpcds.org

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