

Flow Analysis XIII



6–10 July 2015, Diplomat Hotel, Prague, Czech Republic



Final Programme & Book of Abstracts





OP03

Flow injection coupled to electrospray ionization mass spectrometry for non-covalent binding determinations

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Binding determination is of extreme importance in the pharmaceutical field as it tells how efficiently a new drug binds to a target. Several methods exist for binding determination, though electrospray ionization mass spectrometry (ESI-MS) has particularly high sensitivity and specificity. It allows the direct and independent detection of analytes and complexes down to the picomole to femtomole range. In ESI-MS, titration is the most used method for the equilibrium determination between host and guest as it is simple to perform, although it can also be a tedious and time-consuming procedure since it requires the preparation of multiple samples with varied concentrations. Therefore, to improve throughput, Frycák and Schug developed a different titration method, called dynamic titration that uses a single solution of host and guest and is based on the controlled band-dispersion concept obtained by hyphenating ESI-MS with flow injection analysis (FIA). In this work a new MS-based noncovalent binding determination method was developed by using a continuous stirred tank reactor (CSTR) as a flow injection device for exponential dilution of an equimolar host-guest solution over time. By combining an exponential dilution model with a previously established equimolar binding model, binding constants can be determined for host-guest complexes with a single injection. This methodology was applied for the determination of binding constants between vancomycin and Ac-Lys(Ac)-Ala-Ala tripeptide stereoisomers.

Acknowledgements: I. C. Santos thanks FCT, Portugal, and FSE through the program POPH – QREN the grant SFRH/BD/76012/2011. This work was supported by National Funds from FCT through project PEst-OE/EQB/LA0016/2013 and by the US National Science Foundation (CHE-0846310).