

3-Substituted xanthenes as promising candidates for quadruplex formation: computational, synthetic and analytical studies

János Szolomájer,^a Gábor Paragi,^b Gyula Batta,^c Célia Fonseca Guerra,^d F. Matthias Bickelhaupt,^d Zoltán Kele,^a Petra Pádár,^a Zoltán Kupihár^a and Lajos Kovács

^a Department of Medicinal Chemistry, University of Szeged, Szeged, Hungary, Fax: +36 62 545141; Tel: +36 62 545145; E-mail: kovacs@ovrisc.mdche.u-szeged.hu

^b Supramolecular and Nanostructured Materials Research Group of the Hungarian Academy of Sciences, University of Szeged, Szeged, Hungary

^c Department of Organic Chemistry, University of Debrecen, Debrecen, Hungary

^d Department of Theoretical Chemistry and Amsterdam Center for Multiscale Modeling (ACMM), Scheikundig Laboratorium der Vrije Universiteit, Amsterdam, The Netherlands

Nano-ESI-Q-TOF MS spectrum of 3-methylxanthine (M = 166.0491): (a) m/z range: 0-2800, (b) m/z range: 1012-1041

(a) Whole spectrum

ammonium hydrogenkarbonattal telített metanol 99%, a tobbsi 1 a vizes minta

KZ100519_XANTEN_MEOHB 101 (1.871) Cm (99:107)

TOF MS ES+
5.12e3



