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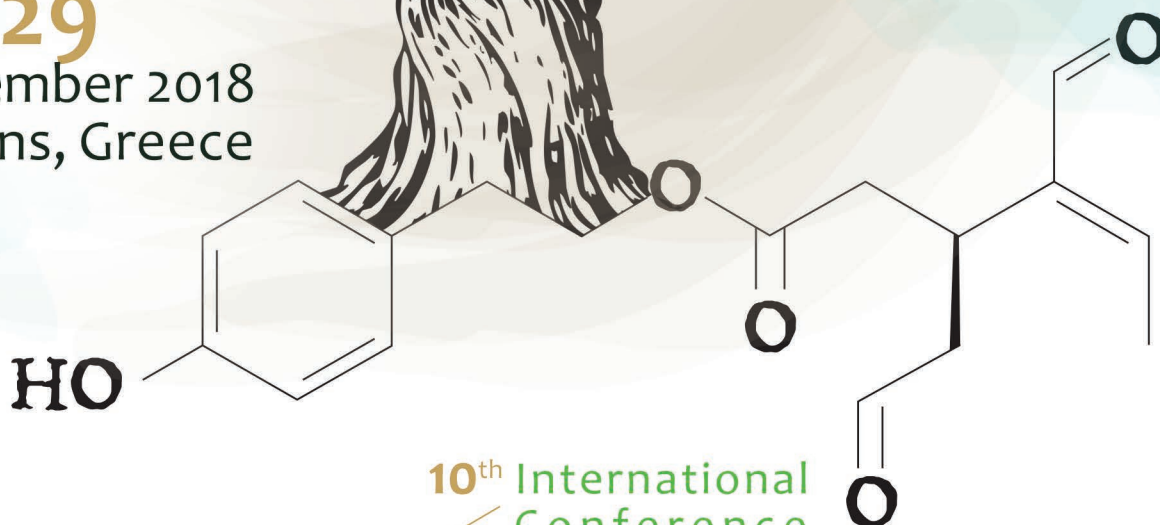


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abstractbook



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SL-002

NMR in natural products: chemical analysis, monitoring of dynamic changes, “in-cell” NMR and DFT calculated structures based on NMR chemical shifts in solution

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A critical overview of recent developments of NMR spectroscopy in natural products will be provided with emphasis in the following applications:

- (i) chemical analysis of extracts without isolation or derivatization steps [1],
- (ii) ‘*in situ*’ monitoring of dynamic changes of metabolites [2], ‘*in situ*’ analysis of enzymatic reaction products [3], and enriching the biological space of natural products, through monitoring in the NMR tube [4],
- (iii) “in-cell” NMR in decoding the apoptotic activity of flavonoids [5] and artemisinin with the Bcl-2 family of proteins and
- (iv) quantum chemical calculations of high-resolution structures in solution based on NMR chemical shifts – comparison with X-ray and neutron diffraction methods [6].

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Keywords: Chemical shifts, DFT, NMR, in-cell NMR

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