

NMR assignment in regioisomeric hydroquinones

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A set of regioisomeric pairs of tricyclic hydroquinones, analogues of antitumor

9,10-dihydroxy-4,4-dimethyl-5,8-dihydroanthracen-1(4H)-one (1) and other derivatives, were

synthesized and their regiochemistry and NMR spectra assigned by using ^1H -detected one-bond

(C-H) HMQC and long-range C-H HMBC, in good agreement with theoretical O3LYP/Alhrichs-pVTZ

calculations. The 5-hydroxymethyl derivatives (11, 15, 19) showed a $^3J_{\text{H}}$, H coupling constant of

methylene protons evidencing the presence of a seven-membered intramolecular hydrogen bonded

ring, not observed for the 8-hydroxymethyl isomers. © 2011 John Wiley & Sons, Ltd.