
**ITAPEJARAFURAN, (5*R*,5*aS*,9*aR*)-4,5,5*a*,6,7,9*a*-HEXAHYDRO-1,5,8-TRIMETHYL
NAPHTHO[2,1-*b*]FURAN FROM *Baccharis punctulata* (Asteraceae) AND
CYTOTOXIC EVALUATION ON MIA PaCa-2 CELL LINE**

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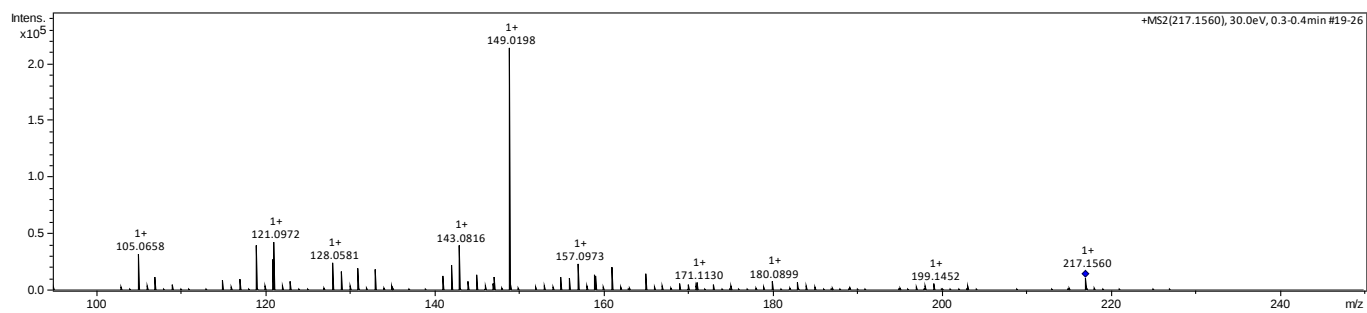


Figure 1S. HRMS (ESI(+)-QTOF) of compound **2**

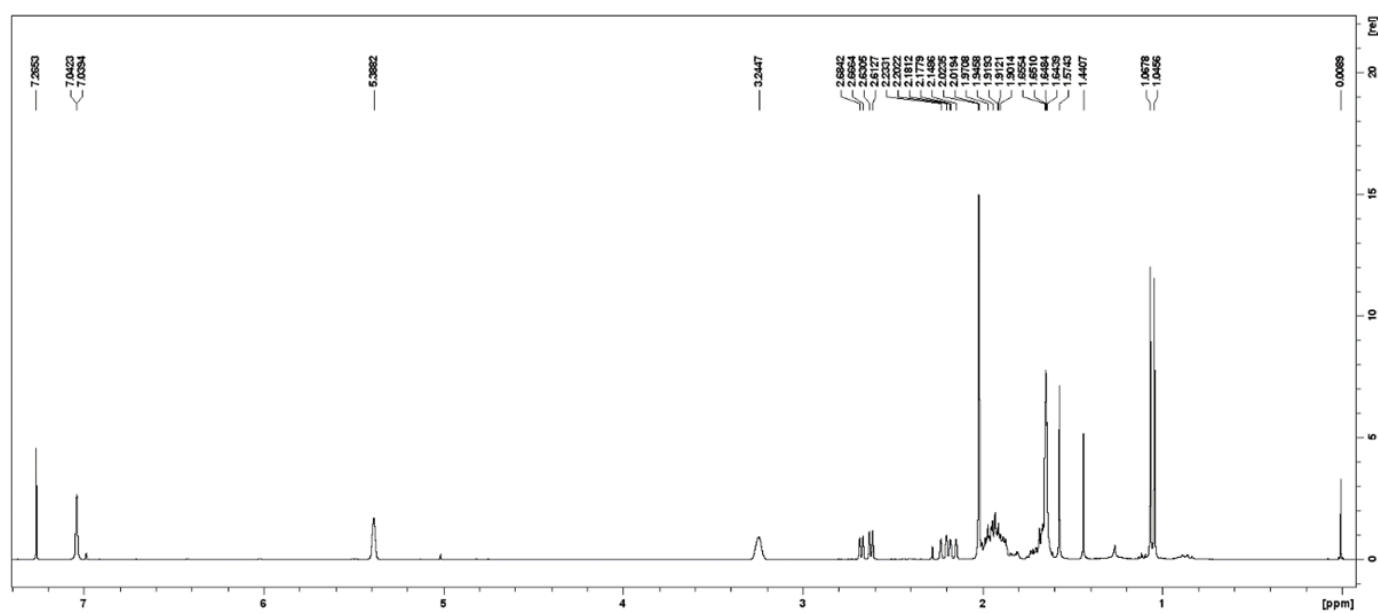


Figure 2S. ¹H NMR of compound **2** (300 MHz, CDCl₃)

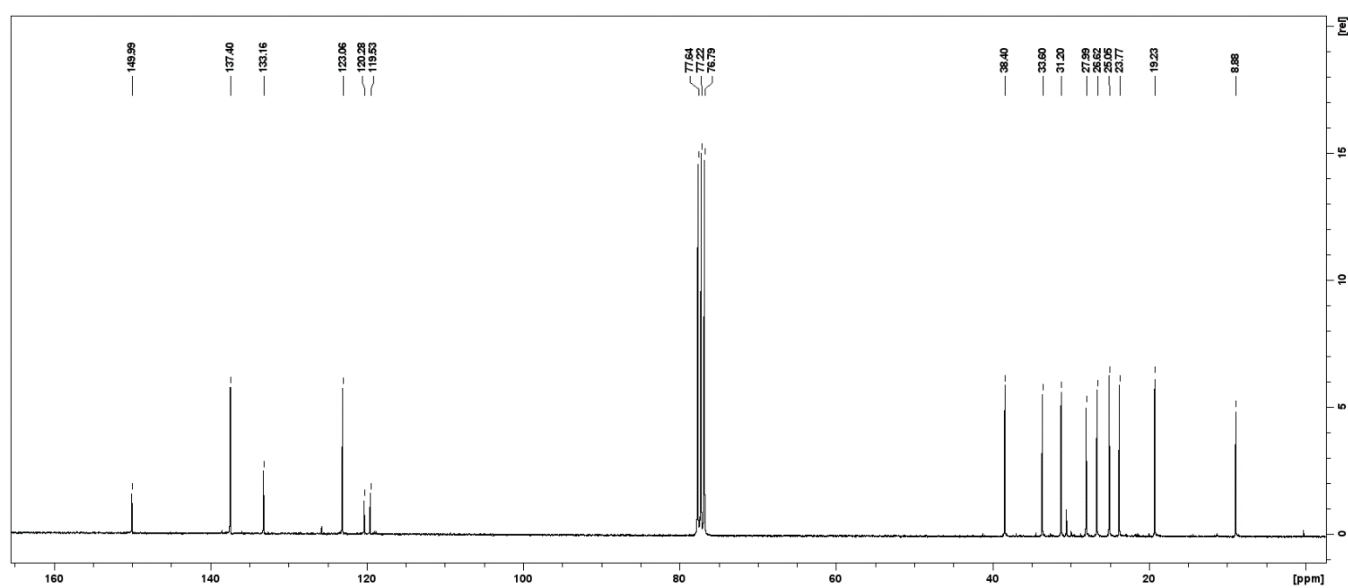


Figure 3S. ¹³C NMR of compound **2** (75 MHz, CDCl₃)

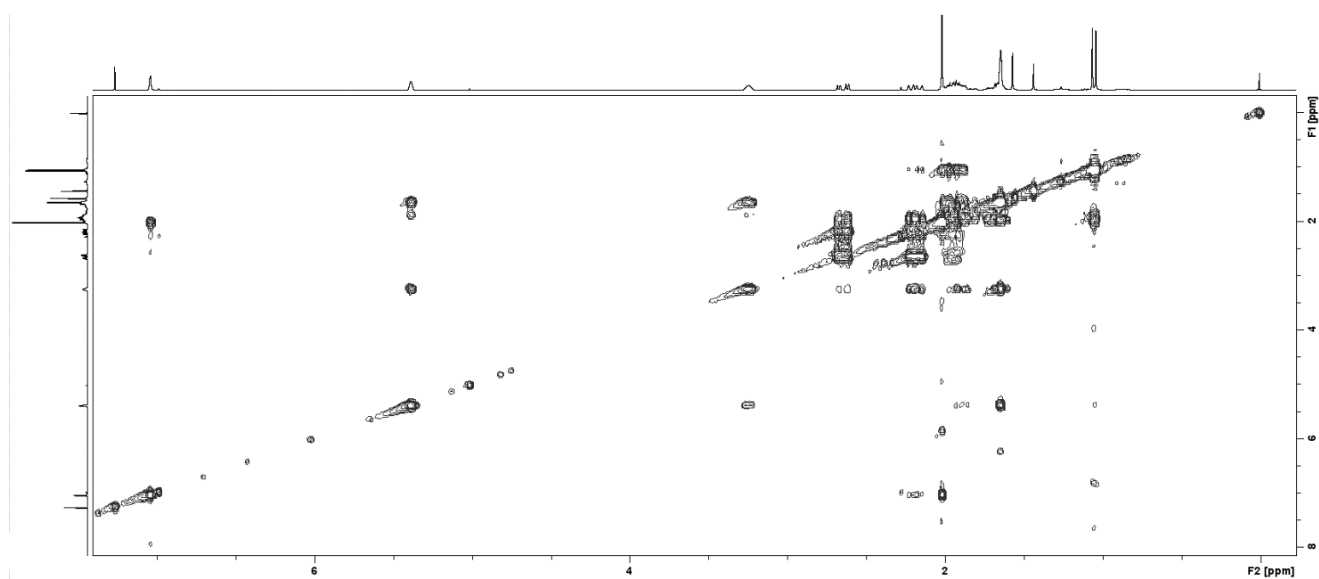


Figure 4S. COSY NMR of compound **2** (300 MHz, CDCl_3)

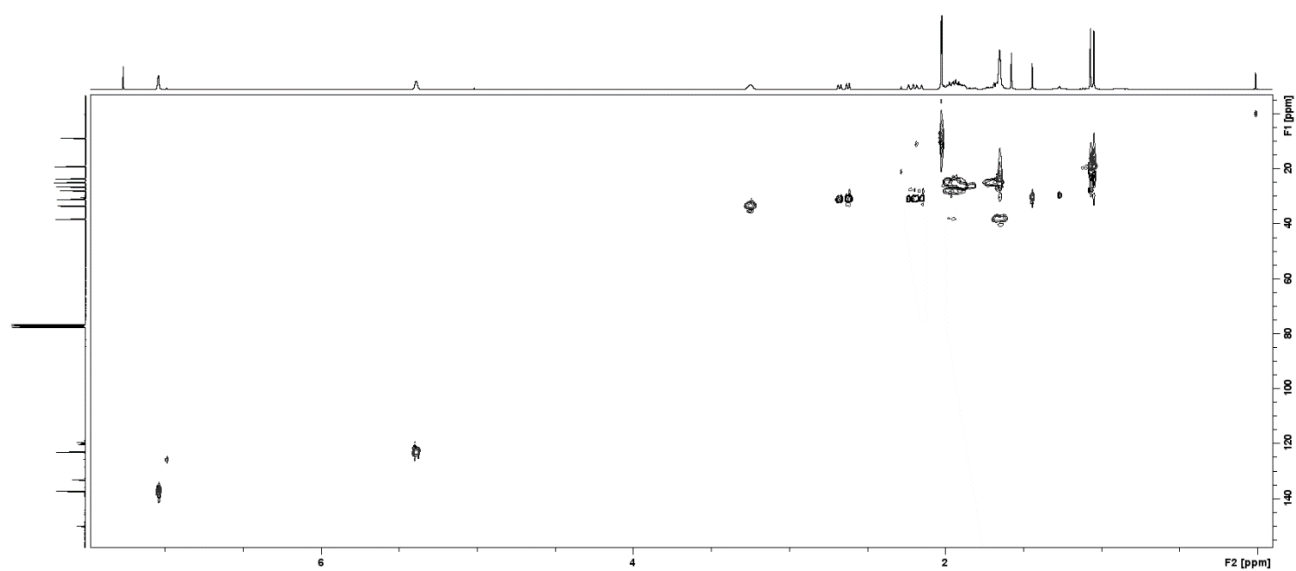


Figure 5S. HSQC NMR of compound **2** (300 MHz, CDCl_3)

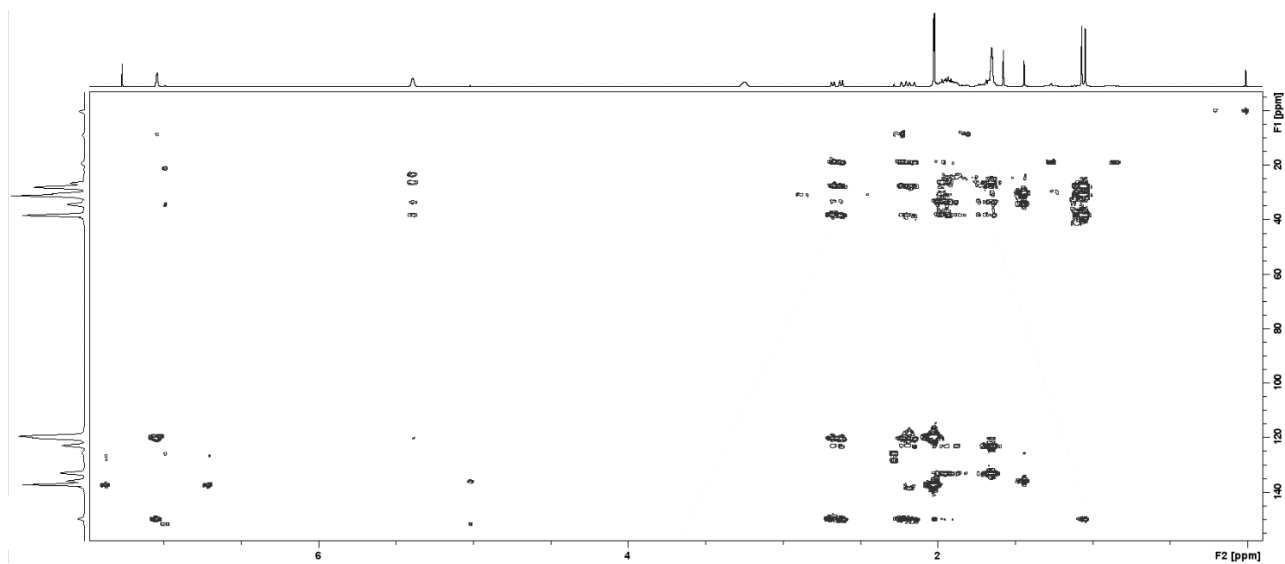


Figure 6S. *HMBC NMR of compound 2 (300 MHz, CDCl₃)*

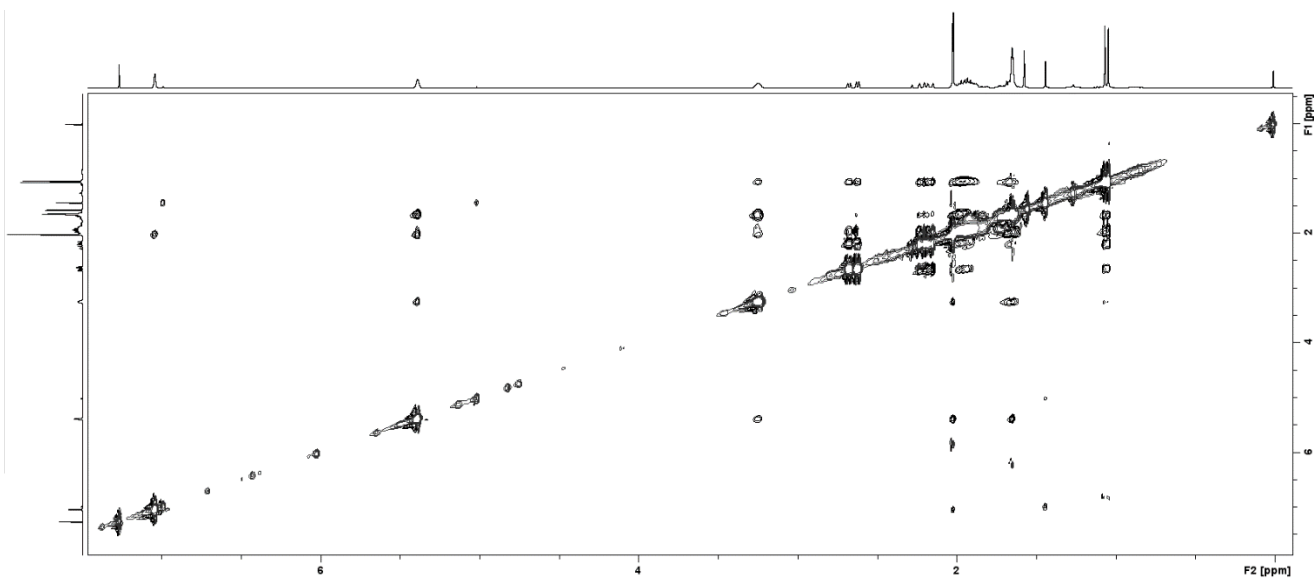


Figure 7S. *NOESY NMR of compound 2 (300 MHz, CDCl₃)*

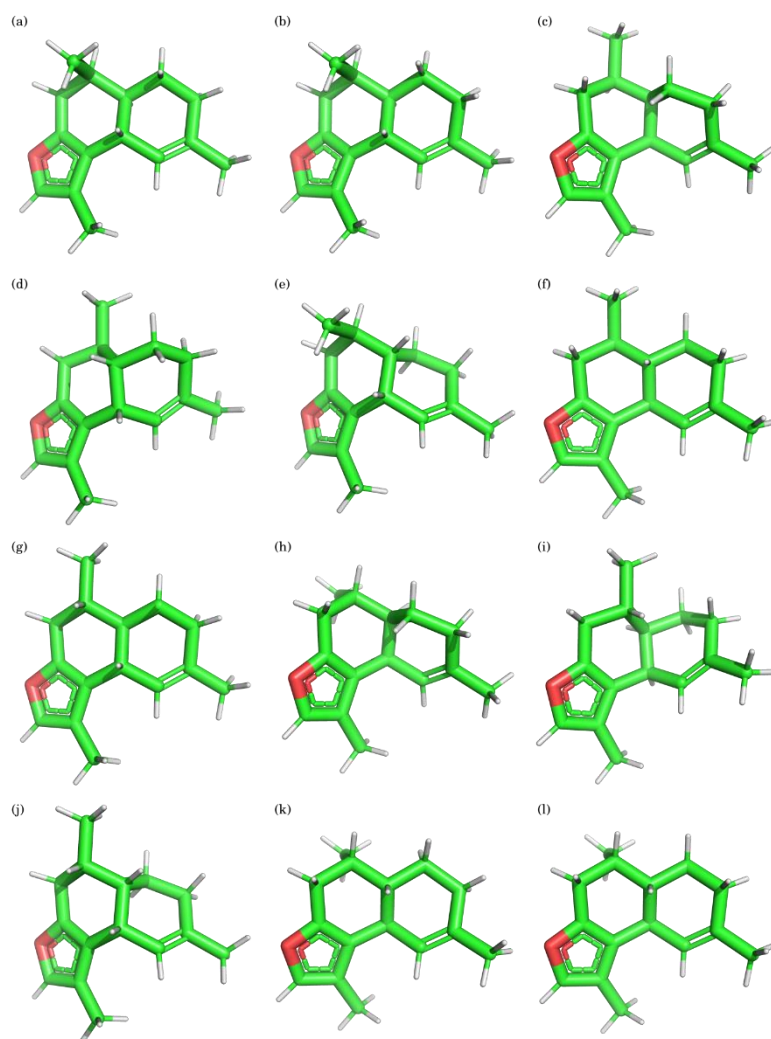


Figure 8S. Conformers with significant population of all isomers. The letter correspondence to the conformers listed in Table 2 is as follows: (a) RRR_i; (b) RRR_ii; (c) RRS_i; (d) RSR_i; (e) RSR_ii; (f) RSS_i; (g) SRR_i; (h) SRS_i; (i) SRS_ii; (j) SSR_i; (k) SSS_i; (l) SSS_ii

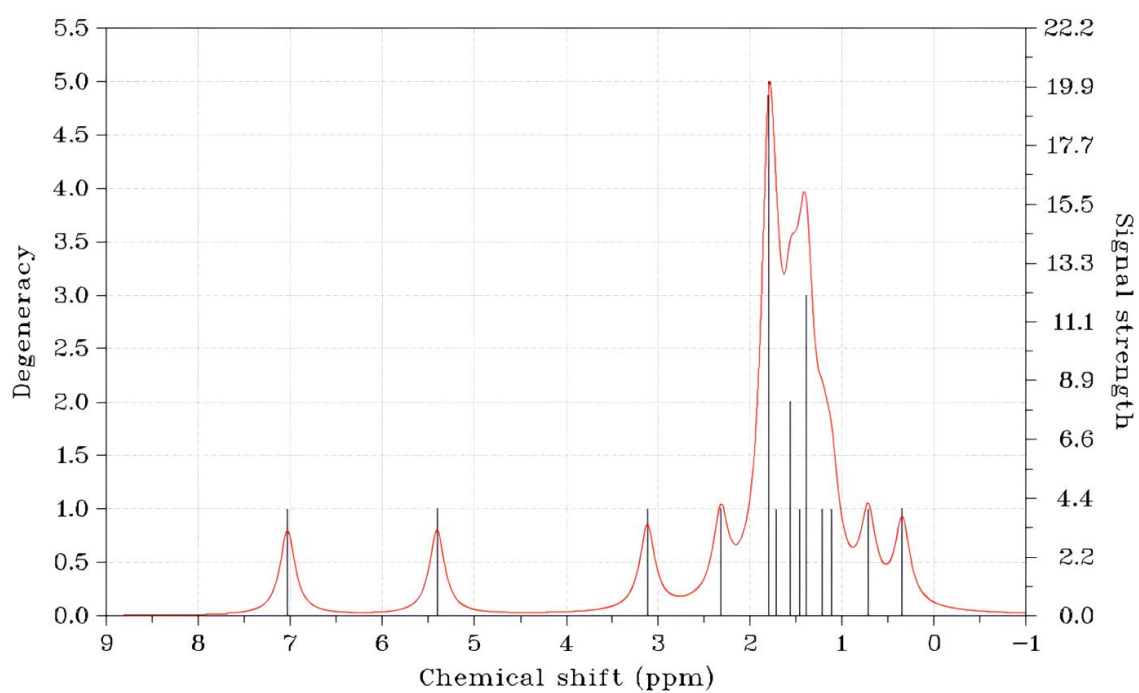


Figure 9S. Calculated ^1H NMR spectrum of compound 2