

The Impact of a Quinone Scaffold on Thermo-TRPs Modulation by Dimethylheptyl Phytocannabinoids

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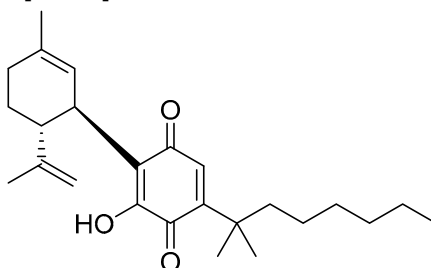
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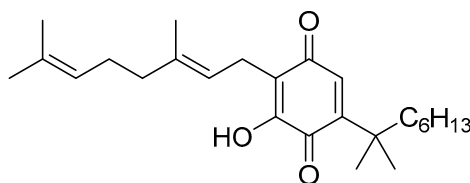
† These authors contributed equally to this work.

Supplementary Information

***para*-3'-Depentyl-3'-(α,α -dimethylheptyl)cannabidiol quinone (*p*-DMHCBQ, **5b**):** dark red solid, 56% yield, R_f= 0.61 in petroleum ether-EtOAc 95:5. IR ν_{max} (KBr disc): 2970, 2918, 2852, 1674, 1136, 1127, 1107, 798 cm⁻¹. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.20 (s, 1H), 6.40 (s, 1H), 5.18 (s, 1H), 4.71–4.50 (m, 2H), 3.74 (dd, *J* = 10.8, 2.1 Hz, 1H), 2.77 (ddd, *J* = 12.1, 10.7, 2.9 Hz, 1H), 2.31–2.19 (m, 1H), 2.02 (dd, *J* = 17.5, 5.3 Hz, 1H), 1.85–1.63 (m, 7H), 1.59 (s, 3H), 1.45–1.17 (m, 12H), 1.08–0.97 (m, 2H), 0.88 (t, *J* = 6.9 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 187.25, 183.49, 151.73, 150.07, 148.43, 135.37, 133.94, 129.50, 122.40, 121.73, 110.62, 44.63, 40.61, 38.17, 35.69, 31.67, 30.46, 29.74, 28.78, 27.27, 27.24, 24.99, 23.45, 22.57, 18.70, 14.05. HR ESI-MS *m/z* 385.5672 [M + H]⁺, calcd for C₂₅H₃₇O₃, 385.5680.



***para*-3'-Depentyl-3'-(α,α -dimethylheptyl)cannabigerol quinone (*p*-DMHCBGQ, **7b**):** dark red solid, 52% yield, R_f= 0.78 in petroleum ether-EtOAc 9:1. IR ν_{max} (KBr disc): 3257, 2948, 2870, 1642, 1633, 1361, 1317, 1176, 1169, 584 cm⁻¹. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.22 (bs, OH, 1H), 6.46 (s, 1H), 5.16 (t, *J* = 7.4 Hz, 1H), 5.05 (t, *J* = 7.2 Hz, 1H), 3.14 (d, *J* = 7.4 Hz, 2H), 2.09–1.93 (m, 4H), 1.78–1.68 (m, 2H), 1.75 (s, 3H), 1.65 (s, 3H), 1.58 (s, 3H), 1.30–1.17 (m, 12H), 1.09–0.99 (m, 2H), 0.86 (t, *J* = 6.8 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 187.60, 183.58, 151.36, 150.52, 137.06, 134.97, 131.34, 124.20, 120.26, 119.58, 119.04, 40.65, 39.70, 38.26, 31.66, 29.79, 27.34, 26.57, 25.67, 25.02, 22.61, 21.79, 17.65, 16.16, 14.03. HR ESI-MS *m/z* 387.2895 [M + H]⁺, calcd for C₂₅H₃₉O₃, 387.2899.



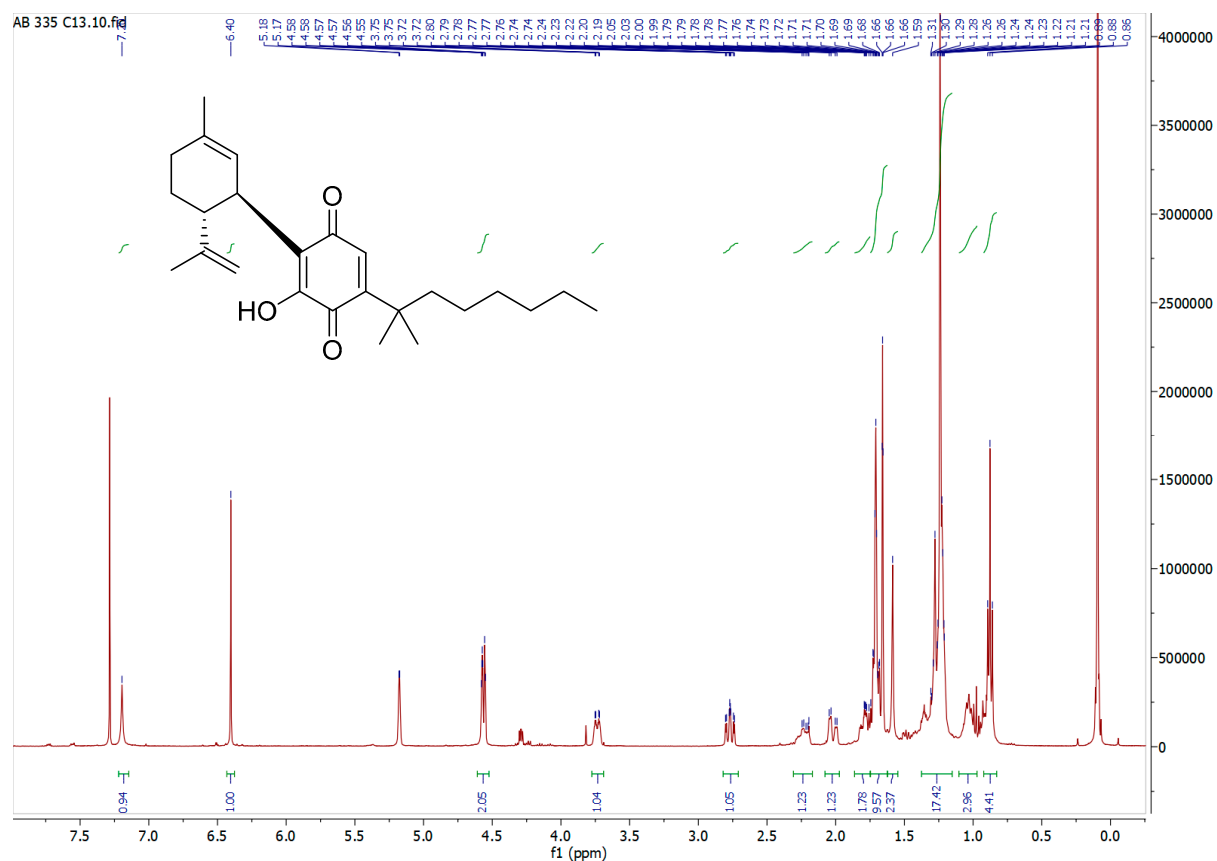


Figure S1. ¹H NMR spectrum (400 MHz) of compound **5b** in CDCl₃.

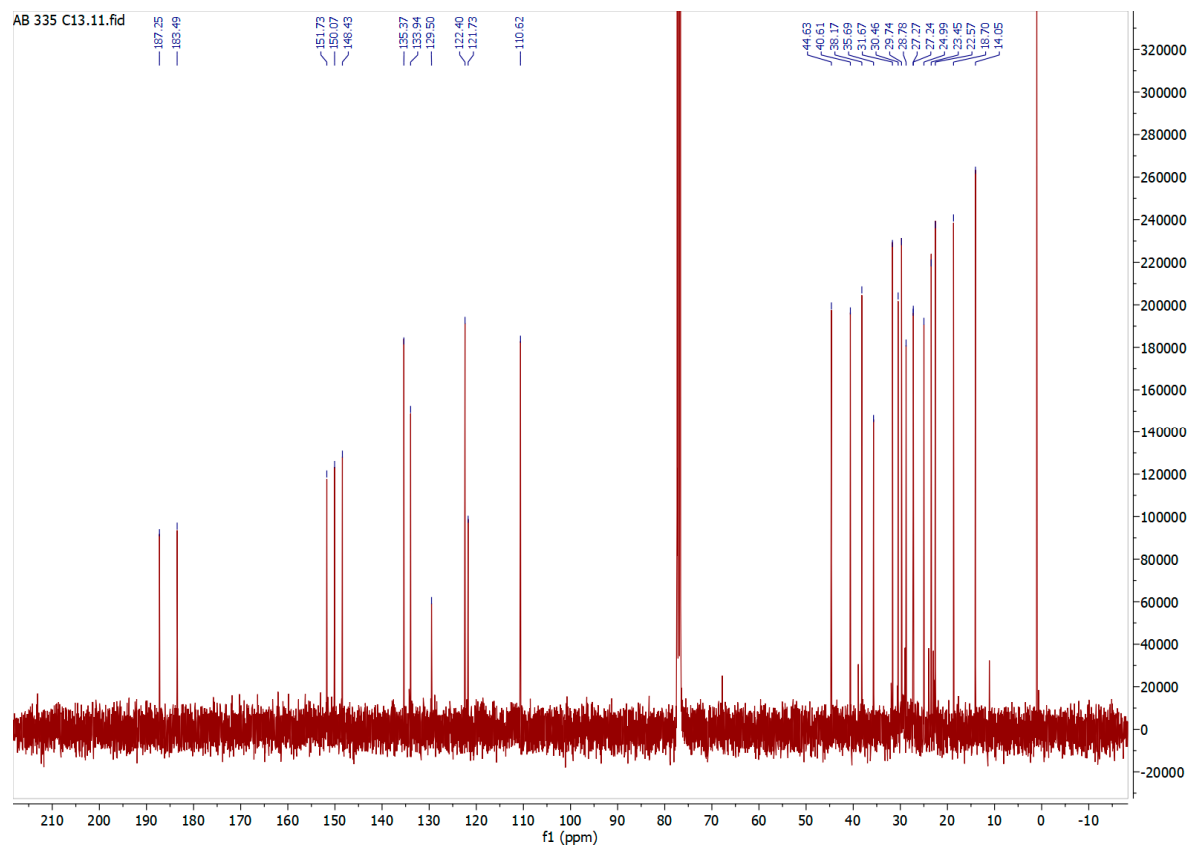


Figure S2. ¹³C NMR spectrum (100 MHz) of compound **5b** in CDCl₃.

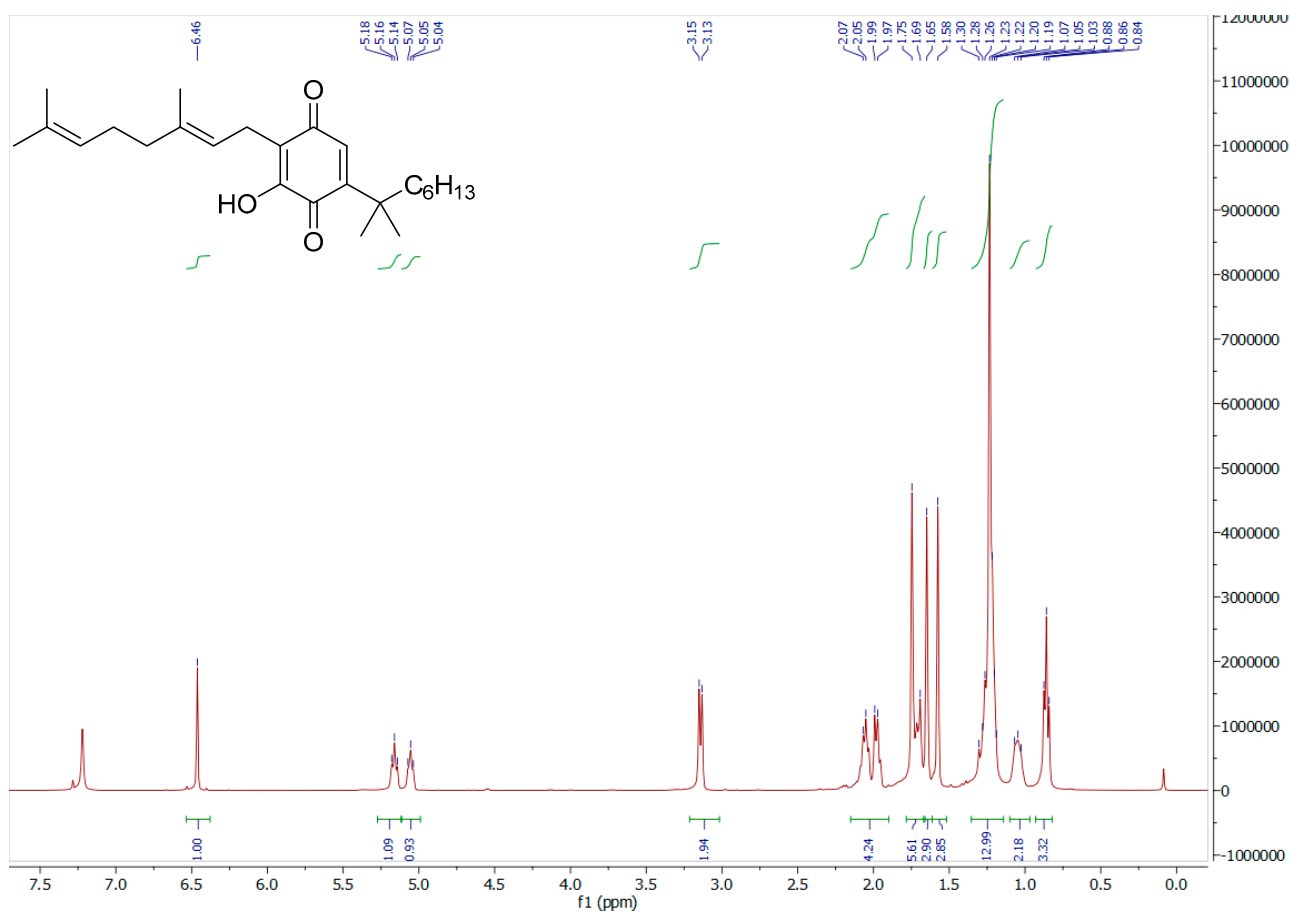


Figure S3. 1H NMR spectrum (400 MHz) of compound **7b** in $CDCl_3$.

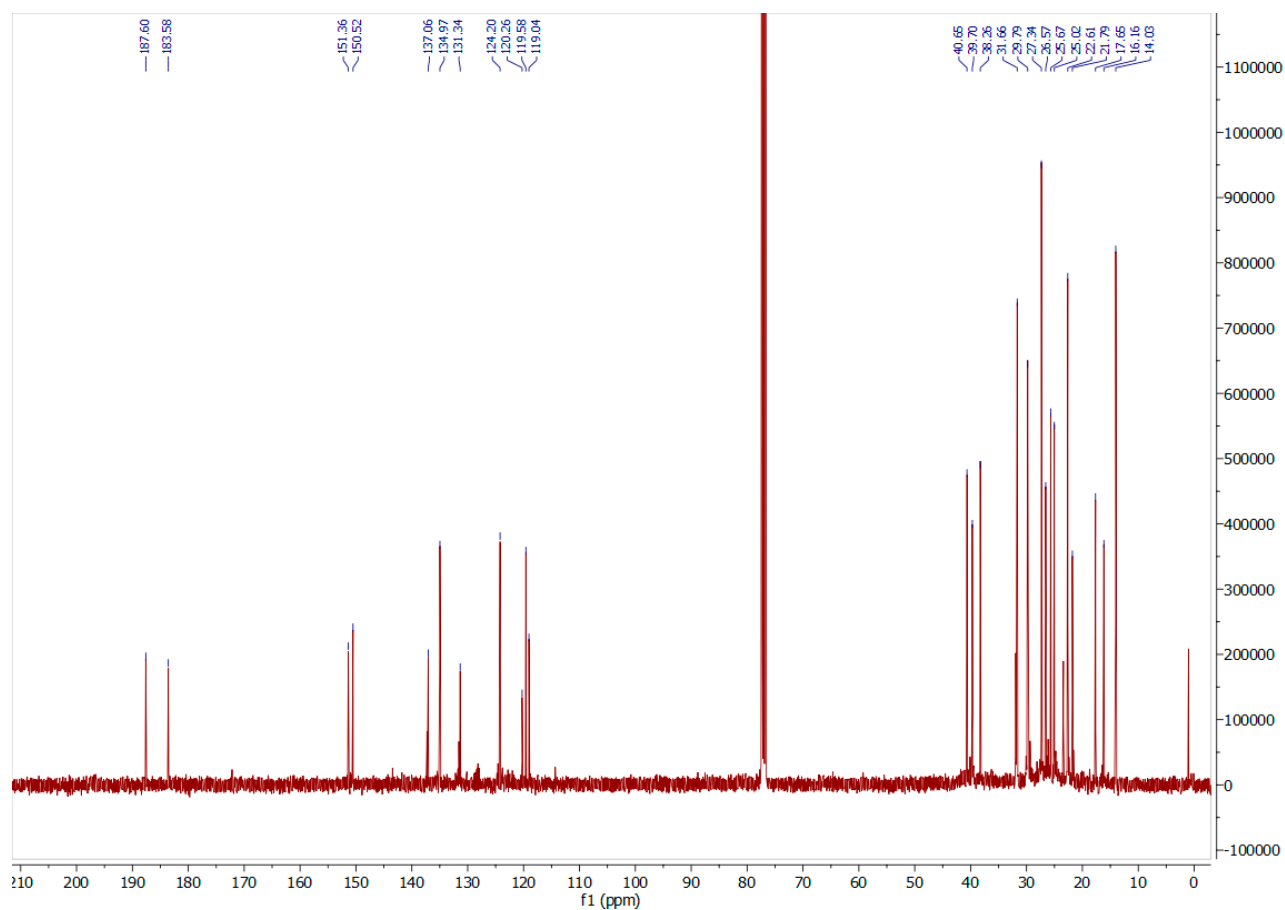


Figure S4. ^{13}C NMR spectrum (100 MHz) of compound **7b** in $CDCl_3$.