

Highly efficient synthesis and characterization of the GPR30 selective agonist G-1 and related tetrahydroquinoline analogs.

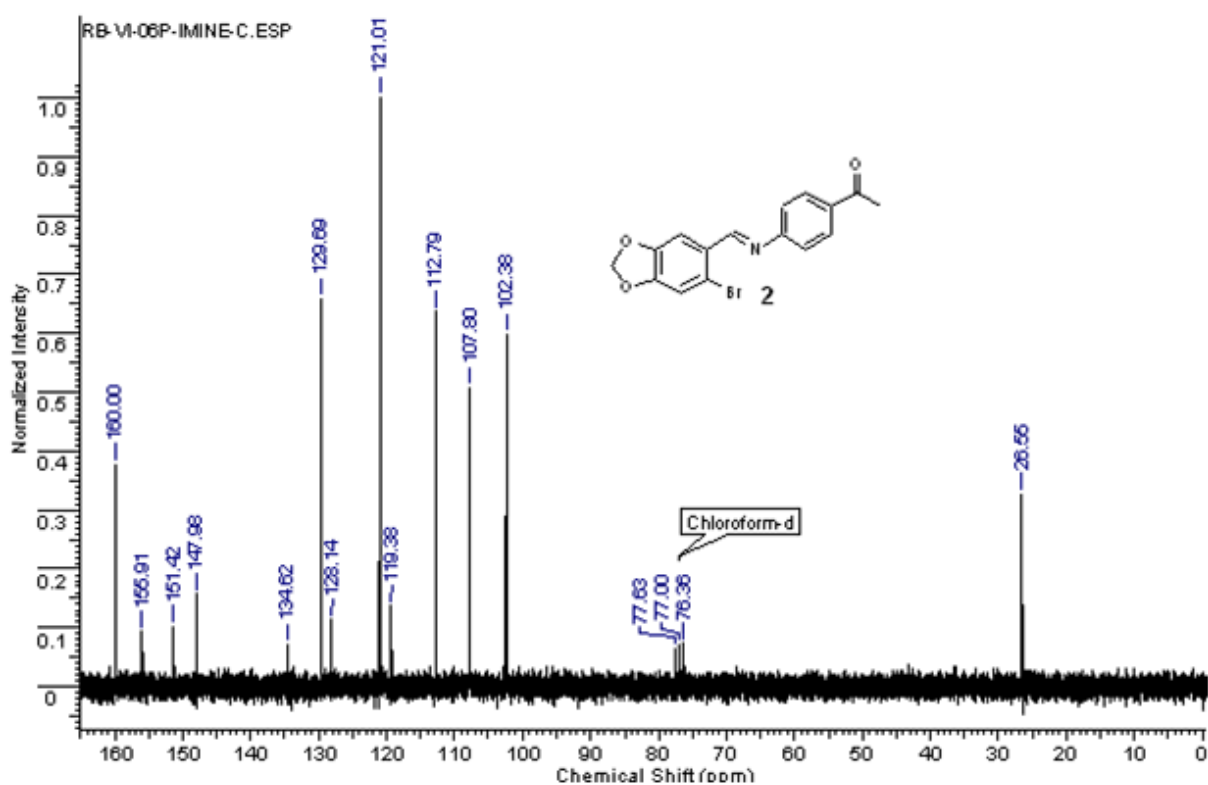
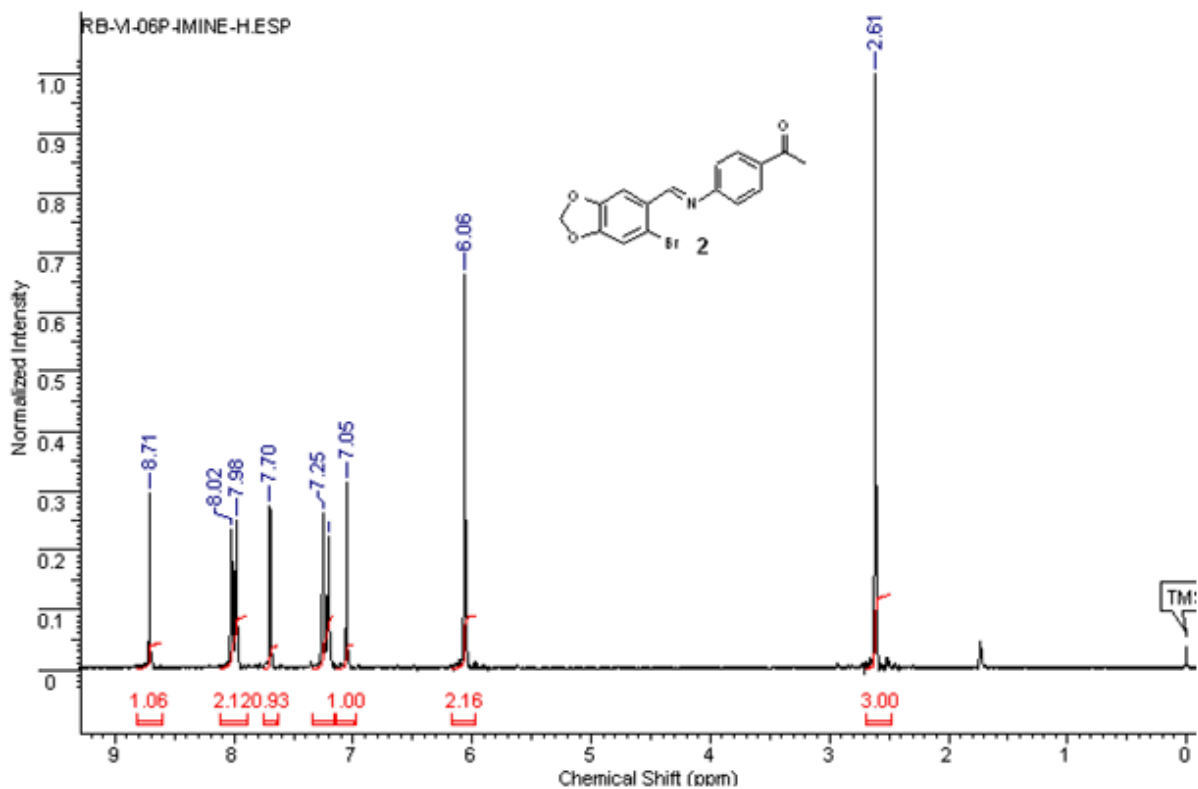
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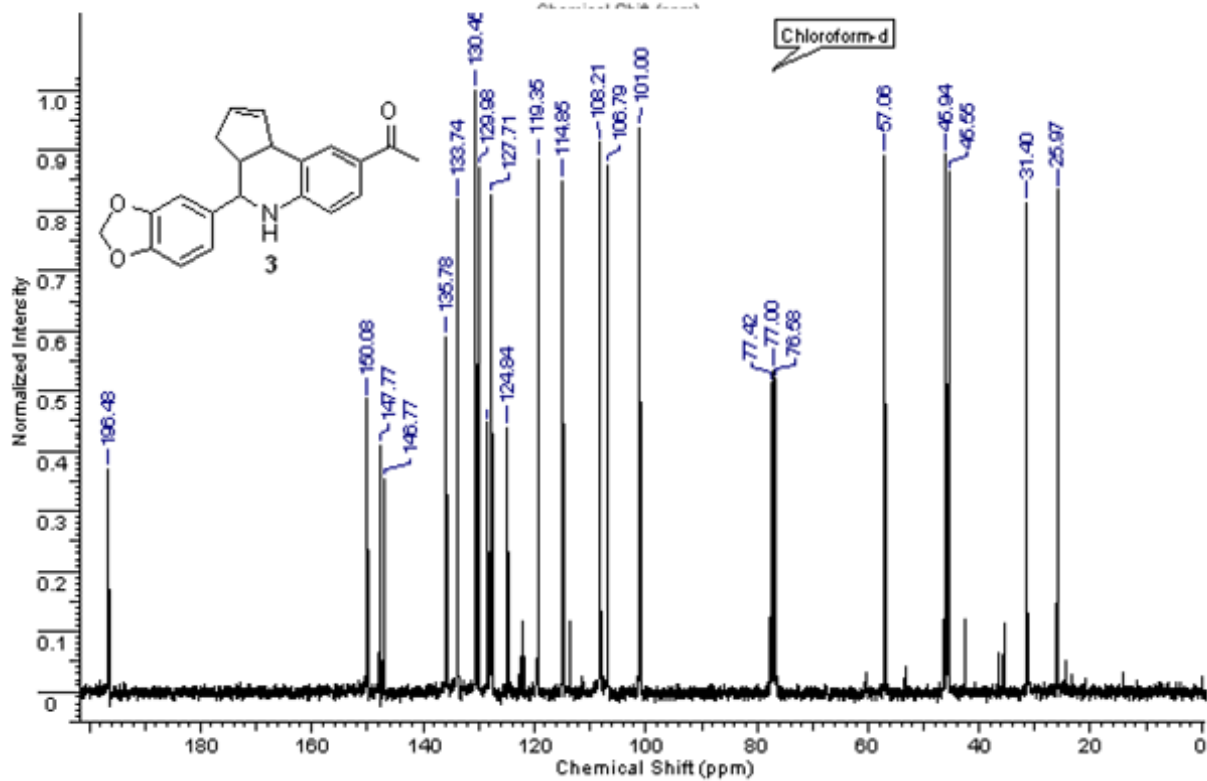
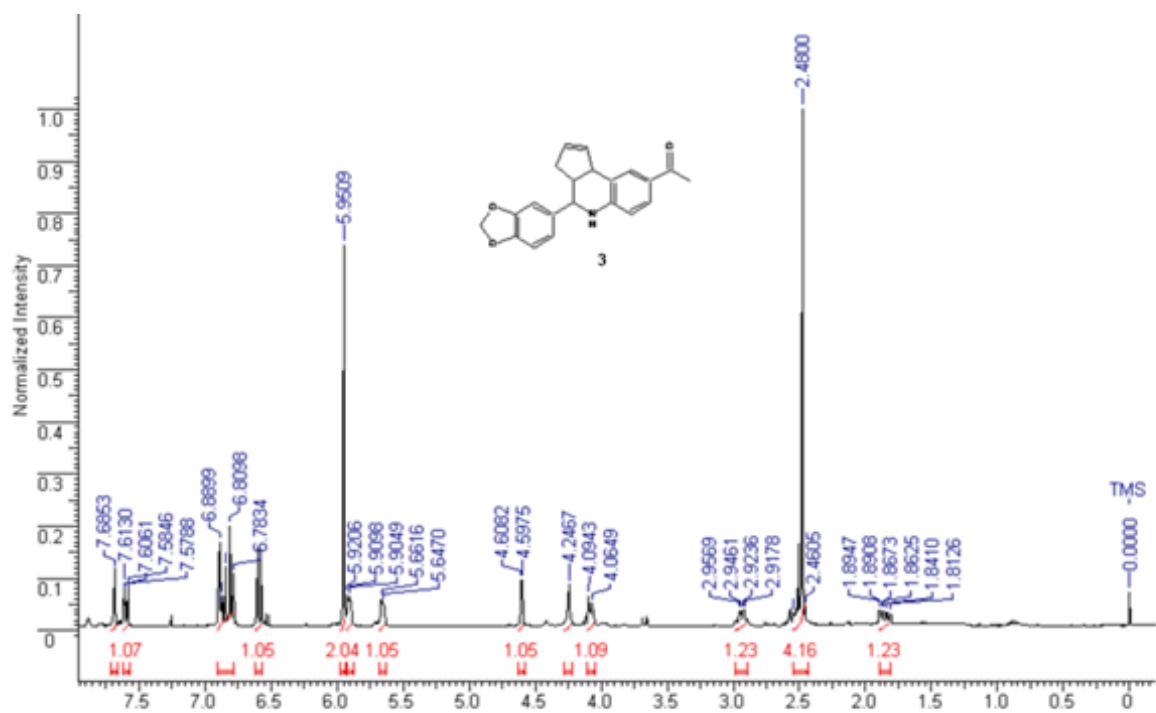
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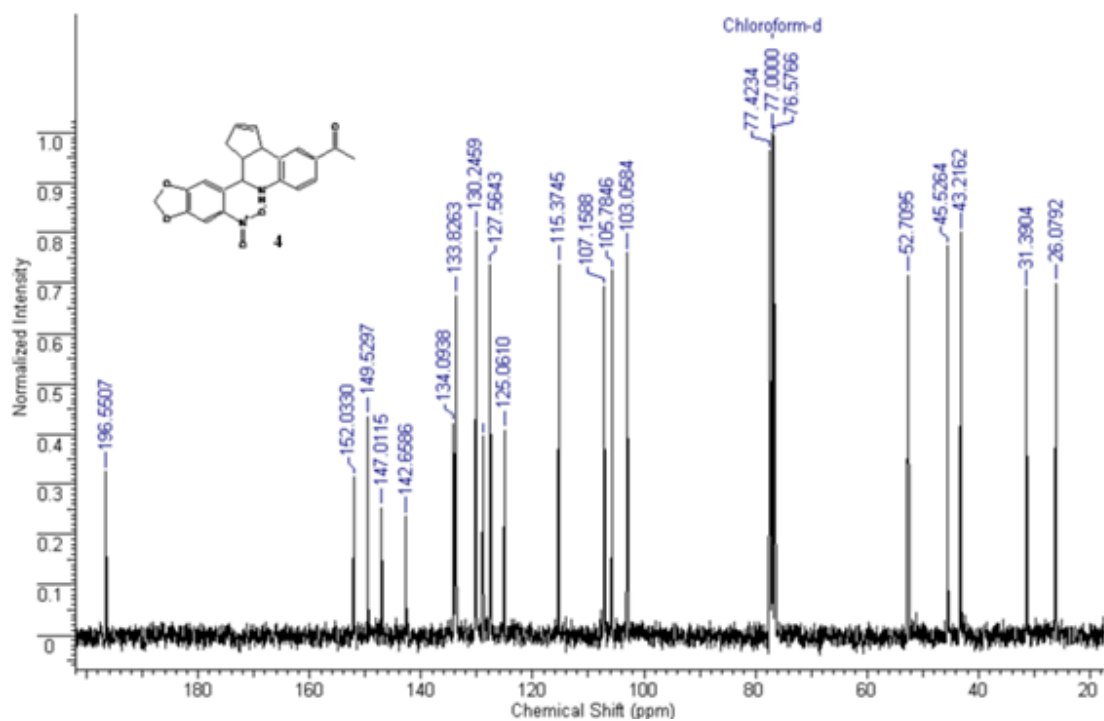
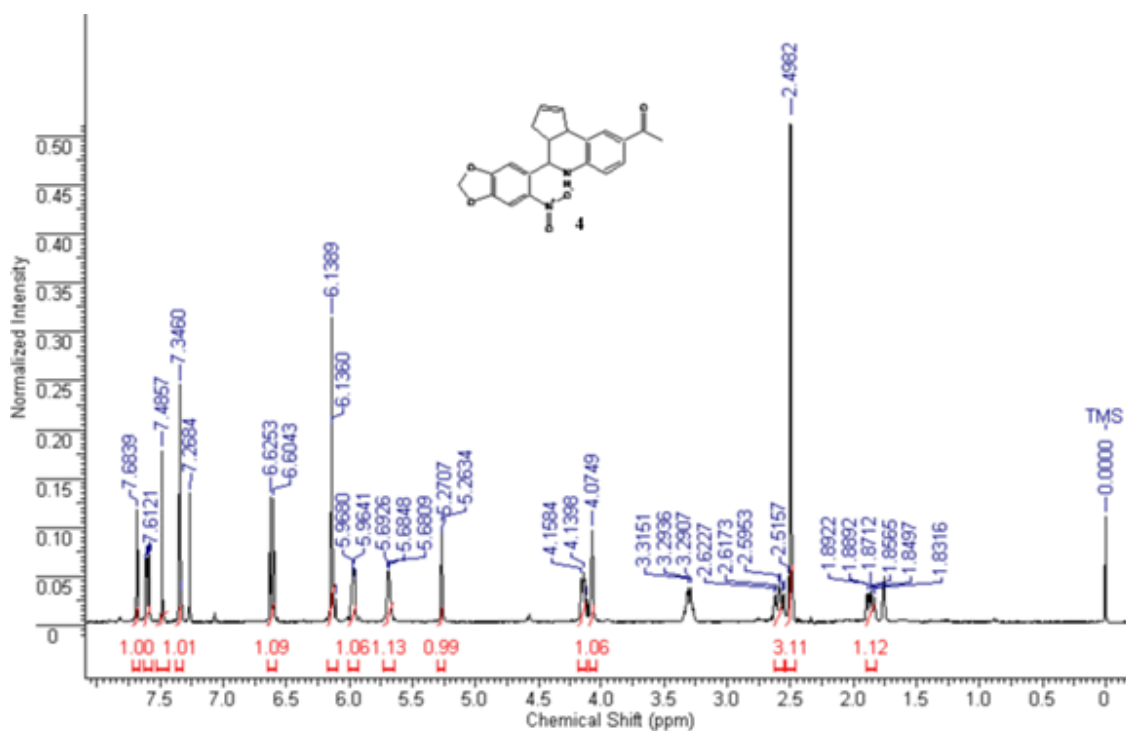
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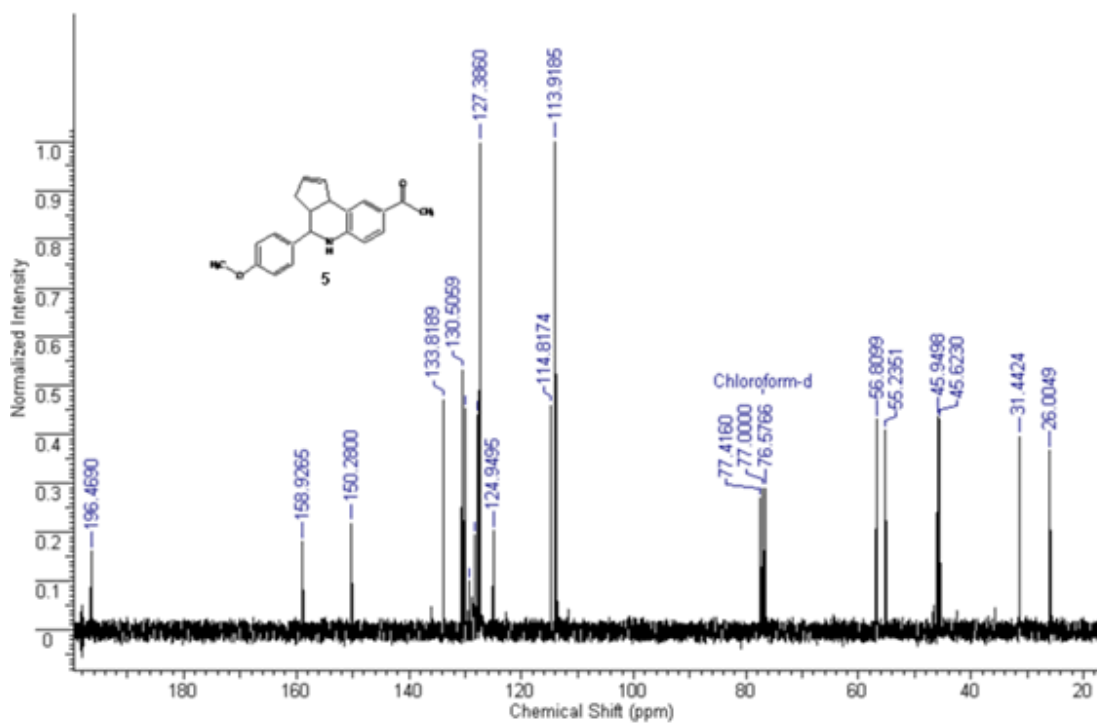
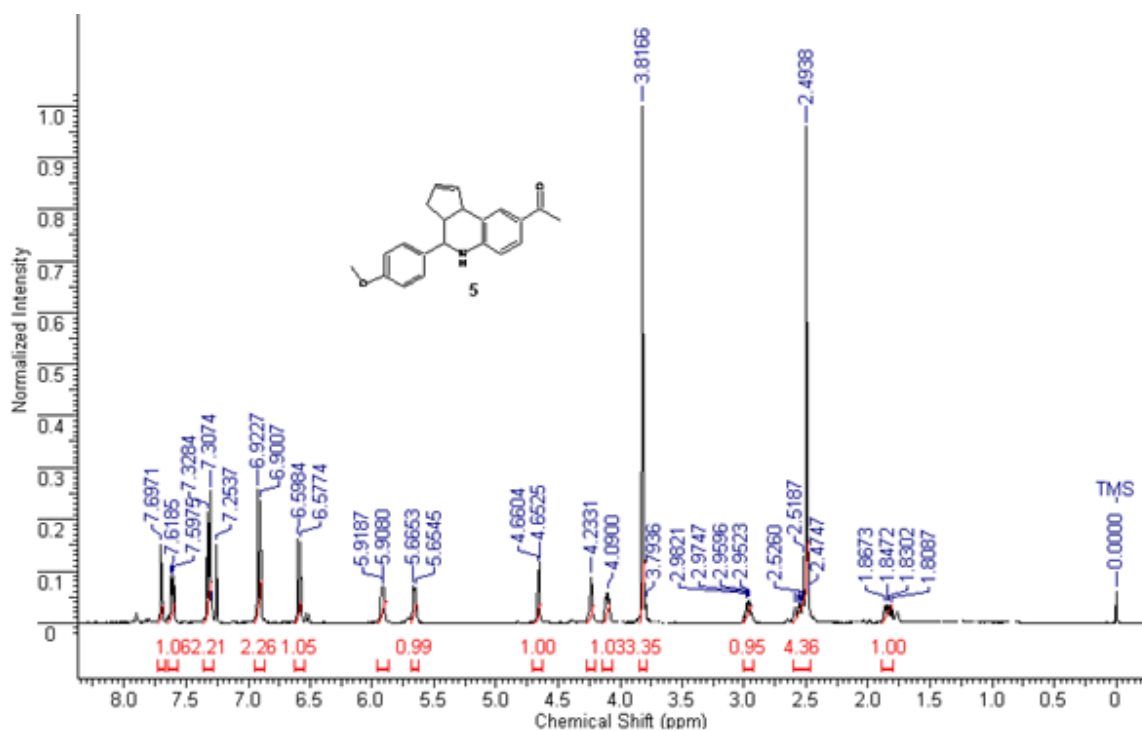
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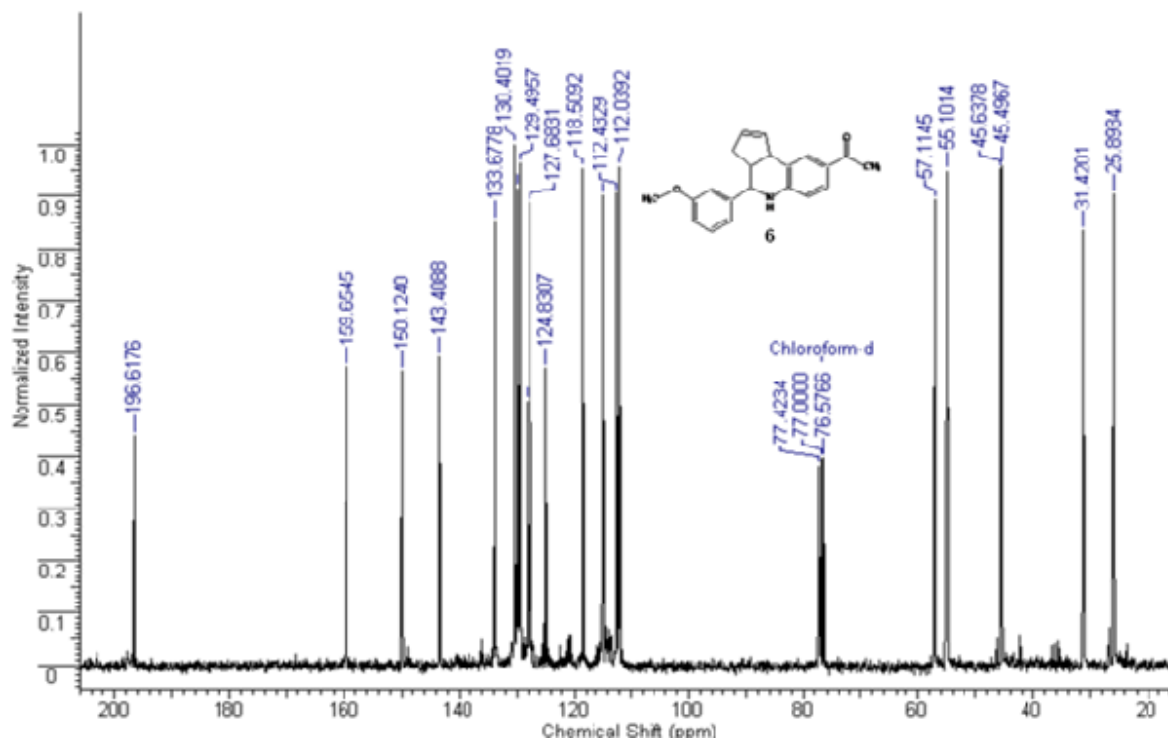
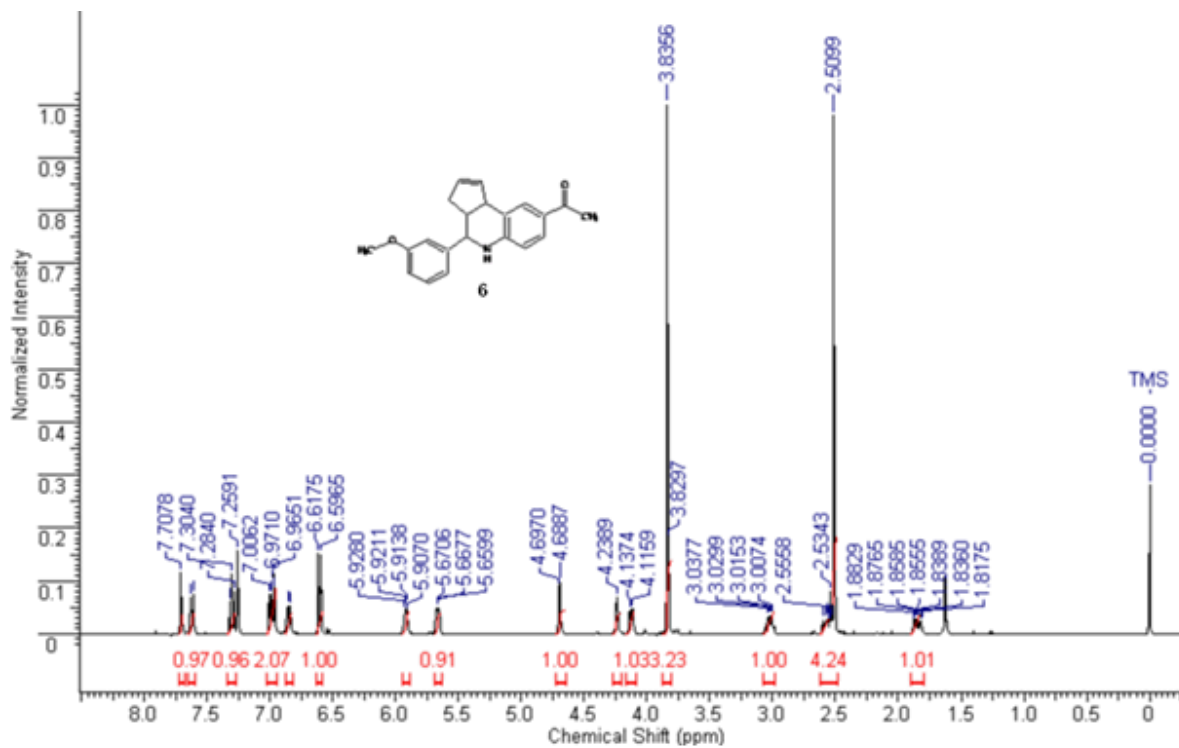
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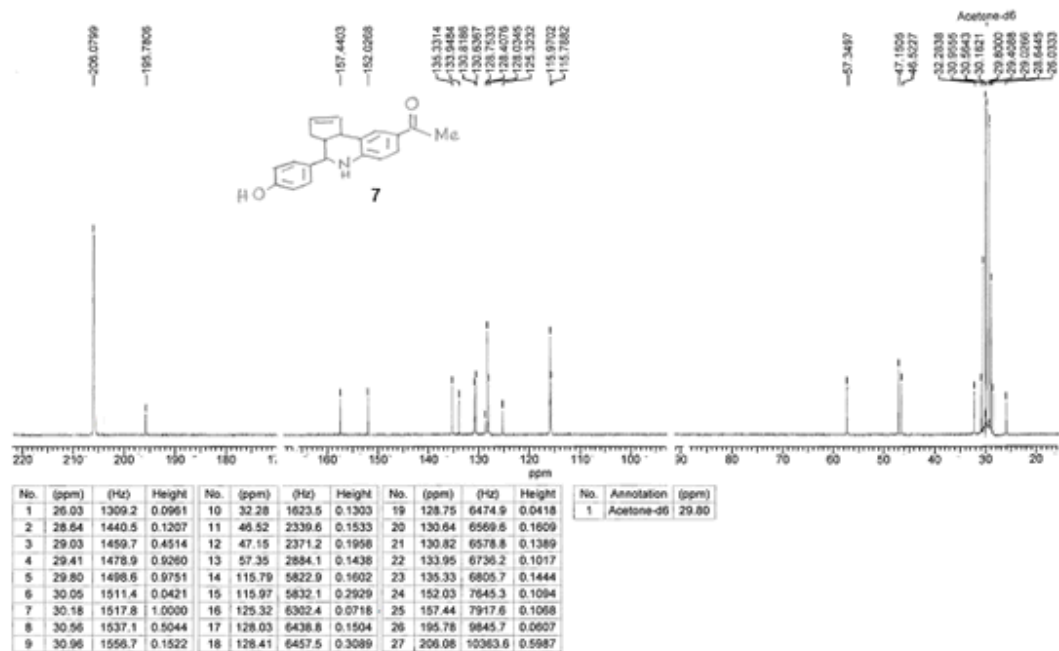
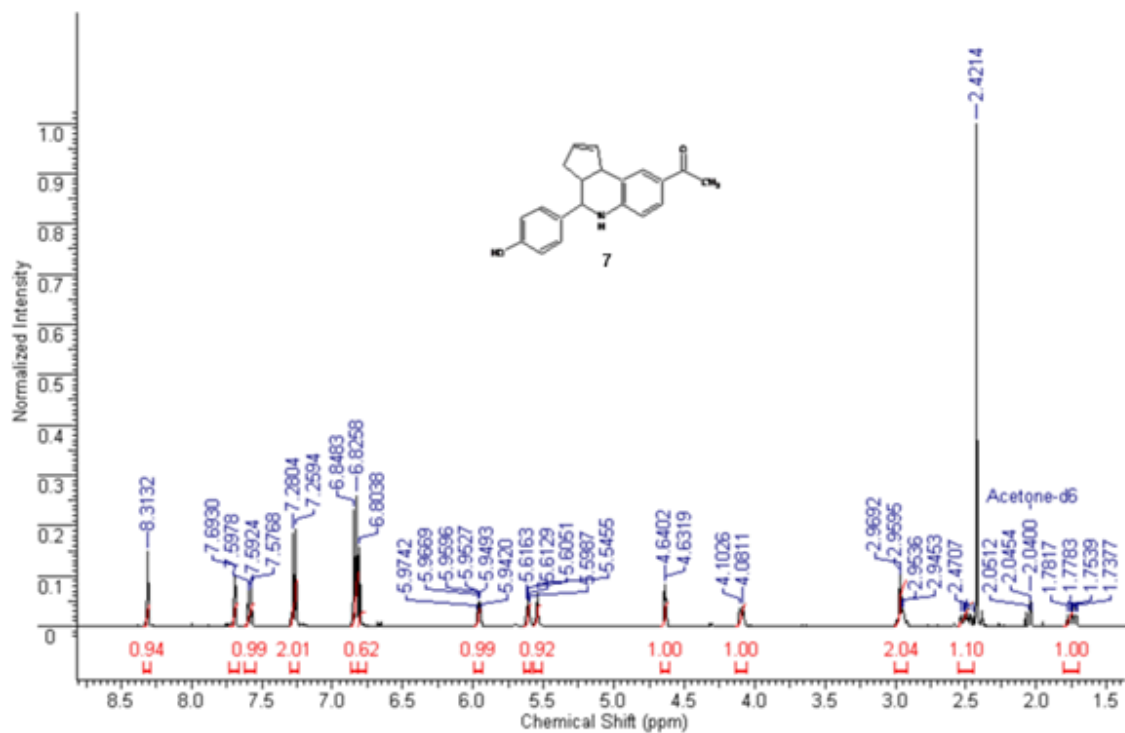


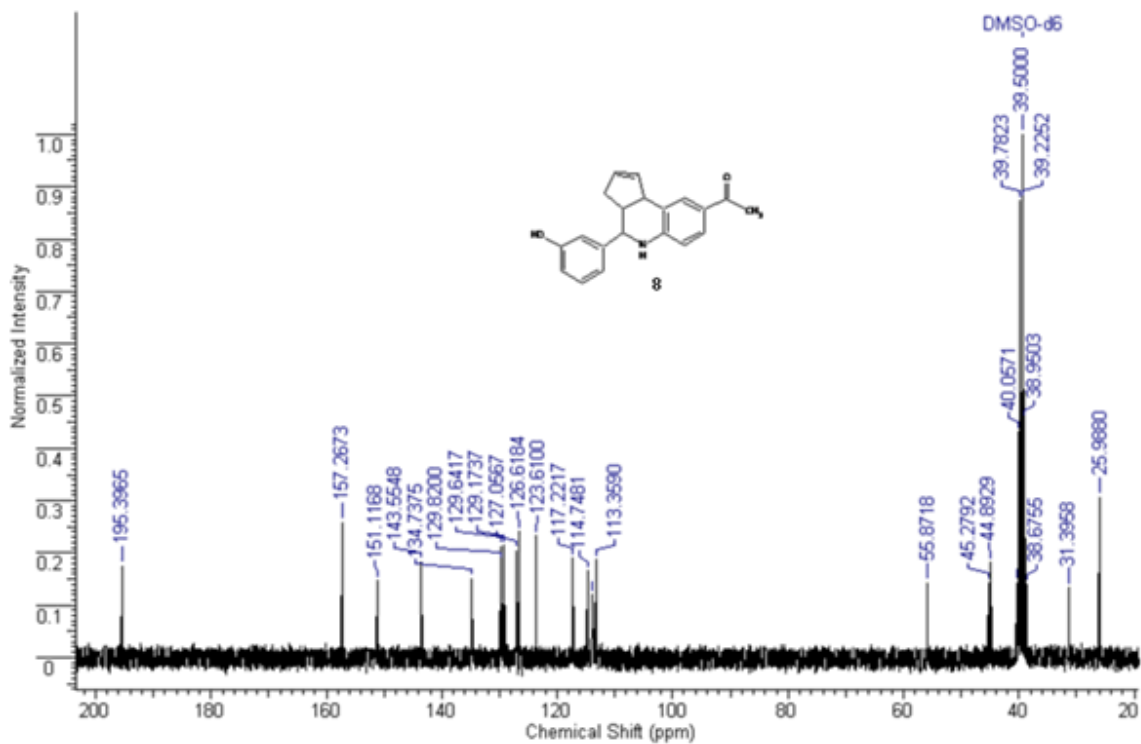
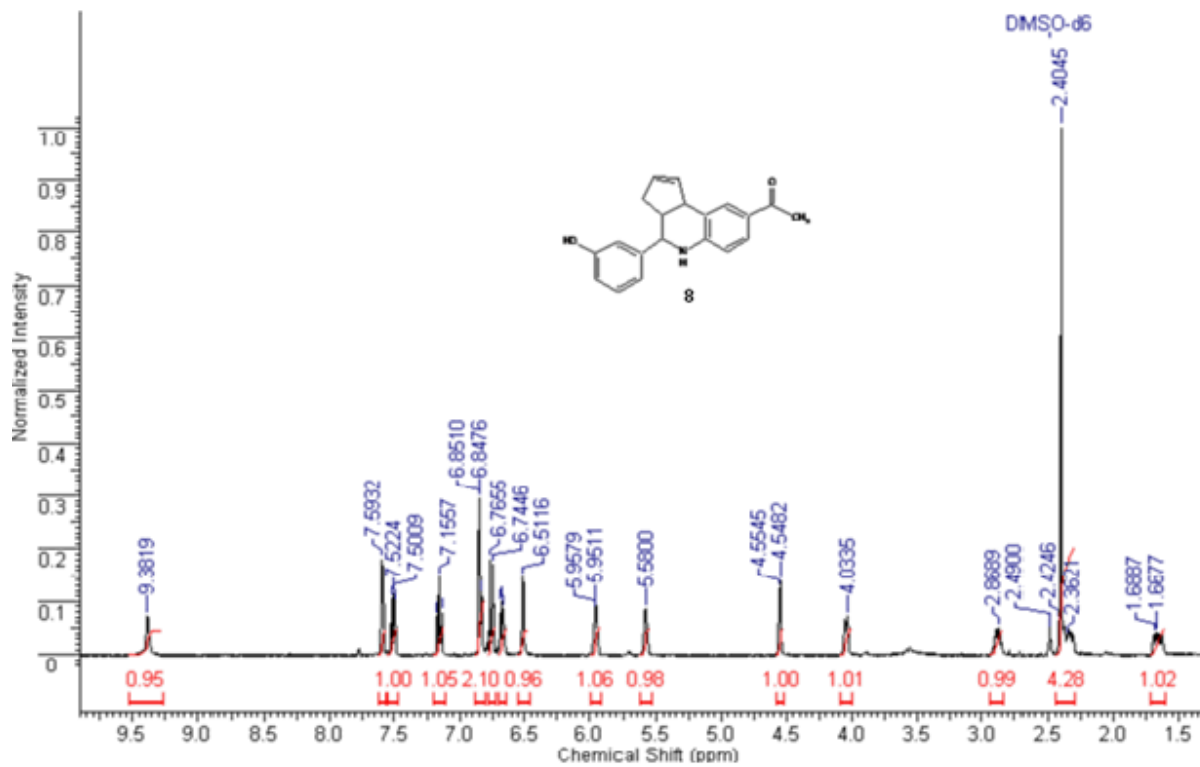


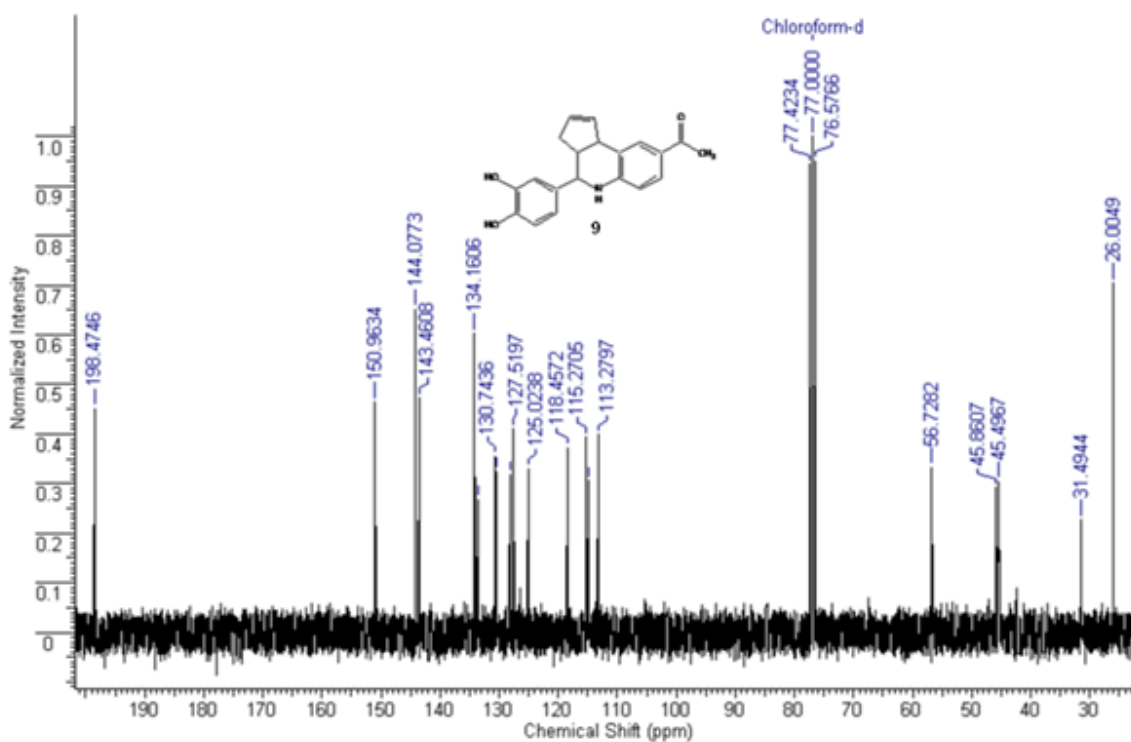
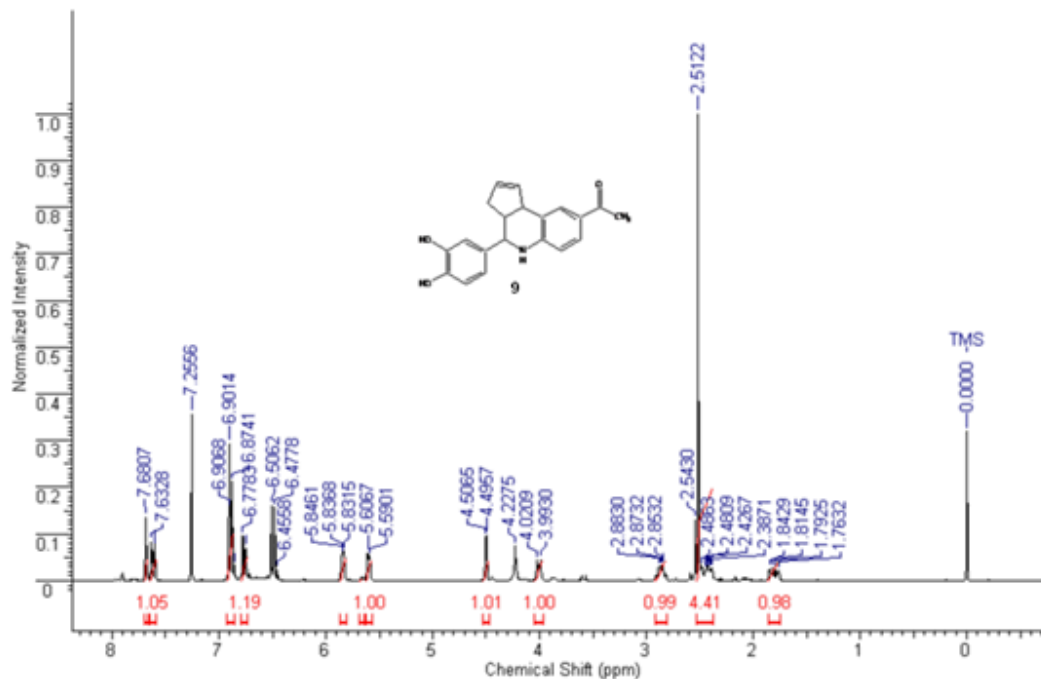


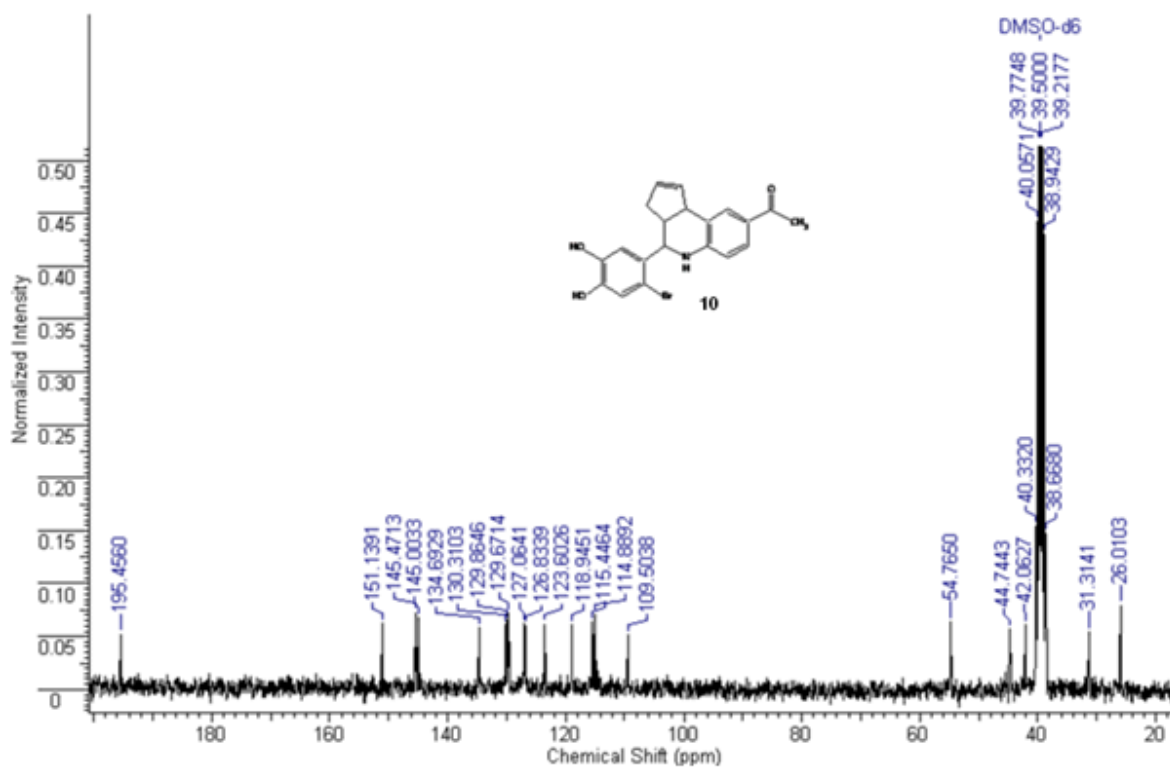
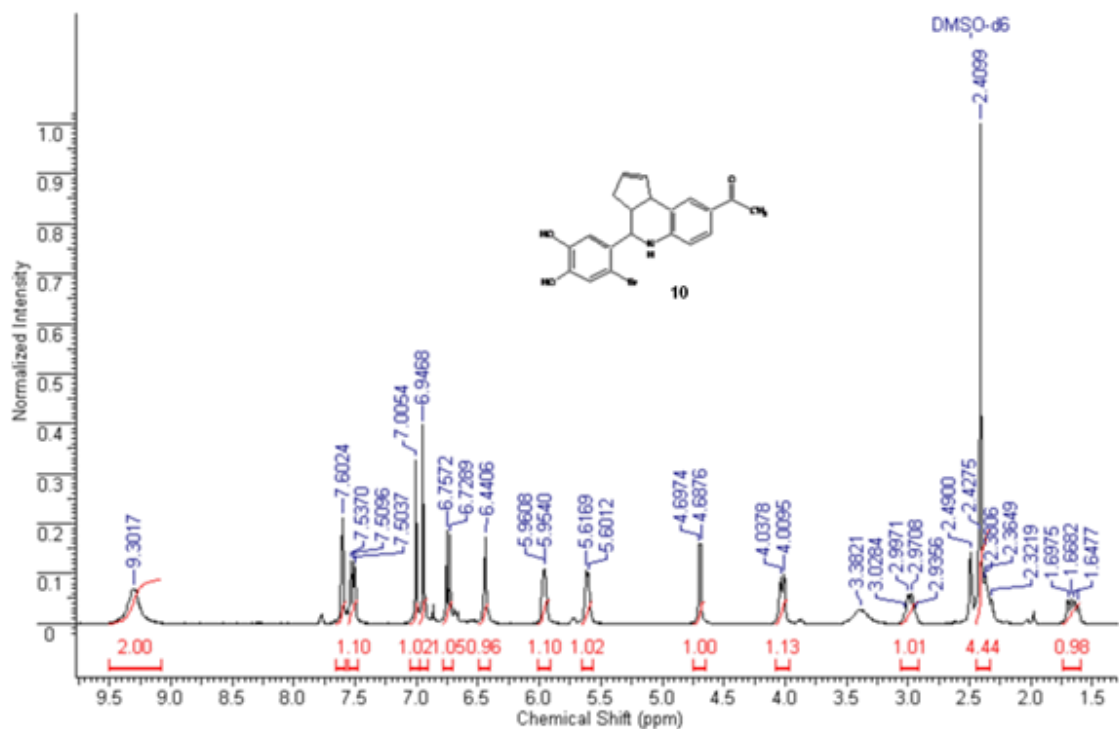


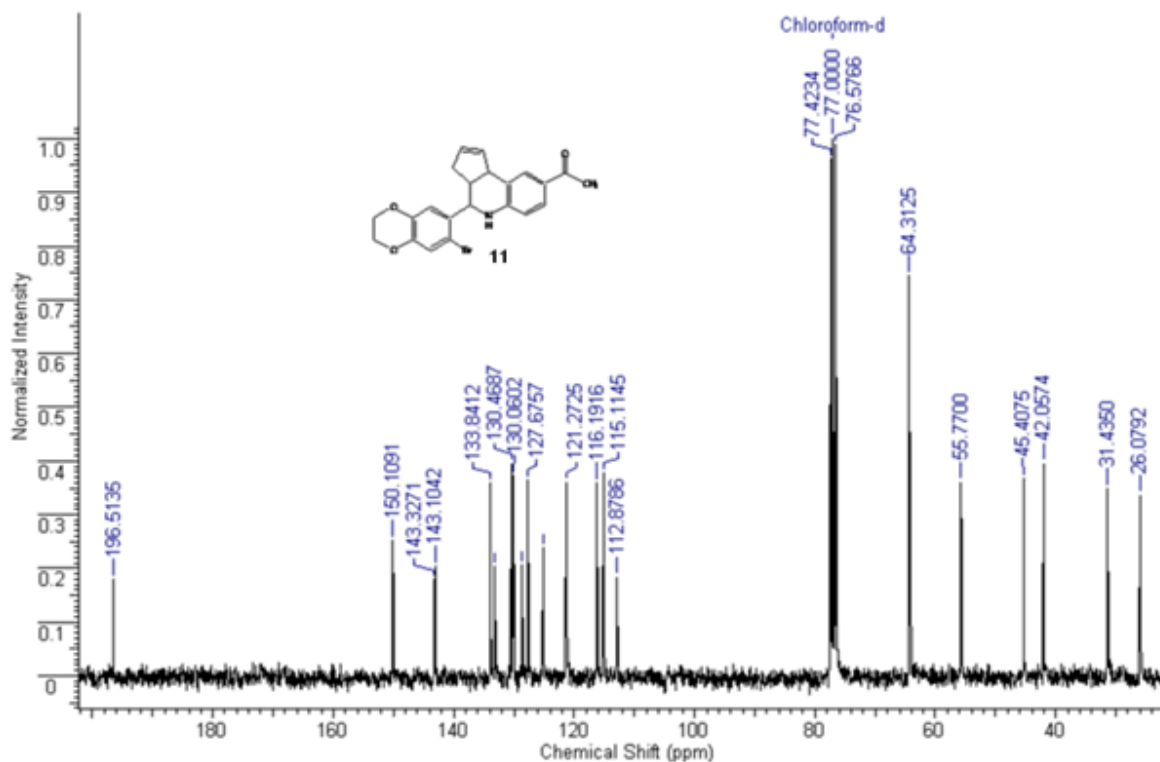
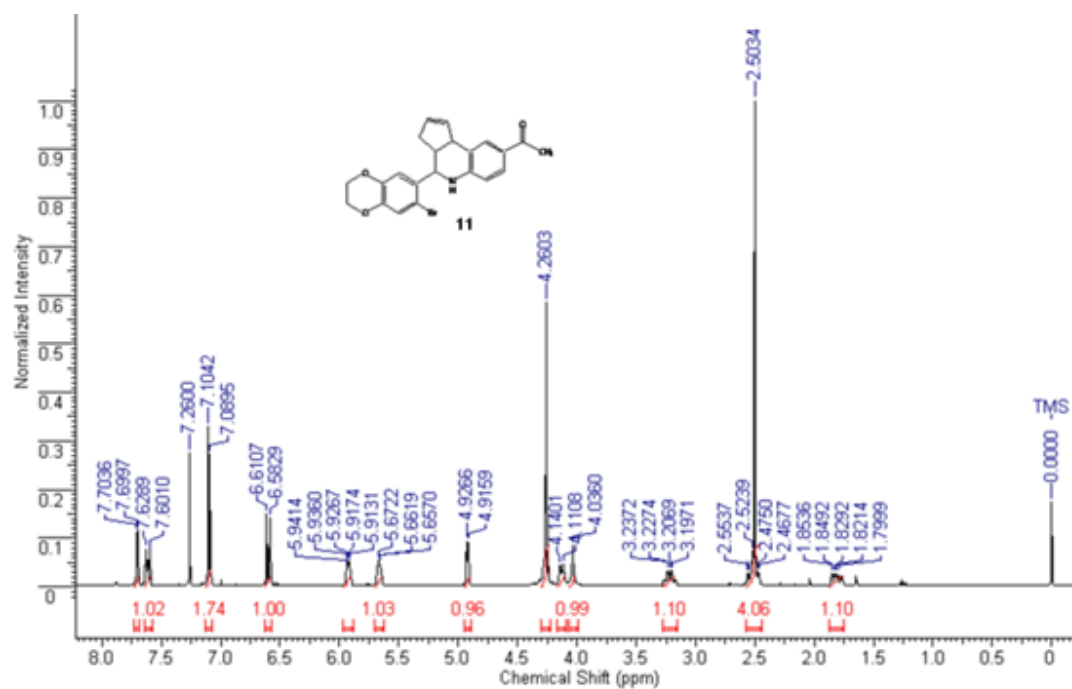


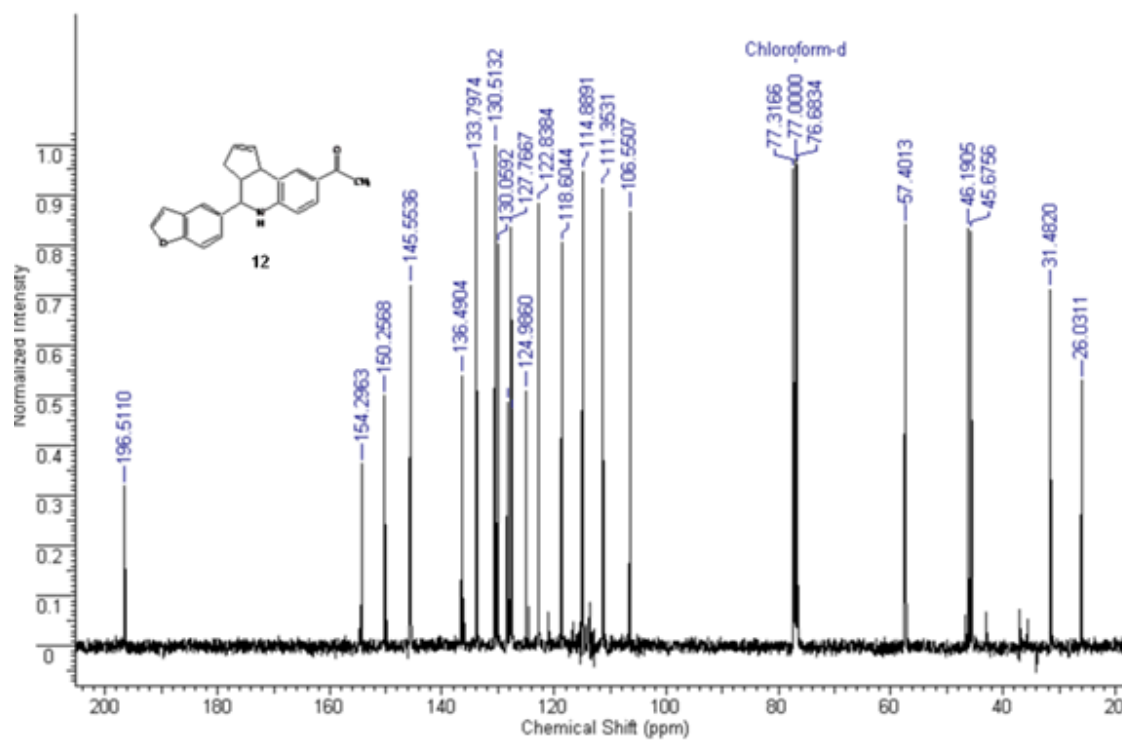
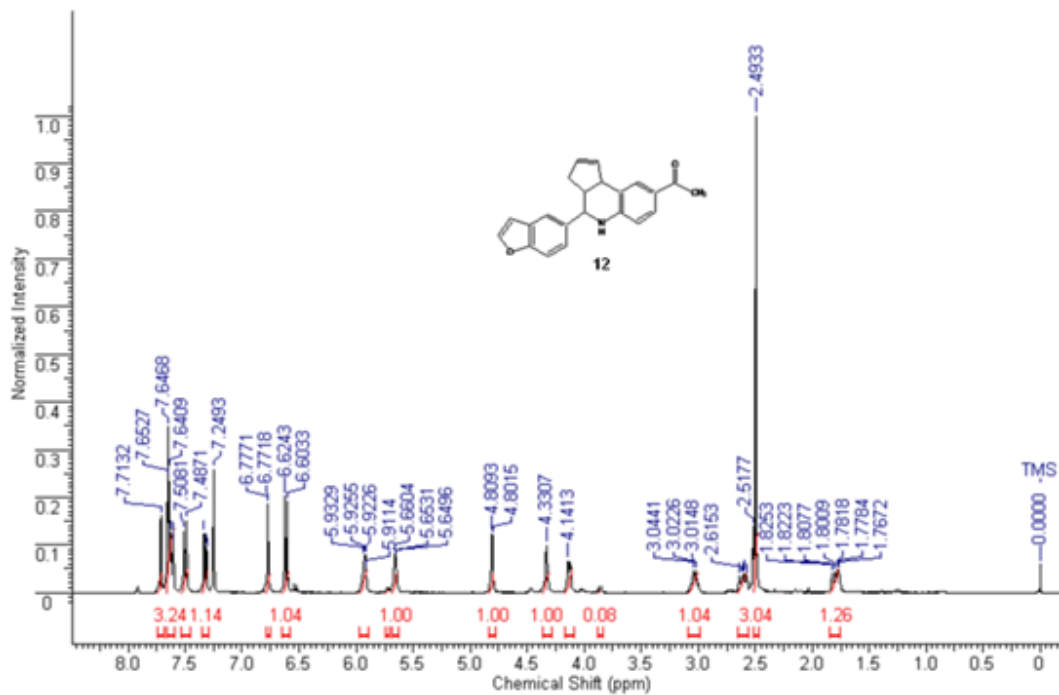


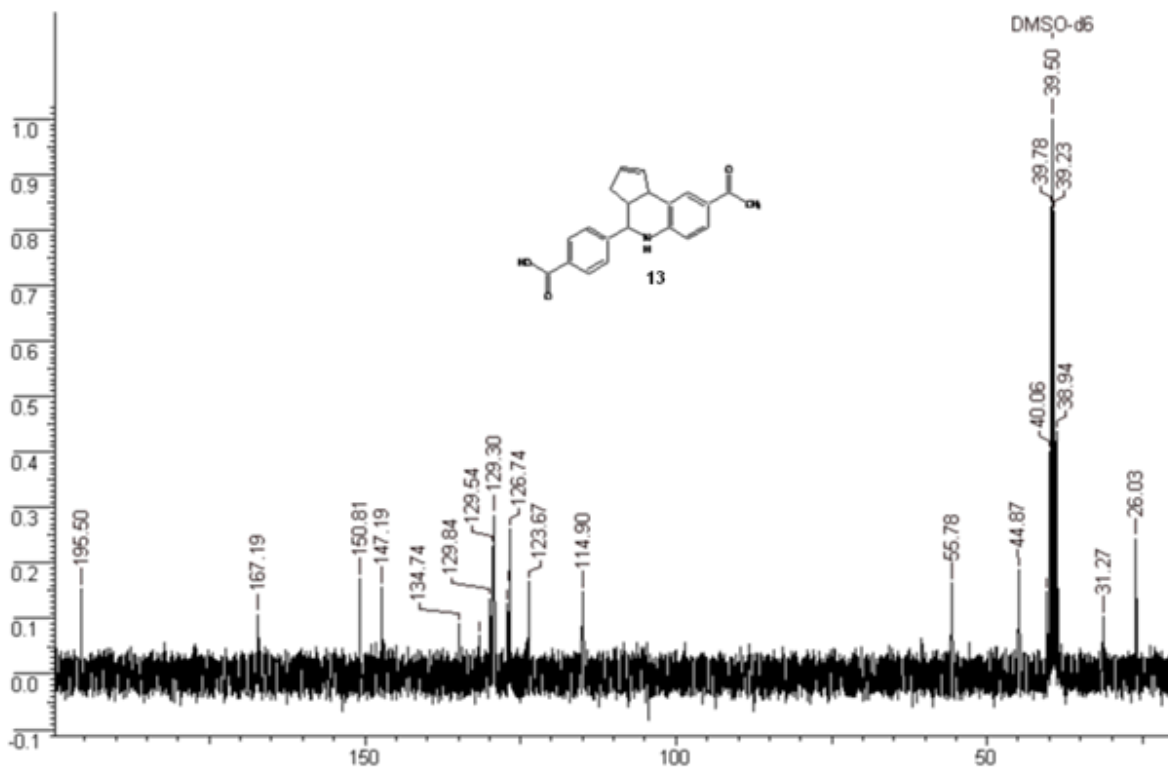
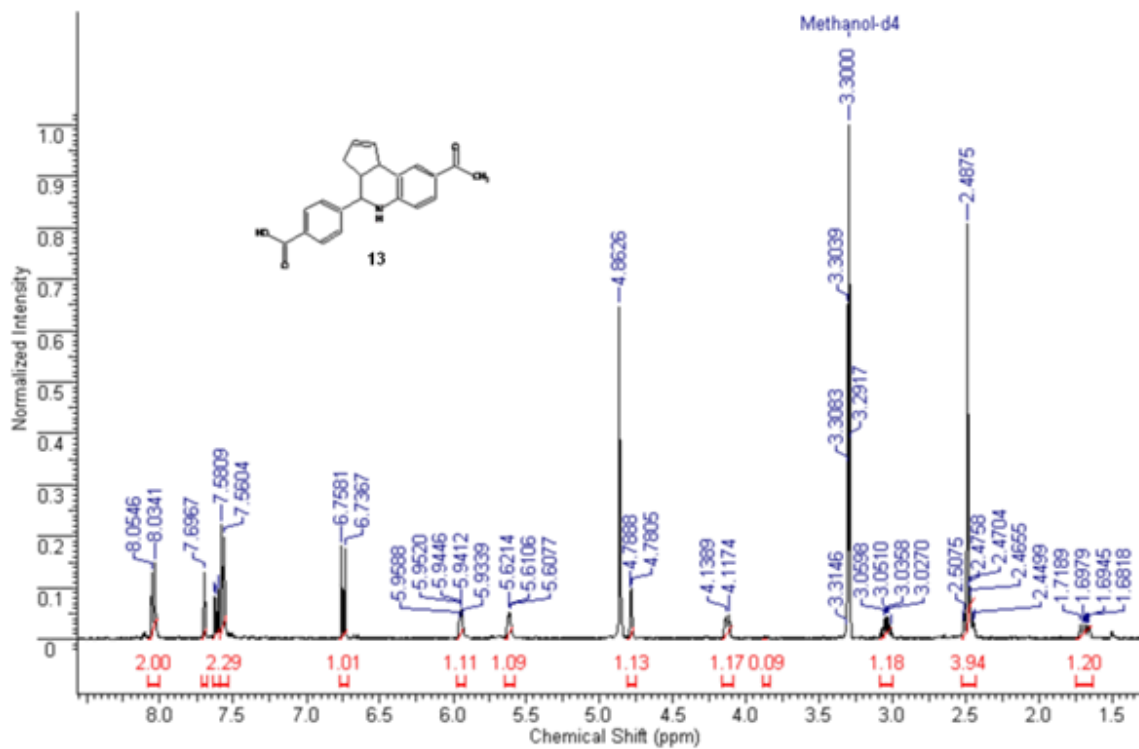


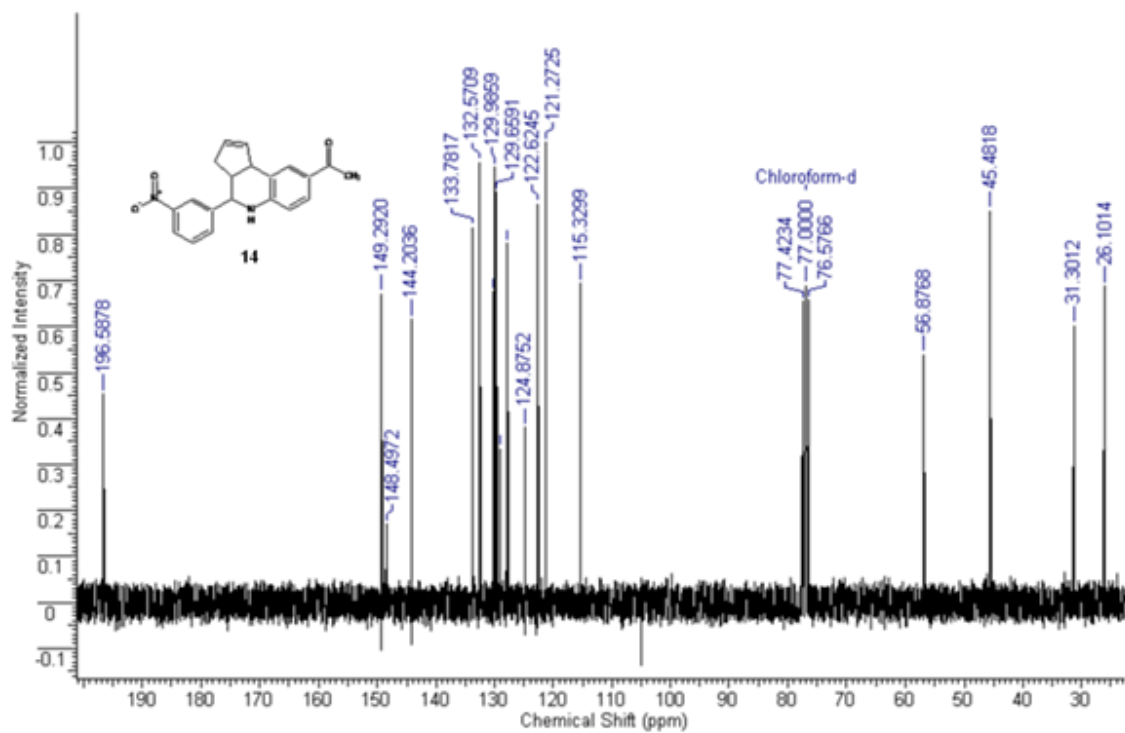
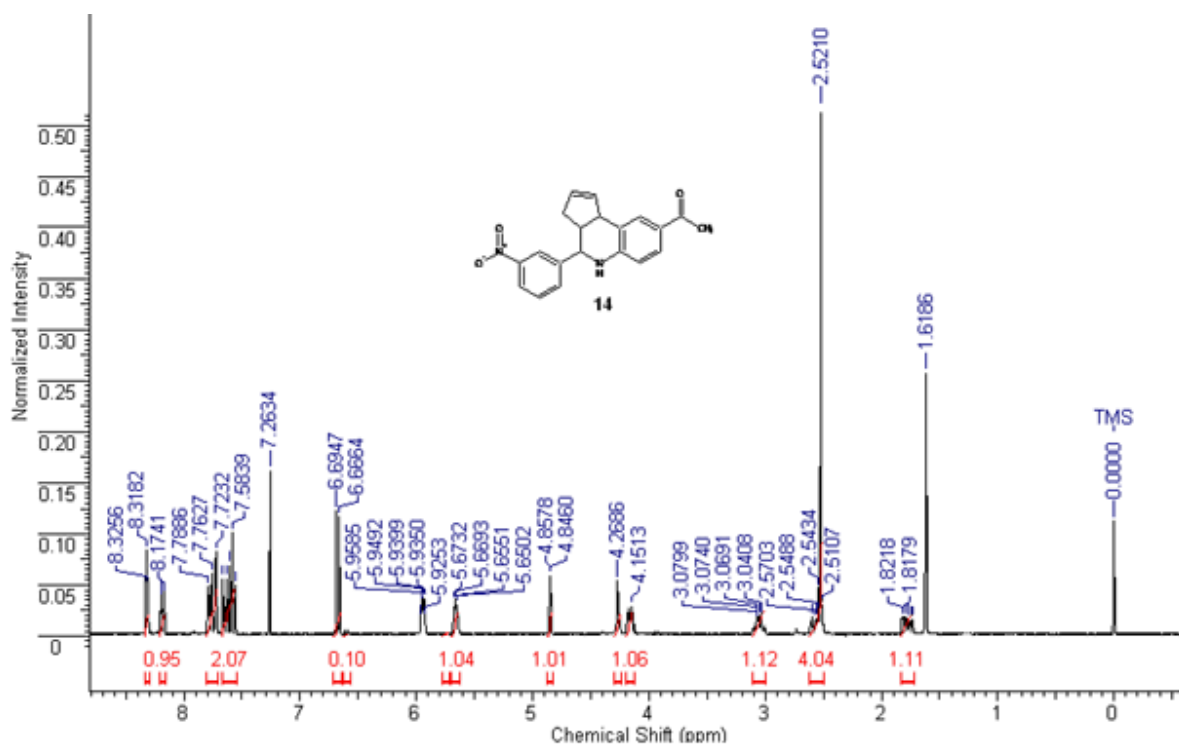


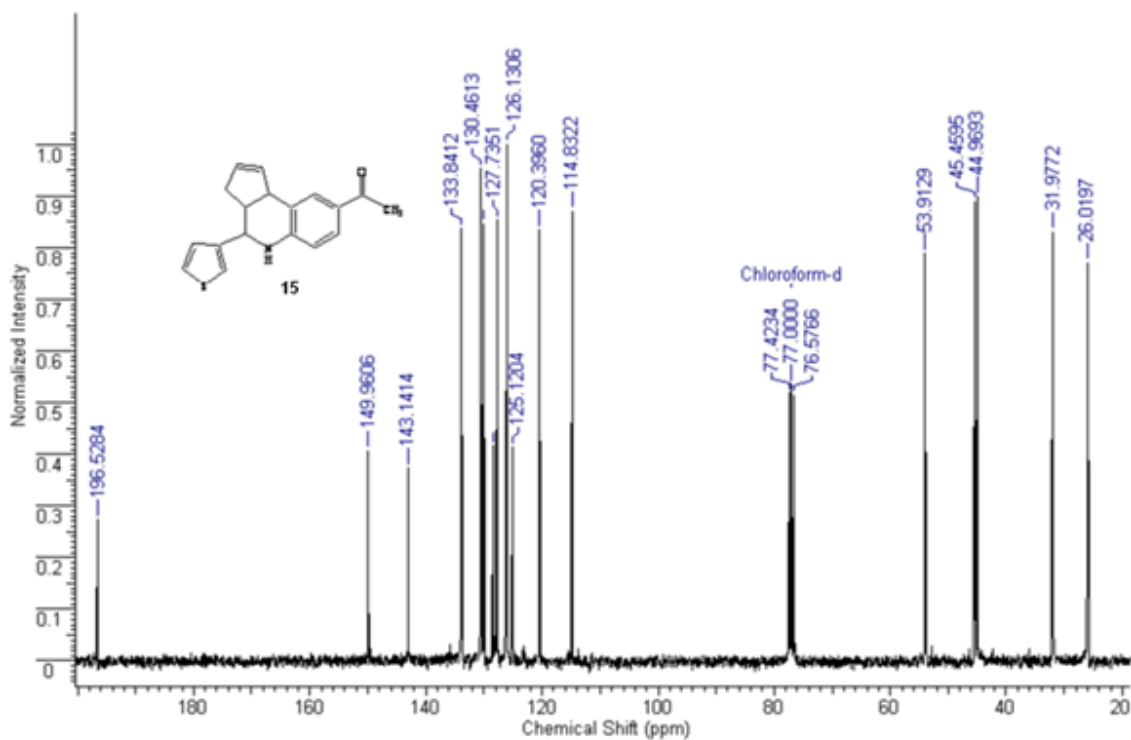
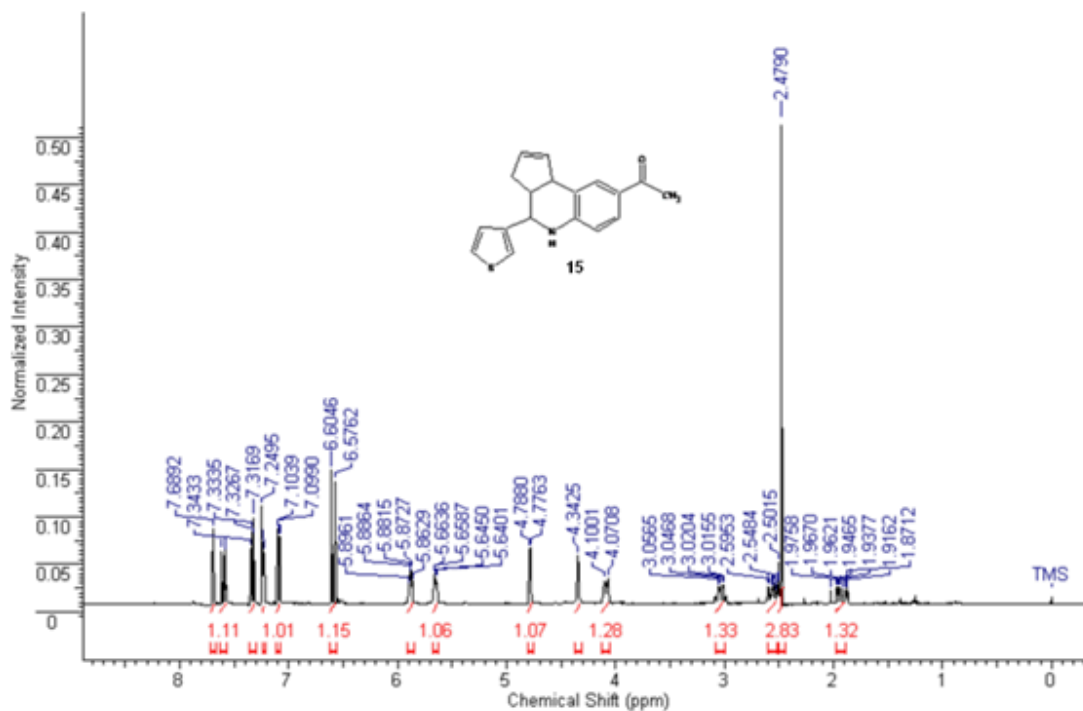


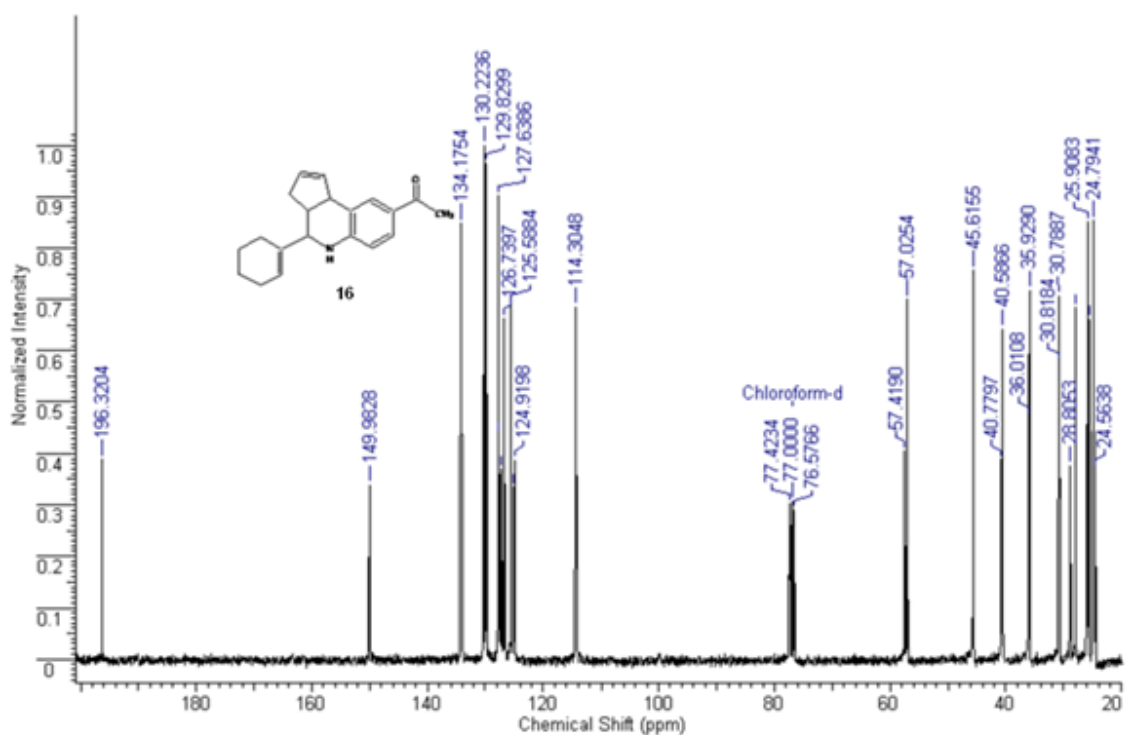
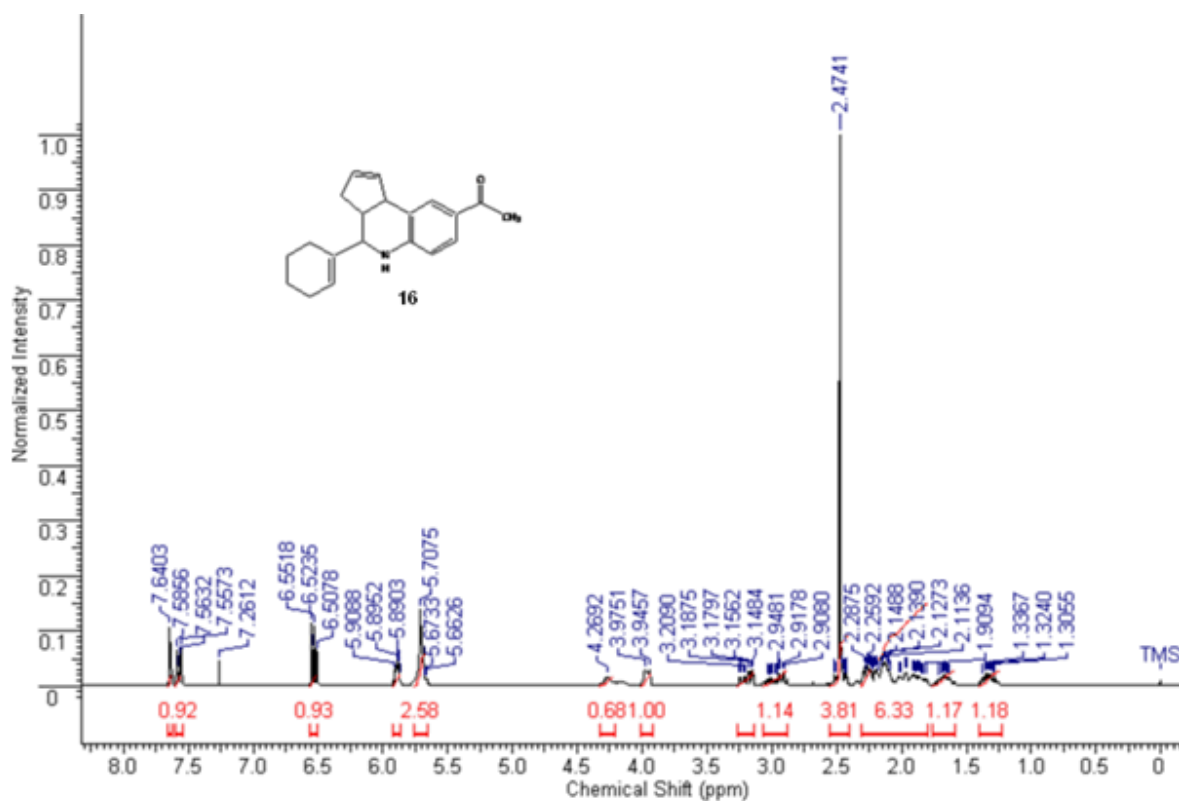


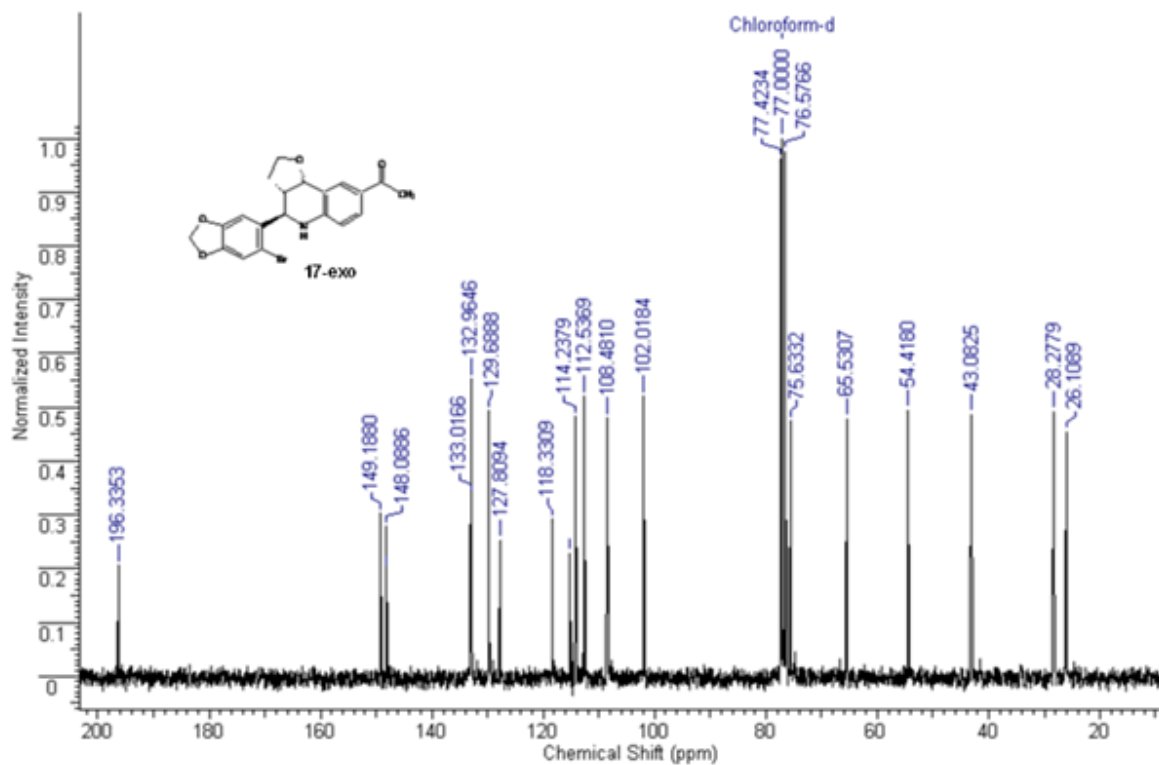
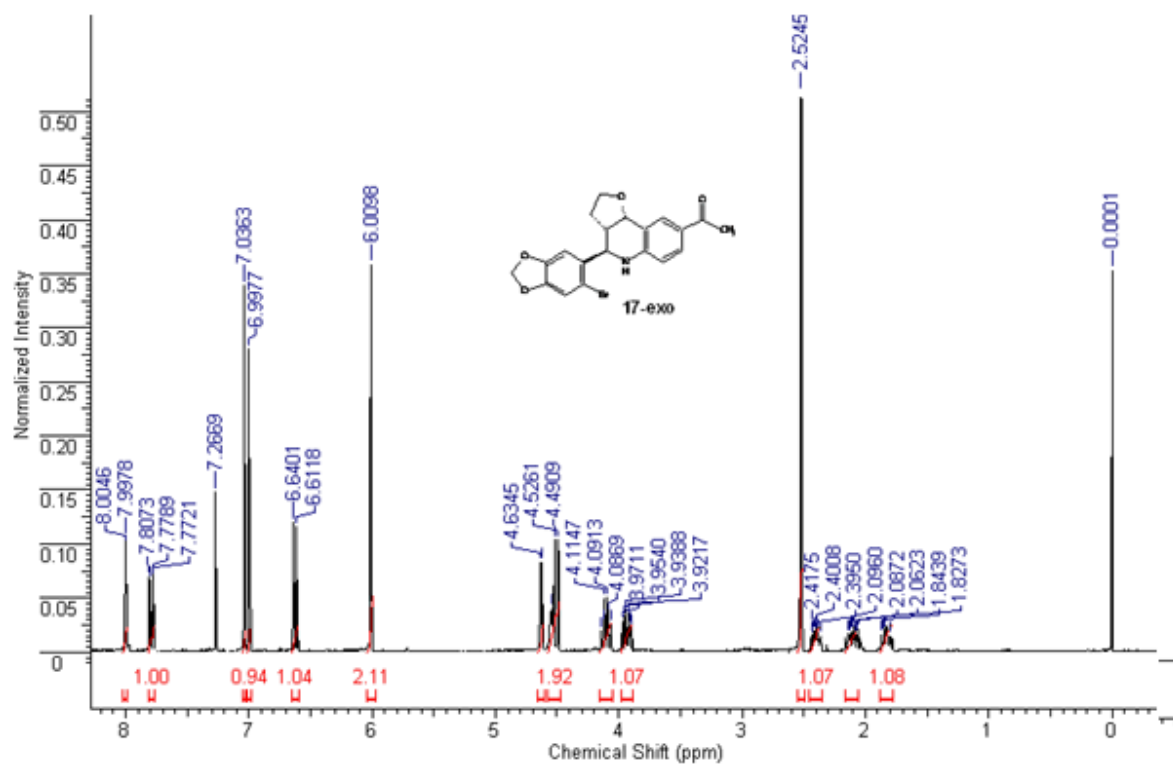


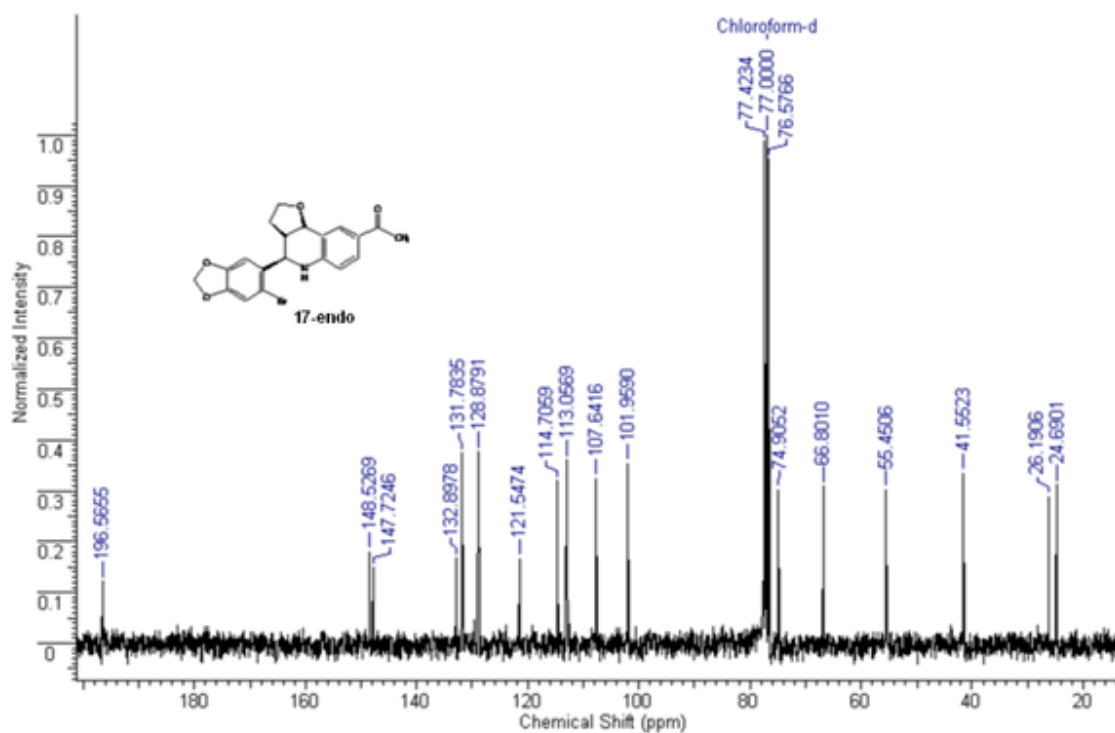
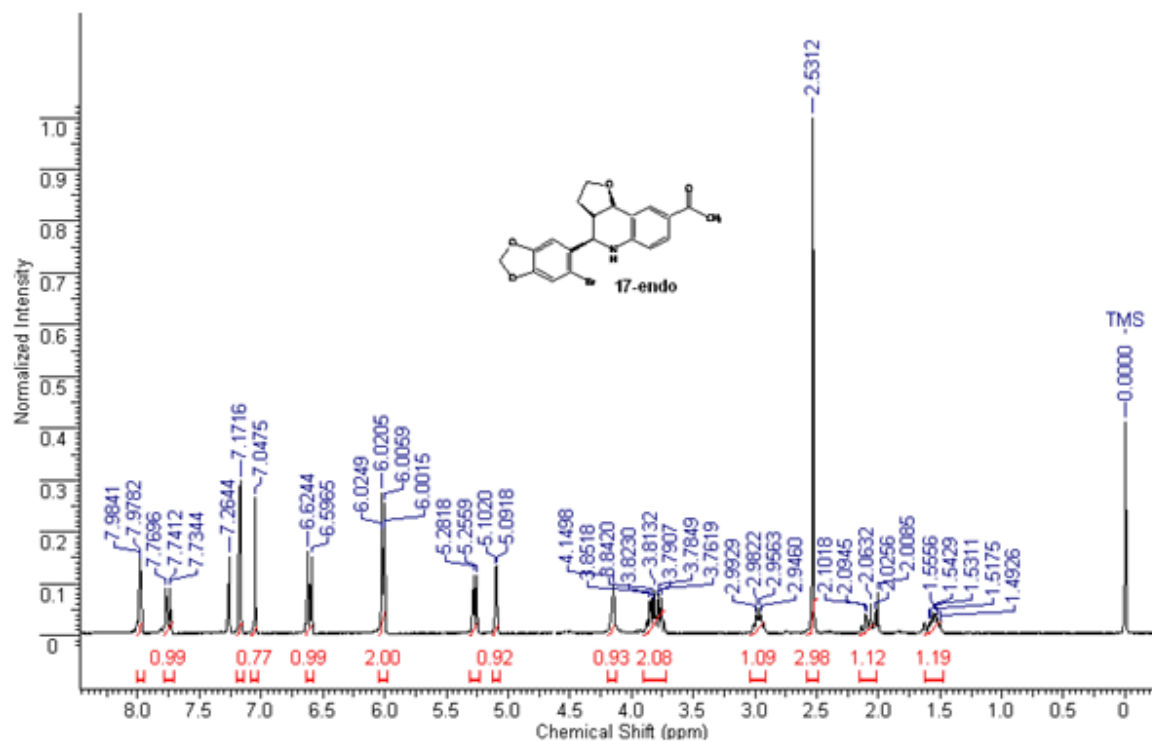






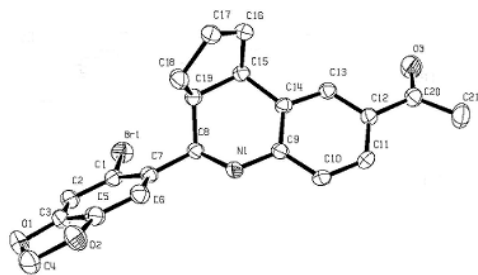






Crystal data and structure refinement for **G-1**.

Identification code	G1
Empirical formula	C ₂₁ H ₁₈ Br N O ₃
Formula weight	412.27
Temperature	228(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 10.0852(9) Å α = 90°. b = 10.6038(9) Å β = 91.353(5)°. c = 31.868(3) Å γ = 90°.
Volume	3407.1(5) Å ³
Z	8
Density (calculated)	1.607 Mg/m ³
Absorption coefficient	2.435 mm ⁻¹
F(000)	1680
Crystal size	0.51 x 0.39 x 0.23 mm ³
Theta range for data collection	2.71 to 31.60°.
Index ranges	-14 ≤ h ≤ 12, -14 ≤ k ≤ 15, -45 ≤ l ≤ 46
Reflections collected	53440
Independent reflections	11402 [R(int) = 0.0431]
Completeness to theta = 31.60°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.568 and 0.350
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	11402 / 0 / 479
Goodness-of-fit on F ²	1.078
Final R indices [I > 2σ(I)]	R1 = 0.0512, wR2 = 0.1143
R indices (all data)	R1 = 0.0835, wR2 = 0.1250
Largest diff. peak and hole	1.426 and -0.563 e.Å ⁻³



X-ray ORTEP Rendition of GPR-30 Agonist G-1.