Supplementary Material (ESI) for Organic and Biomolecular Chemistry

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

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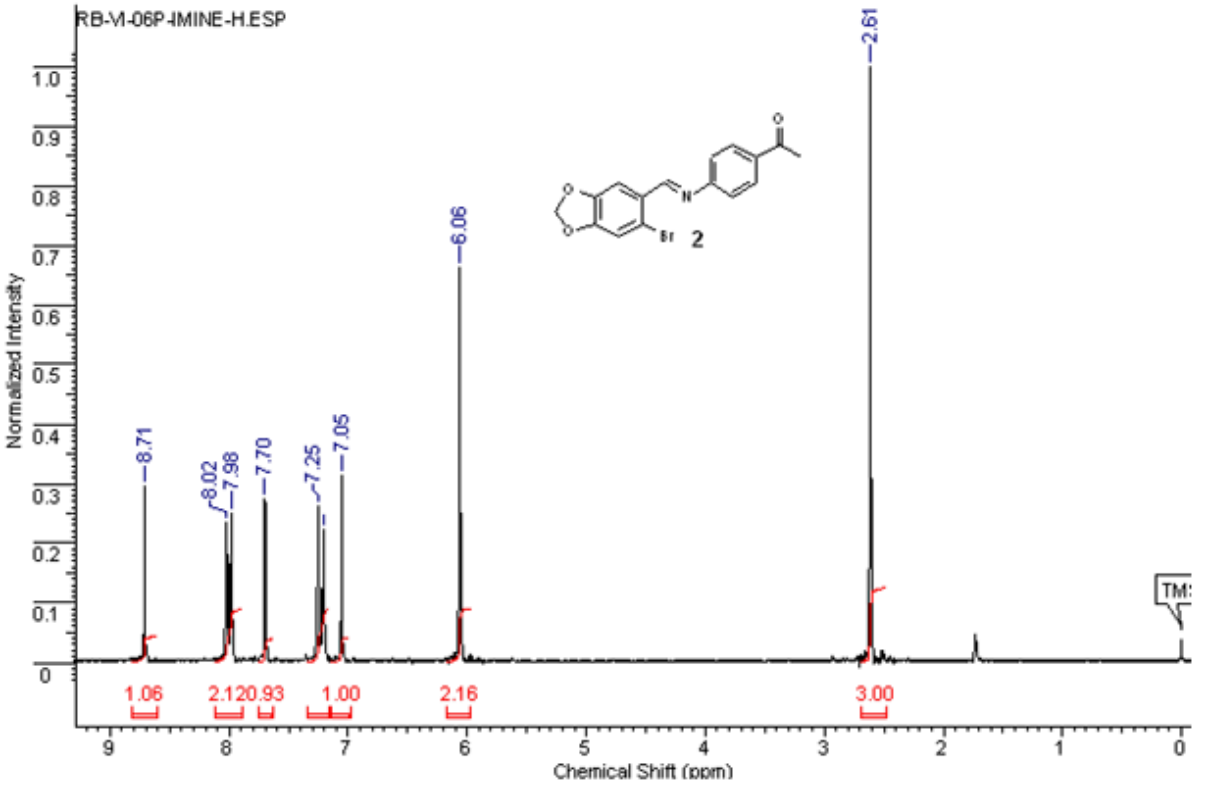

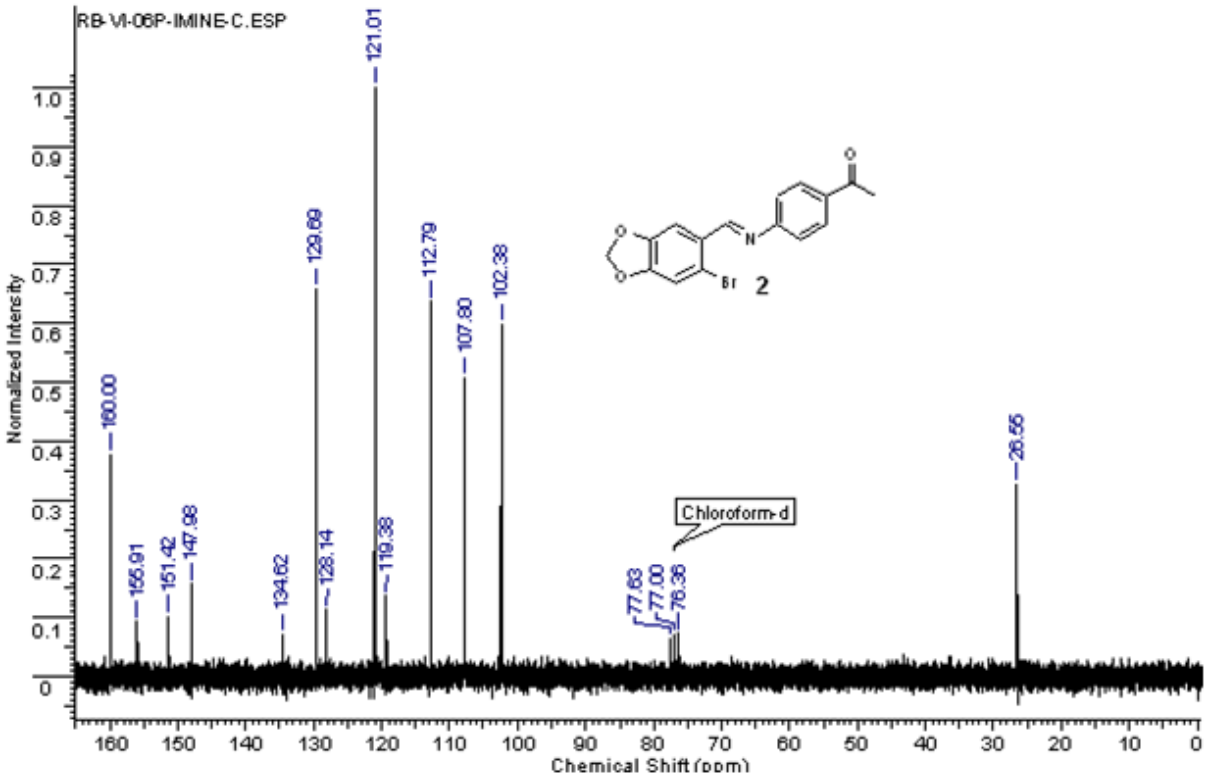

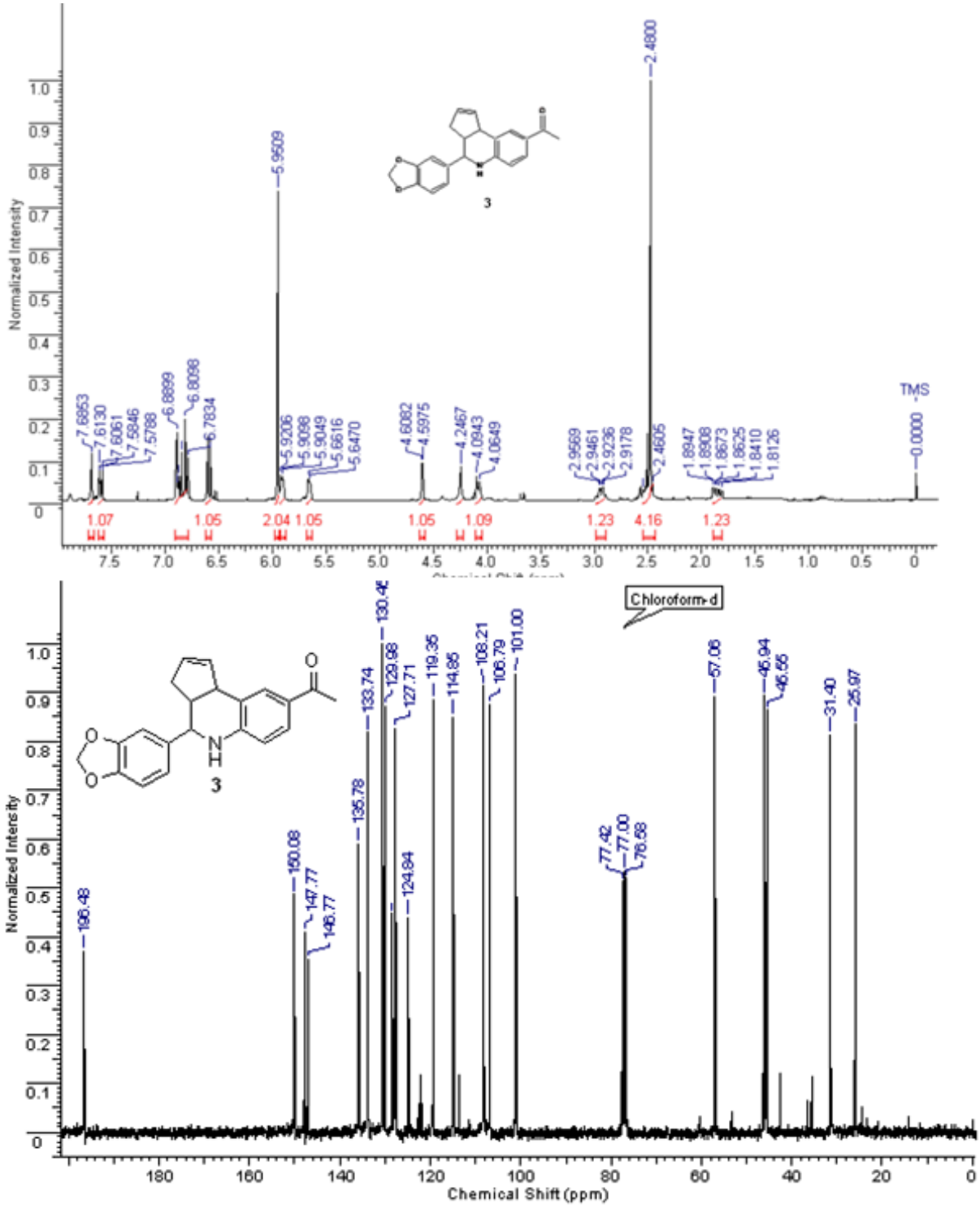

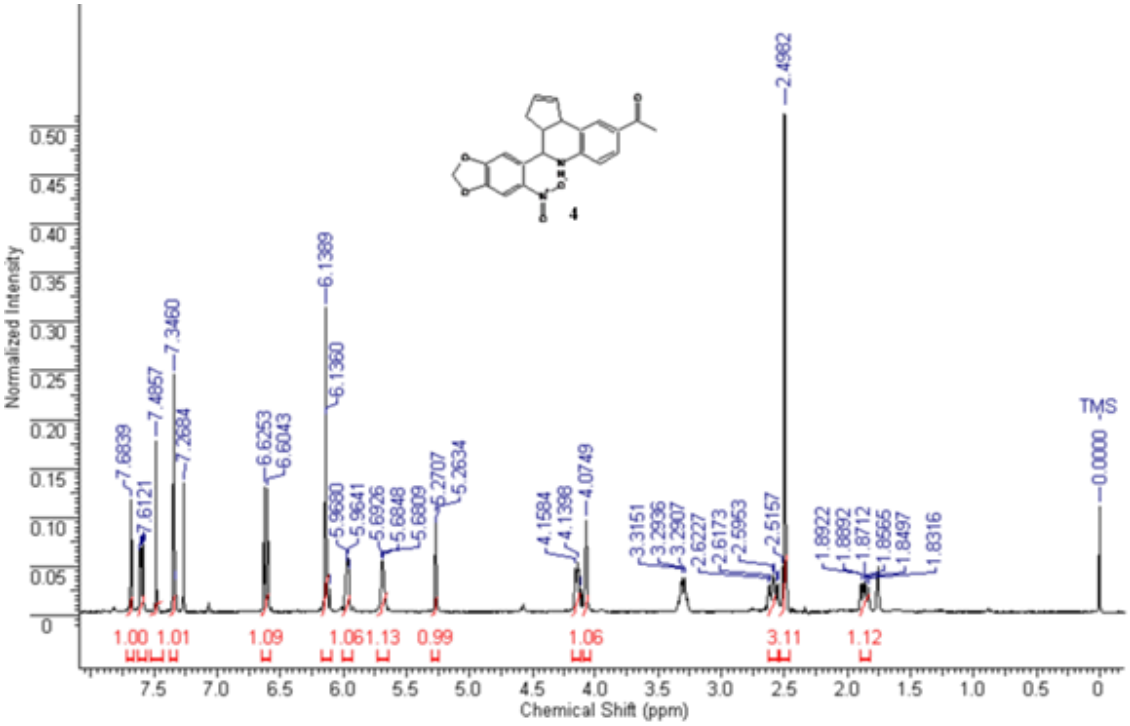

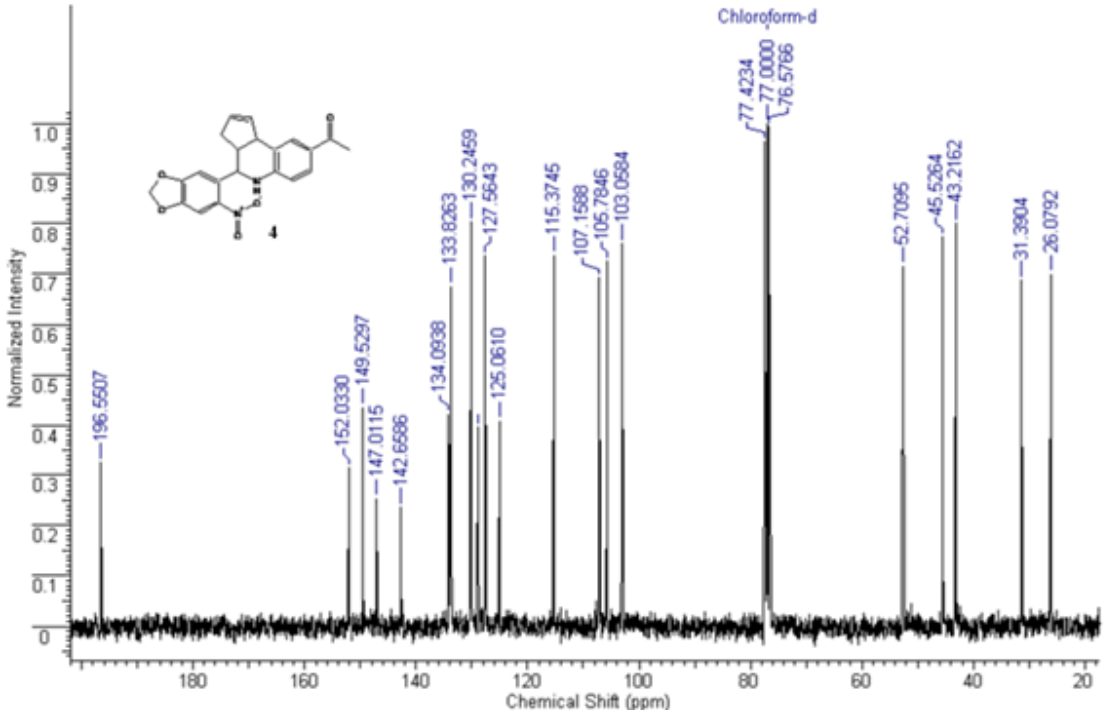

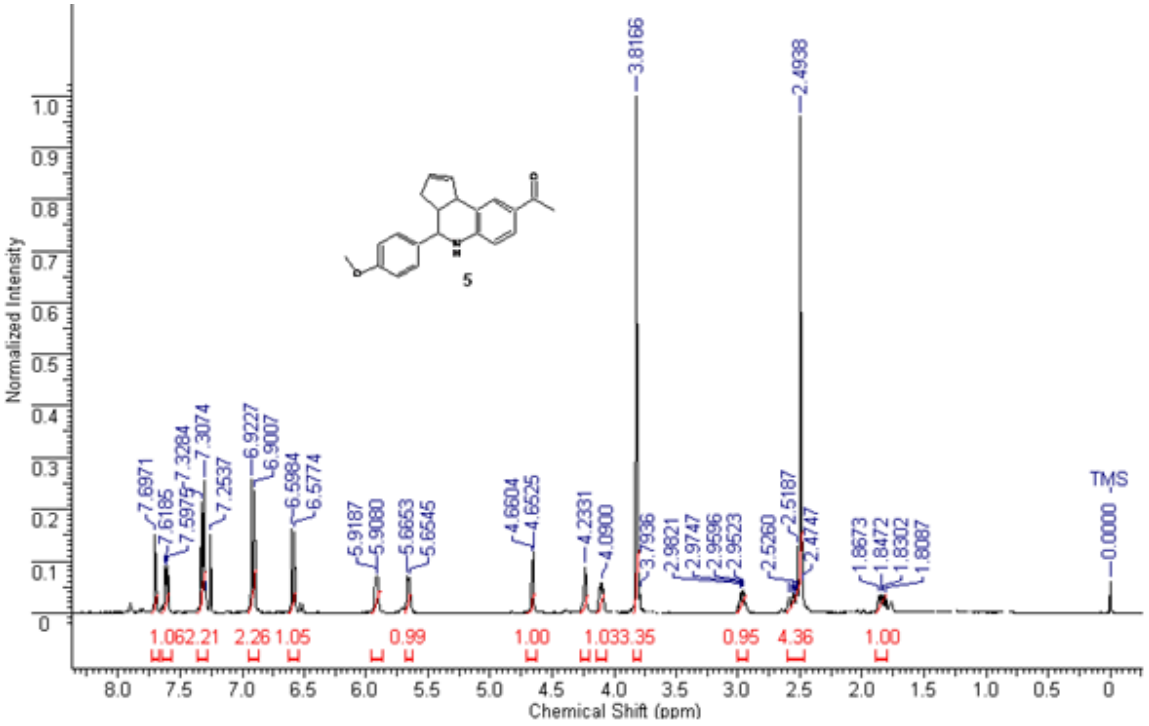

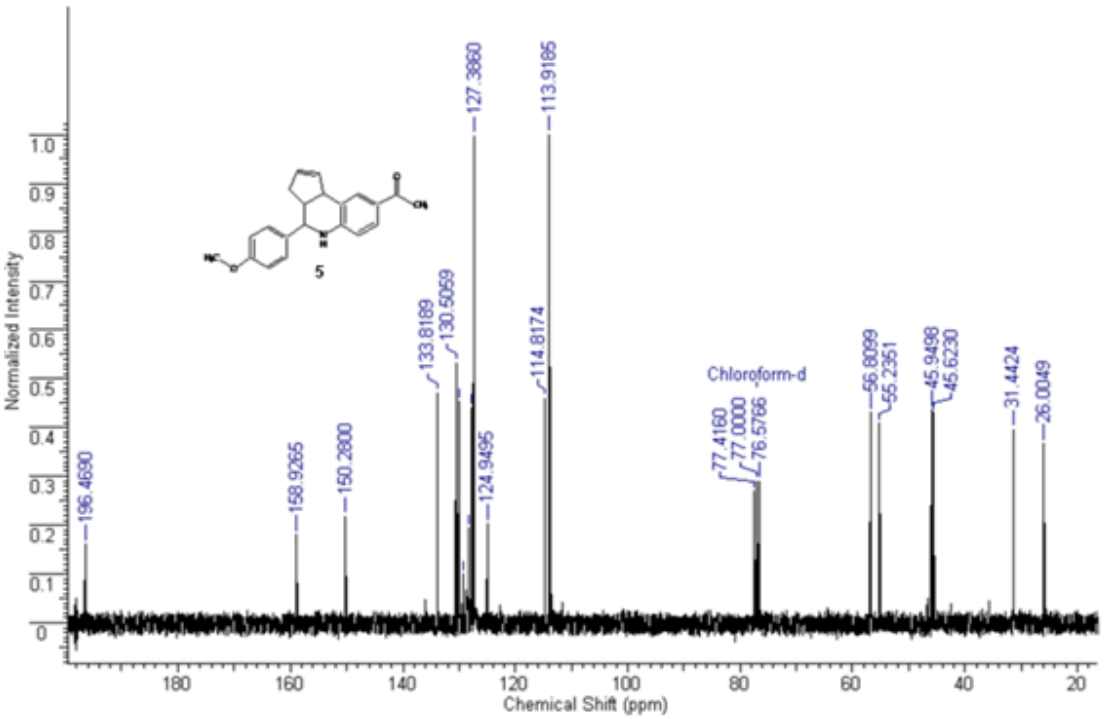

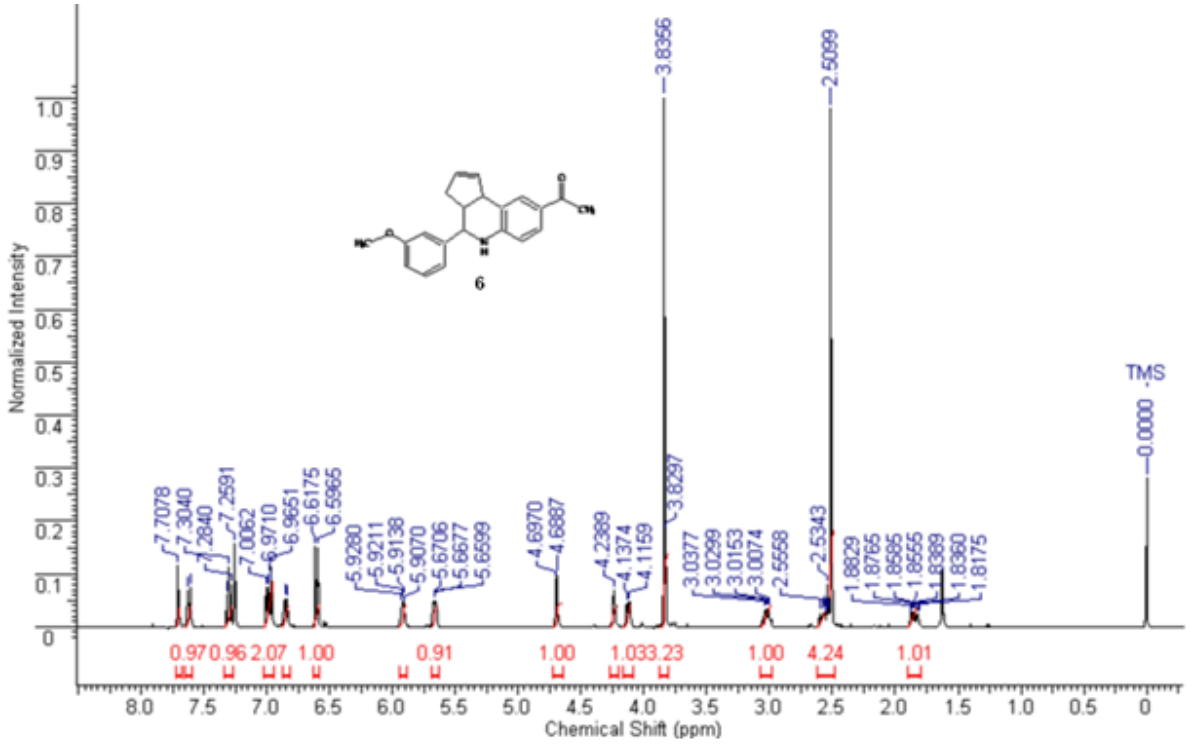

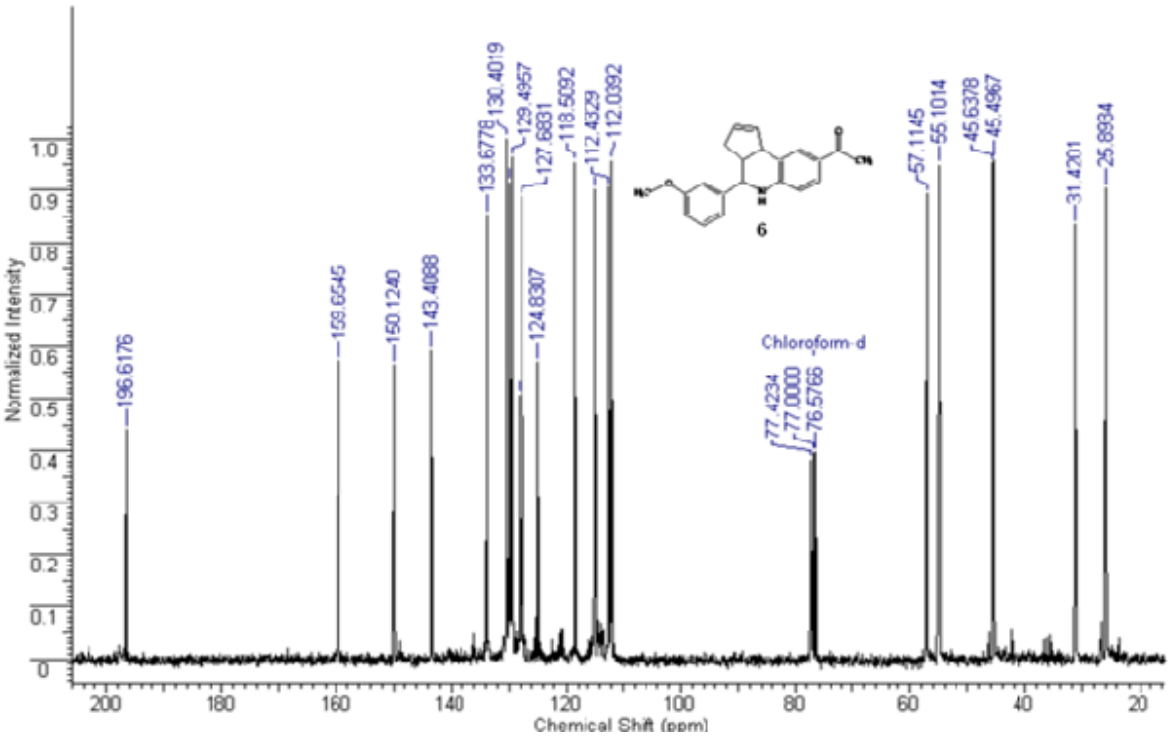

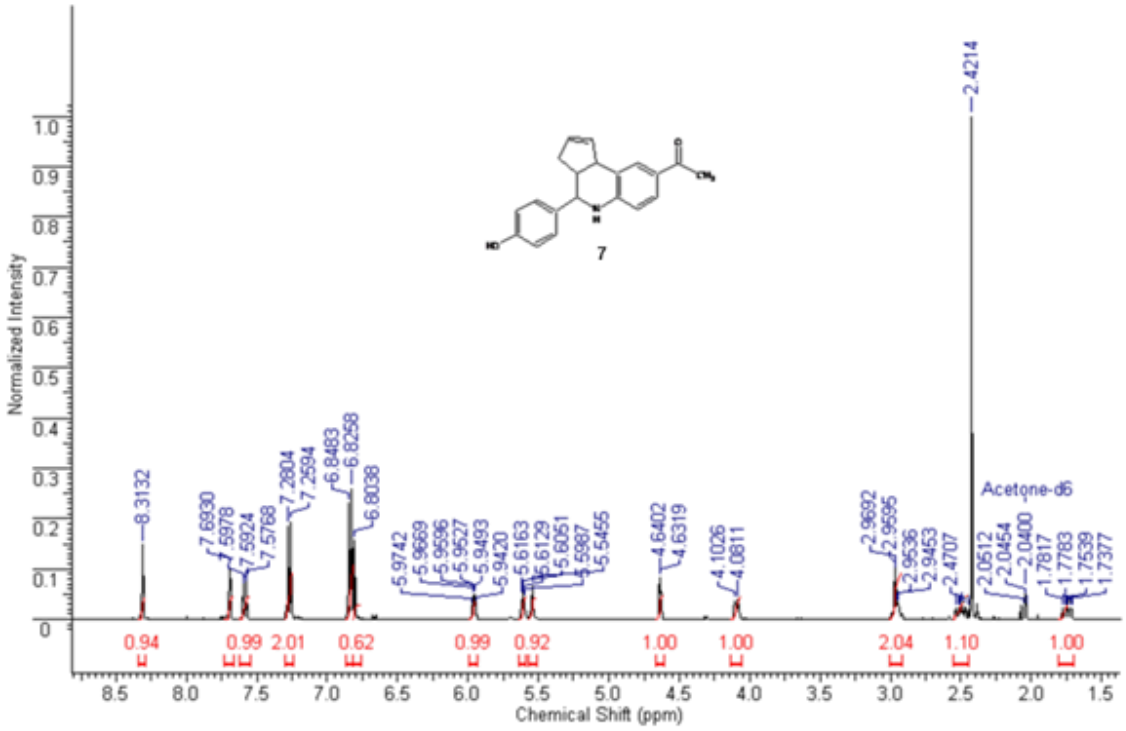

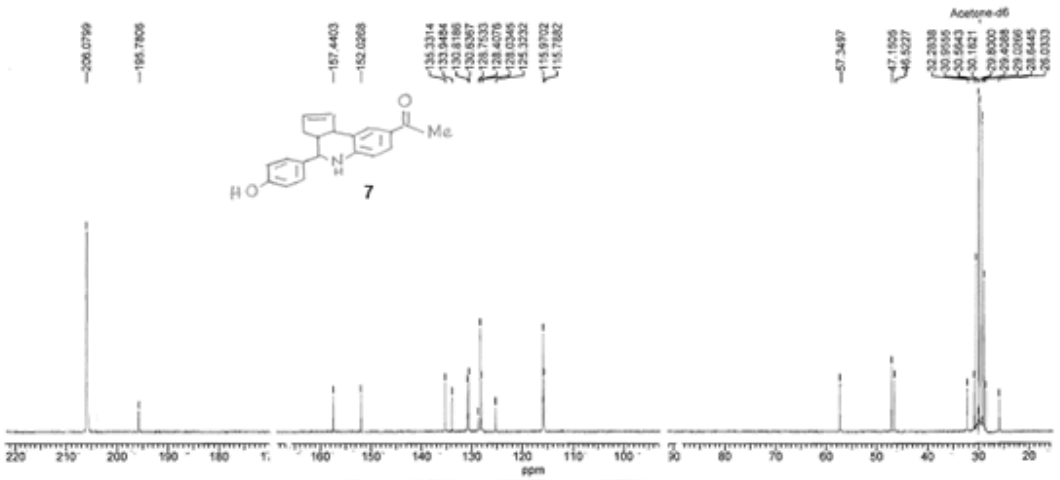

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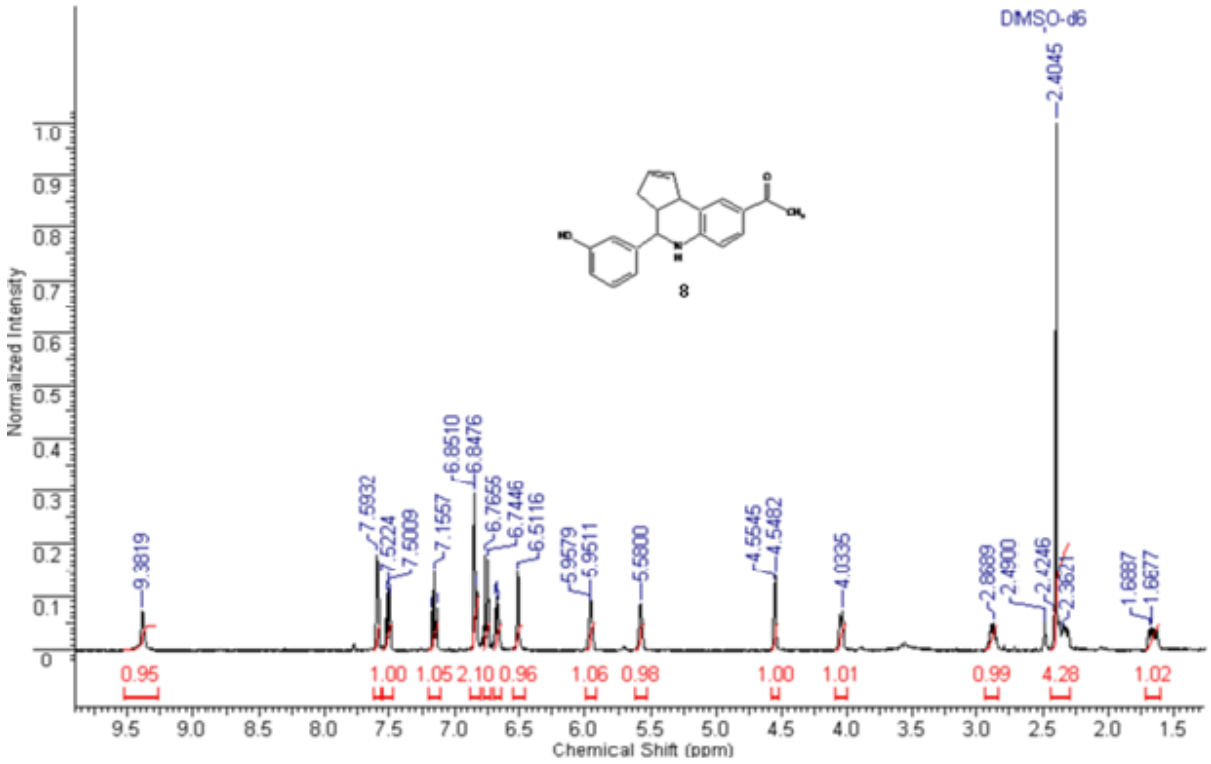
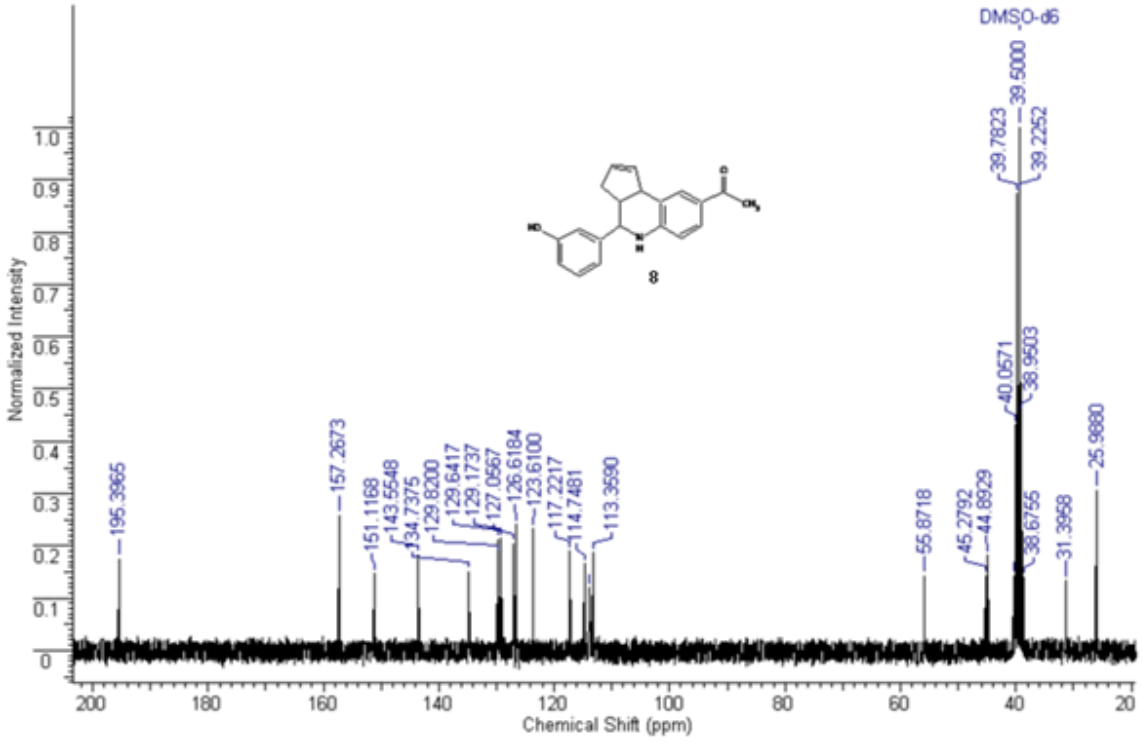
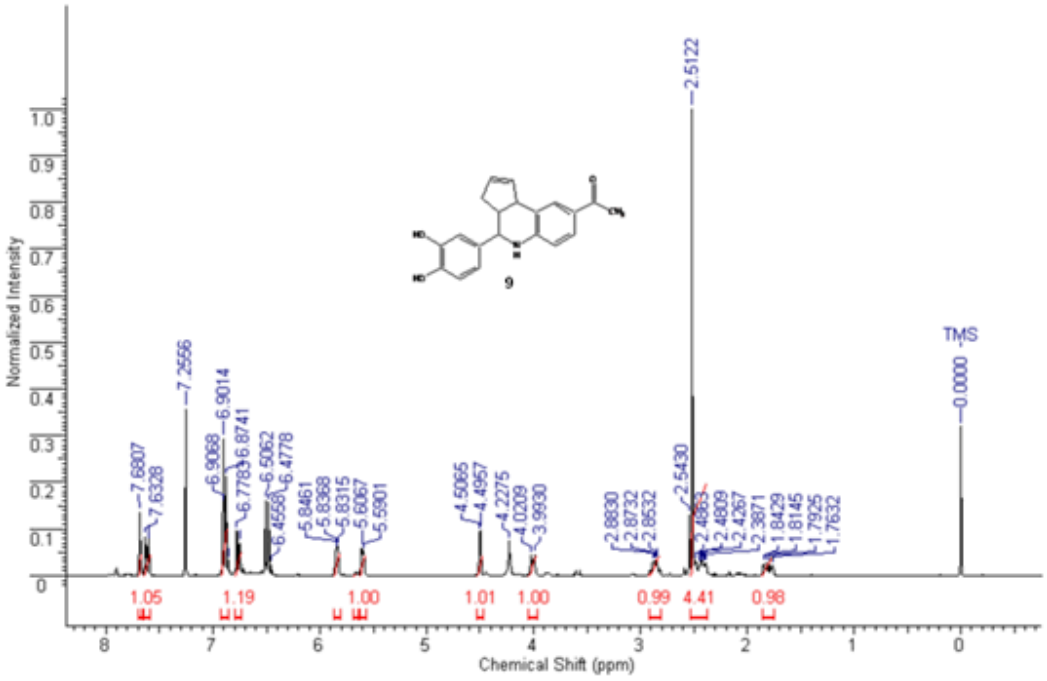
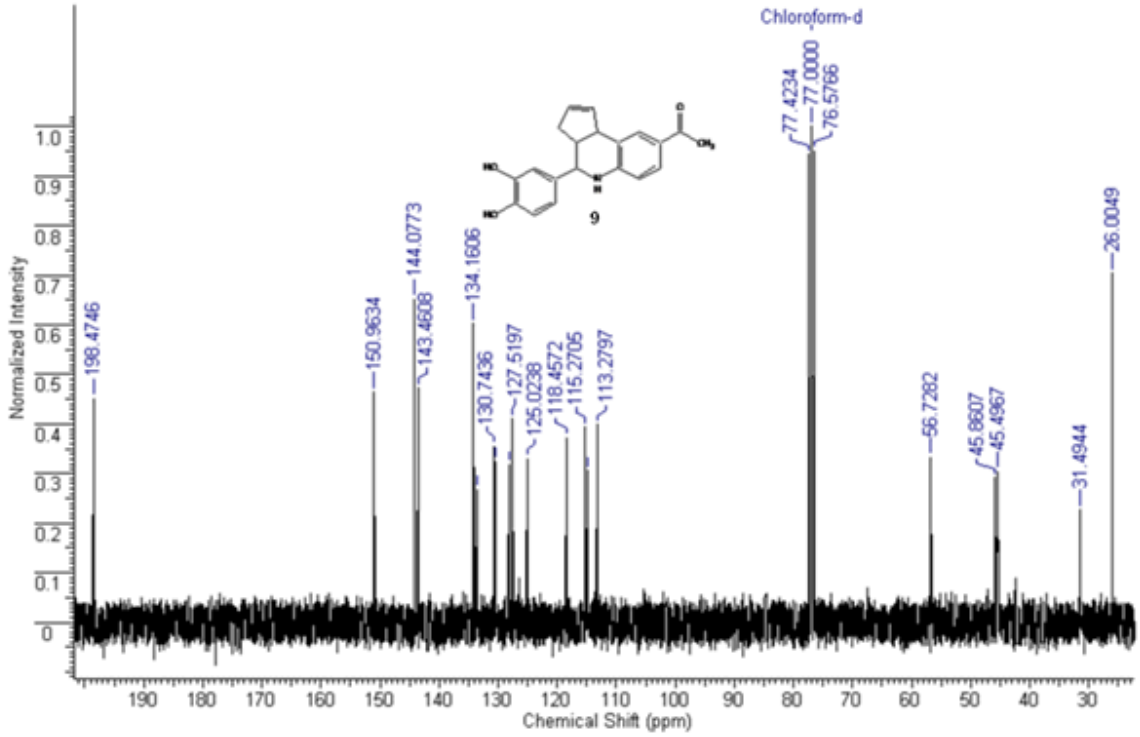
1	26.03	1309.2	0.0961	10	32.28	1623.5	0.1303	19	128.75	6474.9	0.0418
2	28.64	1440.5	0.1207	11	46.52	2339.6	0.1533	20	130.64	6569.6	0.1609
3	29.03	1459.7	0.4514	12	47.15	2371.2	0.1958	21	130.82	6578.8	0.1389
4	29.41	1478.9	0.9260	13	57.35	2884.1	0.1438	22	133.95	6736.2	0.1017
5	29.80	1498.6	0.9751	14	115.79	5822.9	0.1602	23	135.33	6805.7	0.1444
6	30.05	1511.4	0.0421	15	115.97	5832.1	0.2929	24	152.03	7645.3	0.1094
7	30.18	1517.8	1.0000	16	125.32	6302.4	0.0718	25	157.44	7917.6	0.1068
8	30.56	1537.1	0.5044	17	128.03	6438.8	0.1504	26	195.78	9845.7	0.0607
9	30.96	1556.7	0.1522	18	128.41	6457.5	0.3089	27	206.08	10363.6	0.5987

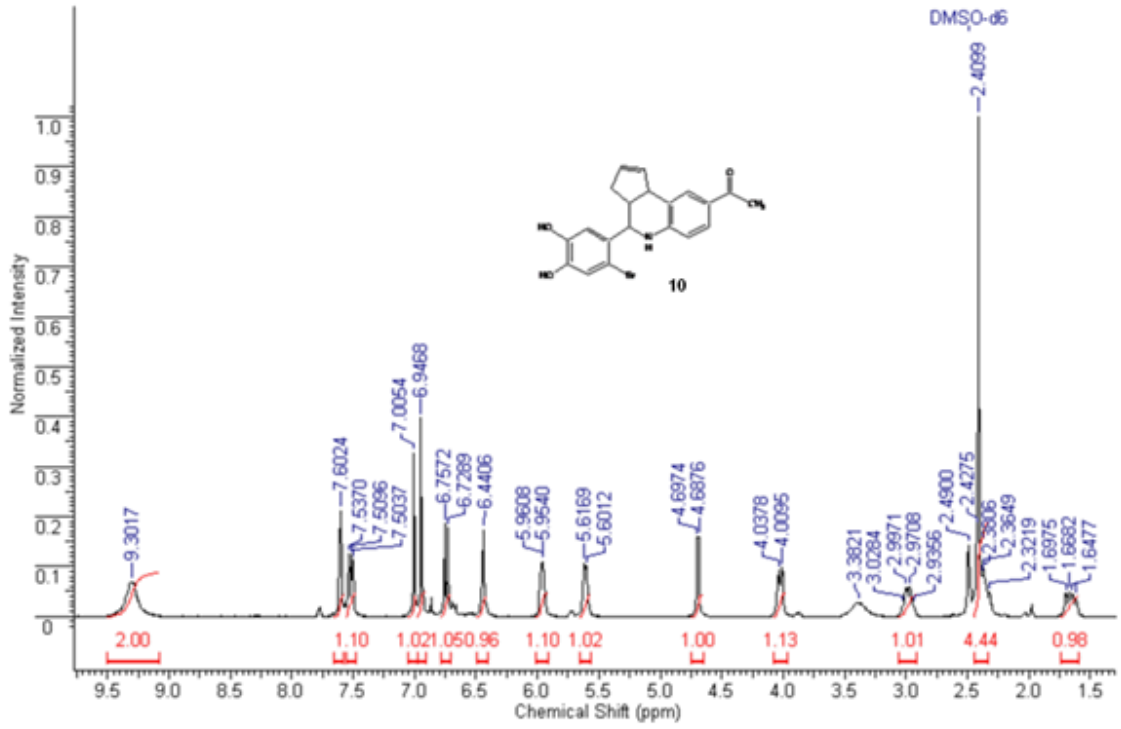
No.	Annotation	(ppm)
1	Acetone-d6	29.80

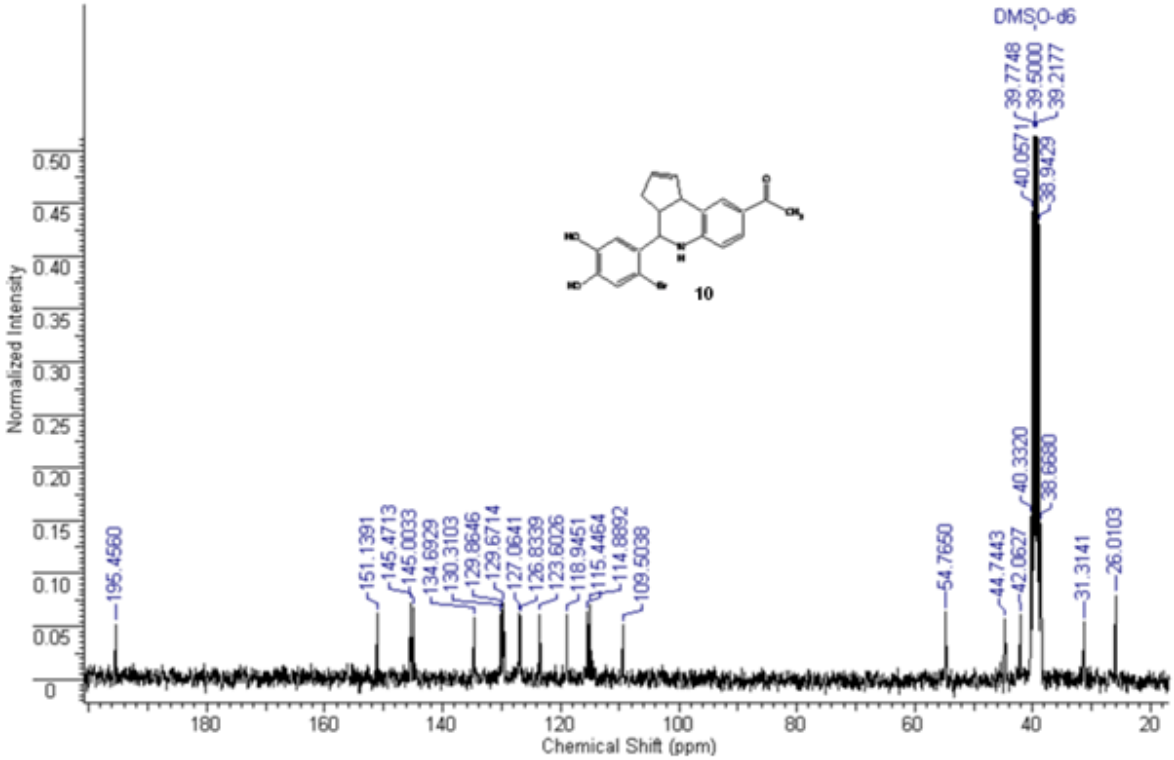


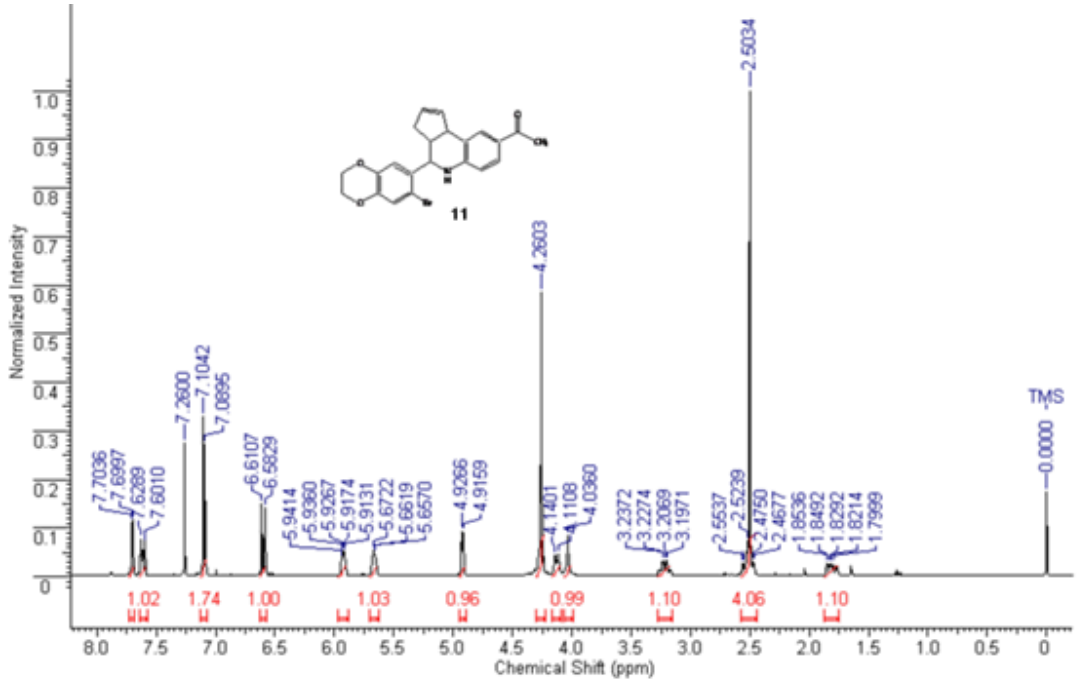


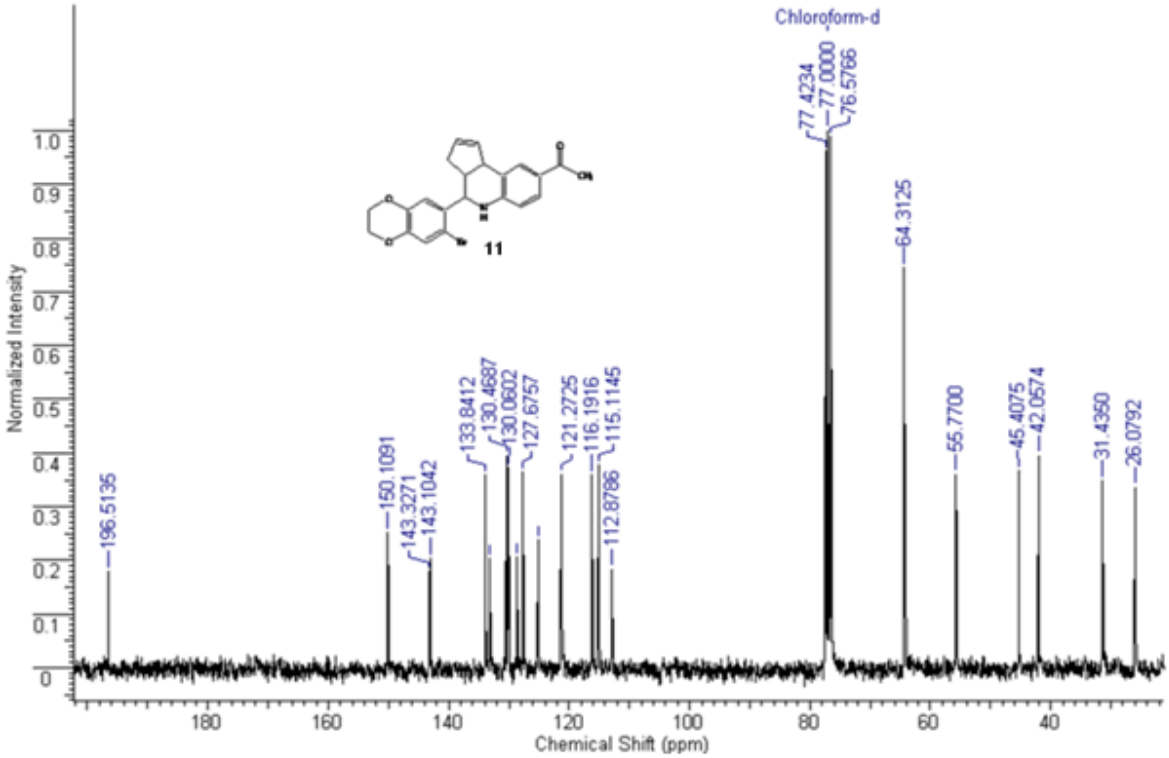


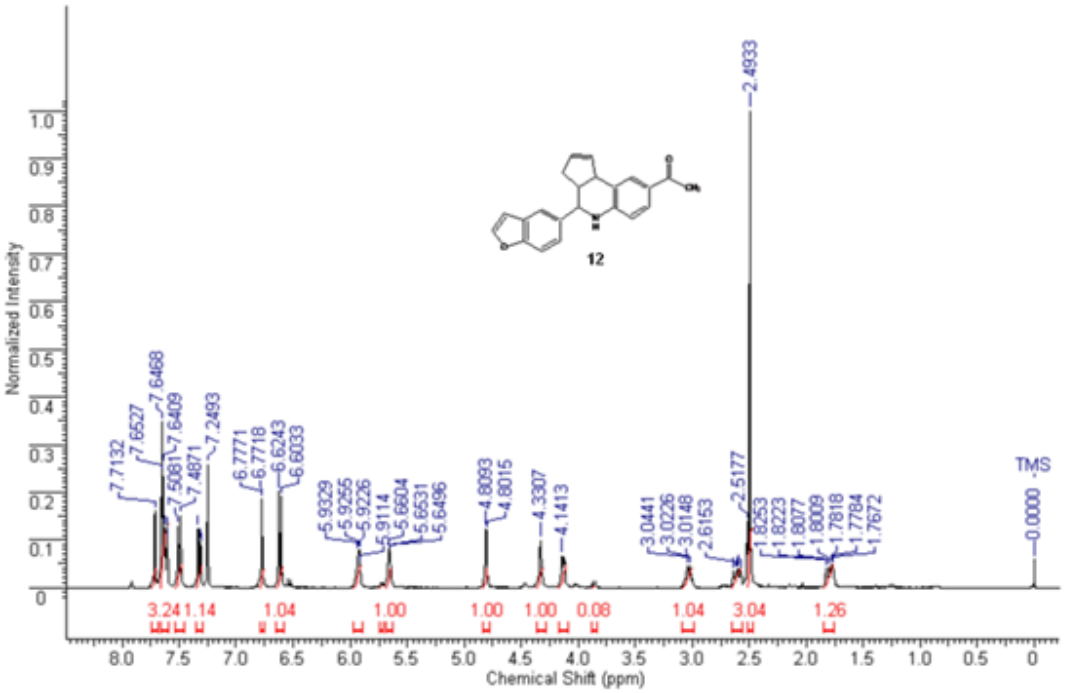


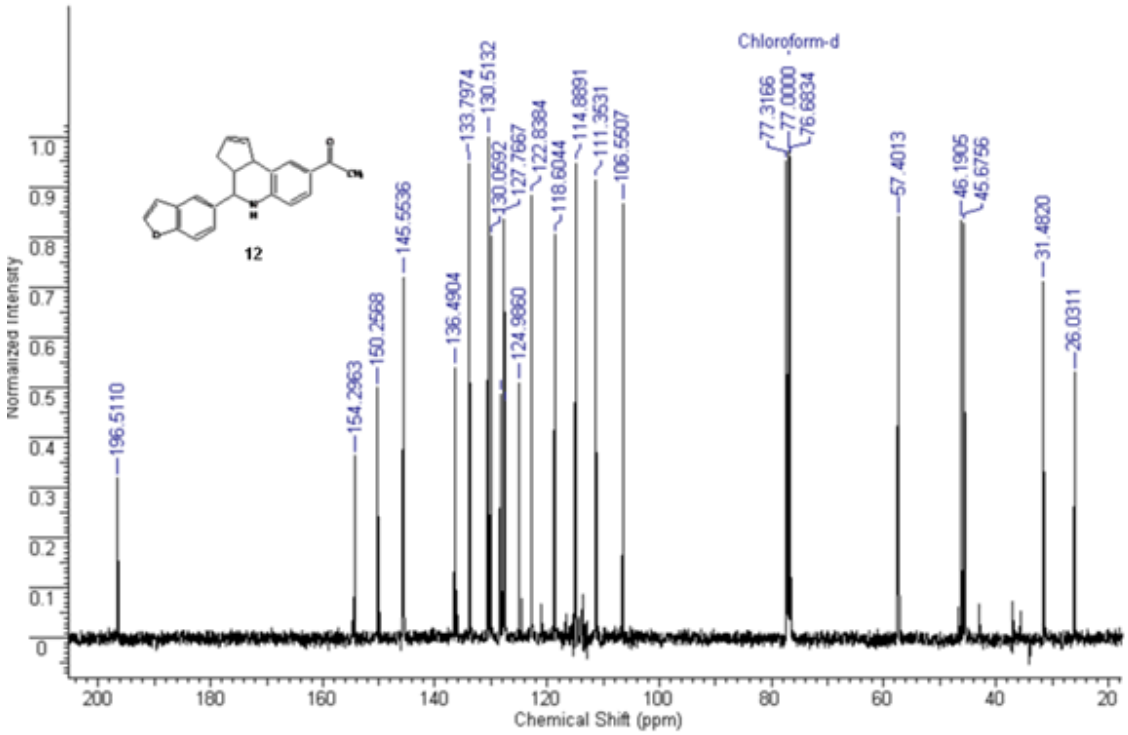


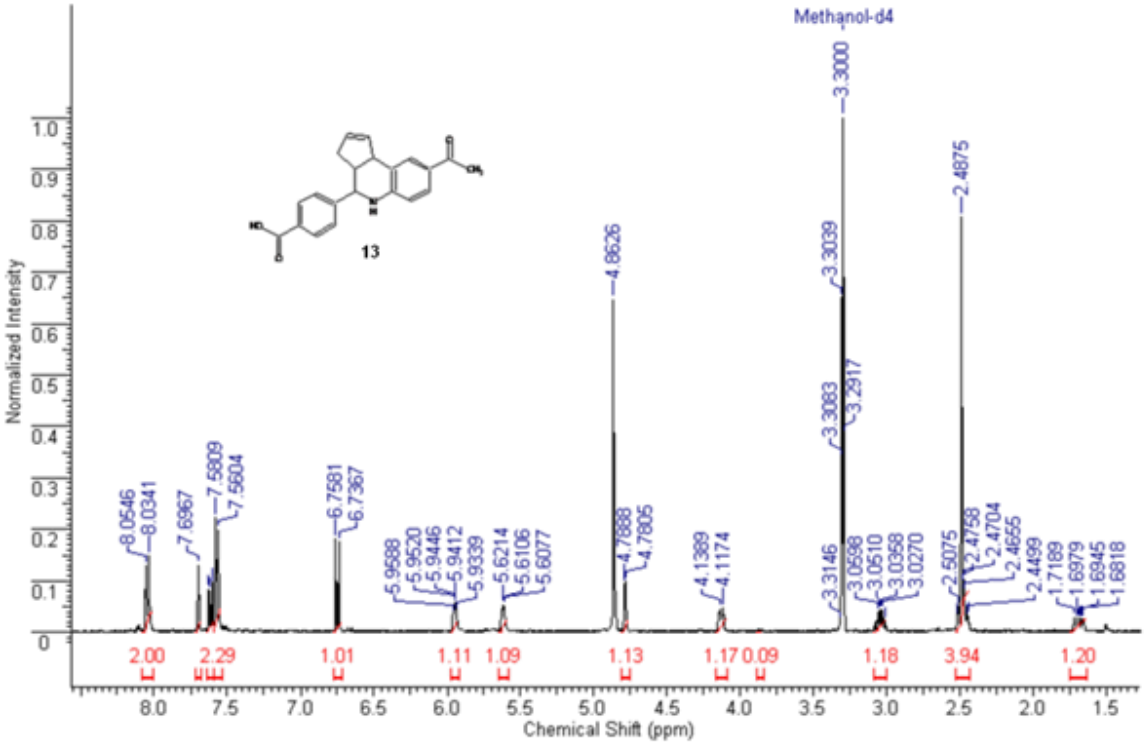


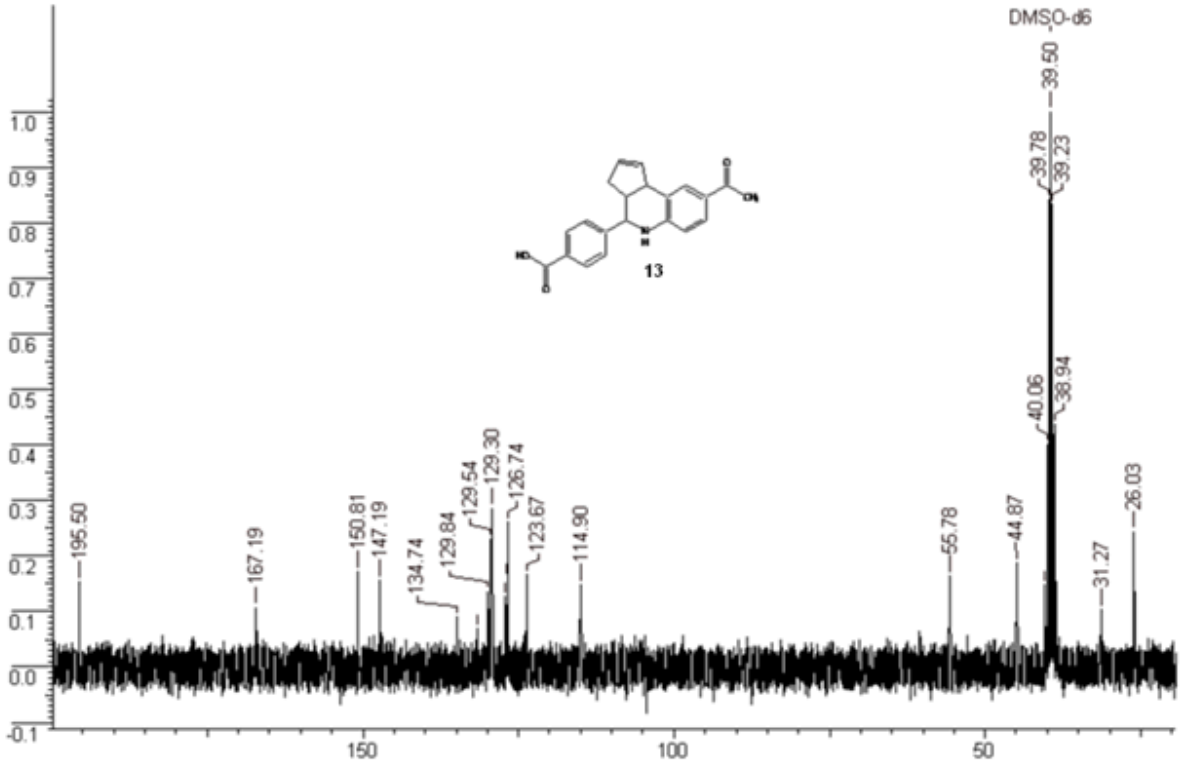


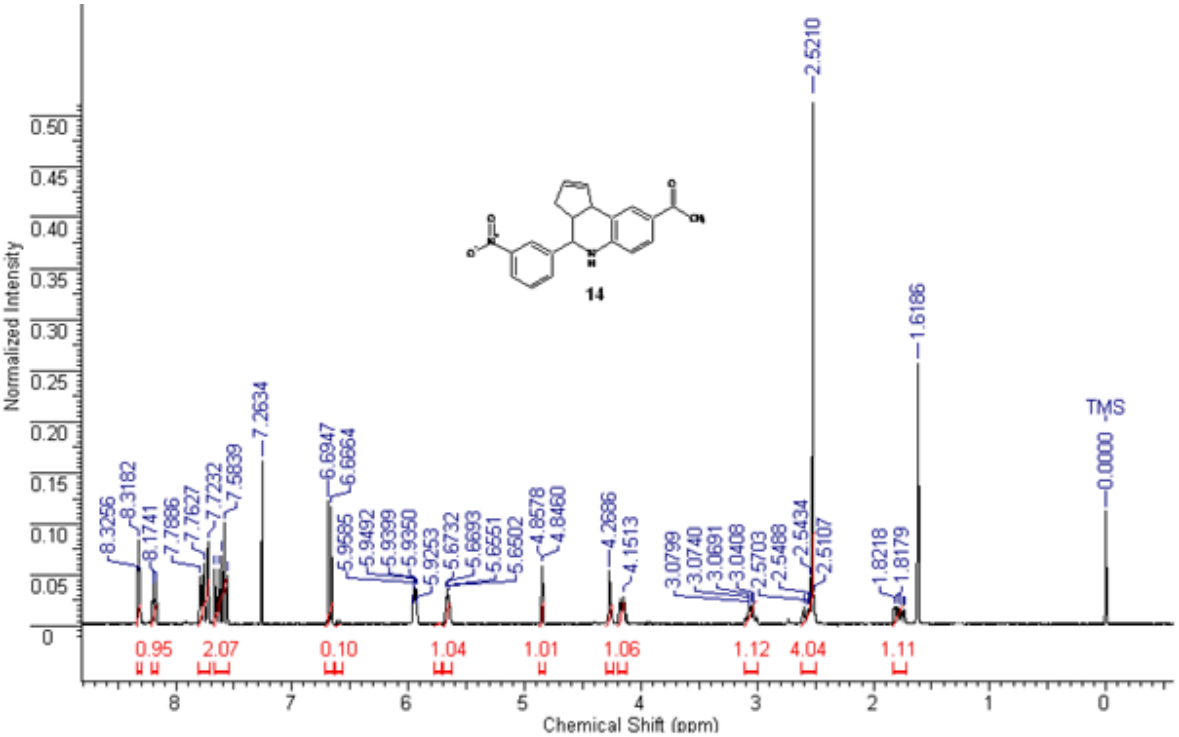


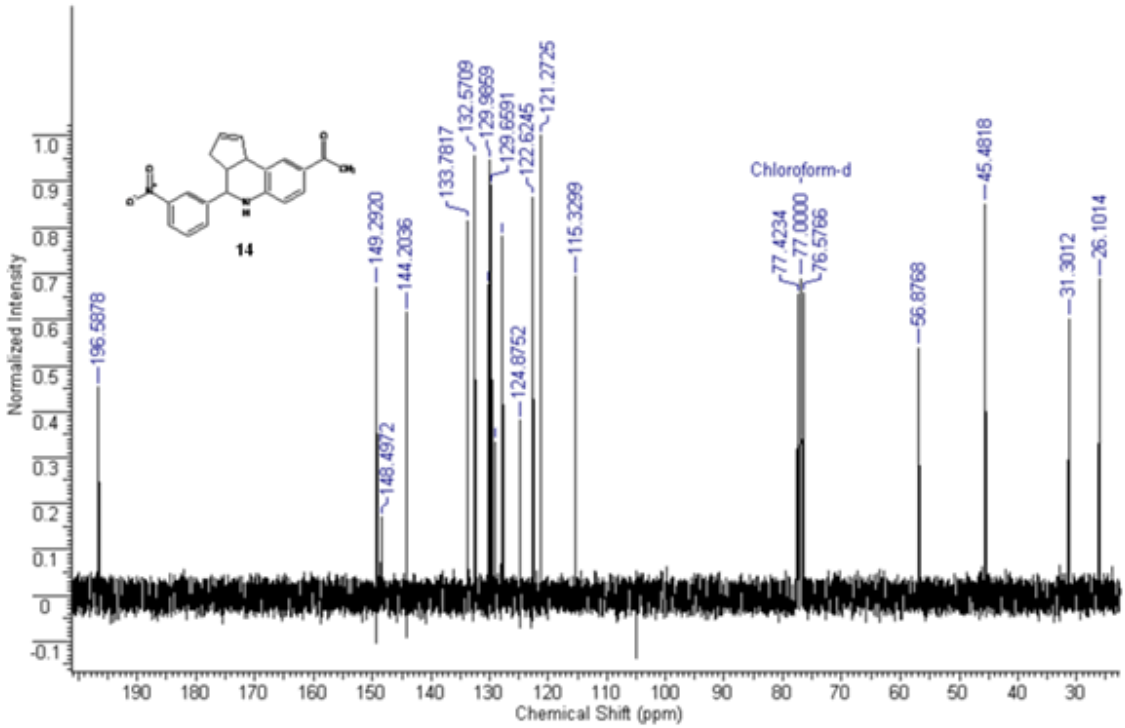


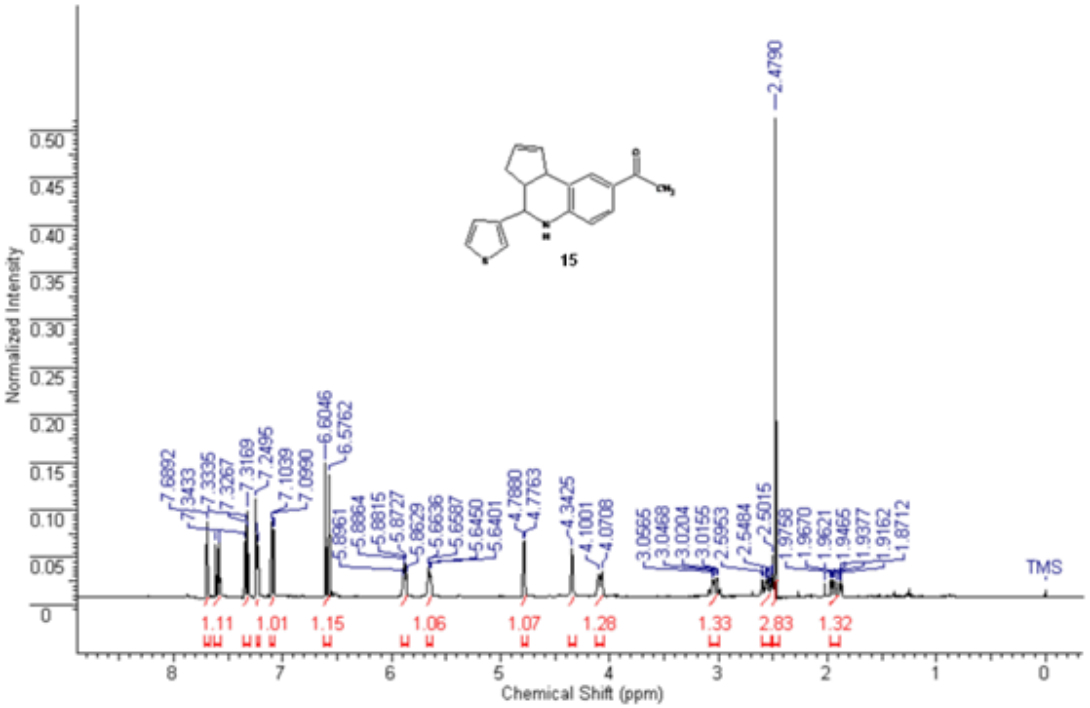


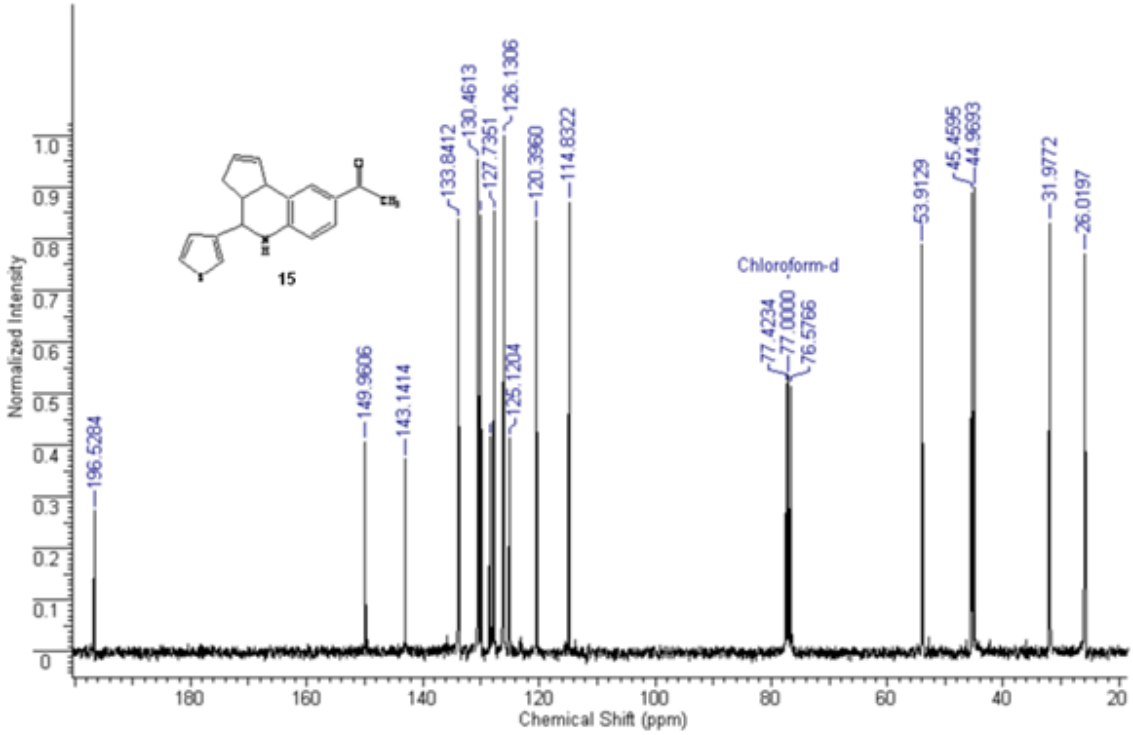


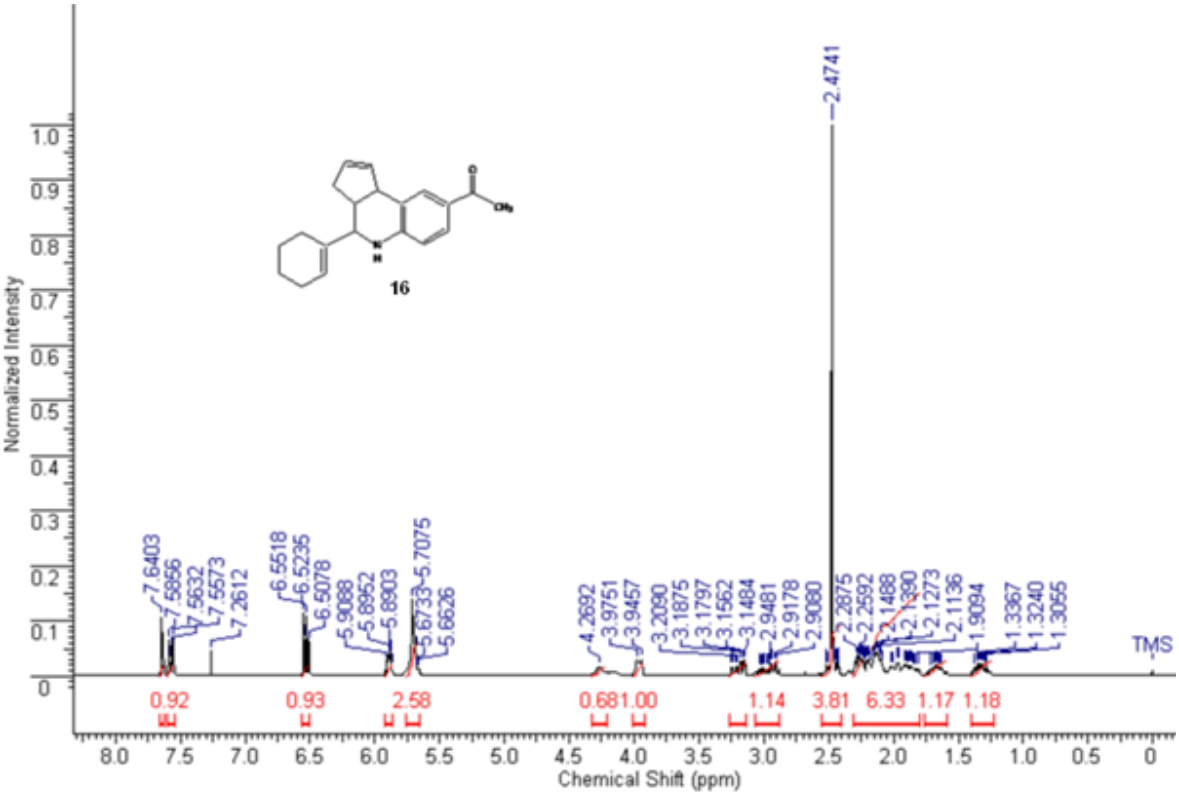


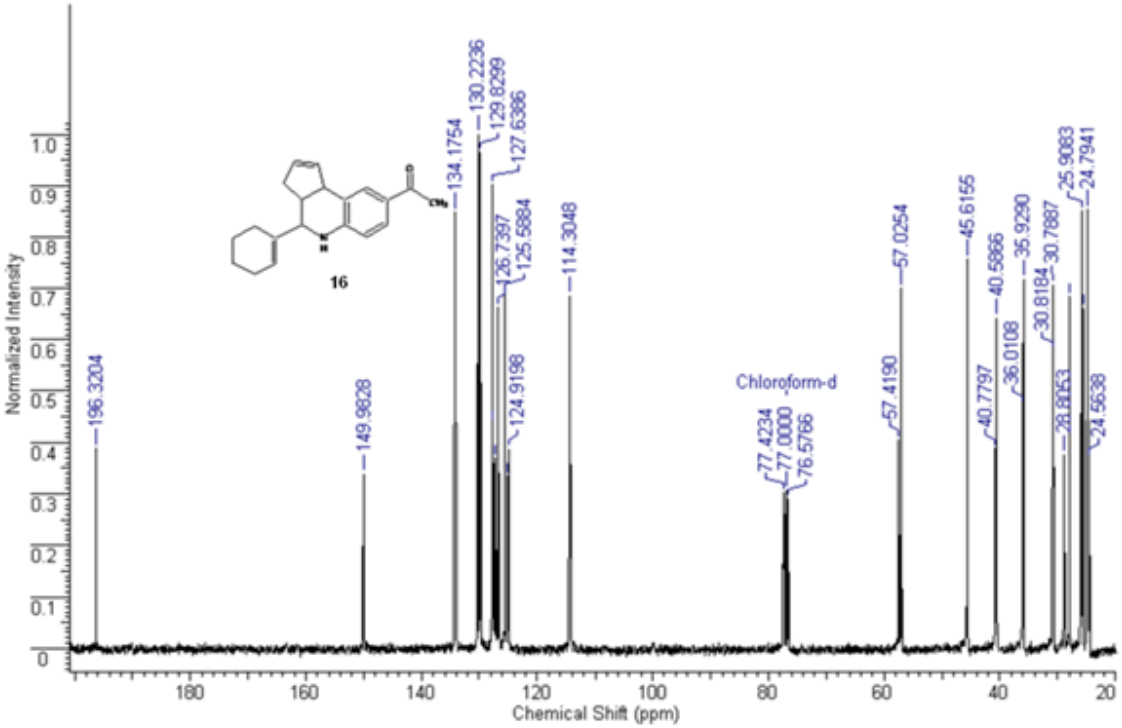


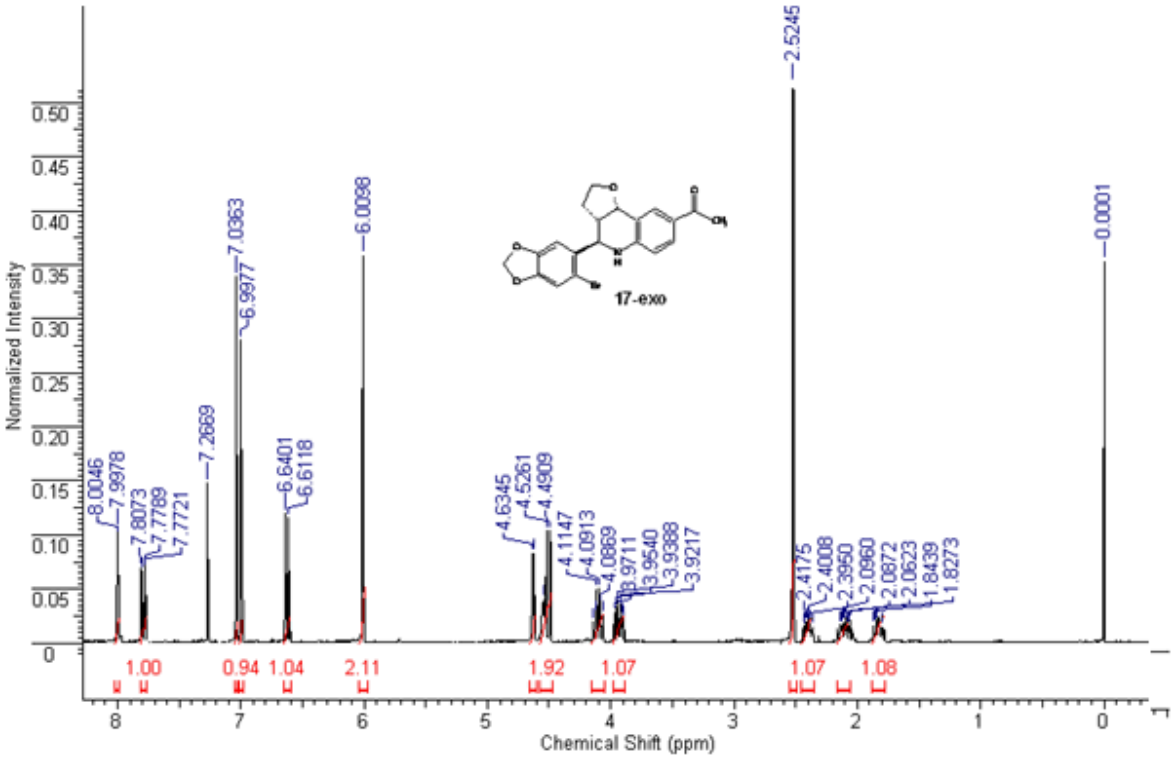


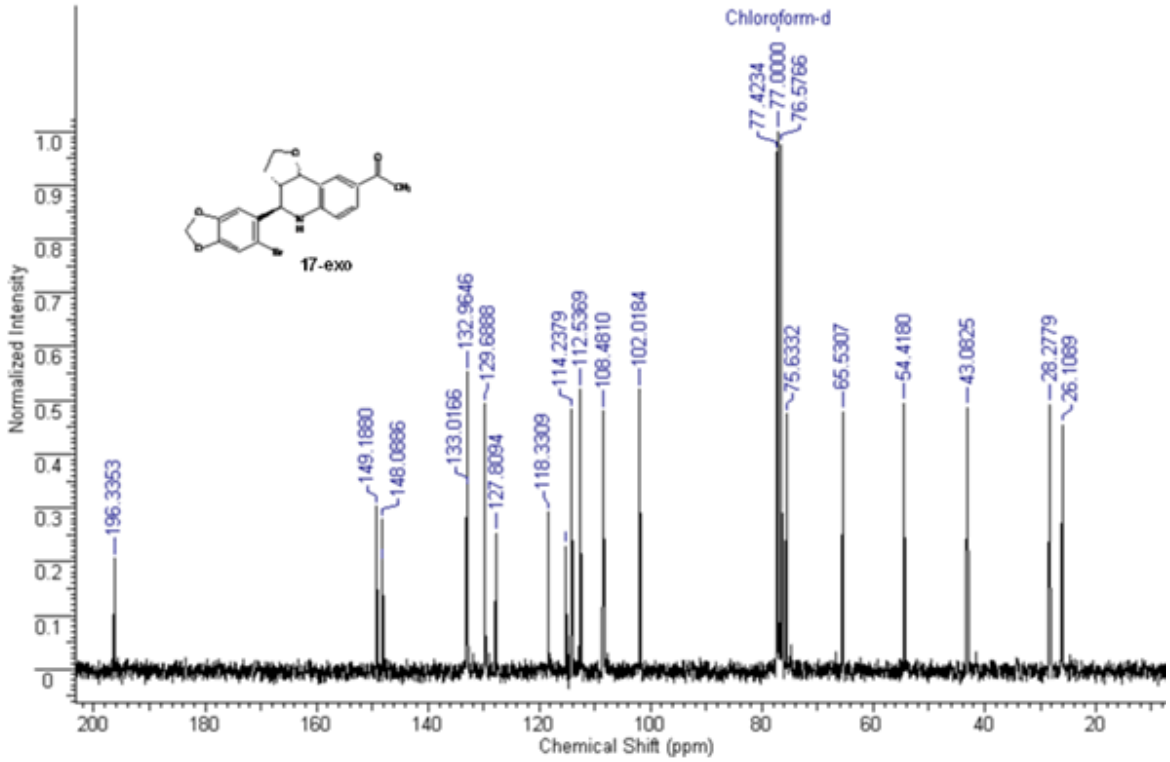


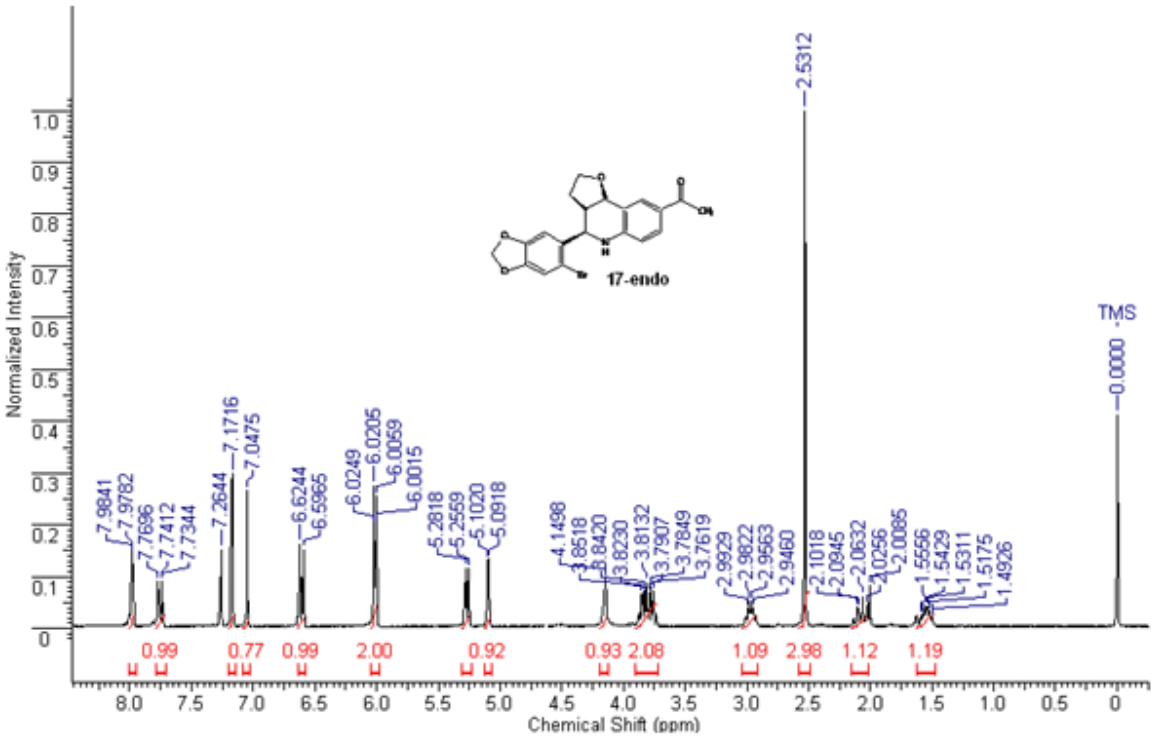


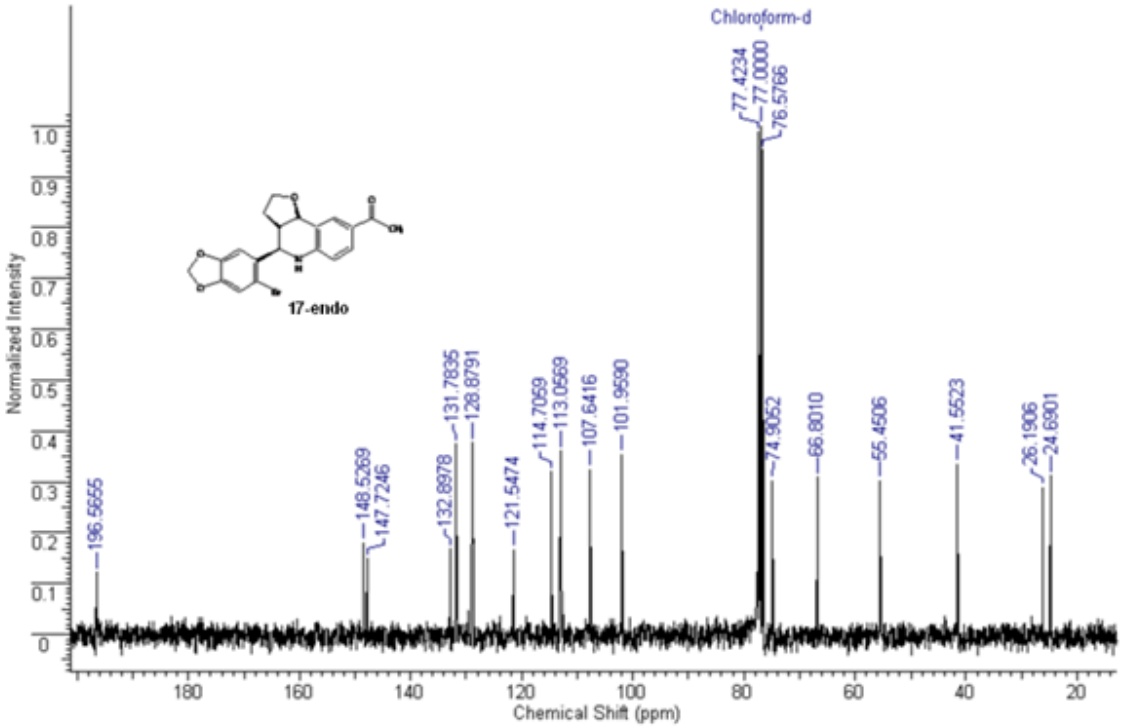






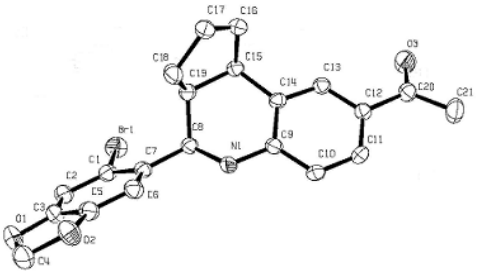






Crystal data and structure refinement for **G-1**.

Identification code	G1	
Empirical formula	C21 H18 Br N O3	
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>2sigma(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.