Supporting information

SYNTHESIS AND RADICAL SCAVENGING ACTIVITIES OF TOCOPHEROL ANALOGS CONTAINING HETEROCYCLIC RINGS

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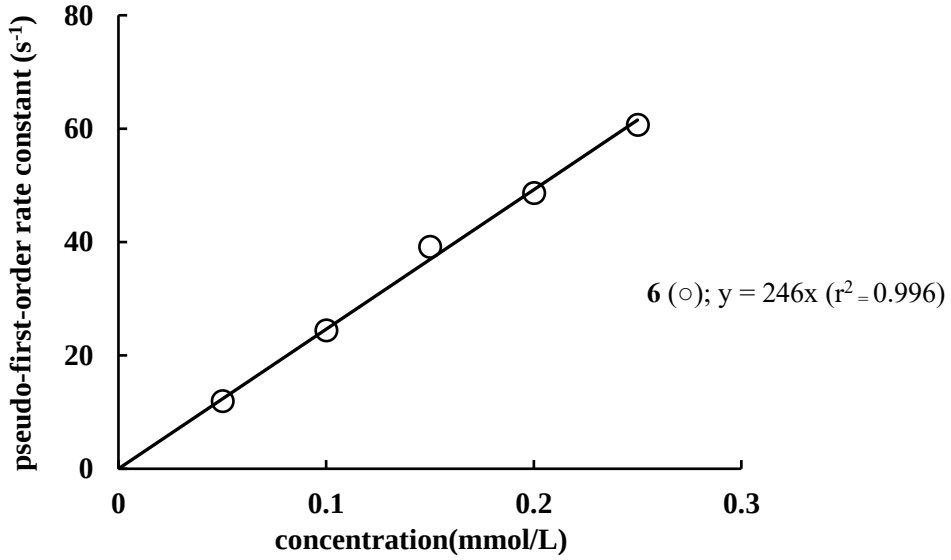


Figure S1 Plot of pseudo-first order rate constant versus concentration of **6** (○)

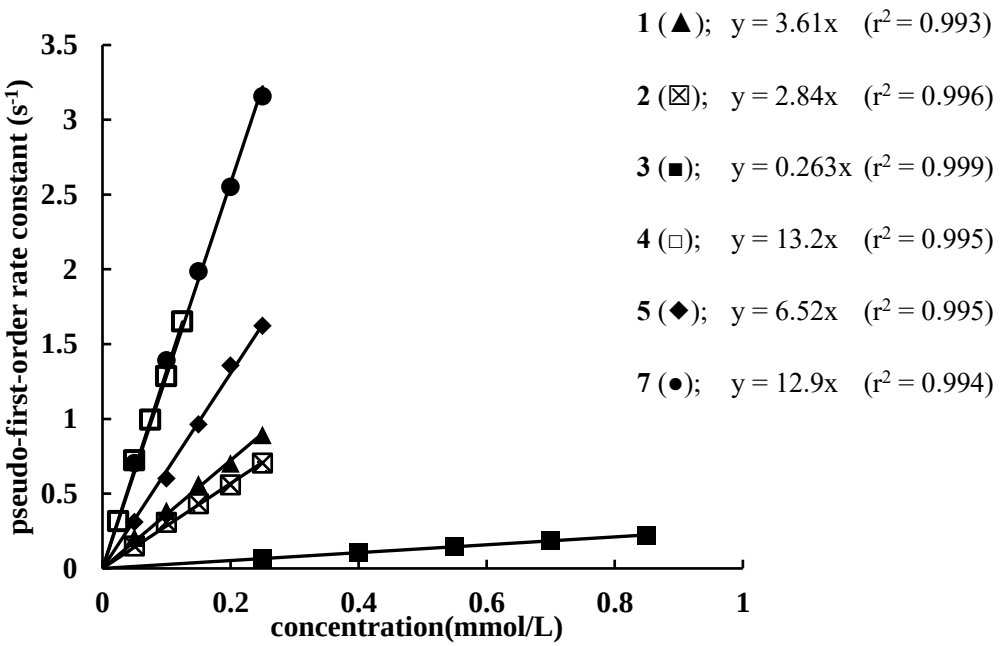


Figure S2 Plot of pseudo-first order rate constant versus concentration of **1** (▲), **2** (☒), **3** (■), **4** (□), **5** (◆), and **7** (●)

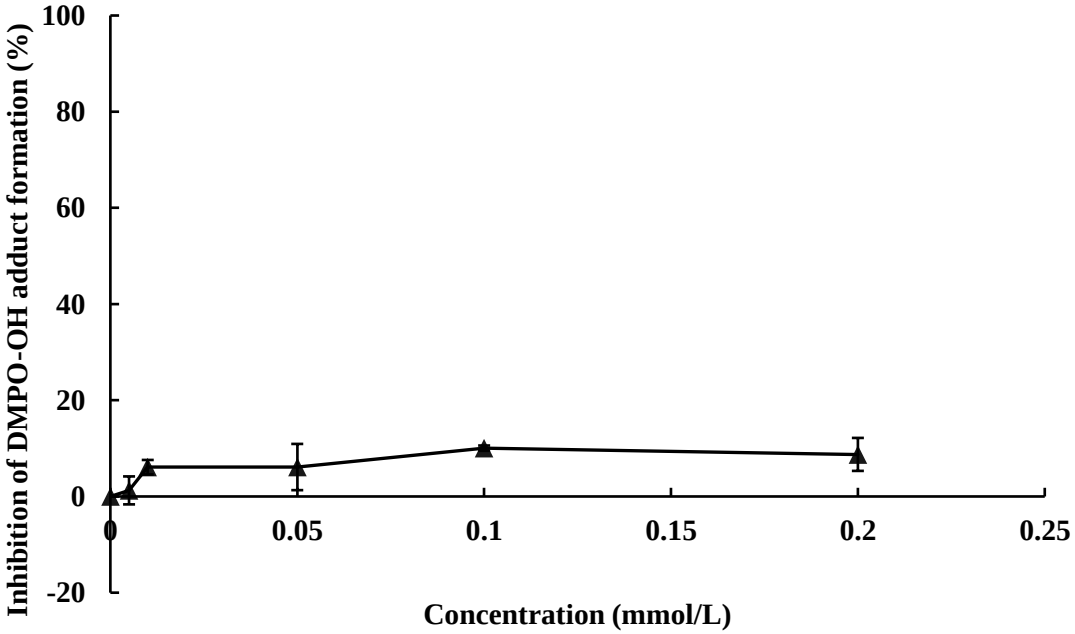


Figure S3 Inhibition (%) of DMPO-OH adduct formation by **1** (▲)

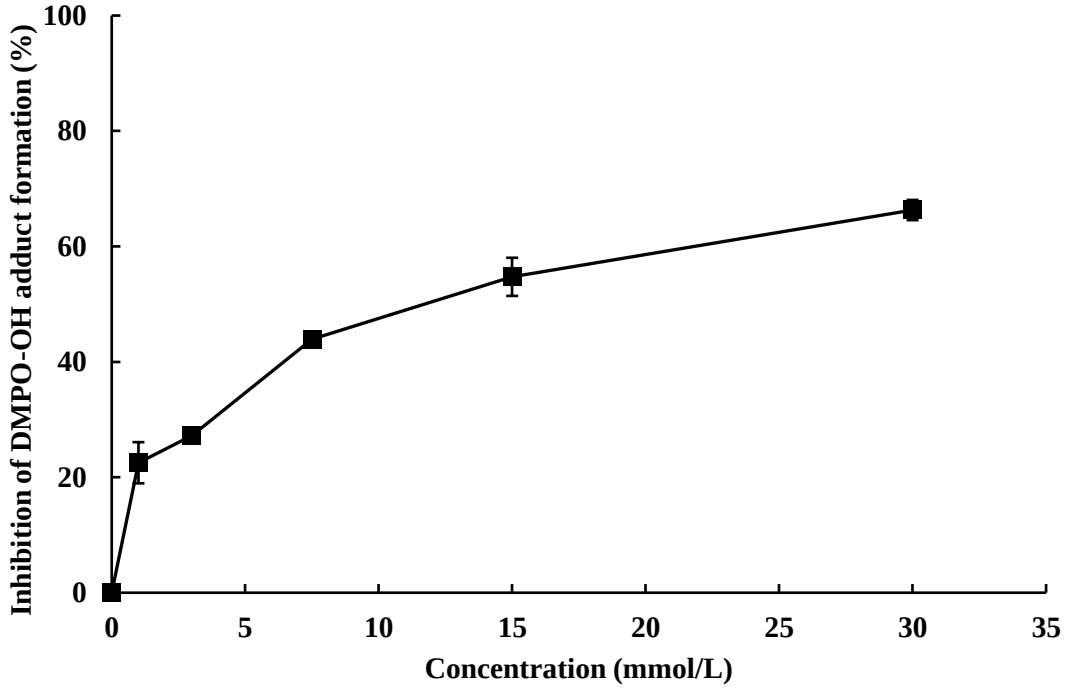


Figure S4 Inhibition (%) of DMPO-OH adduct formation by **3** (■)

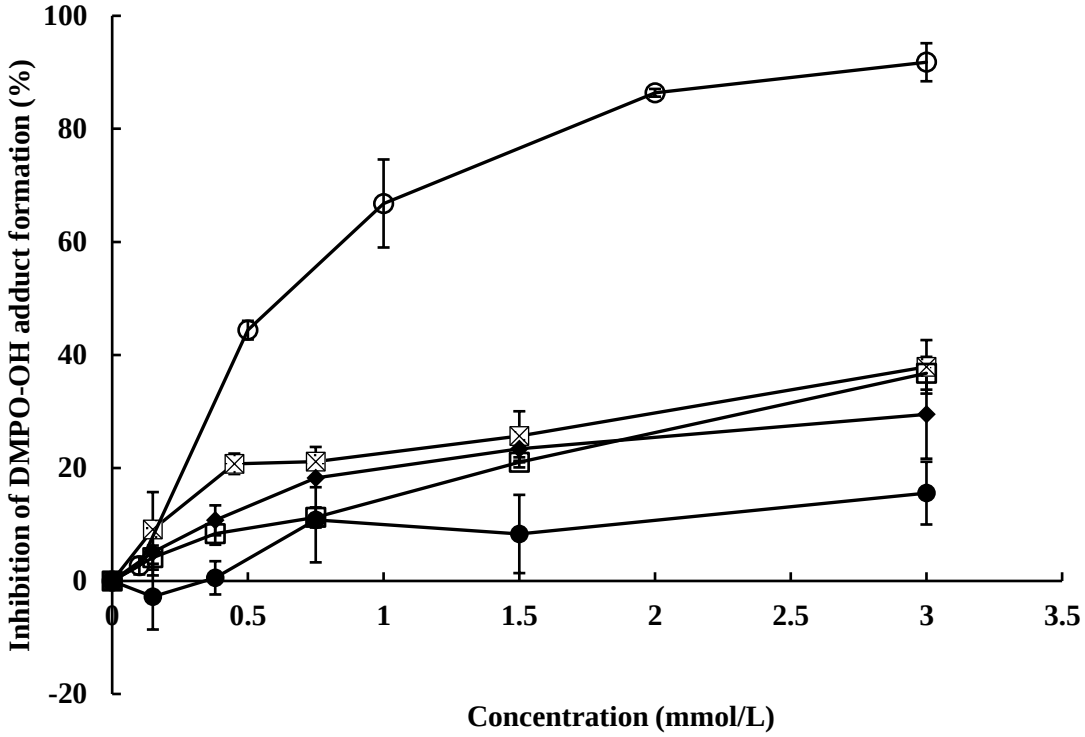


Figure S5 Inhibition (%) of DMPO-OH adduct formation by **2** (☒), **4** (□), **5**, (◆), **6** (○), and **7** (●)

Table S1 CBS-4M Gibbs free energies (in Hartree [a])

	acid	anion
2	-694.934063	-694.378896
3	-577.201734	-576.642827
4	-730.597809	-730.04982
5 (conjugated acid)	-747.011213	-746.630624
5 (hydroxyl group)	-747.011213	-746.087657
6	-708.58983	-708.029482
7 (conjugated acid)	-725.009191	-724.641506
7 (hydroxyl group)	-724.641506	-724.077053

a: optimization with B3LYP/6-31G(d)

Table S2 Solvation energies of acids and their anions (in kcal/mol [a])

	acid	anion
2	-10.81	-72.97
3	-8.40	-78.22
4	-13.85	-72.72
5 (conjugated acid)	-62.83	-20.83
5 (hydroxyl group)	-20.83	-76.01
6	-18.42	-83.23
7 (conjugated acid)	-77.93	-22.07
7 (hydroxyl group)	-22.07	-92.57

a: optimization with HF/6-31G(d) using SMD

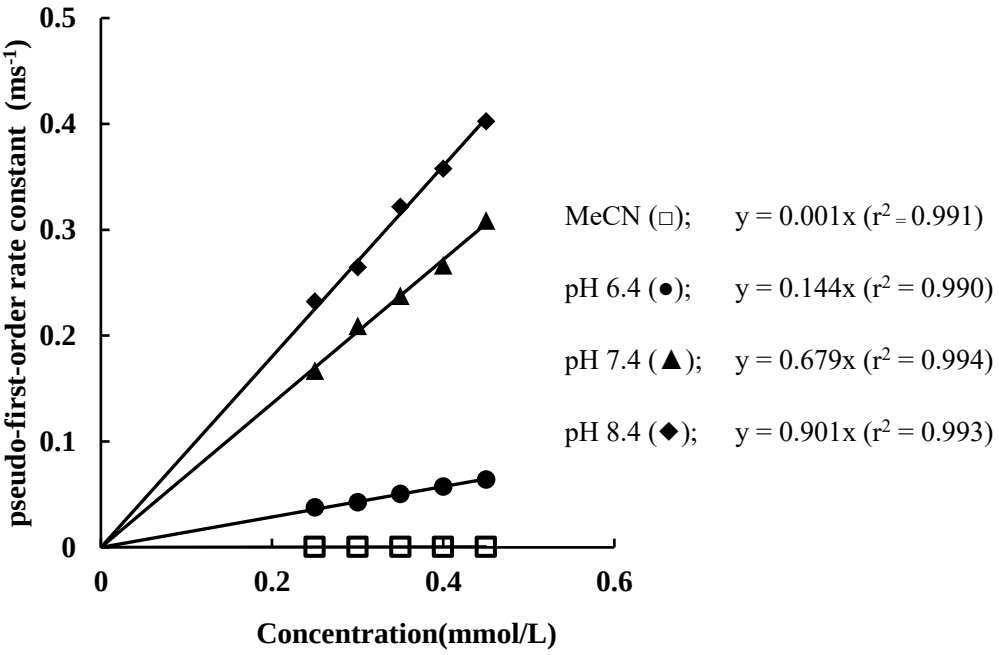
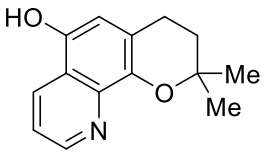
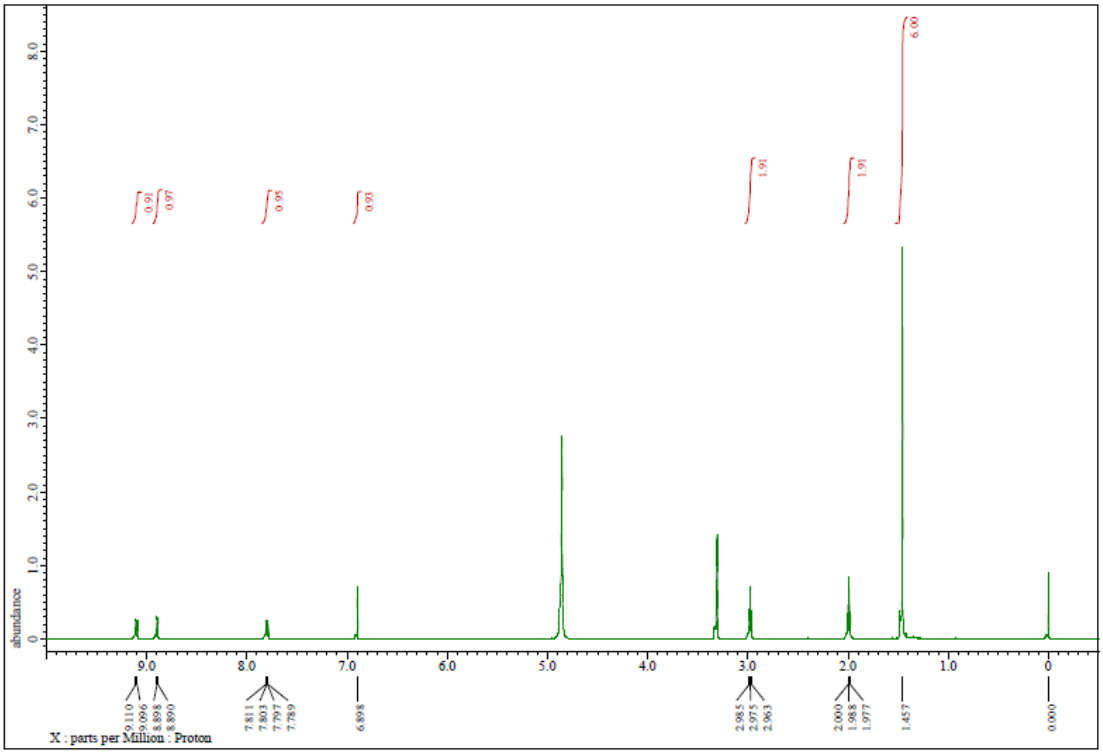
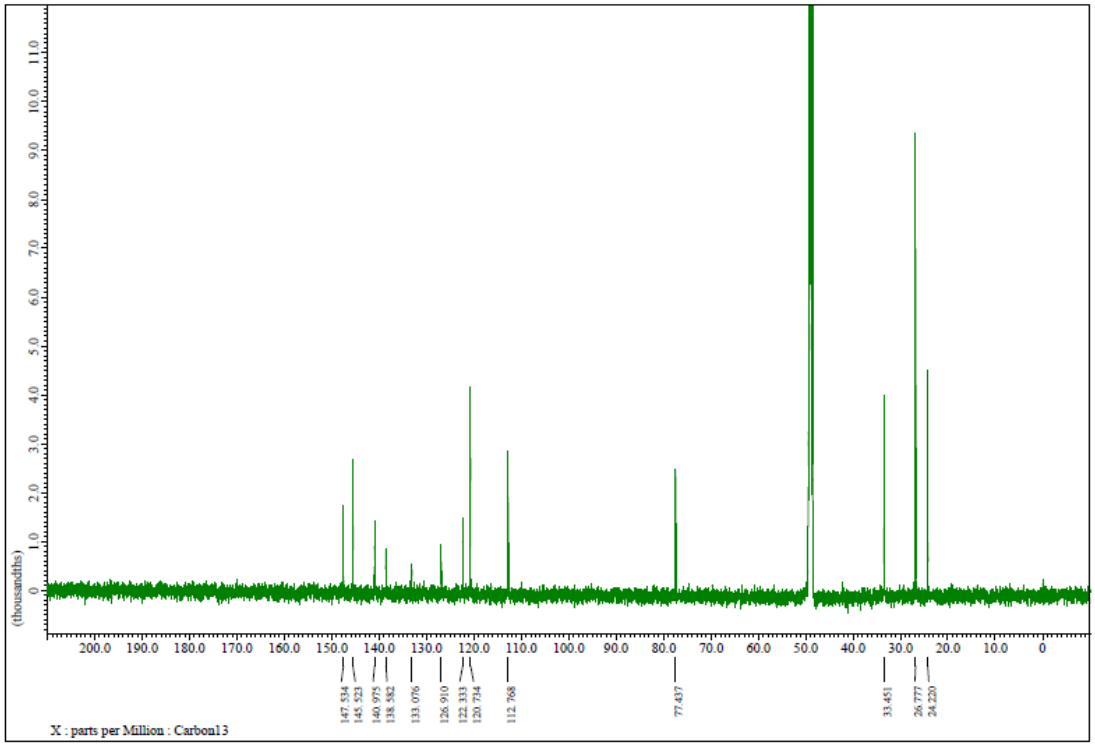


Figure S6 Plot of pseudo-first order rate constant versus concentration of **5** in aqueous solution

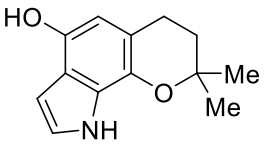
^{1}H and ^{13}C spectra of 2,2-dimethyl-3,4-dihydro-2*H*-pyrano[3,2-*h*]quinolin-6-ol (**5**)

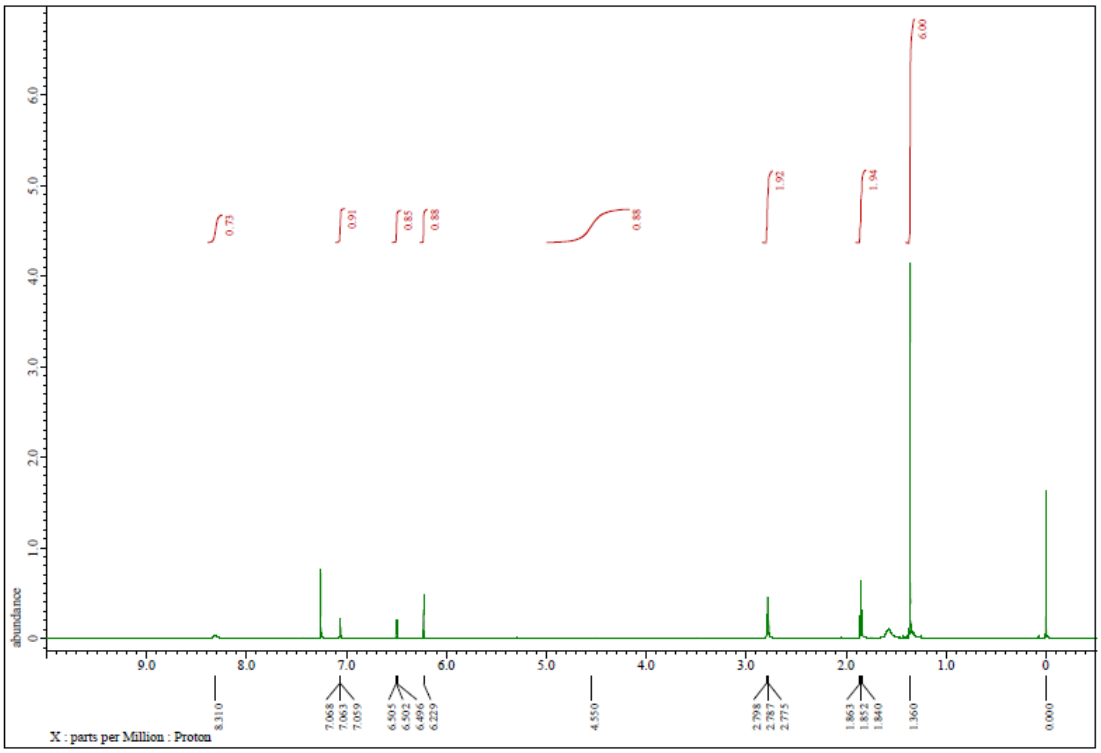


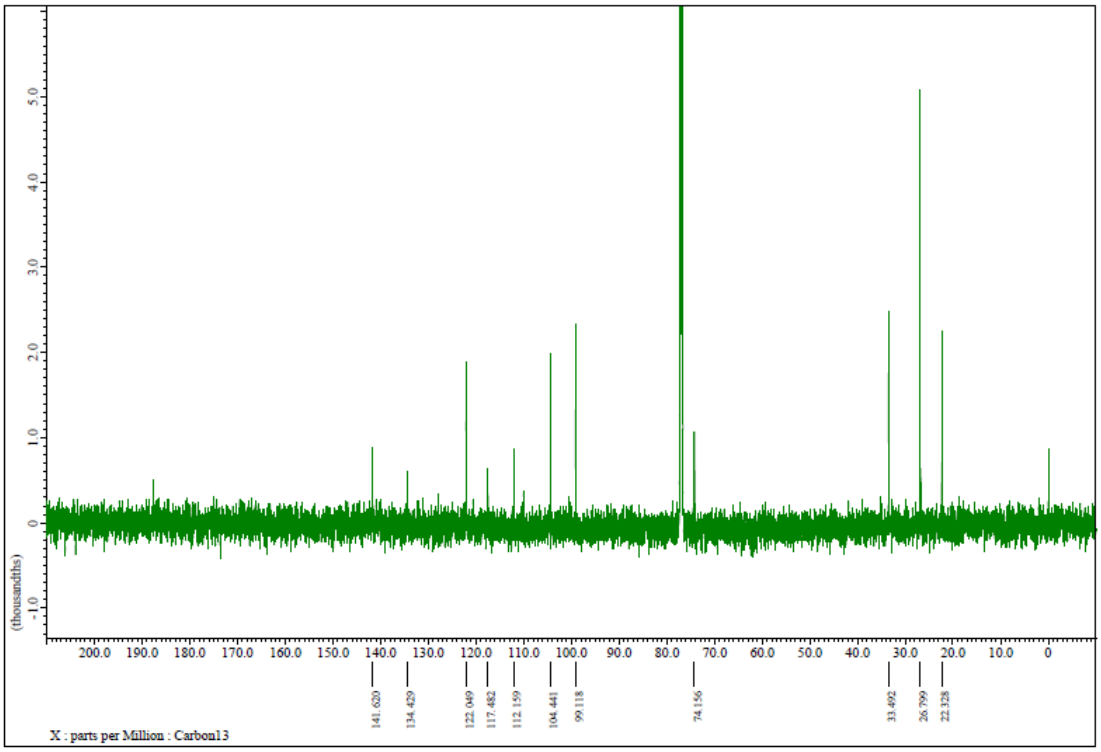




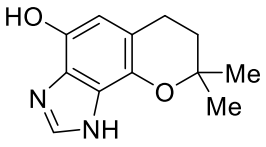
^{1}H and ^{13}C spectra of 2,2-dimethyl-2,3,4,9-tetrahydropyrano[3,2-*g*]indol-6-ol (**6**)

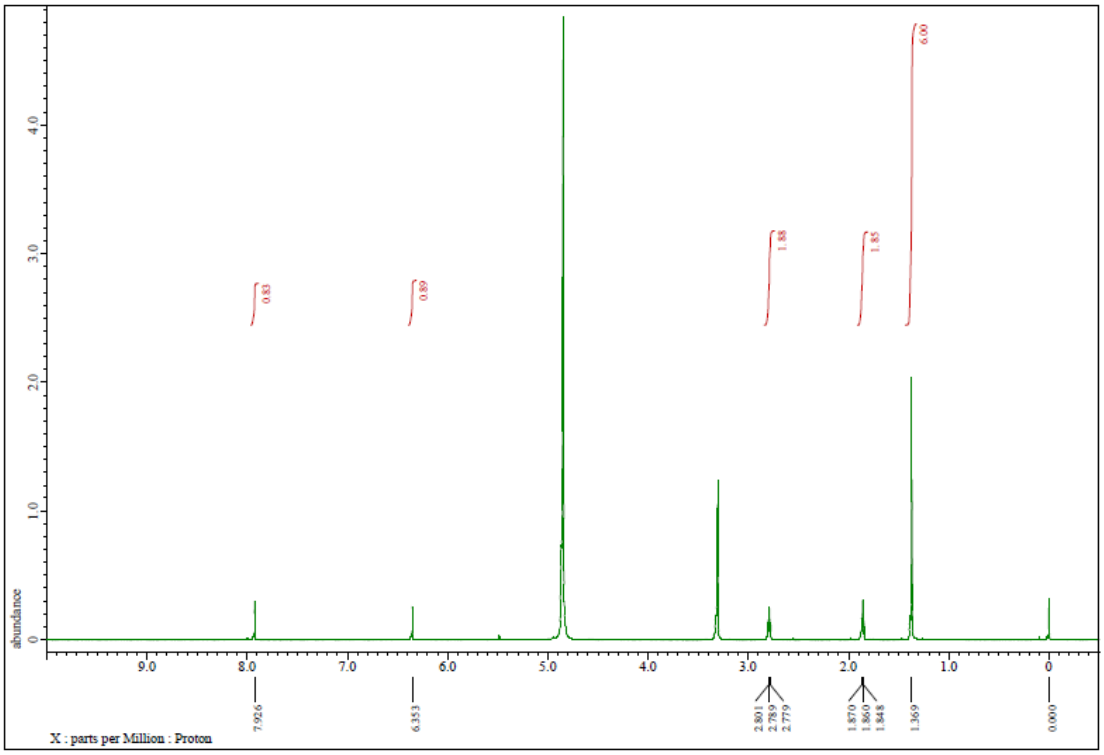


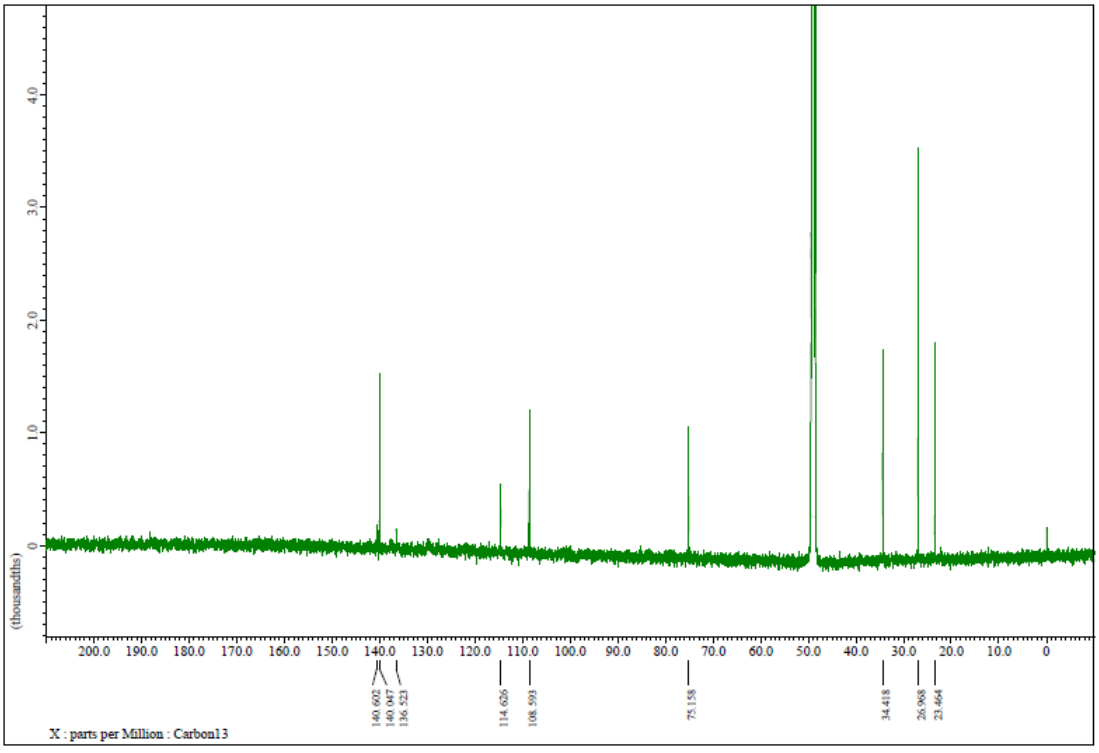




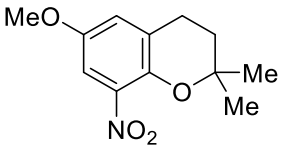
^{1}H and ^{13}C spectra of 8,8-dimethyl-1,6,7,8-tetrahydrochromeno[7,8-*d*]imidazol-4-ol (**7**)

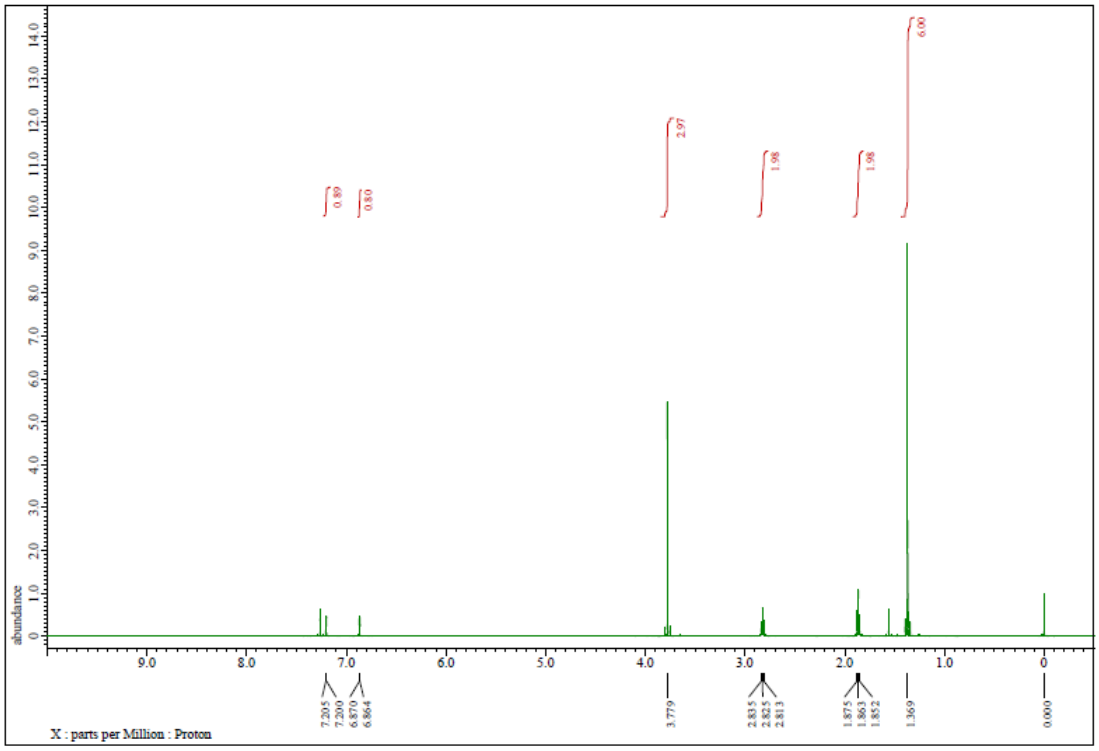


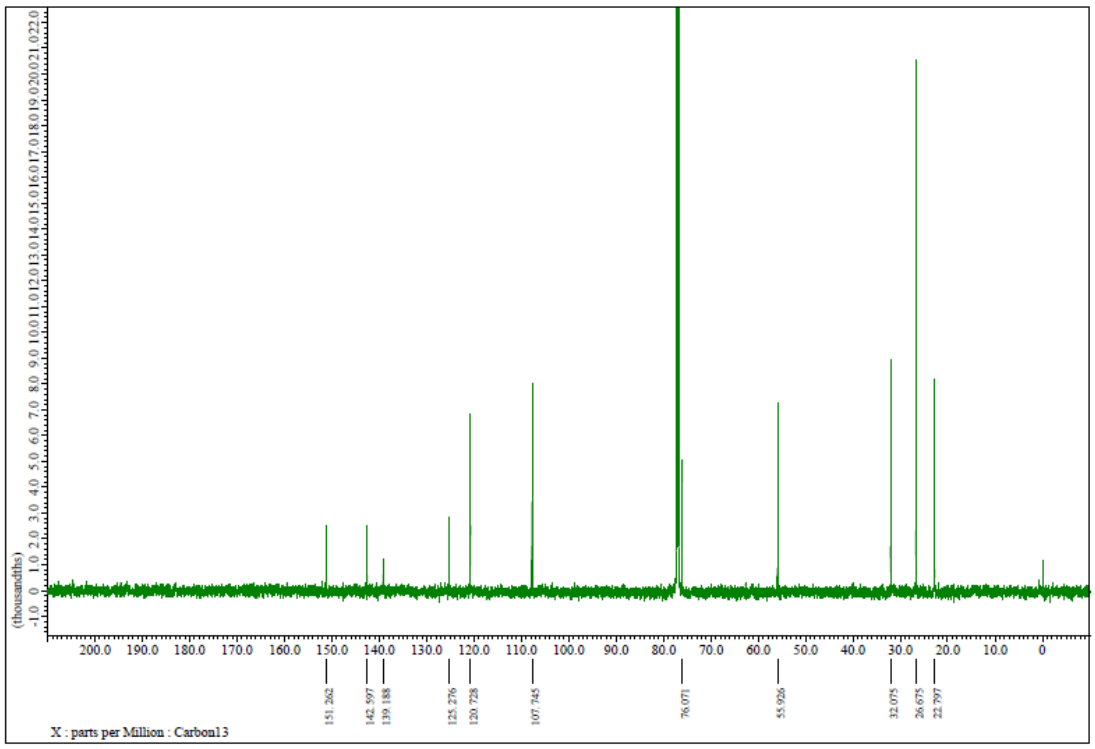




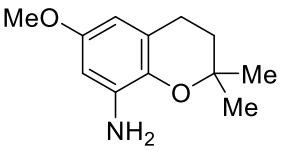
^{1}H and ^{13}C spectra of 6-methoxy-2,2-dimethyl-8-nitrochromane (**8**)

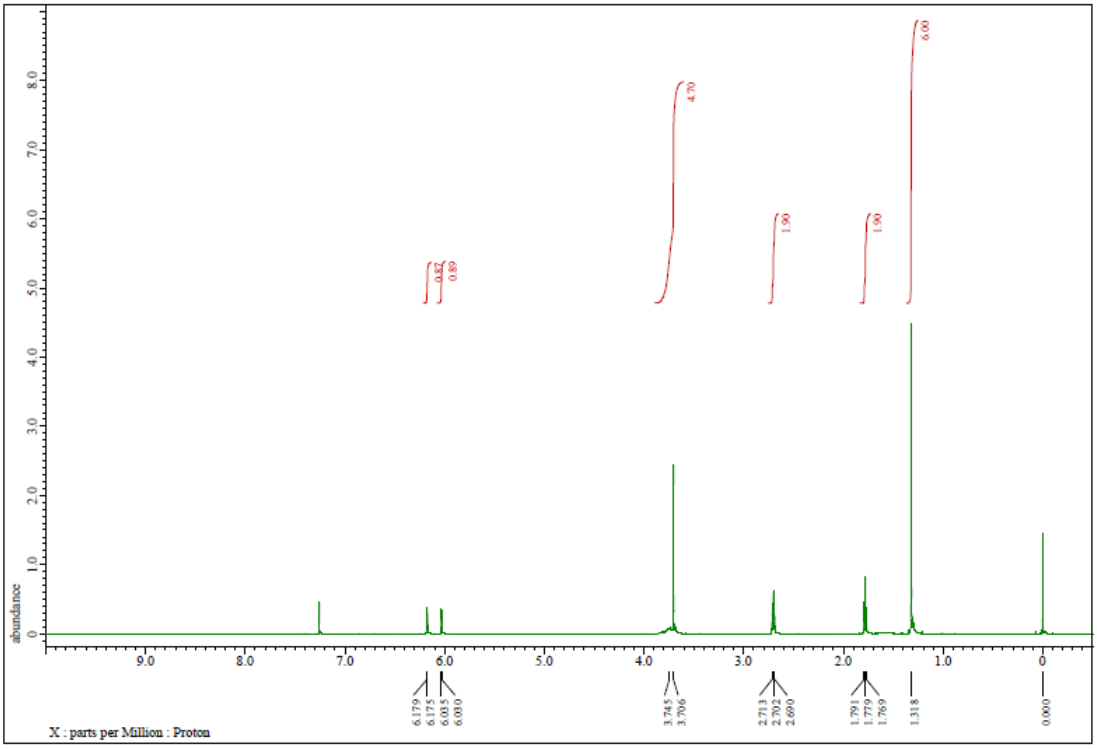


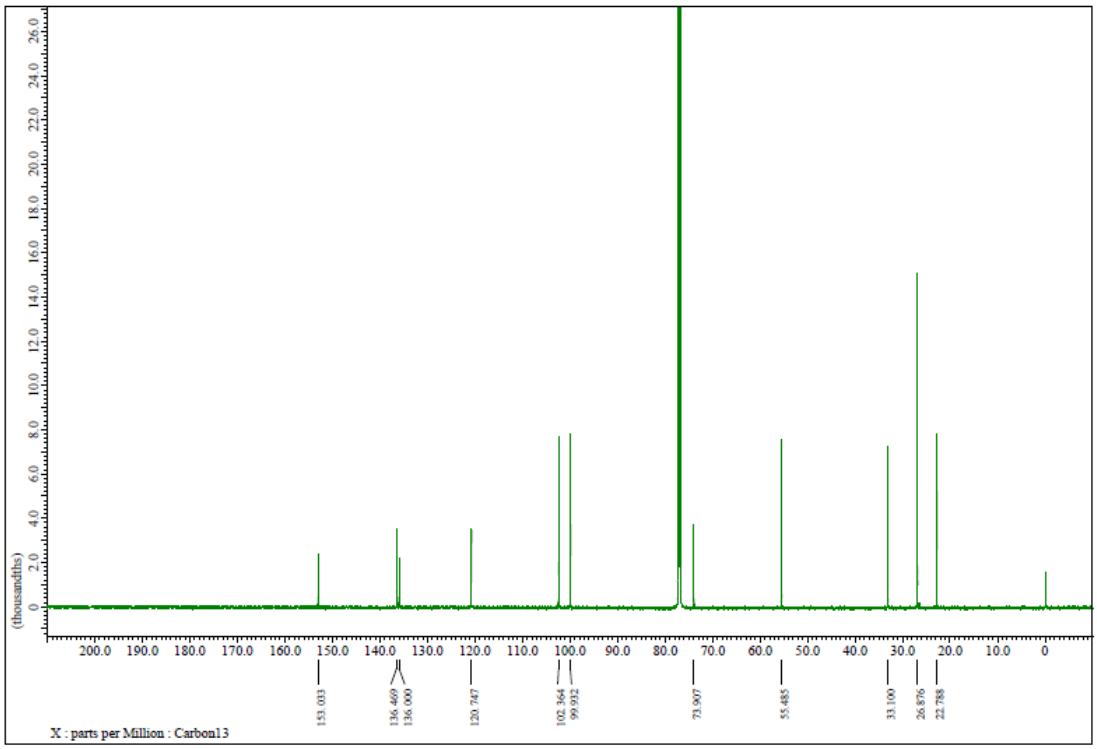




^{1}H and ^{13}C spectra of 8-amino-6-methoxy-2,2-dimethylchroman (**9**)

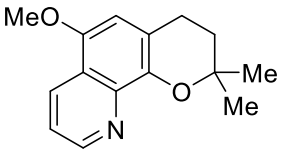


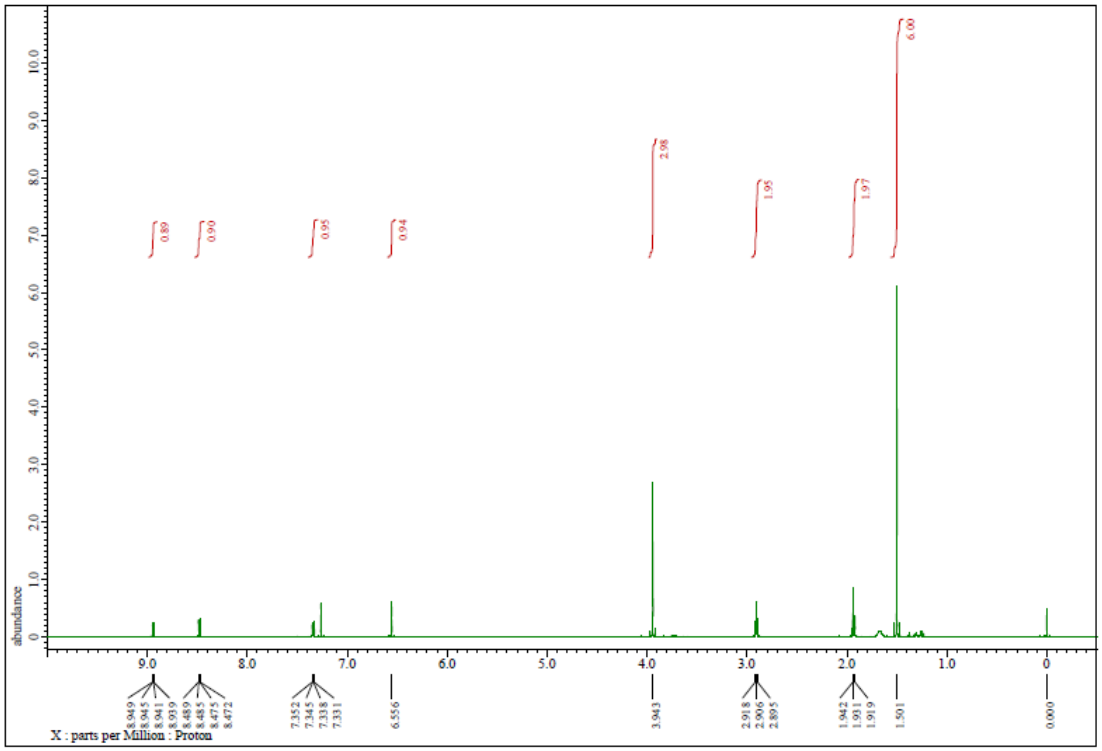


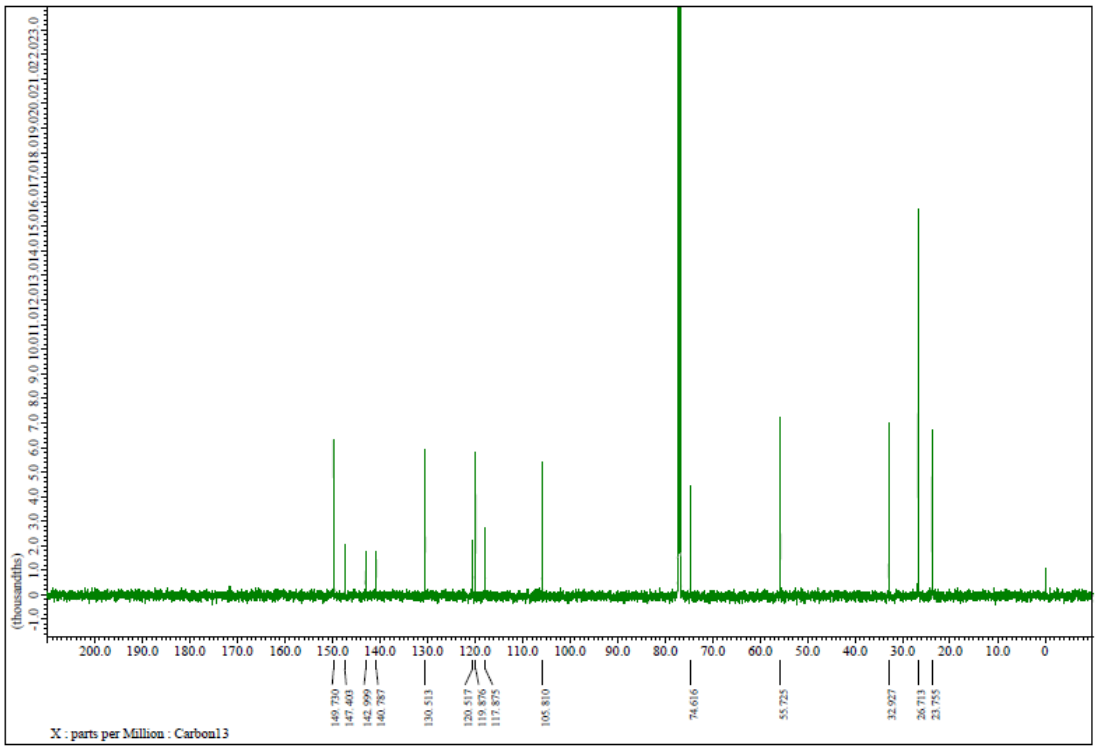


^{1}H and ^{13}C spectra of 6-methoxy-2,2-dimethyl-

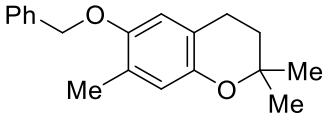
3,4-dihydro-2*H*-pyrano[3,2-*h*]quinoline (**10**)

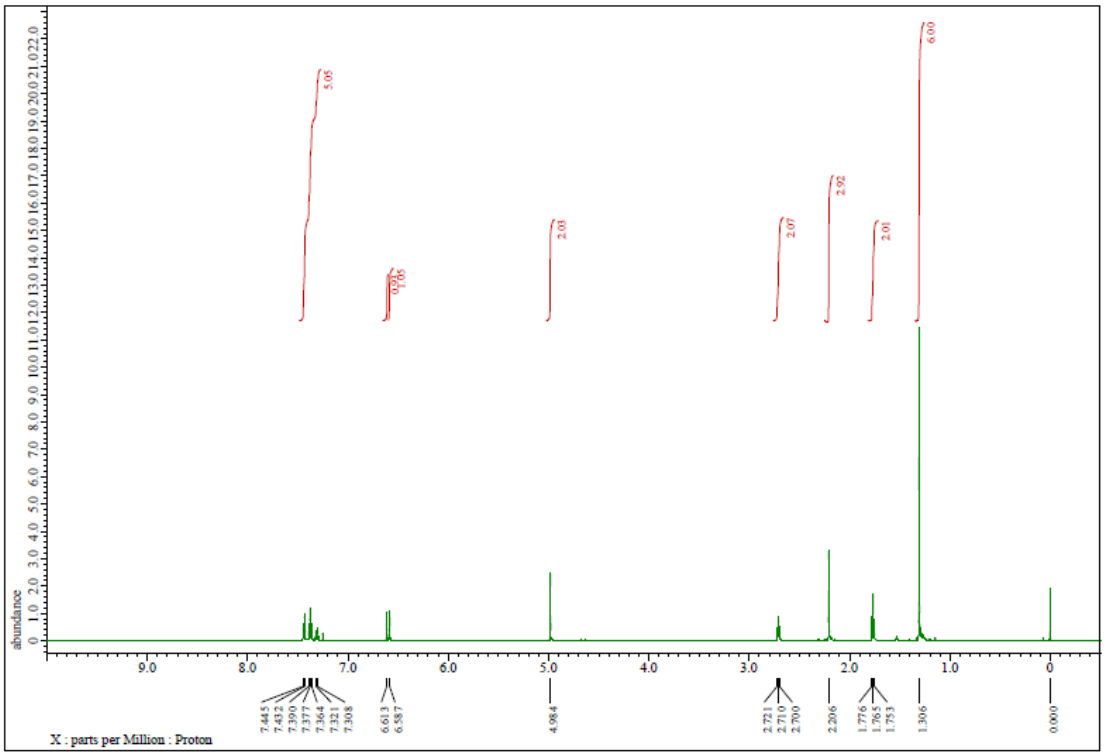


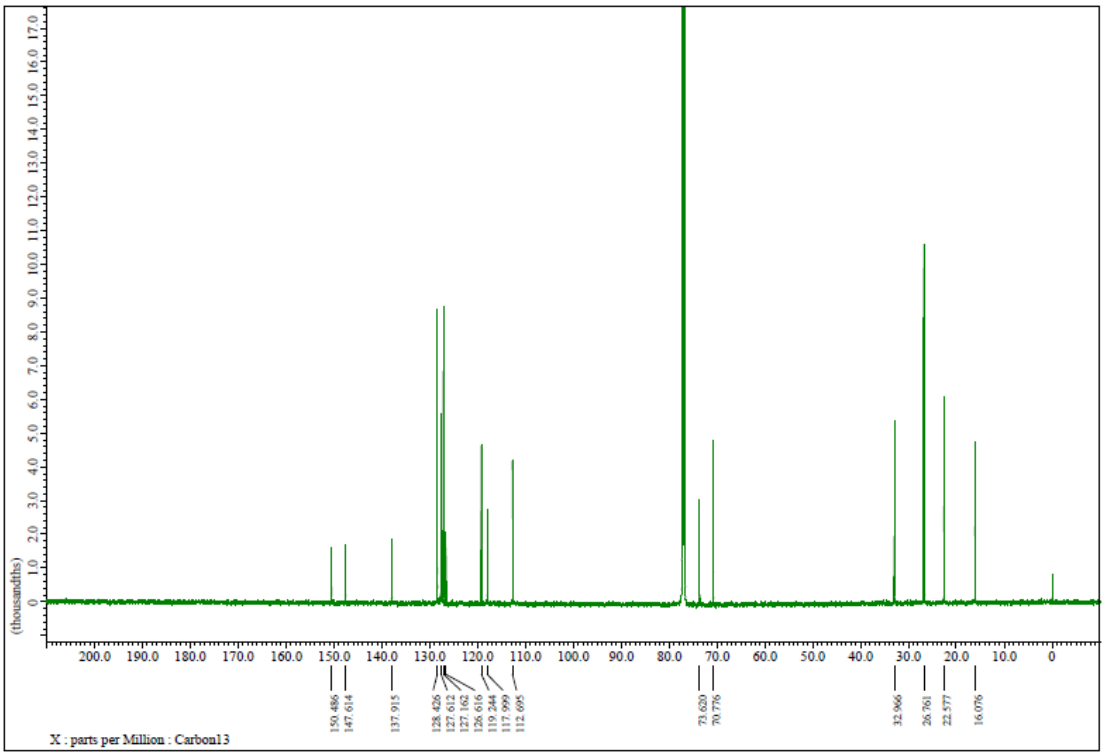




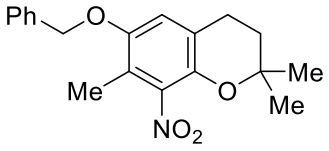
^{1}H and ^{13}C spectra of 6-benzyloxy-2,2,7-trimethylchromane (**11**)

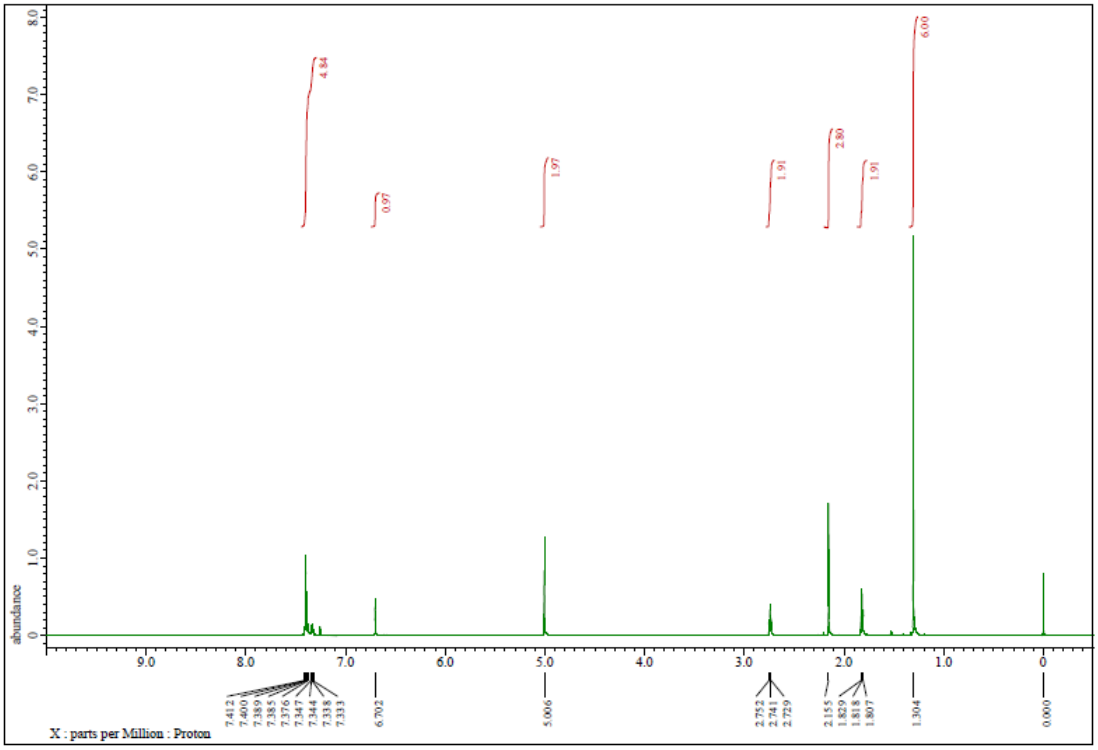


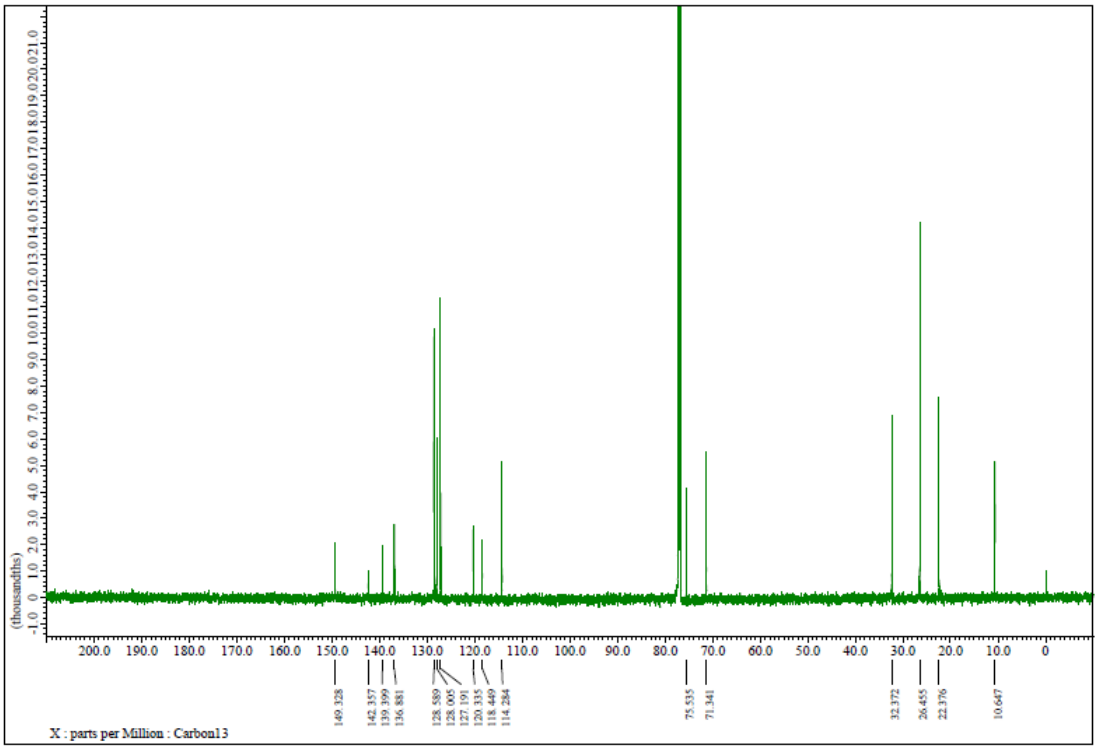




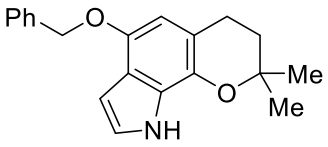
^{1}H and ^{13}C spectra of 6-benzyloxy-2,2,7-trimethyl-8-nitrochromane (**12**)

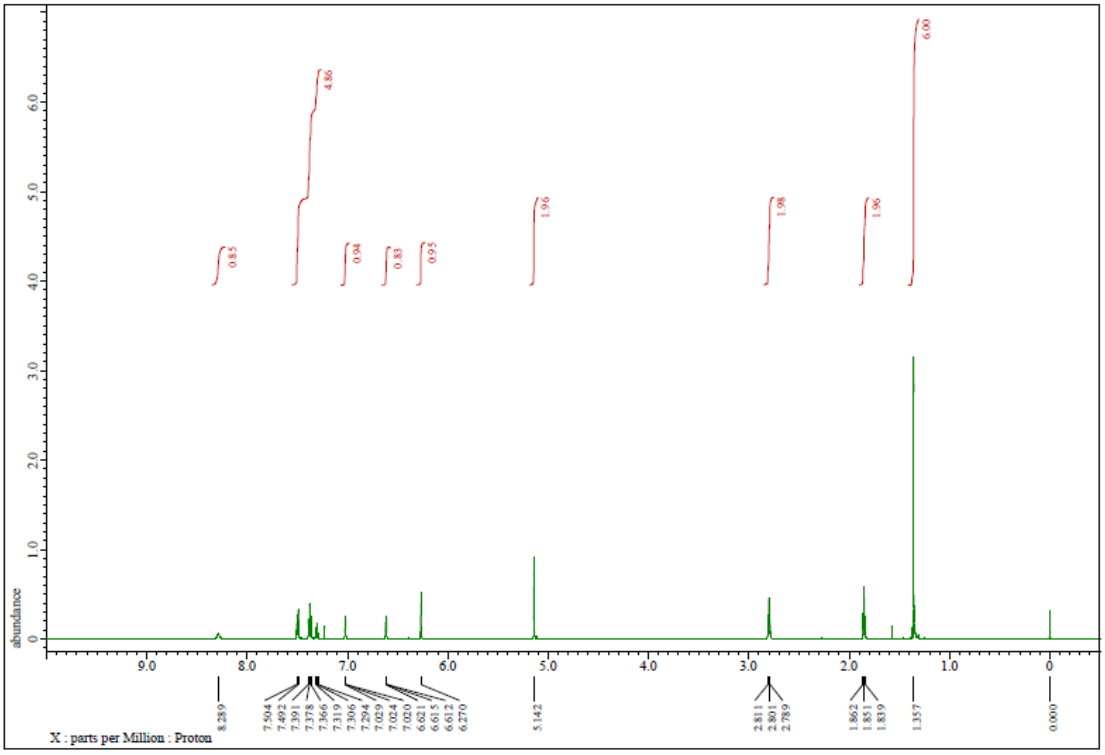


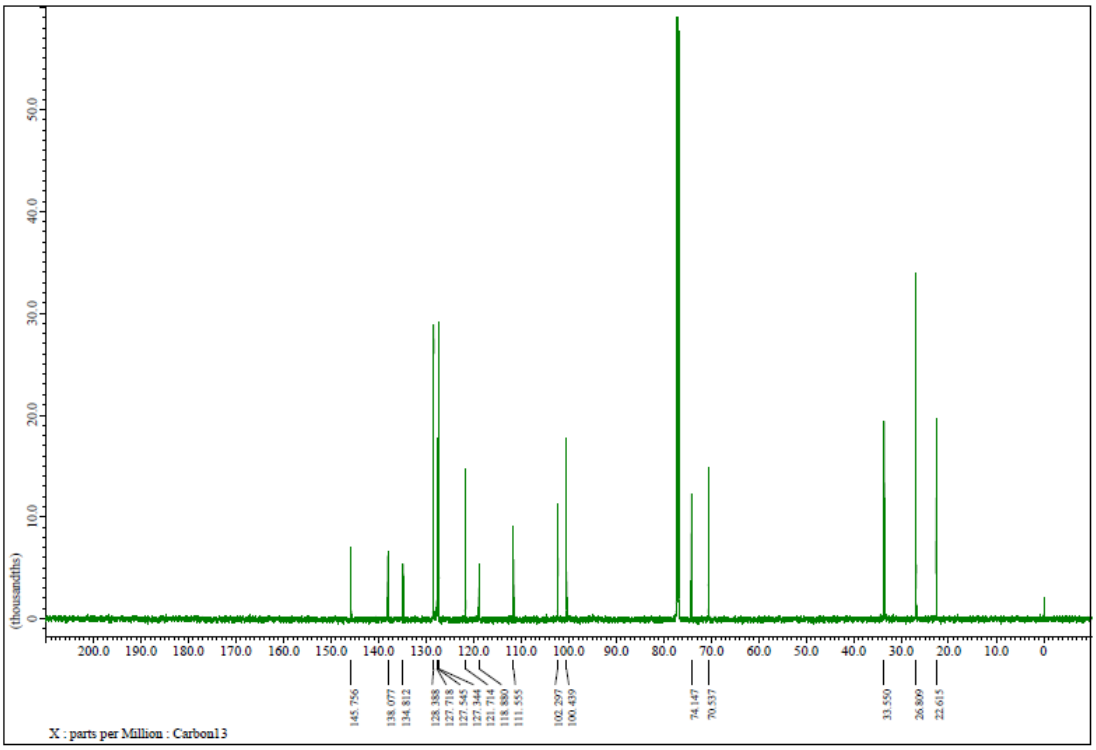




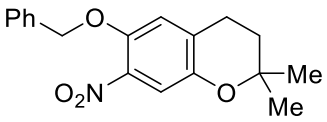
^{1}H and ^{13}C spectra of 6-benzyloxy-2,2-dimethyl-2,3,4,9-tetrahydropyrano[3,2-*g*]indole (**13**)

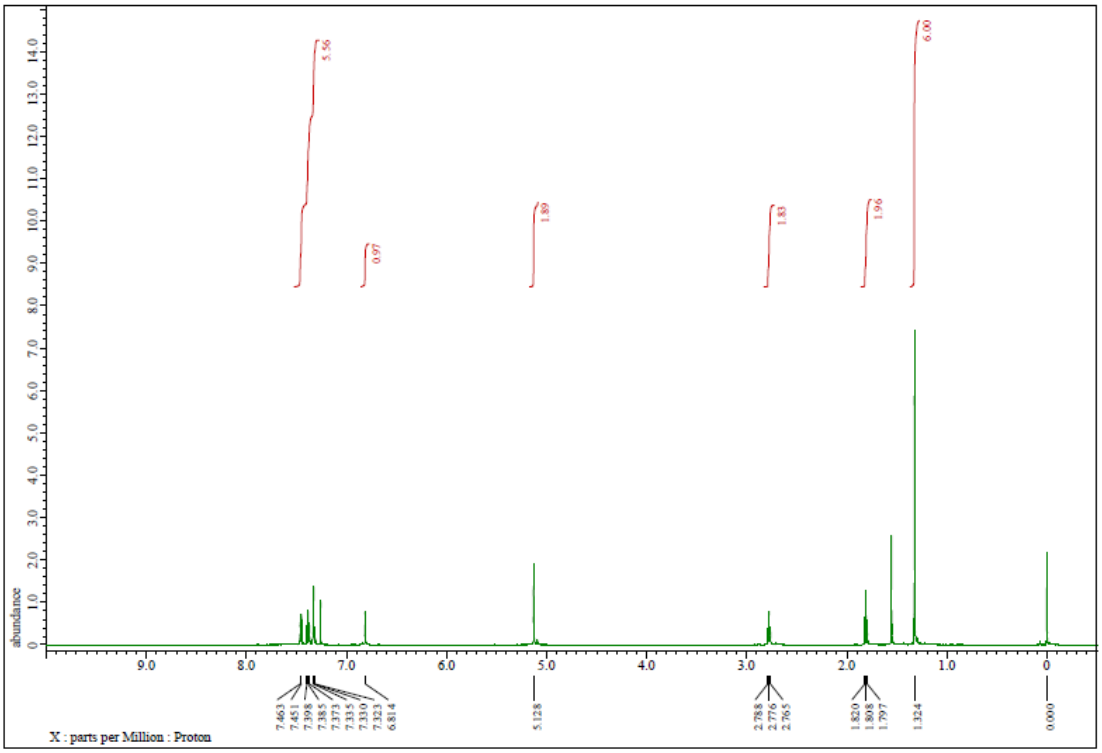


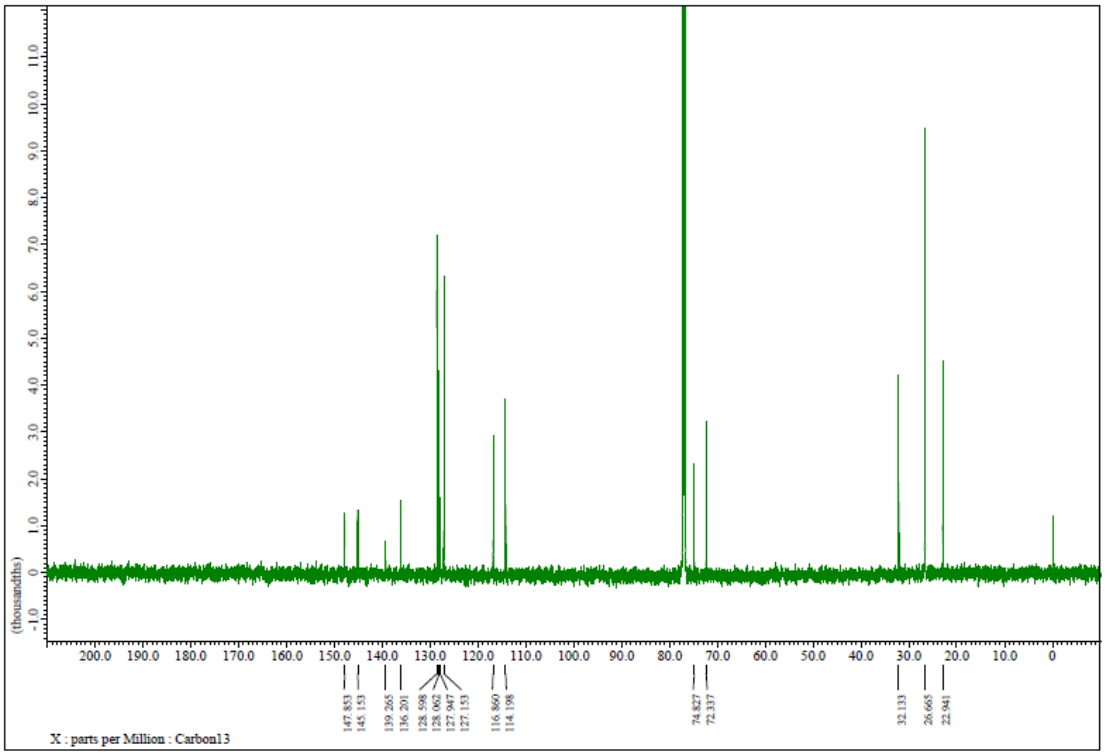




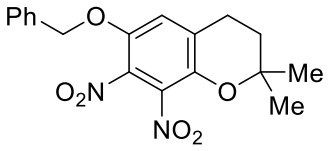
^{1}H and ^{13}C spectra of 6-benzyloxy-2,2-dimethyl-7-nitrochromane (**14**)

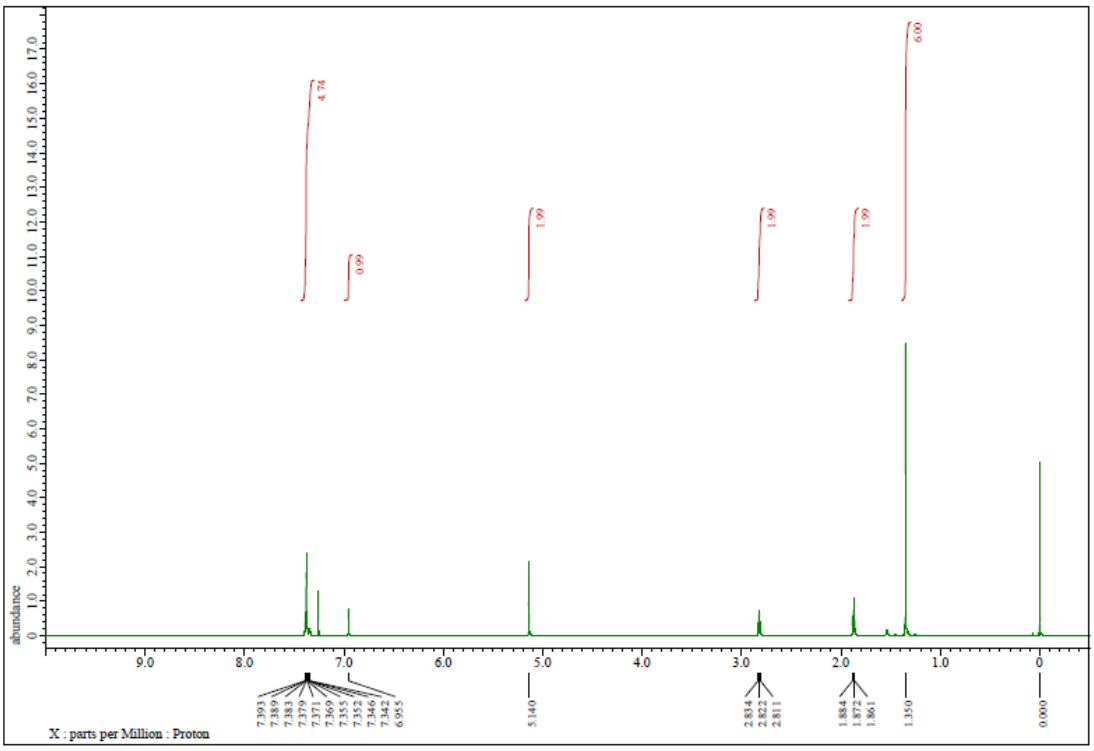


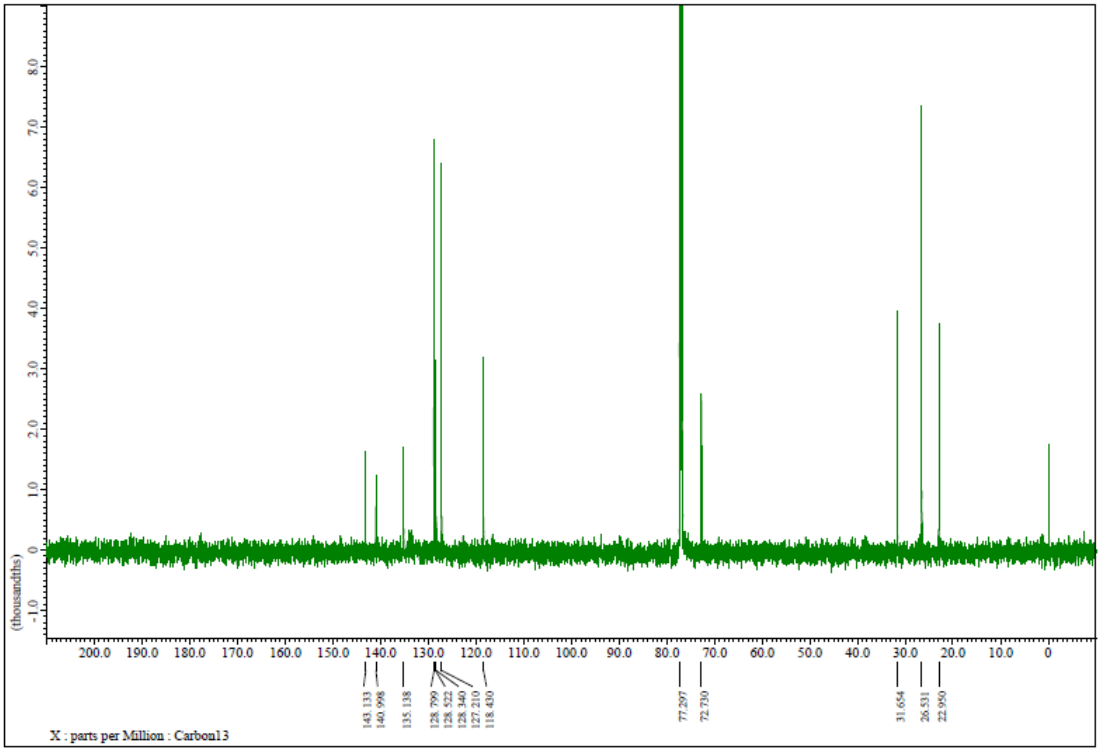




^{1}H and ^{13}C spectra of 6-benzyloxy-2,2-dimethyl-7,8-dinitrochromane (**15**)







^{1}H and ^{13}C spectra of 4-benzyloxy-8,8-dimethyl-1,6,7,8-tetrahydrochromeno[7,8-*d*]imidazole (**16**)