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Deproto-metallation using mixed lithium-zinc and lithium-copper bases and computed CH acidity of 2-substituted quinolines

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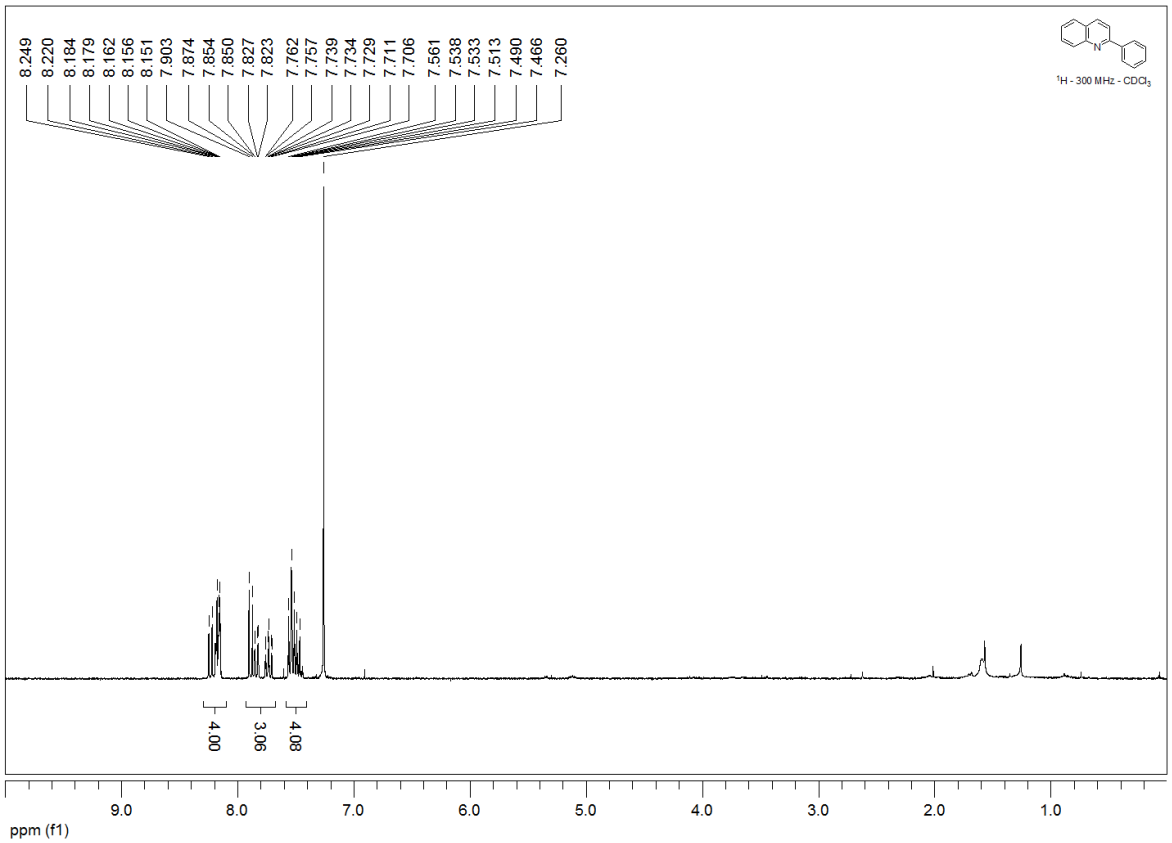
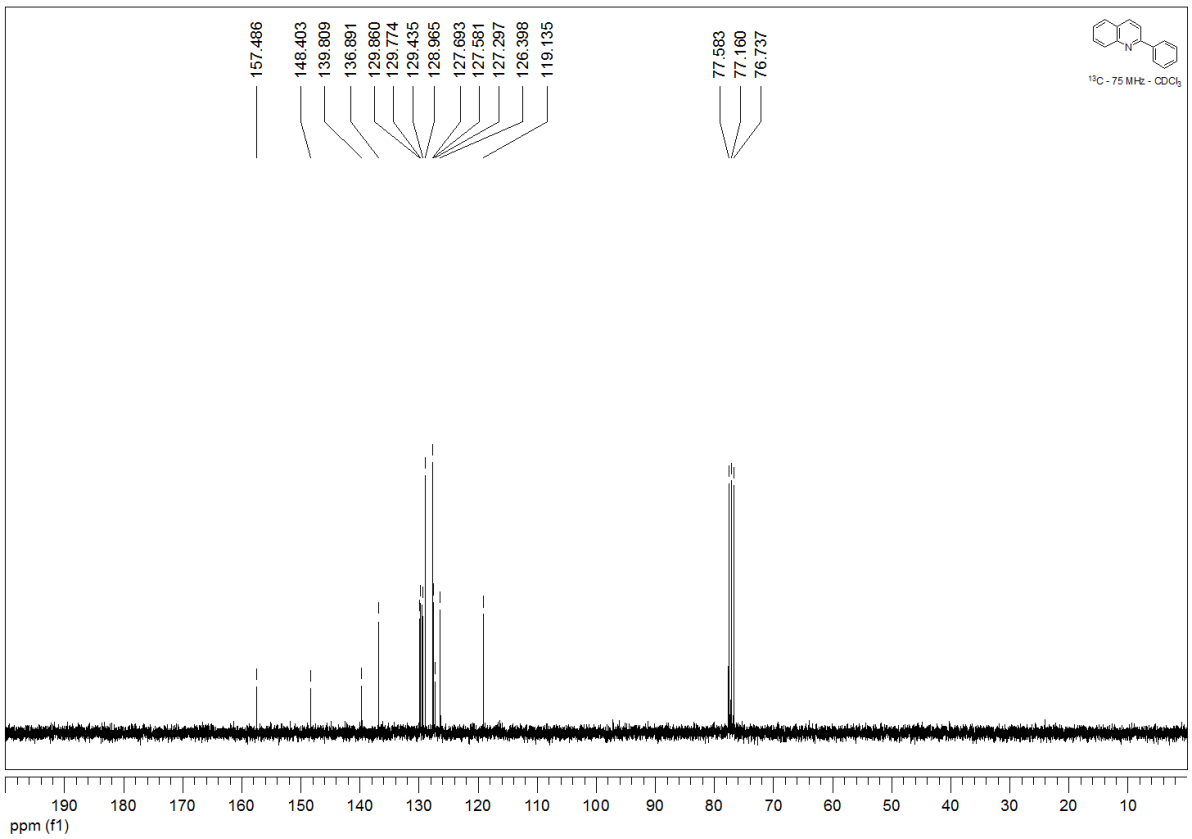
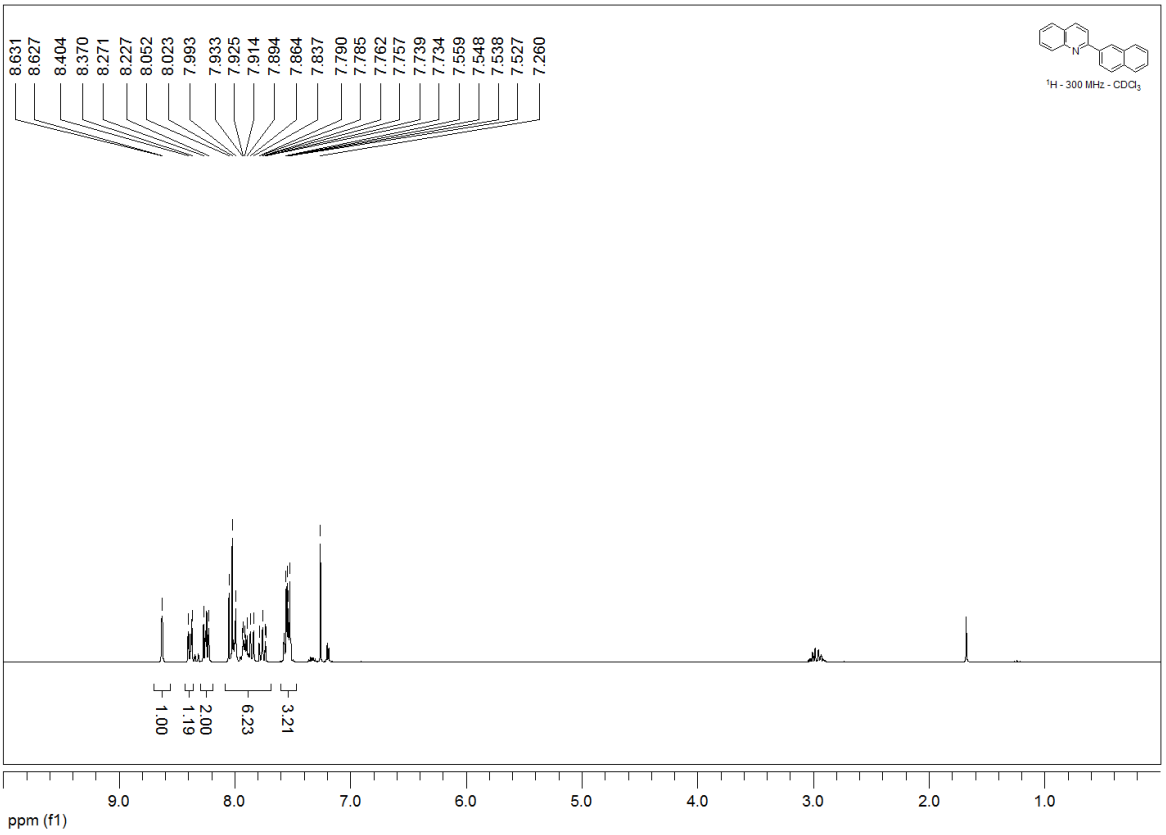
^{1}H and ^{13}C NMR spectra

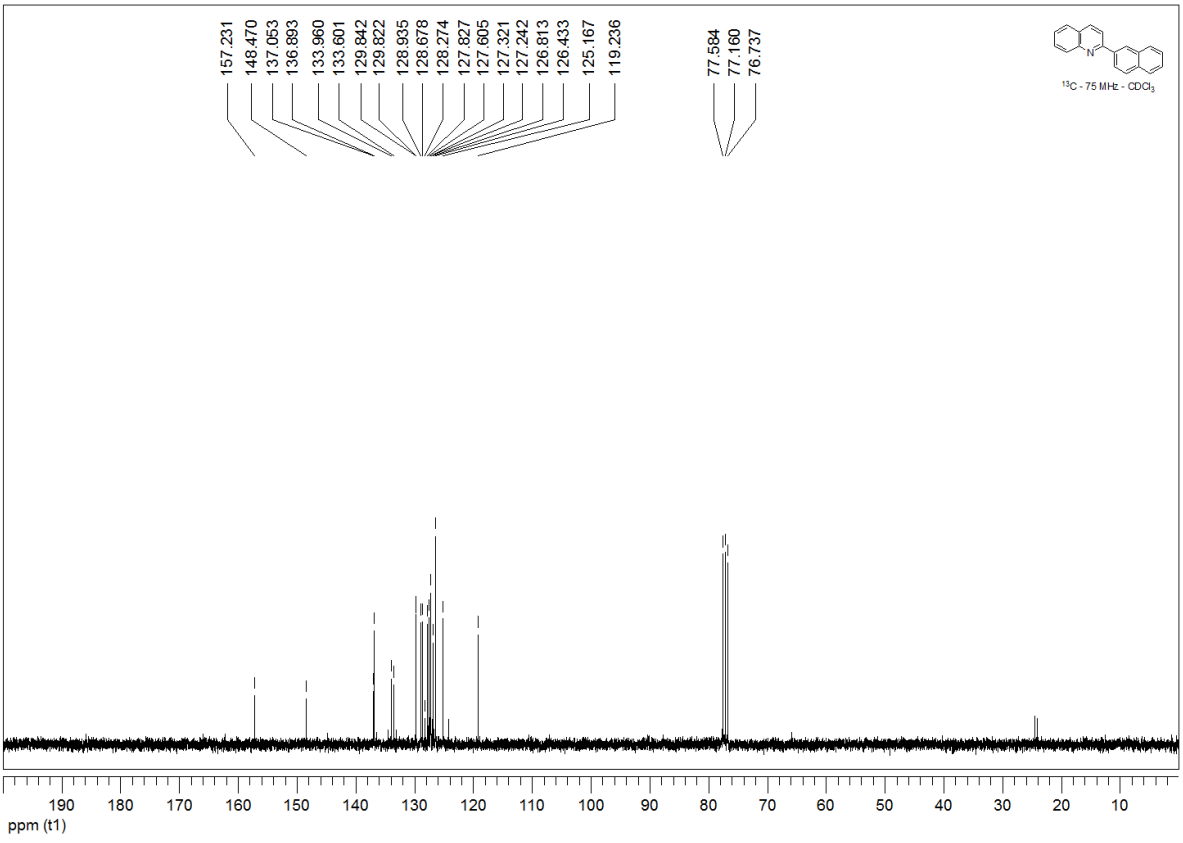
2-Phenylquinoline (1a).



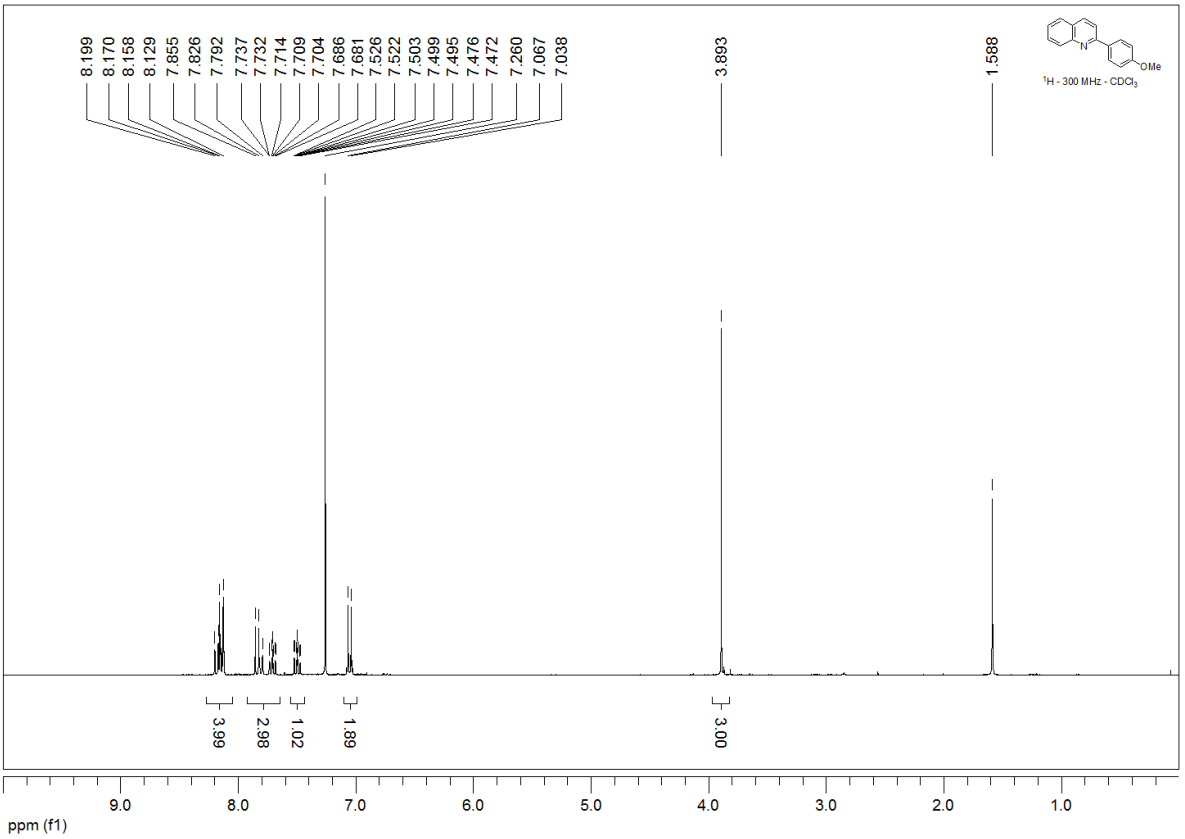


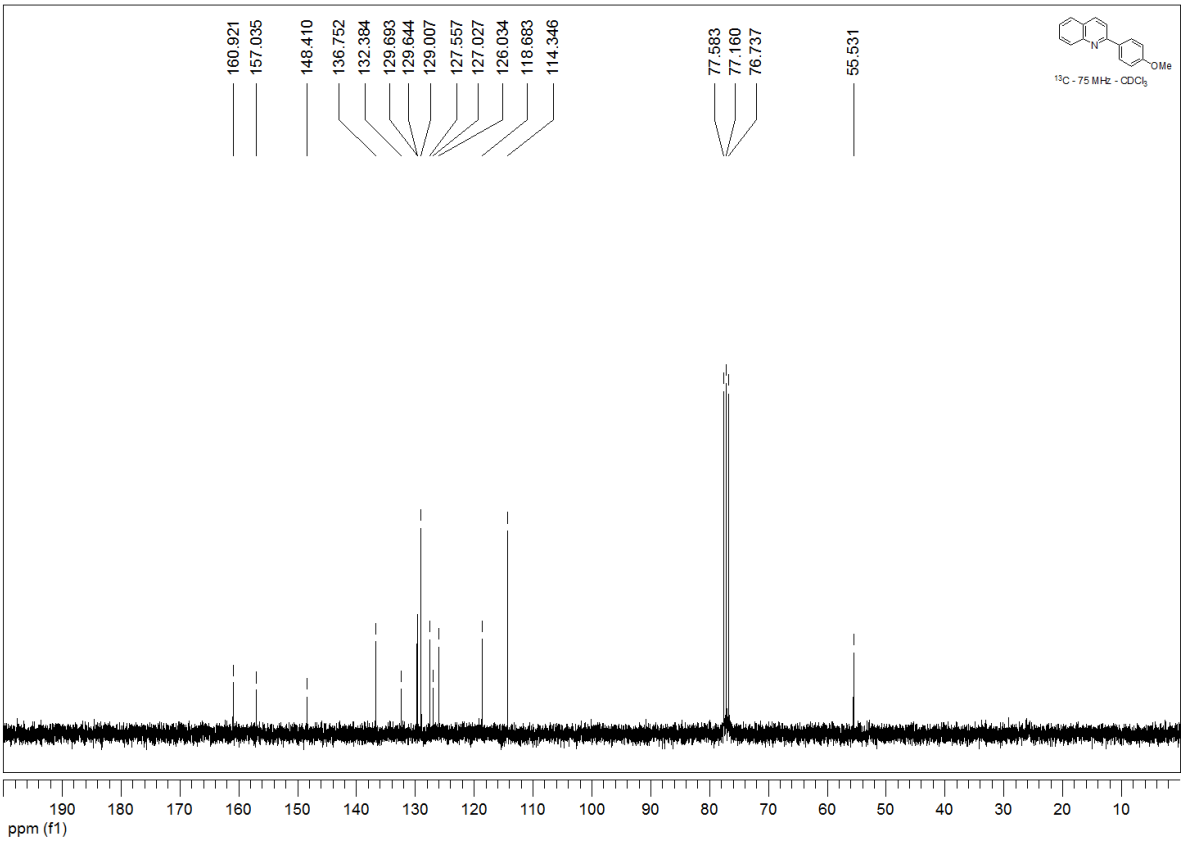
2-(2-Naphthyl)quinoline (1b).



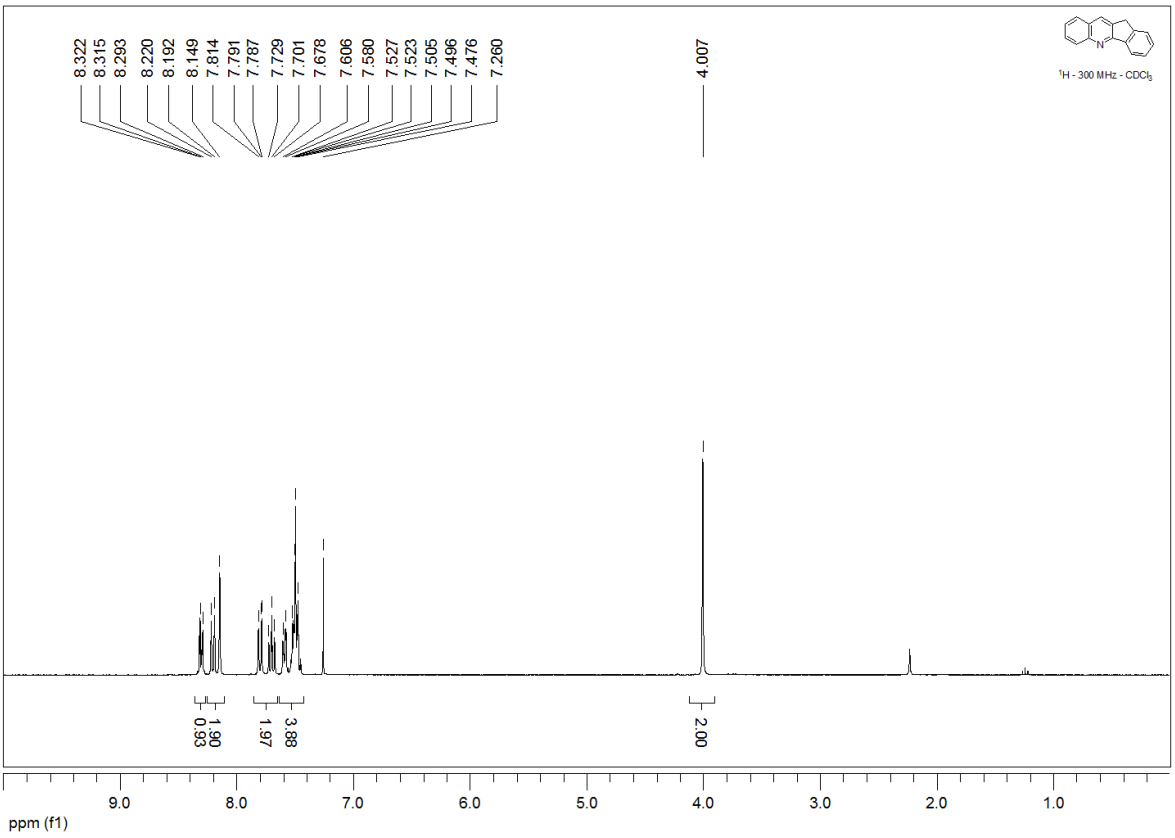


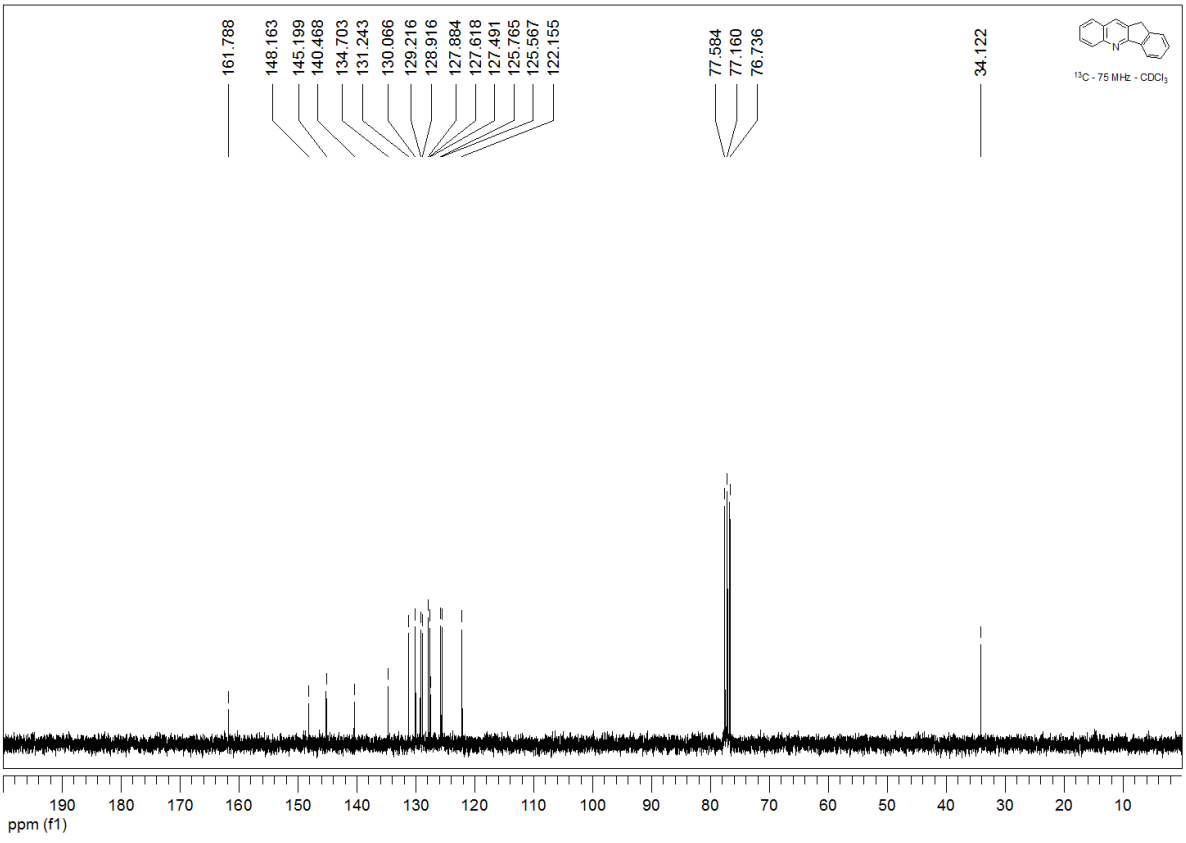
2-(4-Methoxyphenyl)quinoline (1c).



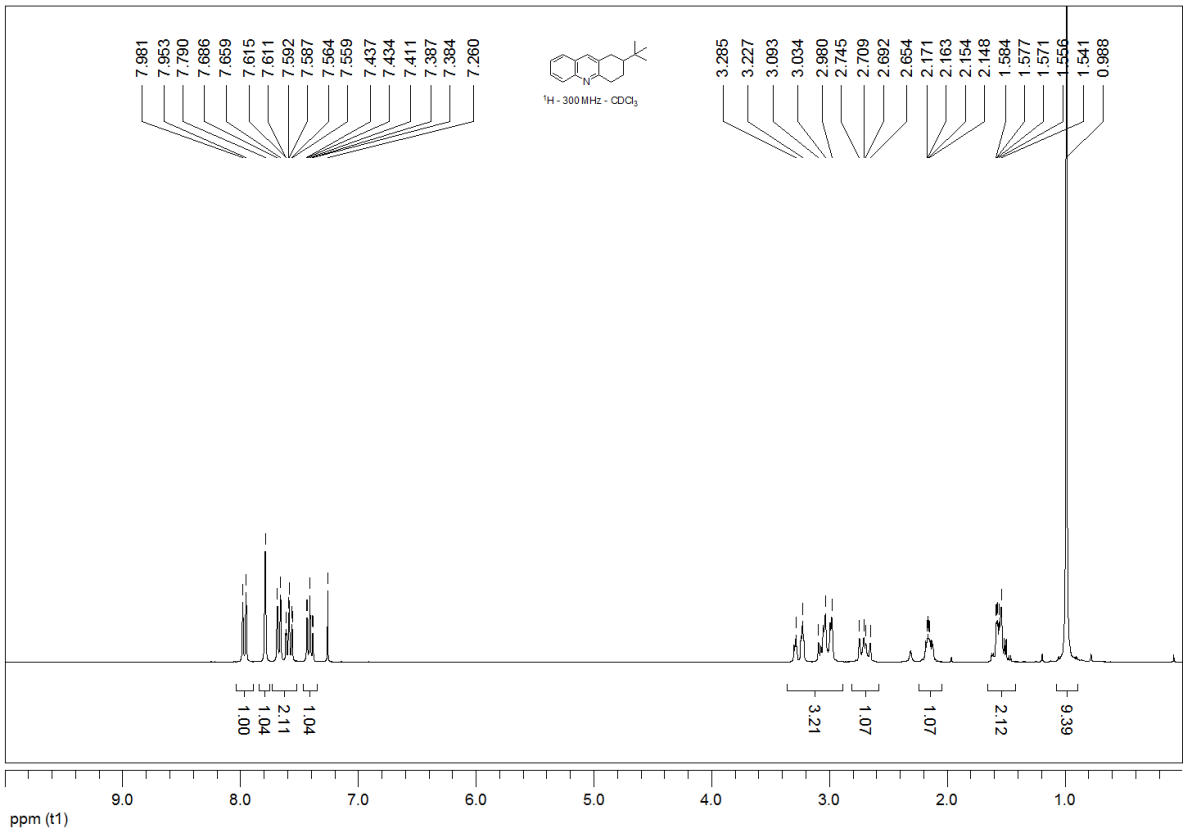


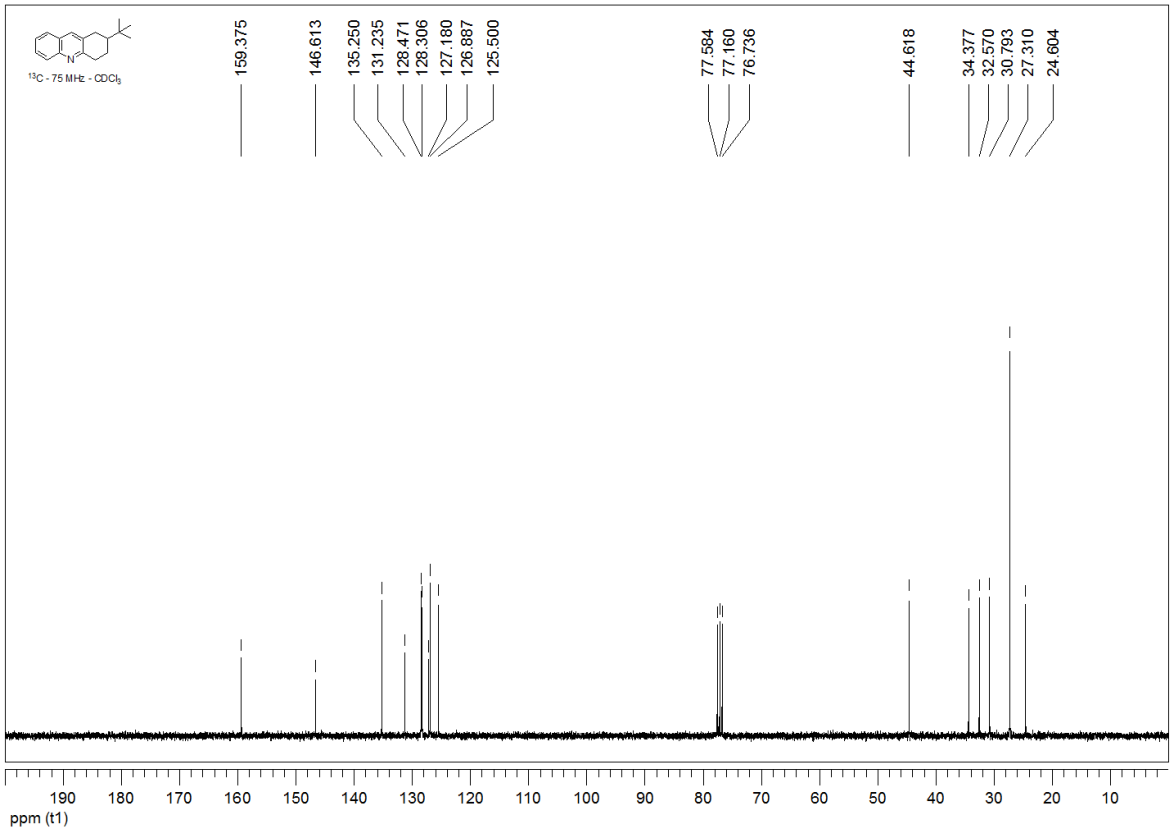
11*H*-Indeno[1,2-*b*]quinoline (1d).



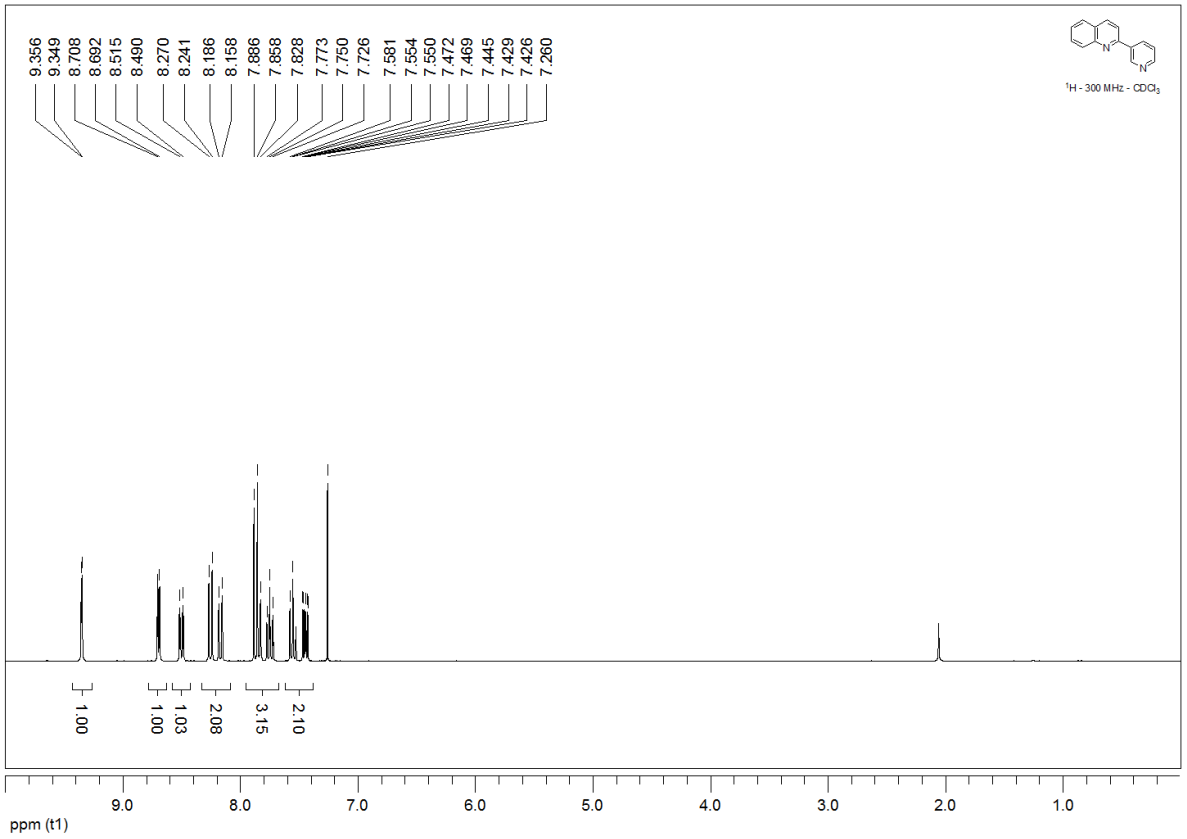


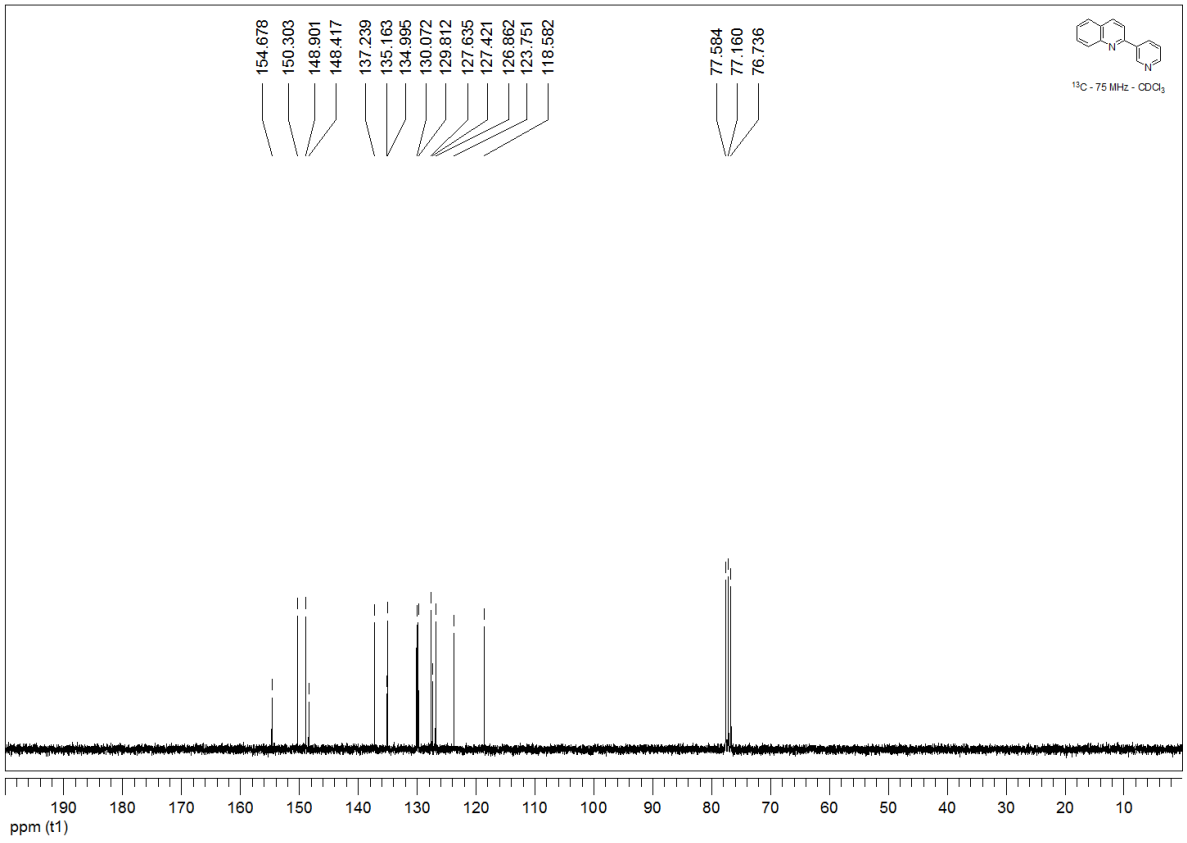
2-*tert*-Butyl-1,2,3,4-tetrahydroacridine (1e).



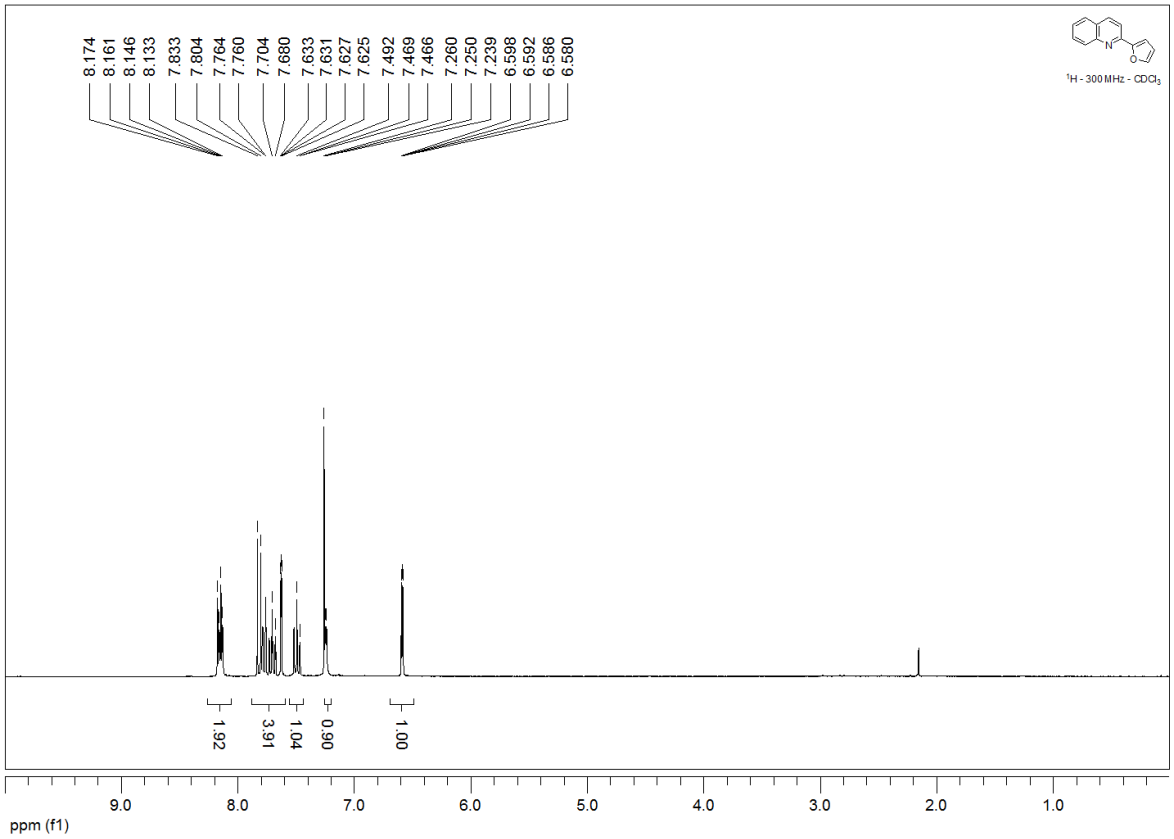


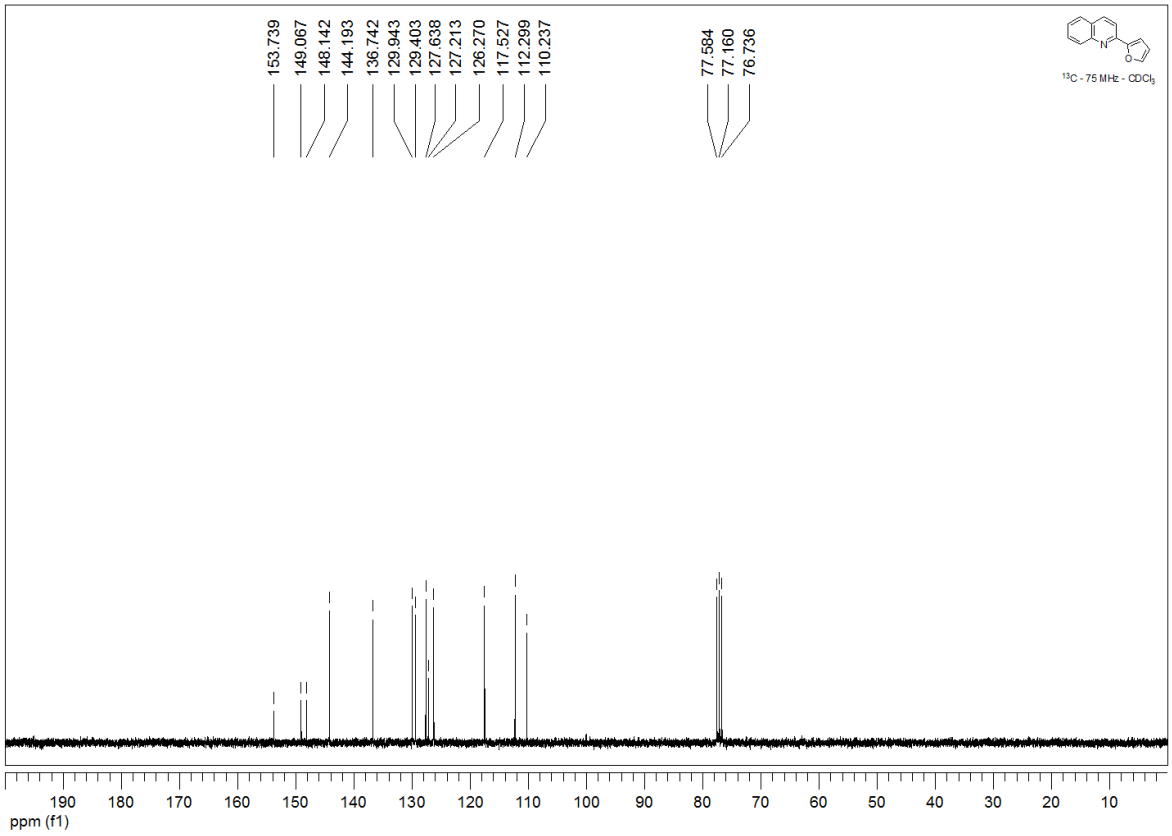
2-(3-Pyridyl)quinoline (1f).



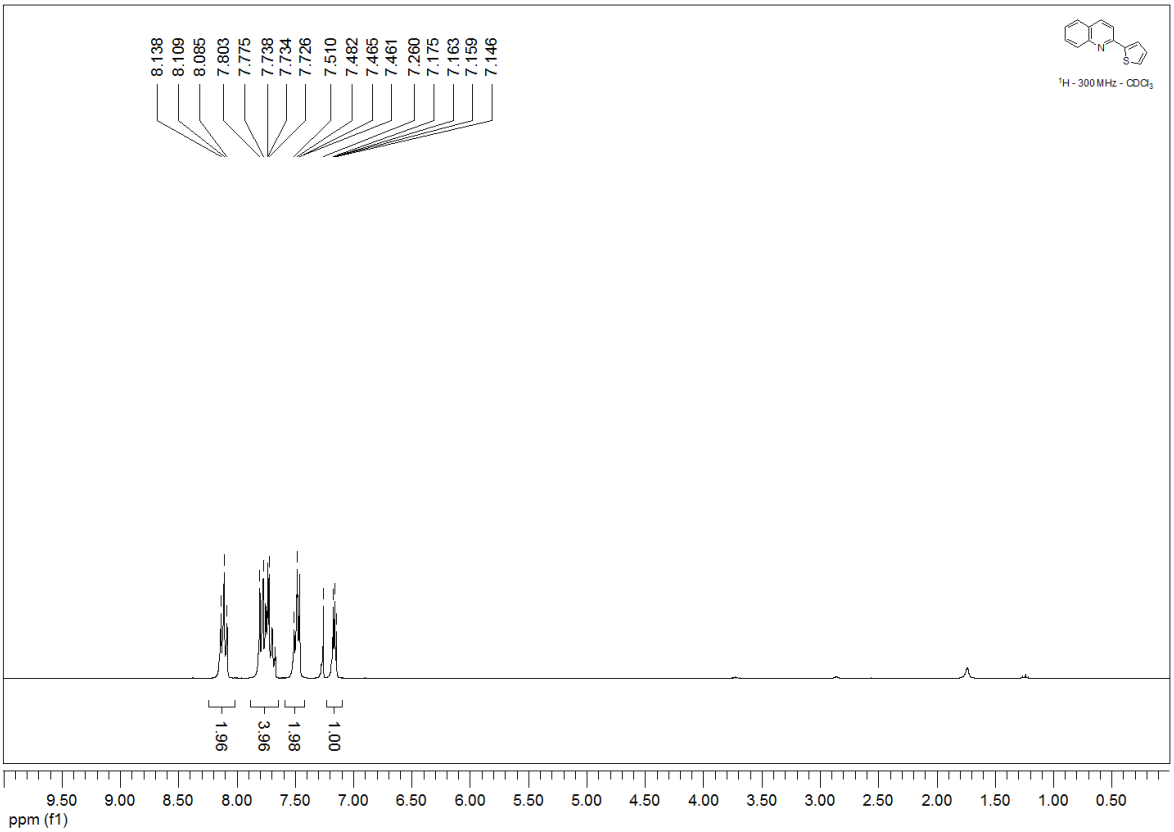


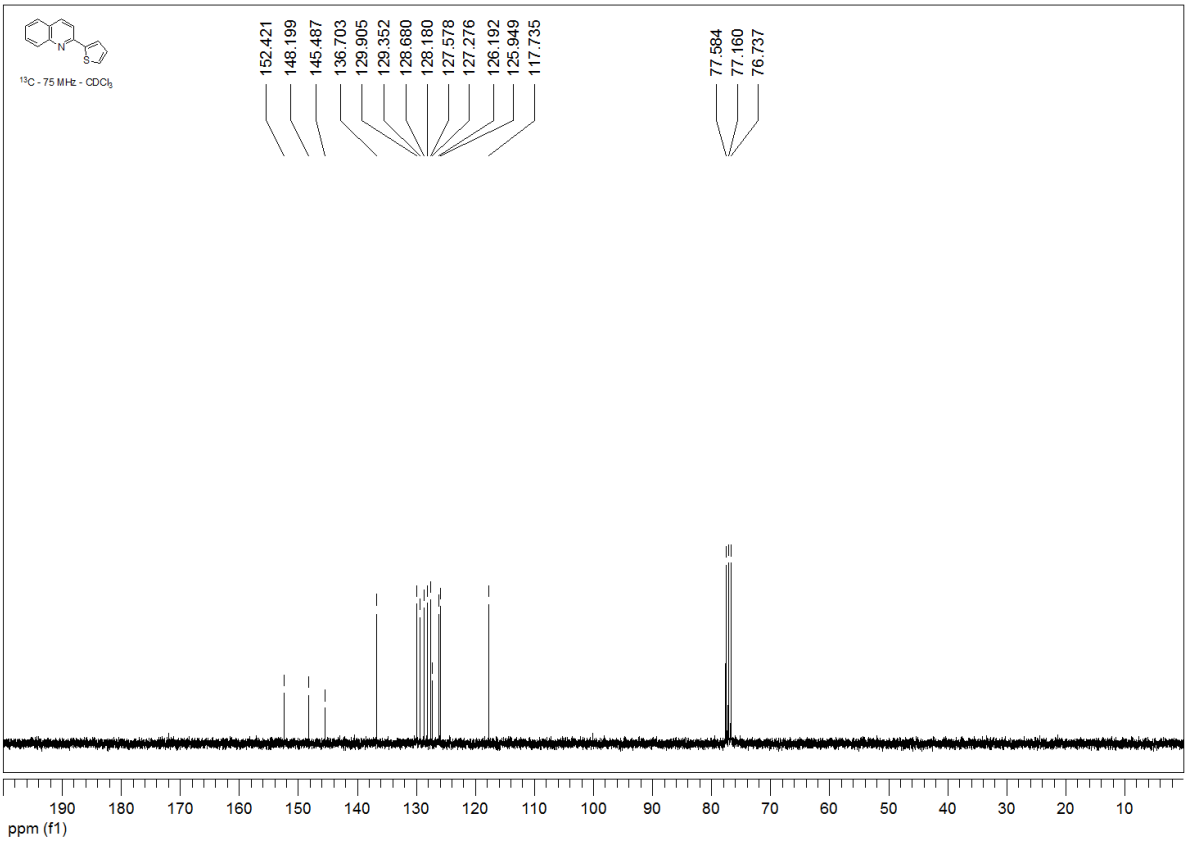
2-(2-Furyl)quinoline (1g).



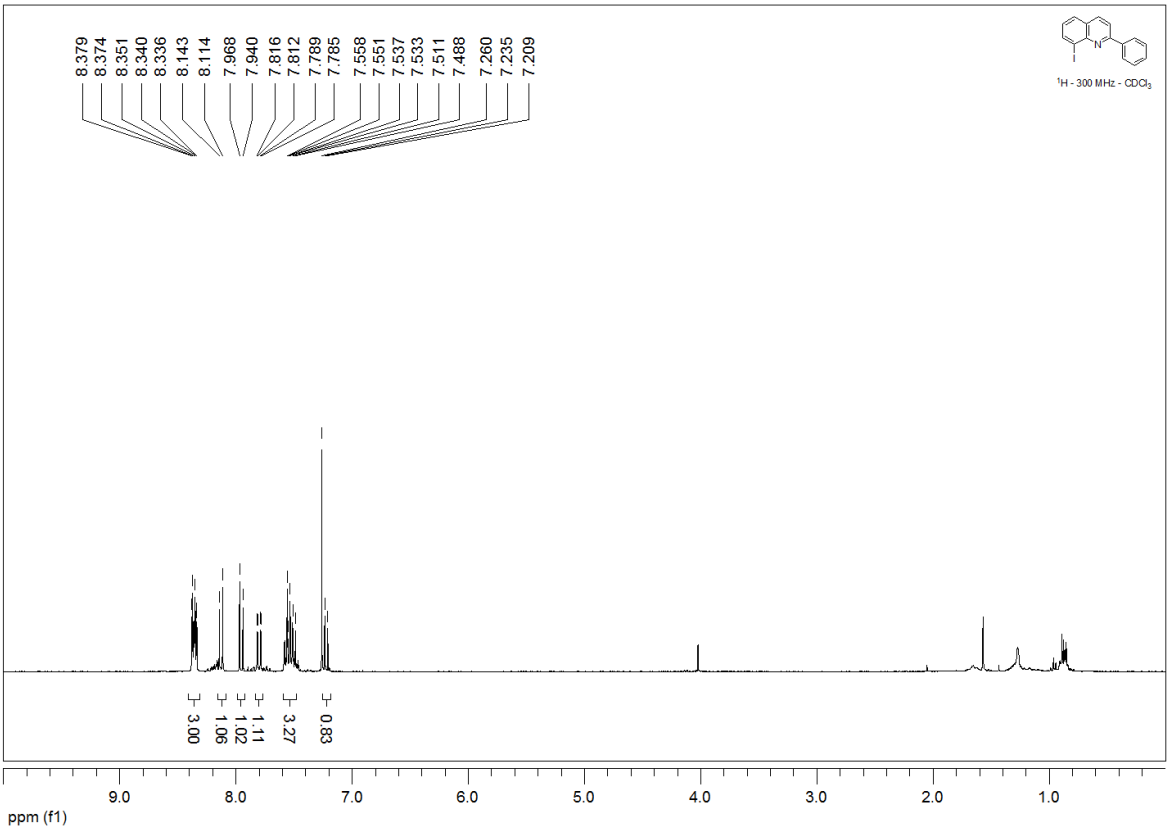


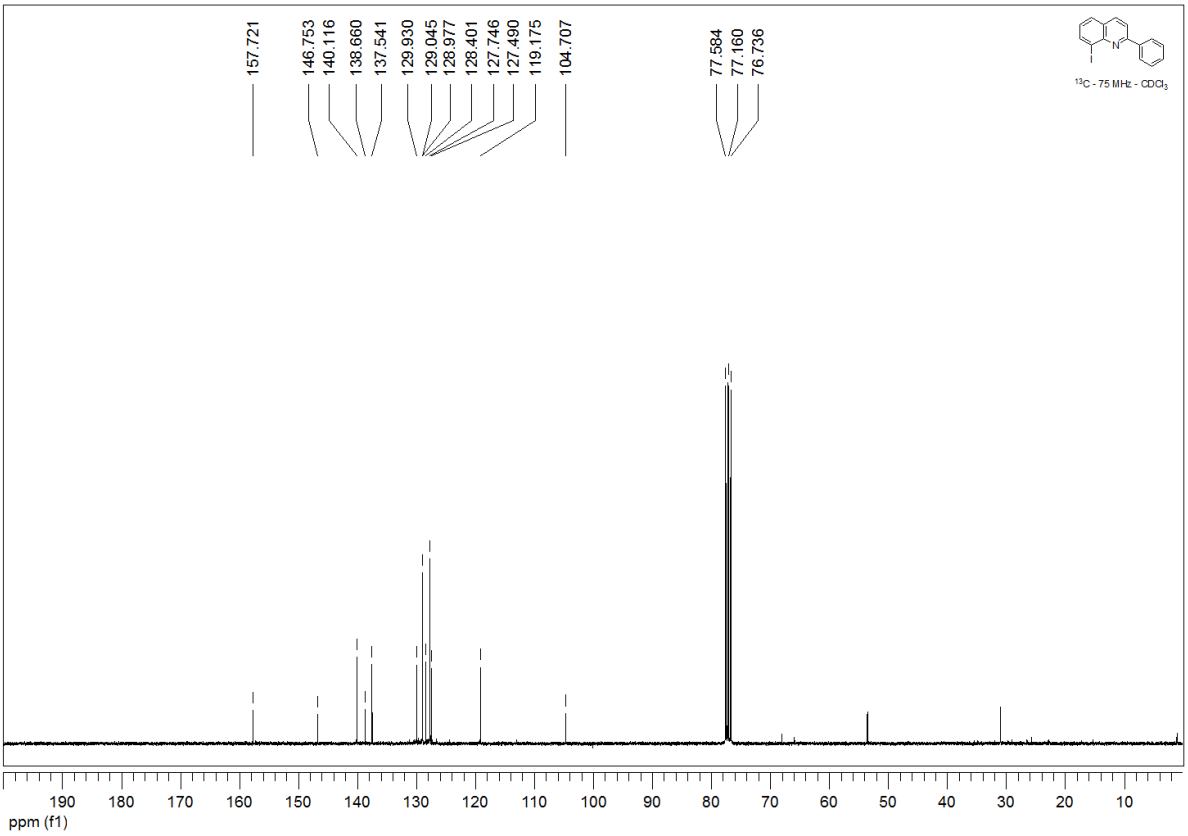
2-(2-Thienyl)quinoline (1h).



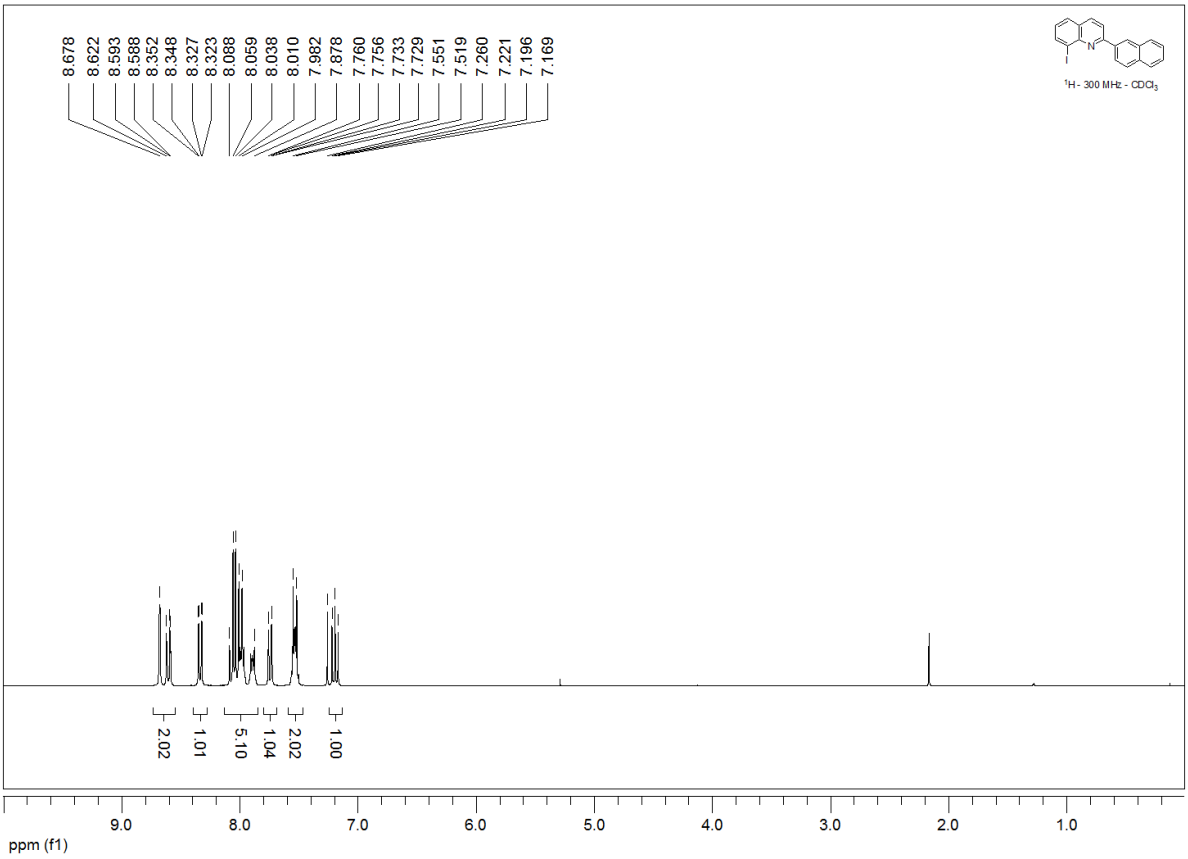


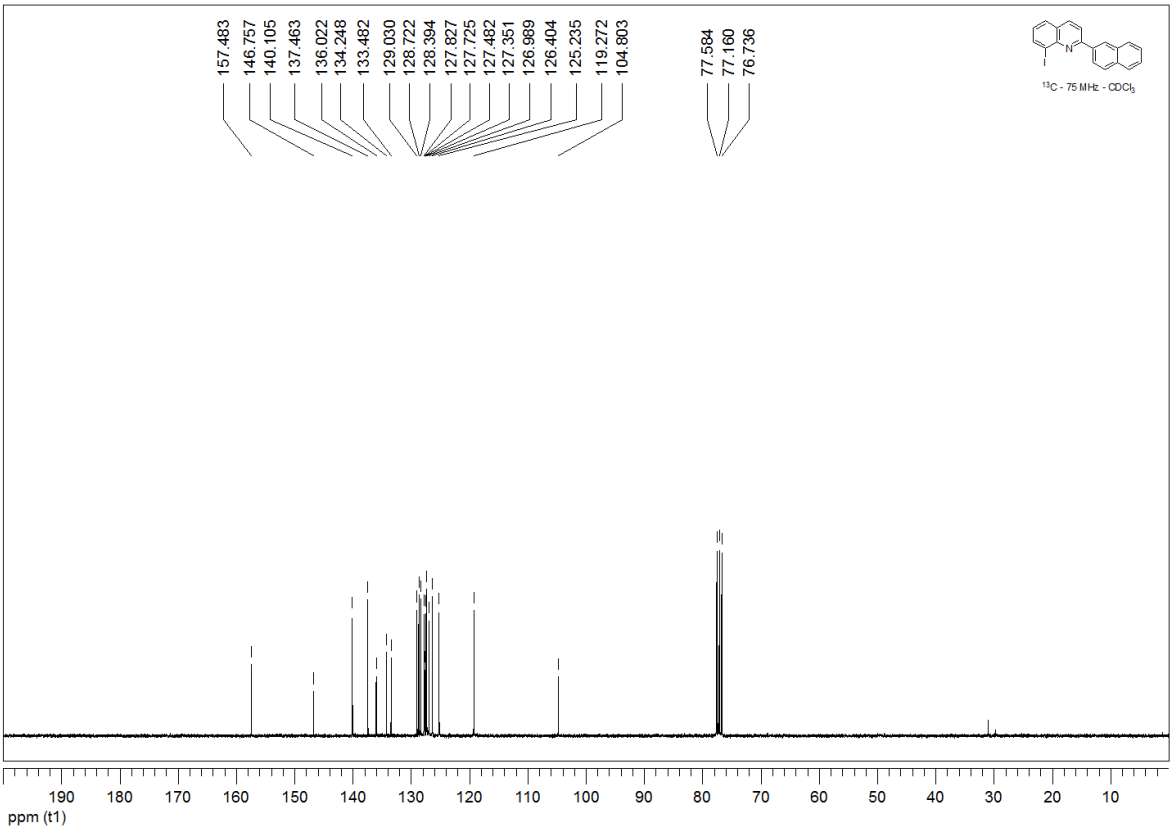
8-Iodo-2-phenylquinoline (2a).



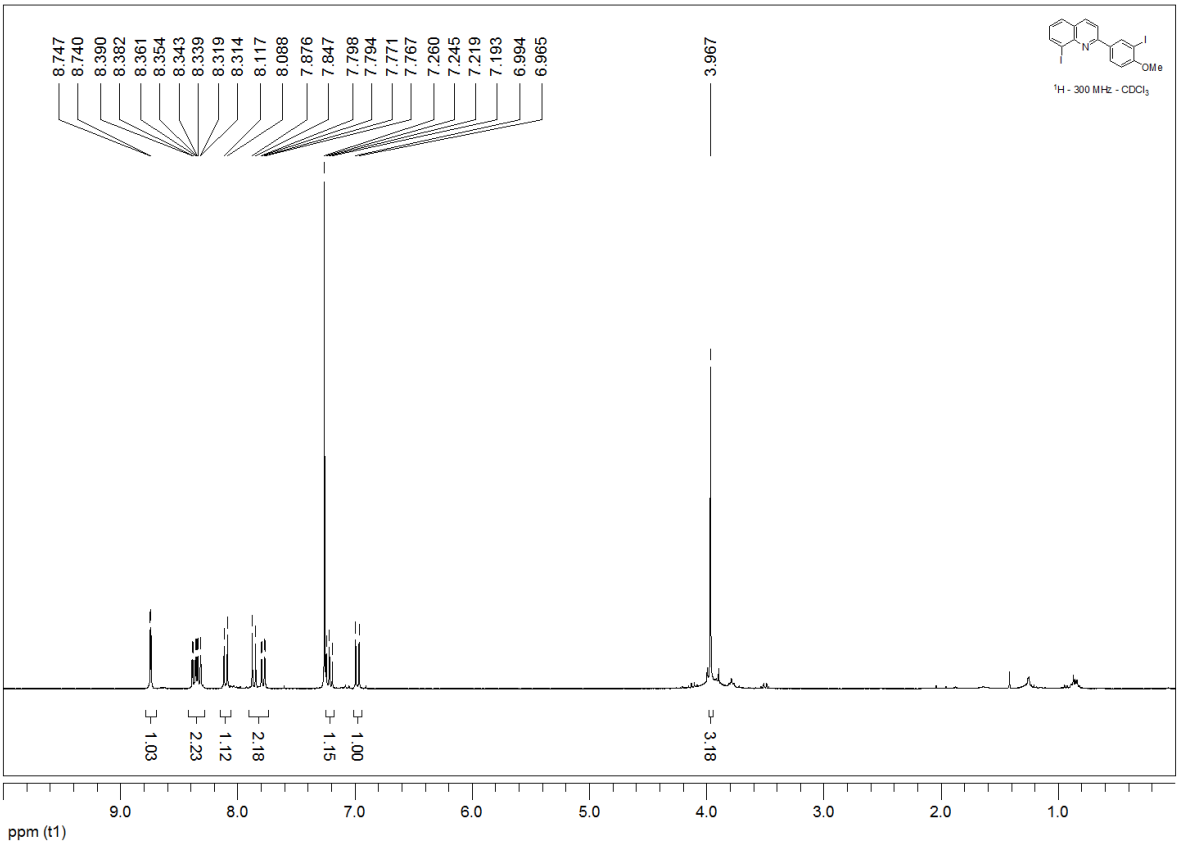


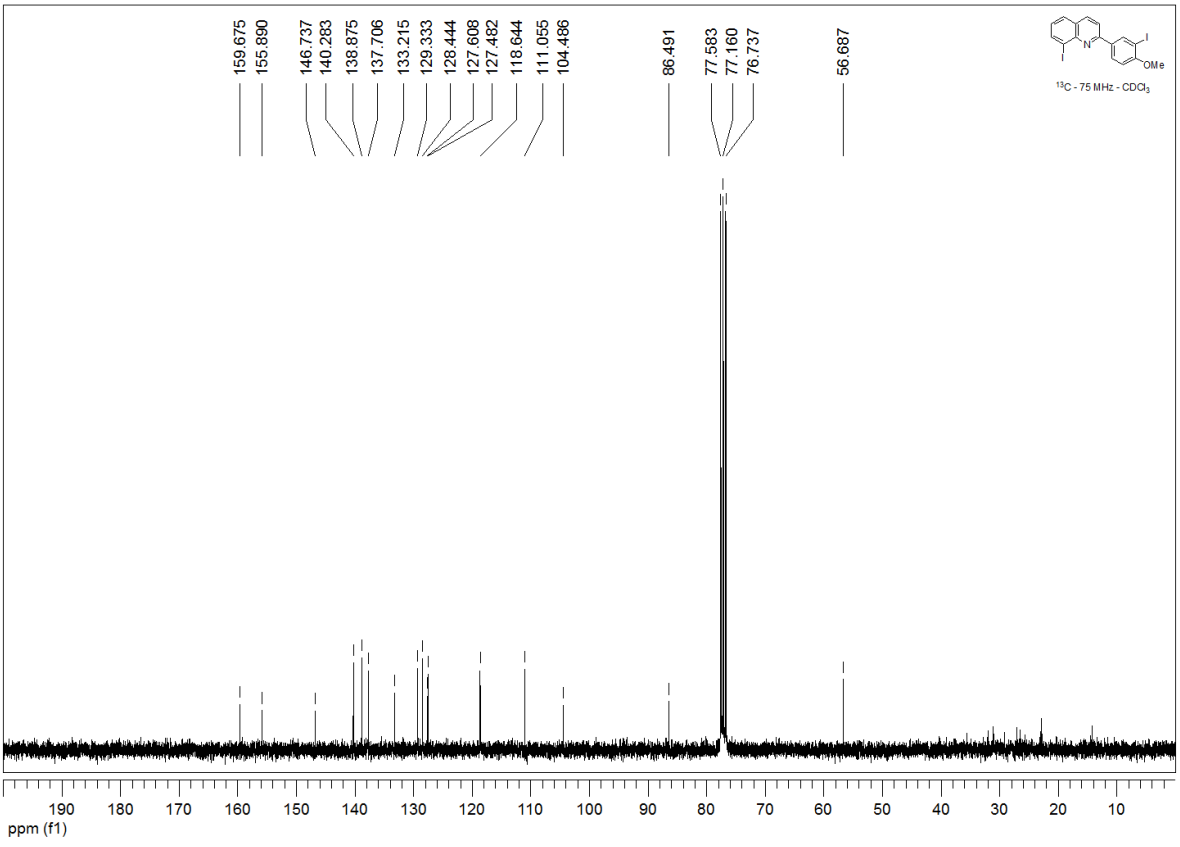
8-Iodo-2-(2-naphthyl)quinoline (2b).



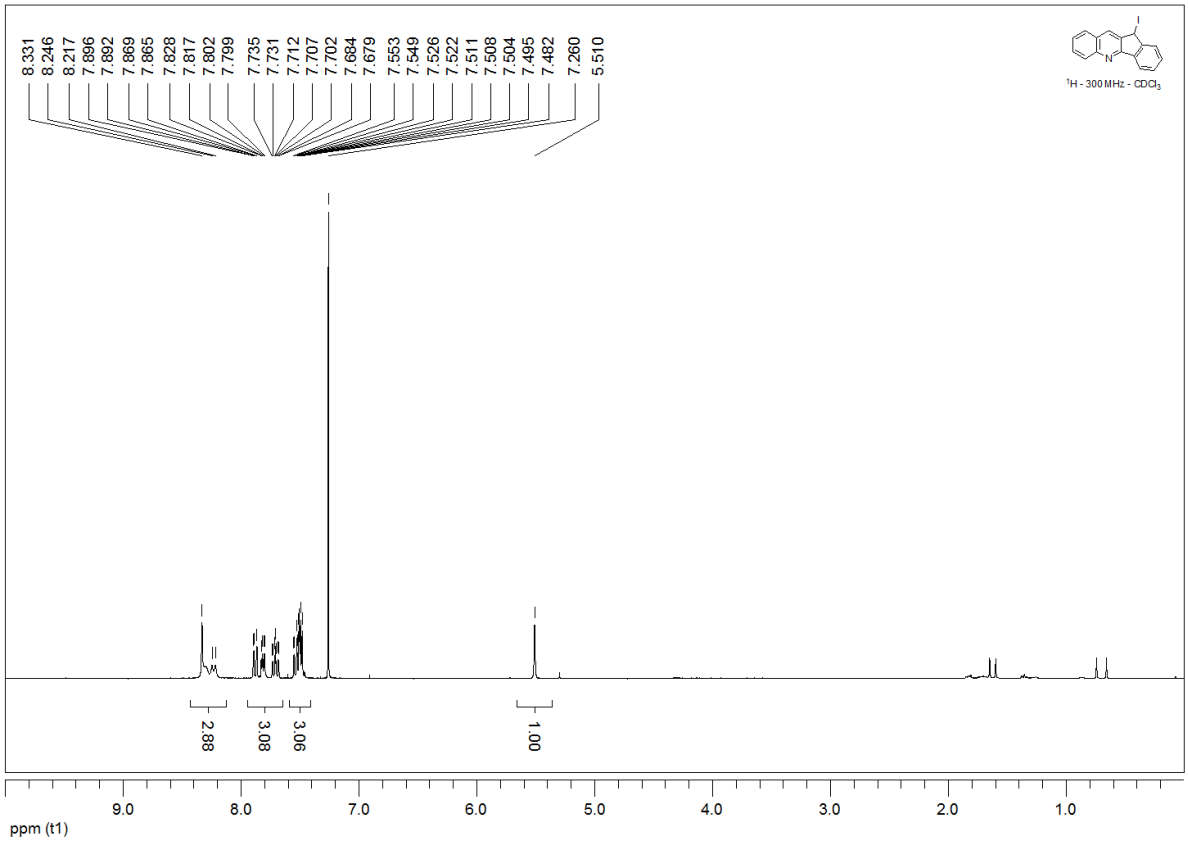


8-Iodo-2-(3-iodo-4-methoxyphenyl)quinoline (3c).

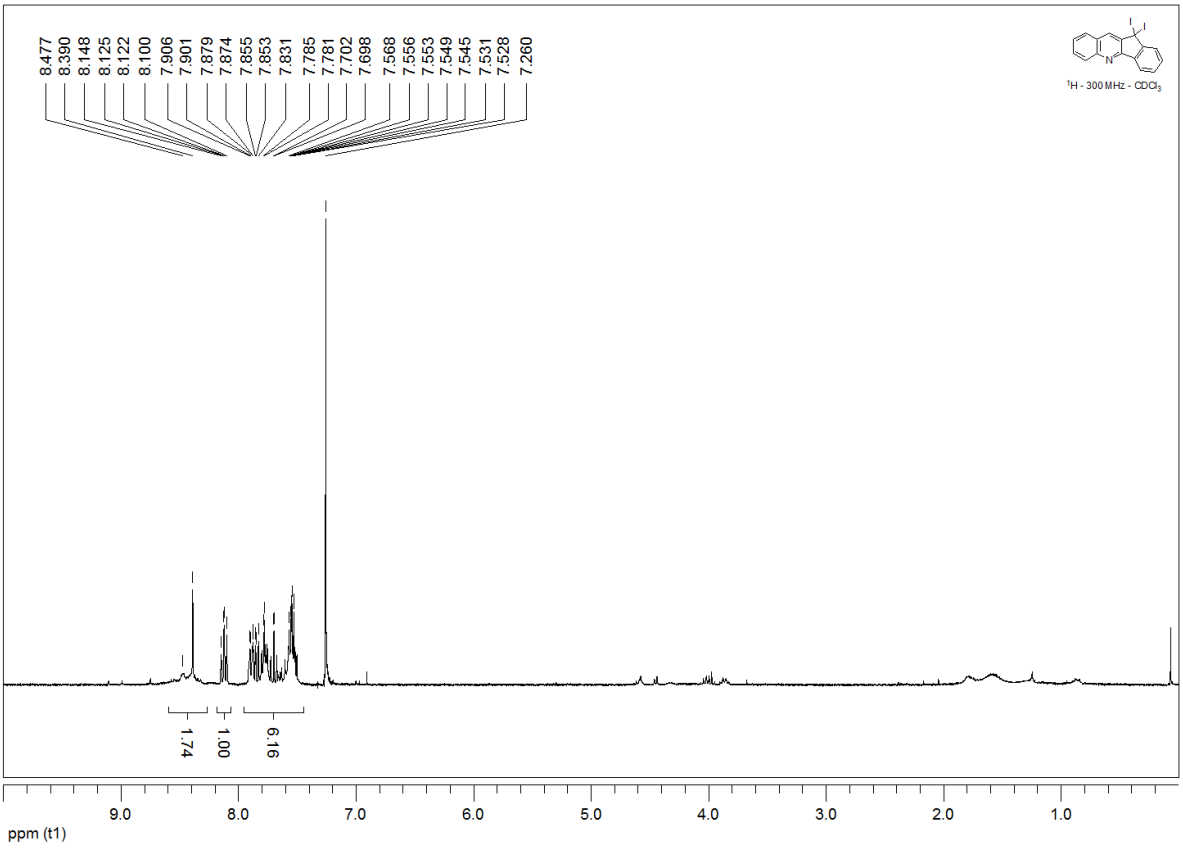


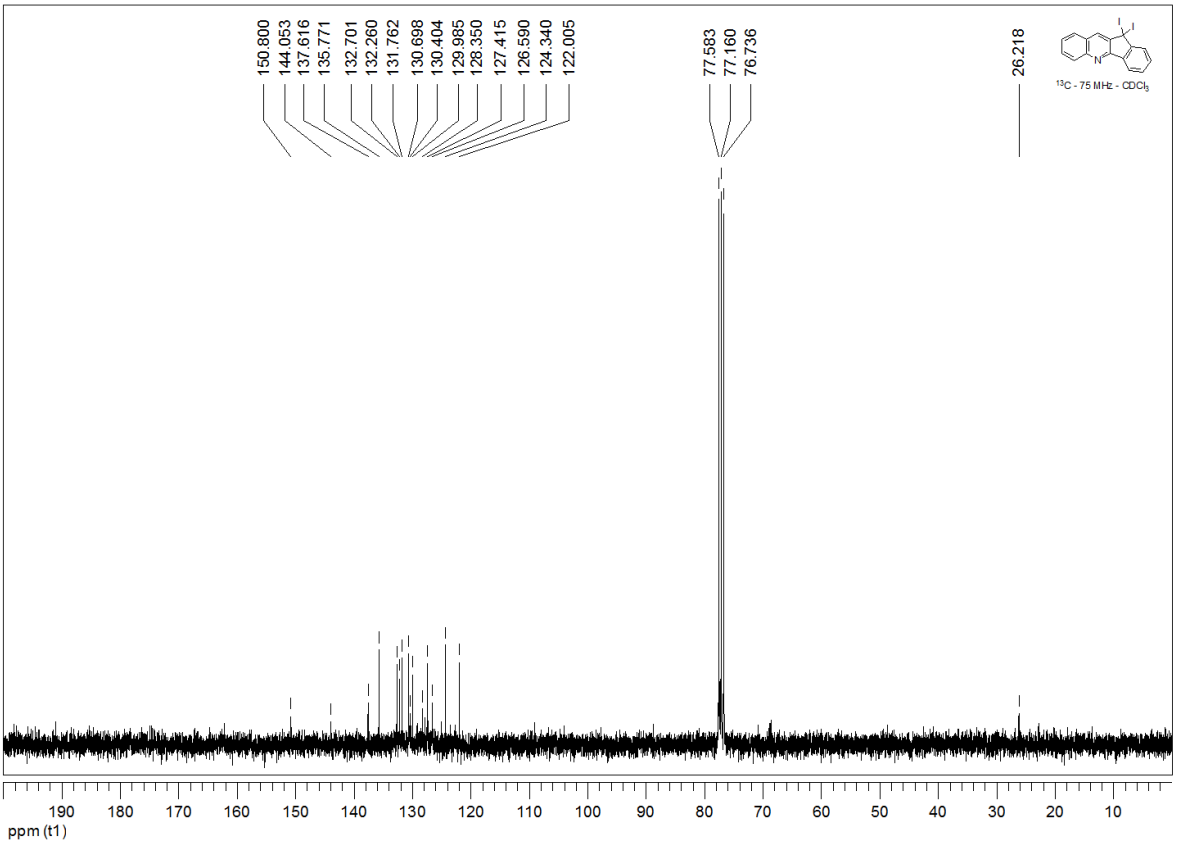


11-Iodo-11*H*-indeno[1,2-*b*]quinoline (2d).

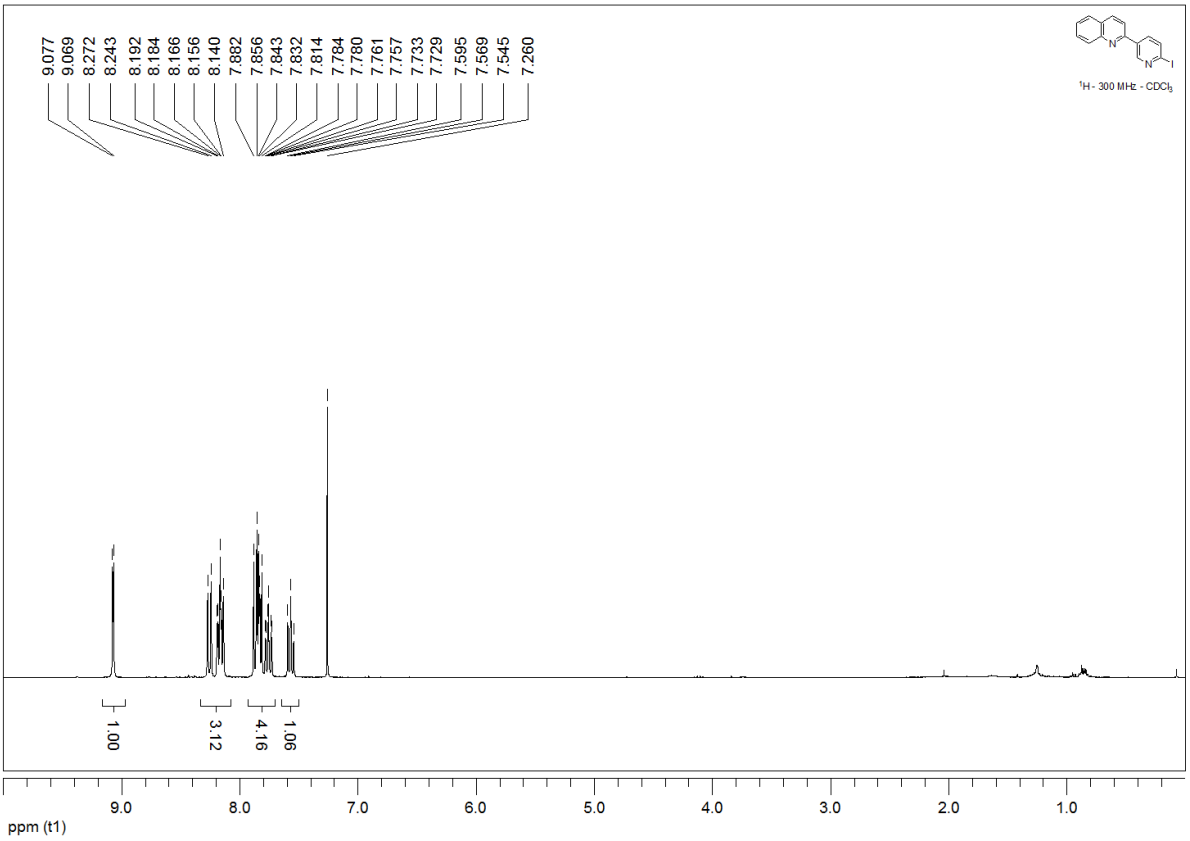


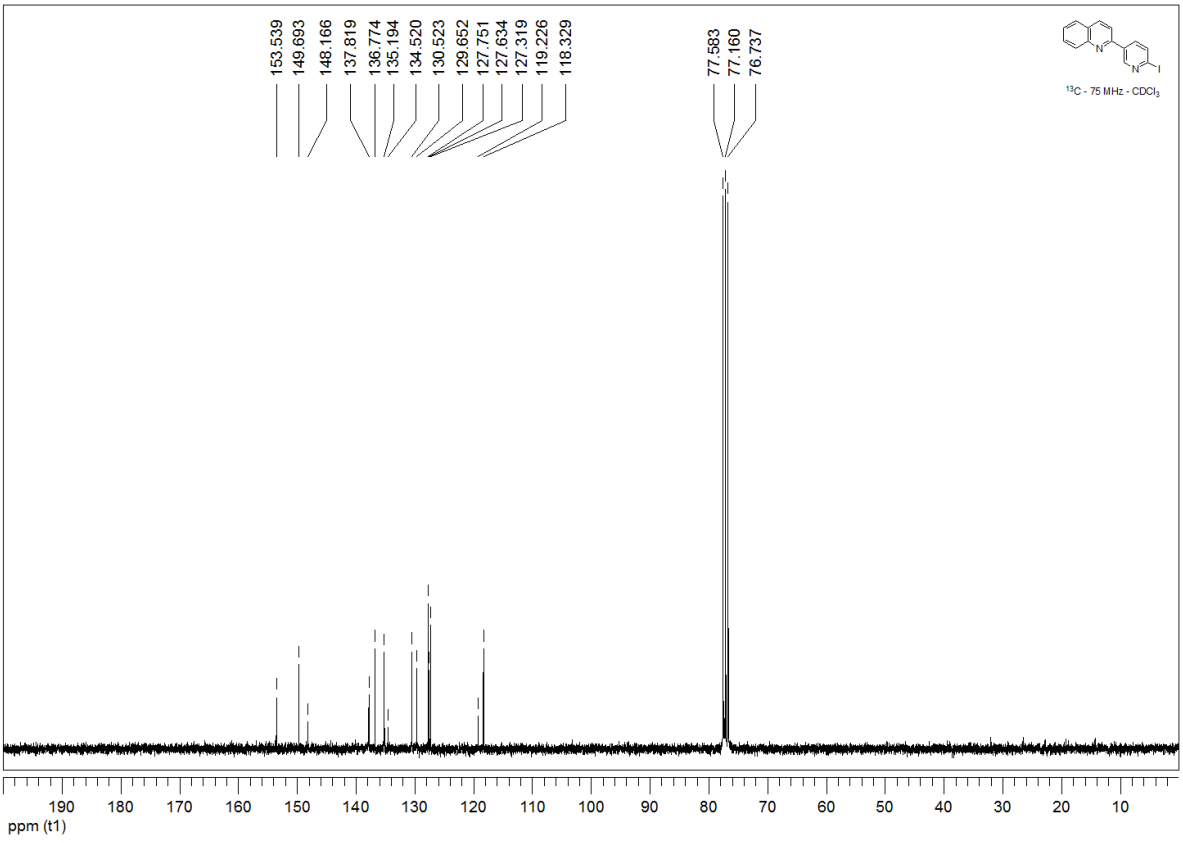
11,11-Diiodo-11*H*-indeno[1,2-*b*]quinoline (3d).



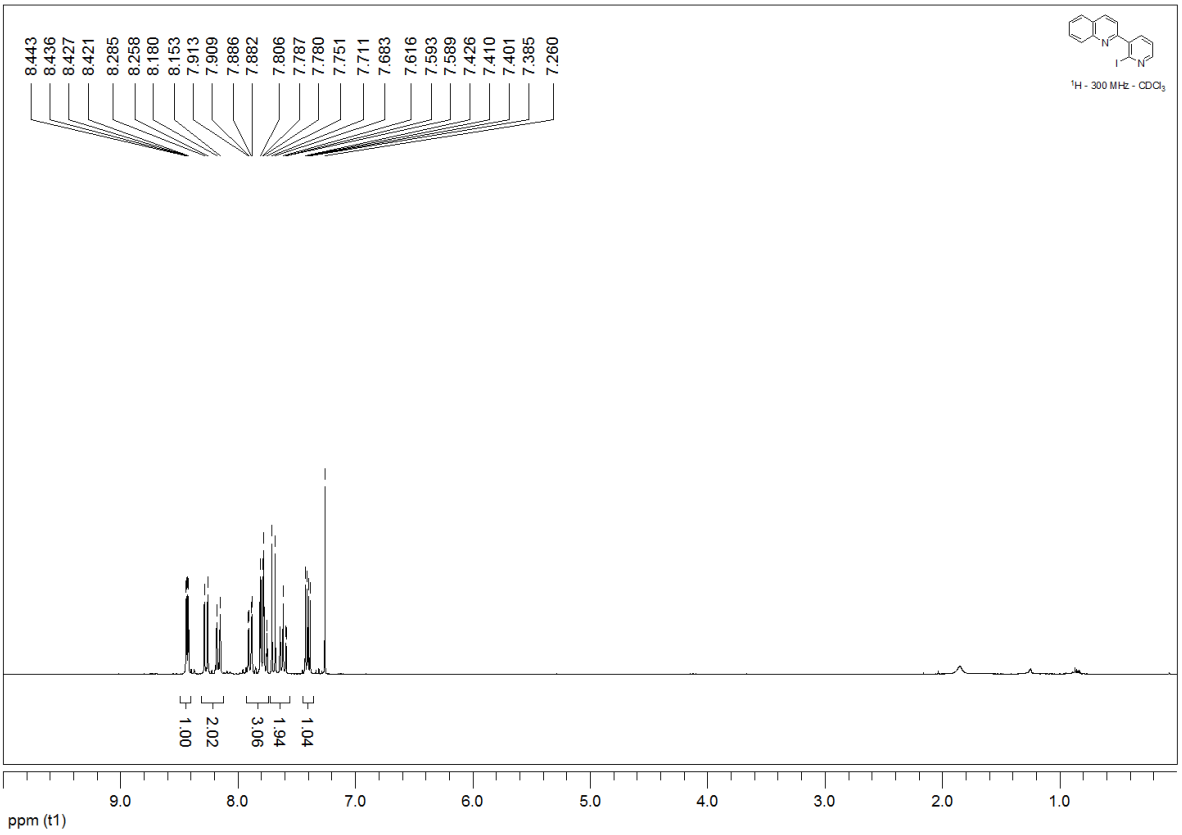


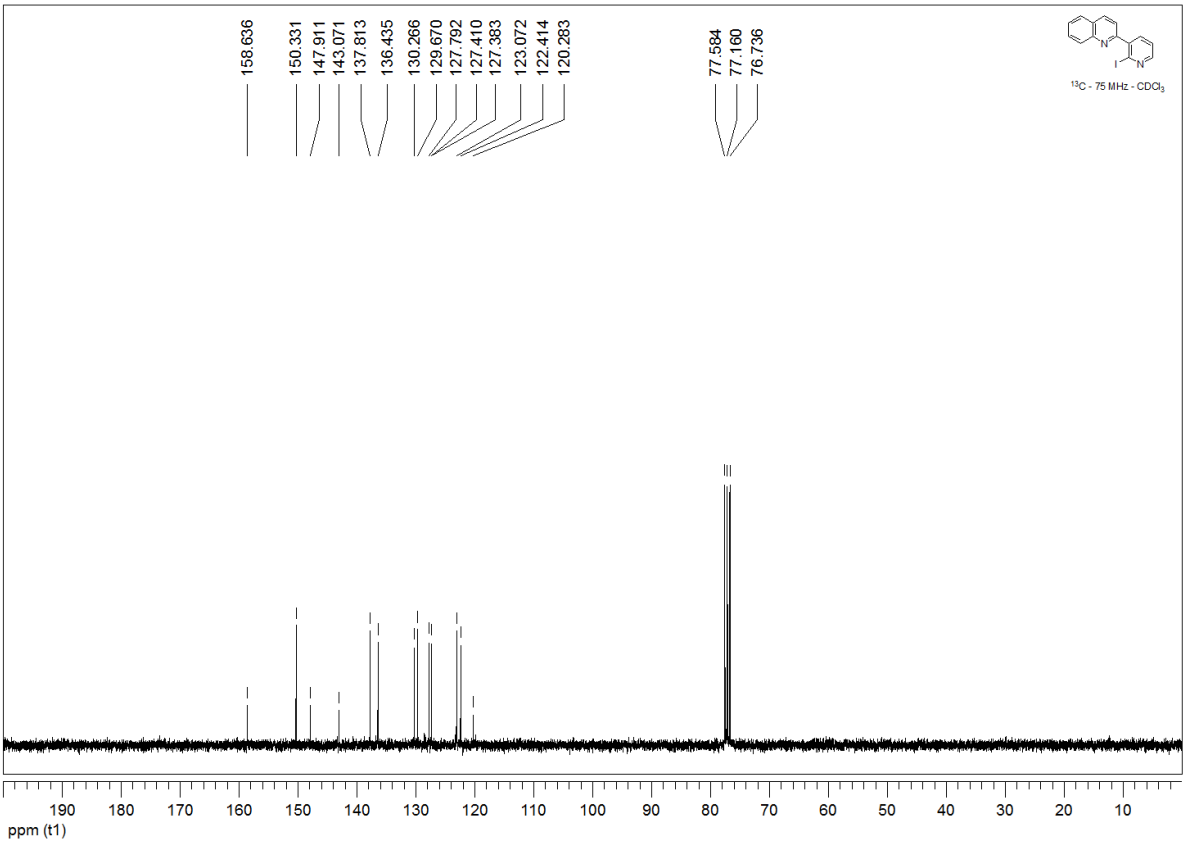
2-(6-Iodo-3-pyridyl)quinoline (2f).



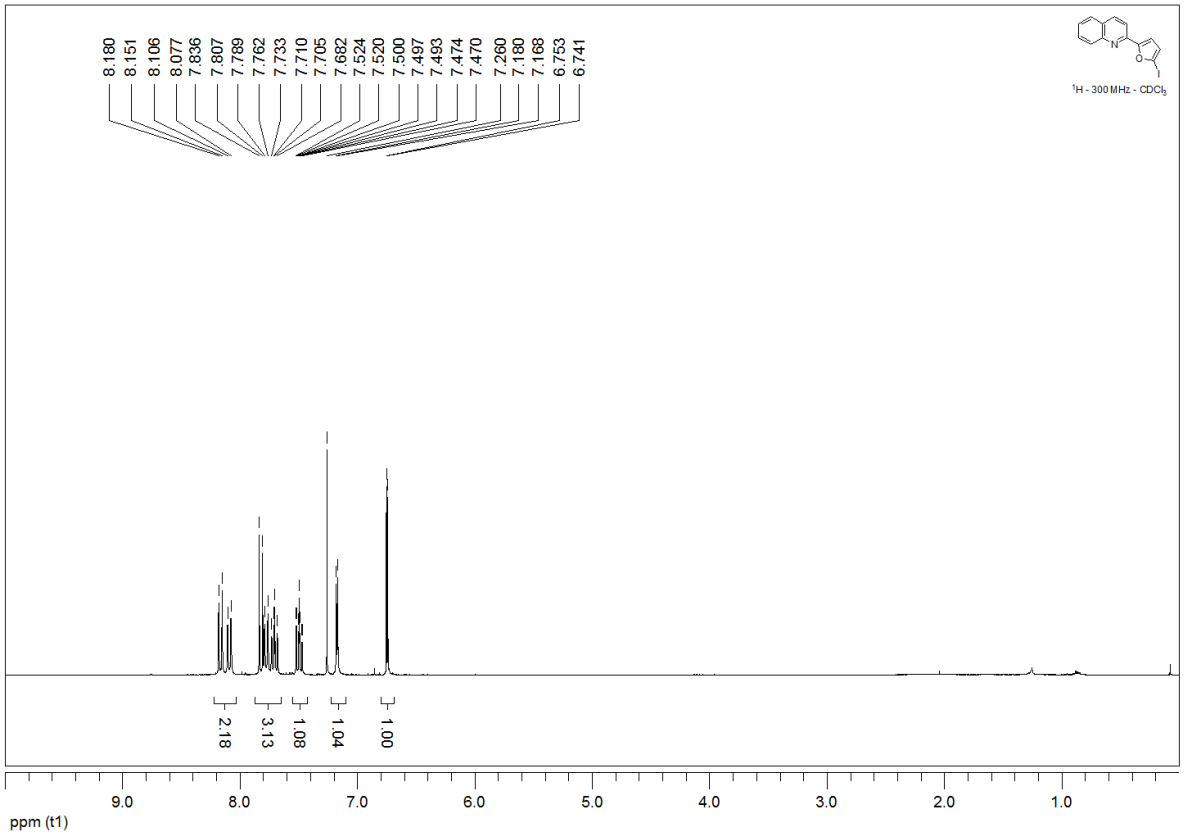


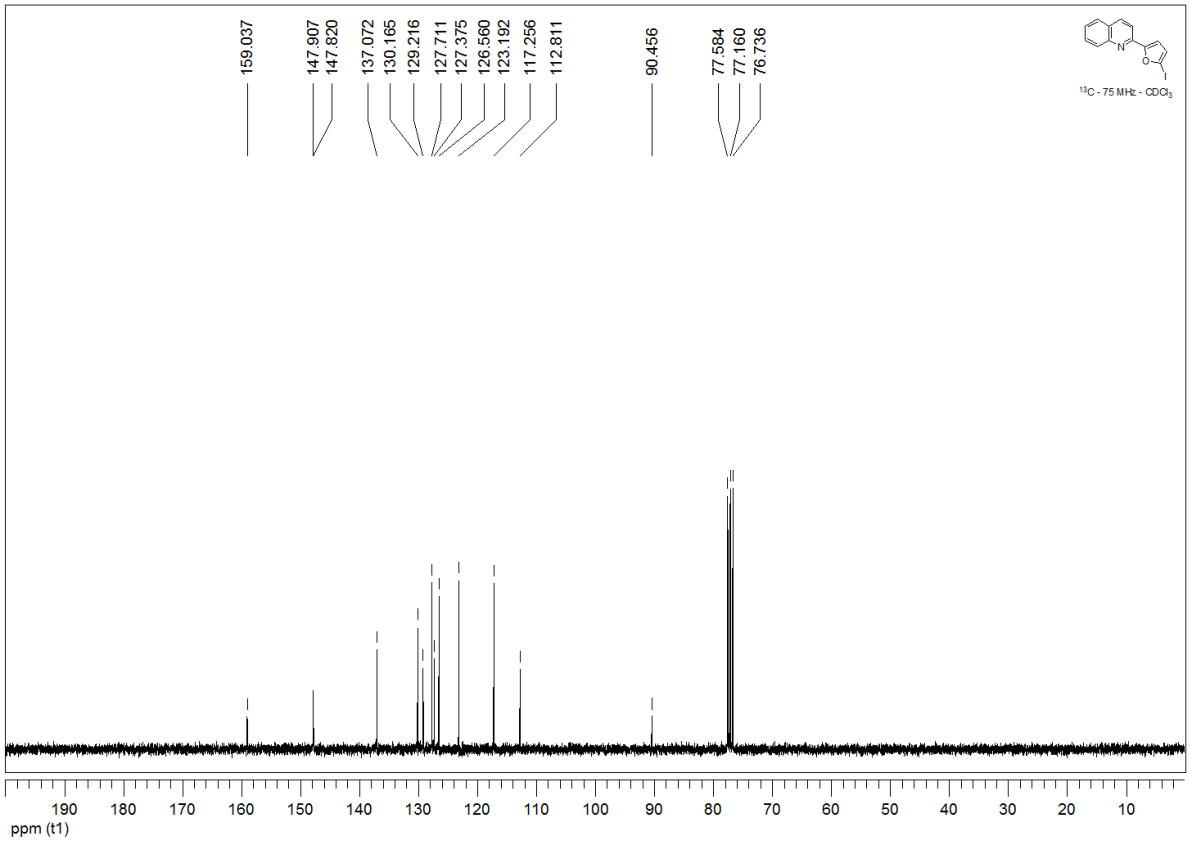
2-(2-Iodo-3-pyridyl)quinoline (2f').



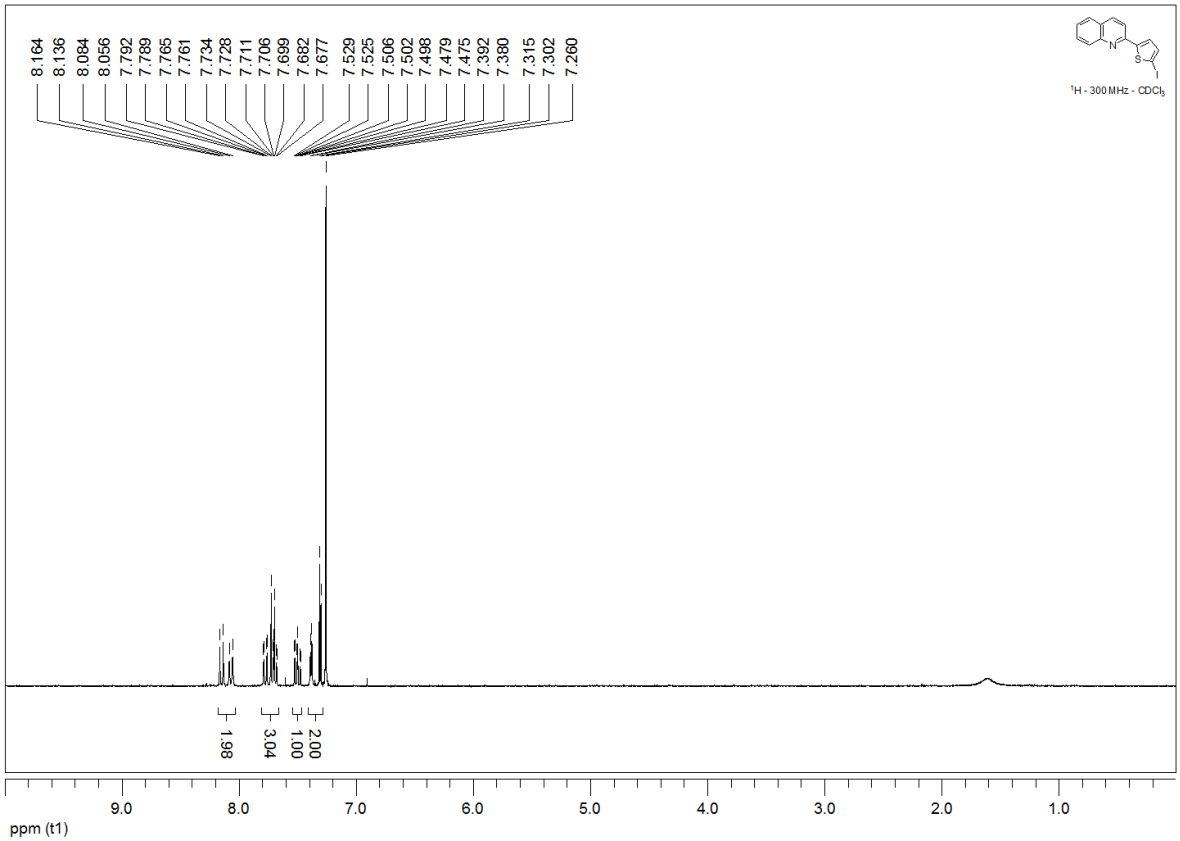


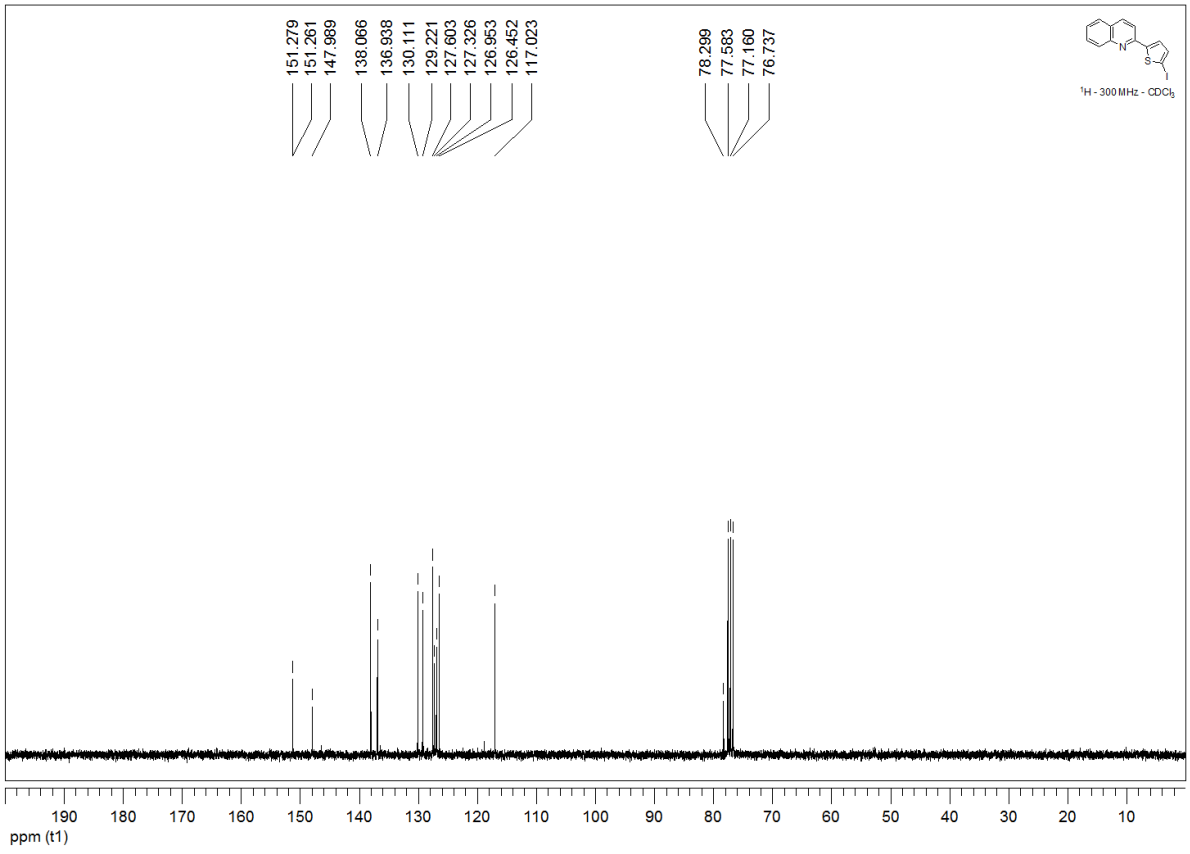
2-(5-Iodo-2-furyl)quinoline (2g).



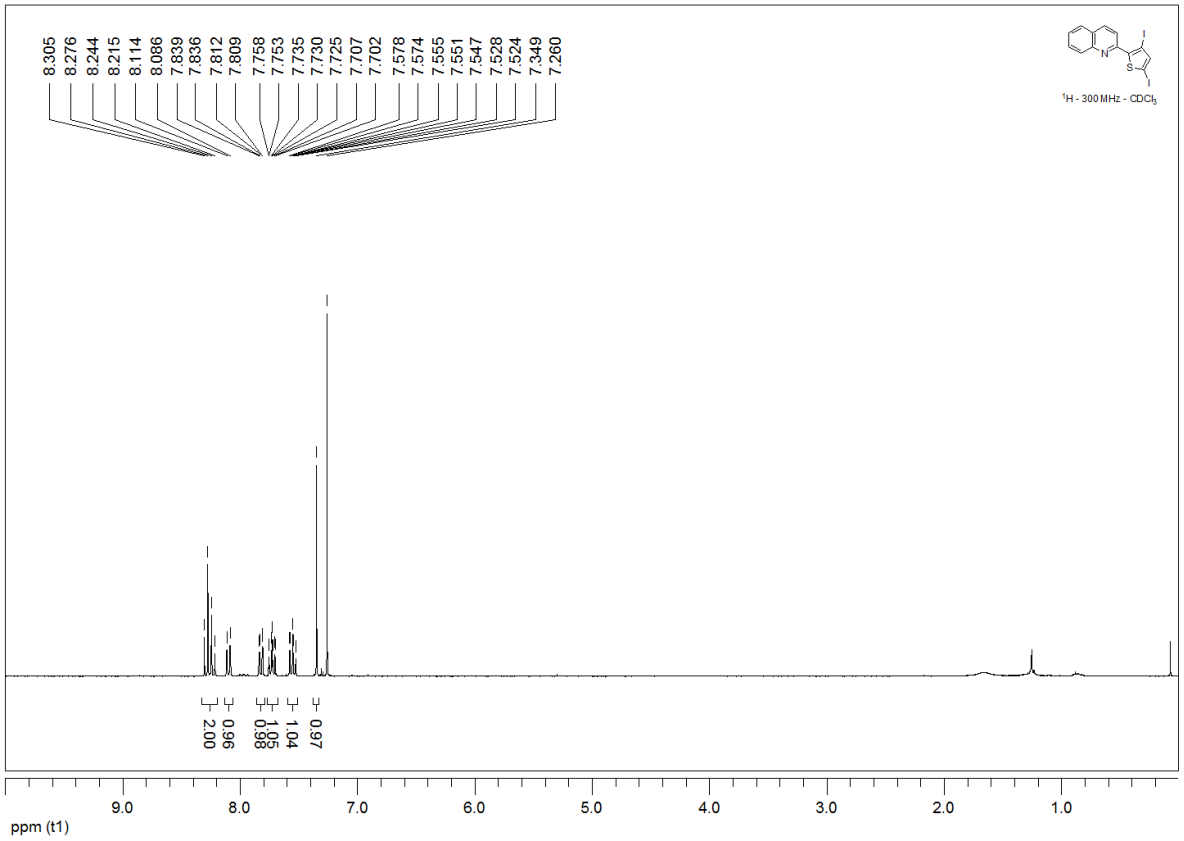


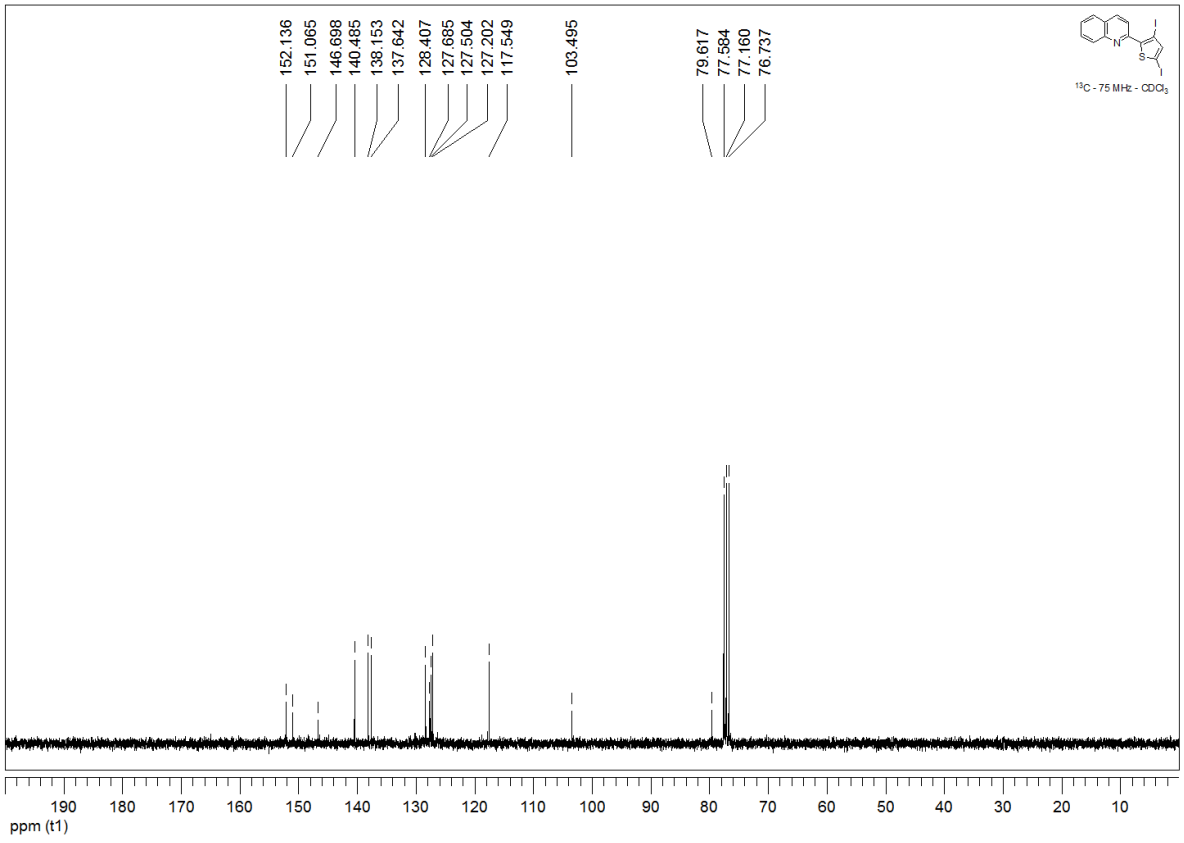
2-(5-Iodo-2-thienyl)quinoline (2h).



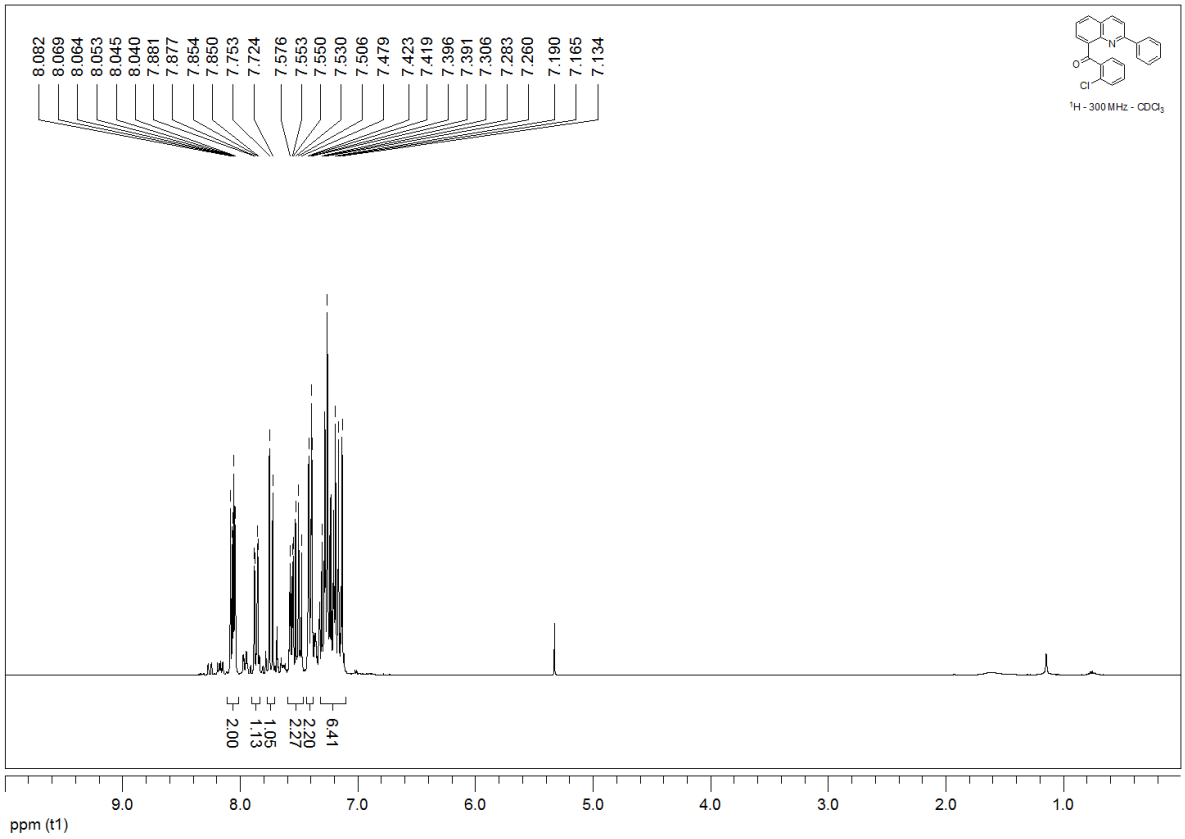


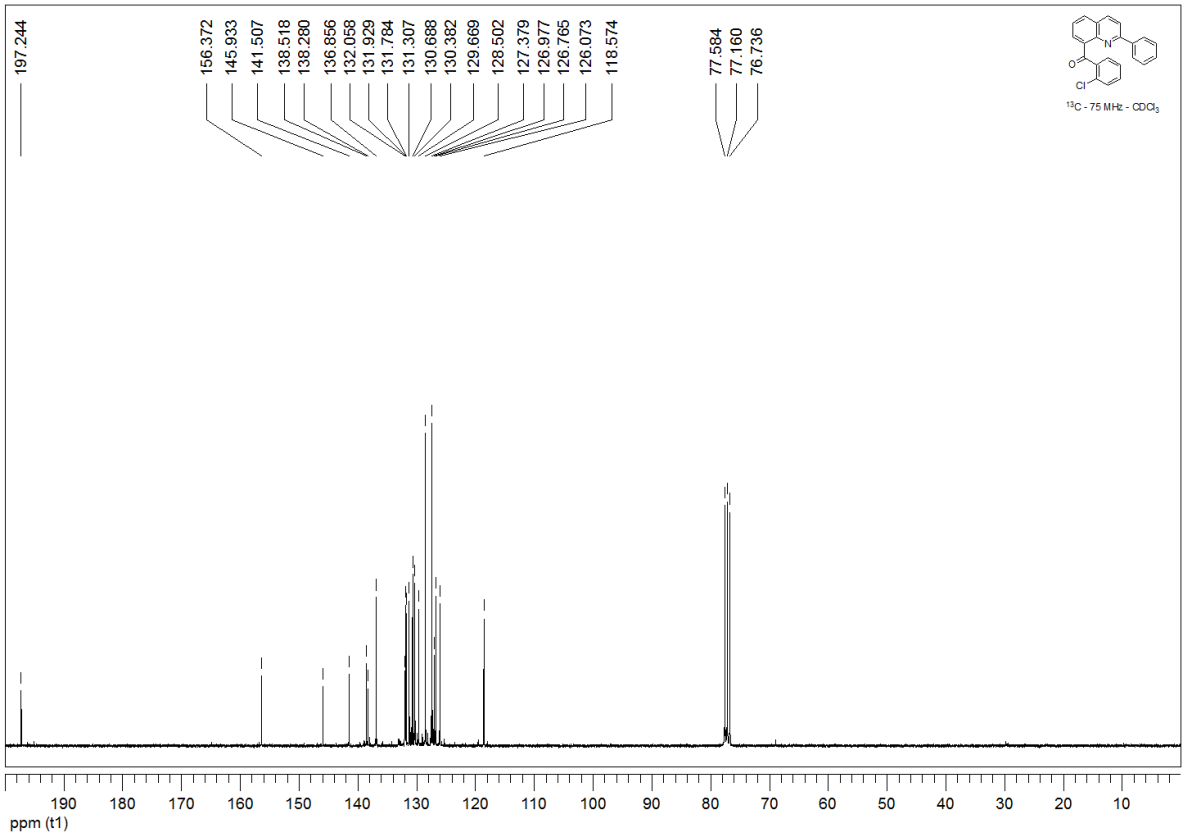
2-(3,5-Diiodo-2-thienyl)quinoline (3h).



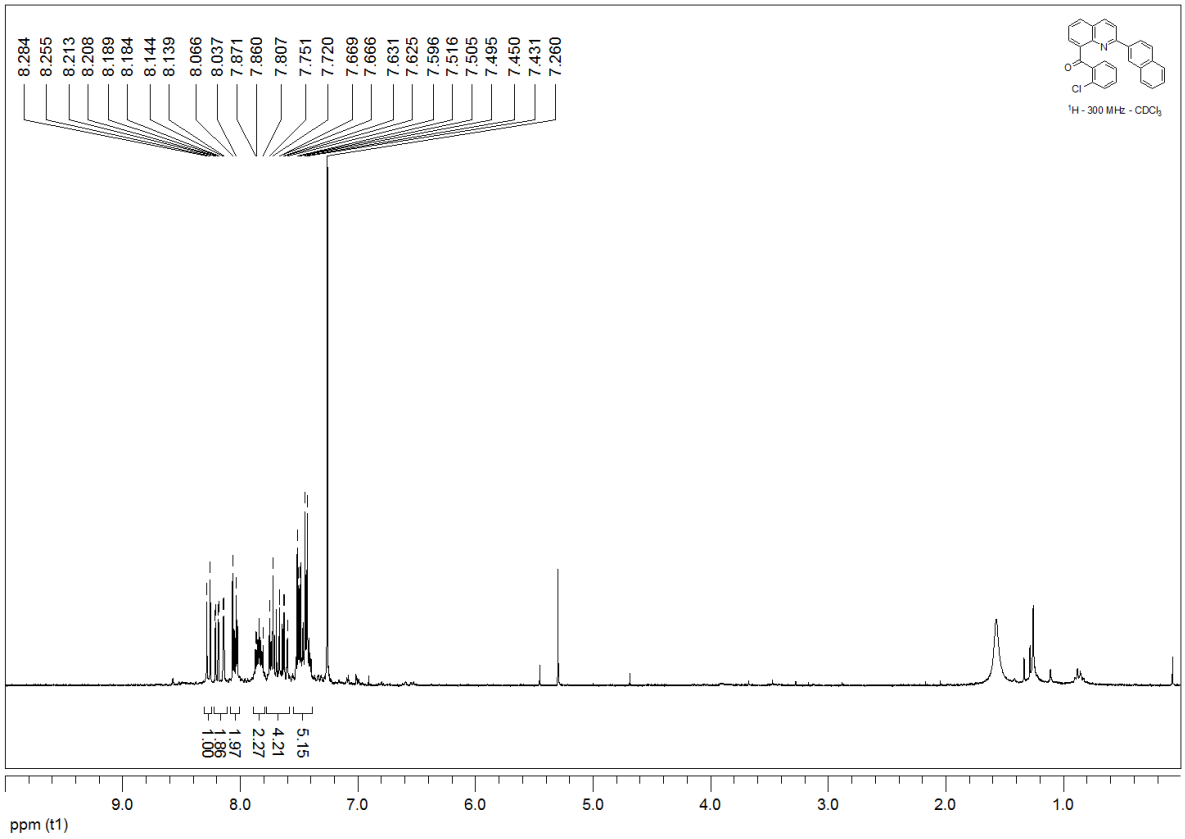


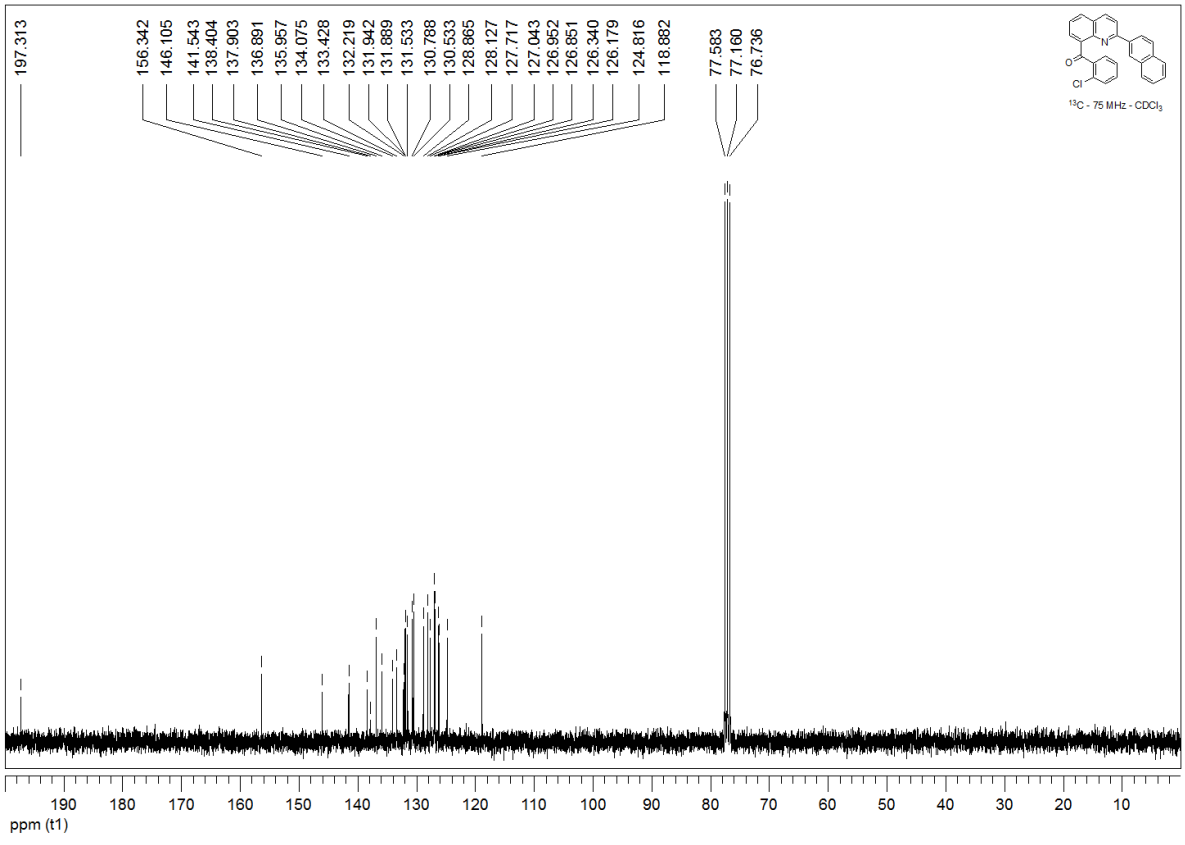
8-(2-Chlorobenzoyl)-2-phenylquinoline (4a).



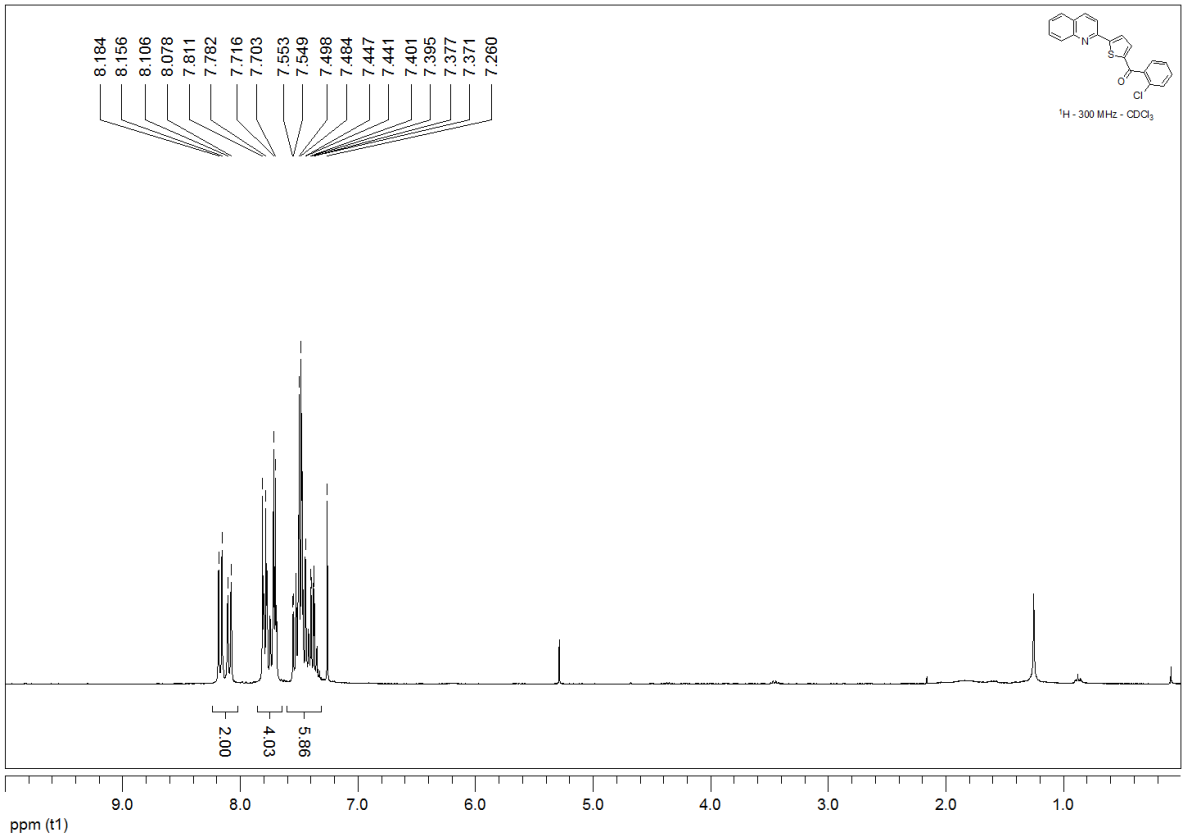


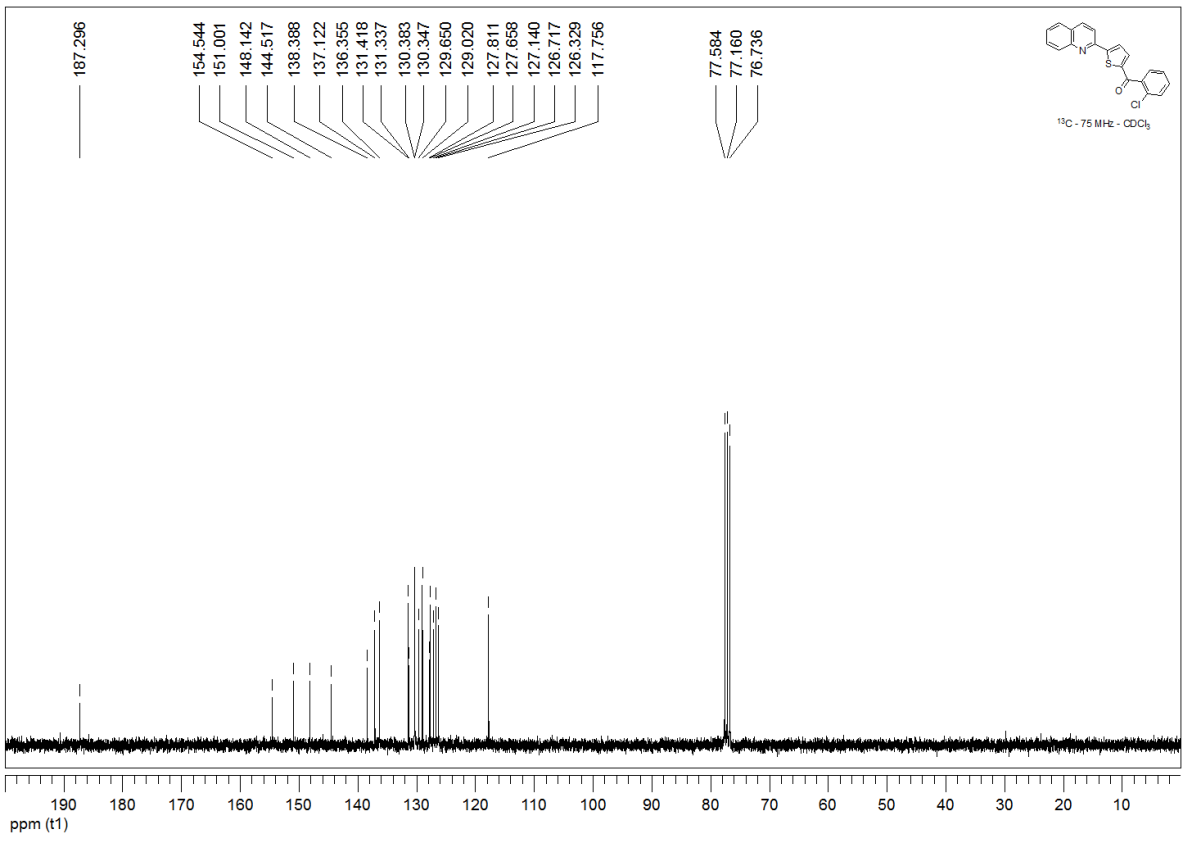
8-(2-Chlorobenzoyl)-2-(2-naphthyl)quinoline (4b).



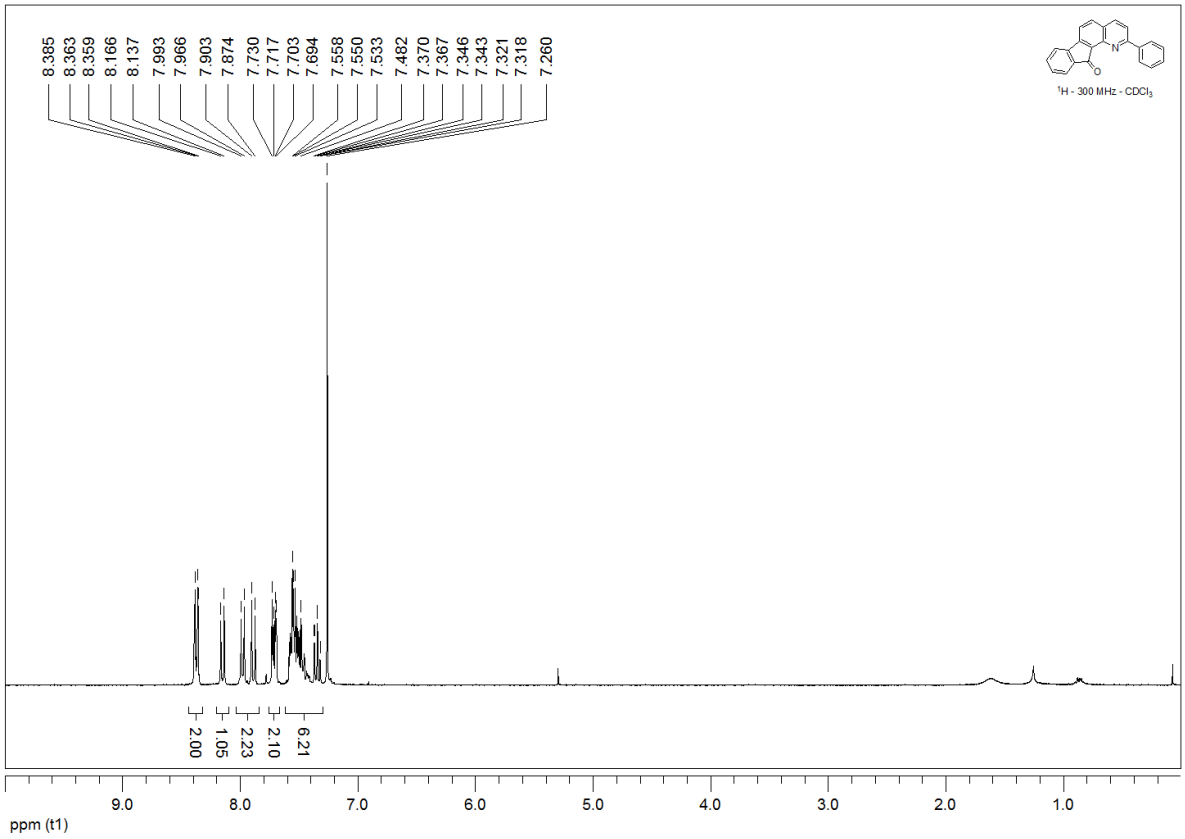


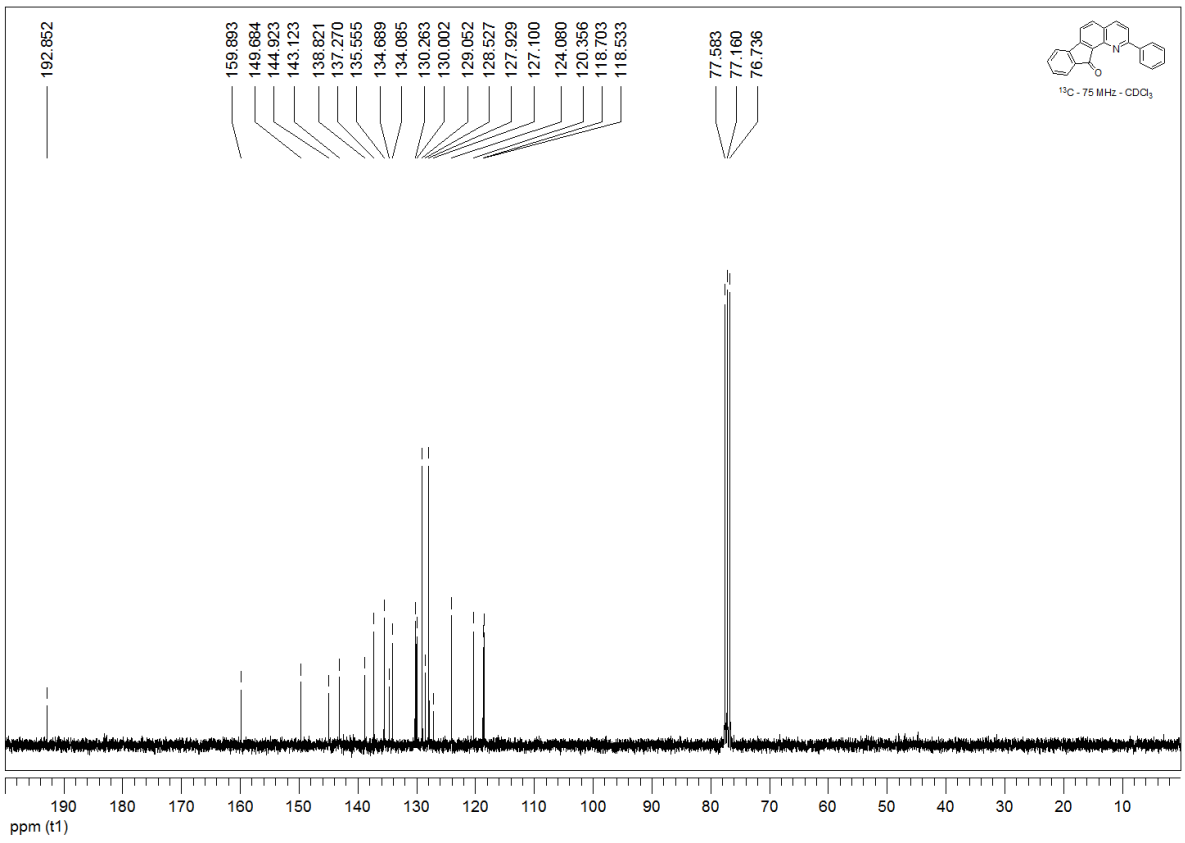
2-(5-(2-Chlorobenzoyl)-2-thienyl)quinoline (4h).



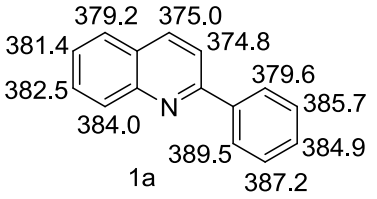


2-Phenyl-11*H*-indeno[1,2-*h*]quinolin-11-one (5a).

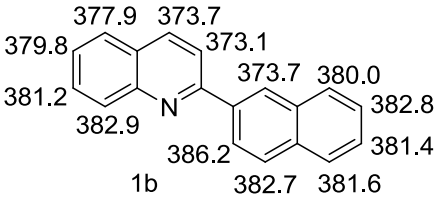




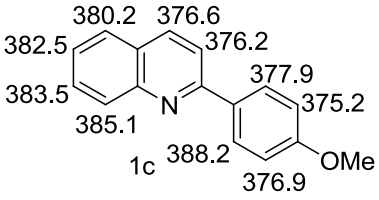
Calculated values of the Gibbs energies $\Delta_{acid}G$ [kcal mol^{-1}] for deprotonation at the corresponding positions of the investigated quinolines



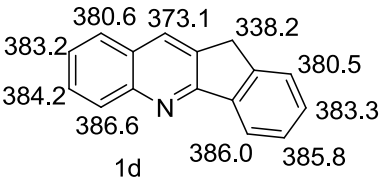
1a



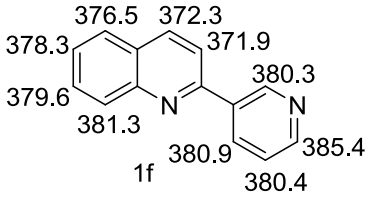
1b



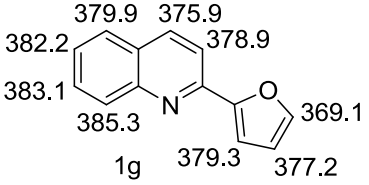
1c



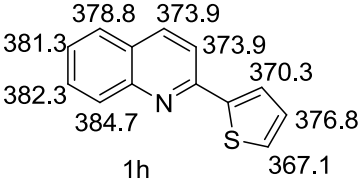
1d



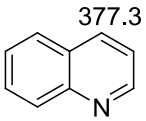
1f



1g

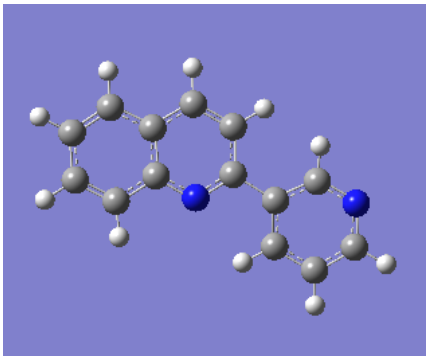


1h



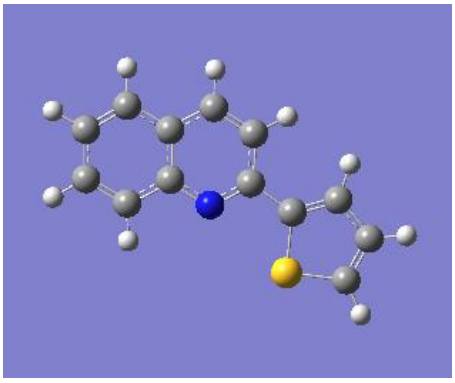
Cartesian coordinates of molecular geometry for the most stable rotamer form of selected quinolines (on example of 1f, 1h) (neutral molecule, gas phase) optimized at B3LYP/6-31G(d) level of theory

1f



C	0.864745	-0.0568	-0.03846
C	1.530703	1.170595	-0.33594
C	2.890335	-1.14499	0.250674
C	2.902177	1.208188	-0.34418
H	0.959426	2.070933	-0.53161
C	3.588755	-2.34303	0.559895
C	3.641967	0.034781	-0.05189
H	3.430426	2.133389	-0.56331
C	4.965334	-2.36492	0.567247
H	3.000245	-3.22691	0.785257
C	5.059084	-0.01895	-0.03627
C	5.707993	-1.19541	0.266916
H	5.492192	-3.28525	0.804331
H	5.622923	0.882089	-0.26669
H	6.793776	-1.23183	0.276884
C	-0.6189	-0.14637	-0.01951
C	-1.2578	-1.212	0.632784
C	-1.44414	0.797411	-0.65205
C	-2.64608	-1.27149	0.640186
H	-0.6512	-1.96881	1.118263
N	-2.78047	0.753917	-0.65374
H	-1.00975	1.626217	-1.20749
C	-3.36277	-0.26411	-0.00963
H	-3.16875	-2.08065	1.142063
H	-4.45156	-0.2755	-0.01761
N	1.529602	-1.16659	0.250598

1h



C	-0.45616	-0.12163	-0.02502
C	0.293607	-0.23683	-1.23639
C	1.398767	-0.67804	1.246601
C	1.618513	-0.58063	-1.1715
H	-0.18366	-0.05368	-2.19293
C	1.96648	-0.90507	2.528676
C	2.228534	-0.81714	0.088417
H	2.211667	-0.67508	-2.07838
C	3.293352	-1.25309	2.651355
H	1.320111	-0.79433	3.393656
C	3.590255	-1.17638	0.247264
C	4.113432	-1.39043	1.504069
H	3.7198	-1.42503	3.635996
H	4.214216	-1.28014	-0.63765
H	5.158038	-1.66564	1.619927
N	0.084584	-0.33606	1.16717
C	-1.87309	0.242935	-0.0469
C	-2.69965	0.522837	-1.11396
S	-2.74893	0.371281	1.463512
C	-4.03184	0.839561	-0.72777
H	-2.37018	0.504225	-2.14704
C	-4.20576	0.797752	0.630518
H	-4.82132	1.08654	-1.4294
H	-5.111	0.994205	1.190141