Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.
This journal is © The Royal Society of Chemistry 2015

Organic & Biomolecular Chemistry

Facile synthesis of benzoindoles and naphthofurans through carbonaceous material catalyzed cyclization of naphthylamines/naphthols with nitroolefins in water

Furen Zhang, Chunmei Li, Chen Wang and Chenze Qi*

School of Chemistry and Chemical Engineering, Zhejiang Key Laboratory of Alternative Technologies for Fine Chemicals Process, Shaoxing University, Shaoxing, Zhejiang Province 312000, China

Electronic Supplementary Information (ESI)

Supplementary Information Available: complete product characterization data, analytical details.

Table of Contents

General information

All the chemicals were commercially available and used without further purification, unless otherwise stated. Analytical thin layer chromatography (TLC) was performed using Merck silica gel GF254 plates. Flash column chromatography was performed on silica gel (200–300 mesh). Melting points were measured on an X-4 melting point apparatus. ^{1}HNMR spectra were recorded on a 400 MHz instrument (Bruker Avance 400 Spectrometer). Chemical shifts (δ) are given in ppm relative to TMS as the internal reference, with coupling constants (J) in Hz. ^{13}C NMR spectra were recorded at 100 MHz. Chemical shift were reported in ppm with the internal chloroform signal at 77.0 ppm as a standard. HRMS (ESI) was measured with a Bruker Daltonics APEXII instrument.

General procedure for the synthesis of 3

In a 10-mL reaction vial, 1-naphthylamine/2-naphthylamine (0.5 mmol), nitroolefin (0.5 mmol), carbonaceous material (C-SO_3H) (10 mg) and water (3.0 mL) were mixed and then capped. The mixture was stirred for a given time at 60 ^{o}C. Upon completion as shown by TLC monitoring, the reaction mixture was cooled to room temperature. The resulting solid precipitate was filtered and dried along with the catalyst. Crude product was further purified by column chromatography on silica gel with the eluent (ethyl acetate/petroleum ether = 1:20~1:4) to give the pure product.

General procedure for the synthesis of 5

In a 10-mL reaction vial, 1-naphthol/2-naphthol (0.5 mmol), nitroolefin (0.5 mmol), carbonaceous material (C-SO_3H) (10 mg) and water (3.0 mL) were mixed and then capped. The mixture was stirred for a given time at 60 ^{o}C. Upon completion as shown by TLC monitoring, the reaction mixture was cooled to room temperature. The resulting solid precipitate was filtered and dried along with the catalyst. Crude product was further purified by column chromatography on silica gel with the eluent (ethyl acetate/petroleum ether = 1:30~1:8) to give the pure product.

Preparation and characterization of the carbonaceous material (C-SO_3H) catalyst

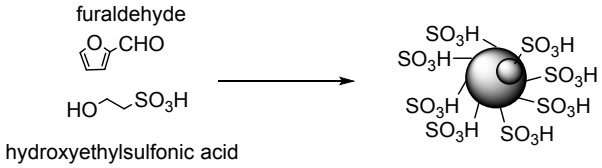


Fig. 1. The synthesis of the carbon functinalized material with sulfonic acid groups

According to literature method,[1] the mixture of the 10 g furaldehyde, 5 g hydroxyethylsulfonic acid and 80 mL deionized water was placed in 100 mL Teflon-lined stainless steel autoclaves, which were heated in an oven at 200 °C for 5 h. The resulting products were filtered, washed with water and methanol, and dried in a vacuum oven at 110 °C for 5 h (Fig. 1). The acidity of the carbonaceous material was 2.4 mmol/g, which was determined through the neutralization titration. This carbonaceous material owned much higher acidity than that of the sulfonated carbonaceous materials, which were obtained via the sulfonation of the inactive carbon. The acid strength of the catalyst was determined by thermodesorption of chemisorbed ammonia (NH_3-TPD). The result showed that the catalyst had great acid strength in which ammonia was desorbed at 400 to 600 °C. IR(KBr) [cm^{-1}] = 3020 (Ar-H), 1704 (C=O), 1604 (C=C), 1204 (C-O), 1040 (S=O), 940 (S-O).

X-ray Crystallography

Single-crystal X-ray diffraction measurement was carried out on a Rigaku Saturn CCD diffractometer at 100(2) K using graphite monochromated Mo Kα radiation (λ = 0.71073 Å). An empirical absorption correction was applied using the SADABS program. The structure was solved by direct methods and refined by full-matrix least squares on F^2 using the SHELXTL-97 program package.

Computational details

All the calculations were carried out using Gaussian 09 programs.[2] The solvation phase geometry optimizations and frequency calculations were performed using the B3LYP functional[3] with the 6-31G+(d) basis set in collaboration with the SMD solvation model.[4] Methanol was used as the solvent. Single-point energy calculations were then performed on the stationary points using M06-2X method[5] with a larger basis set 6-311++G(2df,2p)

and the same solvation model used in the optimization calculation. All the energies correspond to the reference state of 1 mol/L, 298.15 K.

References:

1 X. Z. Liang, M. F. Zeng, C. Z. Qi, *Carbon*, 2010, **48**, 1844-1848.

2 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, Revision D.01, Gaussian, Inc., Wallingford CT, **2009**.

3 (a) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785-789; (b) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648-5652.

4 A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* 2009, 6378-6396.

5 Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* 2008, **120**, 215-241.

Energy properties and Cartesian Coordinates of Reactants, Intermidiates and Transition States

1b

C	-2.363183000	1.109702000	-0.017676000
C	-1.022269000	1.441928000	-0.026135000
C	-0.014146000	0.437309000	-0.004241000
C	-0.418597000	-0.941956000	0.008746000
C	-1.809716000	-1.247025000	0.020708000
C	-2.762150000	-0.249303000	0.010728000
H	-3.115640000	1.894453000	-0.036639000
H	-0.745088000	2.491791000	-0.059860000
C	1.391985000	0.748347000	0.000168000
C	0.563763000	-1.971426000	0.002459000
H	-2.110089000	-2.292831000	0.035179000
H	-3.819725000	-0.502523000	0.019311000
C	1.902906000	-1.639904000	-0.012427000
C	2.317183000	-0.289270000	-0.008335000
H	0.243167000	-3.010579000	0.008839000
H	2.659363000	-2.421722000	-0.017101000
H	3.379247000	-0.051935000	-0.007071000
N	1.821144000	2.078199000	-0.058136000
H	1.246208000	2.752845000	0.436321000
H	2.799885000	2.202687000	0.184004000

TCG = 0.131751 au
E= -441.2154473 au

2a

C	-3.087980000	1.067375000	0.000055000
C	-1.709036000	1.273172000	0.000036000
C	-0.817820000	0.178446000	-0.000022000
C	-1.347256000	-1.131919000	-0.000054000
C	-2.723763000	-1.332190000	-0.000034000
C	-3.597767000	-0.235024000	0.000020000
H	-3.763184000	1.918969000	0.000098000
H	-1.308967000	2.284200000	0.000060000
H	-0.682307000	-1.990369000	-0.000098000
H	-3.121328000	-2.343633000	-0.000058000
H	-4.672471000	-0.398657000	0.000038000
C	0.607291000	0.461592000	-0.000039000
C	1.603775000	-0.451475000	0.000000000
H	0.886872000	1.512483000	-0.000080000
H	1.501739000	-1.527631000	0.000055000
N	2.967856000	-0.037935000	-0.000007000
O	3.830531000	-0.939369000	0.000110000
O	3.271967000	1.168159000	-0.000076000

TCG = 0.101136 au
E= -514.1195079 au

TSA

C	2.180430000	2.087375000	-1.571172000
C	1.000349000	1.320328000	-1.700813000
C	0.898877000	0.079131000	-1.099083000
C	1.975902000	-0.453078000	-0.318224000
C	3.171030000	0.336760000	-0.202292000
C	3.244619000	1.607117000	-0.839070000
H	2.239908000	3.055707000	-2.060657000
H	0.169337000	1.700336000	-2.289606000
H	4.156695000	2.190663000	-0.738936000
N	-0.325631000	-0.645652000	-1.219824000
H	-0.197534000	-1.654350000	-1.320646000
C	-1.615024000	-0.563189000	0.237308000
H	-0.939375000	-1.036349000	0.943219000
C	-2.719559000	-1.356609000	-0.176895000
H	-3.637297000	-0.954695000	-0.580322000
C	-1.803724000	0.889223000	0.457830000
C	-2.668829000	1.666857000	-0.334801000
C	-1.090943000	1.511778000	1.497689000
C	-2.823668000	3.029853000	-0.081601000
H	-3.217597000	1.212064000	-1.155251000
C	-1.253100000	2.875391000	1.754964000
H	-0.417502000	0.920736000	2.113591000
C	-2.119242000	3.637339000	0.965540000
H	-3.494307000	3.619795000	-0.701380000
H	-0.701839000	3.340785000	2.568131000
H	-2.245091000	4.699225000	1.162369000
N	-2.673109000	-2.707411000	-0.103871000
O	-3.703382000	-3.392904000	-0.431857000
O	-1.617110000	-3.316001000	0.284624000
H	-0.888127000	-0.314981000	-2.005057000
C	1.926531000	-1.716462000	0.335528000
C	4.263049000	-0.172657000	0.554857000
C	3.006211000	-2.178323000	1.061926000
H	2.948183000	-3.145209000	1.555297000
C	4.185940000	-1.402481000	1.173462000
H	5.027758000	-1.779590000	1.748737000
H	5.164552000	0.430695000	0.635831000
H	1.034265000	-2.332269000	0.277504000

TCG = 0.25646 au
E= -955.3280105 au

INTA

C	-1.807803000	-2.266458000	-1.655141000
C	-0.733681000	-1.346801000	-1.664552000
C	-0.826022000	-0.164954000	-0.963671000
C	-1.991528000	0.185566000	-0.215824000
C	-3.073670000	-0.762908000	-0.217971000
C	-2.950172000	-1.980865000	-0.941927000
H	-1.718621000	-3.193819000	-2.213612000
H	0.167128000	-1.574143000	-2.228475000
H	-3.780803000	-2.682534000	-0.926458000
N	0.339671000	0.727645000	-0.998340000
H	0.080607000	1.733595000	-1.062813000
C	1.317409000	0.699165000	0.233558000
H	0.661092000	0.954504000	1.070351000
C	2.358799000	1.746453000	0.022286000
H	3.415440000	1.524664000	0.061038000
C	1.895705000	-0.681851000	0.434597000
C	2.829442000	-1.217661000	-0.466592000
C	1.503123000	-1.441289000	1.545063000
C	3.358562000	-2.493422000	-0.259251000
H	3.144870000	-0.640573000	-1.333180000
C	2.037901000	-2.716047000	1.756911000
H	0.781434000	-1.031898000	2.248130000
C	2.964897000	-3.244859000	0.854294000
H	4.079966000	-2.899110000	-0.964266000
H	1.728979000	-3.292920000	2.625114000
H	3.380711000	-4.236273000	1.017013000
N	2.019195000	3.010273000	-0.157364000
O	2.906205000	3.947692000	-0.260668000
O	0.756168000	3.343155000	-0.252601000
H	0.894057000	0.521016000	-1.837568000

C	-2.157262000	1.402592000	0.507106000
C	-4.260359000	-0.461325000	0.506839000
C	-3.325603000	1.660715000	1.194706000
H	-3.431298000	2.596068000	1.738358000
C	-4.386711000	0.722481000	1.200458000
H	-5.298586000	0.941629000	1.749995000
H	-5.069276000	-1.188320000	0.499610000
H	-1.364905000	2.144734000	0.527510000

TCG = 0.25972 au
E= -955.3422196 au

8

C	1.685163000	-1.603923000	2.209259000
C	0.655343000	-0.827300000	1.628405000
C	0.887013000	-0.053353000	0.495592000
C	2.209169000	-0.050647000	-0.092390000
C	3.234448000	-0.862243000	0.503505000
C	2.949094000	-1.635167000	1.664348000
H	1.456384000	-2.191829000	3.095381000
H	-0.327743000	-0.853049000	2.084744000
H	3.737211000	-2.240984000	2.105005000
N	-0.101027000	0.761764000	-0.062459000
H	0.024492000	0.960611000	1.049096000
C	-1.505565000	0.653109000	0.318190000
H	-1.572613000	0.709571000	1.407679000
C	-2.249740000	1.874702000	-0.246016000
H	-2.181754000	1.944230000	-1.331841000
H	-3.293433000	1.875718000	0.074465000
C	-2.227201000	-0.616515000	-0.144081000
C	-3.157567000	-1.230823000	0.705940000
C	-2.002156000	-1.165031000	-1.414568000
C	-3.850301000	-2.374524000	0.297102000
H	-3.335471000	-0.815146000	1.696045000
C	-2.692655000	-2.309585000	-1.825338000
H	-1.282538000	-0.705621000	-2.088564000
C	-3.618851000	-2.917475000	-0.971064000
H	-4.564128000	-2.843208000	0.970460000
H	-2.505770000	-2.725827000	-2.812451000
H	-4.153225000	-3.809129000	-1.290036000
N	-1.657294000	3.151518000	0.293510000
O	-1.203220000	3.969852000	-0.506892000
O	-1.661817000	3.319338000	1.513162000
C	2.547975000	0.728706000	-1.234560000
C	4.532751000	-0.872217000	-0.080634000
C	3.819876000	0.698368000	-1.774170000
H	4.050746000	1.306069000	-2.645714000
C	4.823814000	-0.113921000	-1.195124000
H	5.821787000	-0.133137000	-1.626525000
H	1.811985000	1.376942000	-1.700742000
H	5.298943000	-1.494668000	0.377278000

TCG = 0.255641 au
E= -955.3611012 au

TSB

C	1.659084000	0.207864000	-0.382141000
H	1.711107000	-0.266666000	-1.360415000
C	2.924608000	0.304789000	0.279029000
H	3.162081000	1.048675000	1.026163000
C	0.763754000	1.393930000	-0.357392000
C	0.632338000	2.226293000	0.769723000
C	0.033444000	1.713520000	-1.517985000
C	-0.196412000	3.350039000	0.730365000
H	1.176540000	2.000799000	1.682304000
C	-0.792470000	2.838277000	-1.557467000
H	0.126397000	1.080500000	-2.397621000
C	-0.911210000	3.660448000	-0.431632000
H	-0.285148000	3.982794000	1.610187000
H	-1.341254000	3.072527000	-2.466491000
H	-1.554725000	4.536529000	-0.459794000
N	3.902302000	-0.588599000	0.040024000
O	5.042864000	-0.469316000	0.627540000
O	3.717782000	-1.572165000	-0.766008000
C	0.716589000	-1.359399000	0.428315000
C	-0.339890000	-1.656489000	-0.509026000
C	0.341725000	-0.992548000	1.780587000
C	-1.706323000	-1.283913000	-0.201066000
C	-0.945099000	-0.716987000	2.107415000
H	1.135441000	-0.900020000	2.517457000
C	-1.995393000	-0.824368000	1.121104000
H	-1.215168000	-0.408454000	3.114222000
H	1.596267000	-1.992516000	0.320974000
N	-0.010651000	-2.230180000	-1.669512000
H	0.945455000	-2.524633000	-1.841505000
H	-0.688268000	-2.456892000	-2.387270000
C	-2.757505000	-1.382233000	-1.143660000
C	-3.327171000	-0.487753000	1.446858000
C	-4.341205000	-0.591014000	0.506047000
H	-5.360243000	-0.325121000	0.775547000
C	-4.054723000	-1.037224000	-0.798493000
H	-4.848356000	-1.108706000	-1.537188000
H	-2.564152000	-1.712377000	-2.160070000
H	-3.547545000	-0.142540000	2.454173000

TCG = 0.255255 au
E= -955.3163846 au

INTB

C	1.579260000	0.019219000	-0.328303000
H	1.748731000	-0.231668000	-1.380828000
C	2.897856000	0.014970000	0.366946000
H	3.172619000	0.742665000	1.117835000
C	0.883517000	1.369183000	-0.268761000
C	0.747862000	2.095372000	0.926345000
C	0.359883000	1.923448000	-1.448510000
C	0.101312000	3.335095000	0.940687000
H	1.150496000	1.700352000	1.854742000
C	-0.288052000	3.162702000	-1.436953000
H	0.466226000	1.382881000	-2.386634000
C	-0.421550000	3.872706000	-0.239943000
H	0.008713000	3.881045000	1.876745000
H	-0.682670000	3.573016000	-2.363591000
H	-0.922720000	4.837614000	-0.227059000
N	3.809711000	-0.898257000	0.092964000
O	4.977331000	-0.885500000	0.683481000
O	3.581635000	-1.845450000	-0.774629000
C	0.649798000	-1.213136000	0.208934000
C	-0.502918000	-1.430821000	-0.720438000
C	0.261841000	-1.052825000	1.638450000
C	-1.860179000	-1.119001000	-0.318489000
C	-1.016672000	-0.916608000	2.030650000
H	1.073413000	-1.029139000	2.361038000
C	-2.106661000	-0.889327000	1.066945000
H	-1.269224000	-0.792827000	3.080843000
H	1.325965000	-2.071518000	0.103650000
N	-0.220971000	-1.904373000	-1.913277000
H	0.736558000	-2.140625000	-2.164908000
H	-0.927662000	-2.091591000	-2.618809000
C	-2.932568000	-1.064183000	-1.237565000
C	-3.424850000	-0.635143000	1.485251000
C	-4.468377000	-0.589454000	0.566776000
H	-5.479961000	-0.386636000	0.908831000
C	-4.222094000	-0.796997000	-0.800955000
H	-5.036594000	-0.745648000	-1.517718000
H	-2.762804000	-1.204520000	-2.300972000
H	-3.618451000	-0.468587000	2.541808000

TCG = 0.257044 au
E= -955.3273827 au

9

C	-3.040774000	-1.002224000	-0.455588000
C	-2.856781000	0.246201000	0.226386000
C	-1.516767000	0.725278000	0.472878000

C	-0.415871000	-0.018357000	0.021497000
C	-0.639700000	-1.242221000	-0.659791000
C	-1.903956000	-1.734496000	-0.890015000
H	0.218277000	-1.813395000	-1.000028000
H	-2.044199000	-2.680993000	-1.406582000
N	-1.348812000	1.965332000	1.091585000
H	-2.094822000	2.250462000	1.715874000
H	-0.450419000	2.126870000	1.533654000
C	1.008375000	0.510859000	0.233254000
H	1.047004000	1.002984000	1.210465000
C	1.262054000	1.606449000	-0.827923000
H	0.495330000	2.383929000	-0.767782000
H	1.317435000	1.222966000	-1.844670000
N	2.557985000	2.334700000	-0.583564000
O	3.370174000	2.417521000	-1.506364000
O	2.743609000	2.825100000	0.531773000
C	2.094759000	-0.561721000	0.276198000
C	2.457931000	-1.093788000	1.524191000
C	2.747411000	-1.043995000	-0.869008000
C	3.438577000	-2.083807000	1.628417000
H	1.968007000	-0.724969000	2.423348000
C	3.732737000	-2.032630000	-0.768001000
H	2.494671000	-0.657133000	-1.852288000
C	4.081755000	-2.557012000	0.479697000
H	3.704909000	-2.478151000	2.606323000
H	4.226861000	-2.390270000	-1.668358000
H	4.849575000	-3.323125000	0.556931000
C	-4.017120000	0.970971000	0.624711000
C	-4.361793000	-1.478888000	-0.687919000
C	-5.463419000	-0.757876000	-0.278420000
H	-6.466283000	-1.134736000	-0.464492000
C	-5.286388000	0.482754000	0.380710000
H	-6.154533000	1.057788000	0.693360000
H	-3.926890000	1.933174000	1.119793000
H	-4.485583000	-2.429591000	-1.202601000

TCG = 0.25681 au

E= -955.3685548 au

1c

C	1.174001000	-1.205524000	0.003415000
C	-0.222483000	-1.211039000	-0.004737000
C	-0.941459000	-0.000075000	-0.008657000
C	-0.222426000	1.211035000	-0.004564000
C	1.173931000	1.205596000	0.003324000
C	1.886445000	-0.000018000	0.006953000
H	1.707972000	-2.153568000	0.009297000
H	-0.766095000	-2.154080000	-0.008184000
H	-0.766269000	2.153951000	-0.007747000
H	1.708023000	2.153570000	0.009276000
H	2.973512000	0.000052000	0.014335000
N	-2.339732000	-0.000103000	-0.080488000
H	-2.783726000	-0.836571000	0.287107000
H	-2.783342000	0.837517000	0.284925000

TCG = 0.25681 au

E= -955.3685548 au

TSA for 1c

C	3.574417000	-0.537612000	-0.681819000
C	2.247110000	-0.373233000	-1.084784000
C	1.263936000	-1.243910000	-0.596172000
C	1.602772000	-2.264513000	0.303222000
C	2.932736000	-2.419711000	0.698661000
C	3.922110000	-1.558265000	0.209835000
H	4.337036000	0.133448000	-1.068853000
H	1.975007000	0.415001000	-1.782486000
H	0.831688000	-2.933172000	0.678712000
H	3.195536000	-3.217504000	1.388702000
H	4.956435000	-1.683652000	0.519531000
N	-0.101139000	-1.057246000	-0.960272000
H	-0.621337000	-1.935306000	-0.998488000
C	-1.230497000	-0.019174000	0.294262000
H	-0.902450000	-0.628628000	1.131547000
C	-2.567637000	-0.216384000	-0.127178000
H	-3.147717000	0.508394000	-0.679813000
C	-0.638043000	1.335783000	0.250193000
C	-0.929850000	2.253182000	-0.777378000
C	0.248570000	1.718485000	1.272471000
C	-0.359565000	3.525875000	-0.768619000
H	-1.595505000	1.971884000	-1.588912000
C	0.811206000	2.997261000	1.284680000
H	0.485159000	1.014014000	2.065993000
C	0.508800000	3.903091000	0.264056000
H	-0.591379000	4.225131000	-1.568051000
H	1.486254000	3.282309000	2.087660000
H	0.947644000	4.897796000	0.269436000
N	-3.207904000	-1.385000000	0.130759000
O	-4.434241000	-1.518504000	-0.202690000
O	-2.601944000	-2.357024000	0.695687000
H	-0.219977000	-0.555019000	-1.840940000

TCG = 0.213162 au

E= -801.6975705 au

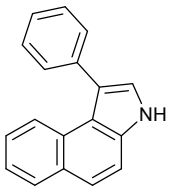
TSB for 1c

C	-0.732597000	-0.491737000	-0.367284000
H	-1.005253000	-0.224342000	-1.388295000
C	-1.765450000	-1.223663000	0.315324000
H	-1.577638000	-1.919363000	1.120947000
C	0.656939000	-1.029146000	-0.271257000
C	1.193166000	-1.537104000	0.925632000
C	1.453703000	-1.057325000	-1.430769000
C	2.485421000	-2.067141000	0.957072000
H	0.604151000	-1.520411000	1.838301000
C	2.744623000	-1.589358000	-1.399520000
H	1.051991000	-0.671934000	-2.364946000
C	3.265344000	-2.095720000	-0.204055000
H	2.883251000	-2.456877000	1.890985000
H	3.340887000	-1.609693000	-2.308588000
H	4.270524000	-2.509411000	-0.177254000
N	-3.061178000	-1.028110000	0.024275000
O	-3.971711000	-1.705098000	0.637858000
O	-3.419400000	-0.164694000	-0.859563000
C	-0.796153000	1.336486000	0.249372000
C	0.043277000	2.079427000	-0.679374000
C	-0.396546000	1.333304000	1.642143000
C	1.321539000	2.533269000	-0.256214000
C	0.817238000	1.820003000	2.036505000
H	-1.072334000	0.874912000	2.359619000
C	1.687254000	2.403443000	1.064407000
H	1.978722000	3.016267000	-0.974765000
H	1.129927000	1.772167000	3.075454000
H	2.660997000	2.770093000	1.380361000
H	-1.865925000	1.422770000	0.054134000
N	-0.372576000	2.276415000	-1.936560000
H	-1.313717000	2.032116000	-2.226002000
H	0.213035000	2.755481000	-2.612216000

TCG = 0.21162 au

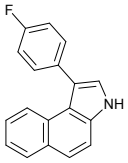
E= -801.6795538 au

Spectral data of the compounds



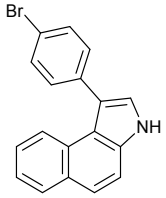
1-phenyl-3H-benzo[e]indole (3a)

Brown oil; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.48 (br, s, 1H), 8.18 (d, J = 8.0 Hz, 1H), 7.96 (d, J = 8.8 Hz, 1H), 7.67-7.69 (m, 3H), 7.52-7.56 (m, 3H), 7.47-7.50 (m, 1H), 7.35-7.45 (m, 2H), 7.19 (d, J = 2.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 137.1, 132.9, 130.2, 129.8, 128.8, 128.7, 128.3, 126.8, 125.4, 123.8, 123.4, 123.2, 121.6, 121.3, 119.5, 112.9; HRMS (ESI) calcd for $C_{18}H_{13}N$ $(M + H)^+$: 244.1121, found: 244.1125.



1-(4-fluorophenyl)-3H-benzo[e]indole (3b)

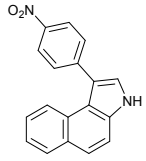
Brown oil; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.47 (br, s, 1H), 8.08 (d, J = 8.4 Hz, 1H), 7.96 (d, J = 8.4 Hz, 1H), 7.68 (d, J = 8.8 Hz, 1H), 7.54-7.62 (m, 3H), 7.35-7.45 (m, 2H), 7.20-7.24 (m, 2H), 7.16 (d, J = 2.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 163.4, 160.9, 133.0, 132.8, 131.7, 129.8, 128.9, 128.6, 125.5, 123.9, 123.3, 123.1, 121.5, 120.1, 119.6, 115.4, 115.2, 112.9; HRMS (ESI) calcd for $C_{18}H_{12}FN$ $(M + H)^+$: 262.1026, found: 262.1029.



1-(4-nitrophenyl)-3H-benzo[e]indole (3c)

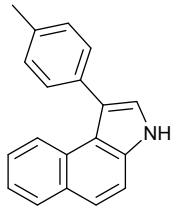
Brown solid, mp: 82-84 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.53 (br, s, 1H), 8.11 (d, J = 8.0 Hz, 1H), 7.95 (d, J = 8.8 Hz, 1H), 7.63-7.69 (m, 3H), 7.51-7.57 (m, 3H), 7.36-

7.45 (m, 2H), 7.17 (d, J = 2.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 136.1, 132.9, 131.8, 131.5, 129.8, 128.9, 128.5, 125.6, 124.1, 123.4, 123.2, 121.6, 120.8, 120.0, 119.3, 112.9; HRMS (ESI) calcd for $C_{18}H_{12}BrN$ $(M + H)^+$: 322.0226, found: 322.0235.



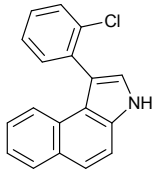
1-(4-nitrophenyl)-3H-benzo[e]indole (3d)

Brown solid, mp: 130-132^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.75 (br, s, 1H), 8.37 (d, J = 8.4 Hz, 2H), 8.07 (d, J = 8.0 Hz, 1H), 7.96 (d, J = 8.0 Hz, 1H), 7.82 (d, J = 8.8 Hz, 2H), 7.71 (d, J = 8.8 Hz, 1H), 7.60 (d, J = 8.8 Hz, 1H), 7.37-7.46 (m, 2H), 7.29 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 146.6, 144.5, 133.4, 130.3, 130.0, 129.1, 128.2, 125.7, 124.6, 123.8, 123.7, 123.0, 122.4, 119.4, 118.9, 112.9; HRMS (ESI) calcd for $C_{18}H_{12}N_2O_2$ $(M + H)^+$: 289.0971, found: 289.0985.



1-(p-tolyl)-3H-benzo[e]indole (3e)

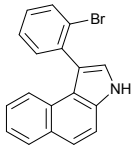
Brown solid, mp: 44-46 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.48 (br, s, 1H), 8.19 (d, J = 8.4 Hz, 1H), 7.94 (d, J = 7.6 Hz, 1H), 7.67 (d, J = 8.8 Hz, 3H), 7.33-7.42 (m, 5H), 7.17 (d, J = 2.4 Hz, 1H), 2.52 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 136.5, 134.1, 132.8, 130.1, 130.0, 129.8, 129.1, 128.8, 128.7, 127.3, 125.3, 123.8, 123.7, 123.4, 123.2, 121.5, 121.2, 119.6, 112.9; HRMS (ESI) calcd for $C_{19}H_{15}N$ $(M + H)^+$: 258.1277, found: 258.1265.



1-(2-chlorophenyl)-3H-benzo[e]indole (3f)

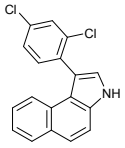
Brown solid, mp: 56-58 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.53 (br, s, 1H), 7.94 (d, J = 7.6 Hz, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.67-7.71 (m, 2H), 7.55-7.58 (m, 2H), 7.33-

7.48 (m, 4H), 7.19 (d, J = 2.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 138.1, 132.9, 132.8, 132.3, 129.7, 129.0, 128.7, 128.6, 127.3, 126.2, 125.7, 123.8, 123.3, 123.1, 121.6, 120.2, 119.6, 112.9; HRMS (ESI) calcd for $C_{18}H_{12}BrN$ $(M + H)^+$: 278.0371, found: 278.0367.



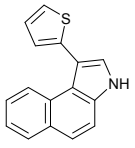
1-(2-bromophenyl)-3H-benzo[e]indole (3g)

Brown solid, mp: 64-66 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.55 (br, s, 1H), 7.94 (d, J = 8.0 Hz, 1H), 7.74 (d, J = 8.0 Hz, 1H), 7.68 (d, J = 9.2 Hz, 1H), 7.62-7.67 (m, 1H), 7.55-7.58 (m, 2H), 7.36-7.45 (m, 4H), 7.20 (d, J = 2.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 136.1, 135.4, 132.9, 132.5, 129.7, 129.6, 128.8, 128.7, 128.6, 126.7, 125.7, 123.8, 123.3, 123.0, 121.8, 120.3, 117.6, 112.9; HRMS (ESI) calcd for $C_{18}H_{12}BrN$ $(M + H)^+$: 322.0226, found: 322.0232.



1-(2,4-dichlorophenyl)-3H-benzo[e]indole (3h)

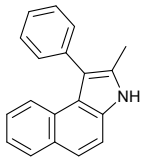
Brown oil; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.59 (br, s, 1H), 7.94 (d, J = 8.4 Hz, 1H), 7.67-7.70 (m, 2H), 7.64 (d, J = 2.0 Hz, 1H), 7.58 (d, J = 8.8 Hz, 3H), 7.49 (d, J = 8.0 Hz, 1H), 7.37-7.42 (m, 3H), 7.20 (d, J = 2.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 136.1, 134.7, 133.8, 133.5, 132.5, 129.7, 129.4, 128.7, 128.5, 127.0, 125.8, 124.0, 123.4, 122.9, 121.8, 116.4, 112.9; HRMS (ESI) calcd for $C_{18}H_{12}Cl_2N$ $(M + H)^+$: 312.0341, found: 312.0348.



1-(thiophen-2-yl)-3H-benzo[e]indole (3i)

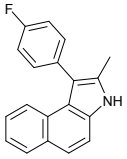
Brown oil; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.49 (br, s, 1H), 8.17-8.19 (m, 1H), 7.93-7.95 (m, 1H), 7.67 (d, J = 8.8 Hz, 1H), 7.51-7.57 (m, 2H), 7.38-7.43 (m, 4H), 7.24 (d, J = 2.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 137.0, 132.8, 130.1, 129.8, 128.7,

125.6, 125.3, 123.8, 123.3, 122.6, 121.7, 120.0, 117.8, 115.5, 112.8; HRMS (ESI) calcd for $C_{16}H_{11}NS$ $(M + H)^+$: 250.0685, found: 250.0690.



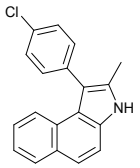
2-methyl-1-phenyl-3H-benzo[e]indole (3j)

Brown solid, mp: 52-54 ^oC; ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.17 (br, s, 1H), 7.94 (t, J_1 = 6.8 Hz, J_2 = 7.2 Hz, 2H), 7.63 (d, J = 8.4 Hz, 1H), 7.55-7.57 (m, 4H), 7.45-7.50 (m, 2H), 7.38-7.42 (m, 1H), 7.29-7.33 (m, 1H), 2.35 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 137.2, 131.3, 131.2, 130.4, 129.8, 128.7, 128.5, 128.3, 126.8, 125.1, 123.3, 122.9, 122.4, 120.9, 117.2, 112.4, 11.9; HRMS (ESI) calcd for $C_{19}H_{15}N$ $(M + H)^+$: 258.1277, found: 258.1273.



1-(4-fluorophenyl)-2-methyl-3H-benzo[e]indole (3k)

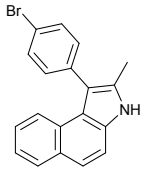
Brown solid, mp: 82-84 ^oC; ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.23 (br, s, 1H), 7.92 (d, J = 7.6 Hz, 1H), 7.83 (d, J = 8.4 Hz, 1H), 7.61 (d, J = 8.8 Hz, 1H), 7.46-7.51 (m, 3H), 7.35-7.39 (m, 1H), 7.25-7.32 (m, 1H), 7.21-7.24 (m, 2H), 2.35 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 163.2, 160.8, 133.0, 132.9, 132.6, 132.5, 131.2, 130.5, 129.8, 128.8, 128.1, 125.2, 123.0, 122.5, 120.9, 116.2, 115.5, 115.3, 112.2, 11.9; HRMS (ESI) calcd for $C_{19}H_{14}FN$ $(M + H)^+$: 276.1183, found: 276.1188.



1-(4-chlorophenyl)-2-methyl-3H-benzo[e]indole (3l)

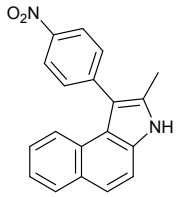
Brown solid, mp: 88-90 ^oC; ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.28 (br, s, 1H), 7.91 (d, J = 8.0 Hz, 1H), 7.84 (d, J = 8.4 Hz, 1H), 7.60 (d, J = 8.8 Hz, 2H), 7.44-7.52 (m, 5H), 7.32-7.39 (m, 1H), 7.28-7.30 (m, 1H), 2.36 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 135.7, 132.7, 132.4, 131.3, 130.4, 129.8, 128.8, 128.6, 128.1, 125.2, 123.0, 122.9, 122.7, 120.8, 116.0, 112.2, 11.9; HRMS (ESI) calcd for $C_{19}H_{14}ClN$ $(M + H)^+$: 292.0887, found:

292.0897.



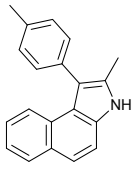
1-(4-bromophenyl)-2-methyl-3H-benzo[e]indole (3m)

Brown solid, mp: 96-98 °C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.29 (br, s, 1H), 7.90 (d, J = 8.0 Hz, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.65 (d, J = 8.4 Hz, 2H), 7.60 (d, J = 8.8 Hz, 1H), 7.50 (d, J = 8.8 Hz, 1H), 7.35-7.41 (m, 3H), 7.31 (d, J = 7.2 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 136.2, 132.8, 131.6, 131.3, 130.4, 129.8, 128.8, 128.1, 125.2, 123.0, 122.9, 122.7, 120.8, 120.7, 116.0, 112.2, 11.9; HRMS (ESI) calcd for $C_{19}H_{14}BrN$ $(M + H)^+$: 336.0382, found: 336.0373.



2-methyl-1-(4-nitrophenyl)-3H-benzo[e]indole (3n)

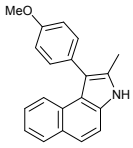
Brown solid, mp: 138-140 °C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.47 (br, s, 1H), 8.39 (d, J = 8.4 Hz, 2H), 7.93 (d, J = 8.0 Hz, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.69 (d, J = 8.4 Hz, 2H), 7.64 (d, J = 8.8 Hz, 1H), 7.52 (d, J = 8.4 Hz, 1H), 7.37-7.41 (m, 1H), 7.32 (d, J = 7.2 Hz, 1H), 2.41 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 146.6, 144.9, 131.7, 131.0, 129.9, 129.0, 127.8, 126.4, 125.8, 125.4, 123.7, 123.3, 123.2, 122.8, 122.5, 120.3, 118.3, 115.3, 112.3, 12.1; HRMS (ESI) calcd for $C_{19}H_{14}N_2O_2$ $(M + H)^+$: 303.1128, found: 303.1133.



2-methyl-1-(p-tolyl)-3H-benzo[e]indole (3o)

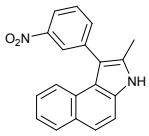
Brown solid, mp: 78-80 °C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.26 (br, s, 1H), 7.90 (t, J_1 = 6.8 Hz, J_2 = 7.2 Hz, 2H), 7.58 (d, J = 8.8 Hz, 1H), 7.50 (d, J = 8.8 Hz, 1H), 7.42 (d, J = 8.0 Hz, 2H), 7.34 (d, J = 8.0 Hz, 3H), 7.25-7.27 (m, 1H), 2.52 (s, 3H), 2.38 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 136.2, 134.0, 131.2, 130.9, 130.3, 129.8, 129.1, 128.6,

128.3, 125.0, 123.2, 122.8, 122.3, 121.0, 117.2, 112.2; HRMS (ESI) calcd for $C_{20}H_{17}N$ $(M + H)^+$: 272.1434, found: 272.1419.



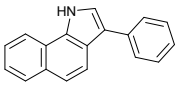
1-(4-methoxyphenyl)-2-methyl-3H-benzo[e]indole (3p)

Brown solid, mp: 92-94 °C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.29 (br, s, 1H), 7.87-7.89 (m, 2H), 7.58 (d, J = 8.8 Hz, 1H), 7.51 (d, J = 8.8 Hz, 1H), 7.42-7.44 (m, 2H), 7.32-7.35 (m, 1H), 7.24-7.26 (m, 1H), 7.07 (d, J = 8.4 Hz, 1H), 3.95 (s, 3H), 2.39 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 158.5, 132.1, 131.2, 130.3, 129.7, 129.2, 128.6, 128.3, 125.0, 123.1, 122.8, 122.3, 113.8, 112.2, 55.3, 12.0; HRMS (ESI) calcd for $C_{20}H_{17}NO$ $(M + H)^+$: 288.1383, found: 288.1381.



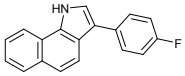
2-methyl-1-(3-nitrophenyl)-3H-benzo[e]indole (3q)

Brown solid, mp: 76-78 °C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.98 (d, J = 8.4 Hz, 1H), 8.34 (br, s, 1H), 8.23 (dd, J_1 = 1.2 Hz, J_2 = 8.8 Hz, 1H), 7.91-8.03 (m, 3H), 7.70-7.75 (m, 2H), 7.52-7.64 (m, 4H), 7.37-7.41 (m, 1H), 6.94 (d, J = 8.8 Hz, 1H), 1.59 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 151.3, 138.5, 134.8, 133.9, 133.7, 129.1, 128.9, 128.0, 127.9, 127.7, 127.4, 127.1, 126.6, 126.5, 124.5, 123.3, 122.1, 119.5, 117.8, 17.6; HRMS (ESI) calcd for $C_{19}H_{14}N_2O_2$ $(M + H)^+$: 303.1128, found: 303.1137.



3-phenyl-1H-benzo[g]indole (3r)

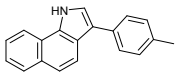
Colorless crystal, mp: 230-232 °C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.94 (br, s, 1H), 8.02 (d, J = 8.4 Hz, 2H), 7.96 (d, J = 8.0 Hz, 1H), 7.30 (m, 2H), 7.54-7.61 (m, 2H), 7.41-7.51 (m, 3H), 7.36 (d, J = 1.2 Hz, 1H), 7.32-7.36 (m, 1H).



3-(4-fluorophenyl)-1H-benzo[g]indole (3s)

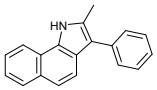
Colorless crystal, mp: 204-206 °C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 9.00 (br, s, 1H),

8.06 (d, J = 8.0 Hz, 1H), 7.94-8.00 (m, 2H), 7.66-7.70 (m, 2H), 7.57-7.63 (m, 2H), 7.48-7.52 (m, 1H), 7.41 (d, J = 2.4 Hz, 1H), 7.18-7.22 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 162.8, 160.4, 131.2, 130.5, 129.2, 129.1, 128.9, 125.7, 124.3, 121.8, 121.6, 121.3, 119.7, 119.4, 119.3, 115.8, 115.6; HRMS (ESI) calcd for $C_{18}H_{12}FN$ $(M + H)^+$: 262.1026, found: 262.1034.



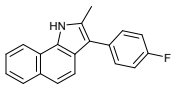
3-(p-tolyl)-1H-benzo[g]indole (3t)

Brown solid, mp: 140-142 °C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.98 (br, s, 1H), 7.93-8.07 (m, 3H), 7.55-7.68 (m, 4H), 7.48-7.50 (m, 1H), 7.44-7.47 (m, 1H), 7.31-7.42 (m, 2H), 2.45 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 135.8, 132.5, 130.5, 129.6, 129.5, 128.8, 127.6, 127.4, 125.6, 124.1, 121.7, 121.0, 120.2, 119.7, 119.6, 119.3, 21.2; HRMS (ESI) calcd for $C_{19}H_{15}N$ $(M + H)^+$: 258.1277, found: 258.1288.



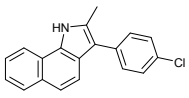
2-methyl-3-phenyl-1H-benzo[g]indole (3u)

Colorless crystal, mp: 80-82 °C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.71 (br, s, 1H), 8.01 (d, J = 8.4 Hz, 1H), 7.96 (d, J = 8.0 Hz, 1H), 7.80 (s, J = 8.8 Hz,1H), 7.51-7.61 (m, 6H), 7.45 (t, J_1 = 7.2 Hz, J_2 = 7.6 Hz, 1H), 7.38 (t, J_1 = 7.2 Hz, J_2 = 7.6 Hz, 1H), 2.64 (s, 3H); HRMS (ESI) calcd for $C_{19}H_{15}N$ $(M + H)^+$: 258.1277, found: 258.1281.



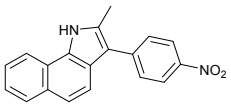
3-(4-fluorophenyl)-2-methyl-1H-benzo[g]indole (3v)

Brown solid, mp: 150-152 °C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.70 (br, s, 1H), 8.01 (d, J = 8.0 Hz, 1H), 7.96 (d, J = 8.0 Hz, 1H), 7.20 (d, J = 8.8 Hz, 2H), 7.50-7.58 (m, 4H), 7.43-7.47 (m, 1H), 7.19-7.24 (m, 2H), 2.60 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 162.6, 160.2, 131.3, 131.0, 130.9, 130.2, 129.4, 128.9, 125.5, 123.6, 123.4, 121.2,120.8, 119.1, 118.9, 115.6, 115.5, 115.3, 12.5; HRMS (ESI) calcd for $C_{19}H_{14}FN$ $(M + H)^+$: 276.1183, found: 276.1179.



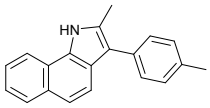
3-(4-chlorophenyl)-2-methyl-1H-benzo[g]indole (3w)

Brown solid, mp: 170-172 °C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.74 (br, s, 1H), 8.01 (d, J = 8.4 Hz, 1H), 7.95 (d, J = 8.0 Hz, 1H), 7.73 (d, J = 8.4 Hz, 1H), 7.53-7.57 (m, 2H), 7.47-7.52 (m, 4H), 7.43-7.46 (m, 1H), 2.61 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 133.9, 131.7, 130.7, 130.2, 129.6, 129.4, 128.9, 128.7, 125.5, 123.7, 123.2, 121.2, 120.9, 119.1, 118.8, 115.3, 12.6; HRMS (ESI) calcd for $C_{19}H_{14}ClN$ $(M + H)^+$: 292.0888, found: 292.0898.



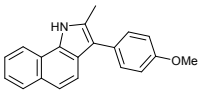
2-methyl-3-(4-nitrophenyl)-1H-benzo[g]indole (3x)

Brown solid, mp: 274-276 °C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.90 (br, s, 1H), 8.38 (d, J = 8.8 Hz, 2H), 8.04 (d, J = 8.4 Hz, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.72-7.78 (m, 3H), 7.57-7.62 (m, 2H), 7.47 (t, J_1 = 7.2 Hz, J_2 = 0.8 Hz, 1H), 2.69 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 130.9, 129.7, 129.5, 129.0, 125.8, 124.1, 124.0, 122.8, 121.6, 119.1, 118.4, 13.0; HRMS (ESI) calcd for $C_{19}H_{14}N_2O_2$ $(M + H)^+$: 303.1128, found: 303.1135.



2-methyl-3-(p-tolyl)-1H-benzo[g]indole (3y)

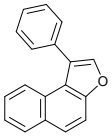
Brown solid, mp: 106-108 °C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.68 (br, s, 1H), 8.01 (d, J = 8.4 Hz, 1H), 7.95 (d, J = 8.4 Hz, 2H), 7.79 (d, J = 8.4 Hz, 2H), 7.53-7.56 (m, 4H), 7.42-7.50 (m, 1H), 7.35 (d, J = 7.6 Hz, 2H), 2.63 (s, 3H), 2.48 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 135.5, 132.4, 130.2, 129.4, 129.3, 128.9, 125.4, 123.5, 121.3, 120.6, 119.3, 119.1, 116.3, 21.3, 12.6; HRMS (ESI) calcd for $C_{20}H_{17}N$ $(M + H)^+$: 272.1434, found: 272.1419.



3-(4-methoxyphenyl)-2-methyl-1H-benzo[g]indole (3z)

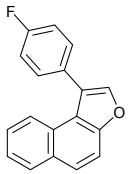
Brown solid, mp: 122-124 °C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.68 (br, s, 1H), 8.01 (d, J = 8.4 Hz, 1H), 7.94 (d, J = 8.0 Hz, 1H), 7.50 (d, J = 8.4 Hz, 1H), 7.48-7.57 (m, 4H), 7.41-7.45 (m, 1H), 7.06-7.09 (m, 2H), 3.92 (s, 3H), 2.62 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 157.9, 130.6, 130.1, 129.3, 129.1, 128.9, 127.7, 125.4, 123.6, 123.5, 121.1, 120.5, 119.2, 119.1, 116.0, 114.0, 55.4, 12.6; HRMS (ESI) calcd for $C_{20}H_{17}NO$ $(M + H)^+$:

288.1383, found: 288.1384.



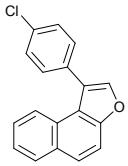
1-phenylnaphtho[2,1-b]furan (5a)

Colorless oil; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.01 (d, J = 8.4 Hz, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.80 (d, J = 8.8 Hz, 1H), 7.30 (d, J = 8.8 Hz, 2H), 7.63-7.65 (m, 2H), 7.50-7.57 (m, 3H), 7.44-7.48 (m, 1H), 7.36-7.40 (m, 1H).



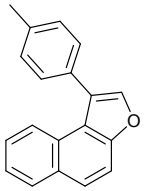
1-(4-fluorophenyl)naphtho[2,1-b]furan (5b)

Yellow oil; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.93-7.97 (m, 2H), 7.80 (d, J = 8.8 Hz, 1H), 7.70-7.74 (m, 2H), 7.58-7.61 (m, 2H), 7.45-7.49 (m, 1H), 7.38-7.42 (m, 1H), 7.22-7.27 (m, 2H).



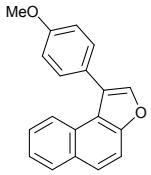
1-(4-chlorophenyl)naphtho[2,1-b]furan (5c)

Yellow oil; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.95-7.99 (m, 2H), 7.81 (d, J = 9.2 Hz, 1H), 7.67-7.76 (m, 2H), 7.53-7.58 (m, 4H), 7.43-7.52 (m, 1H), 7.39-7.41 (m, 1H).



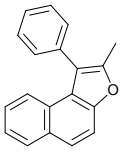
1-(p-tolyl)naphtho[2,1-b]furan (5d)

Yellow oil; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.05 (d, J = 8.8 Hz, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.79 (d, J = 8.8 Hz, 1H), 7.69-7.73 (m, 2H), 7.51-7.54 (m, 2H), 7.46-7.48 (m, 1H), 7.40-7.46 (m, 1H), 7.34-7.39 (m, 2H), 2.51 (s, 3H).



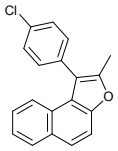
1-(4-methoxyphenyl)naphtho[2,1-b]furan (5e)

Yellow oil; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.03 (d, J = 8.4 Hz, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.79 (d, J = 9.2 Hz, 1H), 7.68-7.73 (m, 2H), 7.53-7.56 (m, 2H), 7.44-7.48 (m, 1H), 7.37-7.41 (m, 1H), 7.08 (d, J = 8.8 Hz, 2H), 3.95 (s, 3H).



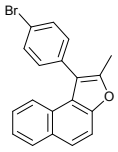
2-methyl-1-phenylnaphtho[2,1-b]furan (5f)

Colorless oil; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.90 (d, J = 8.0 Hz, 1H), 7.76 (d, J = 8.4 Hz, 1H), 7.62-7.70 (m, 2H), 7.36-7.54 (m, 5H), 7.27-7.30 (m, 1H), 7.24-7.26 (m, 1H), 2.42 (s, 3H).



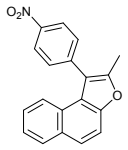
1-(4-chlorophenyl)-2-methylnaphtho[2,1-b]furan (5g)

White solid, mp: 118-120 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.95 (d, J = 8.0 Hz, 1H), 7.72-7.78 (m, 2H), 7.67 (d, J = 8.8 Hz, 1H), 7.53-7.55 (m, 2H), 7.45-7.48 (m, 2H), 7.42-7.44 (m, 3H), 7.33-7.37 (m, 1H), 2.45 (s, 3H).



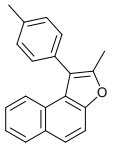
1-(4-bromophenyl)-2-methylnaphtho[2,1-b]furan (5h)

White solid, mp: 132-134 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.95 (d, J = 8.0 Hz, 1H), 7.76 (d, J = 8.4 Hz, 1H), 7.65-7.74 (m, 4H), 7.39-7.45 (m, 3H), 7.32-7.37 (m, 1H), 2.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 151.4, 151.3, 133.2, 132.2, 130.7, 128.9, 127.7, 125.8, 124.8, 124.1, 123.0, 121.9, 121.7, 117.8, 112.1, 12.3; HRMS (ESI) calcd for $C_{19}H_{14}BrO$ $(M + H)^+$: 337.0223, found: 337.0228.



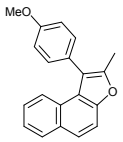
2-methyl-1-(4-nitrophenyl)naphtho[2,1-b]furan (5i)

Yellow solid, mp: 172-174 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.42-8.44 (m, 2H), 7.97 (d, J = 8.0 Hz, 1H), 7.67-7.78 (m, 5H), 7.47 (t, J_1 = 0.8 Hz, J_2 = 6.8 Hz, 3H), 7.44 (t, J_1 = 1.2 Hz, J_2 = 8.0 Hz, 3H), 2.48 (s, 3H).



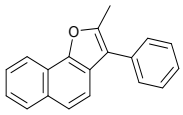
2-methyl-1-(p-tolyl)naphtho[2,1-b]furan (5j)

White solid, mp: 96-98 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.94 (d, J = 8.0 Hz, 1H), 7.85 (d, J = 8.4 Hz, 1H), 7.66-7.73 (m, 2H), 7.40-7.44 (m, 3H), 7.30-7.37 (m, 3H), 2.52 (s, 3H), 2.46 (s, 3H).



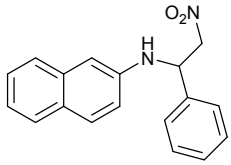
1-(4-methoxyphenyl)-2-methylnaphtho[2,1-b]furan (5k)

White solid, mp: 84-86 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.95 (d, J = 8.0 Hz, 1H), 7.86 (d, J = 8.4 Hz, 1H), 7.66-7.73 (m, 2H), 7.41-7.47 (m, 3H), 7.32-7.36 (m, 1H), 7.09-7.12 (m, 2H), 3.96 (s, 3H), 2.46 (s, 3H).



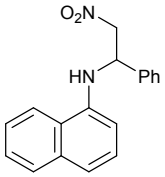
2-methyl-3-phenylnaphtho[1,2-b]furan (5l)

White solid, mp: 66-68 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.34 (d, J = 8.4 Hz, 2H), 7.96 (d, J = 8.0 Hz, 1H), 7.63-7.72 (m, 2H), 7.43-7.62 (m, 6H), 7.40-7.42 (m, 1H), 2.69 (s, 3H).



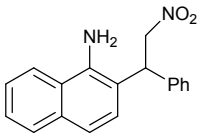
***N*-(2-nitro-1-phenylethyl)naphthalen-2-amine (6)**

Brown oil; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.60-7.67 (m, 2H), 7.55-7.58 (m, 1H), 7.18-7.50 (m, 6H), 7.77-7.99 (m, 1H), 6.91-6.99 (m, 1H), 6.77 (d, J = 2.0 Hz, 1H), 5.31 (t, J = 6.4 Hz, 1H), 4.74-4.82 (m, 2H), 4.56 (s, br, 1H).



***N*-(2-nitro-1-phenylethyl)naphthalen-1-amine (8)**

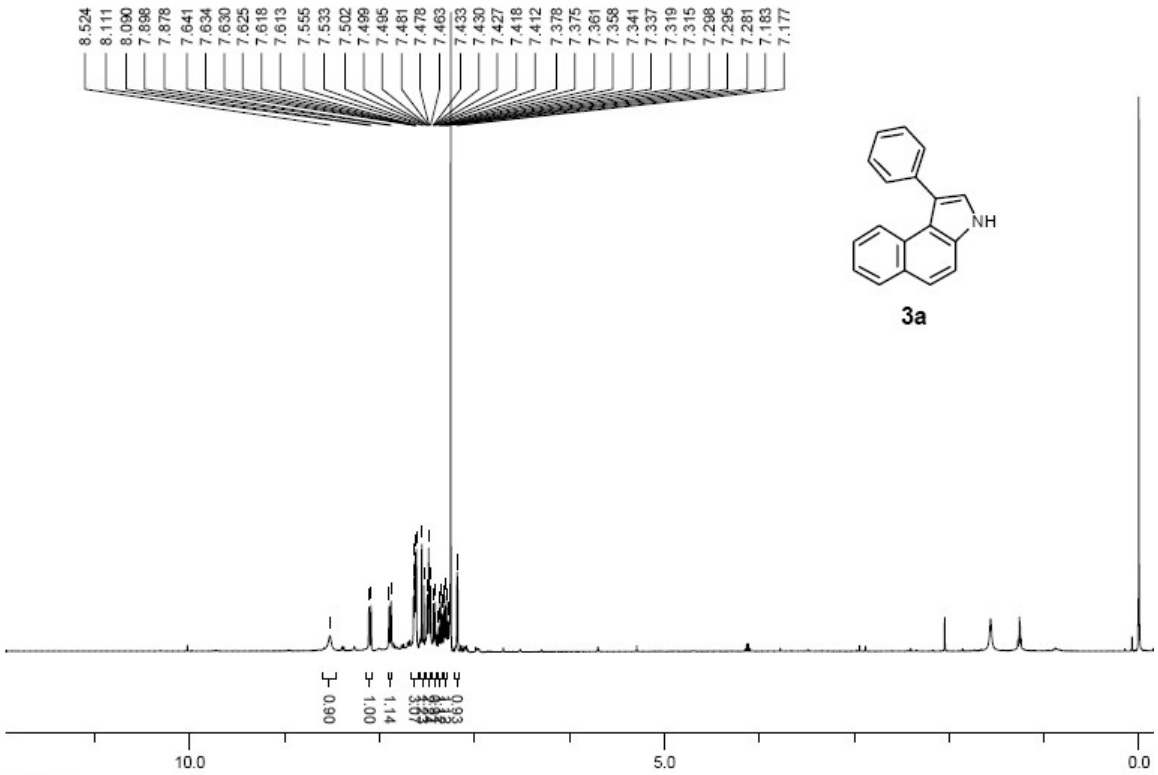
Brown solid, mp: 184-186 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 9.02 (s, br, 1H), 8.15 (d, J = 8.4 Hz, 1H), 8.05 (d, J = 8.0 Hz, 1H), 7.94 (s, 1H), 7.67-7.70 (m, 2H), 7.45-7.58 (m, 4H), 7.22-7.43 (m, 3H), 5.79 (t, J = 8.0 Hz, 1H), 5.22-5.27 (m, 1H), 5.08-5.13 (m, 1H).

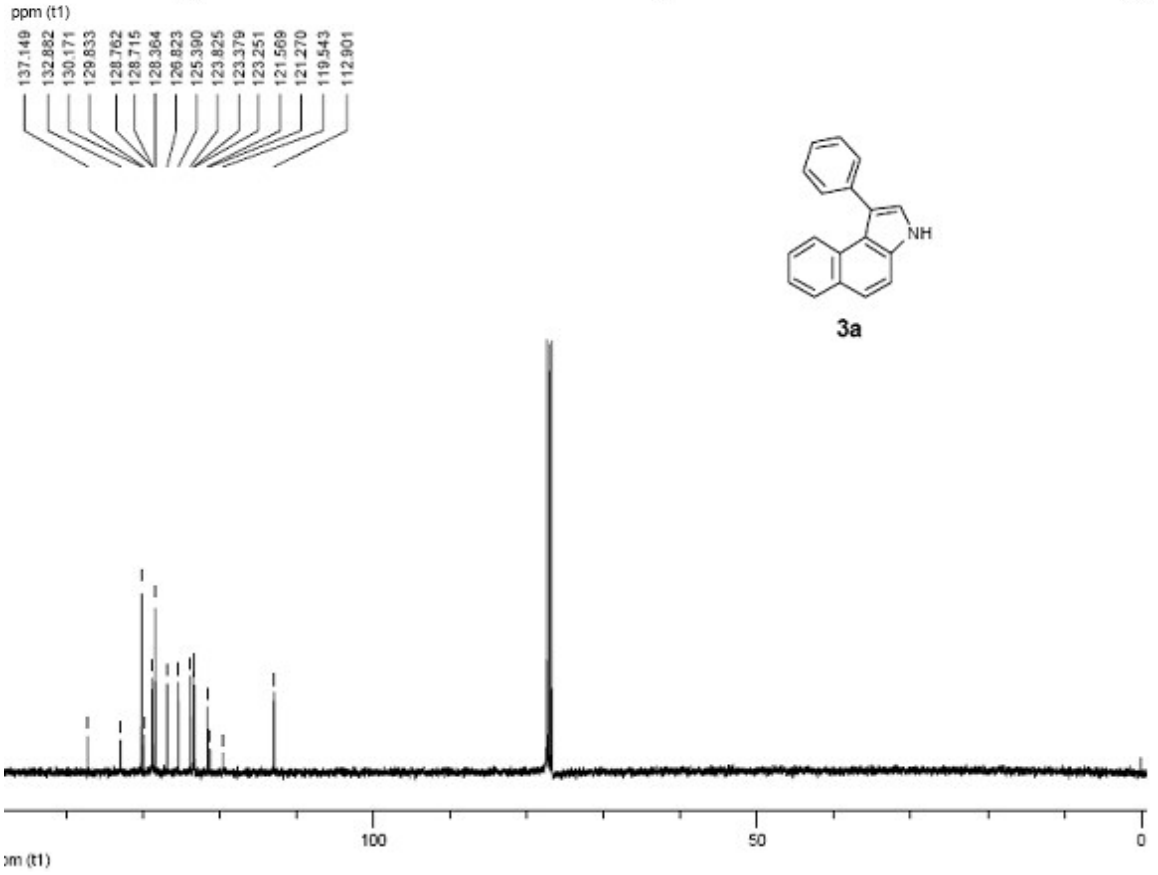


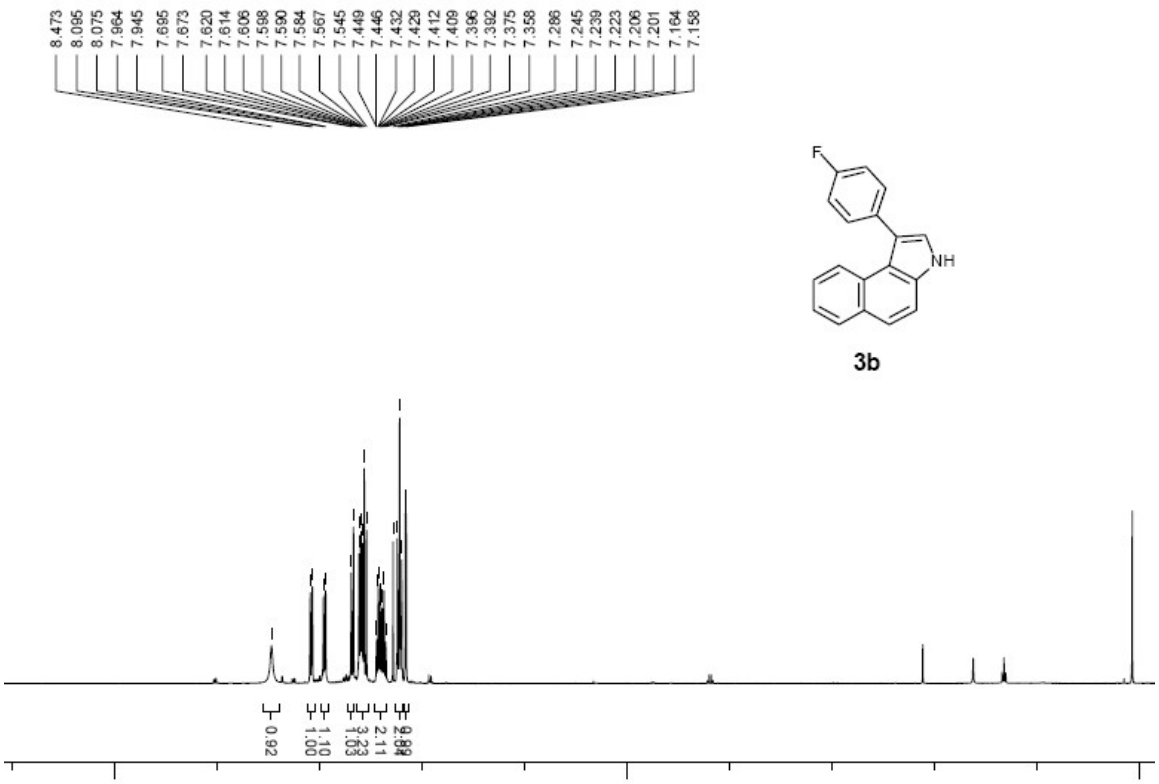
2-(2-nitro-1-phenylethyl)naphthalen-1-amine (9)

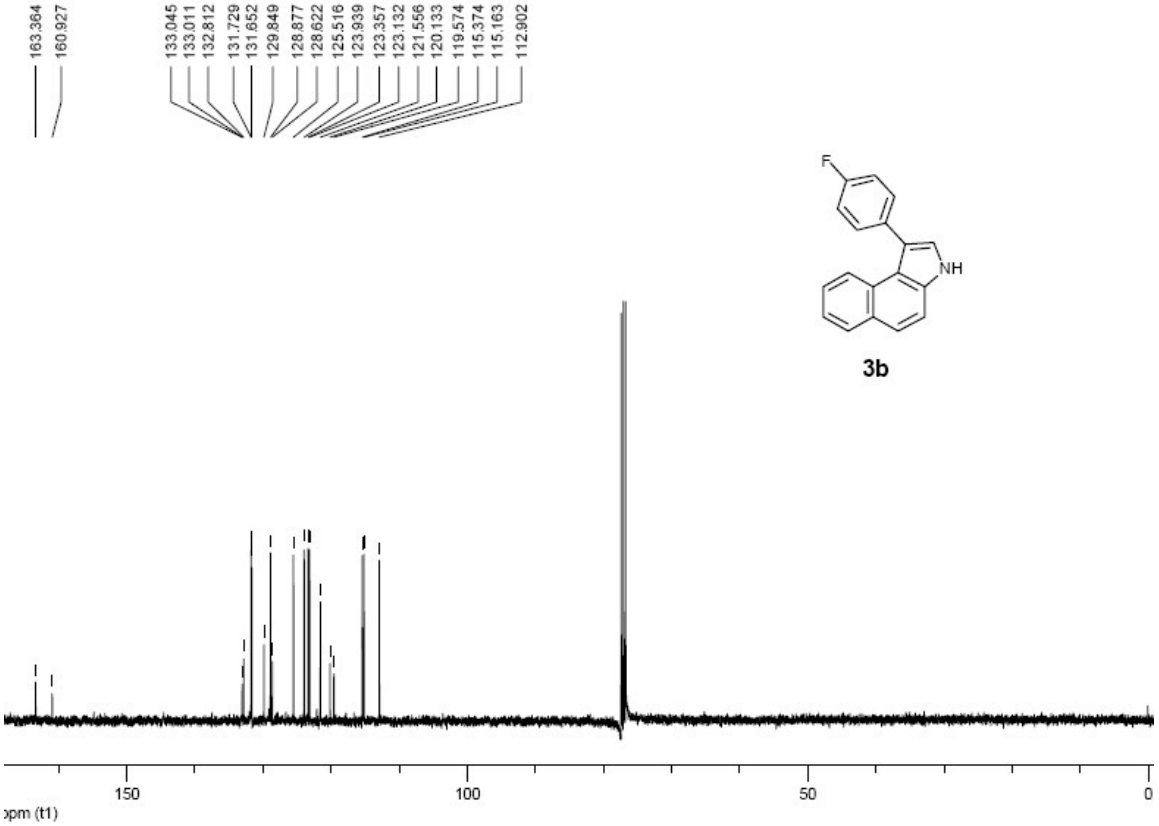
Brown solid, mp: 216-218 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.09 (d, J = 8.8 Hz, 1H), 7.88-7.90 (m, 1H), 7.48-7.56 (m, 2H), 7.31-7.33 (m, 4H), 7.25-7.29 (m, 1H), 7.16 (d, J = 8.0 Hz, 1H), 6.79 (d, J = 7.6 Hz, 1H), 5.66 (t, J = 8.0 Hz, 1H), 5.01-5.13 (m, 2H), 4.42 (s, br, 2H).

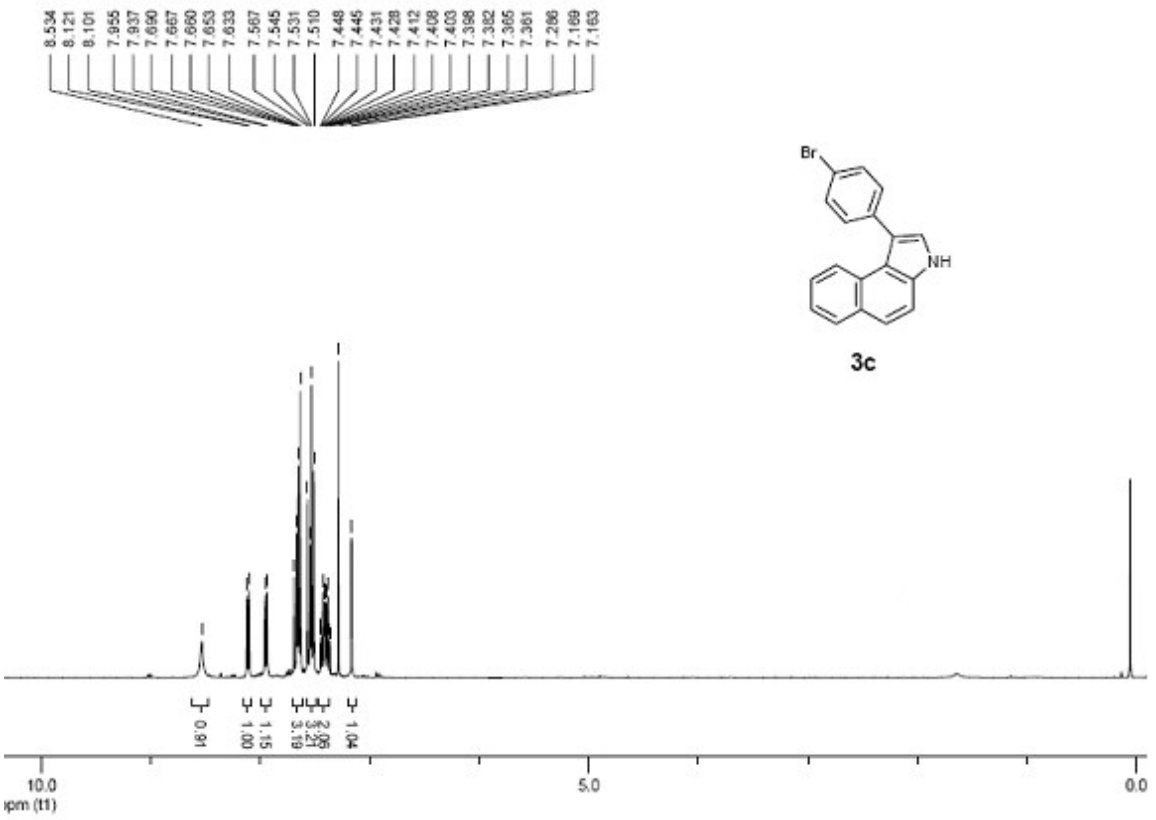
^{1}H and ^{13}C NMR Spectra

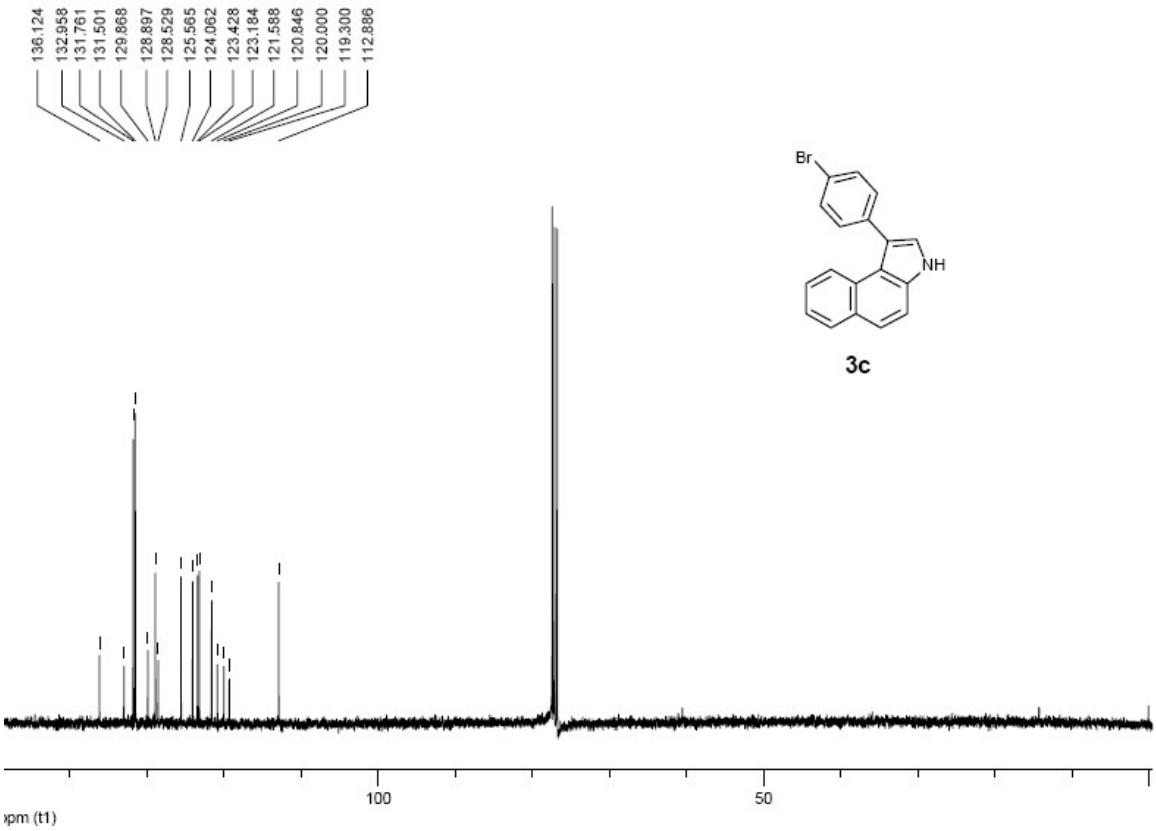


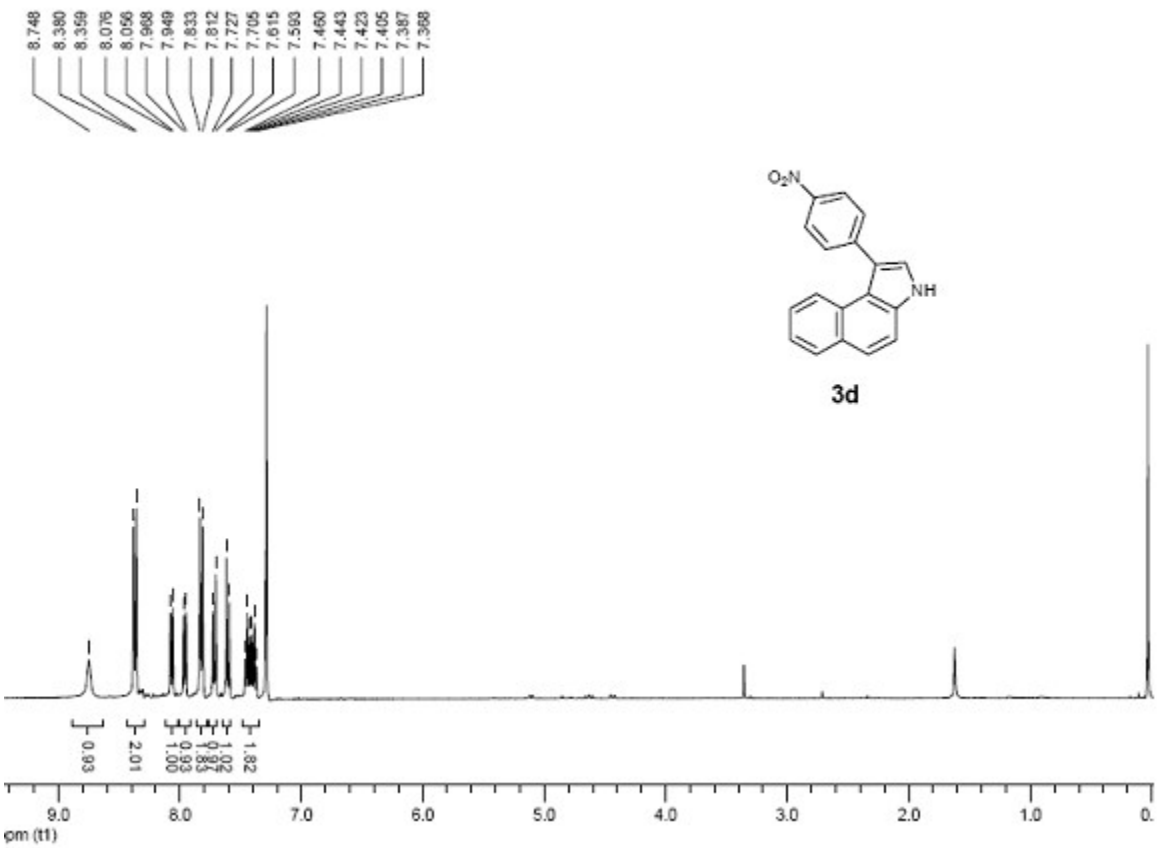


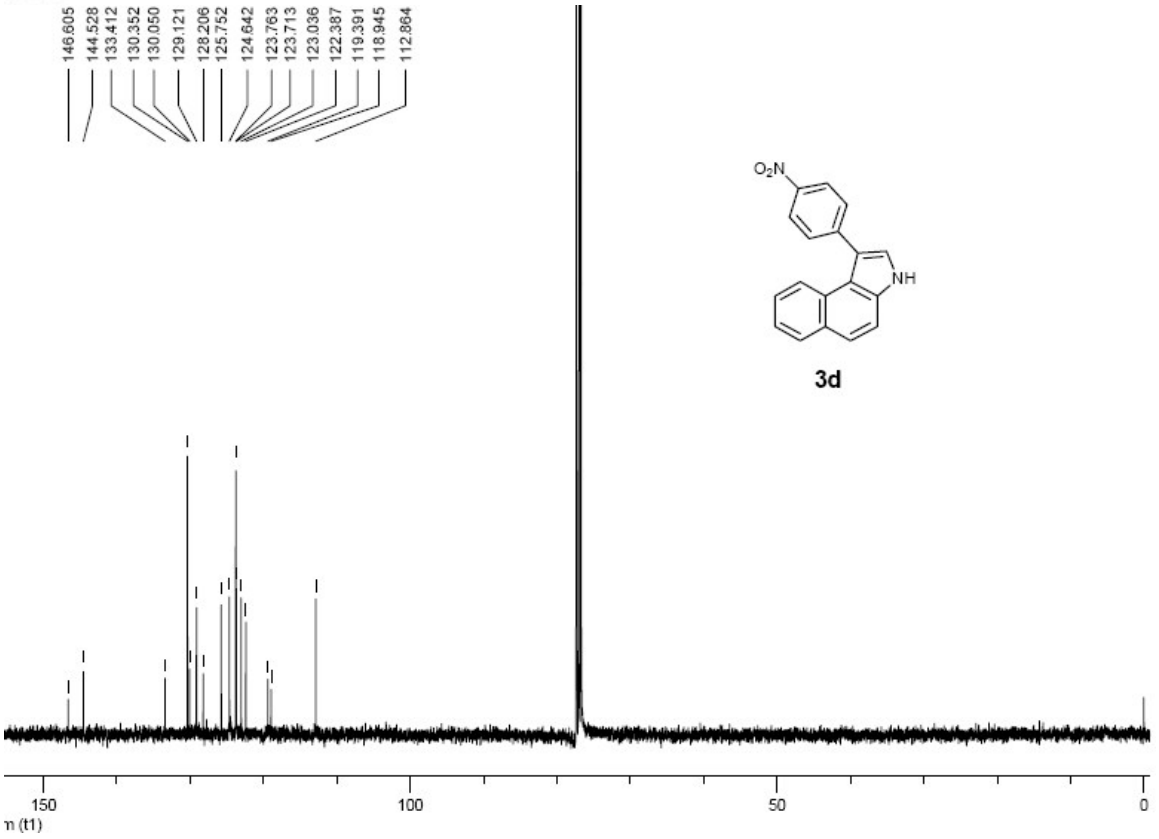

8.473
8.095
8.075
7.964
7.945
7.695
7.673
7.620
7.614
7.606
7.598
7.590
7.584
7.567
7.545
7.449
7.446
7.432
7.429
7.412
7.409
7.396
7.392
7.375
7.358
7.286
7.245
7.239
7.223
7.206
7.201
7.164
7.158
F
NH
3b
0.92
1.00
1.10
3.03
2.11
2.00
2.00
10.0
5.0
0.0
pm (t1)

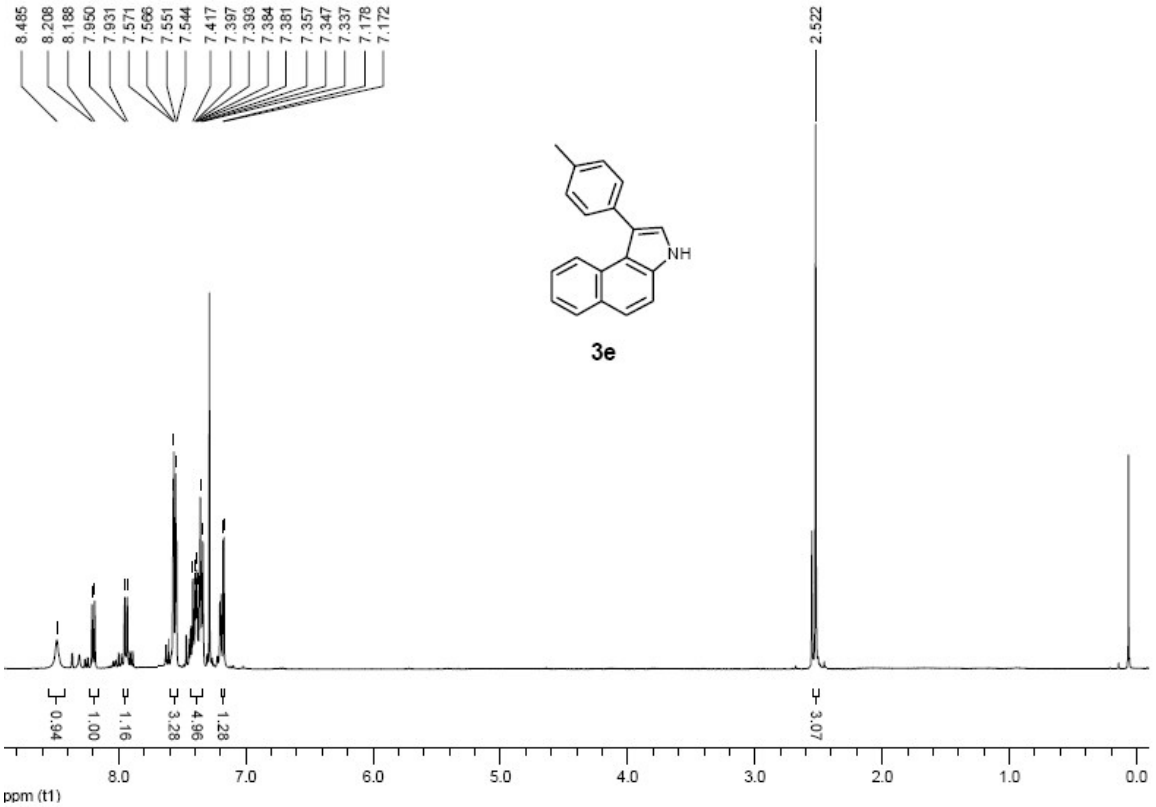

163.364
160.927
133.045
133.011
132.812
131.729
131.652
129.849
128.877
128.622
125.516
123.939
123.357
123.132
121.556
120.133
119.574
115.374
115.163
112.902
F
NH
3b
150
100
50
0
ppm (t1)

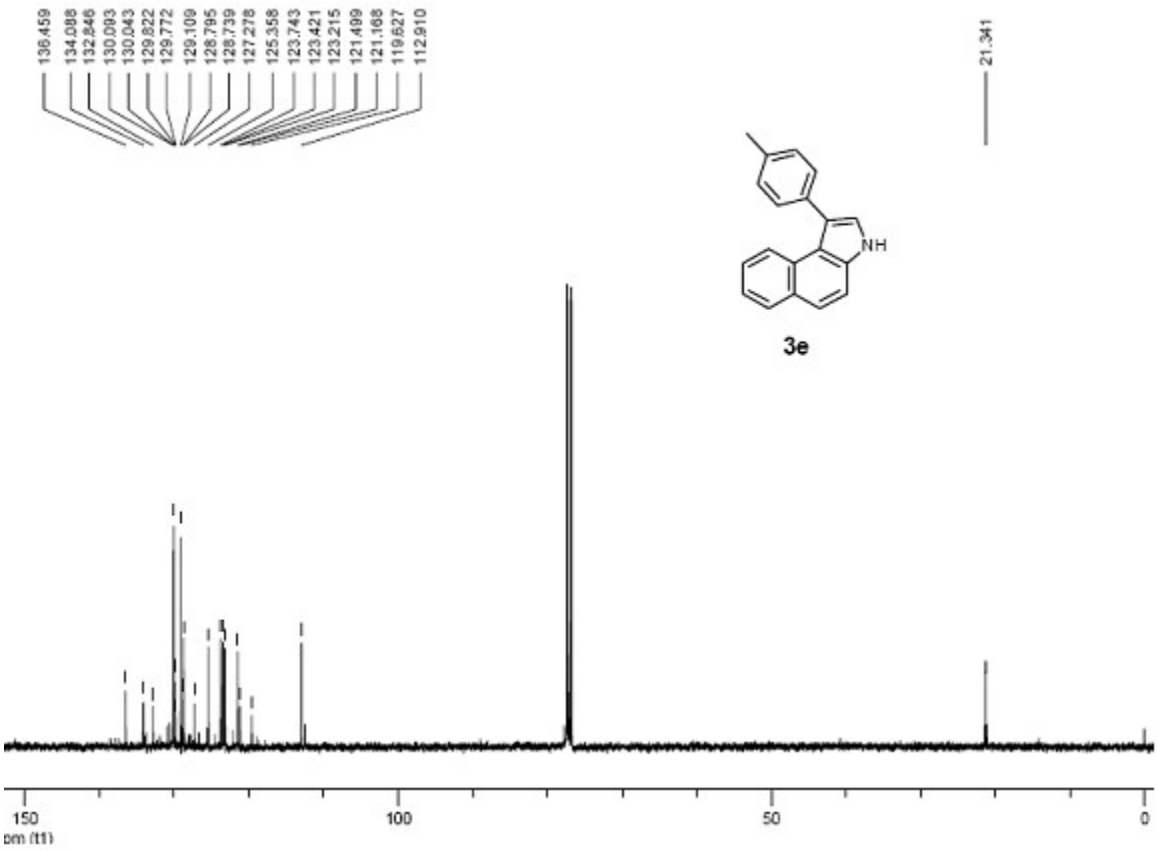

8.534
8.121
8.101
7.955
7.937
7.690
7.667
7.660
7.653
7.633
7.567
7.545
7.531
7.510
7.448
7.445
7.431
7.428
7.412
7.408
7.403
7.398
7.382
7.365
7.361
7.286
7.169
7.163
Br
NH
3c
0.91
1.00
1.15
3.19
2.95
2.27
1.04
10.0
5.0
0.0
ppm (t1)


136.124
132.958
131.761
131.501
129.868
128.897
128.529
125.565
124.062
123.428
123.184
121.588
120.846
120.000
119.300
112.886
Br
NH
3c
100
50
ppm (t1)

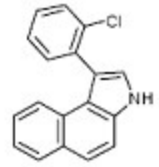

8.748
8.380
8.359
8.076
8.056
7.968
7.949
7.833
7.812
7.727
7.705
7.615
7.593
7.460
7.443
7.423
7.405
7.387
7.368
O2N
NH
3d
0.93
2.01
0.93
1.00
0.97
0.85
1.02
1.82
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
pm (t1)


146.605
144.528
133.412
130.352
130.050
129.121
128.206
125.752
124.642
123.763
123.713
123.036
122.387
119.391
118.945
112.864
O2N
NH
3d
150
100
50
0
n (t1)

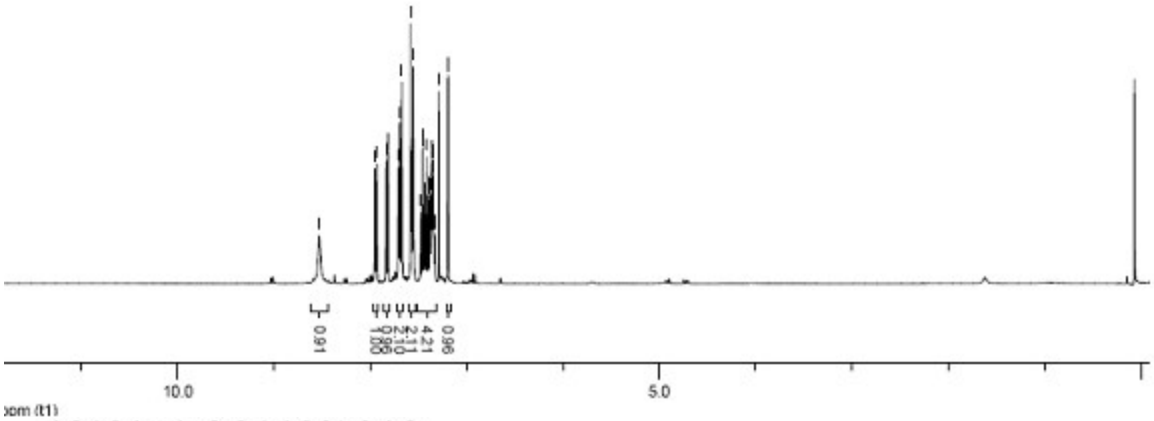

8.485
8.208
8.188
7.950
7.931
7.571
7.566
7.551
7.544
7.417
7.397
7.393
7.384
7.381
7.357
7.347
7.337
7.178
7.172
2.522
NH
3e
0.94
1.00
1.16
3.28
4.96
1.28
3.07
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

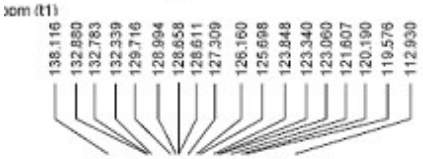

136.459
134.088
132.846
130.093
130.043
129.822
129.772
129.109
128.795
128.739
127.278
125.358
123.743
123.421
123.215
121.499
121.168
119.627
112.910
21.341
NH
3e
150
100
50
0
pm (t1)

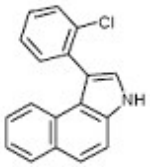

8.529
7.951
7.932
7.835
7.818
7.815
7.708
7.693
7.688
7.672
7.580
7.574
7.570
7.557
7.551
7.475
7.459
7.456
7.440
7.437
7.431
7.414
7.397
7.394
7.382
7.378
7.363
7.359
7.350
7.346
7.340
7.332
7.329
7.286
7.196
7.190


Cl
NH

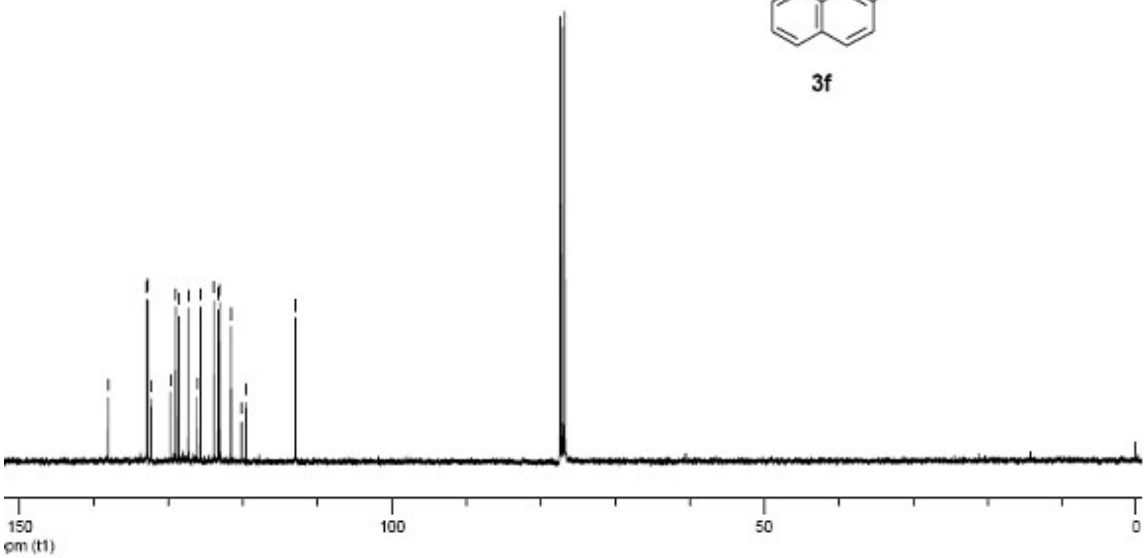
3f

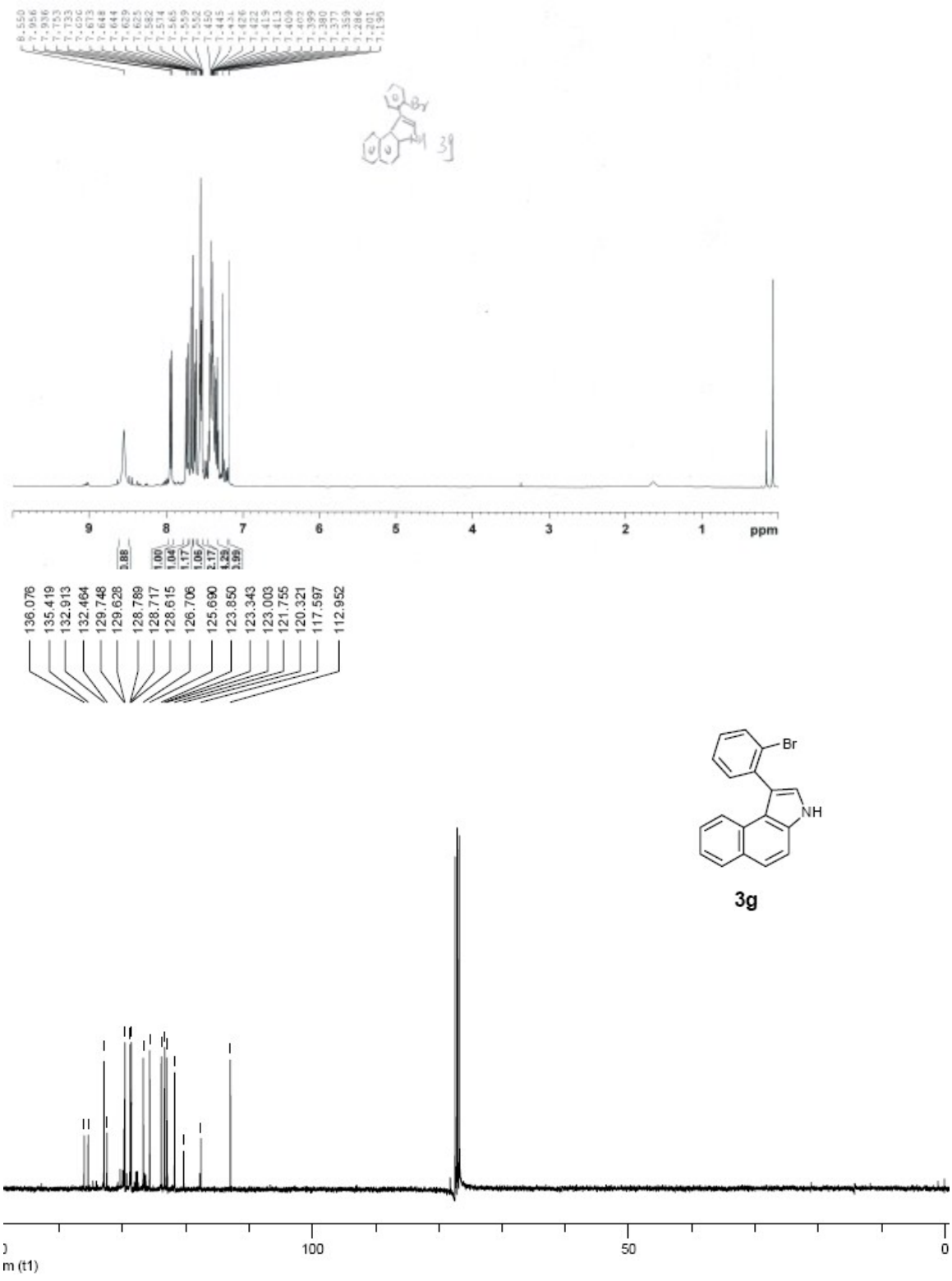

1.00
0.98
2.10
2.11
4.21
0.98
10.0
5.0

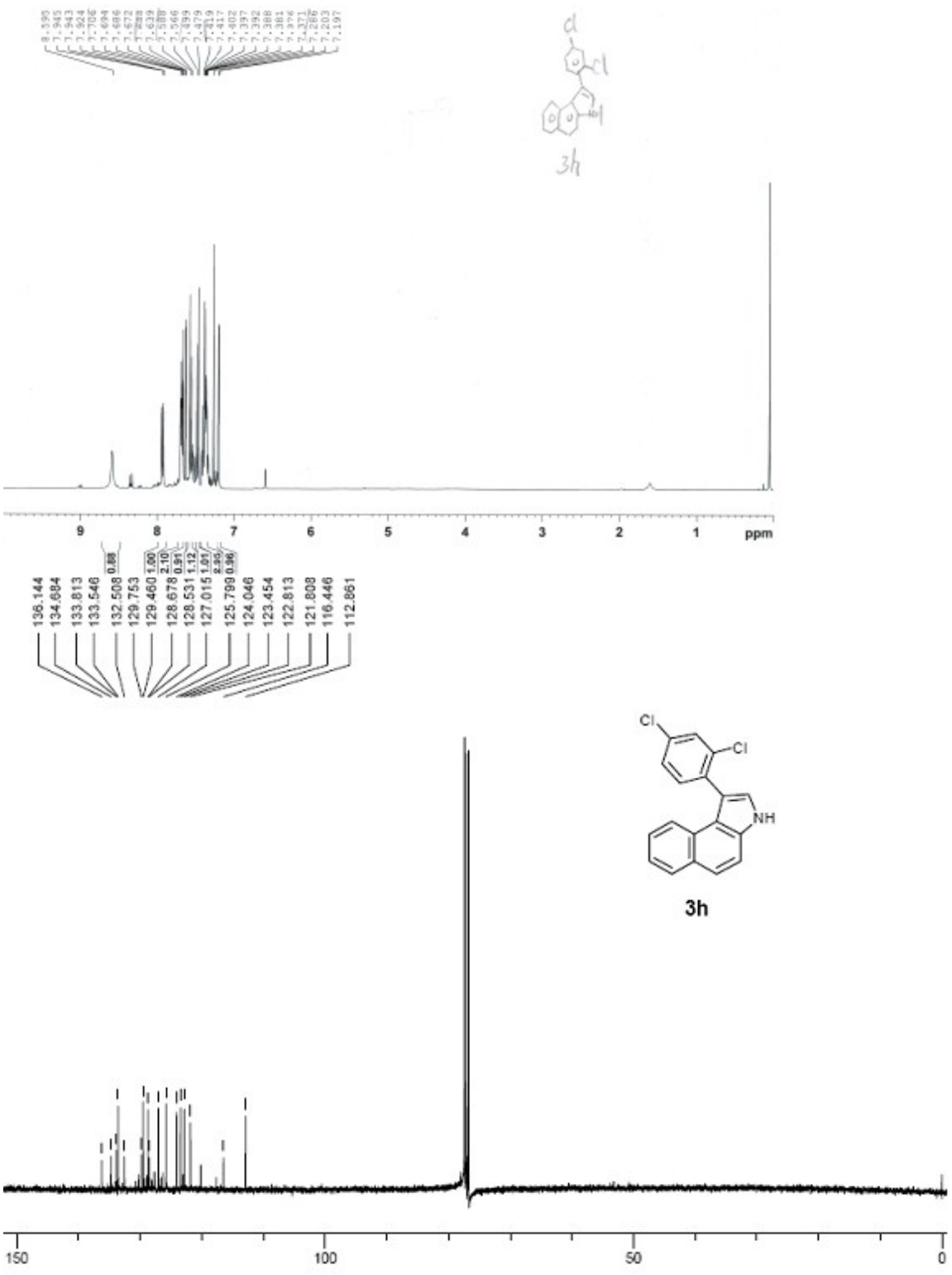

ppm (t1)
138.116
132.880
132.783
132.339
129.716
128.994
128.858
128.611
127.309
126.160
125.698
123.848
123.340
123.060
121.607
120.190
119.576
112.930

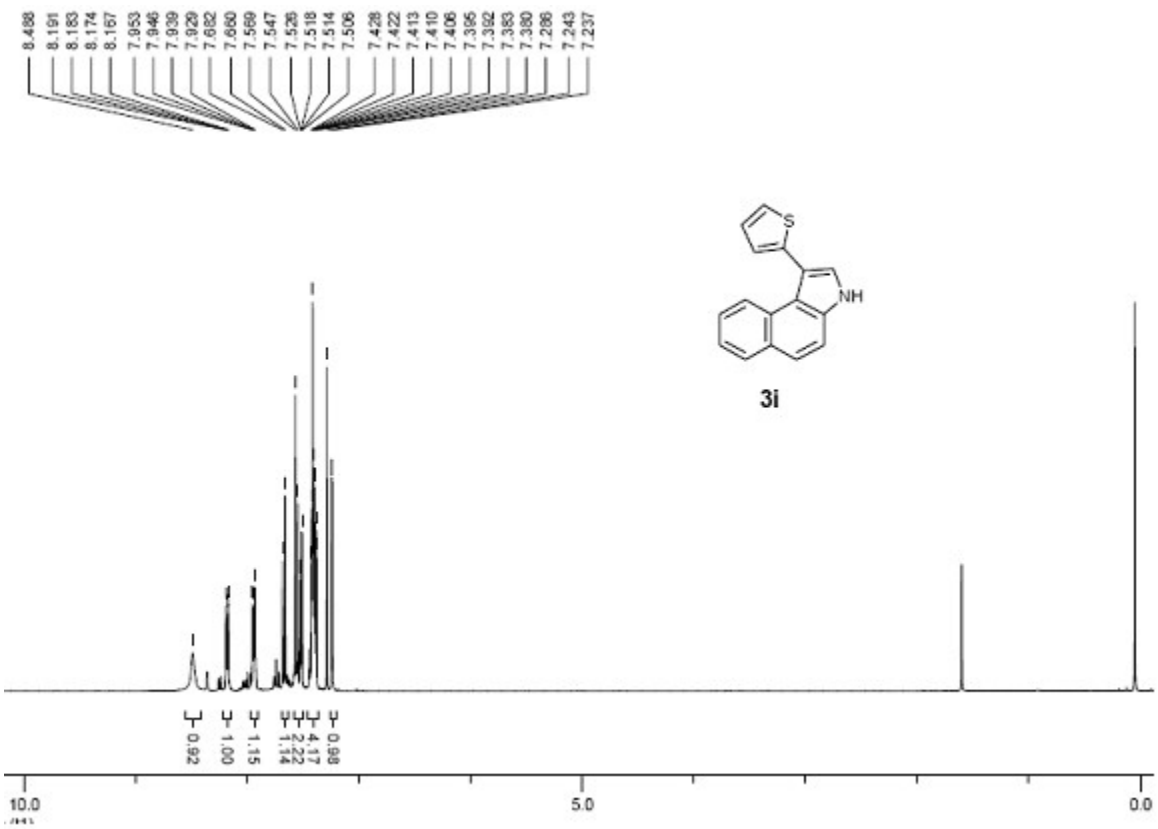

Cl
NH

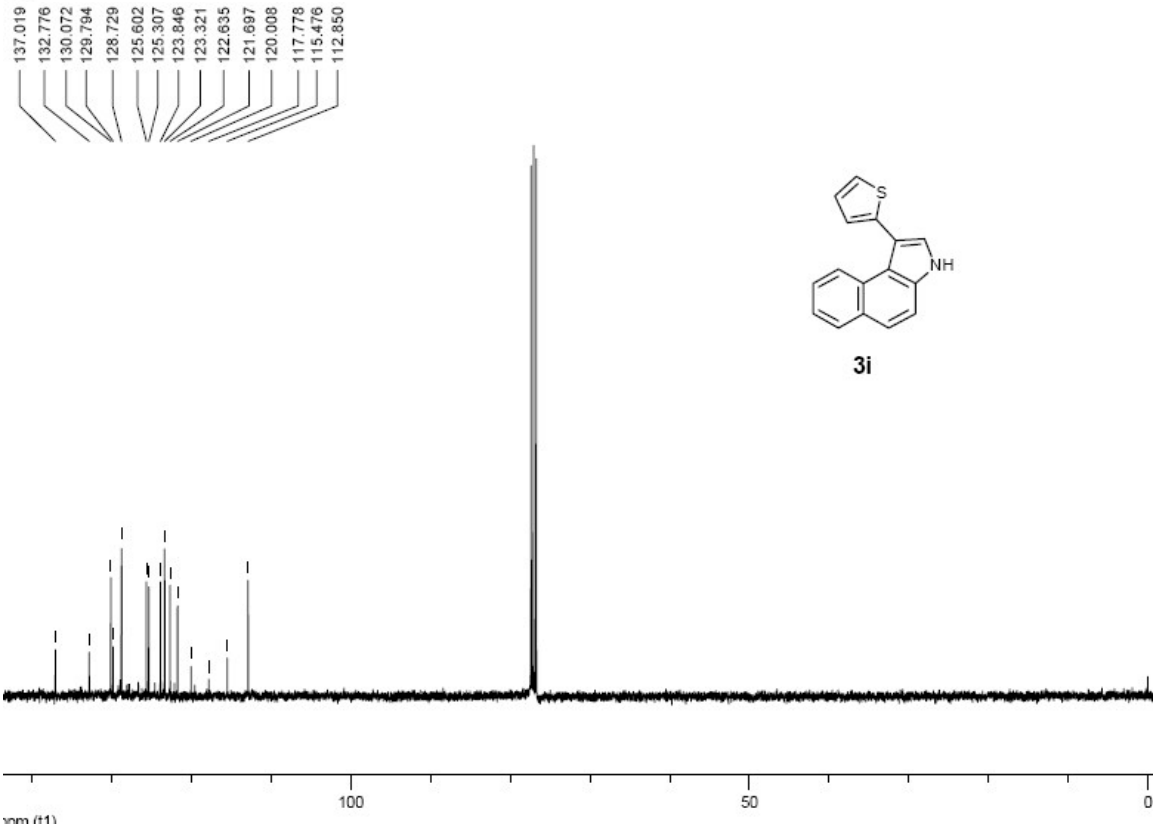
3f

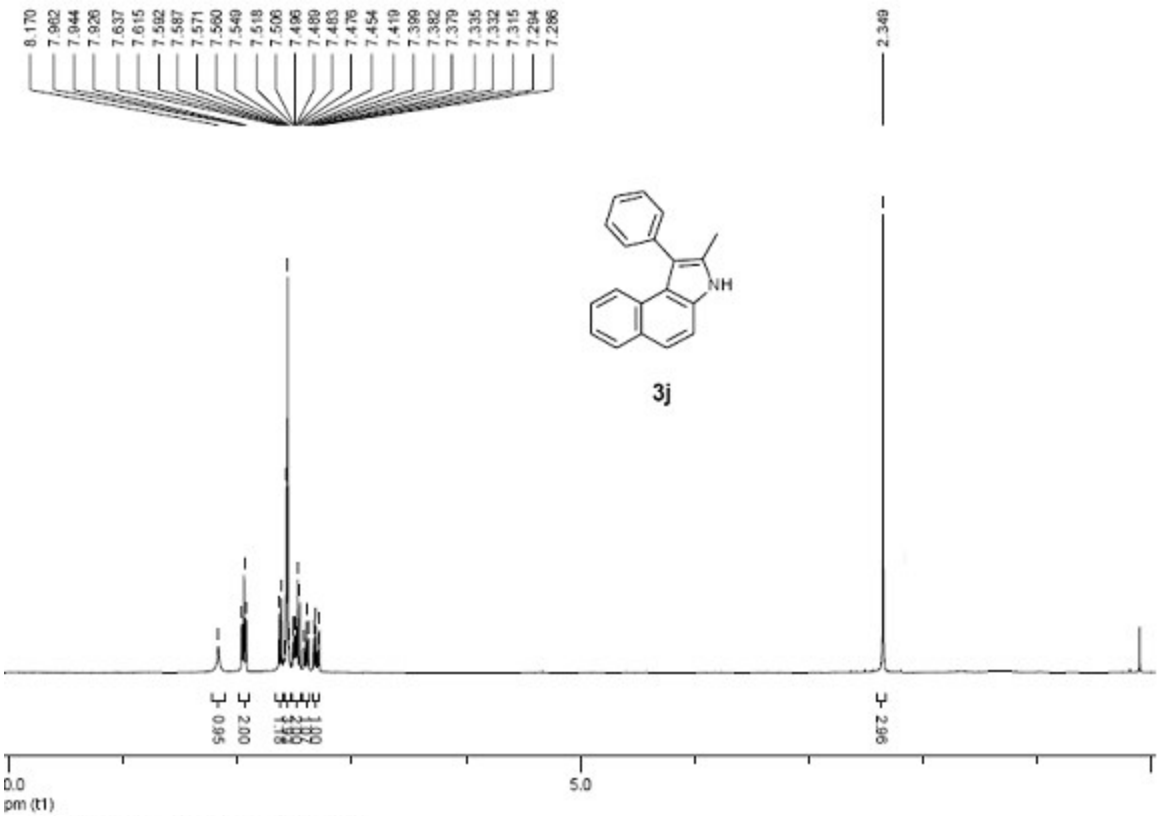

150
100
50
0
ppm (t1)

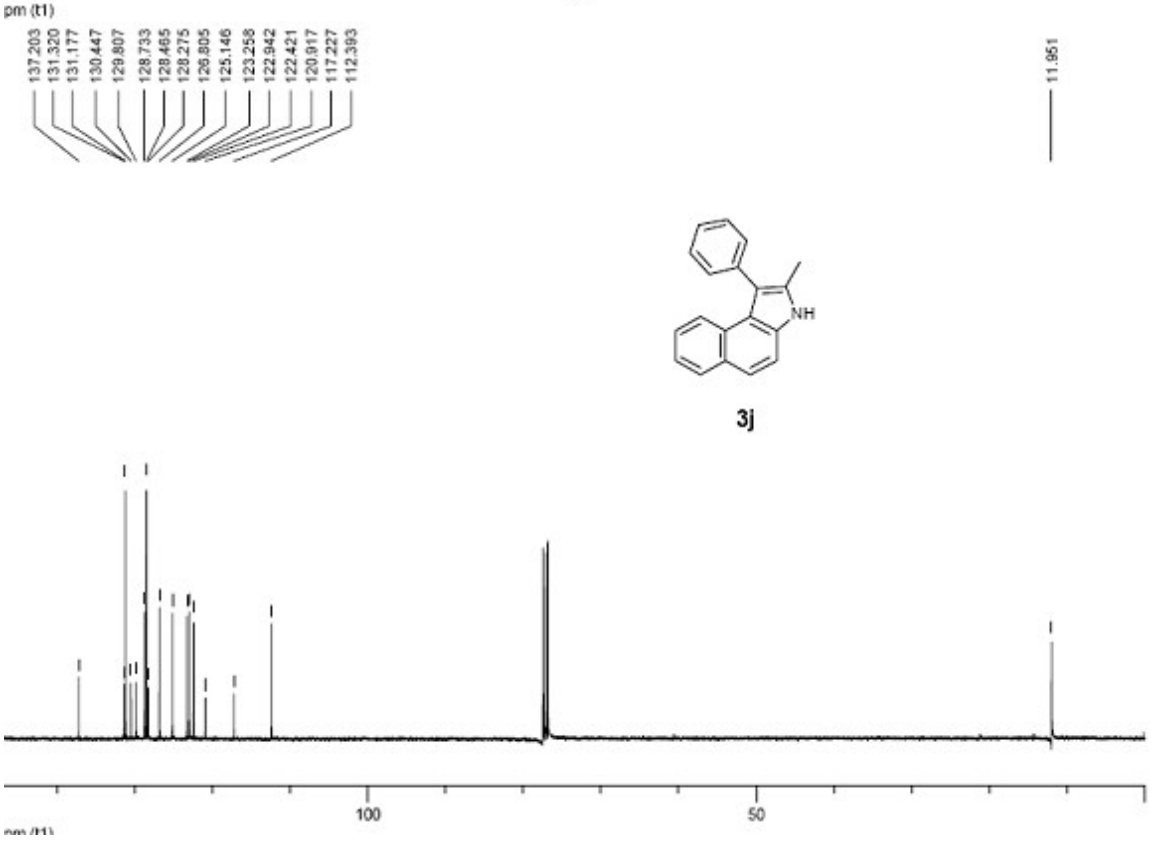

8.550
7.956
7.936
7.753
7.733
7.676
7.673
7.648
7.644
7.629
7.625
7.582
7.574
7.565
7.559
7.552
7.450
7.445
7.426
7.422
7.413
7.409
7.393
7.380
7.370
7.357
7.286
7.201
7.193
Br
NH
3g
9
8
7
6
5
4
3
2
1
ppm
0.88
1.00
1.04
1.17
1.06
2.17
4.29
2.99
136.076
135.419
132.913
132.464
129.748
129.628
128.789
128.717
128.615
126.706
125.690
123.850
123.343
123.003
121.755
120.321
117.597
112.952
100
50
0
m (t1)

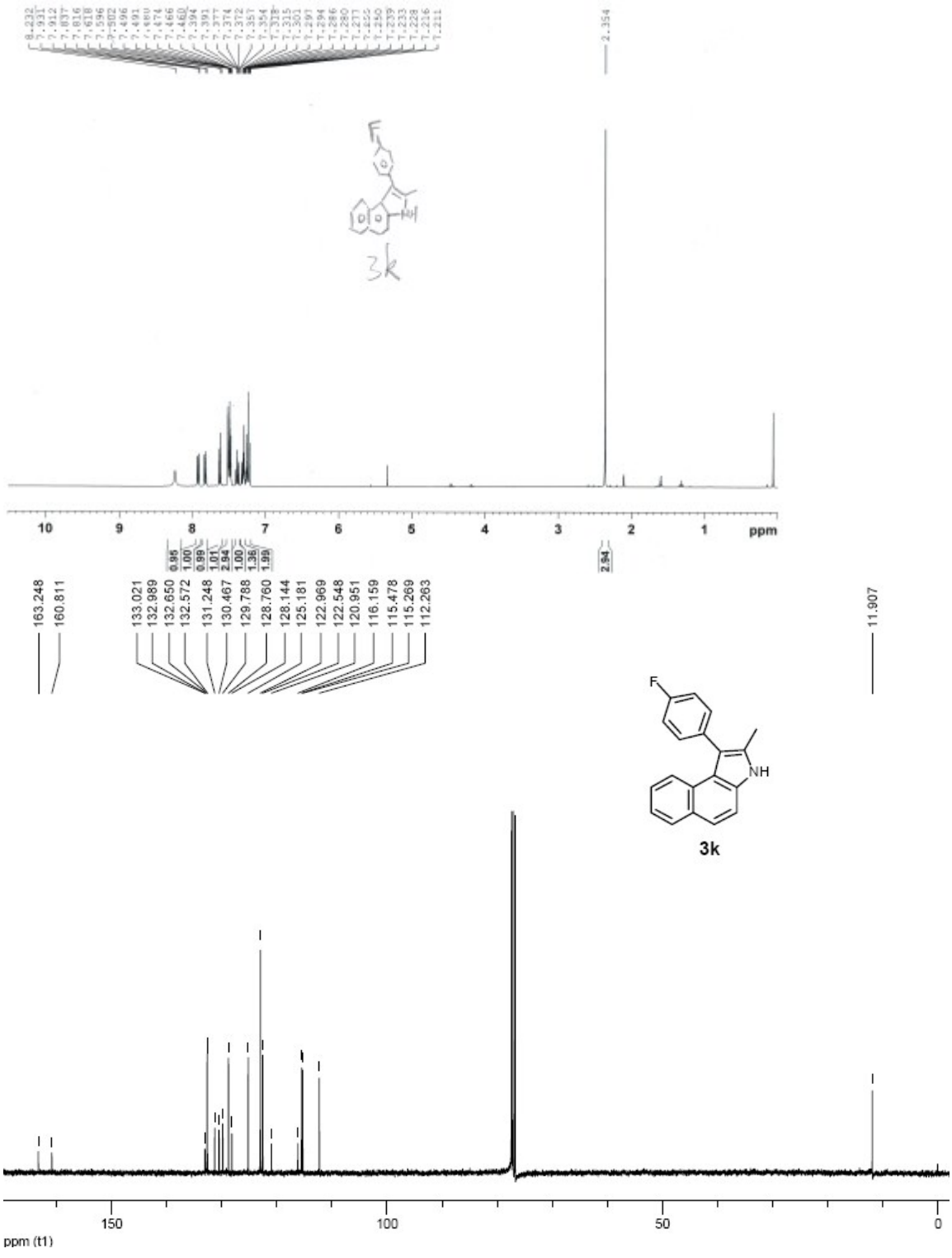

3h
ppm
3h

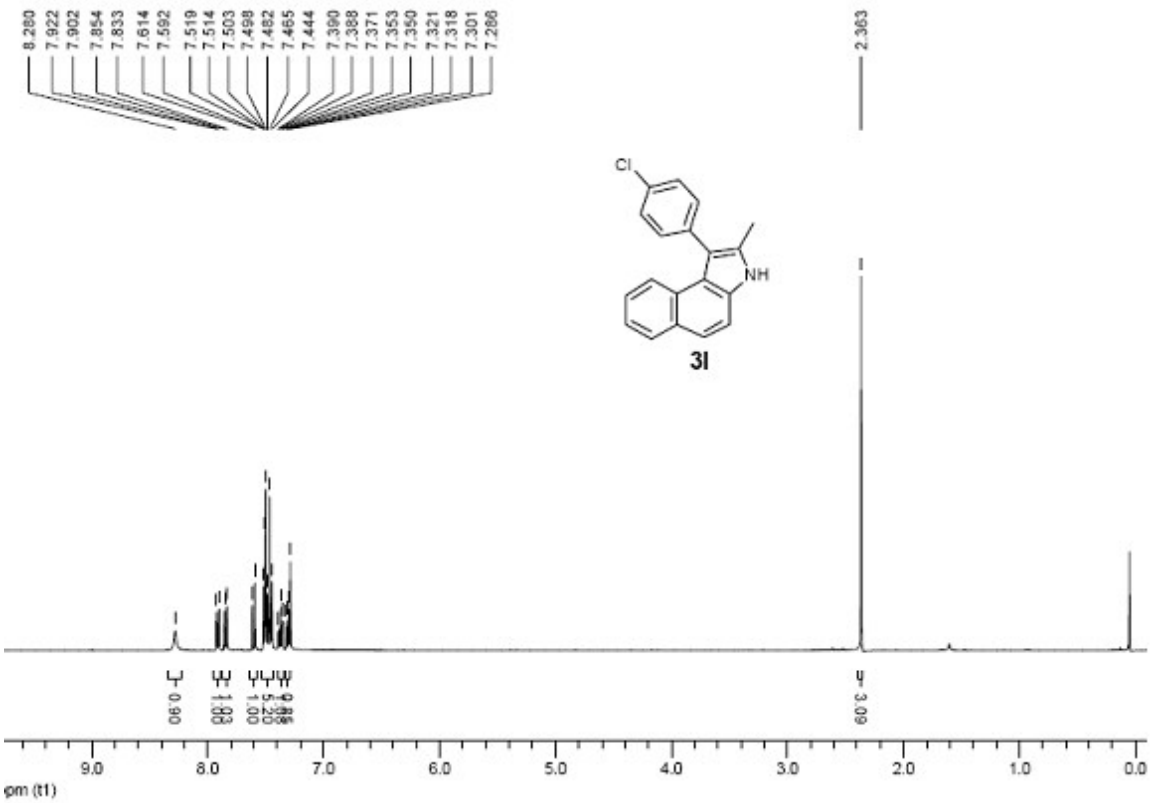

8.488
8.191
8.183
8.174
8.167
7.953
7.946
7.939
7.929
7.682
7.660
7.569
7.547
7.526
7.518
7.514
7.506
7.428
7.422
7.413
7.410
7.406
7.395
7.392
7.383
7.380
7.286
7.243
7.237
S
NH
3i
0.92
1.00
1.15
2.22
1.14
4.17
0.98
10.0
5.0
0.0

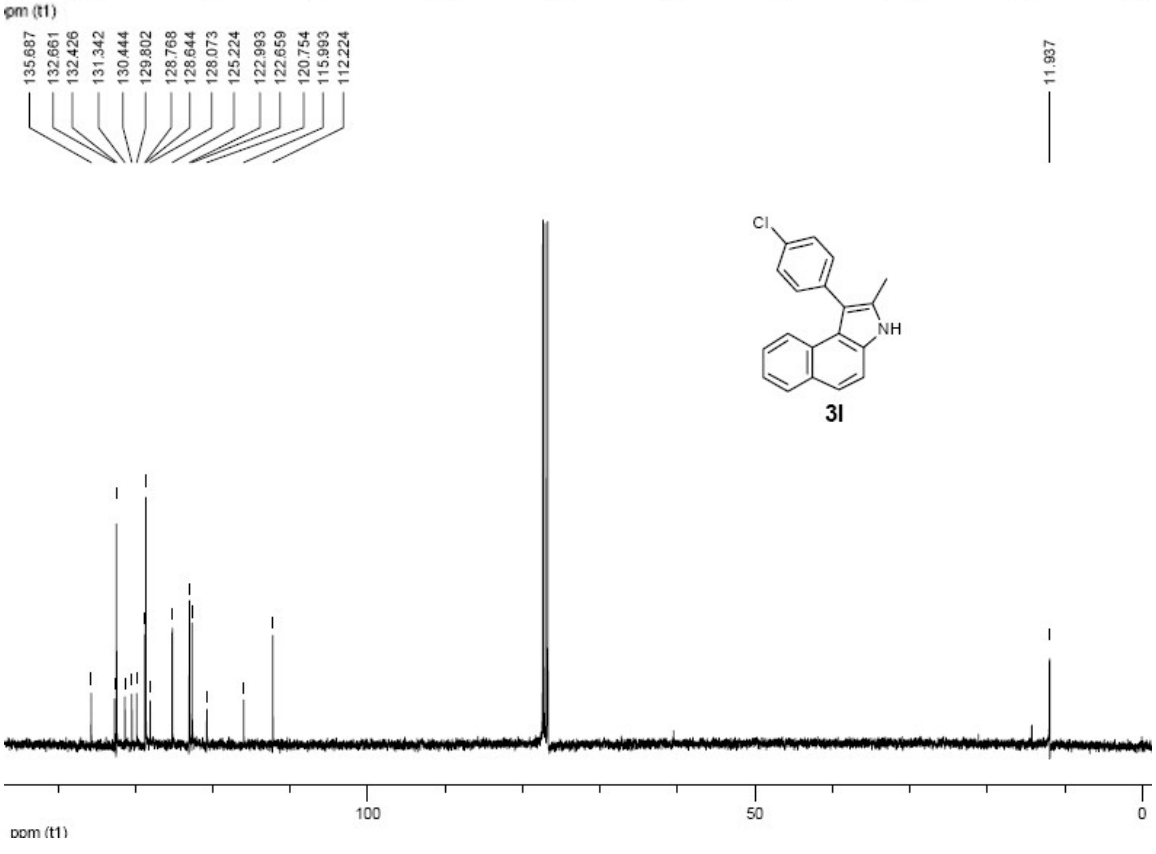

137.019
132.776
130.072
129.794
128.729
125.602
125.307
123.846
123.321
122.635
121.697
120.008
117.778
115.476
112.850
S
NH
3i
100
50
0

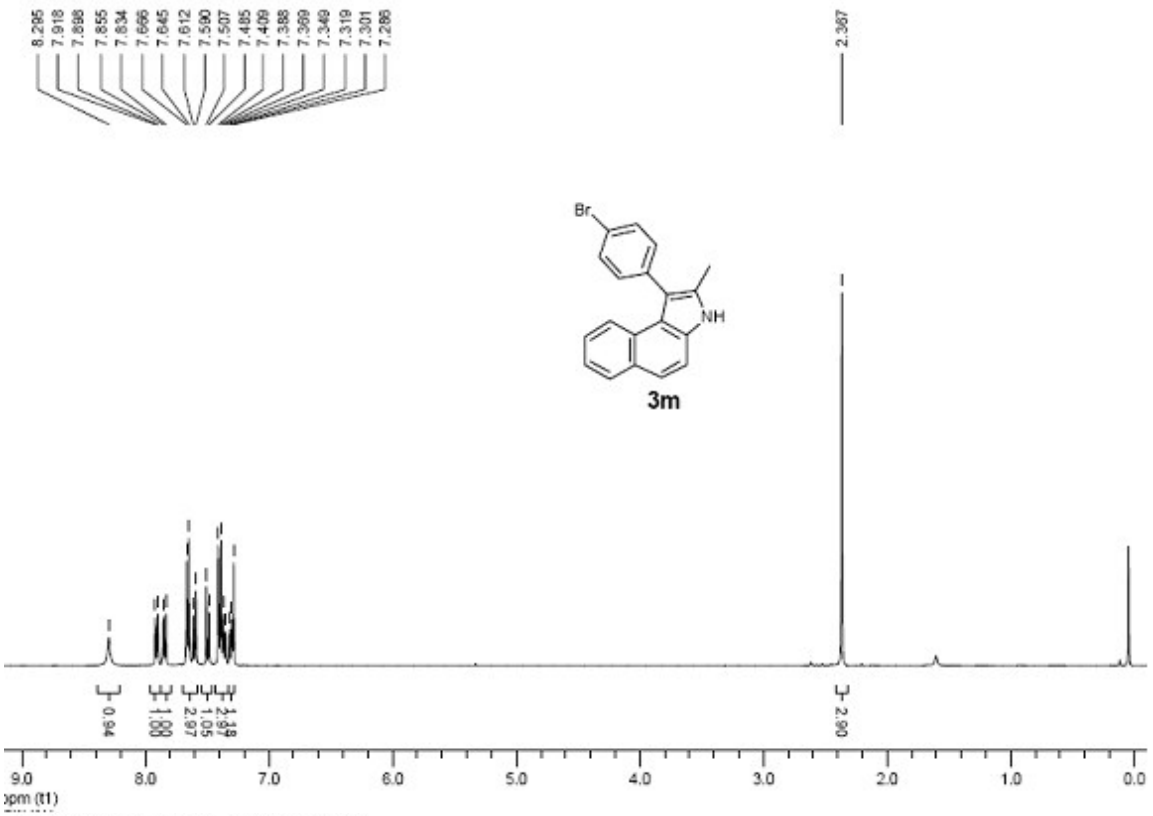

8.170
7.982
7.944
7.926
7.637
7.615
7.592
7.587
7.571
7.560
7.549
7.518
7.506
7.496
7.489
7.483
7.476
7.454
7.419
7.399
7.382
7.379
7.335
7.332
7.315
7.294
7.286
2.349
NH
3j
0.95
2.00
2.96
0.0
5.0
ppm (t1)

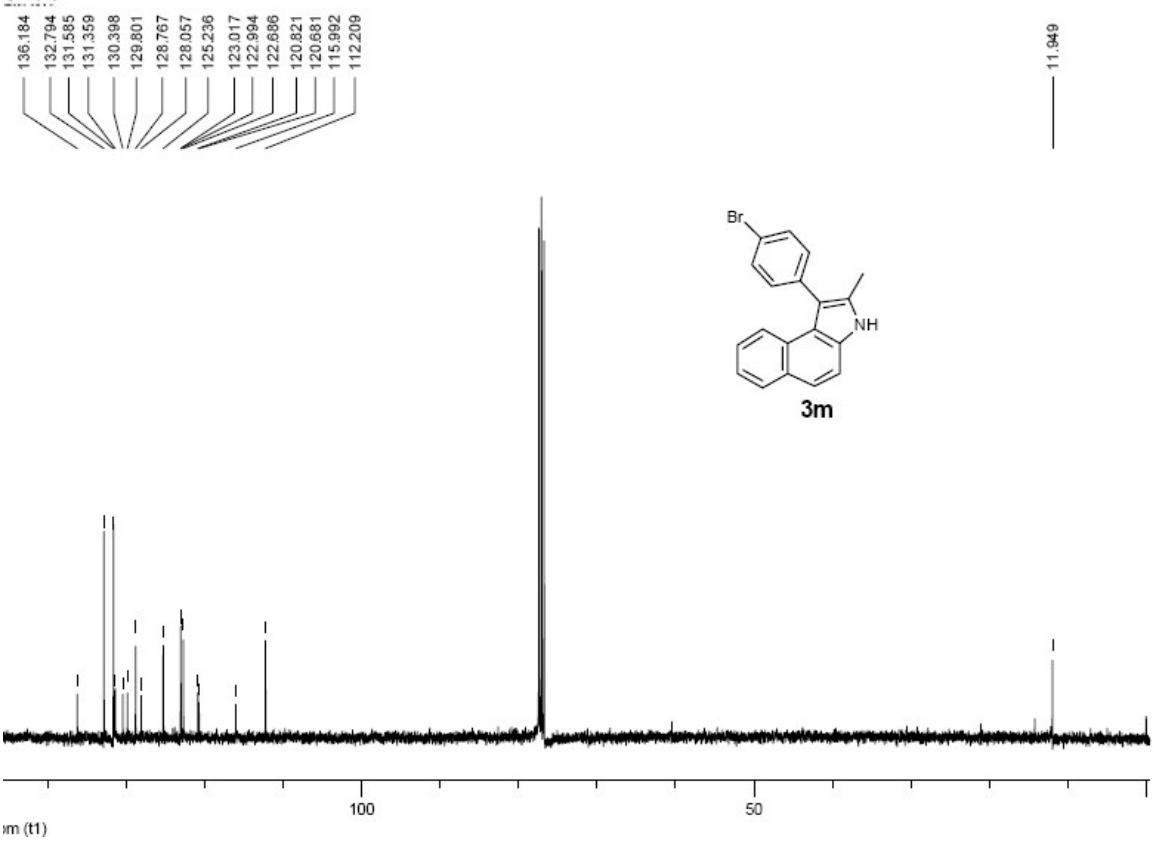

137.203
131.320
131.177
130.447
129.807
128.733
128.465
128.275
126.805
125.146
123.258
122.942
122.421
120.917
117.227
112.393
11.951
NH
3j
100
50

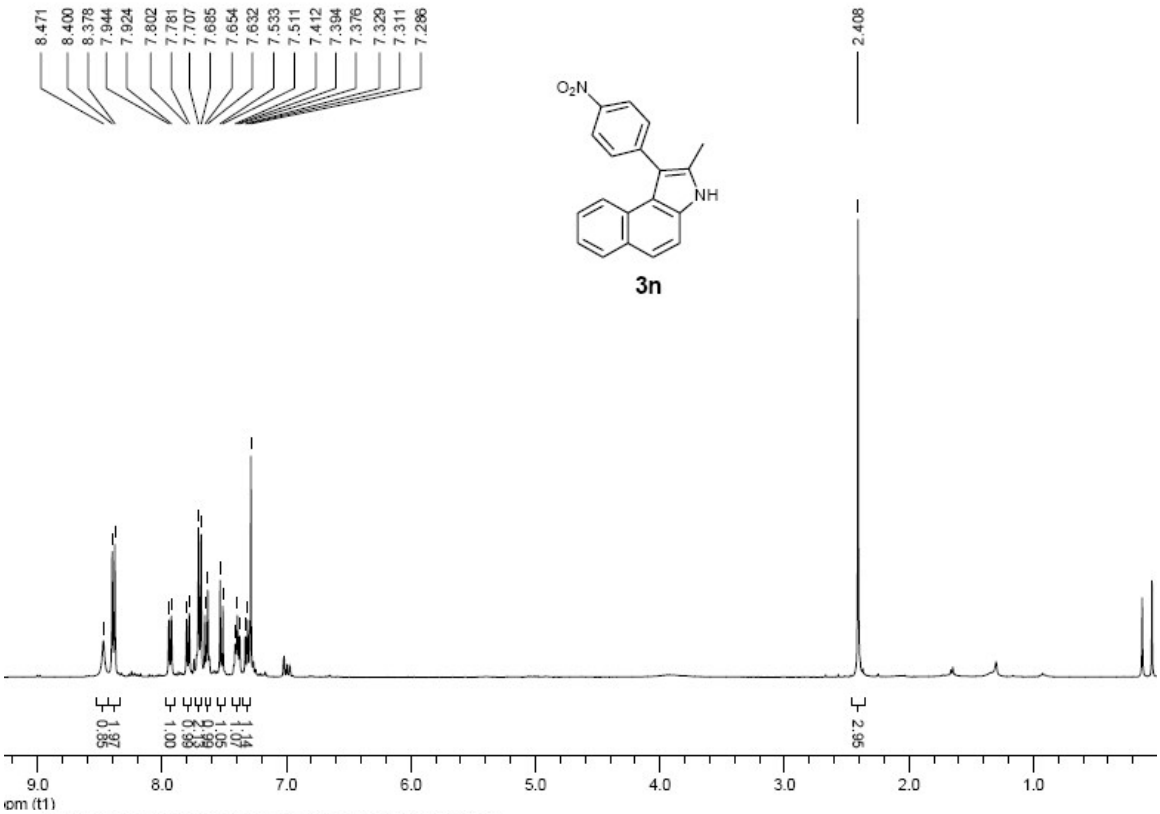

8.232
7.931
7.912
7.837
7.616
7.618
7.596
7.502
7.496
7.491
7.480
7.474
7.466
7.460
7.394
7.391
7.377
7.374
7.372
7.357
7.354
7.318
7.315
7.301
7.297
7.294
7.286
7.280
7.277
7.255
7.250
7.239
7.233
7.228
7.216
7.211
2.354
3k
10
9
8
7
6
5
4
3
2
1
ppm
0.95
1.00
0.99
1.01
2.94
1.00
1.36
1.99
2.94
163.248
160.811
133.021
132.989
132.650
132.572
131.248
130.467
129.788
128.760
128.144
125.181
122.969
122.548
120.951
116.159
115.478
115.269
112.263
11.907
F
NH
3k
150
100
50
0
ppm (t1)

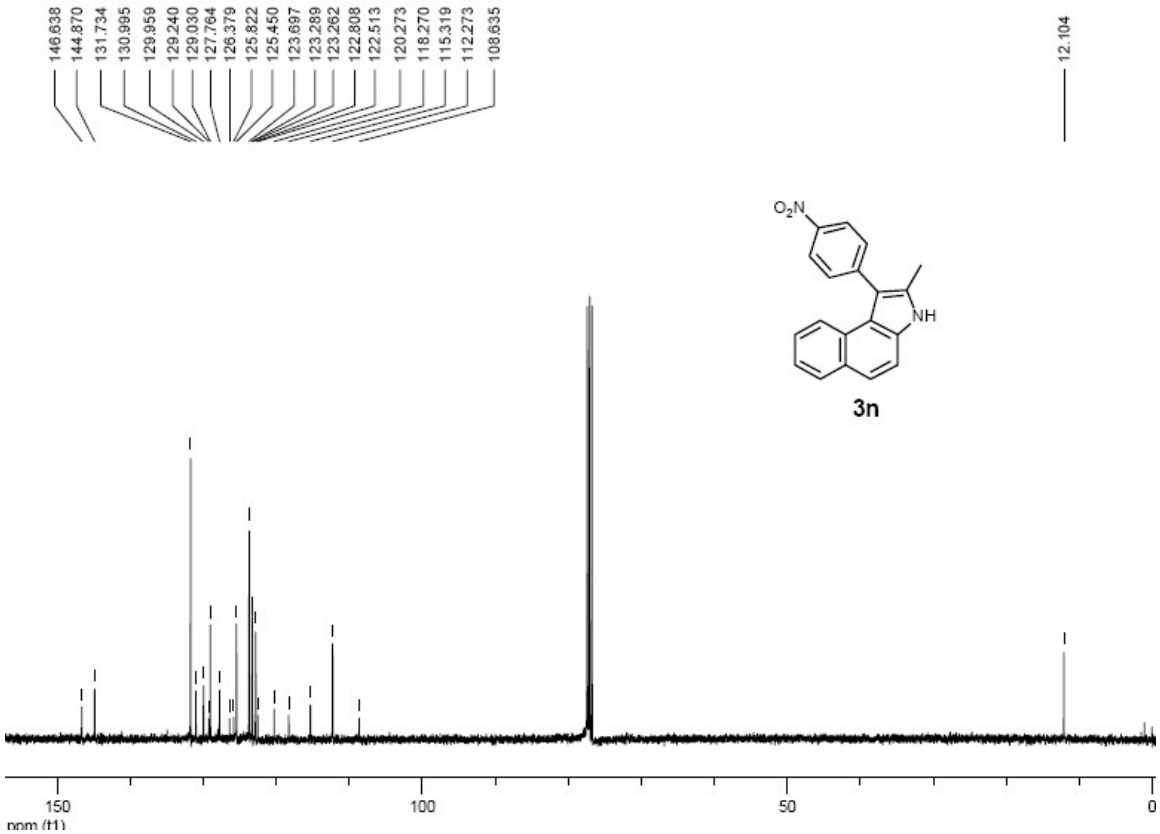

8.280
7.922
7.902
7.854
7.833
7.614
7.592
7.519
7.514
7.503
7.498
7.482
7.465
7.444
7.390
7.388
7.371
7.353
7.350
7.321
7.318
7.301
7.286
2.363
Cl
NH
3l
0.90
1.03
1.00
3.09
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

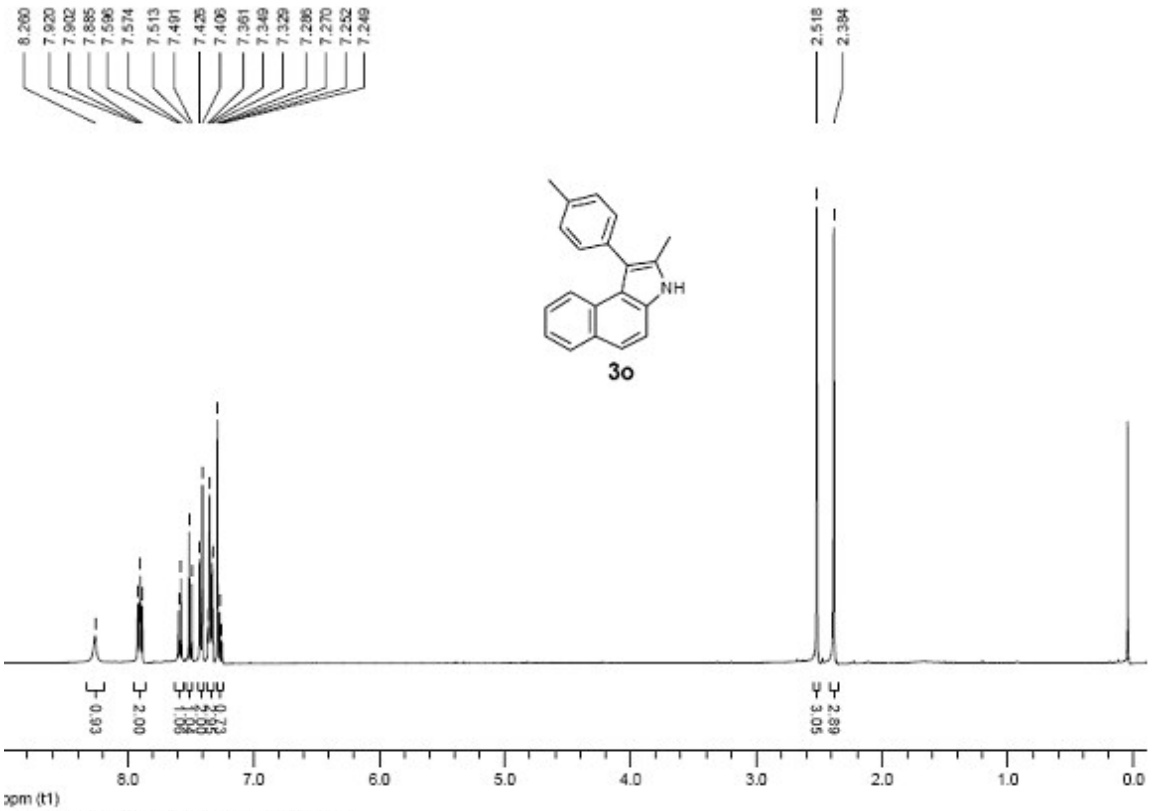

135.687
132.661
132.426
131.342
130.444
129.802
128.768
128.644
128.073
125.224
122.993
122.659
120.754
115.993
112.224
11.937
Cl
NH
3l
100
50
0
ppm (t1)

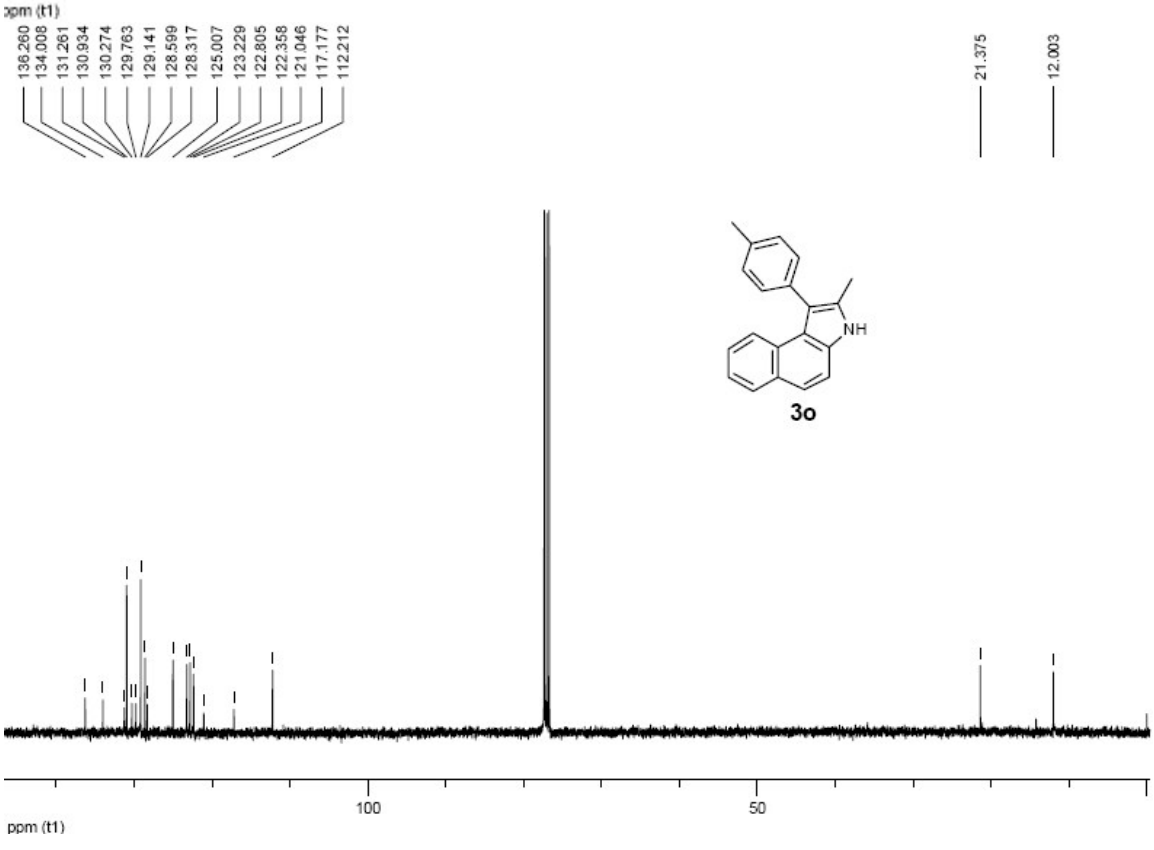

8.285
7.918
7.898
7.855
7.834
7.666
7.645
7.612
7.590
7.507
7.485
7.409
7.388
7.369
7.349
7.319
7.301
7.286
2.367
Br
NH
3m
0.94
1.80
2.97
11.05
21.97
2.90
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

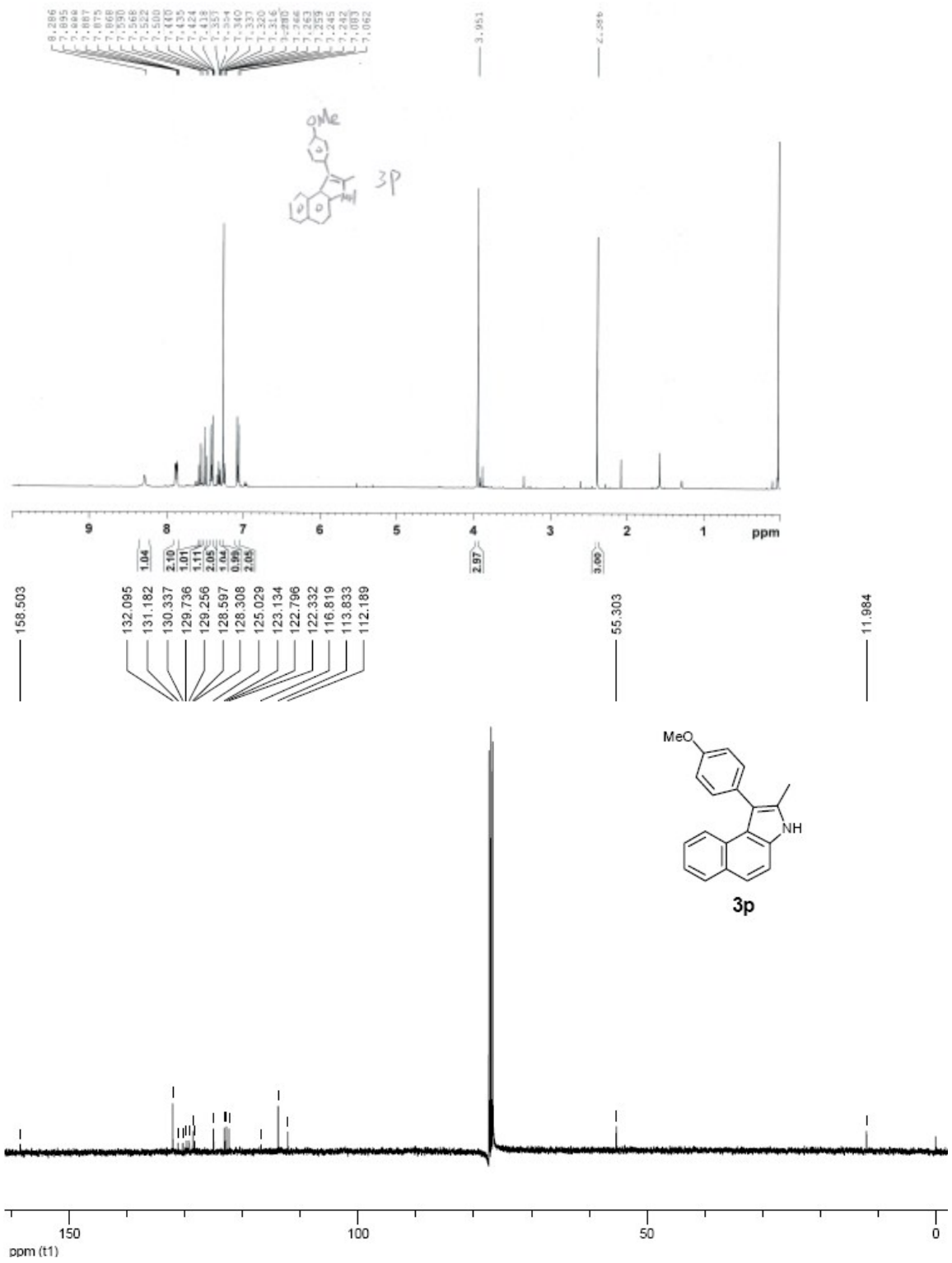

136.184
132.794
131.585
131.359
130.398
129.801
128.767
128.057
125.236
123.017
122.994
122.686
120.821
120.681
115.992
112.209
11.949
Br
NH
3m
100
50
m (t1)

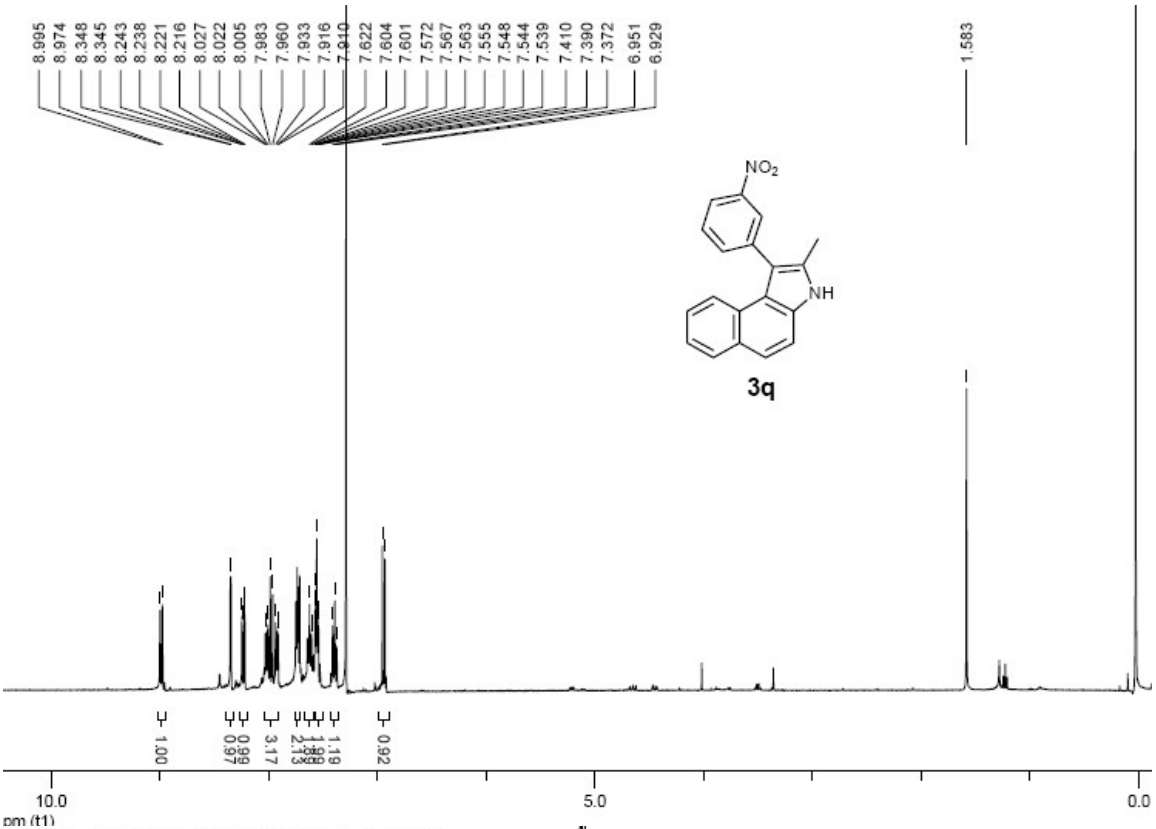

8.471
8.400
8.378
7.944
7.924
7.802
7.781
7.707
7.685
7.654
7.632
7.533
7.511
7.412
7.394
7.376
7.329
7.311
7.286
2.408
O2N
NH
3n
0.85
1.97
1.00
1.05
1.07
1.14
2.96
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)

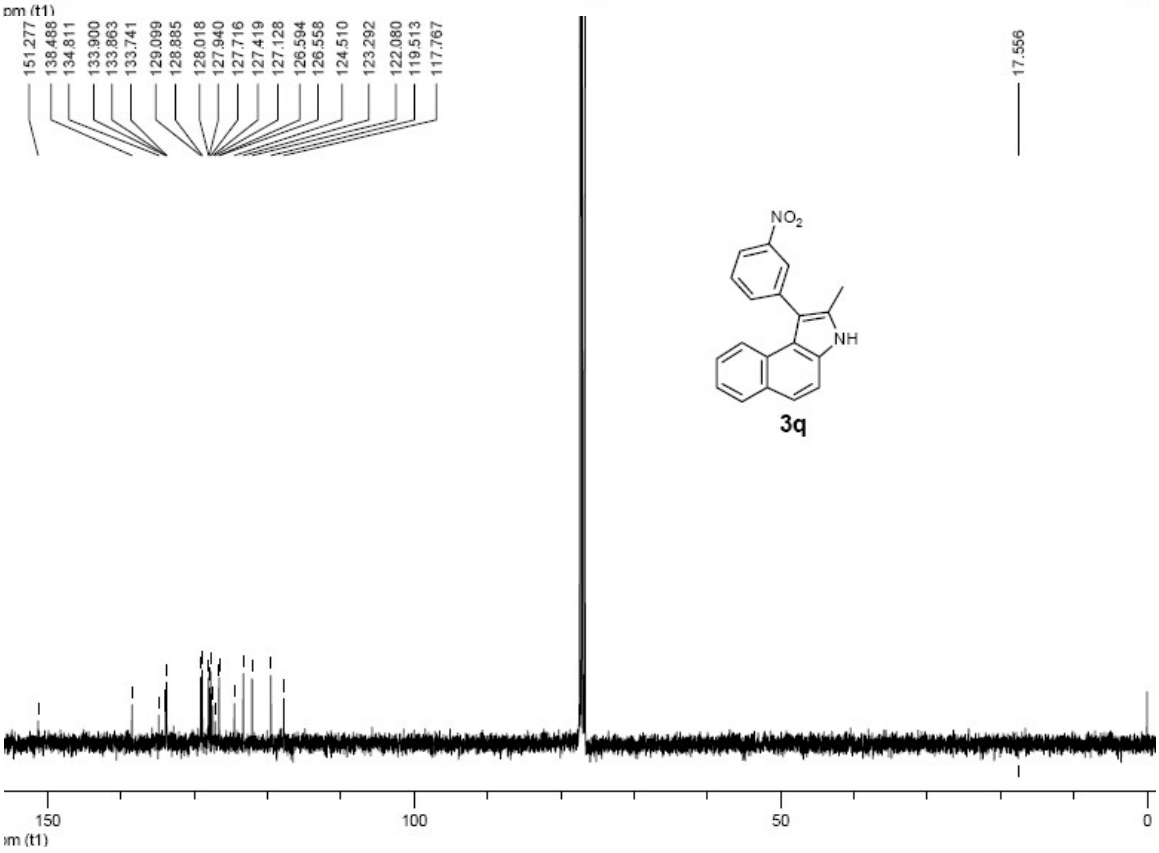

146.638
144.870
131.734
130.995
129.959
129.240
129.030
127.764
126.379
125.822
125.450
123.697
123.289
123.262
122.808
122.513
120.273
118.270
115.319
112.273
108.635
12.104
O2N
NH
3n
150
100
50
0
ppm (t1)

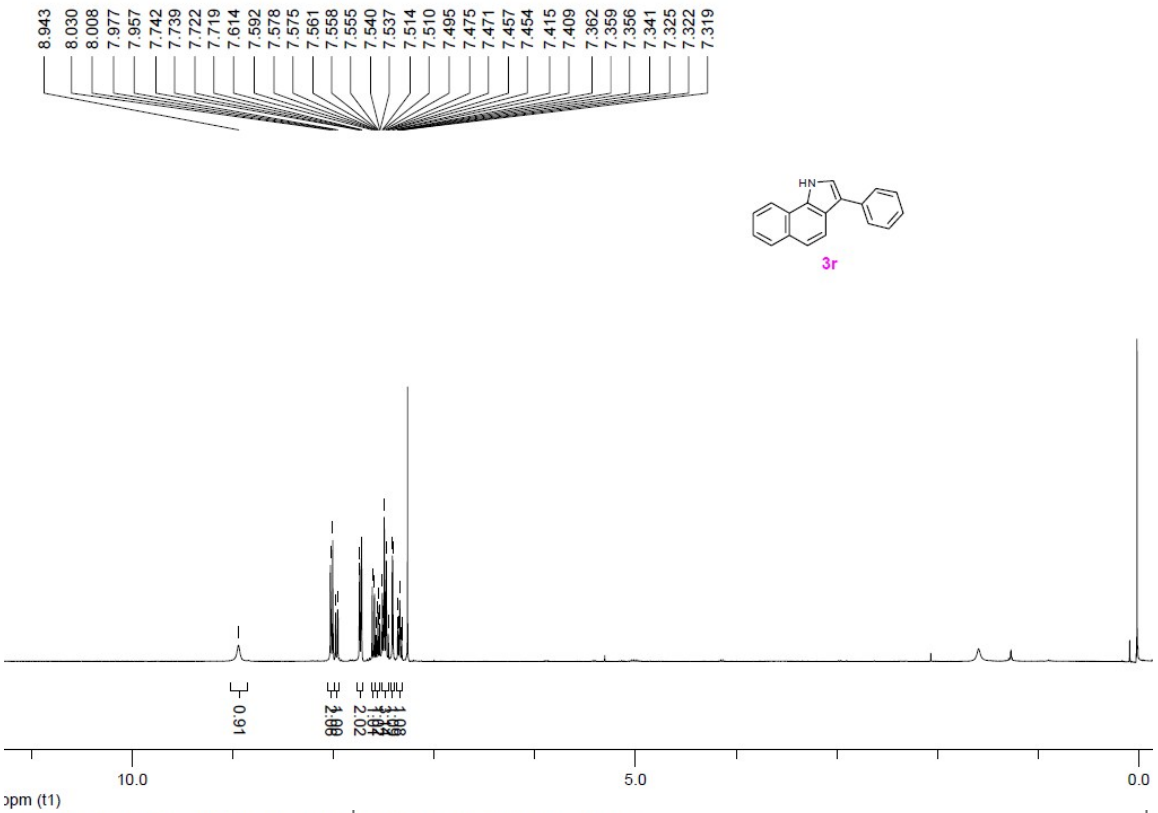

8.260
7.920
7.902
7.885
7.596
7.574
7.513
7.491
7.435
7.406
7.361
7.349
7.329
7.286
7.270
7.252
7.249
2.518
2.384
NH
3o
0.93
2.00
11.08
3.05
2.89
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

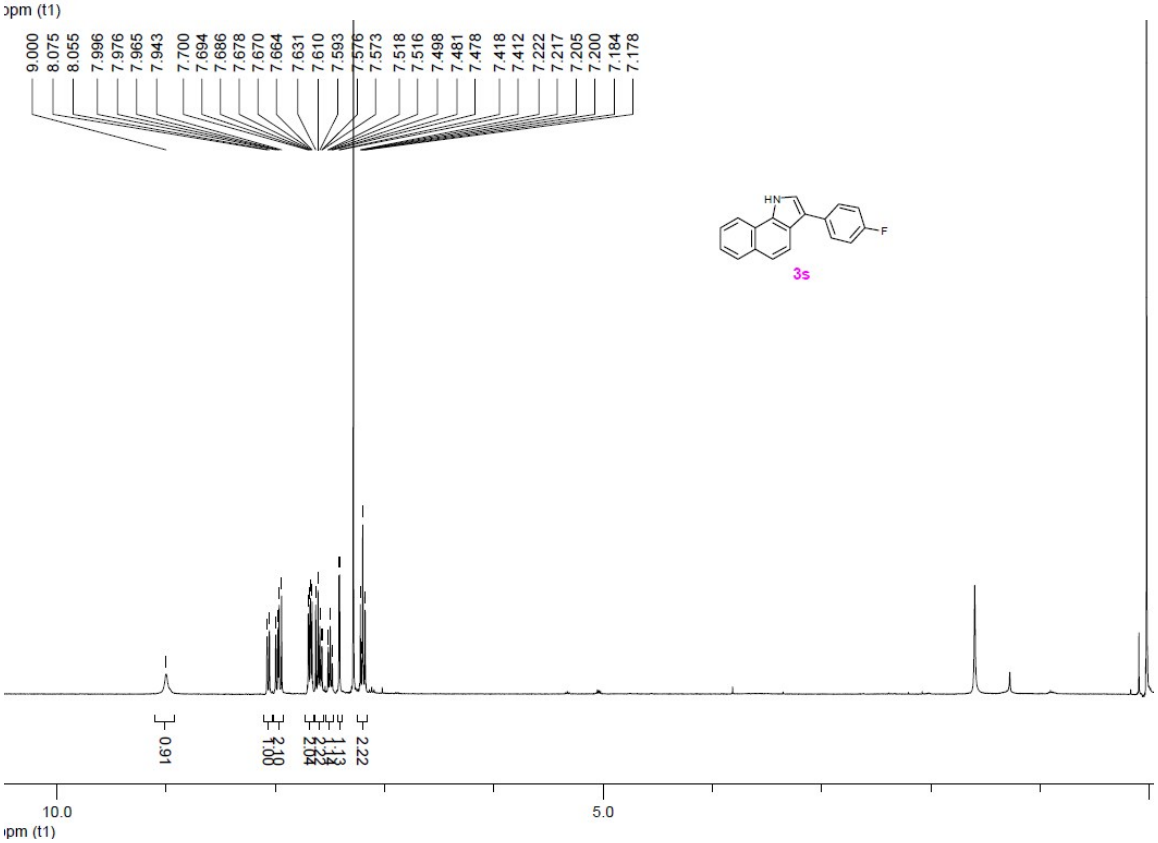

136.260
134.008
131.261
130.934
130.274
129.763
129.141
128.599
128.317
125.007
123.229
122.805
122.358
121.046
117.177
112.212
21.375
12.003
NH
3o
100
50
ppm (t1)

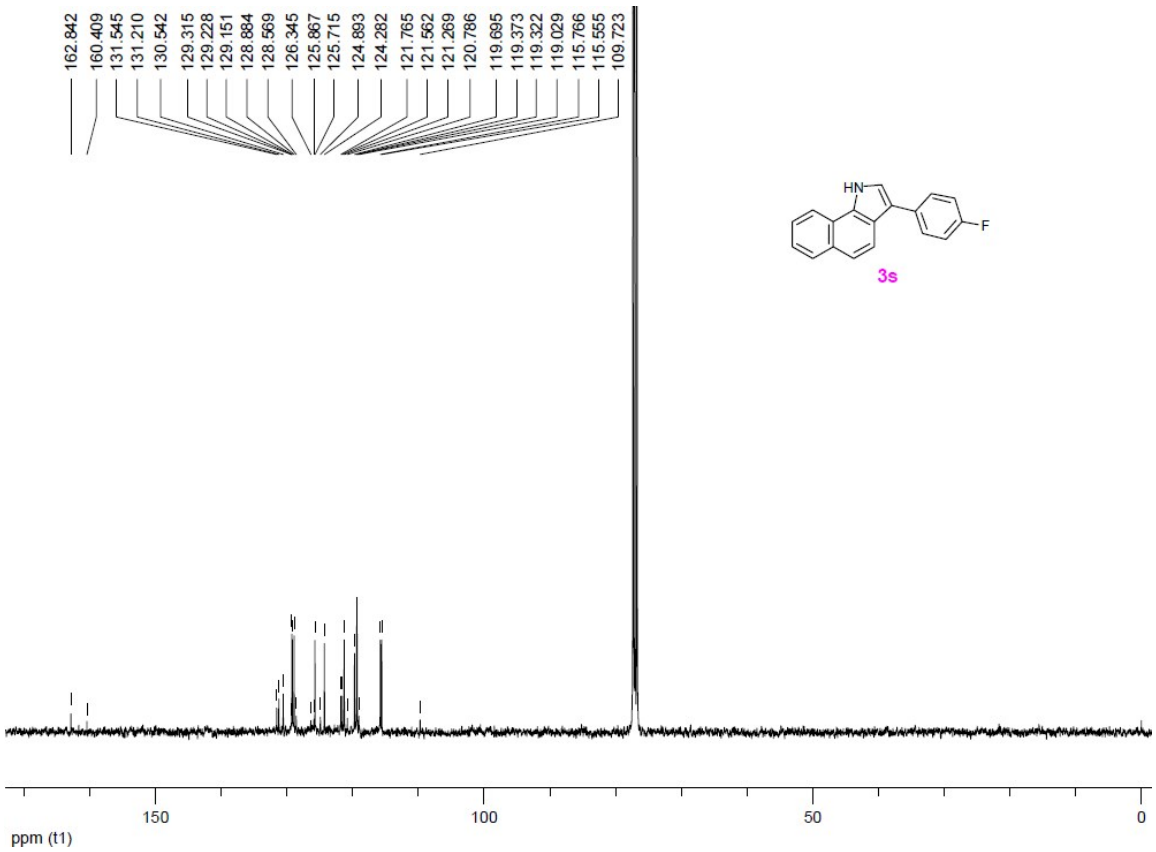

3p
ppm
1.04
2.10
1.01
1.11
2.05
1.04
0.99
2.05
2.97
3.00
158.503
132.095
131.182
130.337
129.736
129.256
128.597
128.308
125.029
123.134
122.796
122.332
116.819
113.833
112.189
55.303
11.984
MeO
NH
3p
150
100
50
0
ppm (t1)

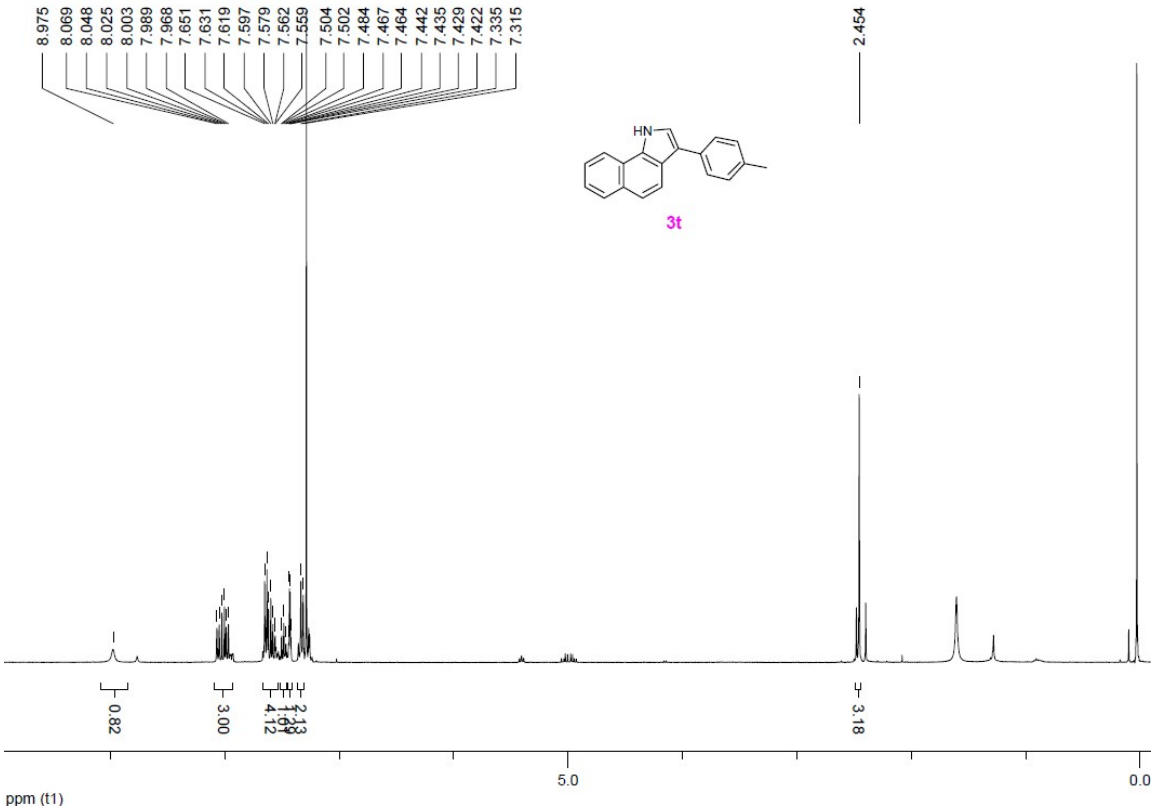

8.995
8.974
8.348
8.345
8.243
8.238
8.221
8.216
8.027
8.022
8.005
7.983
7.960
7.933
7.916
7.910
7.622
7.604
7.601
7.572
7.567
7.563
7.555
7.548
7.544
7.539
7.410
7.390
7.372
6.951
6.929
1.583
NO2
NH
3q
1.00
0.99
0.97
3.17
2.19
1.88
1.19
0.92
10.0
5.0
0.0
pm (t1)

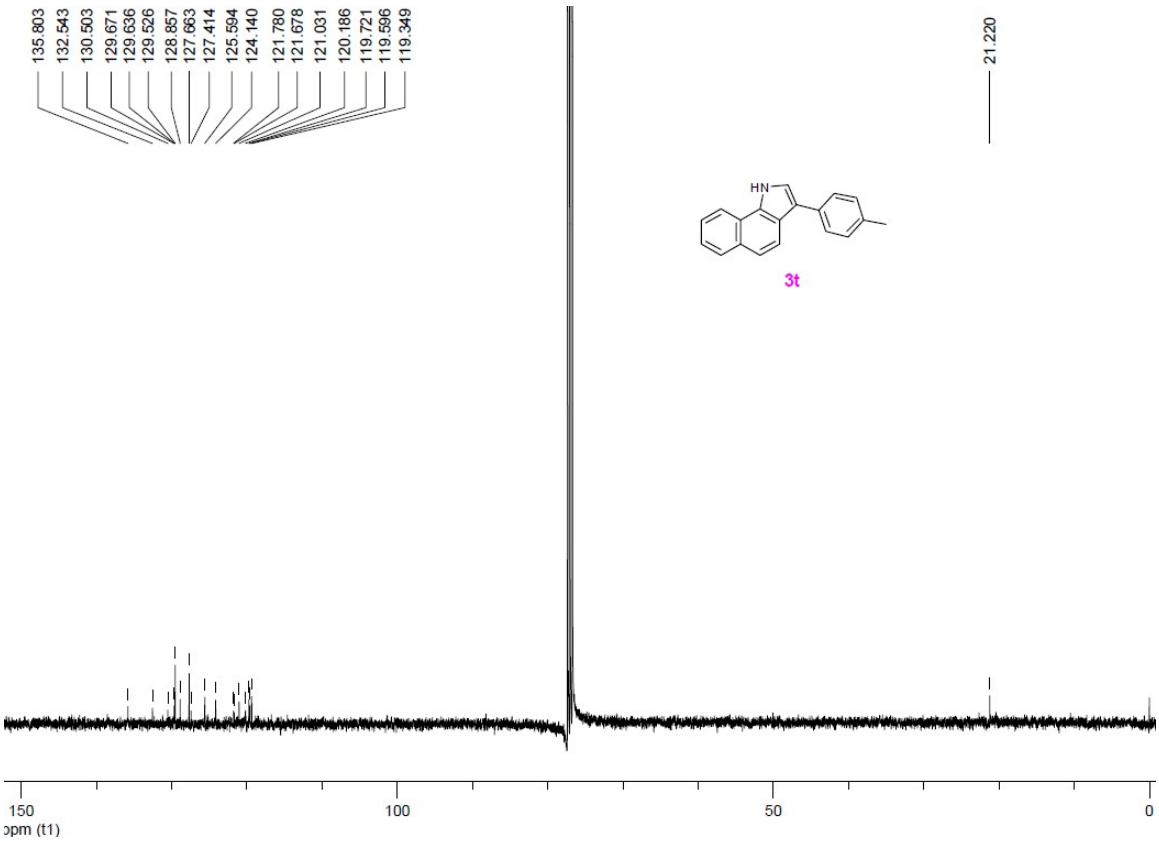

151.277
138.488
134.811
133.900
133.863
133.741
129.099
128.885
128.018
127.940
127.716
127.419
127.128
126.594
126.558
124.510
123.292
122.080
119.513
117.767
17.556
NO2
NH
3q
150
100
50
0
pm (t1)

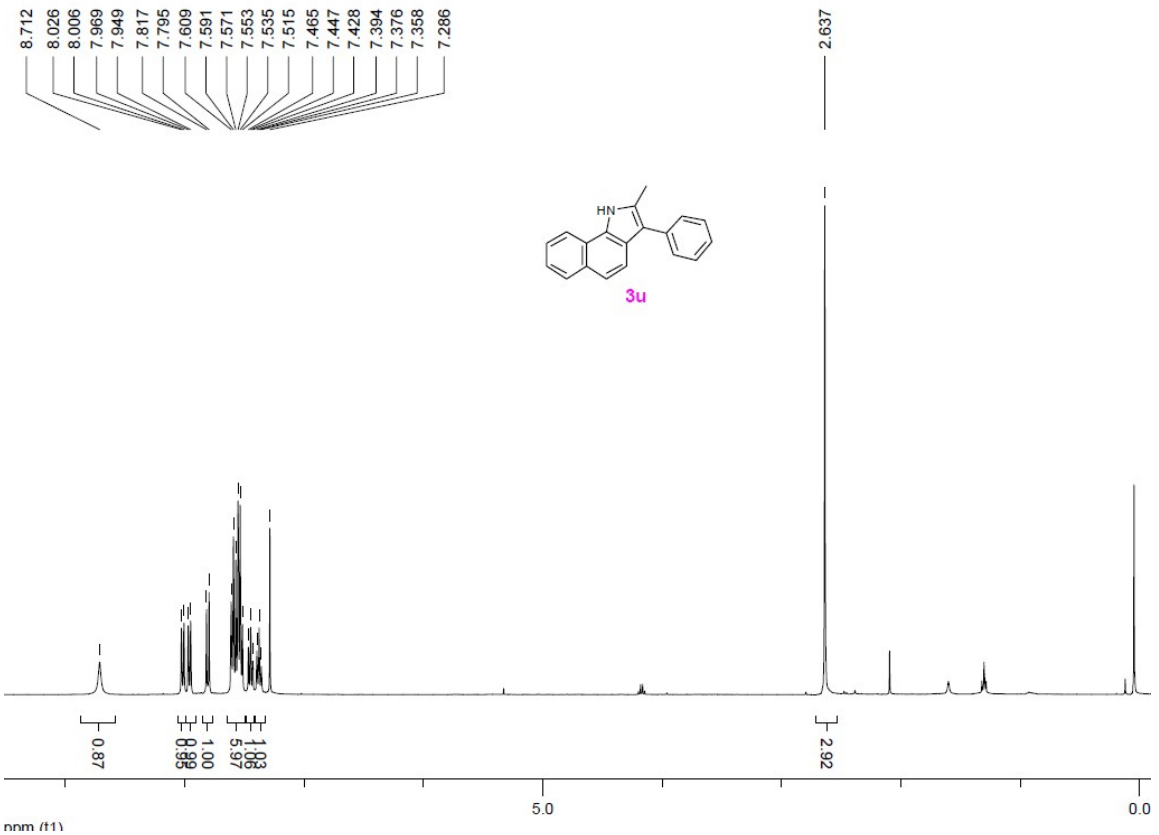

8.943
8.030
8.008
7.977
7.957
7.742
7.739
7.722
7.719
7.614
7.592
7.578
7.575
7.561
7.558
7.555
7.540
7.537
7.514
7.510
7.495
7.475
7.471
7.457
7.454
7.415
7.409
7.362
7.359
7.356
7.341
7.325
7.322
7.319
HN
3r
0.91
10.0
5.0
0.0
ppm (t1)

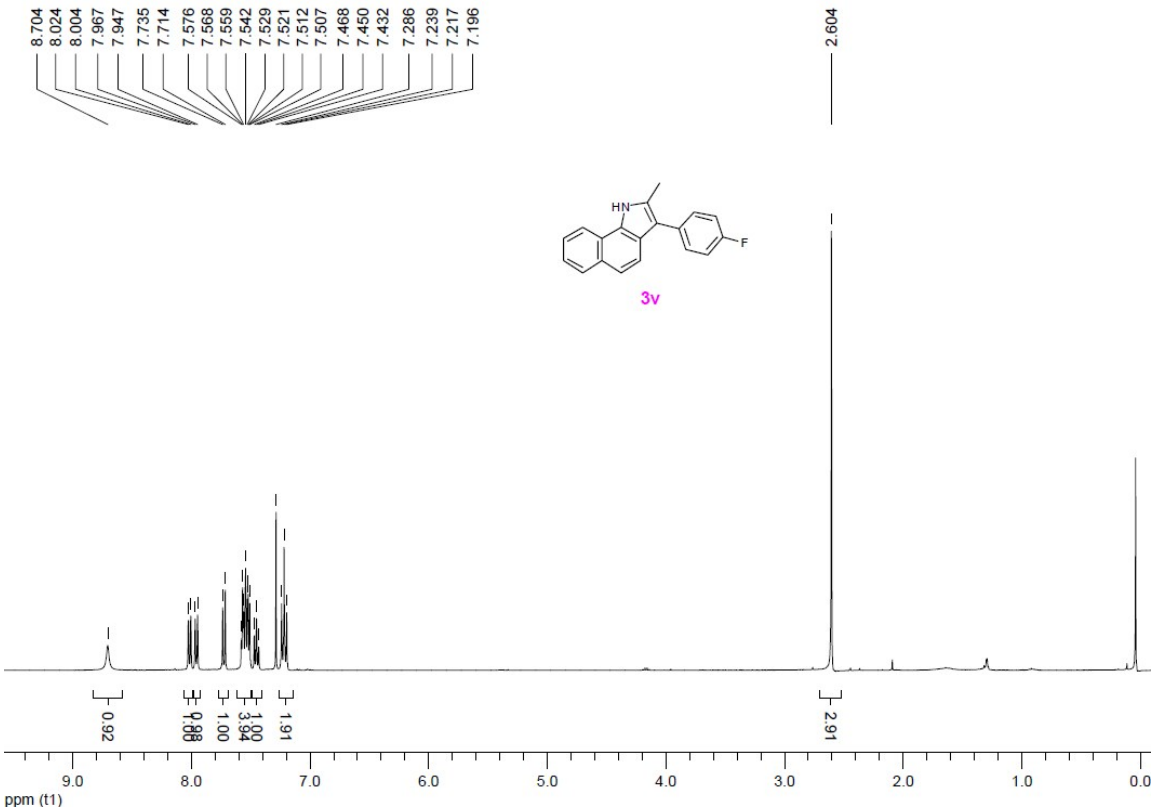

9.000
8.075
8.055
7.996
7.976
7.965
7.943
7.700
7.694
7.686
7.678
7.670
7.664
7.631
7.610
7.593
7.576
7.573
7.518
7.516
7.498
7.481
7.478
7.418
7.412
7.222
7.217
7.205
7.200
7.184
7.178
HN
F
3s
0.91
2.22
10.0
5.0
ppm (t1)

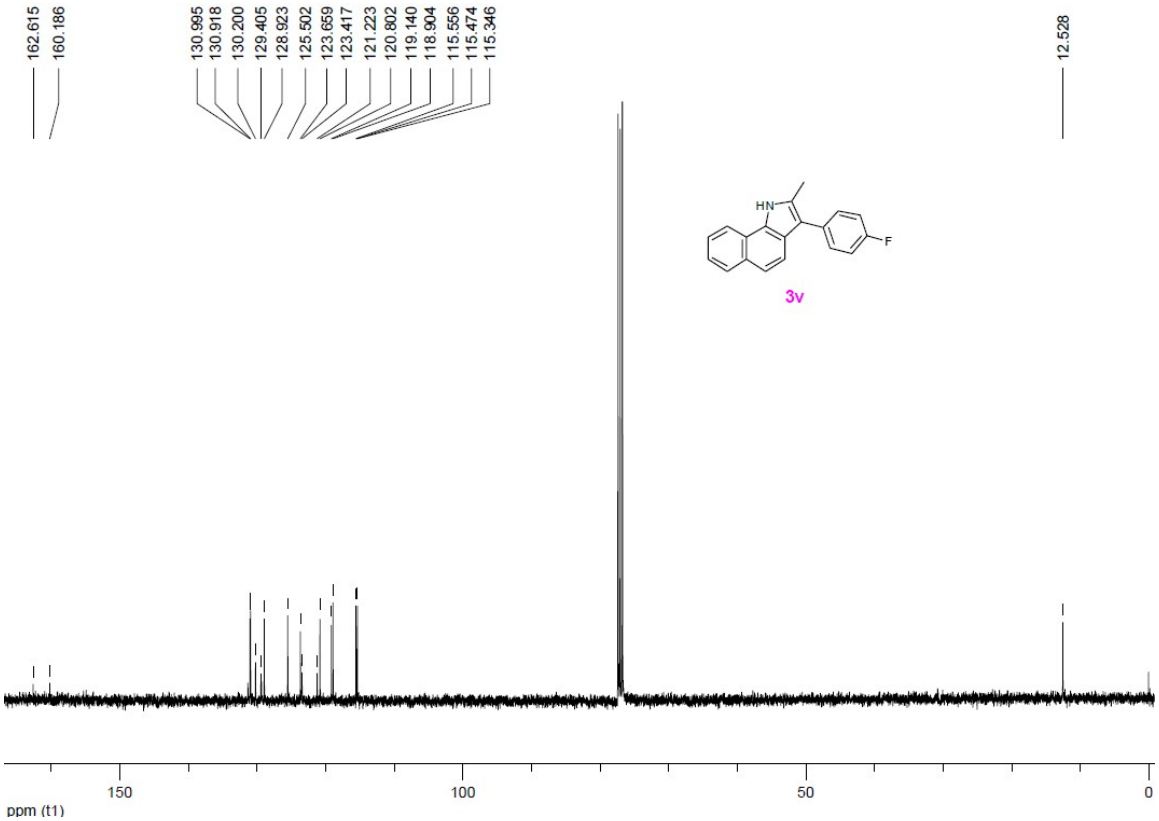

162.842
160.409
131.545
131.210
130.542
129.315
129.228
129.151
128.884
128.569
126.345
125.867
125.715
124.893
124.282
121.765
121.562
121.269
120.786
119.695
119.373
119.322
119.029
115.766
115.555
109.723
HN
F
3s
150
100
50
0
ppm (t1)

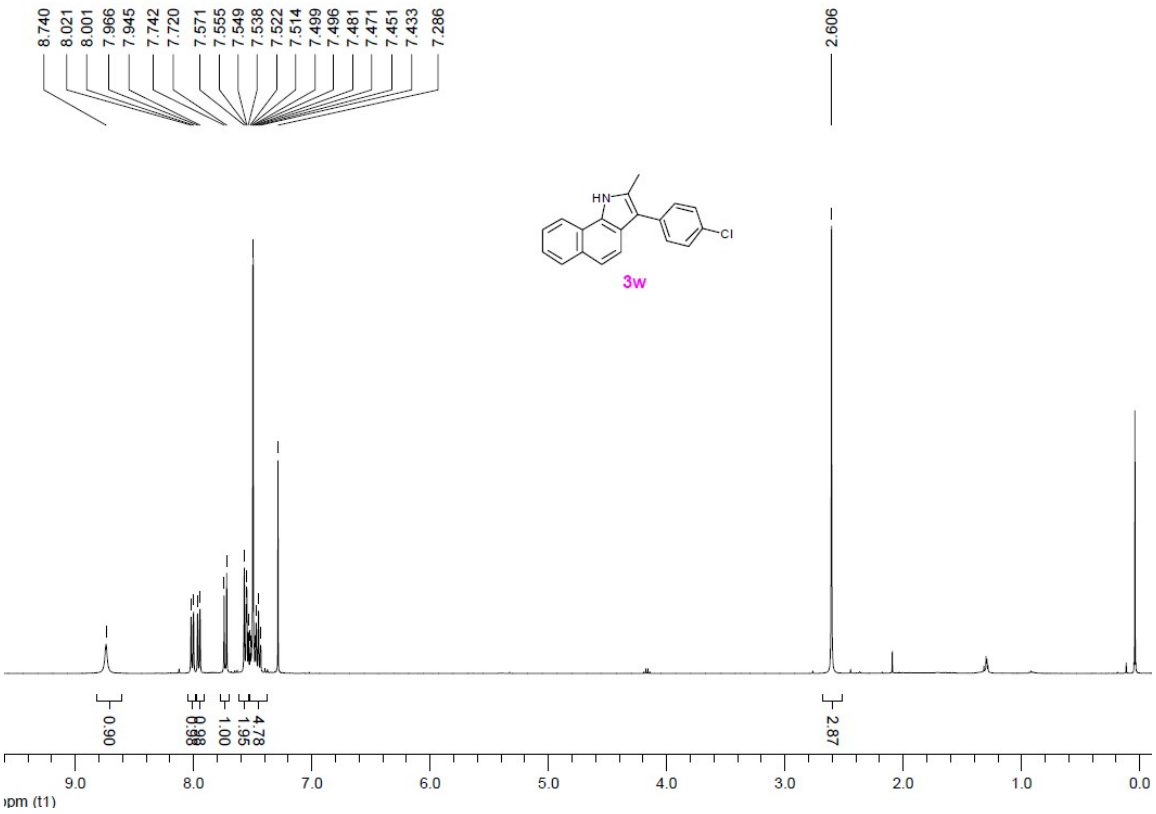

8.975
8.069
8.048
8.025
8.003
7.989
7.968
7.651
7.631
7.619
7.597
7.579
7.562
7.559
7.504
7.502
7.484
7.467
7.464
7.442
7.435
7.429
7.422
7.335
7.315
2.454
HN
3t
0.82
3.00
4.12
3.18
5.0
0.0
ppm (t1)

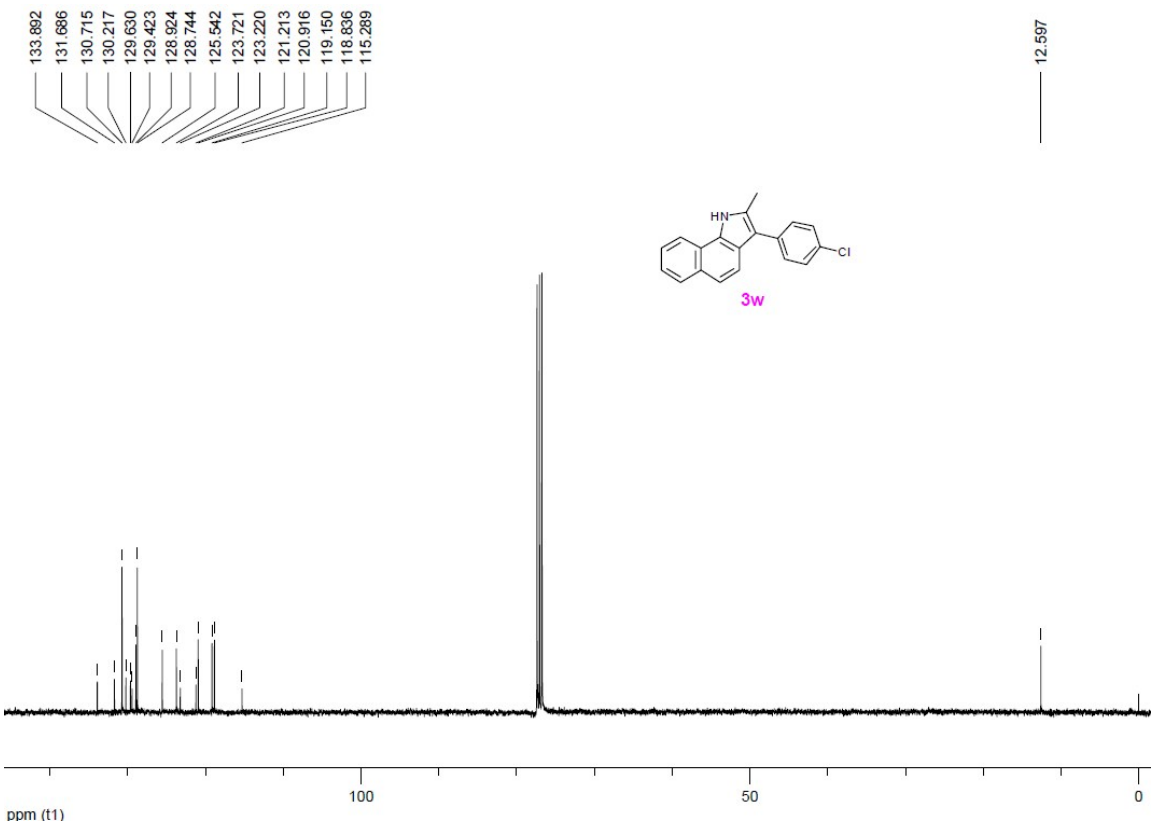

135.803
132.543
130.503
129.671
129.636
129.526
128.857
127.663
127.414
125.594
124.140
121.780
121.678
121.031
120.186
119.721
119.596
119.349
21.220
HN
3t
150
100
50
0
ppm (t1)

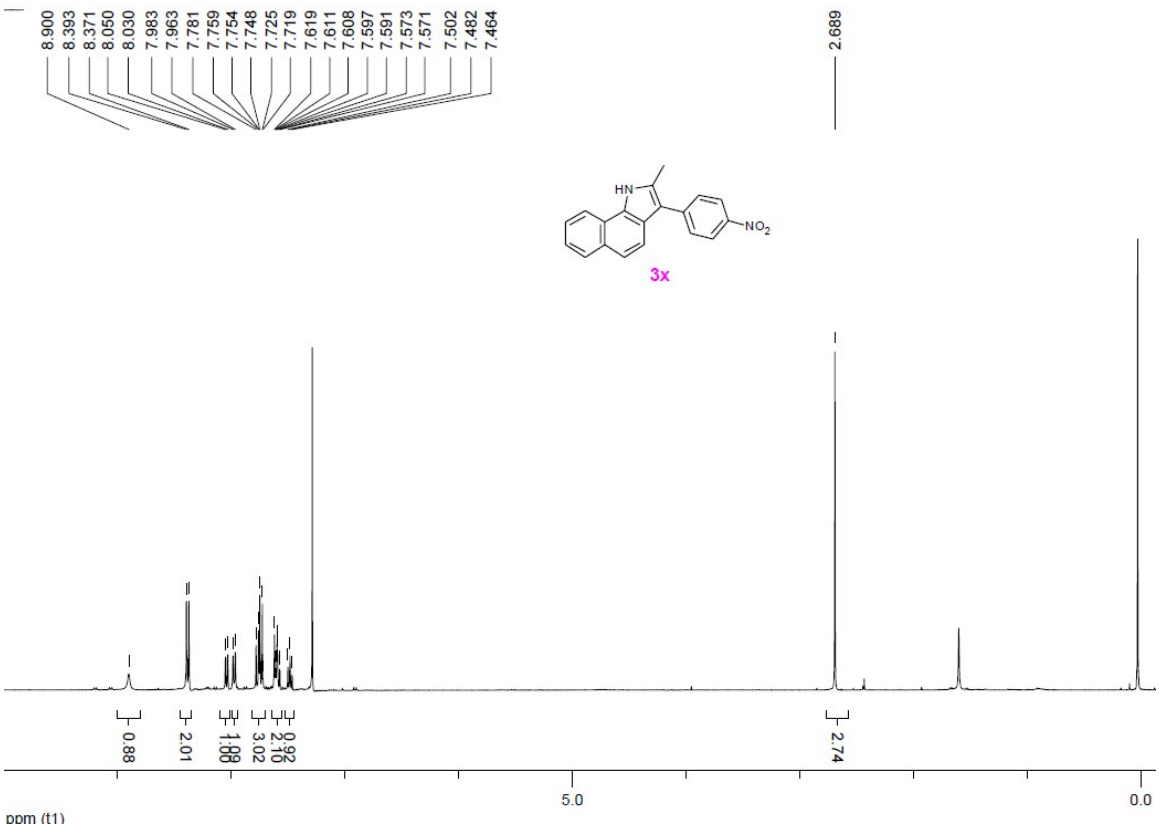

8.712
8.026
8.006
7.969
7.949
7.817
7.795
7.609
7.591
7.571
7.553
7.535
7.515
7.465
7.447
7.428
7.394
7.376
7.358
7.286
2.637
HN
3u
0.87
0.98
0.98
1.00
5.97
1.03
1.06
2.92
5.0
0.0
ppm (t1)

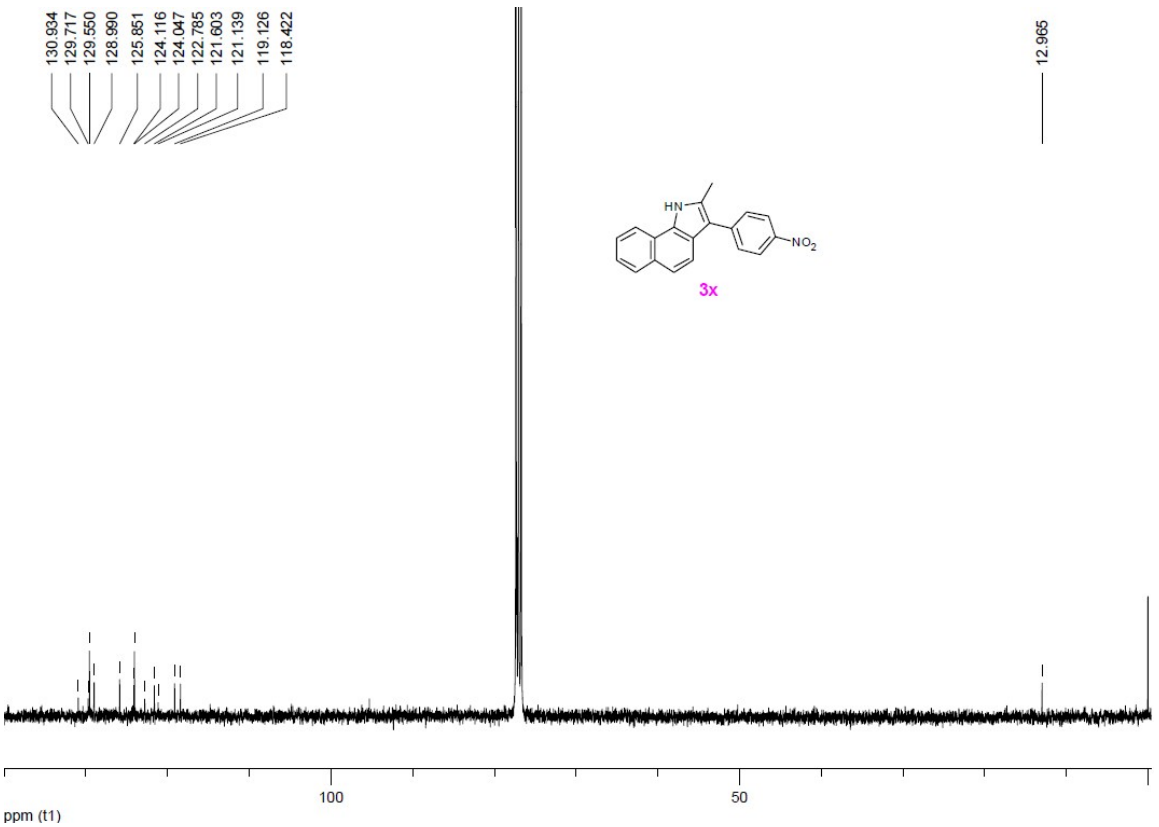

8.704
8.024
8.004
7.967
7.947
7.735
7.714
7.576
7.568
7.559
7.542
7.529
7.521
7.512
7.507
7.468
7.450
7.432
7.286
7.239
7.217
7.196
2.604
HN
F
3v
0.92
0.98
1.00
3.34
3.00
1.91
2.91
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

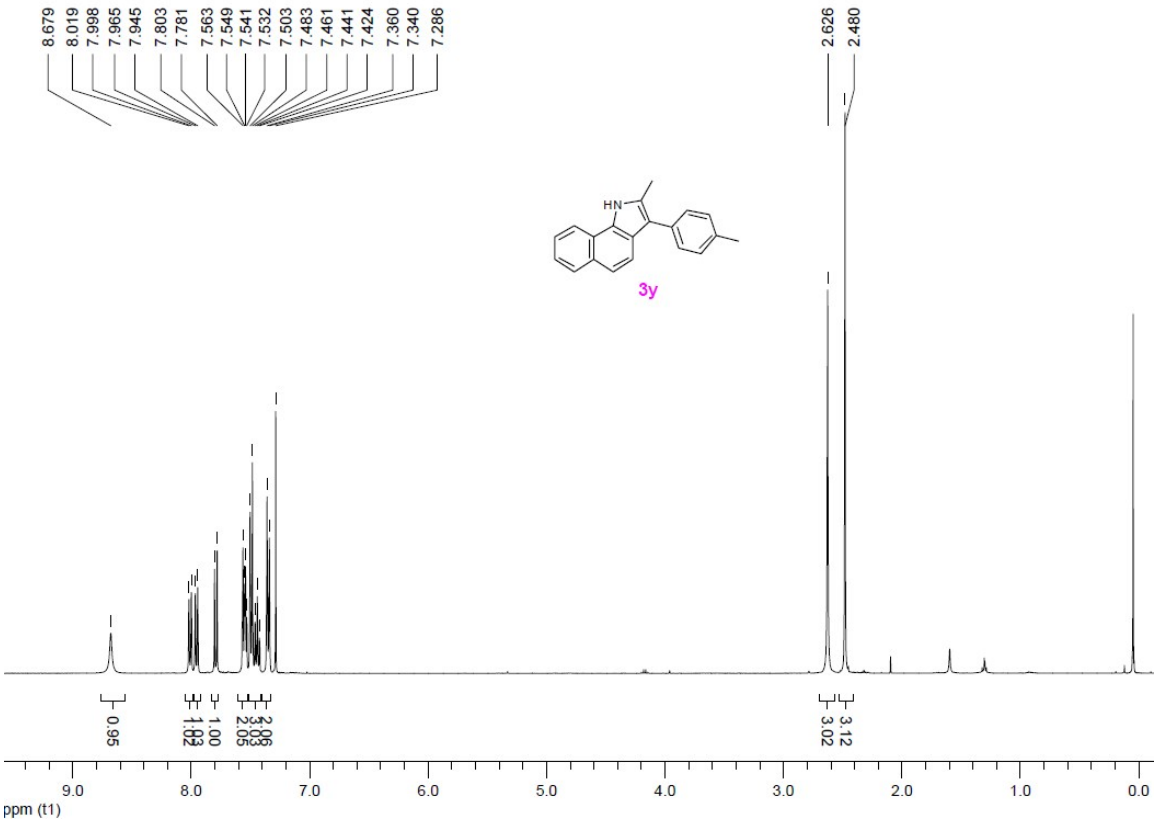

162.615
160.186
130.995
130.918
130.200
129.405
128.923
125.502
123.659
123.417
121.223
120.802
119.140
118.904
115.556
115.474
115.346
12.528
HN
F
3v
150
100
50
0
ppm (t1)

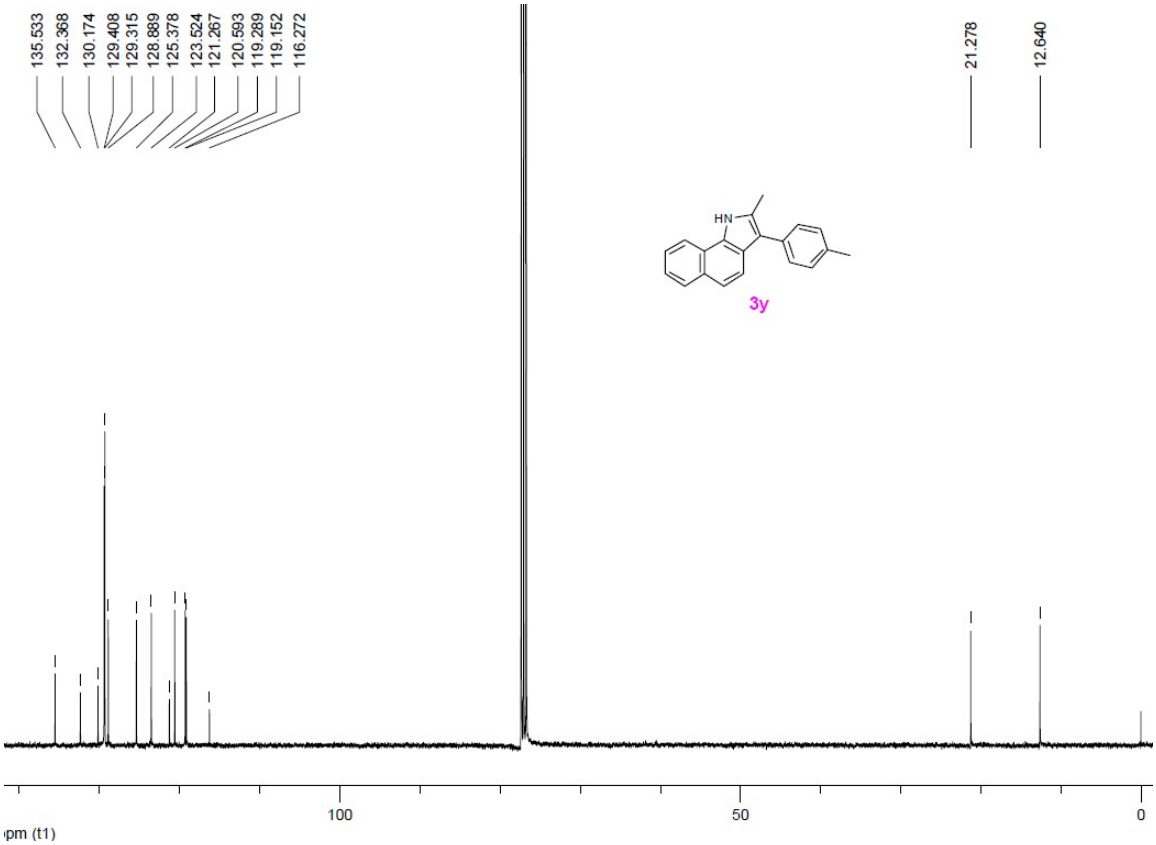

8.740
8.021
8.001
7.966
7.945
7.742
7.720
7.571
7.555
7.549
7.538
7.522
7.514
7.499
7.496
7.481
7.471
7.451
7.433
7.286
2.606
HN
Cl
3w
0.90
1.00
1.96
4.78
2.87
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

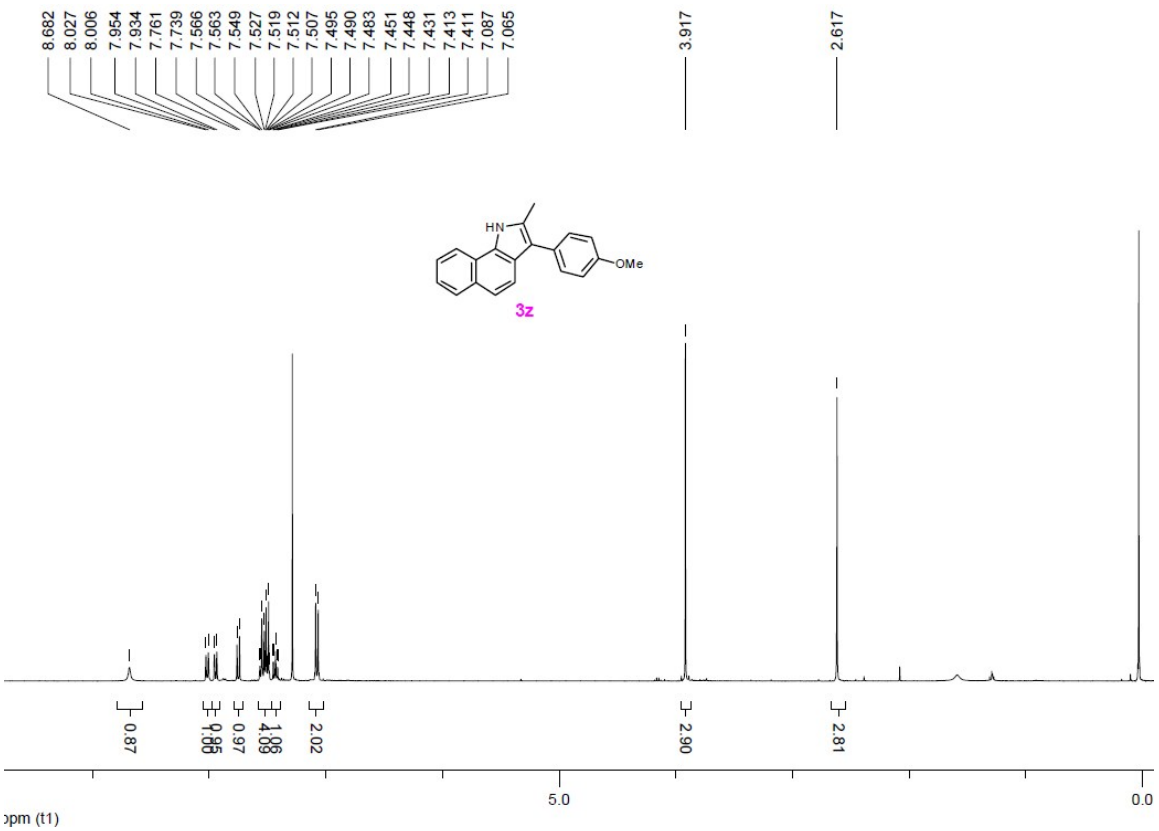

133.892
131.686
130.715
130.217
129.630
129.423
128.924
128.744
125.542
123.721
123.220
121.213
120.916
119.150
118.836
115.289
12.597
HN
Cl
3w
100
50
0
ppm (t1)

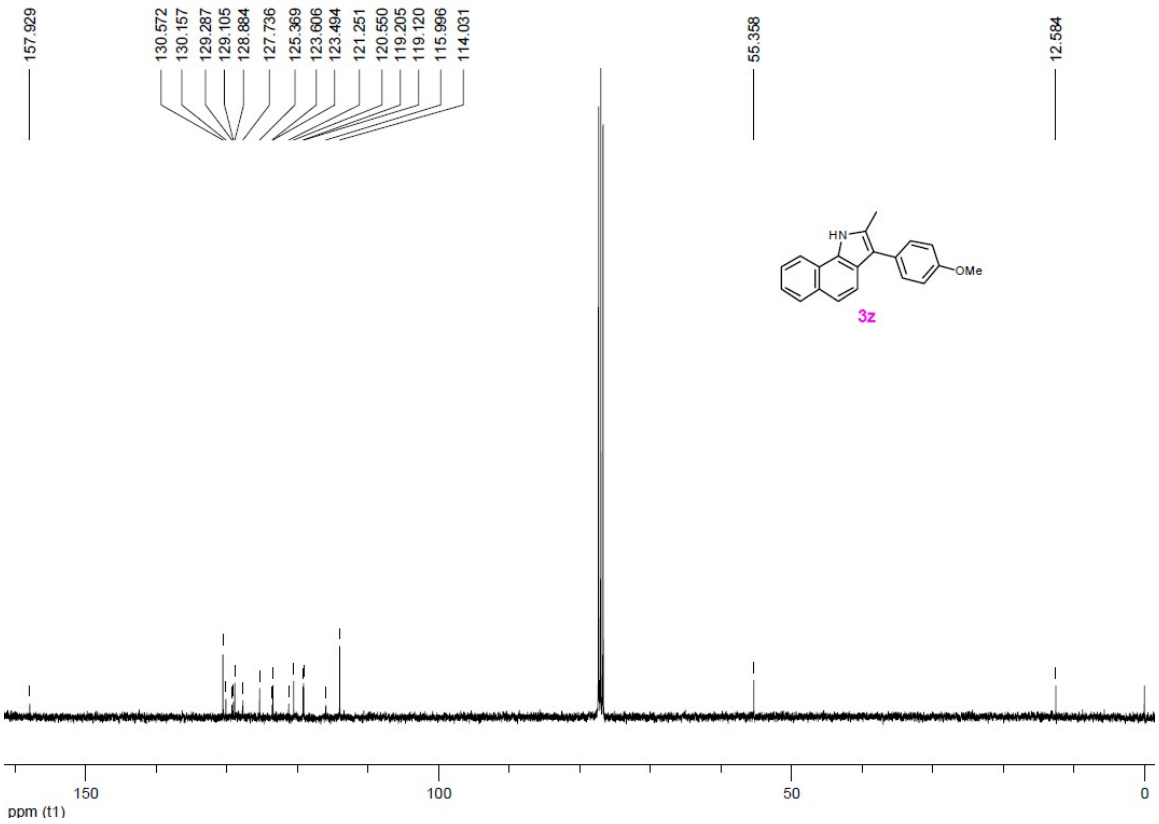

8.900
8.393
8.371
8.050
8.030
7.983
7.963
7.781
7.759
7.754
7.748
7.725
7.719
7.619
7.611
7.608
7.597
7.591
7.573
7.571
7.502
7.482
7.464
2.689
HN
NO2
3x
0.88
2.01
1.00
1.08
3.02
2.10
2.92
2.74
5.0
0.0
ppm (t1)

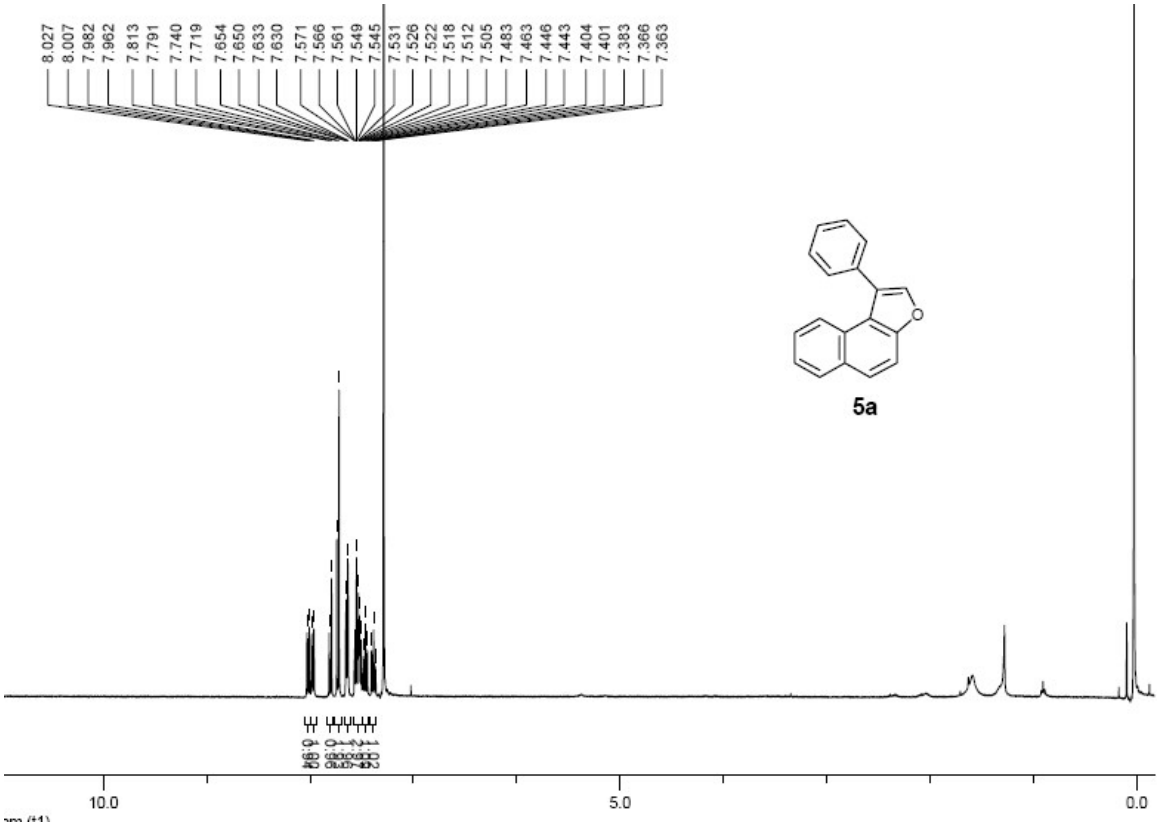

130.934
129.717
129.550
128.990
125.851
124.116
124.047
122.785
121.603
121.139
119.126
118.422
12.965
HN
NO2
3x
100
50
ppm (t1)

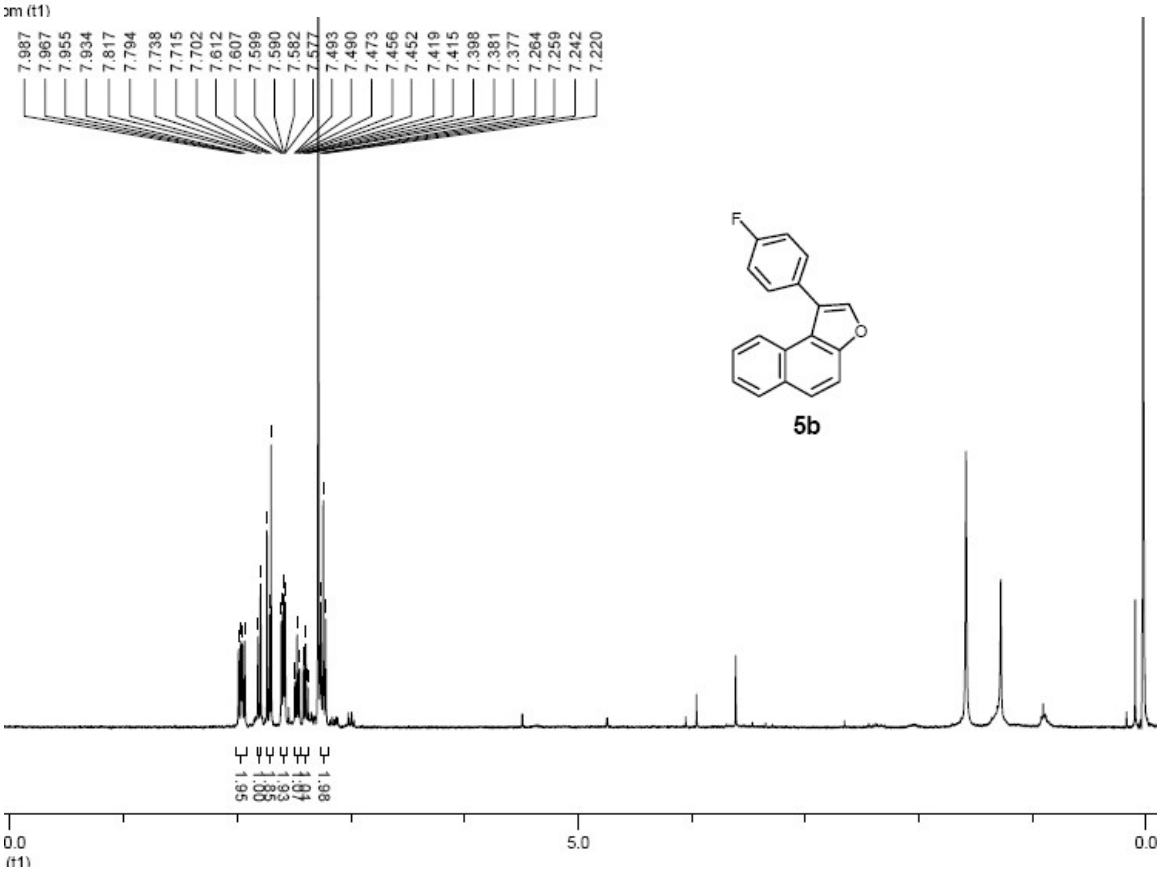

8.679
8.019
7.998
7.965
7.945
7.803
7.781
7.563
7.549
7.541
7.532
7.503
7.483
7.461
7.441
7.424
7.360
7.340
7.286
2.626
2.480
HN
3y
0.95
1.82
1.00
2.05
2.03
2.00
3.02
3.12
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

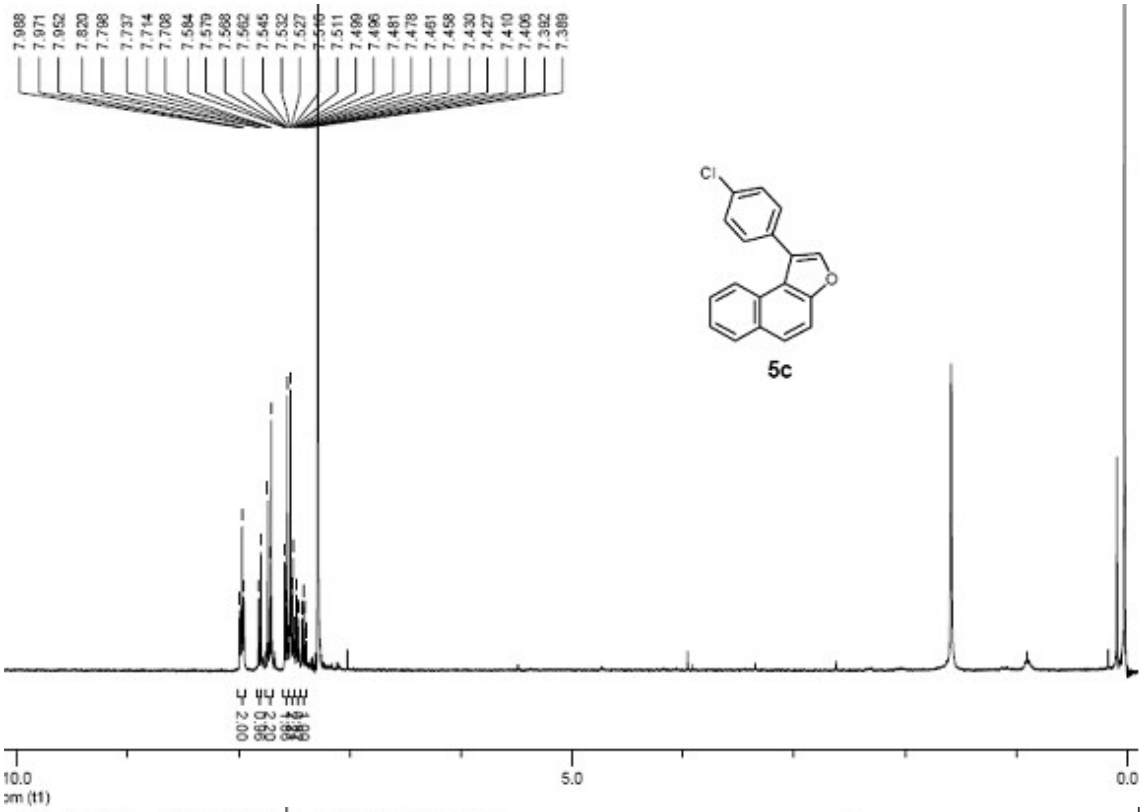

135.533
132.368
130.174
129.408
129.315
128.889
125.378
123.524
121.267
120.593
119.289
119.152
116.272
21.278
12.640
HN
3y
100
50
0
ppm (t1)

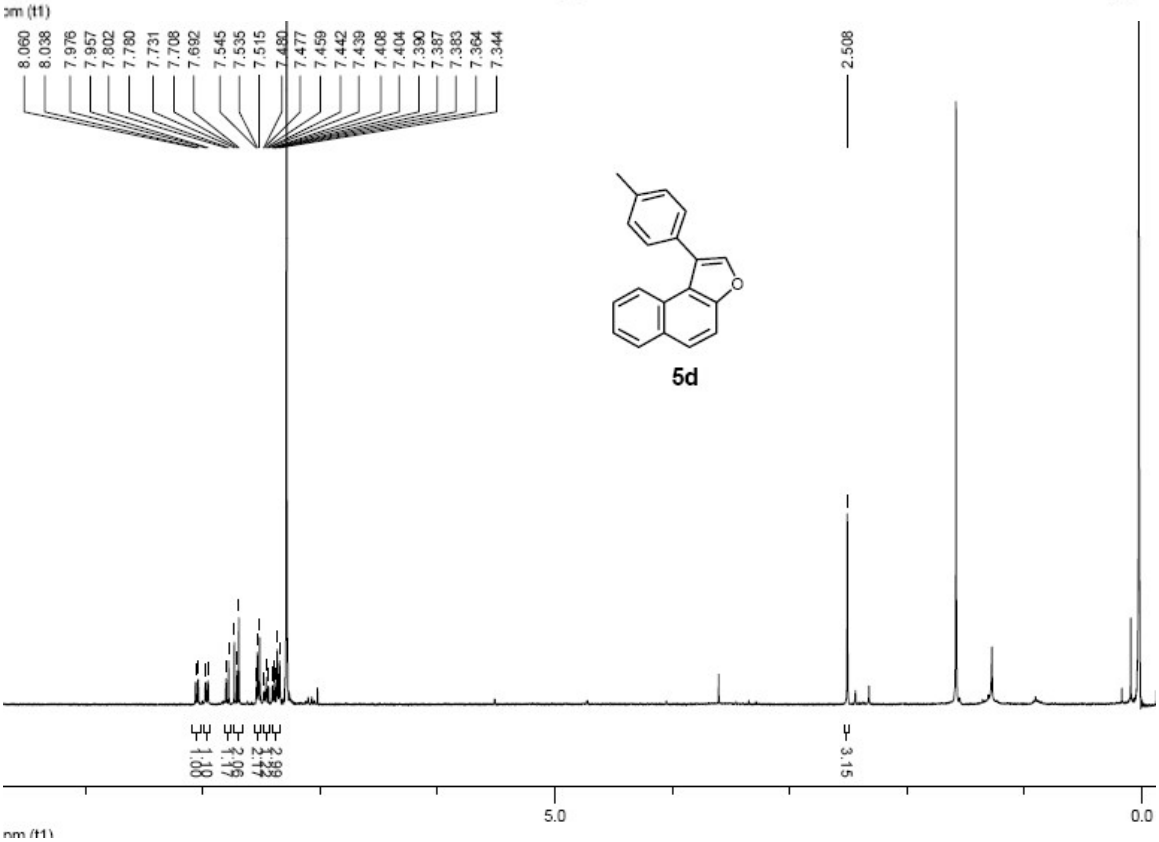

8.682
8.027
8.006
7.954
7.934
7.761
7.739
7.566
7.563
7.549
7.527
7.519
7.512
7.507
7.495
7.490
7.483
7.451
7.448
7.431
7.413
7.411
7.087
7.065
3.917
2.617
HN
OMe
3z
0.87
1.00
0.97
4.08
2.02
2.90
2.81
5.0
0.0
ppm (t1)

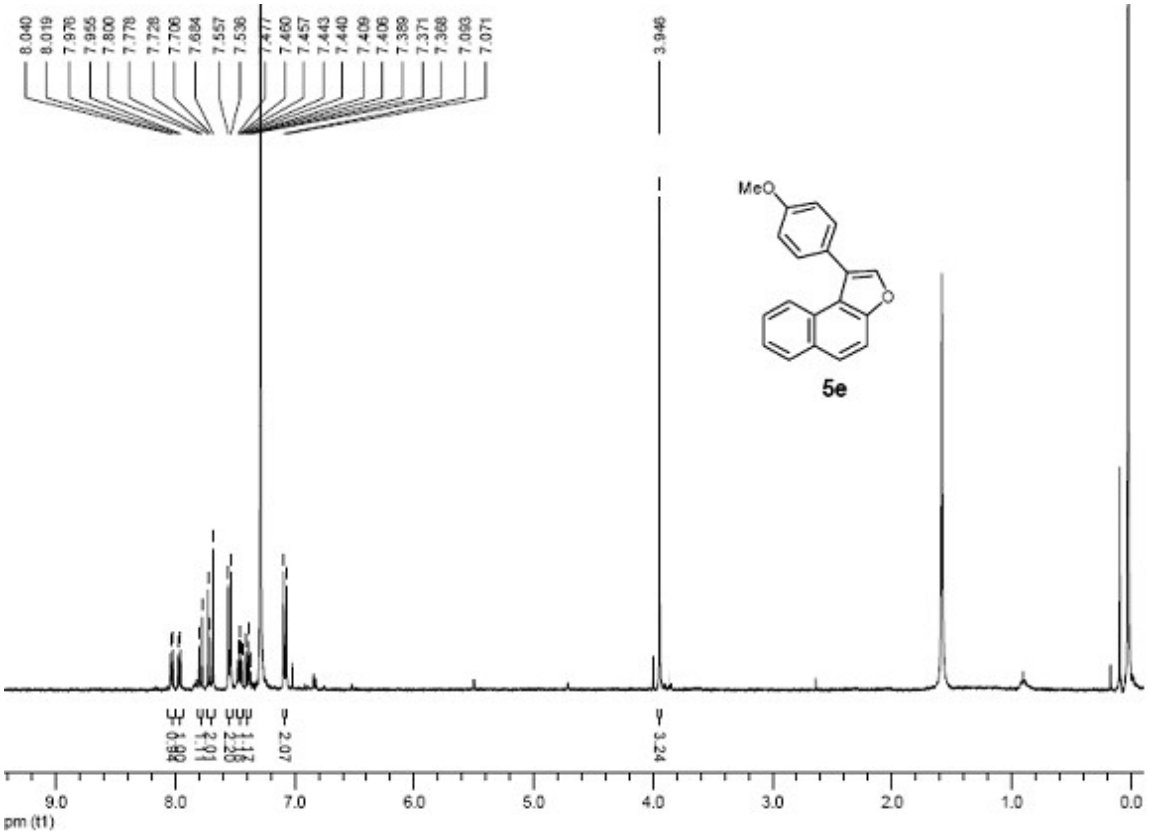

157.929
130.572
130.157
129.287
129.105
128.884
127.736
125.369
123.606
123.494
121.251
120.550
119.205
119.120
115.996
114.031
55.358
12.584
HN
OMe
3z
150
100
50
0
ppm (t1)

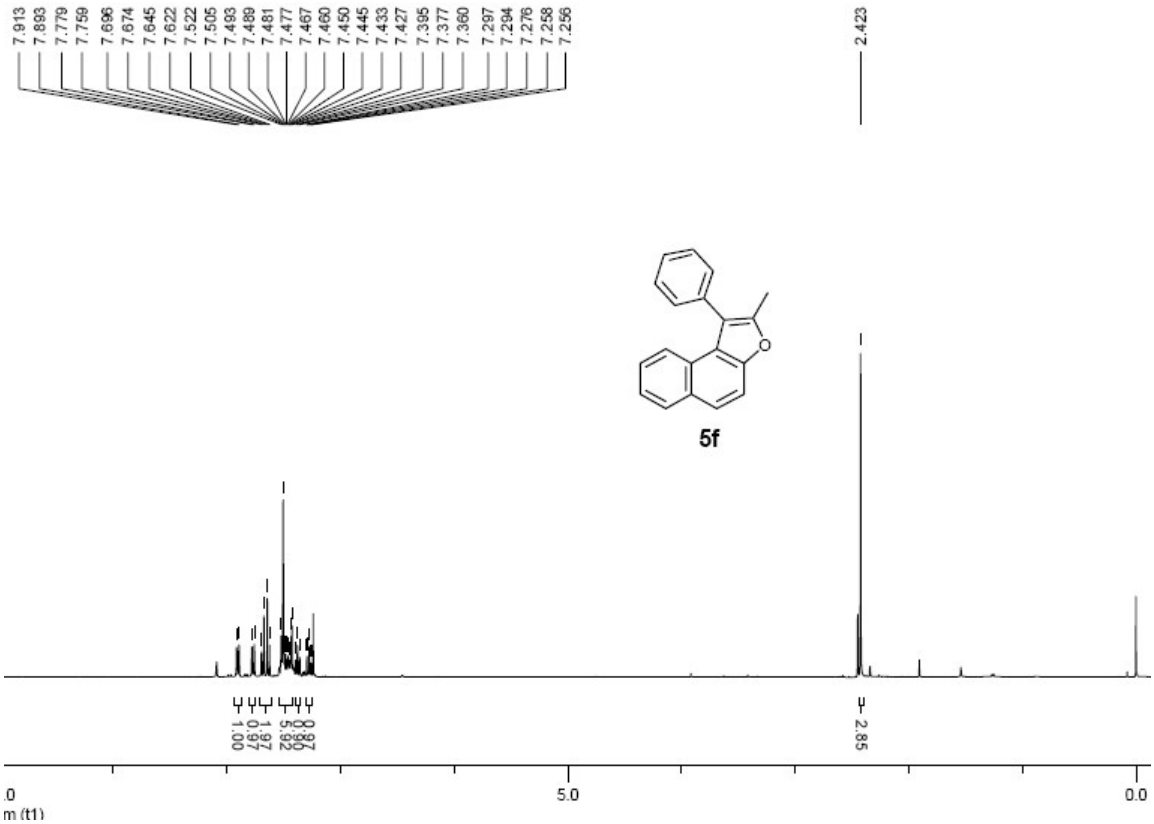

8.027
8.007
7.982
7.962
7.813
7.791
7.740
7.719
7.654
7.650
7.633
7.630
7.571
7.566
7.561
7.549
7.545
7.531
7.526
7.522
7.518
7.512
7.505
7.483
7.463
7.446
7.443
7.404
7.401
7.383
7.366
7.363
5a
10.0
5.0
0.0

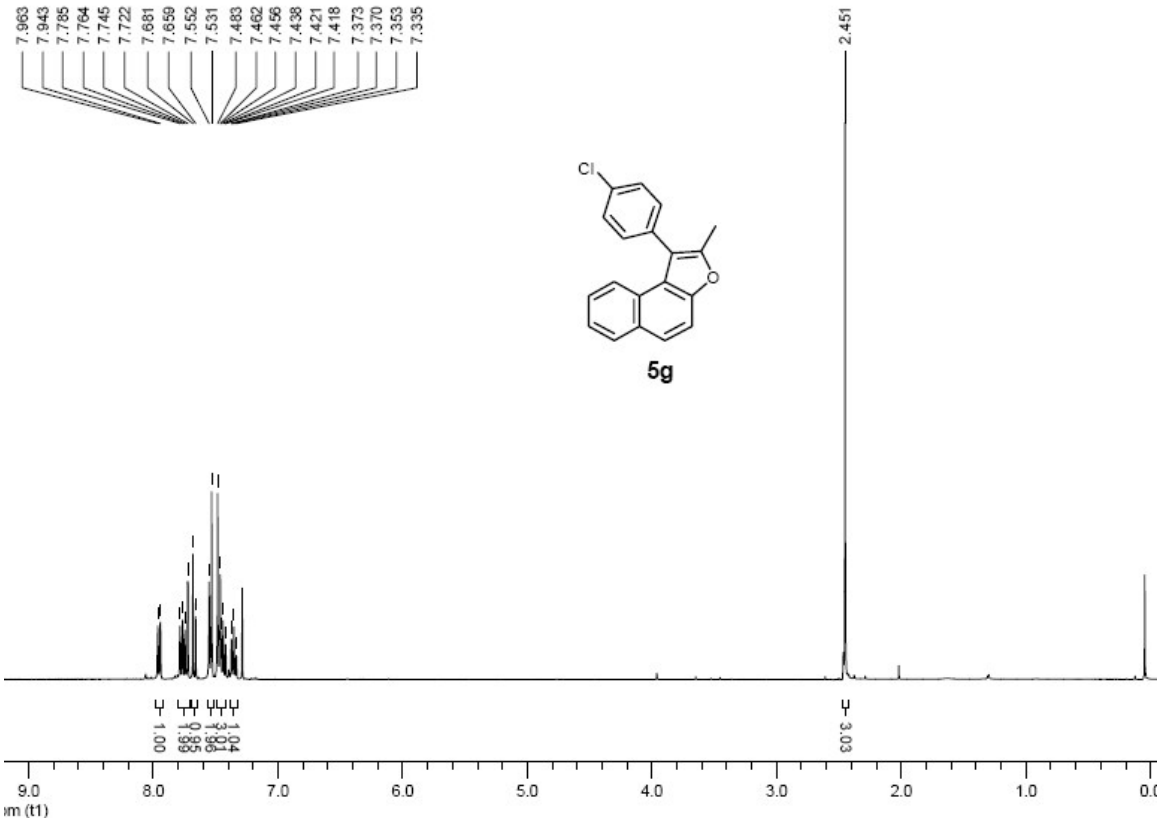

7.987
7.967
7.955
7.934
7.817
7.794
7.738
7.715
7.702
7.612
7.607
7.599
7.590
7.582
7.577
7.493
7.490
7.473
7.456
7.452
7.419
7.415
7.398
7.381
7.377
7.264
7.259
7.242
7.220
F
5b
0.0
5.0
0.0

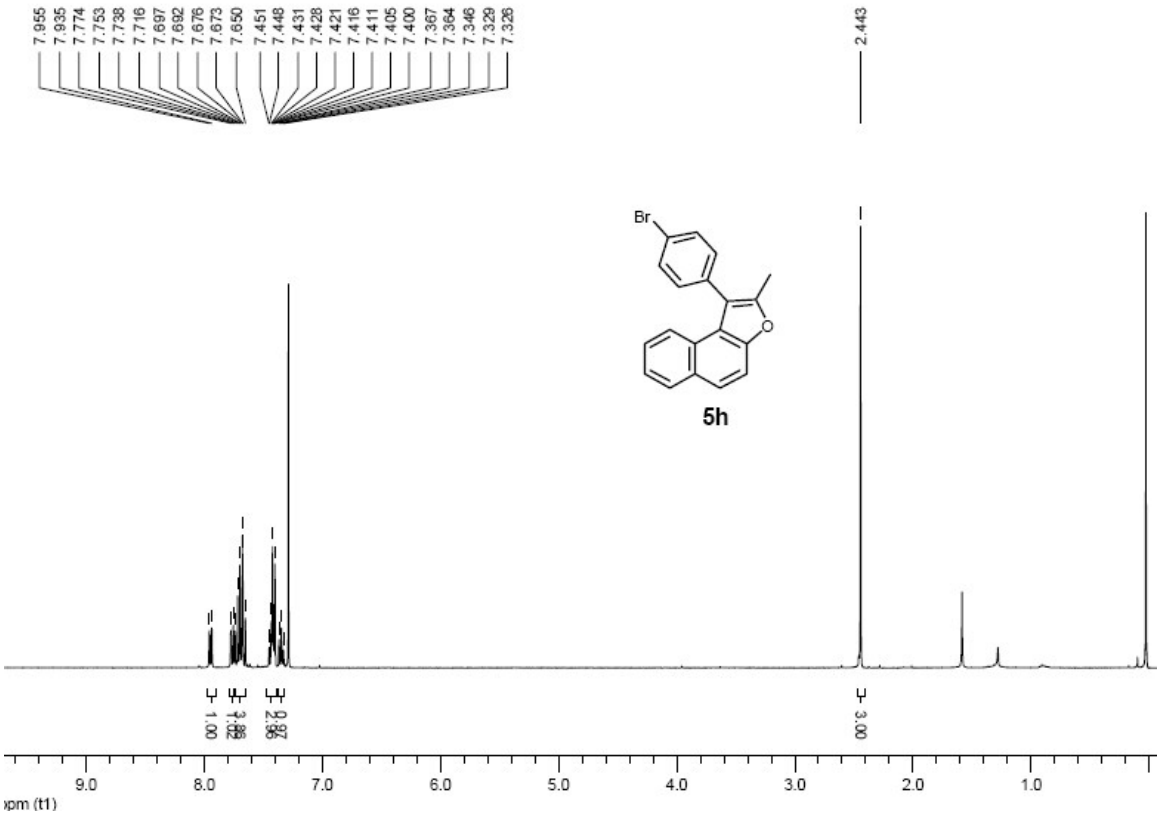

7.988
7.971
7.952
7.820
7.798
7.737
7.714
7.708
7.584
7.579
7.568
7.562
7.545
7.532
7.527
7.511
7.499
7.496
7.481
7.478
7.461
7.458
7.430
7.427
7.410
7.406
7.392
7.389
Cl
O
5c
2.00
6.98
10.0
5.0
0.0

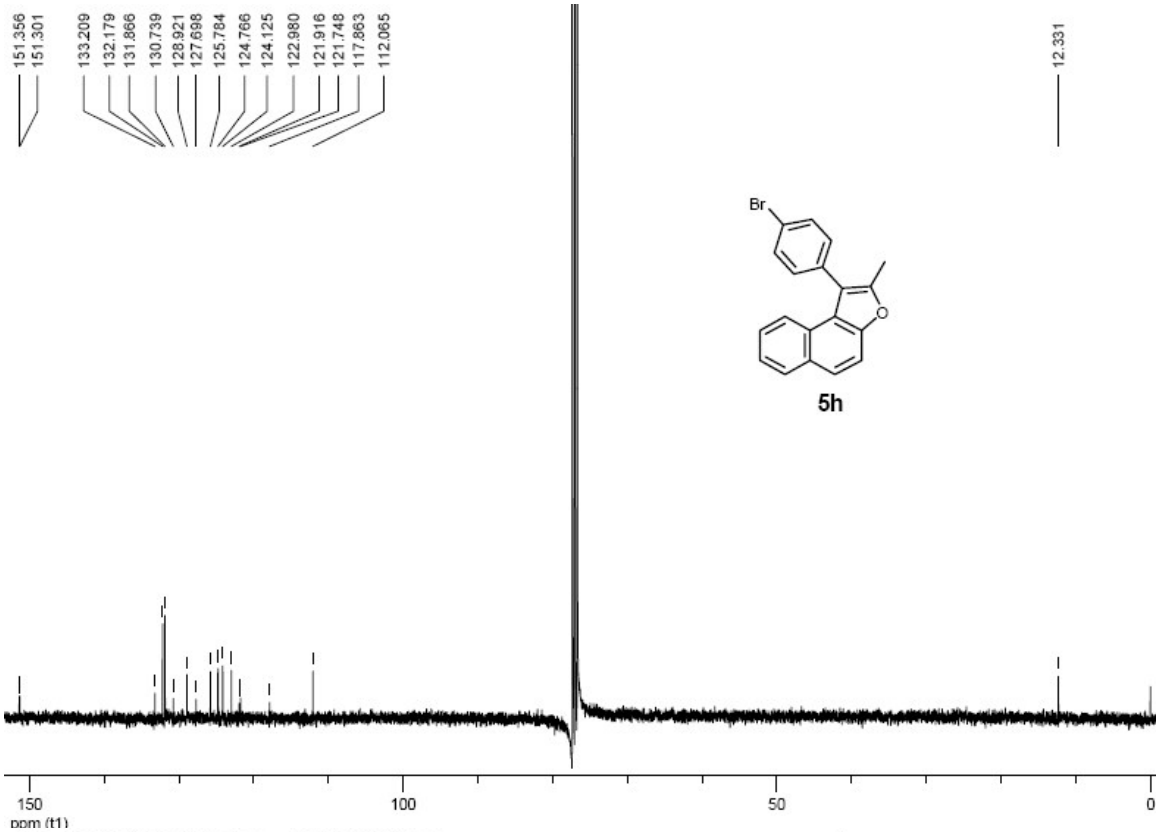

8.060
8.038
7.976
7.957
7.802
7.780
7.731
7.708
7.692
7.545
7.535
7.515
7.480
7.477
7.459
7.442
7.439
7.408
7.404
7.390
7.387
7.383
7.364
7.344
2.508
O
5d
1.00
1.18
7.79
2.44
2.88
3.15
5.0
0.0


8.040
8.019
7.976
7.955
7.800
7.778
7.728
7.706
7.684
7.557
7.536
7.460
7.457
7.443
7.440
7.409
7.406
7.389
7.371
7.368
7.093
7.071
3.946
MeO
O
5e
0.94
1.00
2.01
2.26
1.18
2.07
3.24
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
pm (t1)

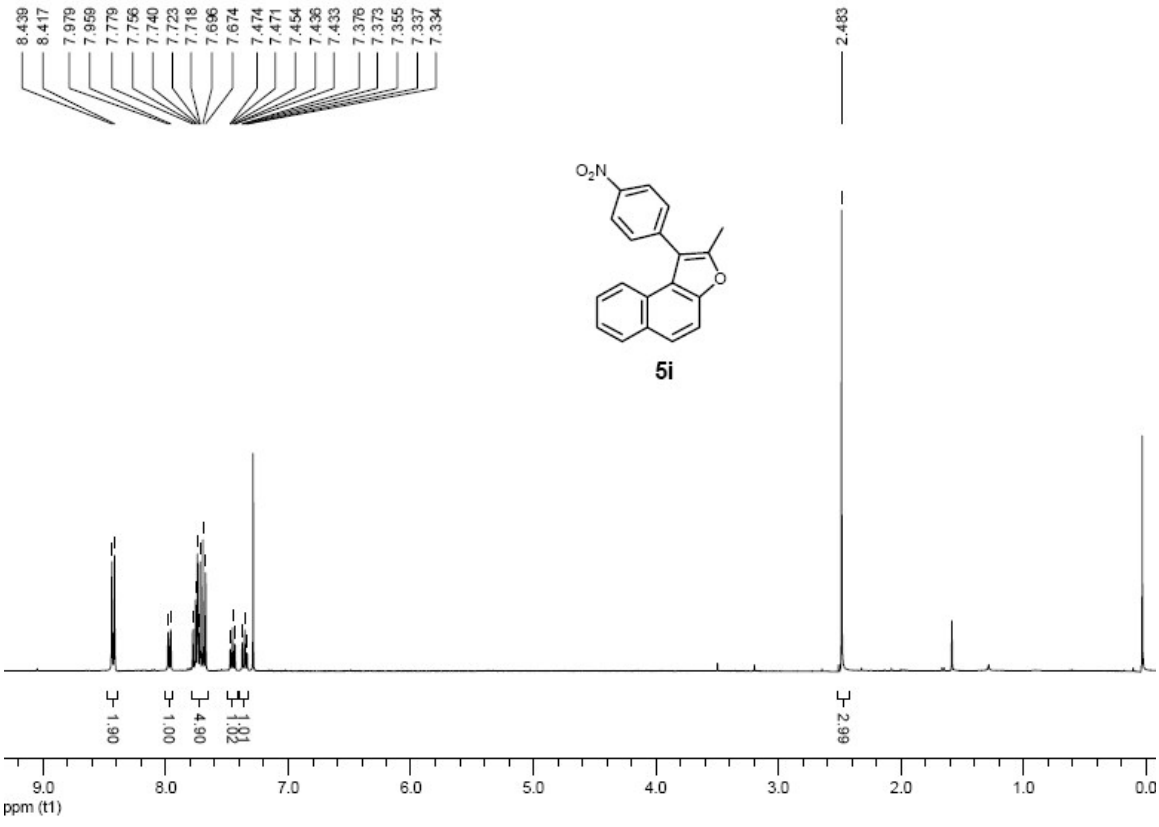

7.913
7.893
7.779
7.759
7.696
7.674
7.645
7.622
7.522
7.505
7.493
7.489
7.481
7.477
7.467
7.460
7.450
7.445
7.433
7.427
7.395
7.377
7.360
7.297
7.294
7.276
7.258
7.256
2.423
O
5f
0.97
1.00
0.97
5.92
0.90
2.85
.0
5.0
0.0
m (t1)


7.963
7.943
7.785
7.764
7.745
7.722
7.681
7.659
7.552
7.531
7.483
7.462
7.456
7.438
7.421
7.418
7.373
7.370
7.353
7.335
2.451
Cl
O
5g
1.00
1.96
0.98
1.96
1.01
1.04
3.03
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

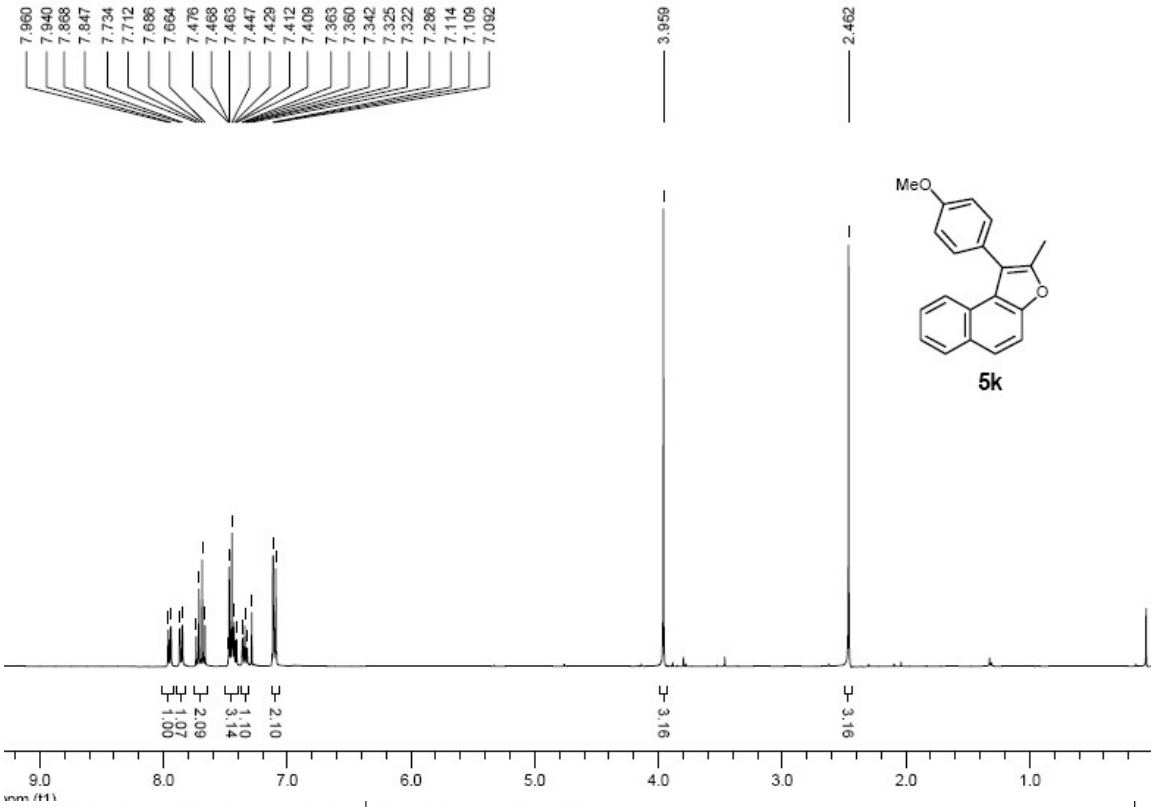

7.955
7.935
7.774
7.753
7.738
7.716
7.697
7.692
7.676
7.673
7.650
7.451
7.448
7.431
7.428
7.421
7.416
7.411
7.405
7.400
7.367
7.364
7.346
7.329
7.326
2.443
Br
O
5h
1.00
1.88
2.98
3.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)

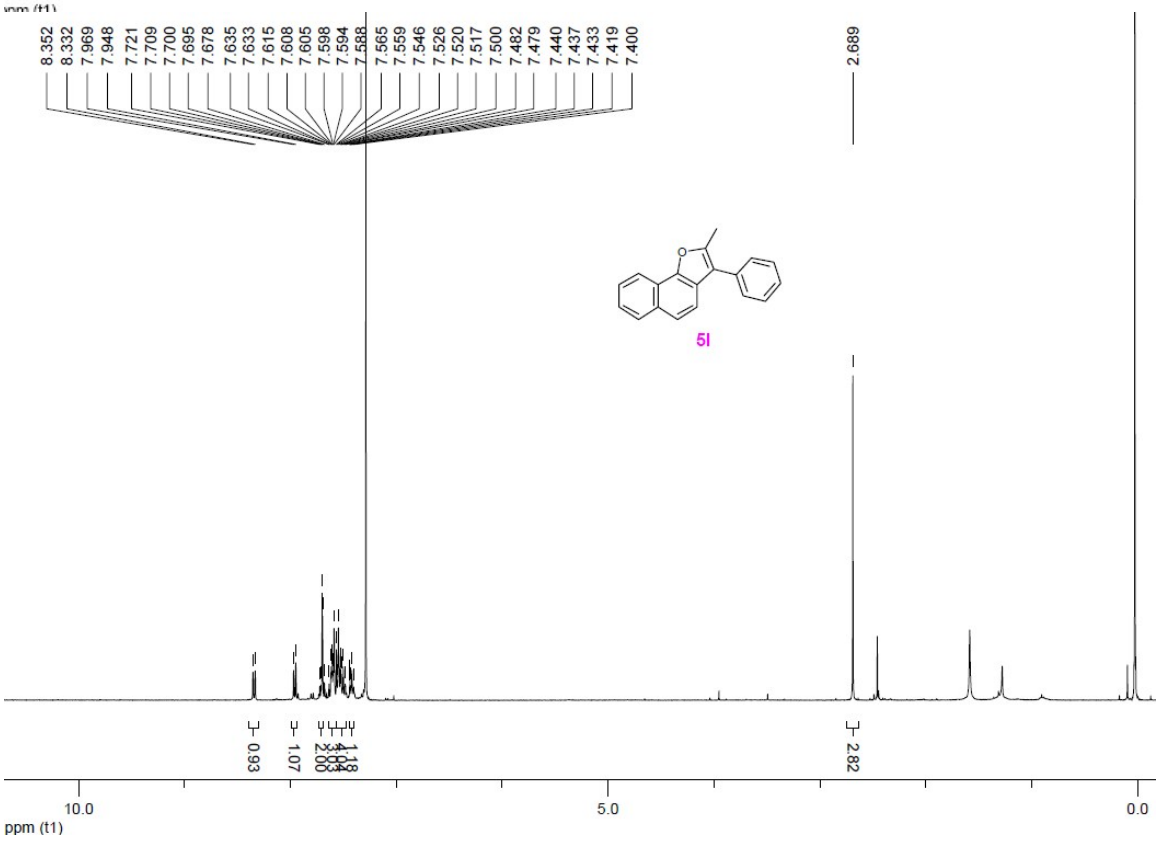

151.356
151.301
133.209
132.179
131.866
130.739
128.921
127.698
125.784
124.766
124.125
122.980
121.916
121.748
117.863
112.065
12.331
Br
O
150
100
50
0
ppm (t1)

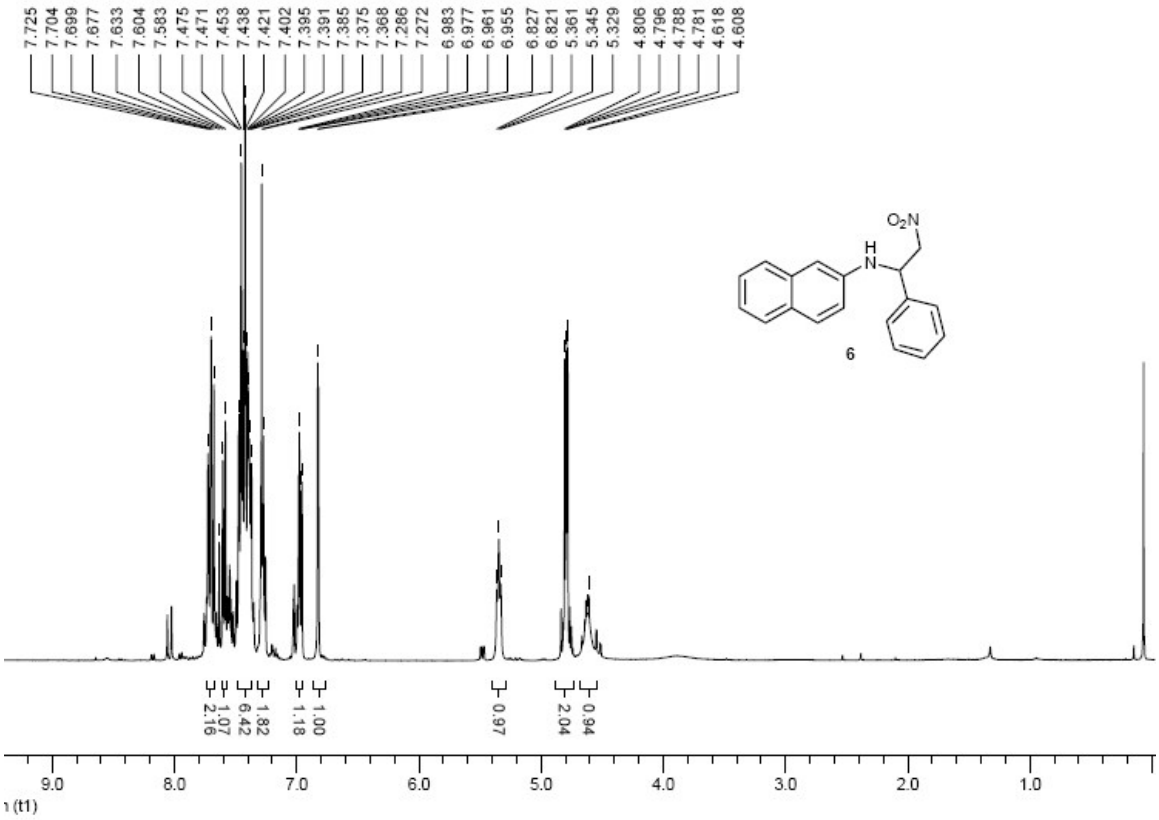
5h

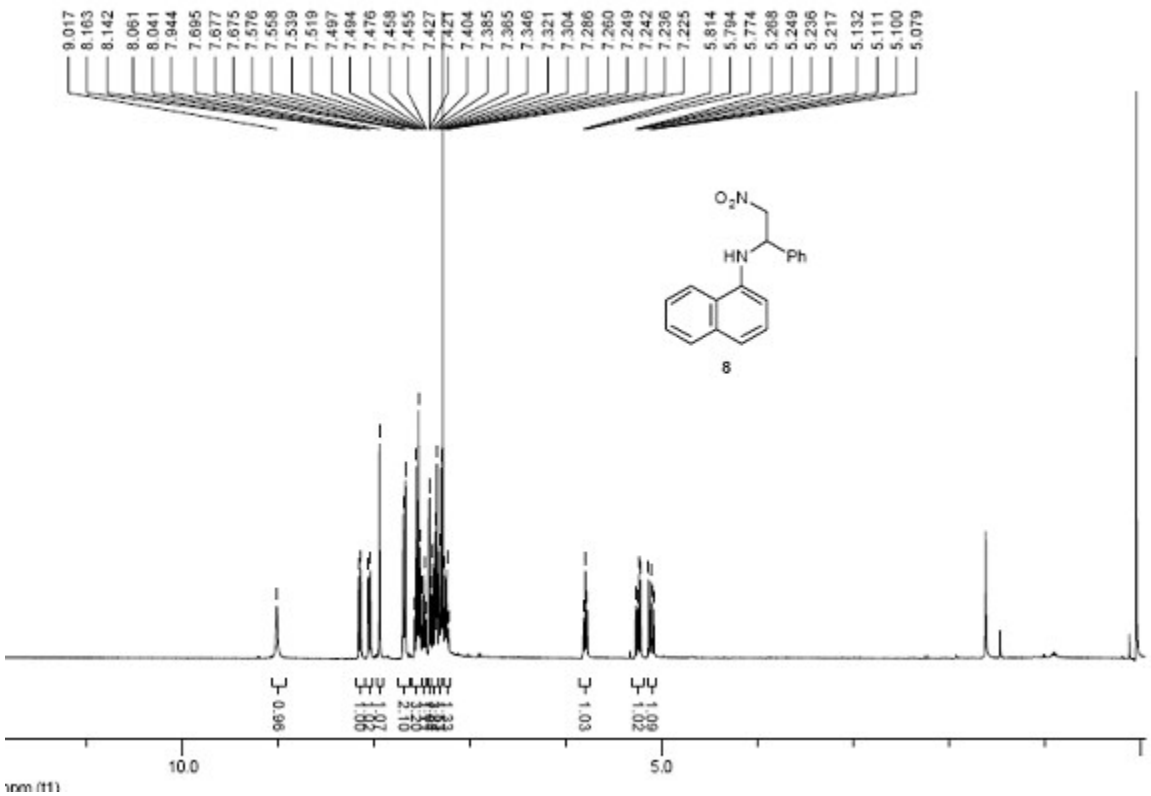

8.439
8.417
7.979
7.959
7.779
7.756
7.740
7.723
7.718
7.696
7.674
7.474
7.471
7.454
7.436
7.433
7.376
7.373
7.355
7.337
7.334
2.483
O2N
O
1.90
1.00
4.90
2.01
2.99
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

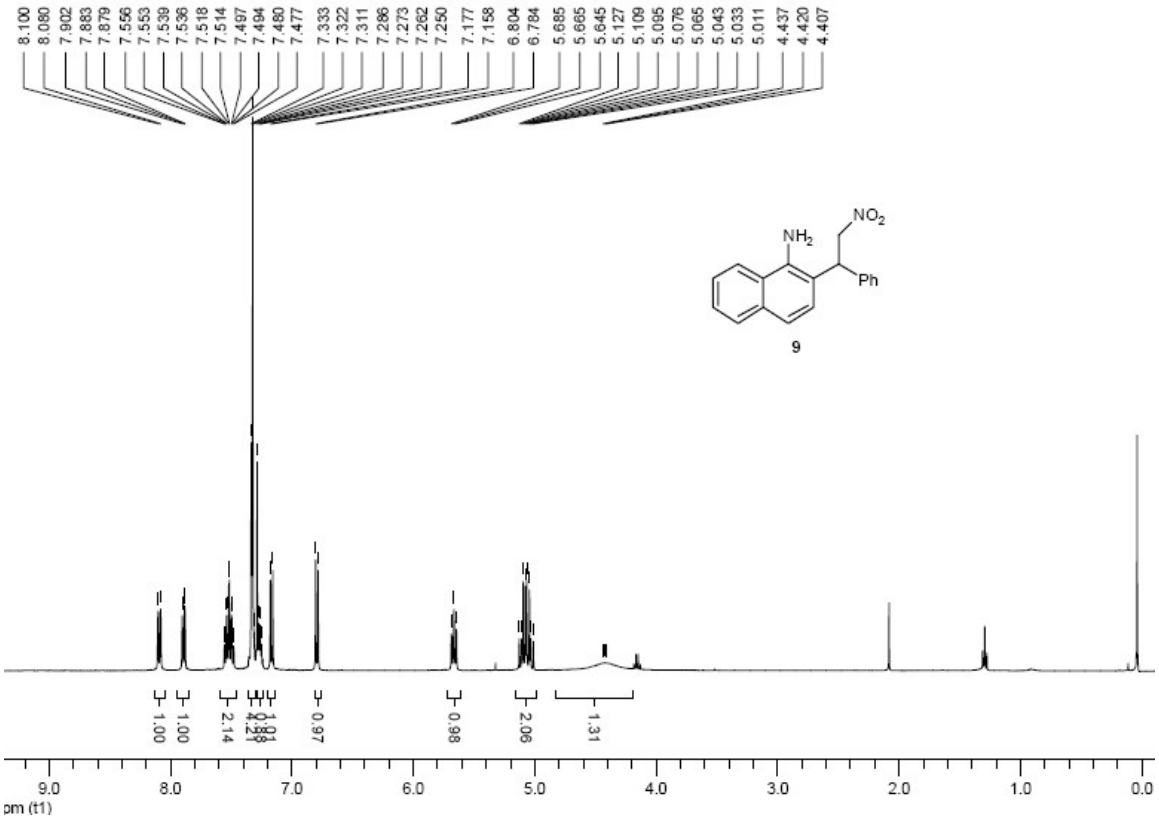
5i


7.960
7.940
7.868
7.847
7.734
7.712
7.686
7.664
7.476
7.468
7.463
7.447
7.429
7.412
7.409
7.363
7.360
7.342
7.325
7.322
7.286
7.114
7.109
7.092
3.959
2.462
MeO
5k
1.00
1.07
2.09
3.14
1.10
2.10
3.16
3.16
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0


8.352
8.332
7.969
7.948
7.721
7.709
7.700
7.695
7.678
7.635
7.633
7.615
7.608
7.605
7.598
7.594
7.588
7.565
7.559
7.546
7.526
7.520
7.517
7.500
7.482
7.479
7.440
7.437
7.433
7.419
7.400
2.689
5l
0.93
1.07
2.00
2.82
10.0
5.0
0.0
ppm (t1)


7.725
7.704
7.699
7.677
7.633
7.604
7.583
7.475
7.471
7.453
7.438
7.421
7.402
7.395
7.391
7.385
7.375
7.368
7.286
7.272
6.983
6.977
6.961
6.955
6.827
6.821
5.361
5.345
5.329
4.806
4.796
4.788
4.781
4.618
4.608
2.16
1.07
6.42
1.82
1.18
1.00
0.97
2.04
0.94
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
(t1)


9.017
8.163
8.142
8.061
8.041
7.944
7.695
7.677
7.675
7.576
7.558
7.539
7.519
7.497
7.494
7.476
7.458
7.455
7.427
7.421
7.404
7.385
7.365
7.346
7.321
7.304
7.286
7.260
7.249
7.242
7.236
7.225
5.814
5.794
5.774
5.268
5.249
5.236
5.217
5.132
5.111
5.100
5.079
0.96
1.02
1.00
2.10
1.03
1.02
10.0
5.0


8.100
8.080
7.902
7.883
7.879
7.556
7.553
7.539
7.536
7.518
7.514
7.497
7.494
7.480
7.477
7.333
7.322
7.311
7.286
7.273
7.262
7.250
7.177
7.158
6.804
6.784
5.685
5.665
5.645
5.127
5.109
5.095
5.076
5.065
5.043
5.033
5.011
4.437
4.420
4.407
NO2
NH2
Ph
9
1.00
1.00
2.14
0.98
0.67
0.98
2.06
1.31
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)