

Synthesis of Benzo[a]carbazoles via Cyanide-catalyzed Imino-Stetter Reaction/ Friedel-Crafts Reaction Sequence

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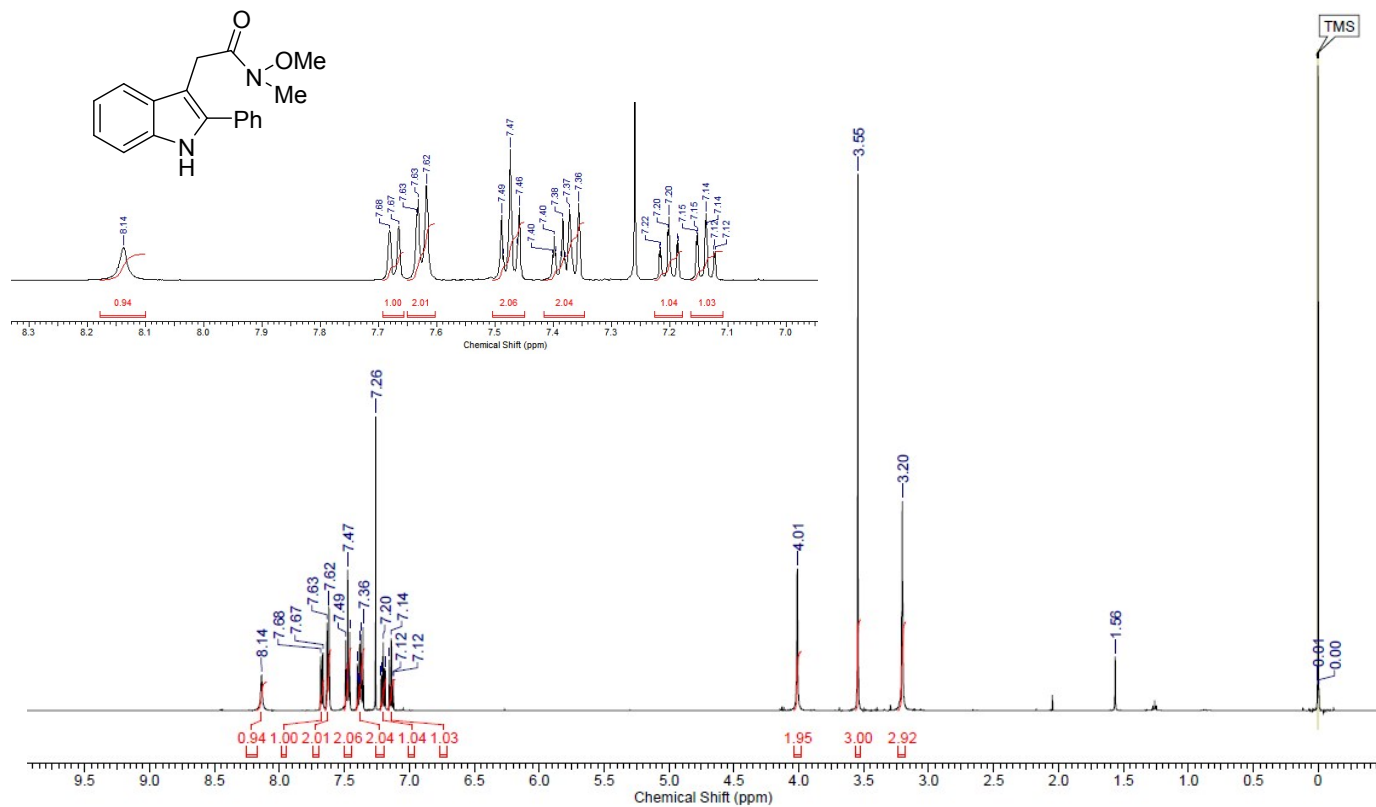
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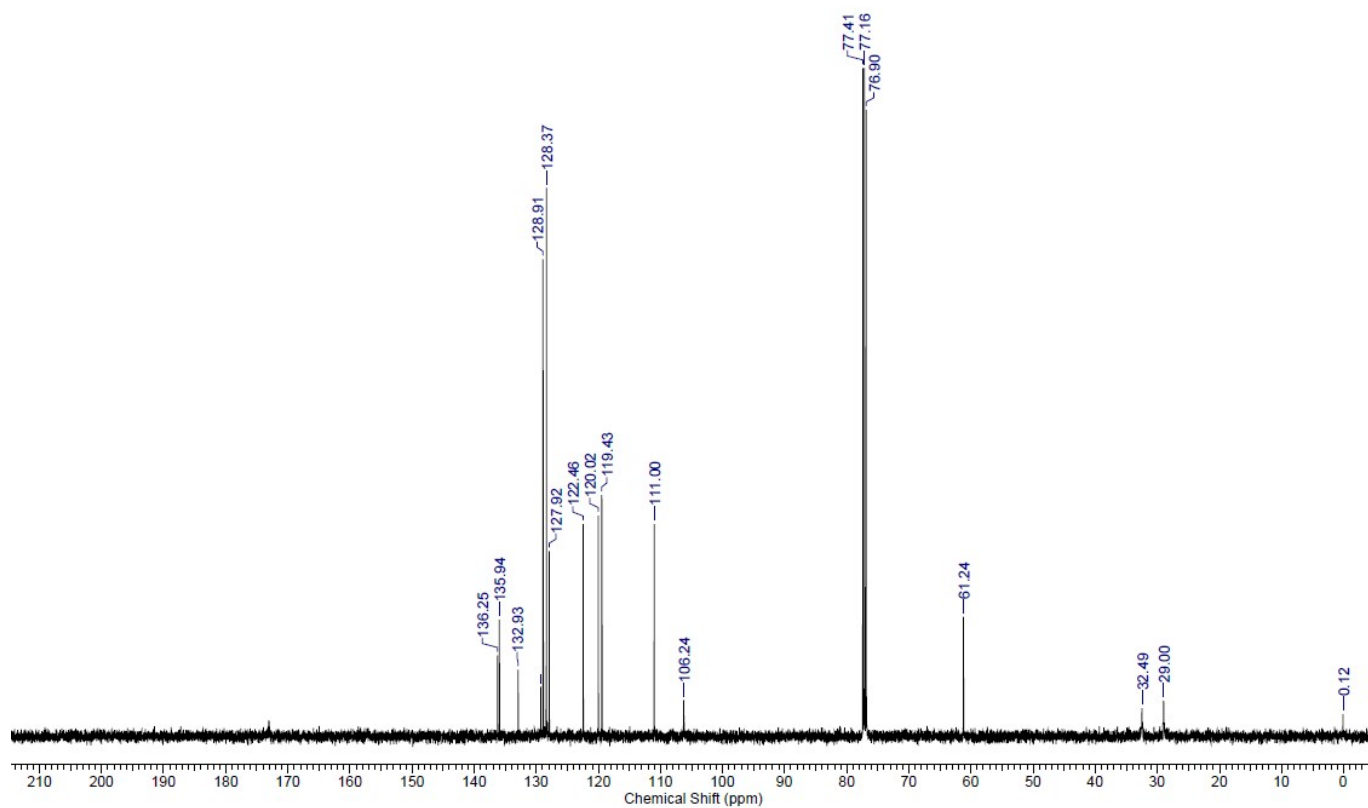
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1. Spectroscopic Data of *N*-Methoxy-*N*-methyl-2-(2-phenyl-1*H*-indol-3-yl)acetamide (**3**)

a) ¹H NMR Spectrum (500 MHz, CDCl₃)



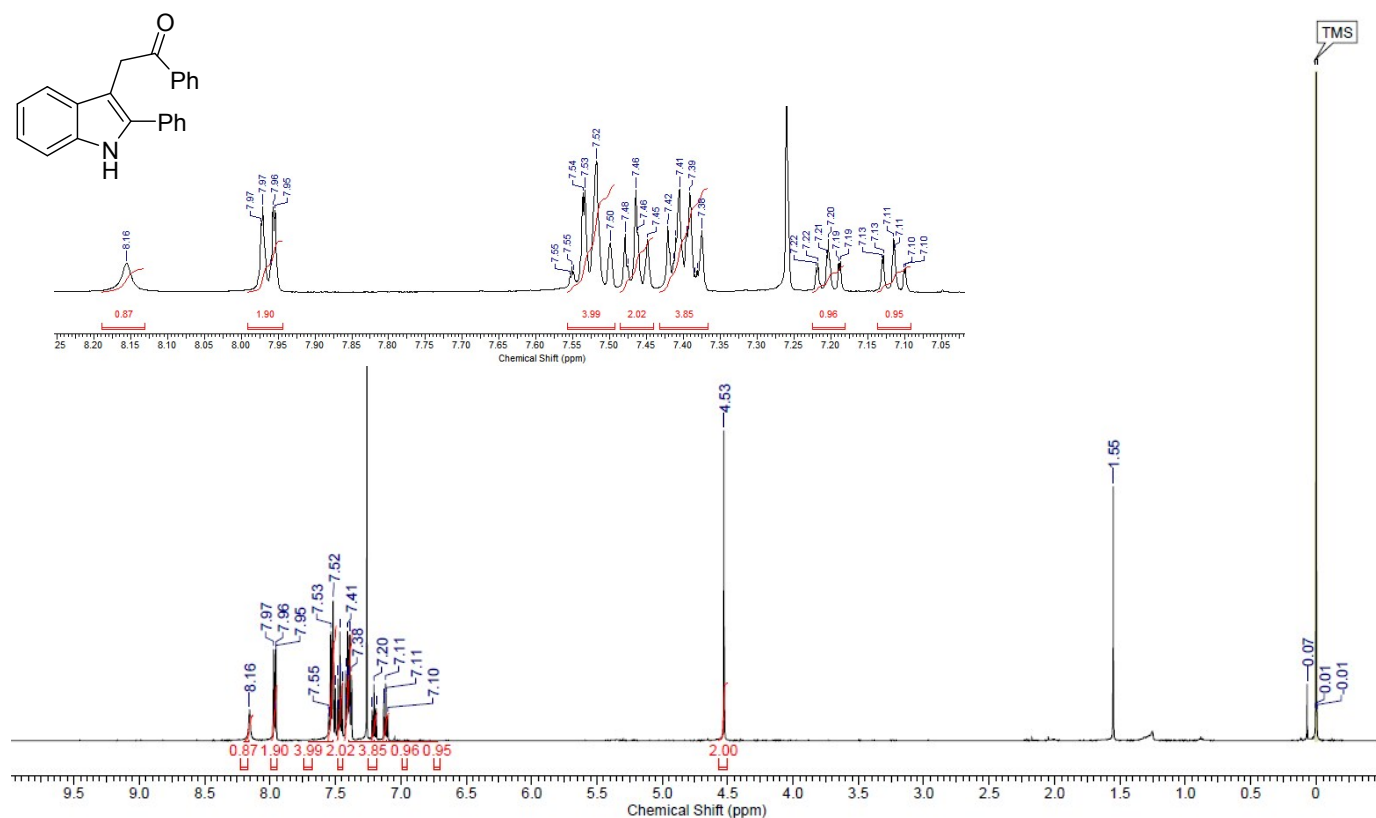
b) ¹³C NMR Spectrum (125 MHz, CDCl₃)



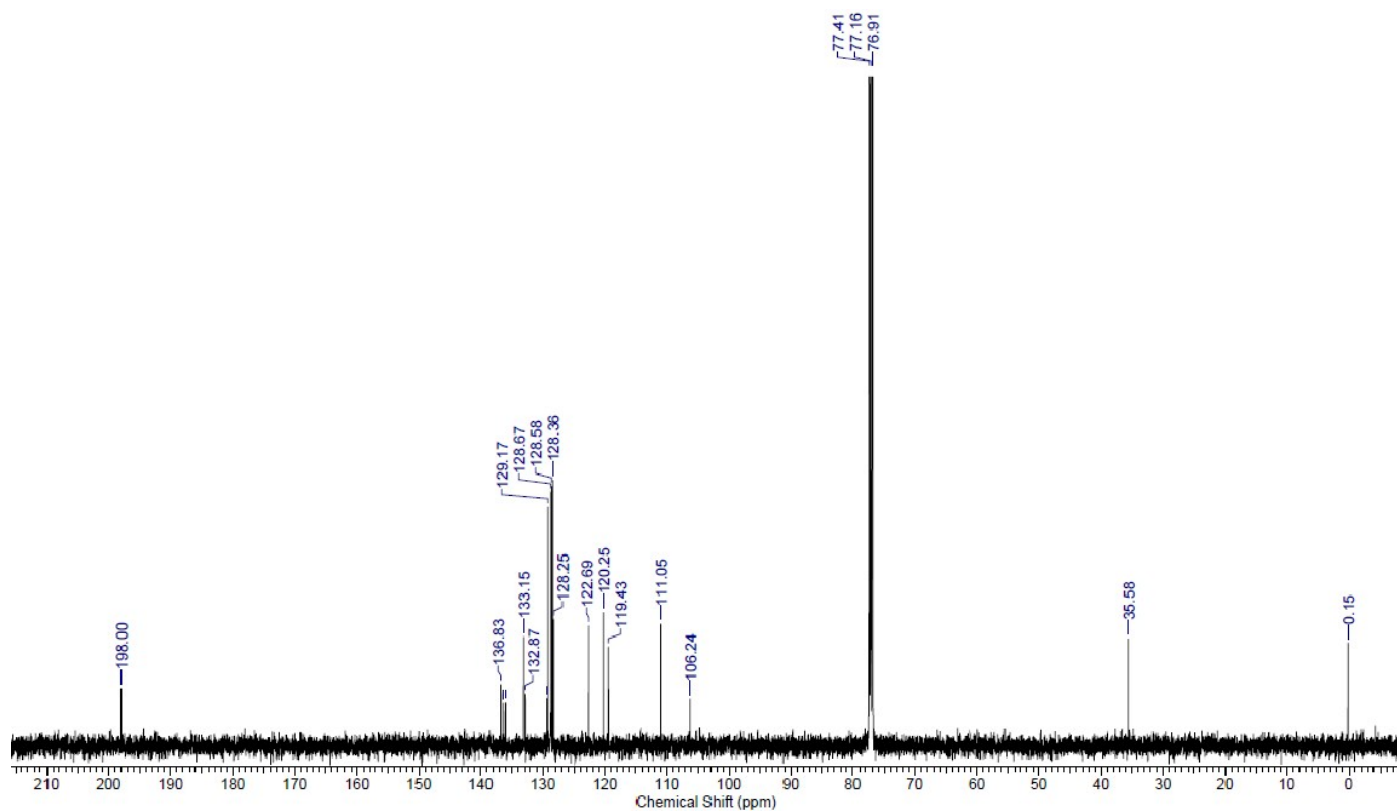
2. Spectroscopic Data of 2-Aryl-3-arenacylindole Derivatives (2)

2-1. NMR Spectra of 2-Phenyl-3-phenacylindole (2a)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

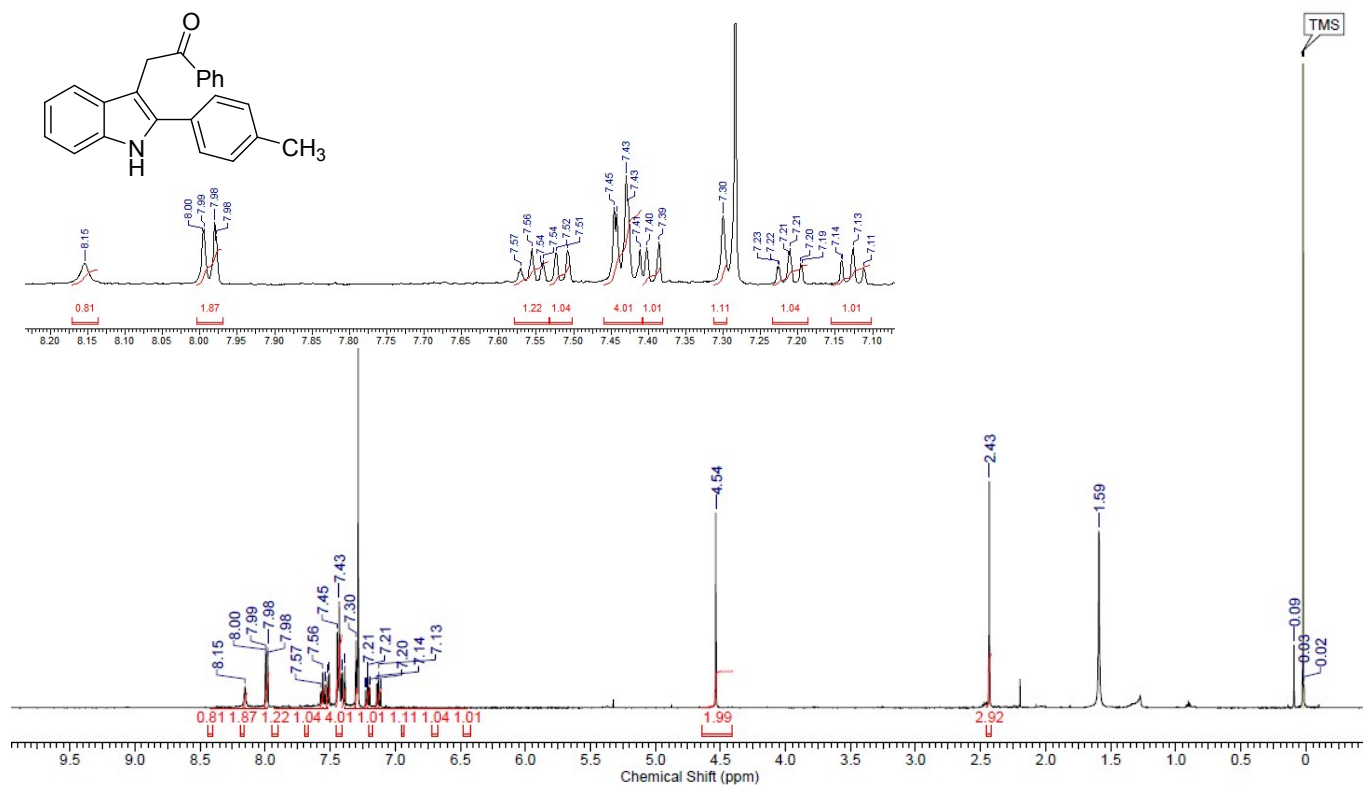


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

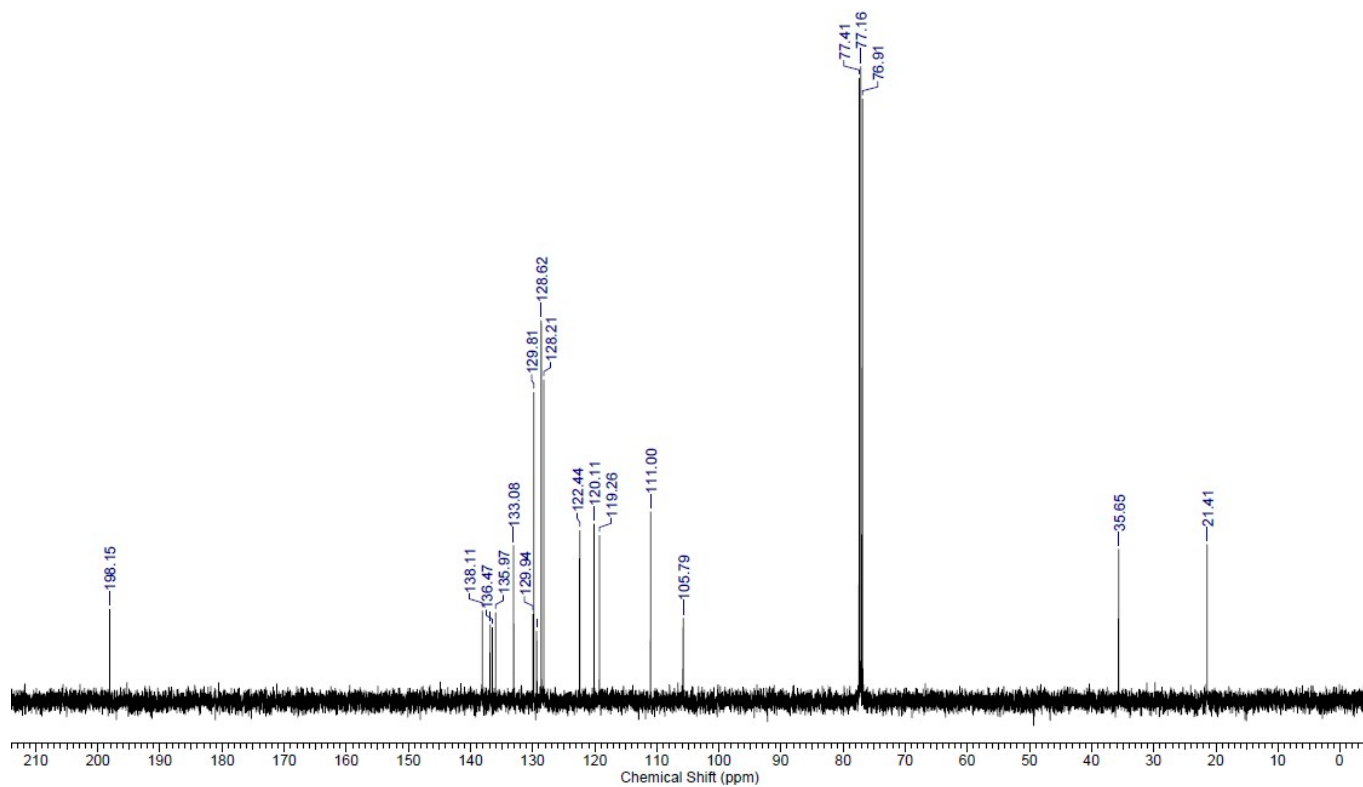


2-2. NMR Spectra of 2-(4-Methylphenyl)-3-phenacylindole (**2b**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

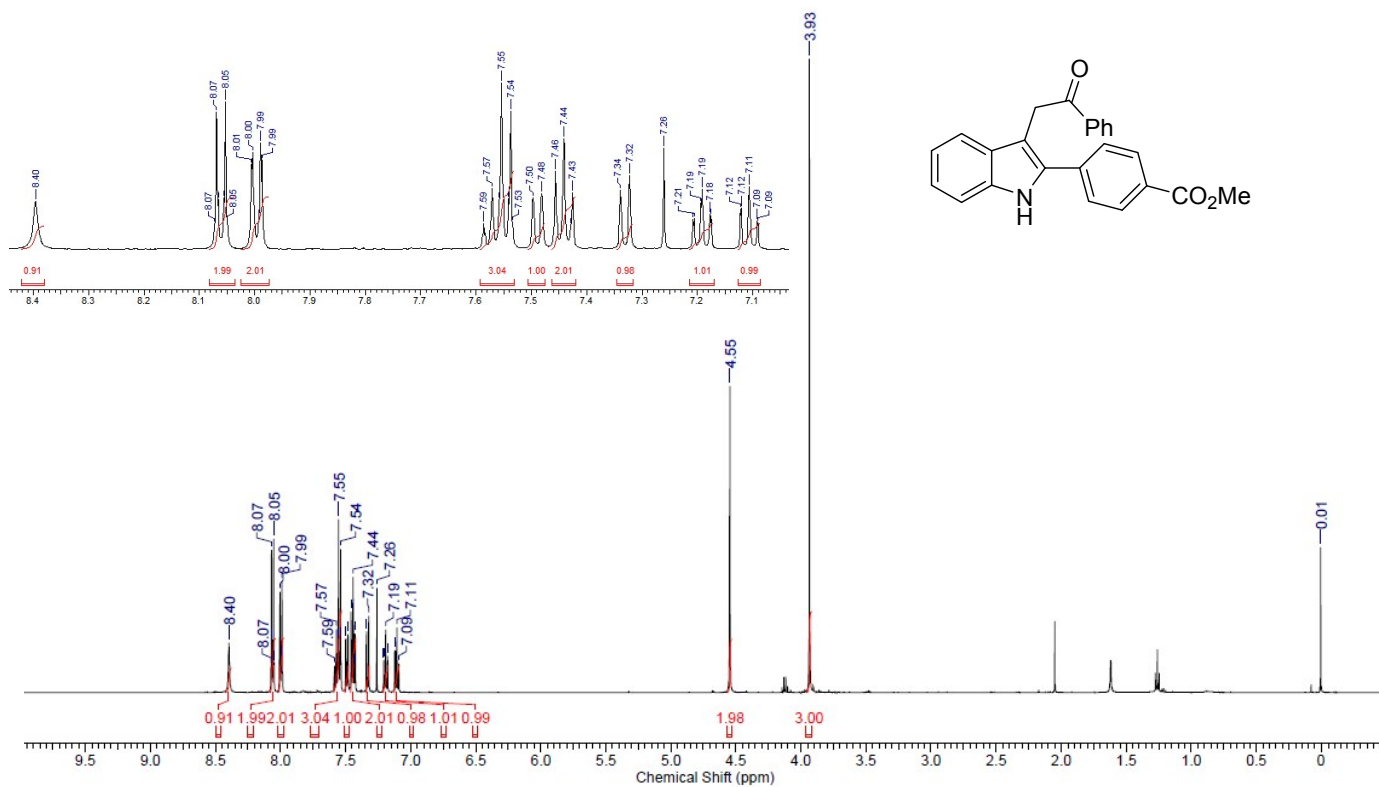


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

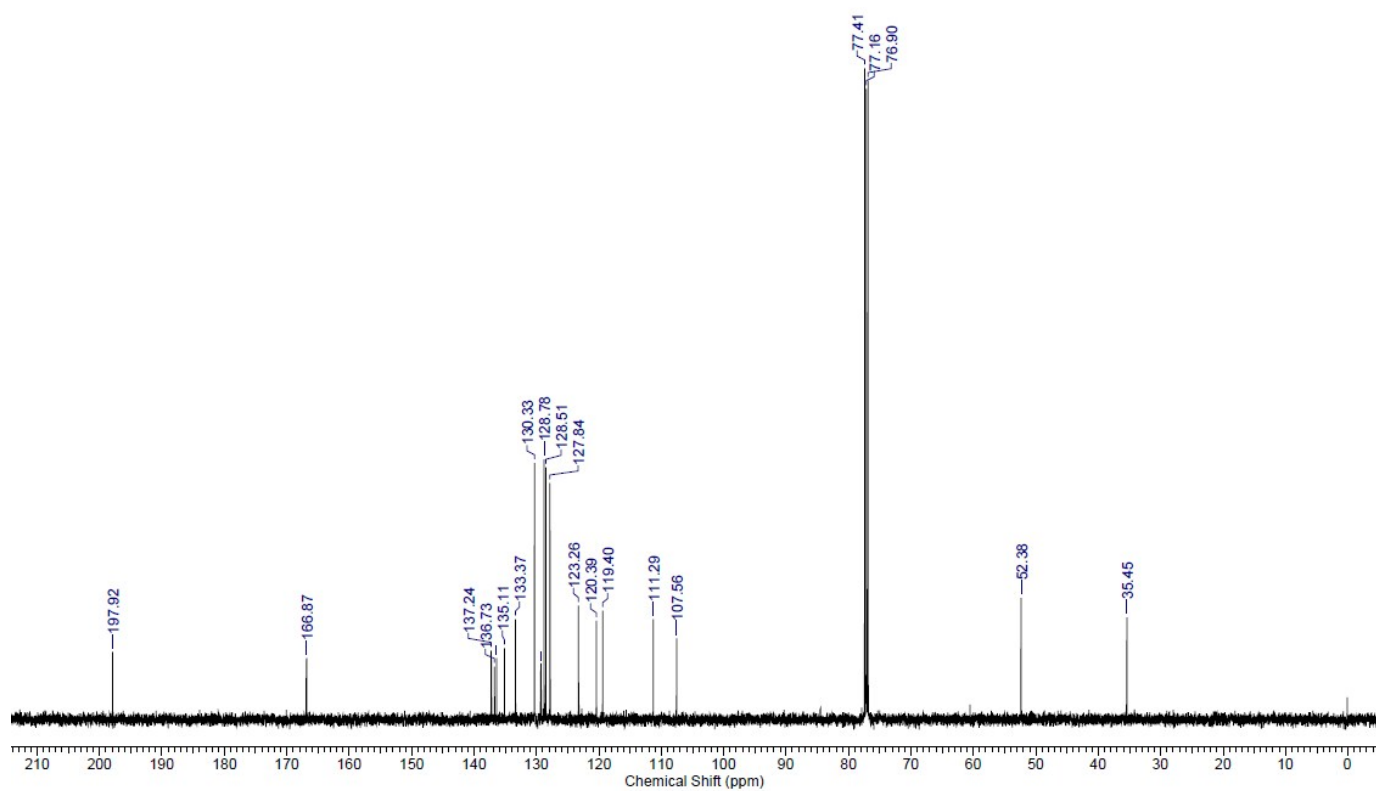


2-3. NMR Spectra of 2-(4-Methoxycarbonylphenyl)-3-phenacylindole (**2c**)

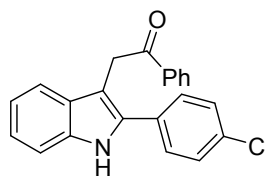
a) ^1H NMR Spectrum (500 MHz, CDCl_3)



b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)



a) ^1H NMR Spectrum (500 MHz, CDCl_3)

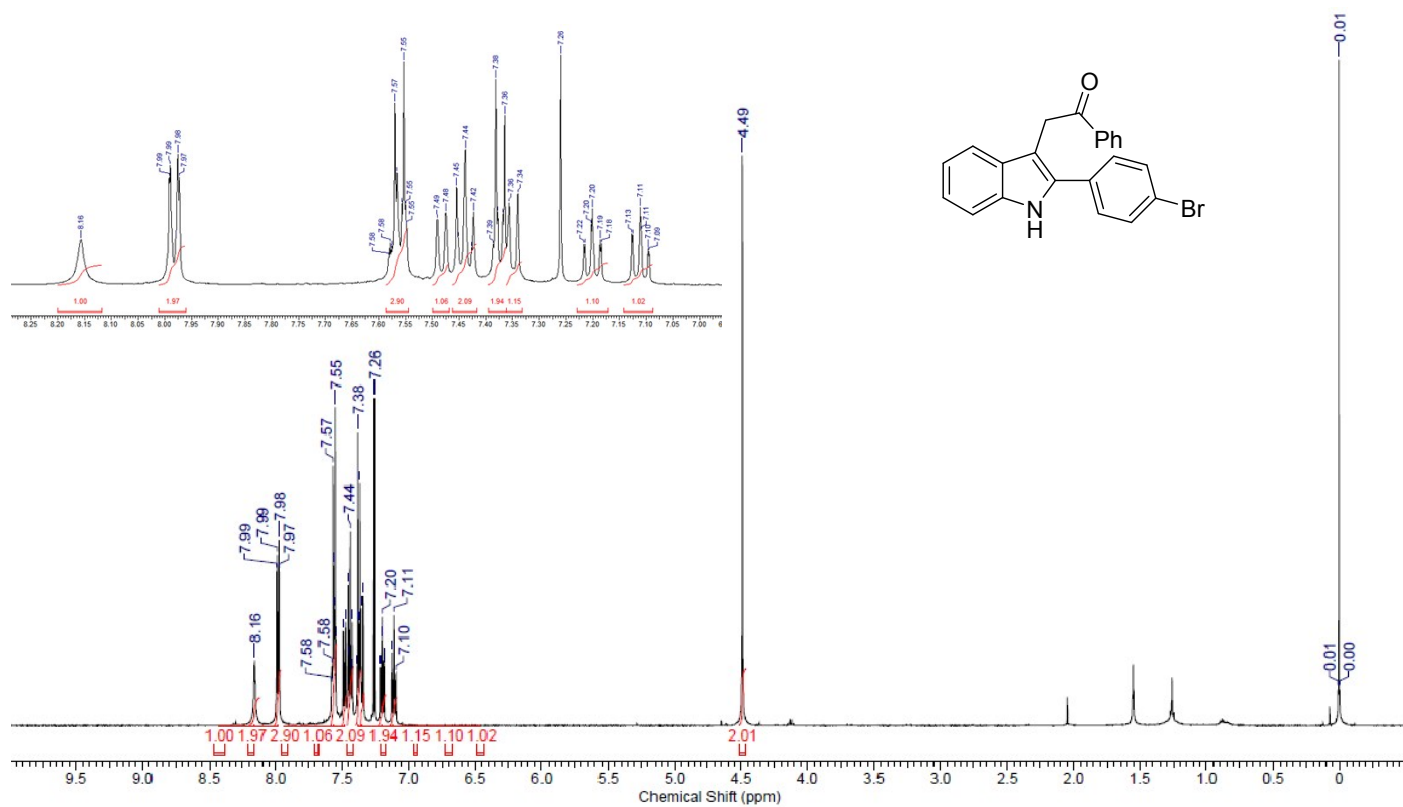


Chemical Shift (ppm)

198.14, 136.75, 135.18, 133.34, 131.22, 129.39, 129.27, 128.76, 128.51, 122.87, 120.27, 119.18, 111.20, 106.52, 77.41, 77.16, 76.91, 35.34, -0.14

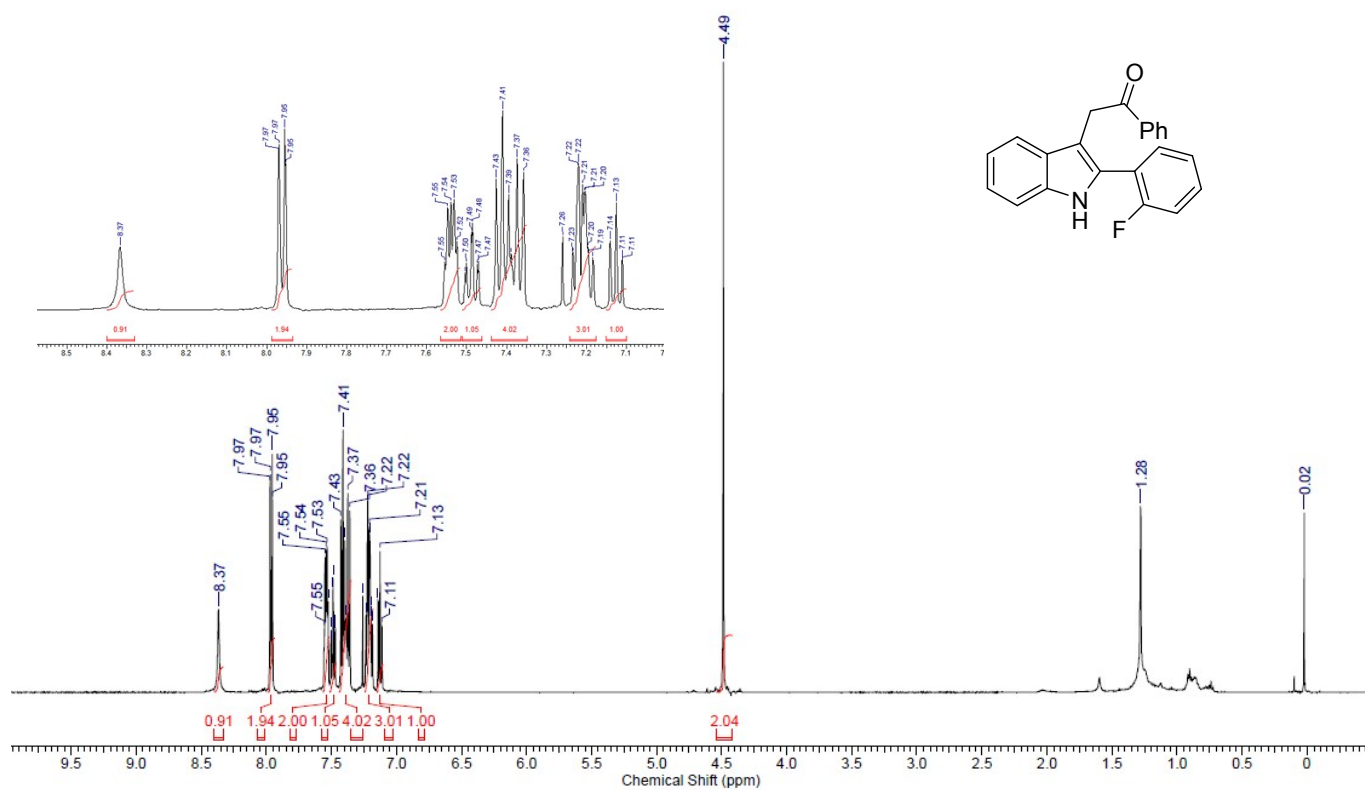
2-5. NMR Spectra of 2-(4-Bromophenyl)-3-phenacylindole (**2e**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

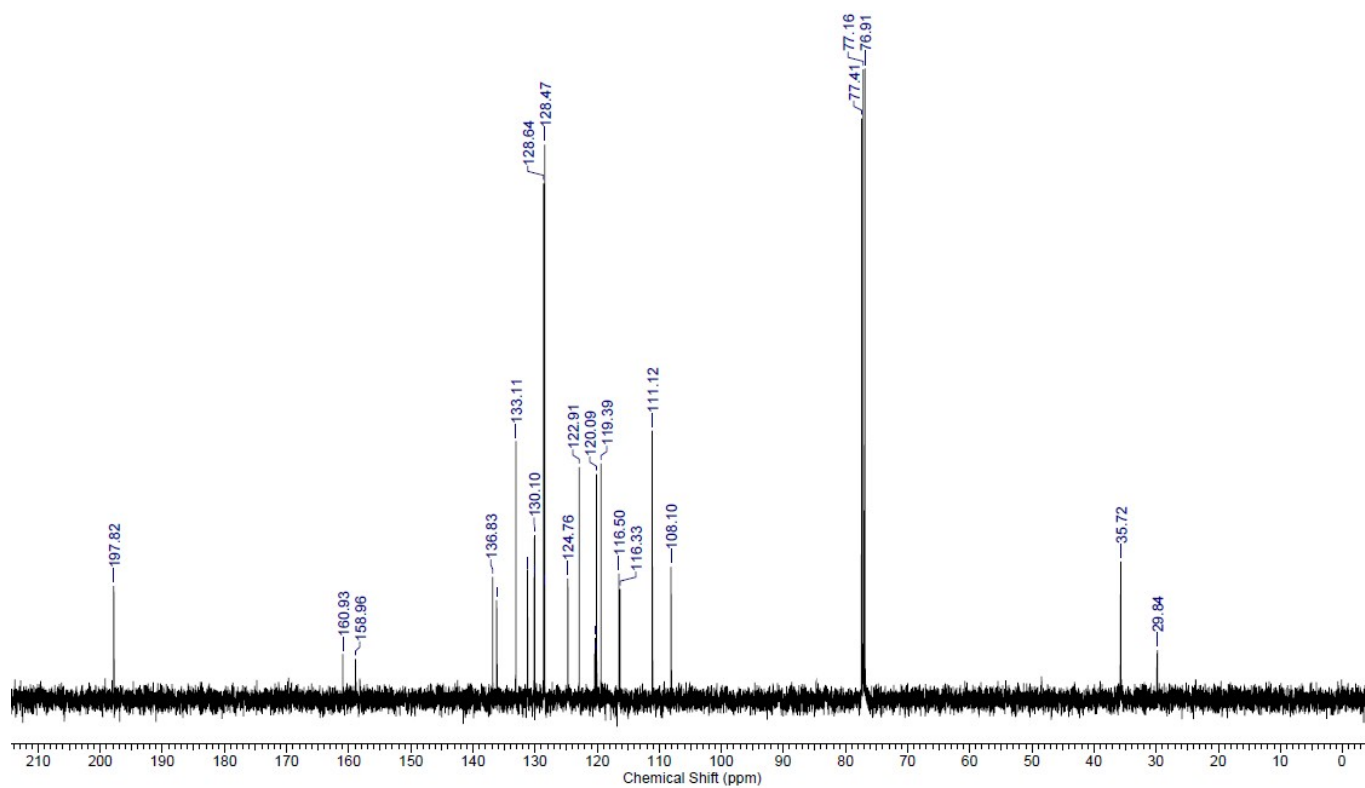


2-6. NMR Spectra of 2-(2-Fluorophenyl)-3-phenacylindole (**2f**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

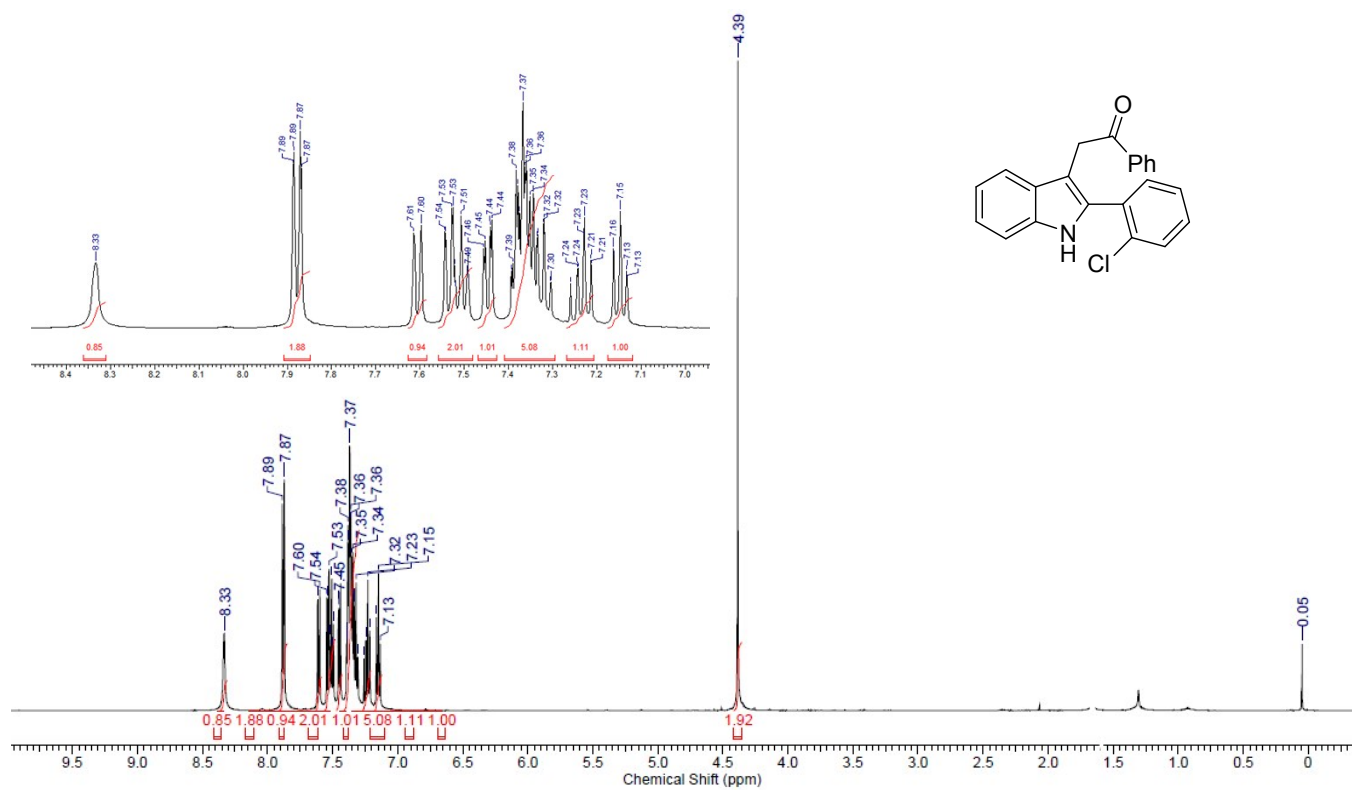


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

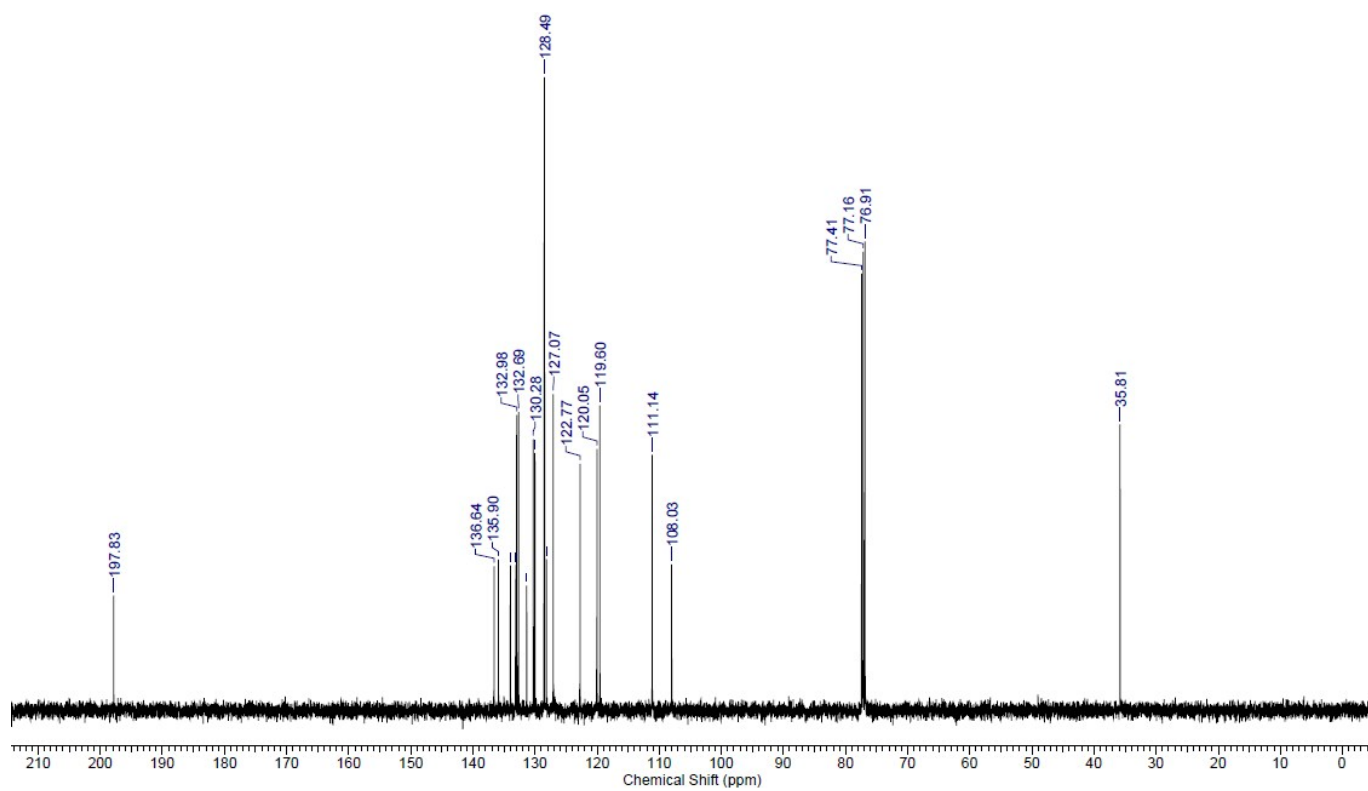


2-7. NMR Spectra of 2-(2-Chlorophenyl)-3-phenacylindole (**2g**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

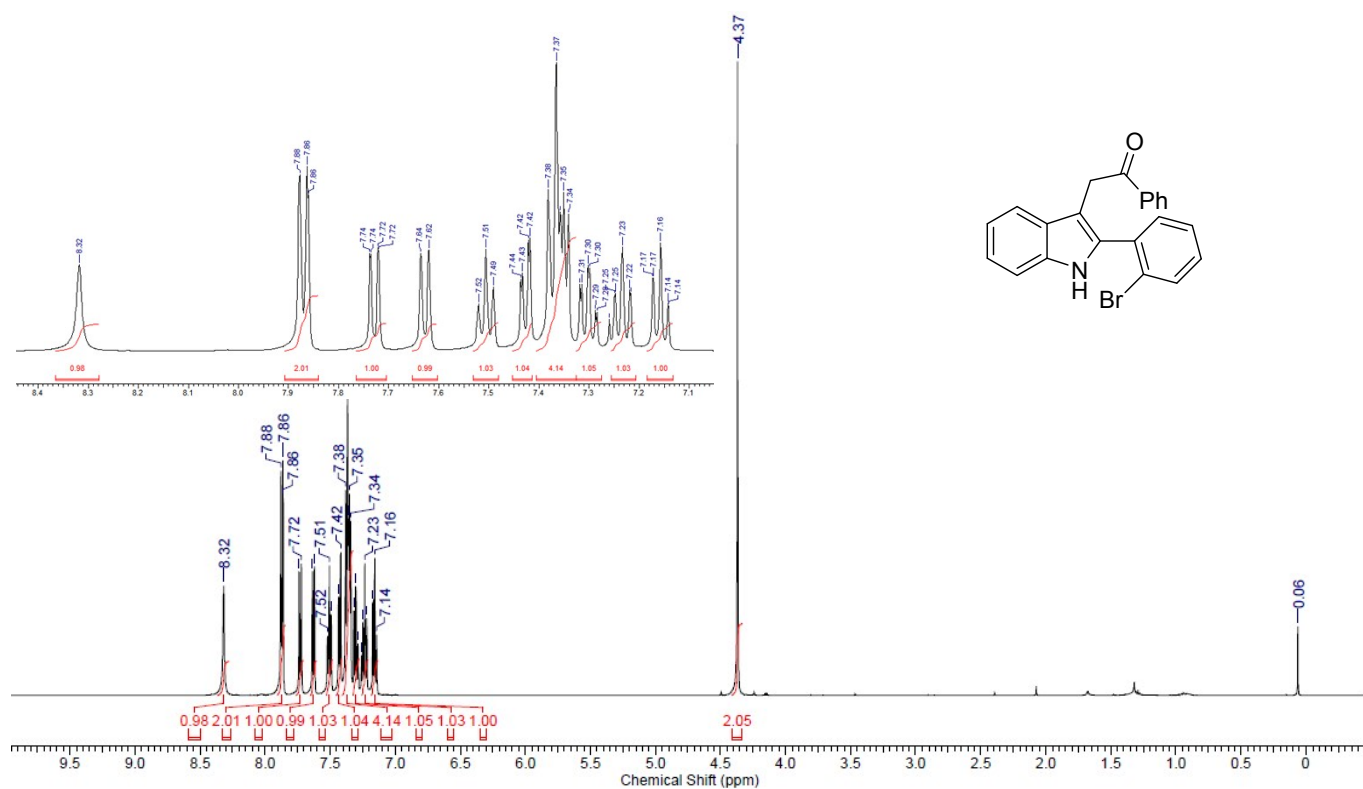


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

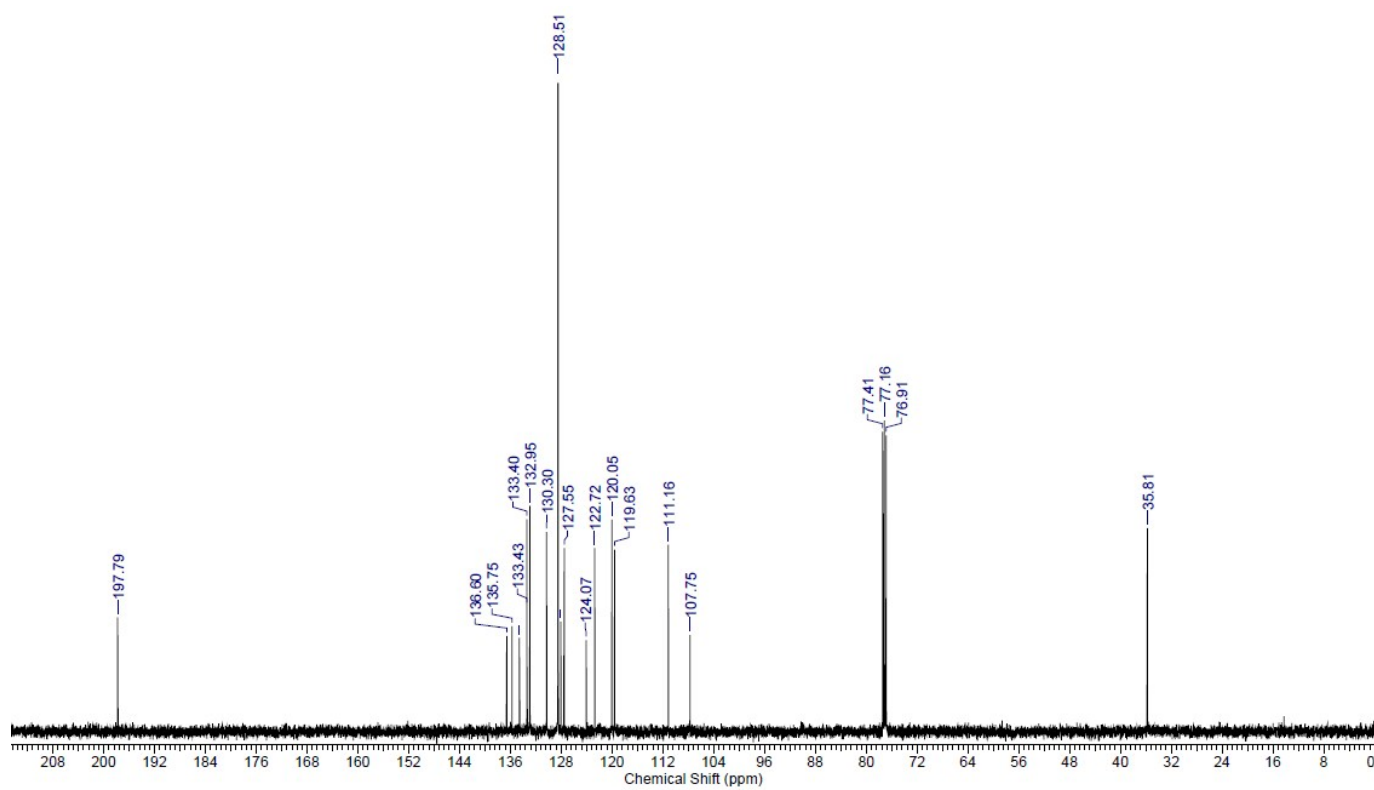


2-8. NMR Spectra of 2-(2-Bromophenyl)-3-phenacylindole (**2h**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

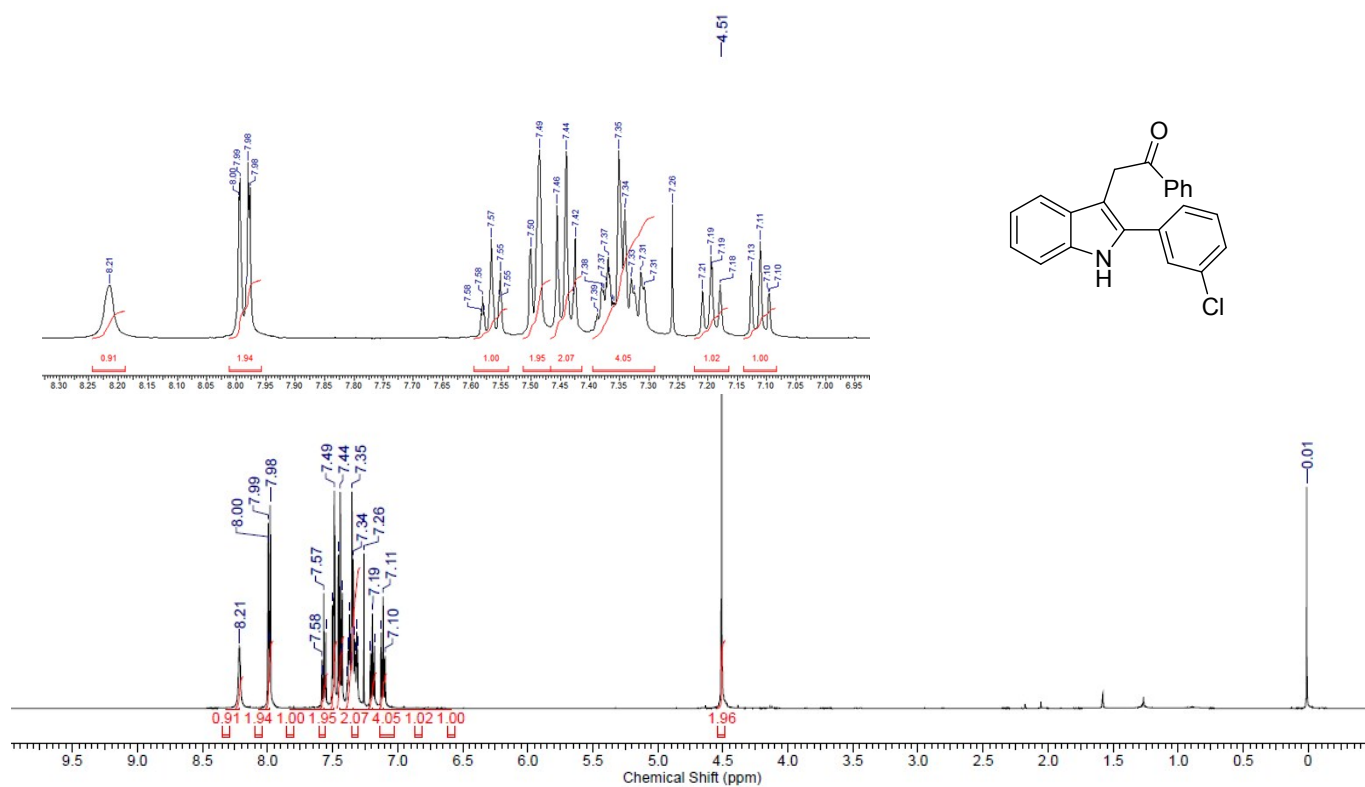


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

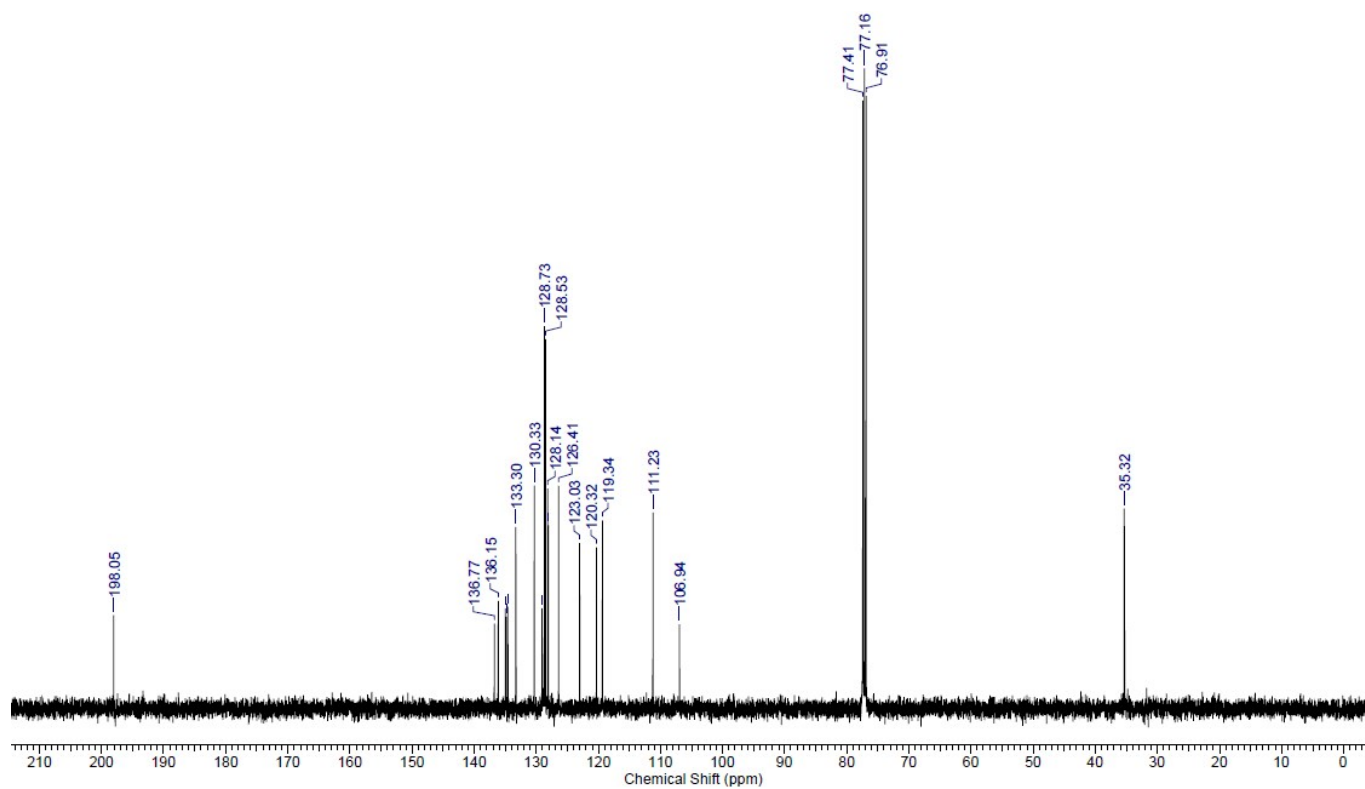


2-9. NMR Spectra of 2-(3-Chlorophenyl)-3-phenacylindole (**2i**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

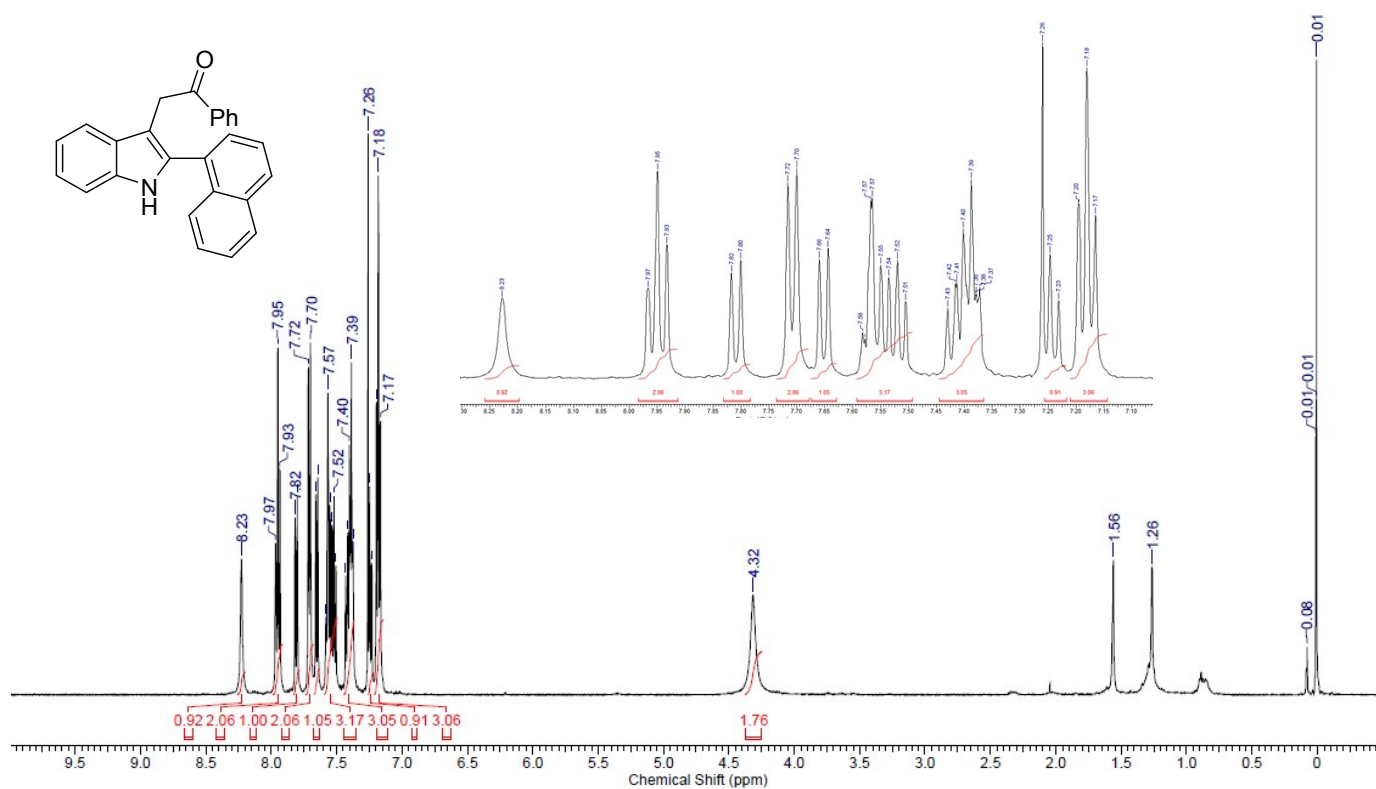


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

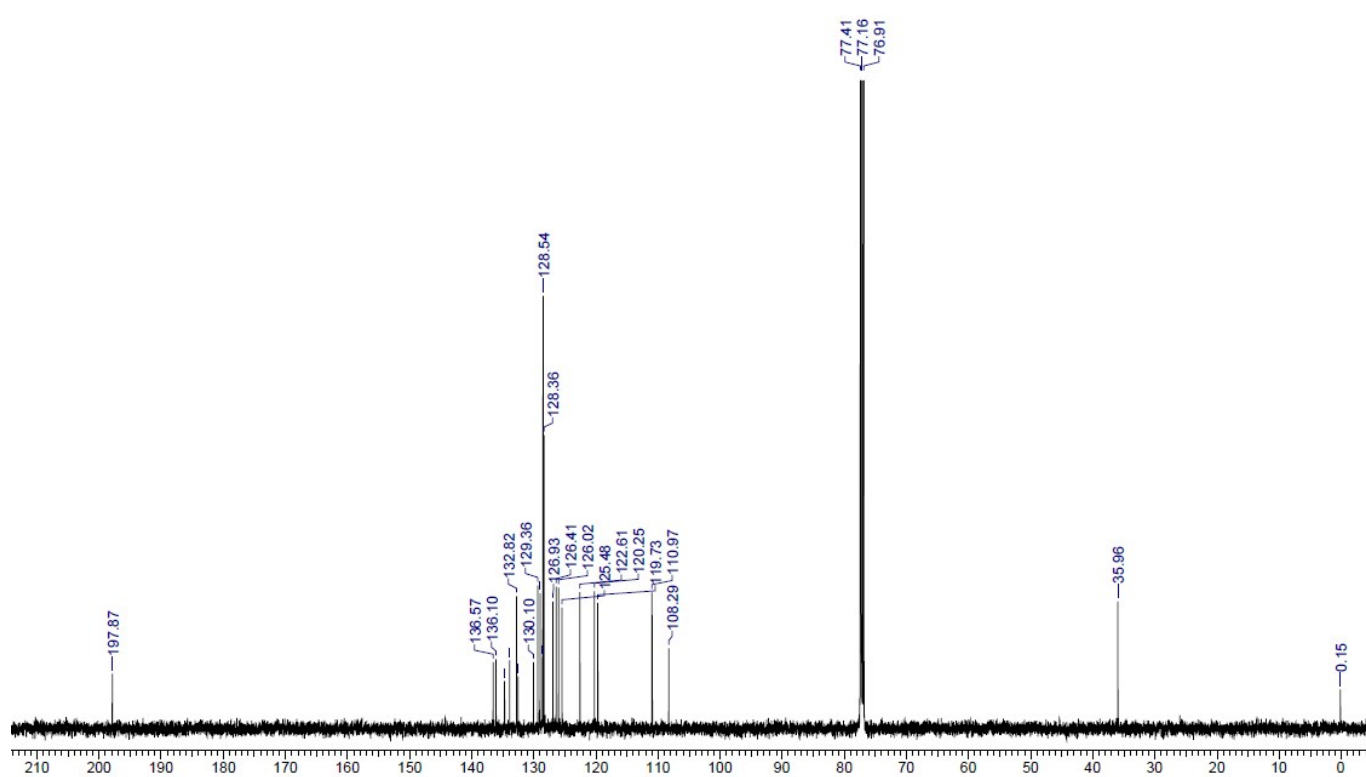


2-10. NMR Spectra of 2-(Naphthalen-1-yl)-3-phenacylindole (**2j**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

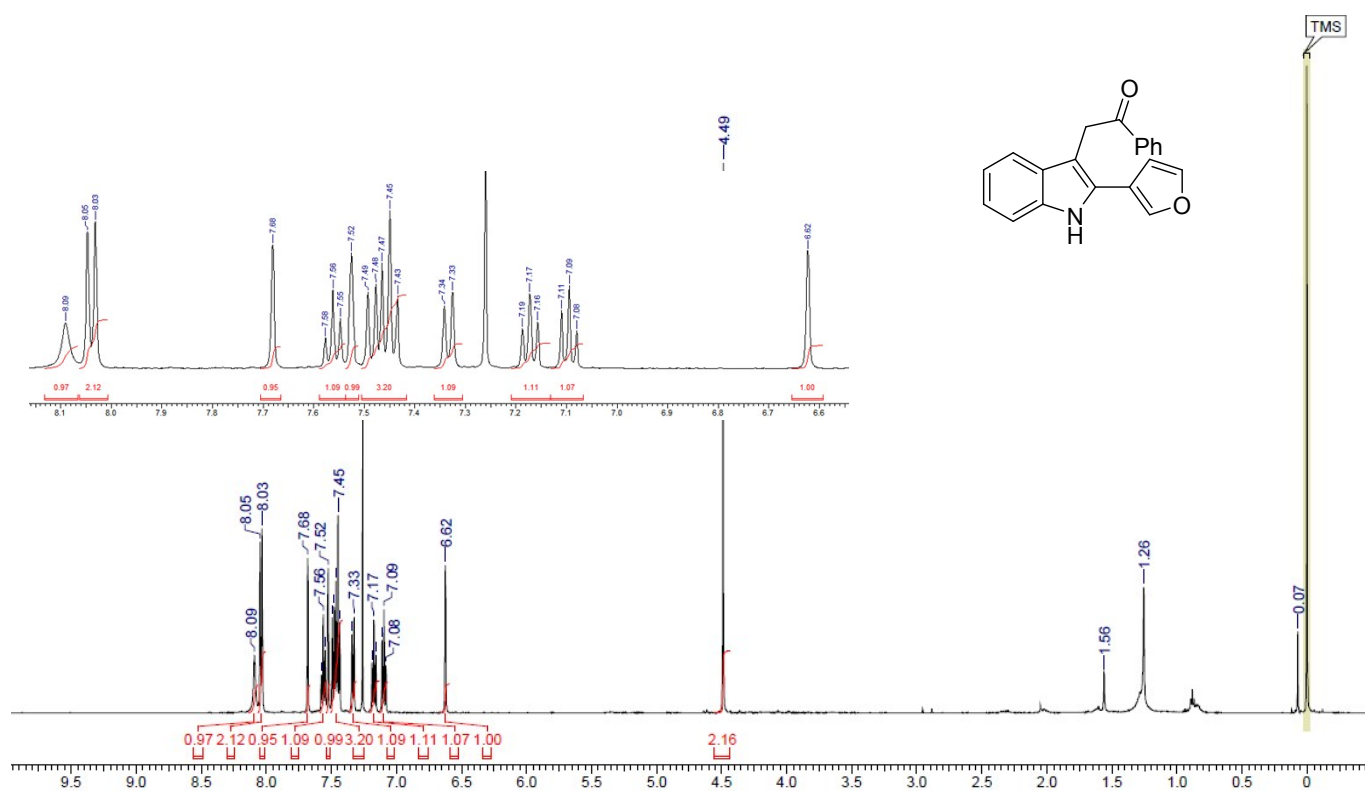


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

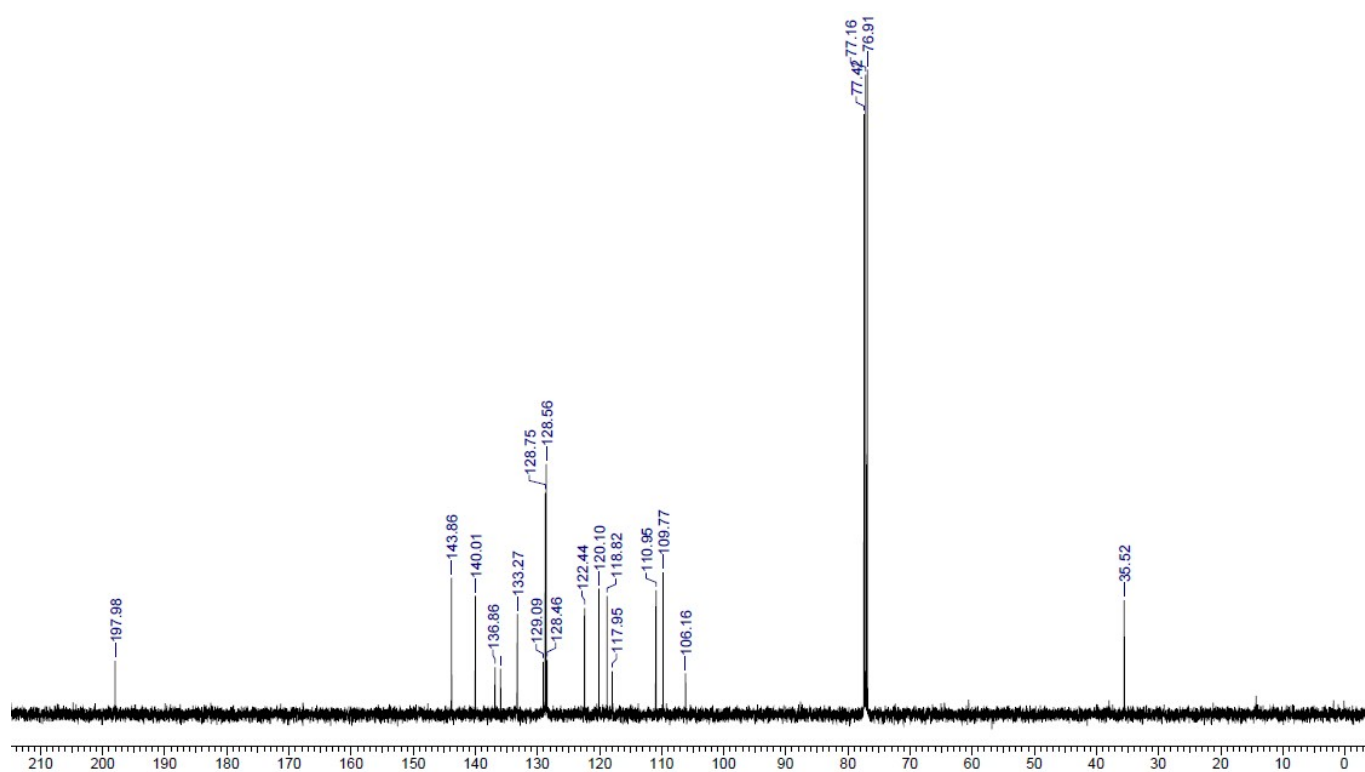


2-11. NMR Spectra of 2-(Furan-3-yl)-3-phenacylindole (**2k**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

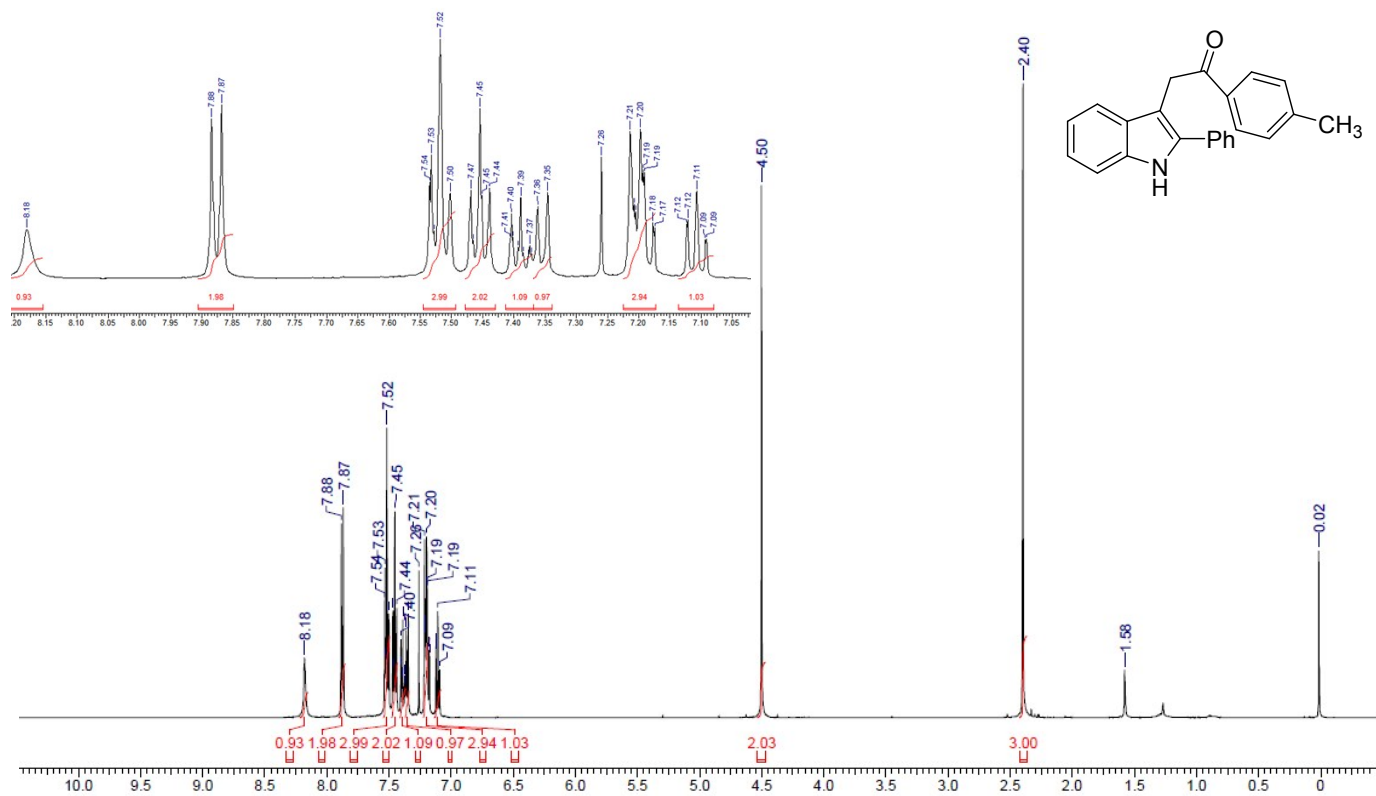


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

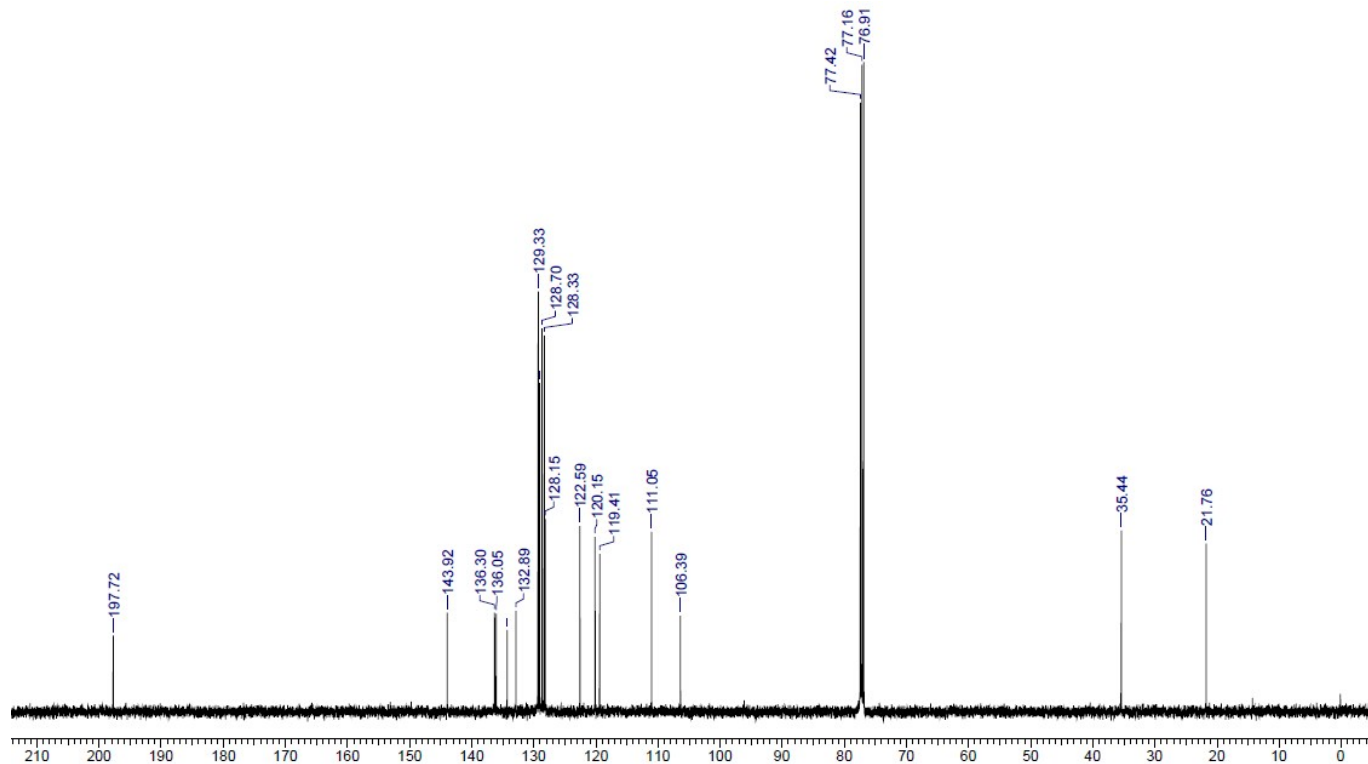


2-12. NMR Spectra of 3-(4-Methylphenacyl)-2-phenylindole (**21**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

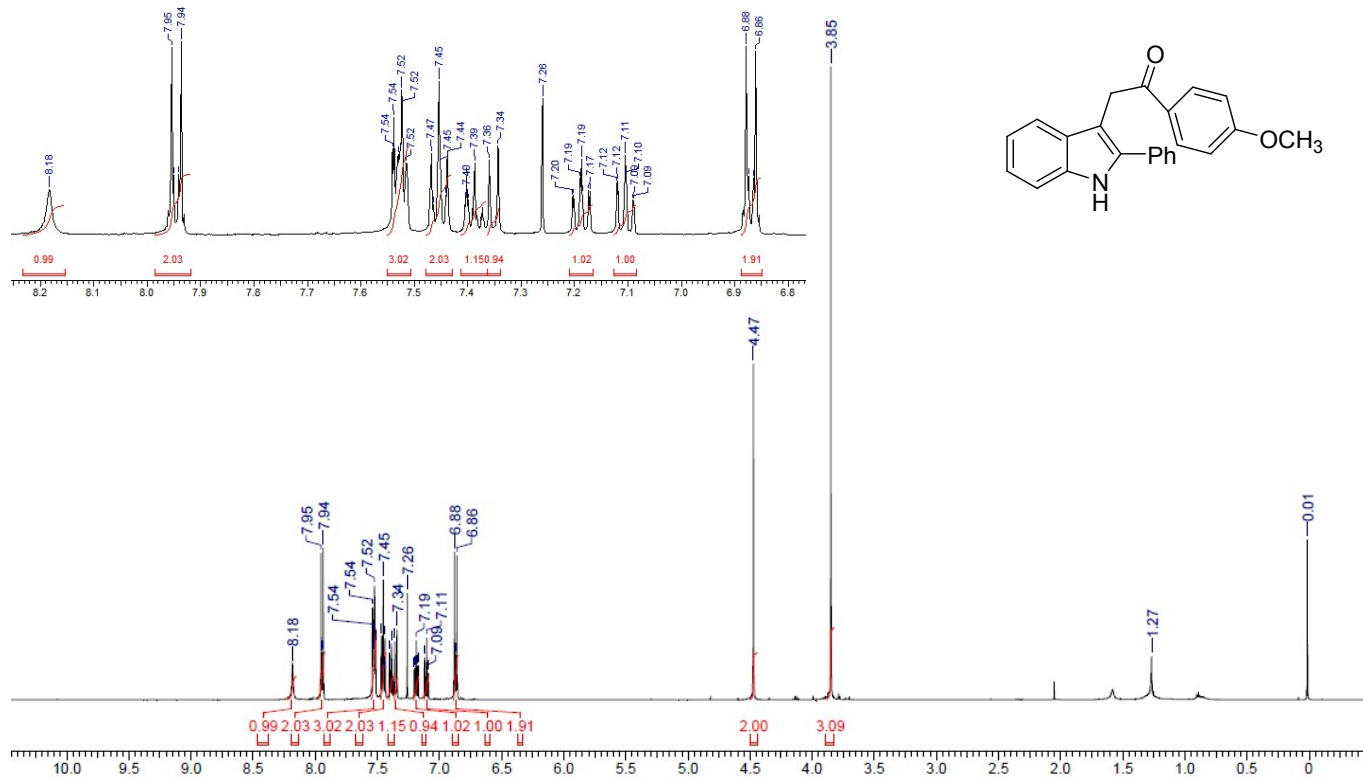


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

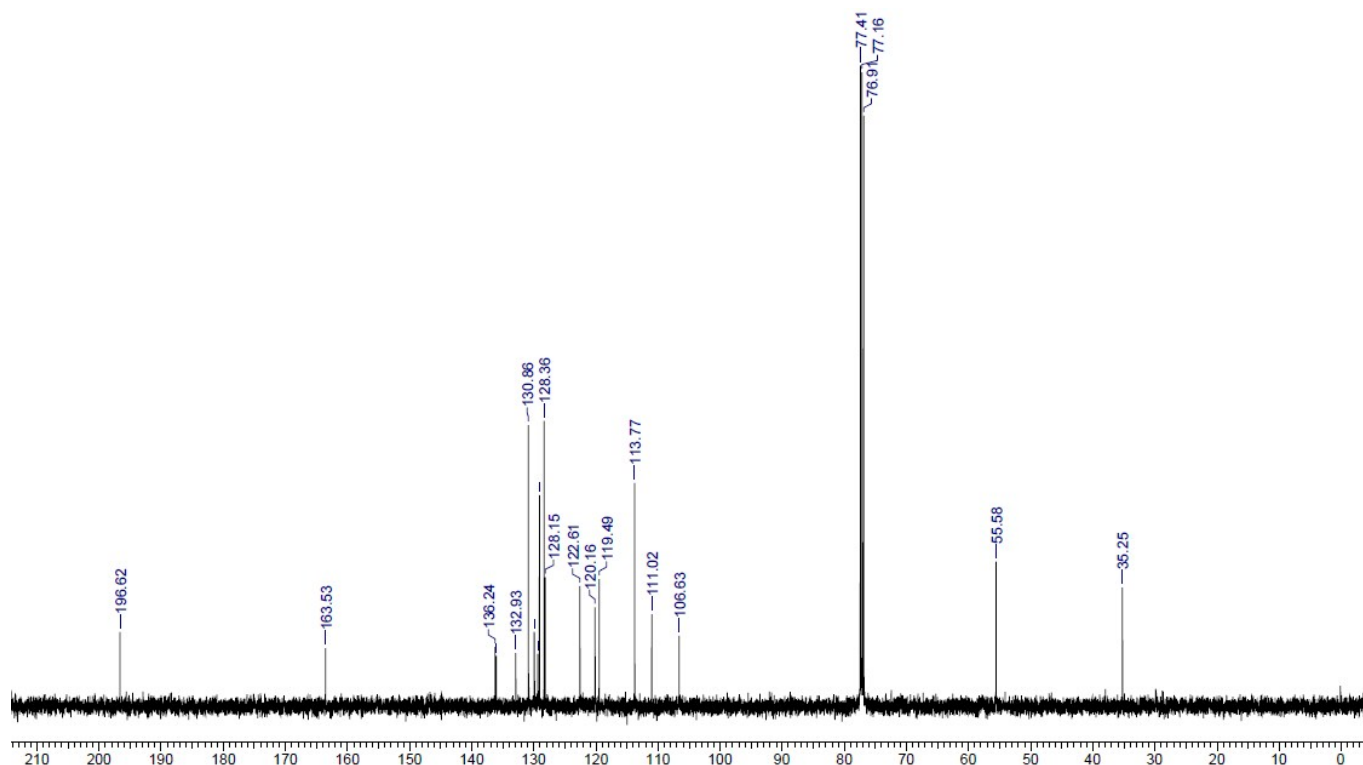


2-13. NMR Spectra of 3-(4-Methoxyphenacyl)-2-phenylindole (**2m**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

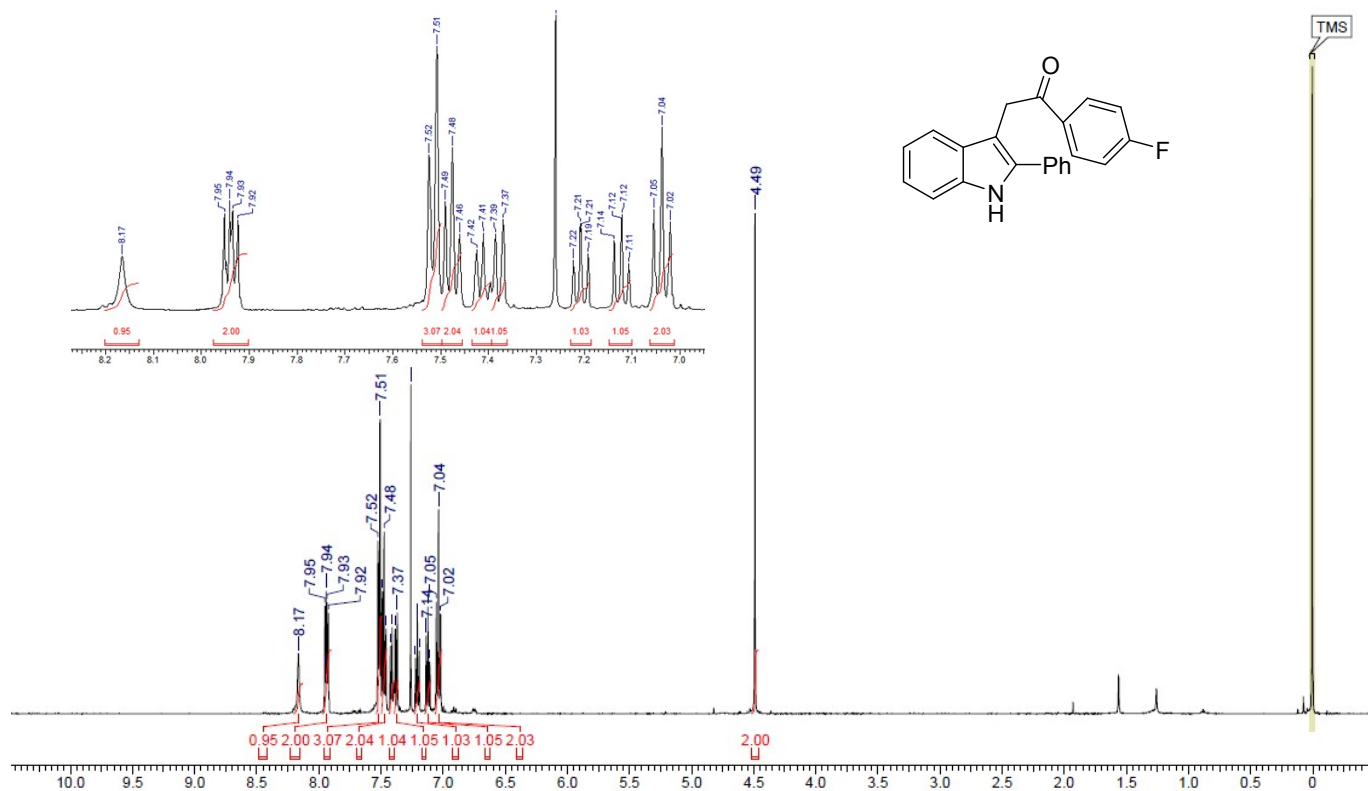


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

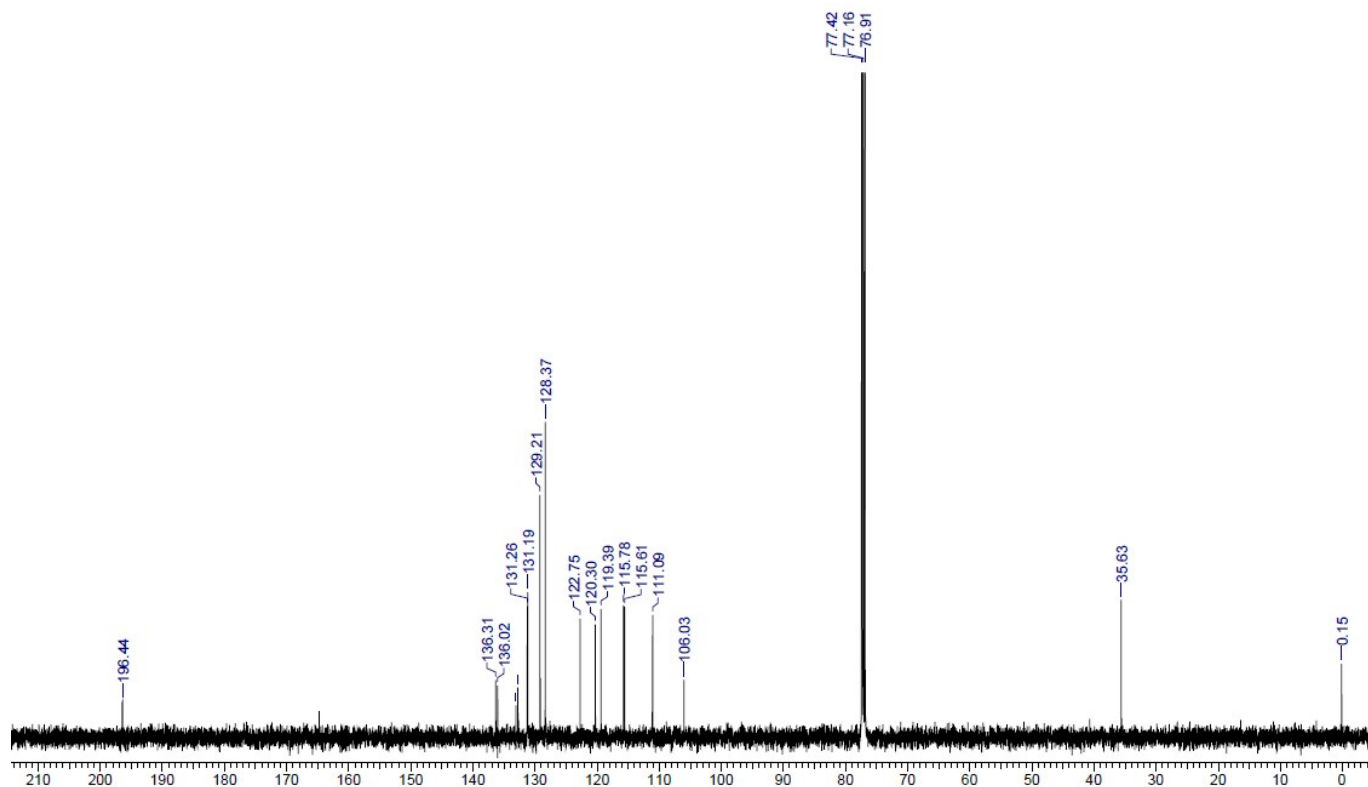


2-14. NMR Spectra of 3-(4-Fluorophenacyl)-2-phenylindole (**2n**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

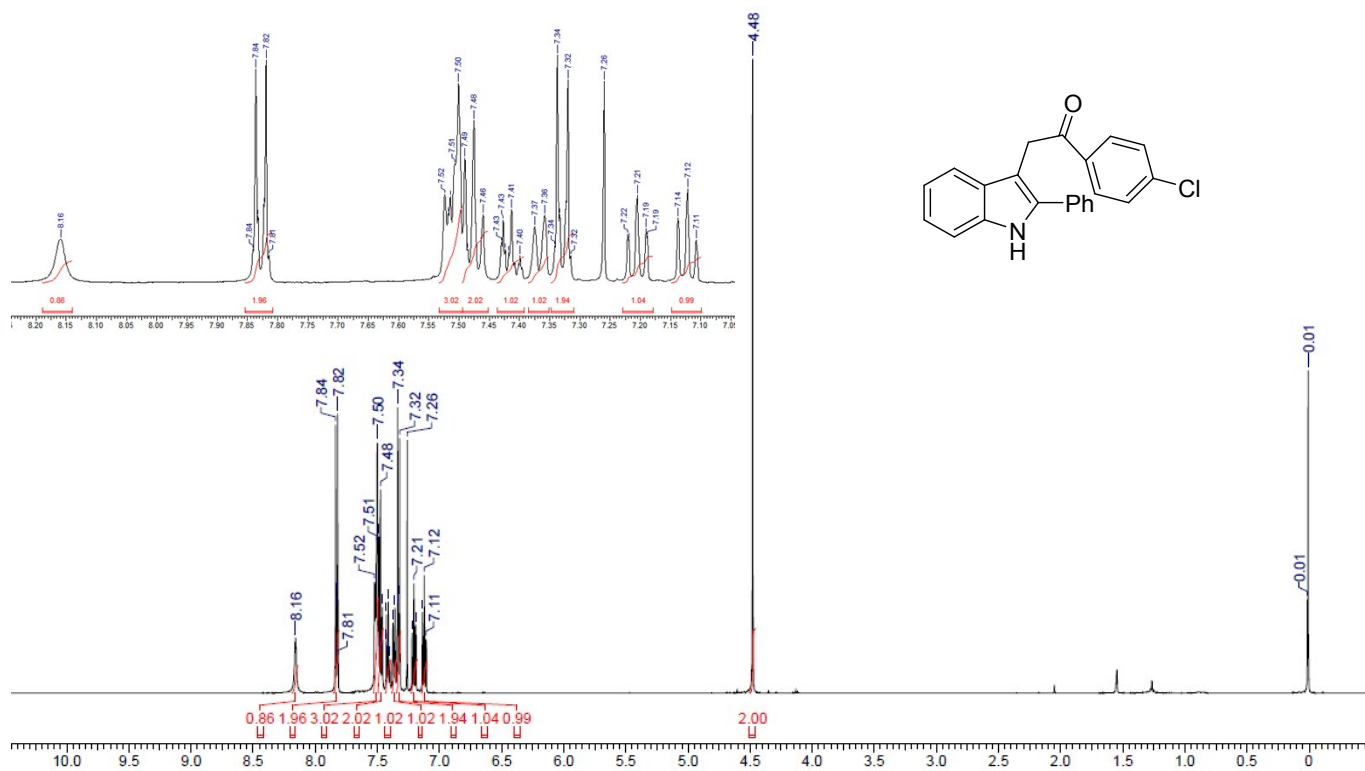


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

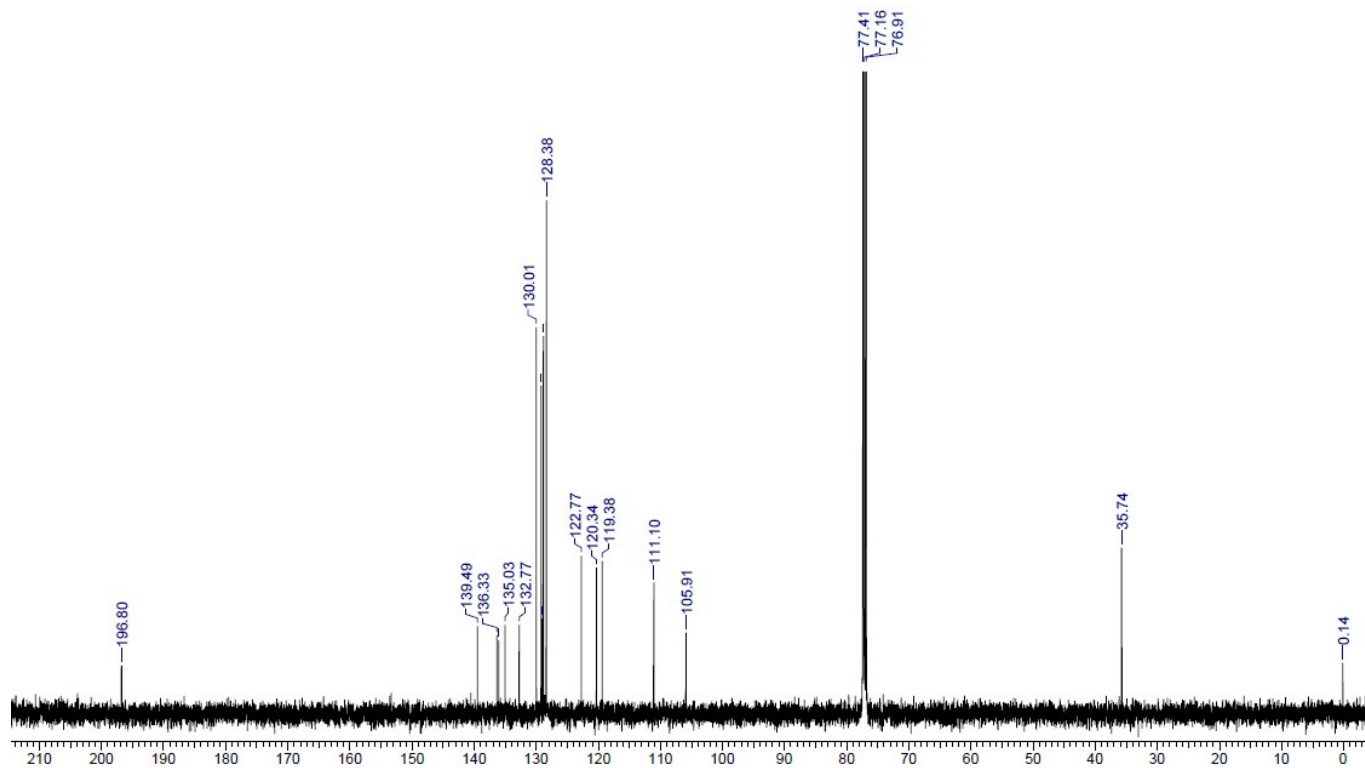


2-15. NMR Spectra of 3-(4-Chlorophenacyl)-2-phenylindole (**2o**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

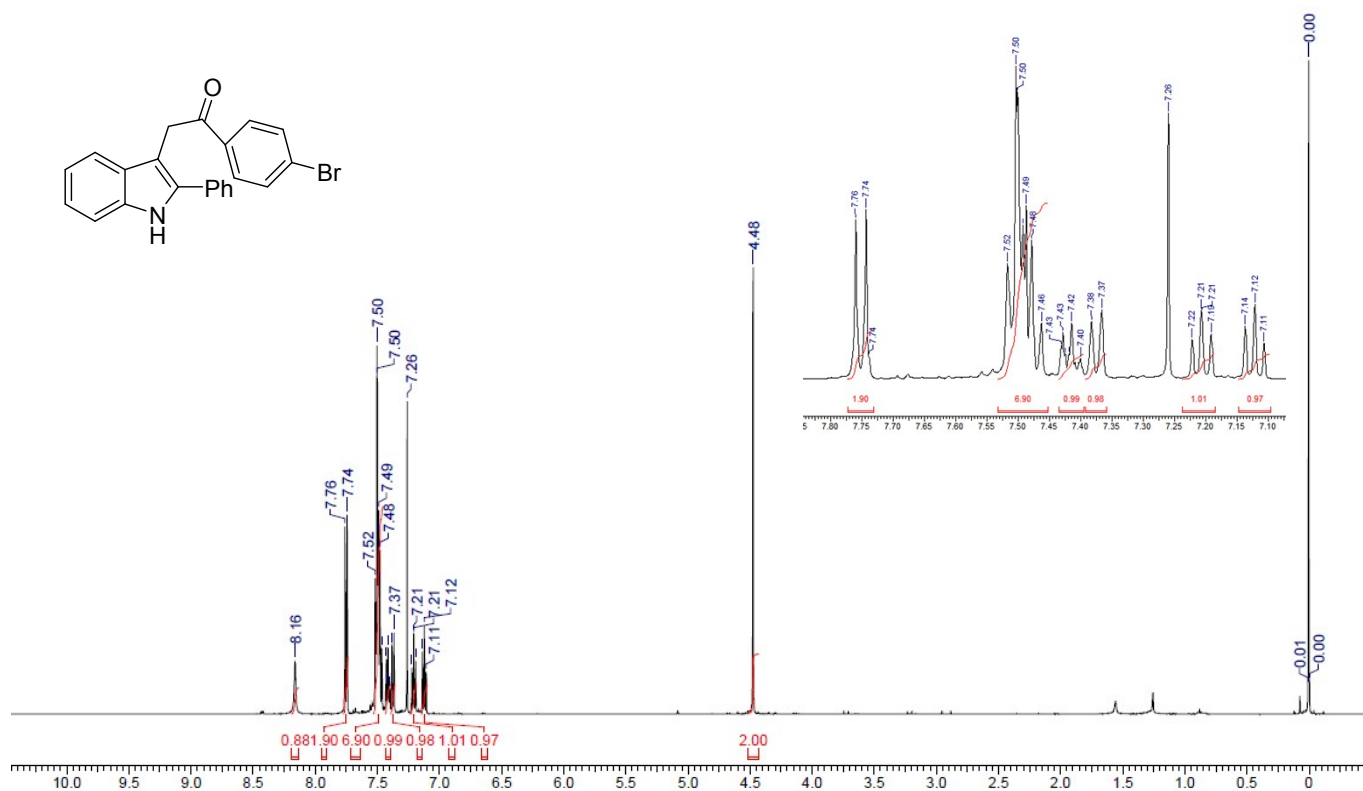


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

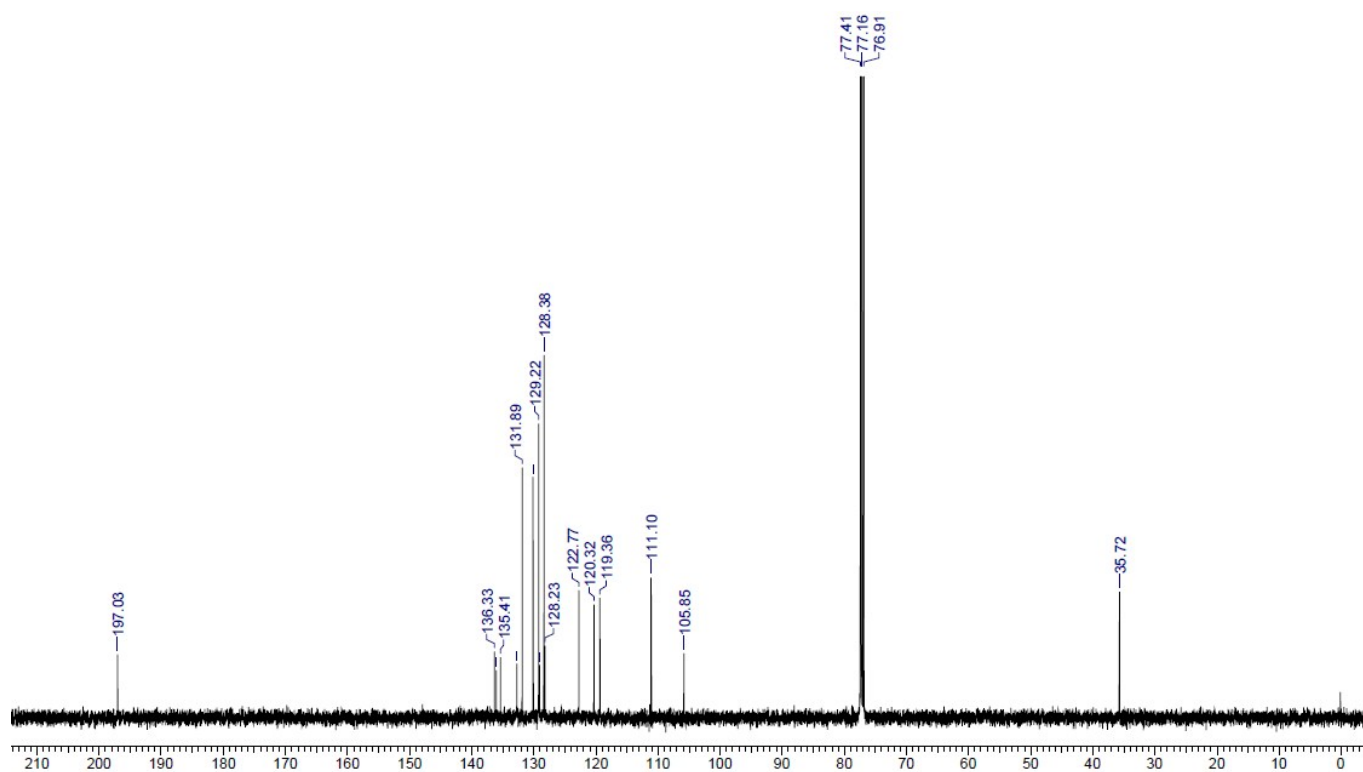


2-16. NMR Spectra of 3-(4-Bromophenacyl)-2-phenylindole (**2p**)

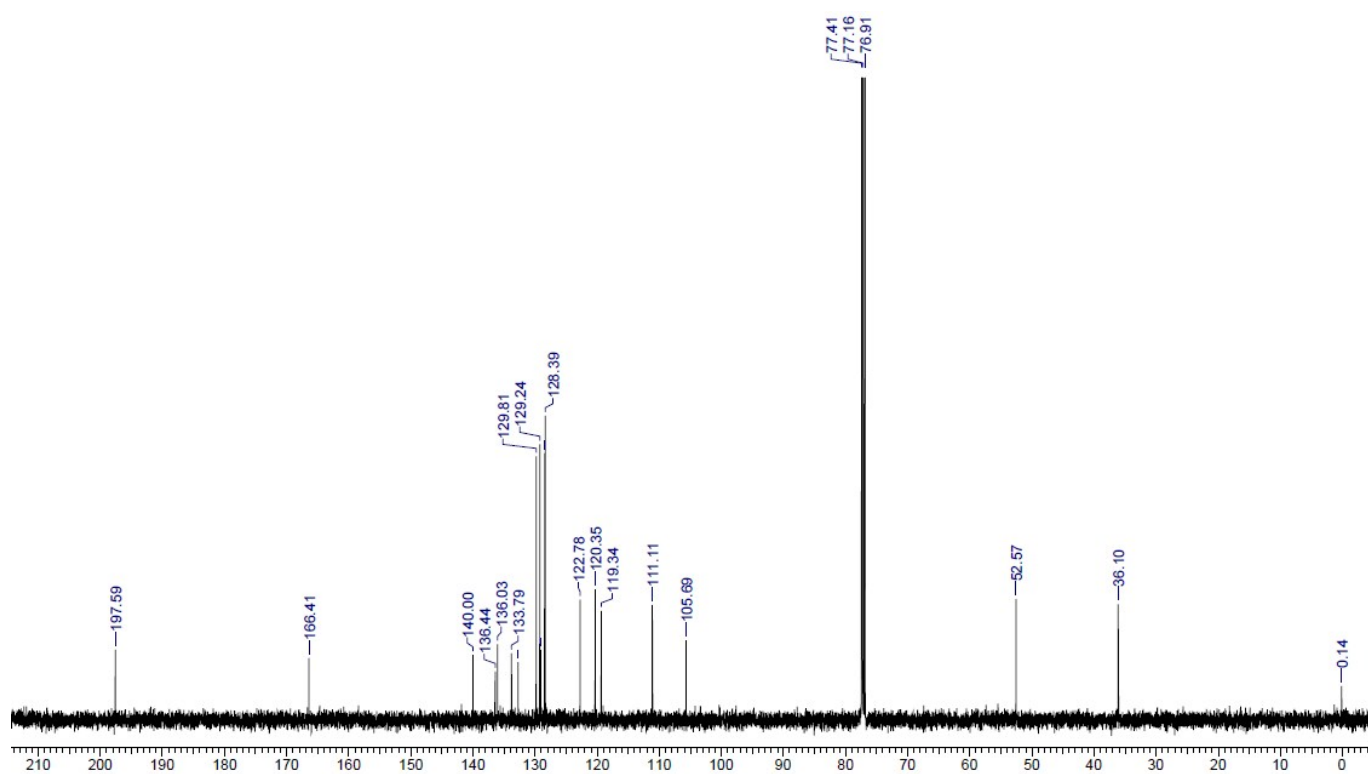
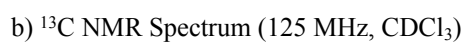
a) ^1H NMR Spectrum (500 MHz, CDCl_3)



b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

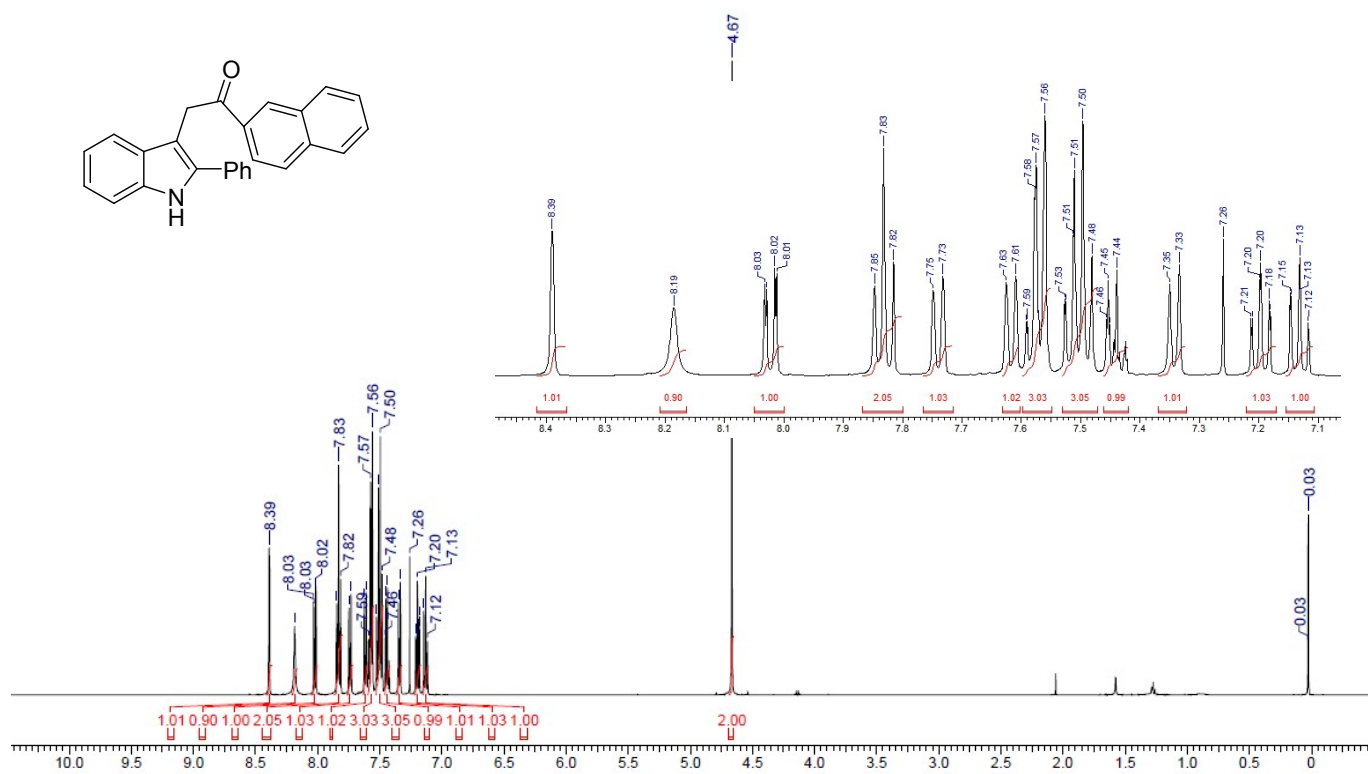


a) ^1H NMR Spectrum (500 MHz, CDCl_3)

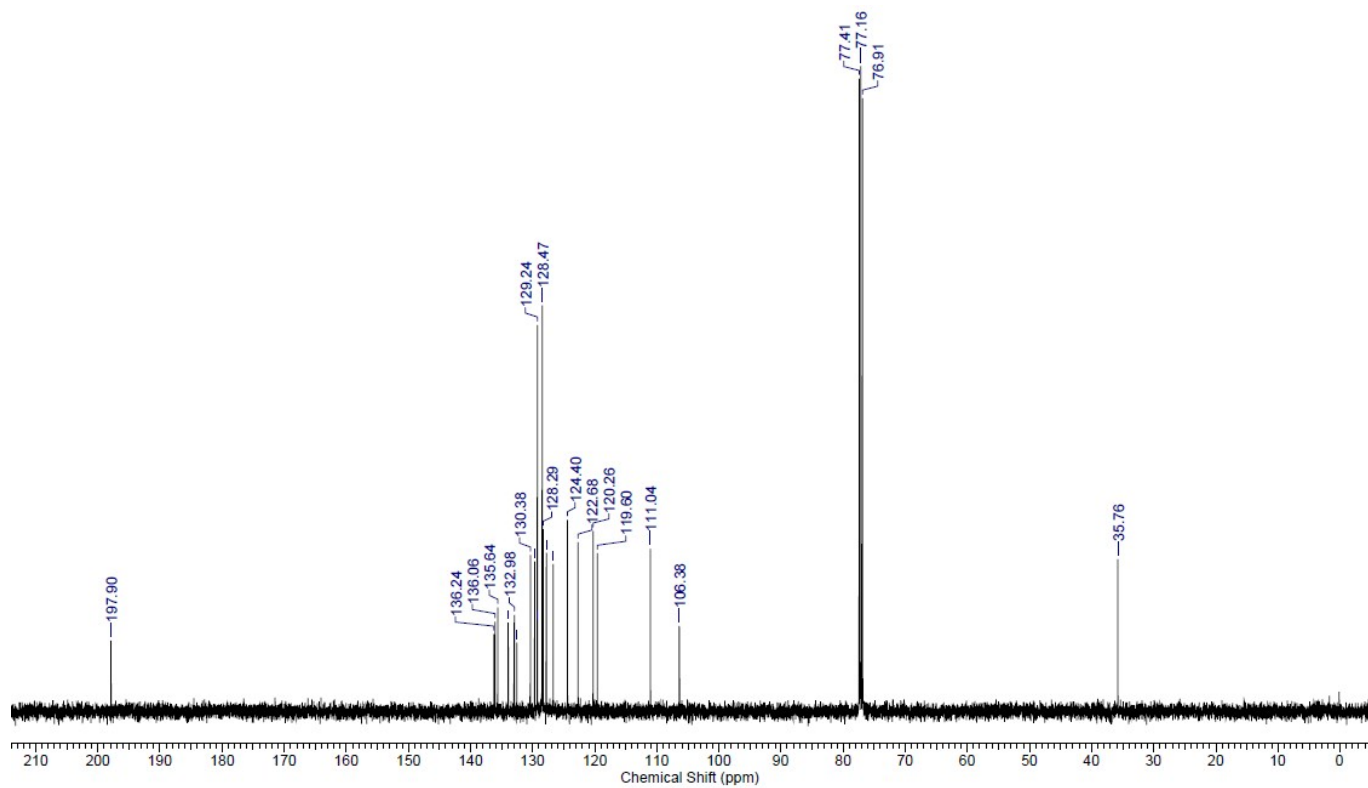


2-18. NMR Spectra of 3-(2-Naphthylacetyl)-2-phenylindole (**2r**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

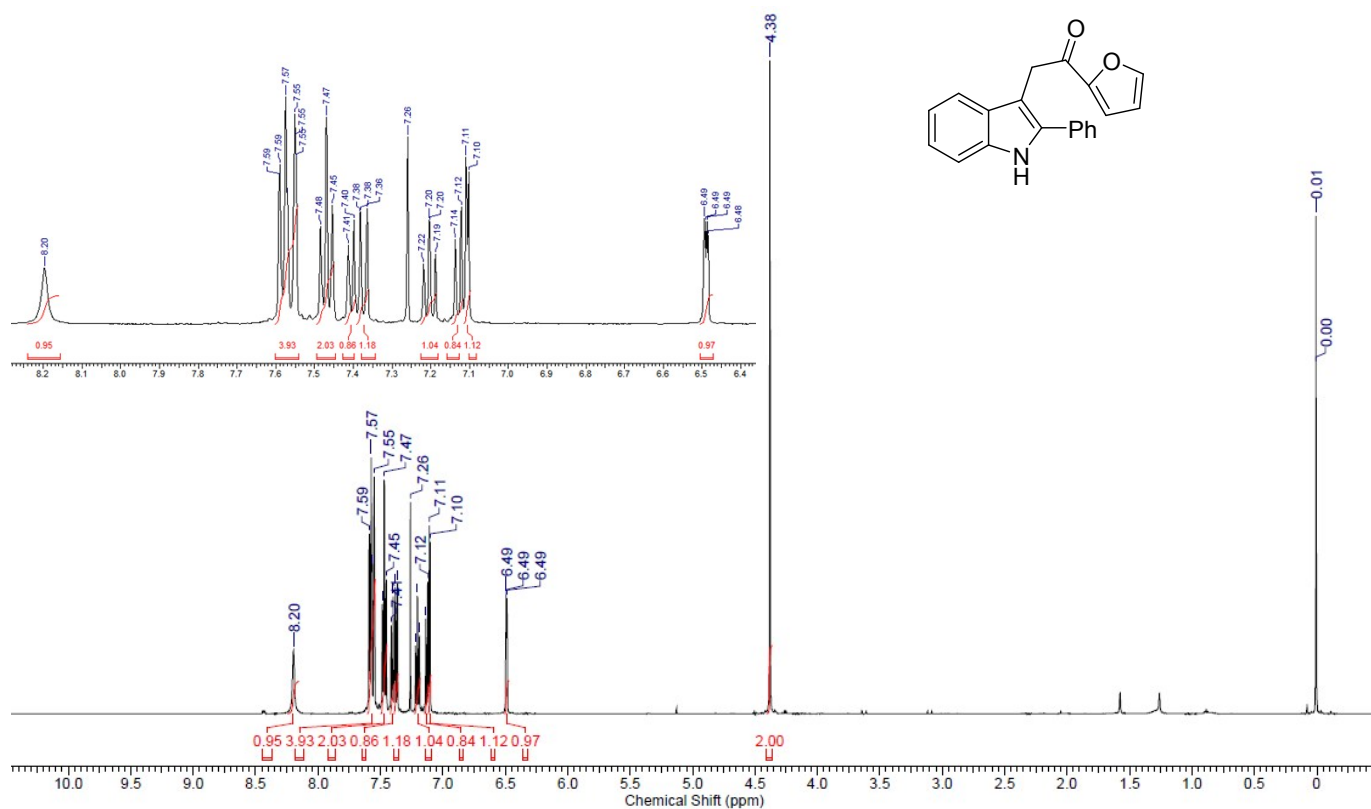


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

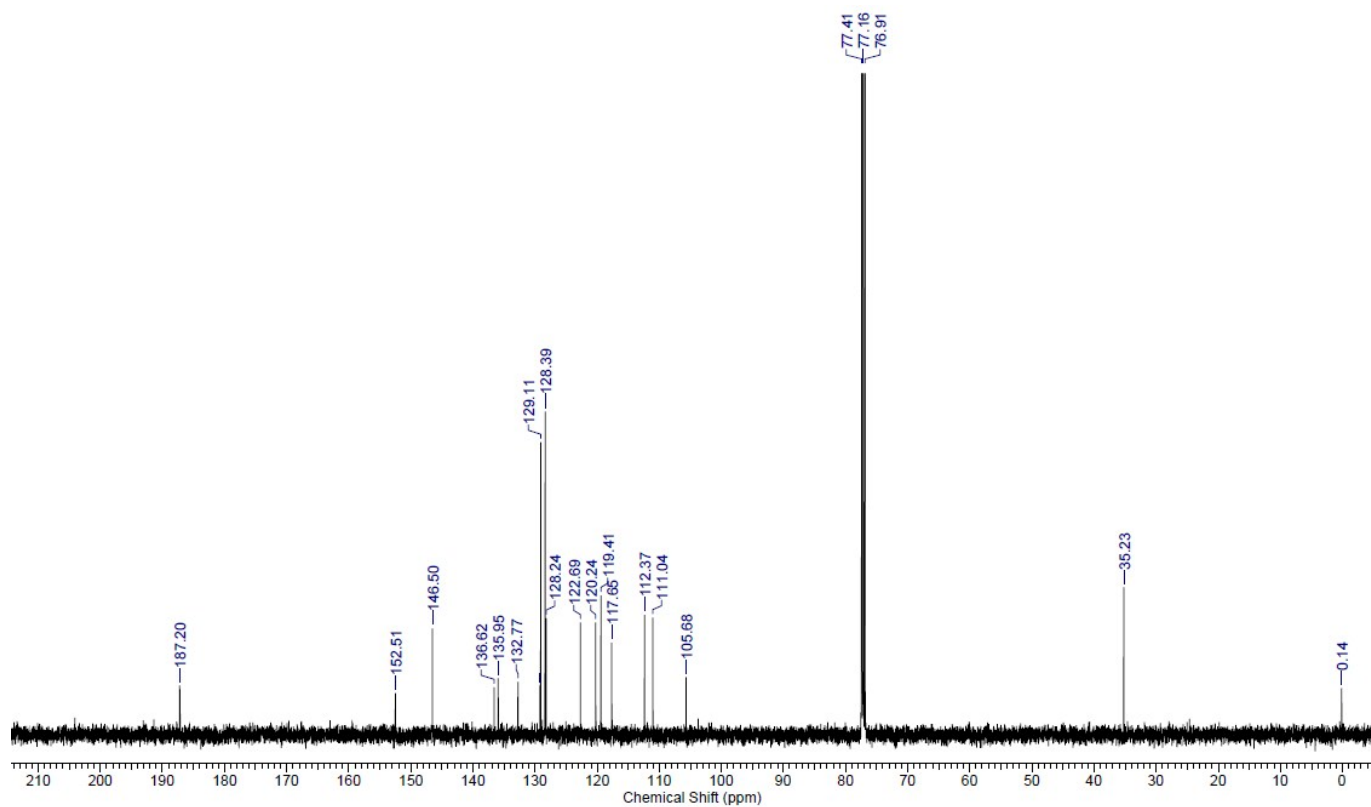


2-19. NMR Spectra of 3-(2-Furanylacetyl)-2-phenylindole (**2s**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

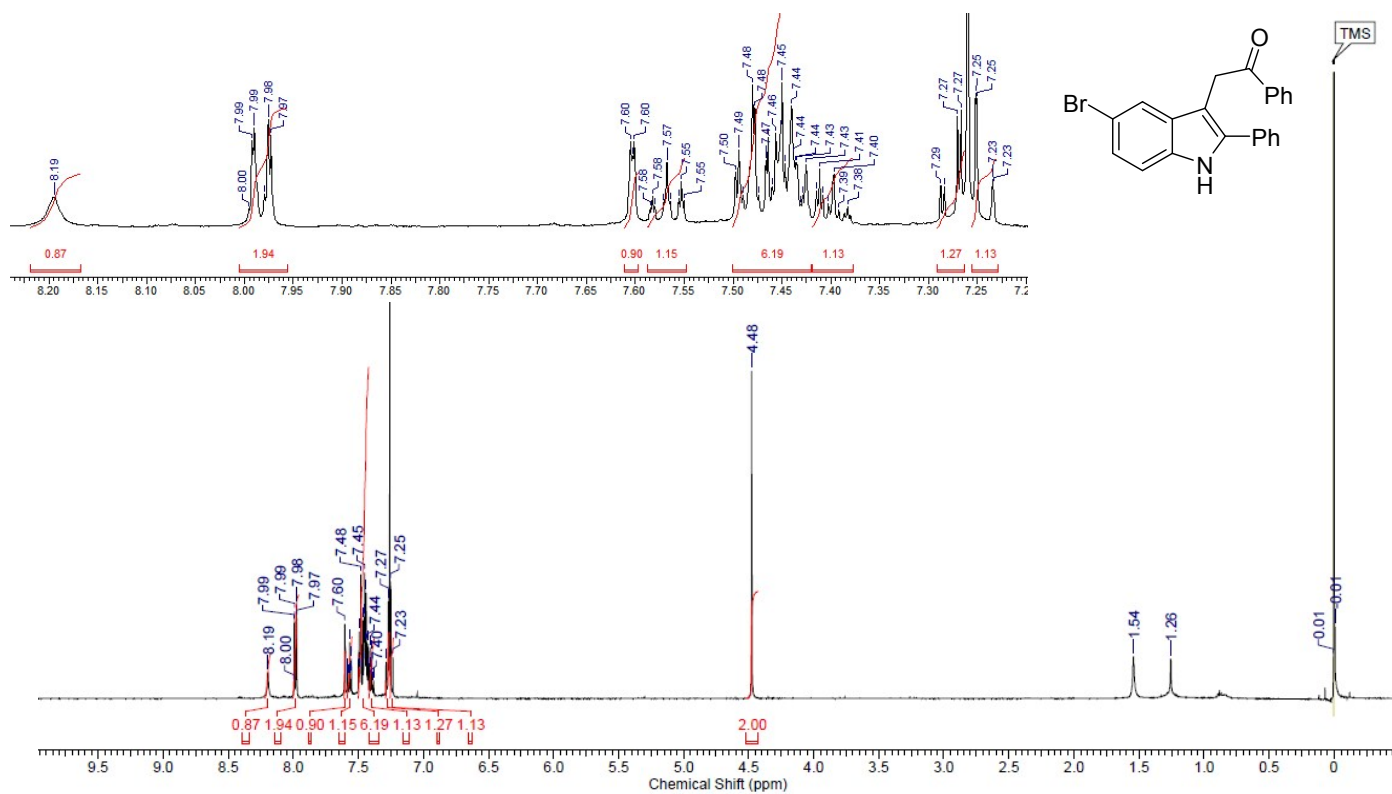


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

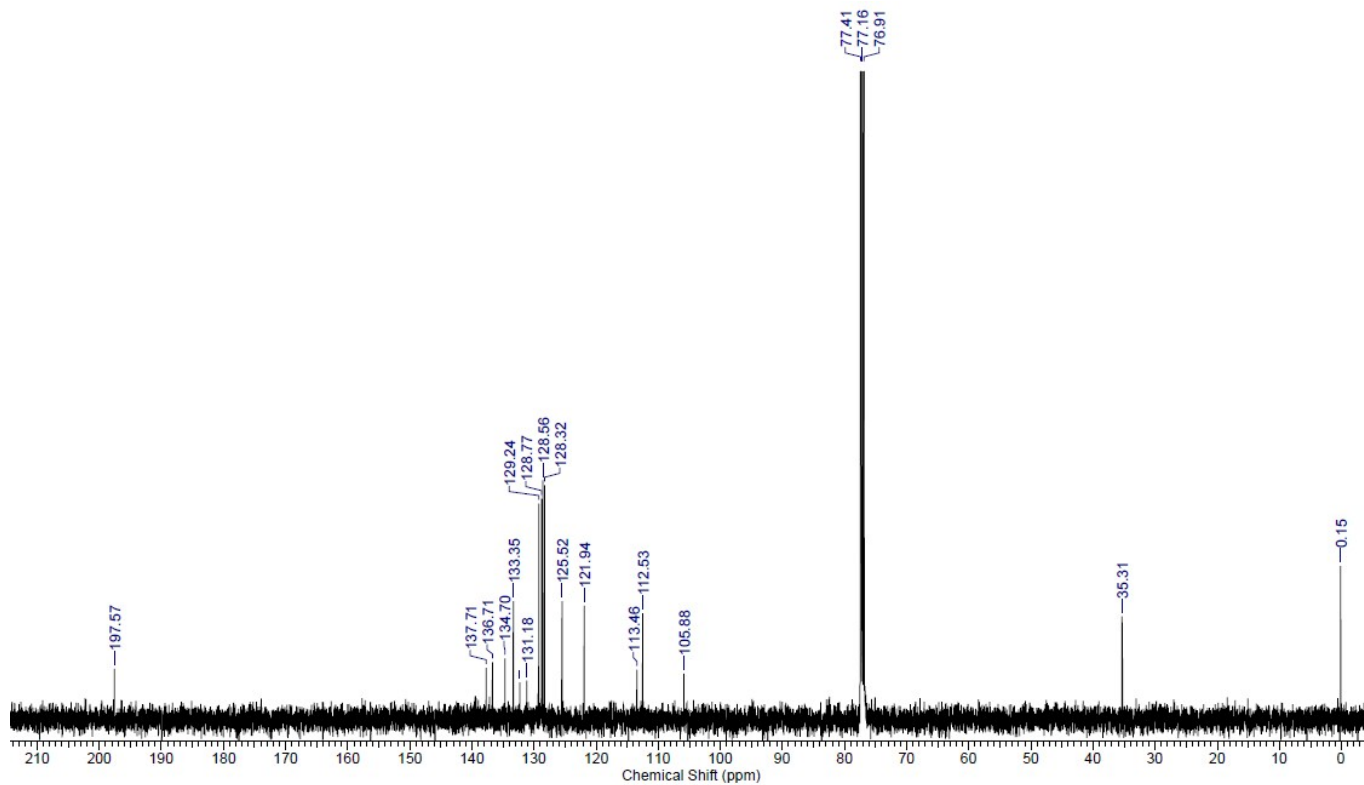


2-20. NMR Spectra of 5-Bromo-3-phenacyl-2-phenylindole (**2t**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)



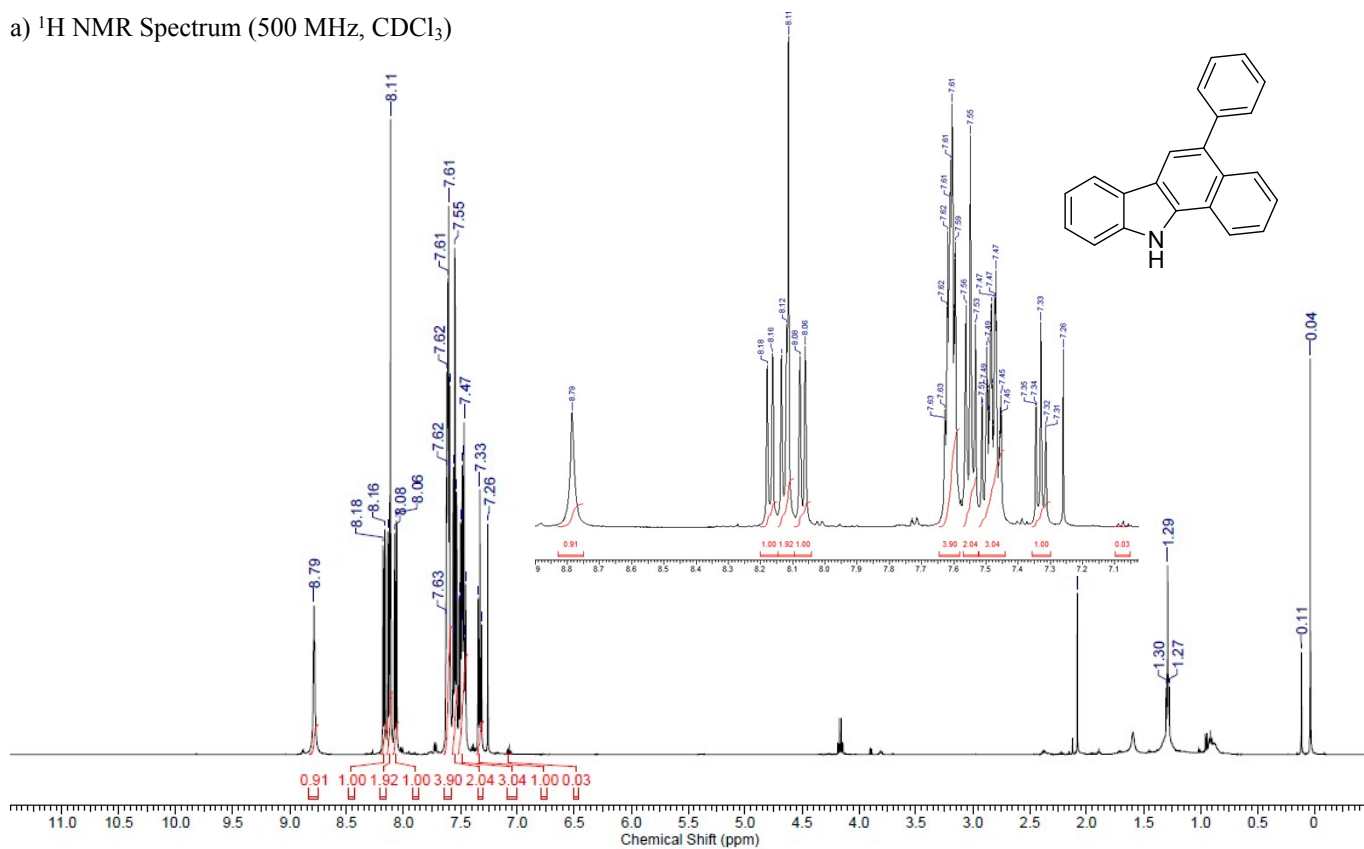
b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)



3. Spectroscopic Data of Benzo[a]carbazoles (**1**)

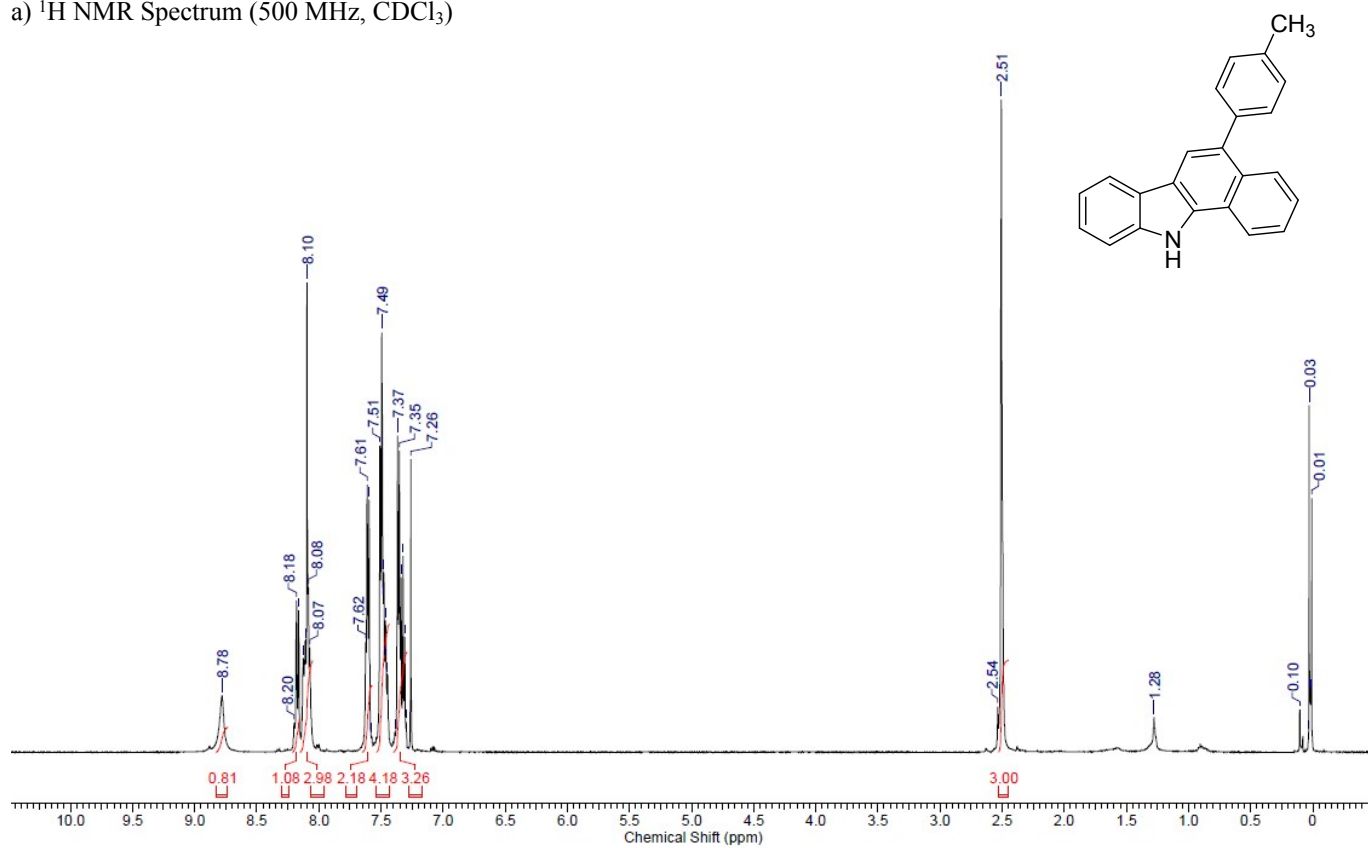
3-1. NMR Spectra of 6-Phenyl-11H-benzo[a]carbazole (**1a**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

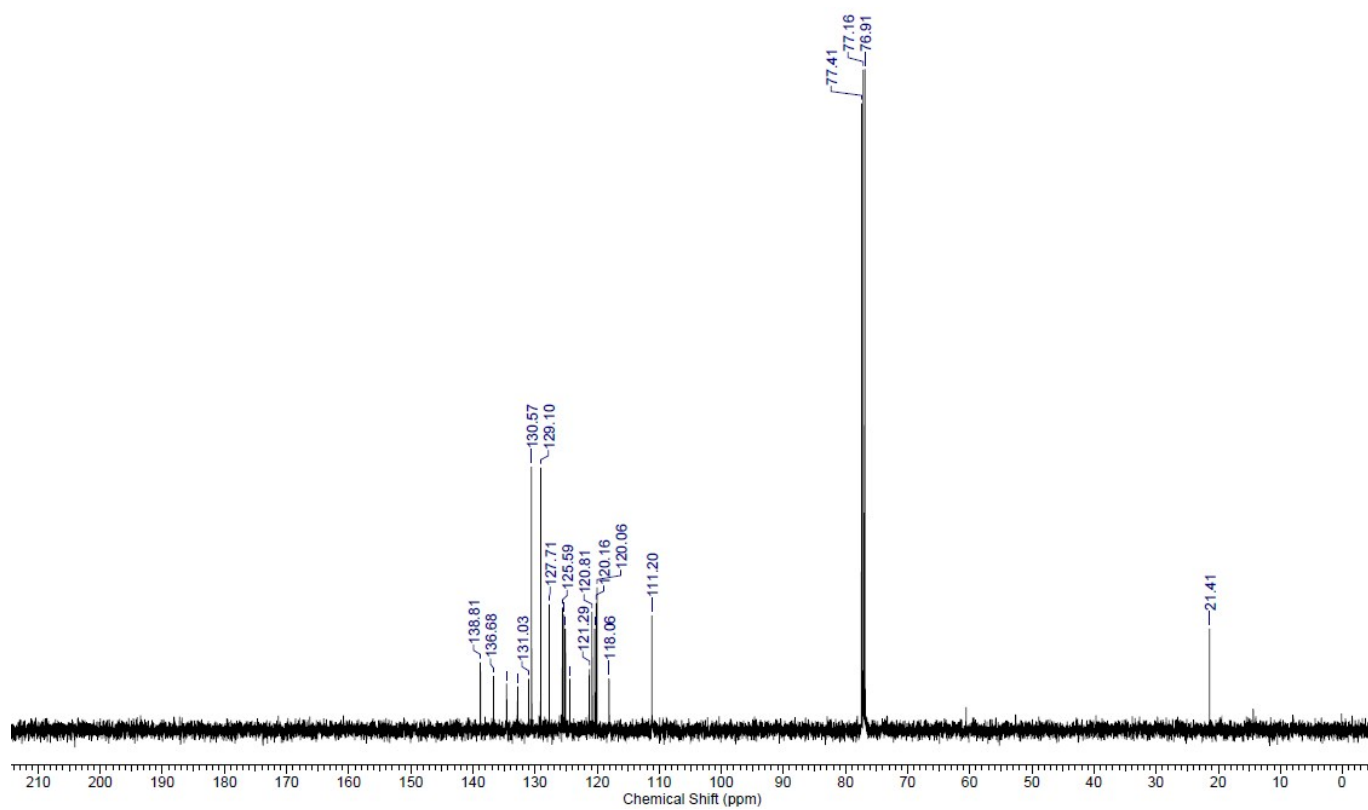


3-2. NMR Spectra of 6-(4-Methylphenyl)-11H-benzo[a]carbazole (**1b**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

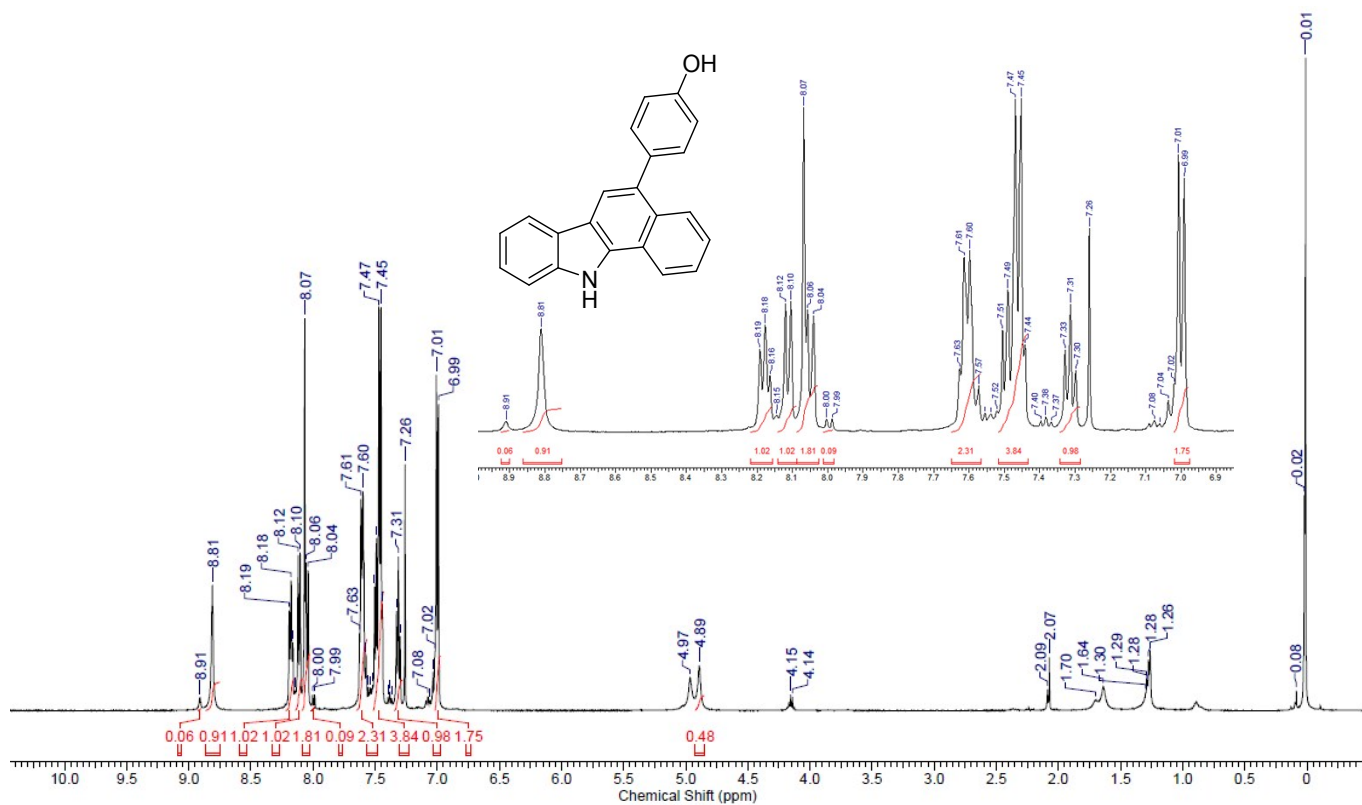


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

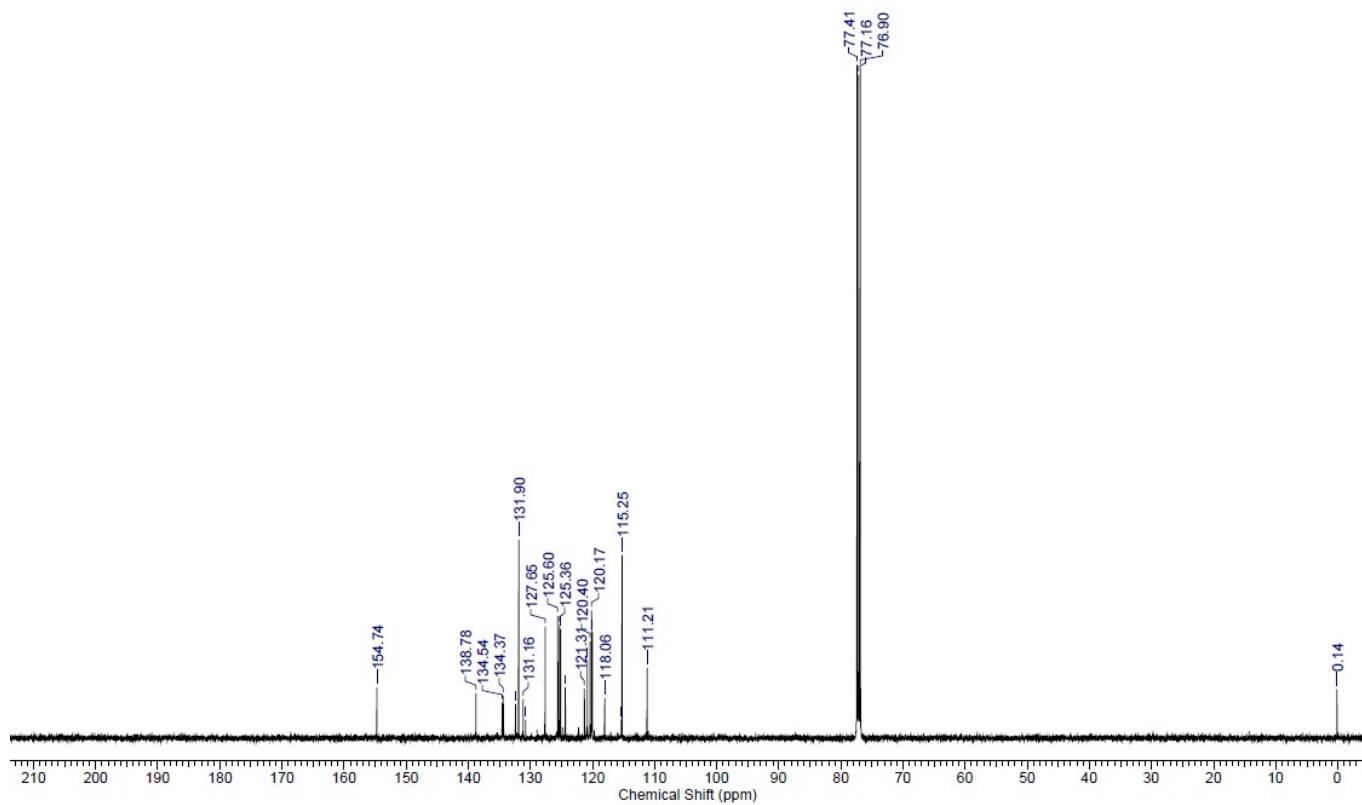


3-3. NMR Spectra of 6-(4-Hydroxyphenyl)-11H-benzo[a]carbazole (**1c**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

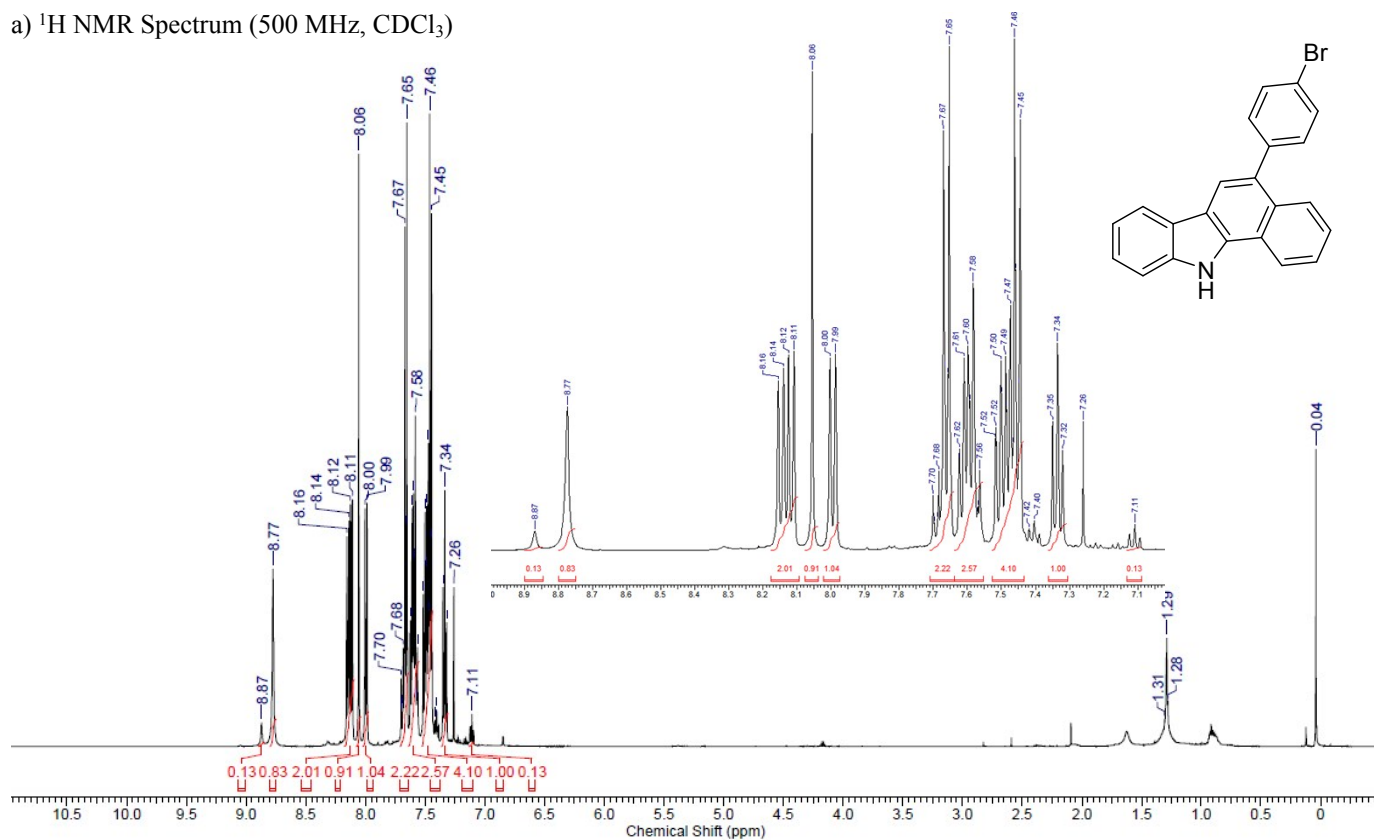


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)



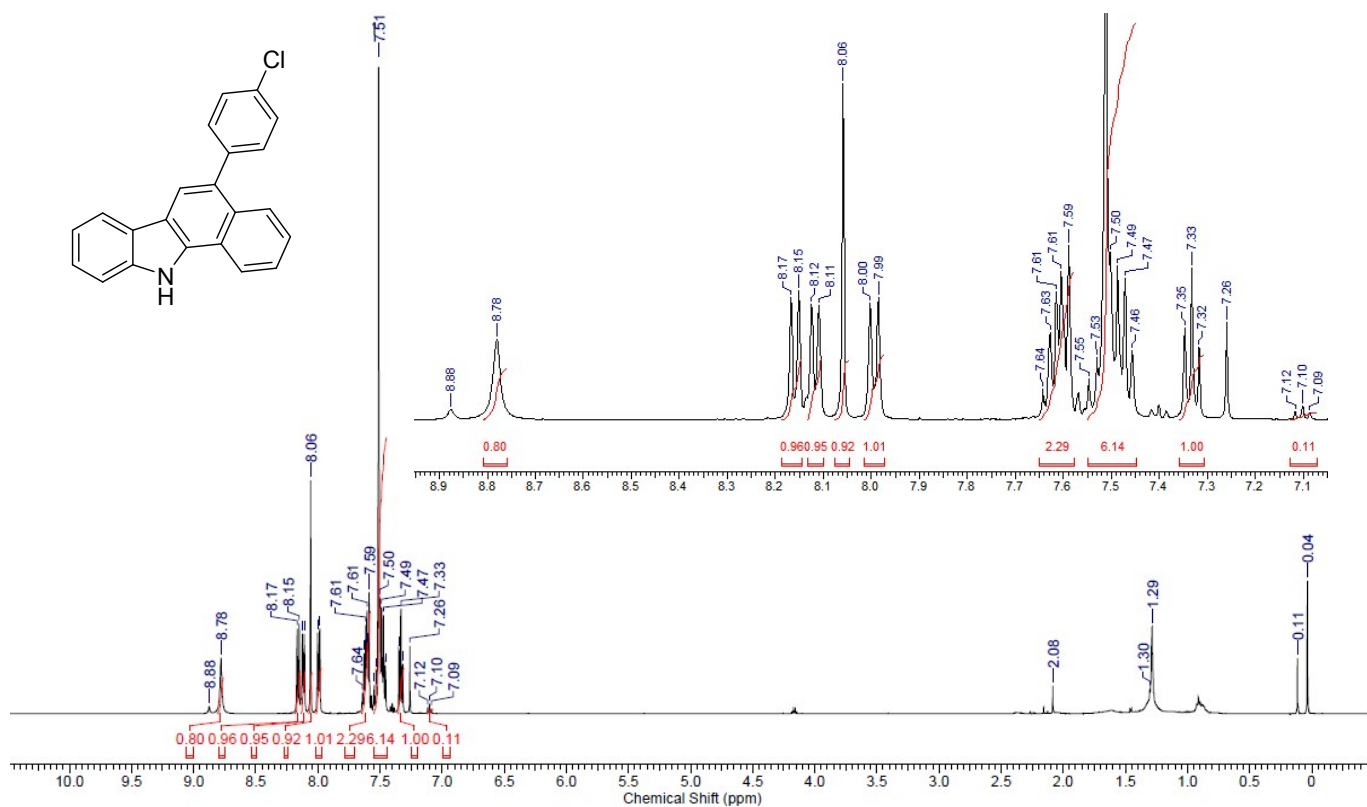
3-4. NMR Spectra of 6-(4-Bromophenyl)-11H-benzo[a]carbazole (**1d**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

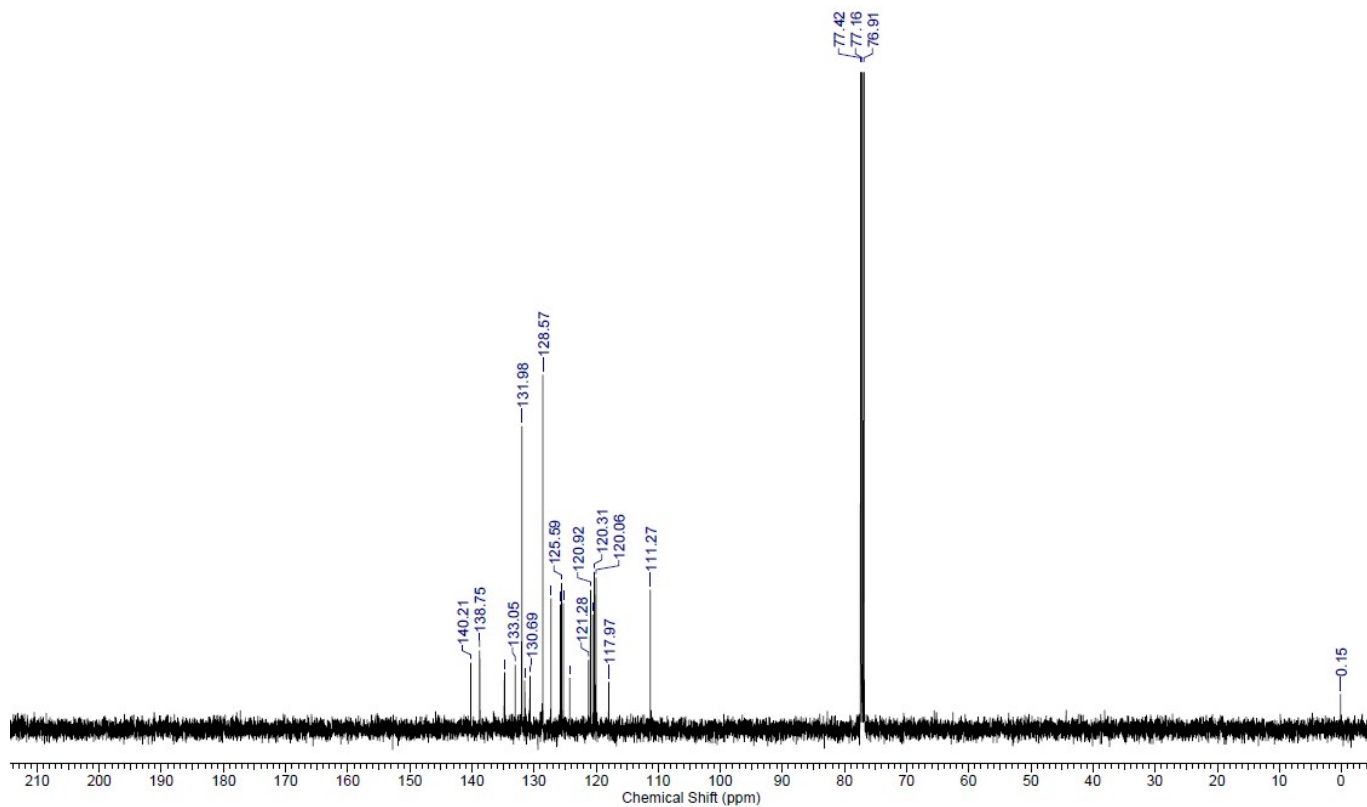


3-5. NMR Spectra of 6-(4-Chlorophenyl)-1*H*-benzo[*a*]carbazole (**1e**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

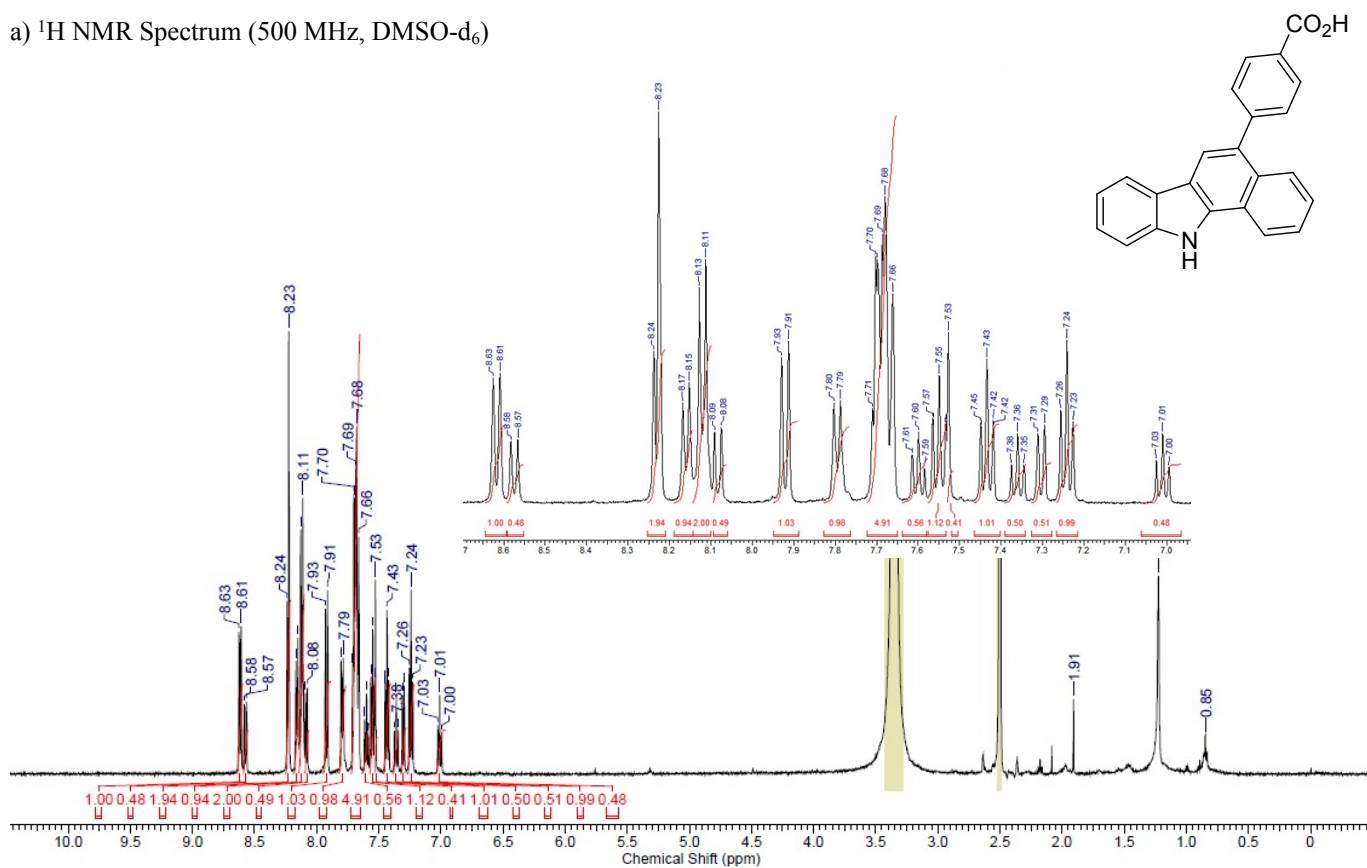


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

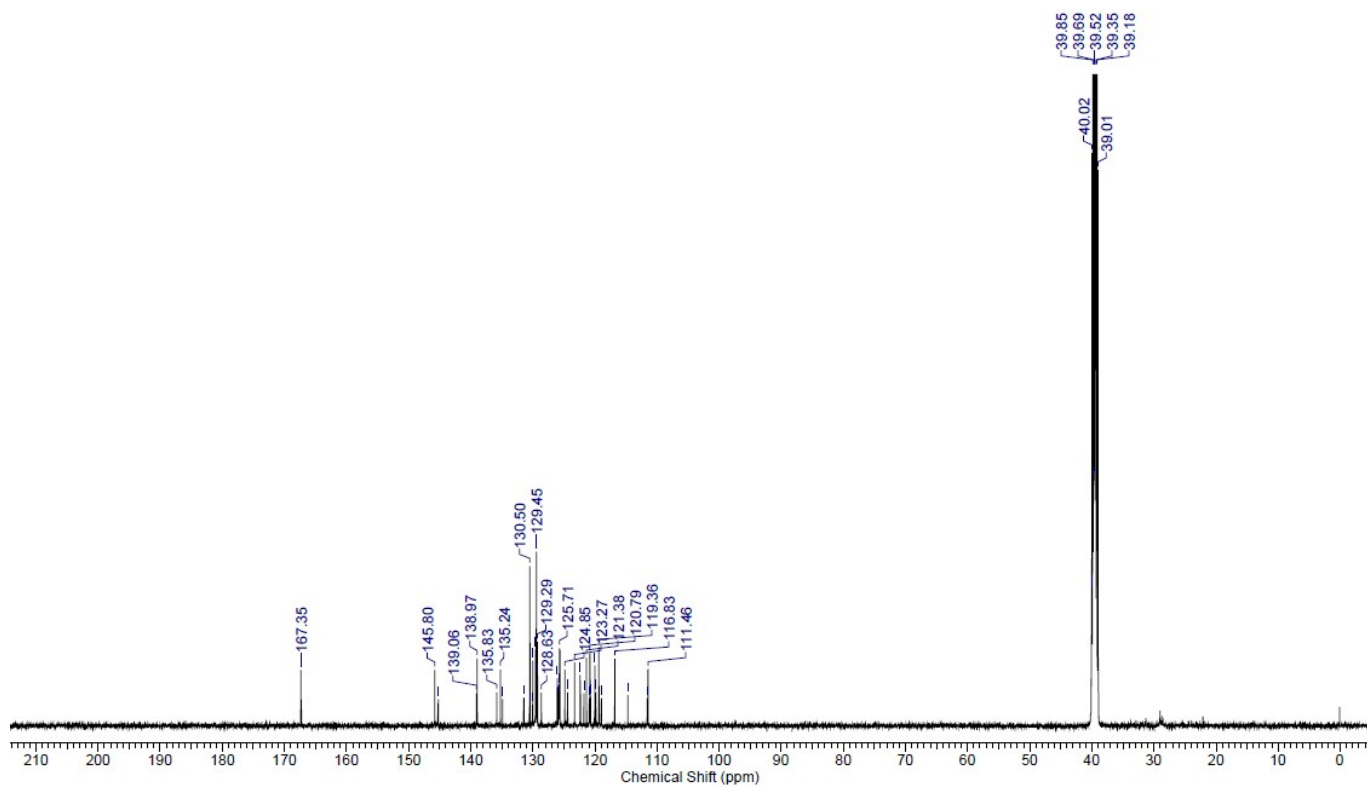


3-6. NMR Spectra of 4-(1*H*-Benzo[*a*]carbazol-6-yl)benzoic acid (**1f**)

a) ¹H NMR Spectrum (500 MHz, DMSO-*d*₆)

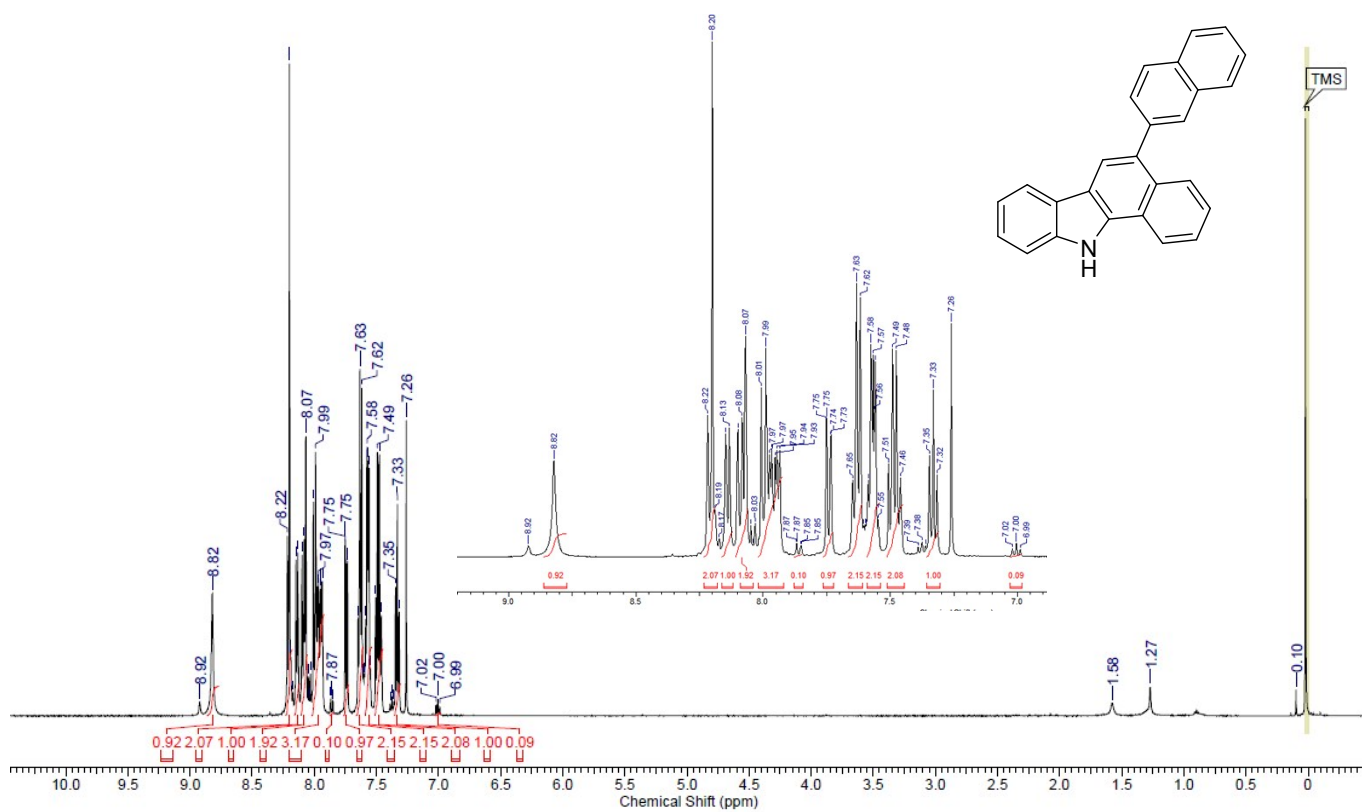


b) ¹³C NMR Spectrum (125 MHz, DMSO-*d*₆)

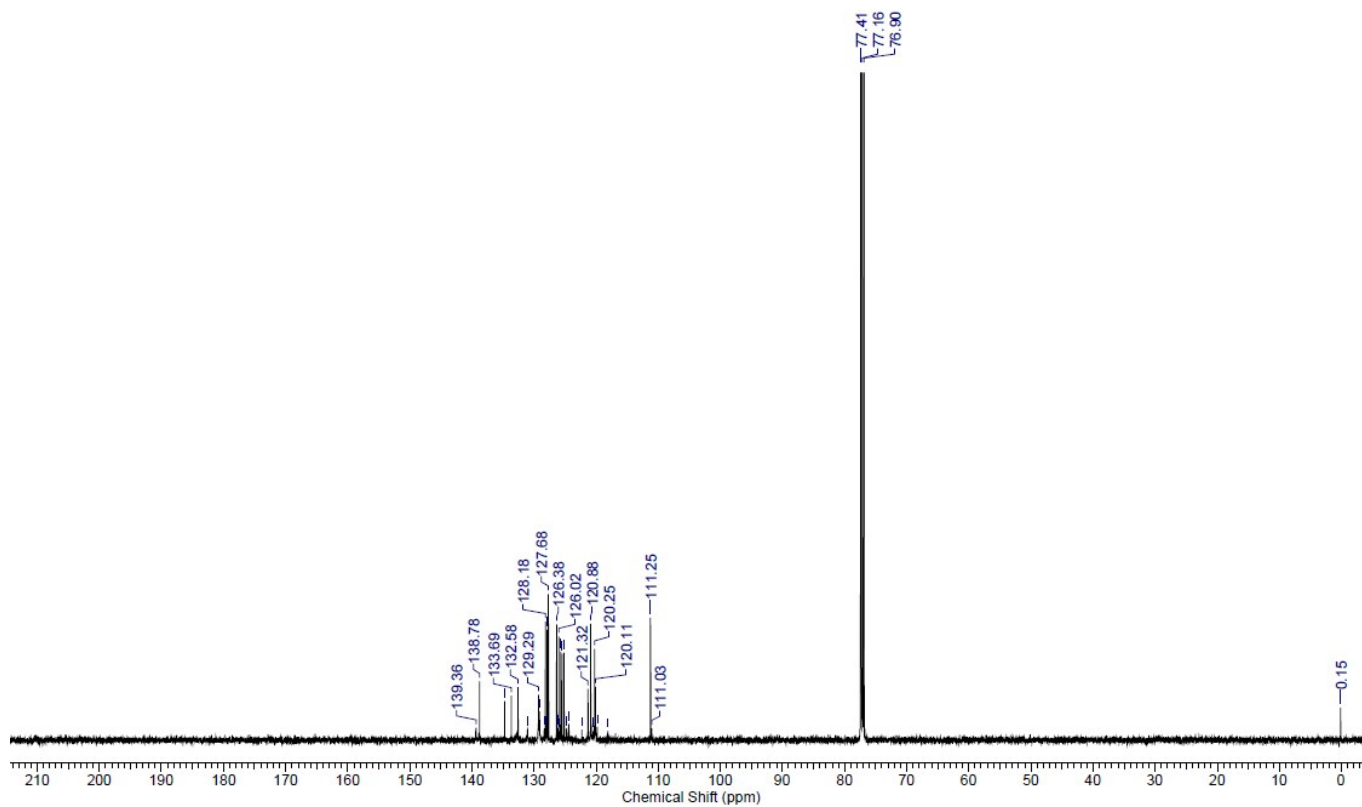


3-7. NMR Spectra of 6-(Naphthalen-2-yl)-11H-benzo[a]carbazole (**1g**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

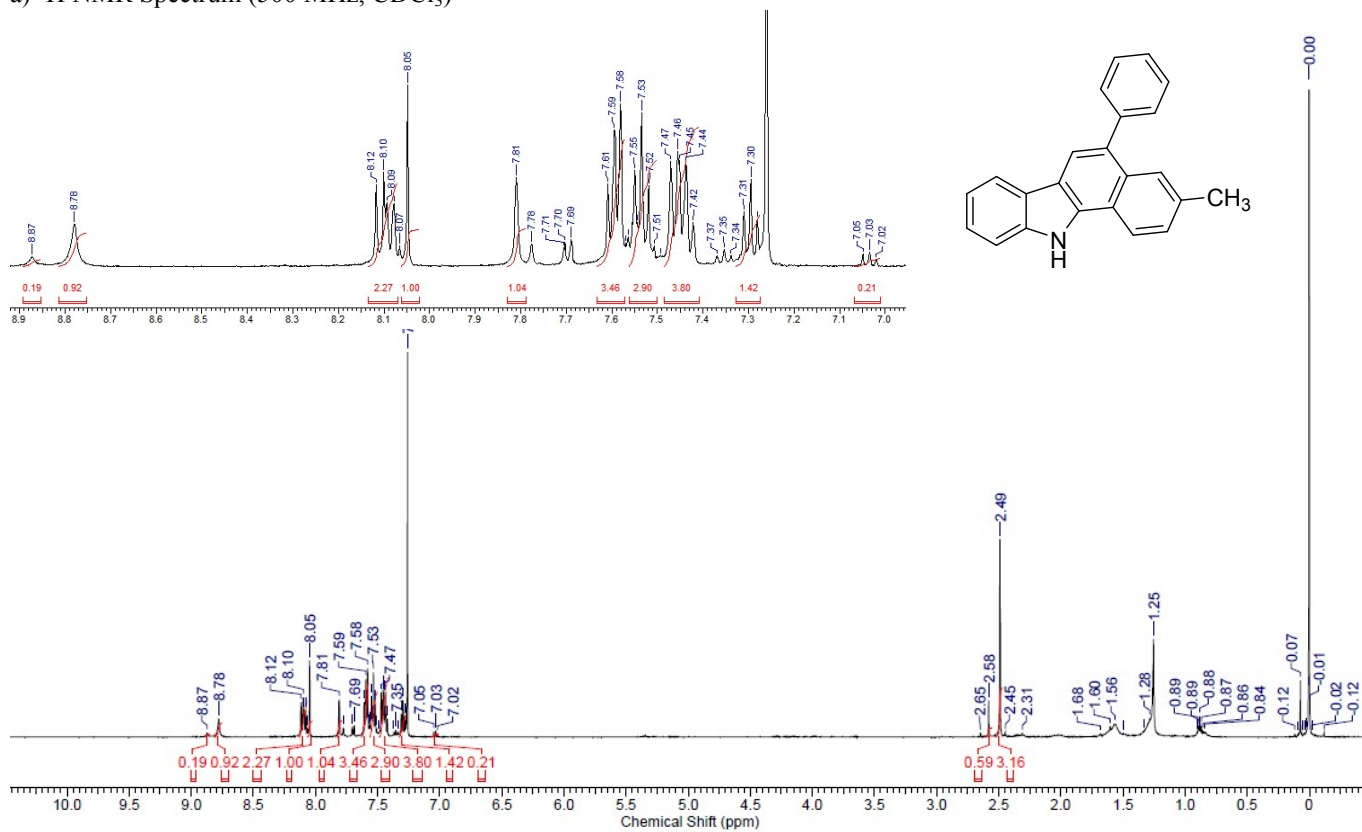


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

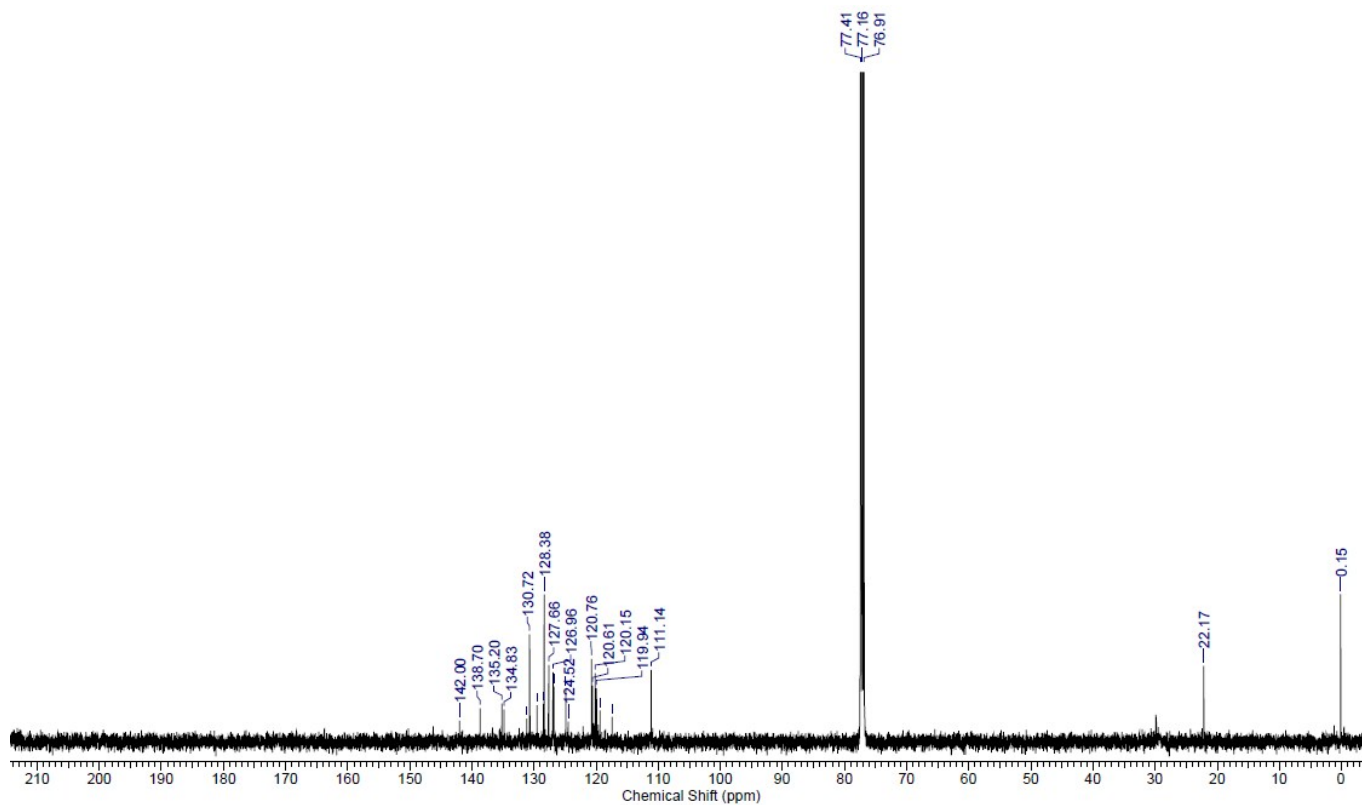


3-8. NMR Spectra of 8-Methyl-6-phenyl-11H-benzo[*a*]carbazole (**1h**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

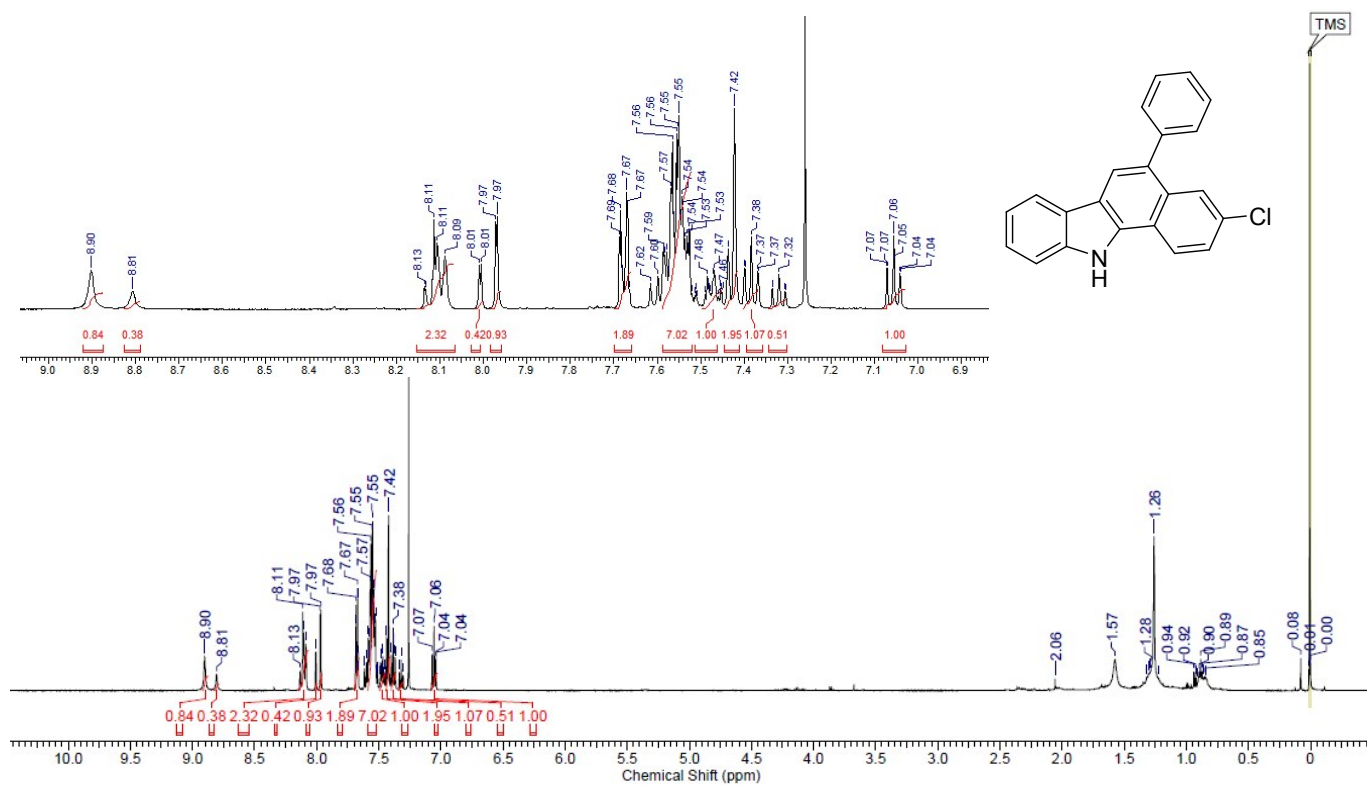


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

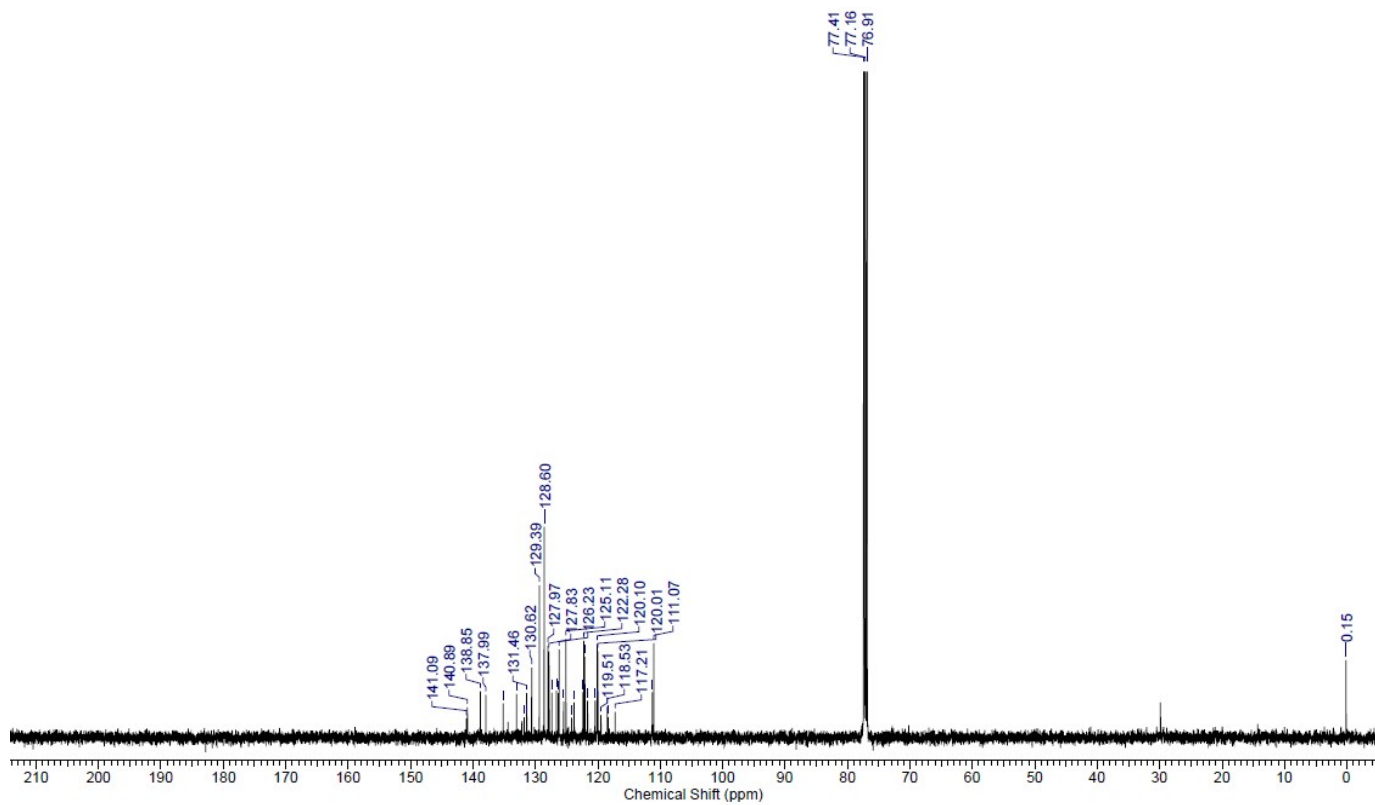


3-9. NMR Spectra of 8-Chloro-6-phenyl-1*H*-benzo[*a*]carbazole (**1i**)

a) ¹H NMR Spectrum (500 MHz, CDCl₃)

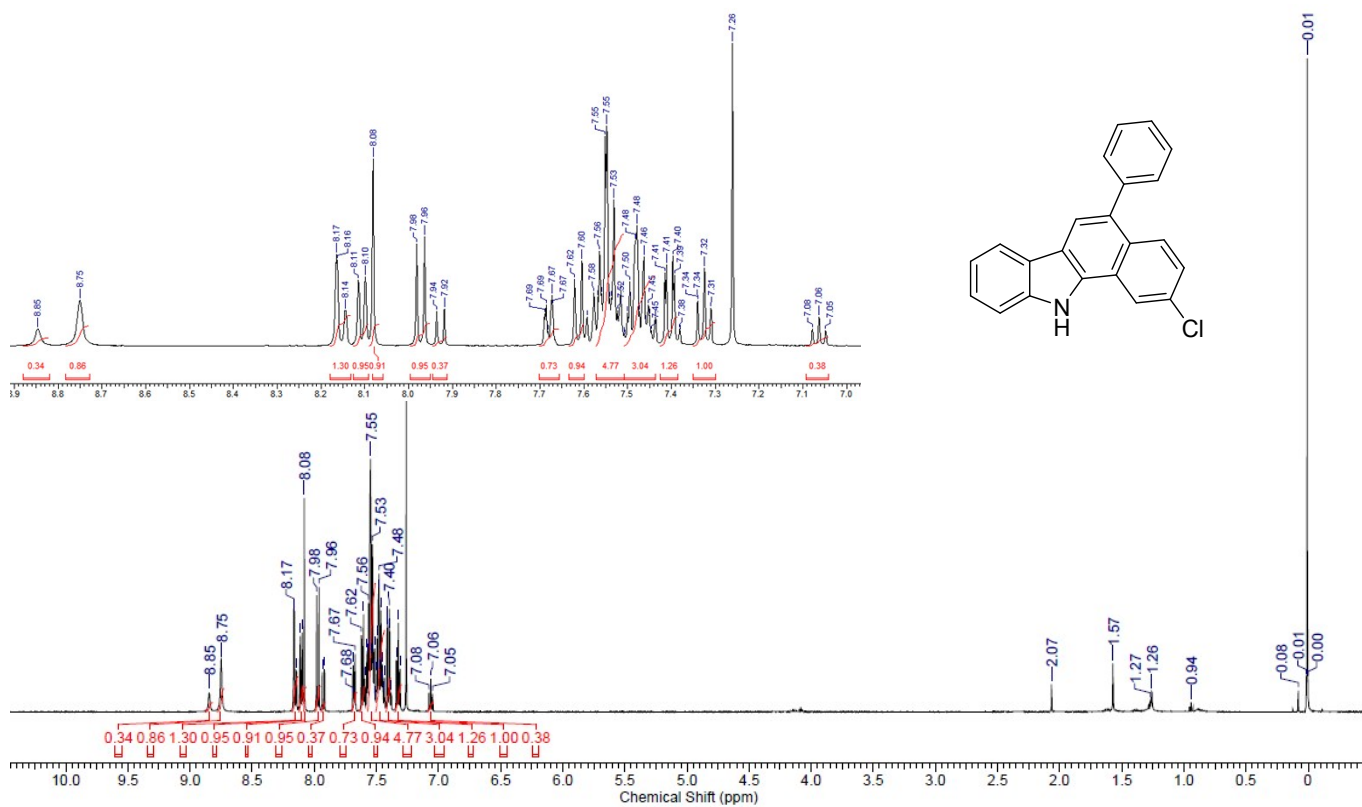


b) ¹³C NMR Spectrum (125 MHz, CDCl₃)

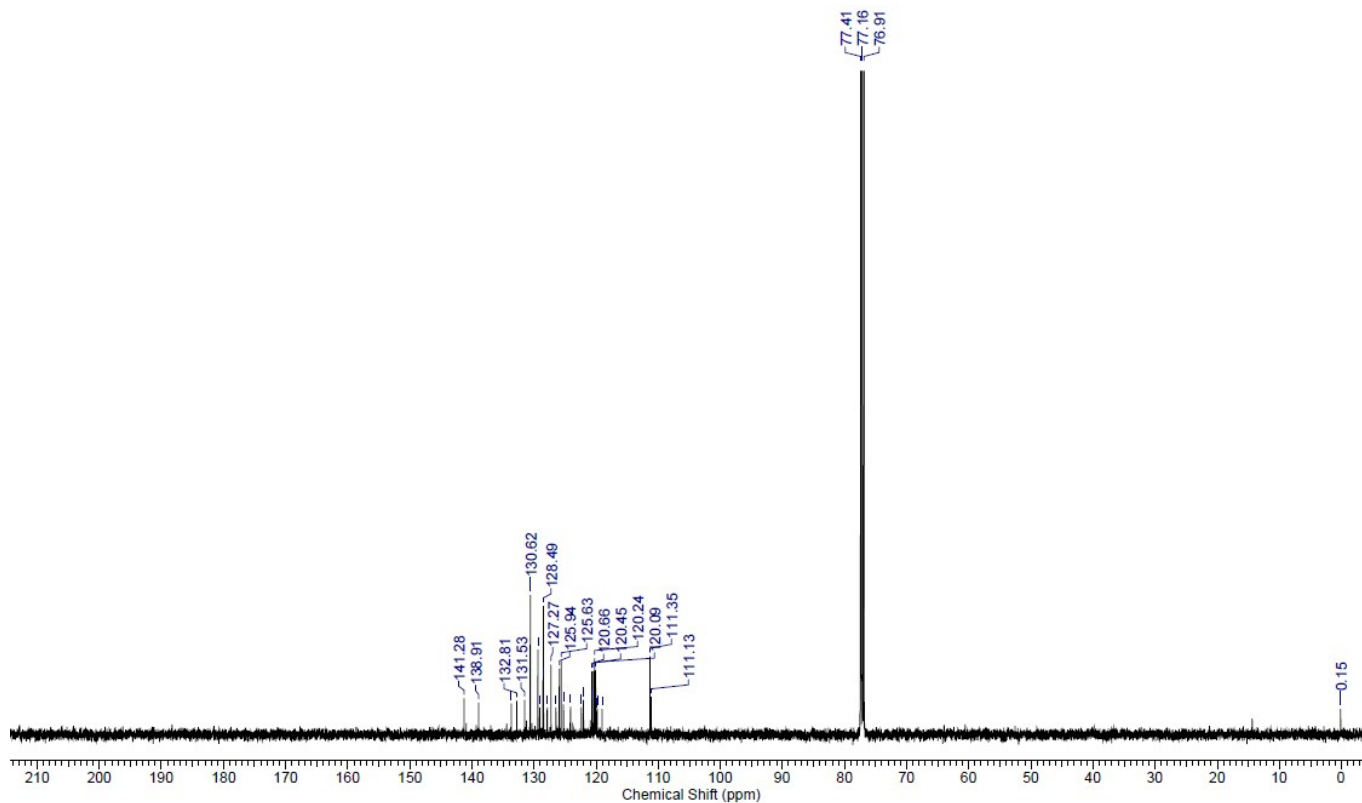


3-10. NMR Spectra of 9-Chloro-6-phenyl-11H-benzo[*a*]carbazole (**1ja**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

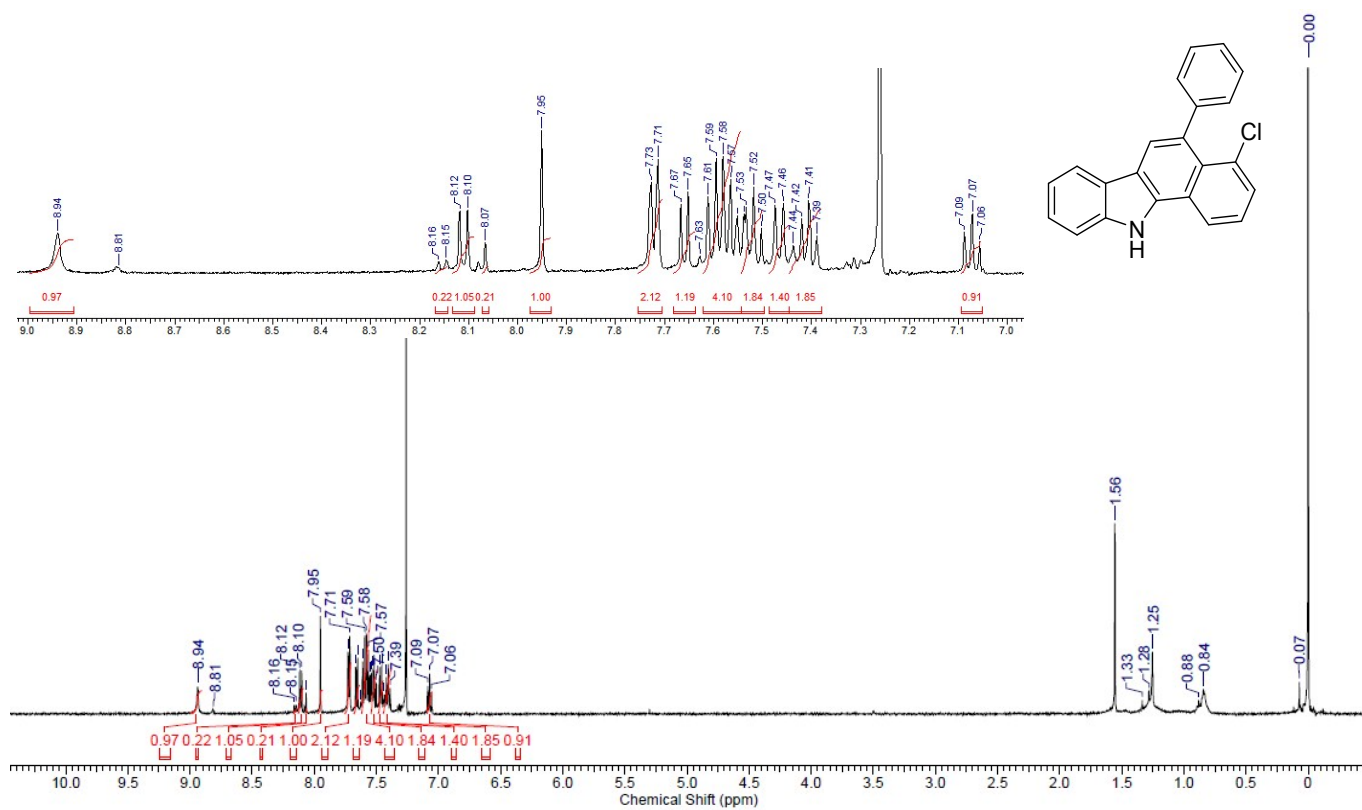


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)



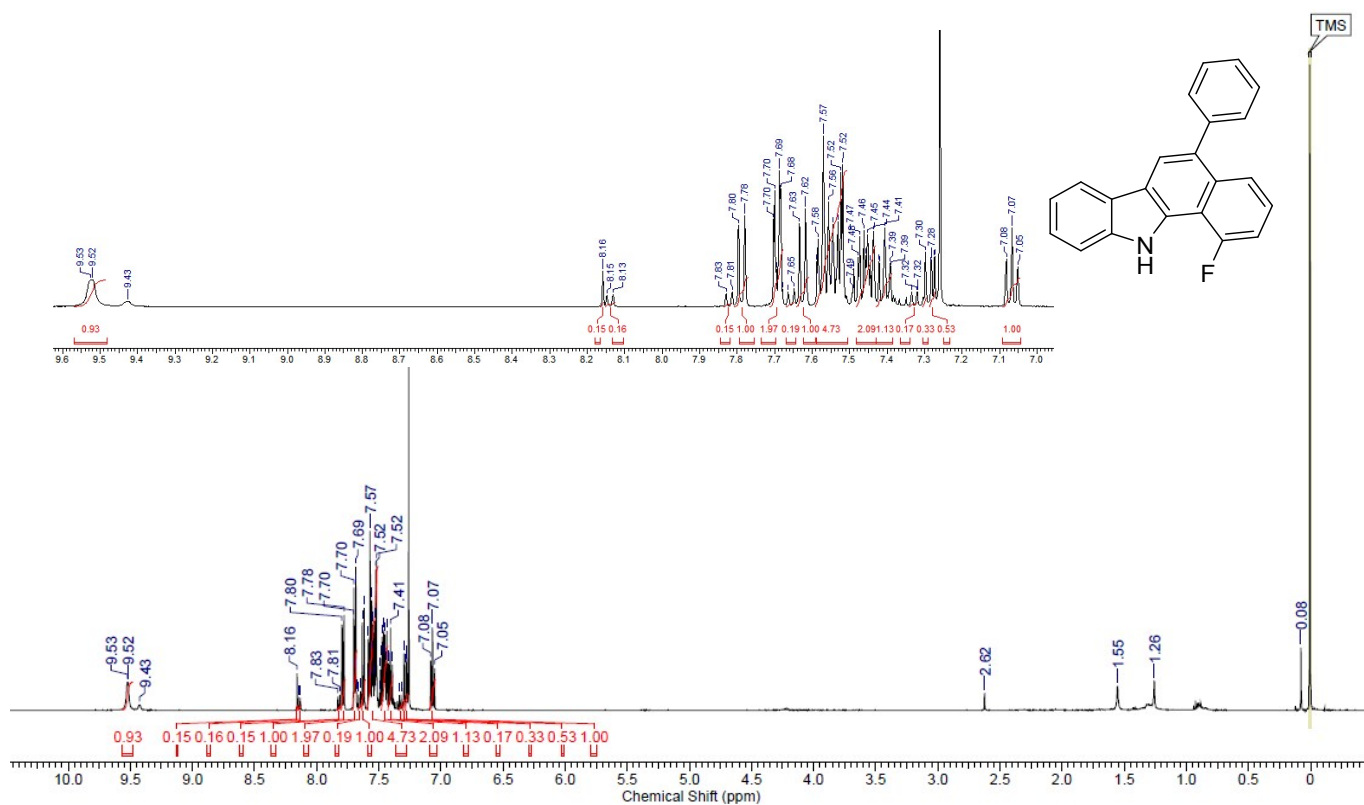
3-11. NMR Spectra of 7-Chloro-6-phenyl-11H-benzo[*a*]carbazole (**1j**b****)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

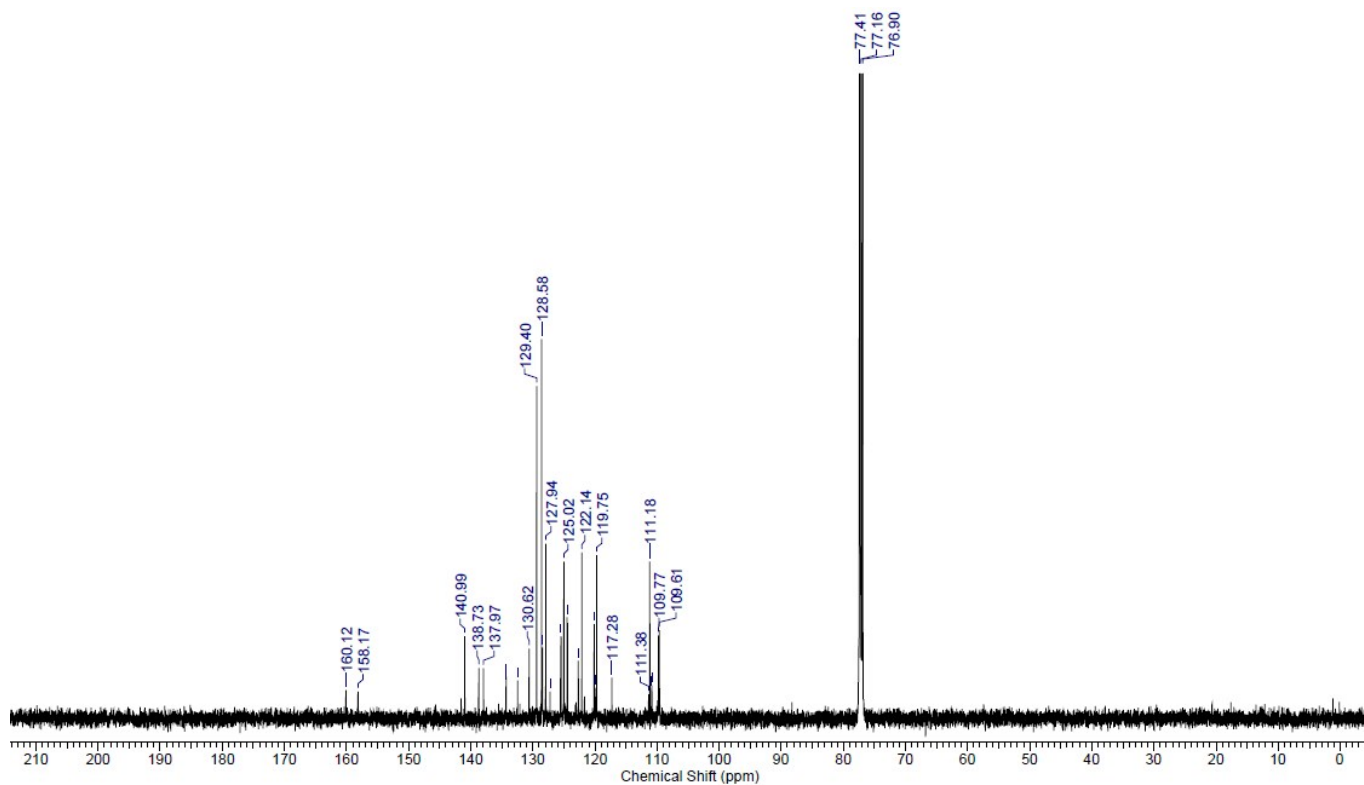


3-12. NMR Spectra of 10-Fluoro-6-phenyl-11H-benzo[a]carbazole (**1k**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

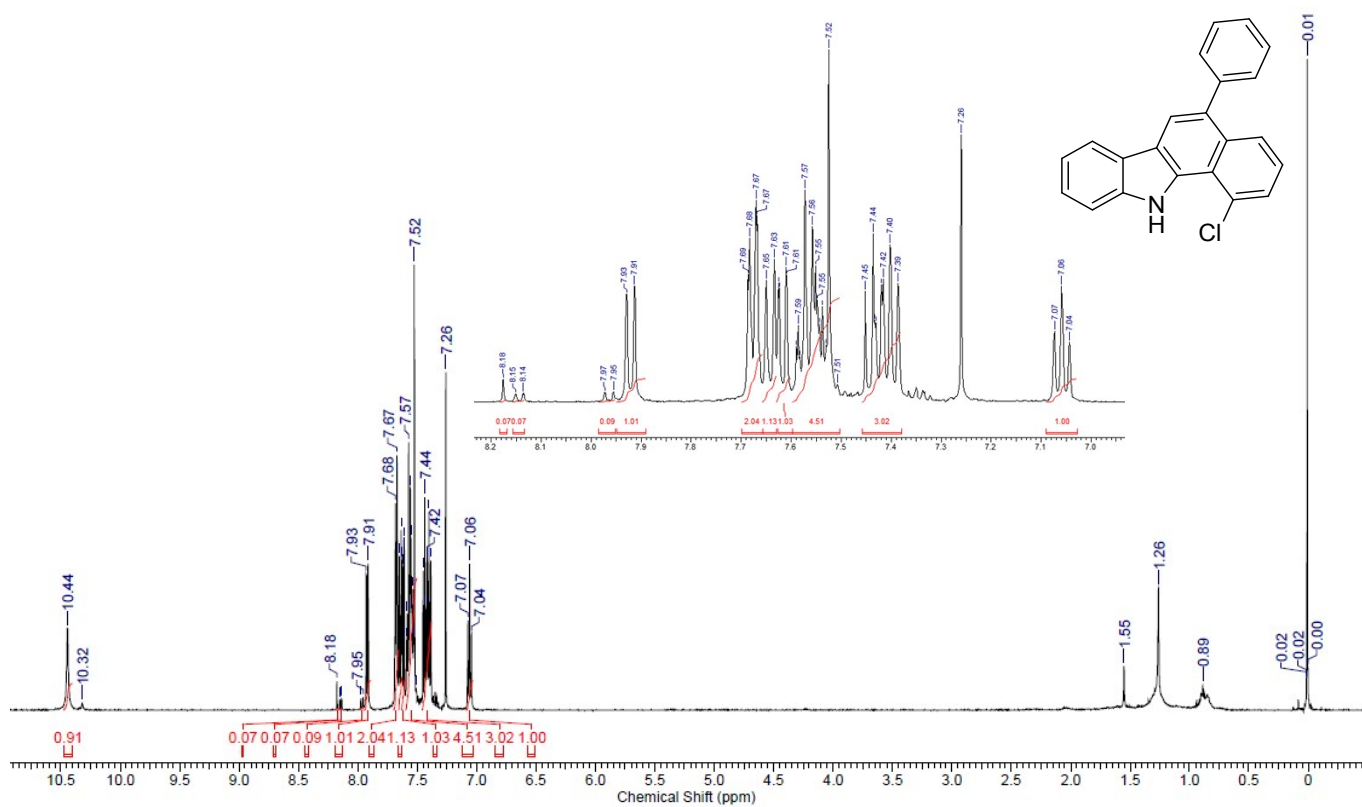


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

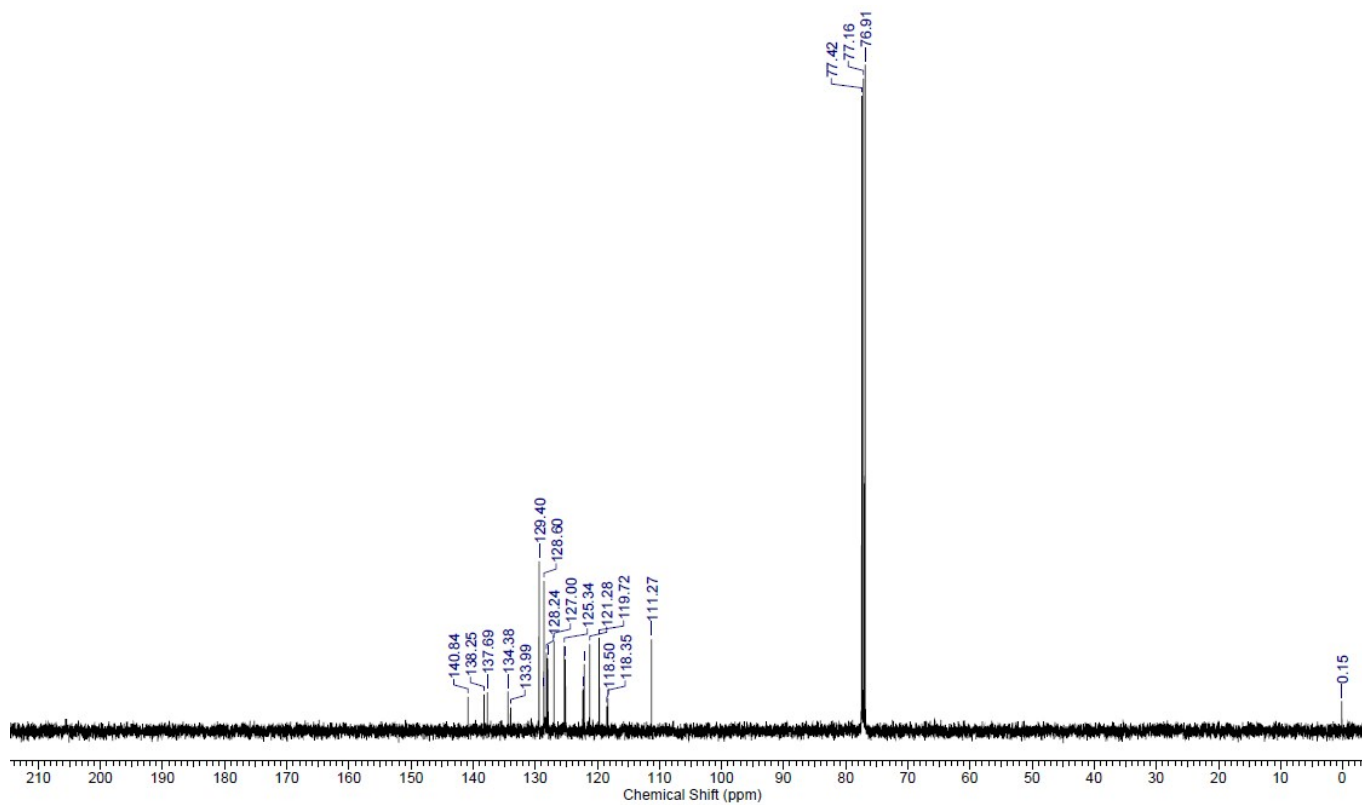


3-13. NMR Spectra of 10-Chloro-6-phenyl-11H-benzo[a]carbazole (**11**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

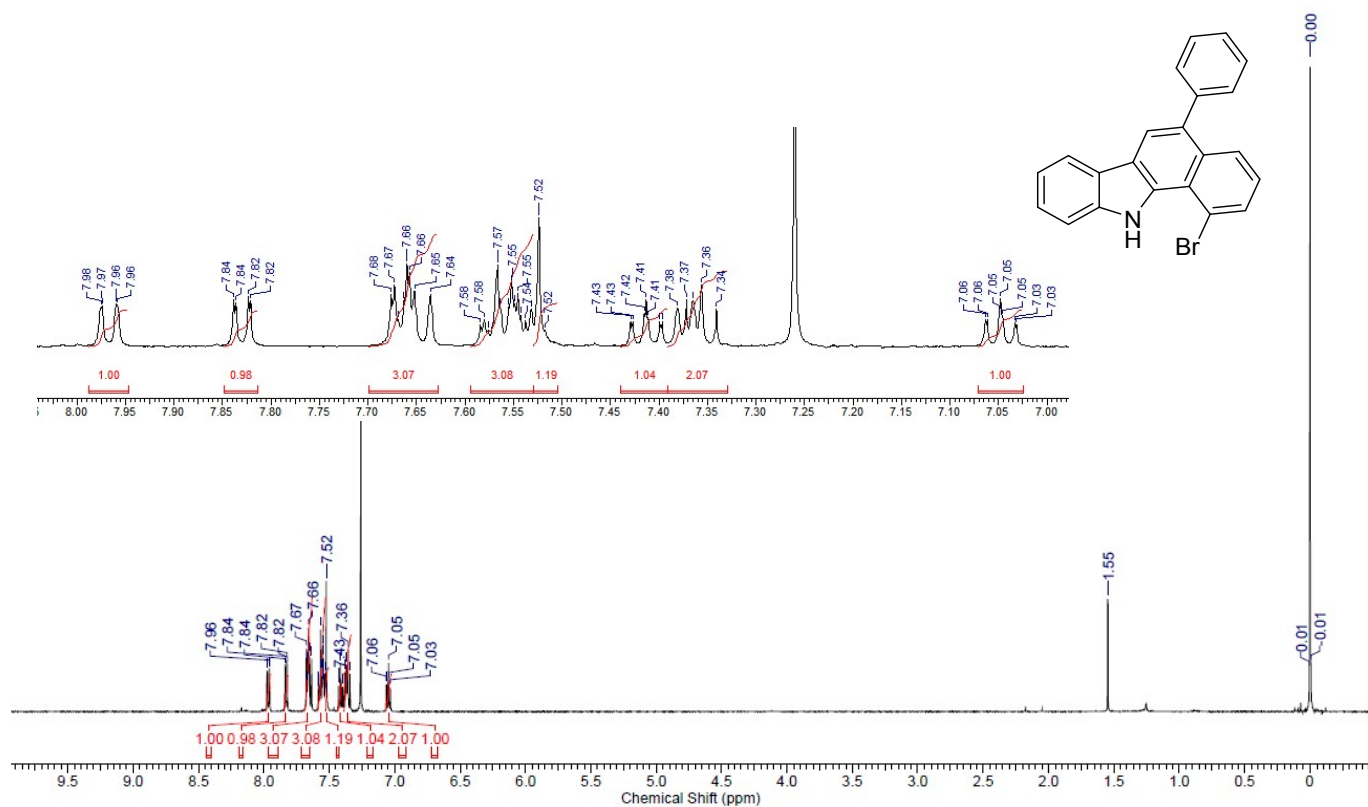


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

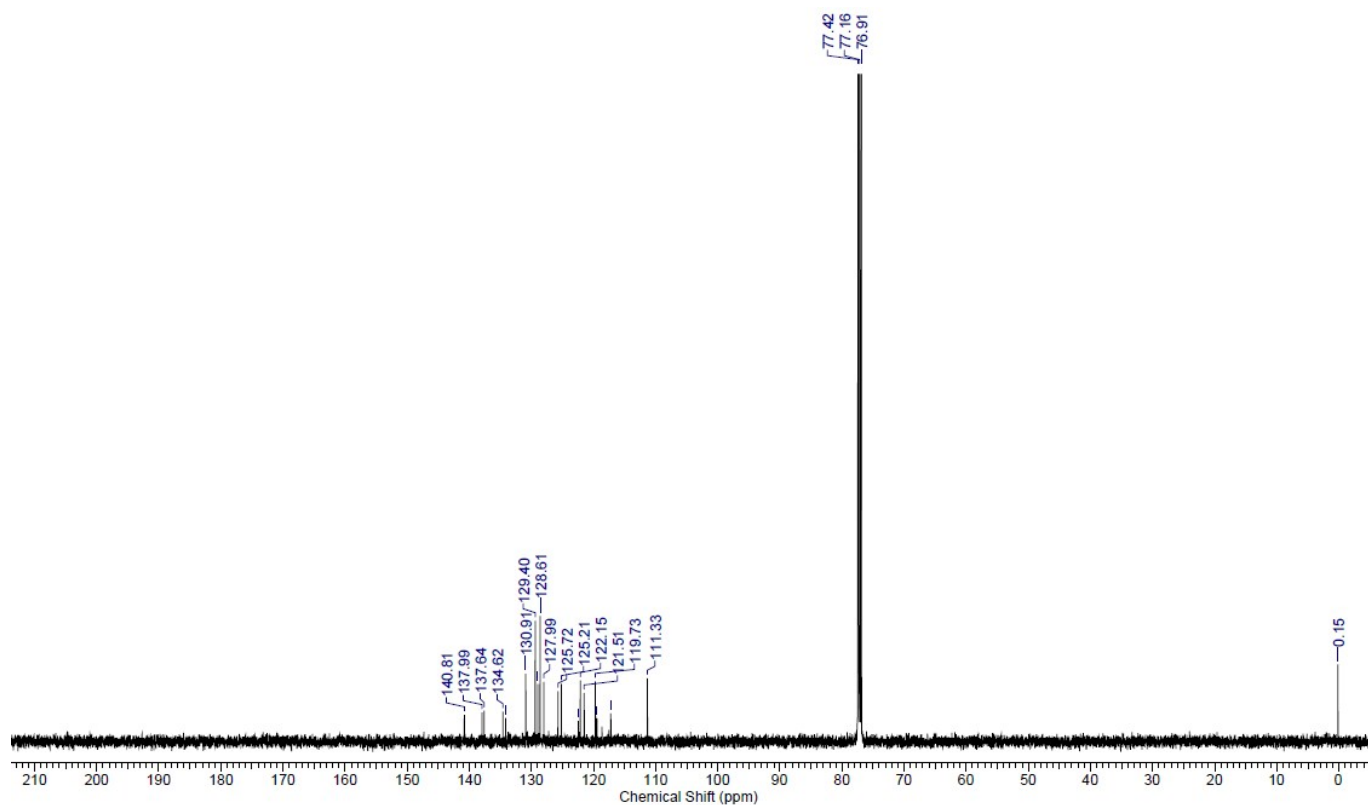


3-14. NMR Spectra of 10-Bromo-6-phenyl-11H-benzo[a]carbazole (**1m**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)



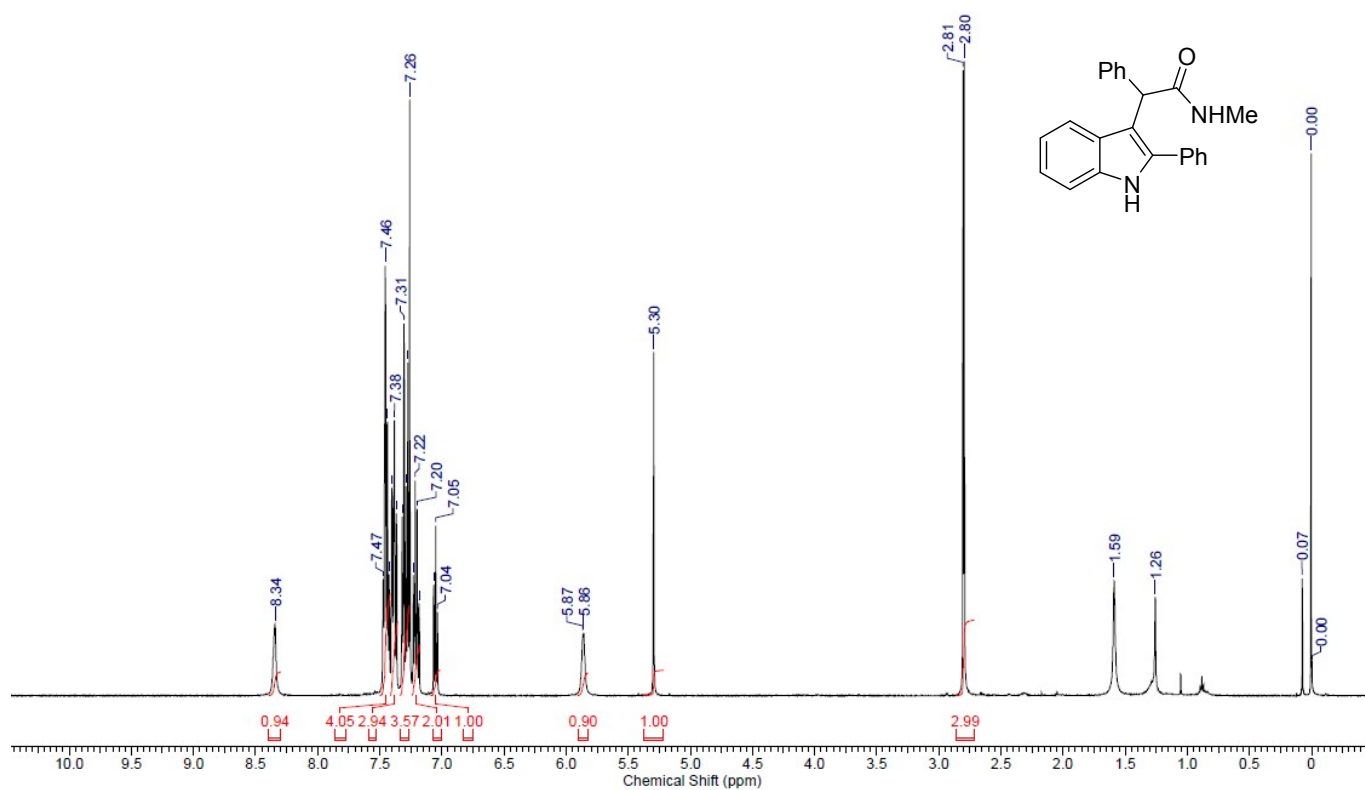
b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)



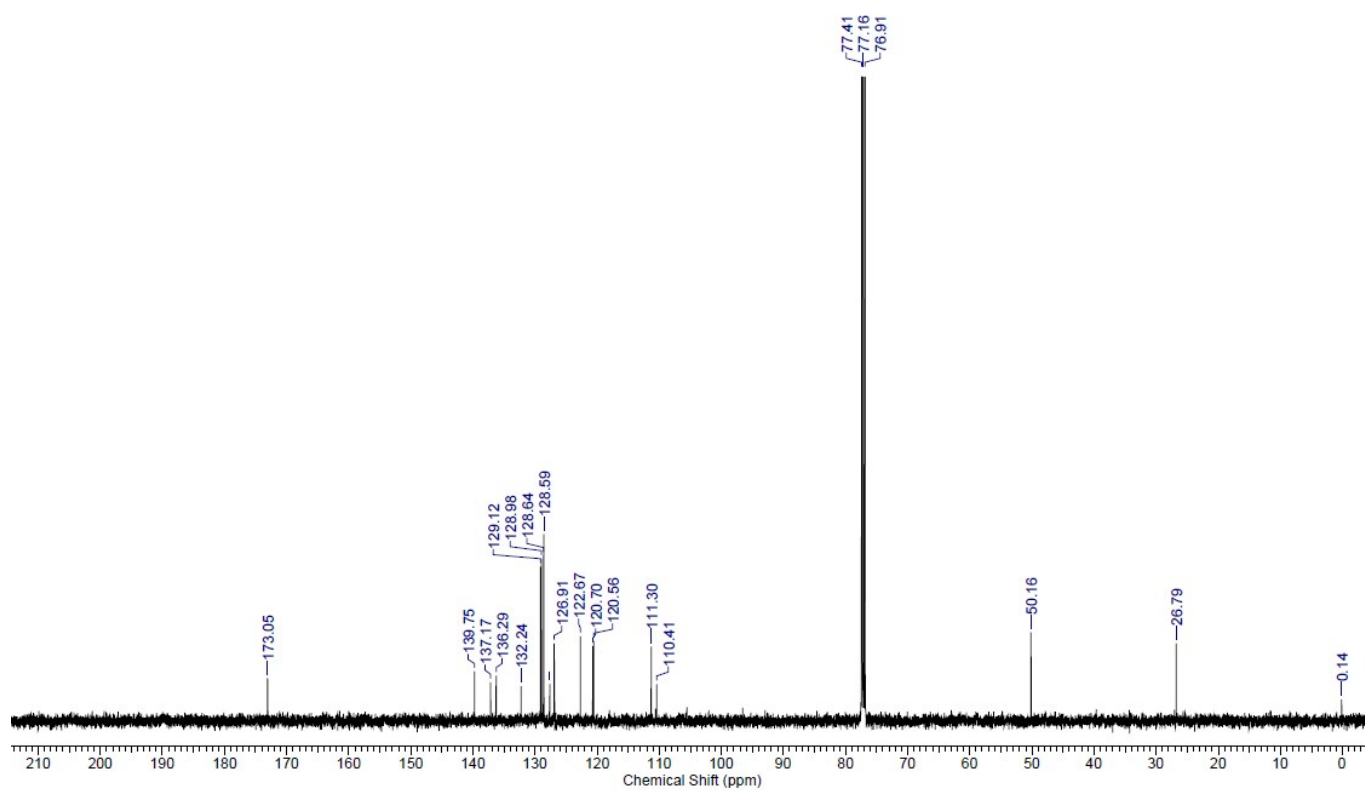
4. Spectroscopic Data of Acetamide Derivatives (9)

4-1. NMR Spectra of *N*-Methyl-2-phenyl-2-(2-phenyl-1*H*-indol-3-yl)acetamide (9a)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

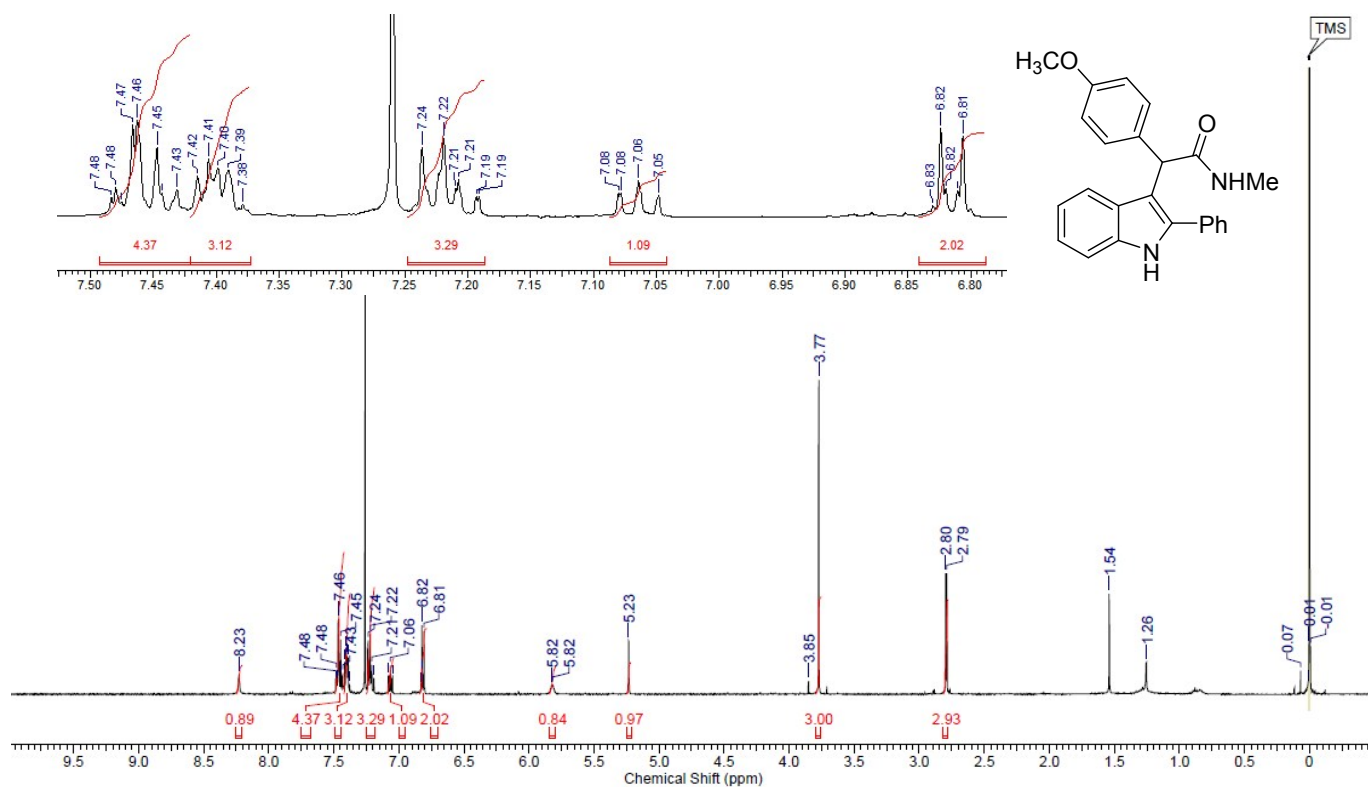


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)

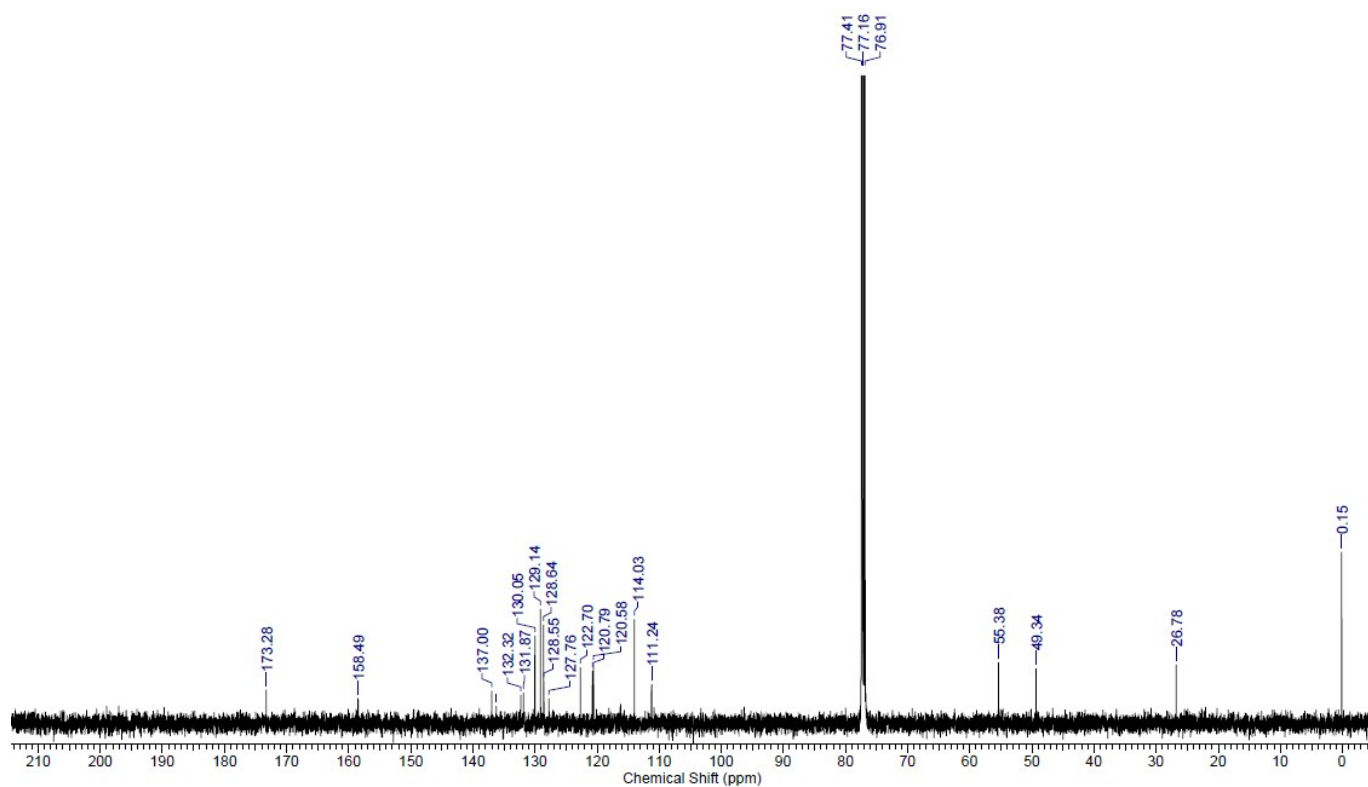


4.2. NMR Spectra of 2-(4-Methoxyphenyl)-N-methyl-2-(2-phenyl-1H-indol-3-yl)acetamide (**9m**)

a) ^1H NMR Spectrum (500 MHz, CDCl_3)

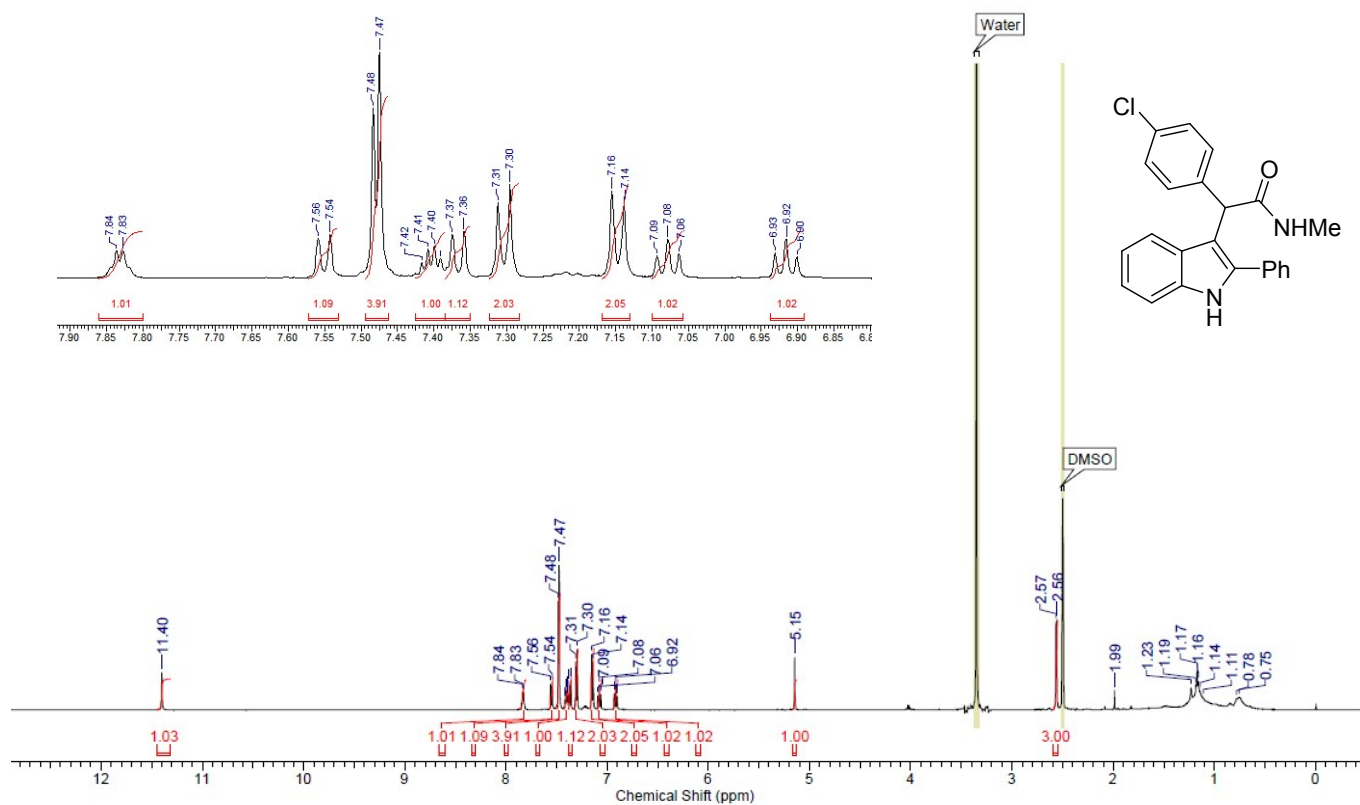


b) ^{13}C NMR Spectrum (125 MHz, CDCl_3)



4-3. NMR Spectra of 2-(4-Chlorophenyl)-N-methyl-2-(2-phenyl-1H-indol-3-yl)acetamide (**9o**)

a) ¹H NMR Spectrum (500 MHz, DMSO-d₆)



b) ¹³C NMR Spectrum (125 MHz, DMSO-d₆)

