

## Supporting Information

# Synthesis of xylyl-linked bis-benzimidazolium salts and their application in the palladium-catalyzed Suzuki–Miyaura cross-coupling reaction of aryl chlorides

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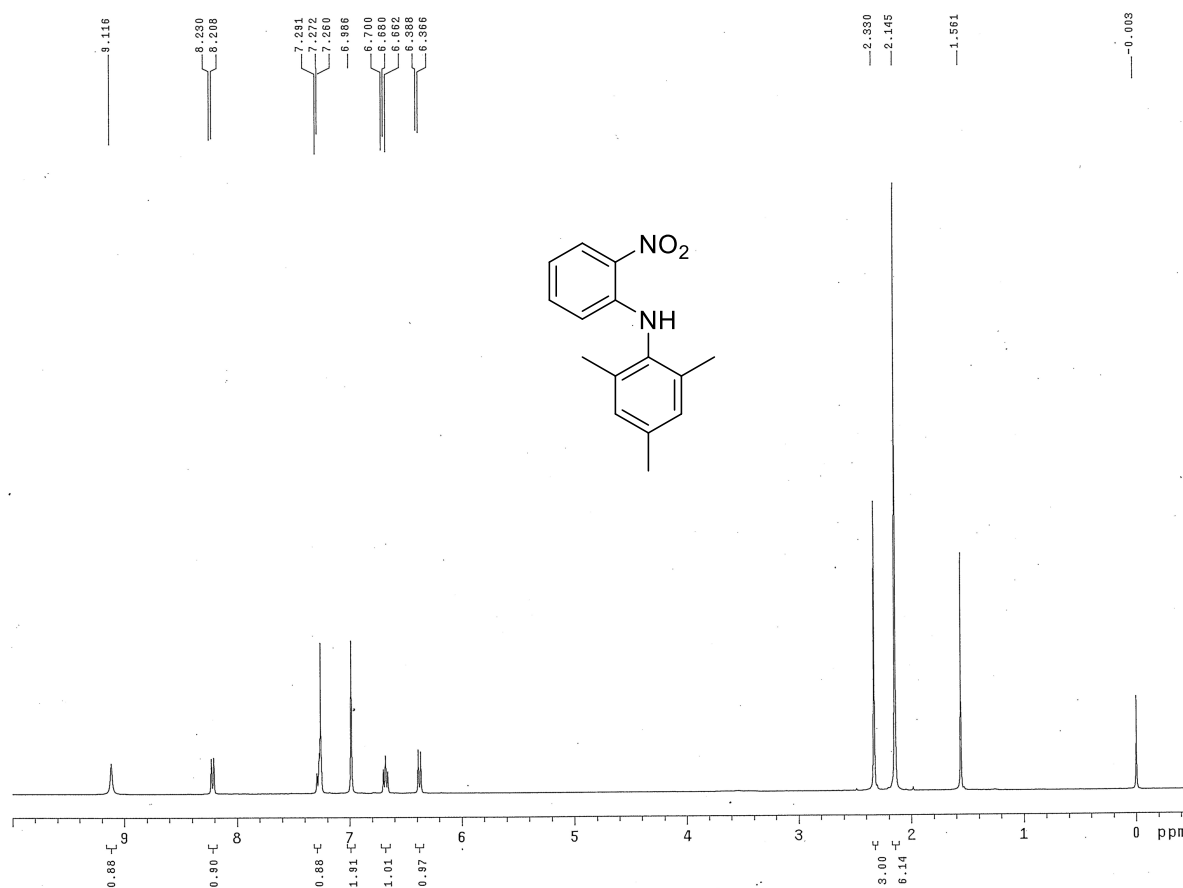


Figure S1: <sup>1</sup>H NMR spectrum of 2-(2',4',6'-trimethylanilido)nitrobenzene **S1** in CDCl<sub>3</sub>.

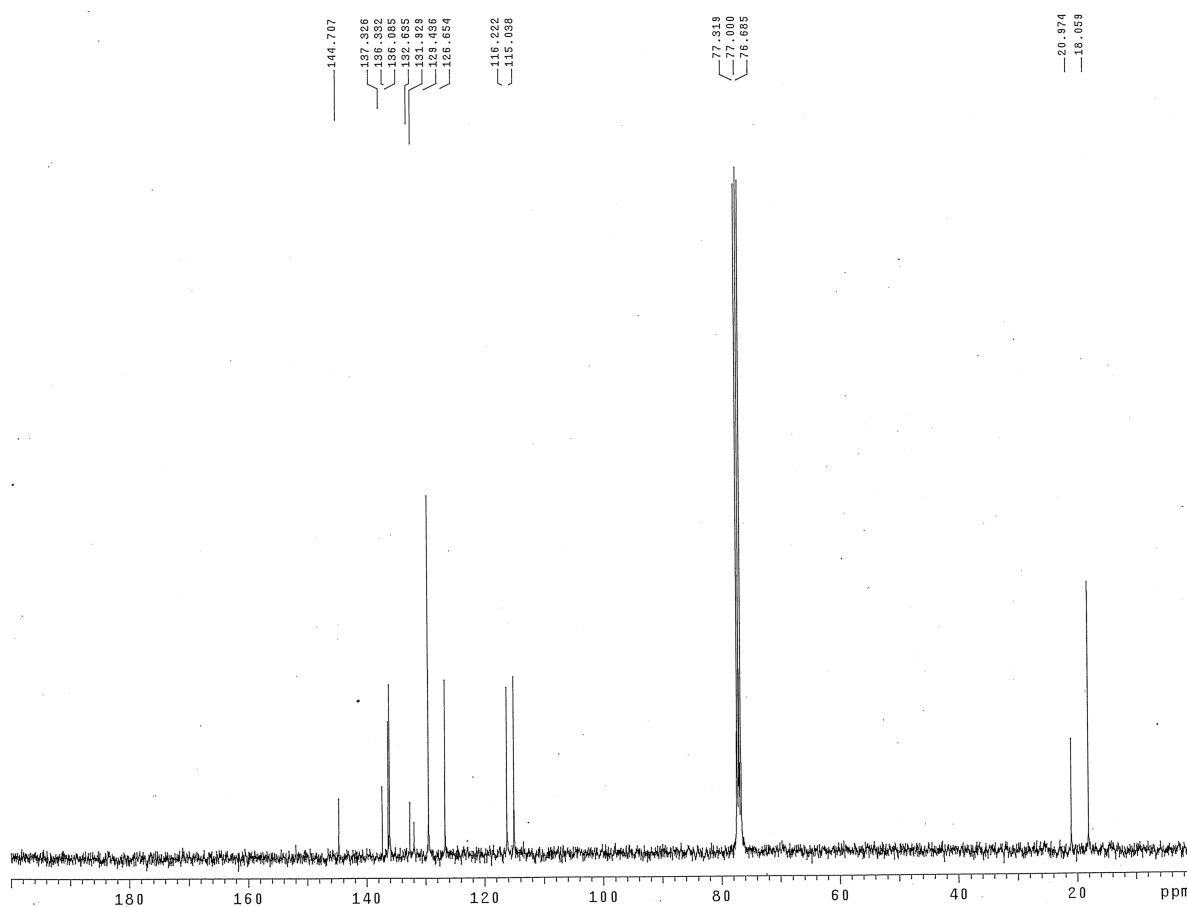


Figure S2: <sup>13</sup>C NMR spectrum of 2-(2',4',6'-trimethylanilido)nitrobenzene **S1** in CDCl<sub>3</sub>.

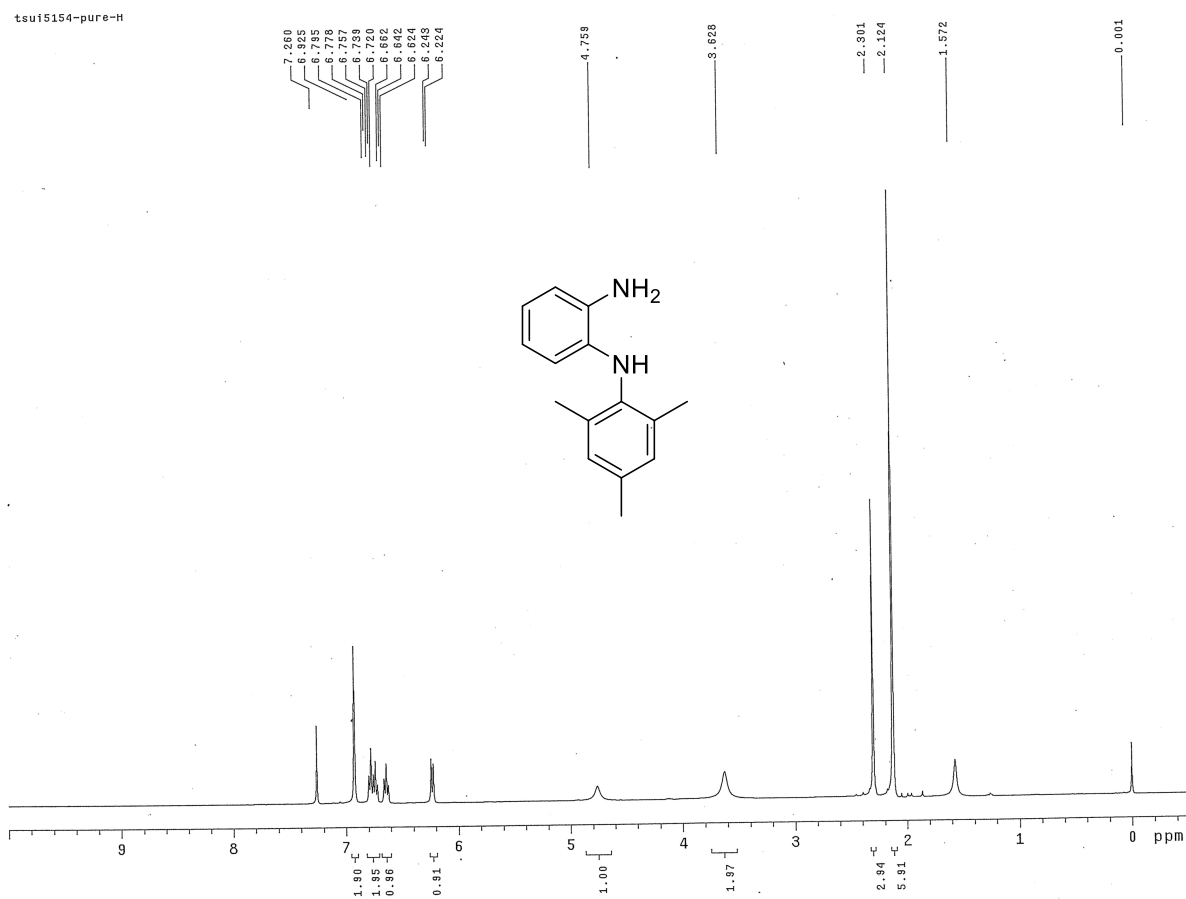


Figure S3: <sup>1</sup>H NMR spectrum of *N*-(2,4,6-trimethylphenyl)-1,2-phenylenediamine **S1** in CDCl<sub>3</sub>.

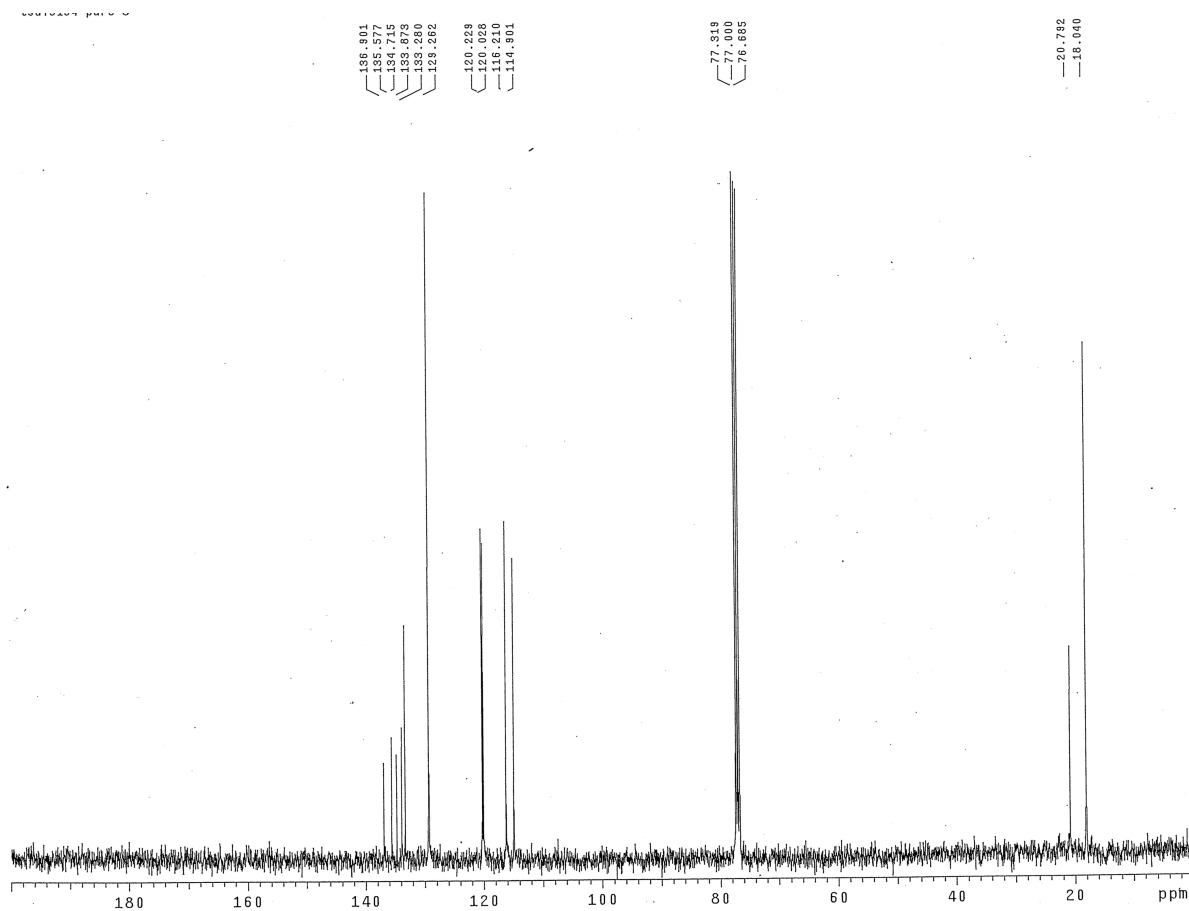


Figure S4: <sup>13</sup>C NMR spectrum of *N*-(2,4,6-trimethylphenyl)-1,2-phenylenediamine **S2** in CDCl<sub>3</sub>.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz) spectrum of compound **2b**

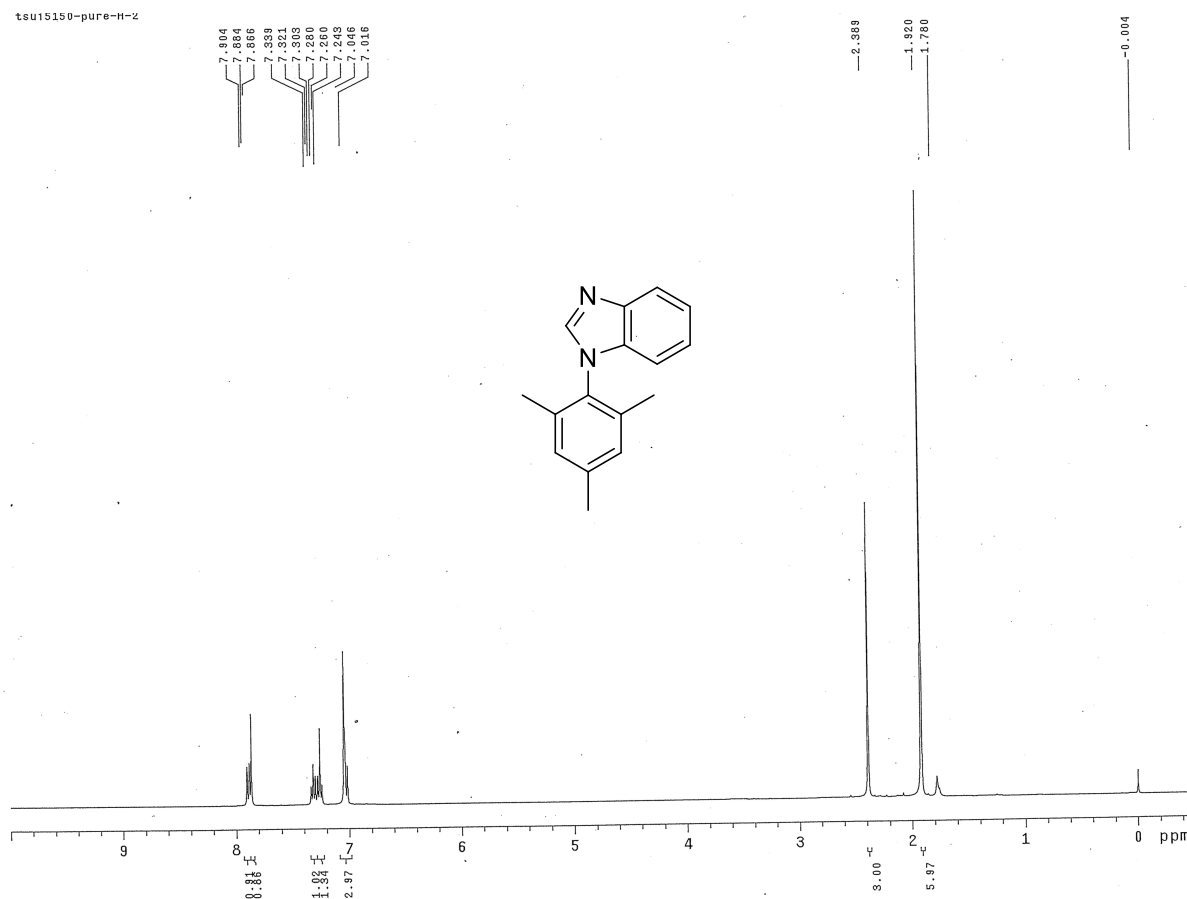


Figure S5:  $^1\text{H}$  NMR spectrum of 1-(2,4,6-trimethylphenyl)-1H-benzimidazole **2b** in  $\text{CDCl}_3$ .

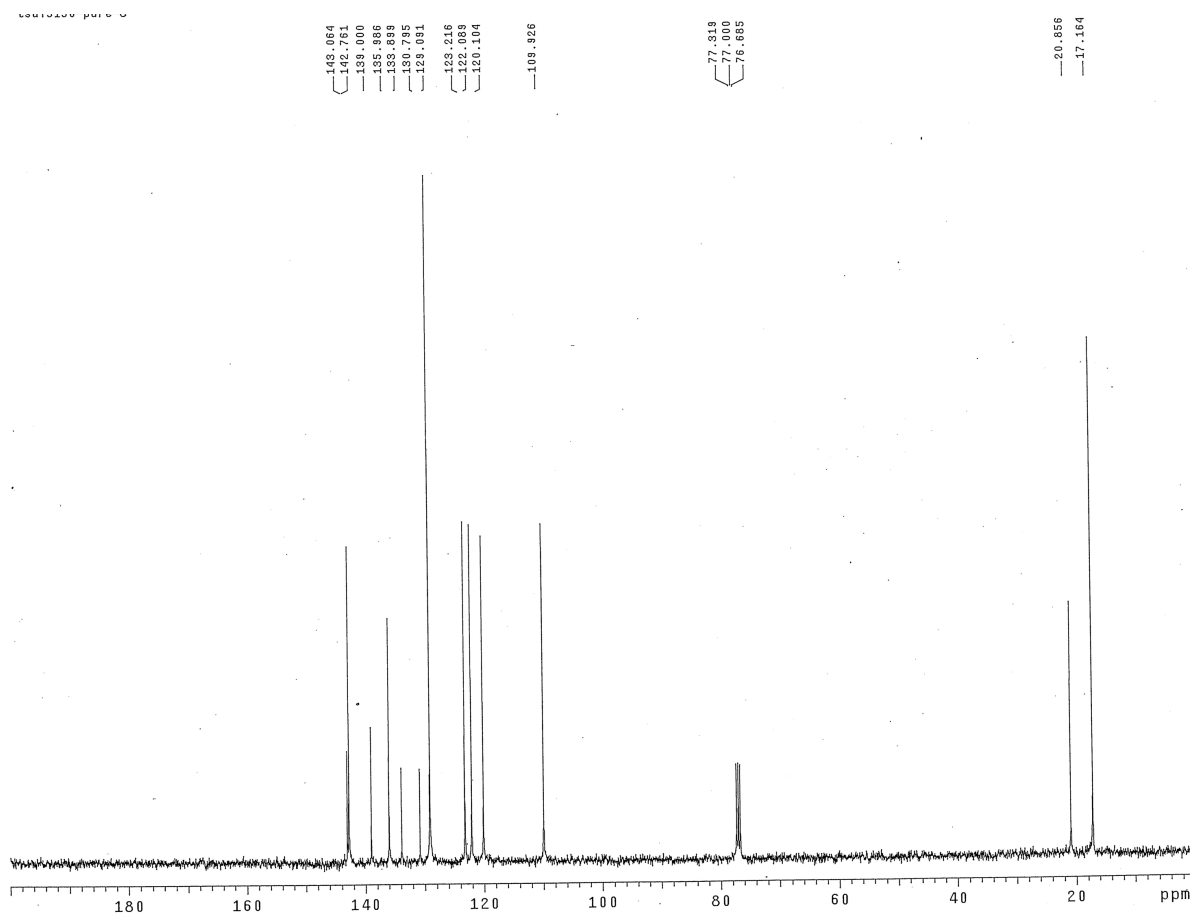


Figure S6:  $^{13}\text{C}$  NMR spectrum of 1-(2,4,6-trimethylphenyl)-1H-benzimidazole **2b** in  $\text{CDCl}_3$ .



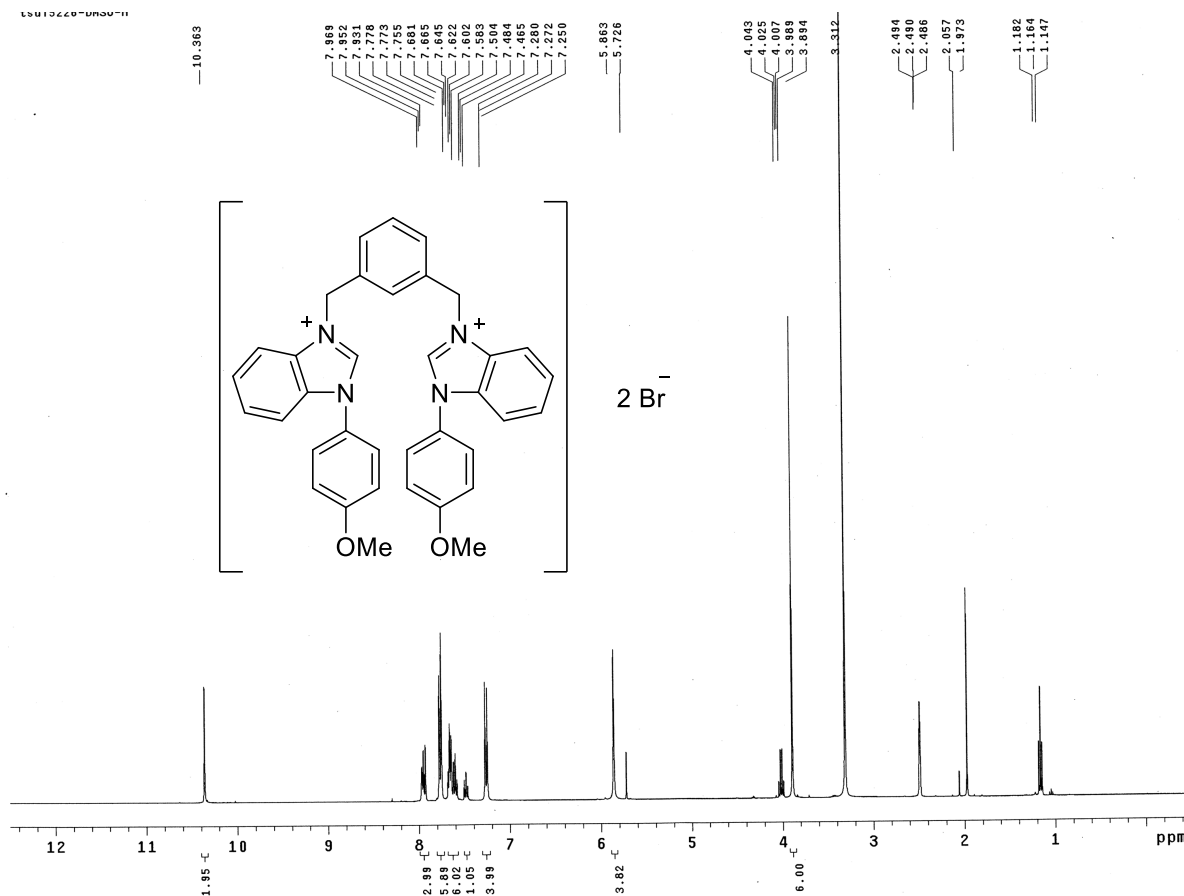


Figure S7: <sup>1</sup>H NMR spectrum of (3,3'-(1,3-phenylenebis(methylene))bis(1-(4-methoxyphenyl)-1H-benzo[d]imidazol-3-ium)) dibromide (**3a**) in DMSO-d<sub>6</sub>.

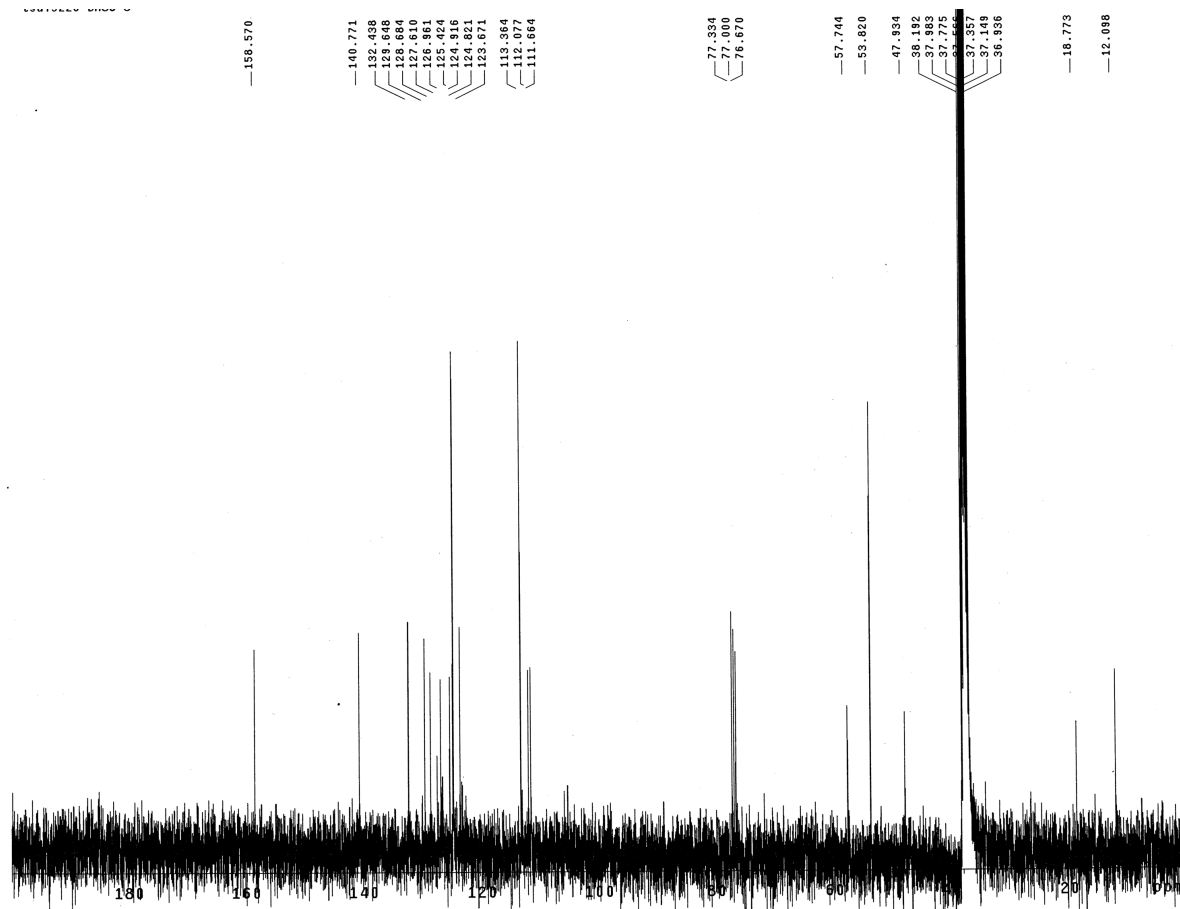


Figure S8: <sup>13</sup>C NMR spectrum of (3,3'-(1,3-phenylenebis(methylene))bis(1-(4-methoxyphenyl)-1H-benzo[d]imidazol-3-ium)) dibromide (**3a**) in DMSO-d<sub>6</sub>.

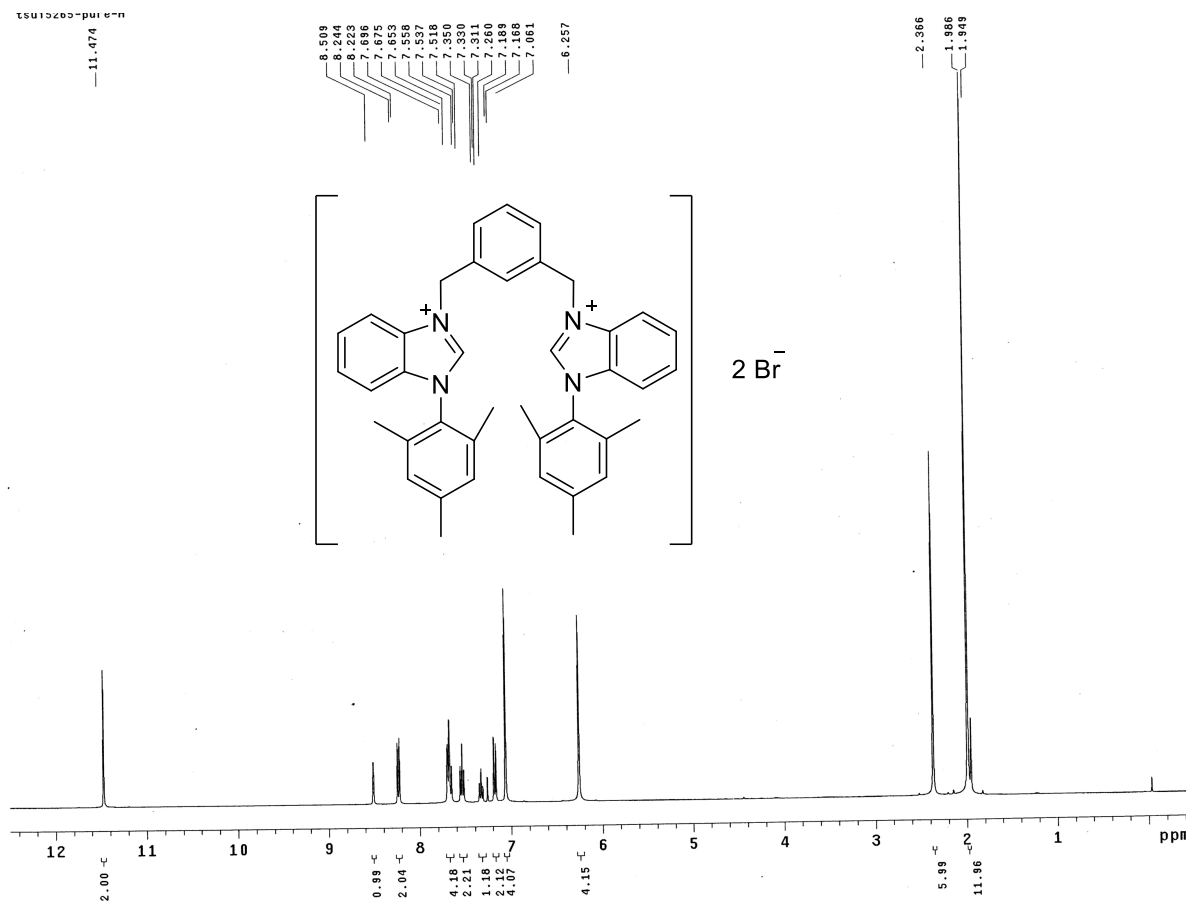


Figure S9: <sup>1</sup>H NMR spectrum of (3,3'-(1,3-phenylenebis(methylene))bis(1-mesityl-1H-benzo[d]imidazol-3-ium)) dibromide (**3b**) in CDCl<sub>3</sub>.

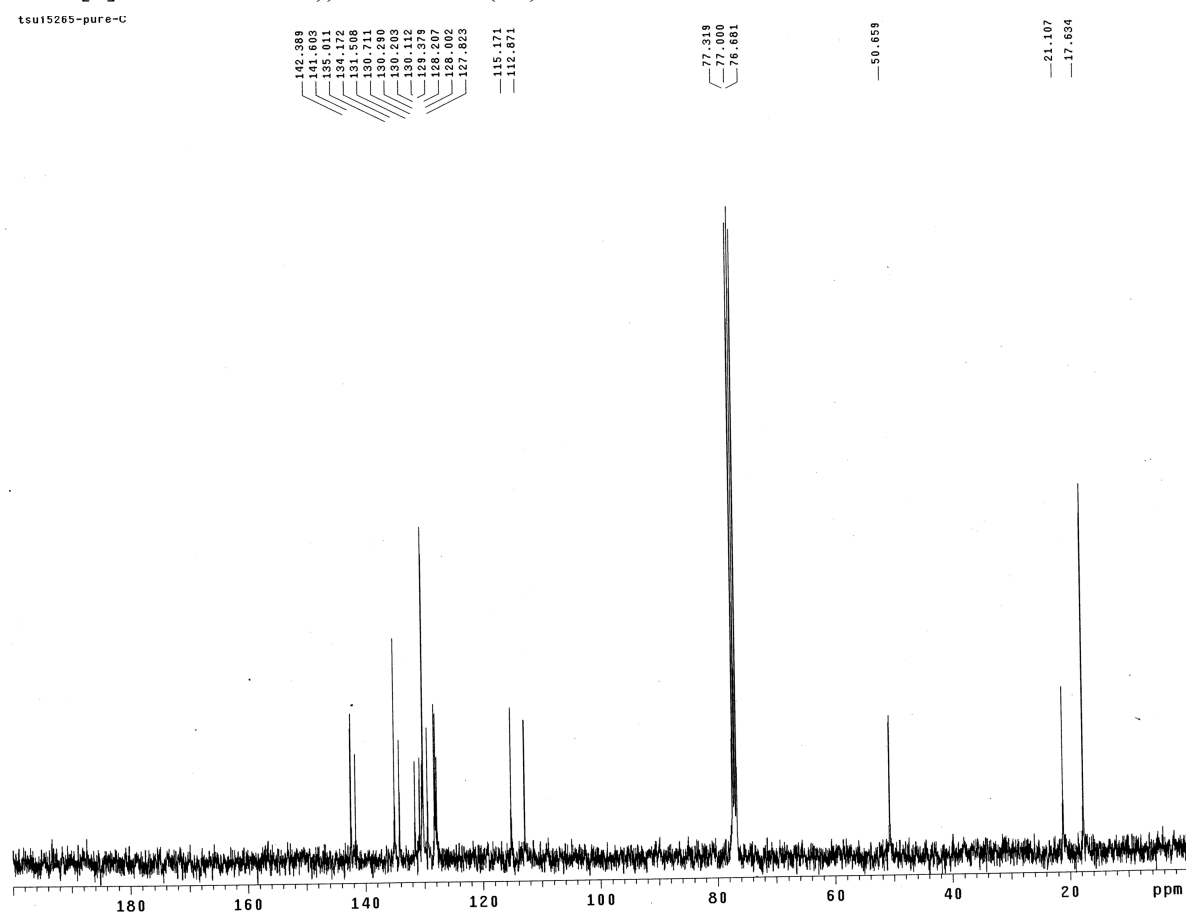


Figure S10: <sup>13</sup>C NMR spectrum of (3,3'-(1,3-phenylenebis(methylene))bis(1-mesityl-1H-benzo[d]imidazol-3-ium)) dibromide (**3b**) in CDCl<sub>3</sub>.

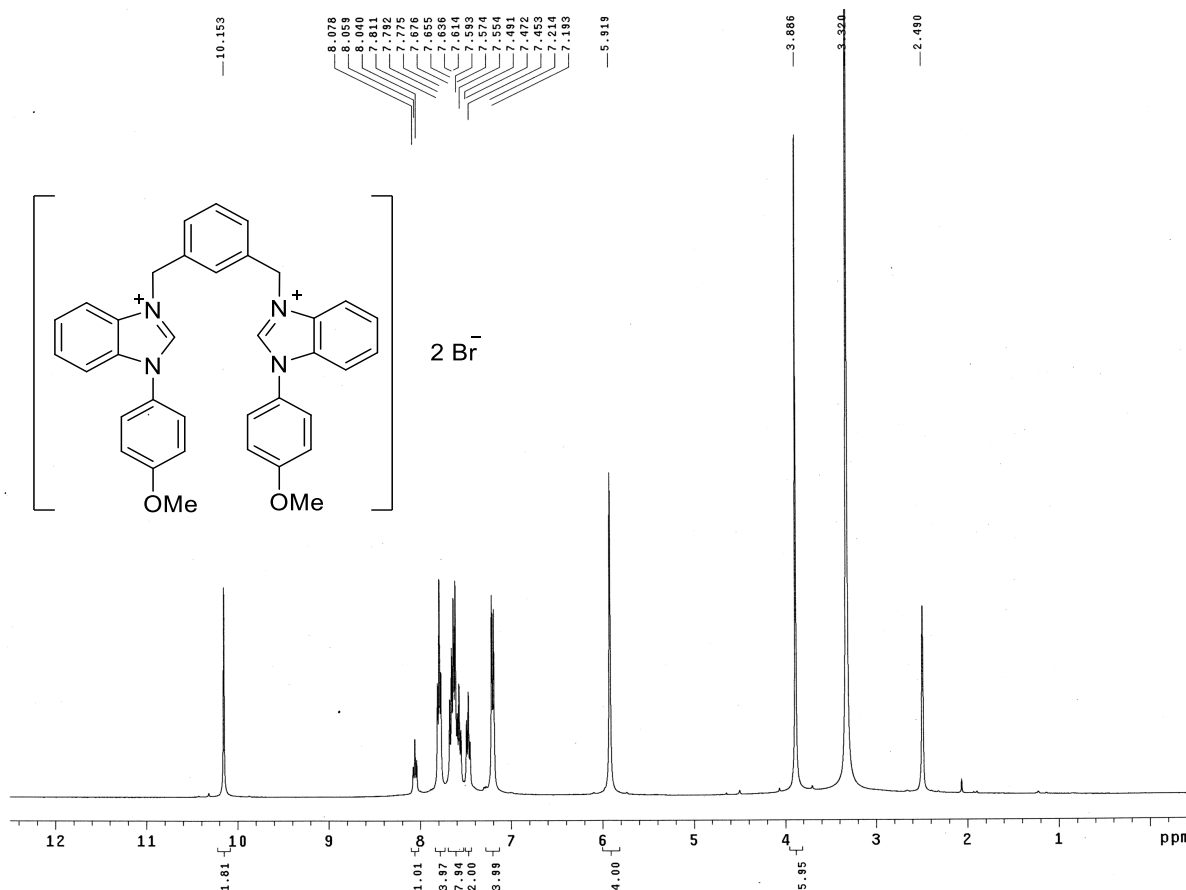


Figure S11: <sup>1</sup>H NMR spectrum of (3,3'-(pyridine-2,6-diylbis(methylene))bis(1-(4-methoxyphenyl)-1H-benzo[d]imidazol-3-ium)) dibromide (**3c**) in DMSO-d<sub>6</sub>.

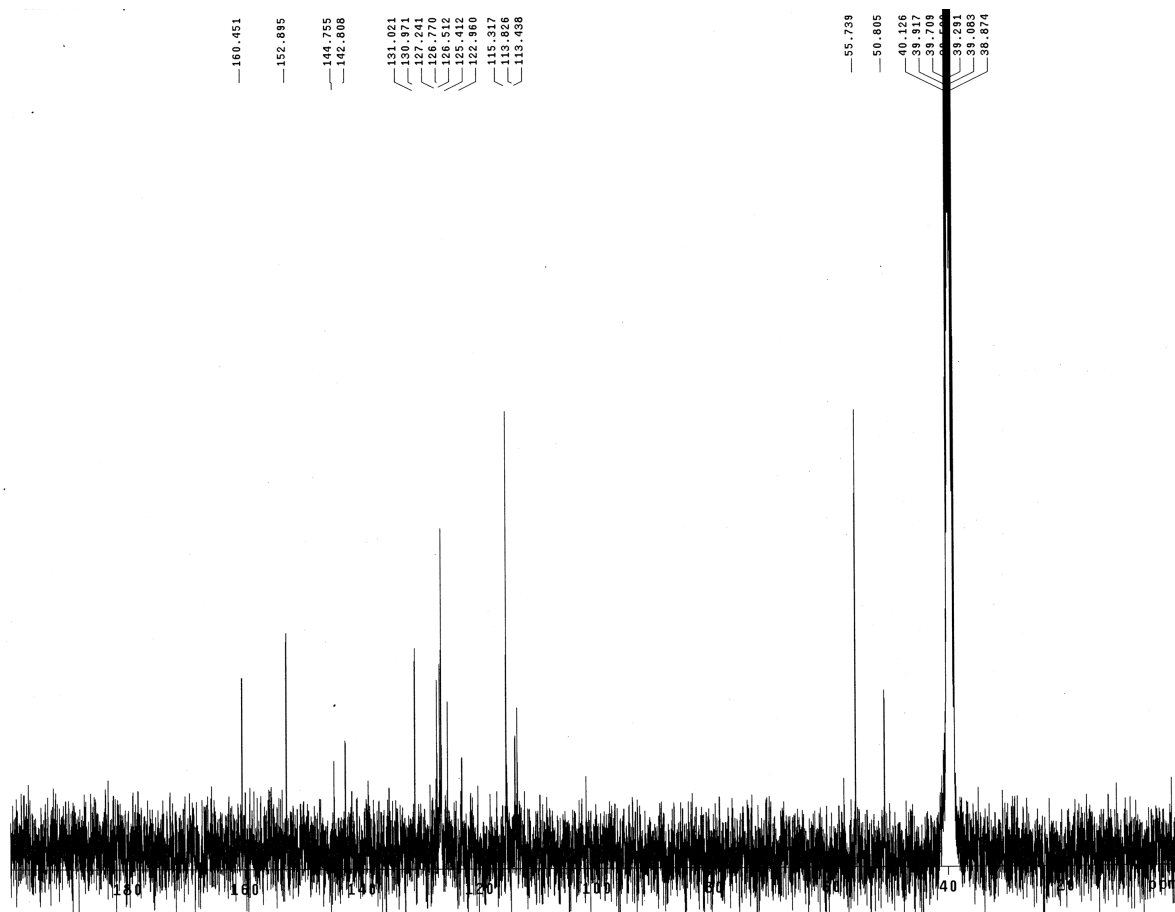


Figure S12: <sup>13</sup>C NMR spectrum of (3,3'-(pyridine-2,6-diylbis(methylene))bis(1-(4-methoxyphenyl)-1H-benzo[d]imidazol-3-ium)) dibromide (**3c**) in DMSO-d<sub>6</sub>.

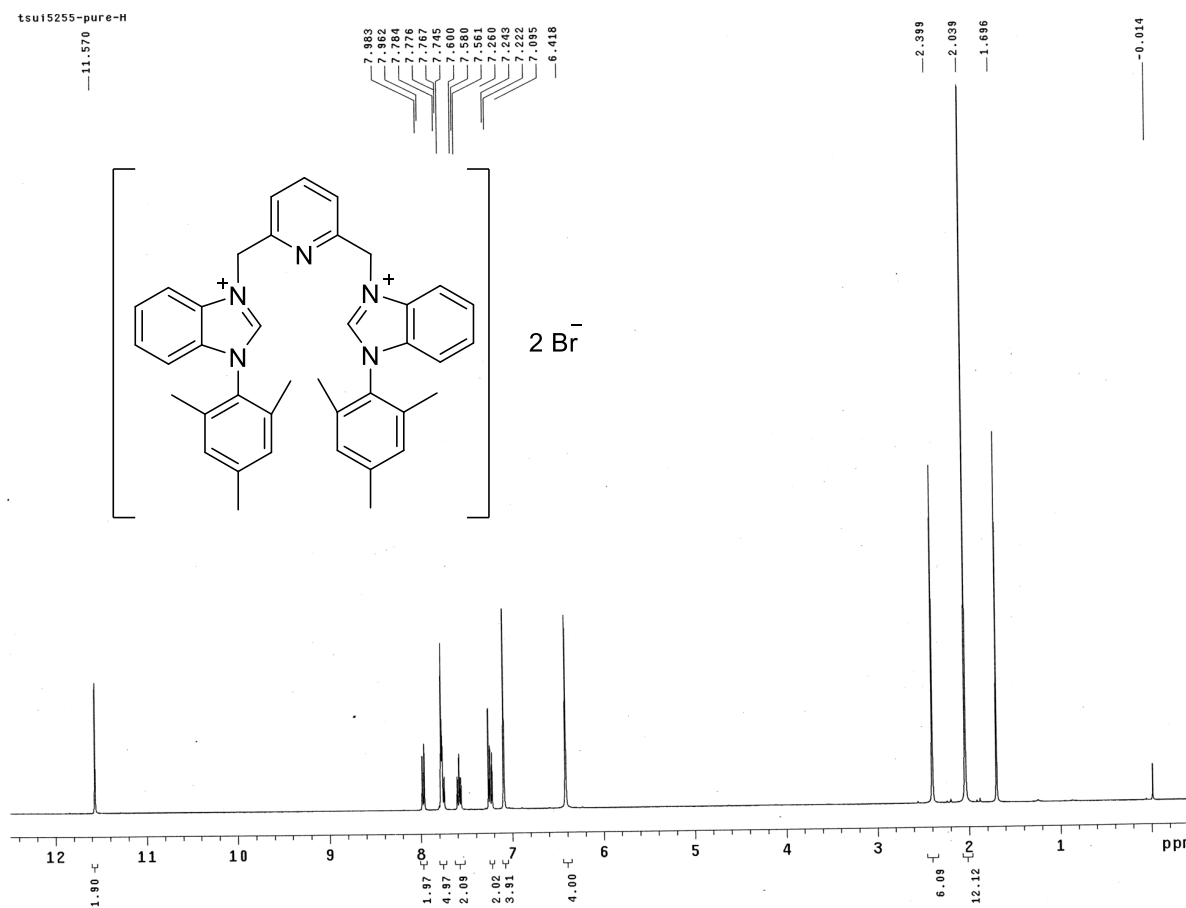


Figure S13:  $^1\text{H}$  NMR spectrum of (3,3'-(pyridine-2,6-diylbis(methylene))bis(1-mesityl-1H-benzo[d]imidazol-3-ium)) dibromide (**3d**) in CDCl<sub>3</sub>.

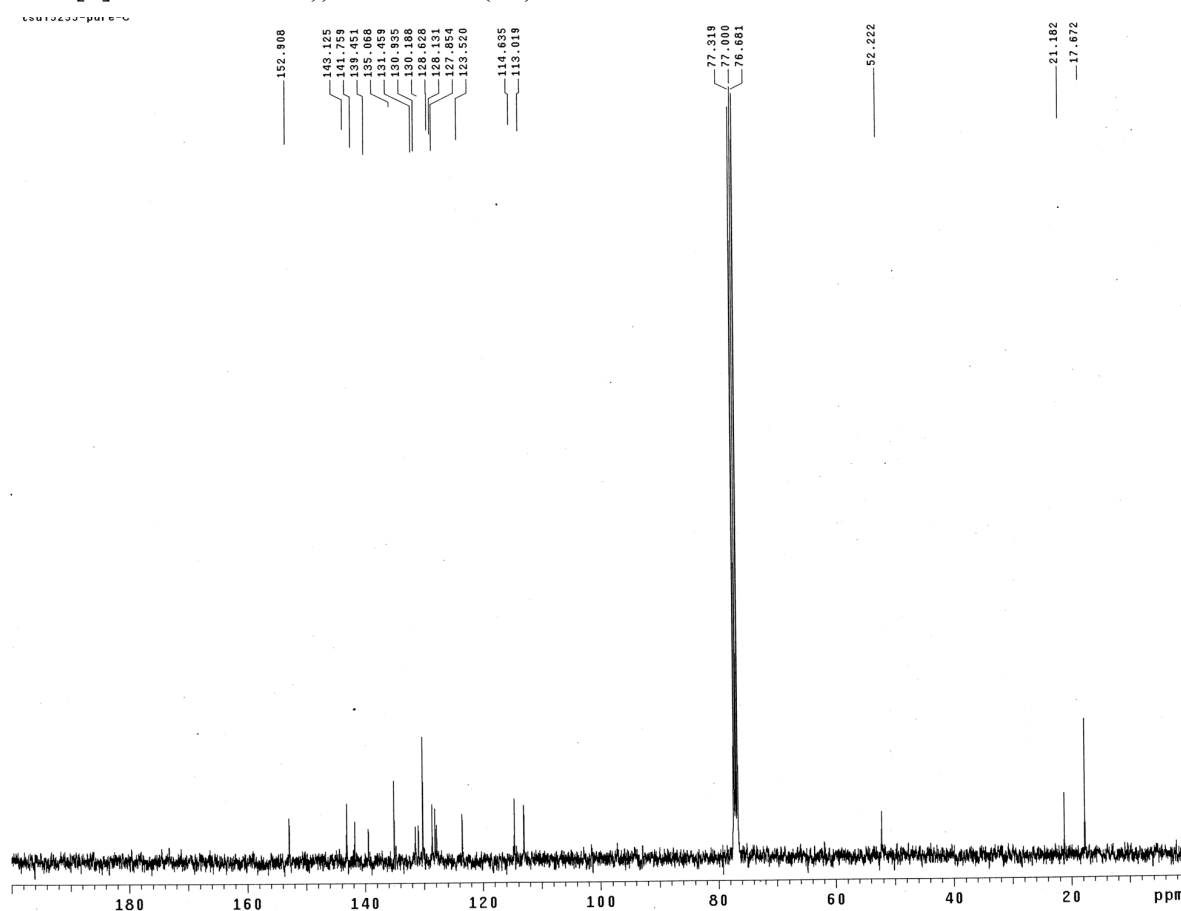


Figure S14:  $^{13}\text{C}$  NMR spectrum of (3,3'-(pyridine-2,6-diylbis(methylene))bis(1-mesityl-1H-benzo[d]imidazol-3-ium)) dibromide (**3d**) in CDCl<sub>3</sub>.

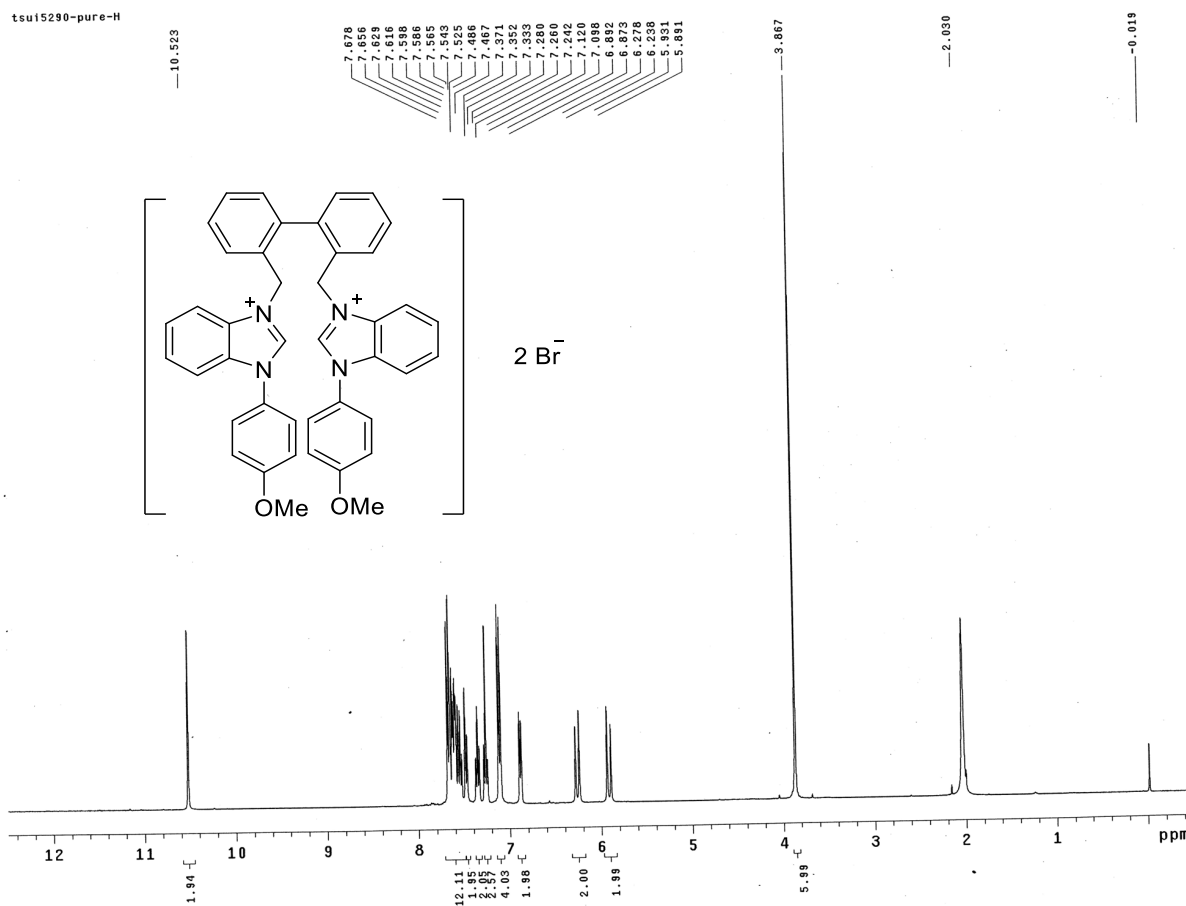


Figure S15: <sup>1</sup>H NMR spectrum of 3,3'-([1,1'-biphenyl]-2,2'-diylbis(methylene))bis(1-(4-methoxyphenyl)-1*H*-benzo[d]imidazol-3-ium) dibromide (**3e**) in CDCl<sub>3</sub>.

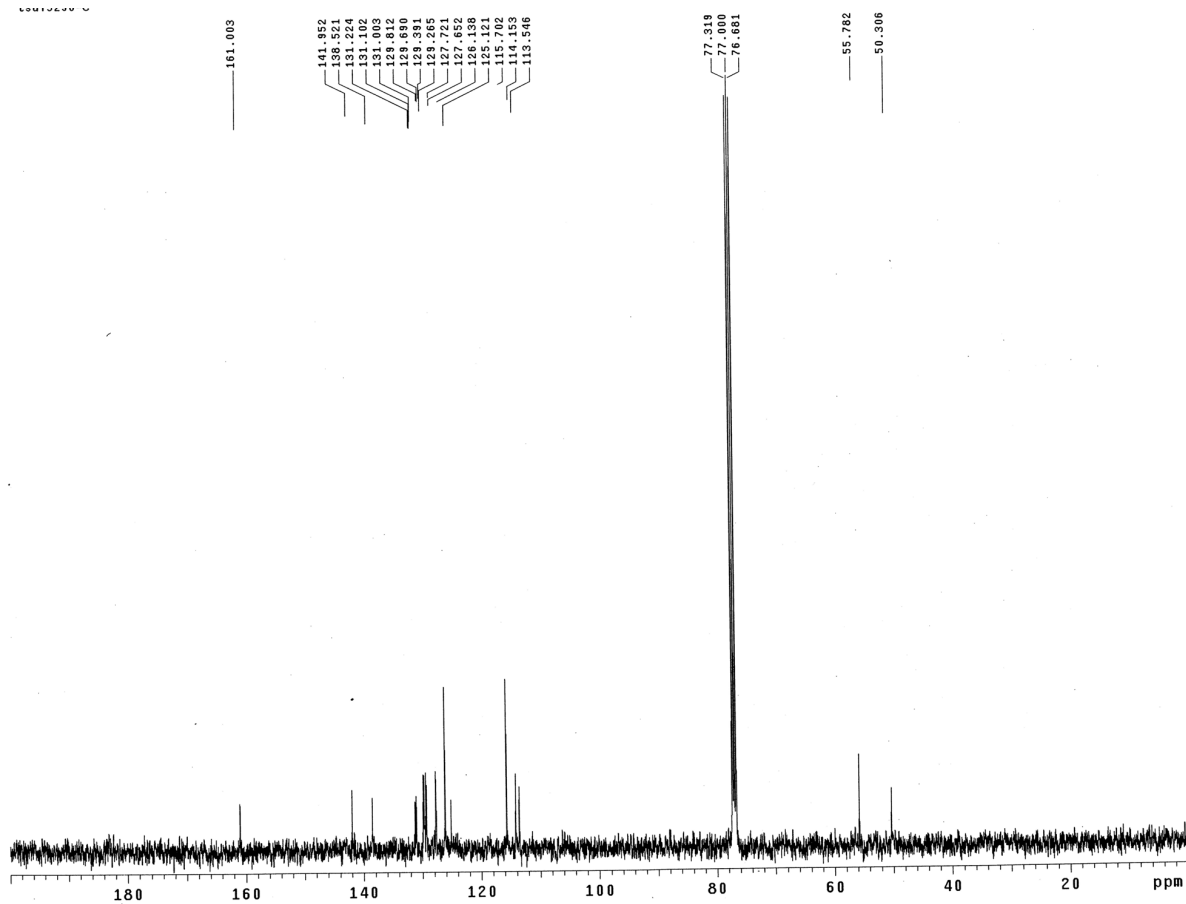


Figure S16: <sup>13</sup>C NMR spectrum of 3,3'-([1,1'-biphenyl]-2,2'-diylbis(methylene))bis(1-(4-methoxyphenyl)-1*H*-benzo[d]imidazol-3-ium) dibromide (**3e**) in CDCl<sub>3</sub>.



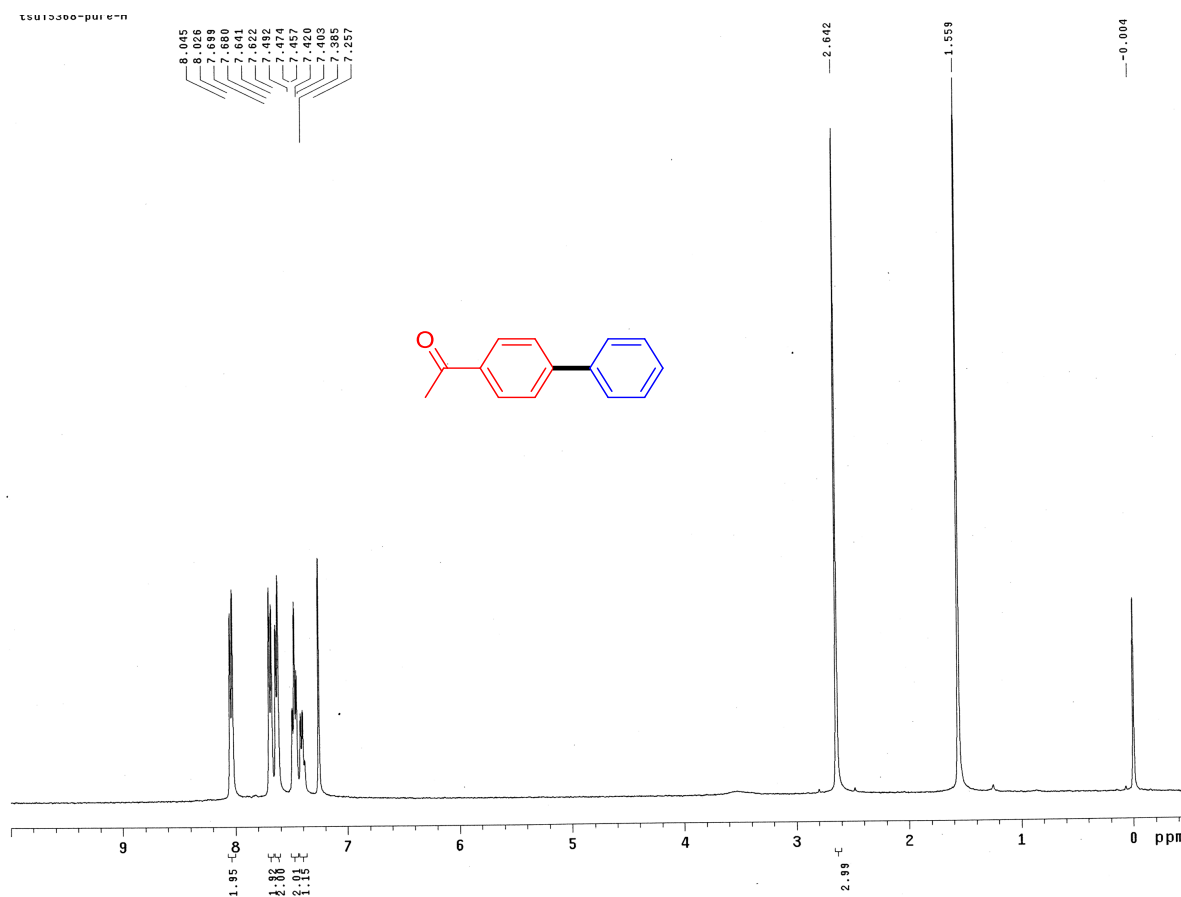


Figure S19: <sup>1</sup>H NMR spectrum of 4-acetylbiphenyl (**6aa**) in CDCl<sub>3</sub>.

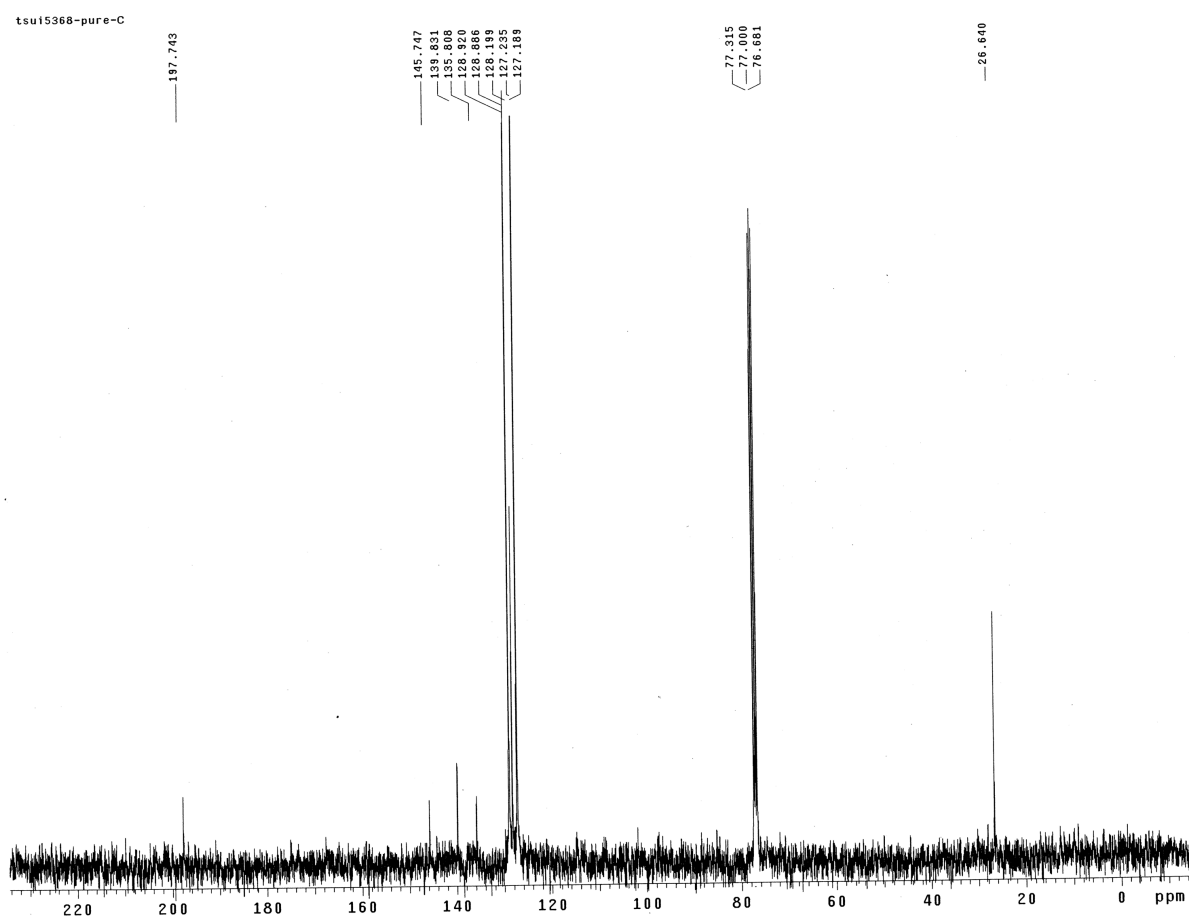


Figure S20: <sup>13</sup>C NMR spectrum of 4-acetylbiphenyl (**6aa**) in CDCl<sub>3</sub>.





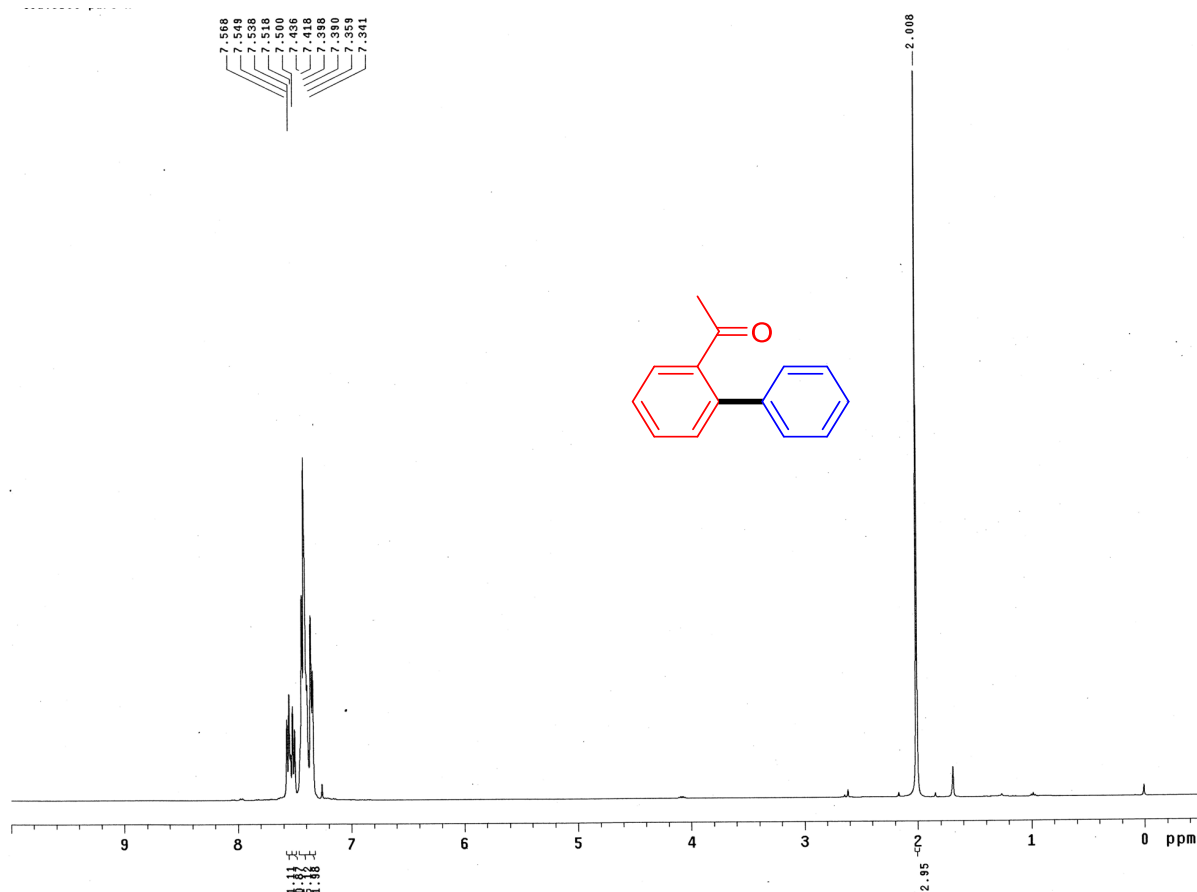


Figure S23: <sup>1</sup>H NMR spectrum of 2-acetylbiphenyl (**6ca**) in CDCl<sub>3</sub>.

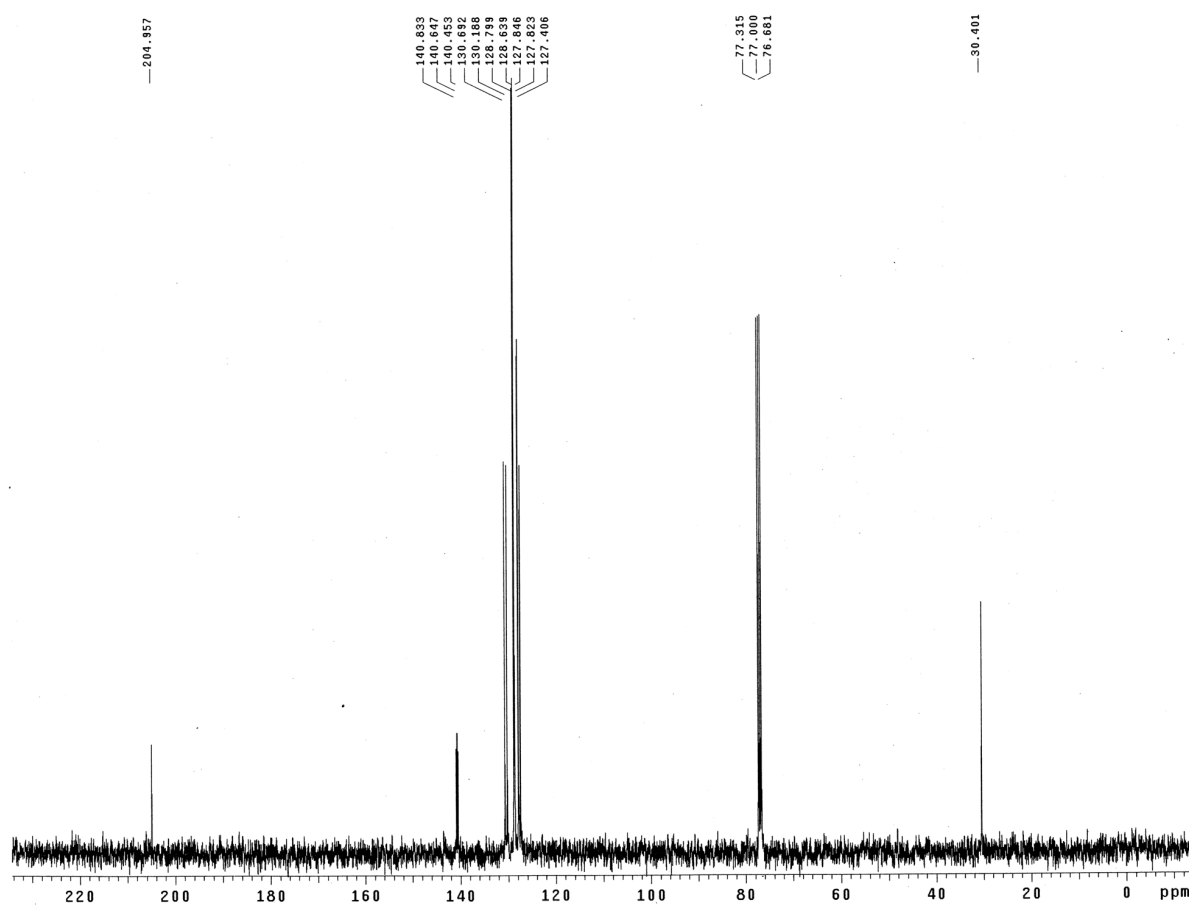


Figure S24: <sup>13</sup>C NMR spectrum of 2-acetylbiphenyl (**6ca**) in CDCl<sub>3</sub>.

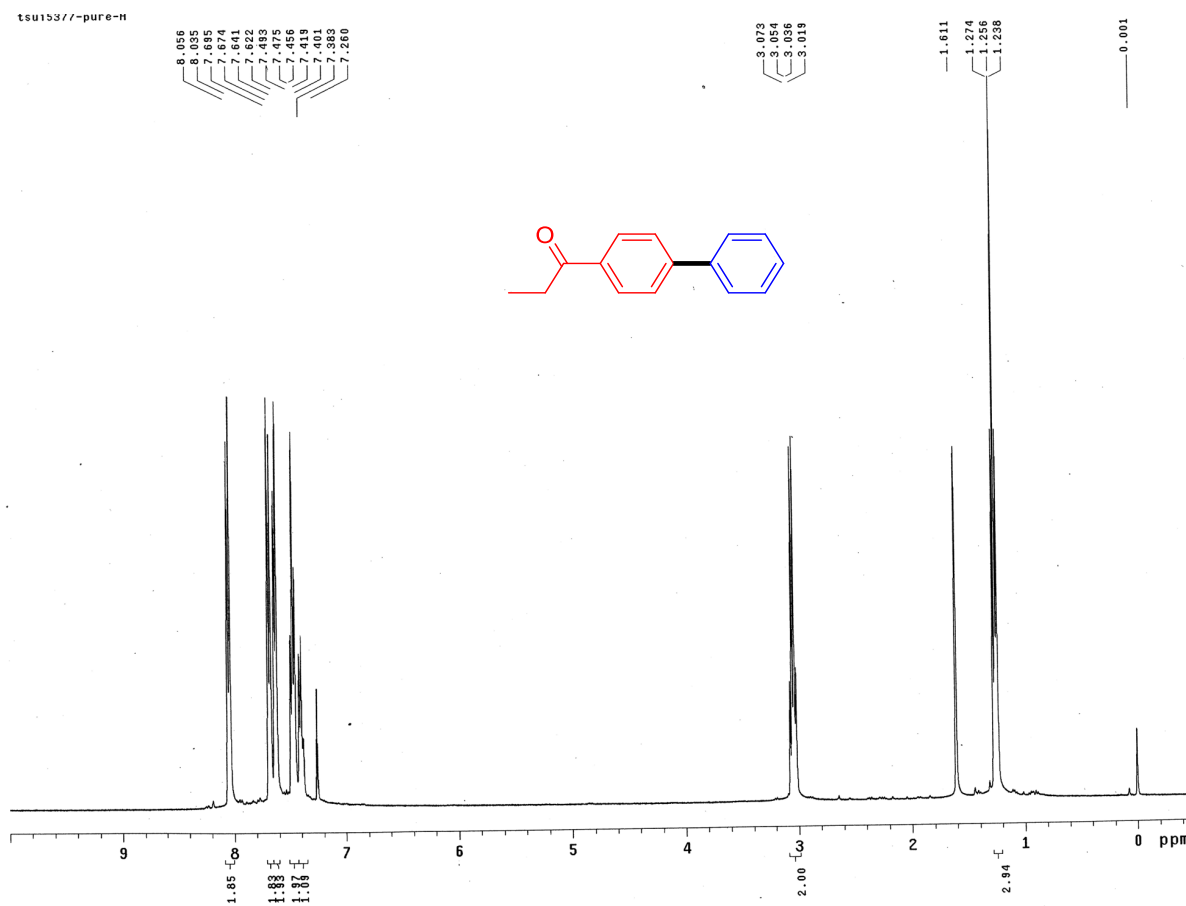


Figure S25: <sup>1</sup>H NMR spectrum of 4'-phenylpropiphenone (**6da**) in CDCl<sub>3</sub>.

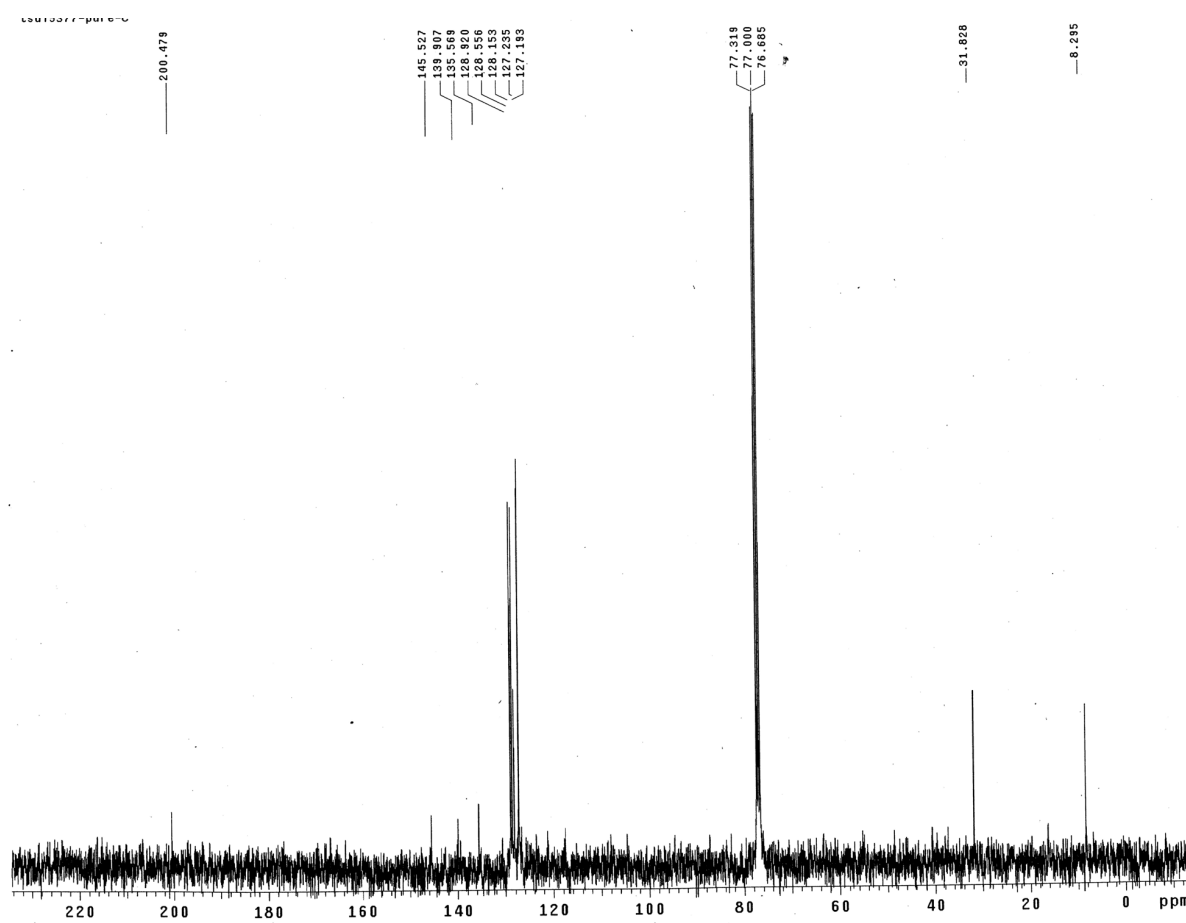


Figure S26: <sup>13</sup>C NMR spectrum of 4'-phenylpropiphenone (**6da**) in CDCl<sub>3</sub>.

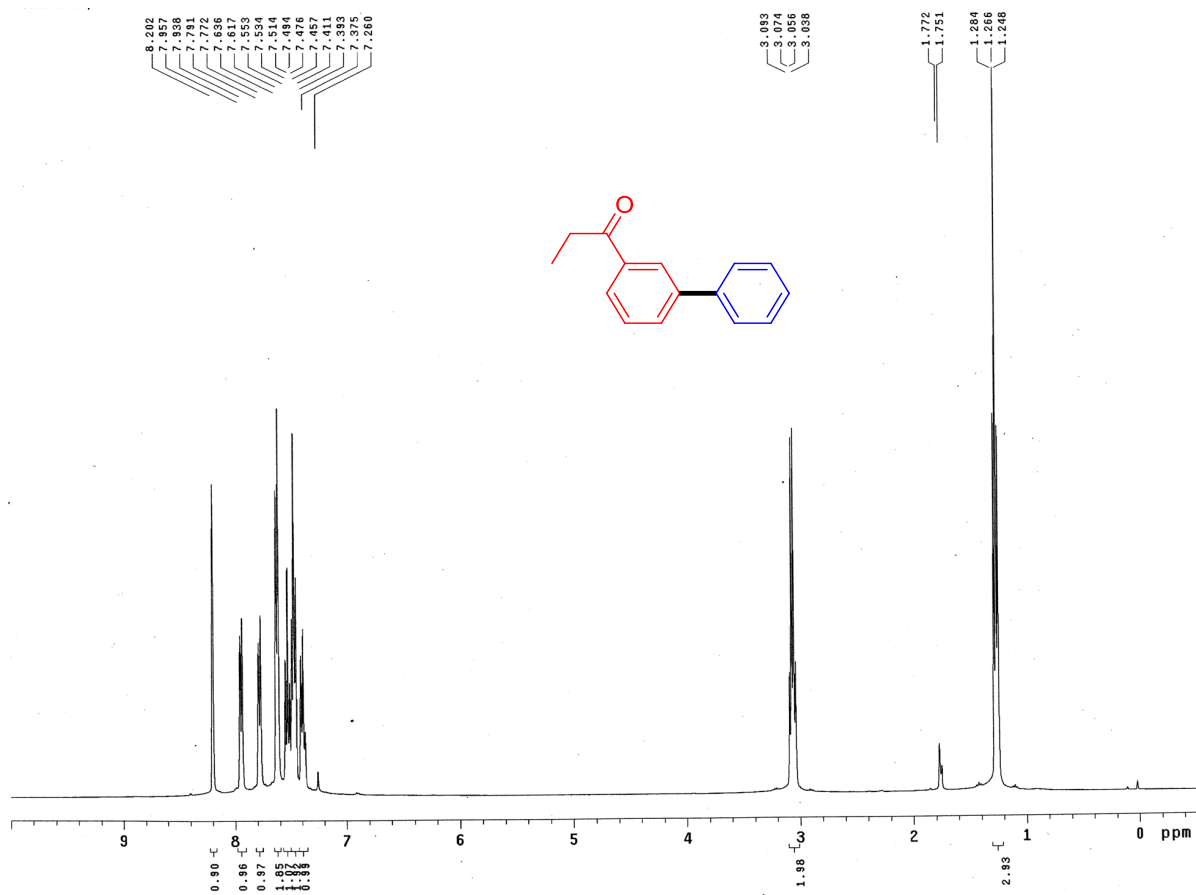


Figure S27: <sup>1</sup>H NMR spectrum of 3'-phenylpropiphenone (**6ea**) in CDCl<sub>3</sub>.

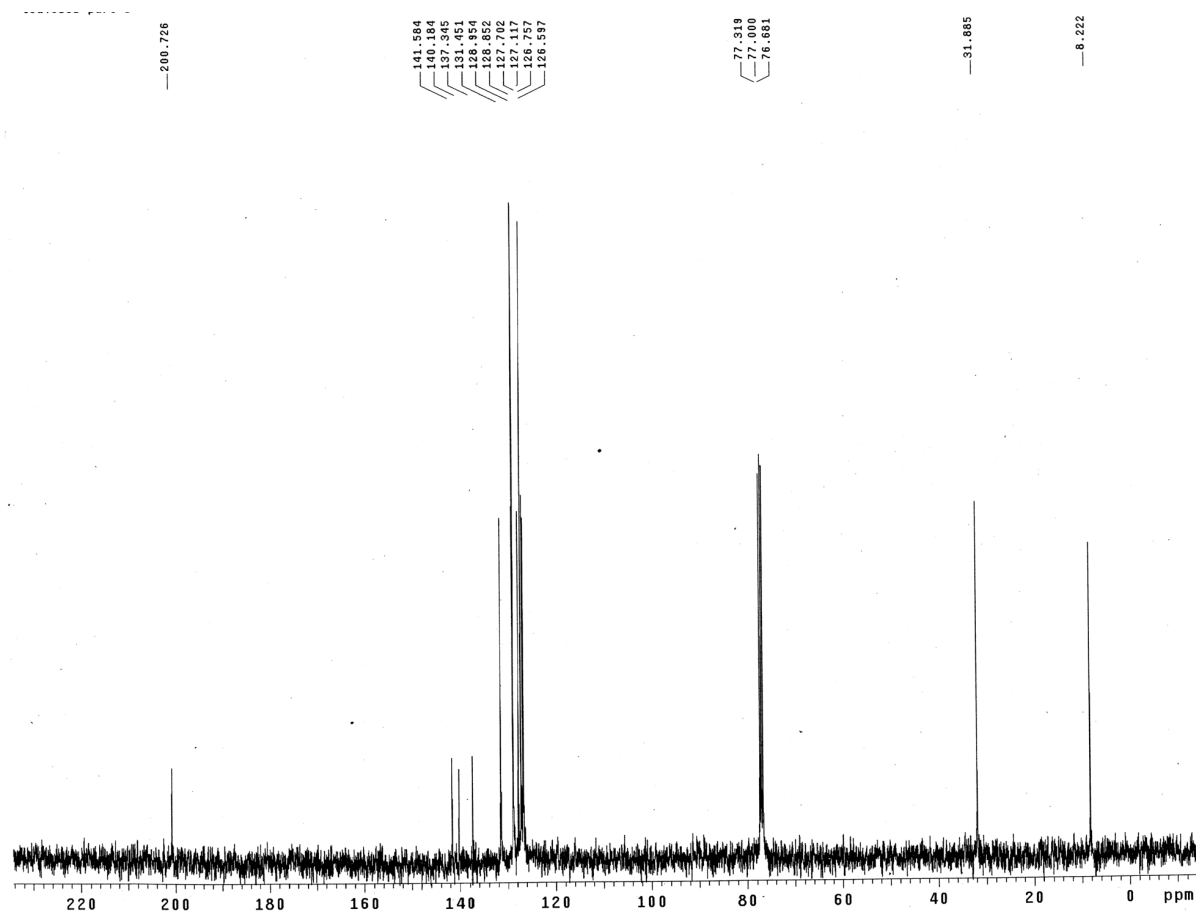


Figure S28: <sup>13</sup>C NMR spectrum of 3'-phenylpropiphenone (**6ea**) in CDCl<sub>3</sub>.

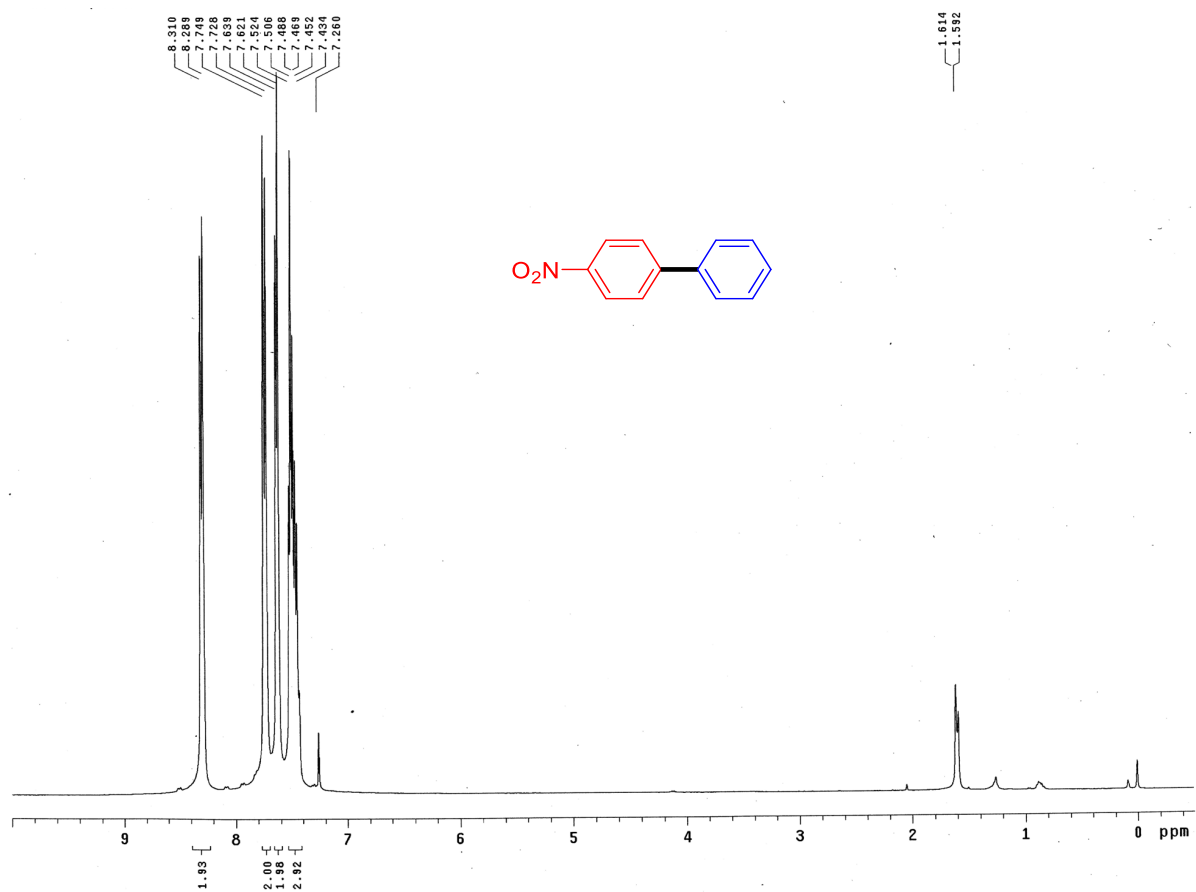


Figure S29: <sup>1</sup>H NMR spectrum of 4-nitrobiphenyl (**6fa**) in CDCl<sub>3</sub>.

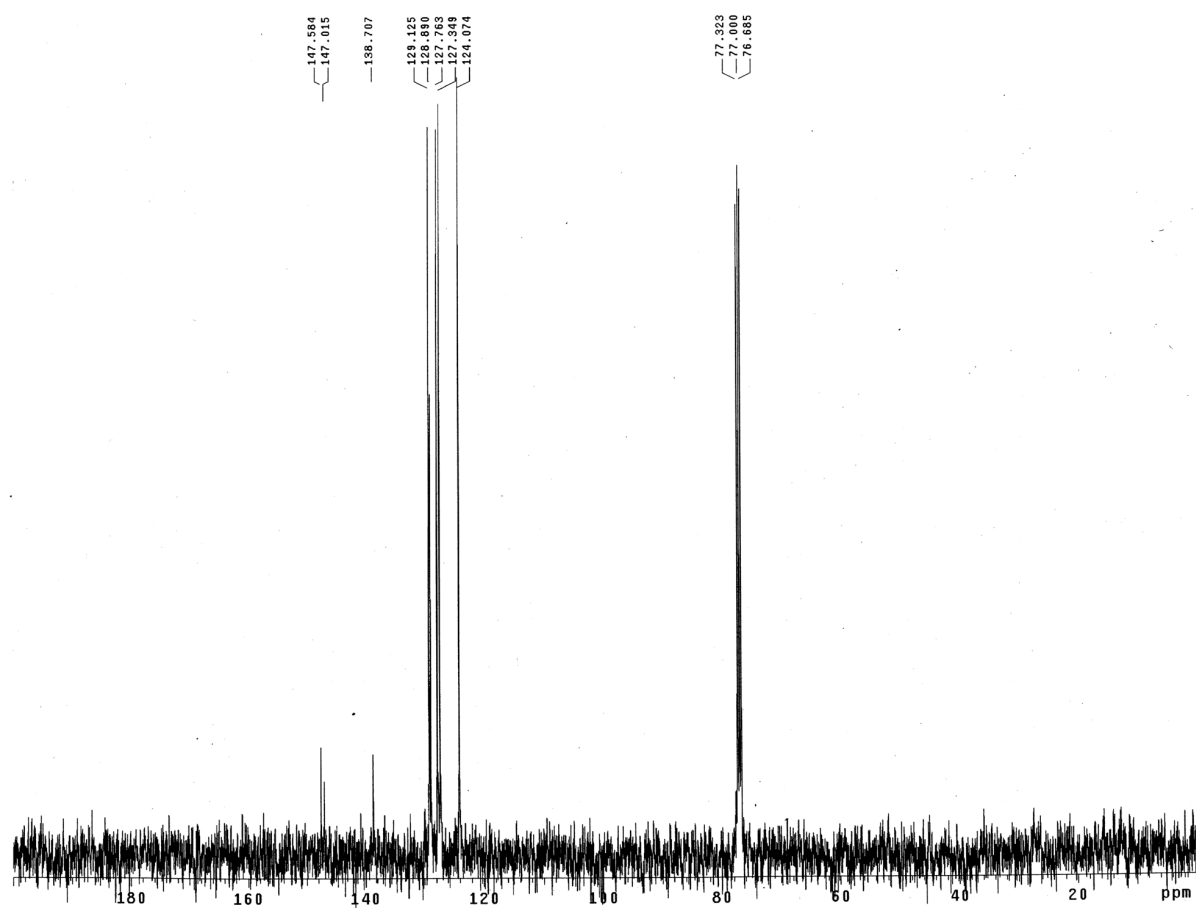


Figure S30: <sup>13</sup>C NMR spectrum of 4-nitrobiphenyl (**6fa**) in CDCl<sub>3</sub>.

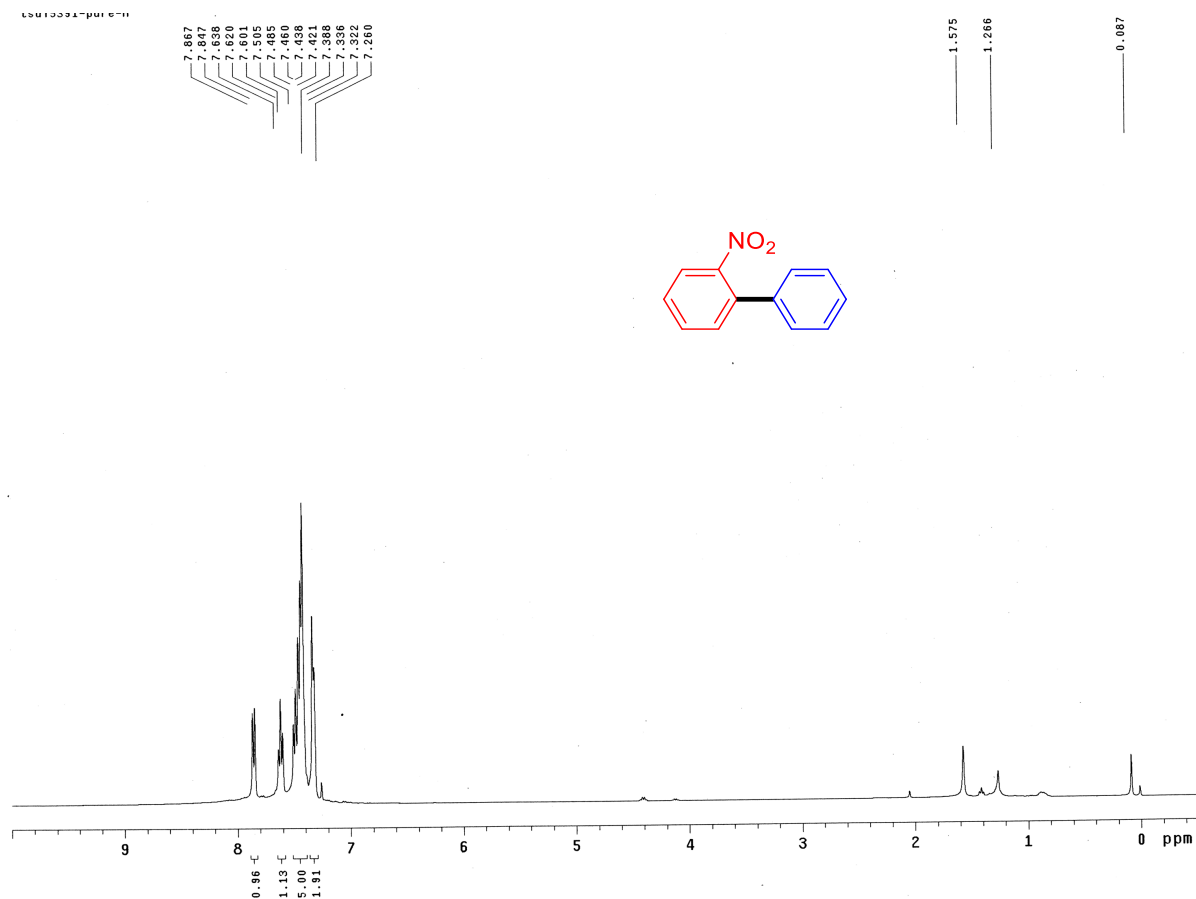


Figure S31: <sup>1</sup>H NMR spectrum of 2-nitrobiphenyl (**6ga**) in CDCl<sub>3</sub>.

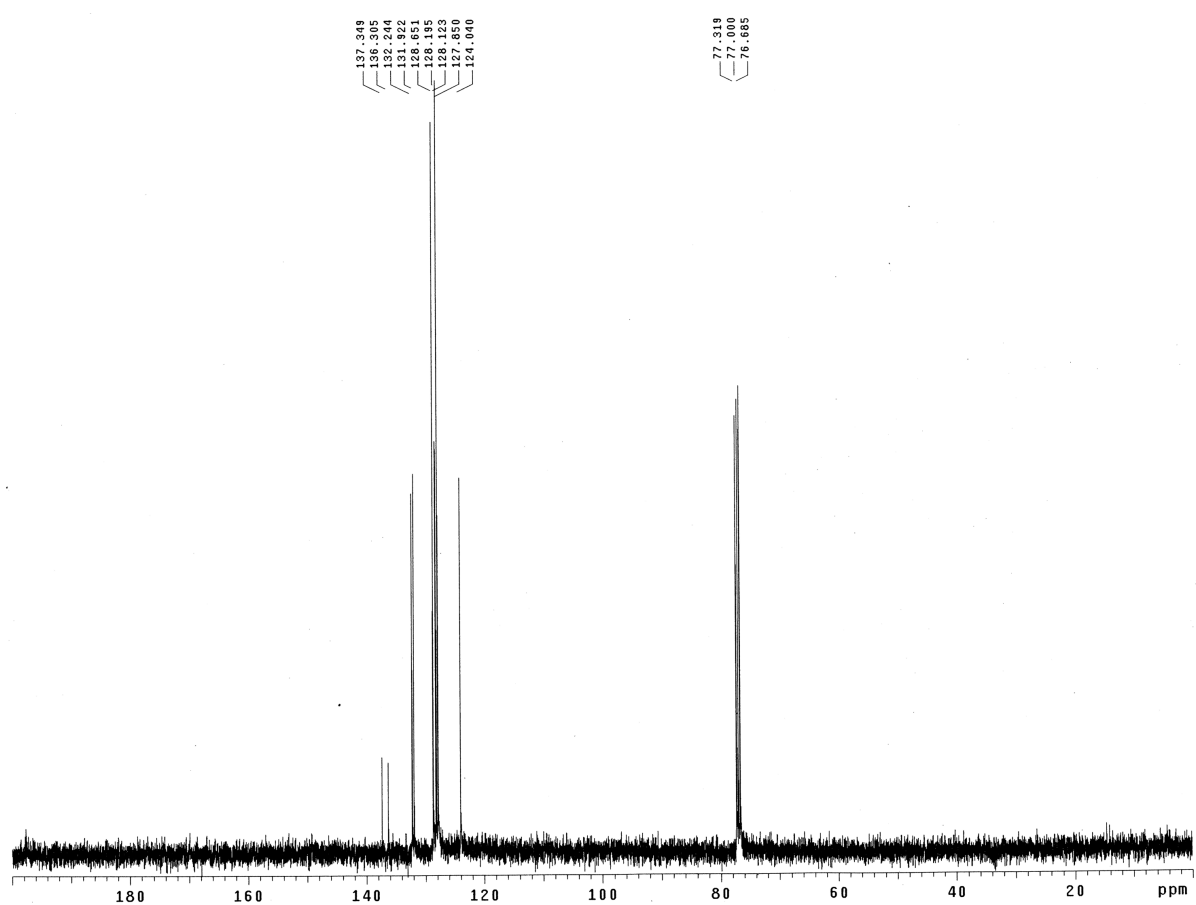


Figure S32: <sup>13</sup>C NMR spectrum of 2-nitrobiphenyl (**6ga**) in CDCl<sub>3</sub>.

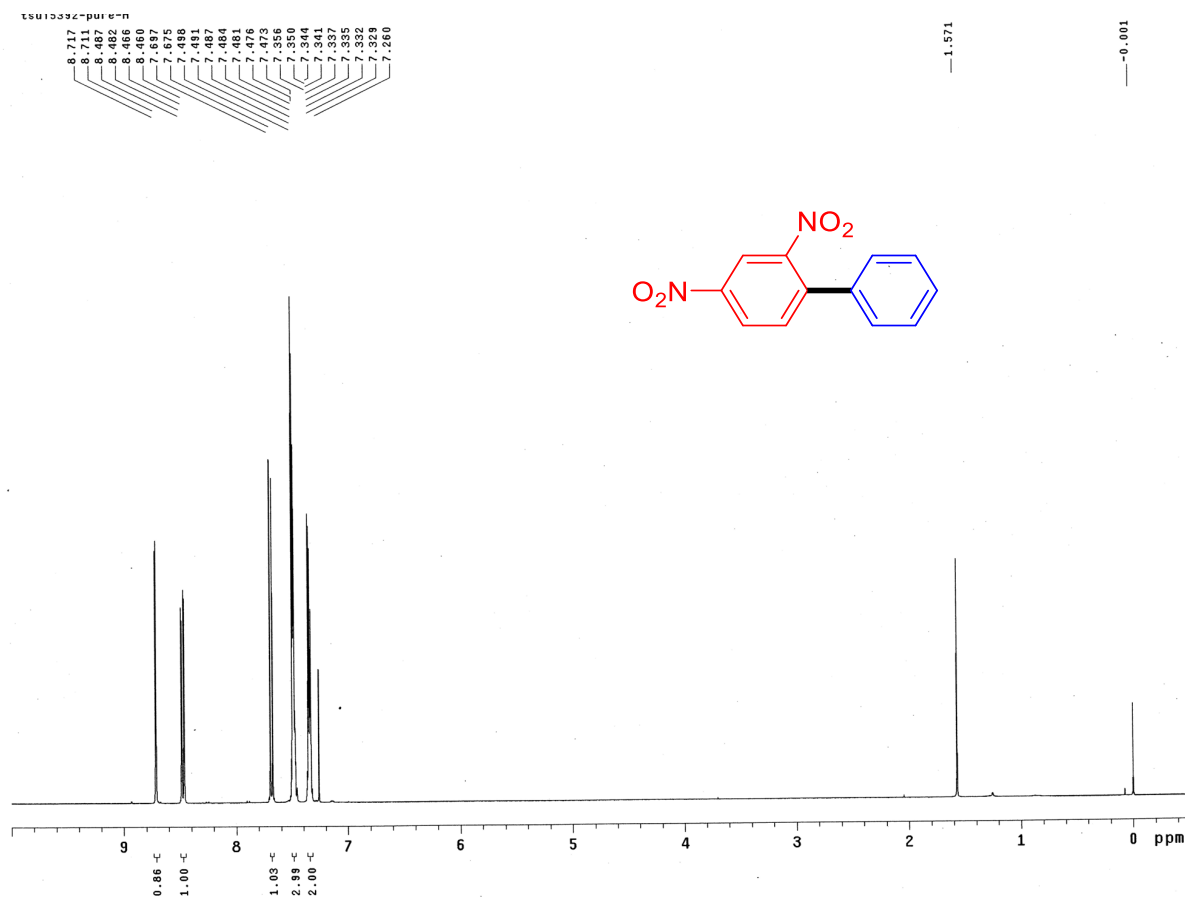


Figure S33: <sup>1</sup>H NMR spectrum of 2,4-dinitrobiphenyl (**6ha**) in CDCl<sub>3</sub>.

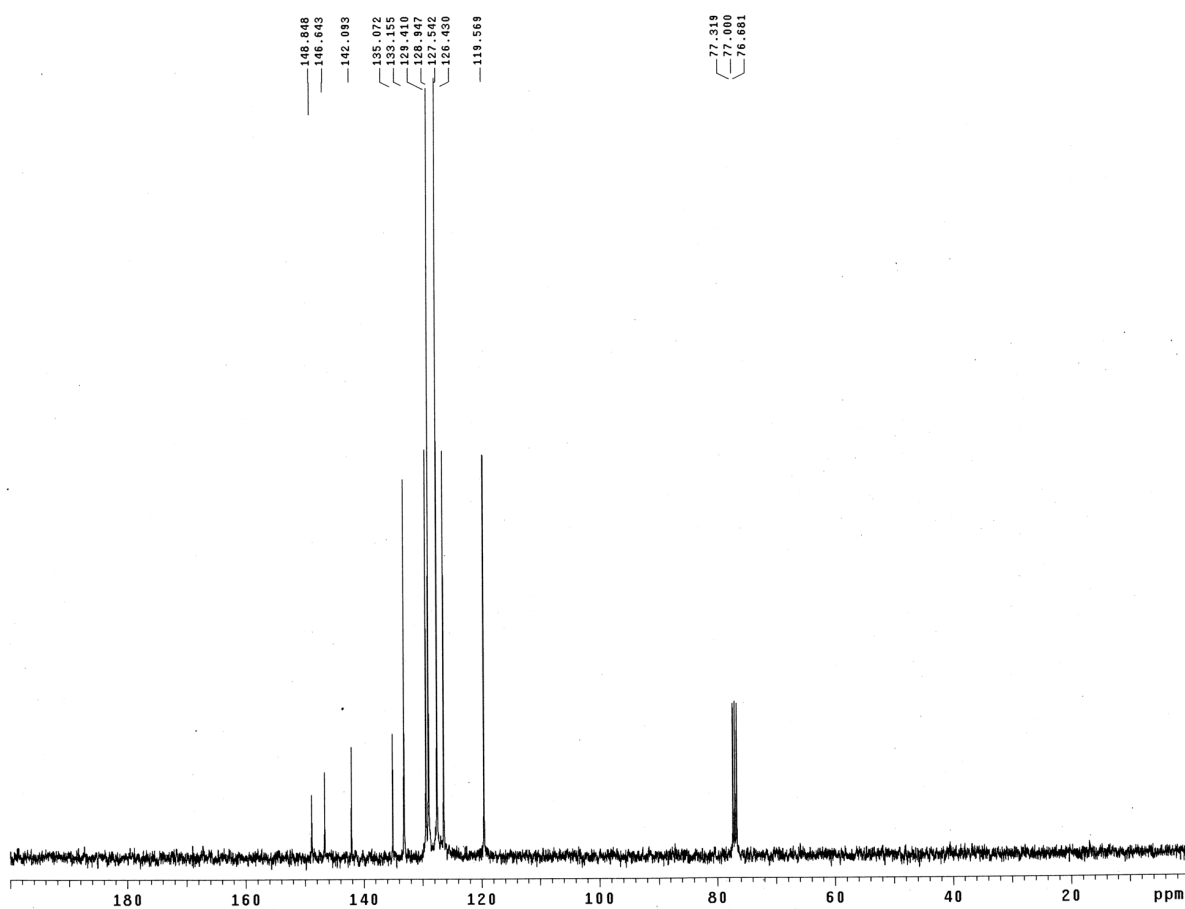


Figure S34: <sup>13</sup>C NMR spectrum of 2,4-dinitrobiphenyl (**6ha**) in CDCl<sub>3</sub>.

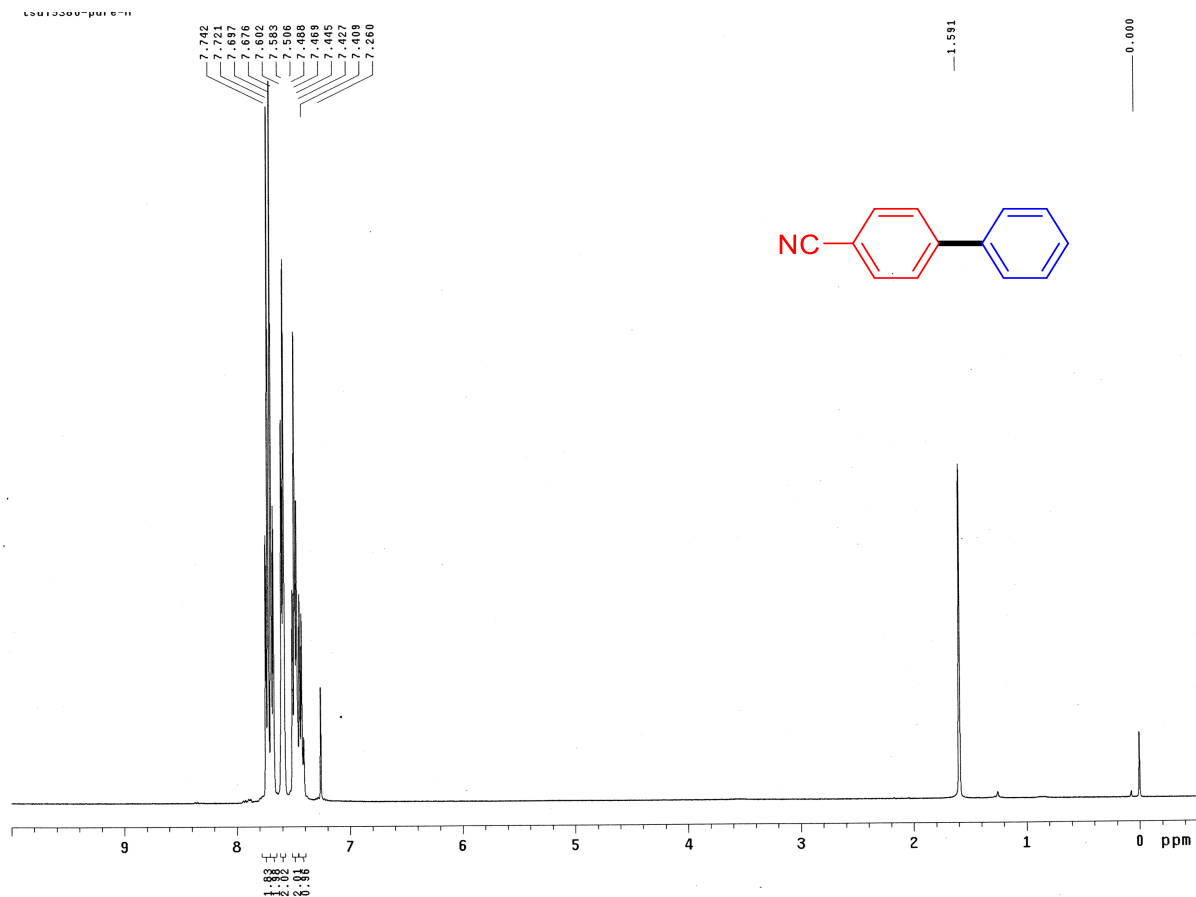


Figure S35: <sup>1</sup>H NMR spectrum of 4-cyanobiphenyl (**6ia**) in CDCl<sub>3</sub>.

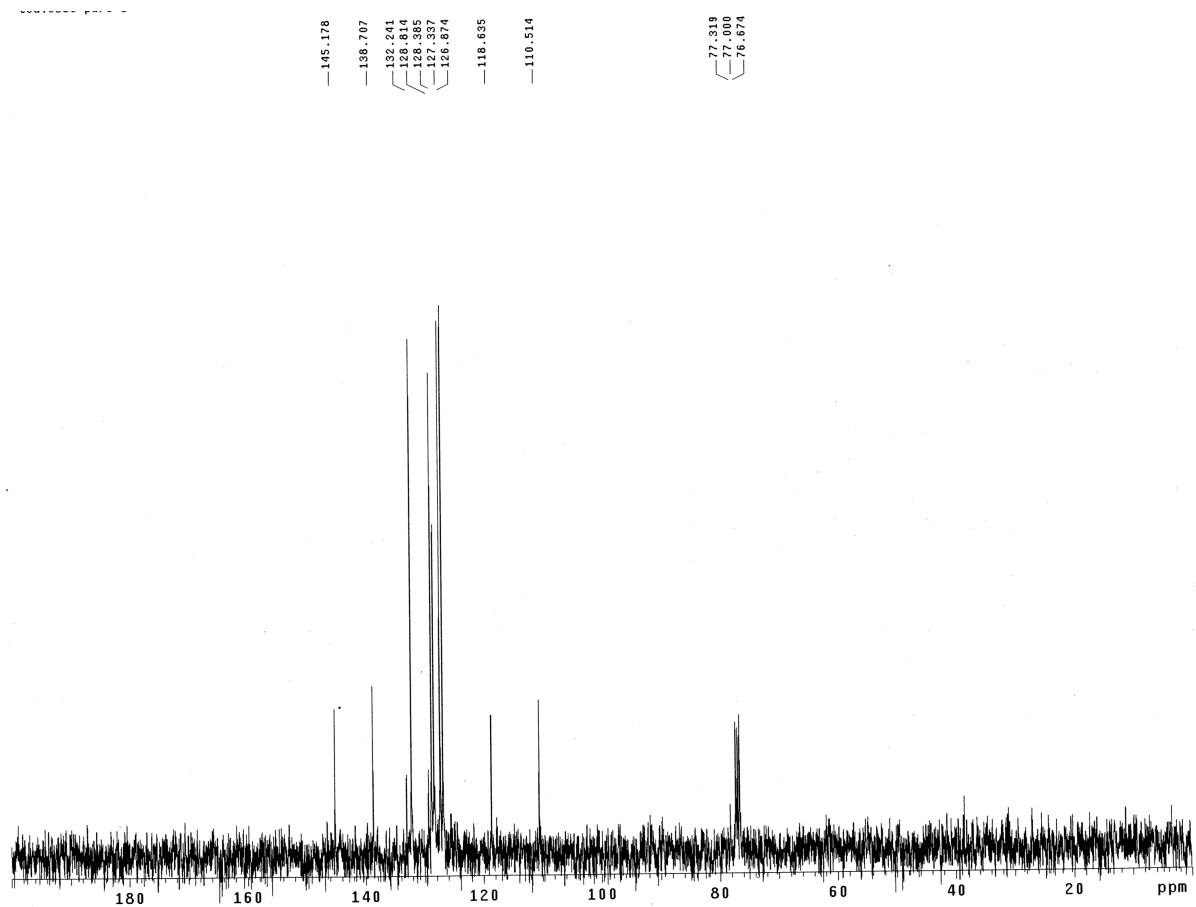


Figure S36: <sup>13</sup>C NMR spectrum of 4-cyanobiphenyl (**6ia**) in CDCl<sub>3</sub>.

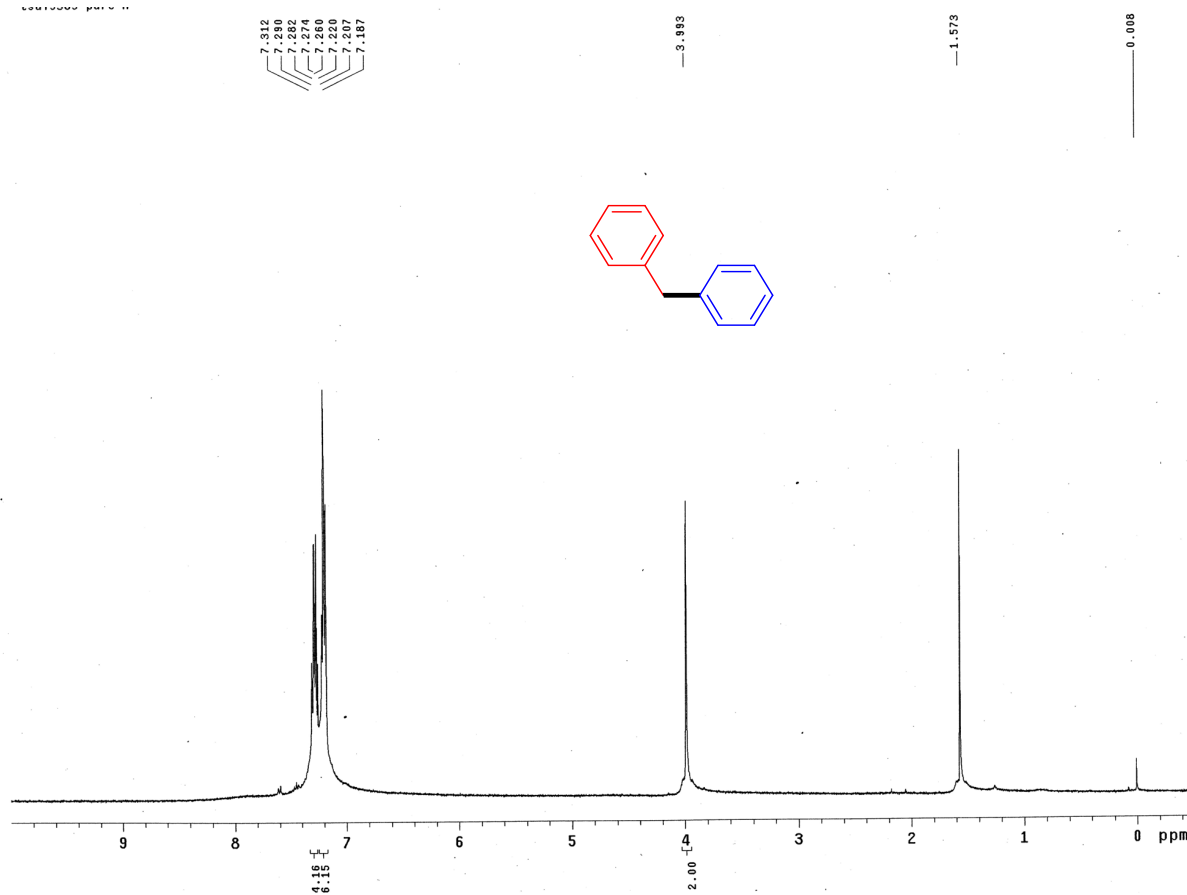


Figure S37: <sup>1</sup>H NMR spectrum of diphenylmethane (**6ja**) in CDCl<sub>3</sub>.

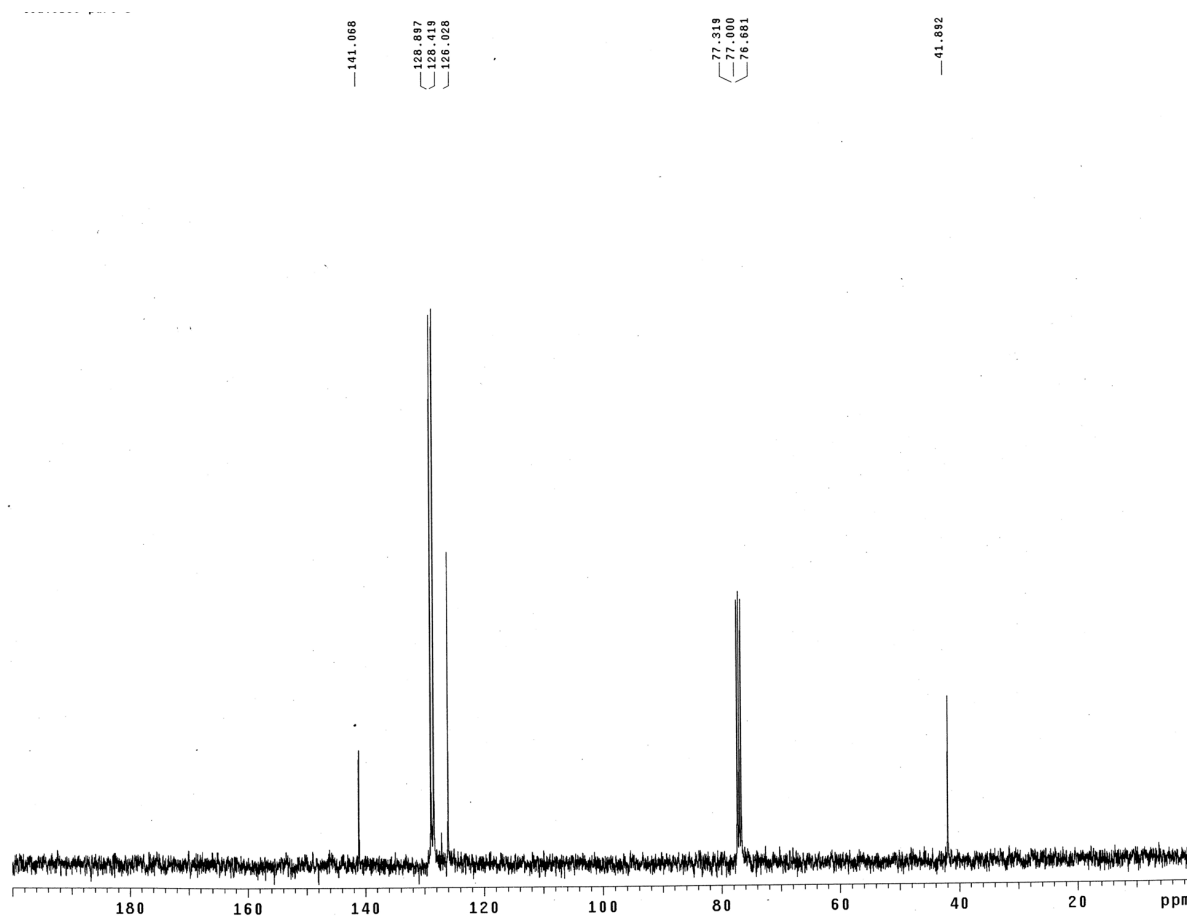


Figure S38: <sup>13</sup>C NMR spectrum of diphenylmethane (**6ja**) in CDCl<sub>3</sub>.



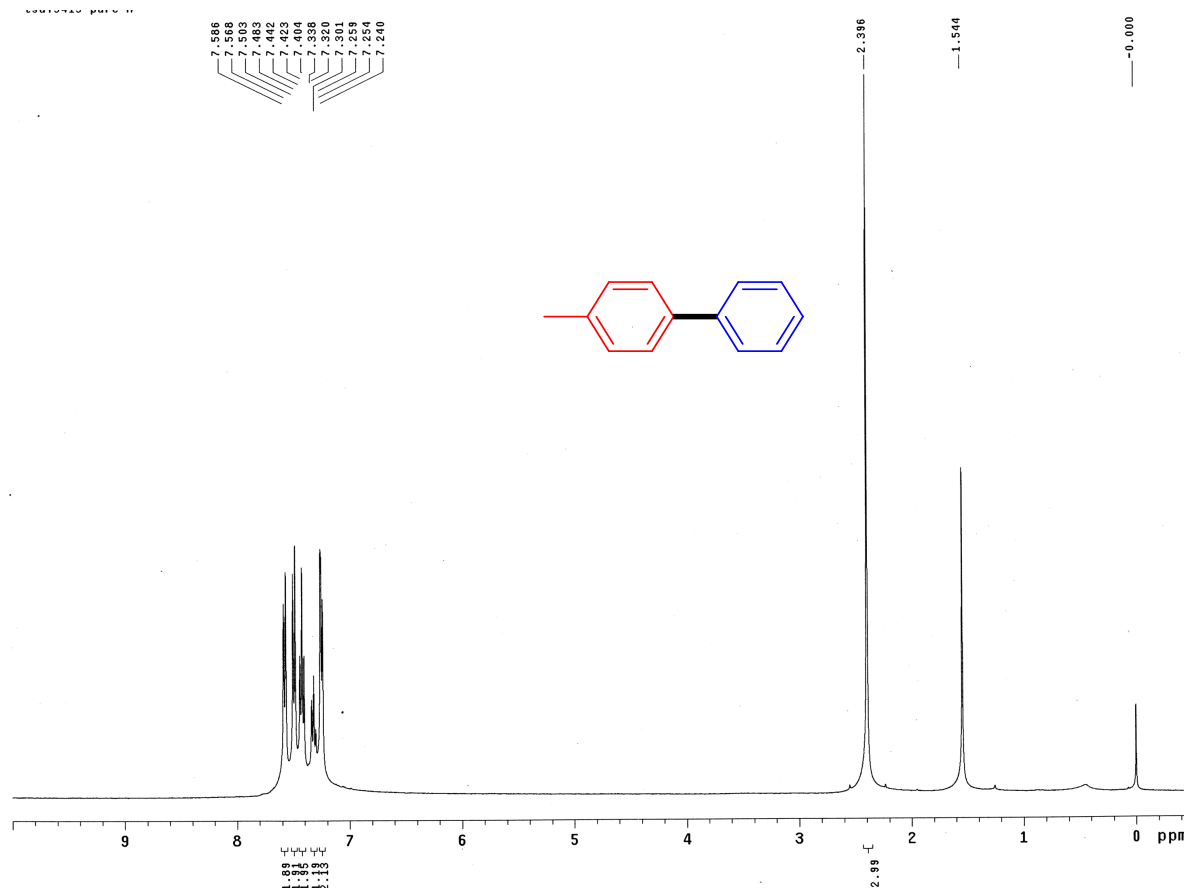


Figure S39: <sup>1</sup>H NMR spectrum of 4-methylbiphenyl (**6ka**) in CDCl<sub>3</sub>.

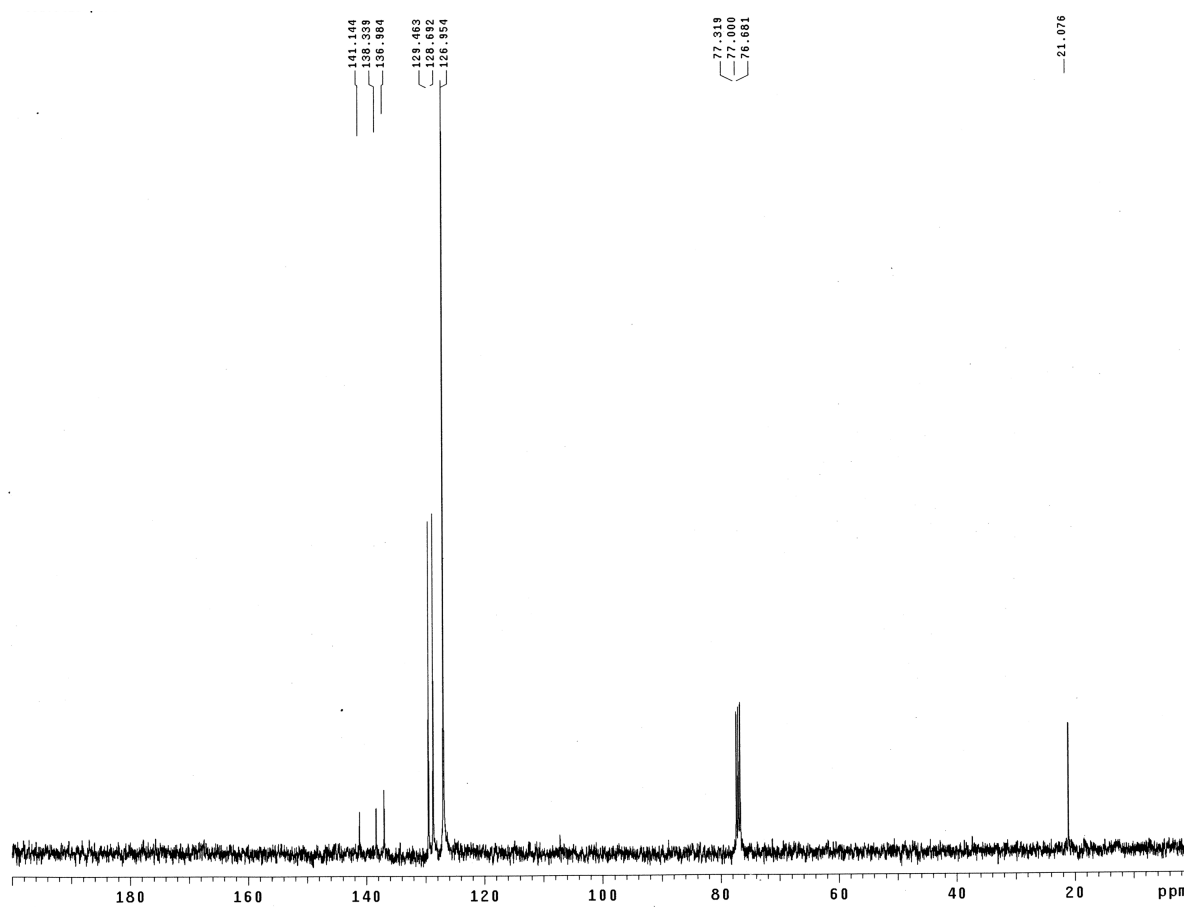


Figure S40: <sup>13</sup>C NMR spectrum of 4-methylbiphenyl (**6ka**) in CDCl<sub>3</sub>.

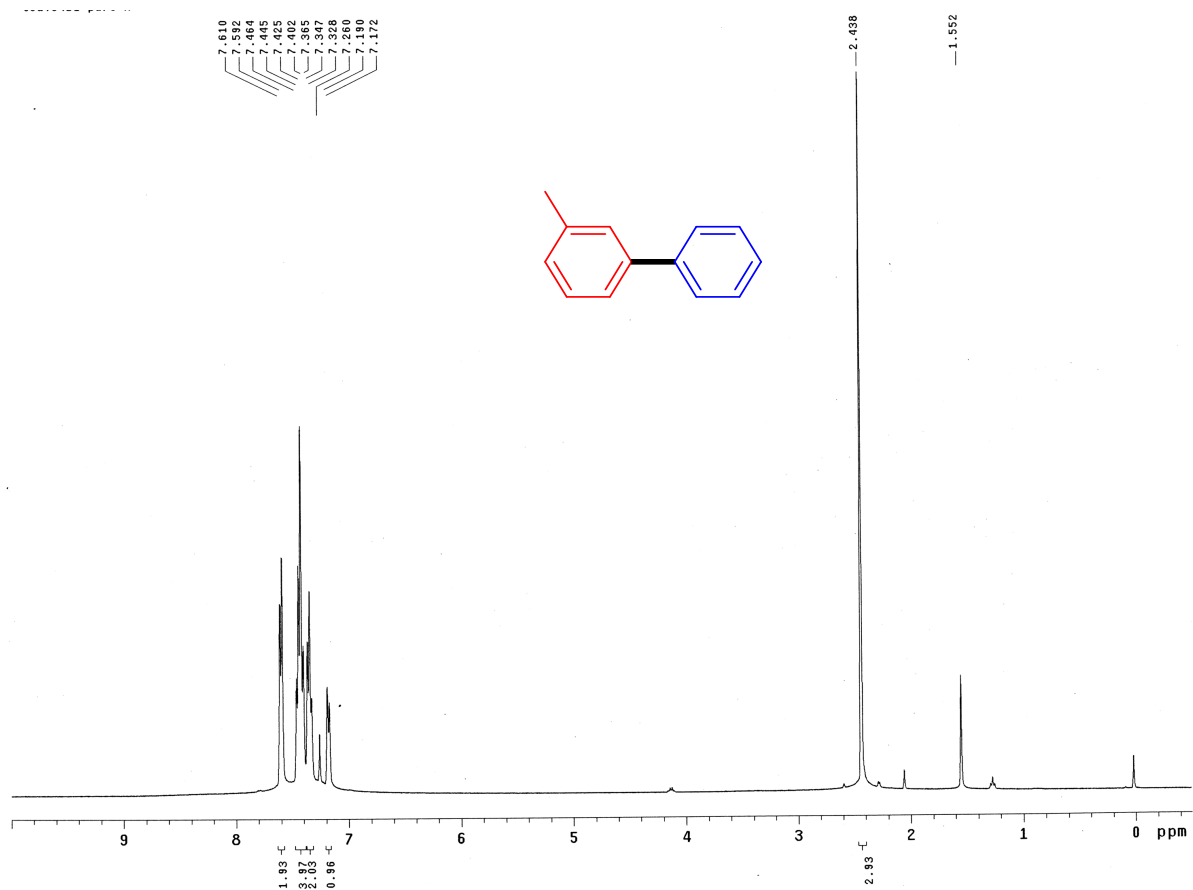


Figure S41: <sup>1</sup>H NMR spectrum of 3-methylbiphenyl (**6la**) in CDCl<sub>3</sub>.

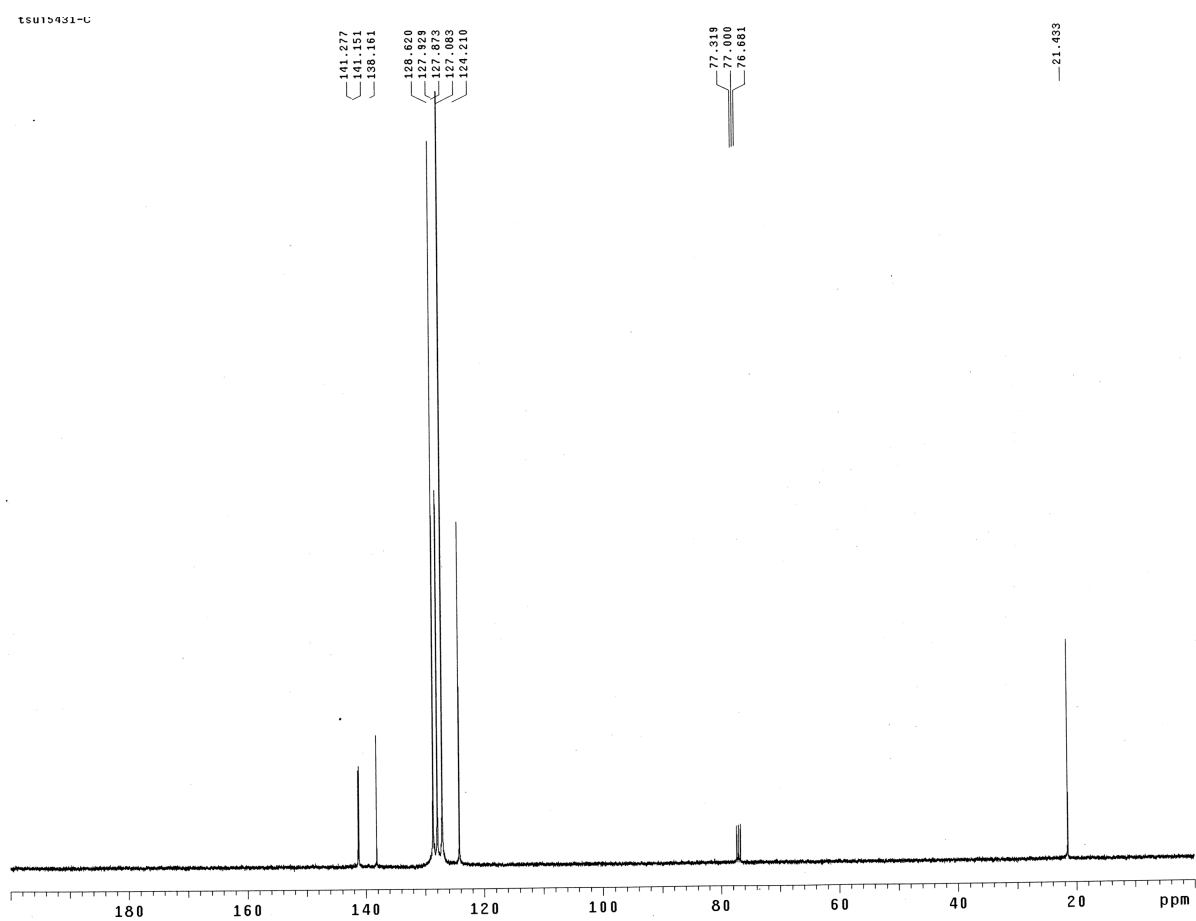


Figure S42: <sup>13</sup>C NMR spectrum of 3-methylbiphenyl (**6la**) in CDCl<sub>3</sub>.

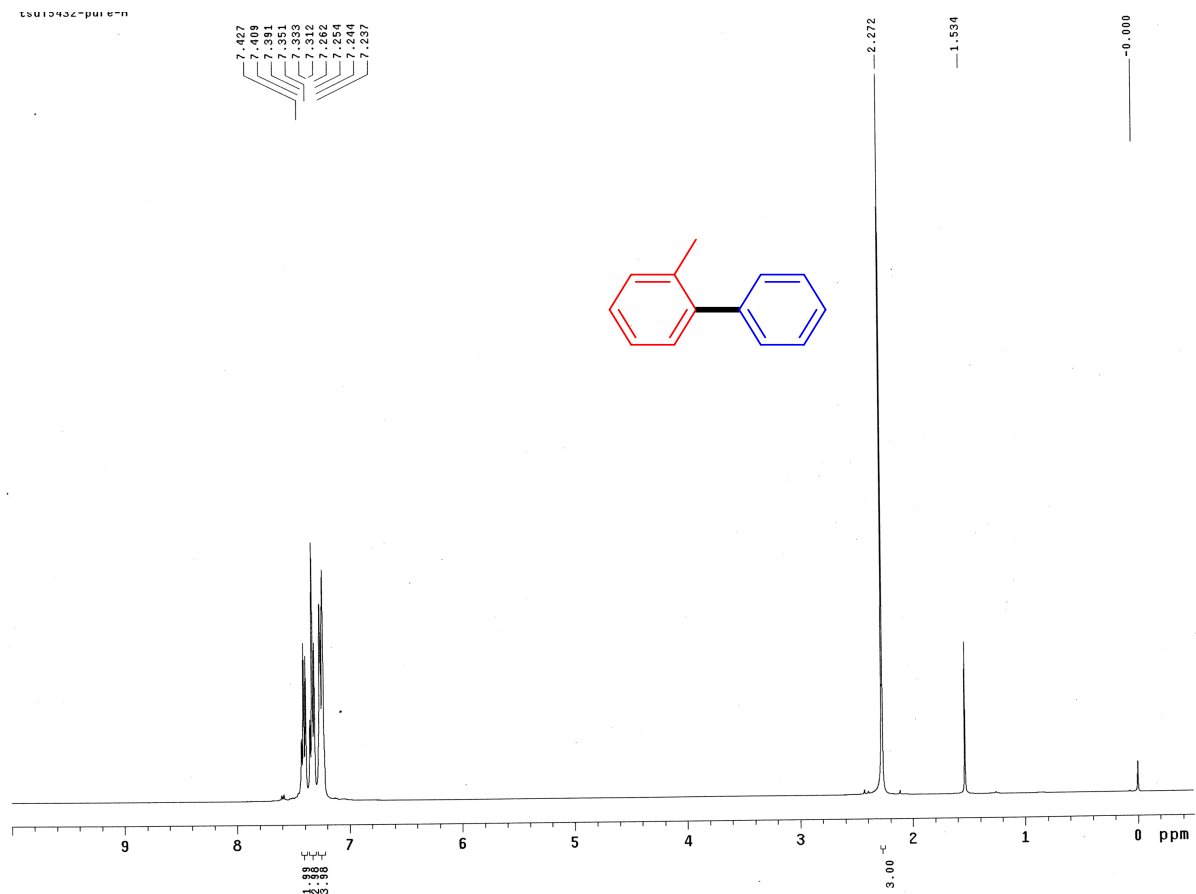


Figure S43: <sup>1</sup>H NMR spectrum of 2-methylbiphenyl (**6ma**) in CDCl<sub>3</sub>.

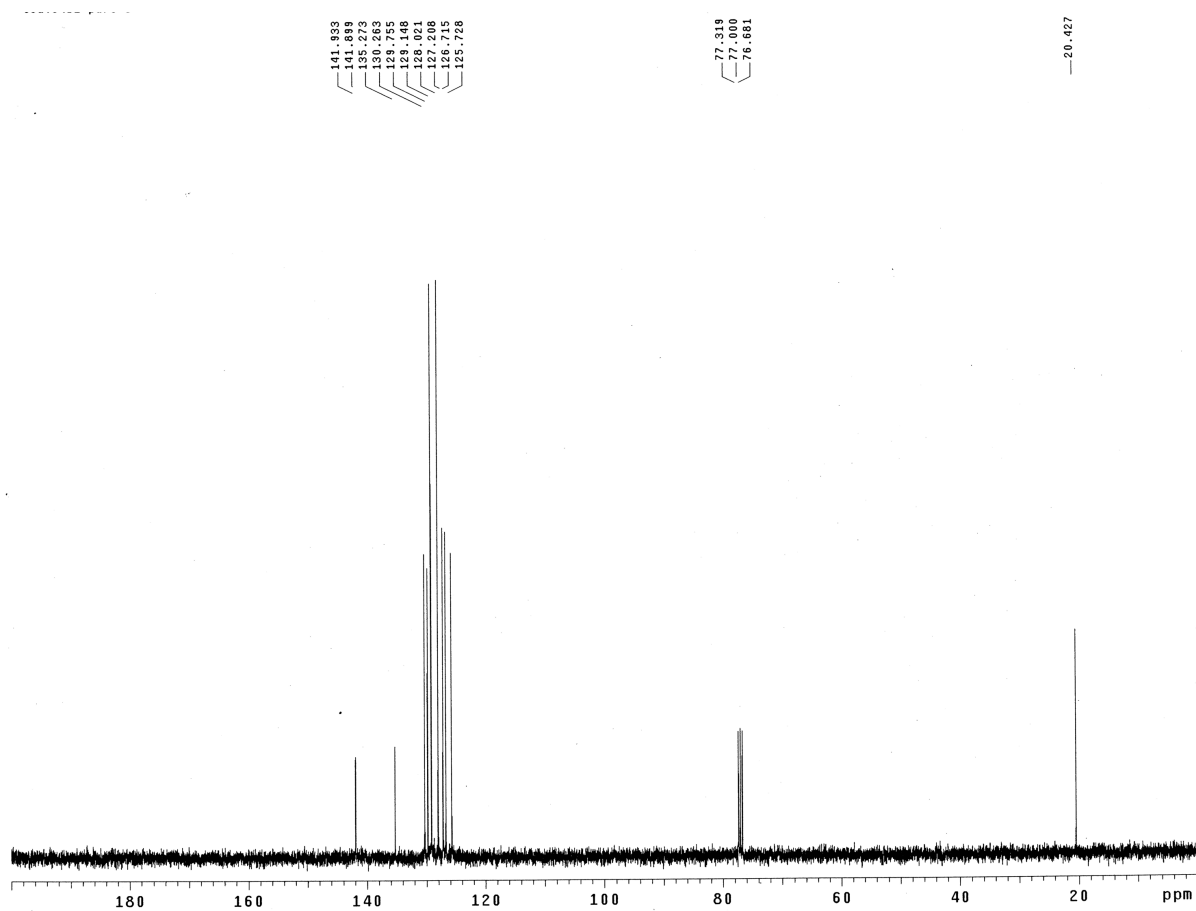


Figure S44: <sup>13</sup>C NMR spectrum of 2-methylbiphenyl (**6ma**) in CDCl<sub>3</sub>.

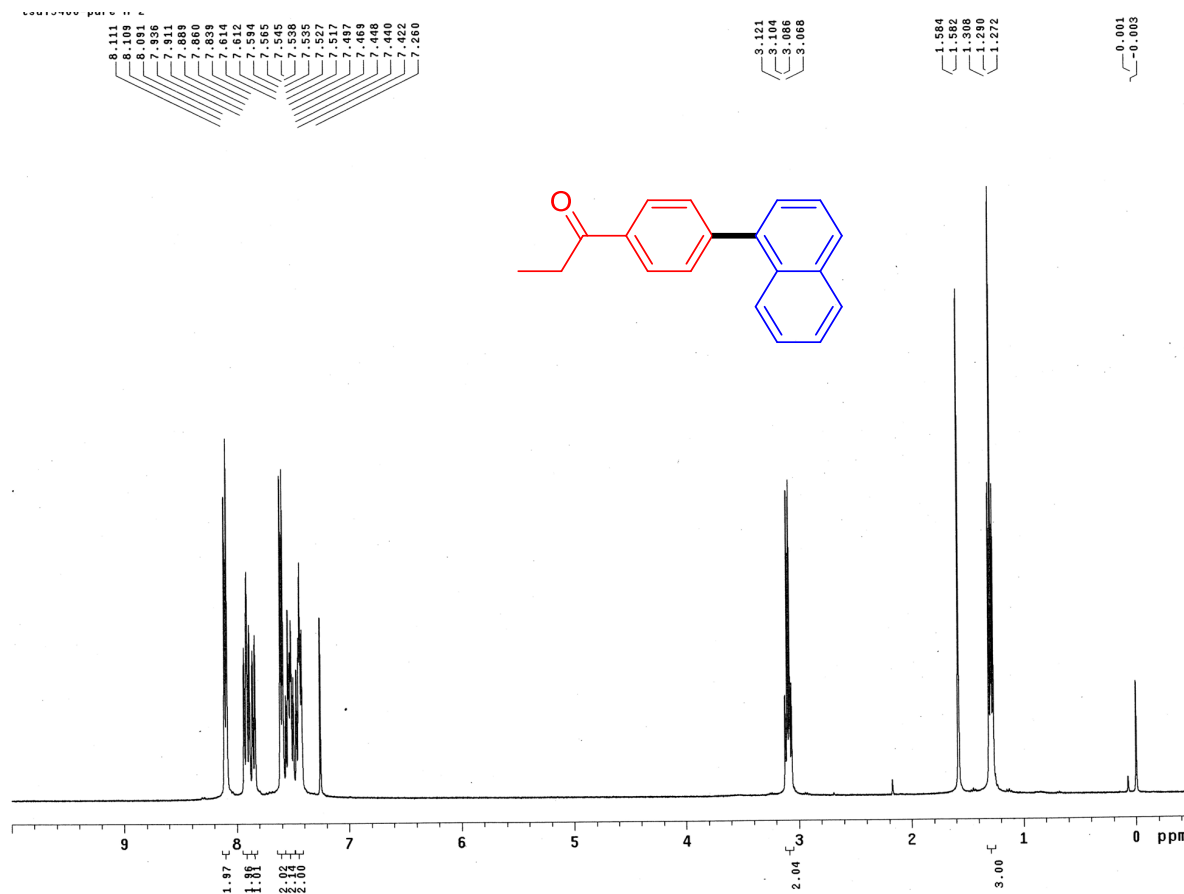


Figure S45: <sup>1</sup>H NMR spectrum of 1-(4-(naphthalen-1-yl)phenyl)propan-1-one (**6db**) in CDCl<sub>3</sub>.

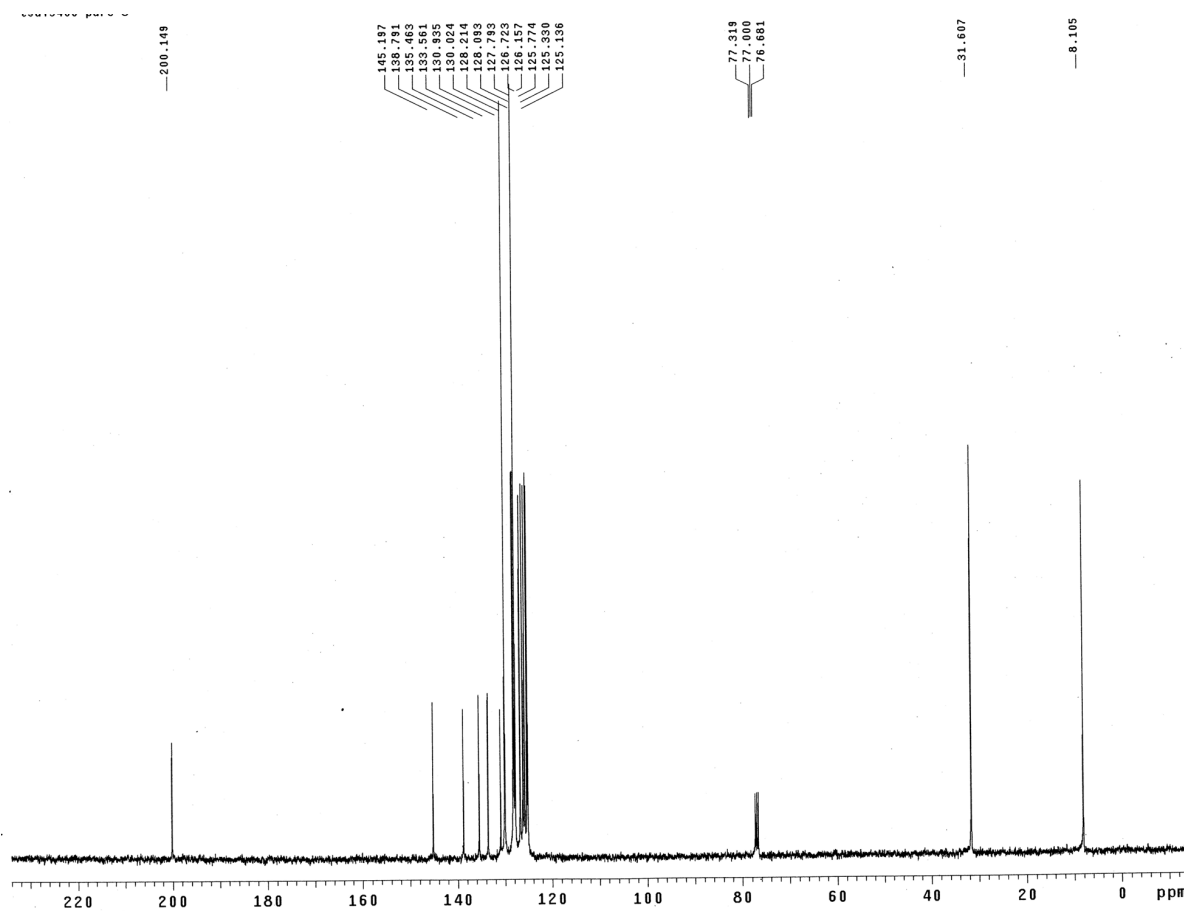


Figure S46: <sup>13</sup>C NMR spectrum of 1-(4-(naphthalen-1-yl)phenyl)propan-1-one (**6db**) in CDCl<sub>3</sub>.

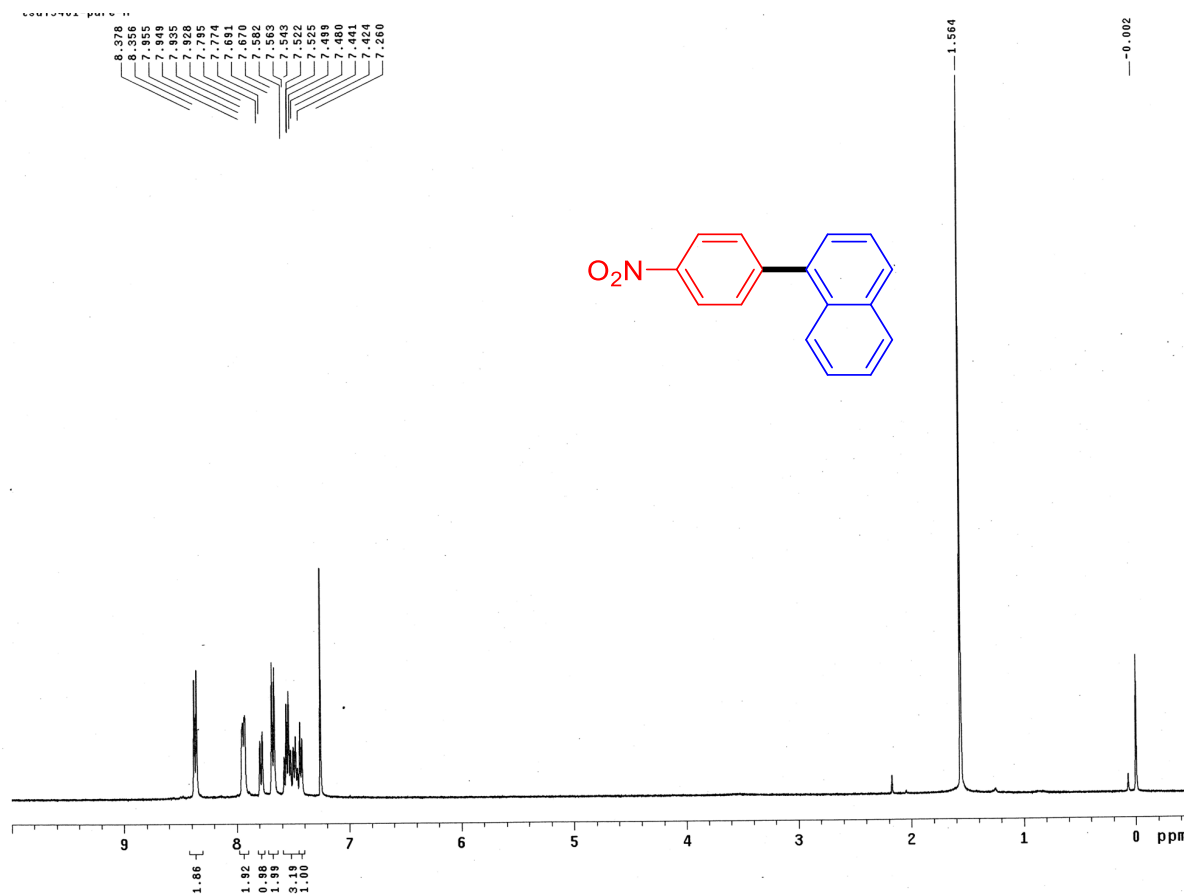


Figure S47: <sup>1</sup>H NMR spectrum of 1-(4-nitrophenyl)naphthalene (**6fb**) in CDCl<sub>3</sub>.

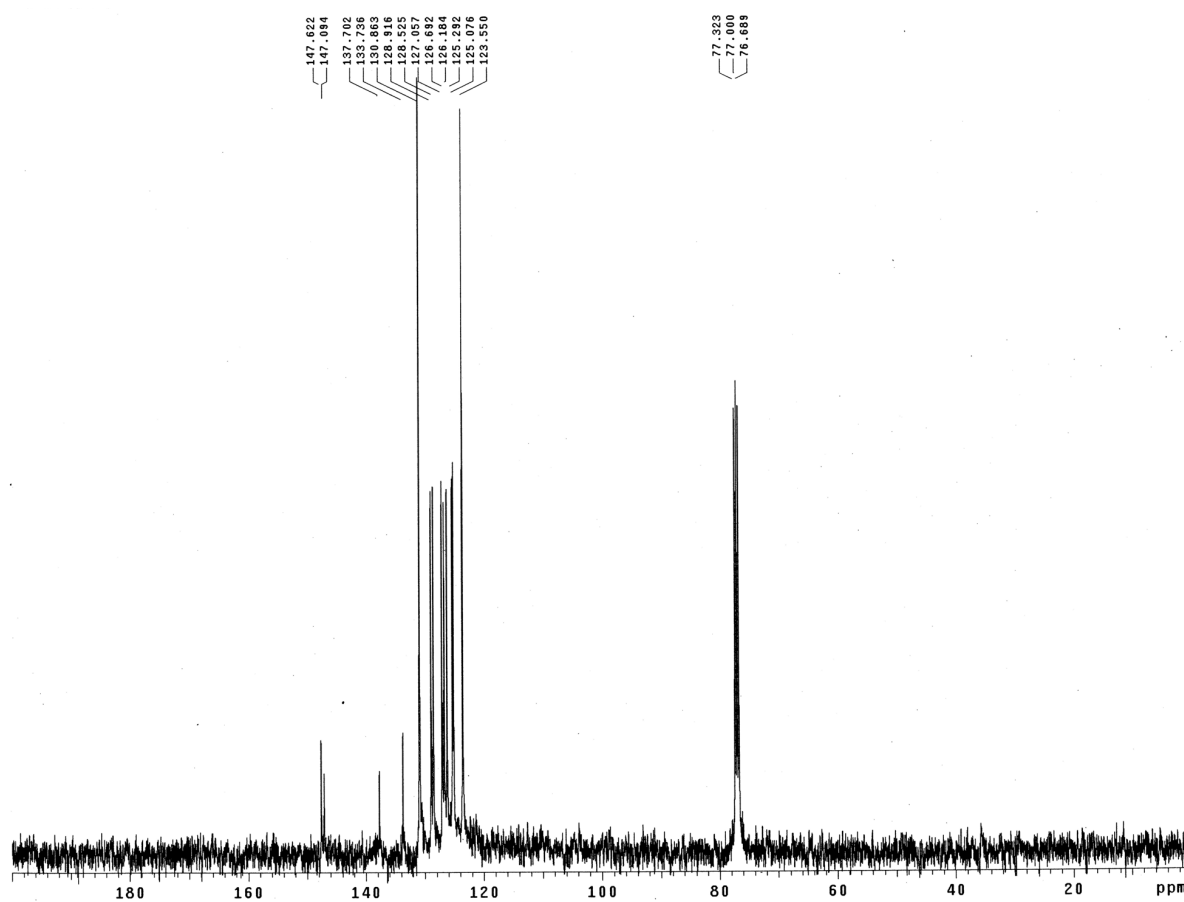


Figure S48: <sup>13</sup>C NMR spectrum of 1-(4-nitrophenyl)naphthalene (**6fb**) in CDCl<sub>3</sub>.

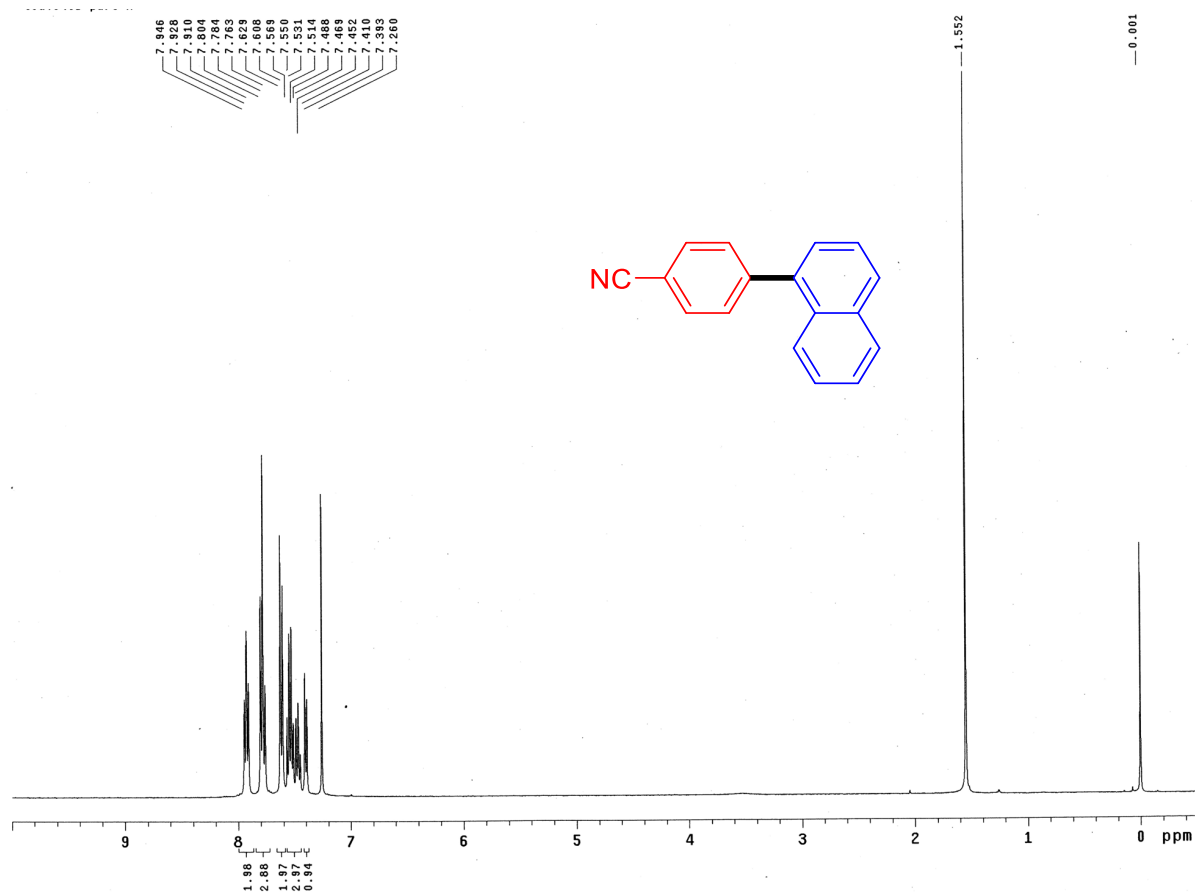


Figure S49: <sup>1</sup>H NMR spectrum of 4-(1-naphthyl)benzonitrile (**6ib**) in CDCl<sub>3</sub>.

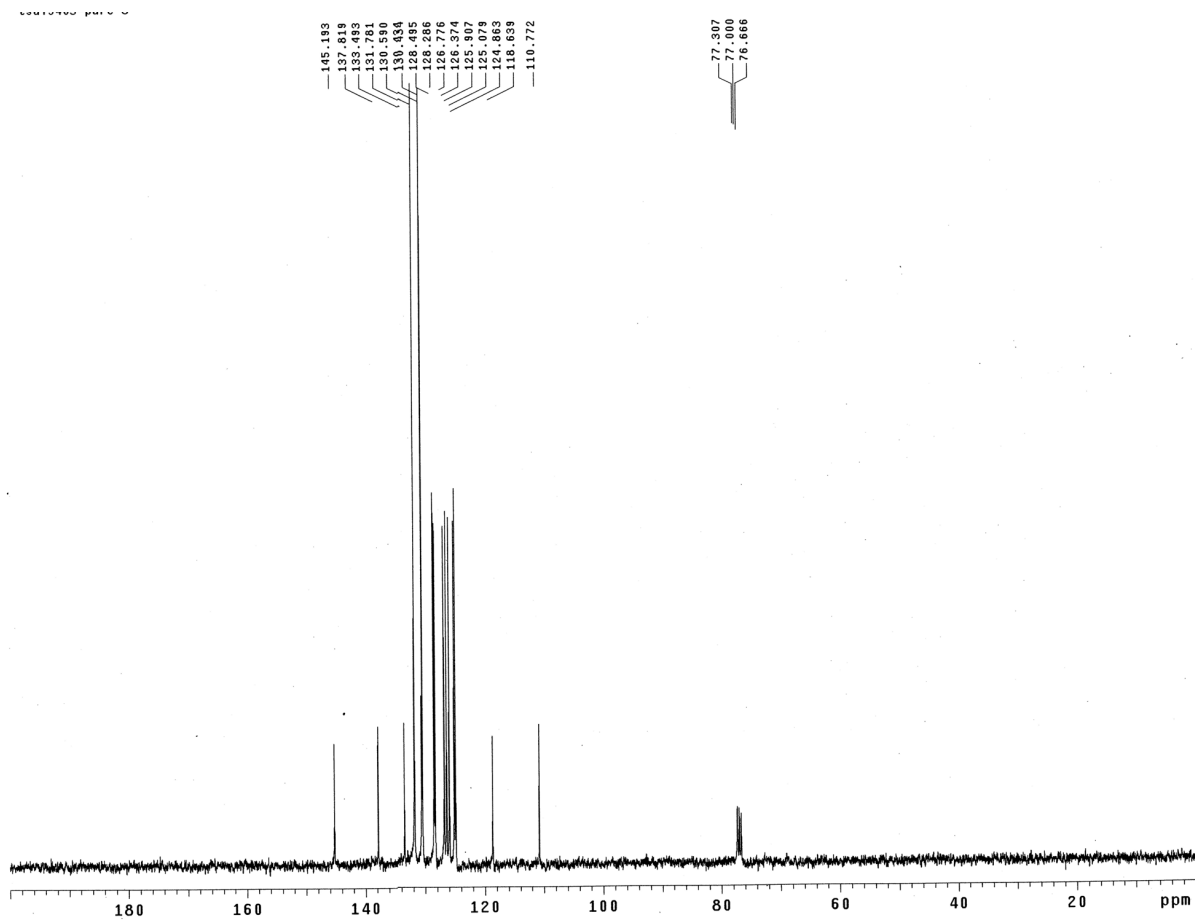
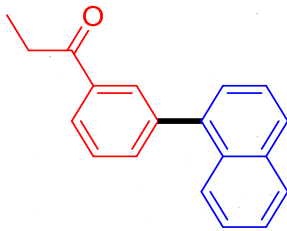


Figure S50: <sup>13</sup>C NMR spectrum of 4-(1-naphthyl)benzonitrile (**6ib**) in CDCl<sub>3</sub>.



13C NMR spectrum (CDCl<sub>3</sub>) of compound 10a. The x-axis represents chemical shift in ppm, ranging from 0 to 220. The spectrum shows several sharp peaks. A peak at 200.081 ppm is labeled. A cluster of peaks between 125 and 141 ppm is labeled with values: 140.719, 138.787, 136.662, 134.028, 133.463, 132.552, 129.170, 128.218, 128.100, 127.785, 126.730, 126.499, 125.813, 125.602, 125.170, and 125.041. A peak at 77.323 ppm is labeled, with a solvent peak at 76.681 ppm indicated by a bracket. A peak at 31.509 ppm is labeled. A peak at 7.892 ppm is labeled. The chemical structure of 10a is shown in the top right corner.

Figure S52:  $^{13}\text{C}$  NMR spectrum of 1-(3-(naphthalen-1-yl)phenyl)propan-1-one (**6e**) in  $\text{CDCl}_3$ .

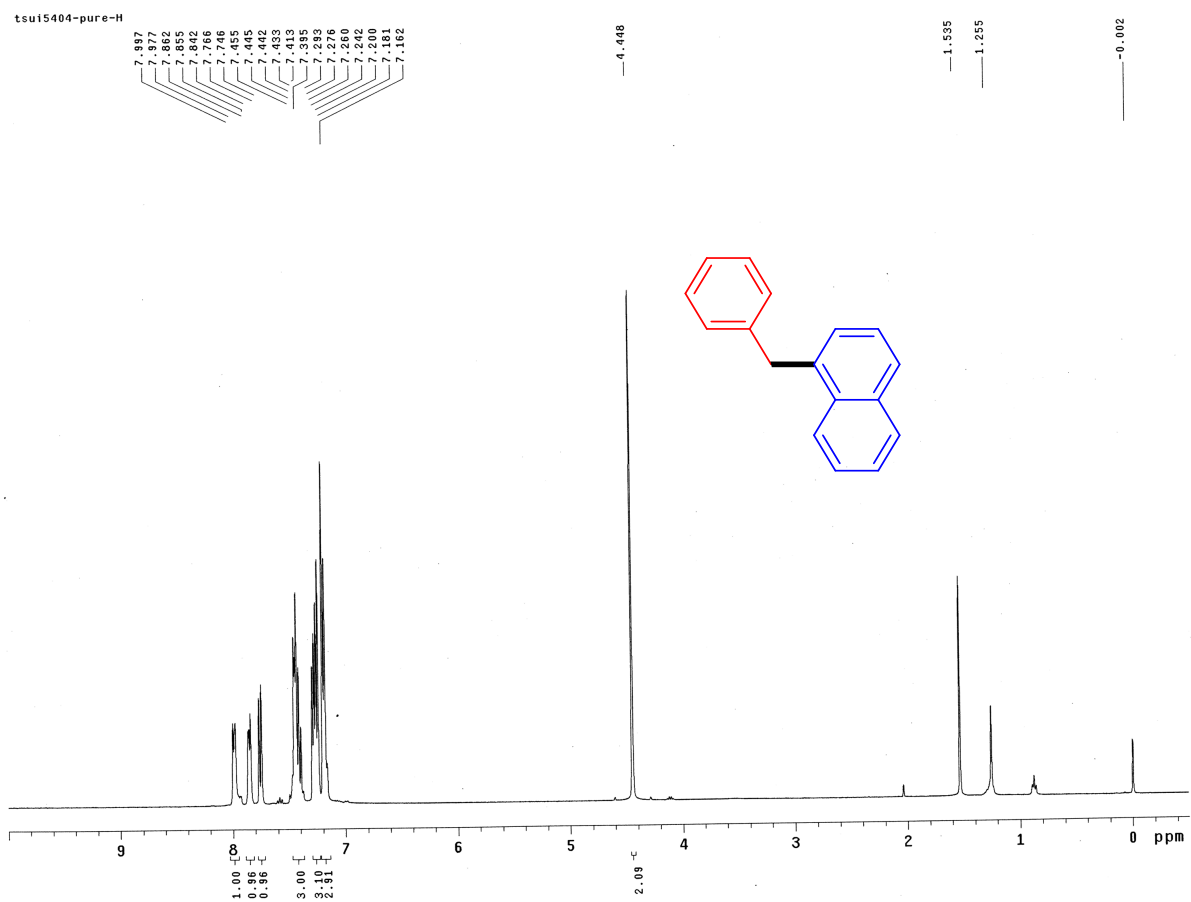


Figure S53: <sup>1</sup>H NMR spectrum of 1-benzyl-naphthalene (**6jb**) in CDCl<sub>3</sub>.

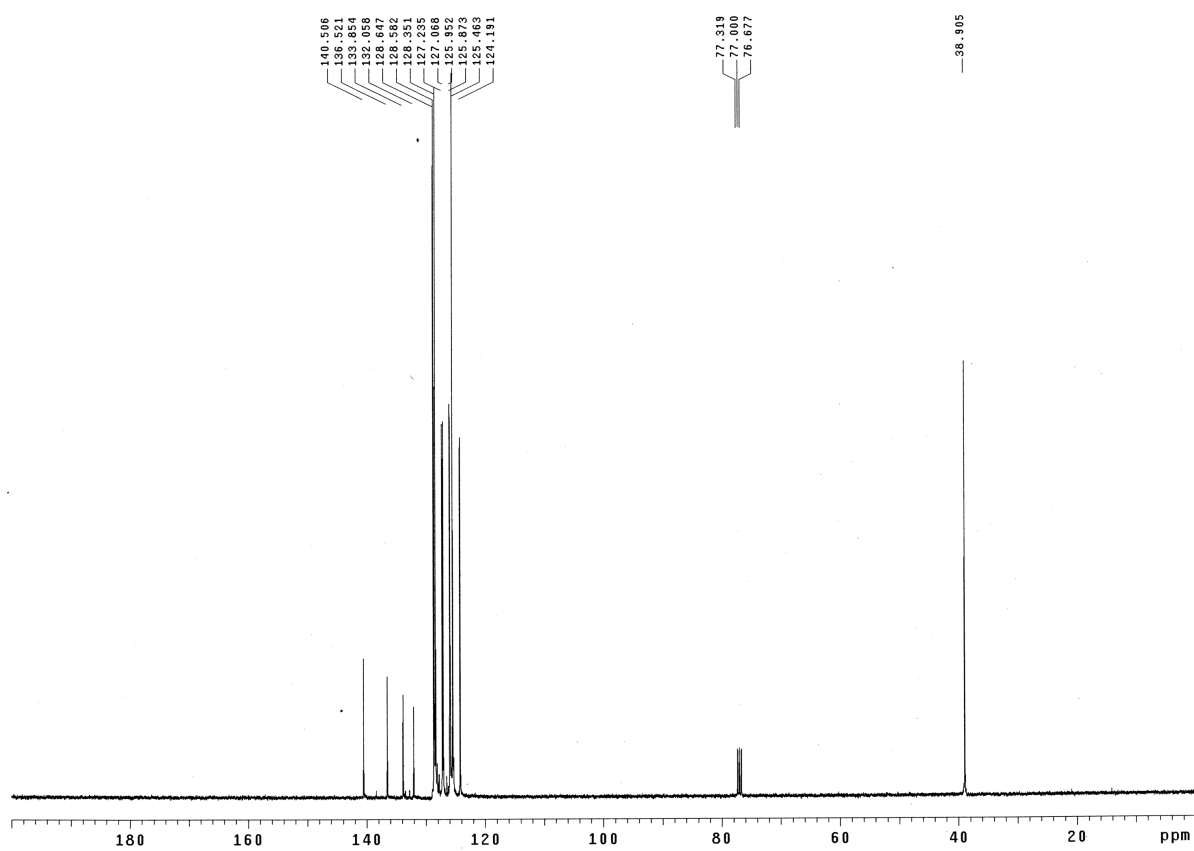


Figure S54: <sup>13</sup>C NMR spectrum of 1-benzyl-naphthalene (**6jb**) in CDCl<sub>3</sub>.



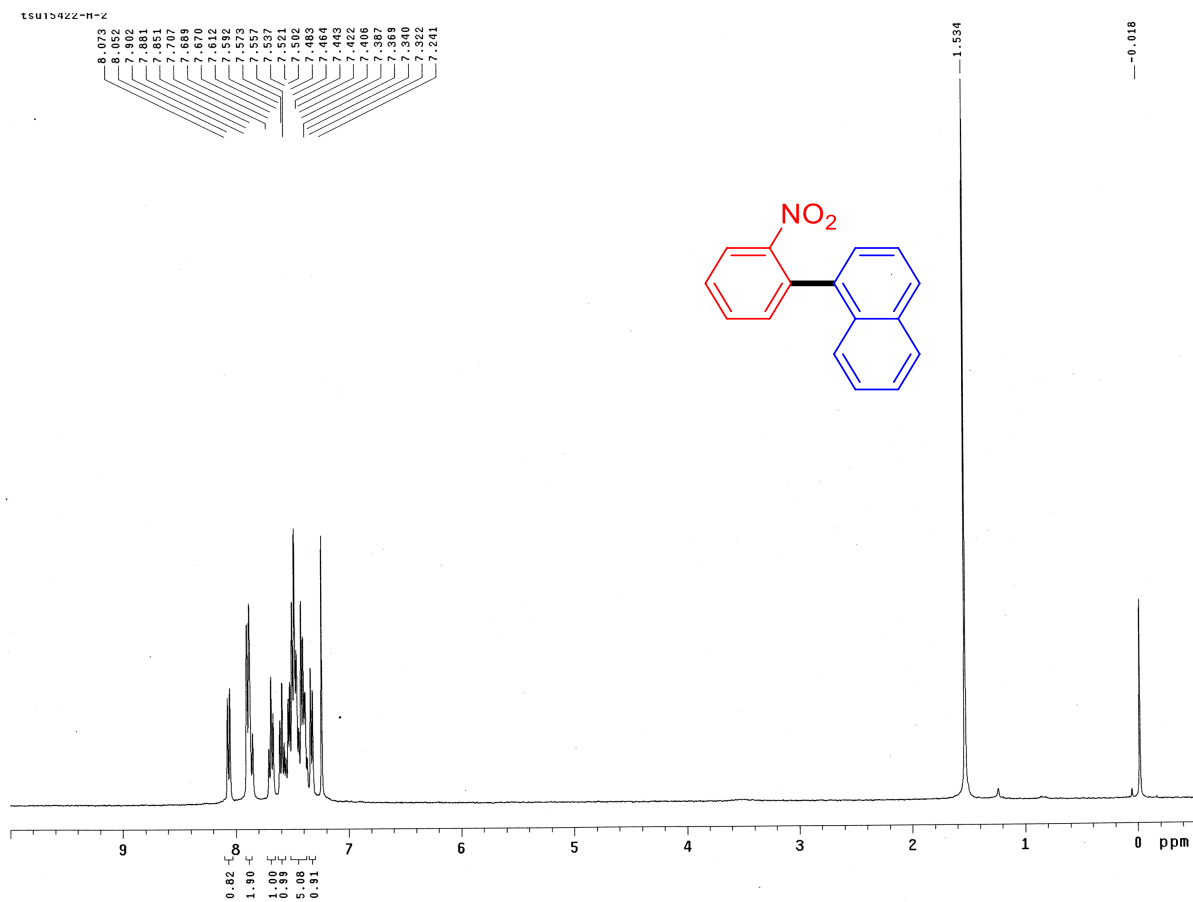


Figure S55: <sup>1</sup>H NMR spectrum of 1-(2-nitrophenyl)naphthalene (**6gb**) in CDCl<sub>3</sub>.

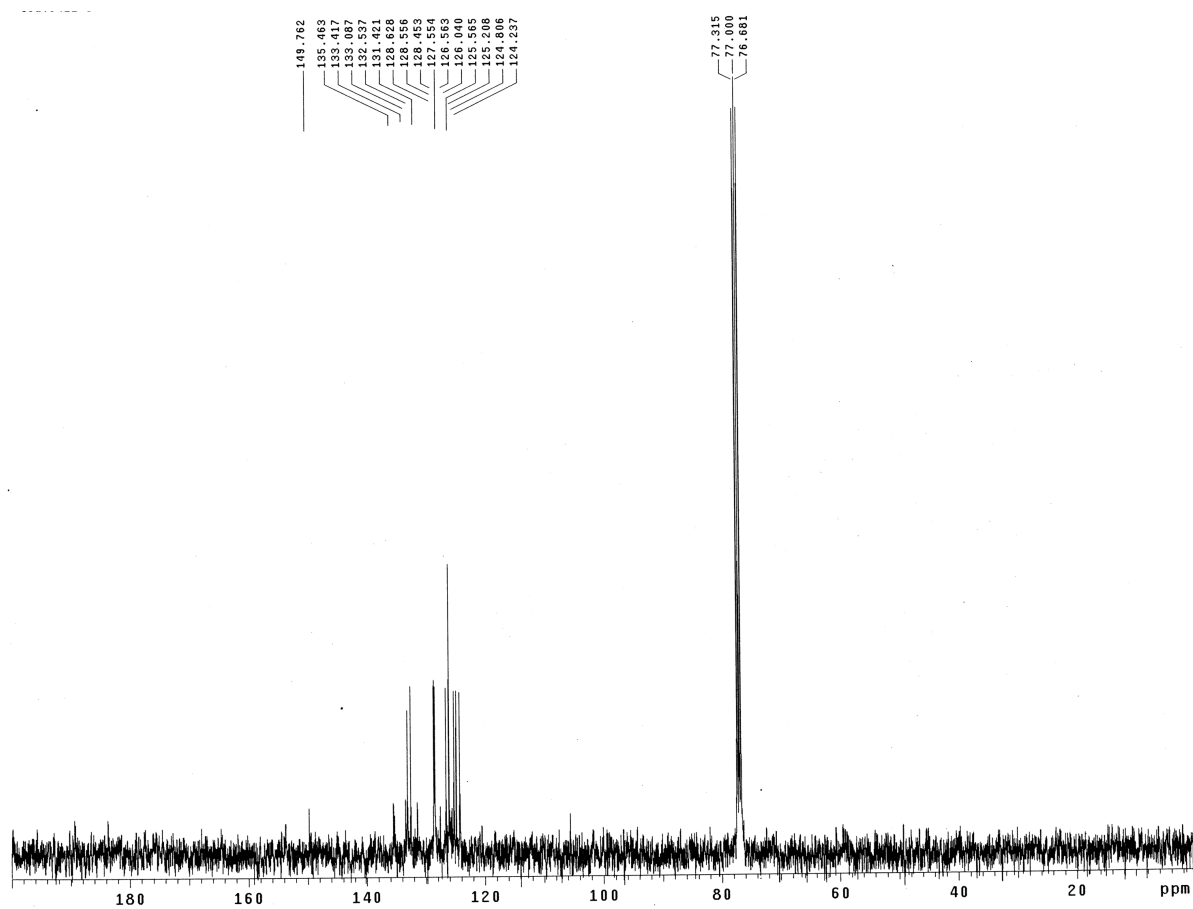


Figure S56: <sup>13</sup>C NMR spectrum of 1-(2-nitrophenyl)naphthalene (**6gb**) in CDCl<sub>3</sub>.

