Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Stabilized Well-dispersed Pd(0) Nanoparticles for Aminocarbonylation of Aryl Halides

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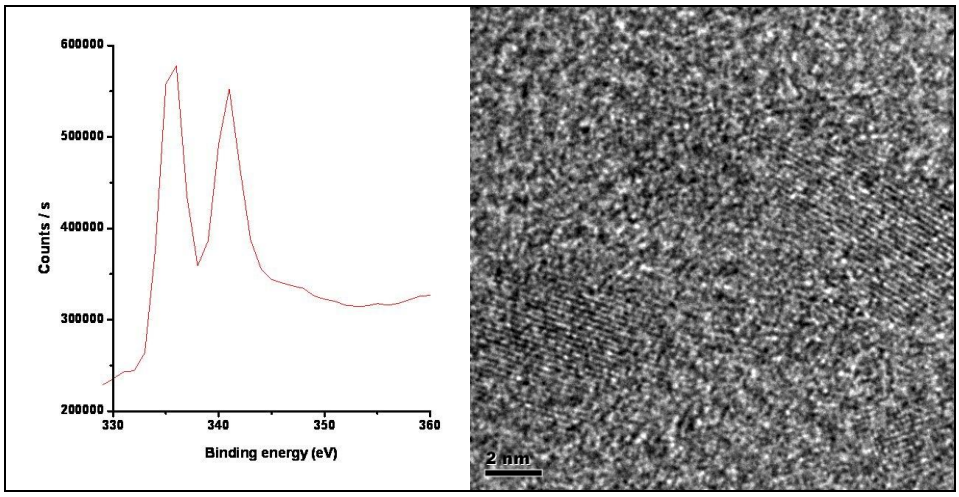
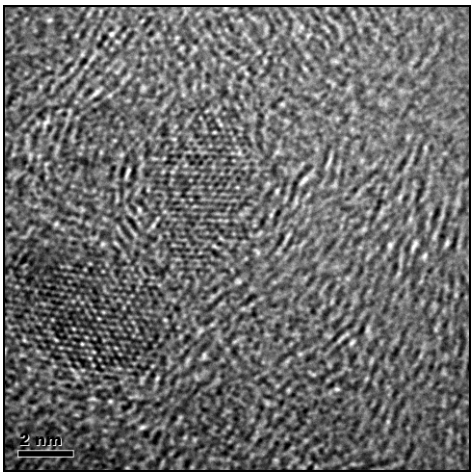
Figure S-1. XPS spectrum (a), TEM image (b) of nano-Pd after 5 runs and TEM image (c) of nano-Pd after storing 4 weeks under argon.

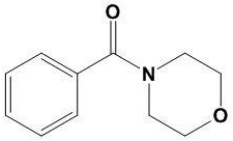


(a) (b)

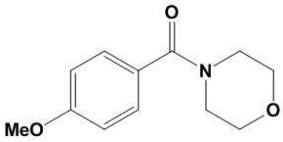


(c)

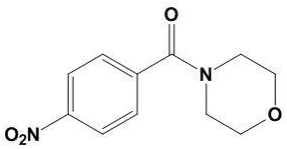
Spectroscopic data for products.



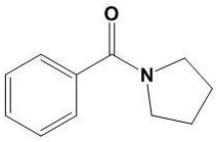
***N*-Benzoylmorpholine.** Yield 142 mg (74%), colorless oil. ^{1}H NMR ($CDCl_3$) δ (ppm): 3.44-3.77 (m, 8H), 7.40 (m, 5H); ^{13}C NMR ($CDCl_3$) δ (ppm): 42.6, 48.2, 66.9, 127.1, 128.6, 129.9, 135.3, 170.4. [3].



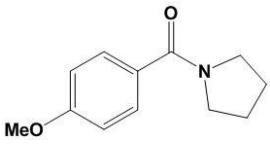
***N*-(*p*-Methoxybenzoyl)morpholine.** Yield 177 mg (80%), colorless oil. ^{1}H NMR ($CDCl_3$) δ (ppm): 3.60-3.67 (m, 8H), 3.81 (s, 3H); 6.79-6.90 (m, 2H); 7.36-7.38 (m, 2H); ^{13}C NMR ($CDCl_3$) δ (ppm): 41.5, 48.4, 55.3, 67.1, 114.4, 127.3, 129.2, 160.9.1, 170.4 [4].



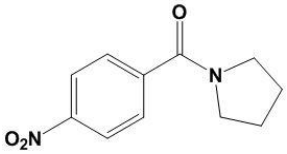
***N*-(*p*-Nitrobenzoyl)morpholine**. Yield 196 mg (83%), yellow solid. ^{1}H NMR ($CDCl_3$) δ (ppm): 3.23-3.85 (m, 8H), 7.53 (d, 2H), 8.22 (d, 2H). ^{13}C NMR ($CDCl_3$) δ (ppm): 42.5, 48.7, 67.3, 123.9, 128.4, 141.5, 148.4, 168.3 [5].



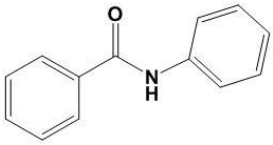
***N*-Benzoylpyrrolidine.** Yield 105 mg (60%), colorless oil. ^{1}H NMR ($CDCl_3$) δ (ppm): 1.68-1.76 (m, 4H), 3.23-3.46 (m, 4H), 7.22-7.30 (m, 5H); ^{13}C NMR ($CDCl_3$) δ (ppm): 23.8, 25.8, 45.5, 48.9, 126.4, 127.6, 129.1, 136.6, 169.0 [6].



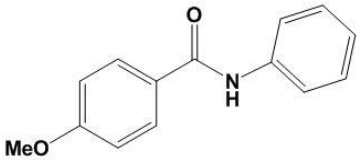
***N*-(*p*-Methoxybenzoyl)pyrrolidine.** Yield 138 mg (67%) colorless solid. ^{1}H NMR ($CDCl_3$) δ (ppm): 1.83 (m, 4H), 3.57 (t, 4H), 3.70 (s, 3H), 6.77-680 (m, 2H), 7.39-7.43 (m, 2H); ^{13}C NMR ($CDCl_3$) δ (ppm): 24.1, 26.3, 46.2, 49.6, 55.1, 113.2, 129.1, 131.9, 160.6, 172.1 [7].



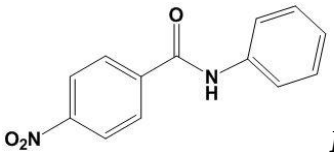
***N*-(*p*-Nitrobenzoyl)pyrrolidine.** Yield 156 mg (71%) yellow solid. ^{1}H NMR ($CDCl_3$) δ (ppm): 1.83-1.87 (m, 4H), 3.31-3.62 (m, 4H), 7.20-8.21 (m, 4H); ^{13}C NMR ($CDCl_3$) δ (ppm): 23.3, 25.4, 45.7, 49.5, 117.1, 127.1, 131.6, 149.7, 165.0 [8].



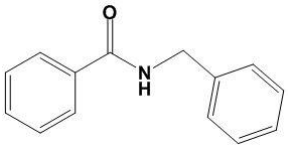
Phenylbenzamide. Yield 152 mg (77%), colorless solid. ^{1}H NMR ($CDCl_3$) δ (ppm): 7.13-7.87 (m, 10H); ^{13}C NMR ($CDCl_3$) δ (ppm): 120.3, 124.6, 127.1, 128.8, 129.1, 131.9, 135.0, 138.0, 165.8 [9].



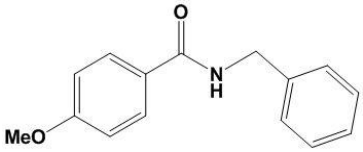
***N*-Phenyl-4-methoxybenzamide.** Yield 208 mg (86%), white solid. ^{1}H NMR ($CDCl_3$) δ (ppm): 3.80 (s, 3H), 6.87-7.94 (m, 9H); ^{13}C NMR ($CDCl_3$) δ (ppm): 55.5, 122.1, 124.1, 126.7, 127.8, 128.7, 130.5, 133.9, 138.4, 165.6 [10].



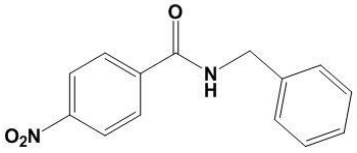
***N*-Phenyl-4-nitrobenzamide**. Yield 215 mg (89%), pale-yellow solid. ^{1}H NMR ($CDCl_3$) δ (ppm): 7.06-8.30 (m, 10H); ^{13}C NMR ($CDCl_3$) δ (ppm): 120.6, 123.5, 124.5, 128.7, 129.3, 131.9, 138.5, 139.4, 150.4, 166.0 [11].



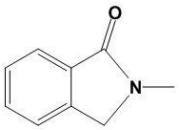
***N*-Benzylbenzamide**. Yield 138 mg (65%) colorless solid. ^{1}H NMR ($CDCl_3$) δ (ppm): 4.60 (d, 2H), 6.70 (s, 1H), 7.30-7.80 (m, 10H); ^{13}C NMR ($CDCl_3$) δ (ppm): 44.1, 127.0, 127.6, 127.9, 128.6, 128.8, 131.5, 134.4, 138.3, 167.4 [9, 10].



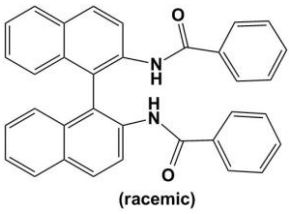
***N*-Benzyl-4-methoxbenzamide**. Yield 178 mg (74%) colorless solid. ^{1}H NMR ($CDCl_3$) δ (ppm): 3.67 (s, 3H), 4.42 (d, 2H), 6.30 (s, 1H), 6.70-7.74 (m, 10H). ^{13}C NMR ($CDCl_3$) δ (ppm): 43.7, 55.4, 113.6, 126.3, 127.6, 127.9, 128.5, 128.7, 138.8, 162.1, 167.2 [10].



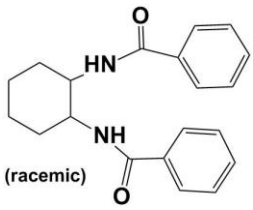
***N*-Benzyl-4-nitrobenzamide**. Yield 174 mg (68%) colorless solid. ^{1}H NMR ($CDCl_3$) δ (ppm): 4.60 (d, 2H), 6.65 (s, 1H), 7.10-8.09 (m, 10H); ^{13}C NMR ($CDCl_3$) δ (ppm): 43.6, 123.4, 127.5, 127.9, 128.2, 128.8, 137.5, 139.8, 149.5, 167.5 [11].



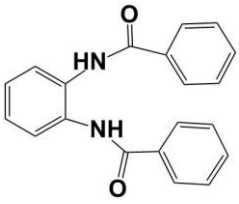
2-Methylisoindolin-1-one. Yield 54 mg (37%) and 13 mg (9%) from bromide and chloride, respectively, colorless solid. ^{1}H NMR ($CDCl_3$) δ (ppm): 3.21 (s, 3H), 4.38 (s, 2H), 7.43-7.85 (m, 4H); ^{13}C NMR ($CDCl_3$) δ (ppm): 29.7, 52.0, 122.6, 123.6, 128.0, 133.0, 141.0, 168.7 [12].



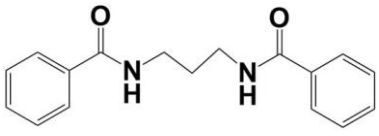
***Racemic-N,N′*-(1,1′-Binaphthyl-2,2′-diyl)dibenzamide.** Yield 375 mg (76%), pale white solid. ^{1}H NMR ($CDCl_3$) δ (ppm): 7.12-7.90 (m, 16H), 7.72 (s, 2H), 7.91 (d, 2H), 8.04 (d, 2H), 8.66 (d, 2H); ^{13}C NMR ($CDCl_3$) δ (ppm): 120.71, 121.43, 125.02, 125.75, 126.74, 127.69, 128.52, 128.65, 130.24, 131.33, 131.83, 132.19, 134.21, 135.26, 165.82 [13].



***Racemic-N,N′*-(cyclohexane-1,2-diyl)dibenzamide**. Yield 220 mg (68%), colorless solid. ^{1}H NMR (DMSO-d_6) δ (ppm): 1.29 (m, 2H), 1.50 (m, 2H), 1.75 (m, 2H), 1.92 (m, 2H), 3.94 (m, 2H), 7.37-7.45 (m, 6H), 7.69-7.72 (m, 4H), 8.25 (m, 2H); ^{13}C NMR (DMSO-d_6) δ (ppm): 24.65, 31.58, 52.92, 127.08, 128.07, 130.85, 134.90, 168.40 [14].



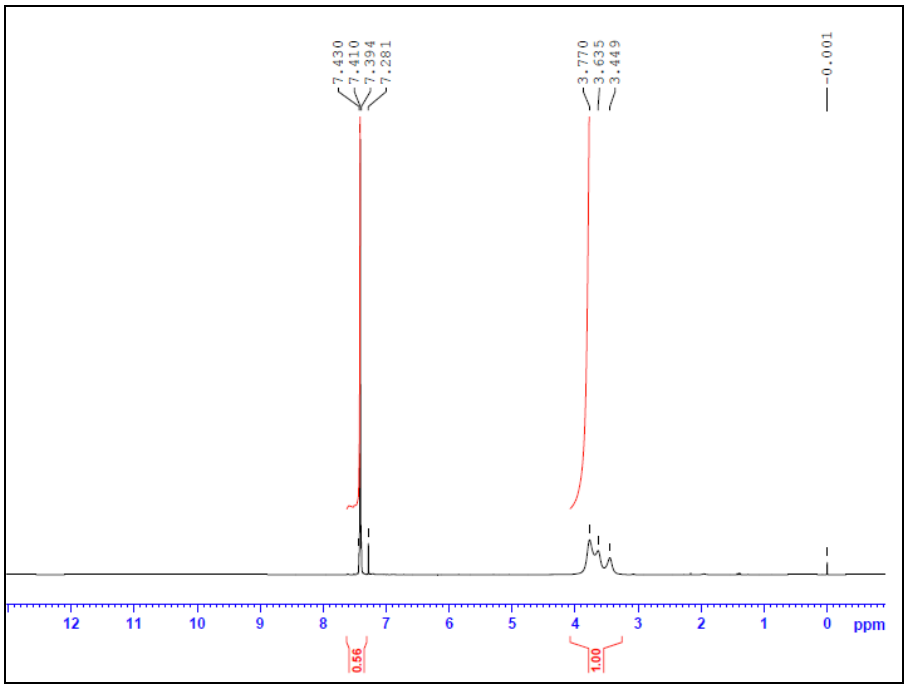
***N,N′*-(1,2-phenylene)dibenzamide.** Yield 228 mg (72%), pale white solid. ^{1}H NMR ($CDCl_3$) δ (ppm): 7.20-7.63 (m, 10H), 8.07-8.12 (m, 6H); ^{13}C NMR ($CDCl_3$) δ (ppm): 128.50, 128.89, 129.32, 130.23, 130.59, 133.84, 134.55, 172.42 [15].



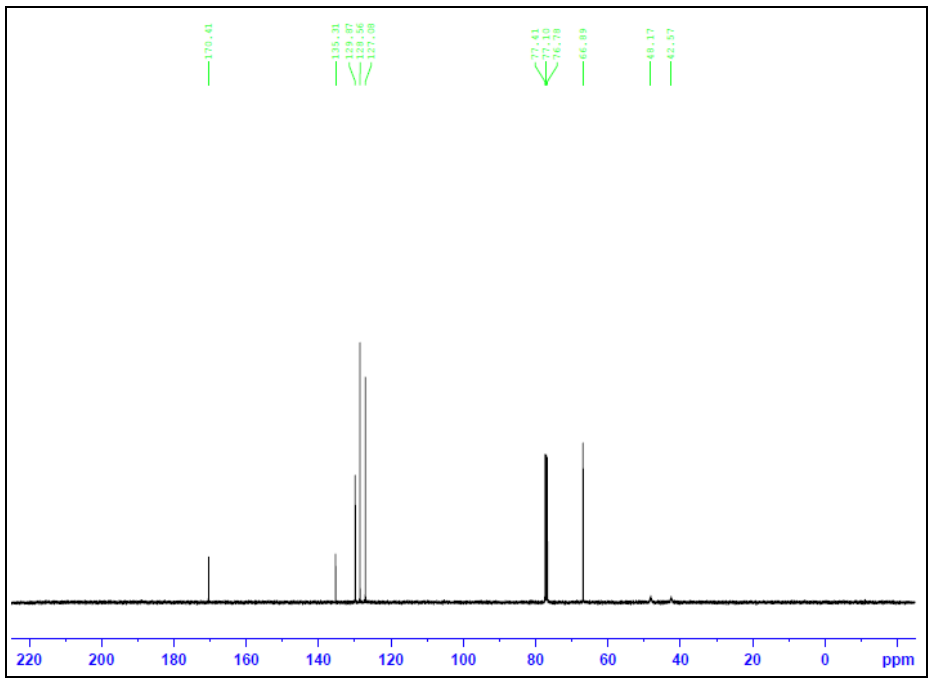
***N,N′*-(propane-1,3-diyl)dibenzamide.** Yield 167 mg (59%), colorless solid. ^{1}H NMR (DMSO-d_6) δ (ppm): 1.78 (t, 2H), 3.33 (m, 4H), 7.44-7.52 (m, 6H), 7.83-7.85 (m, 4H), 8.50 (t, 2H); ^{13}C NMR (DMSO-d_6) δ (ppm): 29.25, 37.00, 127.05, 128.22, 131.03, 134.55, 166.18 [16].

Selected NMR spectra

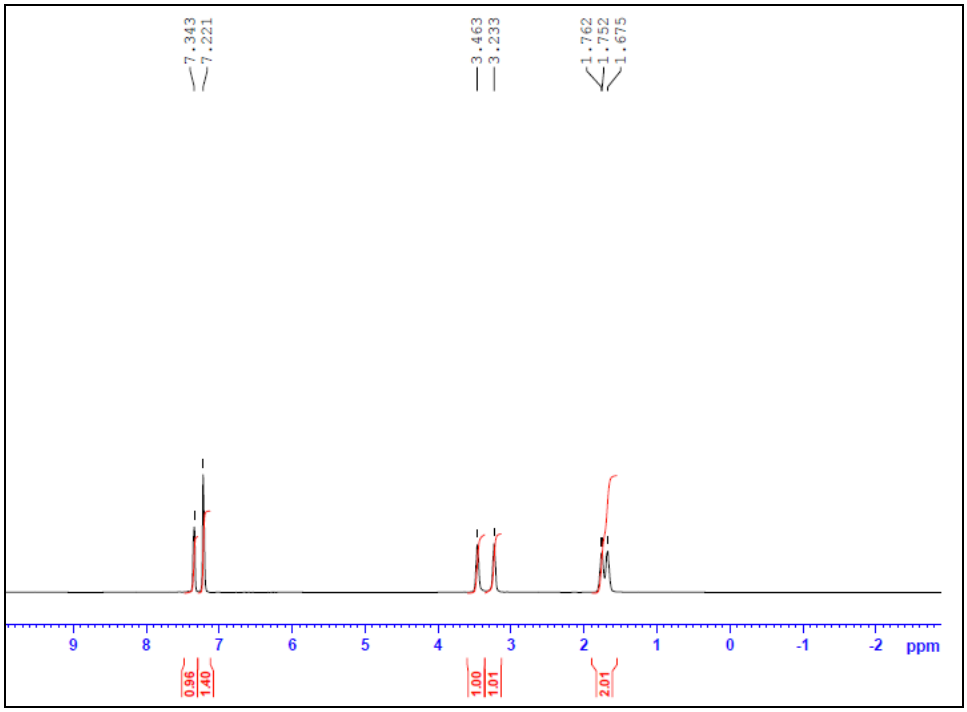
^{1}H NMR ($CDCl_3$) of *N*-benzoylmorpholine



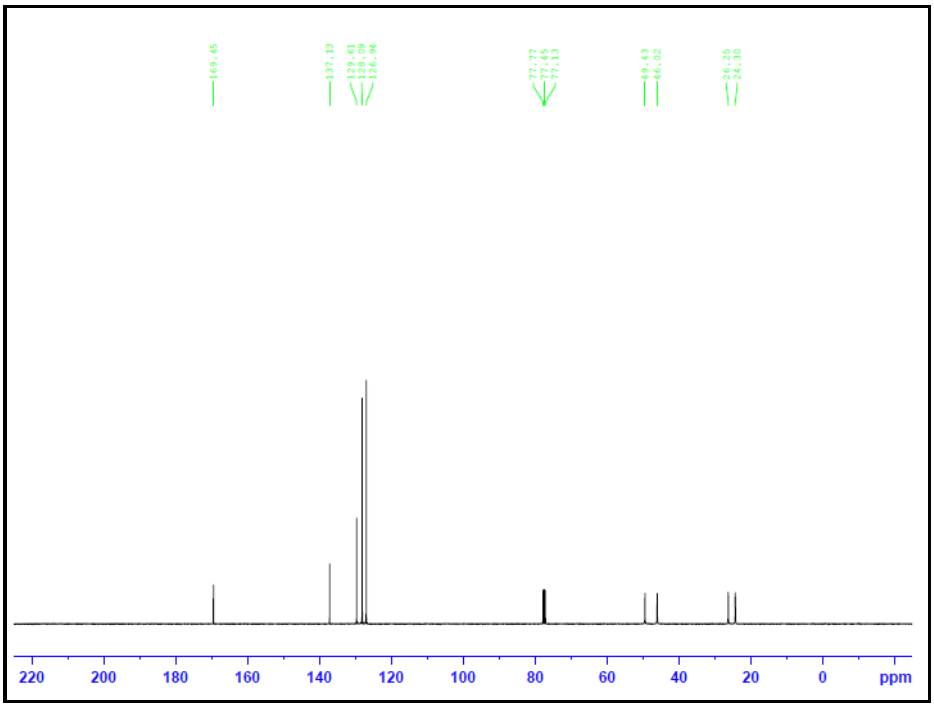
^{13}C NMR ($CDCl_3$) of *N*-benzoylmorpholine



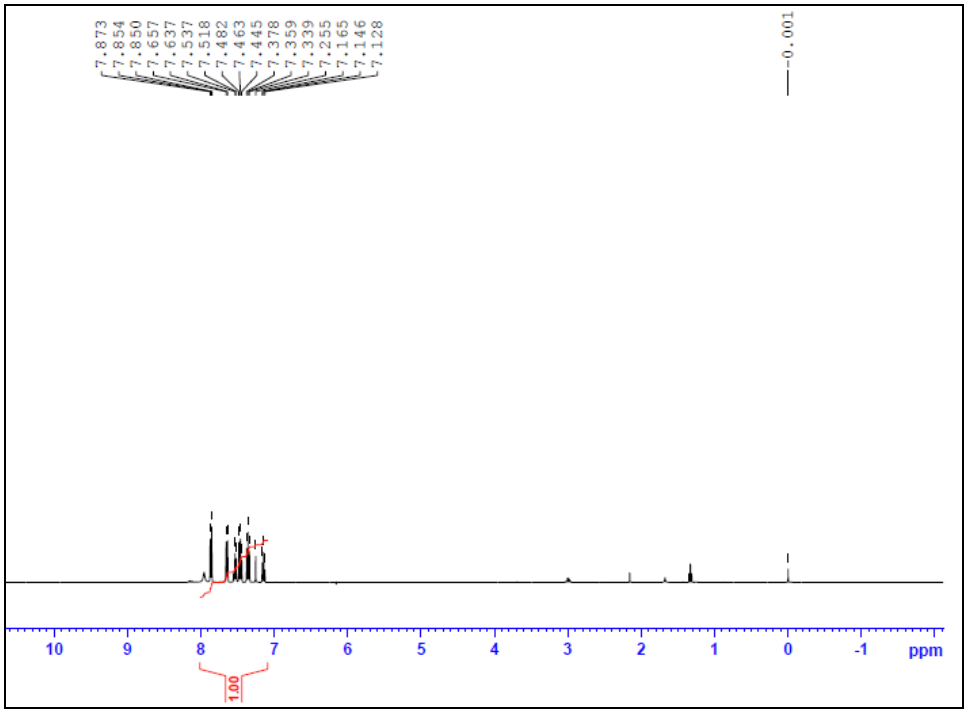
^{1}H NMR ($CDCl_3$) of *N*-benzoylpyrrolidine



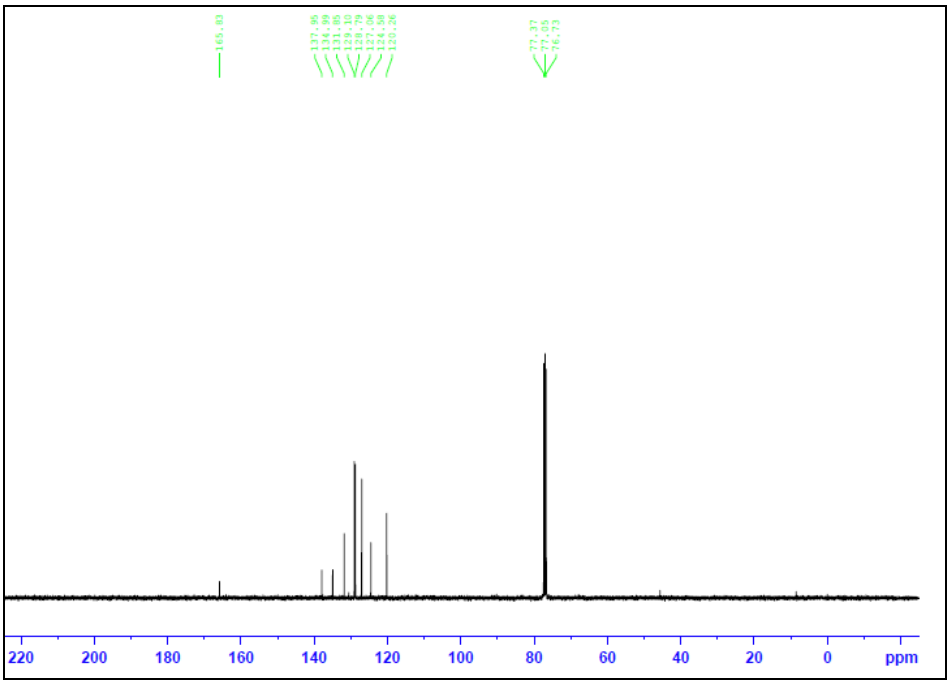
^{13}C NMR ($CDCl_3$) of *N*-benzoylpyrrolidine



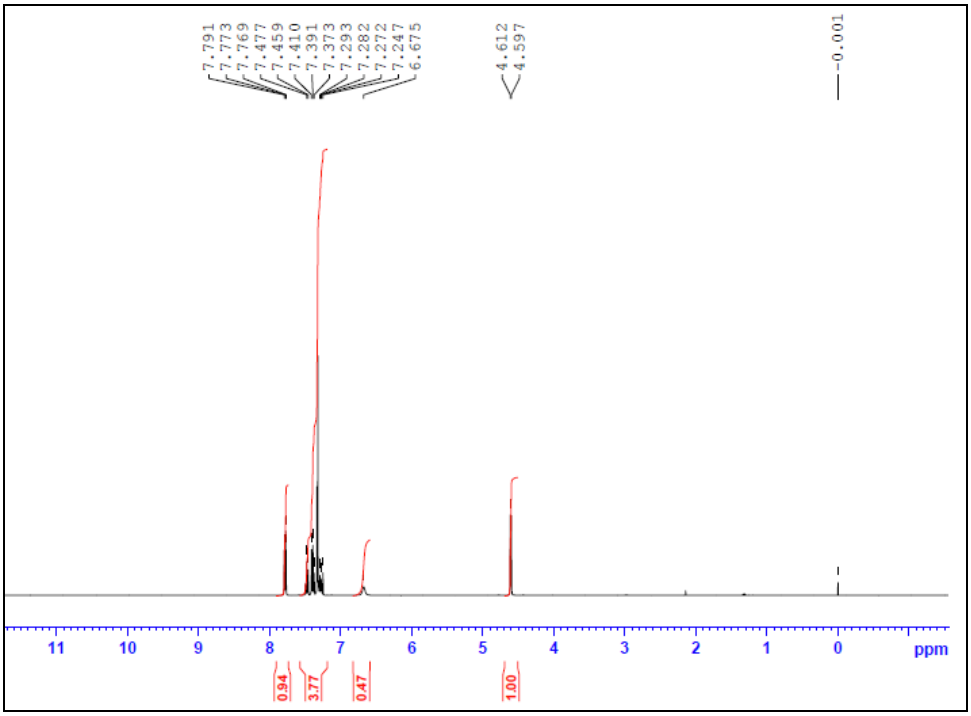
^{1}H NMR ($CDCl_3$) of phenylbenzamide



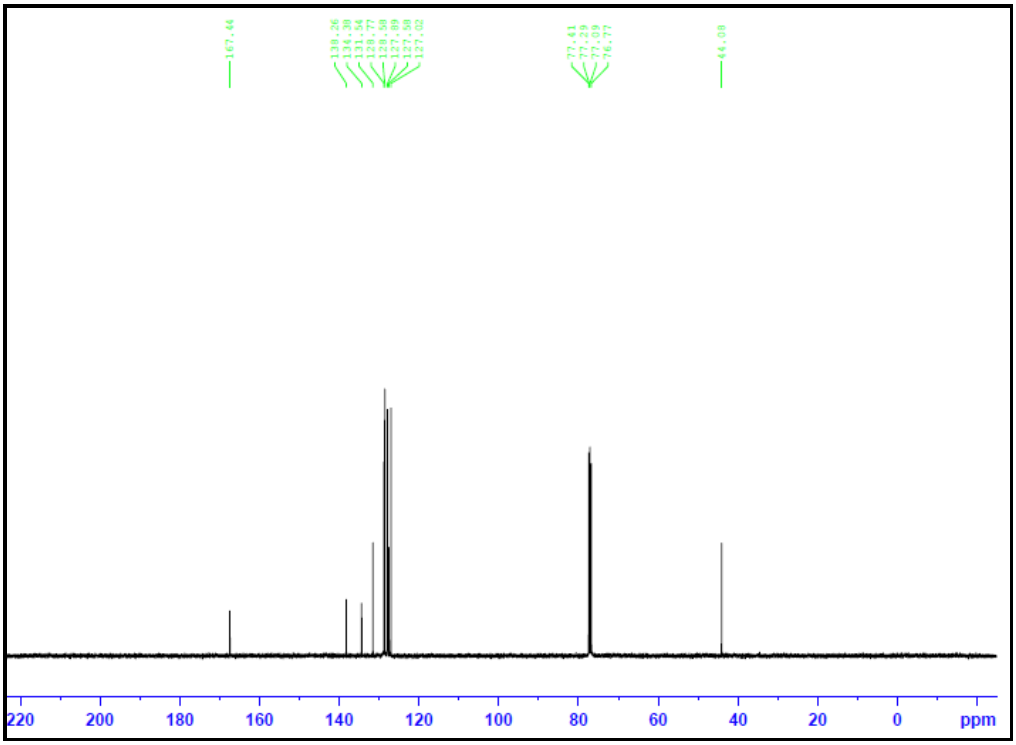
^{13}C NMR ($CDCl_3$) of phenylbenzamide



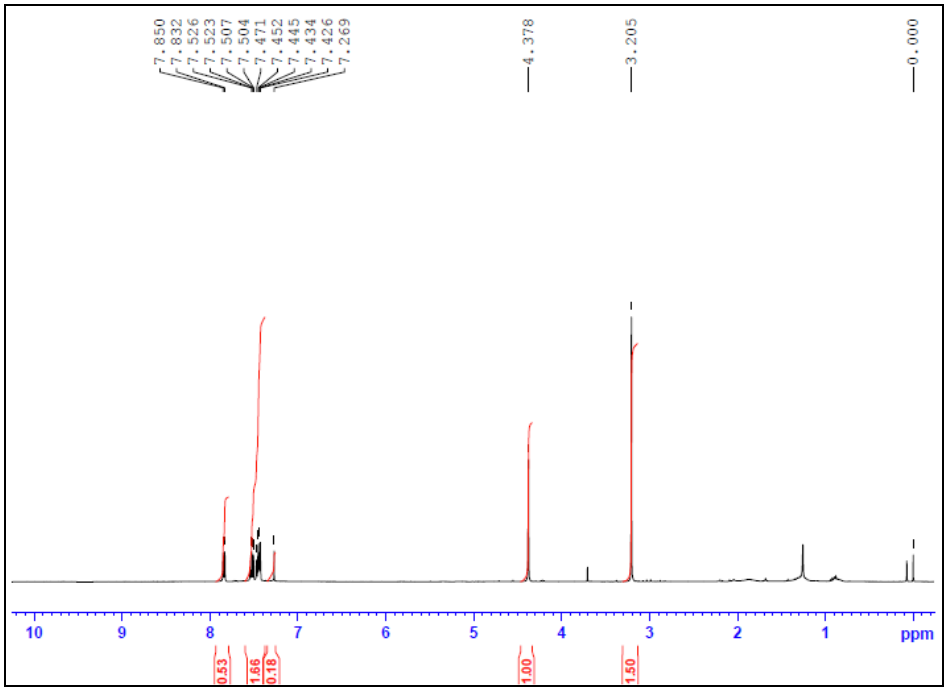
^{1}H NMR ($CDCl_3$) of *N*-benzylbenzamide



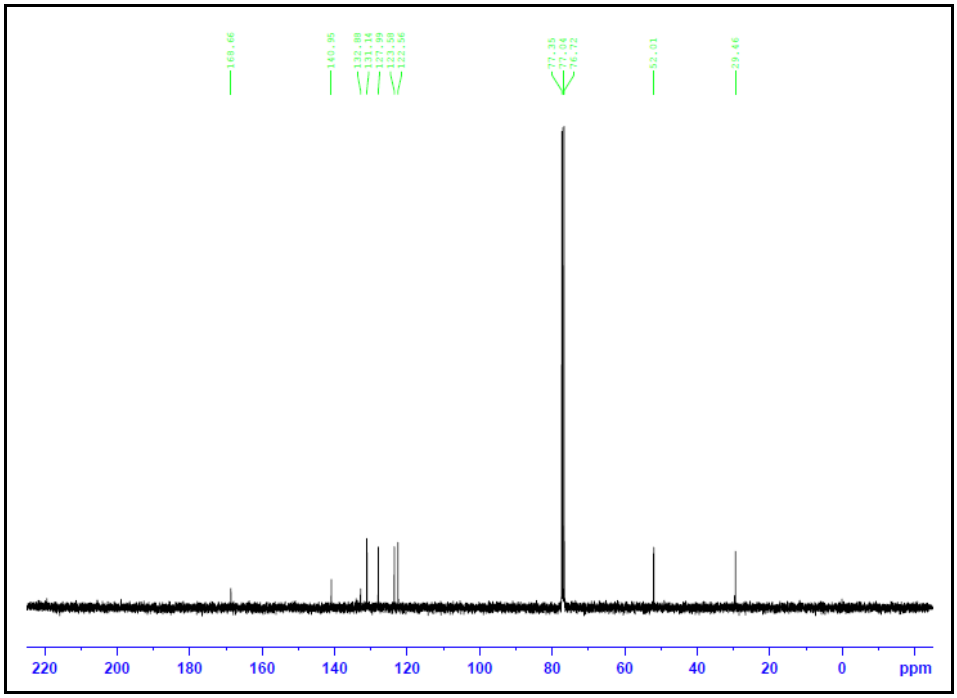
^{13}C NMR ($CDCl_3$) of *N*-benzylbenzamide



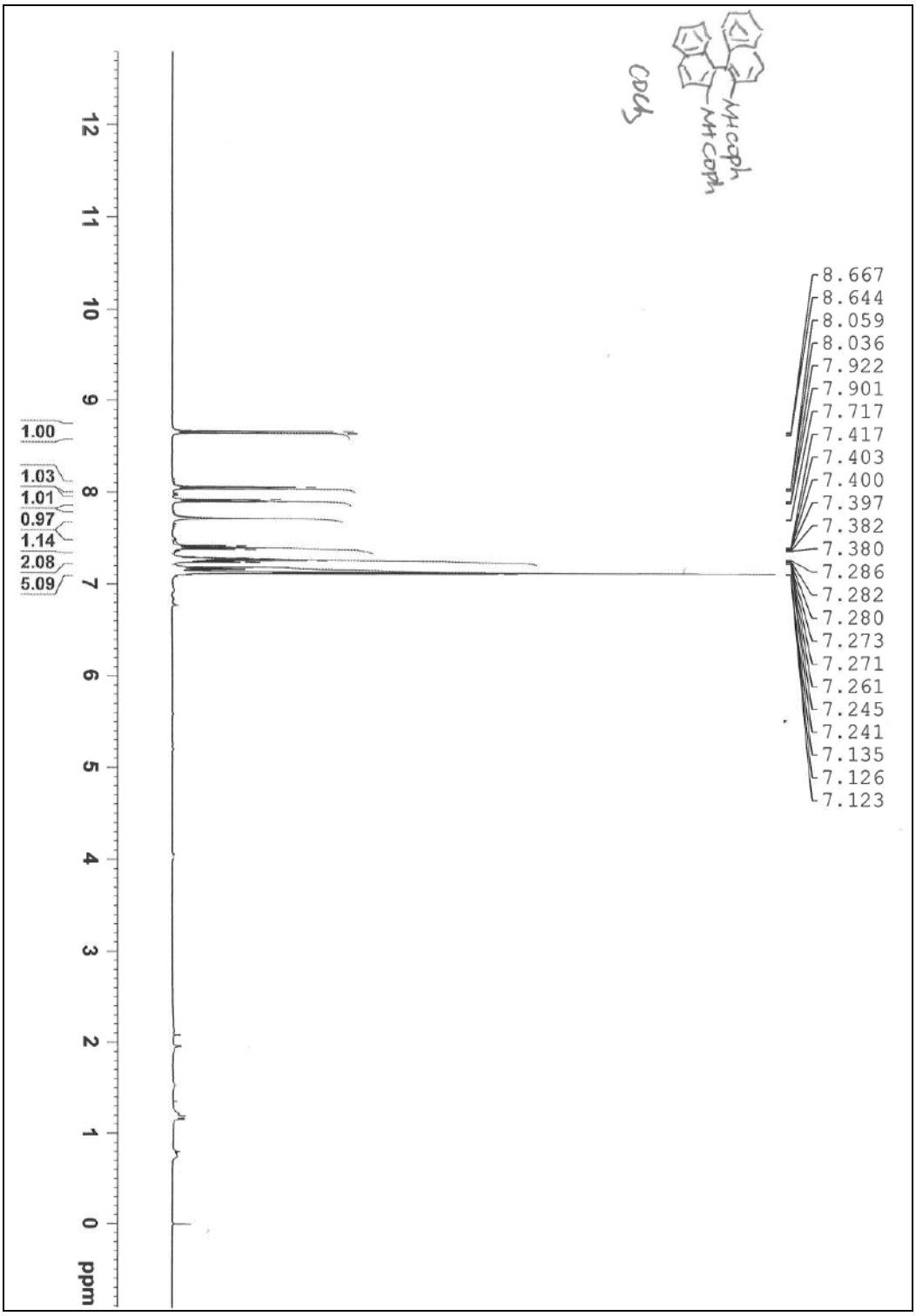
^{1}H NMR ($CDCl_3$) of 2-methylisoindolin-1-one



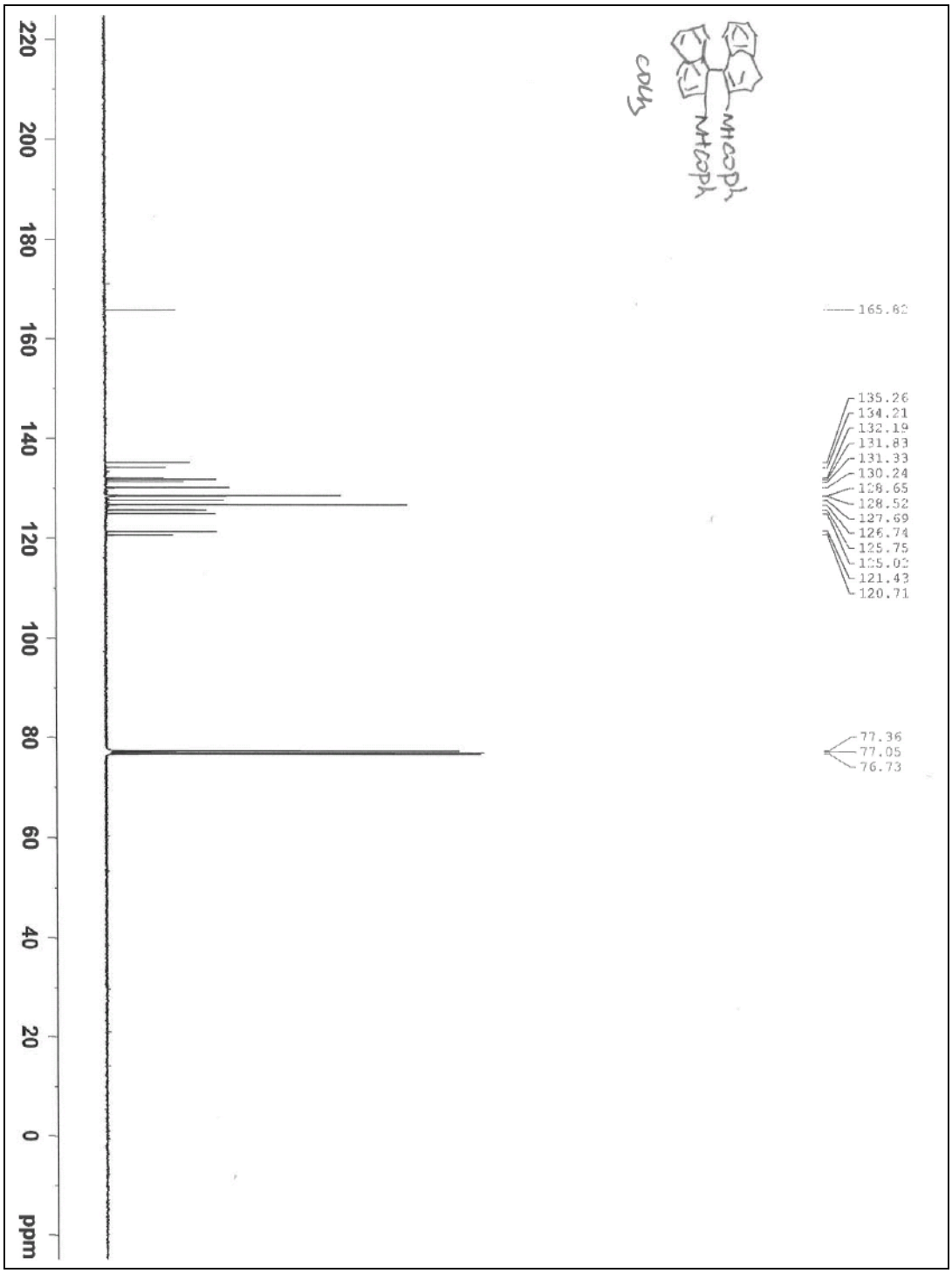
^{13}C NMR ($CDCl_3$) of 2-methylisoindolin-1-one



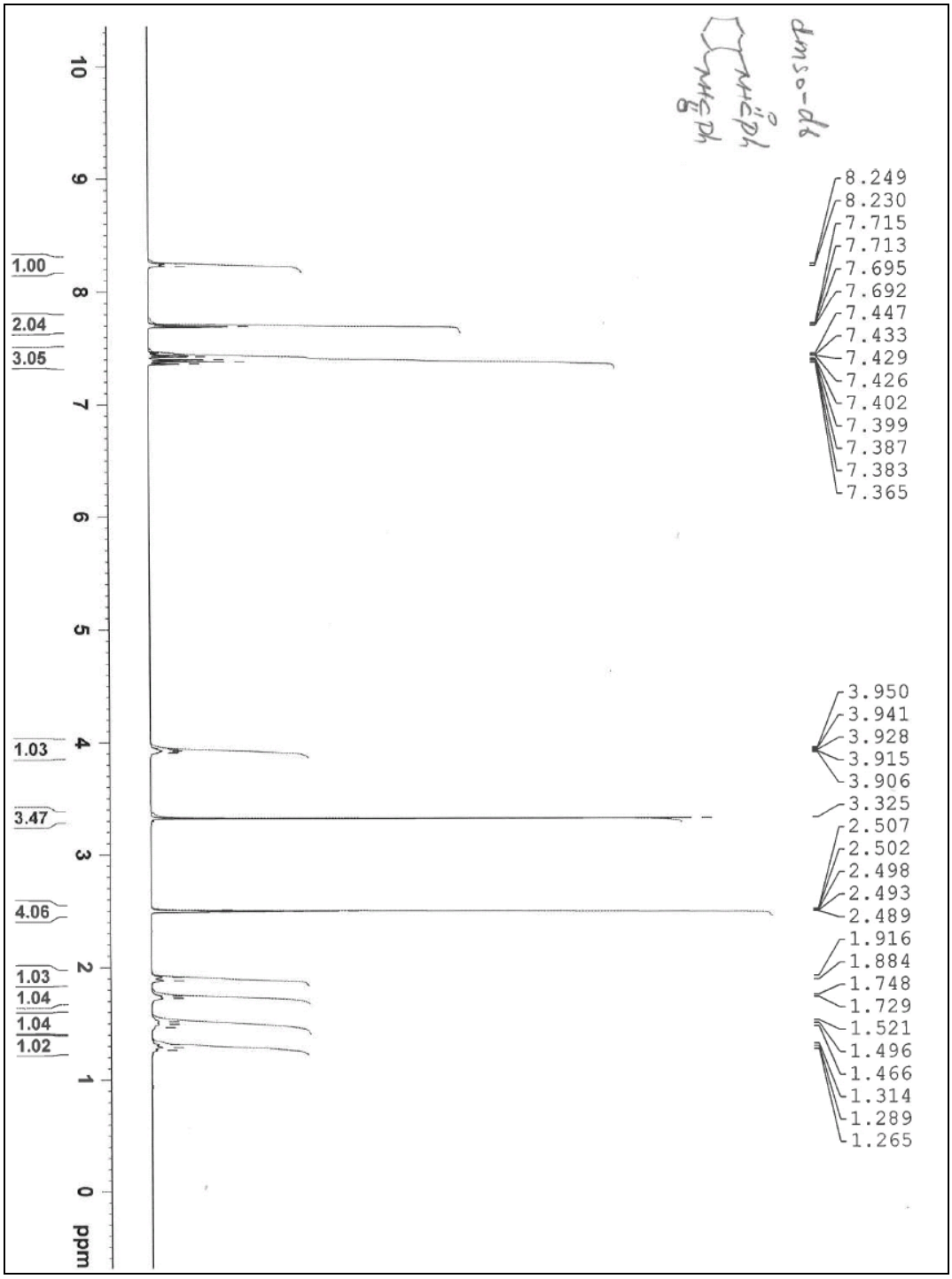
^{1}H NMR ($CDCl_3$) of *Racemic*-*N*,*N*′-(1,1′-Binaphthyl-2,2′-diyl)dibenzamide



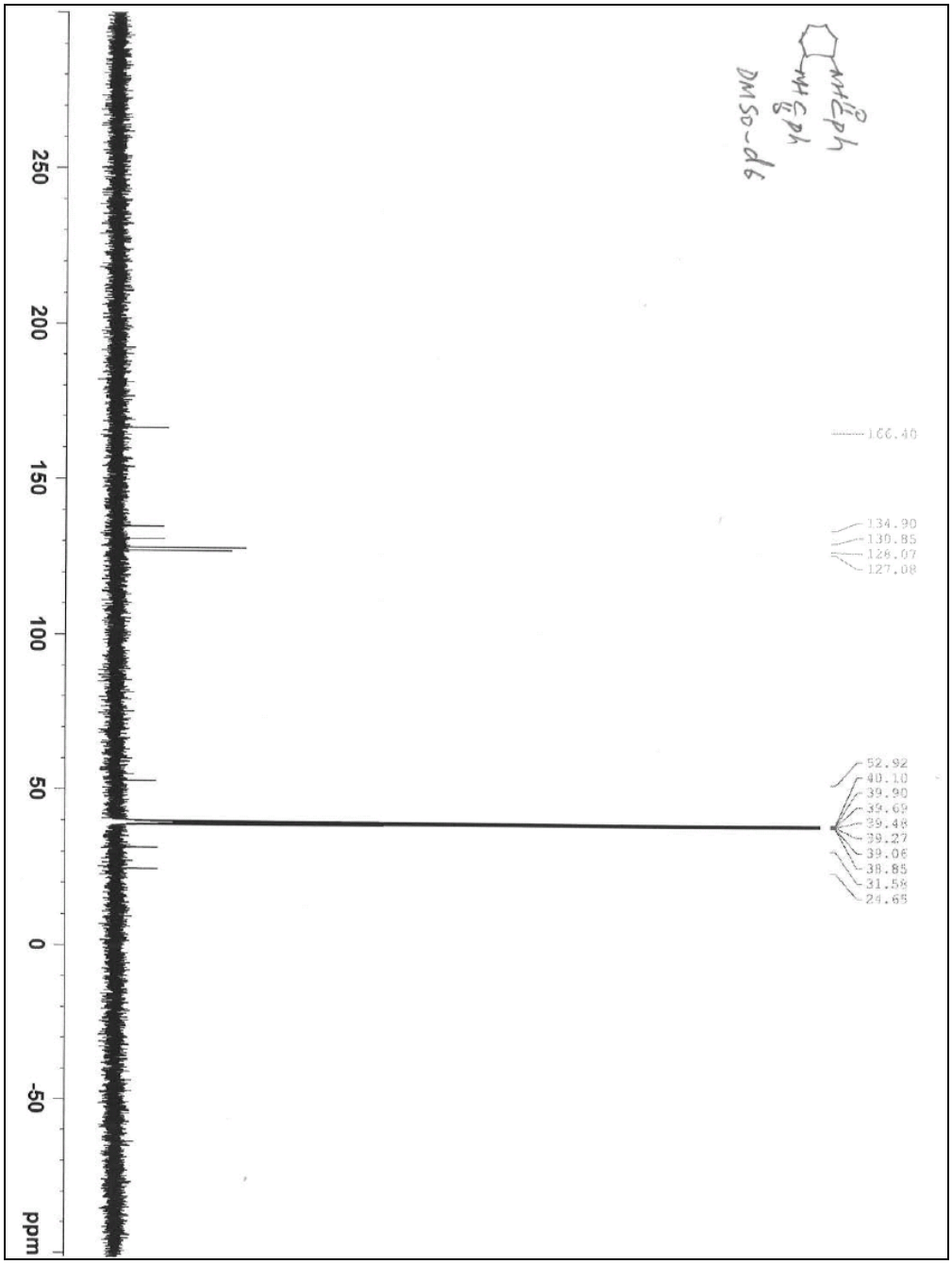
^{13}C NMR ($CDCl_3$) of *Racemic*-*N*,*N*′-(1,1′-Binaphthyl-2,2′-diyl)dibenzamide



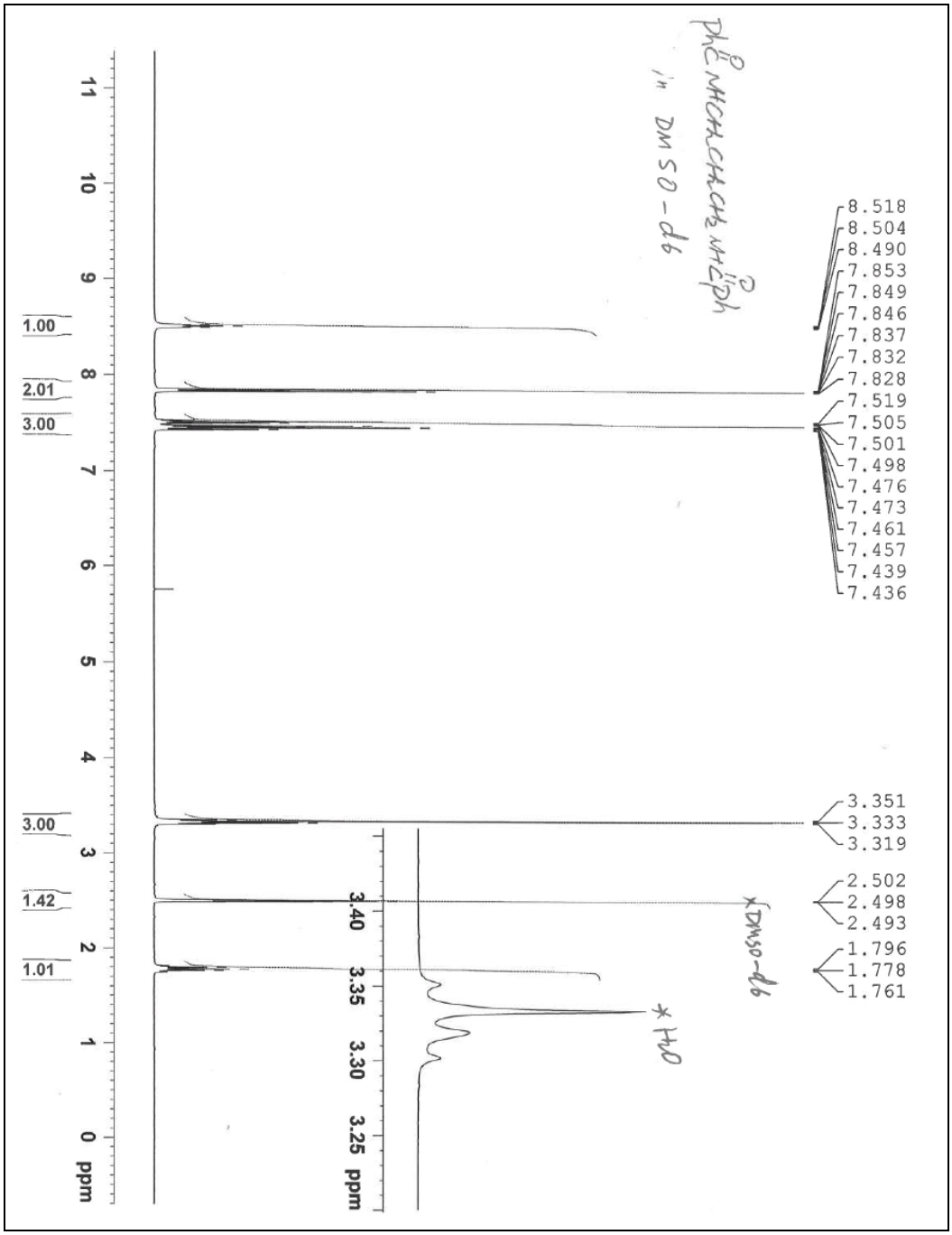
^{1}H NMR (DMSO-d$_6$) of *Racemic-N,N'*-(cyclohexane-1,2-diyl)dibenzamide



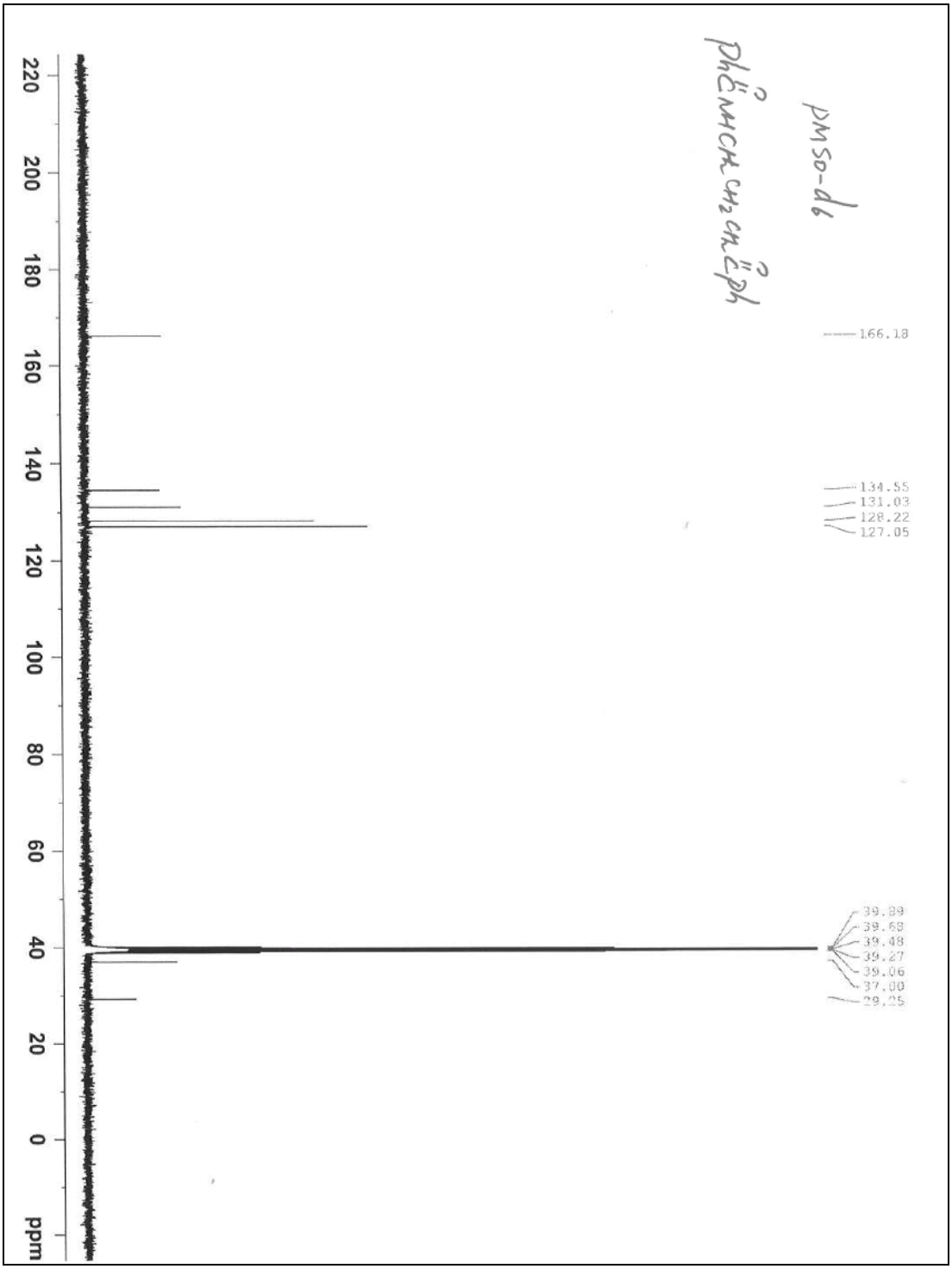
^{13}C NMR (DMSO-d_6) of *Racemic-N,N'*-(cyclohexane-1,2-diyl)dibenzamide



^{1}H NMR (DMSO-d$_6$) of *N,N'*-(propane-1,3-diyl)dibenzamide



^{13}C NMR (DMSO-d$_6$) of *N,N'*-(propane-1,3-diyl)dibenzamide



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