Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

for

Acylative Suzuki coupling of amides: Acyl-nitrogen activation via synergy of independently modifiable activating groups

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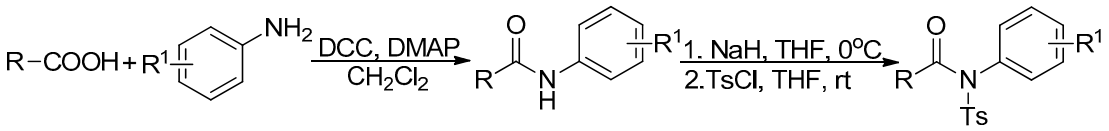
Contents

1. General experimental methods

All reactions were carried out under argon by using standard Schlenk techniques unless otherwise stated. Commercially available chemicals were used as received. Dioxane was dried with sodium/benzophenone and distilled. $Pd(PCy_3)_2Cl_2$[1], **1a**[2], **1b**[3] and **1c**[4] were prepared according to previously reported procedures. Column chromatograph was performed on 200-300 mesh silica gal. ^1H and ^{13}C NMR spectra were recorded in $CDCl_3$ or DMSO-d_6 at ambient temperature. Chemical shifts in NMR are reported in ppm (δ), relative to the internal standard of tetramethylsilane (TMS). The signals observed are described as s (singlet), d (doublet), t (triplet), q (quartet), dd (double doublet), m (multiplets). The number of protons (n) for a given resonance is indicated as nH. Coupling constants are reported as J in Hz. All new compounds were further characterized by HRMS.

2. General procedure for the synthesis of carboxylic amides

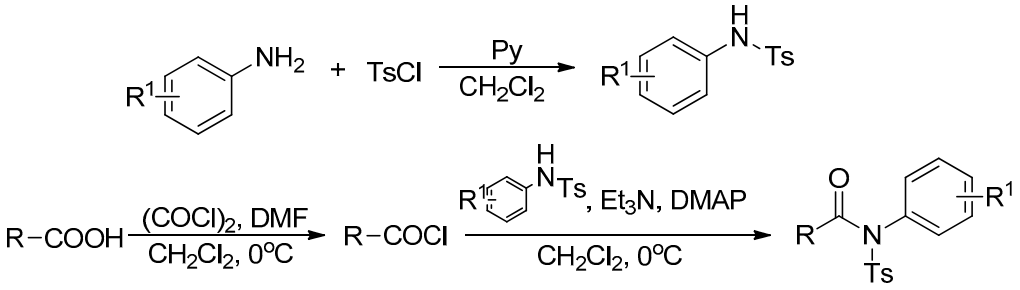
General procedure A:



To a mixture of carboxylic acid (10 mmol) in CH_2Cl_2 (20 ml) were added DCC (11mmol), DMAP (0.2 mmol) and amine (10mmol) at 0°C. The reaction mixture was stirred at room temperature for 5h and washed with brine. The organic layer was dried over Na_2SO_4, filtered and evaporated under reduced pressure to give crude product, which was purified by column chromatography on silica gel to afford N-phenylbenzamide.

To a mixture of NaH (60% dispersion in mineral oil, 6.5 mmol) in dry THF (10 ml) was added a solution of N-phenylbenzamide (10 mmol) in THF (5 ml) at 0°C. The reaction mixture was stirred at 0 °C for 1 h. To this mixture was added a solution of TsCl (6.5 mmol) in dry THF (10 ml) via cannula. The reaction mixture was stirred at room temperature for 5h and quenched with sat.NH_4Cl (aq., 30 ml). The aqueous phase was extracted with CH_2Cl_2, dried over Na_2SO_4, filtered and evaporated under reduced pressure to give crude product, which was purified by column chromatography on silica gel to afford N-tosylcarboxylic amide.

General procedure B:



To a mixture of amine (10 mmol) and pyridine (2 ml, 25 mmol) in CH_2Cl_2 (10 ml) was added slowly TsCl (2.3 g, 12 mmol) in CH_2Cl_2 (10 ml) at 0^oC. The reaction mixture was stirred at room temperature for 1h. The reaction mixture was washed with 5% HCl, brine and H_2O. The organic layer was dried over Na_2SO_4, filtered and evaporated under reduced pressure to give crude product, which was purified by column chromatography on silica gel to afford the sulfonamide.

To a solution of carboxylic acid (5 mmol) in CH_2Cl_2 (10 ml) were added oxalyl chloride (0.5 ml, 6 mmol, 1.2 equiv) and DMF (two drops) at 0^oC. The mixture was stirred until gas evolution stopped. Then it was concentrated under reduced pressure, washed with dichloromethane and concentrated again. The crude acyl chloride was used directly in the next step.

To a mixture of the corresponding sulfonamide (5 mmol), DMAP (0.5 mmol%) and Et_3N (1.5 ml, 10 mmol) in CH_2Cl_2 (10 ml) was added slowly the acyl chloride made above in CH_2Cl_2 (10 ml) at 0^oC. The reaction mixture was stirred at room temperature for 2h. Then the reaction mixture was washed with 5% HCl, brine and H_2O. The organic layer was dried over Na_2SO_4, filtered and evaporated under reduced pressure to give crude product, which was purified by column chromatography on silica gel to afford N-tosylcarboxylic amide.

3. Typical procedure for acylative Suzuki coupling reaction

Under a N_2 atmosphere, to a 10 ml dry flask were added amide **1** (0.5 mmol), boronic acid **2** (0.75 mmol), $Pd(PCy_3)_2Cl_2$ (5 mmol%), PCy_3 (3 mmol%), K_2CO_3 (1 mmol), and dry dioxane (4 ml). The mixture was stirred at 110^oC for a given time or monitored by TLC until the starting material was completely consumed. The reaction mixture was diluted with CH_2Cl_2 (15 ml), followed by washing with H_2O (2×10 ml). The organic layer was dried over Na_2SO_4, filtered, and evaporated under reduced pressure to give crude product, which was purified by column chromatography on silica gel to afford product **3**.

4. Synthesis of 4

Under a N_2 atmosphere, to a 10 ml dry flask were added amide **1w** or **1x** (0.5 mmol), boronic acid **2c** (0.55 mmol), $Pd(PCy_3)_2Cl_2$ (5 mmol%), PCy_3 (3 mmol%), K_2CO_3 (1.5 mmol), and dry dioxane (4 ml). The mixture was stirred at 110^oC for a given time. The reaction mixture was diluted with CH_2Cl_2 (15 ml), followed by washing with H_2O (2×10 ml). The organic layer was dried over Na_2SO_4, filtered, and evaporated under reduced pressure to give crude product, which was purified by column chromatography on silica gel to afford product **4**.

5. Synthesis of 4'-methoxybiphenyl-4-yl(p-tolyl)methanone 5 via sequential reacions in one flask

Under a N_2 atmosphere, to a 10 ml dry flask were added amide **1x** (0.5 mmol), boronic acid **2c** (0.55 mmol), $Pd(PCy_3)_2Cl_2$ (5 mmol%), PCy_3 (3 mmol%), K_2CO_3 (1.5 mmol), and dry dioxane (4 ml). The mixture was stirred at 110^oC for 8h. Then boronic acid **2b** (0.75 mmol) was added, the mixture was stirred at 110^oC for 12h. The reaction mixture was diluted with CH_2Cl_2 (15 ml), followed by washing with H_2O (2×10 ml). The organic layer was dried over Na_2SO_4, filtered, and evaporated under reduced pressure to give crude product, which was purified by column chromatography on silica gel to afford product **5**.

6. Synthesis of 4'-methylbiphenyl-4-yl(p-tolyl)methanone 6 via one-pot reaction

Under a N_2 atmosphere, to a 10 ml dry flask were added amide **1w** or **1x** (0.5 mmol), boronic acid **2b** (1.5 mmol), $Pd(PCy_3)_2Cl_2$ (5 mmol%), PCy_3 (3 mmol%), K_2CO_3 (1.5 mmol), and dry dioxane (4 ml). The mixture was stirred at 110^oC for 12h. The reaction mixture was diluted with CH_2Cl_2 (15 ml), followed by washing with H_2O (2×10 ml). The organic layer was dried over Na_2SO_4, filtered, and evaporated under reduced pressure to give crude product, which was purified by column chromatography on silica gel to afford product **6**.

7. Characterization data of compounds

1-benzoylpyrrolidine-2,5-dione 1a[2]

White solid (92%), mp 129-130°C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.85(d, J=7.2Hz, 2H), 7.67(t, J=7.2Hz, 1H), 7.50 (t, J=7.6Hz, 2H), 2.92(s, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):174.9, 167.9, 135.2, 131.4, 130.5, 129.0, 29.1.

tert-butyl benzoyl(phenyl)carbamate 1b[3]

White solid (85%), mp 98-99°C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.73(d, J=7.2Hz, 2H), 7.52(t, J=7.2Hz, 1H), 7.46-7.41 (m, 4H), 7.34(t, J=7.6Hz, 1H), 7.27(d, J=8.0Hz, 2H), 1.22(s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):172.8, 153.3, 139.1, 137.0, 131.8, 129.2, 128.3, 128.2, 128.0, 127.8, 83.5, 27.5.

N-methyl-N-tosylbenzamide 1c[4]

White solid (90%), mp 62-63°C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.86(d, J=8.0Hz, 2H), 7.58-7.52(m, 3H), 7.43 (t, J=8.0Hz, 2H), 7.36(d, J=8.0Hz, 2H), 3.30(s, 3H), 2.47(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):171.5, 145.0, 135.2, 134.5, 132.0, 129.7, 128.5, 128.4, 128.3, 35.7, 21.7.

N-phenyl-N-tosylbenzamide 1d[5]

Following the general procedure A. White solid (88%), mp 153-154°C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.83(d, J=8.0Hz, 2H), 7.44(d, J=8.0Hz, 2H), 7.33-7.26(m, 6H), 7.18-7.14(m, 4H), 2.45(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):169.9, 144.9, 137.4, 135.2, 133.7, 131.8, 130.4, 129.5, 129.3, 129.2, 129.1, 128.0, 21.7.

4-fluoro-N-phenyl-N-tosylbenzamide 1e

Following the general procedure A. White solid (83%), mp 137-138°C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.81(d, J=8.4Hz, 2H), 7.50-7.46(m, 2H), 7.32-7.26(m, 5H), 7.16-7.13(m, 2H), 6.85(t, J=8.4Hz, 2H), 2.45(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):168.8, 164.5(d, J=252.6Hz), 144.9, 137.4, 135.1, 132.1(d, J=9.3Hz), 130.3, 129.7(d, J=3.0Hz), 129.5, 129.28, 129.27, 129.2, 115.3(d, J=21.9Hz), 21.7. HRMS (ESI) m/z (M^+) calcd for $C_{20}H_{16}NO_3SF$ 370.0835, found 370.1138.

N-phenyl-N-tosyl-4-(trifluoromethyl)benzamide 1f

Following the general procedure B. White solid (80%), mp 147-149°C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.84(d, J=8.4Hz, 2H), 7.53(d, J=8.0Hz, 2H), 7.43(d, J=8.4Hz, 2H), 7.35-7.27(m, 5H), 7.16-7.13(m, 2H), 2.46(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):168.5, 145.2, 137.2, 136.8, 134.9, 133.0(q, J=32.6Hz), 130.4, 129.6, 129.5, 129.4, 125.1(q, J=3.6Hz), 123.4(q, J=279.6Hz), 21.7. HRMS (ESI) m/z (M^+) calcd for $C_{21}H_{17}NO_3SF_3$ 420.0881, found 420.0883.

methyl 4-(phenyl(tosyl)carbamoyl)benzoate 1g

Following the general procedure B. White solid (76%), mp 175-176^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.85-7.81(m, 4H), 7.46(d, J=8.4Hz, 2H), 7.33(d, J=8.0Hz, 2H), 7.29-7.27(m, 3H), 7.15-7.13(m, 2H), 3.84(s, 3H), 2.46(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):169.0, 165.9, 145.2, 137.8, 136.9, 135.0, 132.5, 130.4, 129.5, 129.39, 129.37, 129.3, 129.17, 129.16, 52.4, 21.8. HRMS (ESI) m/z (M^+) calcd for $C_{22}H_{20}NO_5S$ 410.1062, found 410.1059.

4-cyano-N-phenyl-N-tosylbenzamide 1h

Following the general procedure B. White solid (85%), mp 171-172^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.83(d, J=8.4Hz, 2H), 7.48(q, J=8.8Hz, 4H), 7.35-7.28(m, 5H), 7.14-7.11(m, 2H), 2.46(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):168.1, 145.4, 137.9, 136.6, 134.7, 131.8, 130.4, 129.7, 129.6, 129.52, 129.49, 129.45, 117.6, 115.0, 21.8. HRMS (ESI) m/z (M^+) calcd for $C_{21}H_{17}N_2O_3S$ 377.0960, found 377.0977.

4-nitro-N-phenyl-N-tosylbenzamide 1i

Following the general procedure A. Light yellow solid (57%), mp 191-192^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):8.02(d, J=8.8Hz, 2H), 7.85(d, J=8.4Hz, 2H), 7.56 (d, J=8.8Hz, 2H), 7.36-7.28(m, 5H), 7.15-7.13(m, 2H), 2.47(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):167.8, 149.0, 145.5, 139.7, 136.5, 134.6, 130.4, 130.1, 129.8, 129.6, 129.5, 123.2, 21.8. HRMS (ESI) m/z (M^+) calcd for $C_{20}H_{17}N_2O_5S$ 397.0858, found 397.0861.

4-methyl-N-phenyl-N-tosylbenzamide 1j

Following the general procedure B. White solid (88%), mp 137-138^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.81(d, J=8.0Hz, 2H), 7.36(d, J=8.0Hz, 2H), 7.31-7.26 (m, 5H), 7.17-7.15(m, 2H), 6.96(d, J=8.0Hz, 2H), 2.44(s, 3H), 2.23(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):169.9, 144.8, 142.6, 137.6, 135.3, 130.7, 130.3, 129.8, 129.5, 129.2, 129.1, 129.0, 128.8, 21.7, 21.5. HRMS (ESI) m/z (M^+) calcd for $C_{21}H_{20}NO_3S$ 366.1164, found 366.1168.

4-methoxy-N-phenyl-N-tosylbenzamide 1k

Following the general procedure A. White solid (79%), mp 138-139^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.79(d, J=8.0Hz, 2H), 7.47(d, J=8.8Hz, 2H), 7.30-7.28 (m, 5H), 7.18-7.16(m, 2H), 6.66(d, J=9.2Hz, 2H), 3.72(s, 3H), 2.44(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):169.5, 162.5, 144.7, 137.9, 135.3, 132.1, 130.2, 129.4, 129.18, 129.15, 128.9, 125.5, 113.4, 55.3, 21.7. HRMS (ESI) m/z (M^+) calcd for $C_{21}H_{20}NO_4S$ 382.1113, found 382.1111.

tert-butyl (4-(phenyl(tosyl)carbamoyl)phenyl)carbamate 1l

Following the general procedure B. White solid (68%), mp 206-207^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.79(d, J=8.0Hz, 2H), 7.42(d, J=8.4Hz, 2H), 7.37-7.26(m, 5H), 7.17(d, J=8.4Hz, 4H), 6.58(br.s, 1H), 2.43(s, 3H), 1.46(s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):.169.4, 152.2, 144.8, 142.1, 137.7, 135.2, 131.2, 130.2, 129.4, 129.2, 129.0, 127.1, 117.0, 81.1, 28.2, 21.7. HRMS (ESI) m/z (M^+) calcd for $C_{25}H_{27}N_2O_5S$ 467.1641, found 467.1642.

N-phenyl-N-tosylfuran-2-carboxamide 1m

Following the general procedure B. White solid (81%), mp 133-134^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.92(d, J=8.4Hz, 2H), 7.50-7.43(m, 3H), 7.34-7.29(m, 5H), 6.21(dd, J=3.6, 1.6Hz, 1H), 5.95(d, J=3.6Hz, 1H), 2.45(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):157.9, 146.5, 145.4, 145.1, 136.5, 135.6, 130.5, 130.1, 129.53, 129.49, 129.4, 119.8, 111.8, 21.7. HRMS (ESI) m/z (M^+) calcd for $C_{18}H_{16}NO_4S$ 342.0800, found 342.0804.

N-phenyl-N-tosylthiophene-2-carboxamide 1n

Following the general procedure B. White solid (85%), mp 155-156^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.90(d, J=8.4Hz, 2H), 7.53-7.44(m, 3H), 7.39(dd, J=5.2, 1.2Hz, 1H), 7.36-7.33(m, 4H), 6.94(dd, J=4.0, 1.2Hz, 1H), 6.81-6.78(m, 1H), 2.45(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):162.0, 145.0, 136.7, 136.4, 135.7, 135.0, 133.8, 131.0, 130.3, 129.7, 129.5, 129.4, 127.3, 21.8. HRMS (ESI) m/z (M^+) calcd for $C_{18}H_{16}NO_3S_2$ 358.0572, found 358.0572.

N-phenyl-N-tosylcinnamamide 1o

Following the general procedure B. White solid (71%), mp 186-187^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.96(d, J=8.4Hz, 2H), 7.66(d, J=15.6Hz, 1H), 7.56-7.50(m, 3H), 7.37-7.21(m, 9H), 6.04(d, J=15.6Hz, 1H), 2.45(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):165.5, 145.8, 145.0, 136.2, 136.0, 134.1, 130.7, 130.5, 130.1, 129.9, 129.5, 129.3, 128.9, 128.3, 117.8, 21.8. HRMS (ESI) m/z (M^+) calcd for $C_{22}H_{20}NO_3S$ 378.1164, found 378.1161.

N,3-diphenyl-N-tosylpropanamide 1p

Following the general procedure B. Light yellow solid (79%), mp 125-126^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.93(d, J=8.4Hz, 2H), 7.46-7.40(m, 3H), 7.36(d, J=8.4Hz, 2H), 7.18-7.11(m, 5H), 6.95-6.93(m, 2H), 2.81(t, J=8.0Hz, 2H), 2.47(s, 3H), 2.29(t, J=8.0Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):172.1, 145.0, 140.1, 136.22, 136.17, 130.1, 129.9, 129.5, 129.3, 128.5, 128.4, 126.3, 38.5, 30.7, 21.8. HRMS (ESI) m/z (M^+) calcd for $C_{22}H_{21}NO_3SNa$ 402.1140, found 402.1140.

N-phenyl-N-tosylstearamide 1q

Following the general procedure B. White solid (76%), mp 104-105°C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.93(d, J=8.4Hz, 2H), 7.50-7.48(m, 3H), 7.34(d, J=8.0Hz, 2H), 7.27(d, J=4.0Hz, 2H), 2.45(s, 3H), 1.98(t, J=7.2Hz, 2H), 1.25-1.11(m, 30H), 0.89-0.86(m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):172.9, 144.8, 136.5, 136.4, 130.1, 129.9, 129.8, 129.4, 129.2, 36.7, 31.9, 29.7, 29.4, 29.1, 28.8, 24.3, 22.7, 21.7, 14.1. HRMS (EI) m/z (M^+) calcd for $C_{31}H_{47}NO_3S$ 513.3277, found 513.3279.

N-phenyl-N-tosylcyclohexanecarboxamide 1r

Following the general procedure B. White solid (81%), mp 144-145°C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.89(d, J=8.4Hz, 2H), 7.50-7.47(m, 3H), 7.32(d, J=8.0Hz, 2H), 7.28-7.26(m, 2H), 2.44(s, 3H), 2.03-1.97(m, 1H), 1.63-1.33(m, 7H), 1.11-0.84(m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):176.2, 144.7, 136.3, 130.1, 129.9, 129.7, 129.4, 129.1, 43.8, 29.0, 25.4, 25.1, 21.7. HRMS (EI) m/z (M^+) calcd for $C_{20}H_{22}NO_3S$ 356.1320, found 356.1300.

(3r,5r,7r)-N-phenyl-N-tosyladamantane-1-carboxamide 1s

Following the general procedure B. White solid (69%), mp 177-178°C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.63(d, J=8.4Hz, 2H), 7.43-7.36(m, 3H), 7.23(d, J=8.4Hz, 2H), 7.18(d, J=7.6Hz, 2H), 2.40(s, 3H), 1.86-1.47(m, 15H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):181.4, 144.2, 136.1, 135.3, 130.3, 129.5, 129.4, 129.03, 128.97, 46.4, 39.6, 36.1, 28.0, 21.6. HRMS (EI) m/z (M^+) calcd for $C_{24}H_{27}NO_3S$ 409.1712, found 409.1714.

2-methyl-N-phenyl-N-tosylbenzamide 1t

Following the general procedure B. White solid (84%), mp 142-143°C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.91(d, J=8.4Hz, 2H), 7.35(d, J=8.0Hz, 2H), 7.26-7.23 (m, 3H), 7.13-7.11(m, 2H), 7.09-7.05(m, 2H), 6.98(d, J=7.2Hz, 1H), 6.92(t, J=7.2Hz, 1H), 2.47(s, 3H), 2.22(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):170.2, 145.0, 136.5, 135.7, 134.4, 130.5, 130.1, 130.0, 129.4, 129.3, 129.1, 127.6, 125.0, 21.8, 19.4. HRMS (ESI) m/z (M^+) calcd for $C_{21}H_{20}NO_3S$ 366.1164, found 366.1160.

(3r,5r,7r)-N-(3,5-bis(trifluoromethyl)phenyl)-N-tosyladamantane-1-carboxamide 1u

Following the general procedure B. White solid (76%), mp 139-140°C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.95(s, 1H), 7.62(s, 2H), 7.57(d, J=8.0Hz, 2H), 7.26(d, J=8.4Hz, 2H), 2.43(s, 3H), 1.95-1.91(m, 5H), 1.66-1.59(m, 10H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm): 180.0, 144.2, 137.2, 133.3, 131.7(q, J=28.1Hz), 128.9(d, J=2.6Hz), 128.32, 128.29, 121.8-121.7(m), 121.5(q, J=271.4Hz), 45.9, 38.8, 37.3, 35.3, 34.9,

26.8, 26.7, 20.6. HRMS (ESI) m/z (M^+) calcd for $C_{26}H_{25}F_6NO_3SNa$ 568.1352, found 568.1356.

N-(3,5-bis(trifluoromethyl)phenyl)-2-methyl-N-tosylbenzamide 1v

Following the general procedure B. White solid (88%), mp 99-100°C, ^1H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.82-7.77(m, 3H), 7.54(s, 2H), 7.38(d, J=8.0Hz, 2H), 7.18-7.14(m, 1H), 7.06-6.98(m, 3H), 2.50(s, 3H), 2.21(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm): 169.4, 146.0, 138.3, 135.7, 134.8, 133.6, 132.5(q, J=33.9Hz), 130.8, 130.7, 130.4(d, J=2.9Hz), 129.7, 129.2, 127.3, 125.4, 122.9-122.7(m), 122.4(q, J=271.3Hz), 21.8, 19.1. HRMS (ESI) m/z (M^+) calcd for $C_{23}H_{17}F_6NO_3SNa$ 524.0726, found 524.0731.

4-chloro-N-phenyl-N-tosylbenzamide 1w

Following the general procedure B. White solid (88%), mp 138-139°C, ^1H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.81(d, J=8.4Hz, 2H), 7.38(d, J=8.8Hz, 2H), 7.33-7.26 (m, 5H), 7.14(dd, J=8.4, 2.0Hz, 4H), 2.45(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):168.9, 145.1, 138.1, 137.2, 135.0, 132.1, 130.9, 130.3, 129.5, 129.3, 128.4, 21.7. HRMS (ESI) m/z (M^+) calcd for $C_{20}H_{17}NO_3SCl$ 386.0618, found 386.0619.

4-bromo-N-phenyl-N-tosylbenzamide 1x

Following the general procedure B. White solid (86%), mp 148-149°C, ^1H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.81(d, J=8.4Hz, 2H), 7.34-7.27(m, 9H), 7.15-7.12 (m, 2H), 2.45(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):169.0, 145.1, 137.2, 135.0, 132.5, 131.4, 131.0, 130.3, 129.5, 129.3, 126.7, 21.8. HRMS (ESI) m/z (M^+) calcd for $C_{20}H_{17}NO_3SBr$ 430.0113, found 430.0117.

N-(4-acetylphenyl)-2-methyl-N-tosylbenzamide 1t-1

Following the general procedure B. White solid (83%), mp 147-148°C, ^1H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.88(d, J=8.4Hz, 2H), 7.83(d, J=8.4Hz, 2H), 7.36(d, J=8.0Hz, 2H), 7.22(d, J=8.8Hz, 2H), 7.12-7.07(m, 2H), 7.00(d, J=7.6Hz, 1H), 6.93(t, J=7.6Hz, 1H), 2.54(s, 3H), 2.48(s, 3H), 2.23(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):196.9, 169.7, 145.4, 140.6, 137.1, 135.9, 135.3, 134.0, 130.7, 130.4, 130.3, 129.5, 129.3, 129.0, 127.7, 125.2, 26.7, 21.8, 19.4. HRMS (ESI) m/z (M^+) calcd for $C_{23}H_{21}NO_4SNa$ 430.1083, found 430.1085.

N-(2,4-difluorophenyl)-2-methyl-N-tosylbenzamide 1t-2

Following the general procedure B. White solid (76%), mp 147-148°C, ^1H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.94(d, J=8.4Hz, 2H), 7.36-7.31(m, 3H), 7.15-7.11(m, 1H), 7.04(t, J=8.0Hz, 2H), 6.94(t, J=7.6Hz, 1H), 6.84-6.80(m, 1H), 6.77-6.71(m, 1H), 2.47(s, 3H), 2.22(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):169.5, 163.2(qd,

J=12.1, 252.1Hz), 145.4, 136.0, 135.4, 133.5, 133.1, 133.0, 130.6, 130.3, 129.43, 129.39, 126.7, 125.0, 120.9(dd, J=4.2, 13.2Hz), 112.0(dd, J=3.6, 22.4Hz), 104.9(dd, J=24.0, 26.2Hz), 21.8, 19.1. HRMS (ESI) m/z (M^+) calcd for $C_{21}H_{17}F_2NO_3SNa$ 424.0789, found 424.0792.

2-methyl-N-tosyl-N-(3-(trifluoromethyl)phenyl)benzamide 1t-3

Following the general procedure B. White solid (86%), mp 85-86^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.87(d, J=8.4Hz, 2H), 7.51(d, J=7.2Hz, 1H), 7.41-7.31(m, 5H), 7.10(t, J=7.6Hz, 1H), 7.02(q, J=7.6Hz, 2H), 6.94(t, J=7.6Hz, 1H), 2.47(s, 3H), 2.21(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):169.8, 145.5, 137.2, 135.6, 135.2, 134.0, 133.5, 131.5(q, J=33.0Hz), 130.6, 130.3, 129.7, 129.6, 129.2, 127.4, 127.0(q, J=3.6Hz), 126.0(q, J=3.5Hz), 125.2, 123.2(q, J=270.9Hz), 21.7, 19.2. HRMS (ESI) m/z (M^+) calcd for $C_{22}H_{18}F_3NO_3SNa$ 456.0852, found 456.0857.

2-methyl-N-tosyl-N-(4-(trifluoromethyl)phenyl)benzamide 1t-4

Following the general procedure B. White solid (78%), mp 128-129^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.87(d, J=8.0Hz, 2H), 7.52(d, J=8.0Hz, 2H), 7.36(d, J=8.0Hz, 2H), 7.25(d, J=7.2Hz, 2H), 7.15-7.11(m, 1H), 7.08-7.01(m, 2H), 6.95(t, J=7.6Hz, 1H), 2.48(s, 3H), 2.23(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):169.7, 145.5, 139.8, 135.9, 135.3, 133.8, 131.1(q, J=32.8Hz), 130.7, 130.52, 130.46, 129.6, 129.3, 127.7, 126.2(q, J=3.5Hz), 125.3, 123.5(q, J=270.8Hz), 21.7, 19.4. HRMS (ESI) m/z (M^+) calcd for $C_{22}H_{18}F_3NO_3SNa$ 456.0852, found 456.0859.

N-(3,5-difluorophenyl)-2-methyl-N-tosylbenzamide 1t-5

Following the general procedure B. White solid (81%), mp 136-137^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.89(d, J=8.4Hz, 2H), 7.37(d, J=8.0Hz, 2H), 7.18-7.14(m, 1H), 7.09-7.04(m, 2H), 7.00(t, J=7.6Hz, 1H), 6.77-6.69(m, 3H), 2.48(s, 3H), 2.22(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):169.5, 162.4(dd, J=13.8, 249.4Hz), 145.6, 138.6(t, J=12.3Hz), 135.9, 135.2, 133.7, 130.7, 130.5, 129.6, 129.3, 127.5, 125.3, 113.9(dd, J=7.6, 19.1Hz), 105.3(t, J=25.0Hz), 21.8, 19.4. HRMS (ESI) m/z (M^+) calcd for $C_{21}H_{17}F_2NO_3SNa$ 424.0789, found 424.0791.

benzophenone 3aa[6]

Light yellow solid, mp 46-47^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.71-7.69(m, 4H), 7.48(t, J=7.6Hz, 2H), 7.37(t, J=8.0Hz, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):196.8, 137.6, 132.5, 130.1, 128.3.

phenyl(p-tolyl)methanone 3db[6]

Light yellow solid, mp 57-58^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.69-7.67(m, 2H), 7.62(d, J=8.0Hz, 2H), 7.47(t, J=7.6Hz, 1H), 7.36(t,

J=7.6Hz, 2H), 7.17(d, J=8.0Hz, 2H), 2.33(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):196.5, 143.3, 138.0, 134.9, 132.2, 130.3, 130.0, 129.0, 128.2, 21.7.

(4-methoxyphenyl)(phenyl)methanone 3dc[6]

White solid, mp 59-60^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.84-7.81(m, 2H), 7.76-7.74(m, 2H), 7.56(t, J=7.2Hz, 1H), 7.46(t, J=7.6Hz, 2H), 6.98-6.95(m, 2H), 3.87(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):195.6, 163.2, 138.3, 132.6, 131.9, 130.1, 129.7, 128.2, 113.6, 55.5.

(4-fluorophenyl)(phenyl)methanone 3dd[6]

Light yellow oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.86-7.83(m, 2H), 7.78-7.76(m, 2H), 7.61-7.57(m, 1H), 7.50-7.47(m, 2H), 7.18-7.13(m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):195.2, 165.4(d, J=252.4Hz), 137.5, 133.8(d, J=2.9Hz), 132.7, 132.6(d, J=14.5Hz), 129.9, 128.4, 115.5(d, J=21.7Hz).

methyl 4-benzoylbenzoate 3de[7]

White solid, mp 107-108^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):8.15(d, J=8.4Hz, 2H), 7.85-7.79(m, 4H), 7.62(t, J=7.6Hz, 1H), 7.50(t, J=8.0Hz, 2H), 3.97(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):195.9, 166.3, 141.3, 136.9, 133.2, 132.9, 130.1, 129.8, 129.5, 128.5, 52.4.

4-benzoylbenzonitrile 3df[7]

White solid, mp 110-111^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.88(d, J=8.4Hz, 2H), 7.80-7.78(m, 4H), 7.65(t, J=7.6Hz, 1H), 7.52(t, J=7.6Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):195.0, 141.2, 136.3, 133.3, 132.2, 130.2, 130.1, 128.6, 118.0, 115.6.

1-(4-benzoylphenyl)ethanone 3dg[8]

Light yellow solid, mp 82-83^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):8.06(d, J=8.8Hz, 2H), 7.87(d, J=8.4Hz, 2H), 7.82-7.80(m, 2H), 7.65-7.61(m, 1H), 7.53-7.49(m, 2H), 2.67(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):197.5, 195.9, 141.3, 139.5, 136.9, 133.0, 130.1, 130.0, 128.5, 128.2, 26.9.

naphthalen-1-yl(phenyl)methanone 3dh[6]

Light yellow solid, mp 73-74^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):8.09(d, J=8.8Hz, 1H), 7.49(d, J=8.4Hz, 1H), 7.92-7.90(m, 1H), 7.87-7.85(m, 2H), 7.60-7.54(m, 2H), 7.53-7.43(m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):198.1, 138.3, 136.4, 133.8, 133.3, 131.3, 131.0, 130.5, 128.51, 128.48, 127.8, 127.3, 126.5, 125.7, 124.4.

phenyl(o-tolyl)methanone 3di[6]

Light yellow oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.73-7.71(m, 2H), 7.50(t,

J=7.2Hz, 1H), 7.37(t, J=7.6Hz, 2H), 7.33-7.29(m, 1H), 7.24-7.15(m, 3H), 2.25(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):198.7, 138.6, 137.7, 136.8, 133.2, 131.0, 130.3, 130.2, 128.53, 128.48, 125.2, 20.0.

(2-ethylphenyl)(phenyl)methanone 3dj[9]

Light yellow oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.82-7.80(m, 2H), 7.59-7.54(m, 1H), 7.46-7.40(m, 3H), 7.34(d, J=7.2Hz, 1H), 7.28-7.22(m, 2H), 2.67(q, J=7.6Hz, 2H), 1.16(t, J=7.6Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):198.8, 143.0, 138.4, 137.8, 133.2, 130.3, 130.2, 129.5, 128.5, 128.3, 125.2, 26.4, 16.0.

methyl 2-benzoylbenzoate 3dk[10]

Light yellow oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):8.05(d, J=7.6Hz, 1H), 7.75(d, J=7.2Hz, 2H), 7.66-7.62(m, 1H), 7.59-7.53(m, 2H), 7.45-7.41(m, 3H), 3.61(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):197.1, 166.4, 141.7, 137.2, 133.1, 132.4, 130.1, 129.7, 129.3, 128.5, 127.8, 52.2.

phenyl(4-(trifluoromethyl)phenyl)methanone 3fa[6]

White solid, mp 116-117^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.89(d, J=8.0Hz, 2H), 7.82-7.79(m, 2H), 7.76(d, J=8.0Hz, 2H), 7.65-7.61(m, 1H), 7.53-7.49(m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):195.5, 140.7, 136.7, 133.7(q, J=32.4Hz), 133.1, 130.14, 130.10, 128.5, 125.3(q, J=3.6Hz), 122.3(q, J=271.1Hz).

(4-nitrophenyl)(phenyl)methanone 3ia[6]

Light yellow solid, mp 135-136^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):8.35-8.33(m, 2H), 7.96-7.93(m, 2H), 7.82-7.80(m, 2H), 7.66(t, J=7.6Hz, 1H), 7.53(t, J=8.0Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):194.8, 149.8, 142.9, 136.3, 133.5, 130.7, 130.1, 128.7, 123.5.

tert-butyl (4-benzoylphenyl)carbamate 3la[11]

White solid, mp 179-180^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.81-7.75(m, 4H), 7.58-7.55(m, 1H), 7.51-7.45(m, 4H), 6.96(br.s, 1H), 1.53(s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):195.8, 152.4, 142.8, 138.0, 132.1, 131.8, 131.7, 129.9, 128.2, 117.4, 81.2, 28.3.

furan-2-yl(phenyl)methanone 3ma[7]

Light yellow oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.97(d, J=7.2Hz, 2H), 7.71(s, 1H), 7.59(t, J=7.6Hz, 1H), 7.49(t, J=7.6Hz, 2H), 7.23(d, J=3.6Hz, 1H), 6.59-6.58(m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):182.6, 152.3, 147.2, 137.3, 132.6, 129.3, 128.4, 120.6, 112.2.

phenyl(thiophen-2-yl)methanone 3na[7]

Light yellow oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.87-7.85(m, 2H), 7.71(dd,

J=4.8, 1.2Hz, 1H), 7.64(dd, J=4.0, 1.2Hz, 1H), 7.61-7.57(m, 1H), 7.51-7.47(m, 2H), 7.17-7.14(m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):188.3, 143.6, 138.1, 134.9, 134.3, 132.3, 129.2, 128.4, 128.0.

(E)-chalcone 3oa[12]

Light yellow oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):8.02-8.00(m, 2H), 7.81(d, J=15.6Hz, 1H), 7.64-7.62(m, 2H), 7.59-7.47(m, 4H), 7.41-7.38(m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):190.6, 144.9, 138.2, 134.9, 132.9, 130.6, 129.0, 128.7, 128.6, 128.5, 122.1.

1,3-diphenylpropan-1-one 3pa[13]

White solid, mp 71-72^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.93(d, J=8.4Hz, 2H), 7.54-7.50(m, 1H), 7.43-7.40(m, 2H), 7.30-7.17(m, 5H), 3.27(t, J=8.0Hz, 2H), 3.05(t, J=8.0Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):199.3, 141.4, 136.9, 133.1, 128.7, 128.6, 128.5, 128.1, 126.2, 40.5, 30.2.

1-phenyloctadecan-1-one 3qa[14]

White solid, mp 62-63^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.97-7.94(m, 2H), 7.56-7.53(m, 1H), 7.45(t, J=7.6Hz, 2H), 2.96(t, J=7.2Hz, 2H), 1.77-1.67(m, 2H), 1.38-1.26(m, 28H), 0.88(t, J=7.2Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):200.5, 137.1, 132.8, 128.5, 128.0, 38.6, 32.0, 29.8, 29.6, 29.4, 24.4, 22.7, 14.1.

1-(o-tolyl)octadecan-1-one 3qi

White solid, mp 44-45^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.60(d, J=7.6Hz, 1H), 7.37-7.33(m, 1H), 7.24(t, J=7.6Hz, 2H), 2.87(t, J=7.6Hz, 2H), 2.48(s, 3H), 1.73-1.65(m, 2H), 1.36-1.25(m, 28H), 0.88(t, J=7.2Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):204.9, 138.4, 137.8, 131.9, 131.0, 128.3, 125.6, 41.7, 32.0, 29.73, 29.70, 29.6, 29.54, 29.51, 29.40, 29.37, 24.5, 22.7, 21.2, 14.1. HRMS (EI) m/z (M^+) calcd for $C_{25}H_{42}O$ 358.3244, found 358.3236.

1-(2-ethylphenyl)octadecan-1-one 3qj

White solid, mp 47-49^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.53(dd, J=7.6, 1.2Hz, 1H), 7.39-7.35(m, 1H), 7.27-7.21(m, 2H), 2.86(t, J=7.2Hz, 2H), 2.80(q, J=7.2Hz, 2H), 1.73-1.66(m, 2H), 1.30-1.20(m, 31H), 0.88(t, J=7.2Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):205.4, 143.6, 138.7, 130.9, 130.3, 127.9, 125.5, 42.2, 32.0, 29.74, 29.70, 29.66, 29.5, 29.41, 29.36, 26.9, 24.4, 22.7, 16.1, 14.1. HRMS (EI) m/z (M^+) calcd for $C_{26}H_{44}O$ 372.3397, found 372.3392.

cyclohexyl(phenyl)methanone 3ra[15]

White solid, mp 55-56^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.95-7.93(m, 2H), 7.56-7.52(m, 1H), 7.47-7.43(m, 2H), 3.30-3.23(m, 1H), 1.91-1.82(m, 3H),

1.76-1.72(m, 2H), 1.52-1.26(m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):203.9, 136.3, 132.7, 128.6, 128.3, 45.6, 29.4, 26.0, 25.9.

cyclohexyl(o-tolyl)methanone 3ri[16]

Colorless oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.42-7.40(m, 1H), 7.27-7.23(m, 1H), 7.19-7.14(m, 2H), 2.99-2.92(m, 1H), 2.33(s, 3H), 1.80-1.71(m, 5H), 1.38-1.17(m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):208.8, 138.9, 137.2, 131.5, 130.4, 127.3, 125.5, 49.0, 28.8, 26.0, 25.8, 20.6.

(3r,5r,7r)-adamantan-1-yl(phenyl)methanone 3sa[15]

Light yellow oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.55-7.53(m, 2H), 7.44-7.35(m, 3H), 2.07-2.00(m, 10H), 1.78-1.70(m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):210.2, 139.6, 130.2, 128.0, 127.1, 46.9, 39.1, 36.5, 28.1.

(3r,5r,7r)-adamantan-1-yl(o-tolyl)methanone 3ui[17]

Light yellow solid, mp 68-69^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.18-7.14(m, 1H), 7.11-7.05(m, 2H), 7.00(d, J=7.6Hz, 1H), 2.12(s, 3H), 1.95(s, 3H), 1.84-1.83(m, 6H), 1.66-1.58(m, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):214.1, 140.7, 133.9, 130.6, 128.4, 124.68, 124.65, 47.3, 38.6, 36.5, 28.0, 19.9.

(3r,5r,7r)-adamantan-1-yl(2-ethylphenyl)methanone 3uj

Light yellow oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.23-7.17(m, 2H), 7.10-7.06(m, 1H), 7.00(d, J=7.6Hz, 1H), 2.39(q, J=7.6Hz, 2H), 1.95(s, 3H), 1.83-1.82(m, 6H), 1.68-1.58(m, 6H), 1.13(t, J=7.6Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):213.3, 139.1, 127.7, 127.5, 123.7, 123.6, 46.1, 37.7, 35.4, 27.0, 25.7, 14.7. HRMS (EI) m/z (M^+) calcd for $C_{19}H_{24}O$ 268.1830, found 268.1827.

di-*o*-tolylmethanone 3vi[18]

Light yellow oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.27(t, J=7.6Hz, 2H), 7.21-7.13(m, 4H), 7.08(t, J=7.6Hz, 2H), 2.34(s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):200.8, 139.0, 138.2, 131.5, 131.1, 130.3, 125.5, 20.7.

(2-ethylphenyl)(o-tolyl)methanone 3vj

Light yellow oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.33-7.26(m, 2H), 7.23-7.15(m, 4H), 7.10-7.06(m, 2H), 2.70(q, J=7.6Hz, 2H), 2.39(s, 3H), 1.12(t, J=7.6Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):200.9, 144.2, 139.1, 138.8, 138.6, 131.6, 131.3, 131.0, 130.9, 130.0, 129.9, 125.4, 26.7, 20.9, 16.0. HRMS (EI) m/z (M^+) calcd for $C_{16}H_{16}O$ 224.1202, found 224.1201.

4'-methoxy-N-phenyl-N-tosyl-[1,1'-biphenyl]-4-carboxamide 4

White solid, mp 148-149^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.83(d, J=8.0Hz, 2H), 7.51(d, J=8.0Hz, 2H), 7.42(d, J=8.4Hz, 2H), 7.36-7.26(m, 7H),

7.20-7.19(m, 2H), 6.91(d, J=8.4Hz, 2H), 3.81(s, 3H), 2.45(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):169.7, 159.9, 144.8, 144.1, 137.6, 135.3, 131.8, 131.5, 130.4, 130.3, 129.5, 129.3, 129.2, 129.1, 128.2, 126.0, 114.3, 55.4, 21.7. HRMS (EI) m/z (M^+) calcd for $C_{27}H_{23}NO_4S$ 457.1348, found 457.1346.

(4'-methoxy-[1,1'-biphenyl]-4-yl)(p-tolyl)methanone 5

White solid, mp 181-183^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.76(d, J=8.4Hz, 2H), 7.66(d, J=8.0Hz, 2H), 7.56(d, J=8.4Hz, 2H), 7.50(d, J=8.8Hz, 2H), 7.20(d, J=8.0Hz, 2H), 6.92(d, J=8.8Hz, 2H), 3.77(s, 3H), 2.36(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):196.1, 159.9, 144.6, 143.1, 136.0, 135.1, 132.4, 130.7, 130.3, 129.0, 128.4, 126.3, 114.4, 55.4, 21.7. HRMS (EI) m/z (M^+) calcd for $C_{21}H_{18}O_2$ 302.1307, found 302.1309.

(4'-methyl-[1,1'-biphenyl]-4-yl)(p-tolyl)methanone 6

White solid, mp 149-150^{o}C, ^{1}H NMR ($CDCl_3$, 400 MHz) δ(ppm):7.85(d, J=8.0Hz, 2H), 7.74(d, J=8.0Hz, 2H), 7.66(d, J=8.0Hz, 2H), 7.53(d, J=8.0Hz, 2H), 7.29-7.22(m, 4H), 2.43(s, 3H), 2.39(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ(ppm):196.1, 145.0, 143.2, 138.1, 137.1, 136.3, 135.1, 130.7, 130.3, 129.7, 129.0, 127.2, 126.7, 21.7, 21.2. HRMS (EI) m/z (M^+) calcd for $C_{21}H_{18}O$ 286.1357, found 286.1358.

8. References

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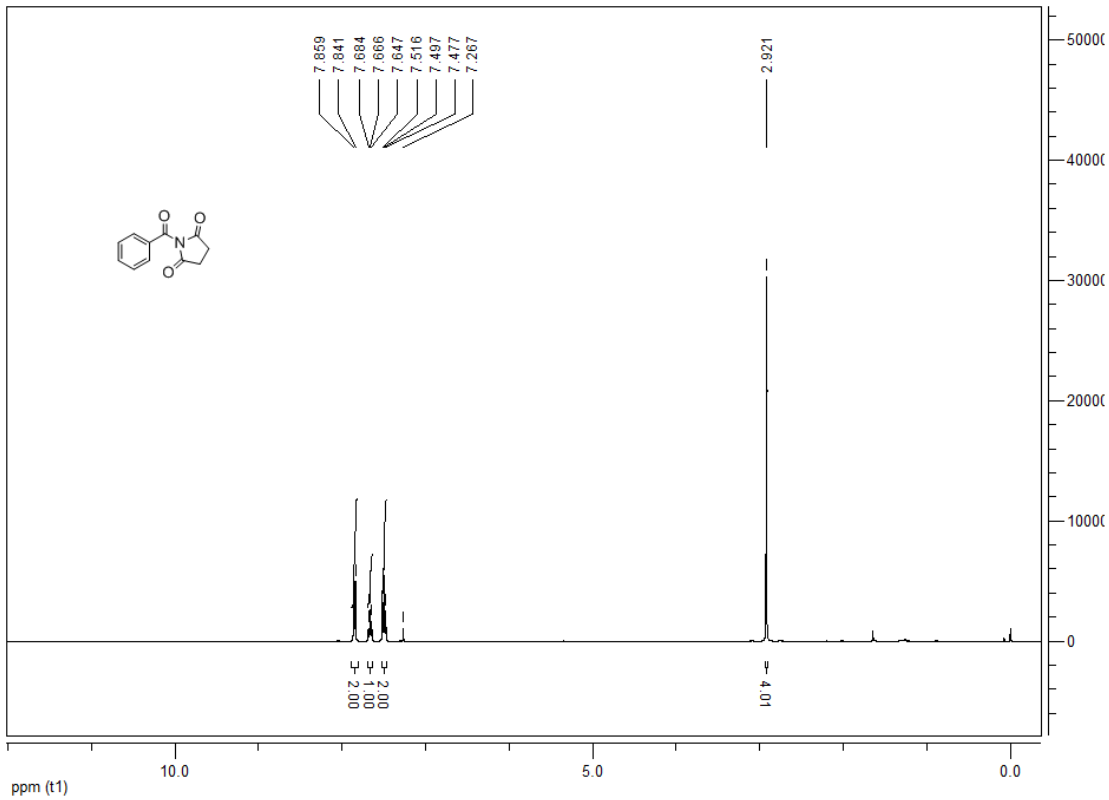
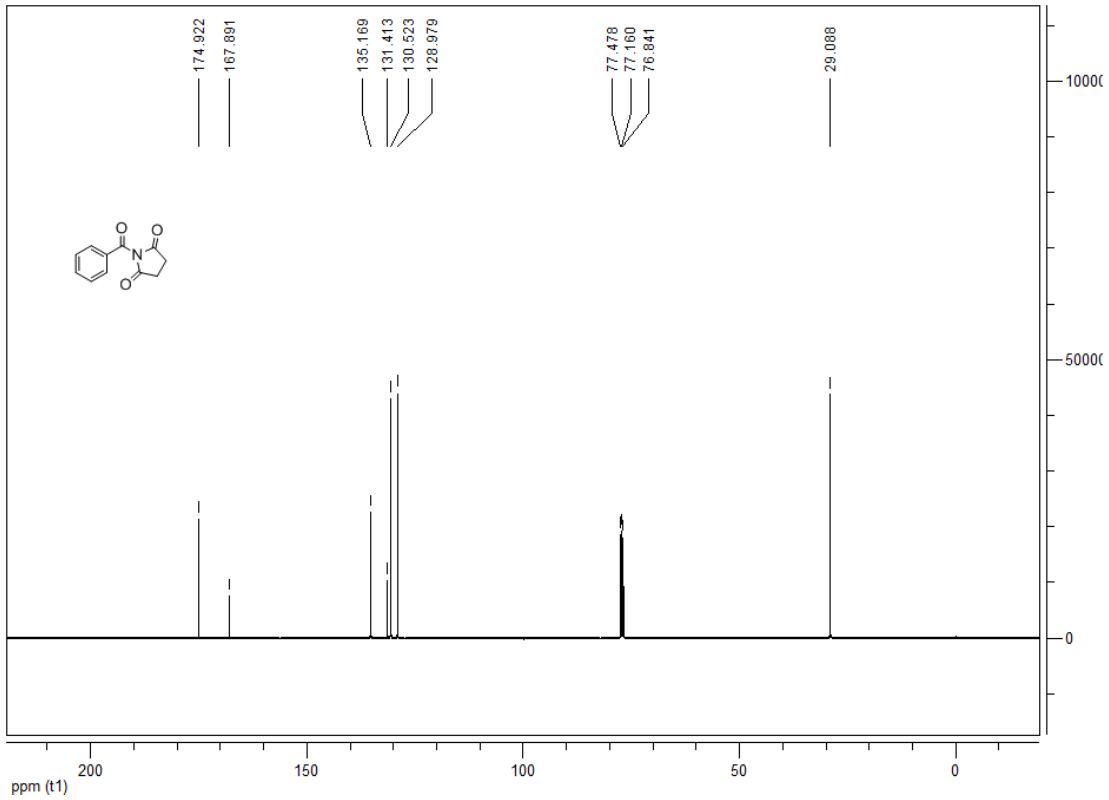
9. ^{1}H and ^{13}CNMR spectra of the carboxylic amide and ketones

1-benzoylpyrrolidine-2,5-dione 1a

^{1}H NMR

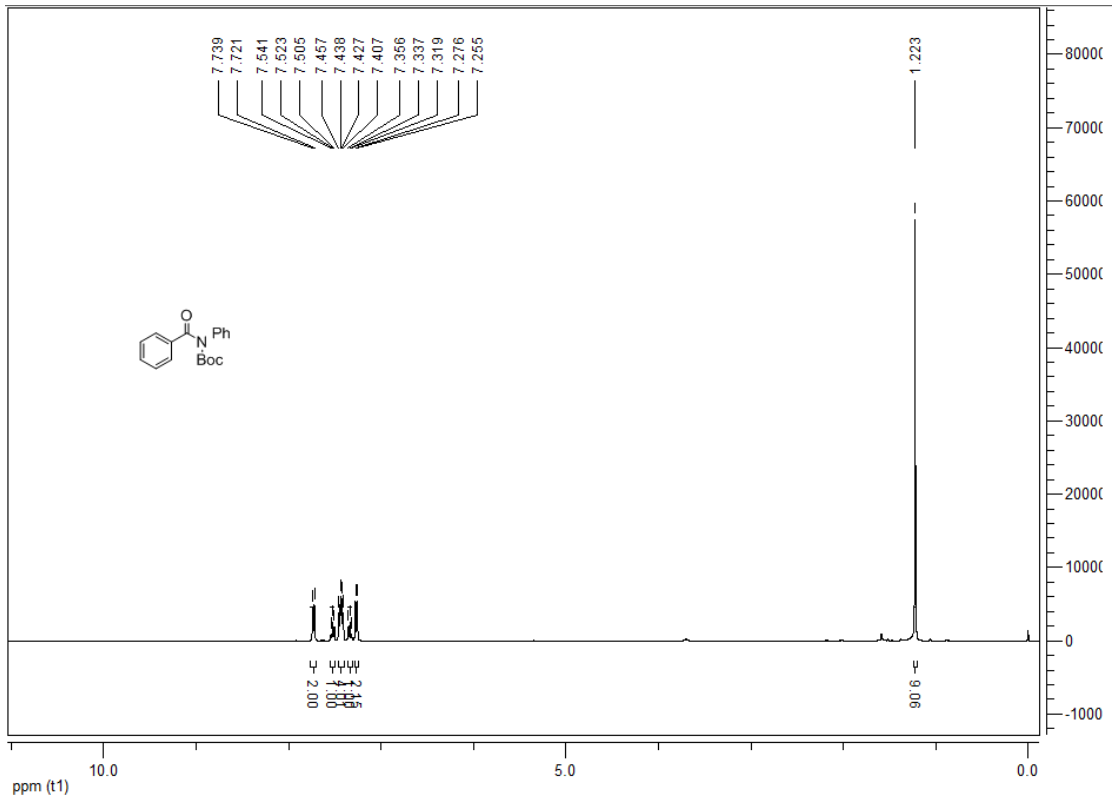


^{13}C NMR

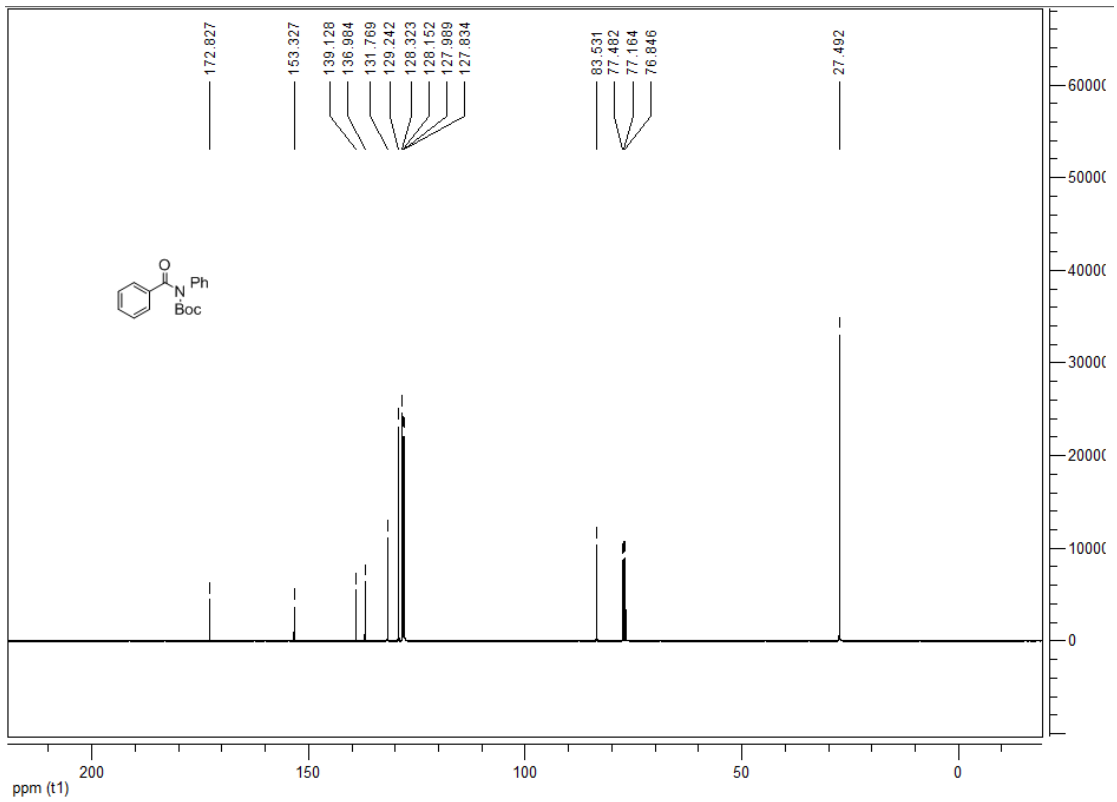


tert-butyl benzoyl(phenyl)carbamate 1b

^{1}H NMR



^{13}C NMR



N-methyl-N-tosylbenzamide 1c

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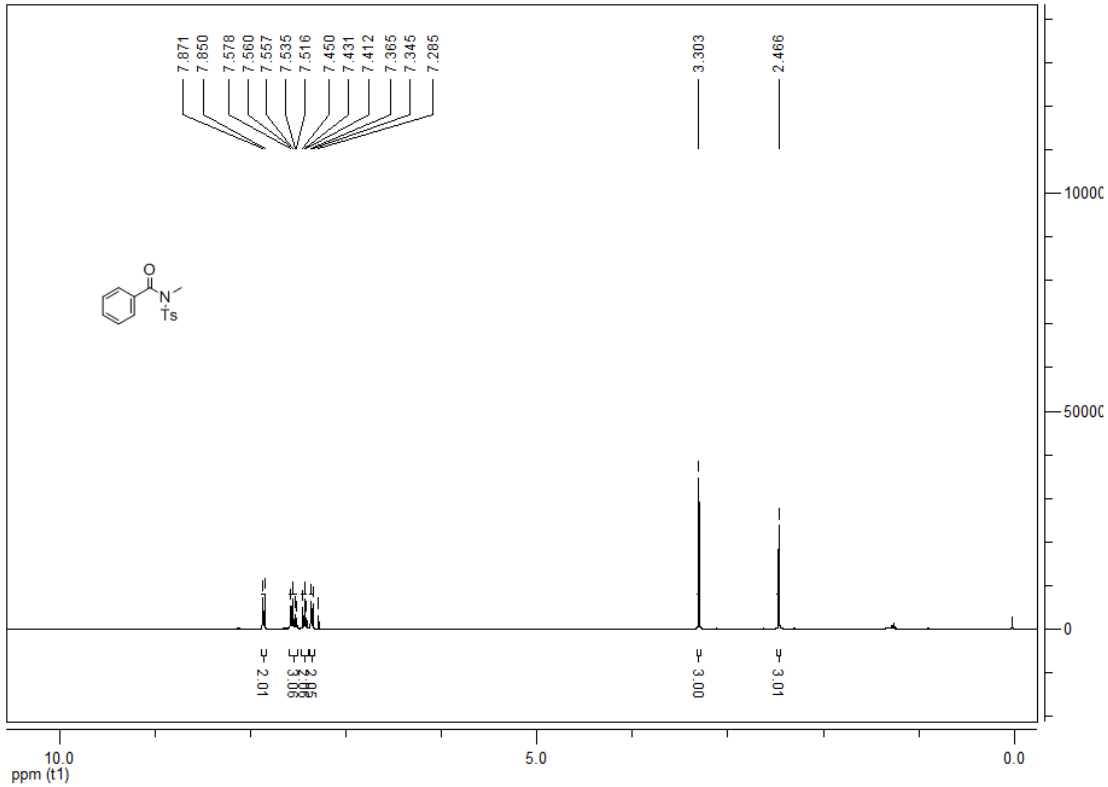
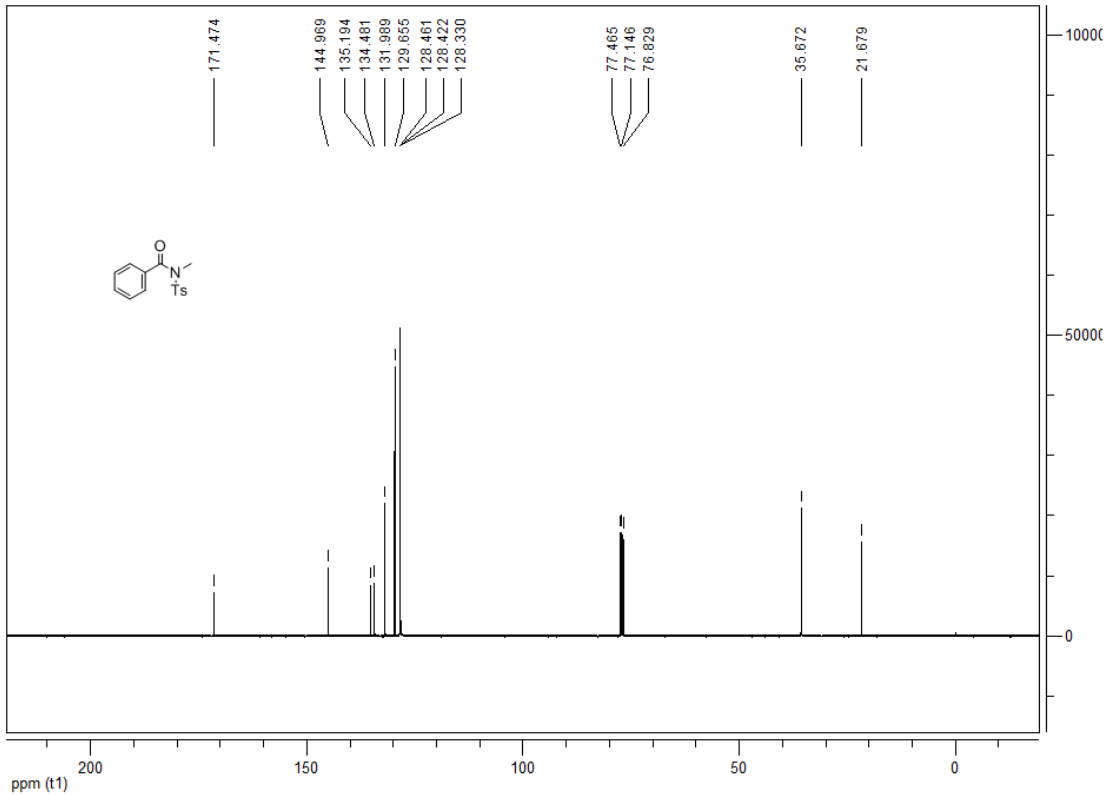
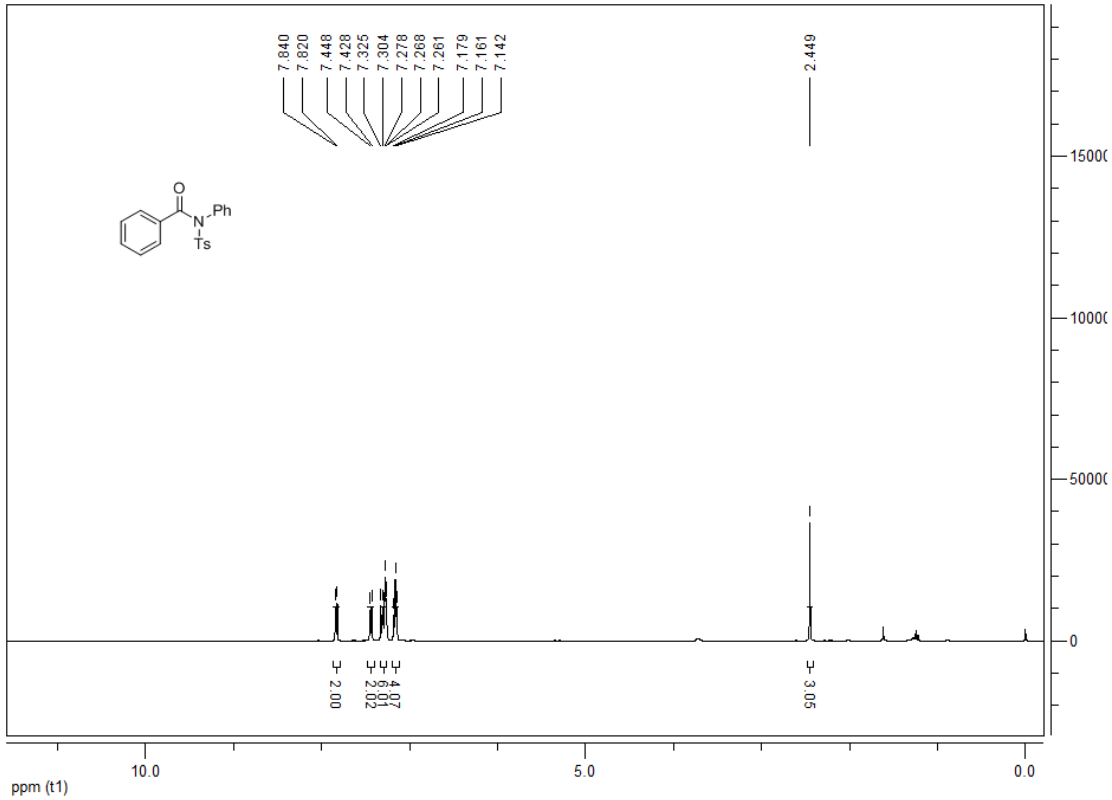


^{13}C NMR

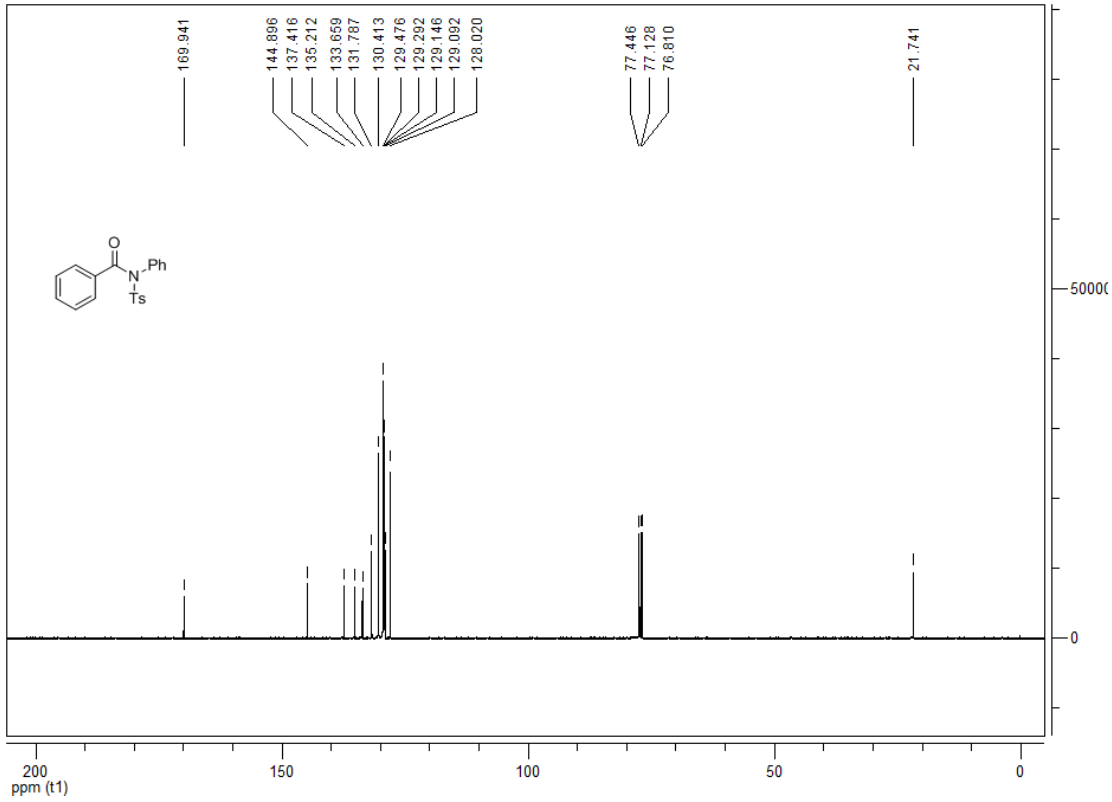


N-phenyl-N-tosylbenzamide 1d

^{1}H NMR

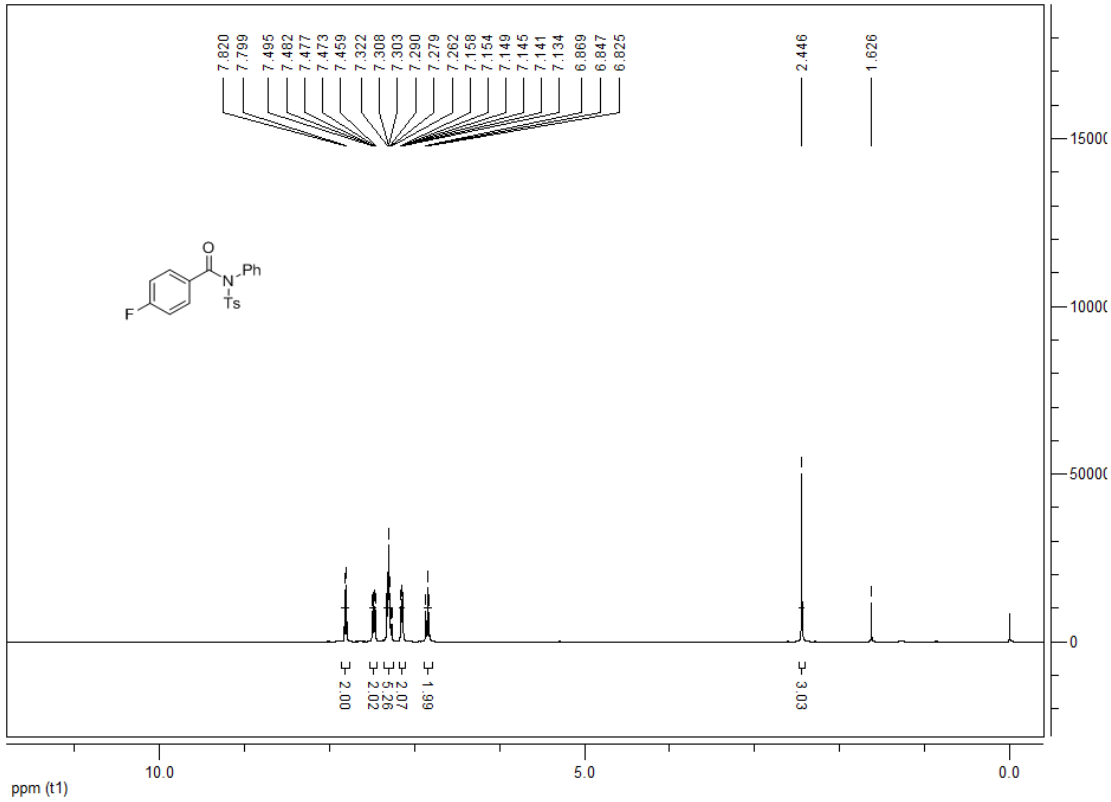


^{13}C NMR

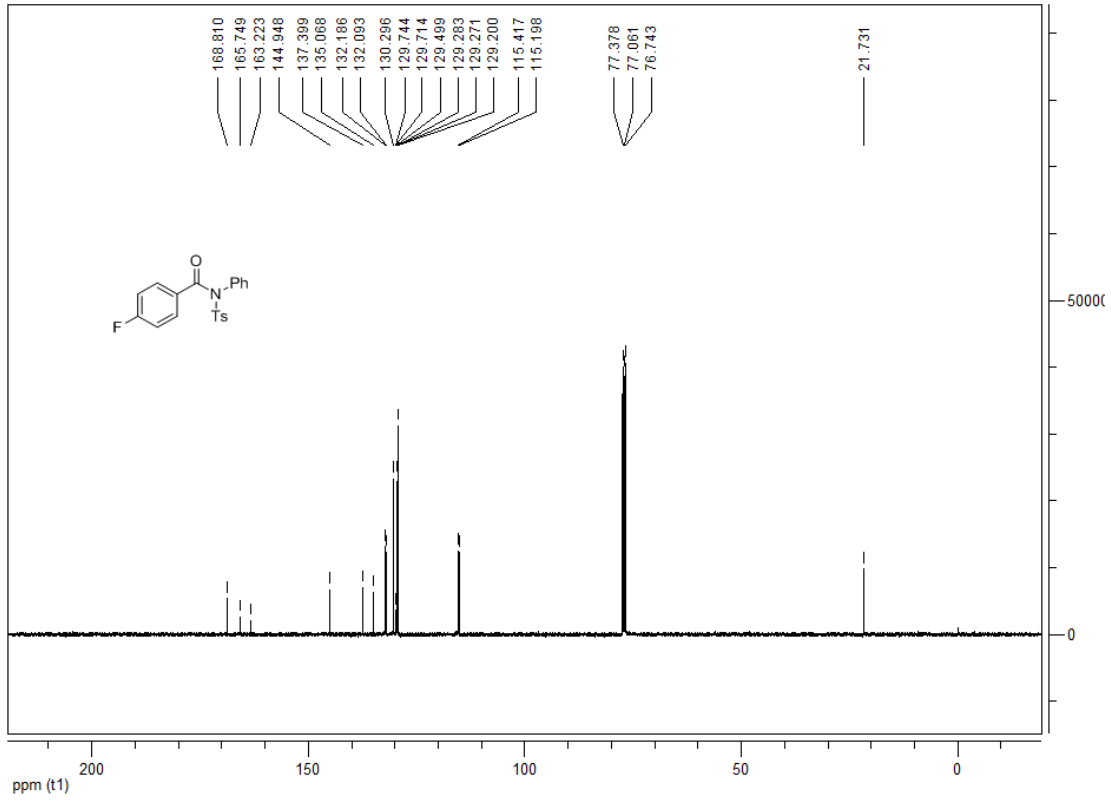


4-fluoro-N-phenyl-N-tosylbenzamide 1e

^{1}H NMR

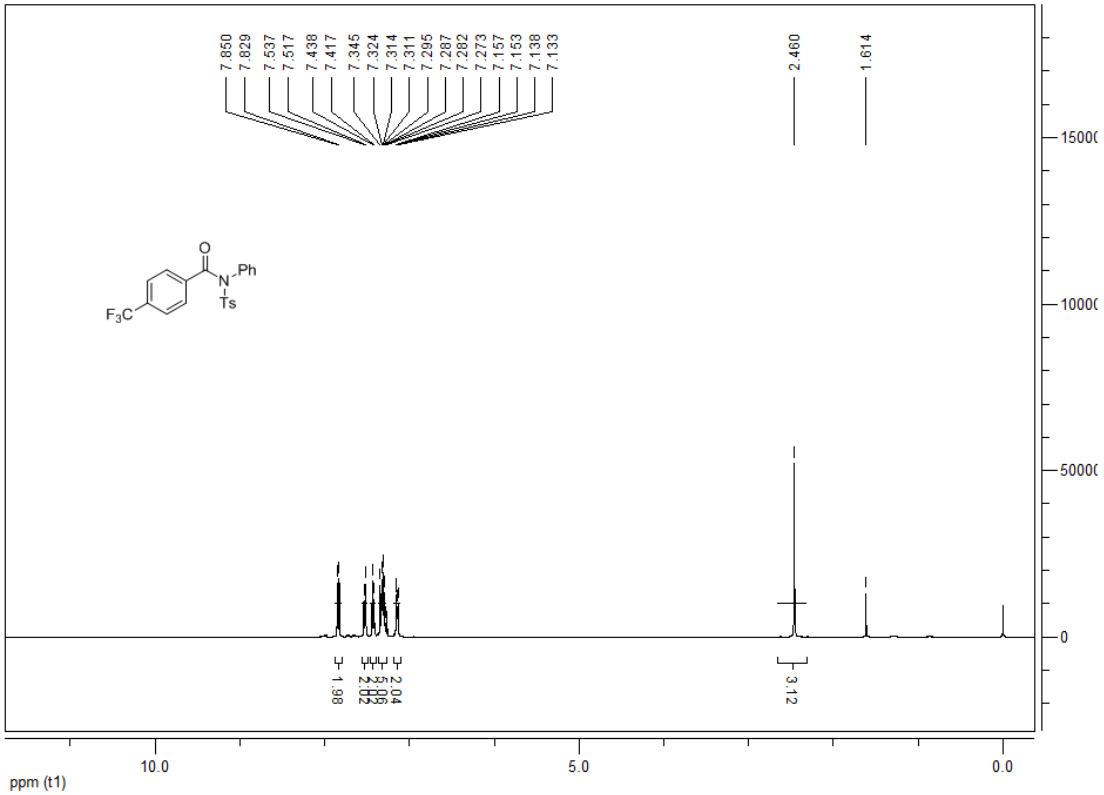


^{13}C NMR

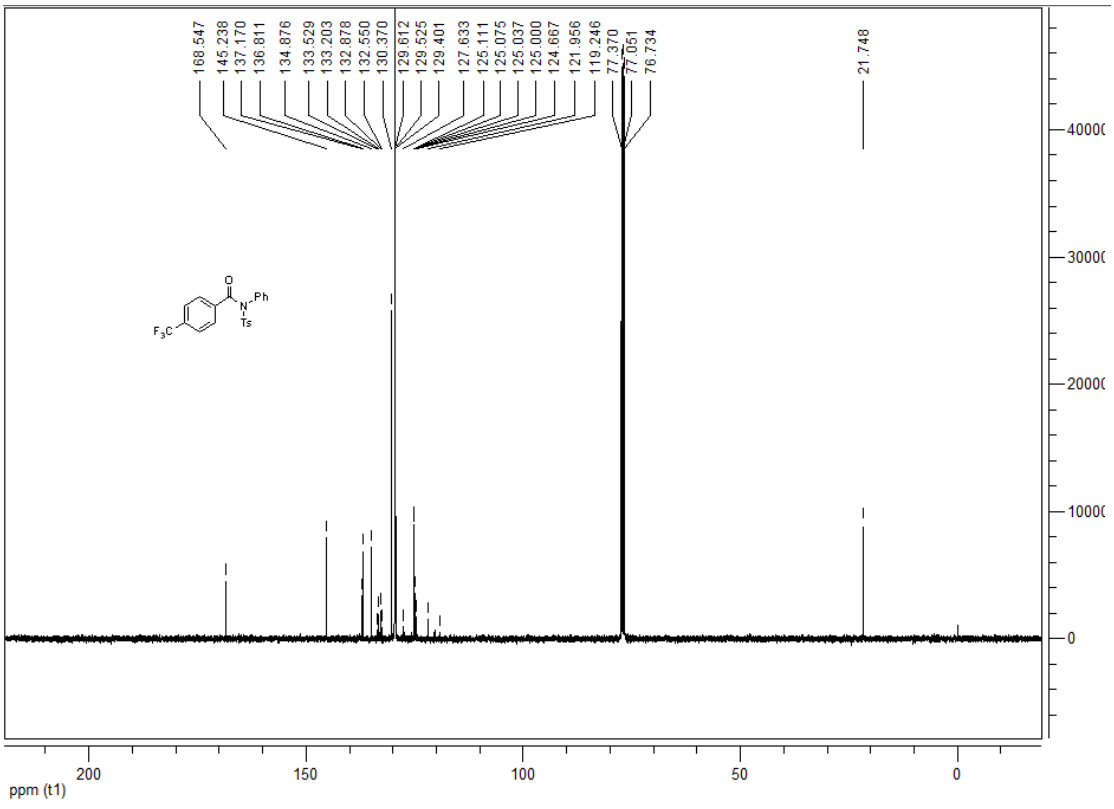


N-phenyl-N-tosyl-4-(trifluoromethyl)benzamide 1f

^{1}H NMR

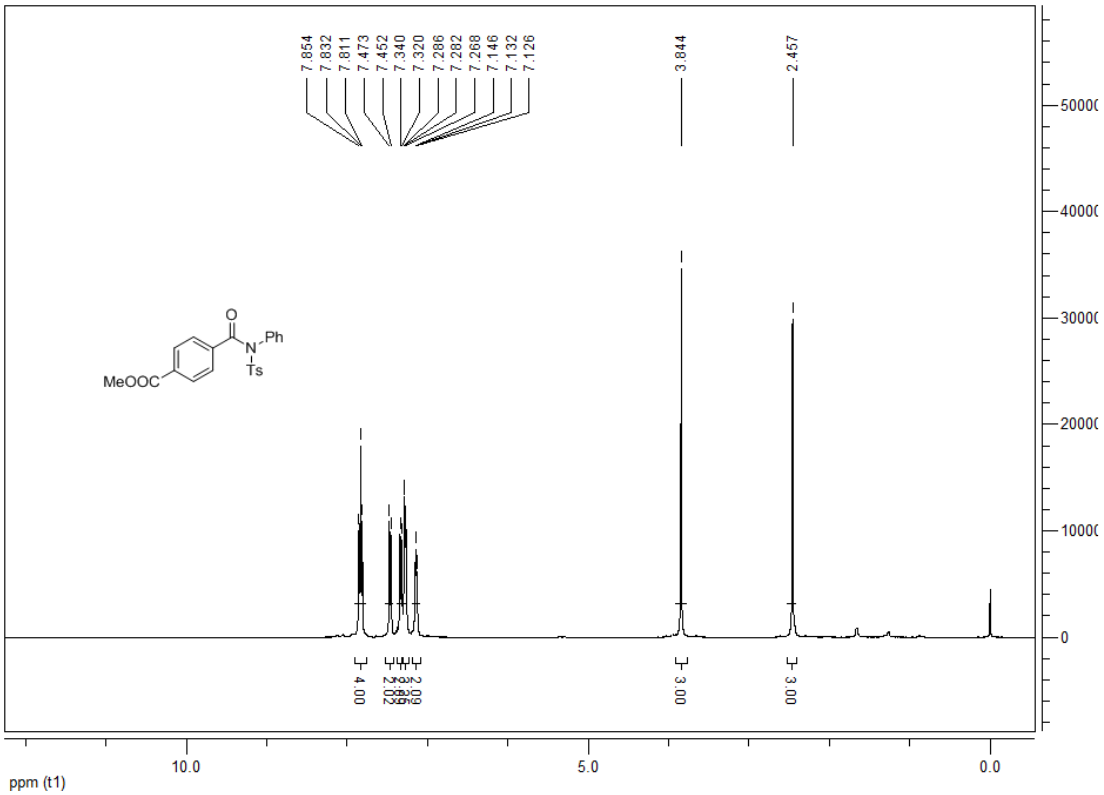


^{13}C NMR

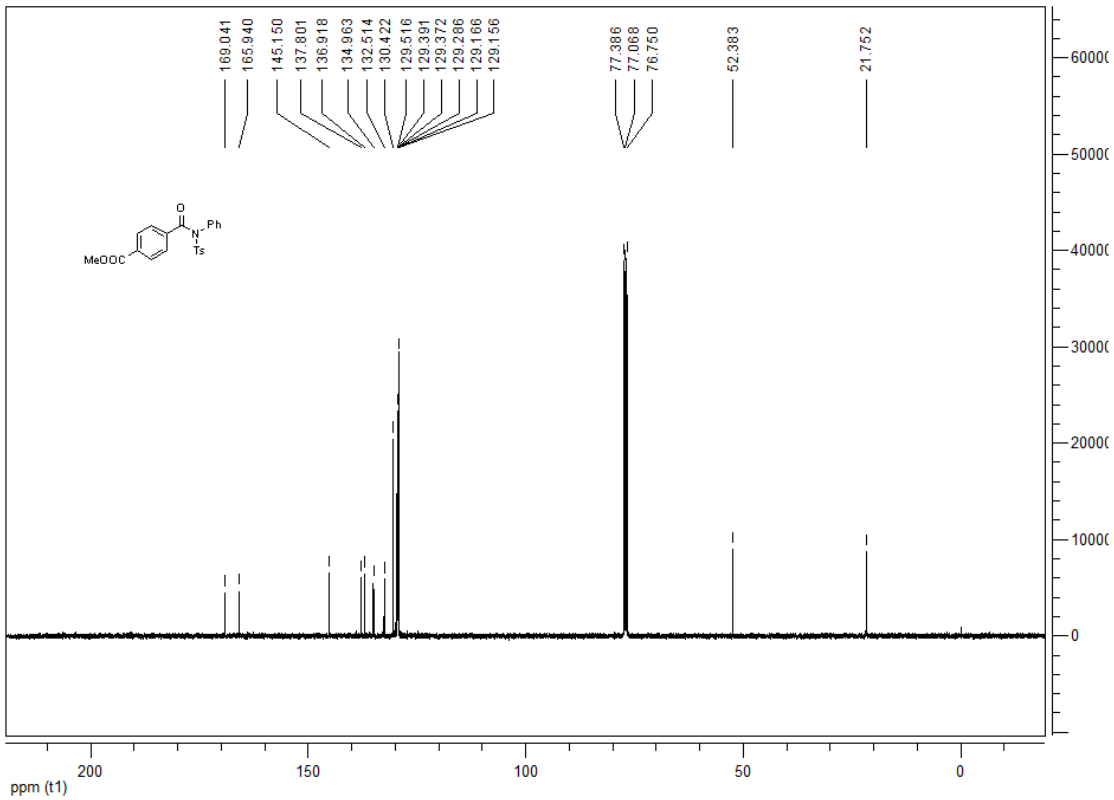


methyl 4-(phenyl(tosyl)carbamoyl)benzoate 1g

^{1}H NMR

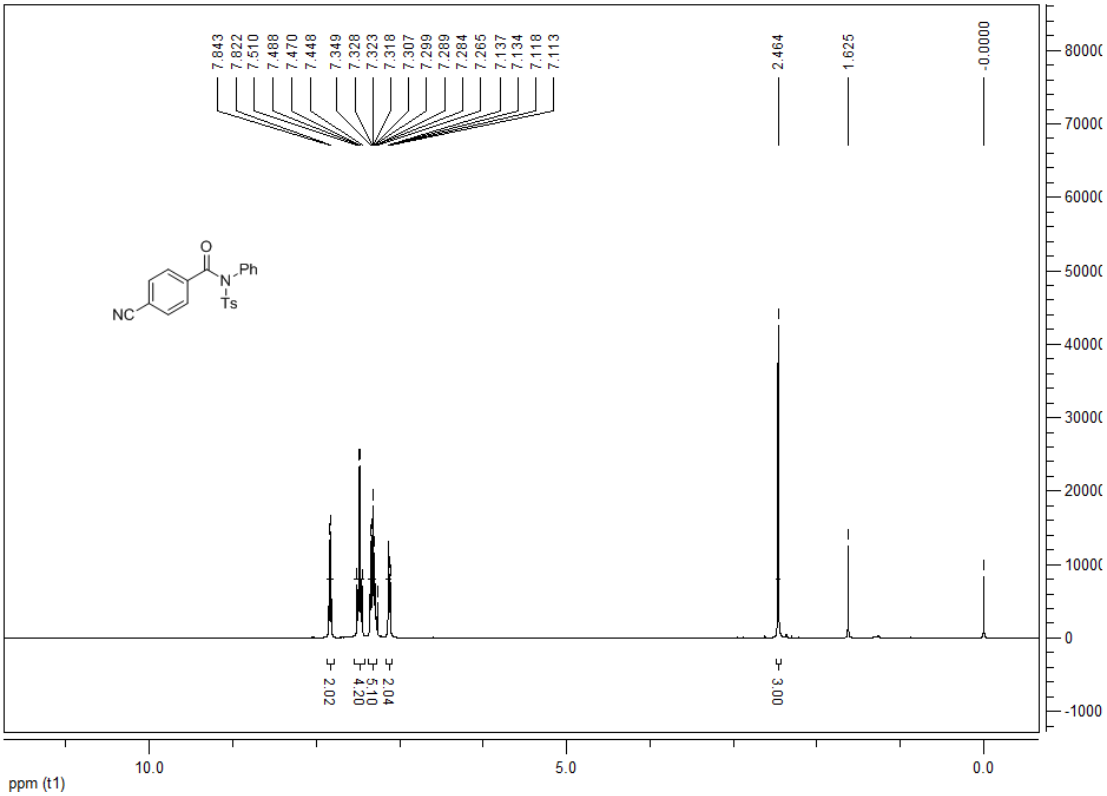


^{13}C NMR

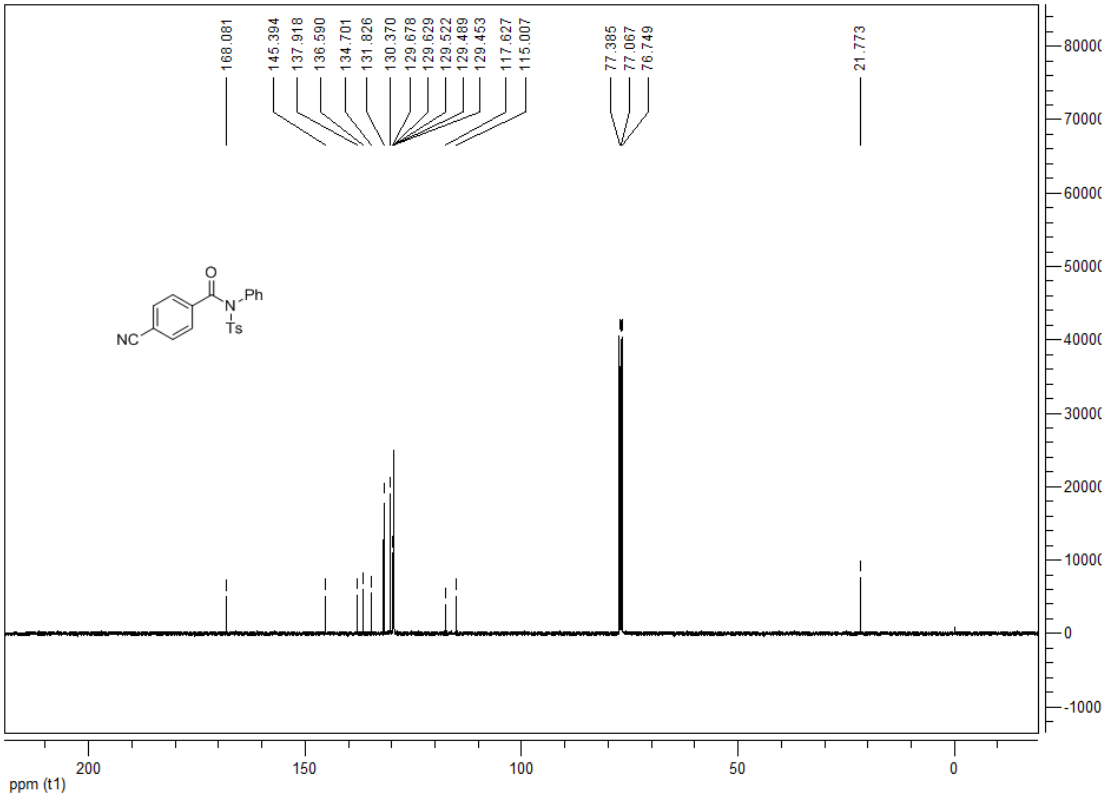


4-cyano-N-phenyl-N-tosylbenzamide 1h

^{1}H NMR

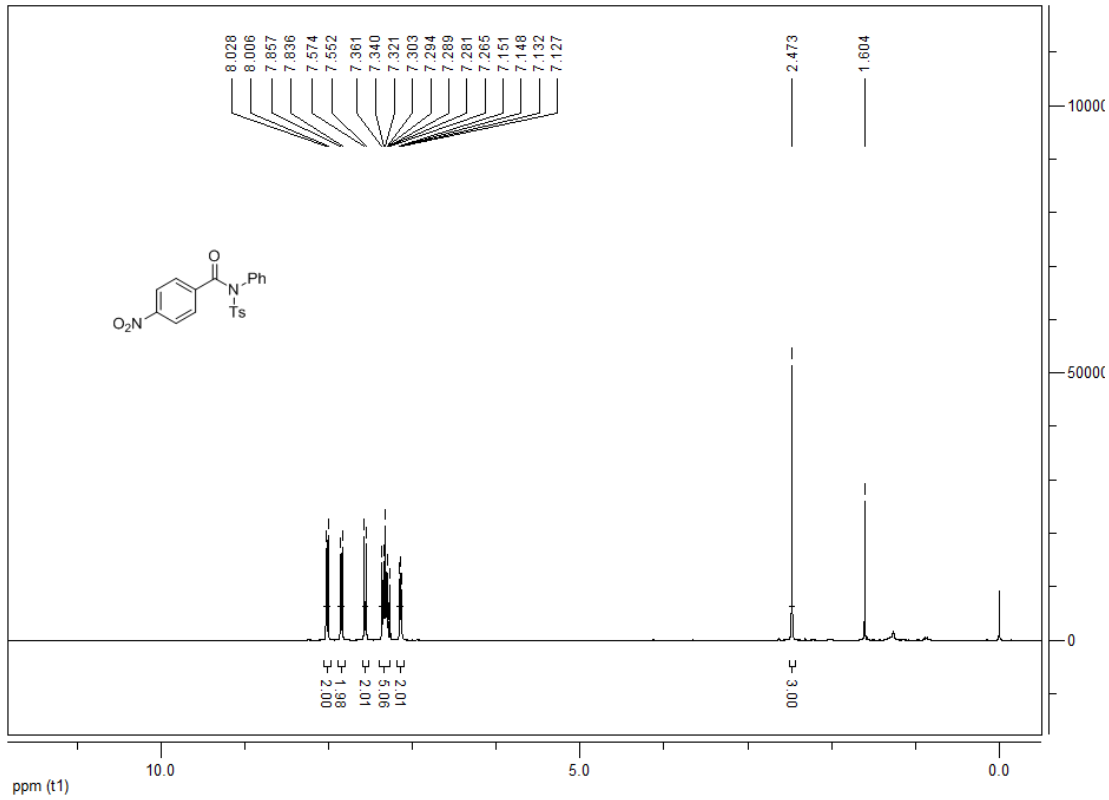


^{13}C NMR

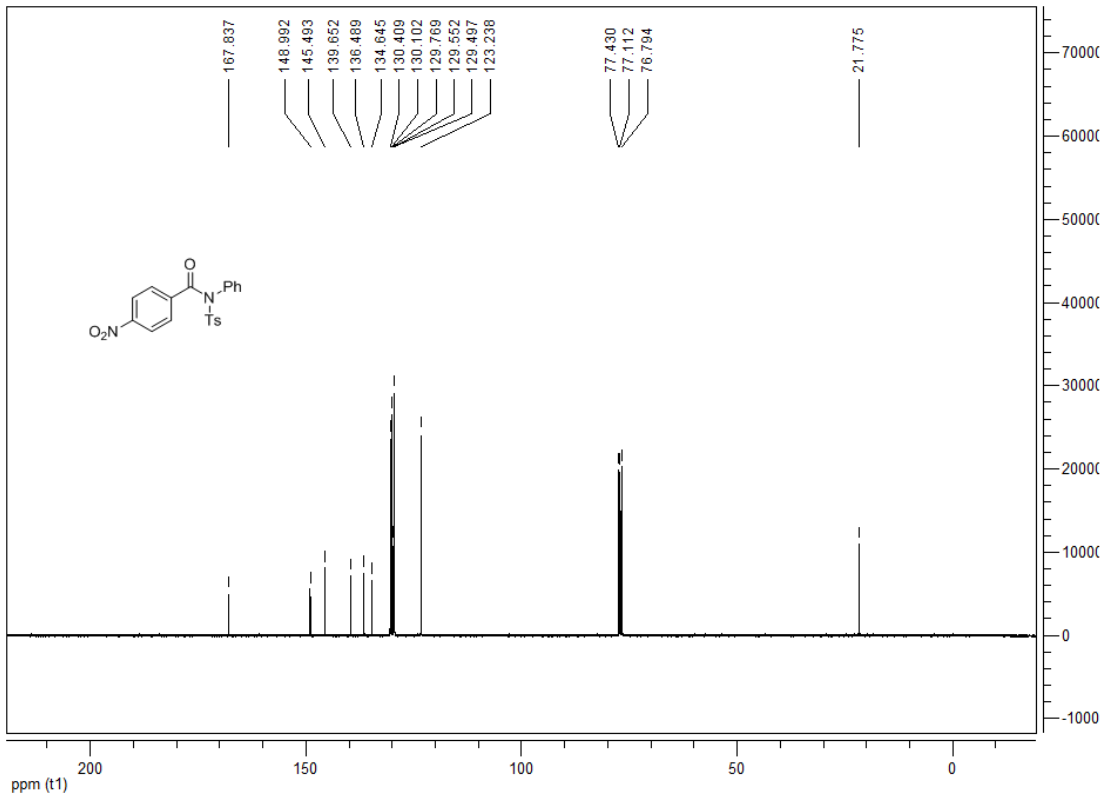


4-nitro-N-phenyl-N-tosylbenzamide 1i

^{1}H NMR

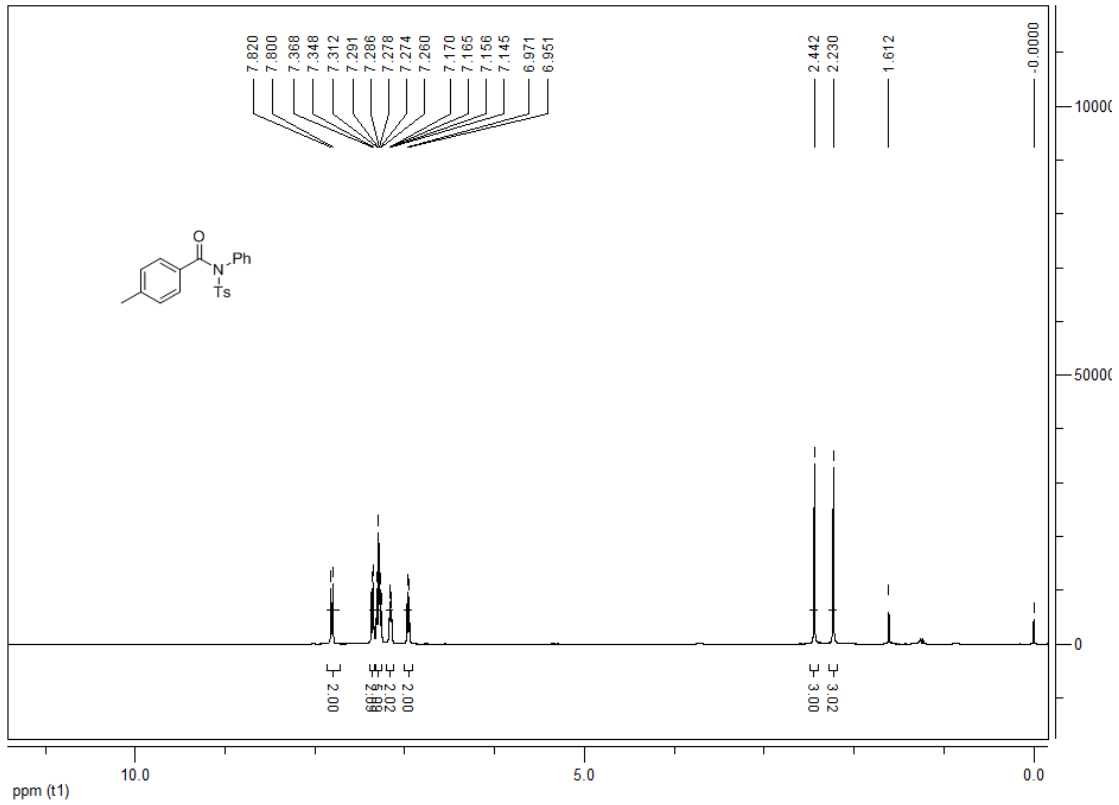


^{13}C NMR



4-methyl-N-phenyl-N-tosylbenzamide 1j

^{1}H NMR



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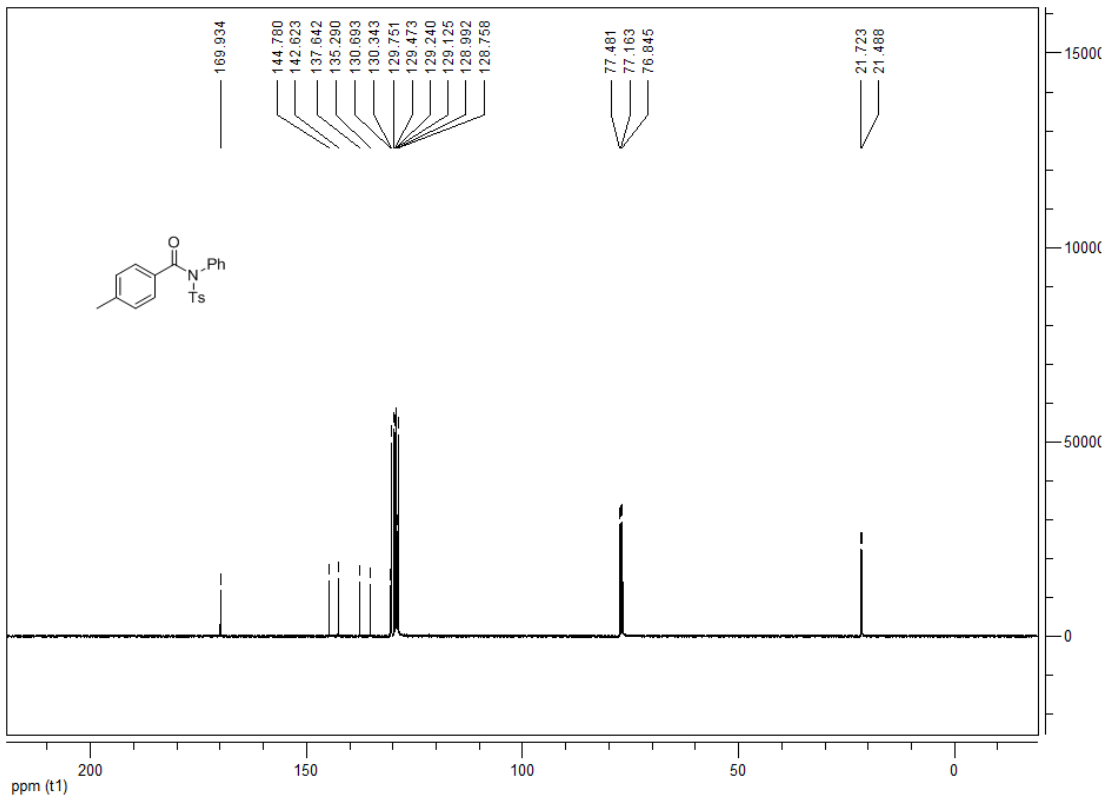
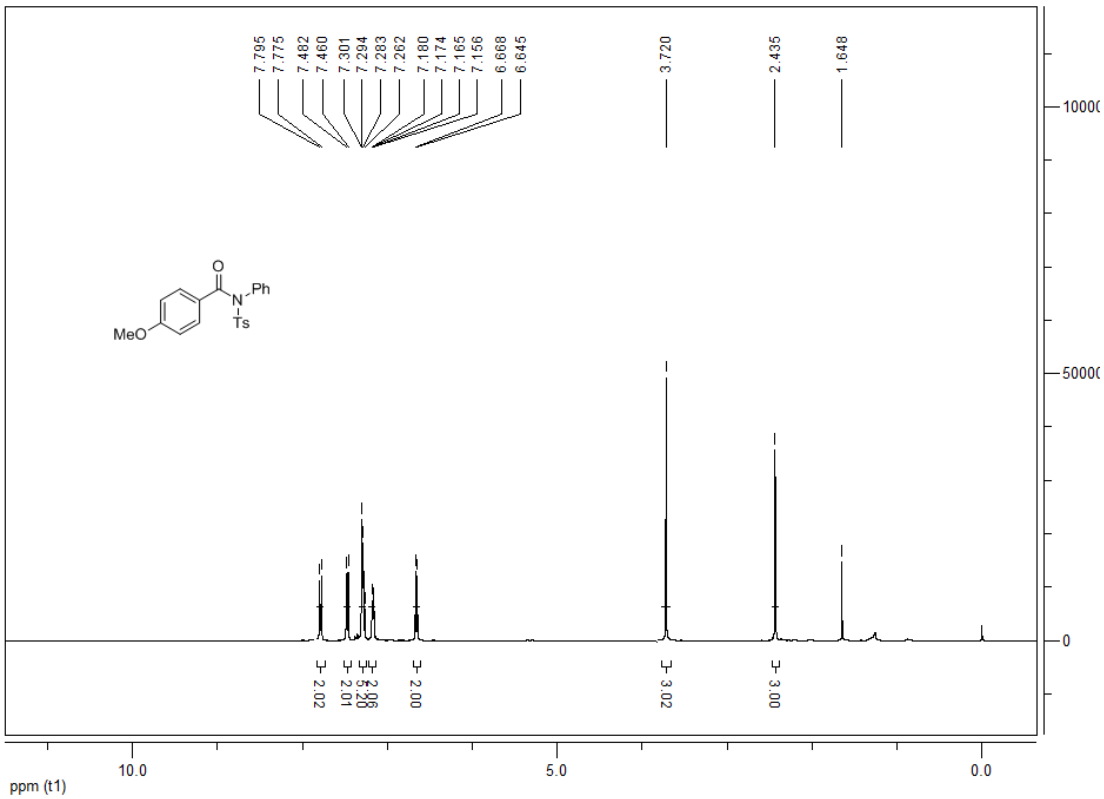
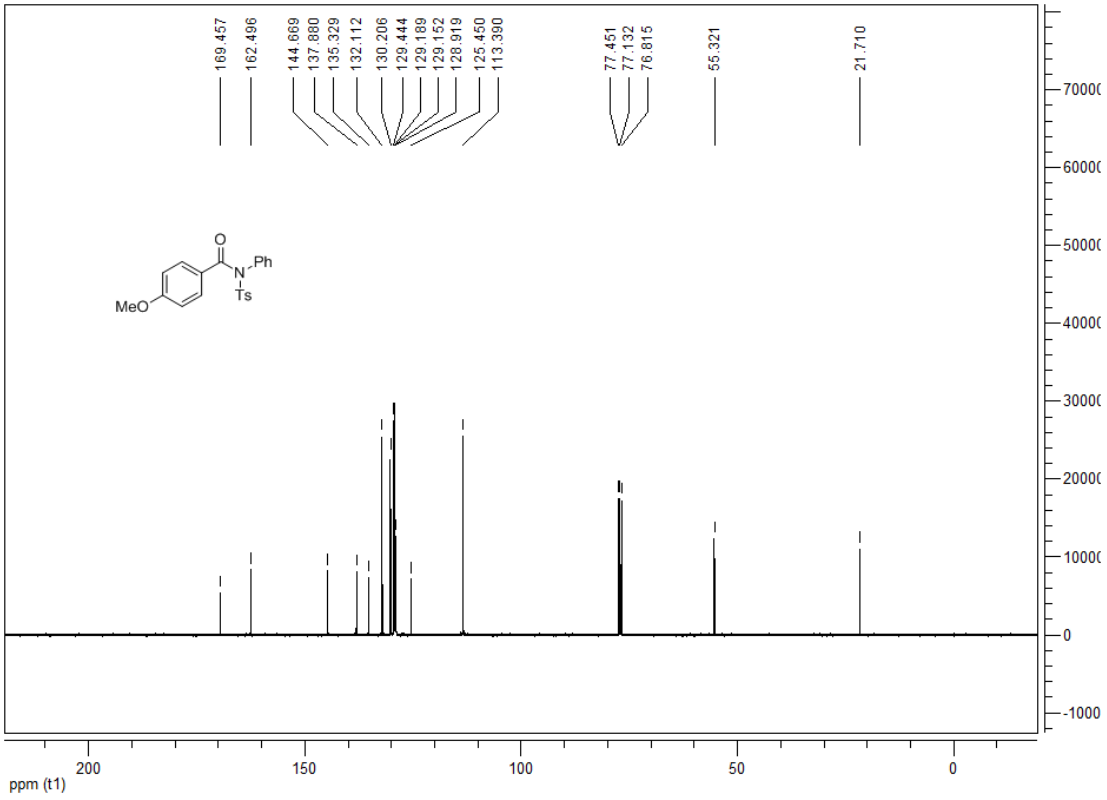


4-methoxy-N-phenyl-N-tosylbenzamide 1k

^{1}H NMR

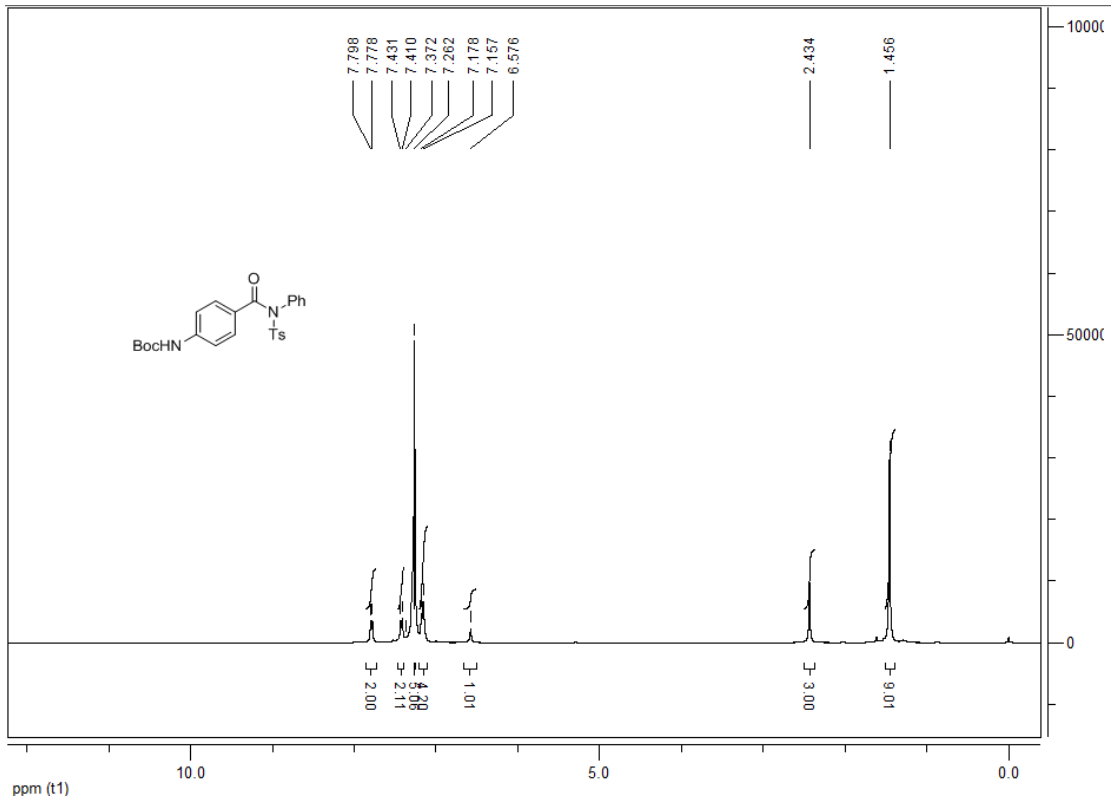


^{13}C NMR

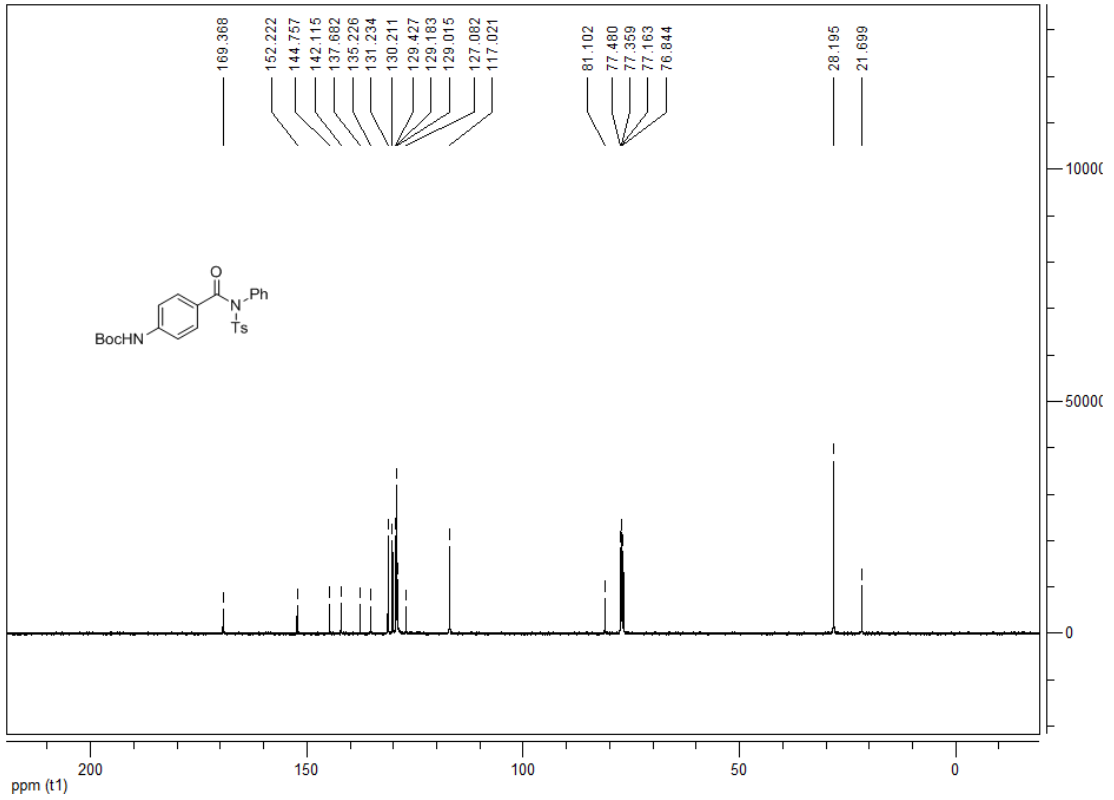


tert-butyl (4-(phenyl(tosyl)carbamoyl)phenyl)carbamate 1l

^{1}H NMR

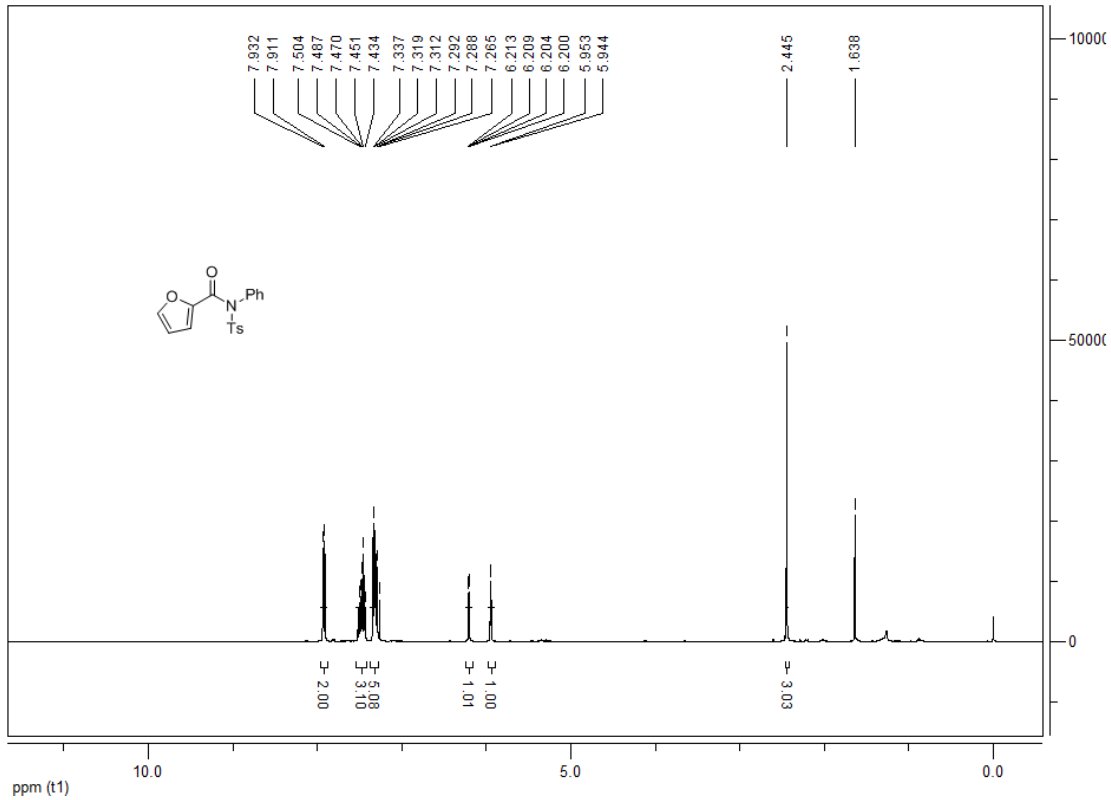


^{13}C NMR



N-phenyl-N-tosylfuran-2-carboxamide 1m

^{1}H NMR



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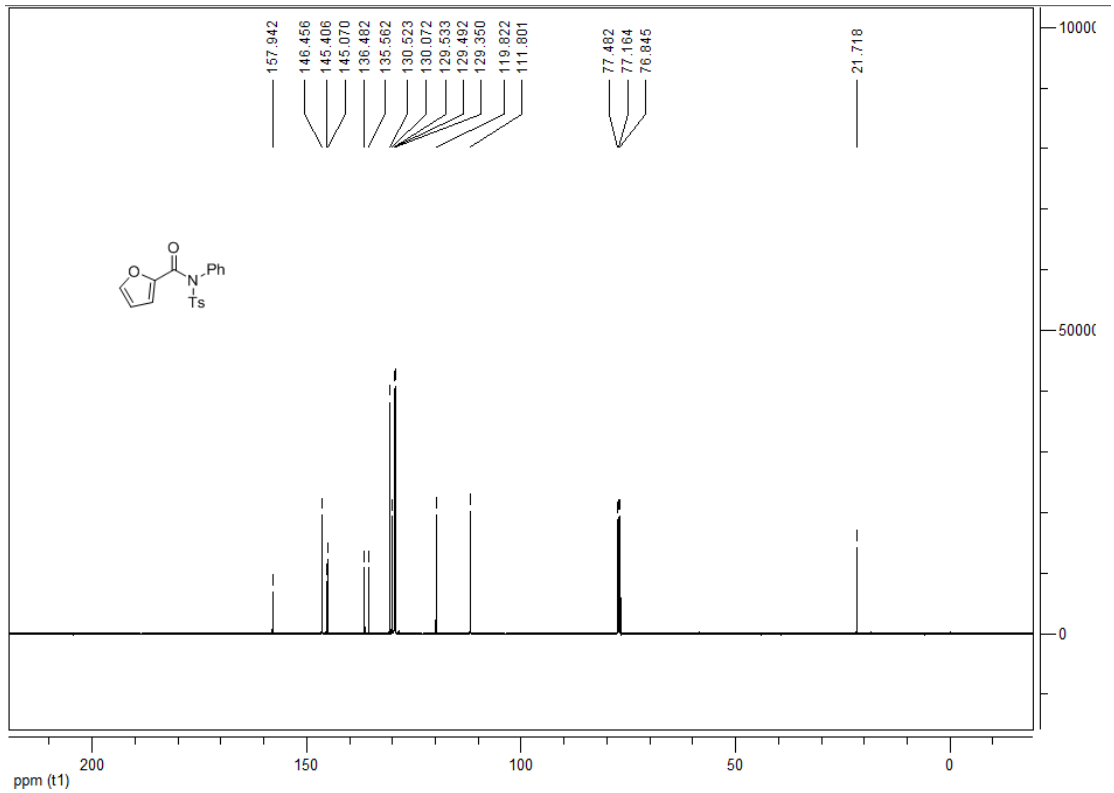
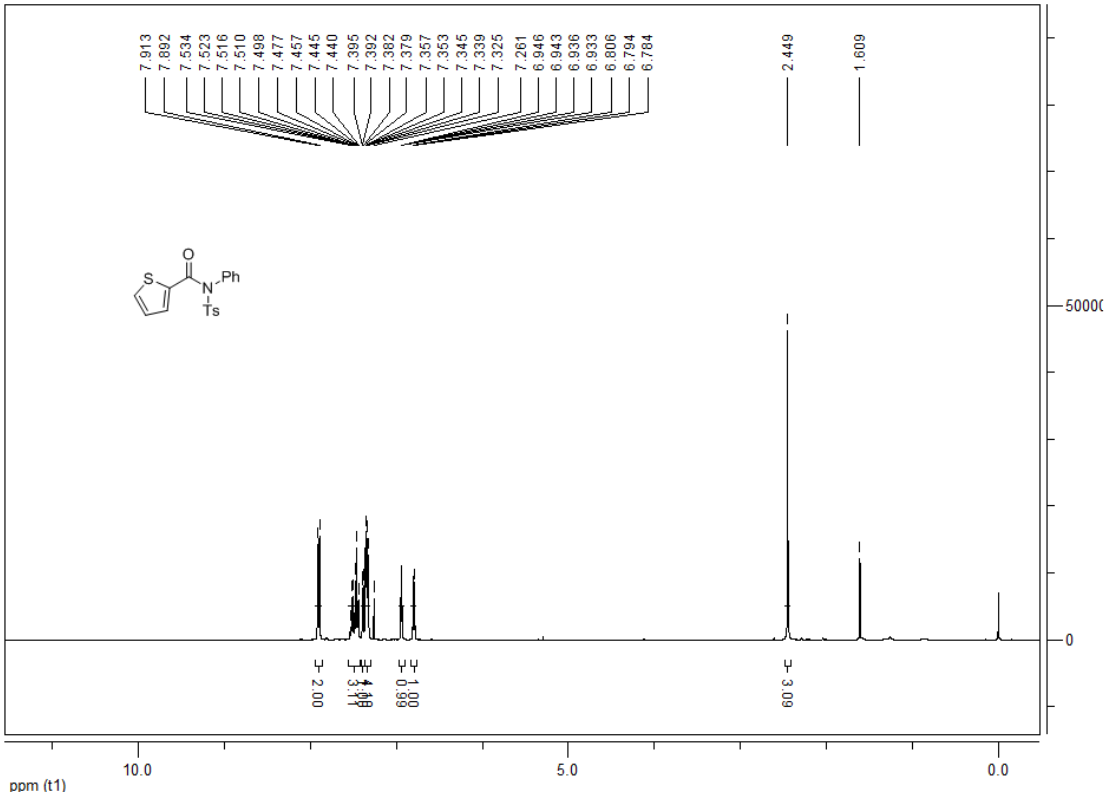
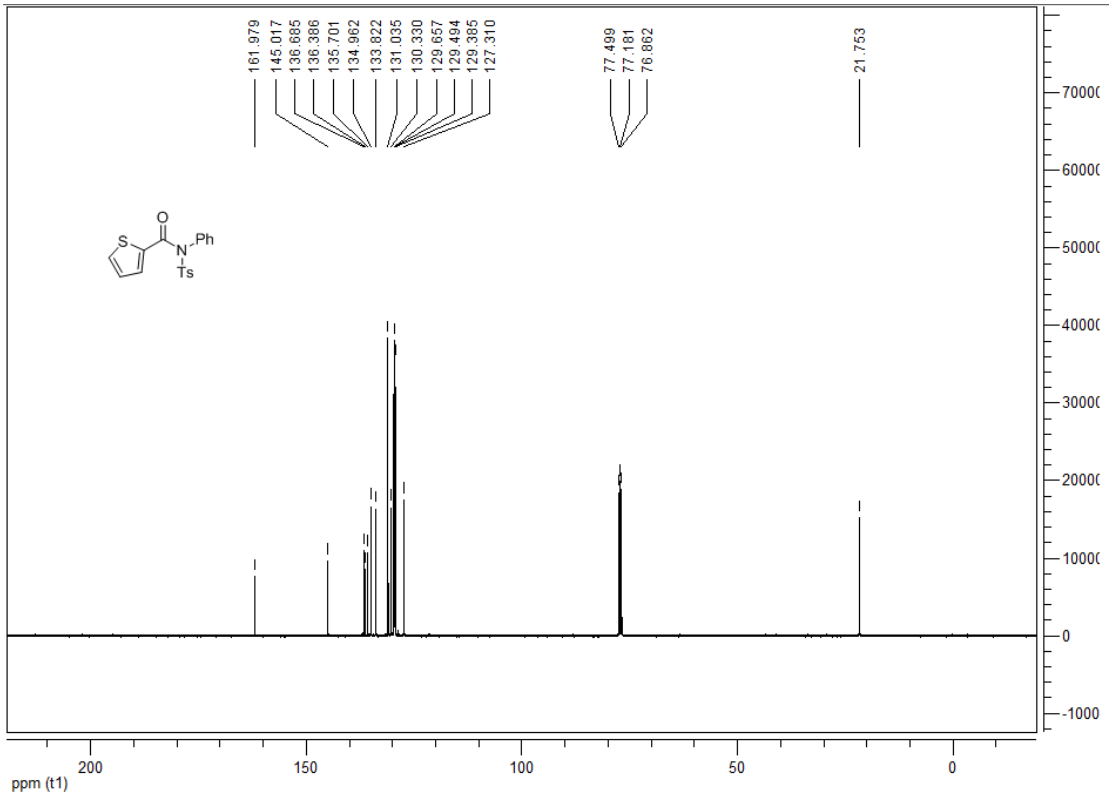


N-phenyl-N-tosylthiophene-2-carboxamide 1n

^{1}H NMR

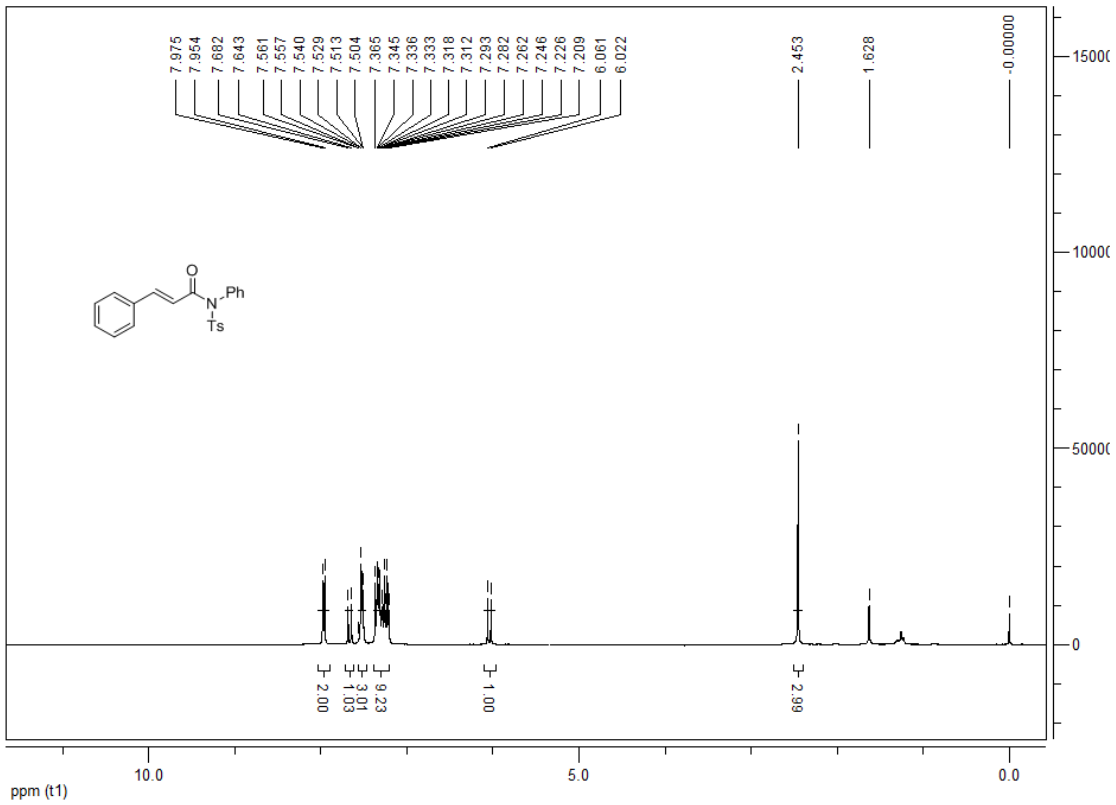


^{13}C NMR

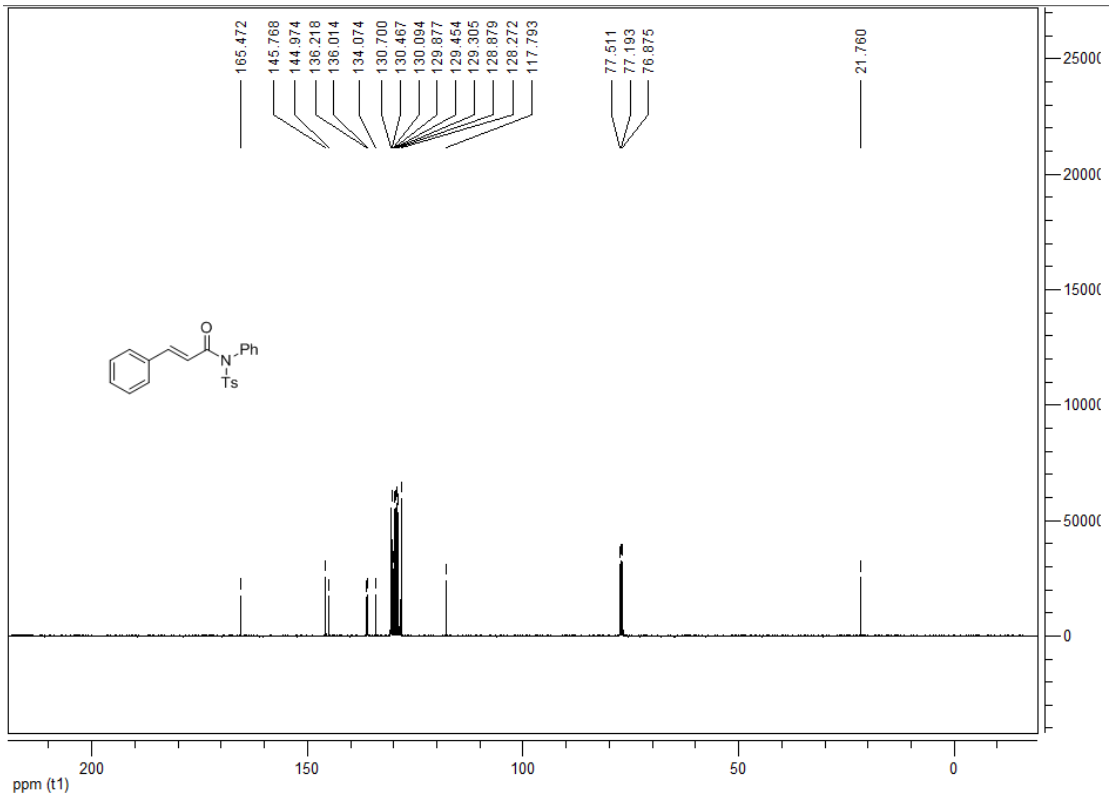


N-phenyl-N-tosylcinnamamide 1o

^{1}H NMR



^{13}C NMR



N,3-diphenyl-N-tosylpropanamide 1p

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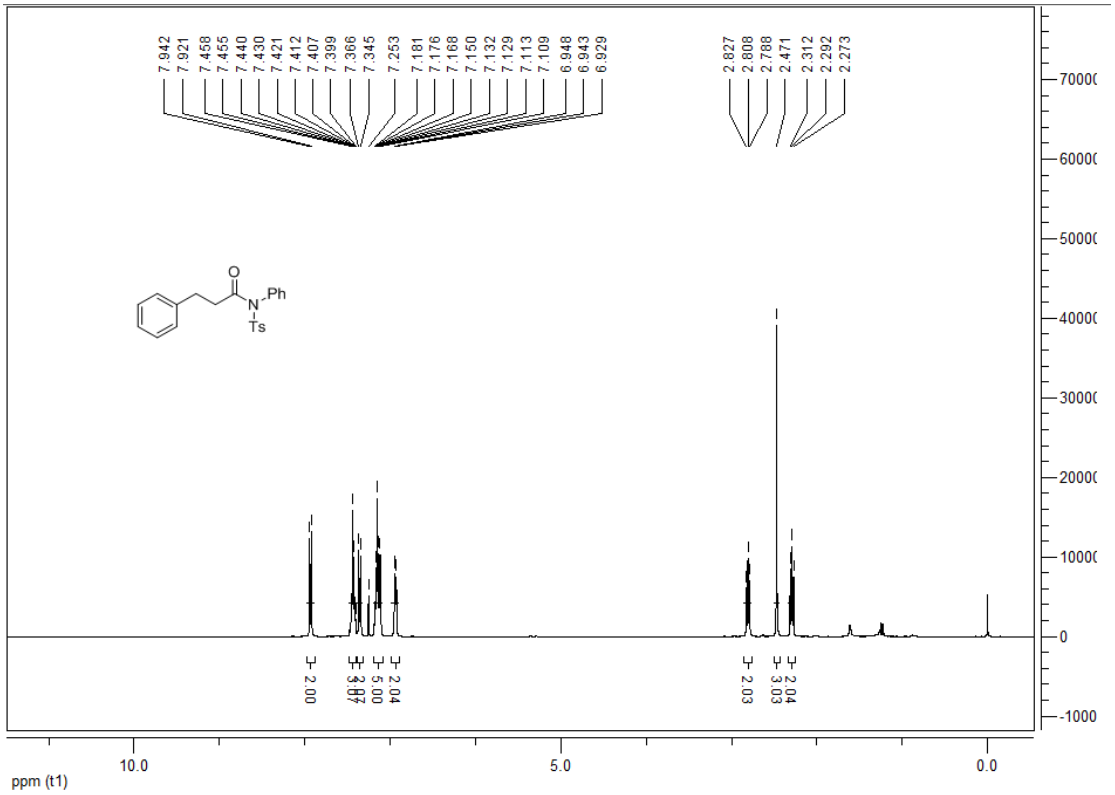

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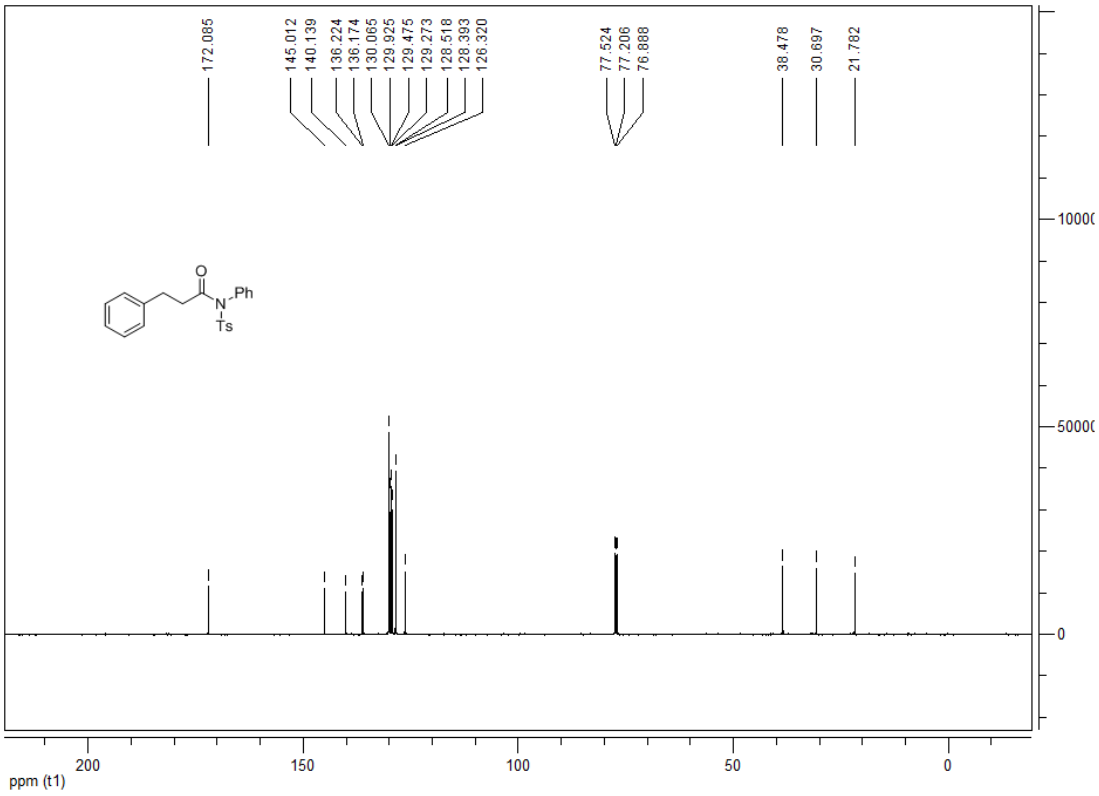
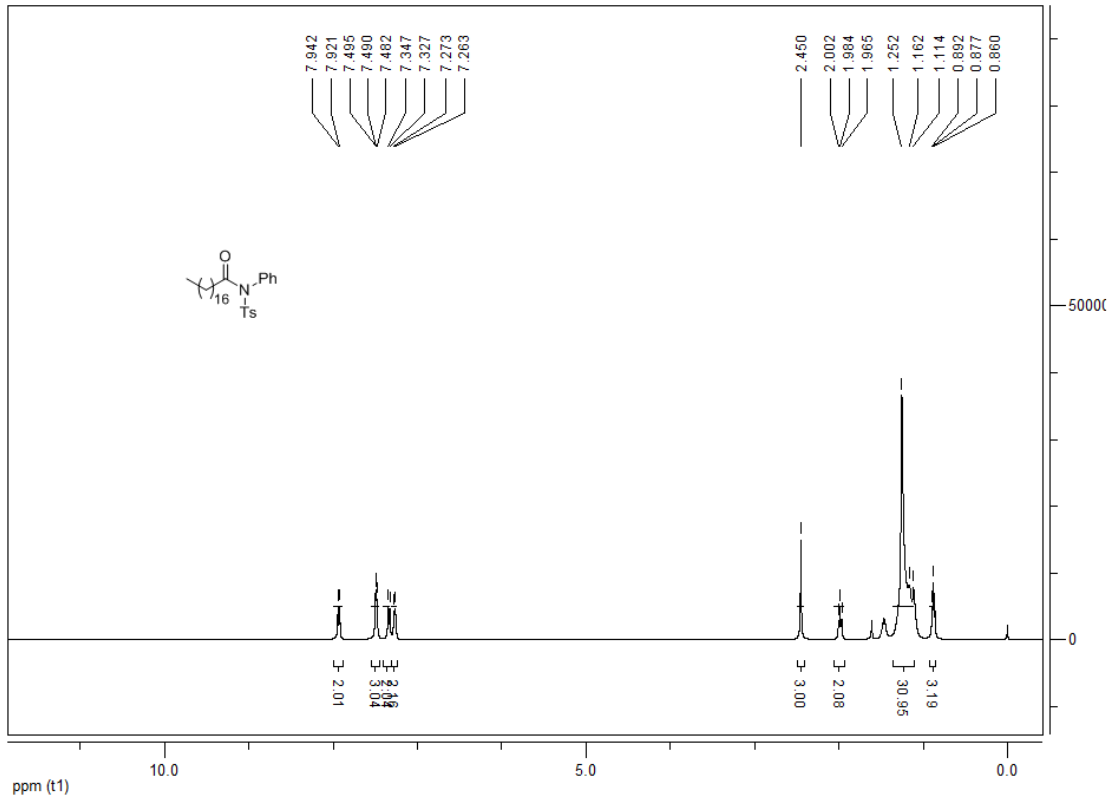


N-phenyl-N-tosylstearamide 1q

^{1}H NMR



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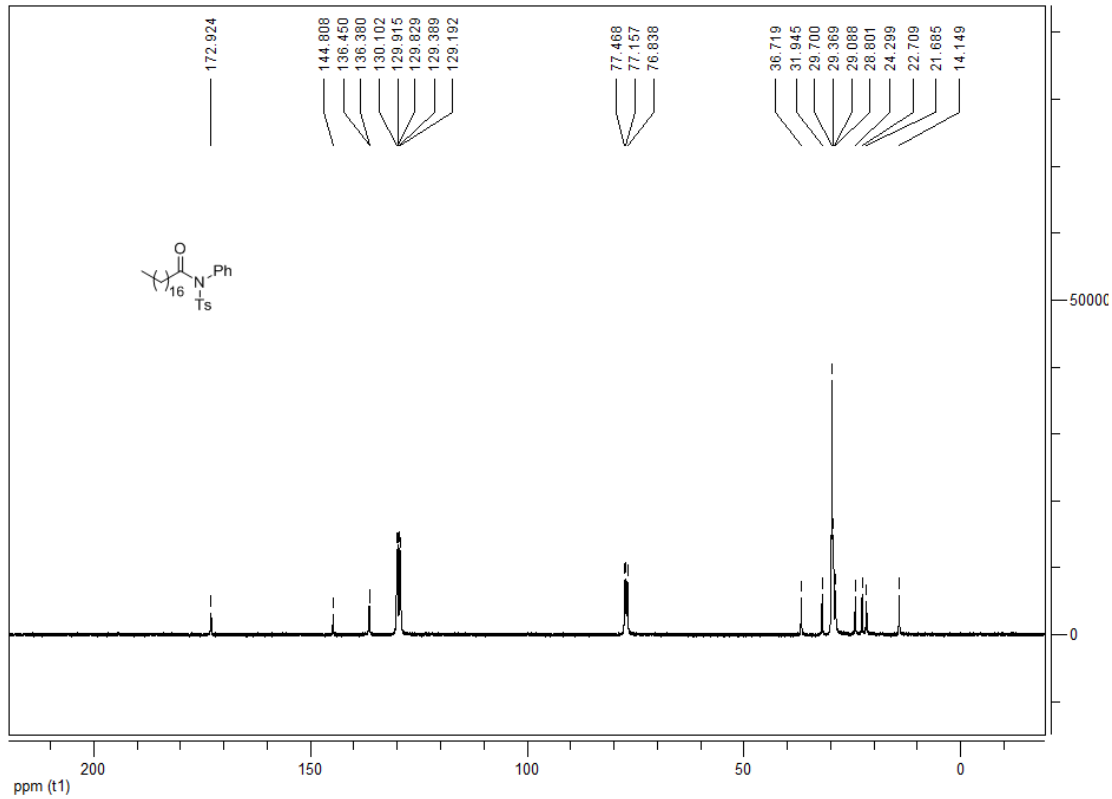
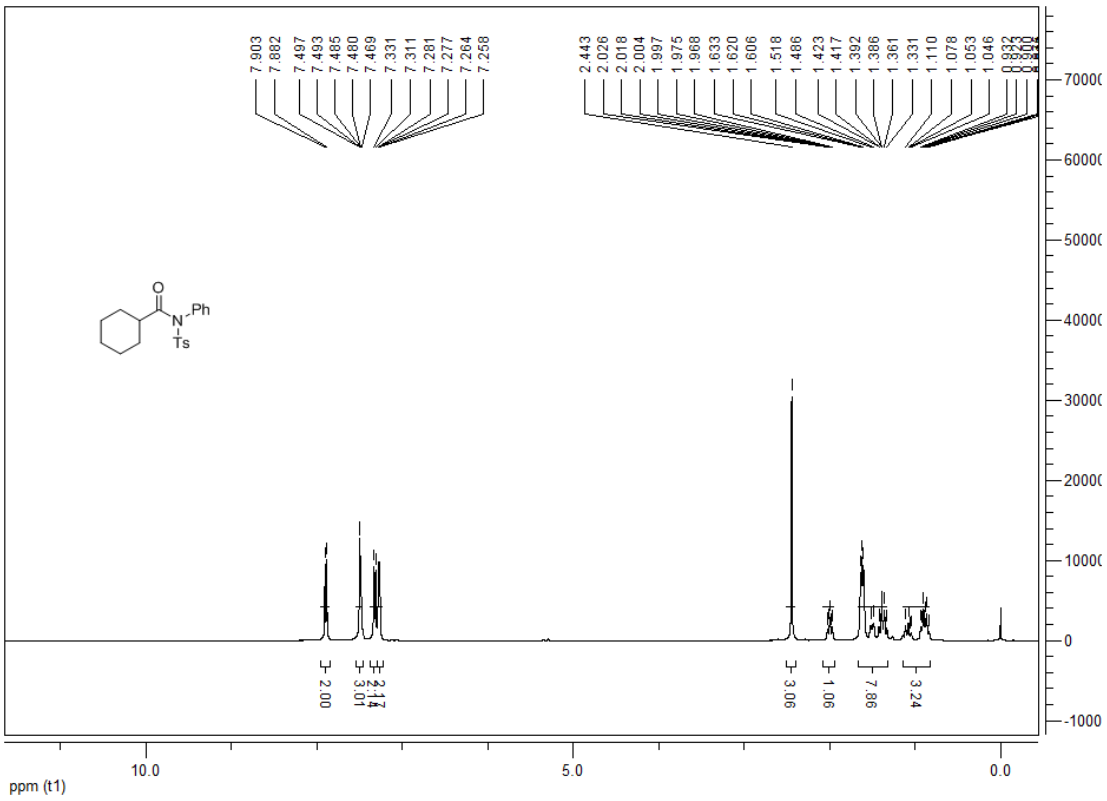


N-phenyl-N-tosylcyclohexanecarboxamide 1r

^{1}H NMR



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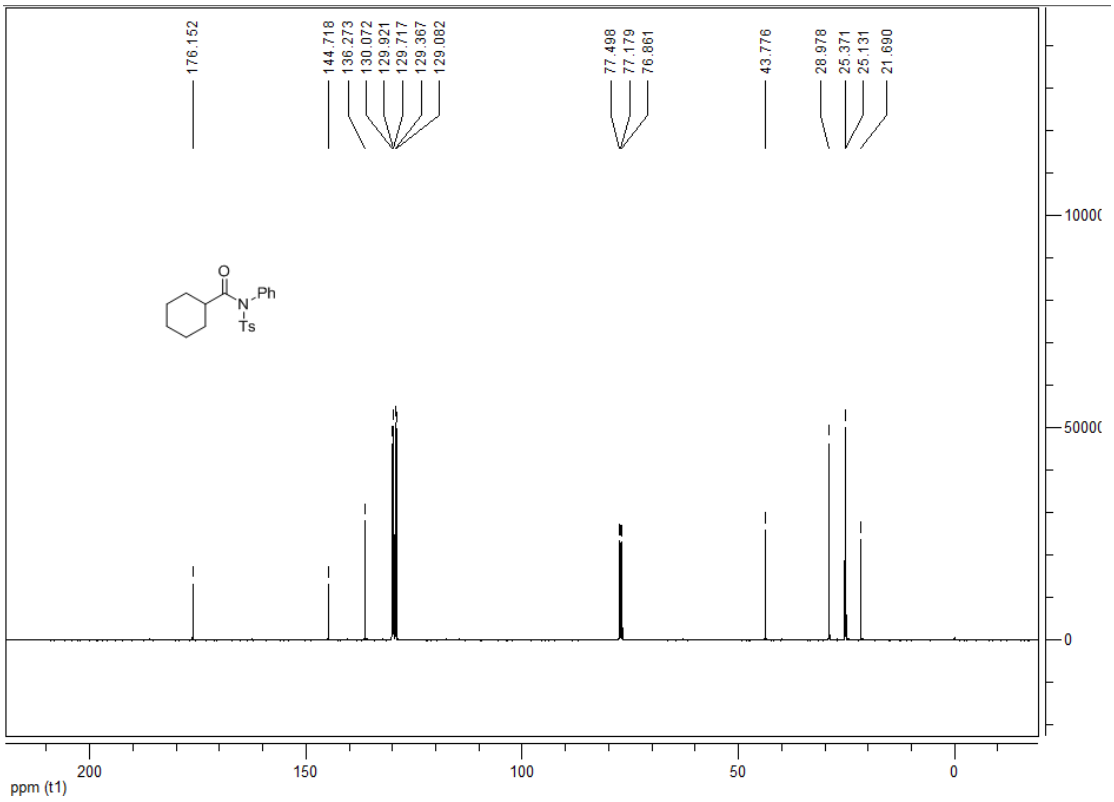
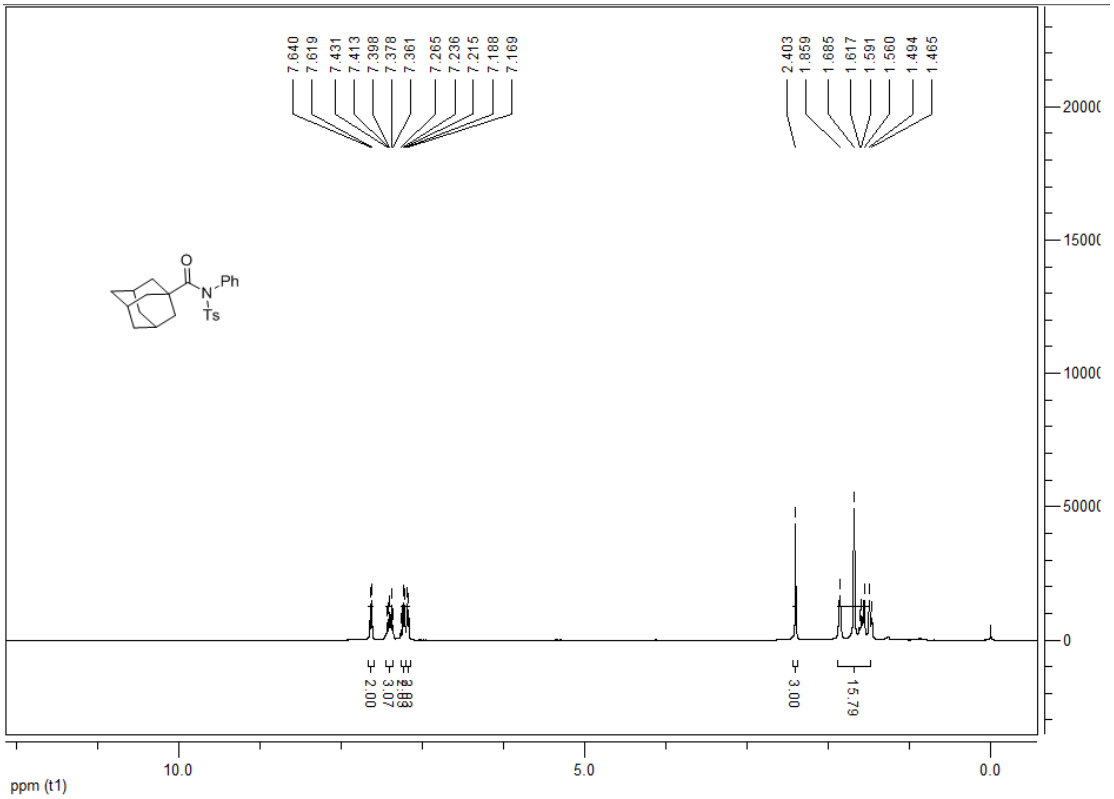
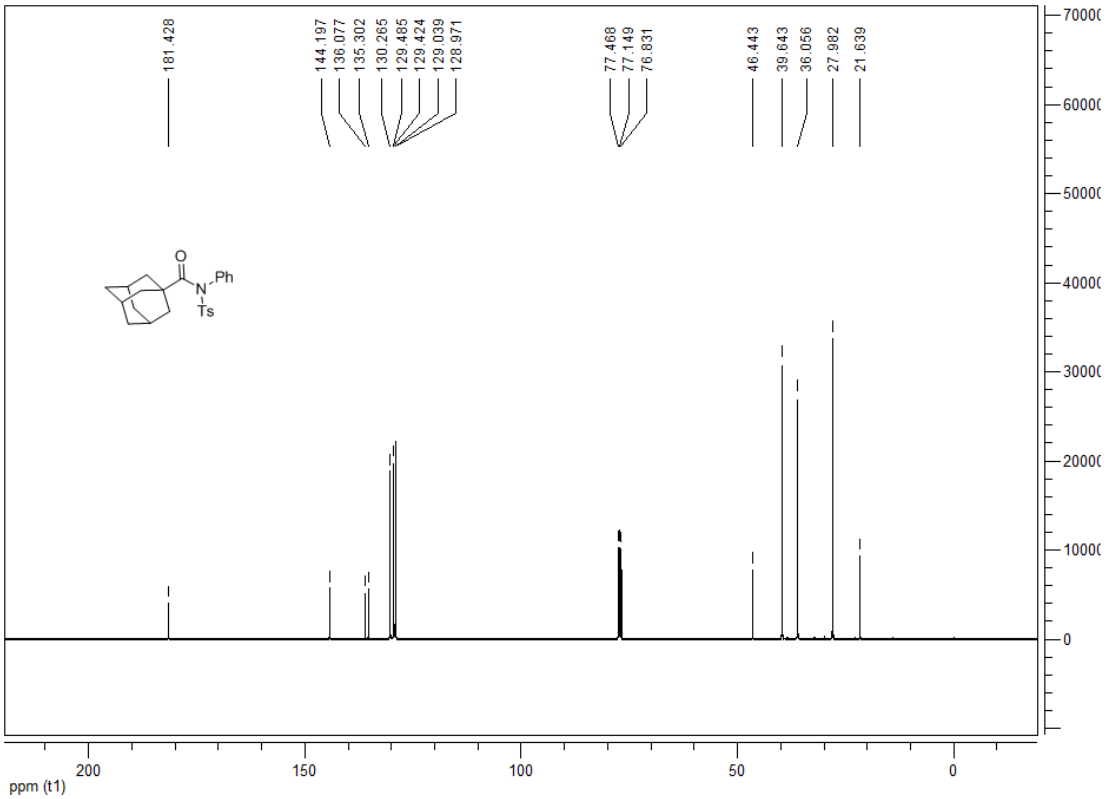


(3r,5r,7r)-N-phenyl-N-tosyladamantane-1-carboxamide 1s

^{1}H NMR

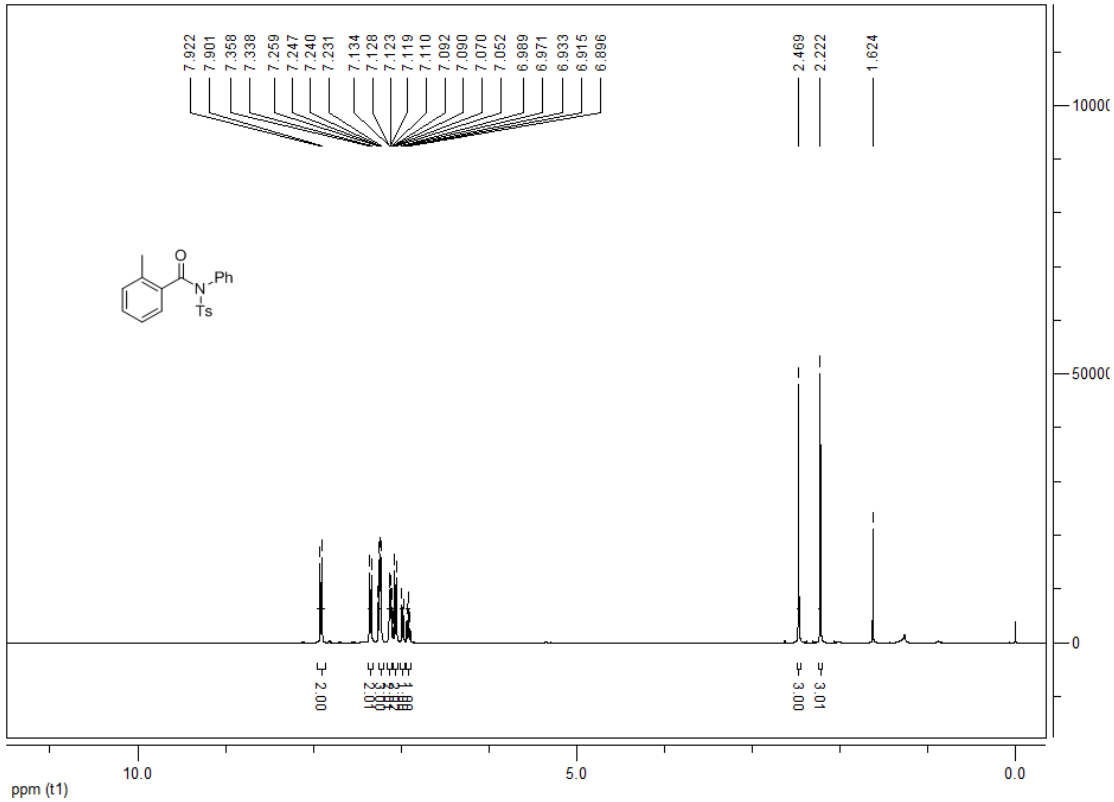


^{13}C NMR

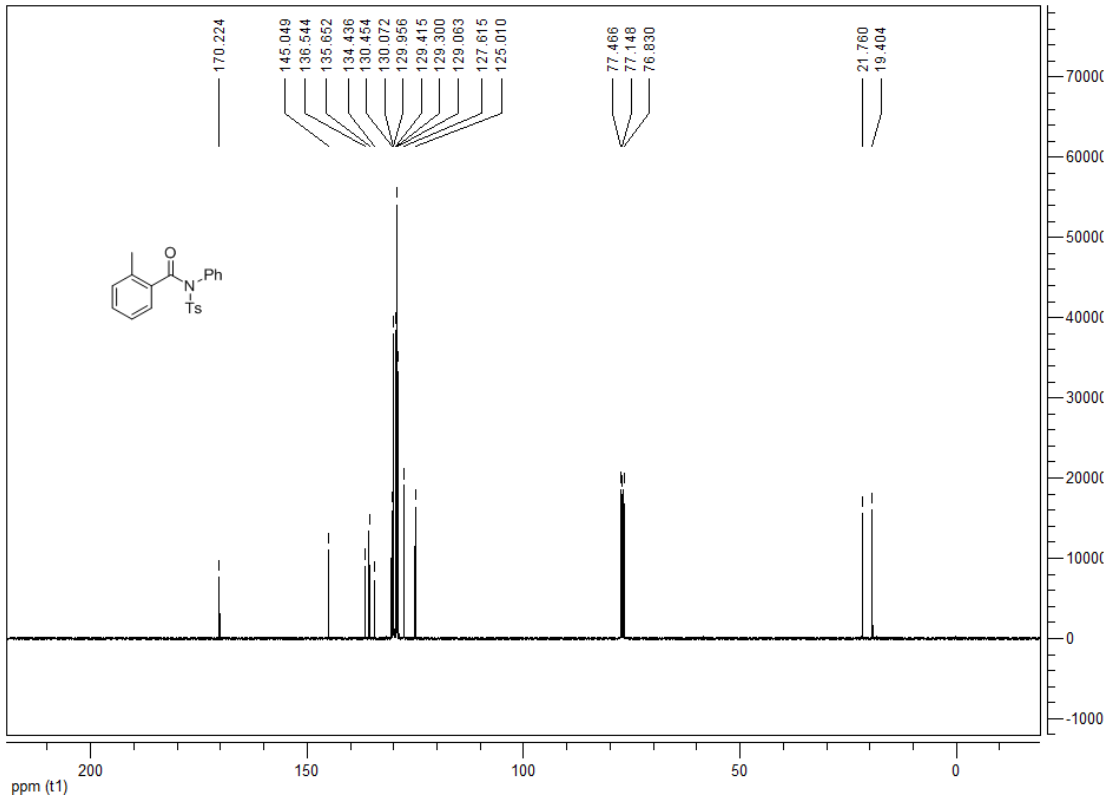


2-methyl-N-phenyl-N-tosylbenzamide 1t

^{1}H NMR



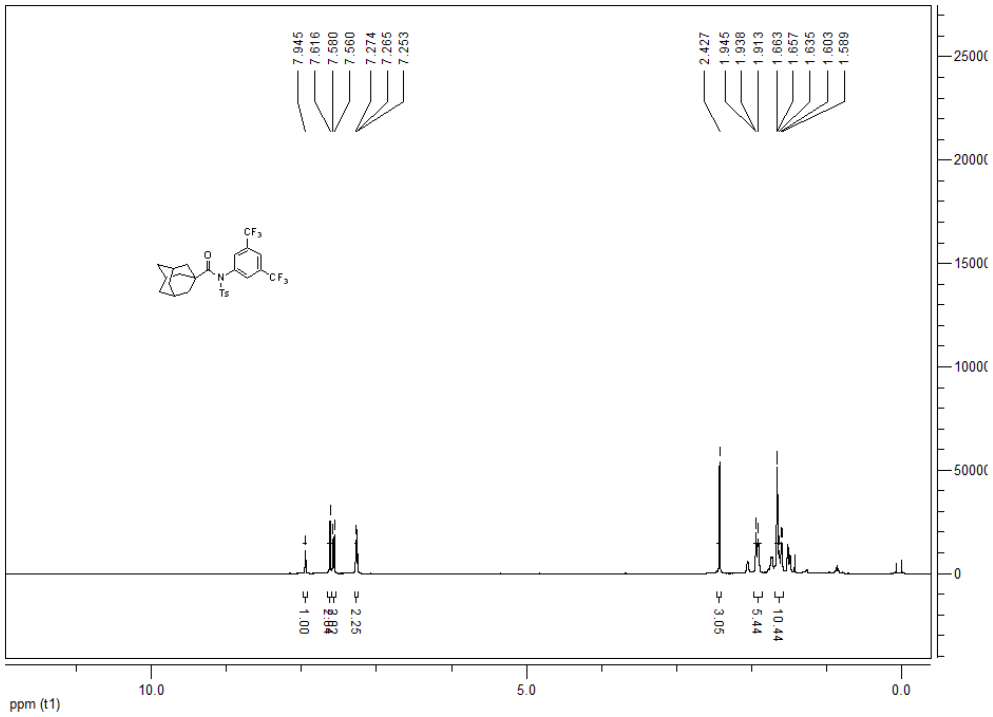
^{13}C NMR



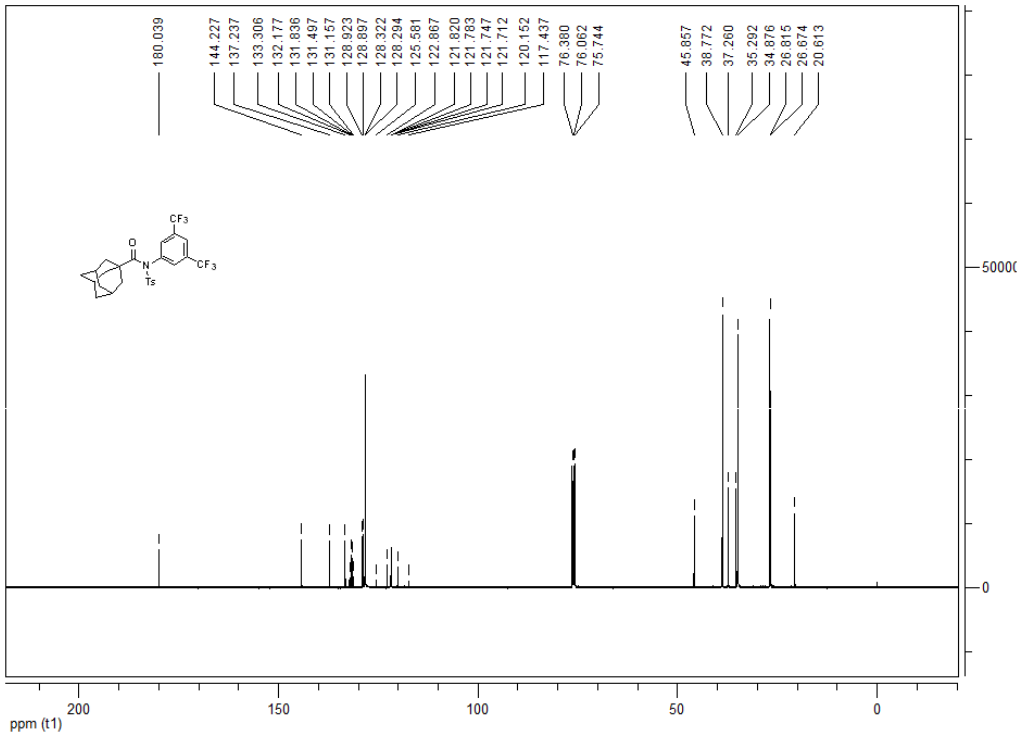
(3r,5r,7r)-N-(3,5-bis(trifluoromethyl)phenyl)-N-tosyladamantane-1-carboxamide

1u

^{1}H NMR

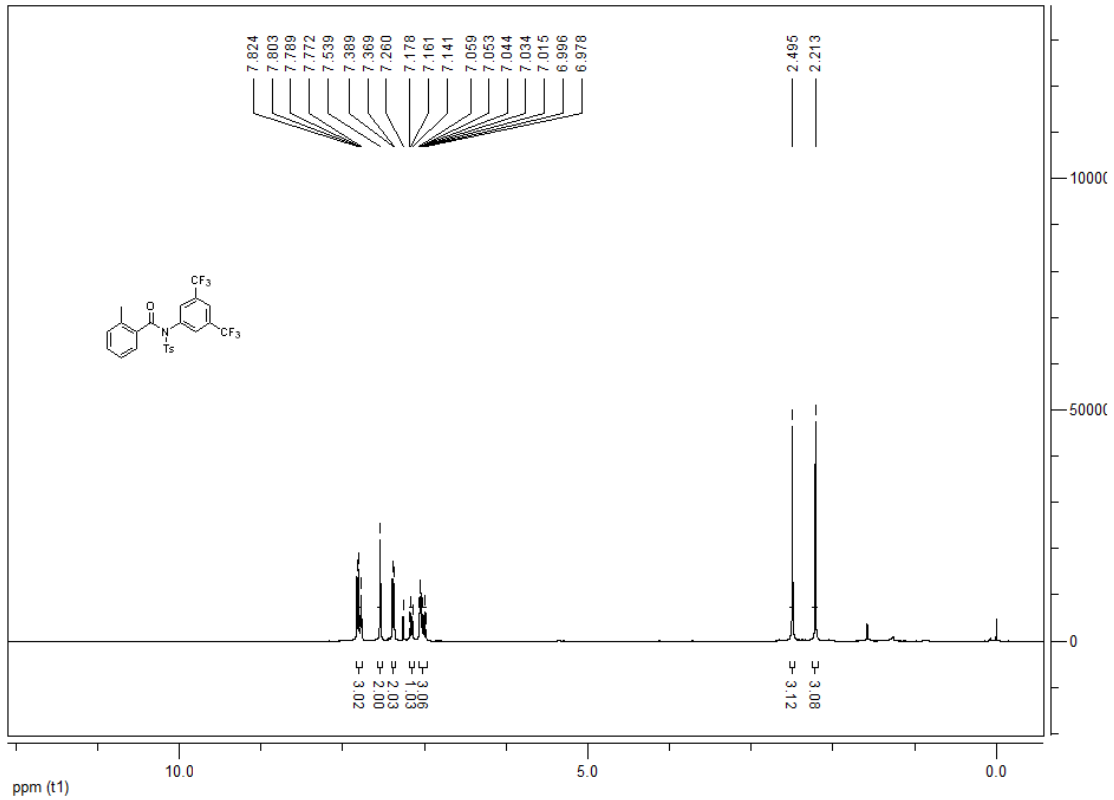


^{13}C NMR

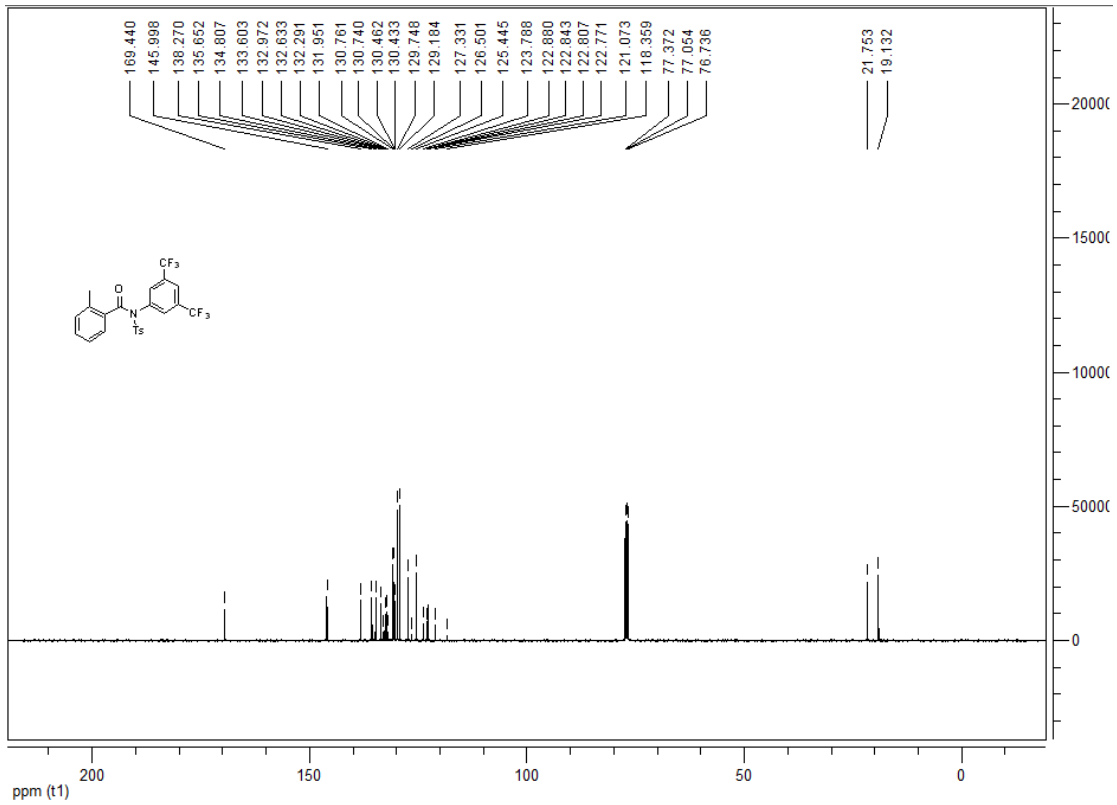


N-(3,5-bis(trifluoromethyl)phenyl)-2-methyl-N-tosylbenzamide 1v

^{1}H NMR

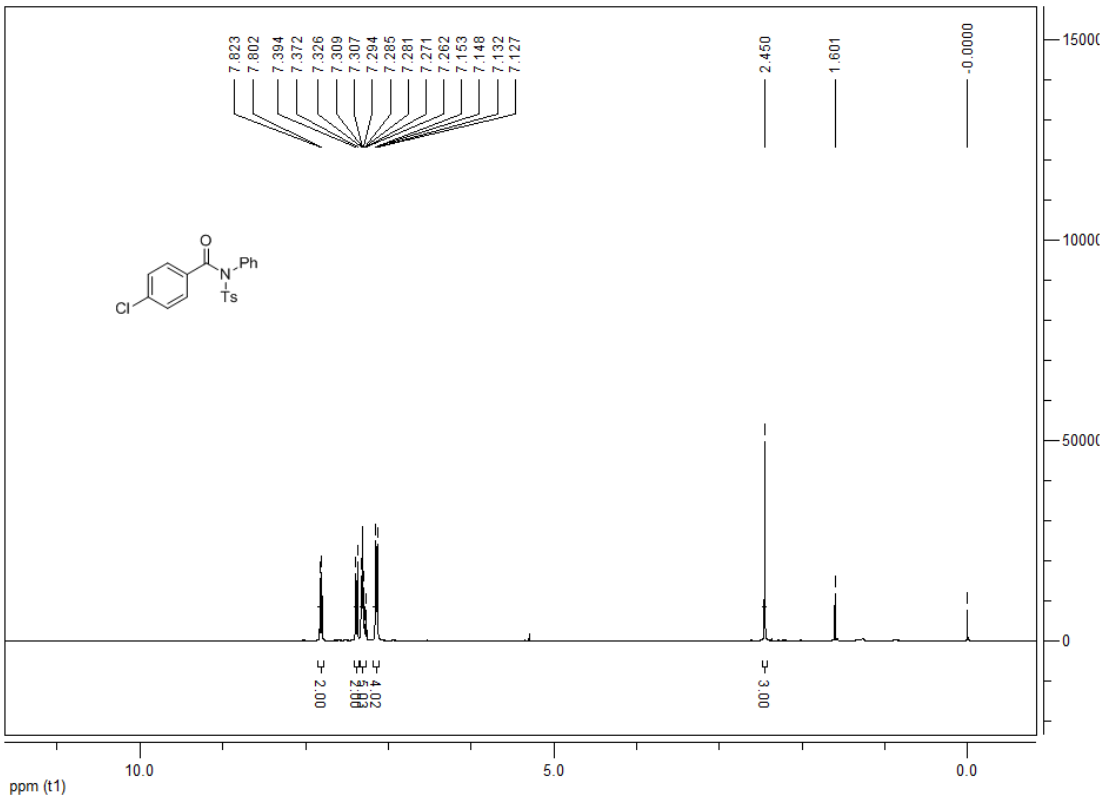


^{13}C NMR

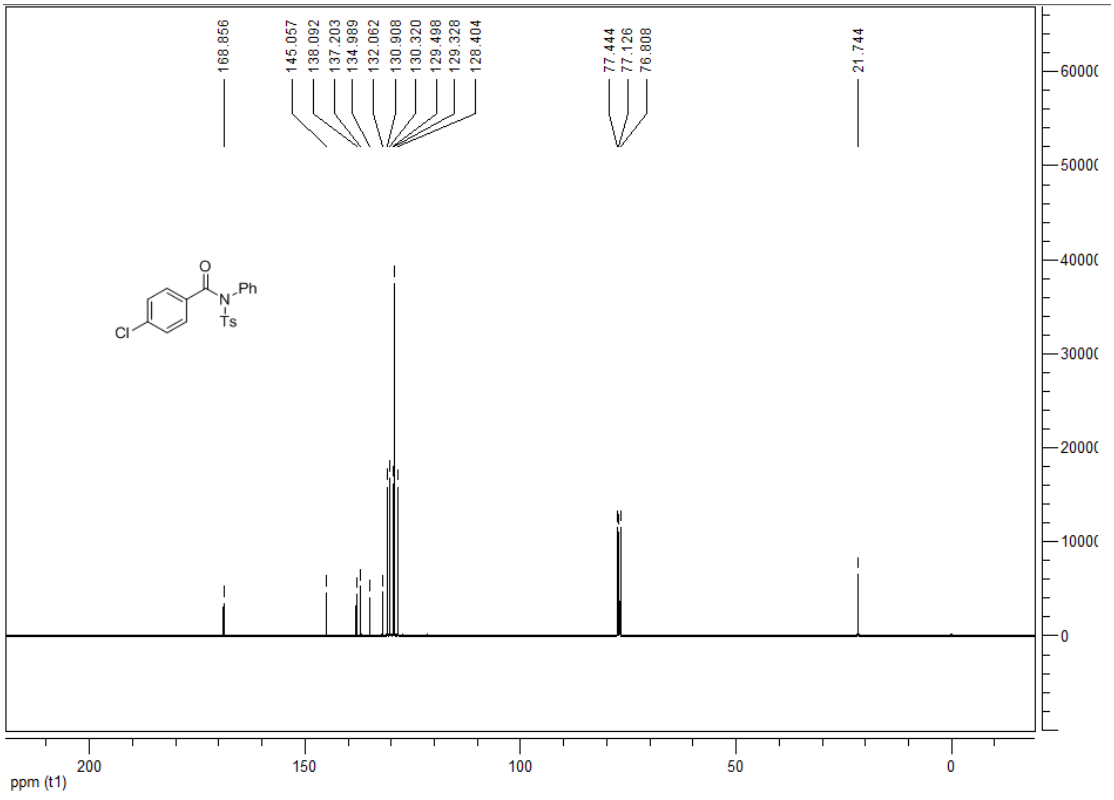


4-chloro-N-phenyl-N-tosylbenzamide 1w

^{1}H NMR

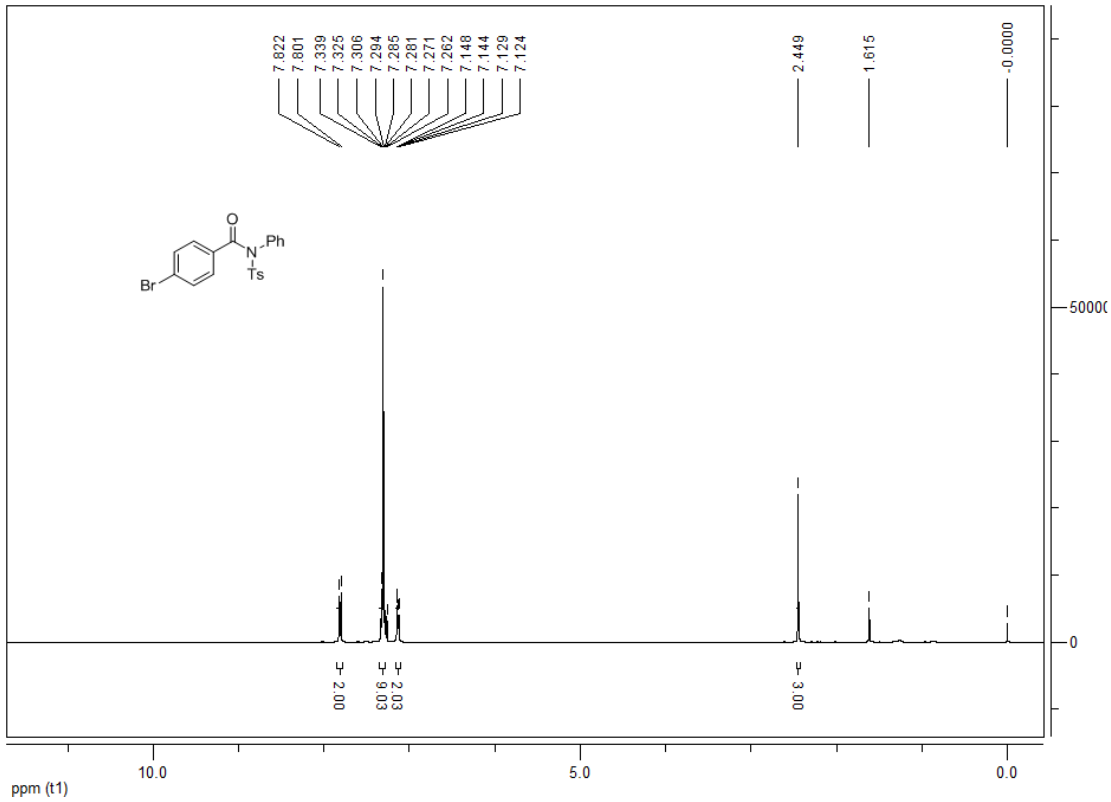


^{13}C NMR

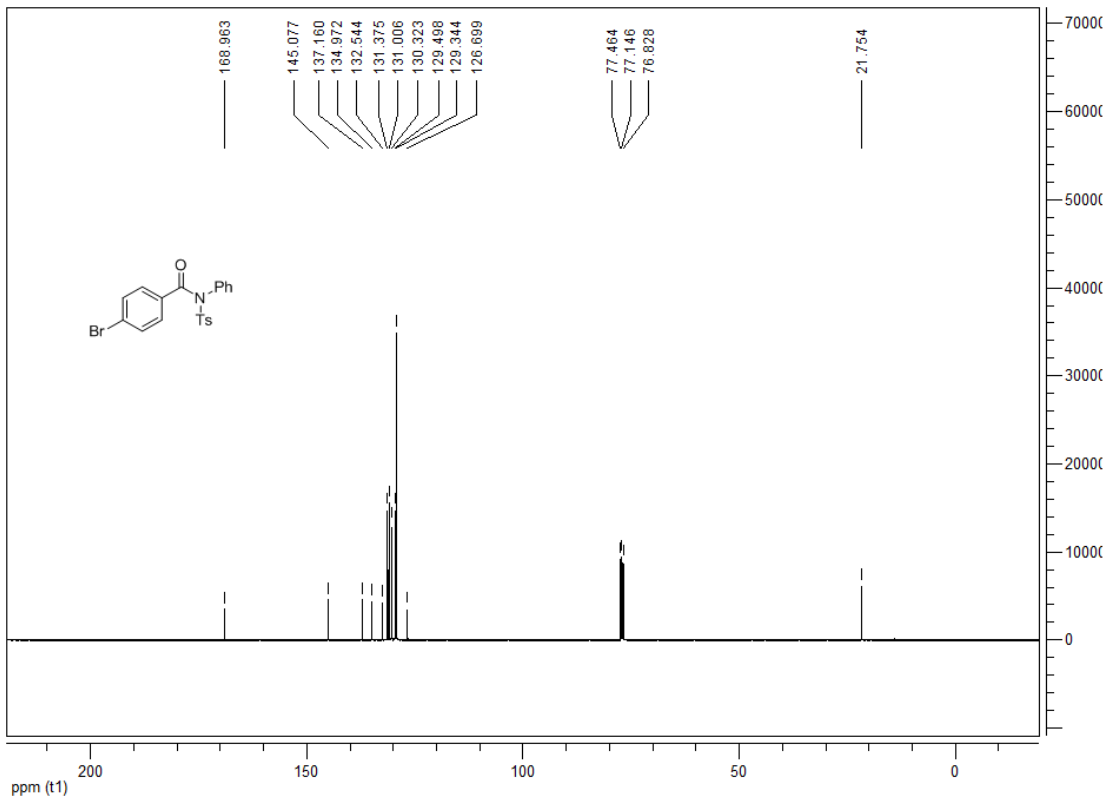


4-bromo-N-phenyl-N-tosylbenzamide 1x

^{1}H NMR

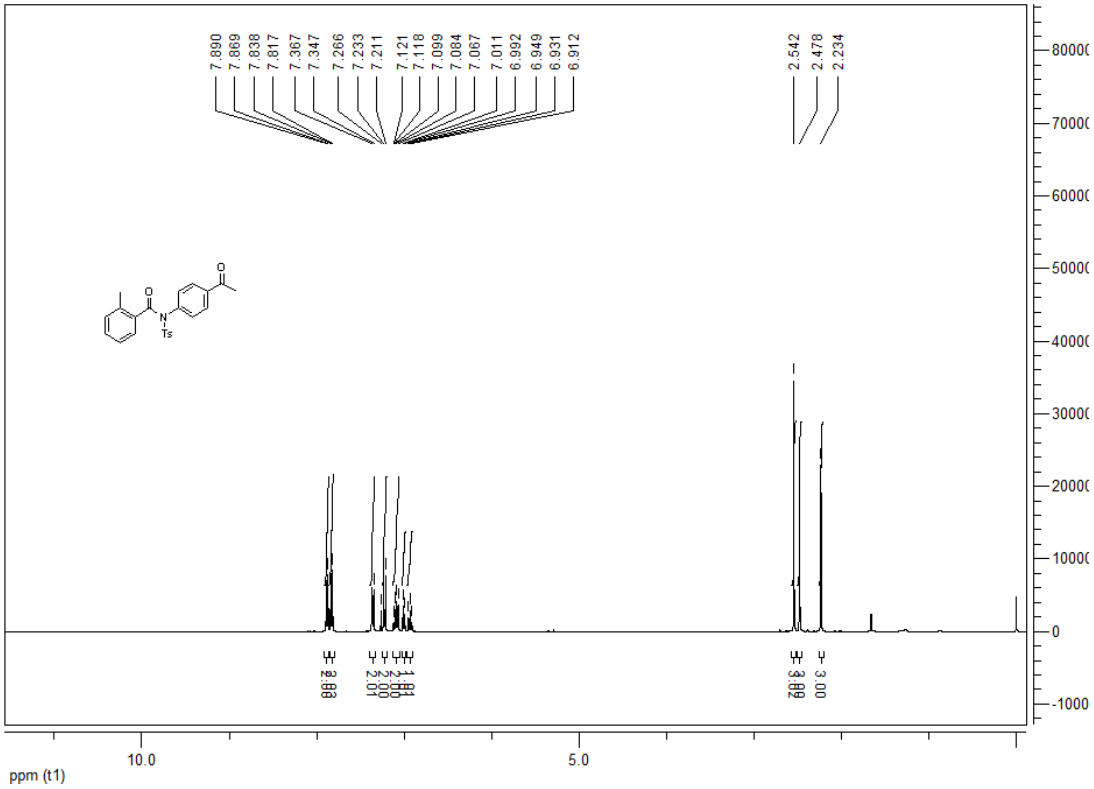


^{13}C NMR

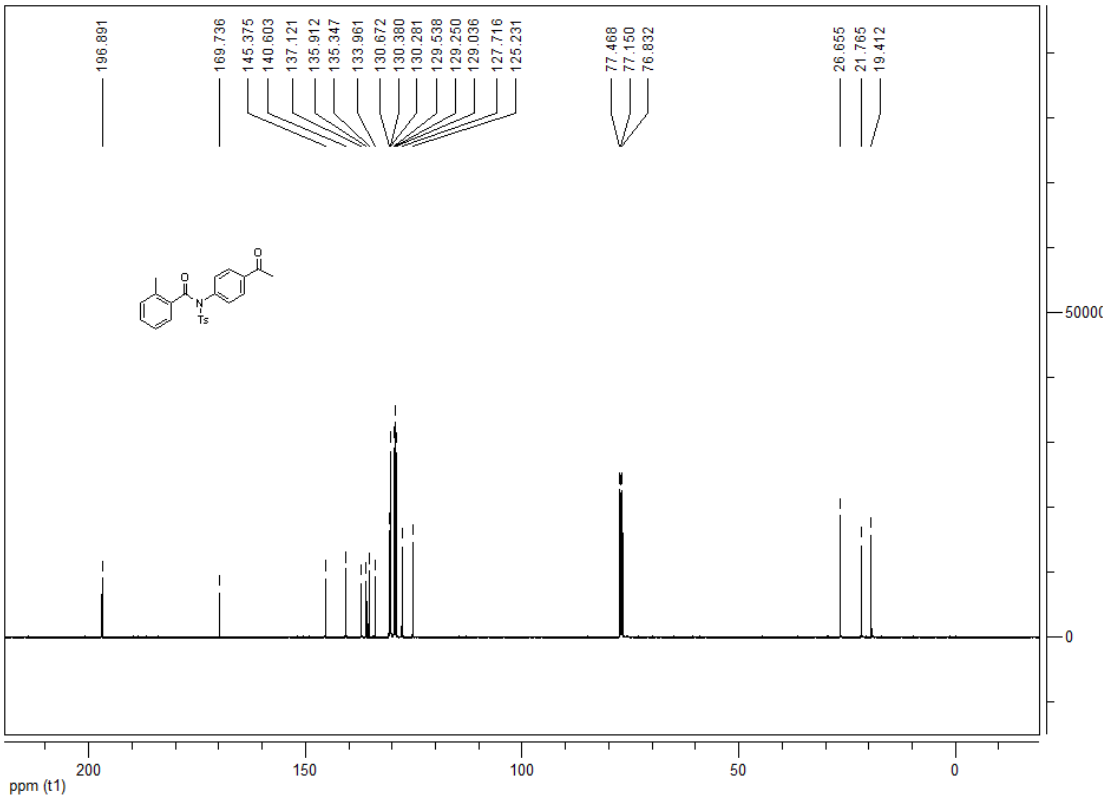


N-(4-acetylphenyl)-2-methyl-N-tosylbenzamide 1t-1

^{1}H NMR

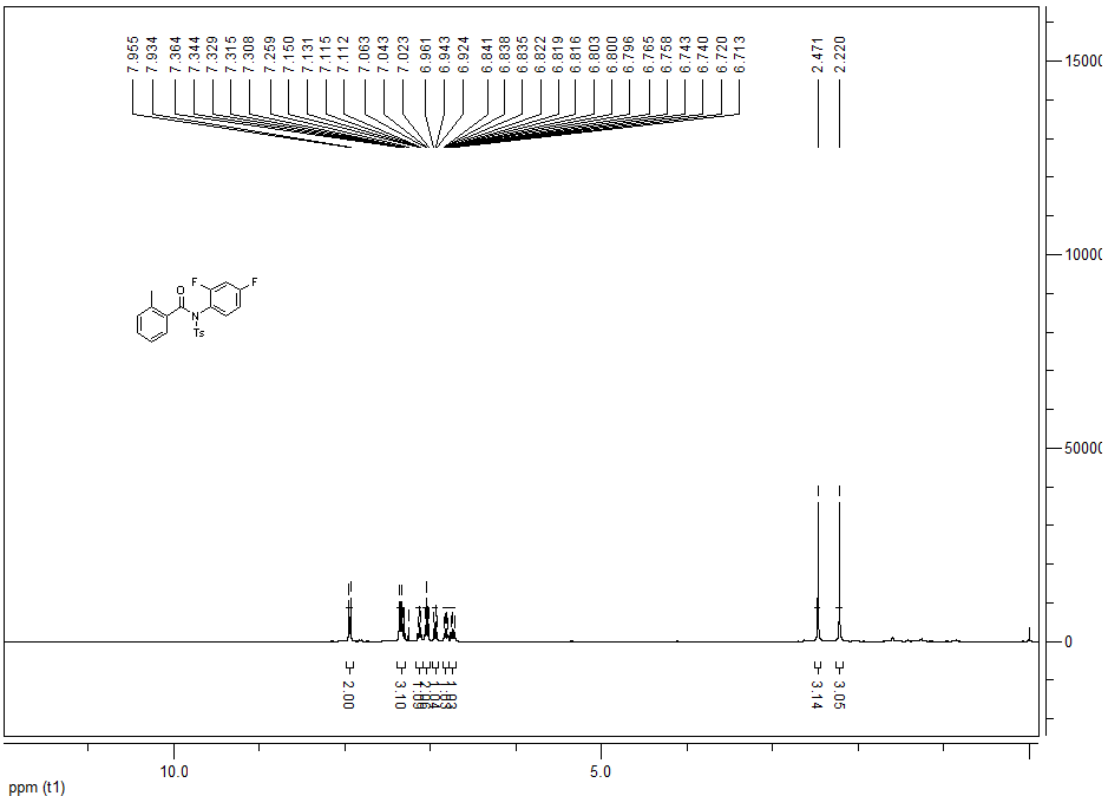


^{13}C NMR

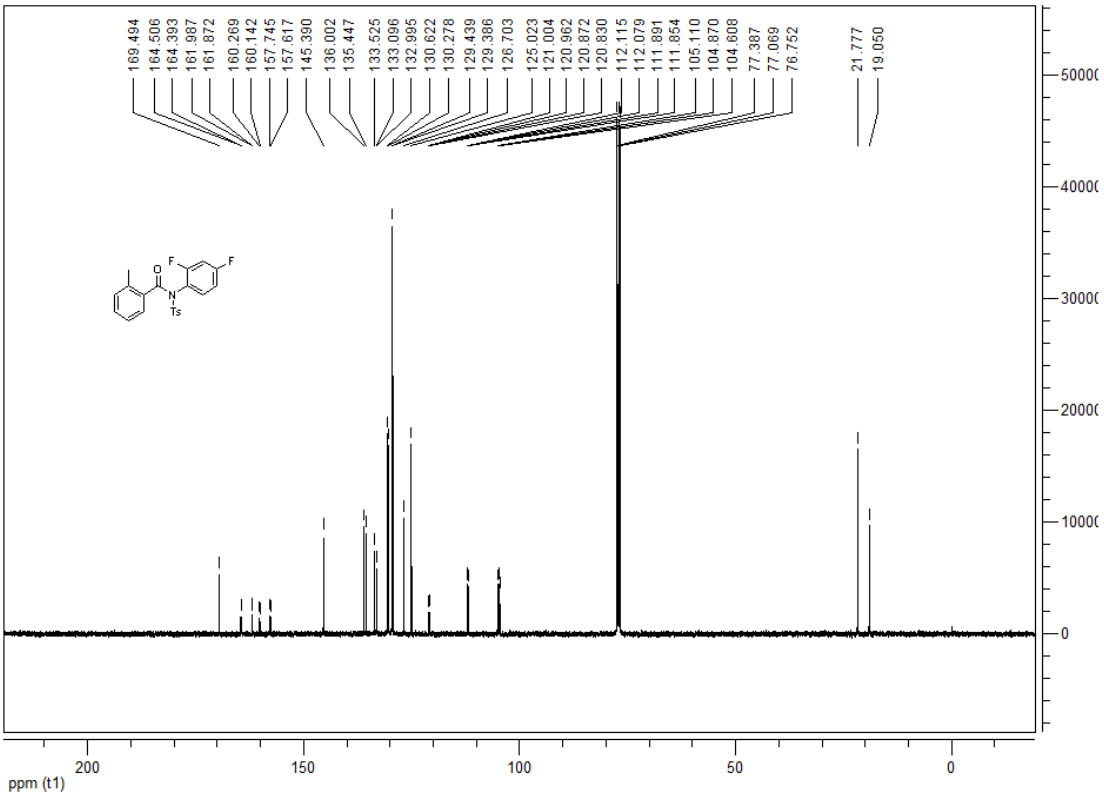


N-(2,4-difluorophenyl)-2-methyl-N-tosylbenzamide 1t-2

^{1}H NMR

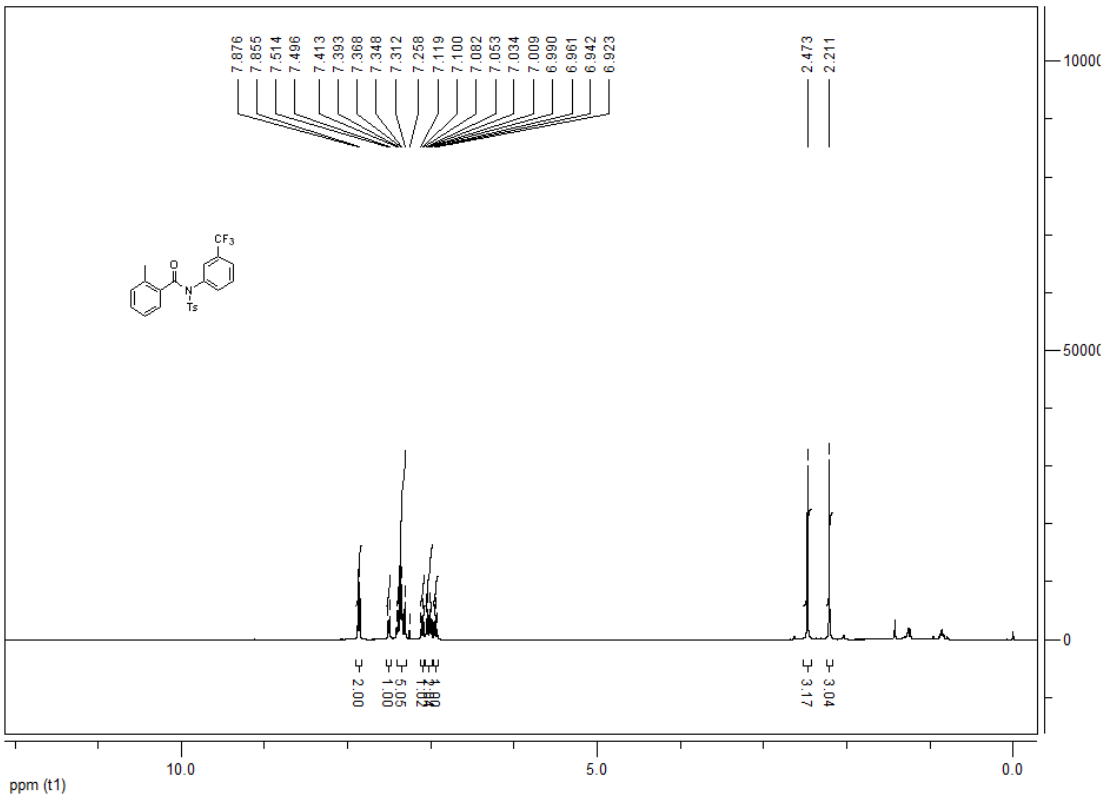


^{13}C NMR

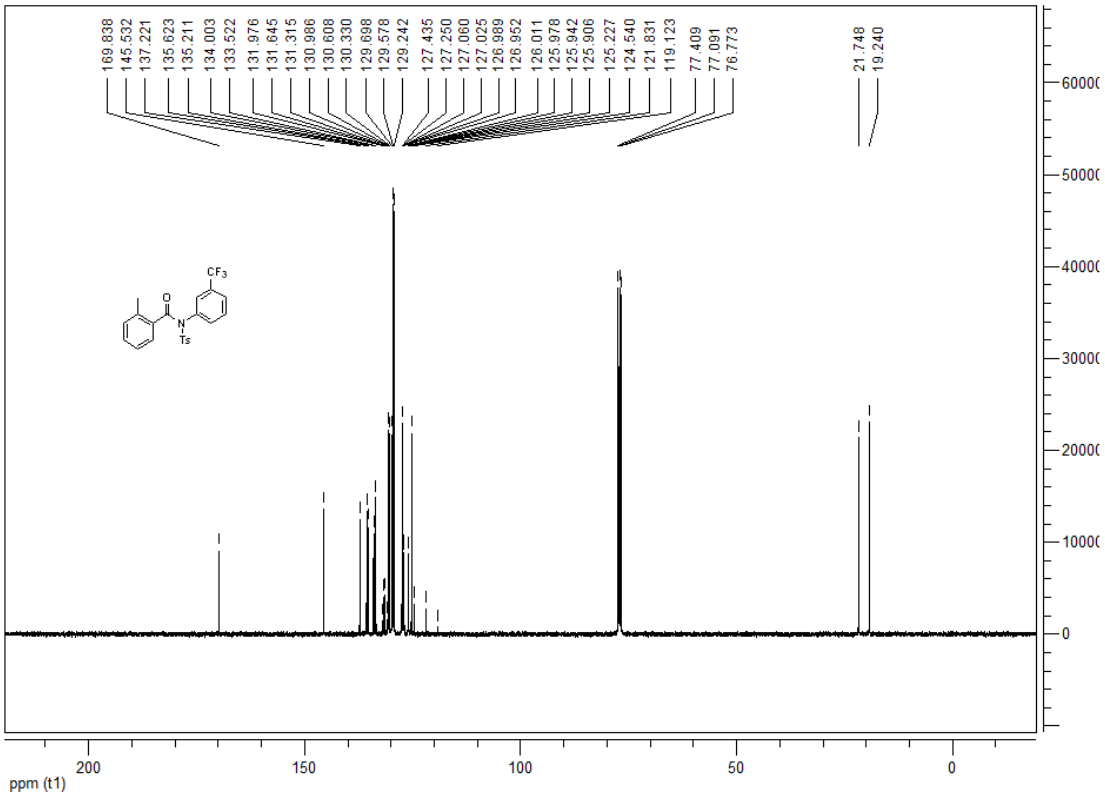


2-methyl-N-tosyl-N-(3-(trifluoromethyl)phenyl)benzamide 1t-3

^{1}H NMR

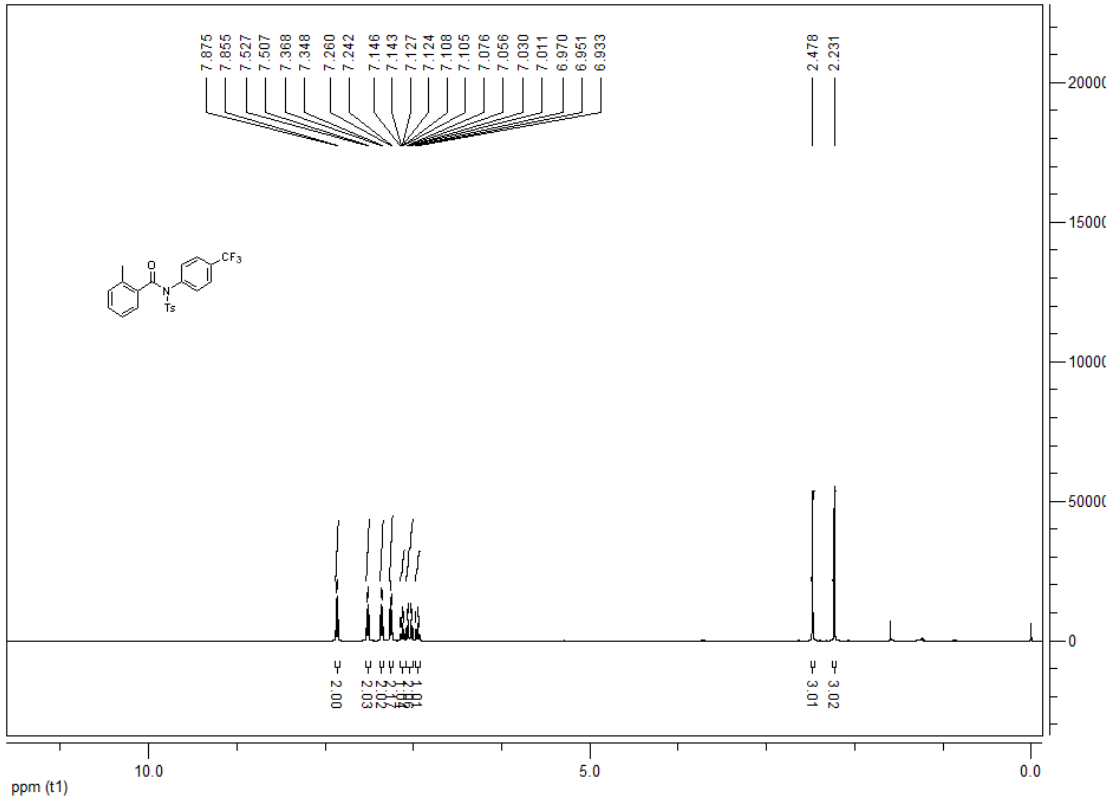


^{13}C NMR

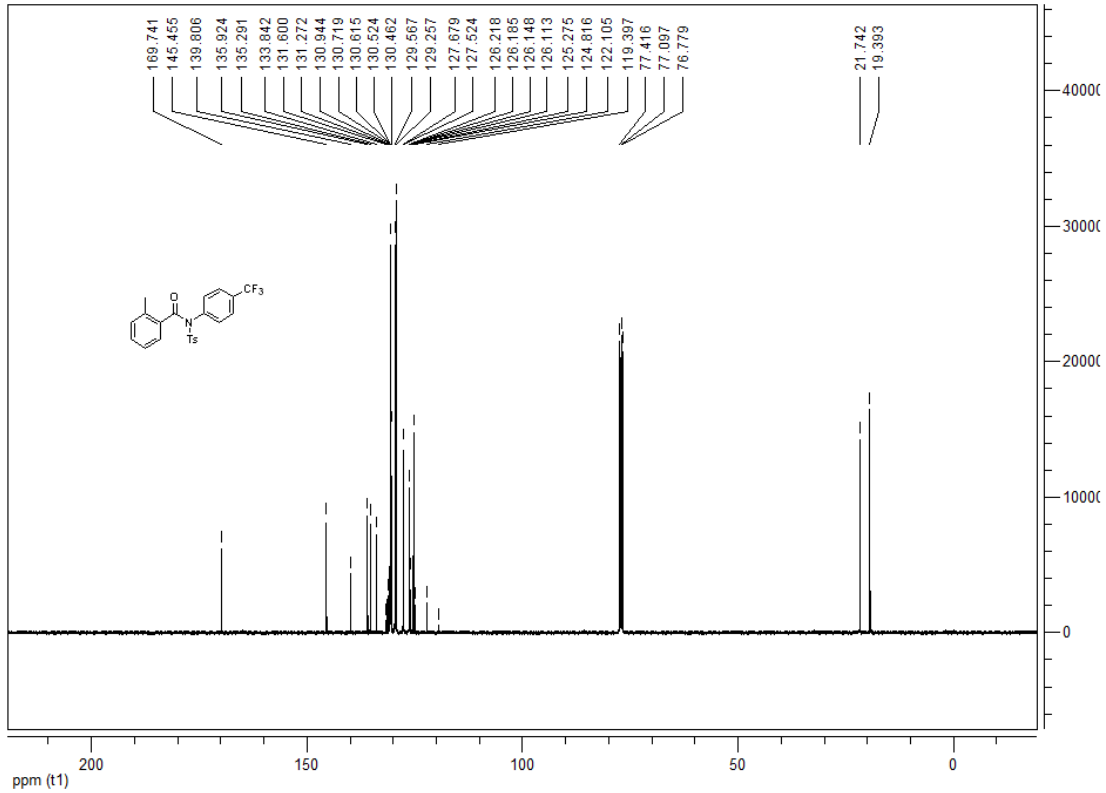


2-methyl-N-tosyl-N-(4-(trifluoromethyl)phenyl)benzamide 1t-4

^{1}H NMR

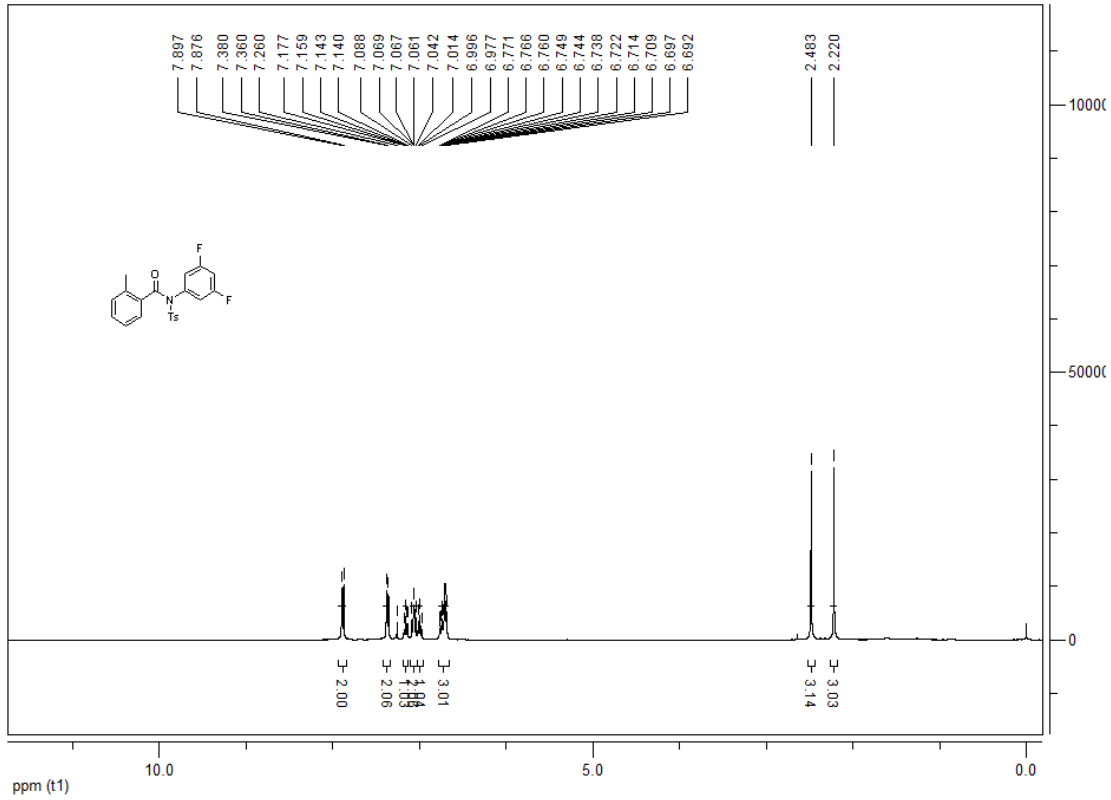


^{13}C NMR

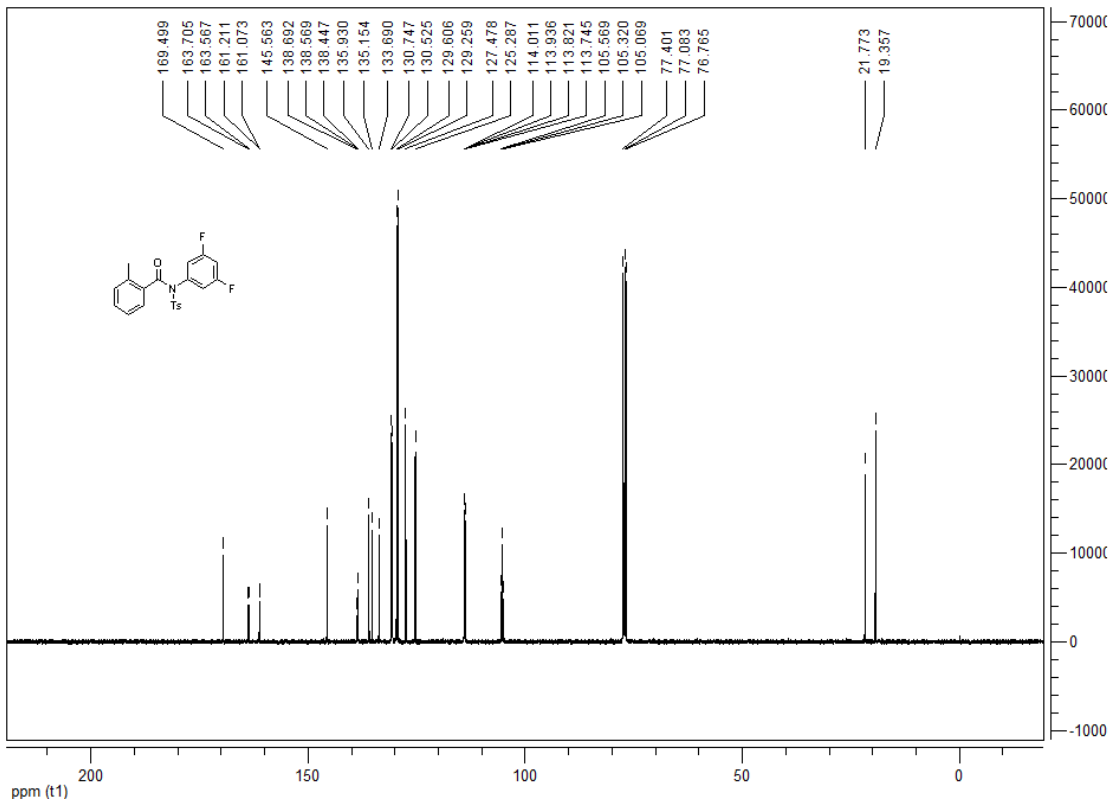


N-(3,5-difluorophenyl)-2-methyl-N-tosylbenzamide 1t-5

^{1}H NMR

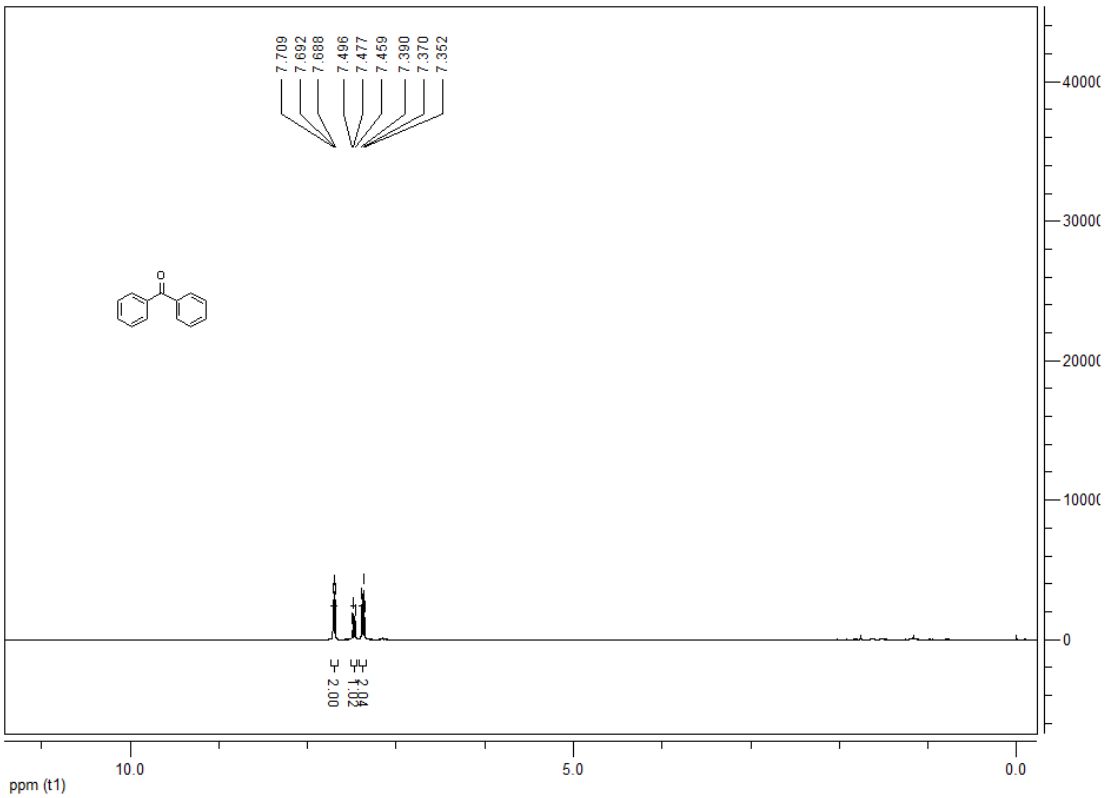


^{13}C NMR

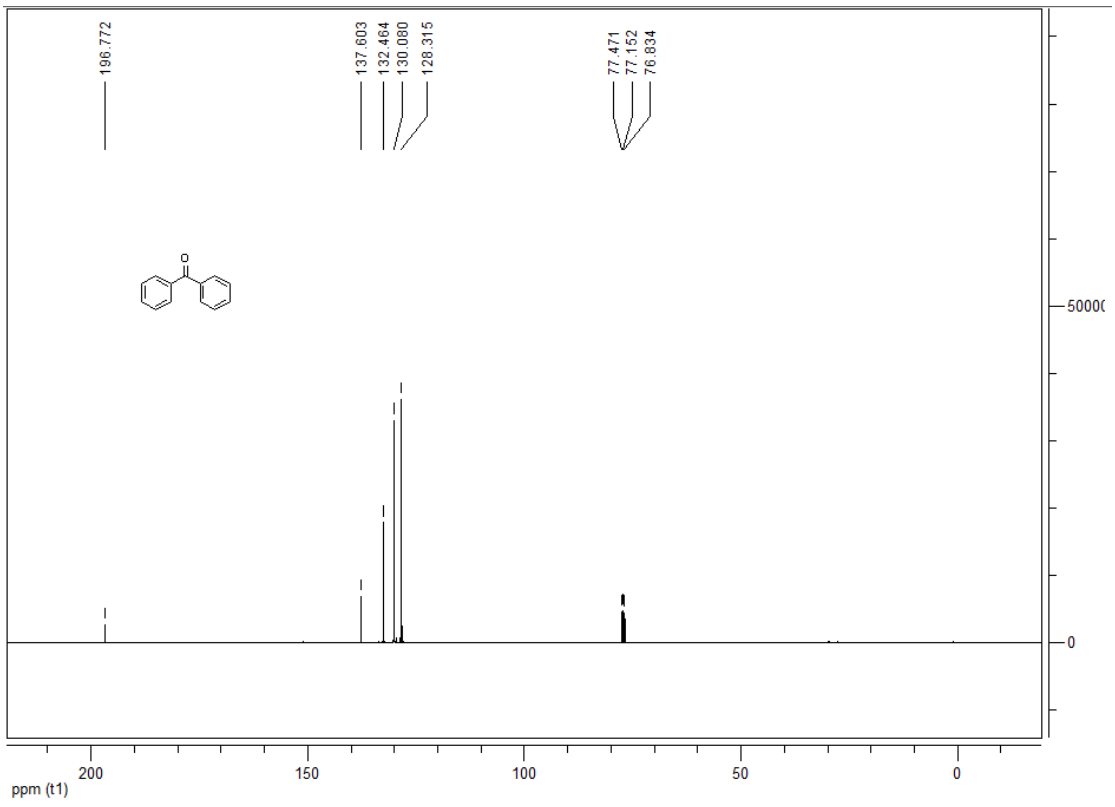


benzophenone 3aa

^{1}H NMR

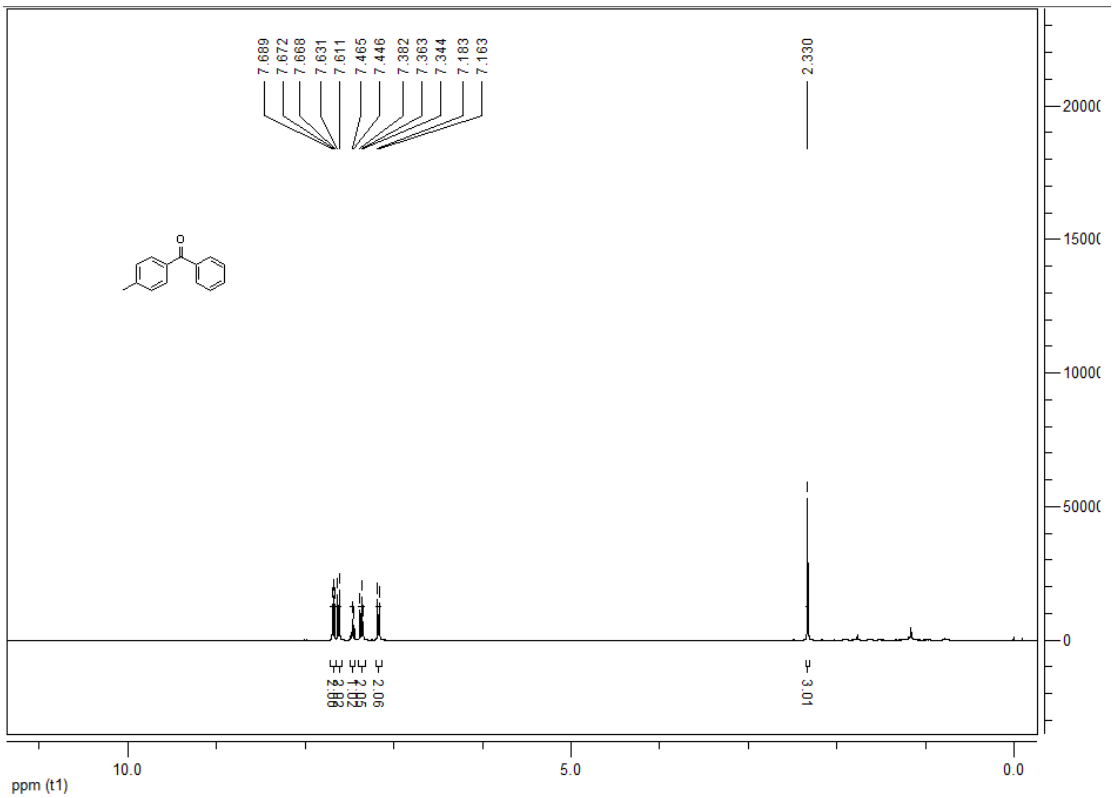


^{13}C NMR

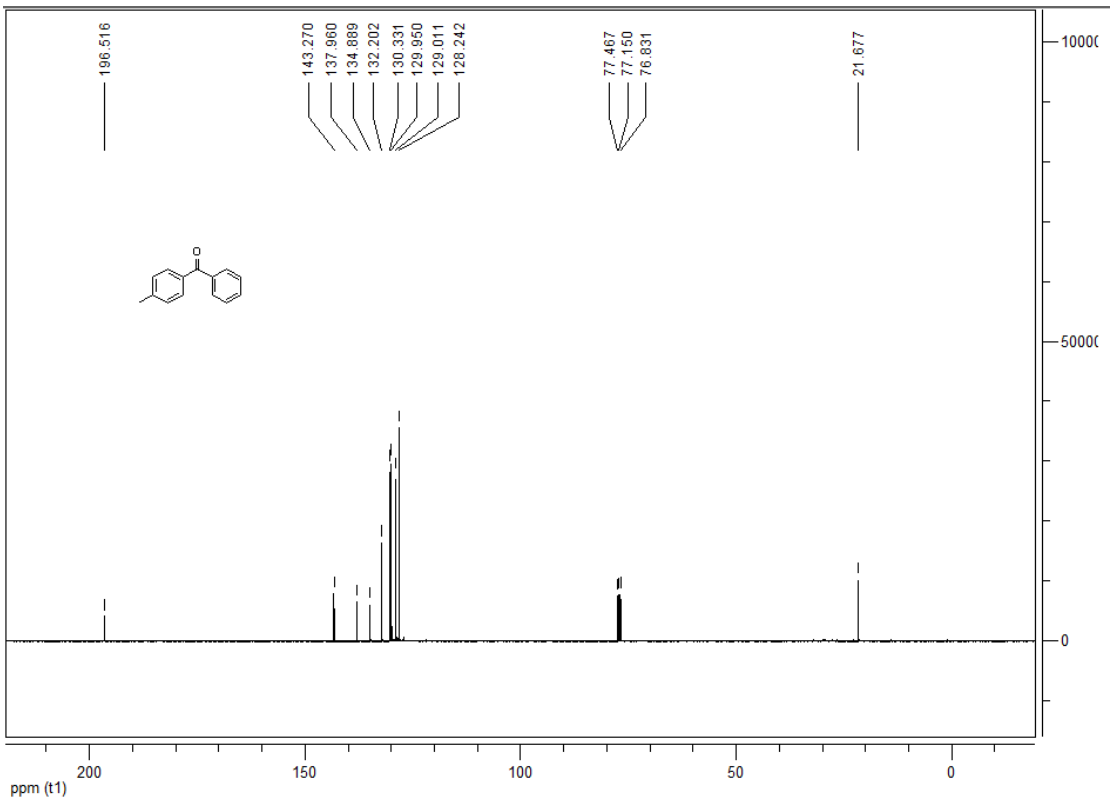


phenyl(p-tolyl)methanone 3db

^{1}H NMR

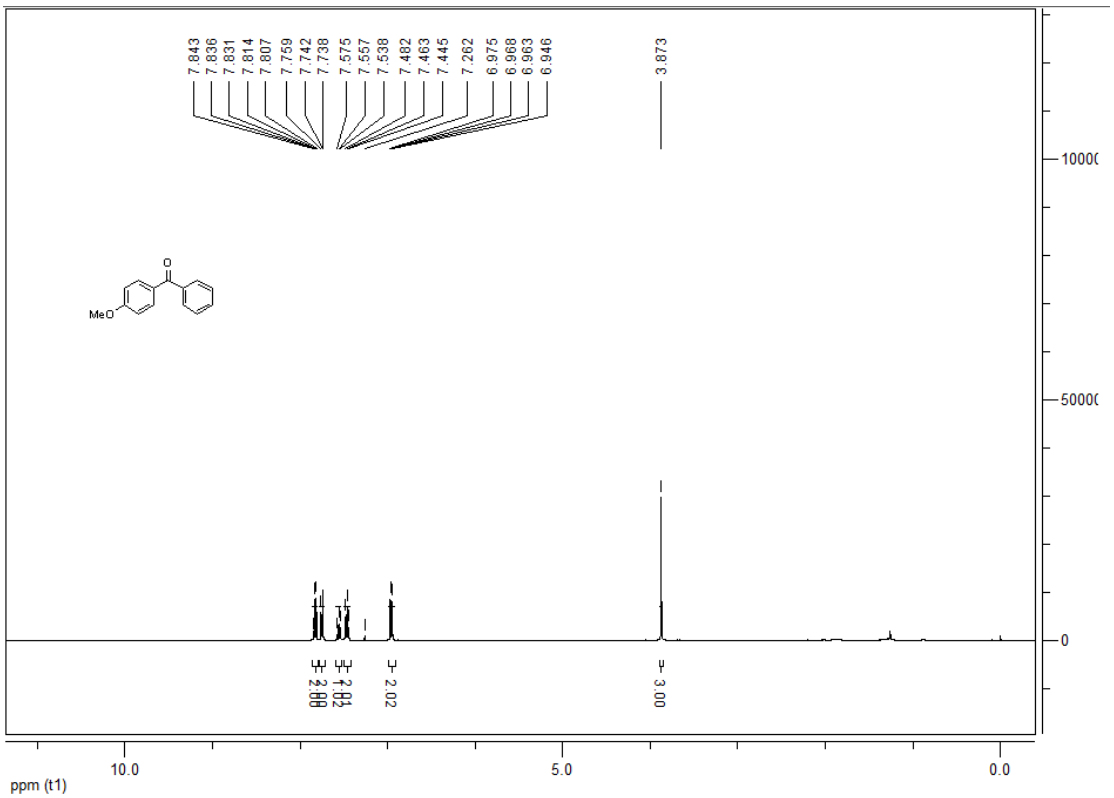


^{13}C NMR

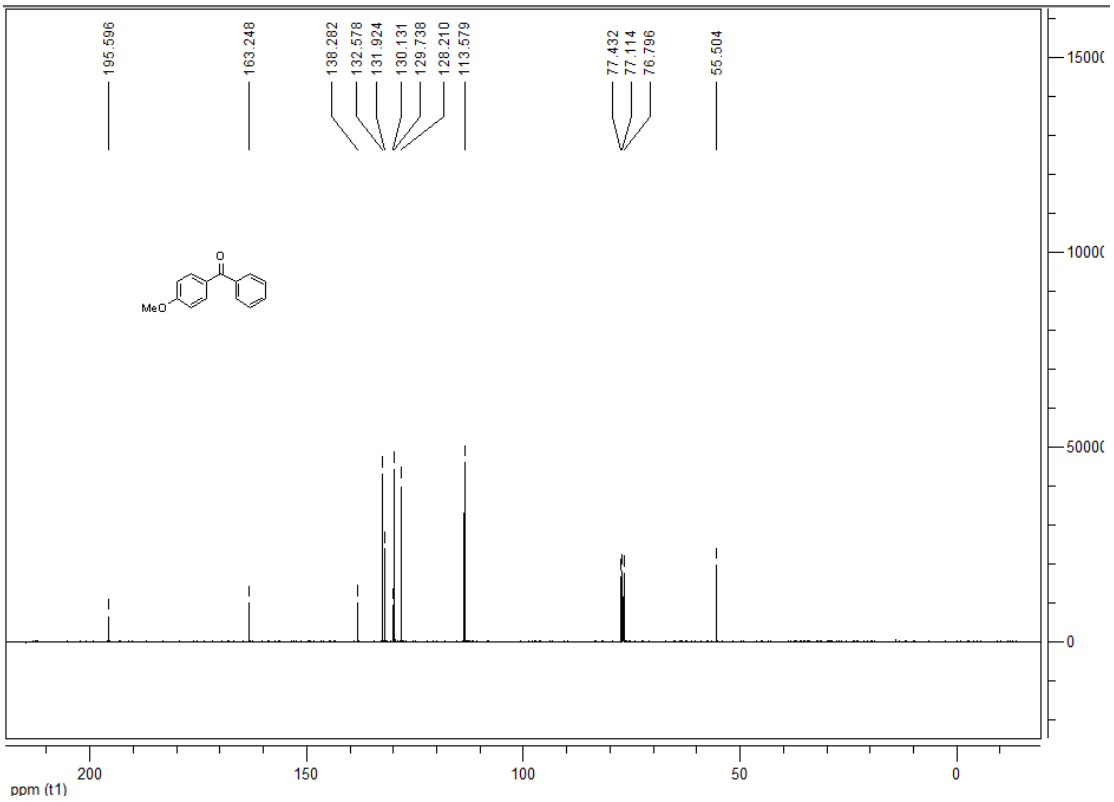


(4-methoxyphenyl)(phenyl)methanone 3dc

^{1}H NMR

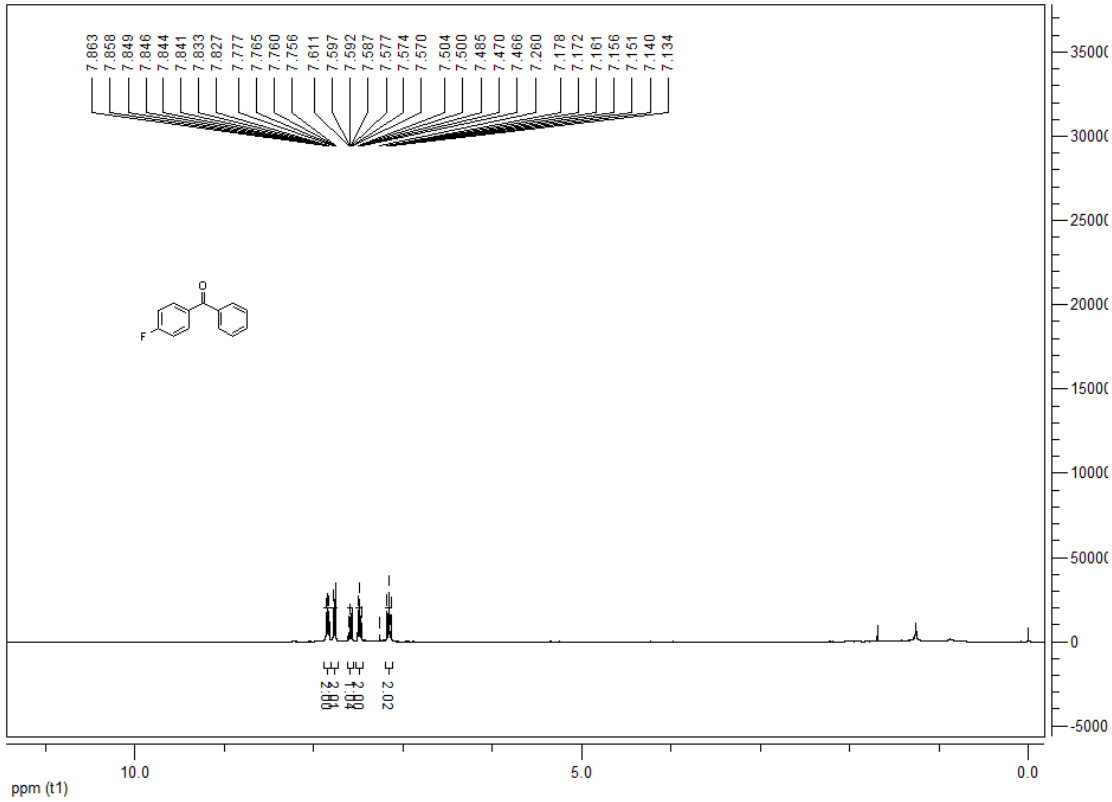


^{13}C NMR

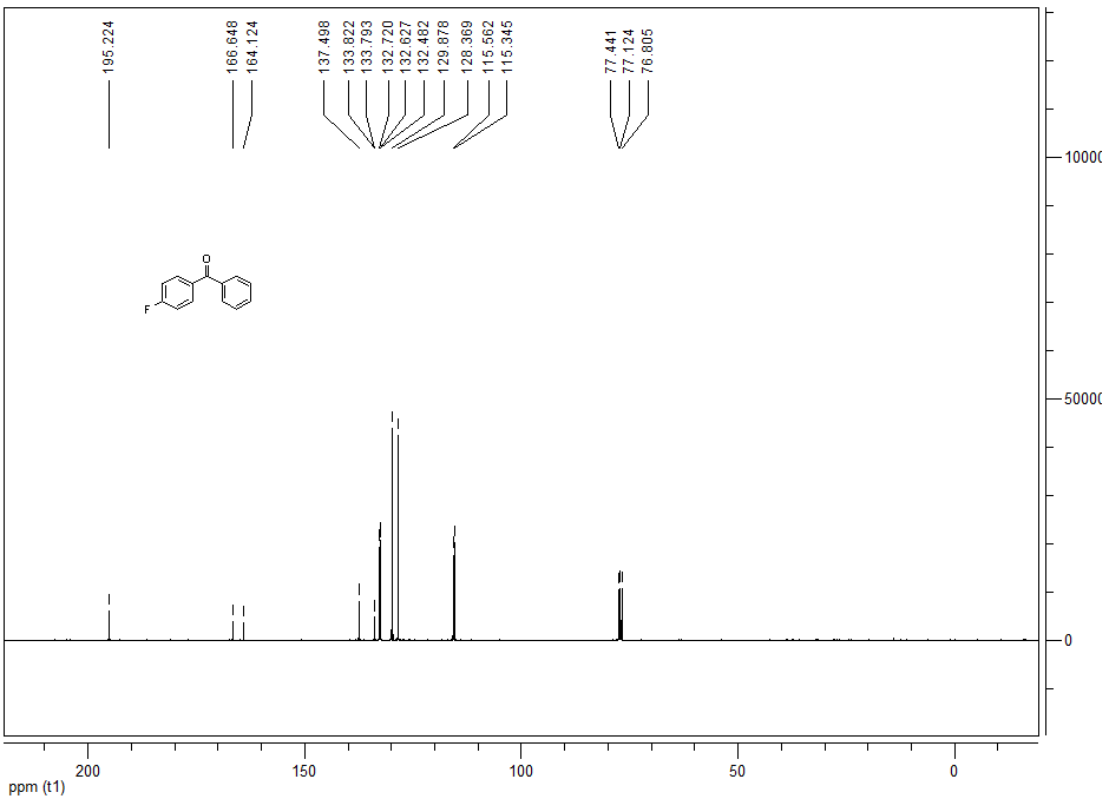


(4-fluorophenyl)(phenyl)methanone 3dd

^{1}H NMR

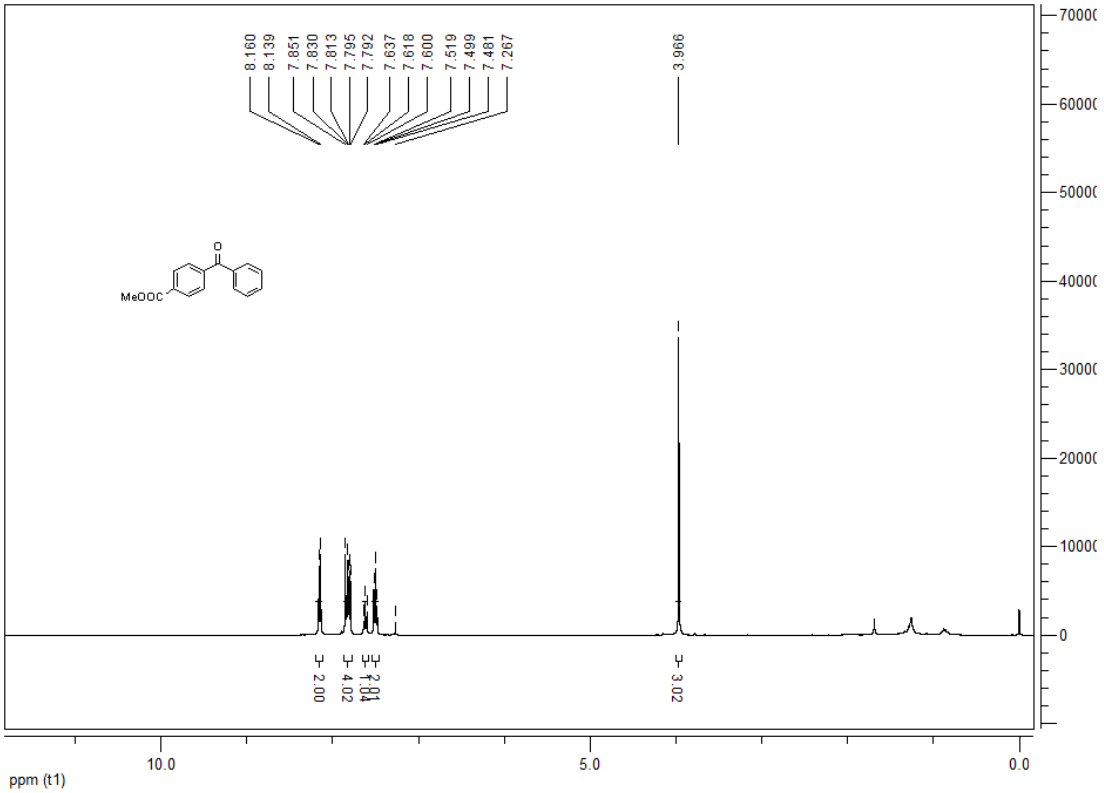


^{13}C NMR

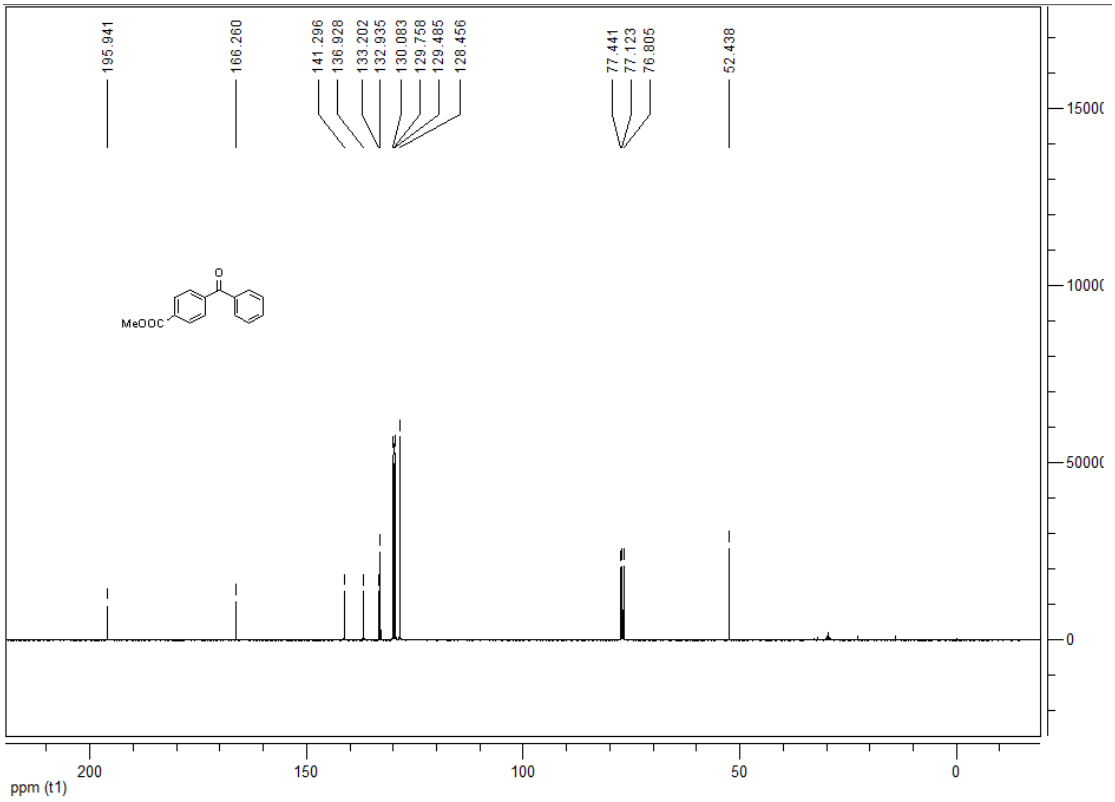


methyl 4-benzoylbenzoate 3de

^{1}H NMR

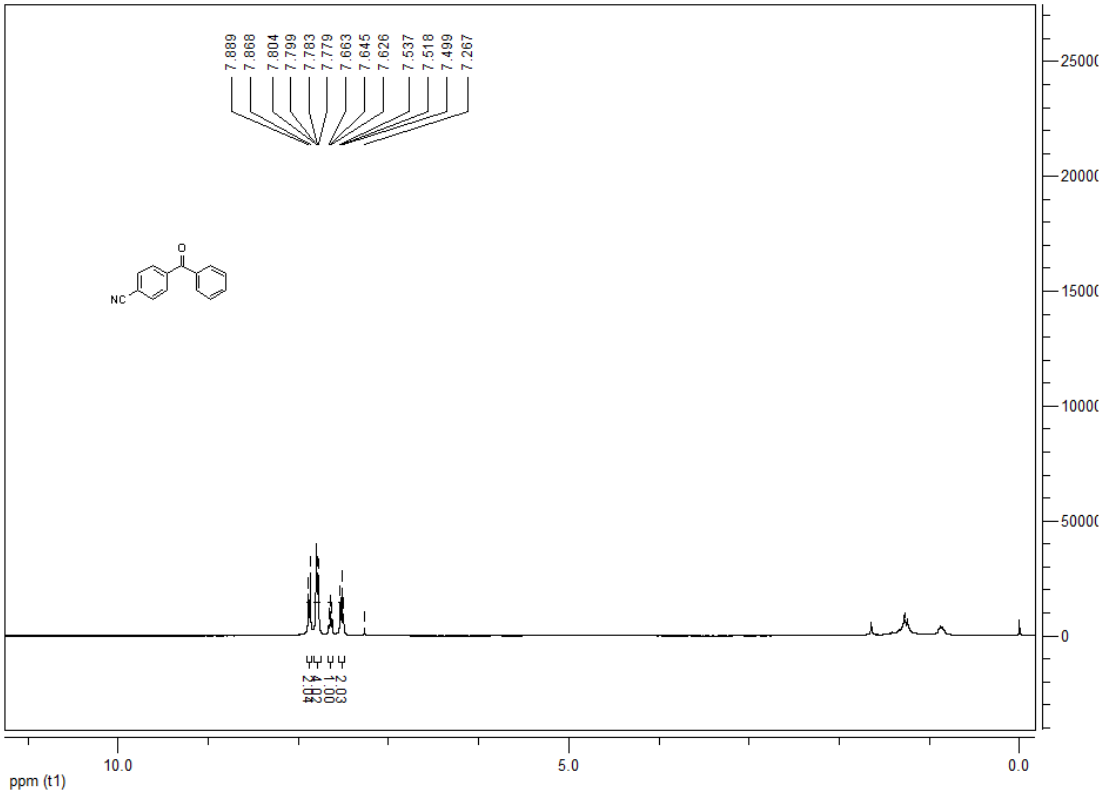


^{13}C NMR

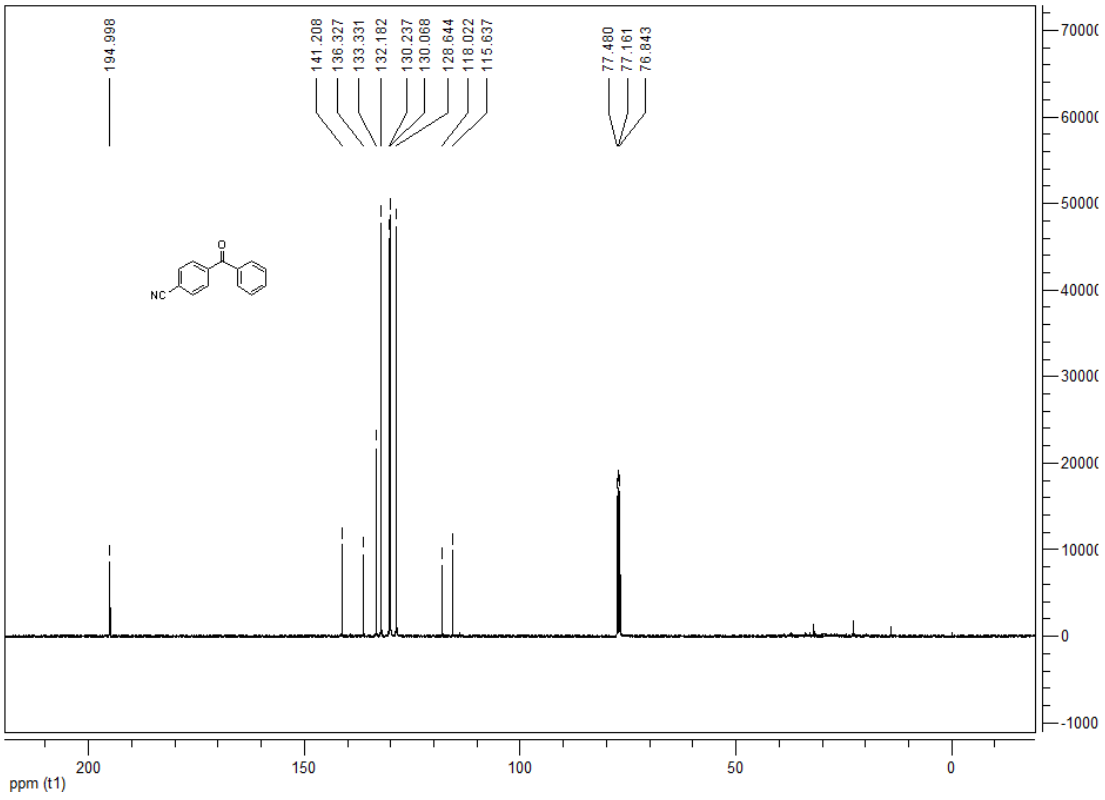


4-benzoylbenzonitrile 3df

^{1}H NMR

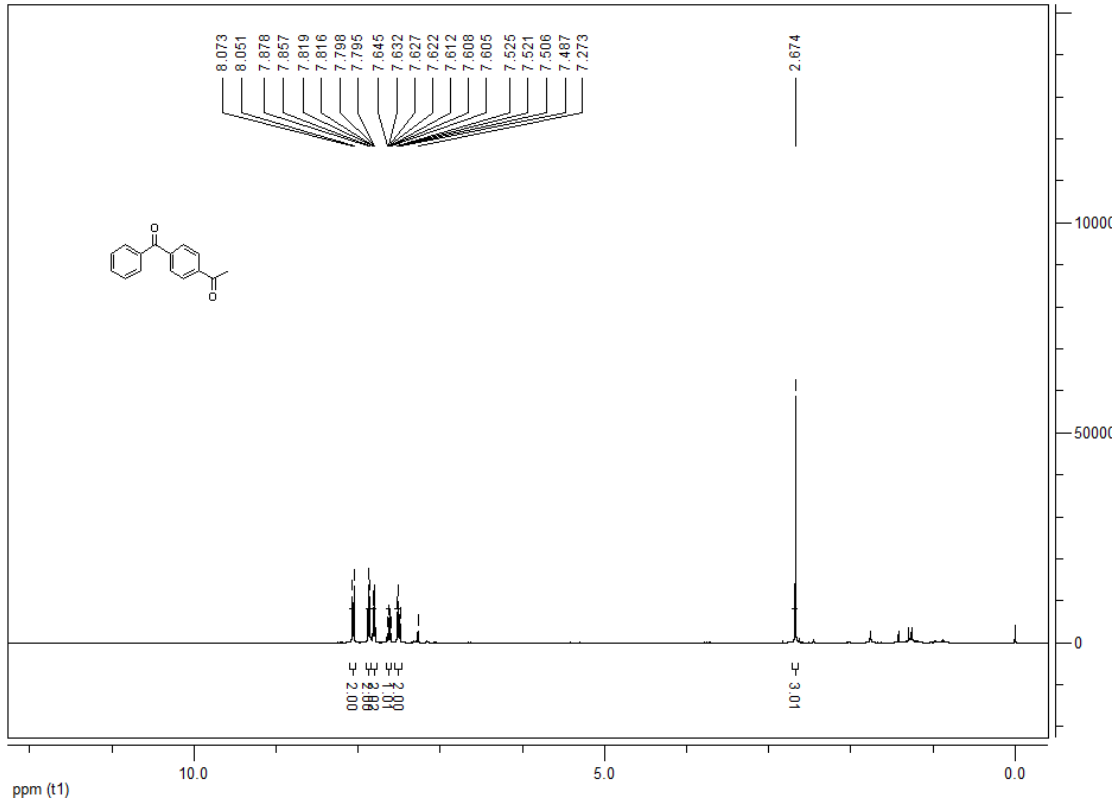


^{13}C NMR

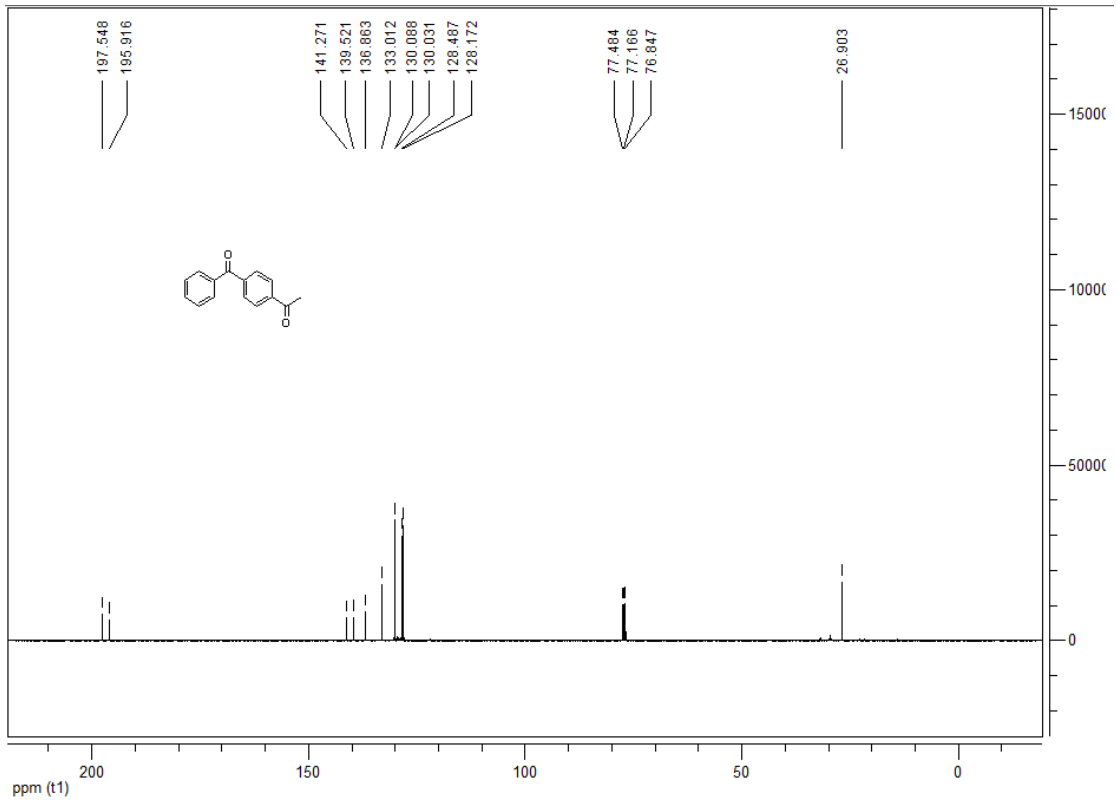


1-(4-benzoylphenyl)ethanone 3dg

^{1}H NMR

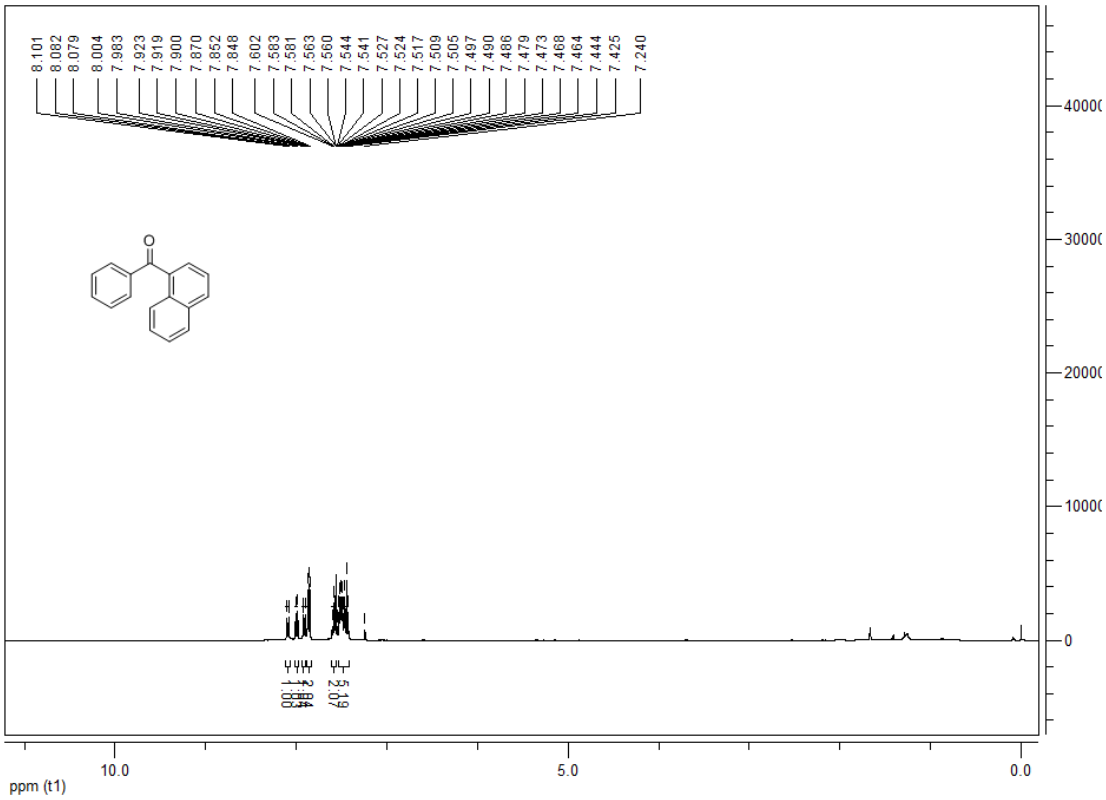


^{13}C NMR

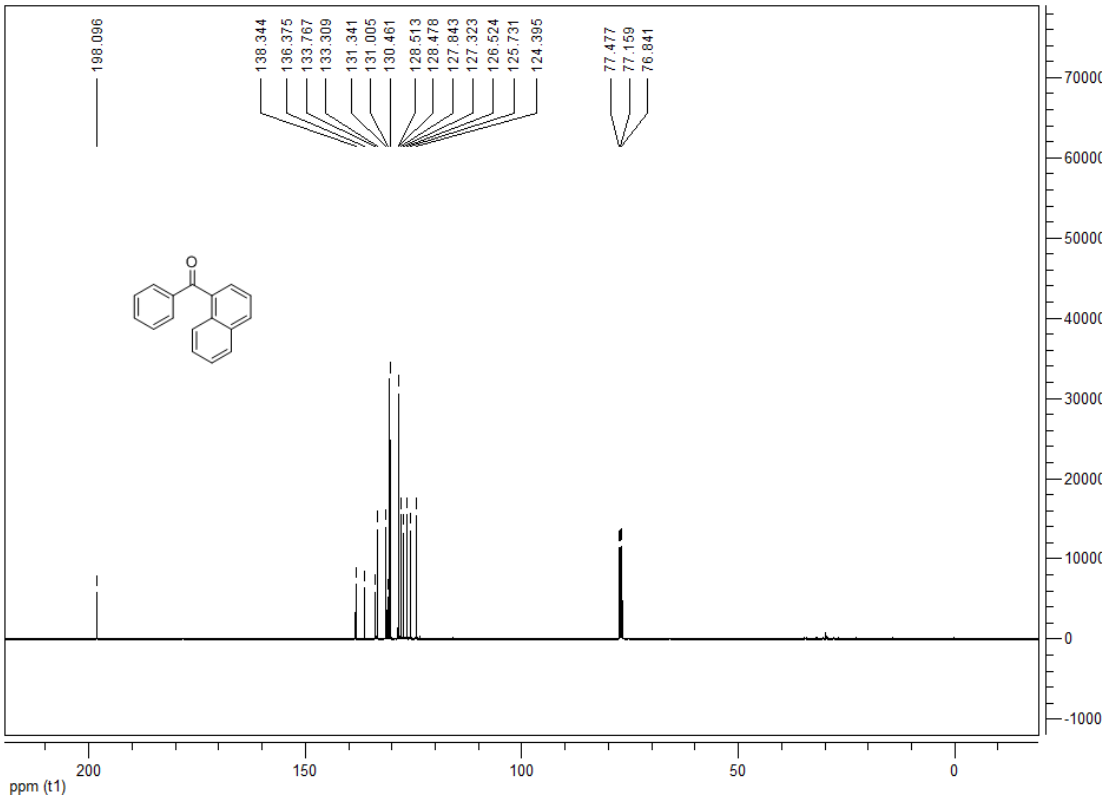


naphthalen-1-yl(phenyl)methanone 3dh

^{1}H NMR

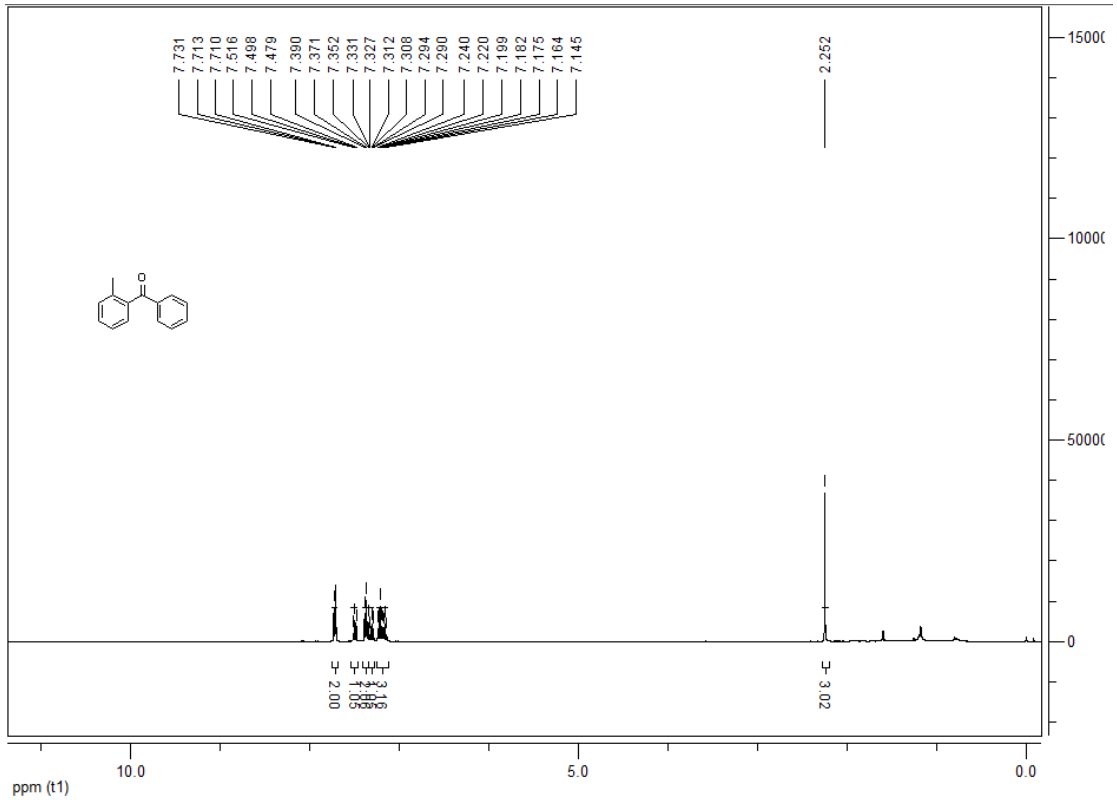


^{13}C NMR

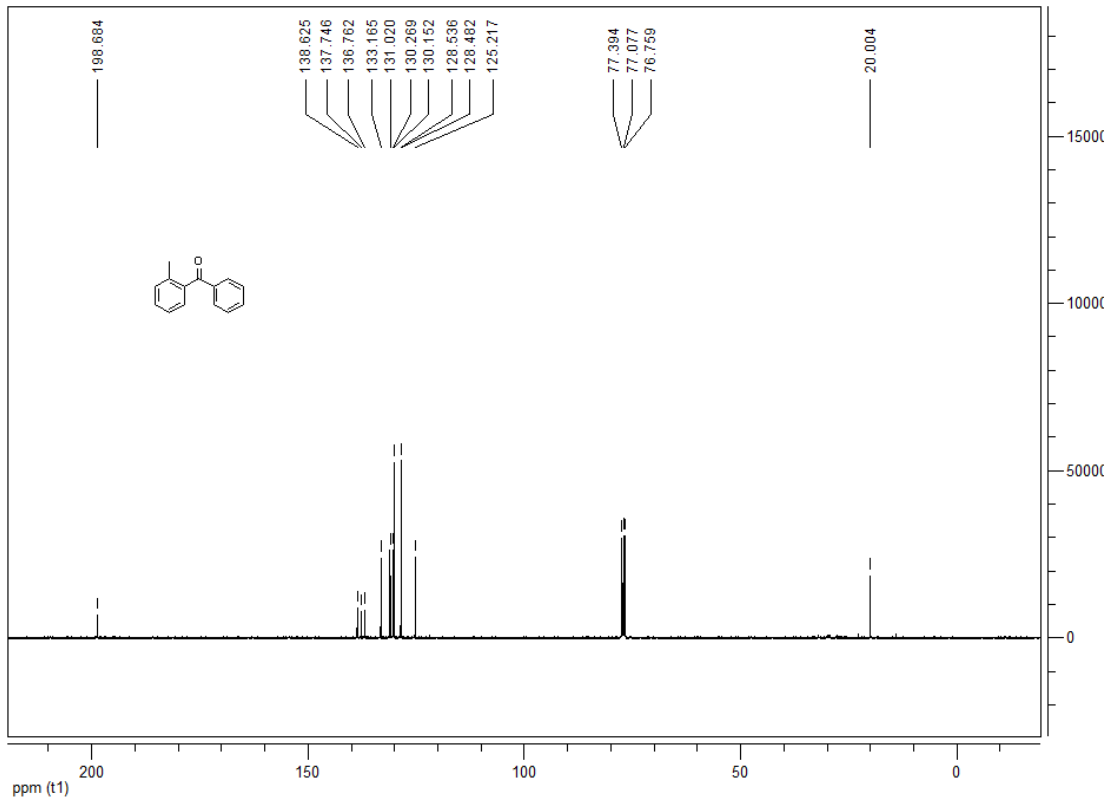


phenyl(o-tolyl)methanone 3di

^{1}H NMR

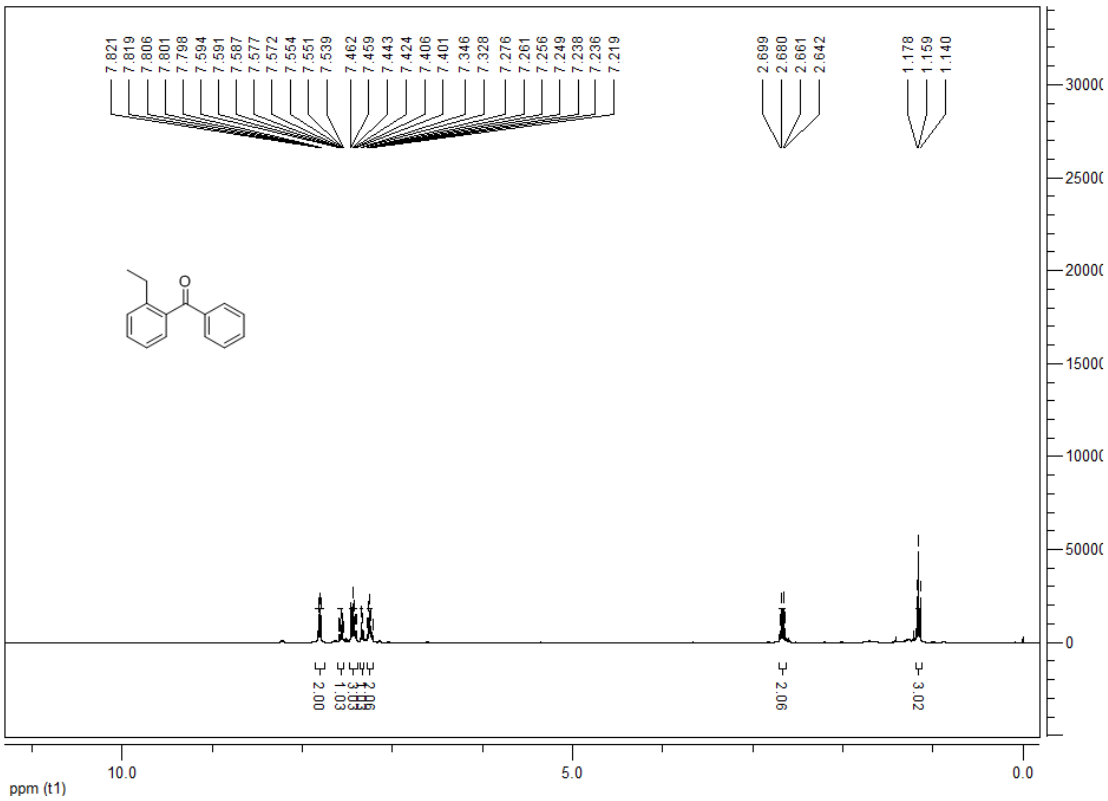


^{13}C NMR

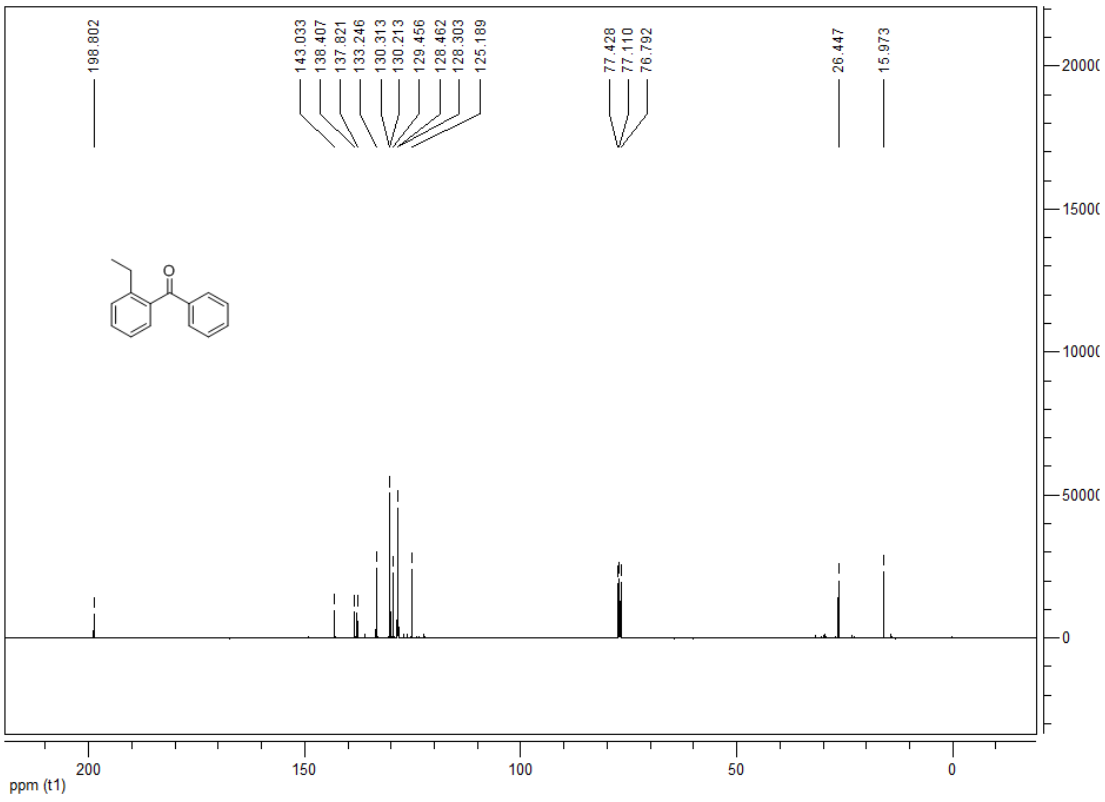


(2-ethylphenyl)(phenyl)methanone 3dj

^{1}H NMR

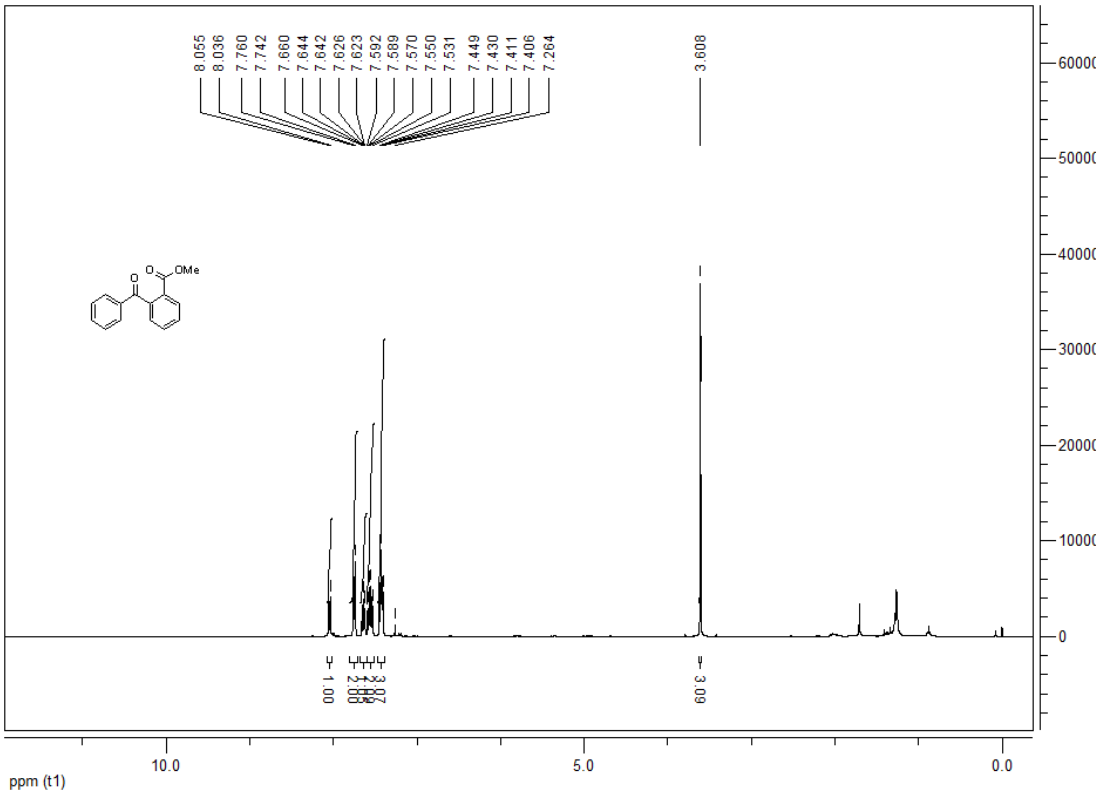


^{13}C NMR

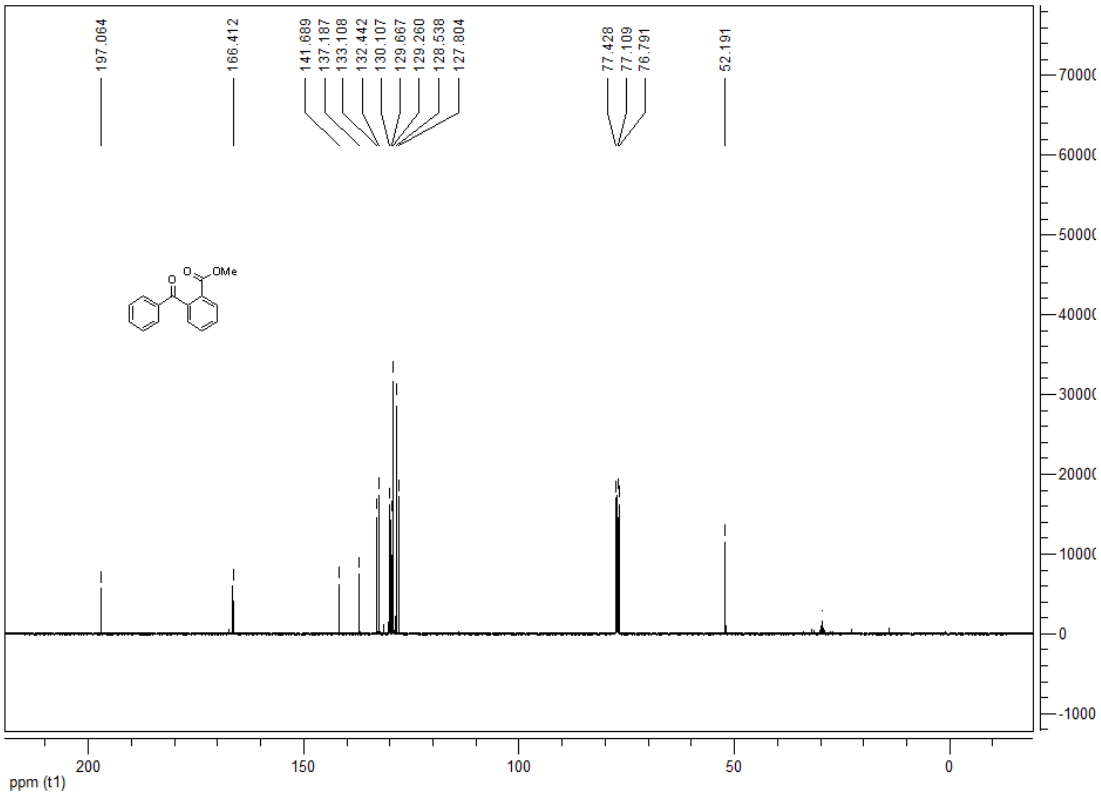


methyl 2-benzoylbenzoate 3dk

^{1}H NMR

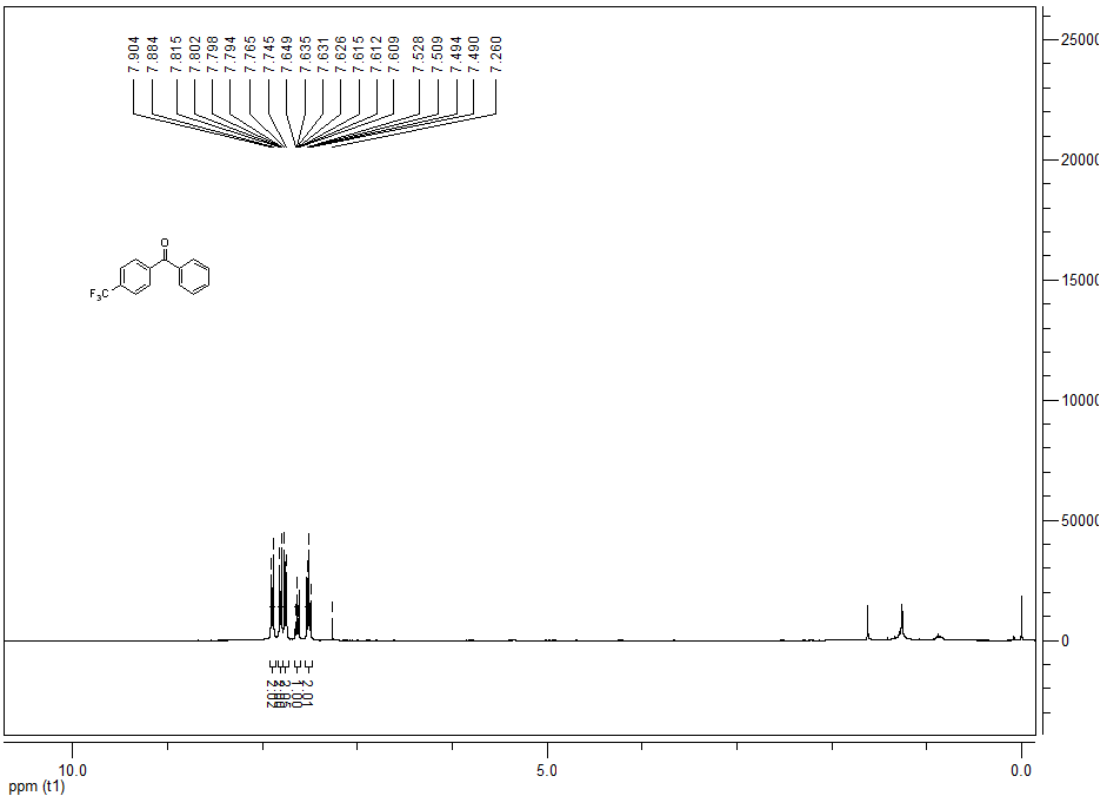


^{13}C NMR

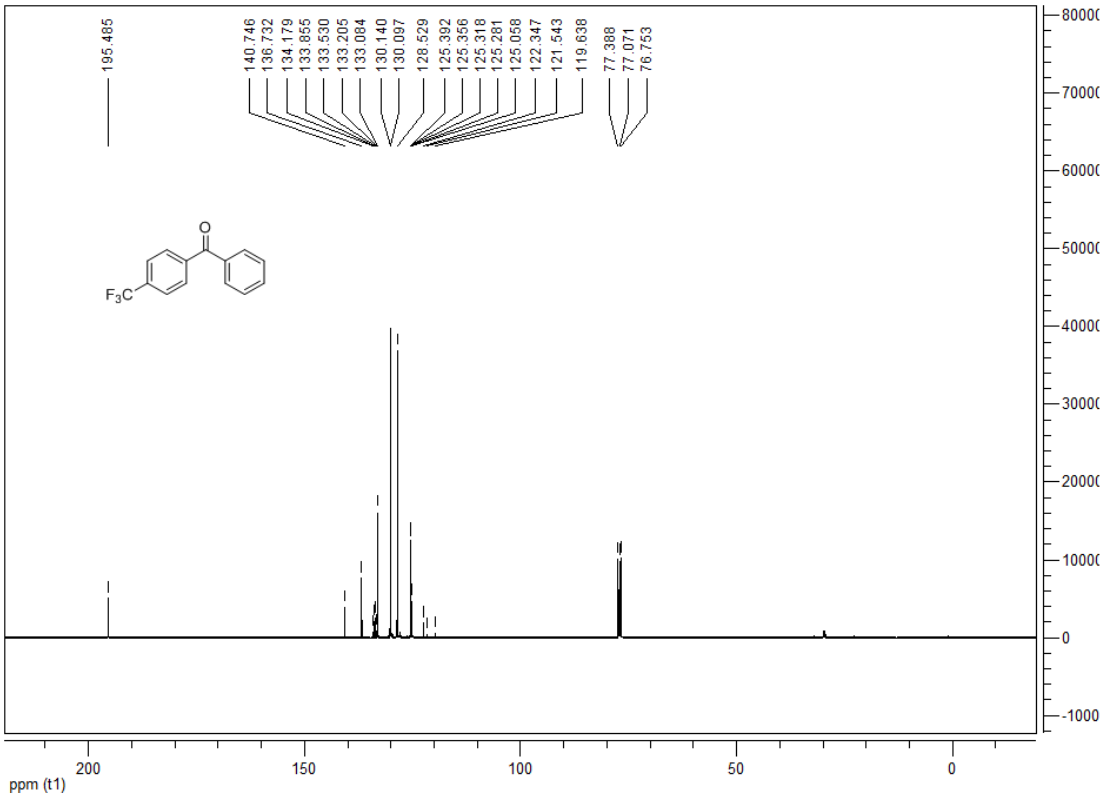


phenyl(4-(trifluoromethyl)phenyl)methanone 3fa

^{1}H NMR

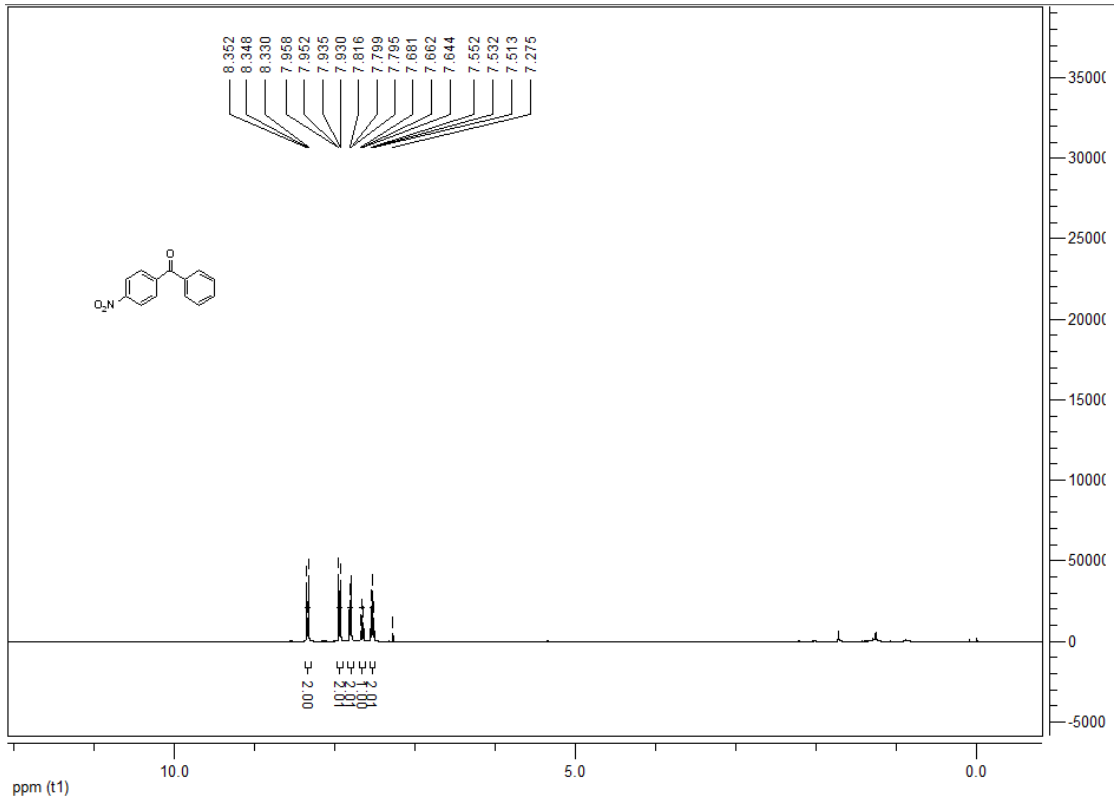


^{13}C NMR

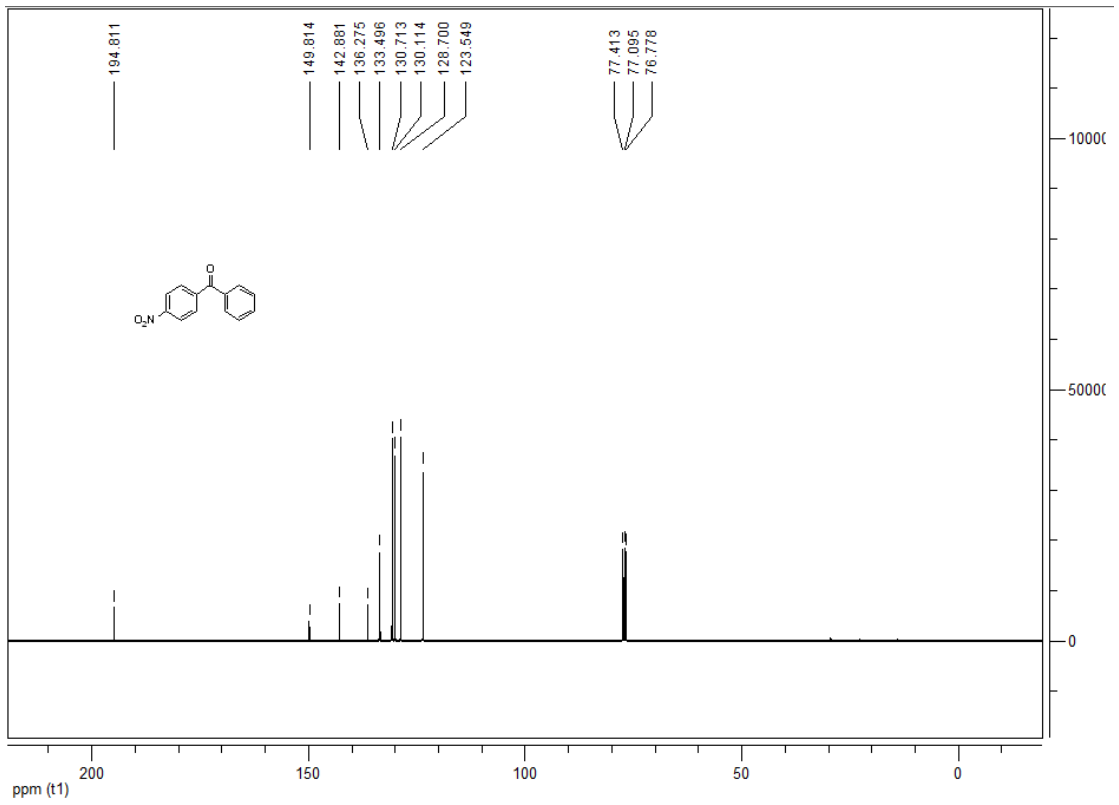


(4-nitrophenyl)(phenyl)methanone 3ia

^{1}H NMR

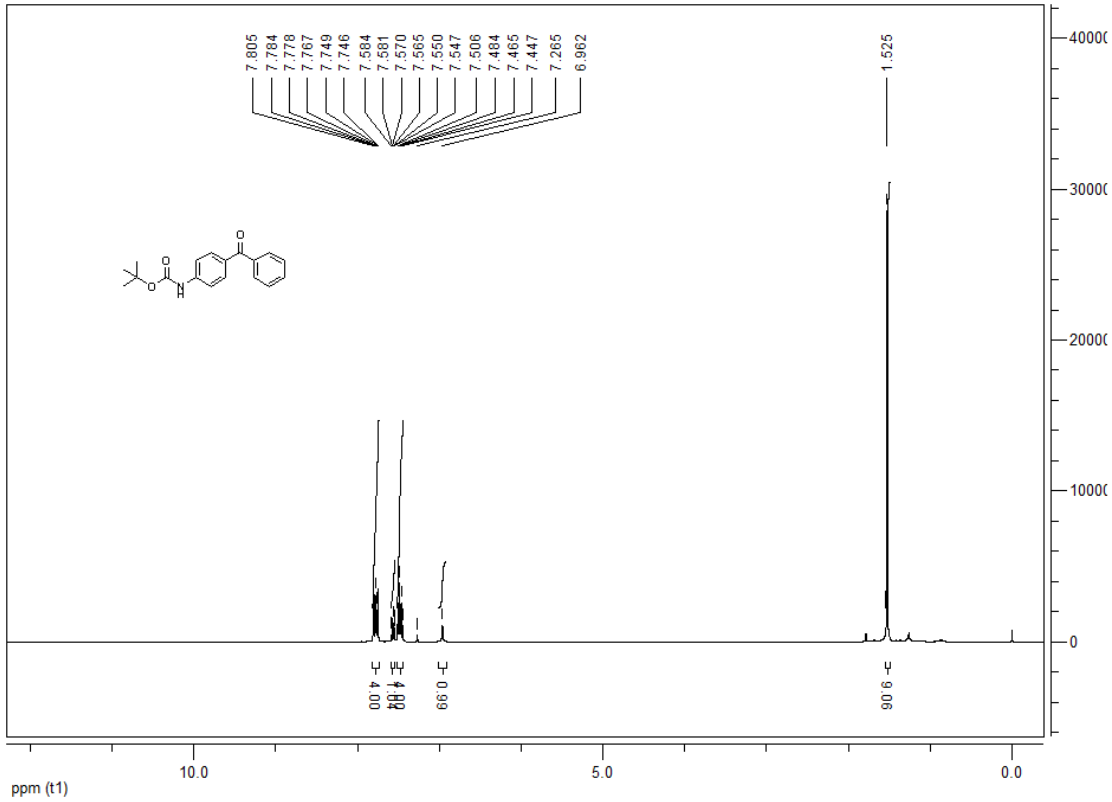


^{13}C NMR

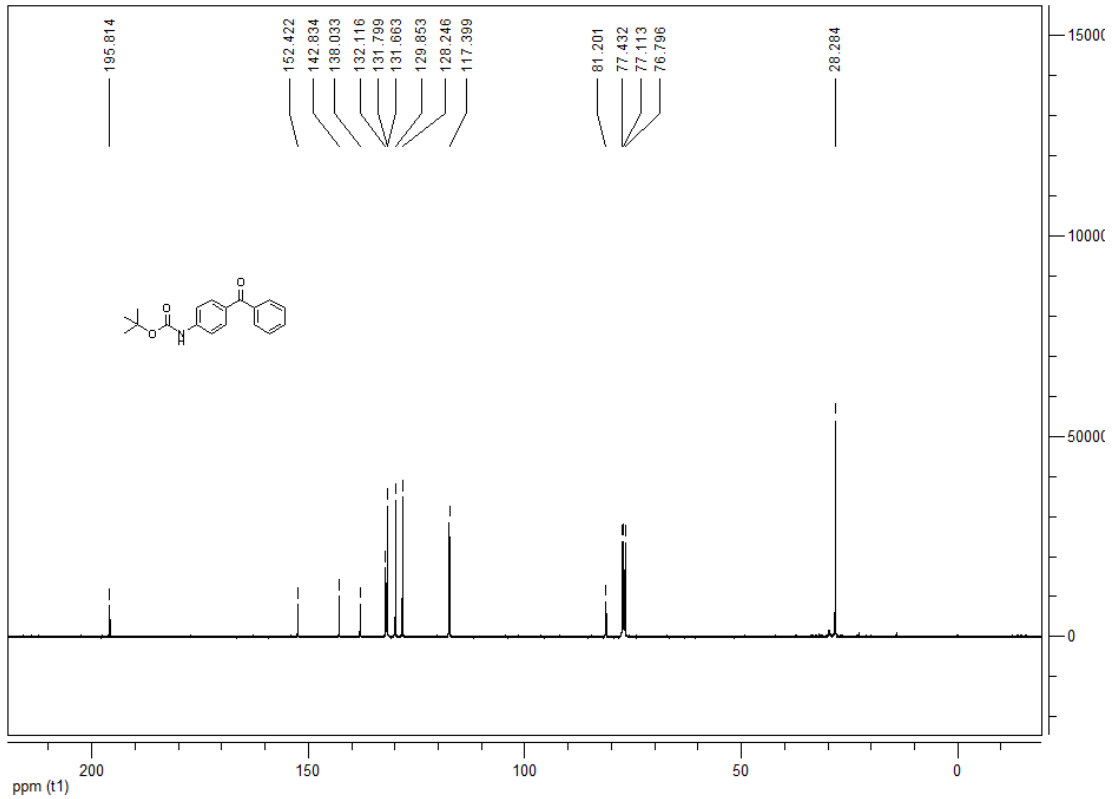


tert-butyl (4-benzoylphenyl)carbamate 3la

^{1}H NMR

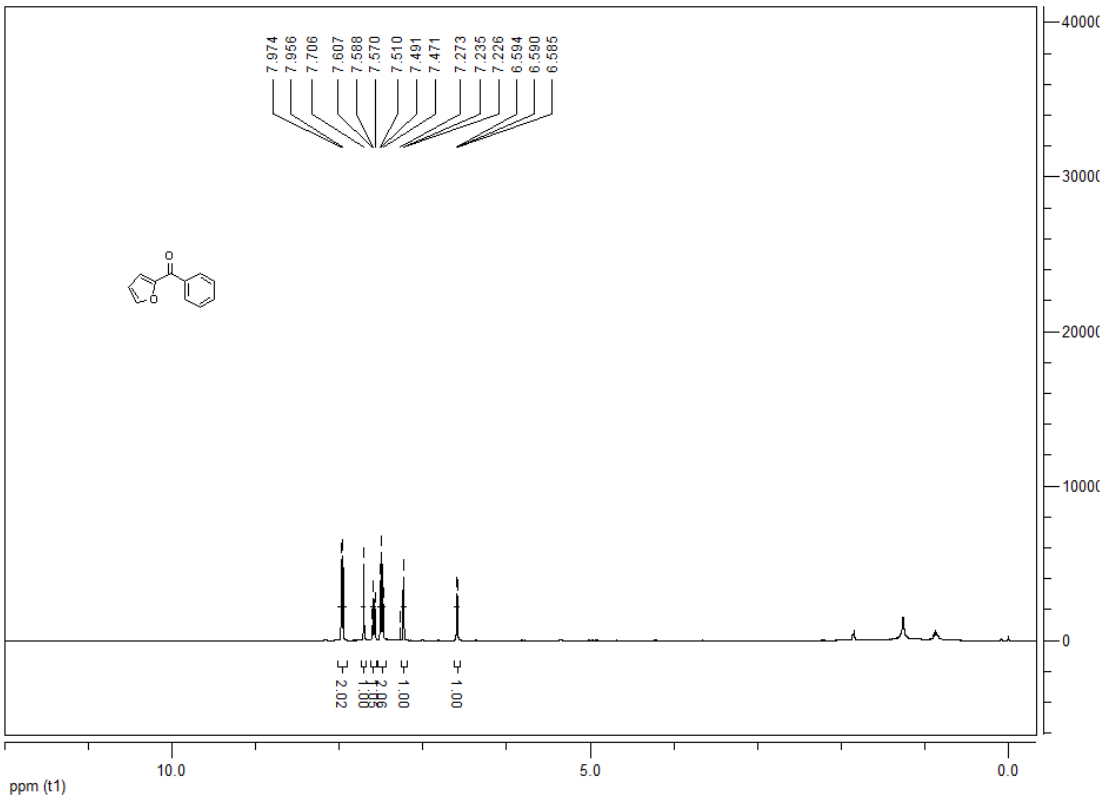


^{13}C NMR

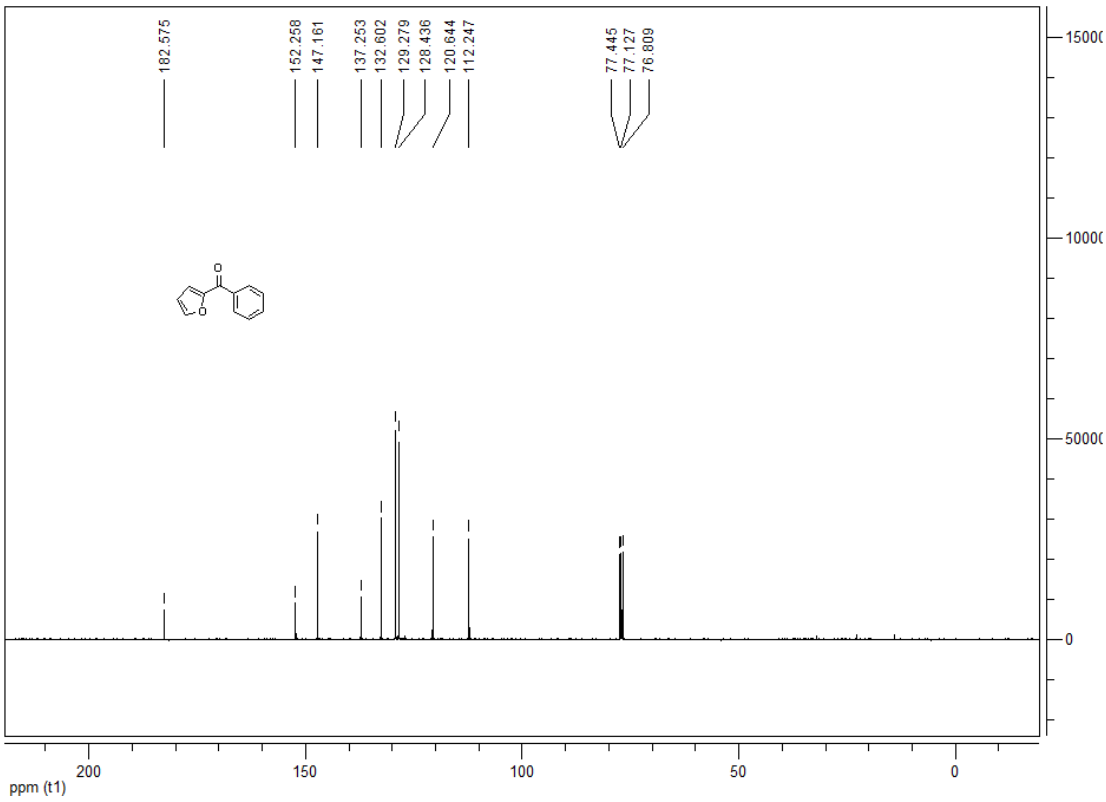


furan-2-yl(phenyl)methanone 3ma

^{1}H NMR

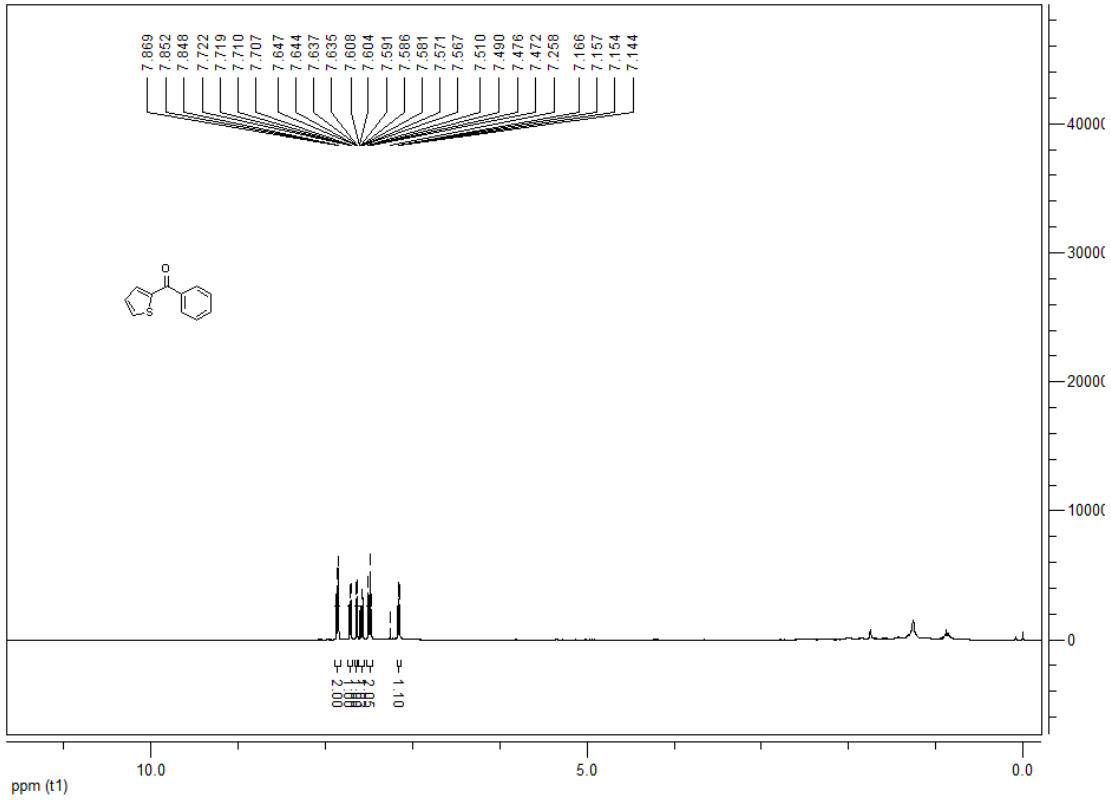


^{13}C NMR

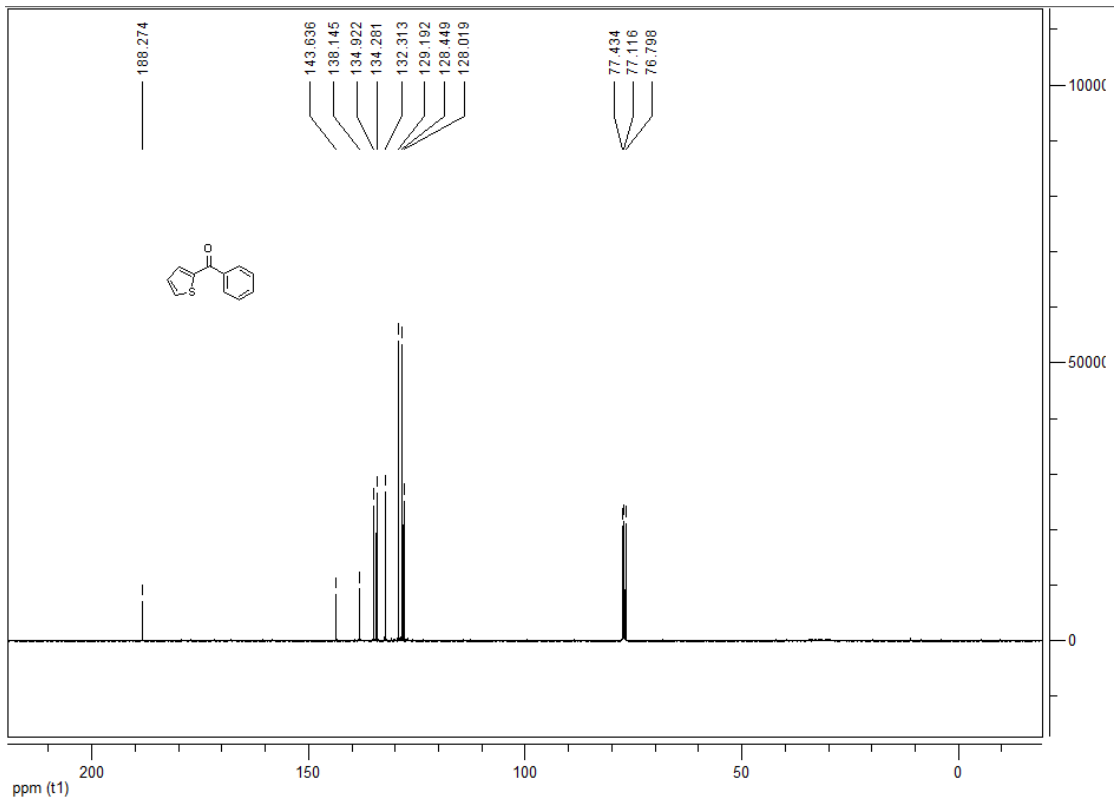


phenyl(thiophen-2-yl)methanone 3na

^{1}H NMR

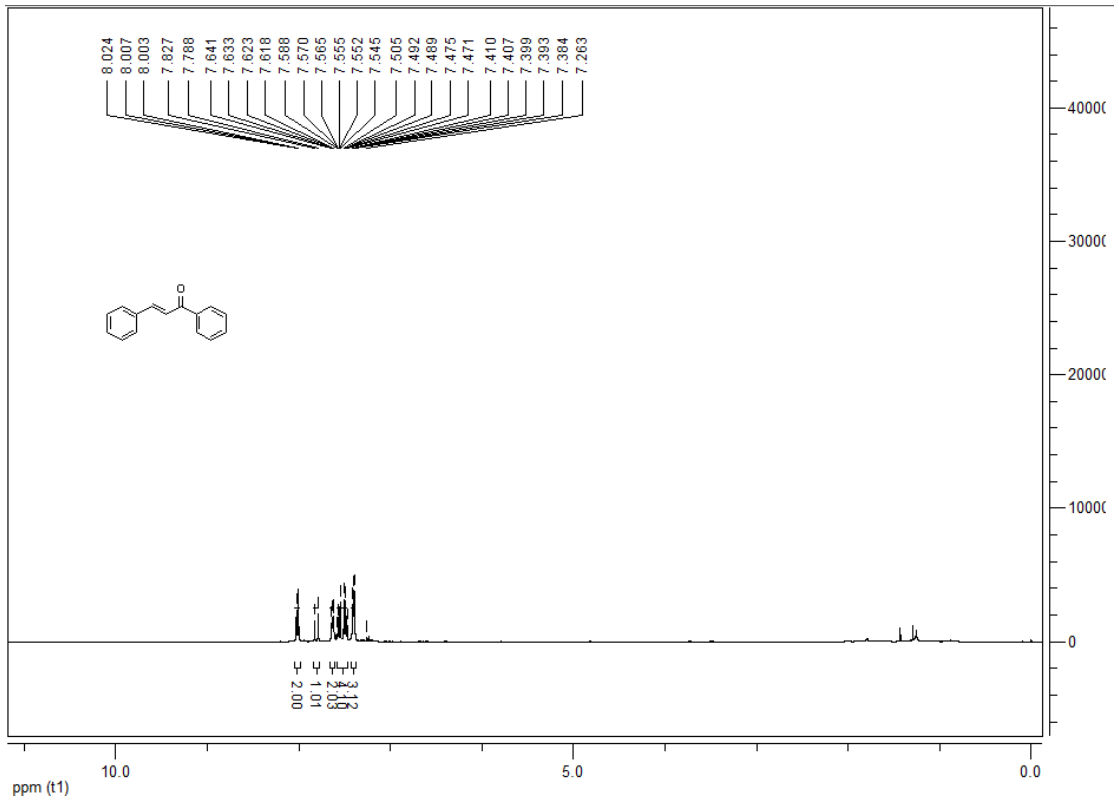


^{13}C NMR

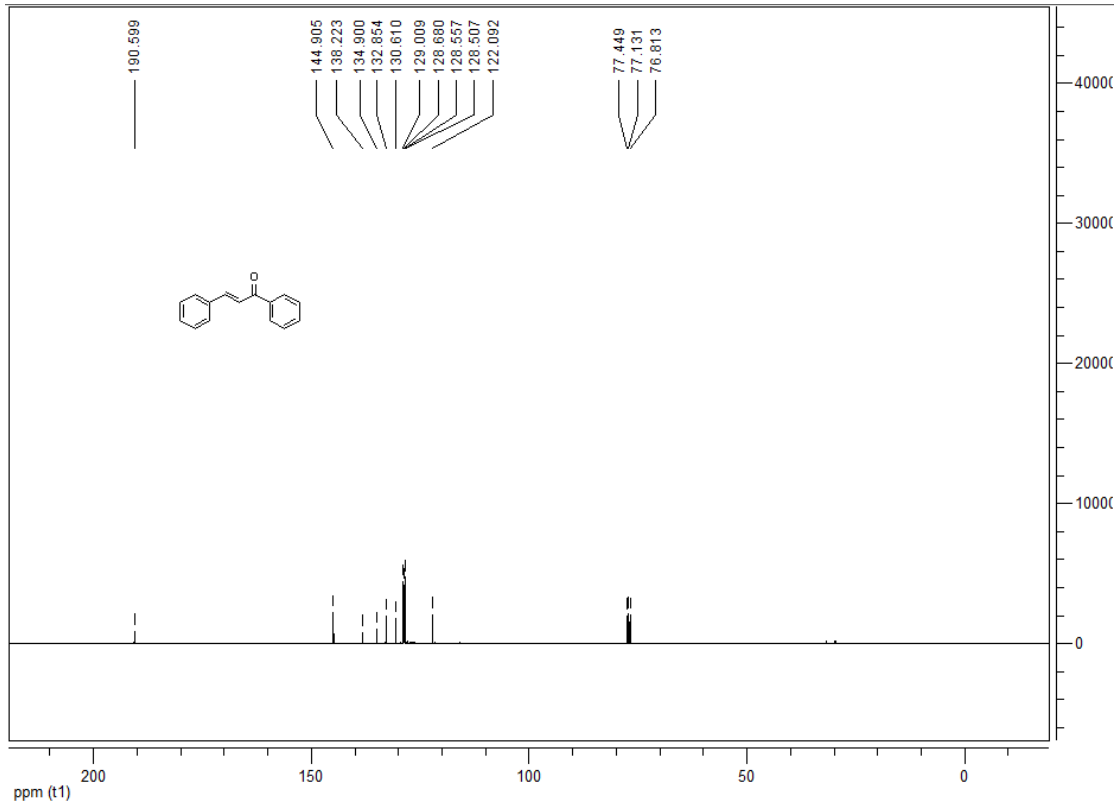


(E)-chalcone 3oa

^{1}H NMR

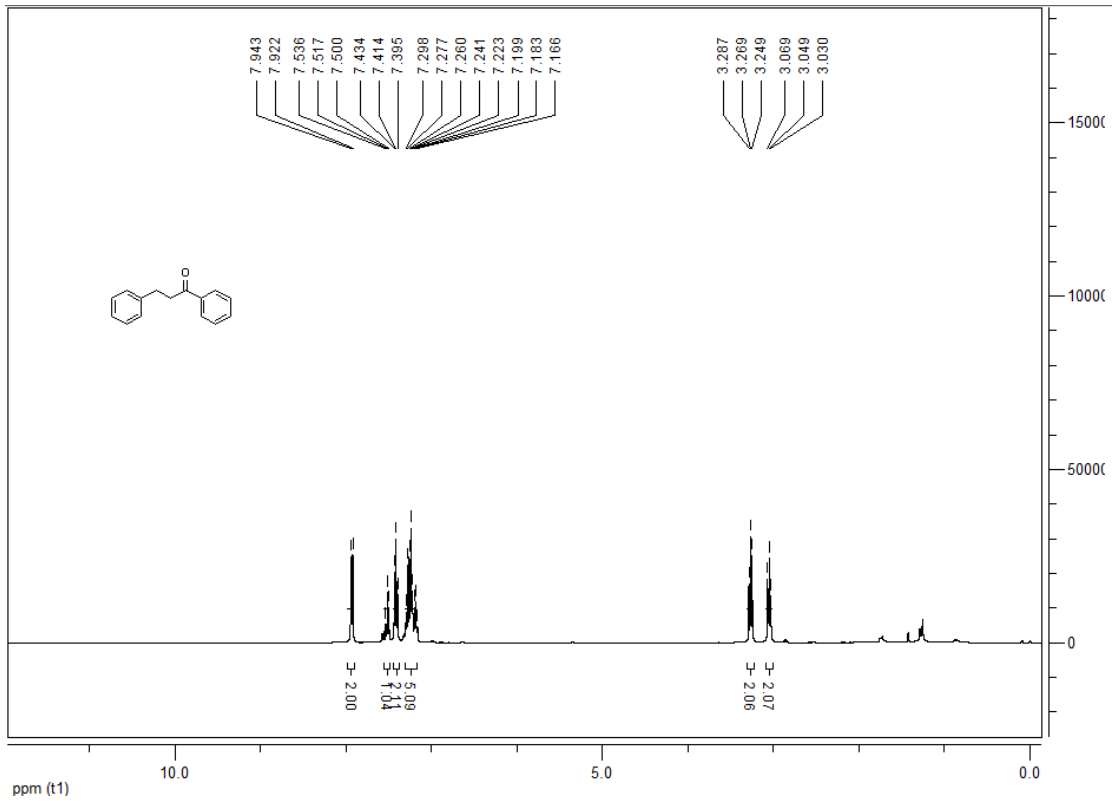


^{13}C NMR

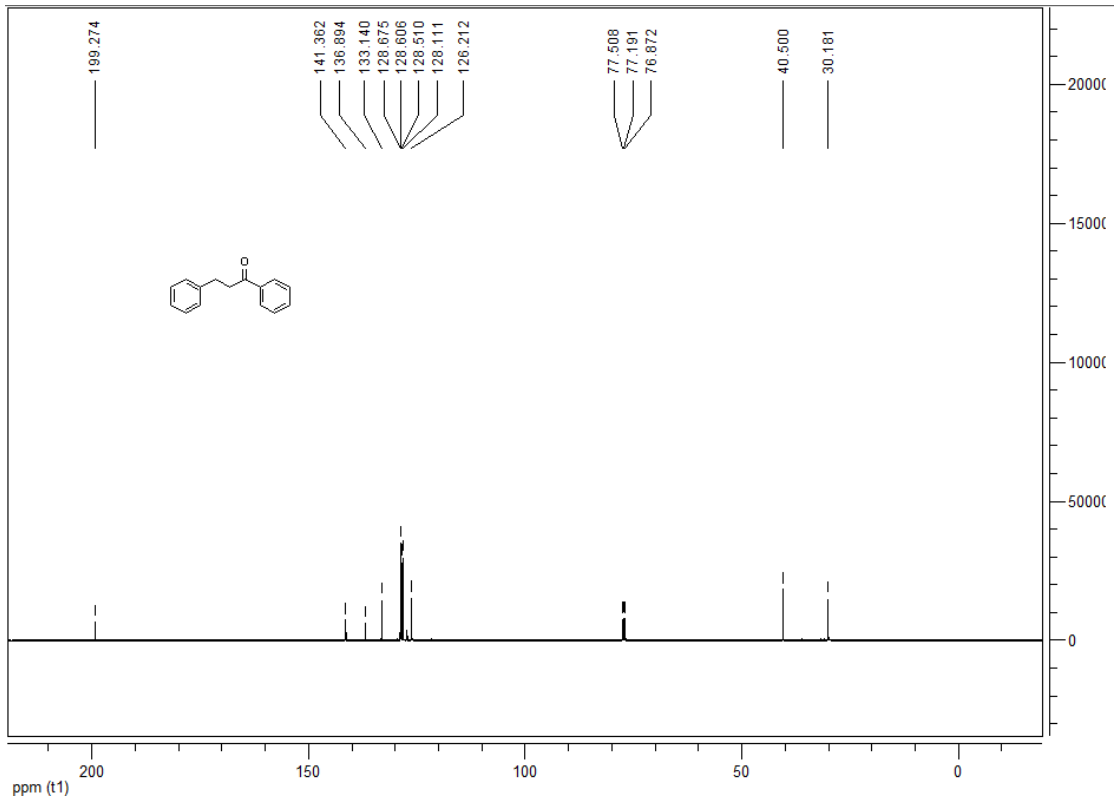


1,3-diphenylpropan-1-one 3pa

^{1}H NMR

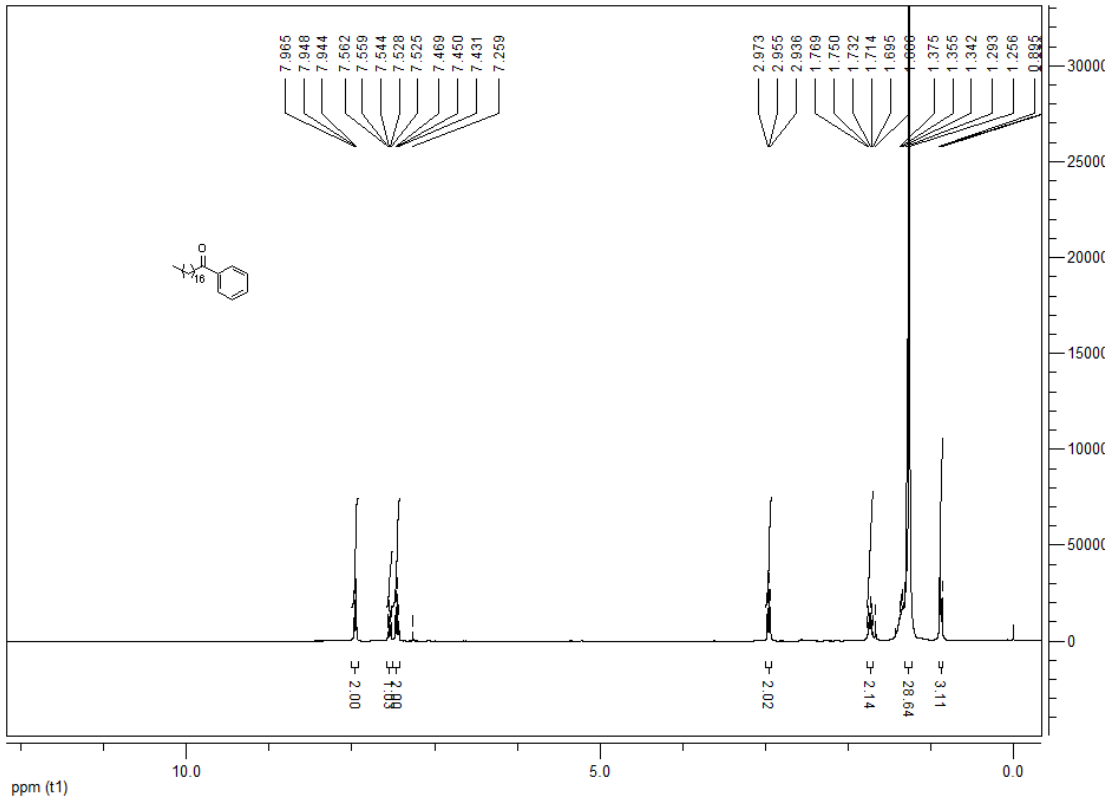


^{13}C NMR

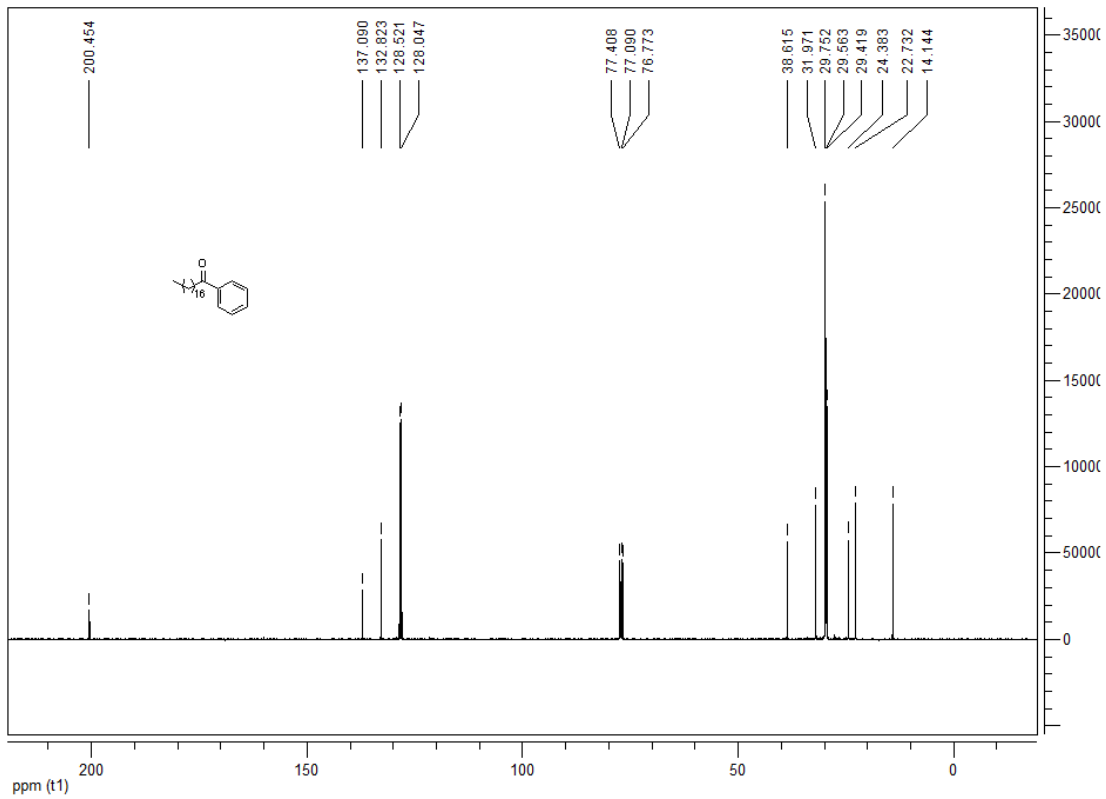


1-phenyloctadecan-1-one 3qa

^{1}H NMR

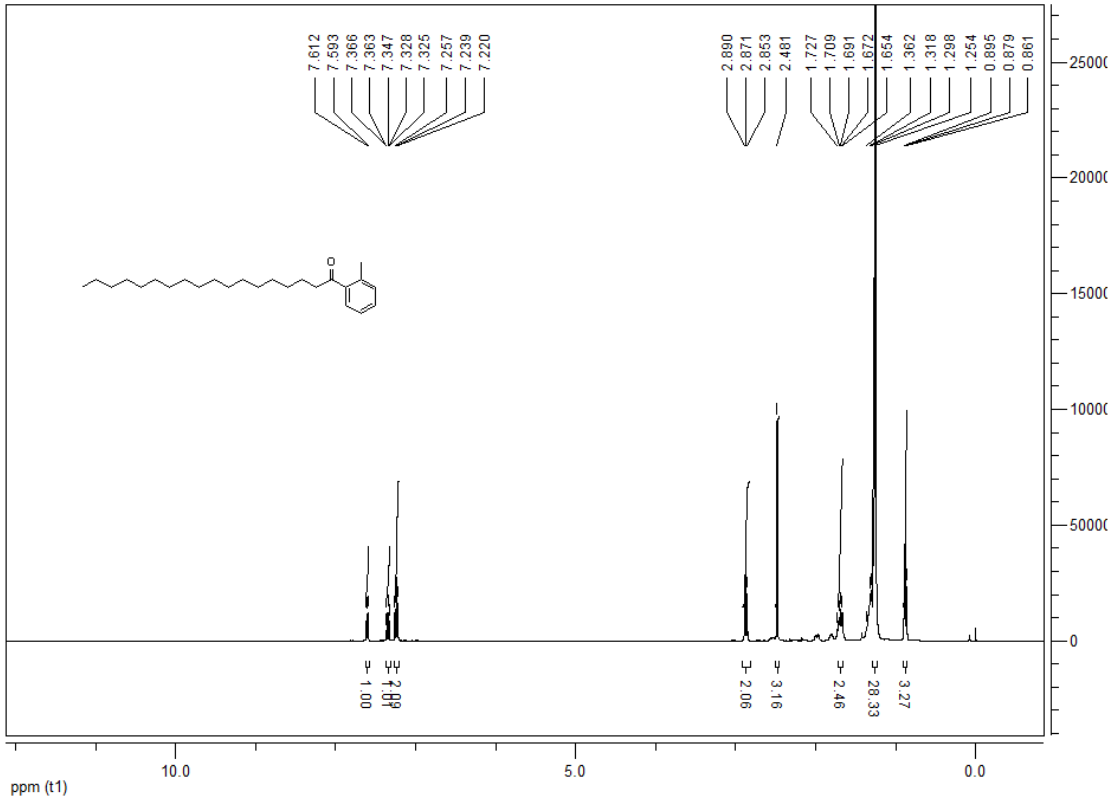


^{13}C NMR

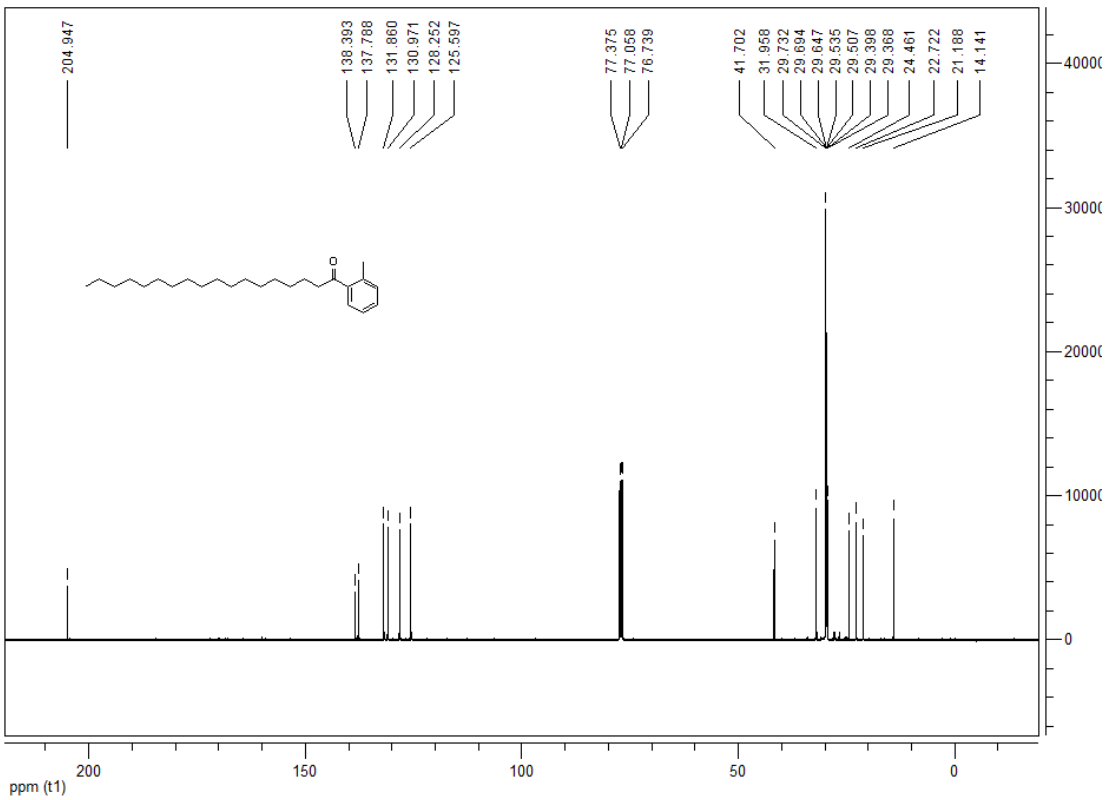


1-(o-tolyl)octadecan-1-one 3qi

^{1}H NMR

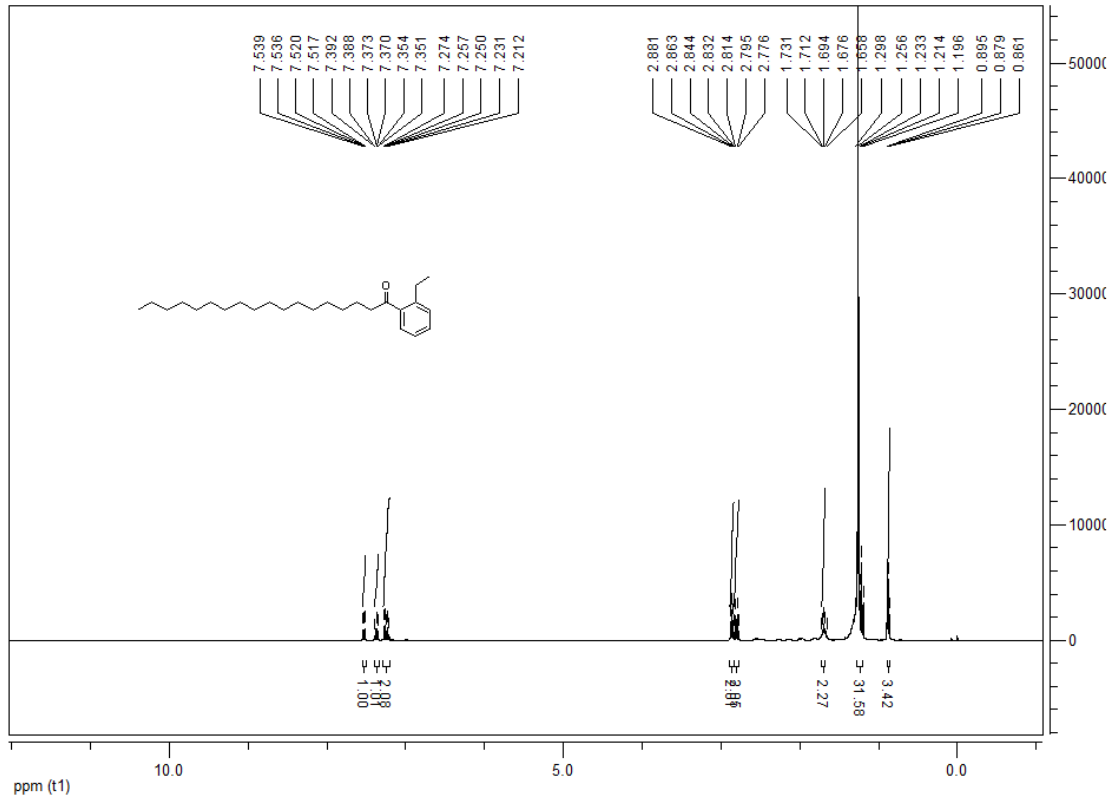


^{13}C NMR

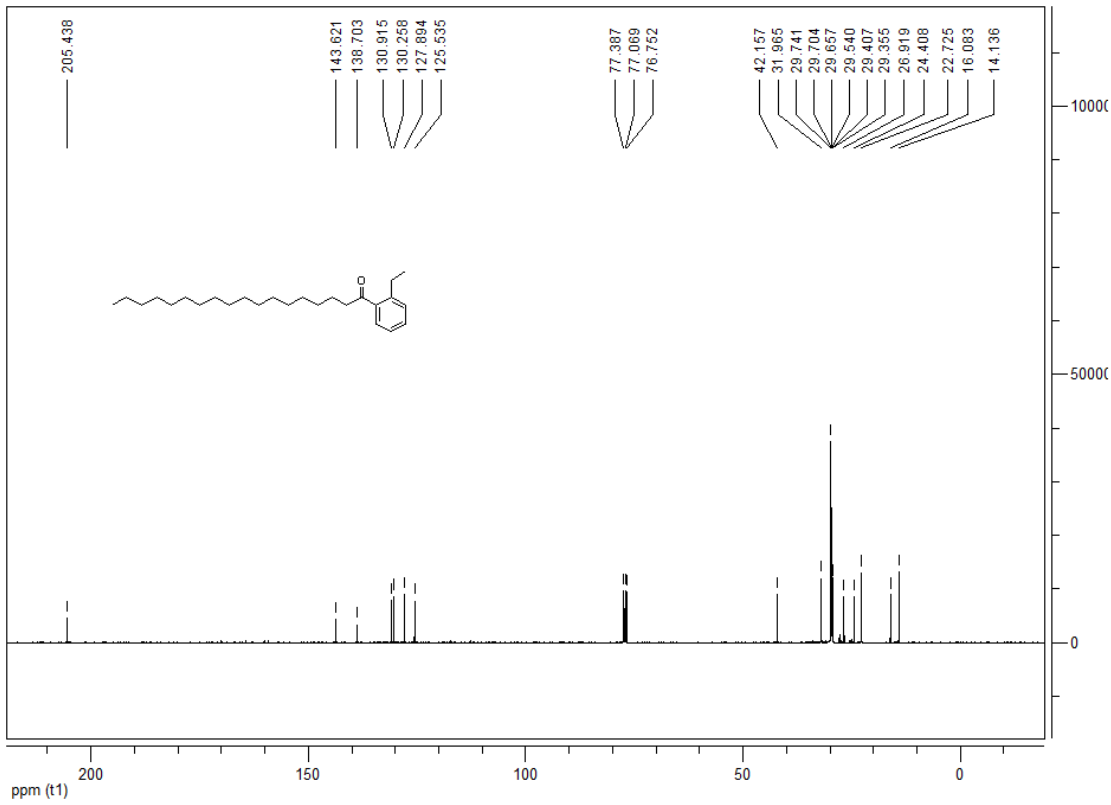


1-(2-ethylphenyl)octadecan-1-one 3qj

^{1}H NMR

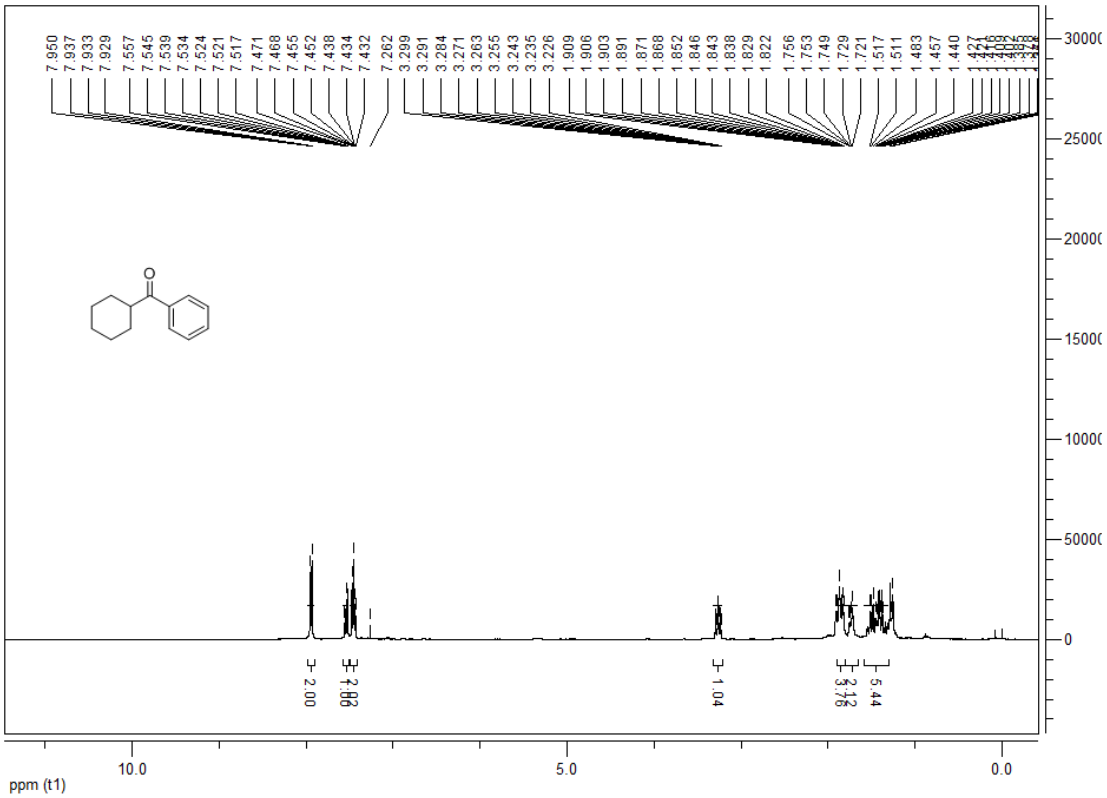


^{13}C NMR

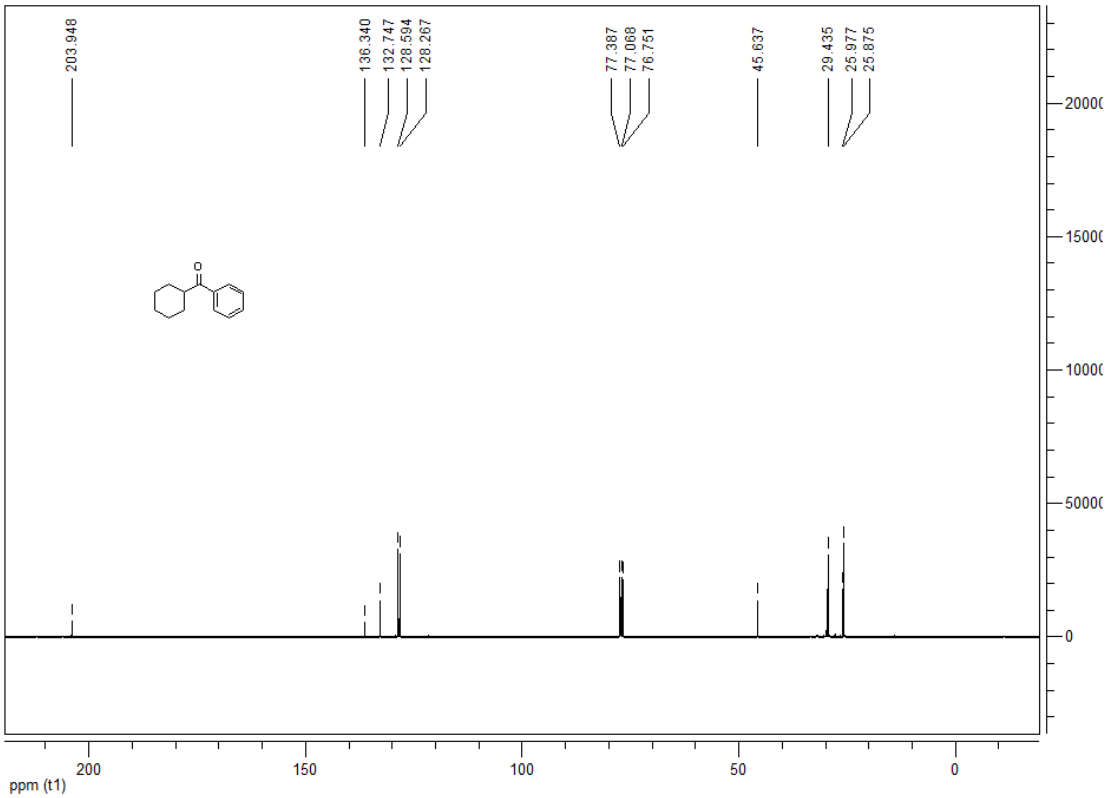


cyclohexyl(phenyl)methanone 3ra

^{1}H NMR

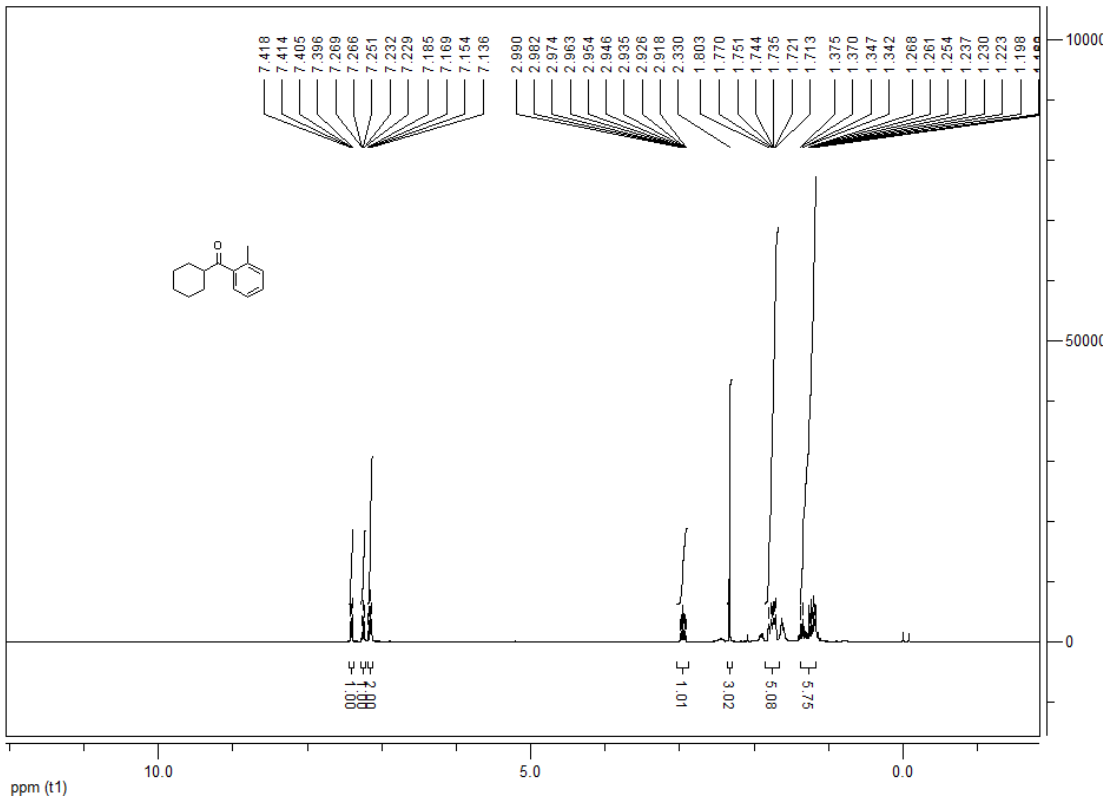


^{13}C NMR

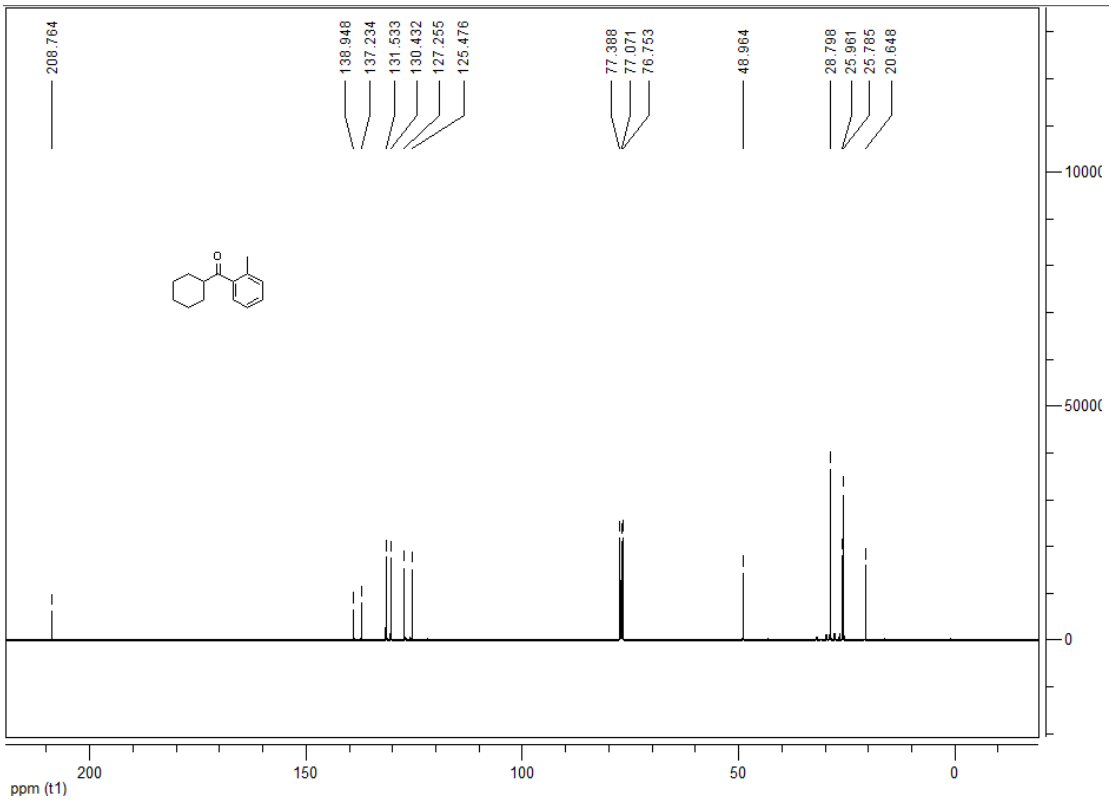


cyclohexyl(o-tolyl)methanone 3ri

^{1}H NMR

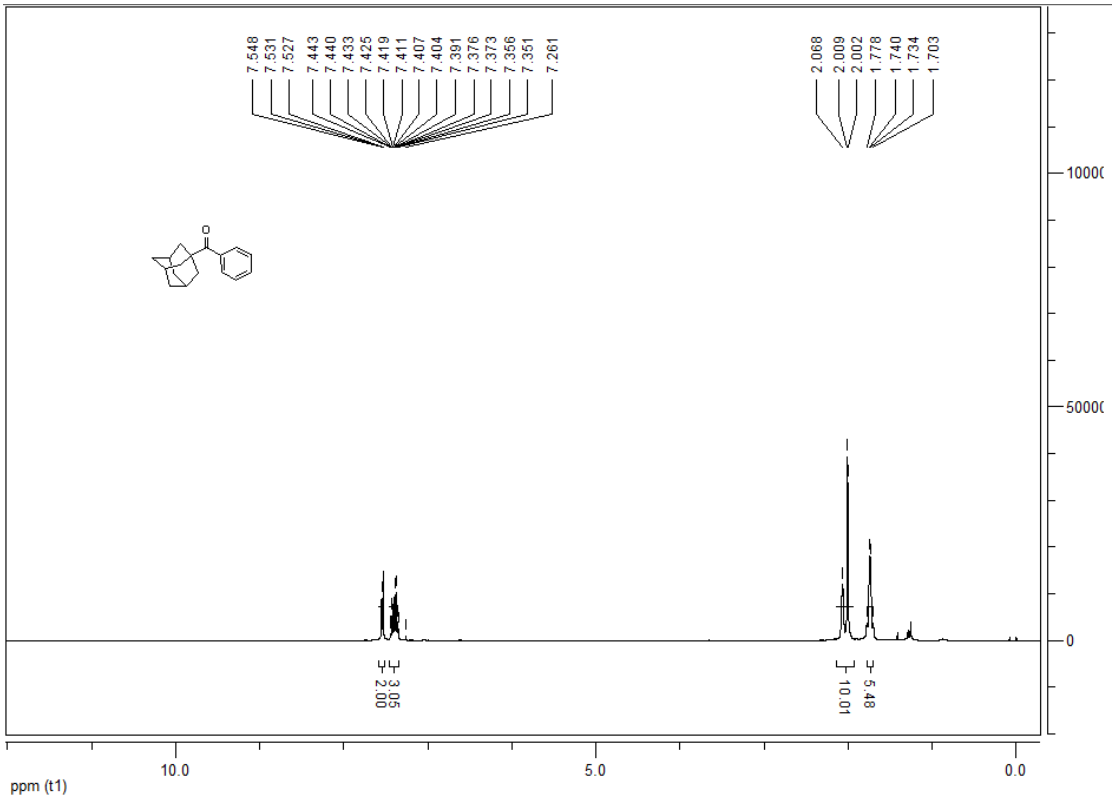


^{13}C NMR

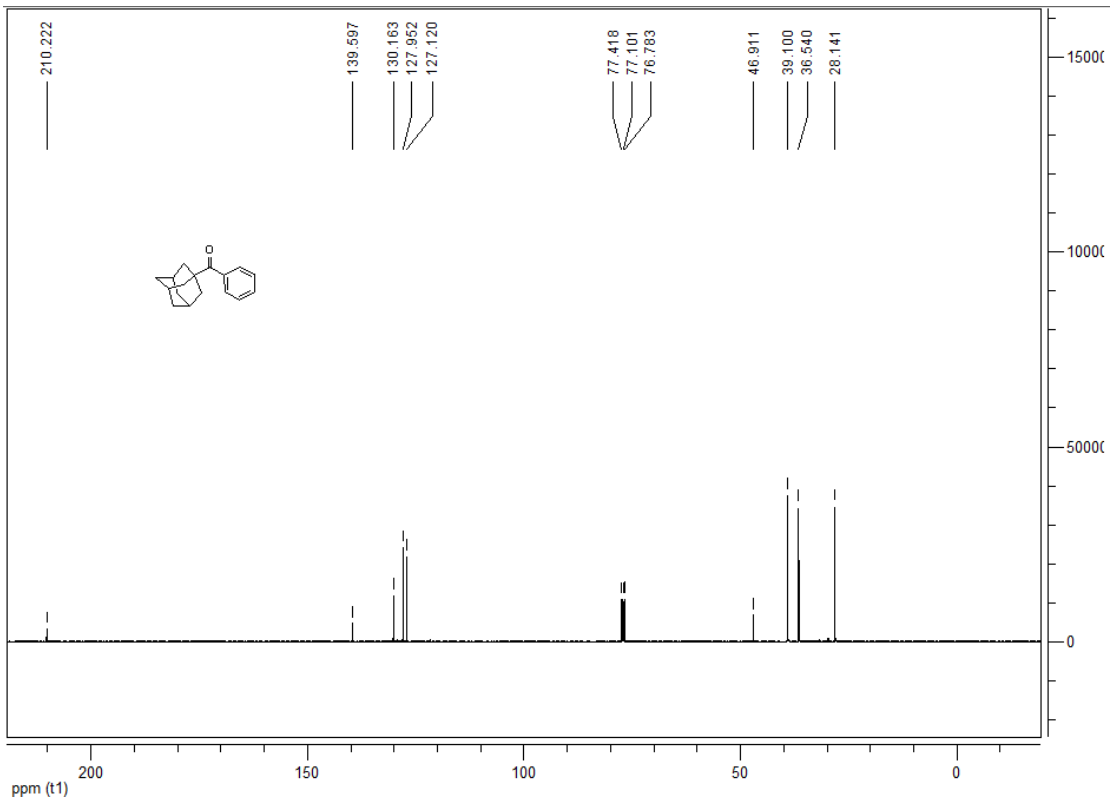


(3r,5r,7r)-adamantan-1-yl(phenyl)methanone 3sa

^{1}H NMR

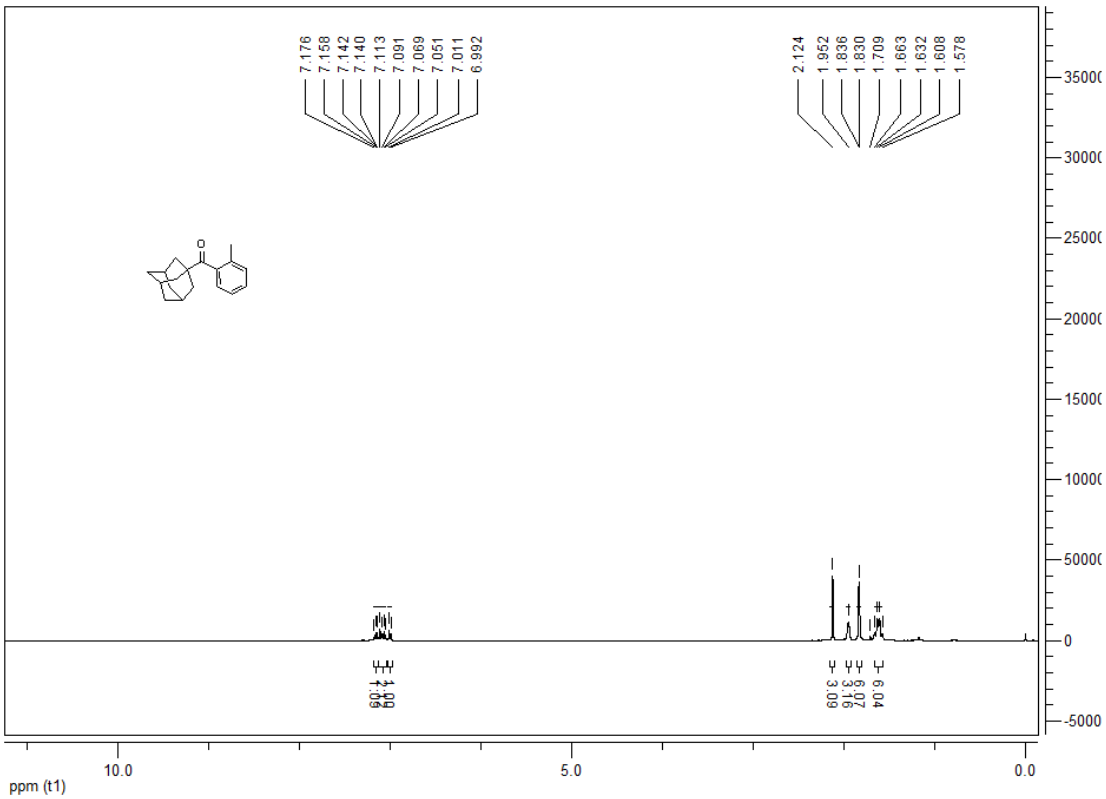


^{13}C NMR

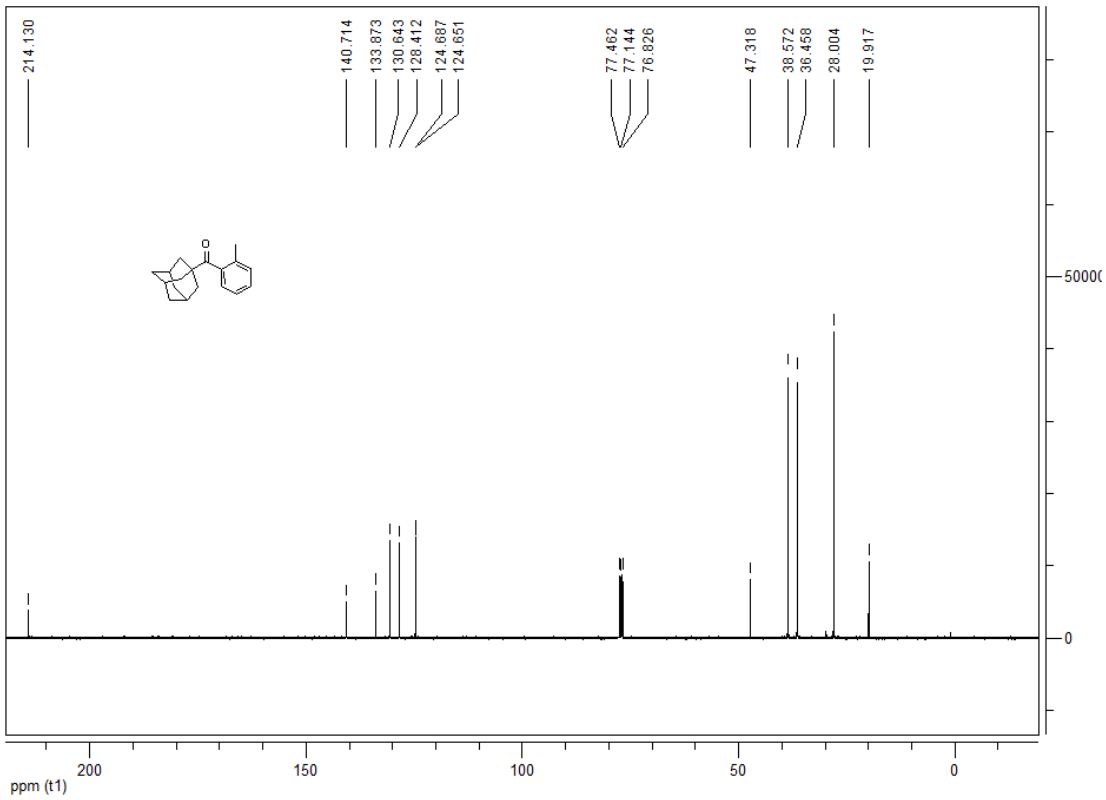


(3r,5r,7r)-adamantan-1-yl(o-tolyl)methanone 3ui

^{1}H NMR

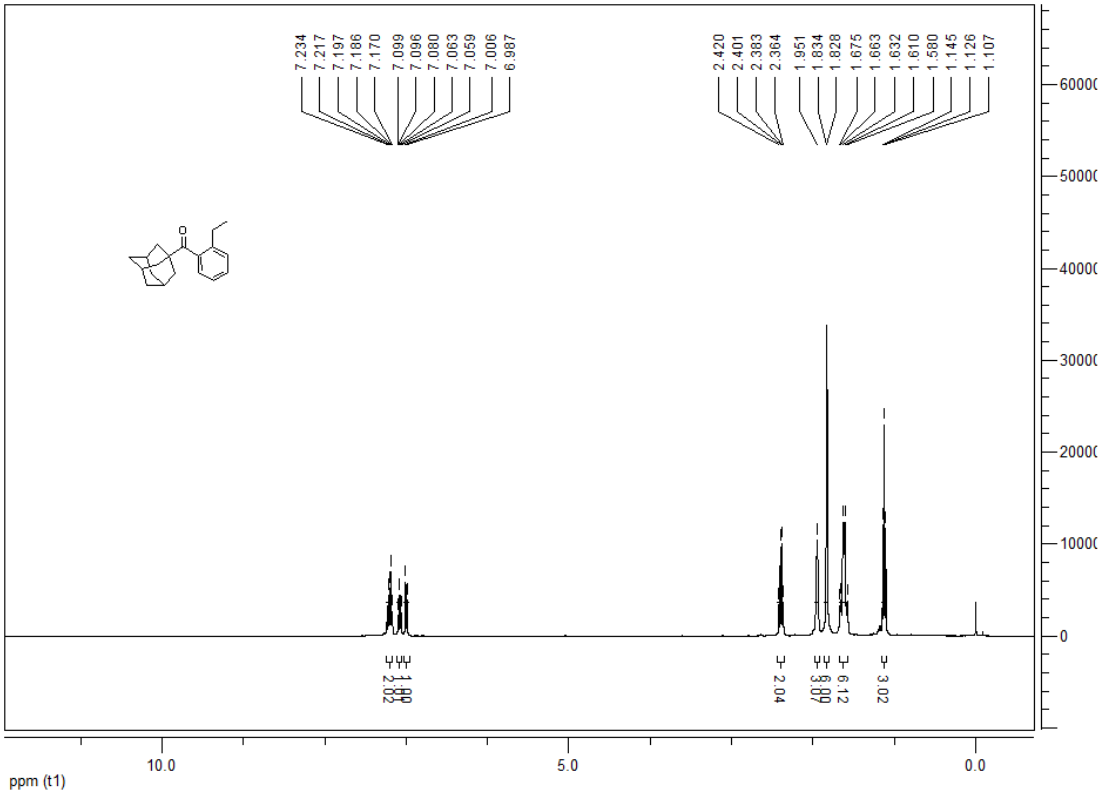


^{13}C NMR

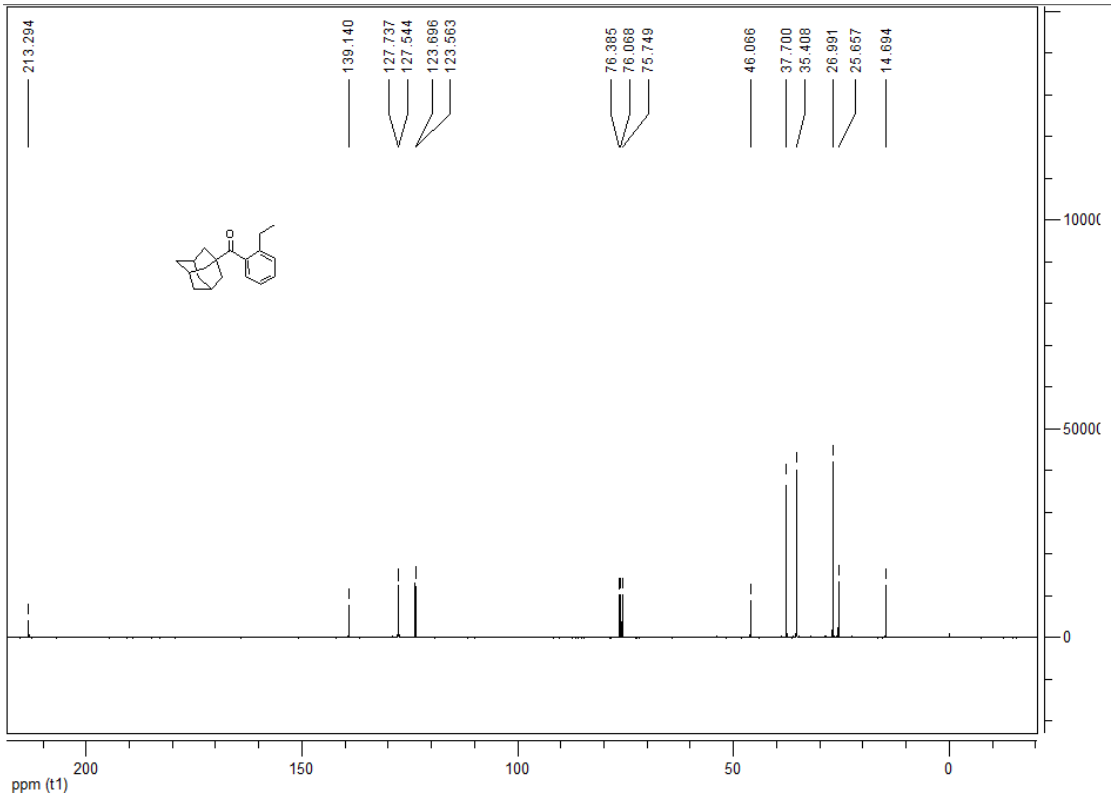


(3r,5r,7r)-adamantan-1-yl(2-ethylphenyl)methanone 3uj

^{1}H NMR

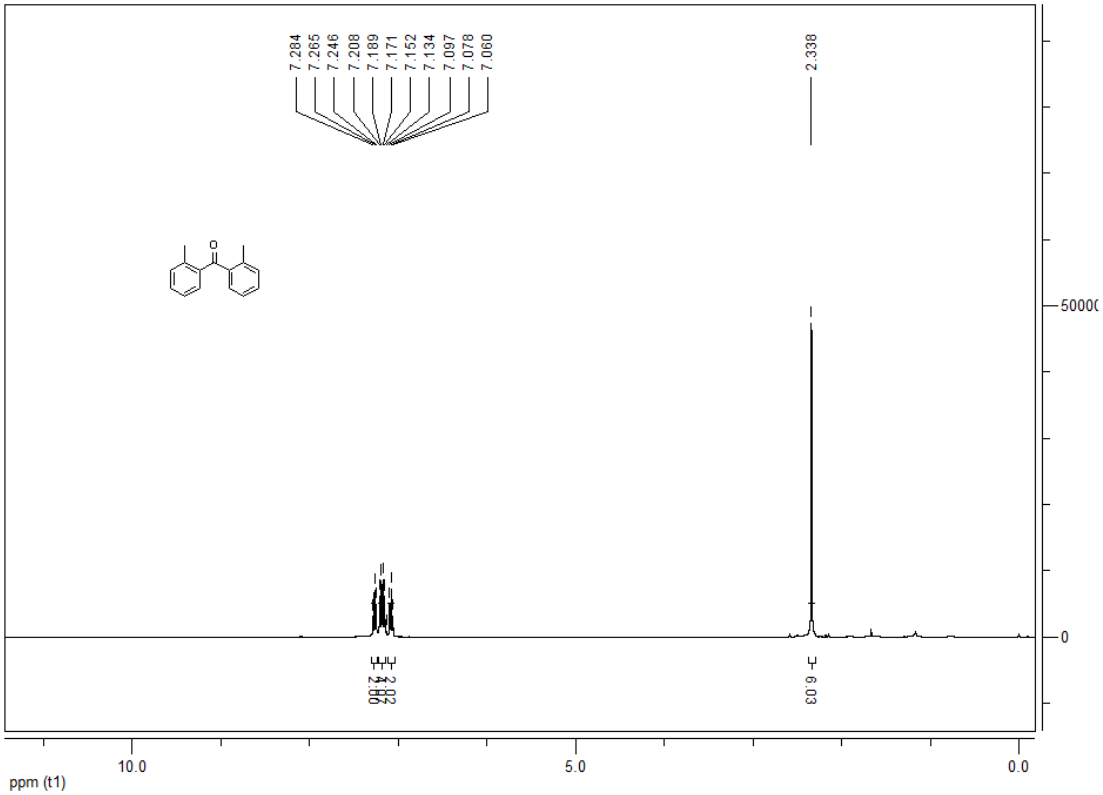


^{13}C NMR

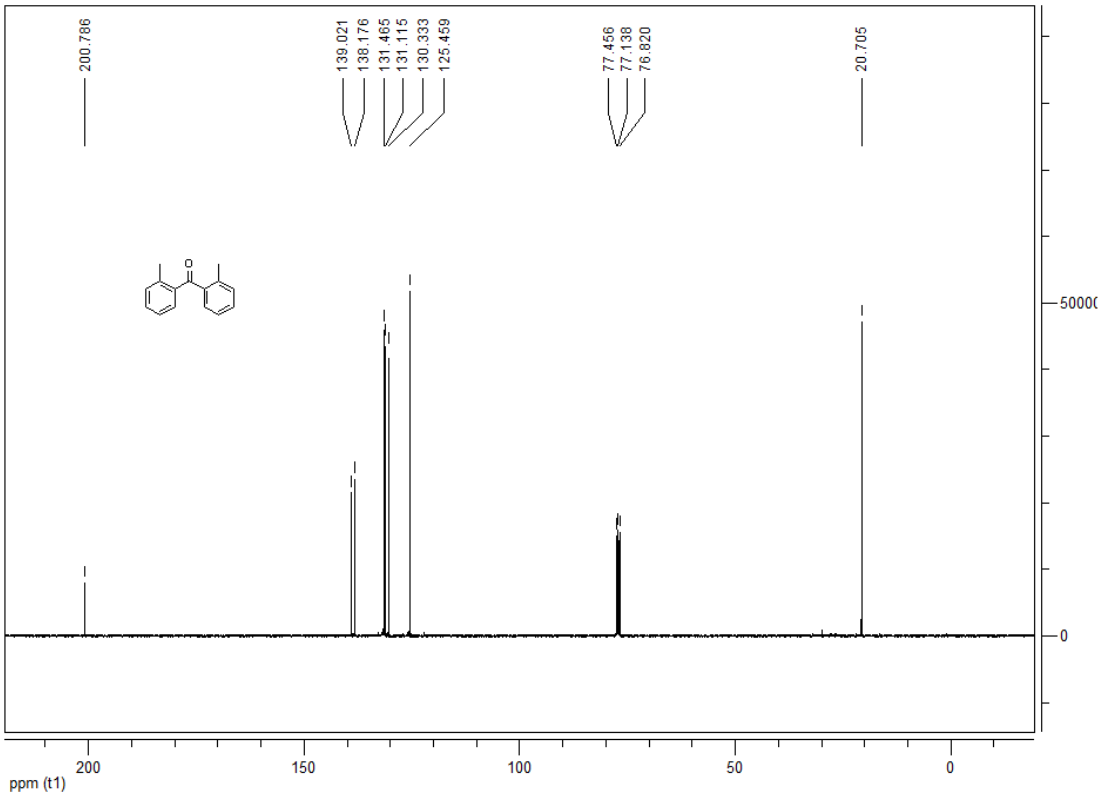


di-*o*-tolylmethanone 3vi

^{1}H NMR

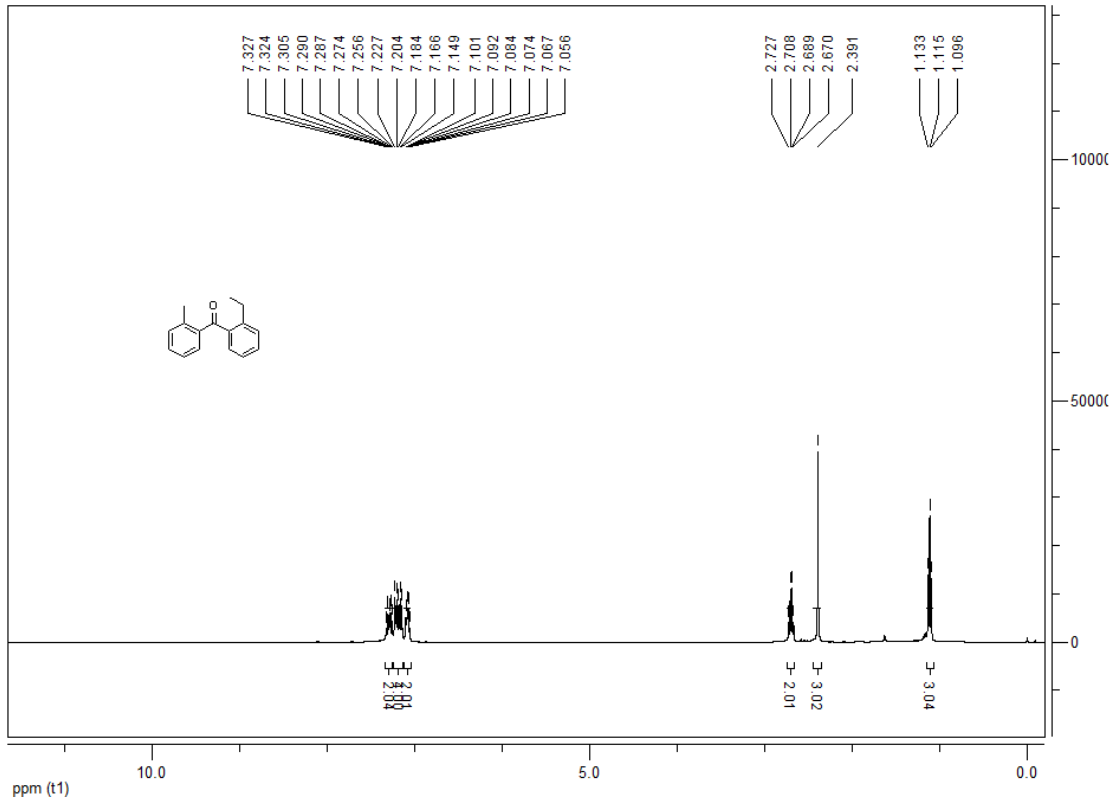


^{13}C NMR

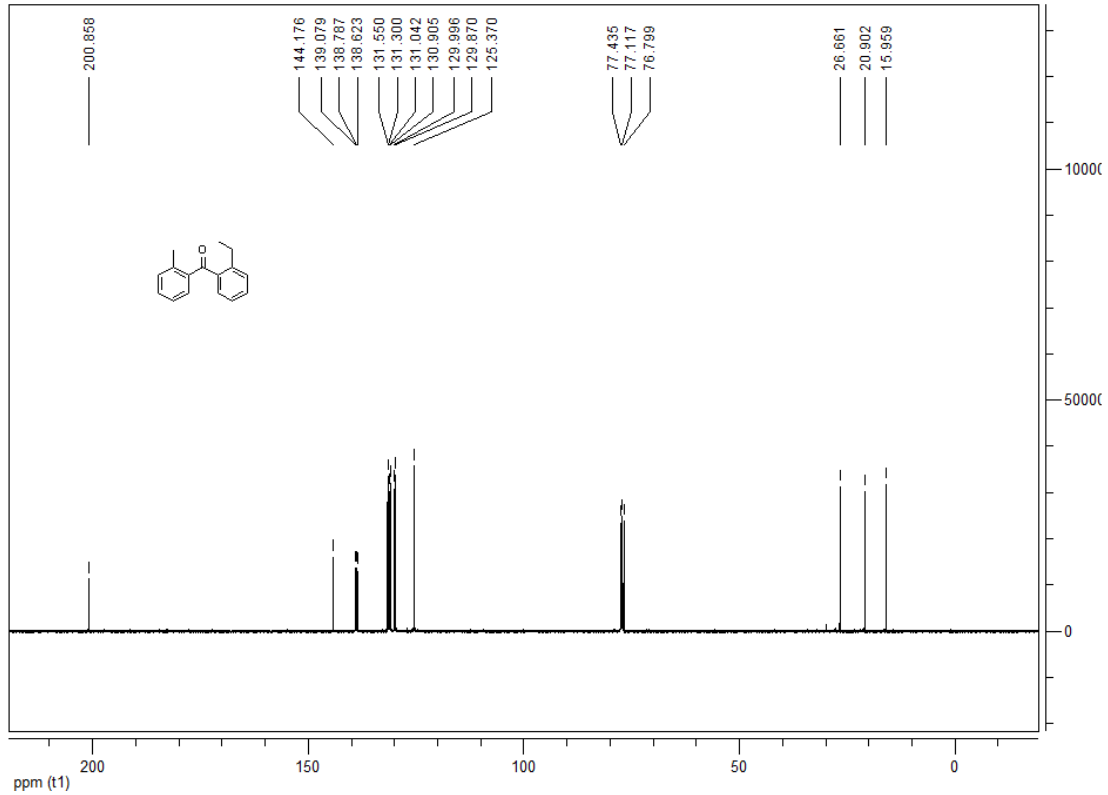


(2-ethylphenyl)(o-tolyl)methanone 3vj

^{1}H NMR

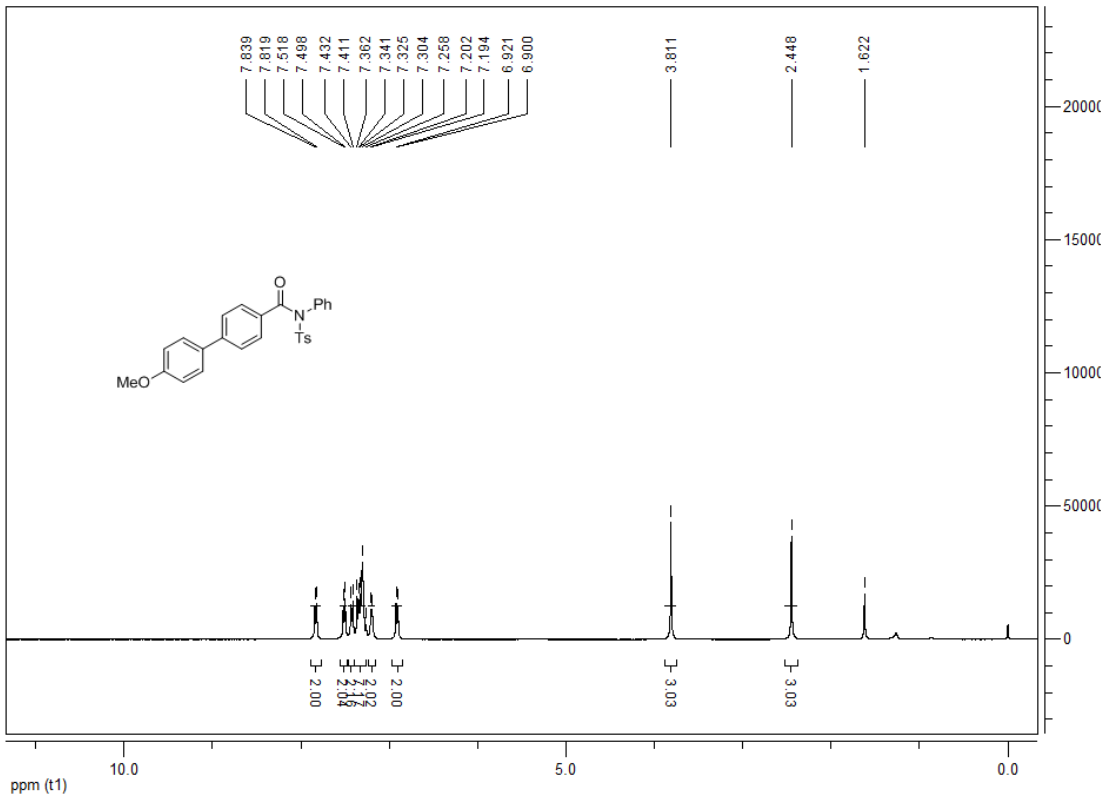


^{13}C NMR

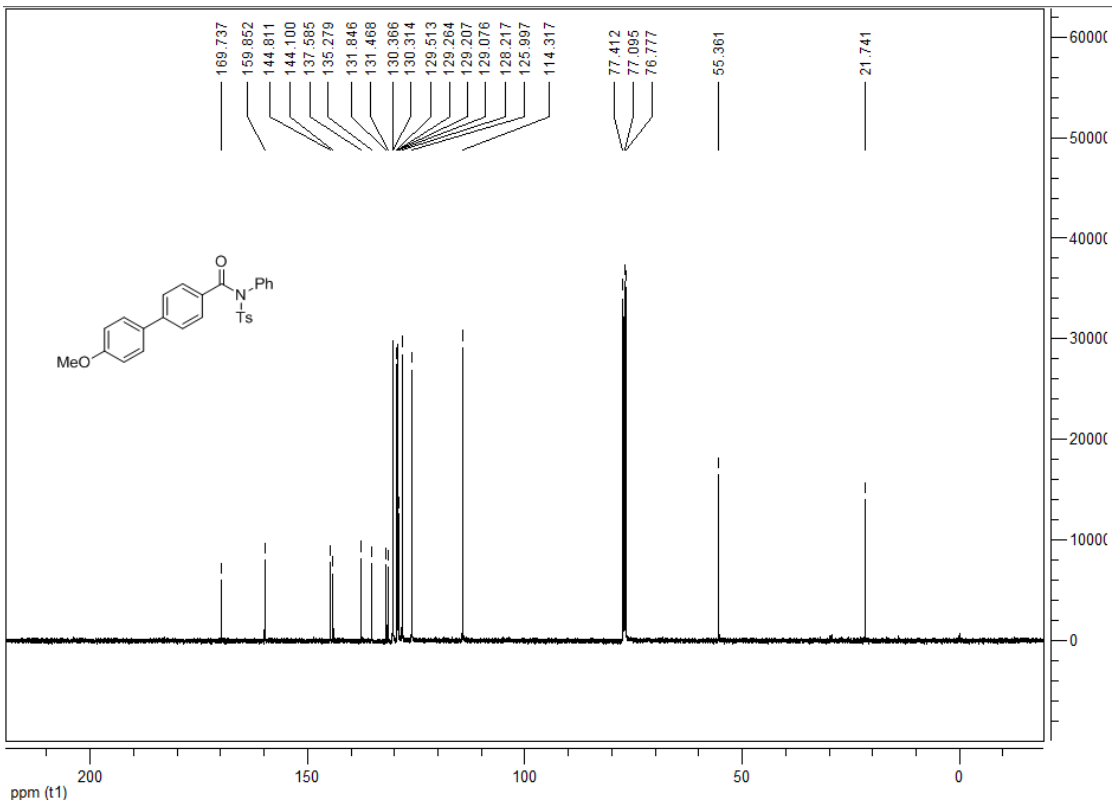


4'-methoxy-N-phenyl-N-tosyl-[1,1'-biphenyl]-4-carboxamide 4

^{1}H NMR

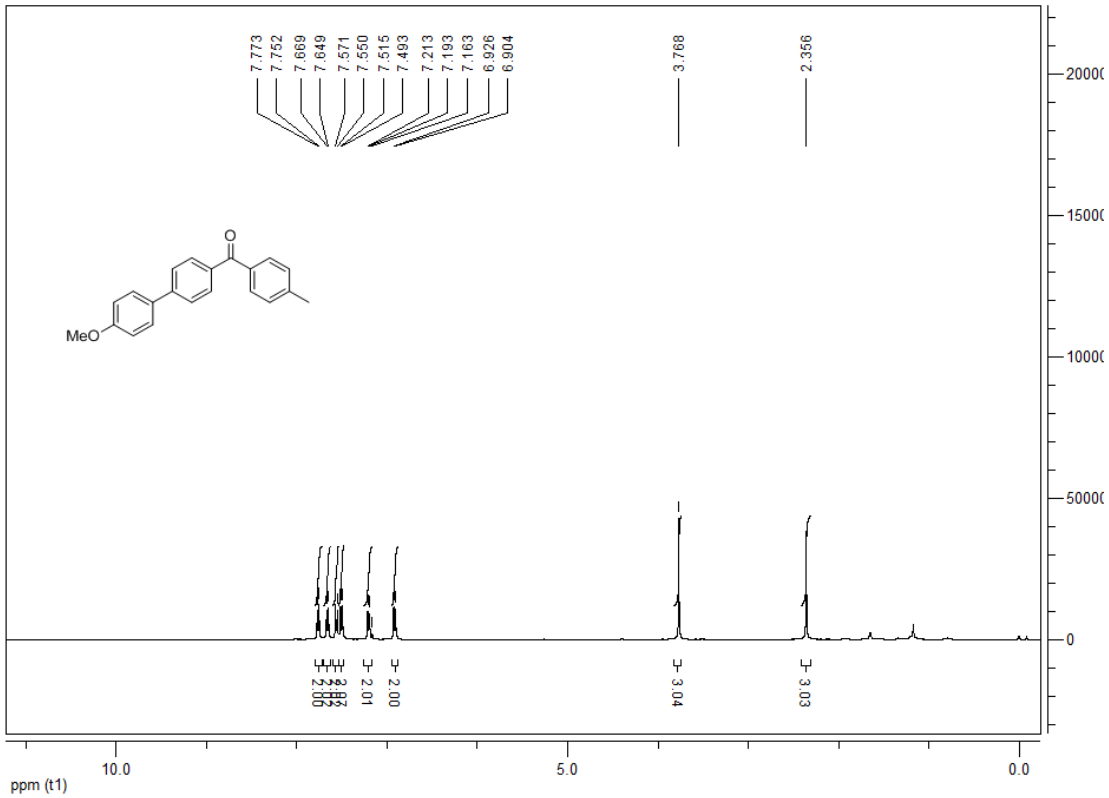


^{13}C NMR

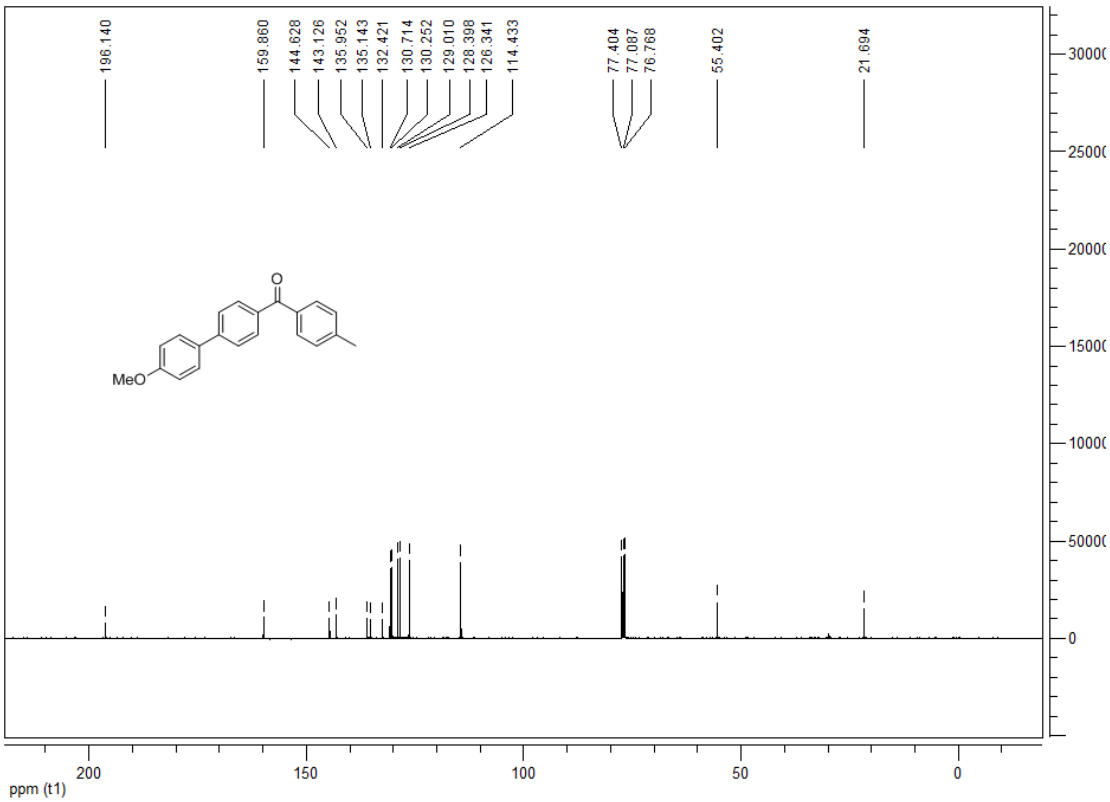


(4'-methoxy-[1,1'-biphenyl]-4-yl)(p-tolyl)methanone 5

^{1}H NMR

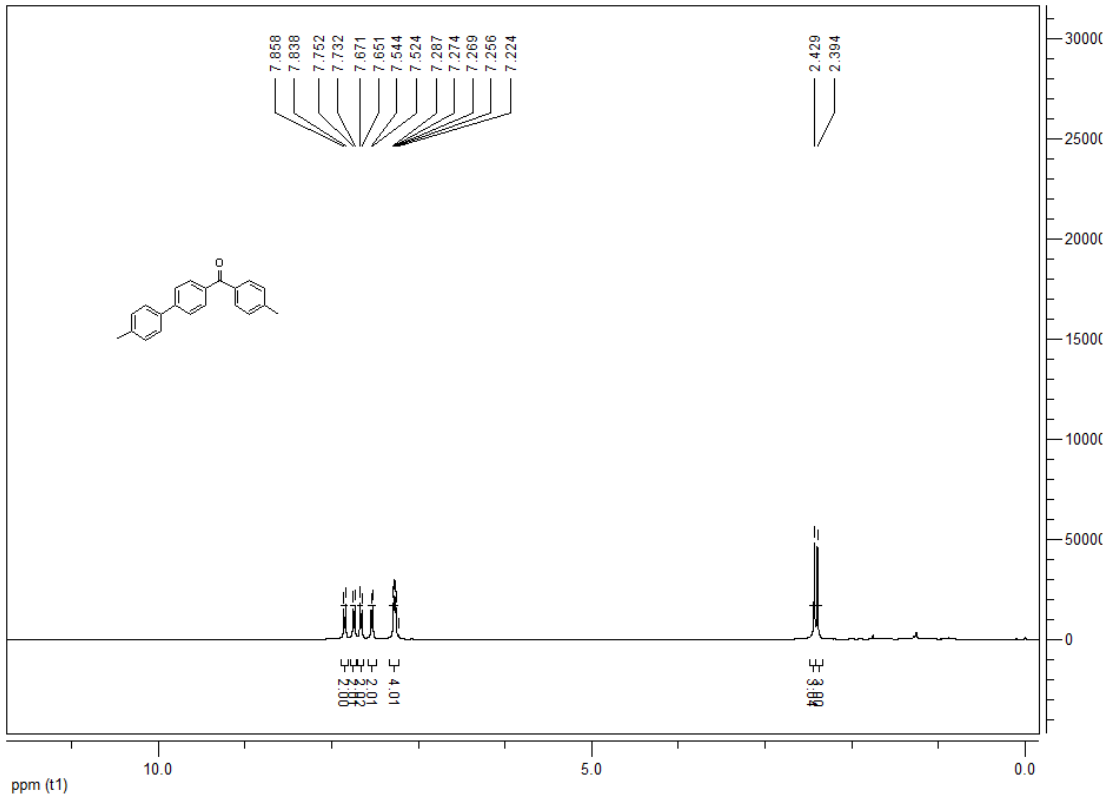


^{13}C NMR

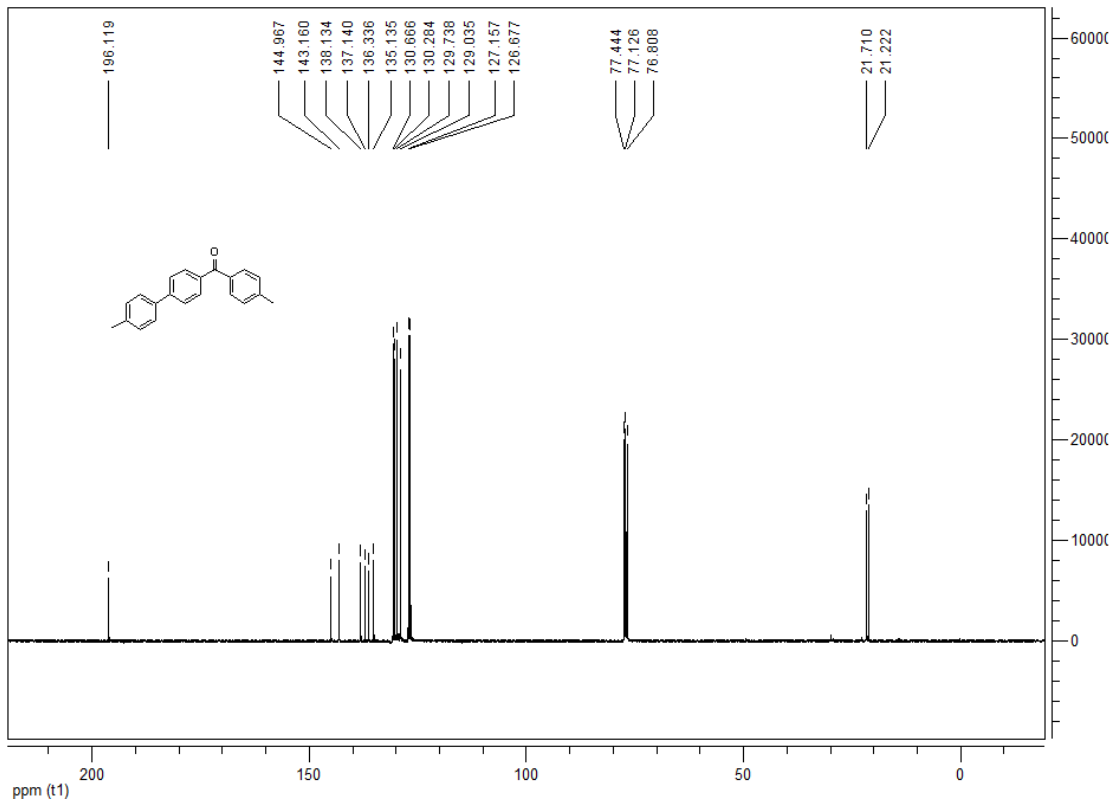


(4'-methyl-[1,1'-biphenyl]-4-yl)(p-tolyl)methanone 6

^{1}H NMR

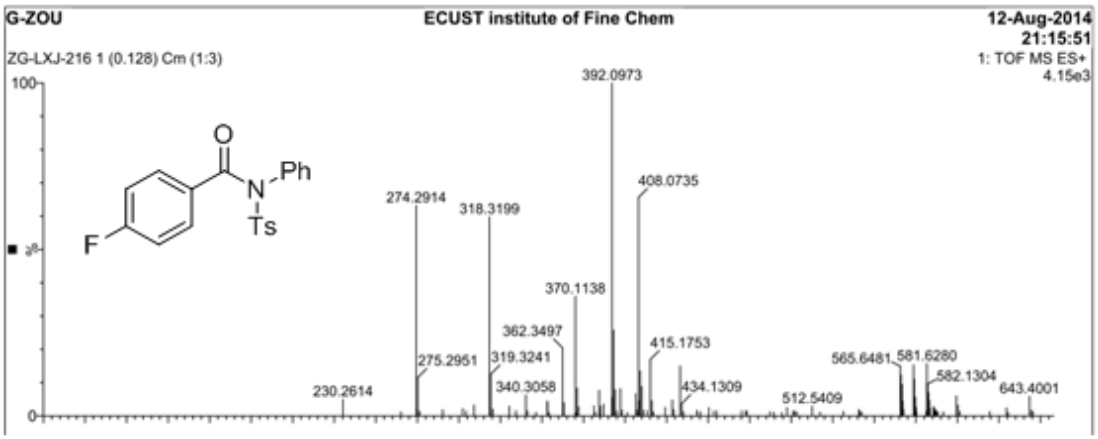


^{13}C NMR

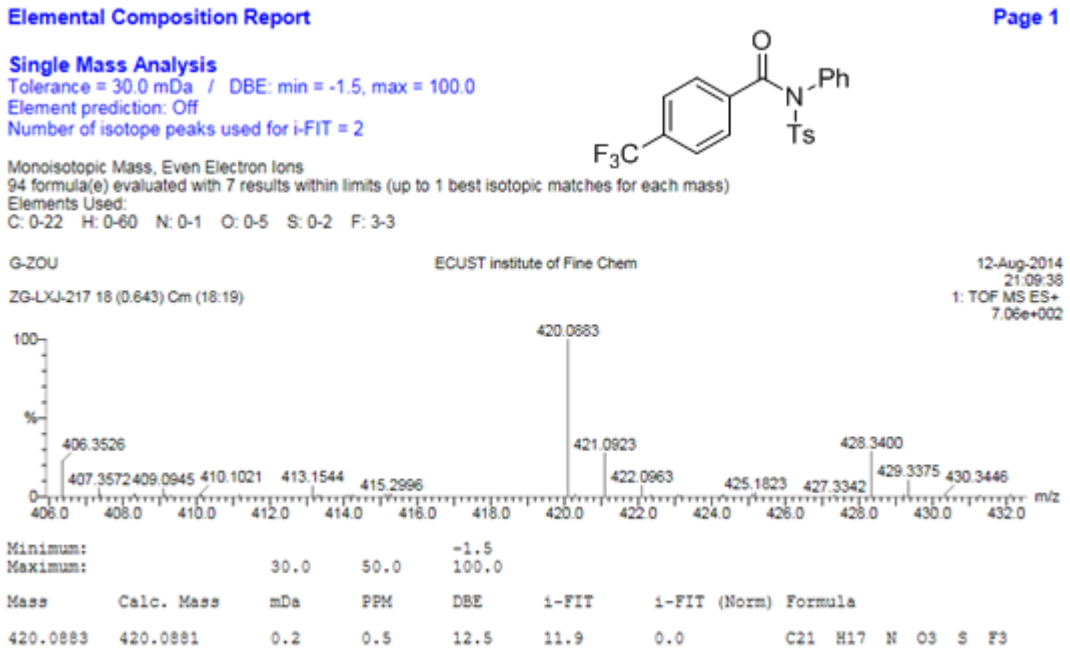


10. HRMS spectra of new compounds

4-fluoro-N-phenyl-N-tosylbenzamide 1e



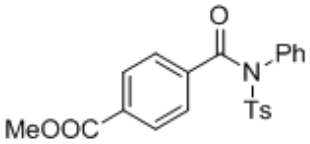
N-phenyl-N-tosyl-4-(trifluoromethyl)benzamide 1f



methyl 4-(phenyl(tosyl)carbamoyl)benzoate 1g

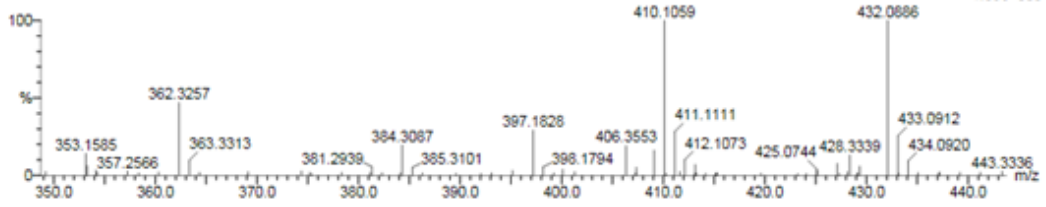
Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions
55 formula(e) evaluated with 3 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-22 H: 0-60 N: 0-1 O: 0-5 S: 0-2

G-ZOU ECUST institute of Fine Chem 12-Aug-2014 21:05:23
ZG-LXJ-219 39 (1.282) Cm (37:40) 1: TOF MS ES+ 1.59e+003

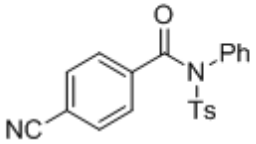


Minimum:				-1.5			
Maximum:		30.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
410.1059	410.1062	-0.3	-0.7	13.5	13.9	0.0	C22 H20 N O5 S

4-cyano-N-phenyl-N-tosylbenzamide 1h

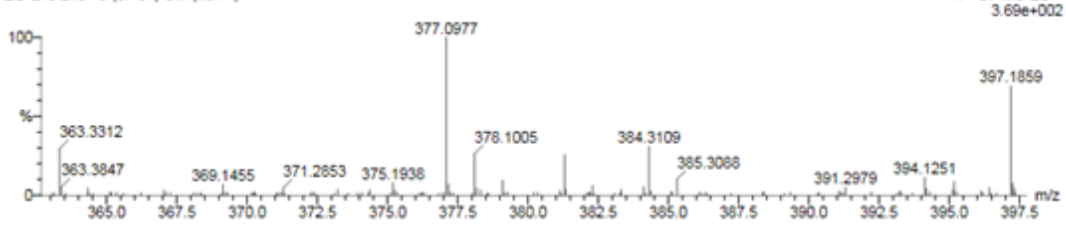
Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions
137 formula(e) evaluated with 10 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-22 H: 0-60 N: 0-2 O: 0-5 S: 0-2

G-ZOU ECUST institute of Fine Chem 12-Aug-2014 21:13:06
ZG-LXJ-218 13 (0.497) Cm (13:14) 1: TOF MS ES+ 3.69e+002

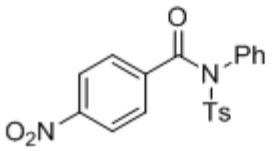


Minimum:				-1.5			
Maximum:		30.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
377.0977	377.0960	1.7	4.5	14.5	37.3	0.0	C21 H17 N2 O3 S

4-nitro-N-phenyl-N-tosylbenzamide 1i

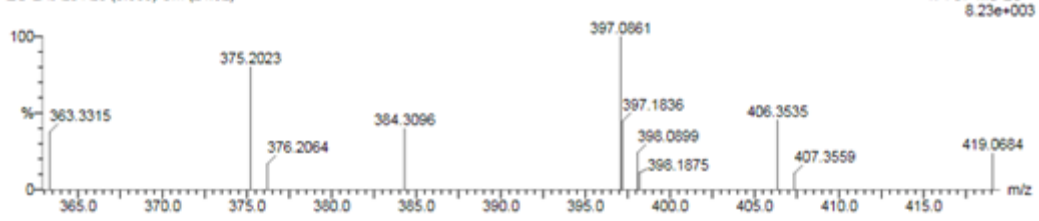
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions
73 formula(e) evaluated with 4 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-23 H: 0-70 N: 0-2 O: 0-5 S: 0-1

G-ZOU ECUST institute of Fine Chem 13-Jul-2014 11:42:20
ZG-LXJ-204 25 (0.866) Cm (24:32) 1: TOF MS ES+ 8.23e+003

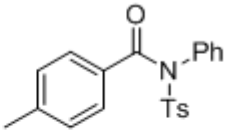


Minimum:				-1.5			
Maximum:		30.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
397.0861	397.0858	0.3	0.8	13.5	37.3	0.0	C20 H17 N2 O5 S

4-methyl-N-phenyl-N-tosylbenzamide 1j

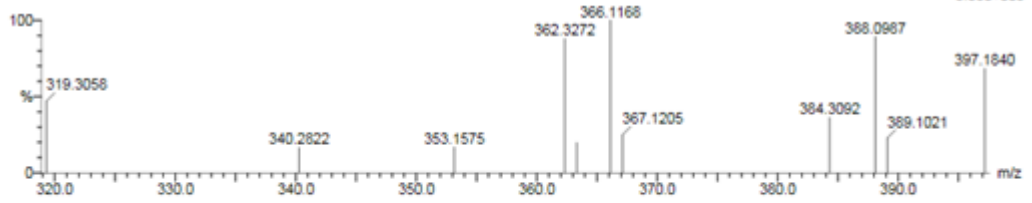
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions
89 formula(e) evaluated with 3 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-22 H: 0-70 N: 0-2 O: 0-5 S: 0-1

G-ZOU ECUST institute of Fine Chem 13-Jul-2014 11:05:44
ZG-LXJ-200 20 (0.691) Cm (17:21) 1: TOF MS ES+ 3.58e+003

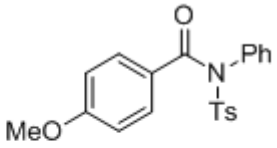


Minimum:				-1.5			
Maximum:		30.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
366.1168	366.1164	0.4	1.1	12.5	6.6	0.0	C21 H20 N O3 S

4-methoxy-N-phenyl-N-tosylbenzamide 1k

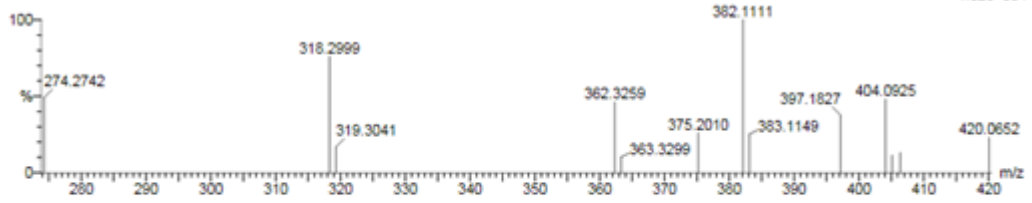
Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions
239 formula(e) evaluated with 10 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-70 N: 0-2 O: 0-8 S: 0-1

G-ZOU ECUST institute of Fine Chem 13-Jul-2014 10:49:46
ZG-LXJ-203 3 (0.176) Cm (1:8) 1: TOF MS ES+ 1.02e+004

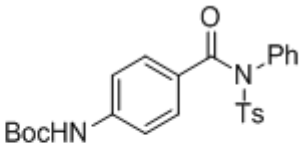


Minimum:				-1.5			
Maximum:		30.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
382.1111	382.1113	-0.2	-0.5	12.5	7.1	0.0	C21 H20 N O4 S

tert-butyl (4-(phenyl(tosyl)carbamoyl)phenyl)carbamate 1l

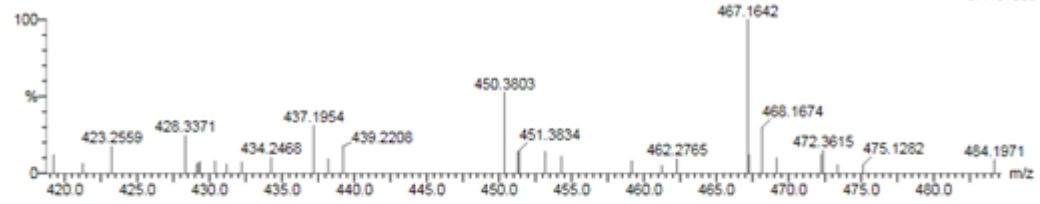
Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions
201 formula(e) evaluated with 15 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-70 N: 0-2 O: 0-8 S: 0-1

G-ZOU ECUST institute of Fine Chem 13-Jul-2014 10:38:46
ZG-LXJ-208 39 (1.282) Cm (37:42) 1: TOF MS ES+ 3.44e+003

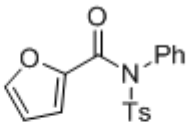


Minimum:				-1.5			
Maximum:		30.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
467.1642	467.1641	0.1	0.2	13.5	19.0	0.0	C25 H27 N2 O5 S

N-phenyl-N-tosylfuran-2-carboxamide 1m

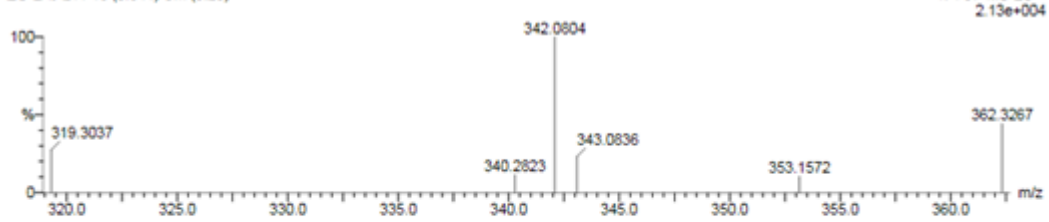
Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions
112 formula(e) evaluated with 4 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-22 H: 0-70 N: 0-2 O: 0-5 S: 0-1

G-ZOU ECUST institute of Fine Chem 13-Jul-2014 11:15:05
ZG-LXJ-211 18 (0.644) Cm (9:23) 1: TOF MS ES+ 2.13e+004

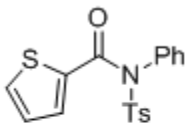


Minimum:				-1.5			
Maximum:		30.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
342.0804	342.0800	0.4	1.2	11.5	9.0	0.0	C18 H16 N O4 S

N-phenyl-N-tosylthiophene-2-carboxamide 1n

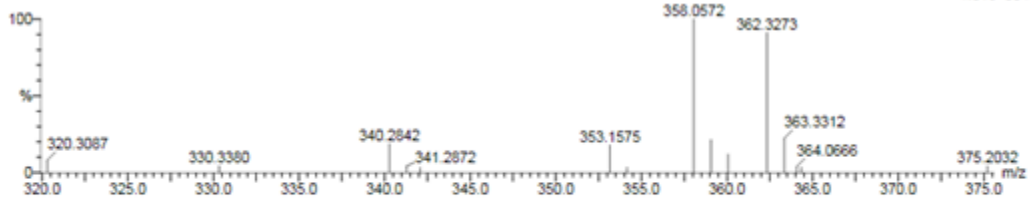
Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions
163 formula(e) evaluated with 7 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-22 H: 0-70 N: 0-2 O: 0-5 S: 0-2

G-ZOU ECUST institute of Fine Chem 13-Jul-2014 11:17:53
ZG-LXJ-212 32 (1.060) Cm (31:44) 1: TOF MS ES+ 1.01e+004

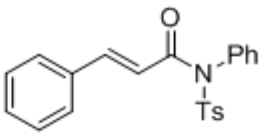


Minimum:				-1.5			
Maximum:		30.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
358.0572	358.0572	0.0	0.0	11.5	7.7	0.0	C18 H16 N O3 S2

N-phenyl-N-tosylcinnamamide 1o

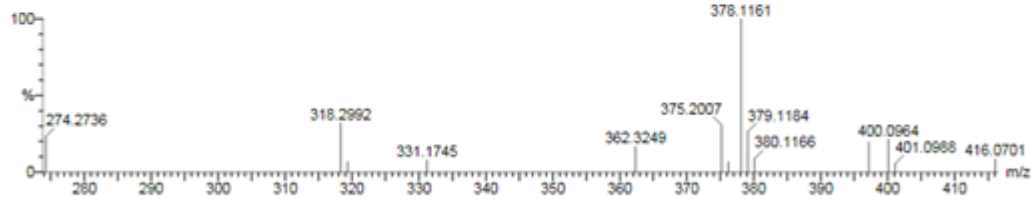
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions
239 formula(e) evaluated with 12 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-70 N: 0-2 O: 0-8 S: 0-1

G-ZOU ECUST institute of Fine Chem 13-Jul-2014 10:43:04
ZG-LXJ-214 27 (0.913) Cm (18:29) 1: TOF MS ES+ 1.65e+004

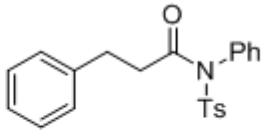


Minimum:				-1.5			
Maximum:		30.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
378.1161	378.1164	-0.3	-0.8	13.5	7.7	0.0	C22 H20 N O3 S

N,3-diphenyl-N-tosylpropanamide 1p

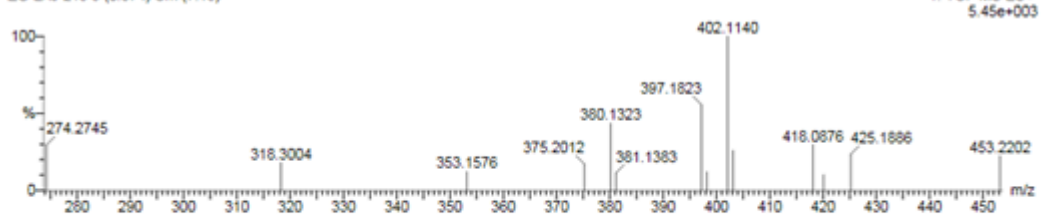
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



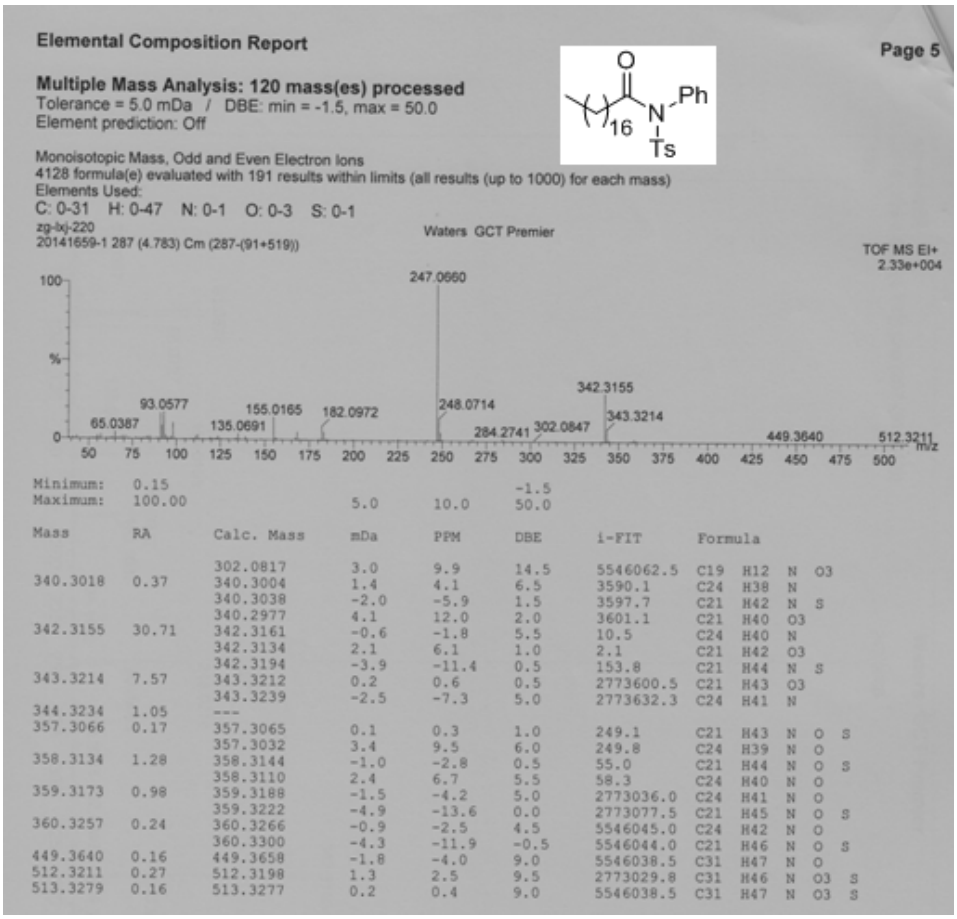
Monoisotopic Mass, Even Electron Ions
487 formula(e) evaluated with 23 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-70 N: 0-2 O: 0-8 S: 0-1 Na: 0-1

G-ZOU ECUST institute of Fine Chem 13-Jul-2014 10:46:51
ZG-LXJ-213 9 (0.374) Cm (7:13) 1: TOF MS ES+ 5.45e+003



Minimum:				-1.5			
Maximum:		30.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
402.1140	402.1140	0.0	0.0	12.5	6.8	0.0	C22 H21 N O3 S Na

N-phenyl-N-tosylstearamide 1q



Elemental Composition Report

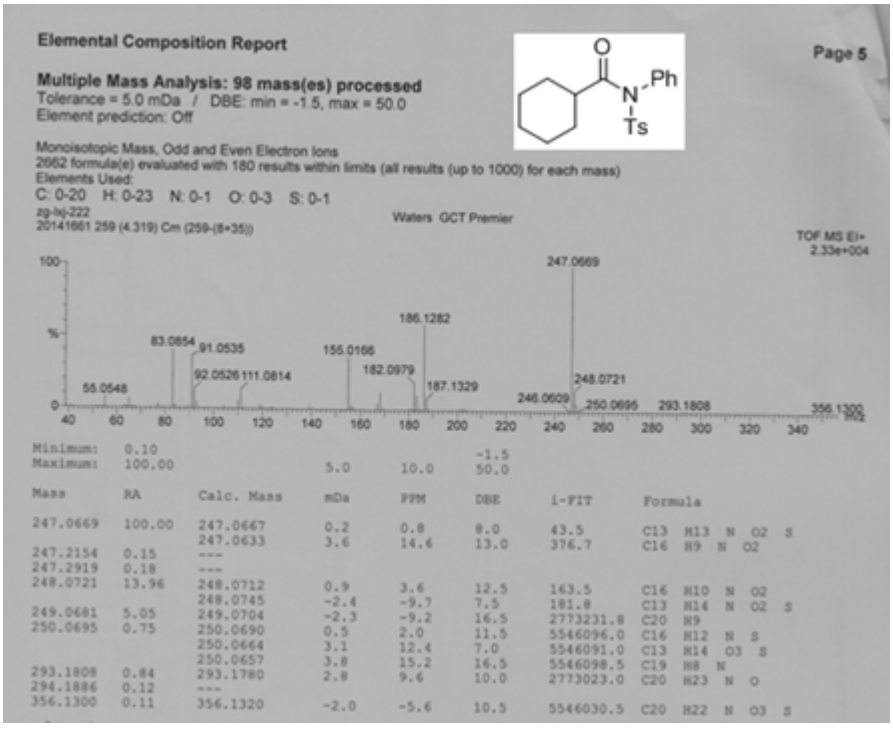
Page 5

Multiple Mass Analysis: 120 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
4128 formula(e) evaluated with 191 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-31 H: 0-47 N: 0-1 O: 0-3 S: 0-1
zg-lxj-220
20141659-1 287 (4.783) Cm (287-(91+519))
Waters GCT Premier
TOF MS EI+
2.33e+004

Minimum:	0.15				-1.5		
Maximum:	100.00		5.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
		302.0817	3.0	9.9	14.5	5546062.5	C19 H12 N O3
340.3018	0.37	340.3004	1.4	4.1	6.5	3590.1	C24 H38 N
		340.3038	-2.0	-5.9	1.5	3597.7	C21 H42 N S
		340.2977	4.1	12.0	2.0	3601.1	C21 H40 O3
342.3155	30.71	342.3161	-0.6	-1.8	5.5	10.5	C24 H40 N
		342.3134	2.1	6.1	1.0	2.1	C21 H42 O3
		342.3194	-3.9	-11.4	0.5	153.8	C21 H44 N S
343.3214	7.57	343.3212	0.2	0.6	0.5	2773600.5	C21 H43 O3
		343.3239	-2.5	-7.3	5.0	2773632.3	C24 H41 N
344.3234	1.05	---					
357.3066	0.17	357.3065	0.1	0.3	1.0	249.1	C21 H43 N O S
		357.3032	3.4	9.5	6.0	249.8	C24 H39 N O
358.3134	1.28	358.3144	-1.0	-2.8	0.5	55.0	C21 H44 N O S
		358.3110	2.4	6.7	5.5	58.3	C24 H40 N O
359.3173	0.98	359.3188	-1.5	-4.2	5.0	2773036.0	C24 H41 N O
		359.3222	-4.9	-13.6	0.0	2773077.5	C21 H45 N O S
360.3257	0.24	360.3266	-0.9	-2.5	4.5	5546045.0	C24 H42 N O
		360.3300	-4.3	-11.9	-0.5	5546044.0	C21 H46 N O S
449.3640	0.16	449.3658	-1.8	-4.0	9.0	5546038.5	C31 H47 N O
512.3211	0.27	512.3198	1.3	2.5	9.5	2773029.8	C31 H46 N O3 S
513.3279	0.16	513.3277	0.2	0.4	9.0	5546038.5	C31 H47 N O3 S

N-phenyl-N-tosylcyclohexanecarboxamide 1r



Elemental Composition Report

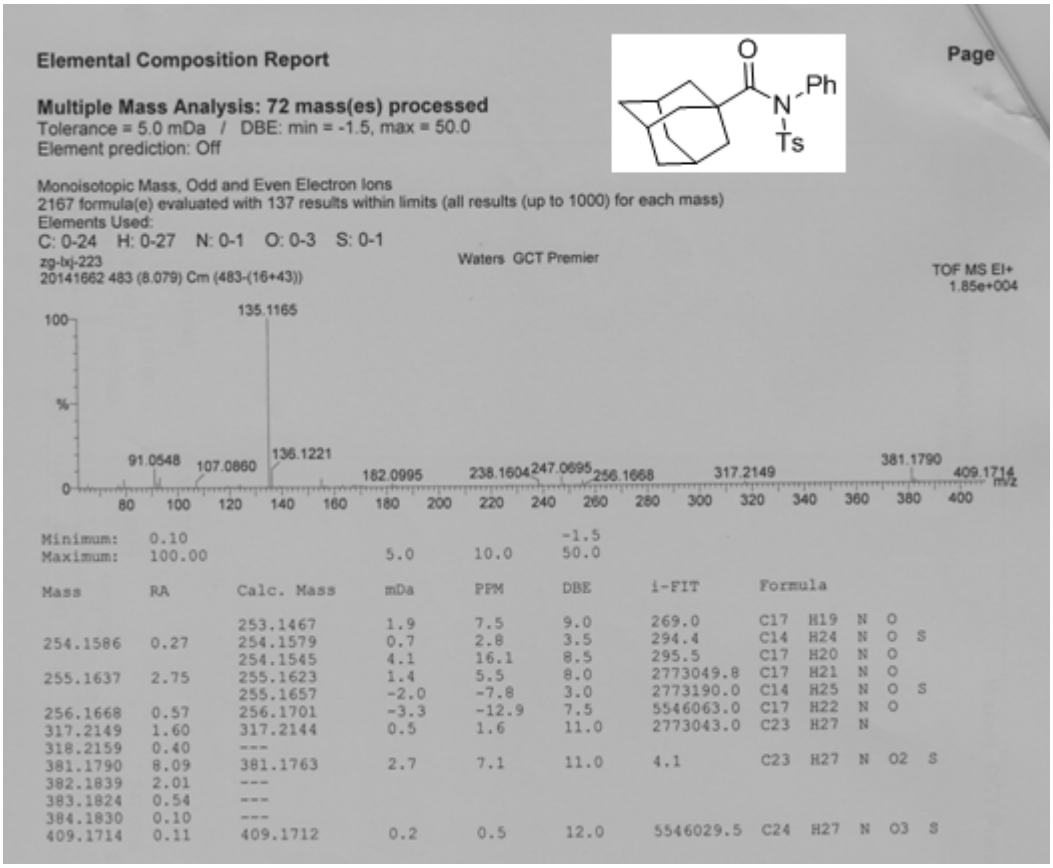
Page 5

Multiple Mass Analysis: 98 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
2662 formula(e) evaluated with 180 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-20 H: 0-23 N: 0-1 O: 0-3 S: 0-1
zg-lxj-222
20141661 259 (4.319) Cm (259-(8+35))
Waters GCT Premier
TOF MS EI+
2.33e+004

Minimum:	0.10				-1.5		
Maximum:	100.00		5.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
247.0669	100.00	247.0667	0.2	0.8	8.0	43.5	C13 H13 N O2 S
		247.0633	3.6	14.6	13.0	376.7	C16 H9 N O2
247.2154	0.15	---					
247.2919	0.18	---					
248.0721	13.96	248.0712	0.9	3.6	12.5	163.5	C16 H10 N O2
		248.0745	-2.4	-9.7	7.5	181.8	C13 H14 N O2 S
249.0681	5.05	249.0704	-2.3	-9.2	16.5	2773231.8	C20 H9
250.0695	0.75	250.0690	0.5	2.0	11.5	5546096.0	C16 H12 N S
		250.0664	3.1	12.4	7.0	5546091.0	C13 H14 O3 S
		250.0657	3.8	15.2	16.5	5546098.5	C19 H8 N
293.1808	0.84	293.1780	2.8	9.6	10.0	2773023.0	C20 H23 N O
294.1886	0.12	---					
356.1300	0.11	356.1320	-2.0	-5.6	10.5	5546030.5	C20 H22 N O3 S

(3r,5r,7r)-N-phenyl-N-tosyladamantane-1-carboxamide 1s



Elemental Composition Report

Page

Multiple Mass Analysis: 72 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
2167 formula(e) evaluated with 137 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-24 H: 0-27 N: 0-1 O: 0-3 S: 0-1

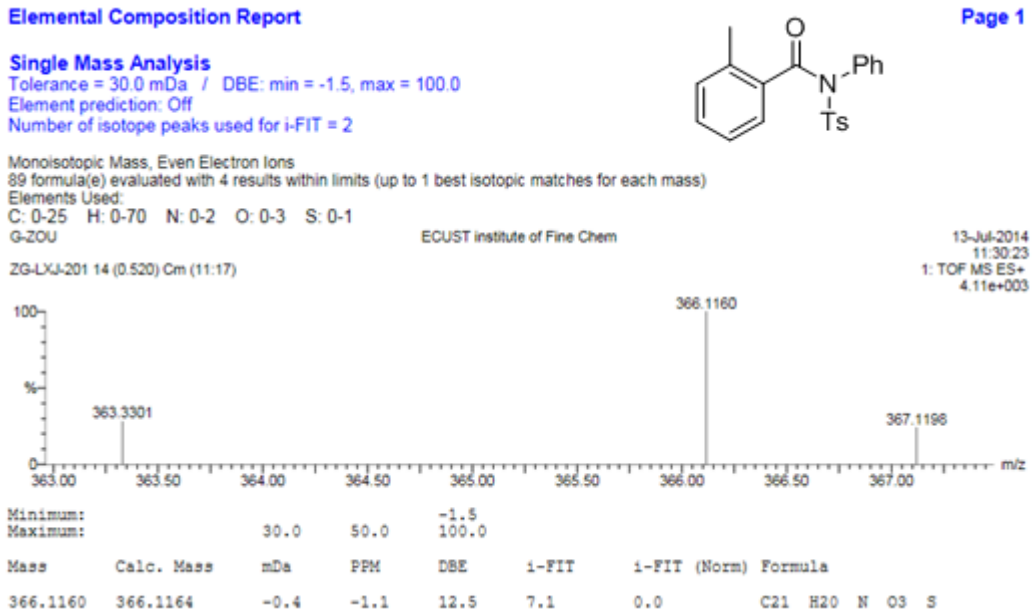
zg-lxj-223
20141662 483 (8.079) Cm (483-(16+43))

Waters GCT Premier

TOF MS EI+
1.85e+004

Minimum:	0.10				-1.5		
Maximum:	100.00		5.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
		253.1467	1.9	7.5	9.0	269.0	C17 H19 N O
254.1586	0.27	254.1579	0.7	2.8	3.5	294.4	C14 H24 N O S
		254.1545	4.1	16.1	8.5	295.5	C17 H20 N O
255.1637	2.75	255.1623	1.4	5.5	8.0	2773049.8	C17 H21 N O
		255.1657	-2.0	-7.8	3.0	2773190.0	C14 H25 N O S
256.1668	0.57	256.1701	-3.3	-12.9	7.5	5546063.0	C17 H22 N O
317.2149	1.60	317.2144	0.5	1.6	11.0	2773043.0	C23 H27 N
318.2159	0.40	---					
381.1790	8.09	381.1763	2.7	7.1	11.0	4.1	C23 H27 N O2 S
382.1839	2.01	---					
383.1824	0.54	---					
384.1830	0.10	---					
409.1714	0.11	409.1712	0.2	0.5	12.0	5546029.5	C24 H27 N O3 S

2-methyl-N-phenyl-N-tosylbenzamide 1t



Elemental Composition Report

Page 1

Single Mass Analysis
Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
89 formula(e) evaluated with 4 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-70 N: 0-2 O: 0-3 S: 0-1

G-ZOU

ECUST institute of Fine Chem

13-Jul-2014
11:30:23
1: TOF MS ES+
4.11e+003

ZG-LXJ-201 14 (0.520) Cm (11:17)

Minimum:				-1.5		
Maximum:		30.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
366.1160	366.1164	-0.4	-1.1	12.5	7.1	0.0	C21 H20 N O3 S

(3r,5r,7r)-N-(3,5-bis(trifluoromethyl)phenyl)-N-tosyladamantane-1-carboxamide 1u

National Center for Organic Mass Spectrometry

Shanghai Institute of Organic Chemistry

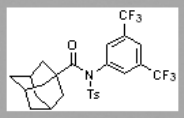
Chinese Academy of Sciences

High Resolution MS Data Report

Instrument

Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS

Card Serial Number	E141918
Analysis Name	D:\Data\zfj2014\20141203_000006.d
Sample Name	lxj-233
Acquisition Date	12/3/2014 9:58:24 AM
Operator:	zfj
Ionization Mode	ESI-Positive
Ion Mass (Measured)	568.1356



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 25 H 24 F 5 N 1 Na 1 O 7	0.164	568.1365	1.67	1.67	0.95	11.50	ok	even
C 25 H 28 F 3 Na 1 O 8 S 1	0.151	568.1349	-1.14	-1.14	-0.65	10.00	ok	odd
C 26 H 25 F 6 N 1 Na 1 O 3 S 1	0.156	568.1352	-0.72	-0.72	-0.41	11.50	ok	even
C 27 H 26 F 1 Na 1 O 11	0.153	568.1351	-0.76	-0.76	-0.43	14.00	ok	odd
C 27 H 29 Na 1 O 10 S 1	0.164	568.1374	3.16	3.16	1.80	13.00	ok	odd

N-(3,5-bis(trifluoromethyl)phenyl)-2-methyl-N-tosylbenzamide 1v

National Center for Organic Mass Spectrometry

Shanghai Institute of Organic Chemistry

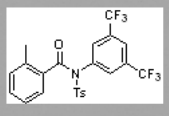
Chinese Academy of Sciences

High Resolution MS Data Report

Instrument

Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS

Card Serial Number	E141921
Analysis Name	D:\Data\zfj2014\20141203_000007.d
Sample Name	lxj-236
Acquisition Date	12/3/2014 10:02:57 AM
Operator:	zfj
Ionization Mode	ESI-Positive
Ion Mass (Measured)	524.0731

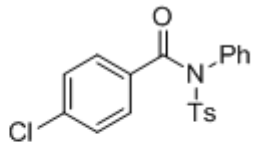


Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 21 H 19 F 2 Na 1 O 12	0.138	524.0737	1.08	1.08	0.56	11.00	ok	odd
C 22 H 16 F 5 N 1 Na 1 O 7	0.144	524.0739	1.53	1.53	0.80	12.50	ok	even
C 22 H 20 F 3 Na 1 O 8 S 1	0.134	524.0723	-1.52	-1.52	-0.80	11.00	ok	odd
C 23 H 17 F 6 N 1 Na 1 O 3 S 1	0.139	524.0726	-1.07	-1.07	-0.56	12.50	ok	even
C 24 H 18 F 1 Na 1 O 11	0.136	524.0725	-1.10	-1.10	-0.58	15.00	ok	odd
C 24 H 21 Na 1 O 10 S 1	0.146	524.0748	3.15	3.15	1.65	14.00	ok	odd

4-chloro-N-phenyl-N-tosylbenzamide 1w

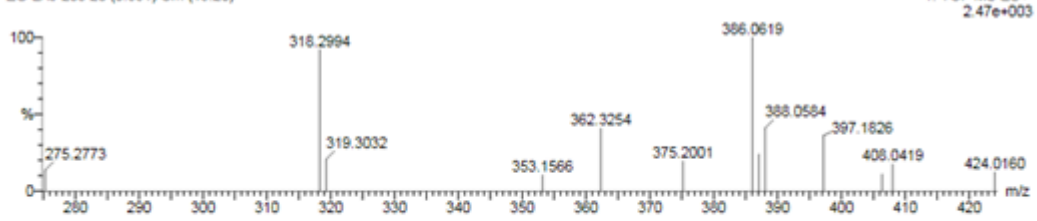
Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions
258 formula(e) evaluated with 11 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-70 N: 0-2 O: 0-3 S: 0-1 Cl: 0-2

G-ZOU ECUST institute of Fine Chem 13-Jul-2014 10:52:58
ZG-LXJ-205 20 (0.691) Cm (19:20) 1: TOF MS ES+ 2.47e+003

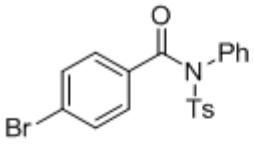


Minimum:				-1.5			
Maximum:		30.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
386.0619	386.0618	0.1	0.3	12.5	6.5	0.0	C20 H17 N O3 S Cl

4-bromo-N-phenyl-N-tosylbenzamide 1x

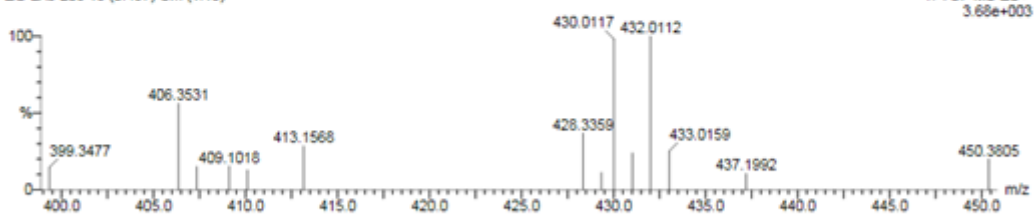
Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2



Monoisotopic Mass, Even Electron Ions
265 formula(e) evaluated with 10 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-22 H: 0-70 N: 0-2 O: 0-5 S: 0-1 Br: 0-2

G-ZOU ECUST institute of Fine Chem 13-Jul-2014 11:02:19
ZG-LXJ-206 13 (0.497) Cm (1:13) 1: TOF MS ES+ 3.68e+003



Minimum:				-1.5			
Maximum:		30.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
430.0117	430.0113	0.4	0.9	12.5	8.5	0.0	C20 H17 N O3 S Br

N-(4-acetylphenyl)-2-methyl-N-tosylbenzamide 1t-1

National Center for Organic Mass Spectrometry

Shanghai Institute of Organic Chemistry

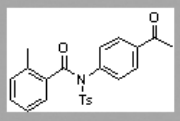
Chinese Academy of Sciences

High Resolution MS Data Report

Instrument

Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS

Card Serial Number	E141917
Analysis Name	D:\Data\zfj2014\20141203_000006.d
Sample Name	lxj-234
Acquisition Date	12/3/2014 9:58:24 AM
Operator:	zfj
Ionization Mode	ESI-Positive
Ion Mass (Measured)	430.1085



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 23 H 21 N 1 Na 1 O 4 S 1	0.139	430.1083	-0.37	-0.37	-0.16	13.50	ok	even

N-(2,4-difluorophenyl)-2-methyl-N-tosylbenzamide 1t-2

National Center for Organic Mass Spectrometry

Shanghai Institute of Organic Chemistry

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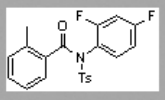
High Resolution MS Data Report

Instrument

Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS

Card Serial Number	E141919
Analysis Name	D:\Data\zfj2014\20141203_000007.d
Sample Name	lxj-239
Acquisition Date	12/3/2014 10:02:57 AM
Operator:	zfj
Ionization Mode	ESI-Positive
Ion Mass (Measured)	424.0792



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 20 H 16 F 1 N 1 Na 1 O 7	0.056	424.0803	2.68	2.49	1.14	12.50	ok	even
C 21 H 17 F 2 N 1 Na 1 O 3 S 1	0.054	424.0789	-0.52	-0.90	-0.22	12.50	ok	even
C 23 H 15 N 1 Na 1 O 6	0.042	424.0792	-0.01	-0.29	-0.00	16.50	ok	even
C 24 H 16 F 1 N 1 Na 1 O 2 S 1	0.048	424.0778	-3.22	-3.62	-1.36	16.50	ok	even

2-methyl-N-tosyl-N-(3-(trifluoromethyl)phenyl)benzamide 1t-3

National Center for Organic Mass Spectrometry

Shanghai Institute of Organic Chemistry

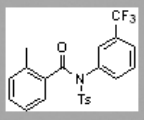
Chinese Academy of Sciences

High Resolution MS Data Report

Instrument

Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS

Card Serial Number	E141916
Analysis Name	D:\Data\zfj2014\20141203_000006.d
Sample Name	lxj-237
Acquisition Date	12/3/2014 9:58:24 AM
Operator:	zfj
Ionization Mode	ESI-Positive
Ion Mass (Measured)	456.0857



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 21 H 17 F 2 N 1 Na 1 O 7	0.138	456.0865	1.83	1.83	0.83	12.50	ok	even
C 21 H 21 Na 1 O 8 S 1	0.129	456.0849	-1.67	-1.67	-0.76	11.00	ok	odd
C 22 H 18 F 3 N 1 Na 1 O 3 S 1	0.133	456.0852	-1.15	-1.15	-0.53	12.50	ok	even
C 24 H 16 F 1 N 1 Na 1 O 6	0.157	456.0854	-0.68	-0.68	-0.31	16.50	ok	even
C 24 H 19 N 1 Na 1 O 5 S 1	0.145	456.0876	4.21	4.21	1.92	15.50	ok	even
C 25 H 17 F 2 N 1 Na 1 O 2 S 1	0.149	456.0840	-3.66	-3.66	-1.67	16.50	ok	even

2-methyl-N-tosyl-N-(4-(trifluoromethyl)phenyl)benzamide 1t-4

National Center for Organic Mass Spectrometry

Shanghai Institute of Organic Chemistry

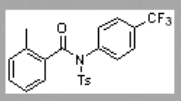
Chinese Academy of Sciences

High Resolution MS Data Report

Instrument

Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS

Card Serial Number	E141920
Analysis Name	D:\Data\zfj2014\20141203_000007.d
Sample Name	lxj-235
Acquisition Date	12/3/2014 10:02:57 AM
Operator:	zfj
Ionization Mode	ESI-Positive
Ion Mass (Measured)	456.0859



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 21 H 17 F 2 N 1 Na 1 O 7	0.041	456.0865	1.42	1.16	0.65	12.50	ok	even
C 21 H 21 Na 1 O 8 S 1	0.053	456.0849	-2.08	-2.43	-0.95	11.00	ok	odd
C 22 H 18 F 3 N 1 Na 1 O 3 S 1	0.046	456.0852	-1.56	-1.95	-0.71	12.50	ok	even
C 24 H 16 F 1 N 1 Na 1 O 6	0.031	456.0854	-1.08	-1.39	-0.49	16.50	ok	even
C 24 H 19 N 1 Na 1 O 5 S 1	0.048	456.0876	3.80	3.48	1.73	15.50	ok	even
C 25 H 17 F 2 N 1 Na 1 O 2 S 1	0.045	456.0840	-4.07	-4.43	-1.85	16.50	ok	even
C 27 H 15 N 1 Na 1 O 5	0.031	456.0842	-3.59	-3.88	-1.64	20.50	ok	even

N-(3,5-difluorophenyl)-2-methyl-N-tosylbenzamide 1t-5

National Center for Organic Mass Spectrometry

Shanghai Institute of Organic Chemistry

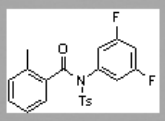
Chinese Academy of Sciences

High Resolution MS Data Report

Instrument

Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS

Card Serial Number	E141915
Analysis Name	D:\Data\zfj2014\20141203_000006.d
Sample Name	lxj-238
Acquisition Date	12/3/2014 9:58:24 AM
Operator:	zfj
Ionization Mode	ESI-Positive
Ion Mass (Measured)	424.0791



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 20 H 16 F 1 N 1 Na 1 O 7	0.062	424.0803	2.85	2.31	1.21	12.50	ok	even
C 21 H 17 F 2 N 1 Na 1 O 3 S 1	0.058	424.0789	-0.36	-1.11	-0.15	12.50	ok	even
C 23 H 15 N 1 Na 1 O 6	0.047	424.0792	0.15	-0.49	0.06	16.50	ok	even
C 24 H 16 F 1 N 1 Na 1 O 2 S 1	0.050	424.0778	-3.06	-3.84	-1.30	16.50	ok	even

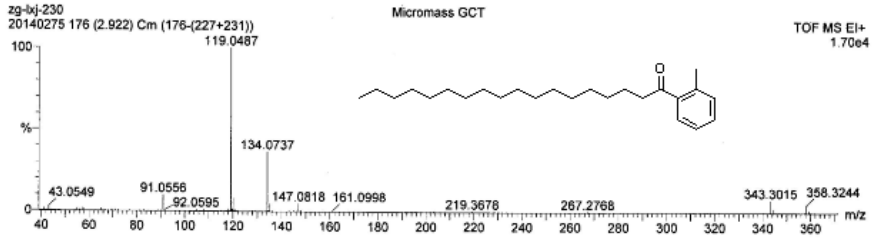
1-(o-tolyl)octadecan-1-one 3qi

Elemental Composition Report Page 1

Multiple Mass Analysis: 8 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
34 formula(e) evaluated with 8 results within limits (up to 50 closest results for each mass)

zg-lxj-230
20140275 176 (2.922) Cm (176-(227+231))
Micromass GCT
TOF MS EI+
1.70e4



Minimum:	3.00				-1.5		
Maximum:	100.00		5.0	5.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
91.0556	9.79	91.0548	0.8	9.1	4.5	1	C7 H7
119.0487	100.00	119.0497	-1.0	-8.3	5.5	1	C8 H7 O
120.0539	7.87	120.0575	-3.6	-30.1	5.0	1	C8 H8 O
134.0737	36.38	134.0732	0.5	4.0	5.0	1	C9 H10 O
135.0782	4.47	135.0810	-2.8	-20.7	4.5	1	C9 H11 O
147.0818	4.87	147.0810	0.8	5.5	5.5	1	C10 H11 O
343.3015	7.45	343.3001	1.4	4.1	5.5	1	C24 H39 O
358.3244	4.37	358.3236	0.8	2.3	5.0	1	C25 H42 O

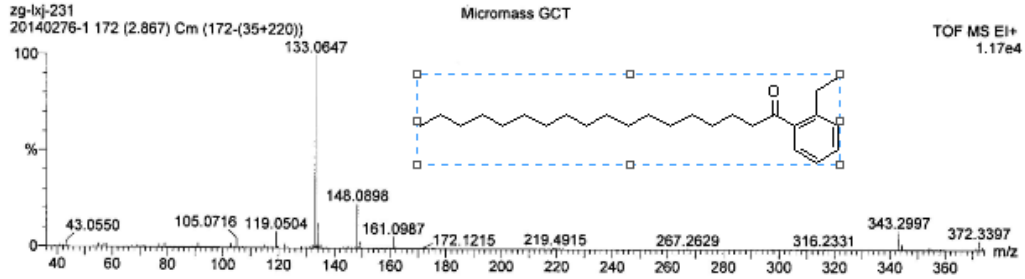
1-(2-ethylphenyl)octadecan-1-one 3qj

Elemental Composition Report Pag

Multiple Mass Analysis: 9 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
43 formula(e) evaluated with 9 results within limits (up to 50 closest results for each mass)

zg-lxj-231
20140276-1 172 (2.867) Cm (172-(35+220))



Minimum:	3.00				-1.5		
Maximum:	100.00		5.0	5.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
105.0716	4.57	105.0704	1.2	11.2	4.5	1	C8 H9
119.0504	8.18	119.0497	0.7	6.0	5.5	1	C8 H7 O
133.0647	100.00	133.0653	-0.6	-4.8	5.5	1	C9 H9 O
134.0706	12.69	134.0732	-2.6	-19.1	5.0	1	C9 H10 O
148.0898	23.00	148.0888	1.0	6.7	5.0	1	C10 H12 O
149.0948	3.22	149.0966	-1.8	-12.3	4.5	1	C10 H13 O
161.0987	5.92	161.0966	2.1	12.8	5.5	1	C11 H13 O
343.2997	9.52	343.3001	-0.4	-1.1	5.5	1	C24 H39 O
372.3397	4.26	372.3392	0.5	1.3	5.0	1	C26 H44 O

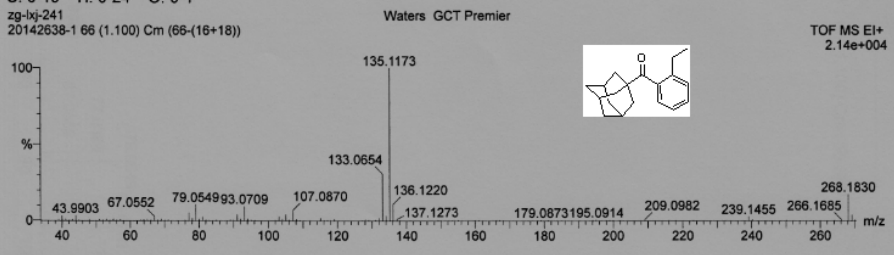
(3r,5r,7r)-adamantan-1-yl(2-ethylphenyl)methanone 3uj

Elemental Composition Report Page 1

Multiple Mass Analysis: 15 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

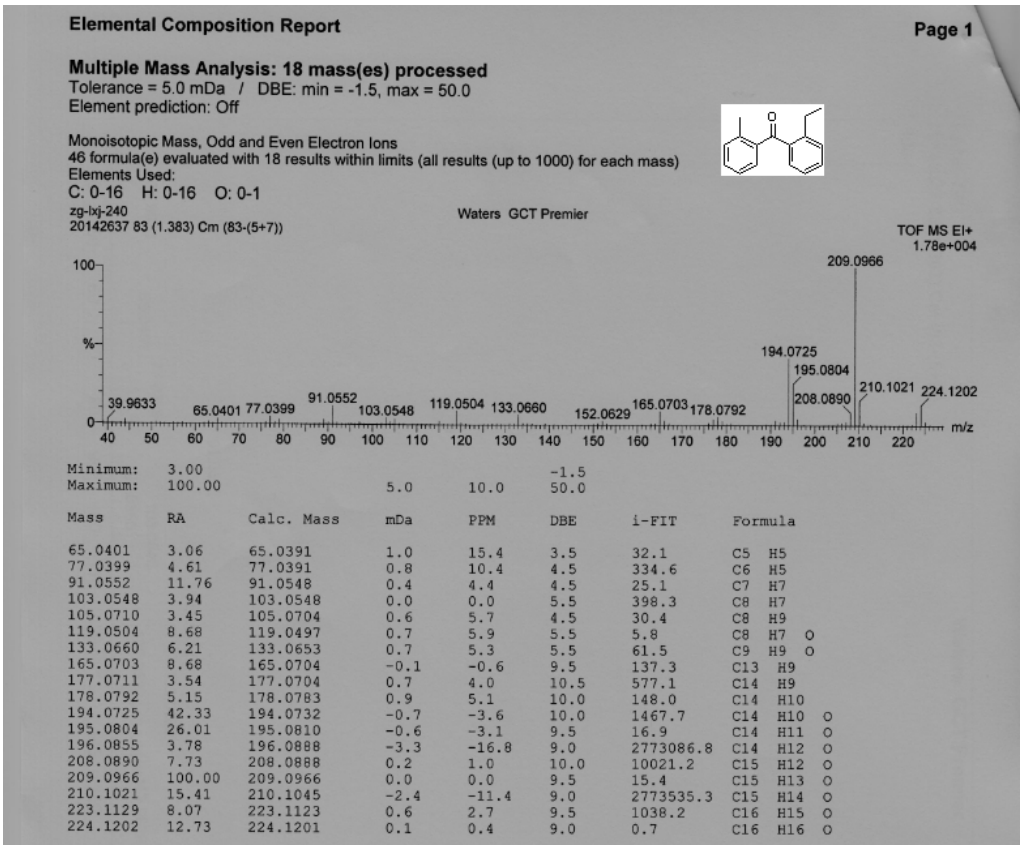
Monoisotopic Mass, Odd and Even Electron Ions
54 formula(e) evaluated with 12 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-19 H: 0-24 O: 0-1

zg-lxj-241
20142638-1 66 (1.100) Cm (66-(16+18))



Minimum:	2.50				-1.5		
Maximum:	100.00		5.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
39.9631	2.85	---					
43.9903	3.04	---					
77.0394	4.89	77.0391	0.3	3.9	4.5	1264.8	C6 H5
79.0549	10.45	79.0548	0.1	1.3	3.5	245.4	C6 H7
91.0553	3.77	91.0548	0.5	5.5	4.5	1092.7	C7 H7
93.0709	9.29	93.0704	0.5	5.4	3.5	28.6	C7 H9
105.0705	3.87	105.0704	0.1	1.0	4.5	735.6	C8 H9
107.0870	6.59	107.0861	0.9	8.4	3.5	13.8	C8 H11
133.0654	30.57	133.0653	0.1	0.8	5.5	17471.7	C9 H9 O
134.0697	3.06	134.0732	-3.5	-26.1	5.0	17744.6	C9 H10 O
135.1173	100.00	135.1174	-0.1	-0.7	3.5	5.5	C10 H15
136.1220	10.67	136.1252	-3.2	-23.5	3.0	54.0	C10 H16
239.1455	2.55	239.1436	1.9	7.9	8.5	2773053.5	C17 H19 O
268.1830	17.15	268.1827	0.3	1.1	8.0	1.1	C19 H24 O
269.1882	3.51	---					

(2-ethylphenyl)(o-tolyl)methanone 3vj



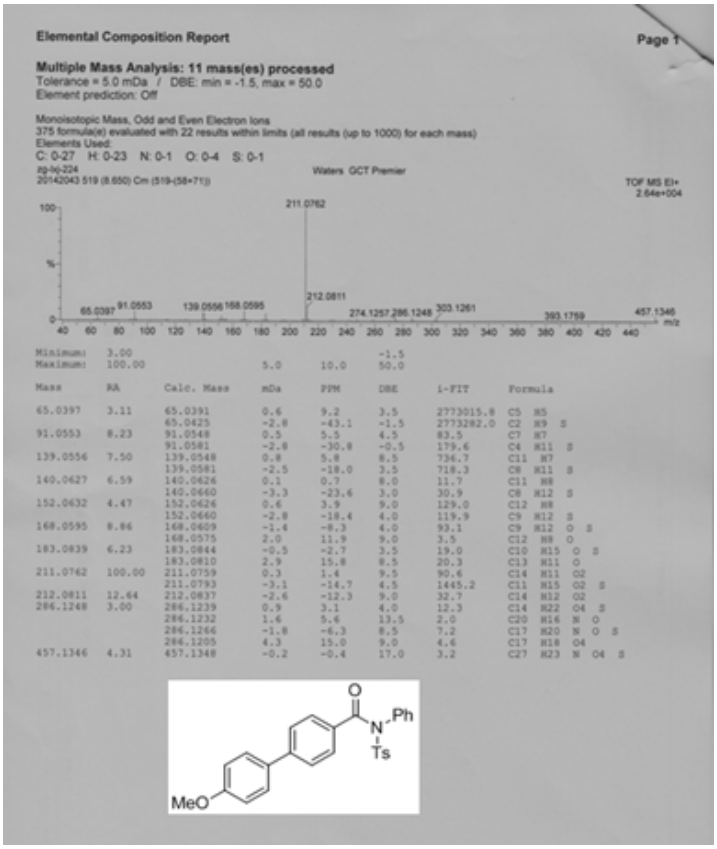
Elemental Composition Report Page 1

Multiple Mass Analysis: 18 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
46 formula(e) evaluated with 18 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-16 H: 0-16 O: 0-1
zg-lxj-240
20142637 83 (1.383) Cm (83-(5+7))
Waters GCT Premier
TOF MS EI+
1.78e+004

Minimum:	3.00				-1.5		
Maximum:	100.00		5.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
65.0401	3.06	65.0391	1.0	15.4	3.5	32.1	C5 H5
77.0399	4.61	77.0391	0.8	10.4	4.5	334.6	C6 H5
91.0552	11.76	91.0548	0.4	4.4	4.5	25.1	C7 H7
103.0548	3.94	103.0548	0.0	0.0	5.5	398.3	C8 H7
105.0710	3.45	105.0704	0.6	5.7	4.5	30.4	C8 H9
119.0504	8.68	119.0497	0.7	5.9	5.5	5.8	C8 H7 O
133.0660	6.21	133.0653	0.7	5.3	5.5	61.5	C9 H9 O
165.0703	8.68	165.0704	-0.1	-0.6	9.5	137.3	C13 H9
177.0711	3.54	177.0704	0.7	4.0	10.5	577.1	C14 H9
178.0792	5.15	178.0783	0.9	5.1	10.0	148.0	C14 H10
194.0725	42.33	194.0732	-0.7	-3.6	10.0	1467.7	C14 H10 O
195.0804	26.01	195.0810	-0.6	-3.1	9.5	16.9	C14 H11 O
196.0855	3.78	196.0888	-3.3	-16.8	9.0	2773086.8	C14 H12 O
208.0890	7.73	208.0888	0.2	1.0	10.0	10021.2	C15 H12 O
209.0966	100.00	209.0966	0.0	0.0	9.5	15.4	C15 H13 O
210.1021	15.41	210.1045	-2.4	-11.4	9.0	2773535.3	C15 H14 O
223.1129	8.07	223.1123	0.6	2.7	9.5	1038.2	C16 H15 O
224.1202	12.73	224.1201	0.1	0.4	9.0	0.7	C16 H16 O

4'-methoxy-N-phenyl-N-tosyl-[1,1'-biphenyl]-4-carboxamide 4



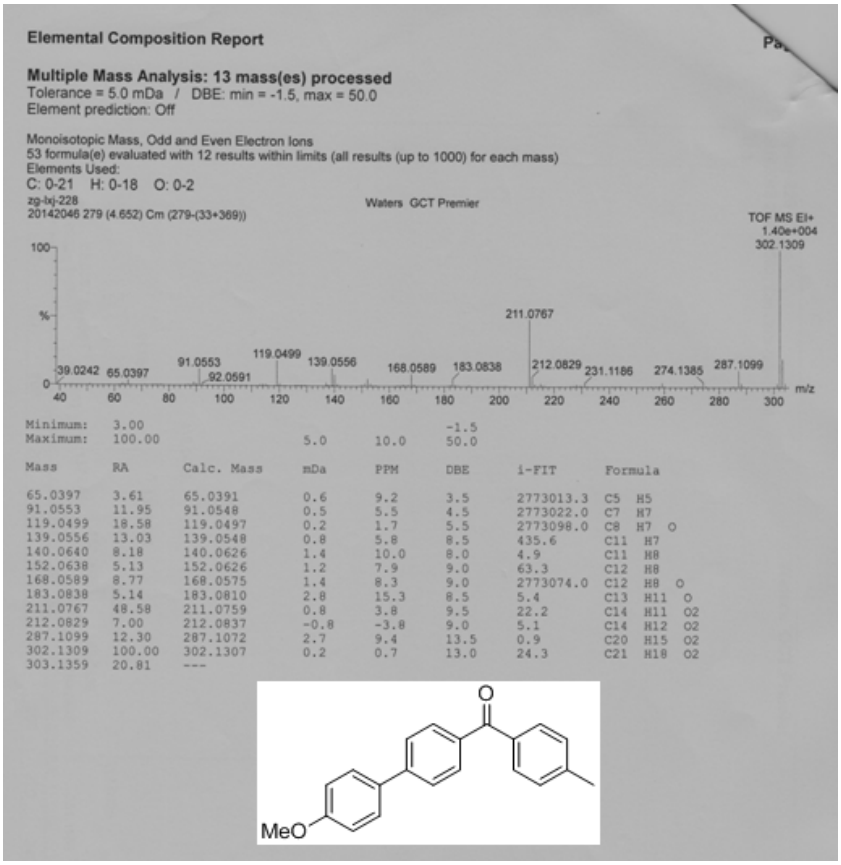
Elemental Composition Report Page 1

Multiple Mass Analysis: 11 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
375 formula(e) evaluated with 22 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-27 H: 0-23 N: 0-1 O: 0-4 S: 0-1
zg-lxj-224
20142043 519 (8.650) Cm (519-(58+71))
Waters GCT Premier
TOF MS EI+
2.64e+004

Minimum:	3.00				-1.5		
Maximum:	100.00		5.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
65.0397	3.11	65.0391	0.6	9.2	3.5	2773015.8	C5 H5
		65.0425	-2.8	-43.1	-1.5	2773282.0	C2 H9 S
91.0553	8.23	91.0548	0.5	5.5	4.5	83.5	C7 H7
		91.0581	-2.8	-30.8	-0.5	179.6	C4 H11 S
139.0556	7.50	139.0548	0.8	5.8	8.5	736.7	C11 H7
		139.0581	-2.5	-18.0	3.5	718.3	C8 H11 S
140.0627	6.59	140.0626	0.1	0.7	8.0	11.7	C11 H8
		140.0660	-3.3	-23.6	3.0	30.9	C8 H12 S
152.0632	4.47	152.0626	0.6	3.9	9.0	129.0	C12 H8
		152.0660	-2.8	-18.4	4.0	119.9	C9 H12 S
168.0595	8.86	168.0609	-1.4	-8.3	4.0	93.1	C9 H12 O S
		168.0575	2.0	11.9	9.0	3.5	C12 H8 O
183.0839	6.23	183.0844	-0.5	-2.7	3.5	19.0	C10 H15 O S
		183.0810	2.9	15.8	8.5	20.3	C13 H11 O
211.0762	100.00	211.0759	0.3	1.4	9.5	90.6	C14 H11 O2
		211.0793	-3.1	-14.7	4.5	1445.2	C11 H15 O2 S
212.0811	12.64	212.0837	-2.6	-12.3	9.0	32.7	C14 H12 O2
286.1248	3.00	286.1239	0.9	3.1	4.0	12.3	C14 H22 O4 S
		286.1232	1.6	5.6	13.5	2.0	C20 H16 N O
		286.1266	-1.8	-6.3	8.5	7.2	C17 H20 N O S
		286.1205	4.3	15.0	9.0	4.6	C17 H18 O4
457.1346	4.31	457.1348	-0.2	-0.4	17.0	3.2	C27 H23 N O4 S

(4'-methoxy-[1,1'-biphenyl]-4-yl)(p-tolyl)methanone 5



Elemental Composition Report

Multiple Mass Analysis: 13 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
53 formula(e) evaluated with 12 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-21 H: 0-18 O: 0-2

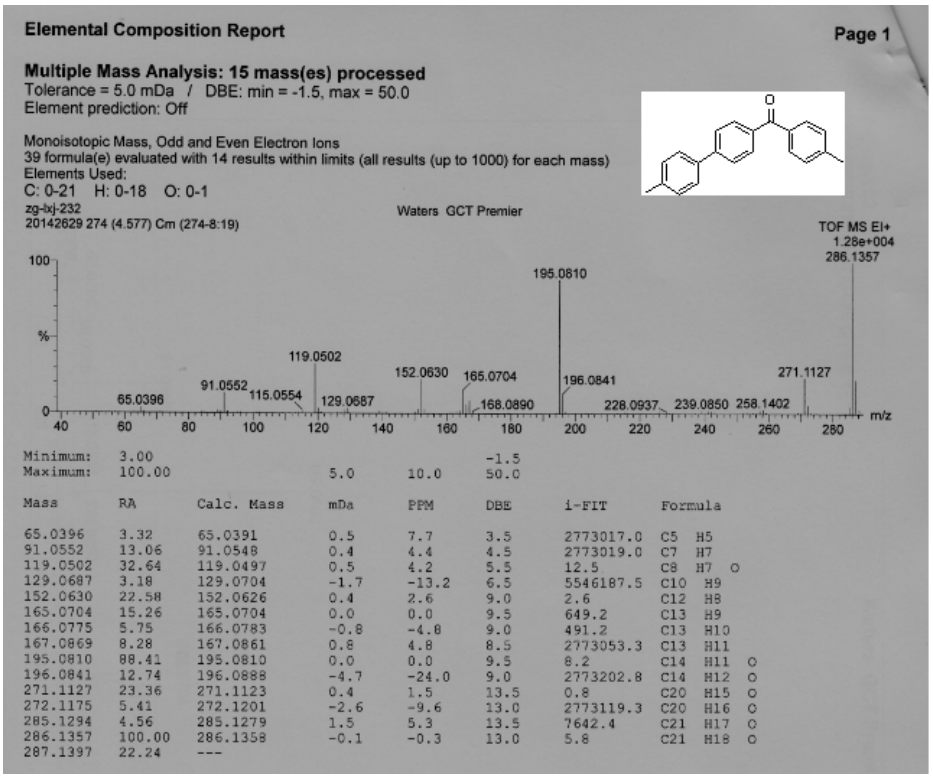
zg-lxj-228
20142046 279 (4.652) Cm (279-(33+369))

Waters GCT Premier

TOF MS EI+
1.40e+004
302.1309

Minimum:	3.00				-1.5		
Maximum:	100.00		5.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
65.0397	3.61	65.0391	0.6	9.2	3.5	2773013.3	C5 H5
91.0553	11.95	91.0548	0.5	5.5	4.5	2773022.0	C7 H7
119.0499	18.58	119.0497	0.2	1.7	5.5	2773098.0	C8 H7 O
139.0556	13.03	139.0548	0.8	5.8	8.5	435.6	C11 H7
140.0640	8.18	140.0626	1.4	10.0	8.0	4.9	C11 H8
152.0638	5.13	152.0626	1.2	7.9	9.0	63.3	C12 H8
168.0589	8.77	168.0575	1.4	8.3	9.0	2773074.0	C12 H8 O
183.0838	5.14	183.0810	2.8	15.3	8.5	5.4	C13 H11 O
211.0767	48.58	211.0759	0.8	3.8	9.5	22.2	C14 H11 O2
212.0829	7.00	212.0837	-0.8	-3.8	9.0	5.1	C14 H12 O2
287.1099	12.30	287.1072	2.7	9.4	13.5	0.9	C20 H15 O2
302.1309	100.00	302.1307	0.2	0.7	13.0	24.3	C21 H18 O2
303.1359	20.81	---					

(4'-methyl-[1,1'-biphenyl]-4-yl)(p-tolyl)methanone 6



Elemental Composition Report Page 1

Multiple Mass Analysis: 15 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
39 formula(e) evaluated with 14 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-21 H: 0-18 O: 0-1

zg-lxj-232
20142629 274 (4.577) Cm (274-8:19)

Waters GCT Premier

TOF MS EI+
1.28e+004
286.1357

Minimum:	3.00				-1.5		
Maximum:	100.00		5.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
65.0396	3.32	65.0391	0.5	7.7	3.5	2773017.0	C5 H5
91.0552	13.06	91.0548	0.4	4.4	4.5	2773019.0	C7 H7
119.0502	32.64	119.0497	0.5	4.2	5.5	12.5	C8 H7 O
129.0687	3.18	129.0704	-1.7	-13.2	6.5	5546187.5	C10 H9
152.0630	22.58	152.0626	0.4	2.6	9.0	2.6	C12 H8
165.0704	15.26	165.0704	0.0	0.0	9.5	649.2	C13 H9
166.0775	5.75	166.0783	-0.8	-4.8	9.0	491.2	C13 H10
167.0869	8.28	167.0861	0.8	4.8	8.5	2773053.3	C13 H11
195.0810	88.41	195.0810	0.0	0.0	9.5	8.2	C14 H11 O
196.0841	12.74	196.0888	-4.7	-24.0	9.0	2773202.8	C14 H12 O
271.1127	23.36	271.1123	0.4	1.5	13.5	0.8	C20 H15 O
272.1175	5.41	272.1201	-2.6	-9.6	13.0	2773119.3	C20 H16 O
285.1294	4.56	285.1279	1.5	5.3	13.5	7642.4	C21 H17 O
286.1357	100.00	286.1358	-0.1	-0.3	13.0	5.8	C21 H18 O
287.1397	22.24	---					