Supporting Information

Inhibitors of the Interaction of Thyroid Hormone Receptor and Coactivators: Preliminary Structure–Activity Relationships

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General experimental section

General Considerations. Unless otherwise noted, all materials were obtained from commercial suppliers and used without further purification. All solvents used were dried using an aluminum oxide column. Thin-layer chromatography was performed on precoated silica gel 60 F254 plates. Purification of compounds was done by reverse-phase high-performance liquid chromatography (HPLC; Flex [Biotage] and RP-C18 Xterra column 5μm, 19 mm × 50 mm [Waters]) or by normal phase column chromatography (SP1 [Biotage], Silica gel 230–400 mesh) followed by evaporation (HT-4X evaporator [Genevac]). The analysis (photodiode array, total ion count, and expected mass [m/z]) was performed using a HPLC-MS (Alliance HT, Micromass ZQ 4000 and RP-C18 Xterra column 5 μm, 6 mm × 50 mm [Waters], flow rate: 1 mL/min; gradient: 30:70 [methanol : water (0.05% TFA)]) to 100% MeOH over 10 min. NMR spectra were recorded on a Bruker 400 MHz and referenced internally to the residual resonance in $CDCl_3$ (δ 7.26 ppm) for hydrogen and (δ = 77 ppm) for carbon atoms.

General procedure for 3a-k: To a suspension of $AlCl_3$ (26.6 g, 200 mmol) in CH_2Cl_2 (200 mL) was added acryloyl chloride (9.78 mL, 100 mmol) at 0°C. The resulting clear solution was treated with 1-phenylhexane (18.9 mL, 100 mmol) and stirred for 2 h at room temperature. The reaction was poured into a mixture of concentrated HCl (40 mL) and ice (200 g). The organic layer was separated, the aqueous layer was extracted with CH_2Cl_2 (100 mL), and the combined organic layers were washed with saturated aqueous $NaHCO_3$ (100 mL) and brine (100 mL) and dried over $MgSO_4$. The filtered solution was concentrated in vacuo to yield compounds **1** and **2** (15.6 g, 70%) as a yellow oil in a ratio of 4:1. Next, 9 g (45 mmol) of the crude product was dissolved in THF (30 mL) to obtain a 1.5 M stock solution. The corresponding amines (3 mmol) were dissolved in THF (8 mL) and treated with 2 mL of the stock solution (1.5 M solution of **1** and **2**) and stirred at room temperature overnight. The reaction mixtures were evaporated, and the residual amines were removed by repeated azeotropic evaporations using ethanol to yield the corresponding β-aminophenylketones in 85–97% yield with a purity of 85–95%, as determined by HPLC-MS.

Subsequent purification by RP-HPLC (flow rate: 20 mL/min; gradient: 0.05% formic acid in water to 0.05% formic acid in 80% acetonitrile over 15 min) resulted in desired product (> 99% purity).

(3a) 1-(4-Hexylphenyl)-3-(methyl(phenethyl)amino)propan-1-one: white solid, mp 147-149°C, yield 84%; ^{1}H-NMR (400 MHz) δ = 7.73 (d, *J* = 8.3 Hz, 2H), 7.19-7.06 (m, 8H), 3.56-3.51 (m, 1H), 3.45-3.33 (m, 3H), 3.08-3.25 (m, 1H), 3.13-3.08 (m, 1H), 2.98-2.94 (m, 2H), 2.75 (s, 3H), 1.49-1.46 (m, 2H), 1.20-1.11 (m, 6H), 0.73 (t, *J* = 6.9 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 195.32, 150.25, 135.37, 133.11, 129.10, 128.97, 128.66, 128.32, 127.51, 58.13, 51.36, 40.47, 36.04, 33.18, 31.61, 30.95, 30.43, 28.86, 22.53, 14.04; MS calcd for $C_{24}H_{33}NO$ (H^+) 352.26, found 352.32.

(3b) 1-(4-Hexylphenyl)-3-((2-hydroxyethyl)(methyl)amino)propan-1-one: White waxy solid, yield 87%; ^{1}H-NMR (400 MHz) δ = 7.73 (d, *J* = 8.3 Hz, 2H), 7.26 (d, *J* = 8.2 Hz, 2H), 3.97 (t, *J* = 4.8 Hz, 2H), 3.69-3.66 (m, 1H), 3.55-3.49 (m, 3H), 3.38-3.33 (m, 1H), 3.13-3.09 (m, 1H), 3.89 (s, 3H), 2.63 (t, *J* = 7.6 Hz, 2H), 1.60-1.55 (m, 2H), 1.31-1.22 (m, 6H), 0.84 (t, *J* = 7.1 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 195.40, 162.35, 150.39, 133.08, 129.01, 128.36, 59.59, 56.14, 52.56, 41.62, 36.06, 33.12, 31.62, 30.97, 28.88, 22.55, 14.05; MS calcd for $C_{17}H_{27}NO_2$ (H^+) 291.22, found 291.22.

(3c) 3-(Diisopropylamino)-1-(4-hexylphenyl)propan-1-one: Pale yellow waxy solid, yield 81%; ^{1}H-NMR (400 MHz) δ = 7.79 (d, *J* = 8.1 Hz, 2H), 7.18 (d, *J* = 8.1 Hz, 2H), 6.06 (s (br), NH), 3.62-3.56 (m, 4H), 3.36-3.31 (m, 2H), 2.57 (t, *J* = 7.6 Hz, 2H), 1.54-1.43 (m, 2H), 1.35 (d, *J* = 6.6 Hz, 6H), 1.31 (d, *J* = 6.7 Hz, 6H), 1.23-1.18 (m, 6H), 0.76 (t, *J* = 6.8 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 195.94, 150.16, 133.17, 128.95, 128.35, 55.01, 42.64, 36.04, 35.25, 31.61, 30.95, 28.86, 22.53, 18.48, 17.12, 14.03; MS calcd for $C_{21}H_{35}NO$ (H^+) 318.27, found 318.33.

(3d) 1-(4-Hexylphenyl)-3-(pyrrolidin-1-yl)propan-1-one: White solid, mp 121-123°C, yield 85%; ^{1}H-NMR (400 MHz) δ = 7.72 (d, *J* = 8.4 Hz, 2H), 7.14 (d, *J* = 8.5 Hz, 2H), 3.75-3.71 (m, 2H), 3.46-3.38 (m, 4H), 2.79-2.75 (m, 2H), 2.54 (t, *J* = 7.6 Hz, 2H), 2.01-1.98 (m, 4H), 1.48-1.46 (m, 2H), 1.19-1.11 (m, 6H), 0.73 (t, *J* = 7.2 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 195.45, 150.26, 133.15, 128.99, 128.36, 54.40, 50.20, 36.06, 34.36, 31.63, 30.97, 28.88, 23.16, 22.55, 14.05; MS calcd for $C_{19}H_{29}NO$ (H^+) 287.22, found 287.28.

(3e) 1-(4-Hexylphenyl)-3-morpholinopropan-1-one: White solid, mp 152-154°C, yield 90%; ^{1}H-NMR (400 MHz) δ = 7.71 (d, *J* = 8.4 Hz, 2H), 7.14 (d, *J* = 8.4 Hz, 2H), 3.88-3.78 (m, 4H), 3.44-3.37 (m, 6H), 2.84-2.81 (m, 2H), 2.52 (t, *J* = 7.6 Hz, 2H), 1.49-1.46 (m, 2H), 1.19-1.09 (m, 6H), 0.72 (t, *J* = 7.2 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 195.28, 162.34, 150.32, 133.05, 129.01, 128.35, 63.92, 52.49, 52.34, 36.05, 32.49, 31.69, 30.96, 28.87, 22.55, 14.05; MS calcd for $C_{19}H_{29}NO_3$ (H^+) 319.21, found 319.19.

(3f) Methyl 1-(3-(4-hexylphenyl)-3-oxopropyl)piperidine-4-carboxylate: White solid, mp 147-149°C, yield 86%; ^{1}H-NMR (400 MHz) δ = 7.73 (d, *J* = 8.3 Hz, 2H), 7.16 (d, *J* = 8.1 Hz, 2H), 3.64 (s, 1.5H), 3.59 (s, 1.5H), 3.44-3.38 (m, 6H), 2.91-2.84 (m, 1H), 2.79-2.72 (m, 0.5H), 2.65-2.57 (m, 1H), 2.54 (t, *J* = 7.8 Hz, 2H), 2.40-2.34 (m, 0.5H), 2.13-2.09 (m, 3H), 2.03-1.95 (m, 1H), 1.51-1.47 (m, 2H), 1.22-1.13 (m, 6H), 0.75 (t, *J* = 6.8 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 195.32, 161.93, 161.56, 150.19, 133.09, 128.97, 128.34, 52.82, 52.33, 51.76, 50.31, 38.93, 36.03, 34.85, 32.85, 31.61, 30.95, 28.86, 25.44, 24.06, 22.53, 14.03; MS calcd for $C_{22}H_{33}NO_3$ (H^+) 359.25, found 291.21.

(3g) 3-(Dibutylamino)-1-(4-hexylphenyl)propan-1-one: White solid, mp 71-73°C, yield 90%; ^{1}H-NMR (400 MHz) δ = 7.75 (d, *J* = 8.3 Hz, 2H), 7.16 (d, *J* = 8.3 Hz, 2H), 3.46-3.36 (m, 4H), 3.00-2.90 (m, 4H), 2.53 (t, *J* = 7.2 Hz, 2H), 1.60-1.47 (m, 6H), 1.29-1.12 (m, 10H), 0.86-0.82 (m, 6H), 0.75 (t, *J* = 7.2 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 195.67, 150.14, 133.27, 128.97, 128.37, 52.45, 48.42, 36.06, 33.18, 31.63, 30.98, 28.88, 24.89, 22.55, 20.01, 14.05, 13.54; MS calcd for $C_{23}H_{39}NO$ (H^+) 345.30, found 345.20.

(3h) 3-(Dimethylamino)-1-(4-hexylphenyl)propan-1-one: White solid, mp 142-144°C, yield 94%; ^{1}H-NMR (400 MHz) δ = 7.85 (d, *J* = 8.3 Hz, 2H), 7.27 (d, *J* = 8.3 Hz, 2H), 3.52 (m, 4H), 2.86 (s, 6H), 2.64 (t, *J* = 7.6 Hz, 2H), 1.61-1.58 (m, 2H), 1.32-1.24 (m, 6H), 0.85 (t, *J* = 7.1 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 195.19, 162.09, 150.31, 133.11, 129.00, 128.36, 53.05, 43.58, 36.06, 33.43, 31.62, 30.97, 28.88, 22.62, 14.05; MS calcd for $C_{17}H_{27}NO$ (H^+) 261.21, found 261.20.

(3i) 3-((Furan-2-ylmethyl)(methyl)amino)-1-(4-hexylphenyl)propan-1-one: Pale brown waxy solid, yield 92%; ^{1}H-NMR (400 MHz) δ = 7.74 (d, *J* = 8.3 Hz, 2H), 7.35 (d, *J* = 1.8 Hz, 1H), 7.16 (d, *J* = 8.3 Hz, 2H), 6.53 (d, *J* = 3.3 Hz, 1H), 6.34 (dd, J_1 = 3.3 Hz, J_2 = 1.8 Hz, 1H), 4.23 (s, 2H), 3.47-3.29 (m, 4H), 2.66 (s, 3H), 2.54 (t, *J* = 7.6 Hz, 2H), 1.51-1.47 (m, 2H), 1.21-1.12 (m, 6H), 0.75 (t, *J* = 7.1 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 195.27, 150.14, 145.09, 142.57, 133.21, 128.94, 128.32, 115.17, 111.44, 99.97, 51.36, 50.19, 39.99, 36.04, 33.29, 31.61, 30.96, 28.87, 22.54, 14.04; MS calcd for $C_{21}H_{29}NO$ (H^+) 327.23, found 327.22.

(3j) 3-(Dicyclohexylamino)-1-(4-hexylphenyl)propan-1-one: White waxy solid, yield 78%; ^{1}H-NMR (400 MHz) δ = 7.79 (d, *J* = 8.2 Hz, 2H), 7.17 (d, *J* = 8.1 Hz, 2H), 5.03 (s (br), NH), 3.57-3.53 (m, 2H), 3.41-3.36 (m, 2H), 3.25-3.18 (m, 2H), 2.57 (t, *J* = 7.4 Hz, 2H), 2.08-2.05 (m, 2H), 1.94-1.91 (m, 2H), 1.83-1.80 (m, 4H), 1.62-1.40 (m, 8H), 1.26-1.05 (m, 12H), 0.76 (t, *J* = 6.8 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 196.18, 150.11, 133.23, 128.94, 128.37, 62.67, 43.71, 36.04, 35.41, 31.61, 30.96, 28.86, 28.27, 27.22, 25.21, 25.06, 24.91, 22.53, 14.04; MS calcd for $C_{27}H_{43}NO$ (H^+) 398.33, found 398.63

(3k) 1-(4-hexylphenyl)-3-(propylamino)propan-1-one: White waxy solid, yield 93%; ^{1}H-NMR (400 MHz) δ = 7.72 (d, *J* = 8.2 Hz, 2H), 7.15 (d, *J* = 8.3 Hz, 2H), 3.39-3.29 (m, 4H), 2.92-2.91 (M, 2H), 2.54 (t, *J* = 7.6 Hz, 2H), 1.71-1.65 (m, 2H), 1.51-1.48 (m, 2H), 1.22-1.14 (m, 6H), 0.91 (t, *J* = 7.3 Hz, 3H), 0.75 (t, *J* = 7.4 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 198.29, 150.45, 133.05, 128.94, 128.35, 49.91, 43.38, 36.06, 33.081, 31.61, 30.93, 28.87, 22.54, 19.64, 14.04, 10.88; MS calcd for $C_{18}H_{29}NO$ (H^+) 275.22, found 275.29.

General procedure for 1, 4a and 4g: see general procedure for **3a-k**.

(1) 1-(4-hexylphenyl)prop-2-en-1-one: Colorless liquid, yield 55%; ^{1}H-NMR (400 MHz) δ = 7.88 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 8.2 Hz, 2H), 7.17 (dd, *J* = 17.1 Hz, *J* = 10.5 Hz, 1H), 6.43 (dd, *J* = 17.1 Hz, *J* = 1.6 Hz, 1H), 5.90 (dd, *J* = 10.5 Hz, *J* = 1.6 Hz, 1H), 2.67 (t, *J* = 7.8 Hz, 2H), 1.63 (p, *J* = 7.1 Hz, 2H), 1.36-1.27 (m, 6H), 0.88 (t, *J* = 6,8 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 190.55, 148.82, 134.94, 132.41, 129.62, 128.86, 128.67, 36.02, 31.65, 31.06, 28.92, 22.56, 14.05; MS calcd for $C_{15}H_{20}O$ (H^+) 216.15, found .

(4a) (E)-4-(4-hexylphenyl)-4-oxobut-2-enoic acid: Yellow solid, mp 90-92°C, yield 45%; (DMSO) ^{1}H-NMR (400 MHz) δ = 7.95 (d, *J* = 8.1 Hz, 2H), 7.87 (d, *J* = 15.5 Hz, 1H), 7.39 (d, *J* = 8.1 Hz, 2H), 6.66 (d, *J* = 15.5 Hz, 1H), 2.66 (t, *J* = 7.6 Hz, 2H), 1.59 (p, *J* = 7.7 Hz, 2H), 1.36-1.20 (m, 6H), 0.85 (t, *J* = 6.9 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 188.78, 166.23, 149.27, 136.19, 133.85, 132.50, 128.88, 35.07, 30.95, 30.39, 28.20, 21.93, 13.84 MS calcd for $C_{16}H_{20}O_3$ (H^+) 261.14, found 261.33.

(4g) 1-(4-hexylphenyl)propan-1-one: Colorless liquid, yield 95%; ^{1}H-NMR (400 MHz) δ = 7.88 (d, *J* = 8.1 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 2.97 (q, *J* = 7.2 Hz, 2H), 2.65 (t, *J* = 7.6 Hz, 2H), 1.62 (p, *J* = 7.5 Hz, 2H), 1.35-1.26 (m, 6H), 1.21 (t, *J* = 7.6 Hz, 3H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 200.53, 148.52, 134.63, 128.55, 128.09, 35.96, 31.64, 31.08, 28.91, 22.55, 14.05, 8.33; MS calcd for $C_{15}H_{22}O$ (H^+) 218.17, found 218.19.

General procedure for 5b-f: To a solution of 1-bromo-4-heptylbenzene (408 μL, 2 mmol) in THF (3 mL) was added n-BuLi (2M in pentane, 1.1 mL, 1.1 equiv.) at –78°C. After stirring for 20 min, aldehyde (2 mmol, 1 equiv.) was added and the solution was stirred for an additional 2 h at –78°C. The reaction mixture was quenched at –78°C with NH_4Cl (aq) (2 mL) and allowed to warm to room temperature. The organic layer was separated. The aqueous layer was extracted with ethyl acetate (3 mL, twice) and the combined organic layers were dried over $MgSO_4$, filtered, and concentrated *in vacuo*. Purification was done by flash column chromatography (SP1, 25M (SiO_2), flow rate: 25 mL/min; gradient: 1% to 30% ethyl acetate in hexanes over 20 CV).

(5b) (E)-1-(4-heptylphenyl)but-2-en-1-ol: Colorless liquid, yield 51%; ^{1}H-NMR (400 MHz) δ = 7.28 (d, *J* = 7.9 Hz, 2H), 7.17 (d, *J* = 8.1 Hz, 2H), 5.82-5.66 (m, 2H), 5.15-5.11 (m, 1H), 2.60 (t, *J* =

7.5 Hz, 2H), 1.95 (m, 1H (OH)), 1.71 (m, 3H), 1.62 (m, 2H), 1.36-1.27 (m, 8H), 0.90 (t, *J* = 6.9 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 142.25, 140.61, 133.68, 128.46, 127.07, 126.02, 75.04, 35.61, 31.79, 31.48, 29.27, 29.15, 22.64, 17.66, 14.07, MS calcd for $C_{17}H_{26}O(H^+)$ 247.20, found 228.80 (-OH).

(5c) 1-(4-heptylphenyl)-3-methylbut-2-en-1-ol: Colorless liquid, yield 67%; ^{1}H-NMR (400 MHz) δ = 7.29 (d, *J* = 8.1 Hz, 2H), 7.16 (d, *J* = 7.9 Hz, 2H), 5.43 (m, 2H), 2.59 (t, *J* = 7.5 Hz, 2H), 1.80 (s, 3H), 1.75 (m, 3H), 1.71 (m, 1H (OH)), 1.60 (m, 2H), 1.34-1.25 (m, 8H), 0.88 (t, *J* = 7.0 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 142.02, 141.46, 134.89, 128/.47, 127.77, 125.48, 70.63, 35.61, 31.79, 31.49, 29.28, 29.15, 25.85, 22.64, 18.24, 14.06; MS calcd for $C_{18}H_{28}O(H^+)$ 261.21, found 244.19 (-OH).

(5d) 1-(4-heptylphenyl)-2-methylprop-2-en-1-ol: Colorless liquid, yield 46%; ^{1}H-NMR (400 MHz) δ = 7.27 (d, *J* = 7.9 Hz, 2H), 7.16 (d, *J* = 7.9 Hz, 2H), 5.21 (m, 1H), 5.11 m, 1H), 4.95 (m, 1H), 2.59 (t, *J* = 7.9 Hz, 2H), 1.91 (m, 1H (OH)), 1.66 (m, 4H), 1.34-1.26 (m, 8H), 0.88 (t, *J* = 6.9 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 146.91, 142.46, 139.19, 128.42, 126.38, 110.78, 77.70, 35.64, 31.80, 31.47, 29.28, 29.16, 22.65, 18.41, 14.08, MS calcd for $C_{17}H_{26}O(H^+)$ 247.20, found 228.80 (-OH).

(5e) (E)-1-(4-heptylphenyl)-2-methylbut-2-en-1-ol: Colorless liquid, yield 67%; ^{1}H-NMR (400 MHz) δ = 7.26 (d, *J* = 7.9 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 5.71 (q, *J* = 6.7 Hz, 1H), 5.10 (d, *J* = 3.0 Hz, 1H), 2.56 (t, *J* = 6.7 Hz, 2H), 1.82 (m, 1H (OH)), 1.66 (d, *J* = 6.7 Hz, 3H), 1.60 (m, 2H), 1.50 (s, 3H), 1.34-1.25 (m, 8H), 0.88 (t, *J* = 6.9 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 141.97, 139.74, 137.64, 128.23, 126.11, 120.85, 79.19, 35.63, 31.80, 31.48, 29.30, 29.17, 22.65, 14.08, 13.14, 11.81, MS calcd for $C_{18}H_{28}O(H^+)$ 261.21, found 244.19 (-OH).

(5f) (E)-1-(4-heptylphenyl)-3-phenylprop-2-en-1-ol: White solid, mp 32-34°C, yield 54%; ^{1}H-NMR (400 MHz) δ = 7.35-7.12 (m, 9H), 6.60 (d, *J* = 15.8 Hz, 1H), 6.32 (dd, *J* = 15.8 Hz, *J* = 6.4 Hz, 1H), 5.27 (dd, *J* = 6.4 Hz, *J* =3.0 Hz, 1H), 2.55 (t, *J* = 7.9 Hz, 2H), 2.20 (d, *J* = 3.0 Hz, 1H(OH)), 1.56 (p, *J* = 7.5 Hz, 2H), 1.34-1.26 (m, 8H), 0.81 (t, *J* = 6.9 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 142.55, 139.99, 136.58, 131.63, 130.17, 128.99, 128.47, 127.62, 126.54, 126.27, 74.90, 35.61, 31.77, 31.46, 29.24, 24.14, 22.63, 14.07, MS calcd for $C_{22}H_{28}O(H^+)$ 309.21, found 291.19 (-OH).

General procedure for 4b-f: To a solution of alcohol (0.36 mmol), 4-methylmorpholine N-oxide (65 mg, 0.54 mmol, 1.5 equiv.), molecular sieves (200 mg) in acetonitrile (3 mL) was added tetrapropylammonium perruthenate (6.5 mg, 0.018 mmol, 0.05 equiv). The reaction mixture was stirred for 1–4 h, absorbed onto silica gel and purified by column chromatography (SP1, 25M (SiO_2) , flow rate: 25 mL/min; gradient: 1–10% ethyl acetate in hexanes over 18 CV).

(4b) (E)-1-(4-heptylphenyl)but-2-en-1-one: Colorless liquid, yield 67%; ^{1}H-NMR (400 MHz) δ = 7.85 (d, *J* = 8.3 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 2H), 7.06 (m, 1H), 6.91 (m, 1H), 2.65 (t, *J* = 8.0 Hz, 2H), 1.99 (d, *J* = 6.8 Hz, 3H), 1.62 (m, 2H), 1.34-1.24 (m, 8H), 0.87 (t, *J* = 7.0 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 190.30, 148.35, 144.42, 135.50, 128.65, 128.55, 127.48, 35.99, 31.76, 31.14, 29.22, 29.12, 22.63, 18.57, 14.7; MS calcd for $C_{17}H_{24}O(H^+)$ 245.77, found 245.77.

(4c) 1-(4-hexylphenyl)-2-methylprop-2-en-1-one: Colorless liquid, yield 46%; ^{1}H-NMR (400 MHz) δ = 7.68 (d, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 7.9 Hz, 2H), 5.86 (m, 1H), 5.60 (m, 1H), 2.65 (t, *J* = 7.9 Hz, 2H), 2.07 (s, 3H), 1.67 (m, 2H), 1.37-1.24 (m, 8H), 0.88 (t, *J* = 6.9 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 198.14, 147.76, 143.85, 135.05, 129.66, 128.19, 126.06, 35.95, 31.77, 31.16, 29.23, 29.12, 22.64, 18.83, 14.08, MS calcd for $C_{17}H_{24}O(H^+)$ 245.77, found .245.18.

(4d) 1-(4-heptylphenyl)-3-methylbut-2-en-1-one: Colorless liquid, yield 67%; ^{1}H-NMR (400 MHz) δ = 7.85 (d, *J* = 8.1 Hz, 2H), 7.24 (d, *J* = 8.1 Hz, 2H), 6.74 (s, 1H), 2.65 (t, *J* = 7.9 Hz, 2H), 2.20 (s, 3H), 2.01 (s, 3H), 1.62 (d, *J* = 7.6 Hz, 3H), 1.35-1.23 (m, 8H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 191.25, 155.80, 147.89, 136.86, 128.44, 128.30, 121.29, 35.94, 31.76, 31.15, 29.20, 29.11, 27.90, 22.62, 21.07, 14.06; MS calcd for $C_{18}H_{26}O(H^+)$ 259.20, found 259.76.

(4e) (E)-1-(4-heptylphenyl)-2-methylbut-2-en-1-one: Colorless liquid, yield 67%; ^{1}H-NMR (400 MHz) δ = 7.55 (d, *J* = 7.9 Hz, 2H), 7.21 (d, *J* = 7.9 Hz, 2H), 6.38 (q, *J* = 6.7 Hz, 1H), 2.64 (t, *J* = 7.3

Hz, 2H), 1.96 (s, 3H), 1.87 (d, *J* = 6.9 Hz, 3H), 1.62 (p, *J* = 7.3 Hz, 2H), 1.36-1.21 (m, 8H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 198.77, 146.85, 140.42, 137.60, 136.12, 129.45, 128.03, 35.91, 31.78, 31.22, 29.23, 29.13, 22.64, 14.65, 14.08, 12.32, MS calcd for $C_{18}H_{26}O(H^+)$ 259.20, found 259.76.

(4f) (E)-1-(4-heptylphenyl)-3-phenylprop-2-en-1-one: Pale yellow solid, mp 58-60°C, yield 54%; ^{1}H-NMR (400 MHz) δ = 7.96 (d, *J* = 8.1 Hz, 2H), 7.81 (d, *J* = 15.7 Hz, 1H), 7.64 (m, 2H), 7.53 (d, *J* = 15.7 Hz, 1H), 7.43 (m, 3H), 7.31 (d, *J* = 8.0 Hz, 2H), 2.69 (t, *J* = 7.9 Hz, 2H), 1.65 (p, *J* = 7.4 Hz, 2H), 1.35-1.26 (m, 8H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 190.06, 148.61, 144.34, 135.82, 135.02, 130.39, 128.92, 128.68, 128.65, 128.39, 122.15, 36.04, 31.77, 31.15, 29.23, 29.12, 22.64, 14.08; MS calcd for $C_{22}H_{26}O(H^+)$ 307.20, found 307.72.

General procedure for 6a-m: A solution of triethylamine (83 μL, 0.6 mmol, 1.1 equiv) and alcohol (0.5 mmol) in DCM (2 mL) was treated with acryloyl chloride (49 μL, 0.6 mmol, 1.1 equiv.) and stirred for 1 h at rt. The reaction mixture absorbed on silica cartridge and purified by flash column chromatography (SP1, 25S (SiO_2), flow rate: 25 mL/min; gradient: 1% to 20% ethyl acetate in hexanes over 20 CV).

(6a) 4-propylphenyl acrylate: Colorless liquid, yield 85%; ^{1}H-NMR (400 MHz) δ = 7.18 (d, *J* = 8.6 Hz, 2H), 7.03 (d, *J* = 8.5 Hz, 2H), 6.59 (dd, *J* = 17.3 Hz, *J* = 1.3 Hz, 1H), 6.31 (dd, *J* = 17.3 Hz, *J* = 10.4 Hz, 1H), 6.00 (dd, *J* = 10.4 Hz, *J* = 1.3 Hz, 1H), 2.58 (t, *J* = 7.4 Hz, 2H), 1.64 (h, *J* = 7.4 Hz, 2H), 0.94 (t, *J* = 7.3 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 164.71, 148.51, 140.26, 132.26, 129.31, 128.08, 121.10, 39.44, 24.51, 13.78; MS calcd for $C_{12}H_{14}O_2$ (H^+) 191.10, found 191.37.

(6b) 4-butylphenyl acrylate: Colorless liquid, yield 86%; ^{1}H-NMR (400 MHz) δ = 7.18 (d, *J* = 8.6 Hz, 2H), 7.03 (d, *J* = 8.5 Hz, 2H), 6.59 (dd, *J* = 17.3 Hz, *J* = 1.3 Hz, 1H), 6.31 (dd, *J* = 17.3 Hz, *J* = 10.4 Hz, 1H), 6.00 (dd, *J* = 10.4 Hz, *J* = 1.3 Hz, 1H), 2.61 (t, *J* = 7.6 Hz, 2H), 1.60 (p, *J* = 7.6 Hz, 2H), 1.34 (h, *J* = 7.7 Hz, 2H), 0.93 (t, *J* = 7.3 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 164.71, 148.46, 140.48, 132.26, 129.26, 128.08, 121.10, 35.03, 33.57, 22.30, 13.91; MS calcd for $C_{13}H_{16}O_2$ (H^+) 205.11, found 205.12.

(6c) 4-pentylphenyl acrylate: Colorless liquid, yield 88%; ^{1}H-NMR (400 MHz) δ = 7.18 (d, *J* = 8.5 Hz, 2H), 7.02 (d, *J* = 8.5 Hz, 2H), 6.58 (dd, *J* = 17.3 Hz, *J* = 1.3 Hz, 1H), 6.31 (dd, *J* = 17.3 Hz, *J* = 10.4 Hz, 1H), 5.99 (dd, *J* = 10.4 Hz, *J* = 1.3 Hz, 1H), 2.59 (t, *J* = 7.9 Hz, 2H), 1.61 (p, *J* = 7.4 Hz, 2H), 1.35-1.28 (m, 4H), 0.89 (t, *J* = 7.0 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 164.71, 148.47, 140.52, 132.26, 129.26, 128.08, 121.10, 35.32, 31.45, 31.11, 22.51, 14.00; MS calcd for $C_{14}H_{18}O_2$ (H^+) 219.30, found 220.10.

(6d) 4-*tert*-pentylphenyl acrylate: Colorless liquid, yield 94%; ^{1}H-NMR (400 MHz) δ = 7.34 (d, *J* = 8.6 Hz, 2H), 7.06 (d, *J* = 8.6 Hz, 2H), 6.60 (dd, *J* = 17.3 Hz, *J* = 1.3 Hz, 1H), 6.32 (dd, *J* = 17.3 Hz, *J* = 10.4 Hz, 1H), 6.00 (dd, *J* = 10.4 Hz, *J* = 1.3 Hz, 1H), 1.64 (q, *J* = 7.4 Hz, 2H), 1.28 (m, 6H), 0.69 (t, *J* = 7.4 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 164.66, 148.18, 147.03, 132.24, 128.12, 126.94, 120.70, 37.71, 36.90, 28.48, 9.09; MS calcd for $C_{14}H_{18}O_2$ (H^+) 219.30, found 219.78.

(6e) 4-hexylphenyl acrylate: Colorless liquid, yield 89%; ^{1}H-NMR (400 MHz) δ = 7.19 (d, *J* = 8.5 Hz, 2H), 7.03 (d, *J* = 8.5 Hz, 2H), 6.60 (dd, *J* = 17.3 Hz, *J* = 1.3 Hz, 1H), 6.31 (dd, *J* = 17.3 Hz, *J* = 10.4 Hz, 1H), 5.99 (dd, *J* = 10.4 Hz, *J* = 1.3 Hz, 1H), 2.60 (t, *J* = 7.8 Hz, 2H), 1.61 (p, *J* = 7.7 Hz, 2H), 1.34-1.26 (m, 6H), 0.89 (t, *J* = 7.1 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 164.71, 148.46, 140.53, 132.26, 129.25, 128.08, 121.10, 35.36, 31.70, 31.40, 28.94, 22.59, 14.02; MS calcd for $C_{15}H_{20}O_2$ (Na^+) 255.31, found 255.75.

(6f) 4-heptylphenyl acrylate: Colorless liquid, yield 76%; ^{1}H-NMR (400 MHz) δ = 7.19 (d, *J* = 8.3 Hz, 2H), 7.03 (d, *J* = 8.3 Hz, 2H), 6.59 (dd, *J* = 17.3 Hz, *J* = 1.3 Hz, 1H), 6.31 (dd, *J* = 17.3 Hz, *J* = 10.4 Hz, 1H), 5.99 (dd, *J* = 10.4 Hz, *J* = 1.3 Hz, 1H), 2.60 (t, *J* = 7.8 Hz, 2H), 1.61 (p, *J* = 7.7 Hz, 2H), 1.35-1.26 (m, 8H), 0.89 (t, *J* = 6.9 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 164.71, 148.46, 140.53, 132.26, 129.25, 128.08, 121.10, 35.36, 31.80, 31.45, 29.24, 29.15, 22.65, 14.08; MS calcd for $C_{16}H_{22}O_2$ (H^+) 247.16, found 248.80.

(6g) 4-octylphenyl acrylate: Colorless liquid, yield 81%; ^{1}H-NMR (400 MHz) δ = 7.19 (d, *J* = 8.2 Hz, 2H), 7.03 (d, *J* = 8.2 Hz, 2H), 6.59 (dd, *J* = 17.3 Hz, *J* = 1.3 Hz, 1H), 6.31 (dd, *J* = 17.3 Hz, *J* = 10.4 Hz, 1H), 5.99 (dd, *J* = 10.4 Hz, *J* = 1.3 Hz, 1H), 2.60 (t, *J* = 7.8 Hz, 2H), 1.61 (p, *J* = 7.7 Hz, 2H), 1.35-1.26 (m, 10H), 0.89 (t, *J* = 6.9 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 164.71, 148.46, 140.53, 132.25, 129.25, 128.08, 121.10, 35.36, 31.87, 31.45, 29.45, 29.28, 28.24, 22.66, 14.08; MS calcd for $C_{17}H_{24}O_2$ (H^+) 261.18, found 262.80.

(6h) (*trans*)-4-tert-pentylcyclohexyl acrylate: Colorless liquid, yield 62%; ^{1}H-NMR (400 MHz) δ = 6.38 (dd, *J* = 17.3 Hz, *J* = 1.5 Hz, 1H), 6.09 (dd, *J* = 17.3 Hz, *J* = 10.4 Hz, 1H), 5.78 (dd, *J* = 10.4 Hz, *J* = 1.5 Hz, 1H), 4.71 (m, 1H), 2.05 (m, 2H), 1.77 (m, 2H), 1.40-1.22 (m, 4H), 1.20-1.09 (m, 3H), 0.79 (t, *J* = 6.8 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 165.81, 130.06, 129.15, 73.89, 44.35, 34.59, 32.74, 32.18, 25.00, 24.28, 8.08; MS calcd for $C_{14}H_{24}O_2$ (H^+) 225.18, found .

(6i) Propyl 4-(acryloyloxy)benzoate: Colorless liquid, yield 85%; ^{1}H-NMR (400 MHz) δ = 8.10 (d, *J* = 8.9 Hz, 2H), 7.22 (d, *J* = 8.9 Hz, 2H), 6.63 (dd, *J* = 17.3 Hz, *J* = 1.3 Hz, 1H), 6.33 (dd, *J* = 17.3 Hz, *J* = 10.4 Hz, 1H), 6.05 (dd, *J* = 10.4 Hz, *J* = 1.3 Hz, 1H), 4.28 (t, *J* = 6.6 Hz, 2H), 1.79 (h, *J* = 7.4 Hz, 2H), 1.03 (t, *J* = 7.4 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 165.85, 163.93, 154.13, 133.13, 131.11, 128.14, 127.60, 121.49, 66.65, 22.10, 10.49; MS calcd for $C_{13}H_{14}O_4$ (H^+) 235.09, found 235.71.

(6j) Pentyl 4-(acryloyloxy)benzoate: White solid, mp 33-35°C, yield 75%; ^{1}H-NMR (400 MHz) δ = 8.09 (d, *J* = 8.8 Hz, 2H), 7.22 (d, *J* = 8.8 Hz, 2H), 6.63 (dd, *J* = 17.3 Hz, *J* = 1.3 Hz, 1H), 6.33 (dd, *J* = 17.3 Hz, *J* = 10.4 Hz, 1H), 6.05 (dd, *J* = 10.4 Hz, *J* = 1.3 Hz, 1H), 4.32 (t, *J* = 6.6 Hz, 2H), 1.77 (p, *J* = 7.2 Hz, 2H), 1.46-1.36 (m, 4H), 0.93 (t, *J* = 7.1 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 165.85, 163.92, 154.12, 133.12, 131.10, 128.15, 127.60, 121.49, 66.24, 28.41, 28.17, 22.34, 13.96; MS calcd for $C_{15}H_{18}O_4$ (H^+) 263.12, found 263.78.

(6k) 4-butyramidophenyl acrylate: White solid, mp 87-89°C, yield 73%; ^{1}H-NMR (400 MHz) δ = 7.51 (d, *J* = 8.8 Hz, 2H), 7.34 (s, br (NH)), 7.06 (d, *J* = 8.8 Hz, 2H), 6.59 (dd, *J* = 17.3 Hz, *J* = 1.3 Hz, 1H), 6.31 (dd, *J* = 17.3 Hz, *J* = 10.4 Hz, 1H), 6.01 (dd, *J* = 10.4 Hz, *J* = 1.3 Hz, 1H), 2.31 (t, *J* = 7.6 Hz, 2H), 1.75 (h, *J* = 7.4 Hz, 2H), 0.99 (t, *J* = 7.4 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 171.22, 164.72, 146.57, 135.73, 132.61, 127.85, 121.86, 120.73, 39.55, 19.02, 13.72; MS calcd for $C_{13}H_{15}NO_3$ (H^+) 235.23, found 234.11.

(6l) Hexyl 2-(acryloyloxy)benzoate: Colorless liquid, yield 71%; ^{1}H-NMR (400 MHz) δ = 8.03 (d, *J* = 7.9 Hz, 1H), 7.57 (t, *J* = 7.8 Hz, 1H), 7.33 (t, *J* = 7.9 Hz, 1H), 7.14 (d, *J* = 7.8 Hz, 1H), 6.64 (dd, *J* = 17.3 Hz, *J* = 1.3 Hz, 1H), 6.39 (dd, *J* = 17.3 Hz, *J* = 10.4 Hz, 1H), 6.05 (dd, *J* = 10.4 Hz, *J* = 1.3 Hz, 1H), 4.24 (t, *J* = 6.8 Hz, 2H), 1.69 (p, *J* = 7.0 Hz, 2H), 1.42-1.28 (m, 6H), 0.89 (t, *J* = 6.7 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 164.68, 164.50, 150.28, 133.61, 132.67, 131.82, 127.79, 126.05, 123.83, 123.74, 65.40, 31.43, 28.55, 25.60, 22.51, 13.98; MS calcd for $C_{16}H_{20}O_4$ (H^+) 277.14, found 277.81.

(6m) 5,6,7,8-tetrahydronaphthalen-2-yl acrylate: Colorless liquid, yield 77%; ^{1}H-NMR (400 MHz) δ = 7.07 (d, *J* = 7.7 Hz, 1H), 6.84 (m, 2H), 6.84 (dd, *J* = 17.3 Hz, *J* = 1.5 Hz, 1H), 6.31 (dd, *J* = 17.3 Hz, *J* = 10.4 Hz, 1H), 5.99 (dd, *J* = 10.4 Hz, *J* = 1.5 Hz, 1H), 2.77 (m, 2H), 1.79 (m, 2H); ^{13}C-NMR (100 MHz) δ = 164.87, 148.12, 138.43, 134.75, 132.16, 129.92, 128.11, 121.54, 118.50, 29.42, 28.88, 23.09, 22.86; MS calcd for $C_{13}H_{14}O_2$ (H^+) 203.10, found 203.31.

General procedure for 7a-g: To a solution of 4-hexylaniline (216 µL, 1 mmol), triethylamine (209 µL, 1.5 mmol, 1.5 equiv.) in DCM (5 mL) was added acid chloride (1.1 mmol) or acid anhydride (1 mmol). The reaction mixture was stirred for 1 h, poured into NH_4Cl (aq) (10 mL), diluted with ethyl acetate (10 mL), and the organic layer was separated. The aqueous layer was extracted with ethyl acetate (10 mL, twice) and the combined organic layers were dried over $MgSO_4$, filtered, and concentrated *in vacuo*. Purification was done by flash column chromatography (SP1, 25M (SiO_2), flow rate: 25 mL/min; gradient: 1–30% ethyl acetate in hexanes over 20 CV).

(7a) N-(4-hexylphenyl)acrylamide: White solid, mp 91-93°C, yield 88%; ^{1}H-NMR (400 MHz) δ = 7.37 (d, *J* = 8.1 Hz, 2H), 7.30 (s, NH), 7.02 (d, *J* = 8.1 Hz, 2H), 6.30 (dd, *J* = 16.8 Hz, *J* = 1.2 Hz, 1H), 6.13 (dd, *J* = 16.8 Hz, *J* = 10.4 Hz, 1H), 5.62 (dd, *J* = 10.6 Hz, *J* = 1.2 Hz, 1H), 2.46 (t, *J* = 7.6 Hz, 2H), 1.47 (p, *J* = 7.1 Hz, 2H), 1.22-1.16 (m, 6H), 0.76 (t, *J* = 6.8 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 163.44, 139.31, 135.30, 131.26, 128.86, 127.44, 120.00, 35.36, 31.69, 31.42, 28.89, 22.58, 14.06 MS calcd for $C_{15}H_{21}NO$ (H^+) 231.33, found 231.16.

(7b) (Z)-4-(4-hexylphenylamino)-4-oxobut-2-enoic acid: Yellow solid, mp 143-145°C, yield 85%; (DMSO-d_6) ^{1}H-NMR (400 MHz) δ = 13.3 (s, br, OH), 10.4 (s, br, NH), 7.56 (d, *J* = 8.3 Hz, 2H), 7.17 (d, *J* = 8.3 Hz, 2H), 6.49 (d, *J* = 12.0, 1H), 6.32 (d, *J* = 12.0 Hz, 1H), 2.56 (t, *J* = 7.5 Hz, 2H), 1.57 (p, *J* = 7.1 Hz, 2H), 1.32-1.26 (m, 6H), 0.88 (t, *J* = 6.7 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 166.65, 162.93, 137.94, 136.00, 131.56, 130.56, 128.43, 119.49, 34.49, 31.01, 30.86, 28.17, 21.96, 13.85 MS calcd for $C_{16}H_{21}NO_3$ (H^+) 276.15, found 276.87.

(7c) (E)-N-(4-hexylphenyl)but-2-enamide: White solid, mp 81-84°C, yield 78 %; ^{1}H-NMR (400 MHz) δ = 7.45-7.37 (m, 2H), 7.13 (d, *J* = 8.3 Hz, 2H), 7.05 (s, NH), 6.96 (m, 1H), 5.93 (d, *J* = 15.0 Hz, 1H), 2.56 (t, *J* = 7.8 Hz, 2H), 1.90 (s, 3H), 1.58 (m, 2H), 1.36-1.28 (m, 6H), 0.87 (t, *J* = 6.6 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 163.97, 141.08, 138.93, 135.62, 128.79, 125.53, 119.97, 35.35, 31.43, 28.89, 22.57, 17.77, 14.05; MS calcd for $H_{16}C_{23}NO$ (H^+) 246.18, found 246.0.

(7d) N-(4-hexylphenyl)-3-methylbut-2-enamide: White solid, mp 67-69°C, yield 84 %; ^{1}H-NMR (400 MHz) δ = 7.42 (d, *J* = 8.3 Hz, 2H), 7.11 (d, *J* = 8.3 Hz, 2H), 7.06 (s, NH), 5.96 (m, 1H), 2.55 (t, *J* = 7.8 Hz, 2H), 2.21 (s, 3H), 1.89 (s, 3H), 1.57 (p, *J* = 8.1 Hz, 2H), 1.36-1.27 (m, 6H), 0.87 (t, *J* = 6.5 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 164.93, 152.77, 138.67, 135.78, 128.74, 120.16, 119.81, 118.78, 35.33, 32.72, 31.69, 31.44, 28.87, 22.28, 19.89, 14.05, MS calcd for $C_{17}H_{25}NO$ (H^+) 260.19, found 260.70.

(7e) N-(4-hexylphenyl)cinnamamide: White solid, mp 117-119°C, yield 89 %; ^{1}H-NMR (400 MHz) δ = 7.74 (d, *J* = 15.5 Hz, 1H), 7.57-7.49 (m, 5H), 7.36-7.35 (m, 3H), 7.15 (d, *J* = 8.2 Hz, 2H), 6.58 (d, *J* = 15.5 Hz, 1H), 2.57 (t, *J* = 7.8 Hz, 2H), 1.59 (p, *J* = 7.6 Hz, 2H), 1.36-1.24 (m, 6H), 0.89 (t, *J* = 6.7 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 1643.17, 141.93, 139.17, 135.70, 134.67, 129.74, 128.85, 128.74, 127.89, 121.14, 120.37, 120.16, 114.36, 35.37, 31.68, 31.41, 28.91, 22.57, 14.06; MS calcd for $C_{21}H_{25}NO$ (H^+) 308.19, found 309.00.

(7f) 4-(4-hexylphenylamino)-2-methylene-4-oxobutanoic acid: White solid, mp 185-187°C, yield 80%; (DMSO-d_6) ^{1}H-NMR (400 MHz) δ = 12.50 (s(br), CO2H, 1H), 9.89 (s, NH, 1H), 7.46 (d, *J* = 7.6 Hz, 2H), 7.09 (d, *J* = 7.8 Hz, 2H), 6.16 (m, 1H), 5.13 (m, 1H), 2.55 (m, 2H), 2.50 (t, *J* = 7.4 Hz, 2H), 1.52 (m, 2H), 1.28-1.23 (m, 6H), 0.85 (t, *J* = 6.6 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 168.07, 167.49, 136.85, 136.83, 135.79, 128.29, 127.32, 118.86, 34.45, 31.02, 30.91, 28.16, 21.97, 13.86 calcd for $C_{17}H_{23}NO_3$ (H^+) 289.17, found 289.95.

(7g) 4-(4-hexylphenylamino)-4-oxobutanoic acid: White solid, mp 154-156°C, yield 78%; (DMSO-d_6) ^{1}H-NMR (400 MHz) δ = 12.1 (s, br, OH), 9.84 (s, br, NH), 7.46 (d, *J* = 8.3 Hz, 2H), 7.08 (d, *J* = 8.3 Hz, 2H), 2.55-2.47 (m, 6H), 1.52 (p, *J* = 6.4 Hz, 2H), 1.28-1.22 (m, 6H), 0.84 (t, *J* = 6.8 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 173.73, 169.68, 136.88, 136.71, 128.26, 118.81, 34.44, 31.01, 30.90, 30.87, 28.74, 28.15, 21.97, 13.85 MS calcd for $C_{16}H_{23}NO_3$ (H^+) 278.17, found 278.89.

General procedure for 8a-b: To a solution of 4-hexylaniline (178 µL, 1 mmol) or 4-hexylphenol (179 µL, 1 mmol), propiolic acid (70 µL, 1.3 mmol, 1.3 equiv.), 4-dimethylaminopyridine (0.01 mmol, 1.2 mg, 0.01 equiv) in DCM (5 mL) was added N,N'-diisopropylcarbodiimide (126 µL, 1.3 mmol, 1.3 equiv.). The resulting reaction mixture was stirred at rt for 5 h, poured into NH_4Cl (aq) (10 mL), diluted with ethyl acetate (10 mL) and the organic layer was separated. The aqueous layer was extracted with ethyl acetate (10 mL, twice) and the combined organic layers were dried over $MgSO_4$, filtered, and concentrated *in vacuo*. Purification was done by flash column chromatography (SP1, 25M (SiO_2), flow rate: 25 mL/min; gradient: 1% to 15% ethyl acetate in hexanes over 15 CV).

(8a) N-(4-hexylphenyl)propiolamide: White solid, mp 62-64°C, yield 79%; ^{1}H-NMR (400 MHz) δ = 7.53 (s (br), NH), 7.41 (d, *J* = 8.4 Hz, 2H), 7.14 (d, *J* = 8.4 Hz, 2H), 2.91 (s, 1H), 3.57 (t, *J* = 7.5 Hz, 2H), 1.58 (p, *J* = 7.4 Hz, 2H), 1.35-1.23 (m, 6H), 0.88 (t, *J* = 6.7 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 154.70, 140.19, 134.38, 129.00, 120.07, 75.64, 74.02, 35.38, 31.68, 31.37, 28.87, 22.58, 14.07; MS calcd for $C_{15}H_{19}O$ (H^+) 229.15, found 229.8.

(8b) 4-hexylphenyl propiolate: Colorless liquid, yield 68%; ^{1}H-NMR (400 MHz) δ = 7.19 (d, *J* = 8.2 Hz, 2H), 7.04 (d, *J* = 8.2 Hz, 2H), 3.05 (s, 1H), 2.60 (t, *J* = 7.8 Hz, 2H), 2.05 (p, *J* = 7.2 Hz, 2H), 1.36-1.24 (m, 6H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 151.15, 147.71, 141.38, 129.48, 120.83, 76.52, 74.37, 35.35, 31.67, 31.36, 28.42, 22.58, 14.57; MS calcd for $C_{15}H_{18}O_2$ (Na^+) 253.29, found 253.68. MS calcd for $C_{17}H_{26}O_4$ (reaction with MeOH) (H^+) 296.39, found 296.63.

General procedure for **8c** and **8e**: see general procedure for **3a-k**.

(8c) 2-chloro-1-(4-hexylphenyl)ethanone: White solid, mp 42-44°C, yield 84%; ^{1}H-NMR (400 MHz) δ = 7.88 (d, *J* = 8.3 Hz, 2H), 7.30 (d, *J* = 8.3 Hz, 2H), 4.69 (s, 2H), 2.67 (t, *J* = 7.8 Hz, 2H), 1.63 (p, *J* = 7.7 Hz, 2H), 1.36-1.27 (m, 6H), 0.88 (t, *J* = 7.0 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 190.69, 149.99, 131.93, 128.92, 128.66, 45.95, 36.07, 31.62, 30.98, 28.90, 22.55, 14.05; MS calcd for $C_{14}H_{19}ClO$ (H^+) 238.11, found 238.8.

(8d) 2-fluoro-1-(4-hexylphenyl)ethanone: Colorless liquid, yield 41%; ^{1}H-NMR (400 MHz) δ = 7.81 (d, *J* = 8.3 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H), 5.51 (d, *J* (H, F) = 47.0 Hz, 2H), 2.67 (t, *J* = 7.8 Hz, 2H), 1.63 (p, *J* = 7.7 Hz, 2H), 1.36-1.27 (m, 6H), 0.88 (t, *J* = 7.0 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 192.08, 150.10, 131.40, 128.94, 127.96, 83.50 (d, *J* (C, F) = 183 Hz), 36.09, 31.61, 30.98, 28.88, 22.54, 14.04; MS calcd for $C_{14}H_{19}FO$ (H^+) 223.14, found 223.03.

(8e) 3-bromo-1-(4-hexylphenyl)propan-1-one: White solid, mp 48-50°C, yield 69% ; ^{1}H-NMR (400 MHz) δ = 7.87 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 8.2 Hz, 2H), 3.74 (t, *J* = 6.9 Hz, 2H), 3.55 (t, *J* = 6.9 Hz, 2H), 2.66 (t, *J* = 7.7 Hz, 2H), 1.63 (p, *J* = 7.7 Hz, 2H), 1.36-1.24 (m, 6H), 0.88 (t, *J* = 6.9 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 196.60, 149.42, 133.97, 128.76, 128.18, 41.43, 36.01, 31.63, 31.03, 28.90, 25.94, 22.55, 14.05; MS calcd for $C_{15}H_{21}BrO$ (H^+) 297.08, found 297.58.

4-bromo-1-(4-hexylphenyl)butan-1-one: Colorless liquid, yield 95% ; ^{1}H-NMR (400 MHz) δ = 7.90 (d, *J* = 8.1 Hz, 2H), 7.25(d, *J* = 8.1 Hz, 2H), 3.55 (t, *J* = 6.4 Hz, 2H), 3.16 (t, *J* = 6.6 Hz, 2H), 2.66 (t, *J* = 7.5 Hz, 2H), 2.31 (p, *J* = 6.5 Hz, 2H), 1.63 (p, *J* = 7.7 Hz, 2H), 1.35-1.24 (m, 6H), 0.88 (t, *J* = 6.9 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 198.46, 148.99, 134.46, 128.66, 128.14, 36.42, 35.99, 33.69, 31.64, 31.05, 28.90, 26.97, 22.55, 14.05; MS calcd for $C_{16}H_{23}BrO$ (H^+) 311.09, found 311.68.

General procedure for 8f: To a solution of **8e** (296 mg, 1 mmol) in benzene (3 mL) was added DBU (1,8-Diazabicyclo[5.4.0]undec-7-ene) (150 µL, 1.1 mmol, 1.1 equiv.) and the reaction mixture was stirred 2 h at room temperature, filtered, and evaporated to yield crude **1**. The crude product was resuspended in MeOH (5 mL) and treated with H_2O_2 (30% in H_2O) (0.3 mL, 3 mmol, 3 equiv.) and NaOH (1M in H_2O) (1 mL). The reaction mixture was evaporated, dissolved in water, and extracted with ethyl acetate (20 mL, twice) and the combined organic layers were dried over $MgSO_4$, filtered, and concentrated *in vacuo*. Purification was done by flash column chromatography (SP1, 25M (SiO_2), flow rate: 25 mL/min; gradient: 1% to 15% ethyl acetate in hexanes over 15 CV).

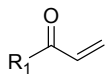
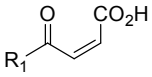
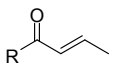
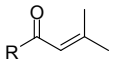
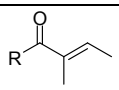
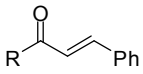
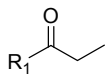
(8f) (4-hexylphenyl)(oxiran-2-yl)methanone: Colorless liquid, yield 74%; ^{1}H-NMR (400 MHz) δ = 7.97 (d, *J* = 8.1 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H), 4.23 (m, 1H), 3.11 (m, 1H), 2.97 (m, 1H), 2.67 (t, *J* = 7.9 Hz, 2H), 1.63 (p, *J* = 7.1 Hz, 2H), 1.36-1.27 (m, 6H), 0.88 (t, *J* = 6.9 Hz, 3H); ^{13}C-NMR (100 MHz) δ = 194.12, 149.91, 133.14, 128.85, 128.46, 50.97, 47.49, 36.06, 31.60, 30.97, 28.87, 22.57, 14.03; MS calcd for $C_{15}H_{20}O_2$ (H^+) 233.15, found 233.15.

Table 1. Summary of β-aminophenylketones 3a–k data: Yield, inhibition (IC_{50}) of the interaction between coregulatory peptide SRC2-2 and TRα/TRβ, viability (LD_{50}) of U2OS and ARO cells in the presence of compound, solubility in PBS buffer containing 5% DMSO, and permeability across an artificial membrane (PAMPA).

					Potency			Cytotoxicity		Property	
Entry	R_1	R_2	Com-pound	Yield[a] (%)	TRα[b] IC_{50} (μM)	TRβ[b] IC_{50} (μM)	TRα :TRβ ratio	ARO[c] LD_{50} (μM)	U2OS[c] LD_{50} (μM)	Solu-bility[c] (μM)	Perme-ability[c] (10^{-6} cm/s)
1	2-phenylethyl	methyl	**3a**	84	3.6 ±0.6	1.5 ±0.4	2.4	2.5 ±1.7	18.4 ±4.1	15 ±7	57 ±39
2	2-hydroxyethyl	methyl	**3b**	87	3.0 ±0.5	1.6 ±0.2	1.9	13.2 ±3.2	13.2 ±3.1	97 ±13	965 ±212
3	isopropyl	isopropyl	**3c**	81	4.1 ±0.4	2.0 ±0.4	2.1	15.4 ±2.9	20.7 ±2.7	55 ±12	747 ±336
4	pyrroline		**3d**	85	4.3 ±0.3	2.7 ±0.3	1.6	19.0 ±6.0	38.4 ±3.2	341 ±29	2144 ±516
5	morpholine		**3e**	90	4.1 ±0.6	2.7 ±0.4	1.5	7.2 ±3.1	20.8 ±1.9	110 ±17	1210 ±317
6	methyl piperidine-4-carboxylate		**3f**	86	6.3 ±0.7	3.9 ±0.4	1.6	8.2 ±2.8	19.7 ±2.5	27 ±6	145 ±8
7	*n*-butyl	*n*-butyl	**3g**	90	6.9 ±0.7	4.2 ±0.8	1.6	5.4 ±2.1	25.5 ±3.1	152 ±23	1957 ±575
8	methyl	methyl	**3h**	94	10.6 ±0.8	4.3 ±0.7	2.5	11.0 ±4.1	34.9 ±3.8	321 ±31	2323 ±713
9	furan-2-ylmethyl	methyl	**3i**	92	22.6 ±2.1	12.1 ±1.3	1.9	15.5 ±4.2	18.6 ±2.9	47 ±5	681 ±172
10	cyclohexyl	cyclohexyl	**3j**	78	16.5 ±1.8	12.7 ±2.4	1.3	25.6 ±6.7	27.3 ±4.1	32 ±3	104 ±73
11	*n*-propyl	hydrogen	**3k**	93	25.8 ±1.9	15.2 ±2.8	1.7	102 ±18.1	160 ±29.3	354 ±26	254 ±6

[a]Isolated yield; [b]values are means of two independent experiments done in quadruplicate; [c]values are means of two independent experiments done in triplicate.

Table 2. Summary of enones 1 and 4a–e and allylic alcohols 5b–e: Yield, IC_{50} values of the inhibition between coregulatory peptide SRC2-2 and TRα/TRβ, viability (LD_{50}) of U2OS and ARO cells in the presence of compound, solubility in PBS buffer containing 5% DMSO, and permeability across an artificial membrane (PAMPA).

					Potency			Cytotoxicity		Property	
Entry	R_1 = 4-hexylbenzene and R = 4-heptylbenzene	Compound	Yield[a] **5** (%)	Yield[a] **4** (%)	TRα[b] IC_{50} (μM)	TRβ[b] IC_{50} (μM)	TRα:TRβ ratio	ARO[c] LD_{50} (μM)	U2OS[c] LD_{50} (μM)	Solubility[c] (μM)	Permeability[c] (10^{-6} cm/s)
1		**1**	-	55	28.1 ±2.1	1.5 ±0.7	18.7	4.5 ±1.5	10.1 ±3.6	36 ±7	38 ±19
2		**4a**	-	45	19.2 ±1.8	17.7 ±2.4	1.1	5.5 ±1.3	57.4 ±19.5	252 ±19	66 ±15
3		**4b**	67	57	18.9 ±2.5	7.6 ±1.8	2.5	1.4 ±0.6	11.6 ±10.2	41 ±10	7 ±5
4		**4c**	67	67	52.9 ±5.6	23.2 ±3.5	2.3	10.7 ±4.0	18.7 ±3.1	37 ±11	43 ±14
5		**4d**	51	64	>100	>100	-	>200	>200	24 ±14	0
6		**4e**	46	59	>100	>100	-	>200	>200	36 ±9	0
7		**4f**	54	77	>100	>100	-	>200	57.0 ±8.9	30 ±5	0
8		**4g**	-	85	>100	>100	-	>200	>200	14 ±2	0

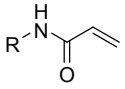
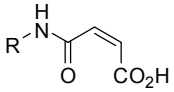
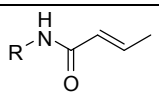
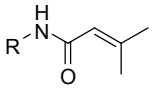
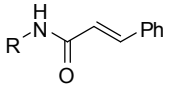
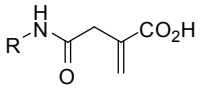
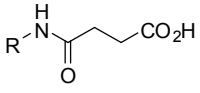
[a]Isolated yield; [b]values are means of two independent experiments done in quadruplicate; [c]values are means of two independent experiments done in triplicate.

Table 3. Summary of IC50 values of 6a–m: Yields; inhibition of coregulatory peptide SRC2-2 and TRα/TRβ binding; viability (LD_{50}) of U2OS and ARO cell in the presence of compounds**.**

				Potency			Cytotoxicity	
Entry	 R =	Com-pound	Yield[a] (%)	TRα[b] IC_{50} (μM)	TRβ[b] IC_{50} (μM)	TRα: TRβ ratio	ARO[c] LD_{50} (μM)	U2OS[c] LD_{50} (μM)
1	4- *n*-propylphenyl	**6a**	85	>100	100	-	20.2 ±6.1	43.9 ±5.1
2	4- *n*-butylphenyl	**6b**	86	71.0 ±7.3	66.0 ±8.4	1.1	9.9 ±2.6	25.6 ±4.0
3	4- *n*-pentylphenyl	**6c**	88	60.9 ±6.8	33.9 ±5.5	1.8	20.0 ±6.1	22.7 ±3.1
4	4- *tert*-pentylphenyl	**6d**	94	69.6 ±9.1	43.5 ±7.3	1.6	5.8 ±1.9	27.5 ±3.2
5	4-*n*-hexylphenyl	**6e**	89	45.2 ±4.3	18.6 ±2.1	2.4	29.5 ±6.3	18.8 ±3.9
6	4-*n*-heptylphenyl	**6f**	76	23.0 ±3.8	10.5 ±1.9	2.2	69.2 ±8.1	36.7 ±5.3
7	4-*n*-octylphenyl	**6g**	81	21.4 ±2.1	11.4 ±2.9	1.9	111 ±12.3	50.5 ±10.1
8	(*trans*) 4-*tert*-pentylcyclohexyl	**6h**	62	75.6 ±10.3	69.1 ±6.9	1.1	92.8 ±21.8	50.2 8.9
9	4-*n*-propylbenzoate	**6i**	75	>100	61.0 ±7.5	-	4.8 ±1.1	121 ±15.3
10	4-*n*-pentylbenzoate	**6j**	71	>100	55.8 ±7.1	-	21.2 ±3.9	36.5 ±9.1
11	2-*n*-hexylbenzoate	**6k**	85	39.1 ±6.9	8.2 ±3.4	4.8	14.6 ±2.2	19.4 ±2.9
12	4-*n*-butyramidophenyl	**6l**	73	>100	85.9 ±10.0	-	8.6 ±2.0	242 ±39.1
13	5,6,7,8-tetrahydronaphthyl	**6m**	77	85.3 ±9.4	69.8 ±9.0	1.2	54.7 ±11.3	101 ±20.6

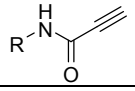
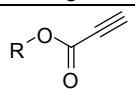
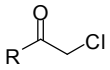
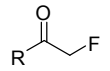
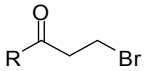
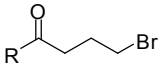
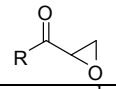
[a]Isolated yield; [b]values are means of two independent experiments done in quadruplicate; the general error limits are 10%; [c]values are means of two independent experiments done in triplicate; the general error limits are 10-15%.

Table 4. Summary of acrylamides 7a–g: Yield, IC_{50} values of the inhibition between coregulatory peptide SRC2-2 and TRα/TRβ, viability (LD_{50}) of U2OS and ARO cells in the presence of compound, solubility in PBS buffer containing 5% DMSO, and permeability across an artificial membrane (PAMPA).

				Potency			Cytotoxicity		Property	
Entry	R = 4-hexylbenzene	Compound	Yield[a] (%)	TRα[b] IC_{50} (μM)	TRβ[b] IC_{50} (μM)	TRα: TRβ ratio	ARO[c] LD_{50} (μM)	U2OS[c] LD_{50} (μM)	Solubility (μM)	Permeability (10^{-6} cm/s)
1		**7a**	88	21.6 ±1.5	20.3 ±1.8	1.1	113 ±21.3	66.5 ±13.9	47 ±8	833 ±71
2		**7b**	85	17.5 ±2.1	17.9 ±1.9	1.0	>200	148 ±24.3	418 ±38	29 ±4
3		**7c**	78	>100	>100	-	>200	>200	42 ±8	432 ±61
4		**7d**	84	>100	>100	-	>200	>200	37 ±7	98 ±16
5		**7e**	89	>100	>100	-	174 ±23.4	69.4 ±8.3	105 ±18	14 ±6
6		**7f**	80	>100	>100	-	183 ±29.1	124 ±15.3	286 ±36	57 ±4
7		**7g**	78	>100	>100	-	.>200	>200	372 ±31	48 ±13

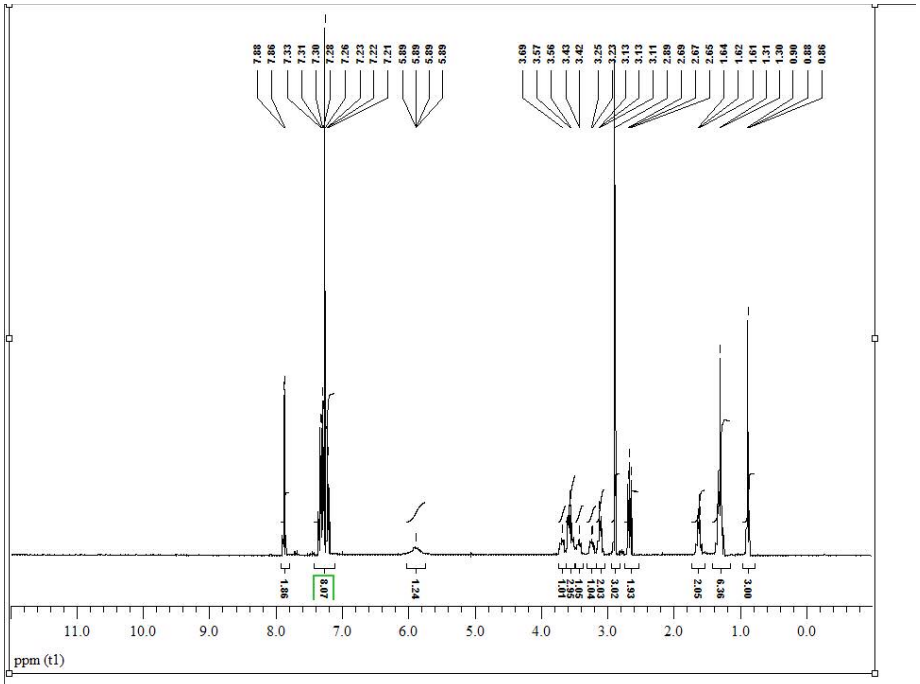
[a]Isolated yield; [b]values are means of two independent experiments done in quadruplicate; [c]values are means of two independent experiments done in triplicate.

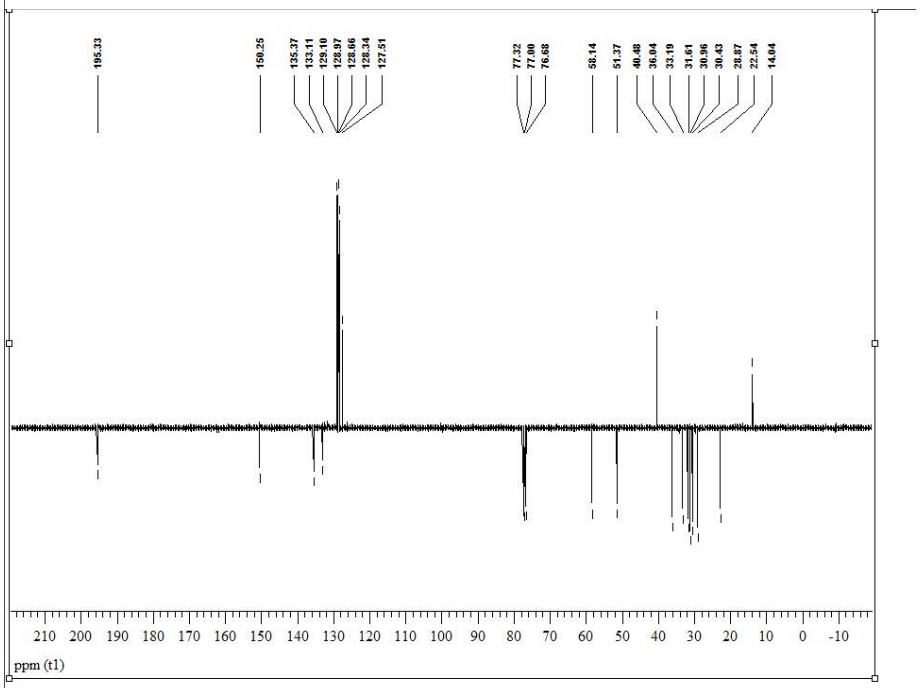
Table 5. Summary of electrophilic compounds 8a–f: Yield, IC_{50} values of the inhibition between coregulatory peptide SRC2-2 and TRα/TRβ, viability (LD_{50}) of U2OS and ARO cells in the presence of compound, solubility in PBS buffer containing 5% DMSO, and permeability across an artificial membrane (PAMPA).

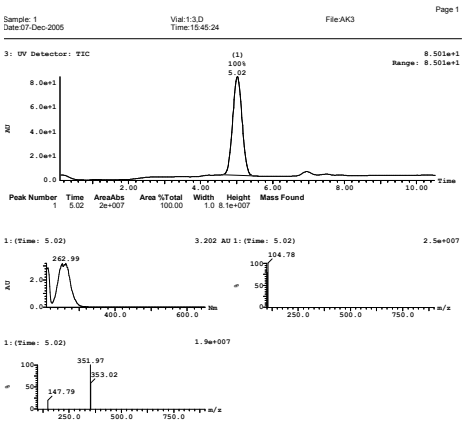
				Potency			Cytotoxicity		Property	
Entry	R = 4-hexylbenzene	Compound	Yield[a] (%)	TRα[b] IC_{50} (μM)	TRβ[b] IC_{50} (μM)	TRα: TRβ ratio	ARO[c] LD_{50} (μM)	U2OS[c] LD_{50} (μM)	Solubility (μM)	Permeability (10^{-6} cm/s)
1		**8a**	63	68.9 ±7.1	35.1 ±5.1	2.0	8.0 ±2.1	17.1 ±2.3	60 ±21	621 ±62
2		**8b**	57	16.7 ±1.3	6.2 ±0.9	2.7	7.9 ±2.5	13.9 ±2.9	18 ±7	21 ±9
3		**8c**	84	47.7 ±4.1	23.1 ±1.6	2.1	12.2 ±3.1	8.3 ±2.1	103 ±23	1029 ±225
4		**8d**	41	>100	>100	-	2.4 ±0.7	69 ±9.1	95 ±18	974 ±88
5		**8e**	69	4.2 ±0.9	3.0 ±0.8	1.4	40.1 ±6.3	17 ±4.3	85 ±29	1190 ±41
6		**8f**	95	>100	>100	-	28.7 ±5.4	25.3 ±4.1	26 ±11	58 ±5
7		**8g**	74	33.2 ±5.3	19.1 ±4.8	1.7	>200	58 ±6.0	204 ±19	1117 ±41

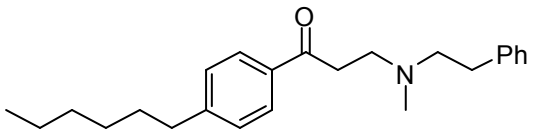
[a]Isolated yield; [b]values are means of two independent experiments done in quadruplicate; [c]values are means of two independent experiments done in triplicate.

Spectral data 3a



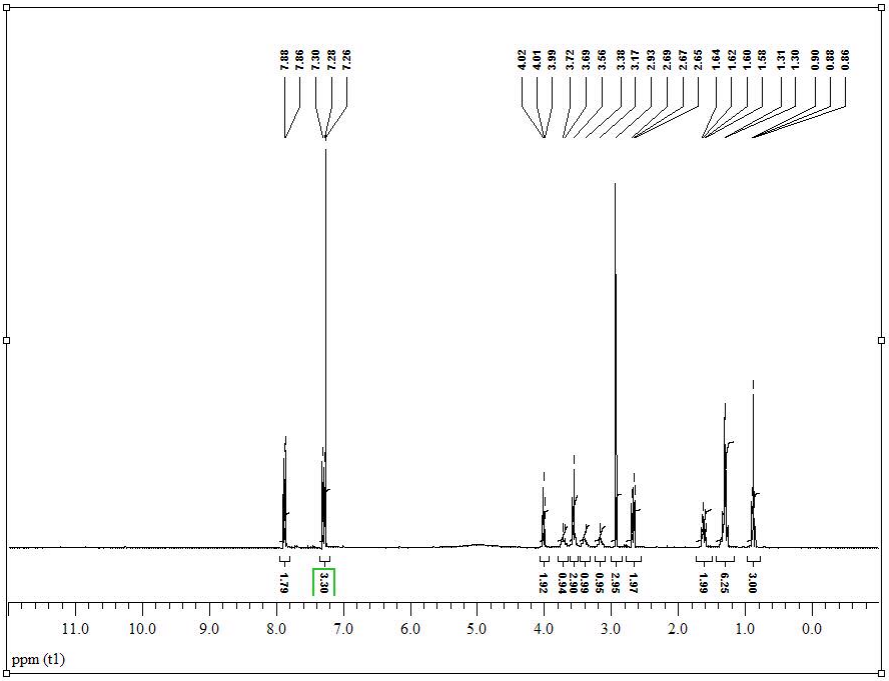


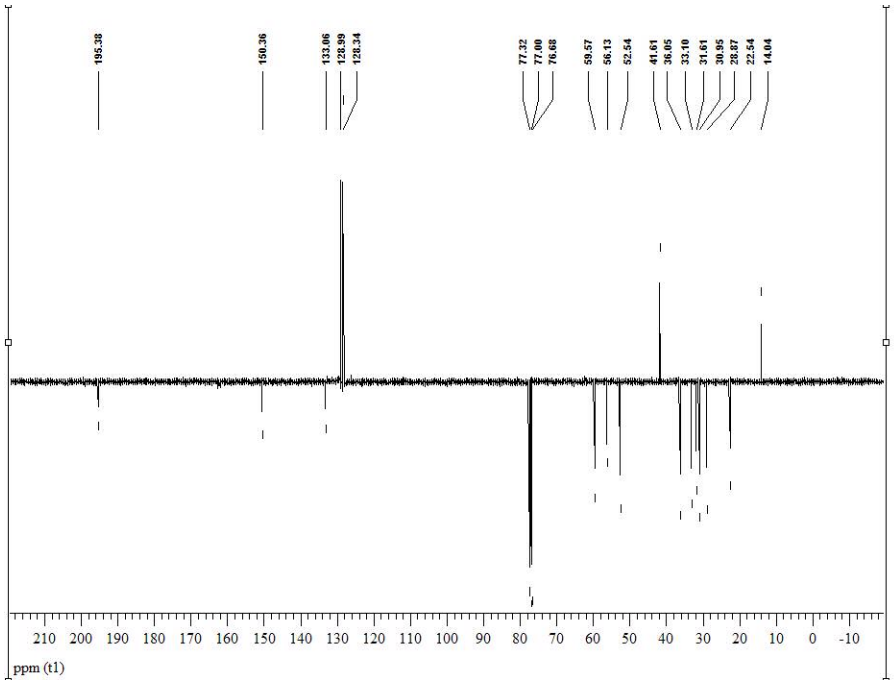


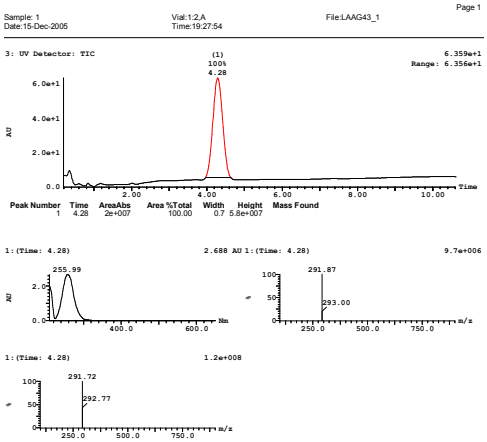


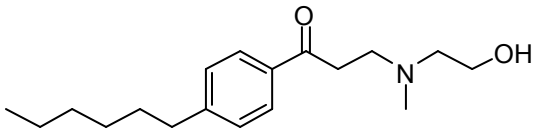
1-(4-hexylphenyl)-3-(methyl(phenethyl)amino)propan-1-one

Spectral data 3b



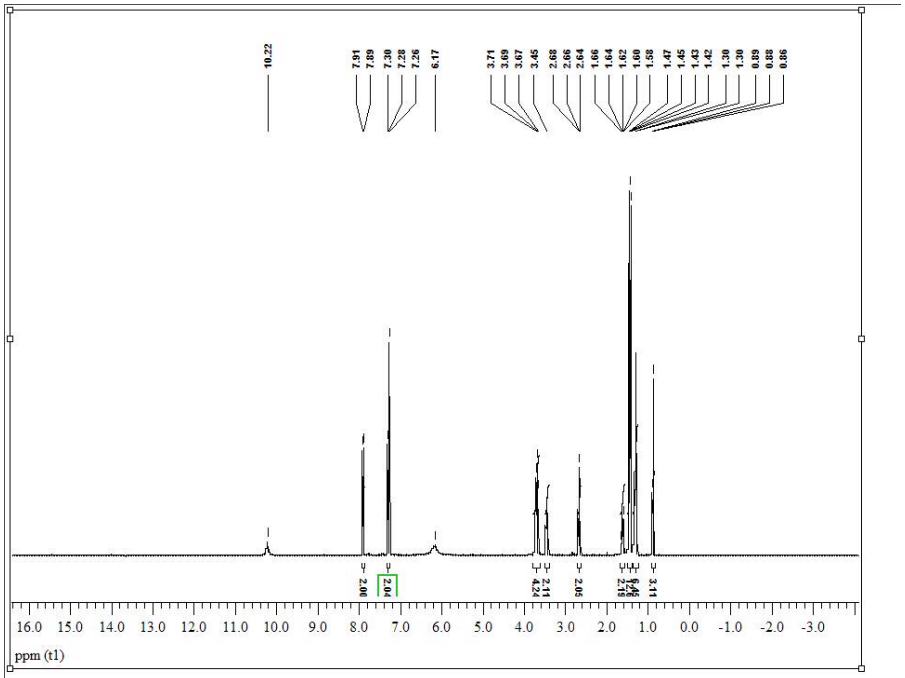


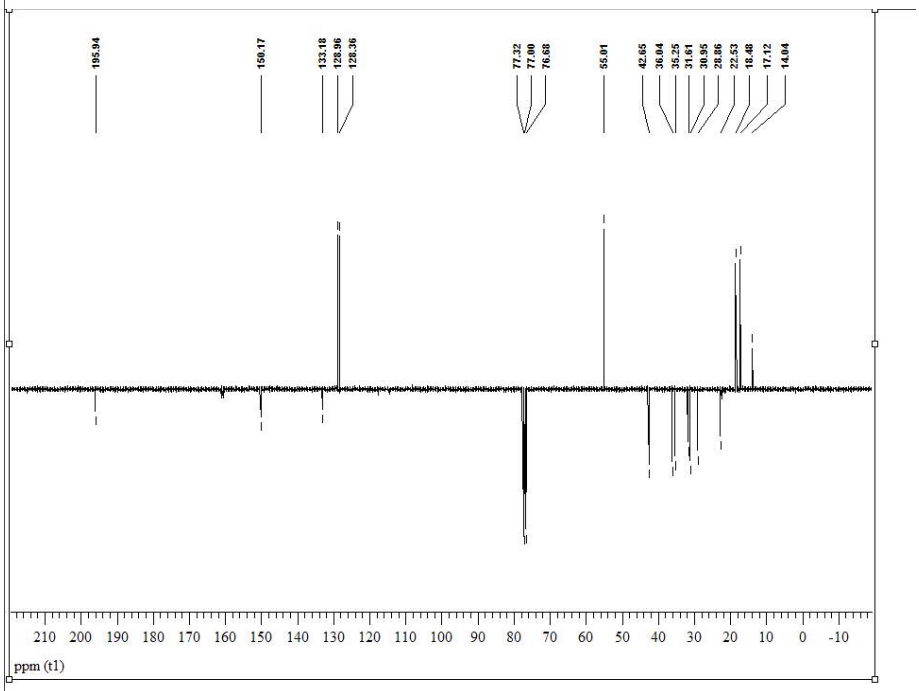


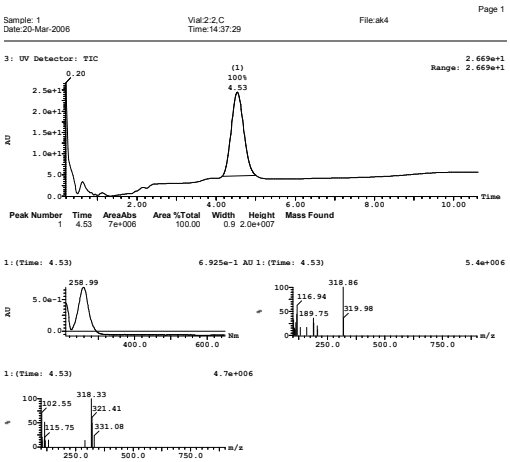


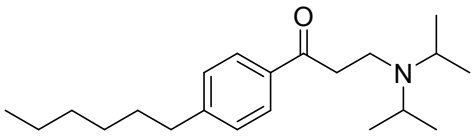
1-(4-hexylphenyl)-3-((2-hydroxyethyl)(methyl)amino)propan-1-one

Spectral data 3c



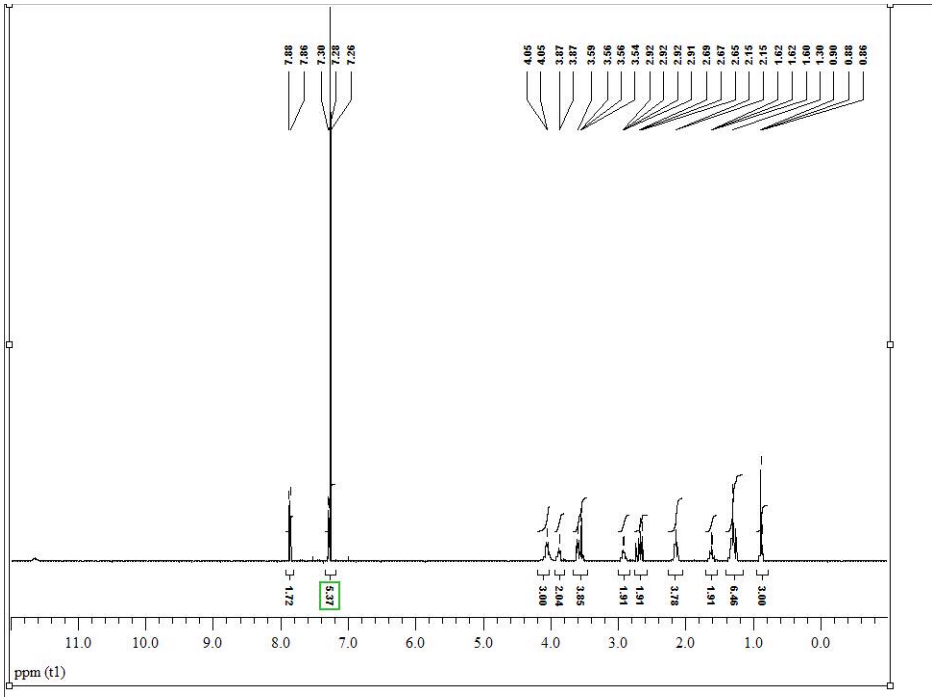


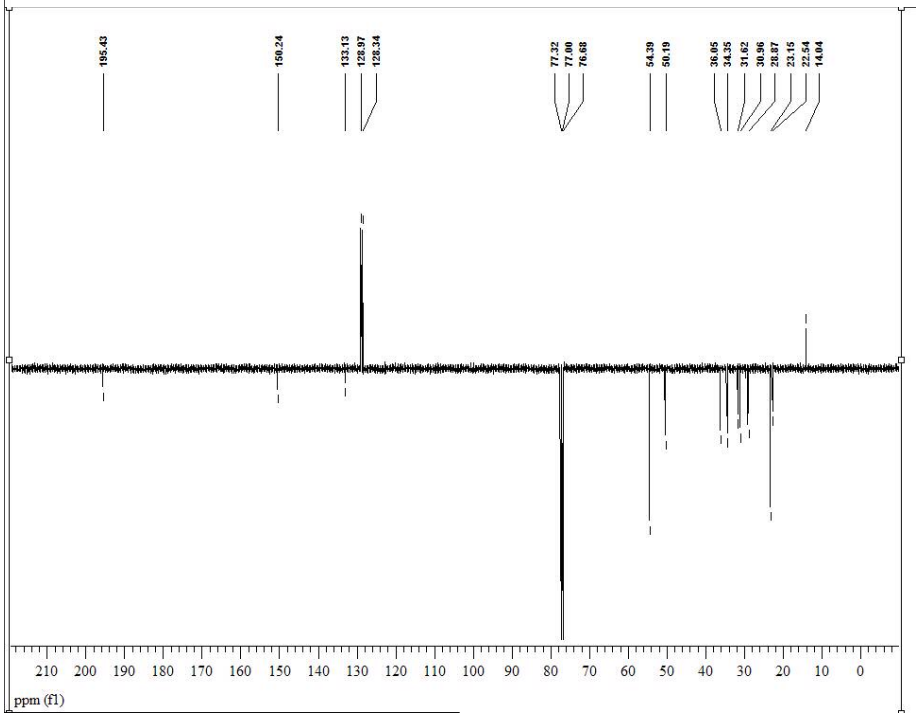


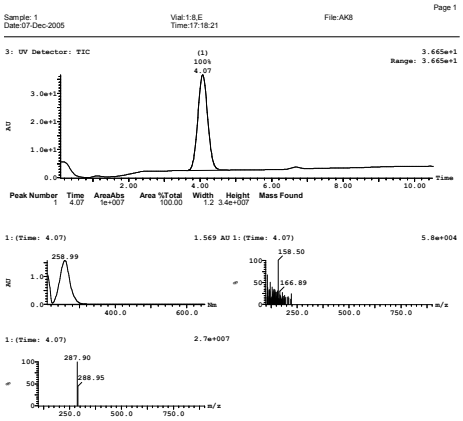


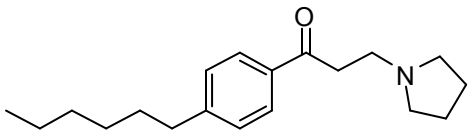
3-(diisopropylamino)-1-(4-hexylphenyl)propan-1-one

Spectral data 3d



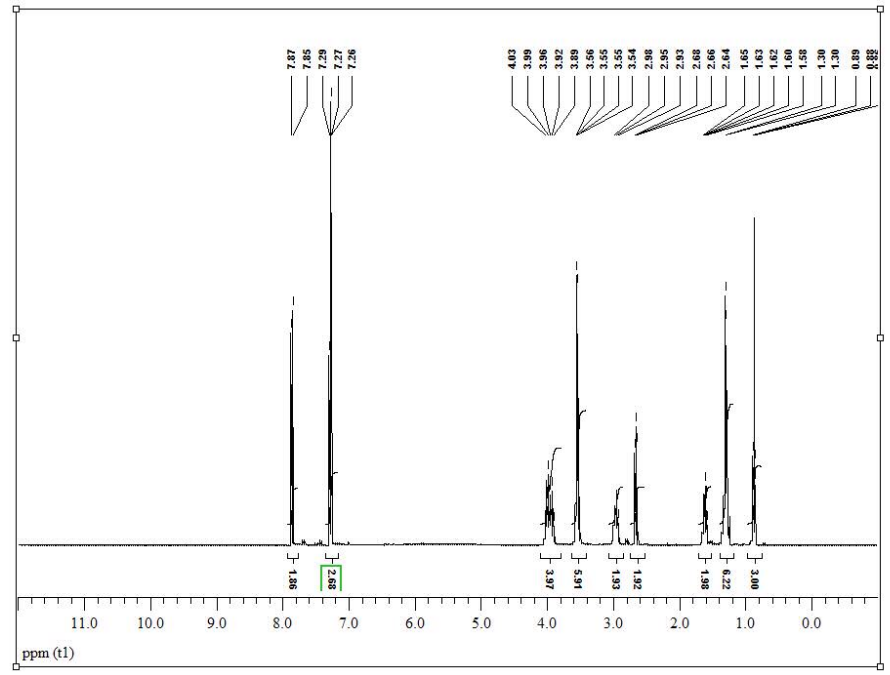


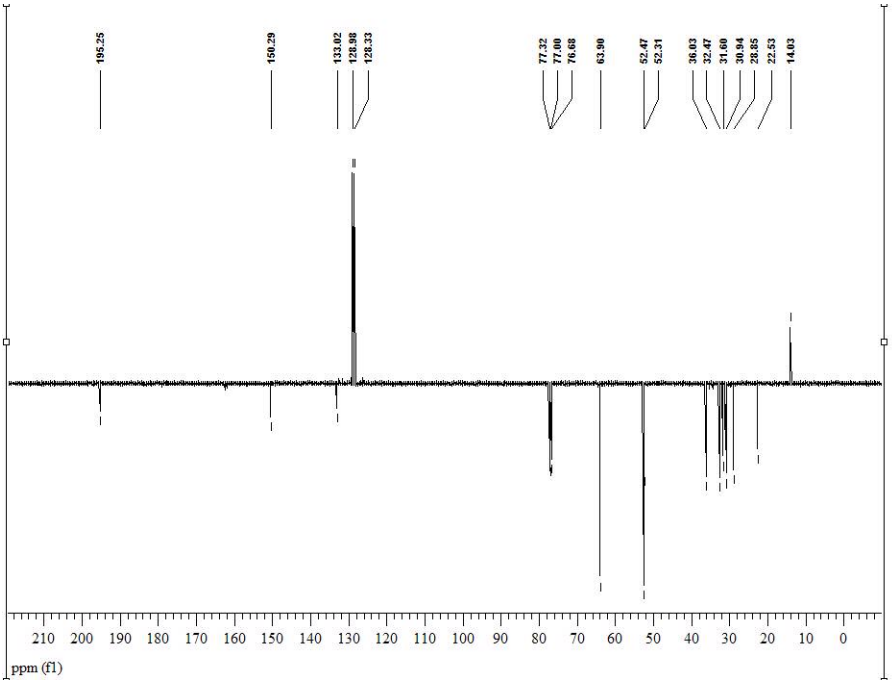


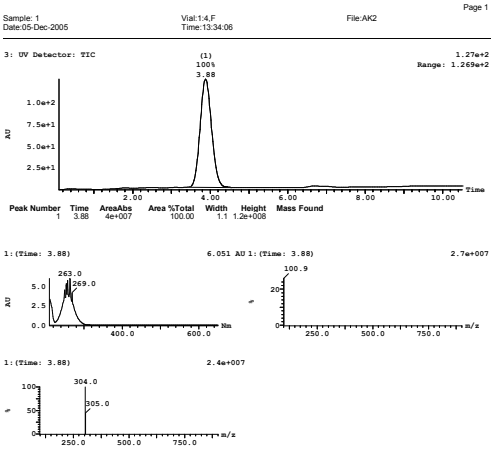


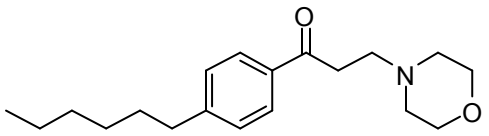
1-(4-hexylphenyl)-3-(pyrrolidin-1-yl)propan-1-one

Spectral data 3e



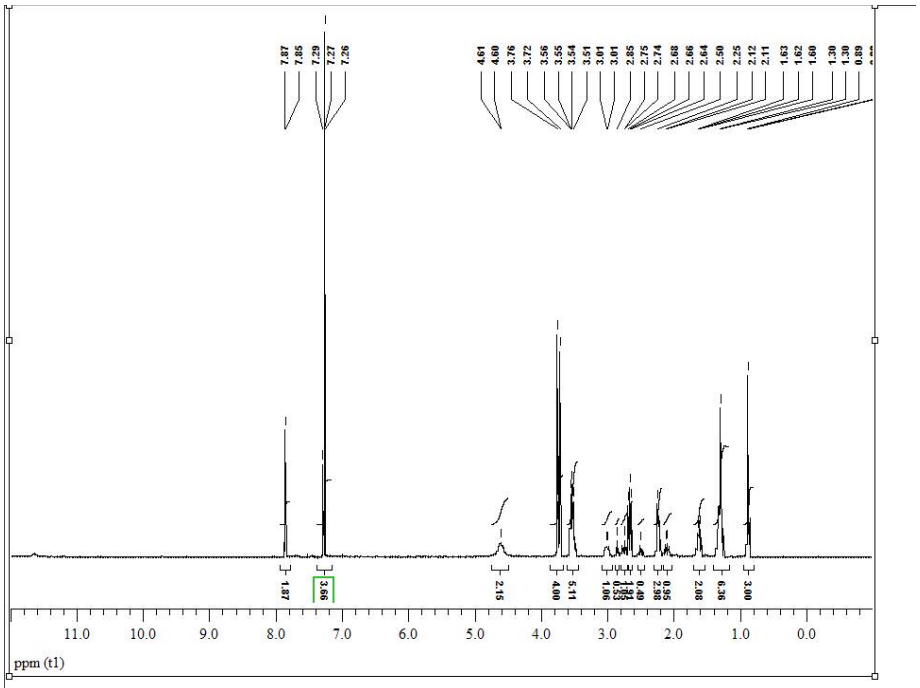


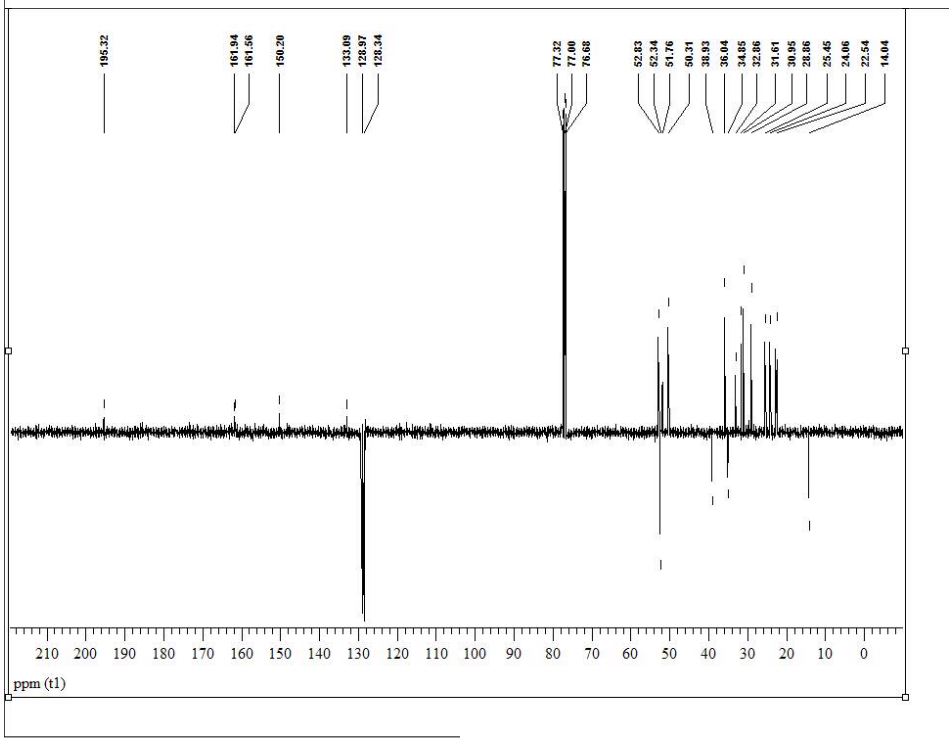


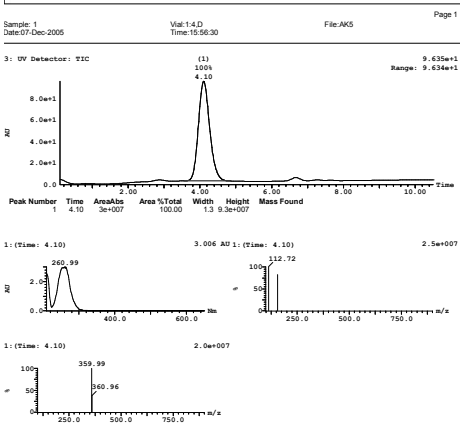


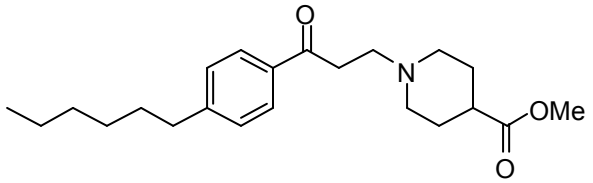
1-(4-hexylphenyl)-3-morpholinopropan-1-one

Spectral data 3f



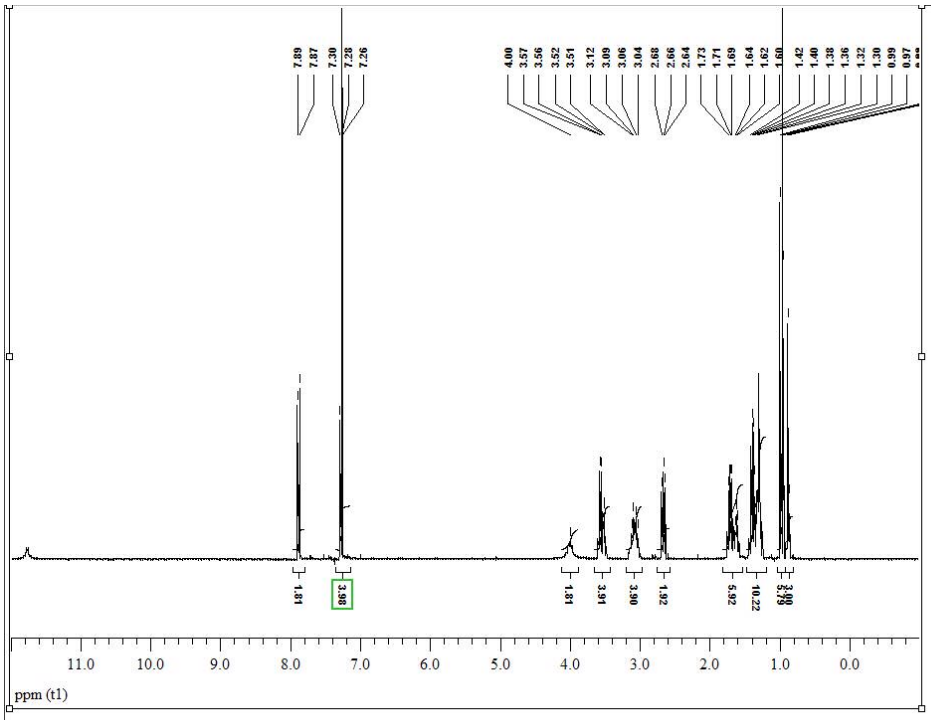


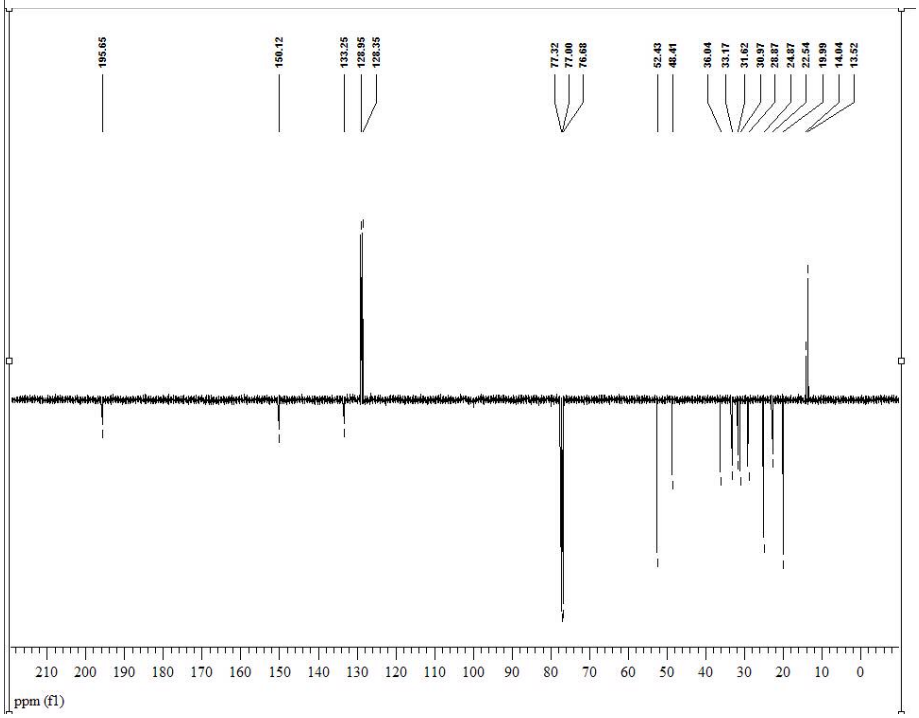


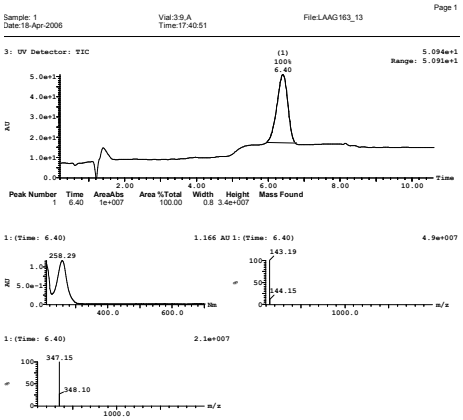


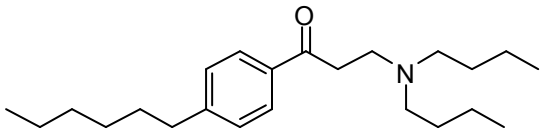
methyl 1-(3-(4-hexylphenyl)-3-oxopropyl)piperidine-4-carboxylate

Spectral data 3g



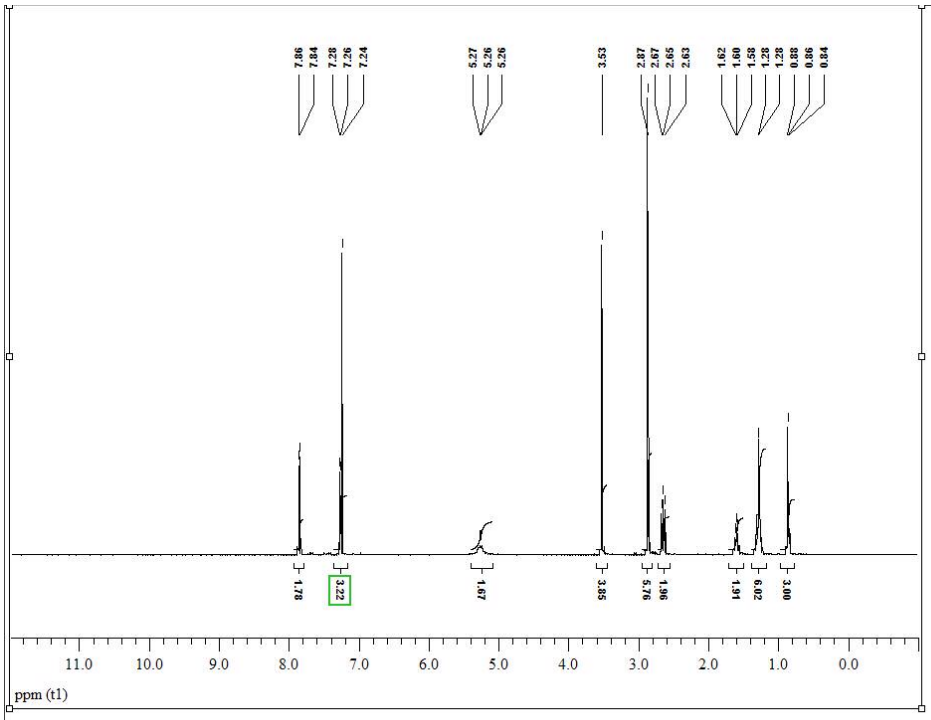


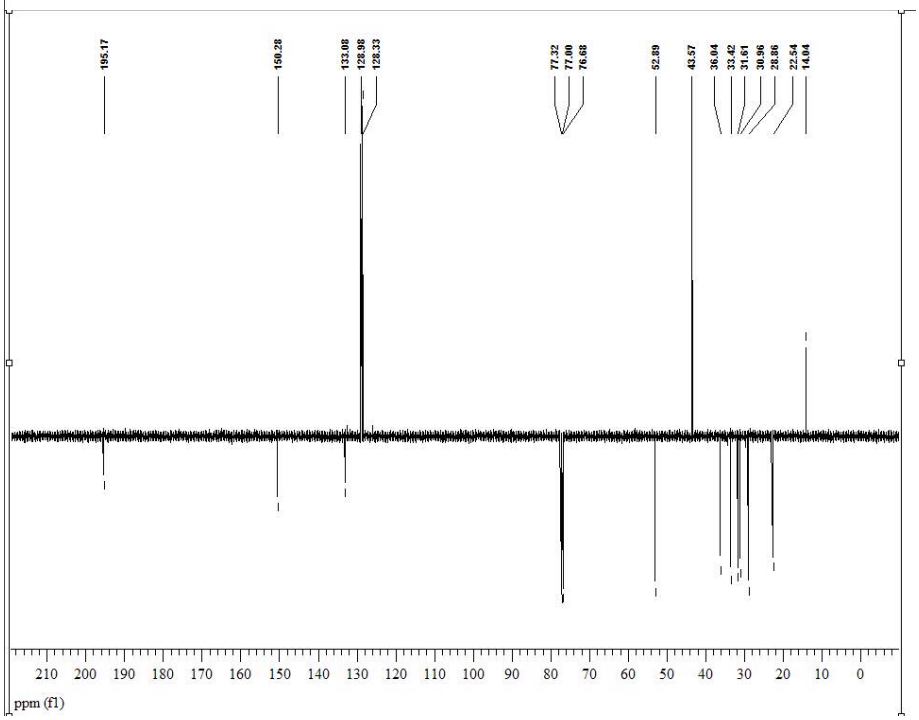


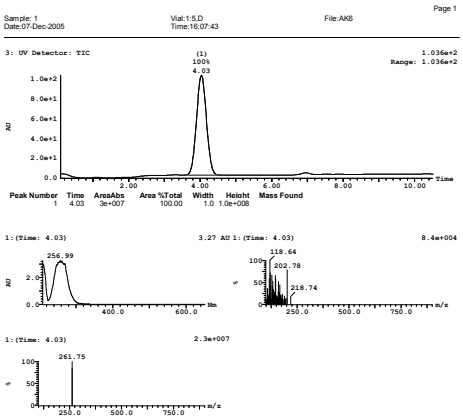


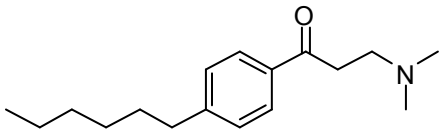
3-(dibutylamino)-1-(4-hexylphenyl)propan-1-one

Spectral data 3h



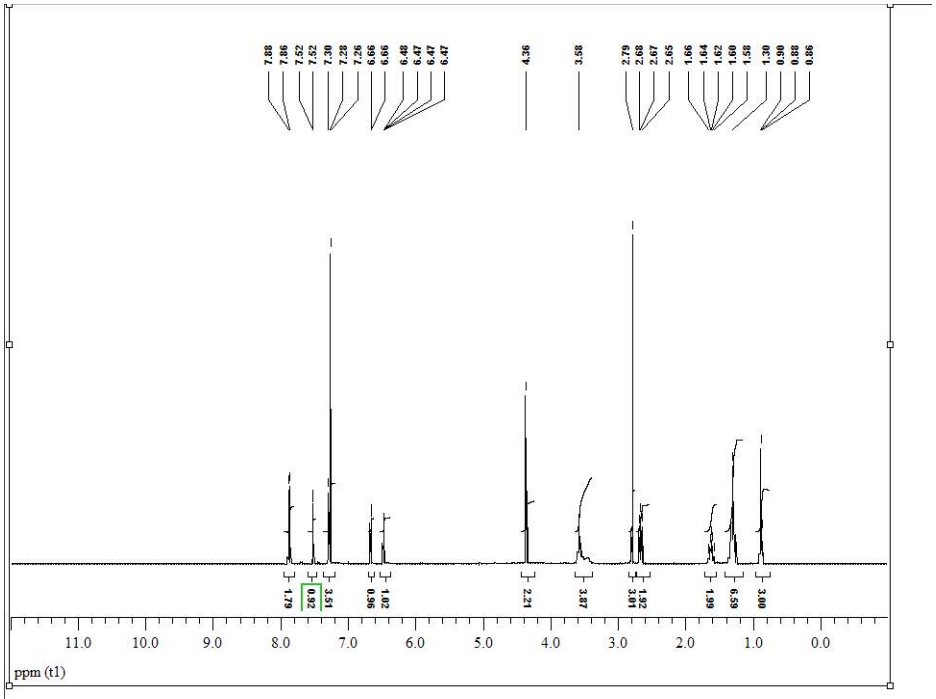


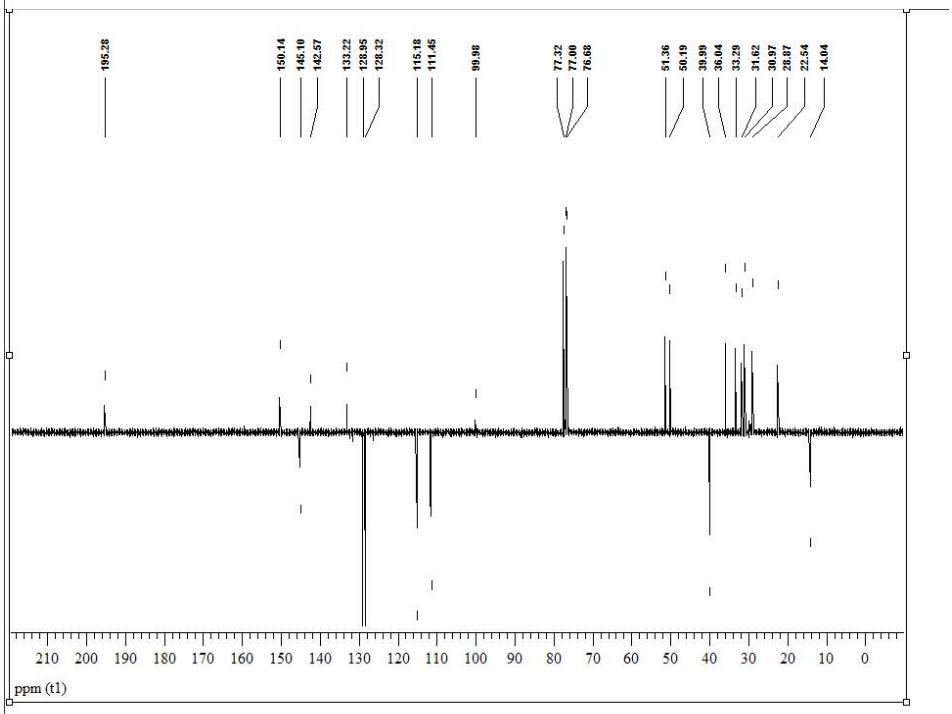


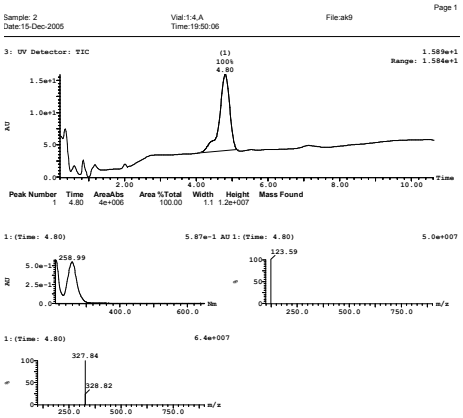


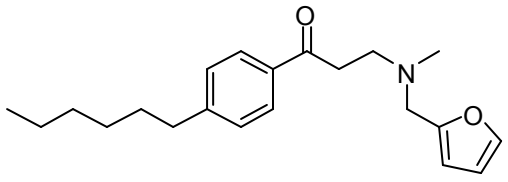
3-(dimethylamino)-1-(4-hexylphenyl)propan-1-one

Spectral data 3i



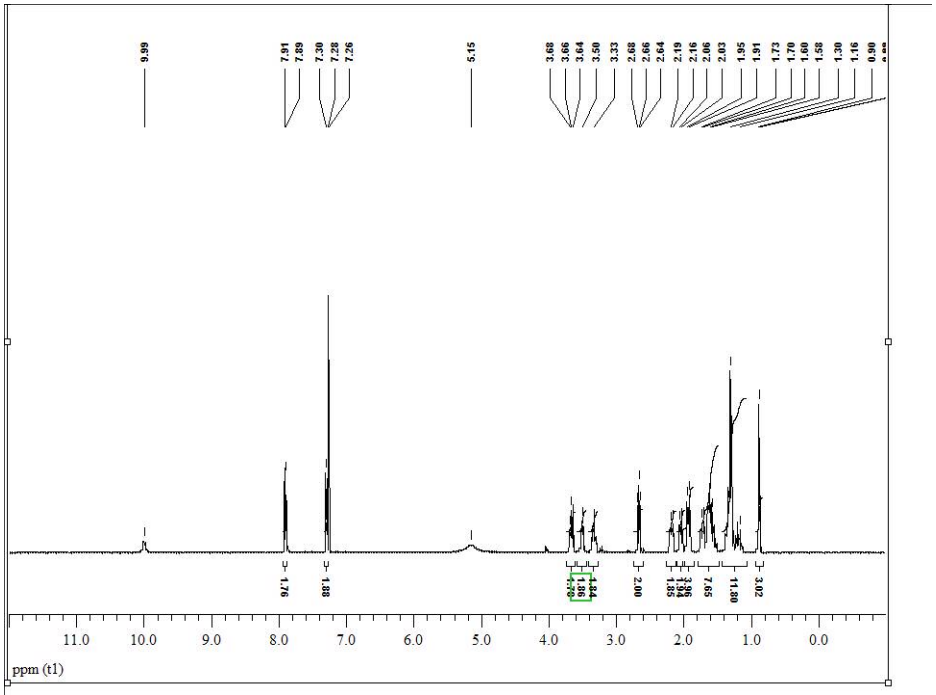


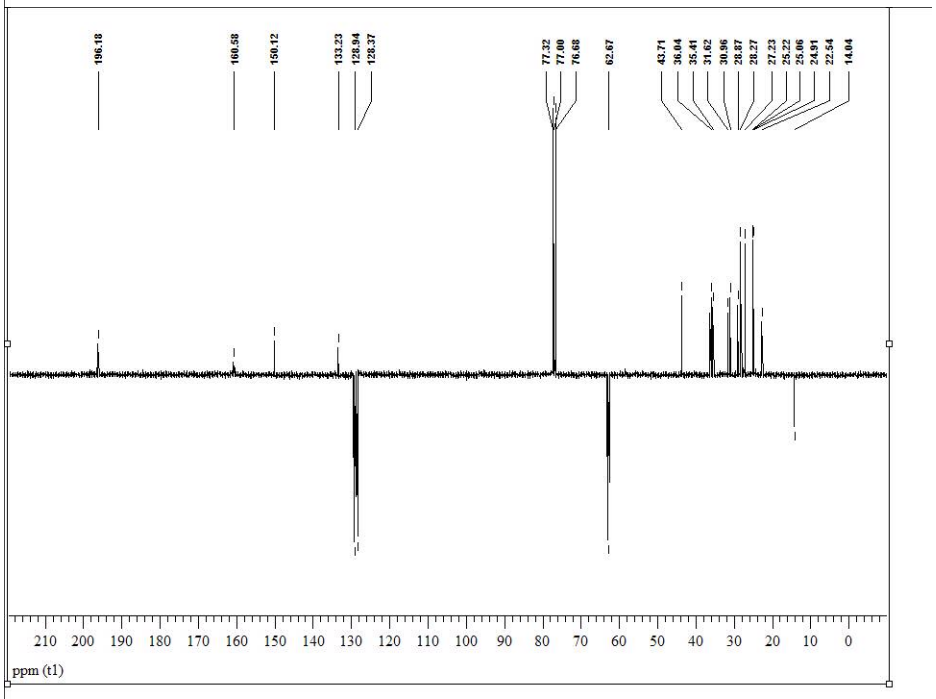


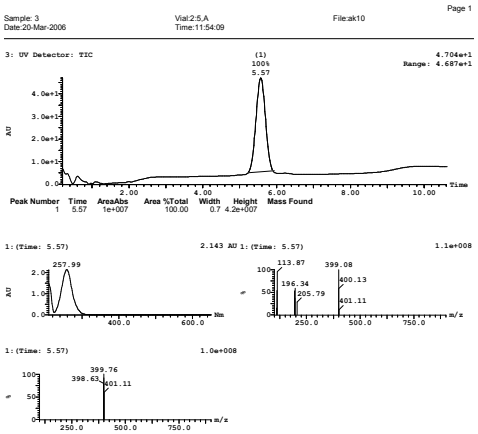


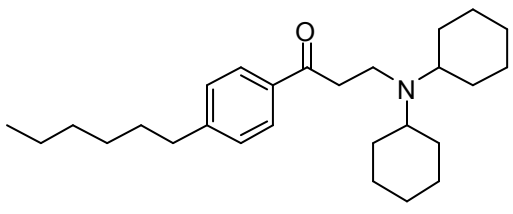
3-((furan-2-ylmethyl)(methyl)amino)-1-(4-hexylphenyl)propan-1-one

Spectral data 3j



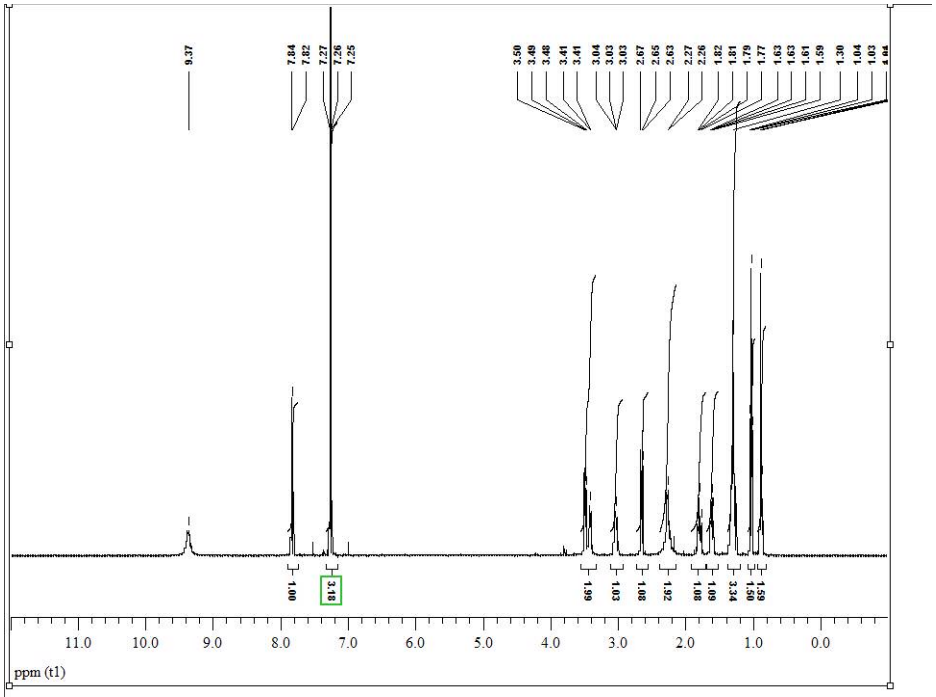


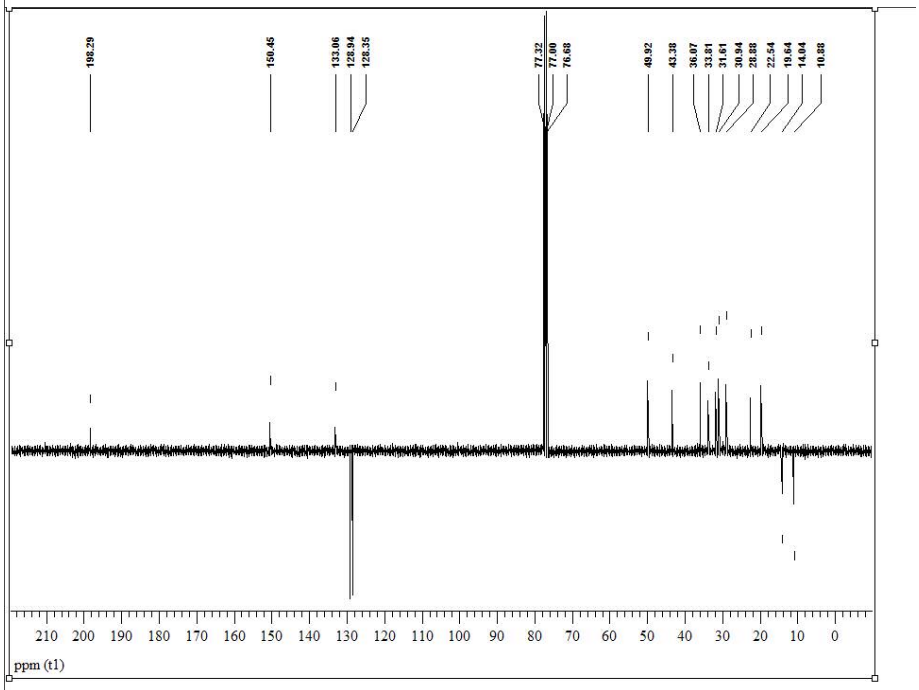


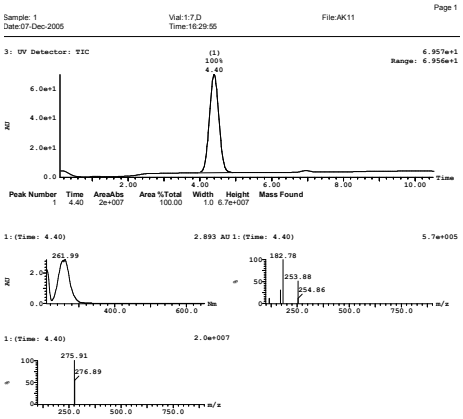


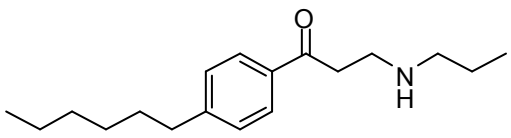
3-(dicyclohexylamino)-1-(4-hexylphenyl)propan-1-one

Spectral data 3k



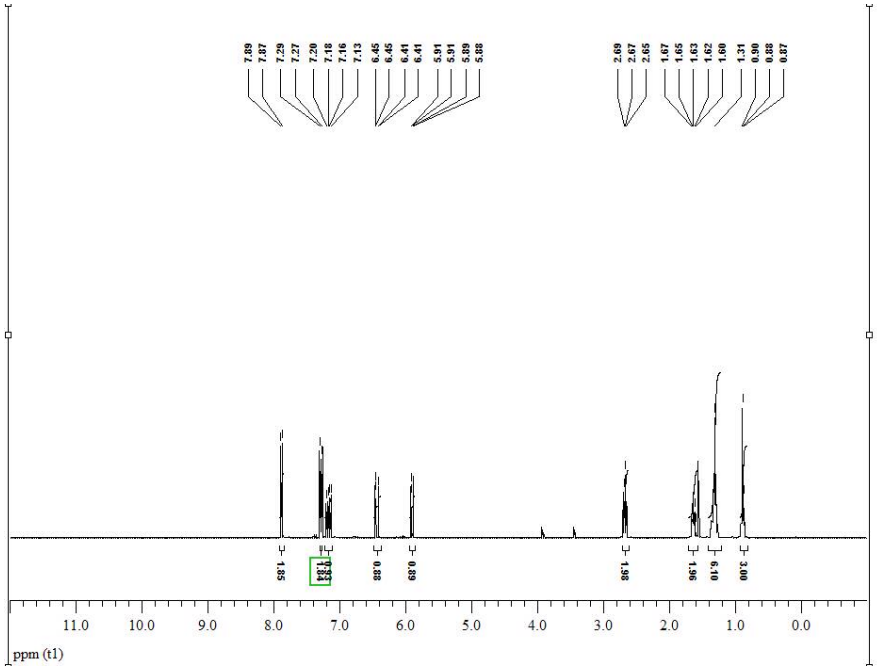


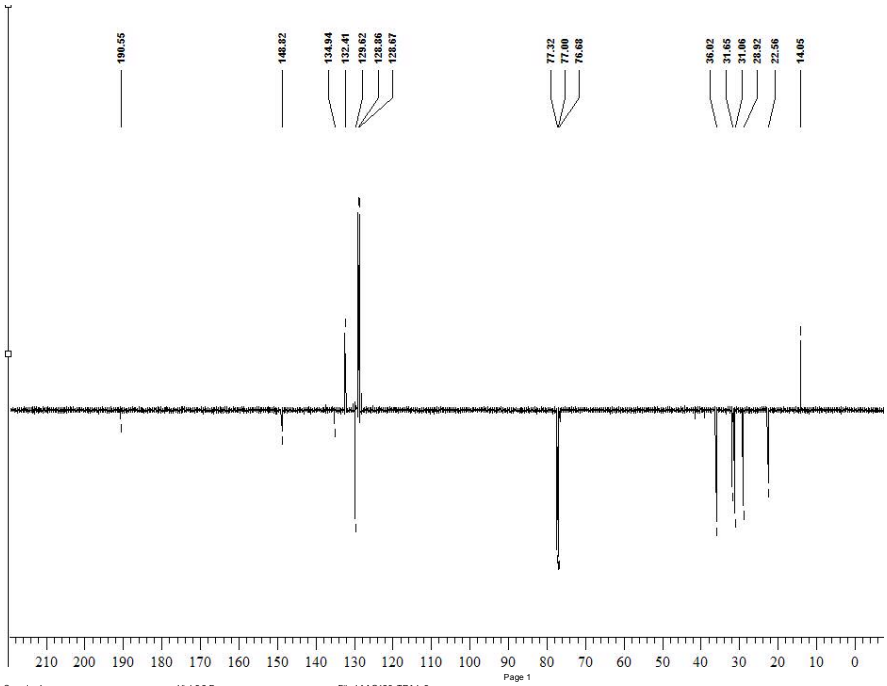


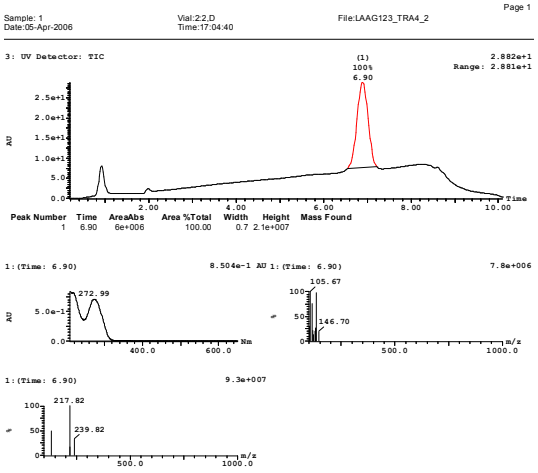


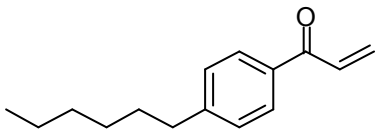
1-(4-hexylphenyl)-3-(propylamino)propan-1-one

Spectral data 1



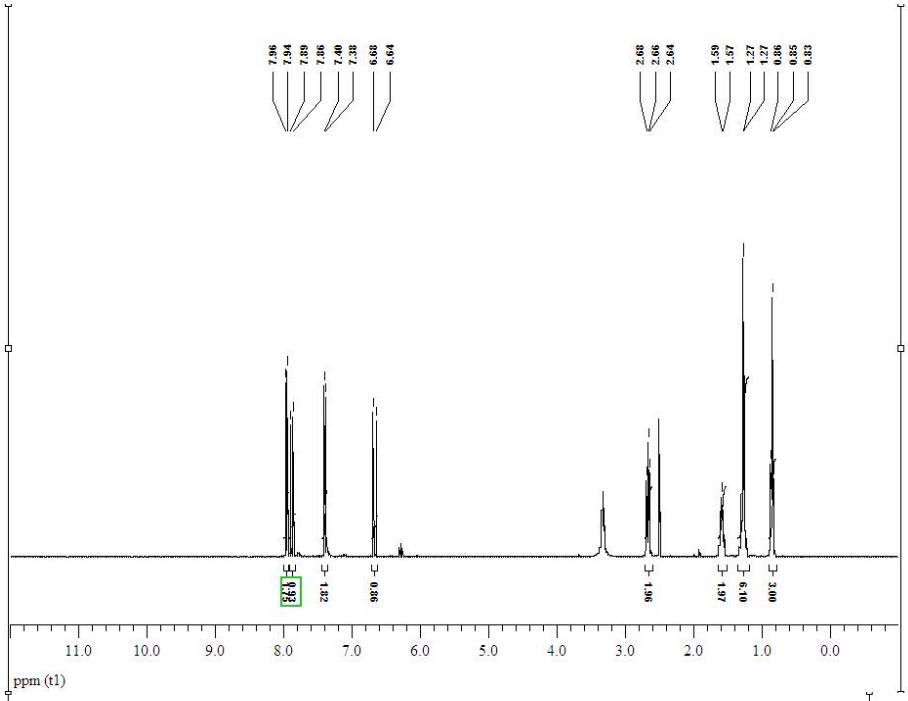


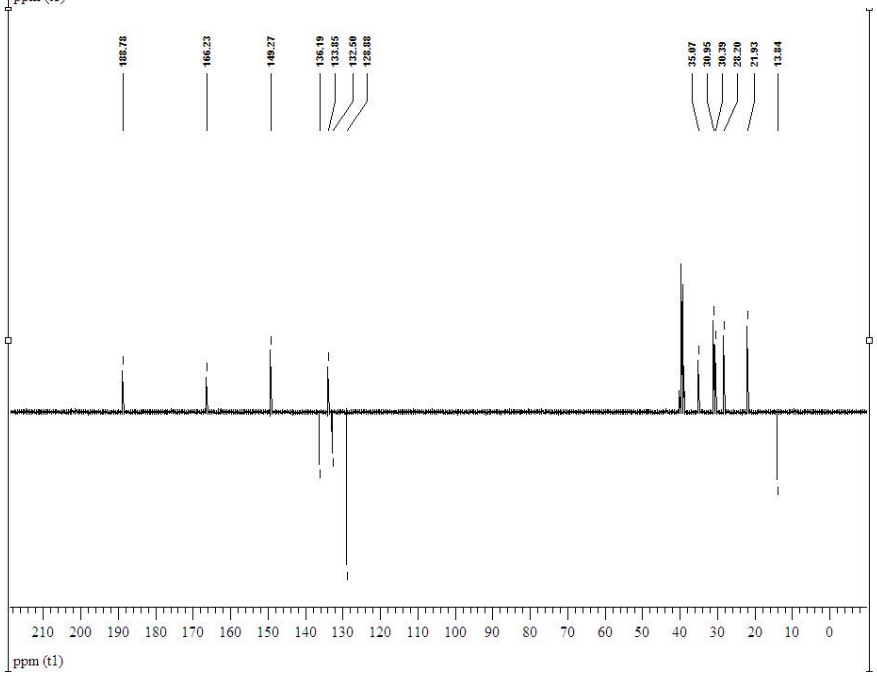


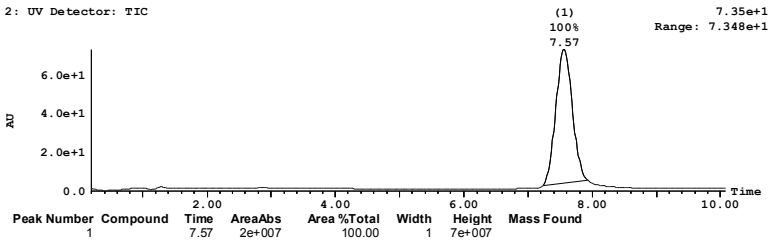


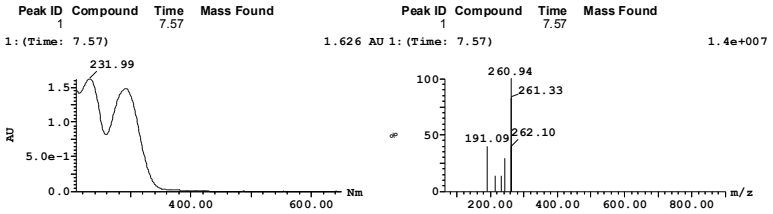
1-(4-hexylphenyl)prop-2-en-1-one

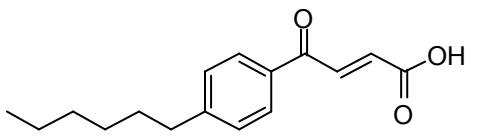
Spectral data 4a





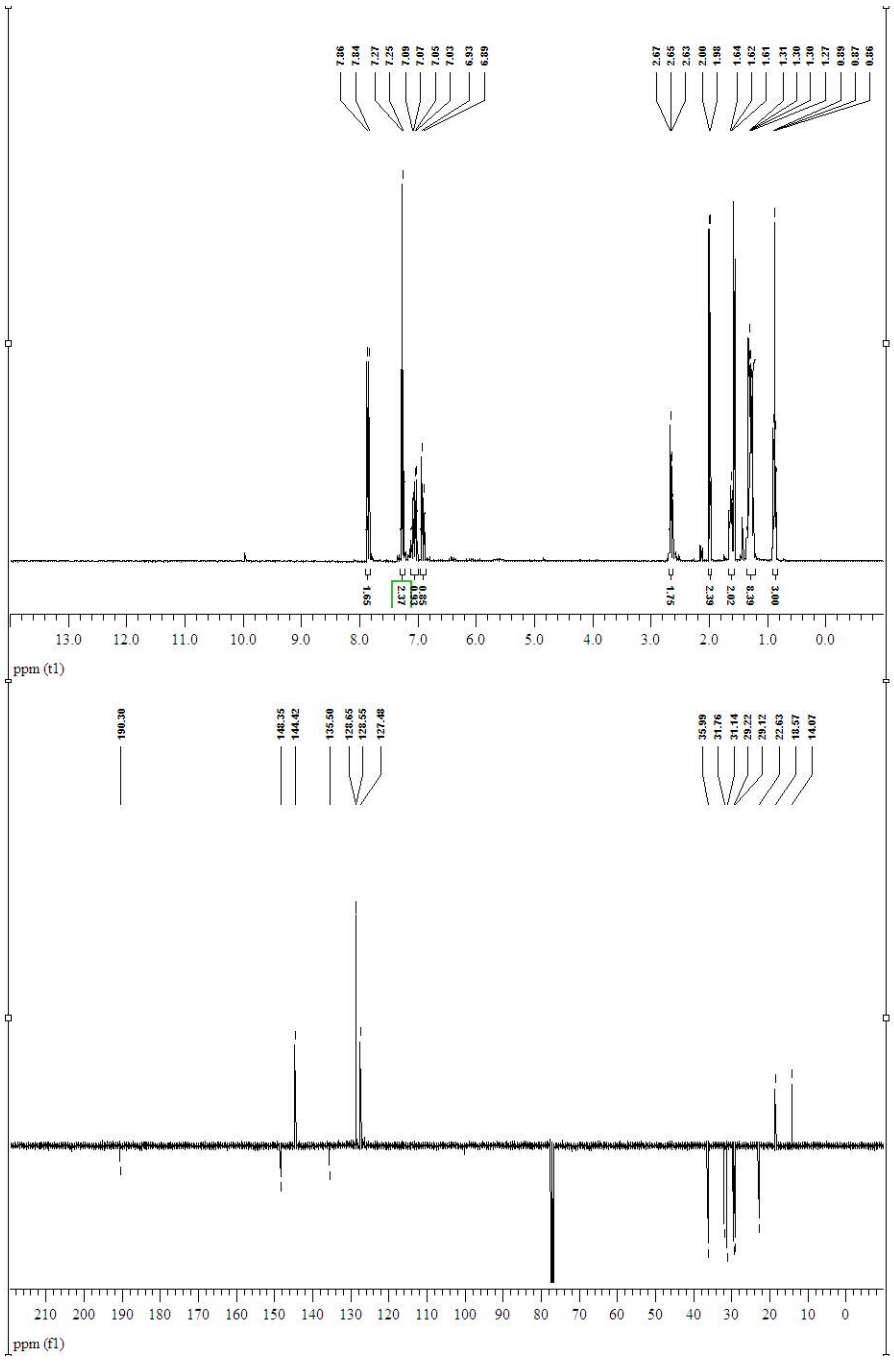






(*E*)-4-(4-hexylphenyl)-4-oxobut-2-enoic acid

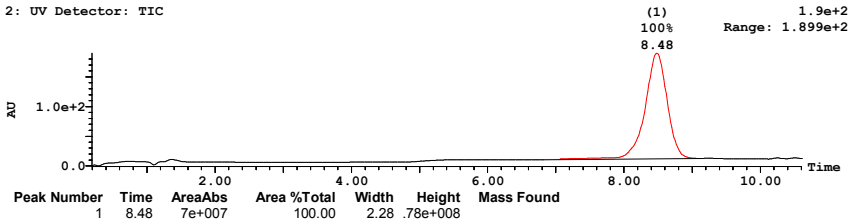
Spectral data 4b



Sample: 3
Date:02-Oct-2006

Vial:1:5,F
Time:11:14:21

File:LAAH171_3



Peak Number	Time	AreaAbs	Area %Total	Width	Height	Mass Found
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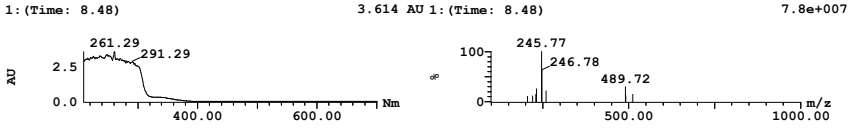
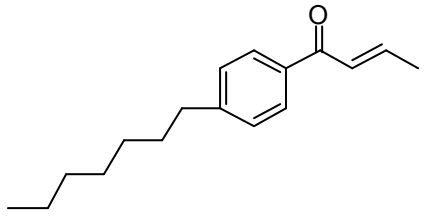
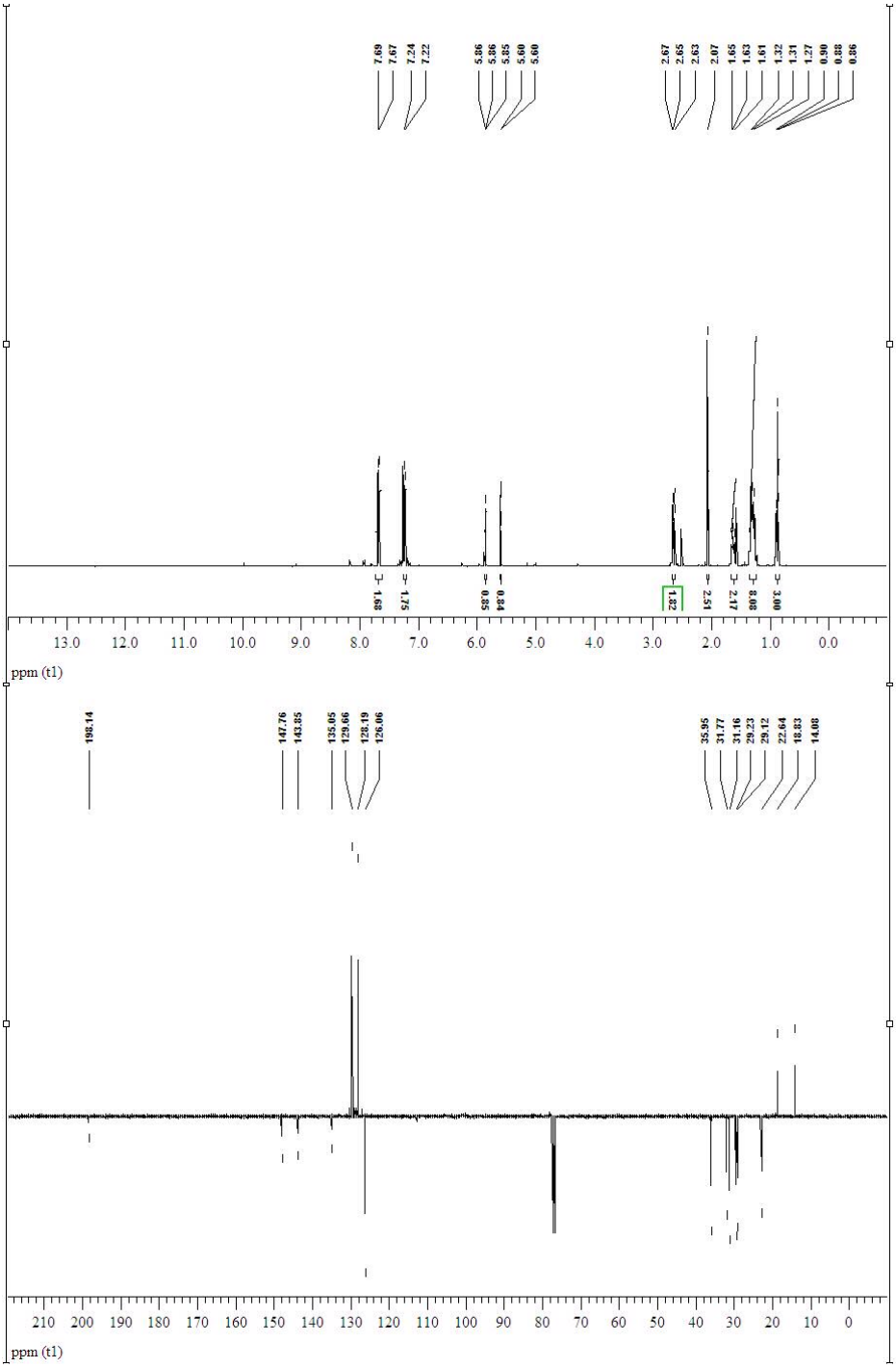
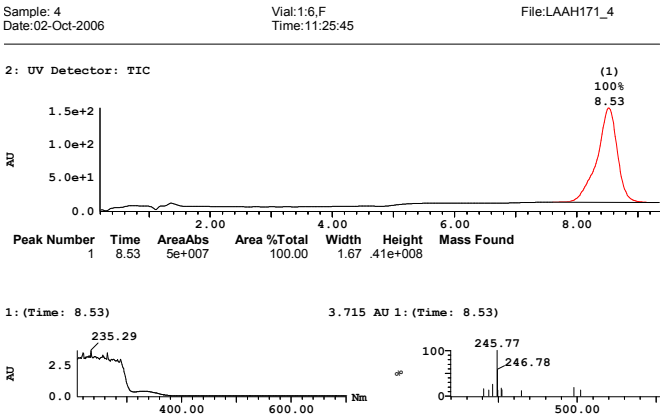


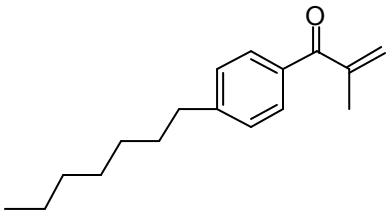


(*E*)-1-(4-heptylphenyl)but-2-en-1-one

Spectral data 4c

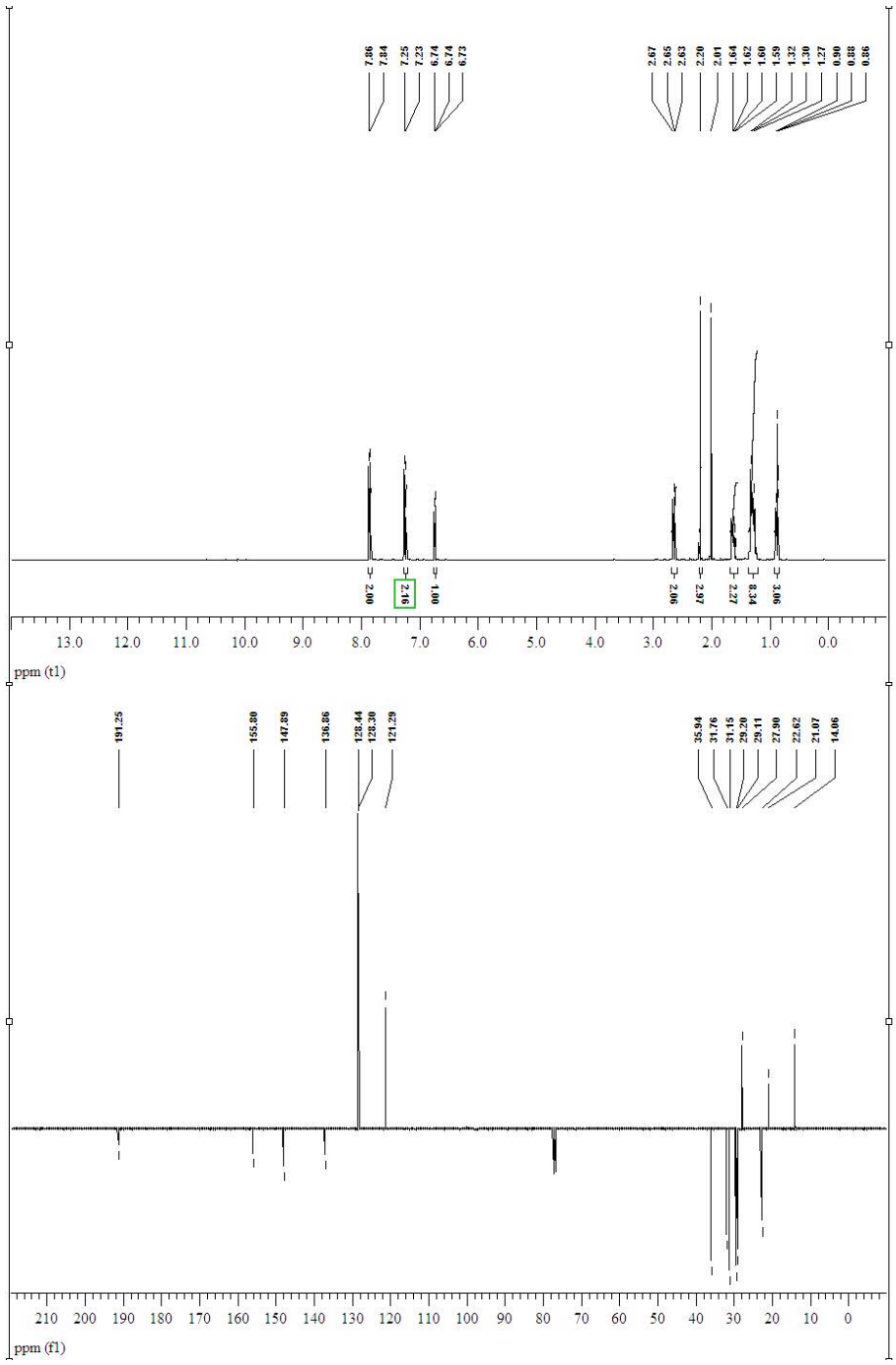






1-(4-heptylphenyl)-2-methylprop-2-en-1-one

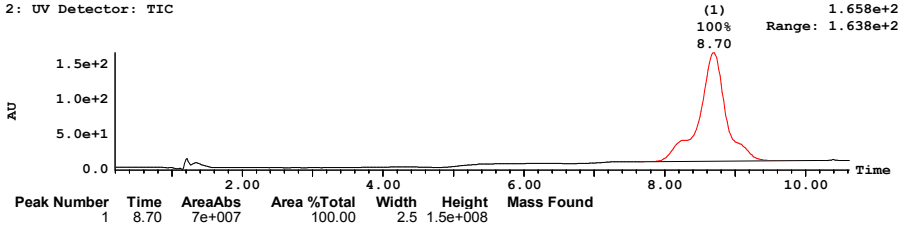
Spectral data 4d



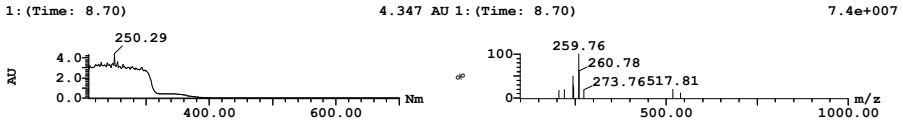
Sample: 1
Date:02-Oct-2006

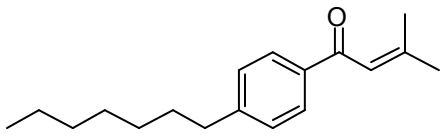
Vial:1:3,F
Time:10:50:36

File:LAAH171_1



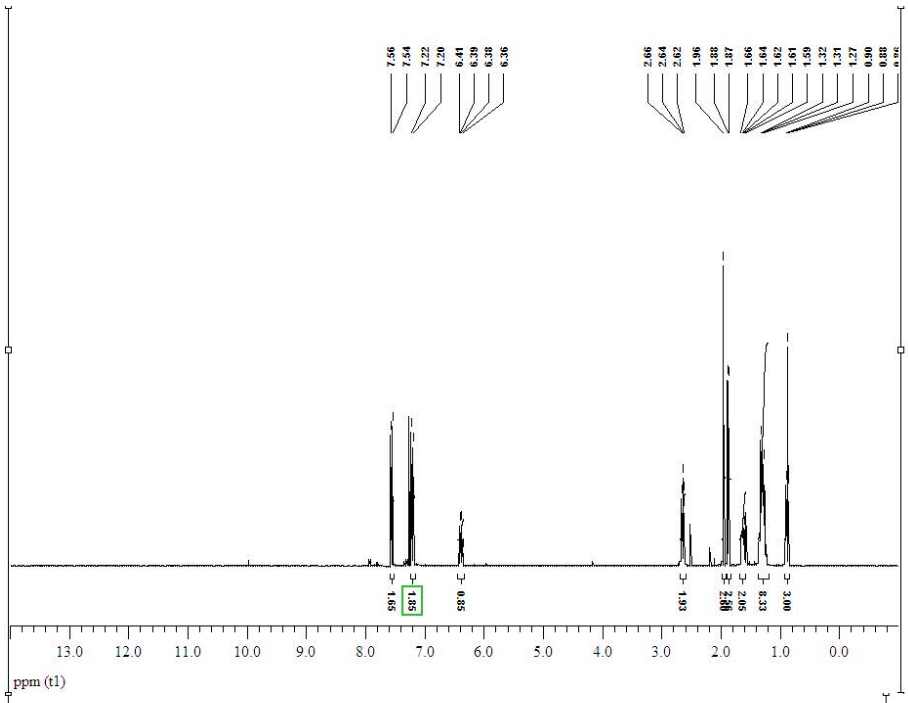
Peak Number	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1	8.70	7e+007	100.00	2.5	1.5e+008	

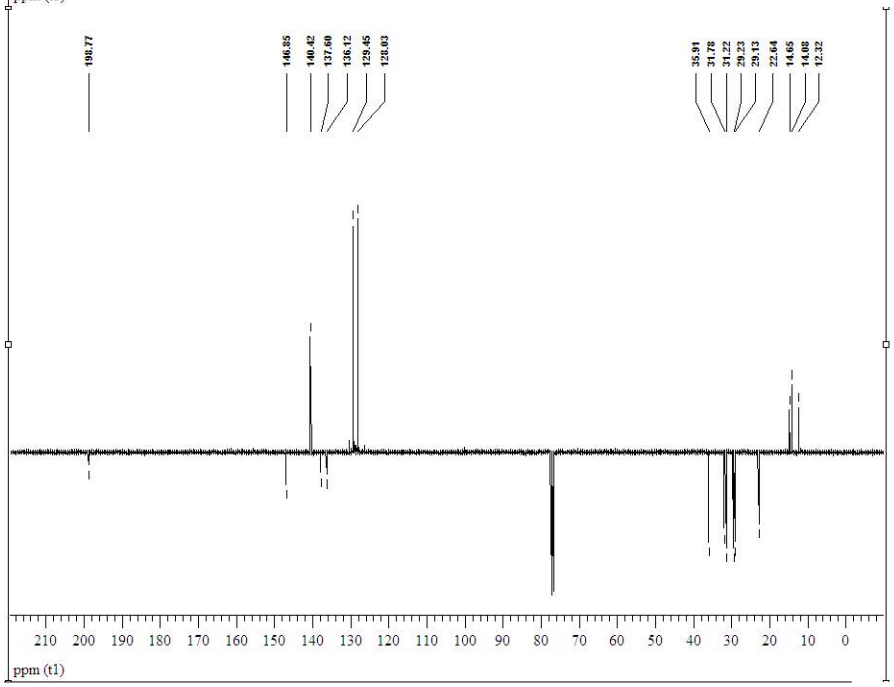


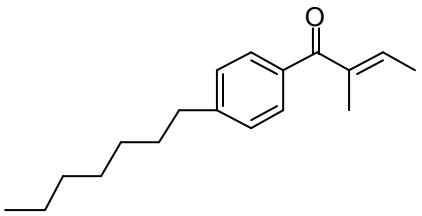


1-(4-heptylphenyl)-3-methylbut-2-en-1-one

Spectral data 4e







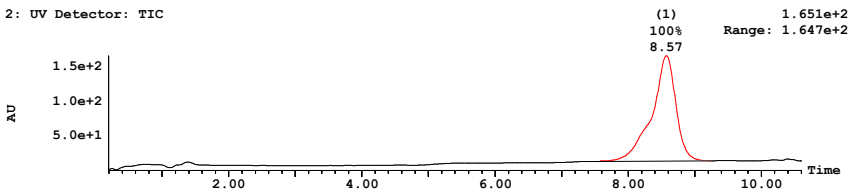
(*E*)-1-(4-heptylphenyl)-2-methylbut-2-en-1-one

Page 1

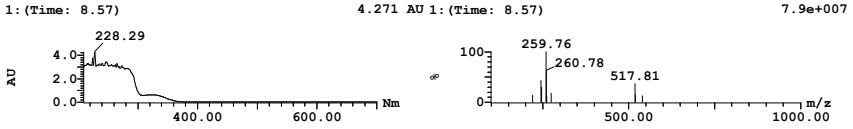
Sample: 2
Date:02-Oct-2006

Vial:1:4,F
Time:11:02:58

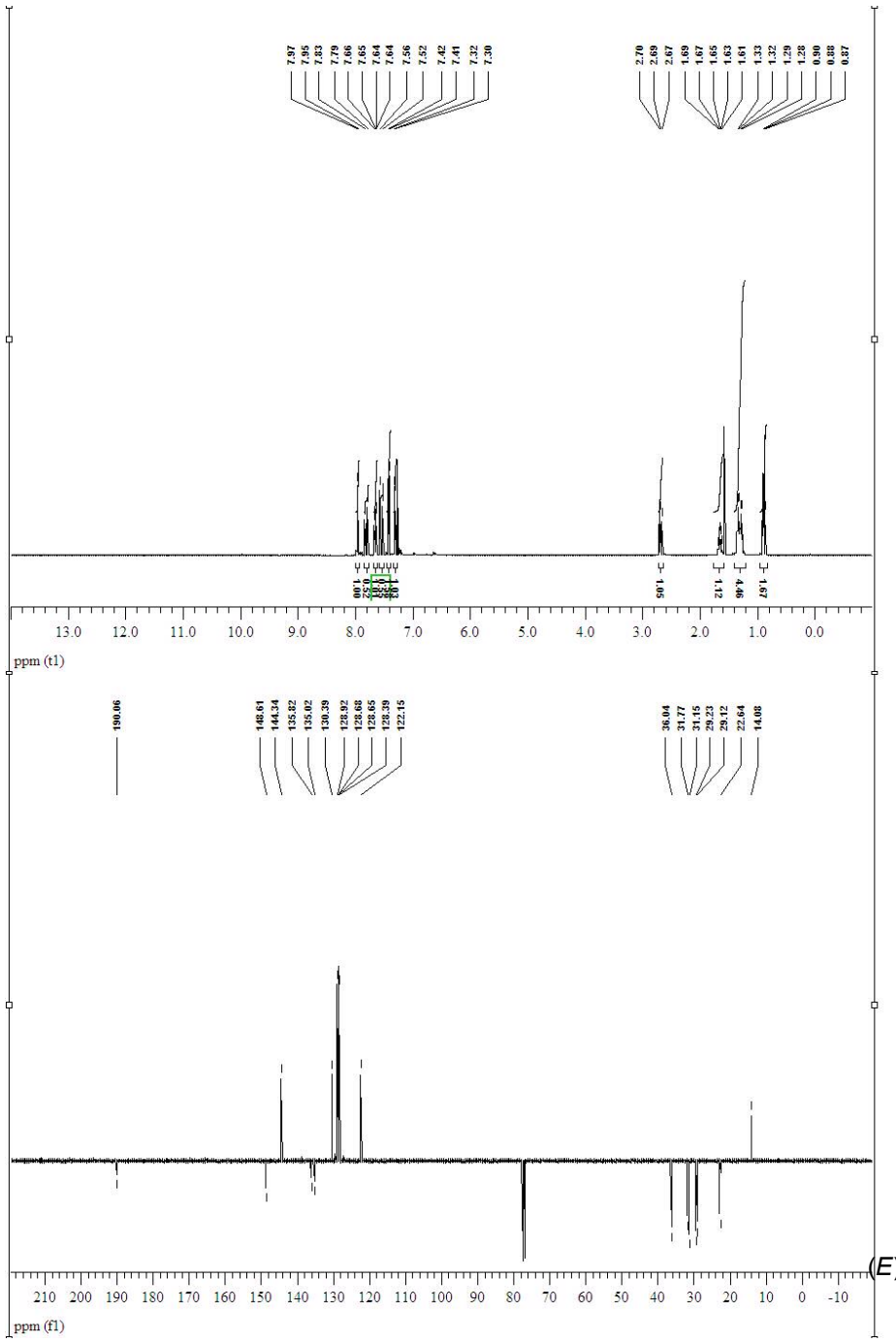
File:LAAH171_2

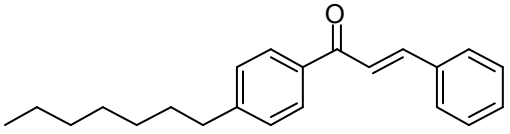


Peak Number	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1	8.57	6e+007	100.00	1.72	.52e+008	



Spectral data 4f





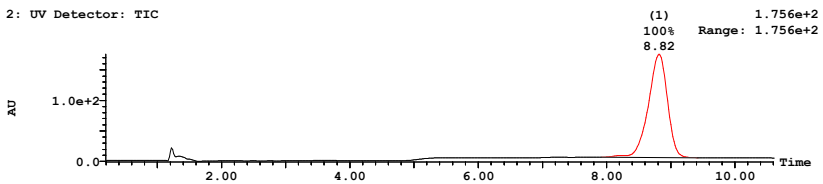
(*E*)-1-(4-heptylphenyl)-3-phenylprop-2-en-1-one

Page 1

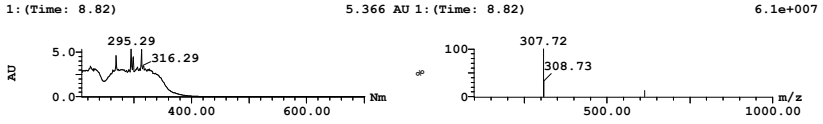
Sample: 1
Date:03-Oct-2006

Vial:1:3,F
Time:10:58:45

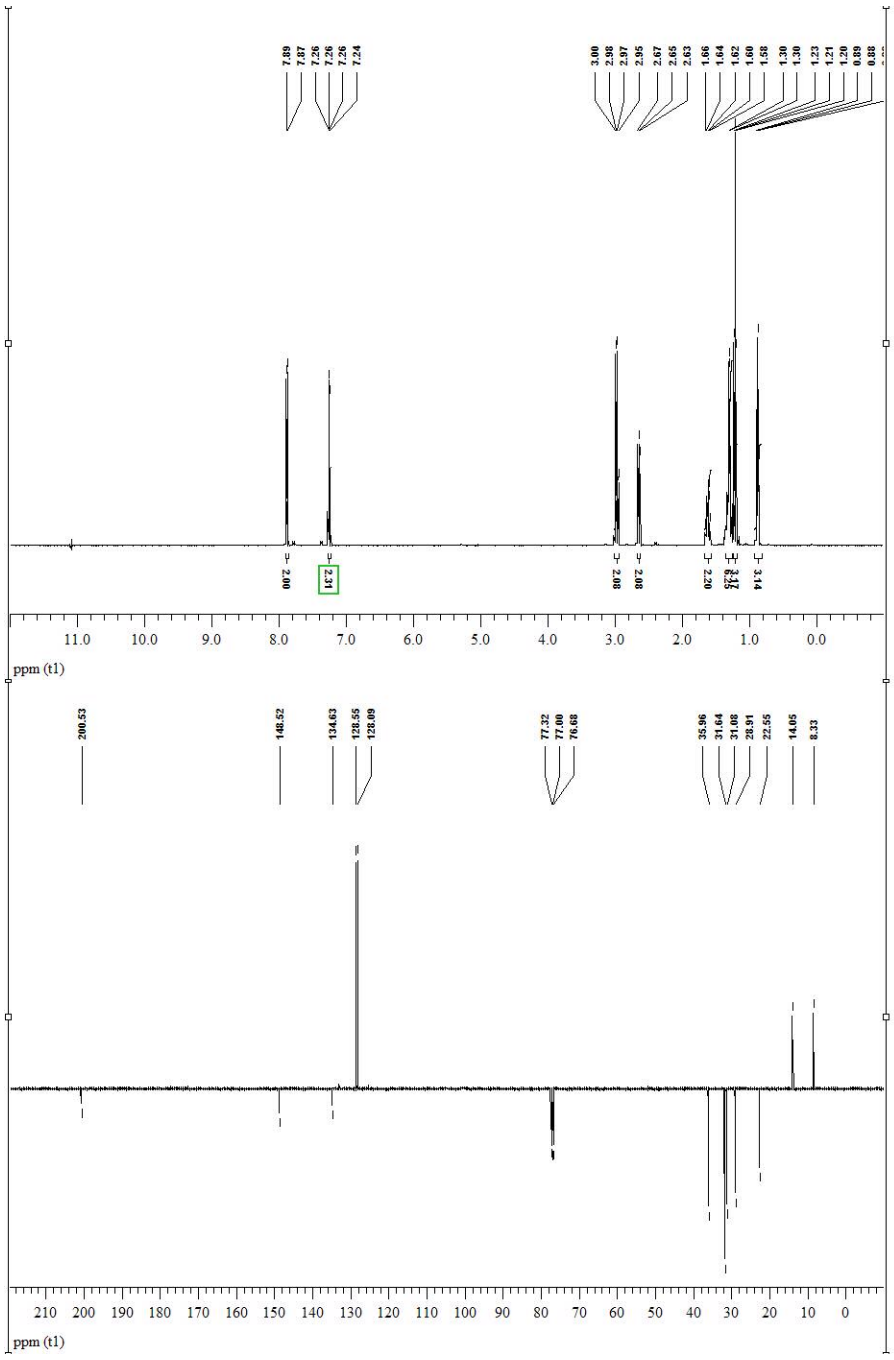
File:LAAH171_5



Peak Number	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1	8.82	6e+007	100.00	1.50	.69e+008	



Spectral data 4g

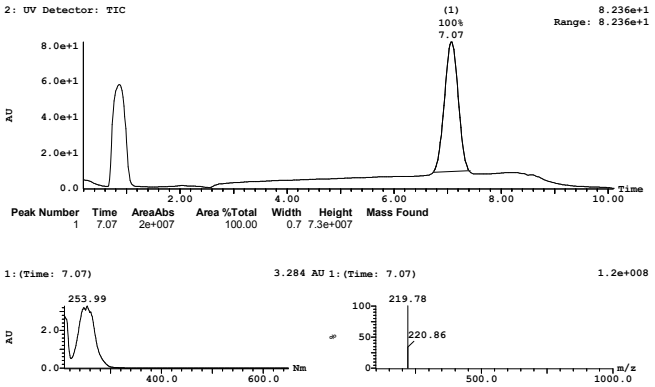


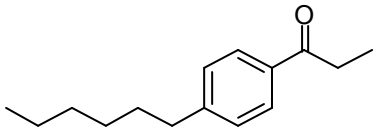
Page 1

Sample: 1
Date:23-Apr-2006

Vial:3:1,C
Time:16:32:38

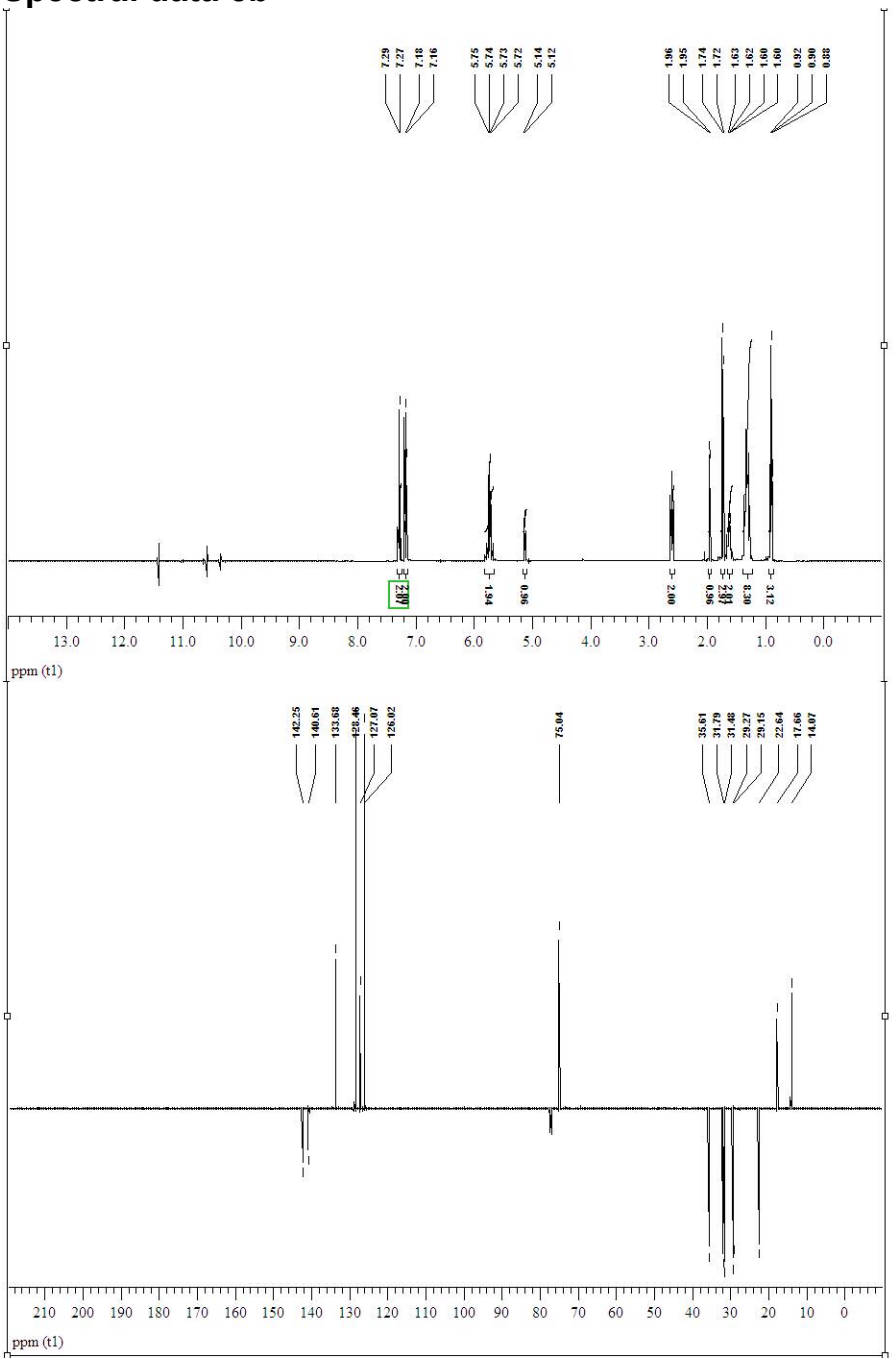
File:LAAG37_5

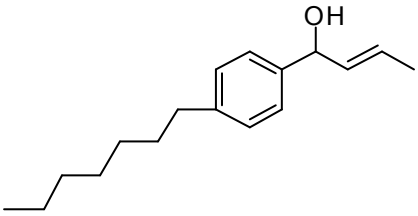




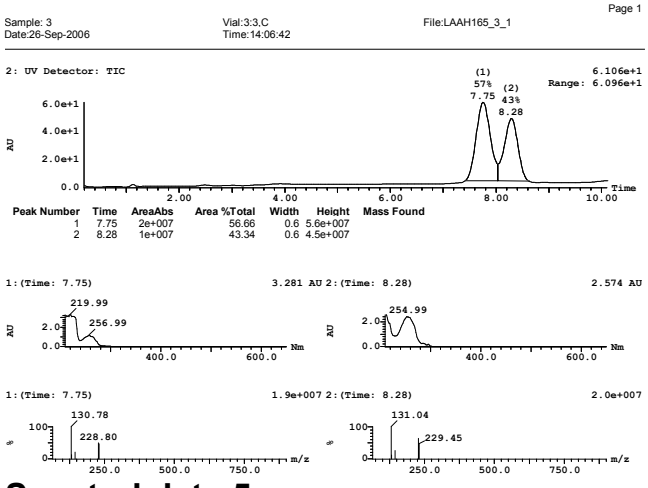
1-(4-hexylphenyl)propan-1-one

Spectral data 5b

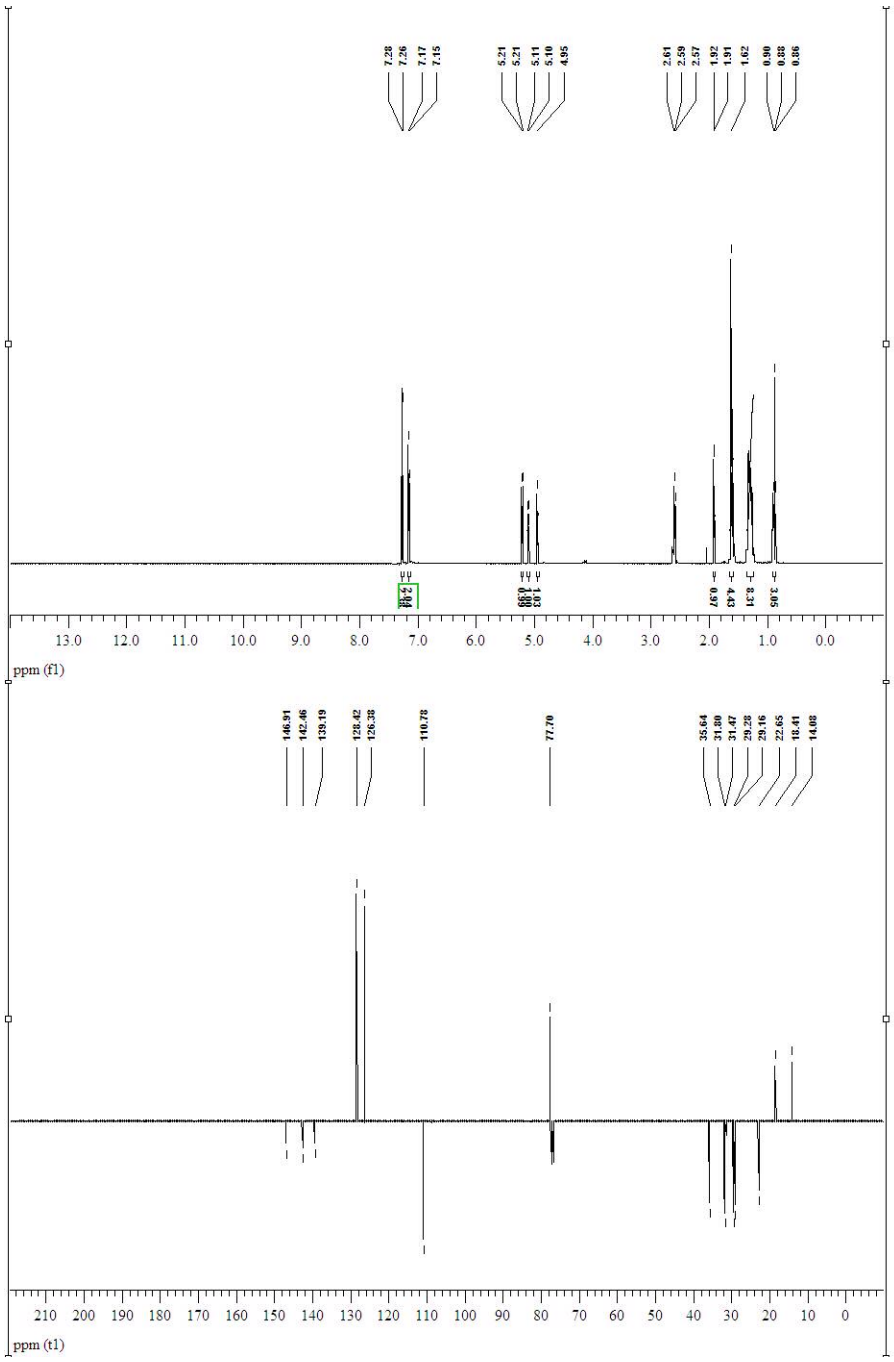


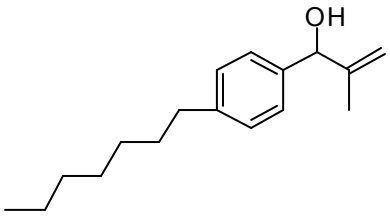


(*E*)-1-(4-heptylphenyl)but-2-en-1-ol



Spectral data 5c





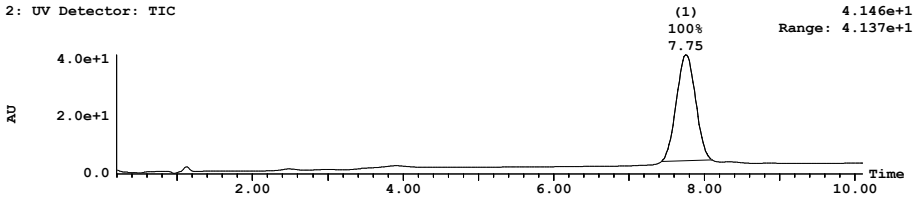
1-(4-heptylphenyl)-2-methylprop-2-en-1-ol

Page 1

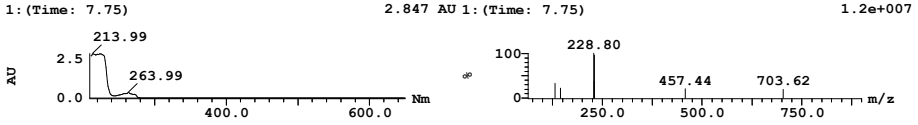
Sample: 4
Date:26-Sep-2006

Vial:3:4,C
Time:14:17:28

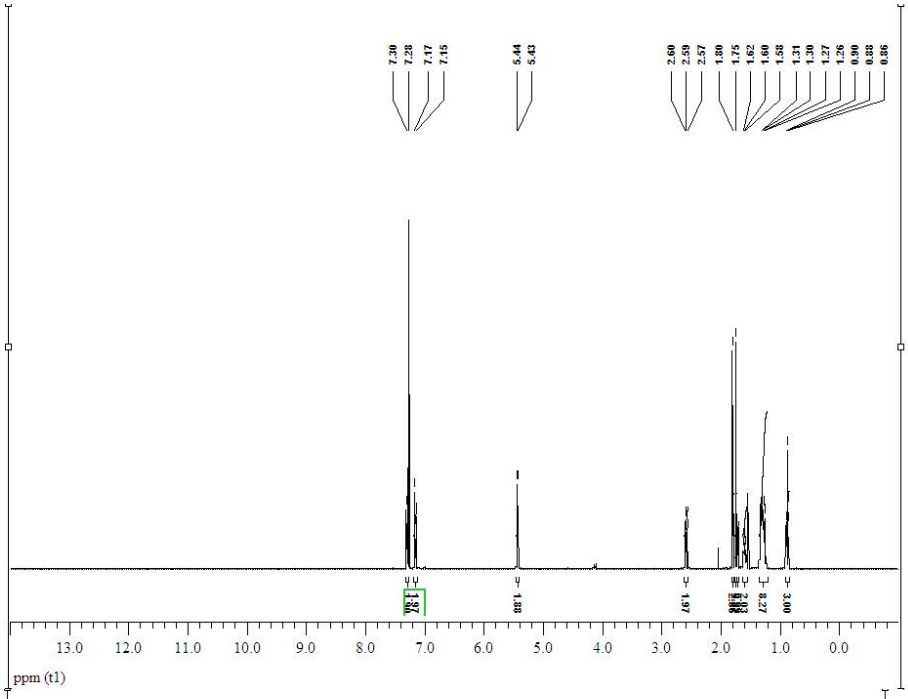
File:LAAH165_4_1

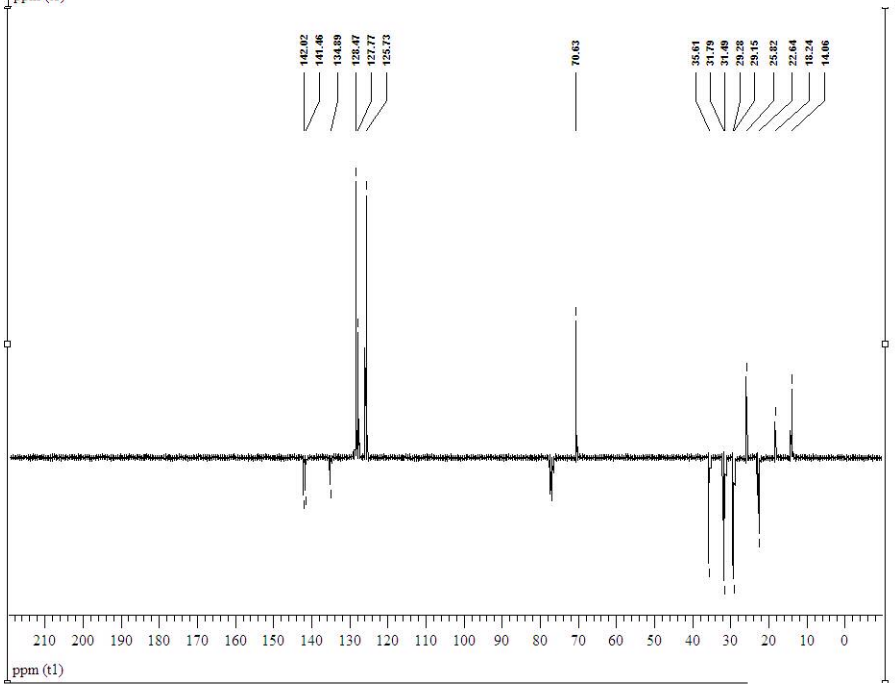


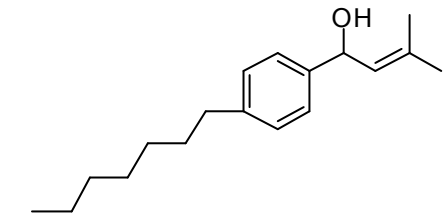
Peak Number	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1	7.75	1e+007	100.00	0.7	3.7e+007	



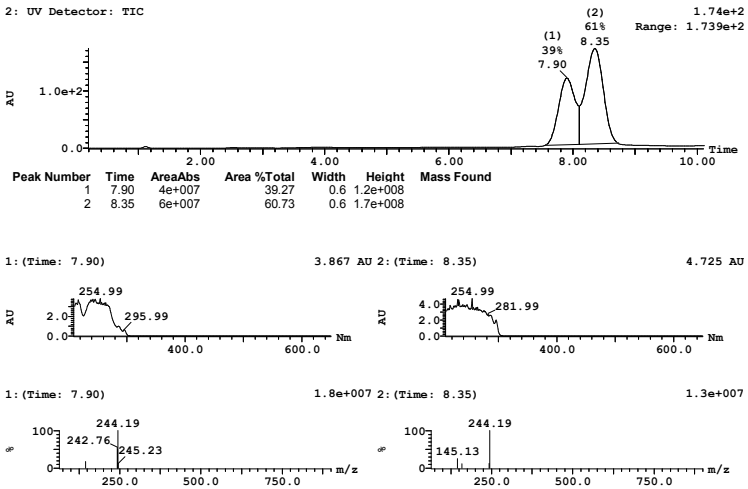
Spectral data 5d



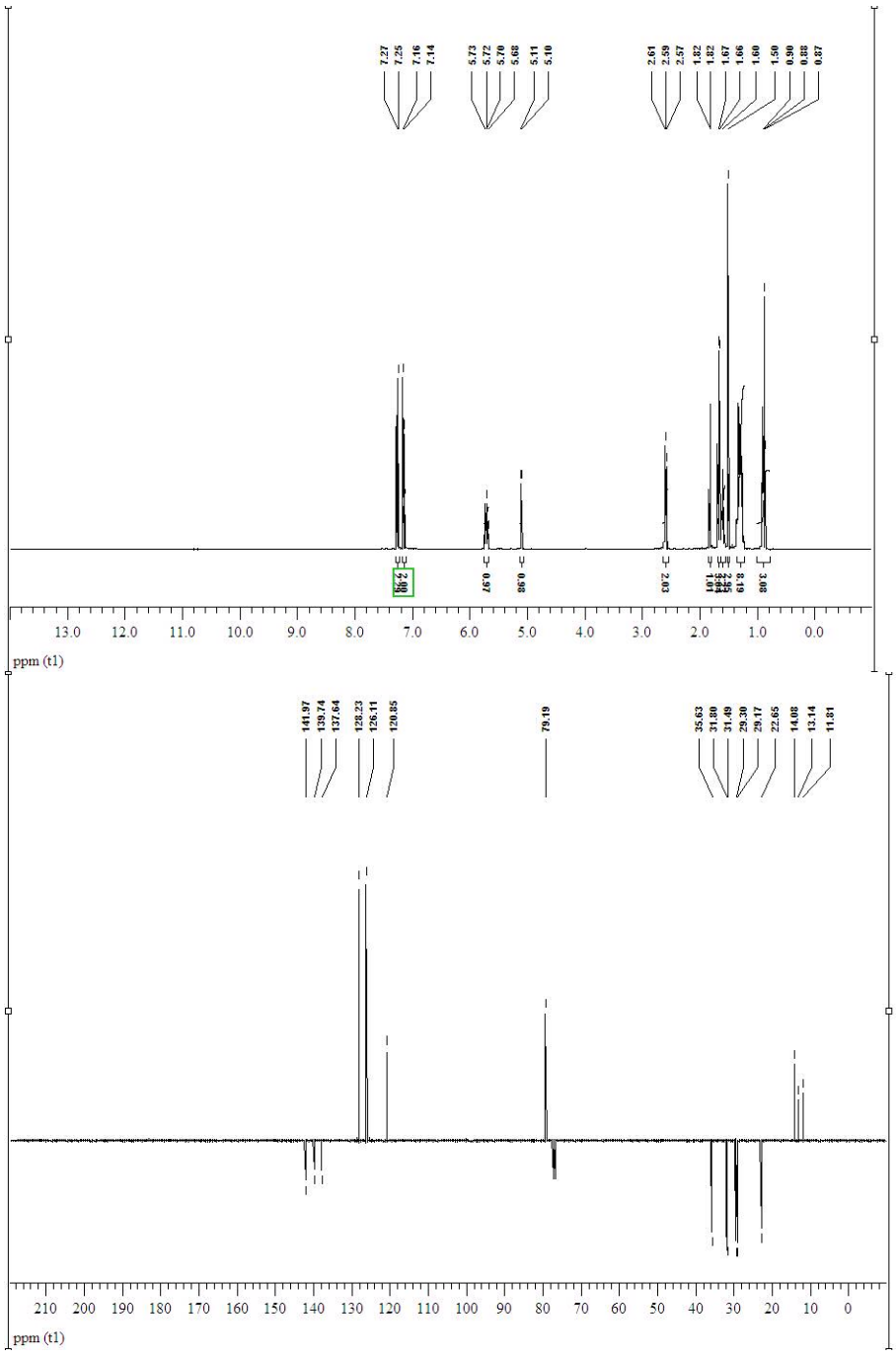


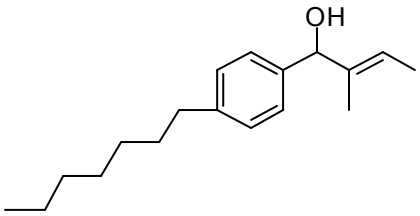


1-(4-heptylphenyl)-3-methylbut-2-en-1-ol



Spectral data 5e



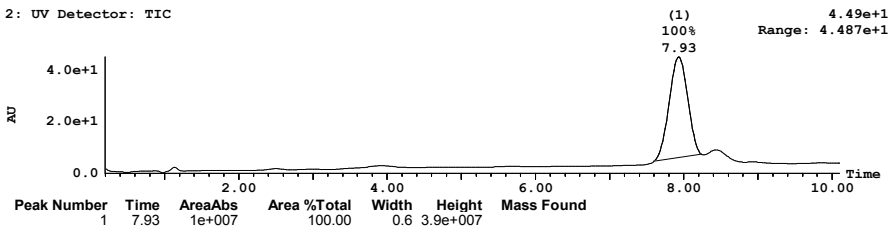


(*E*)-1-(4-heptylphenyl)-2-methylbut-2-en-1-ol

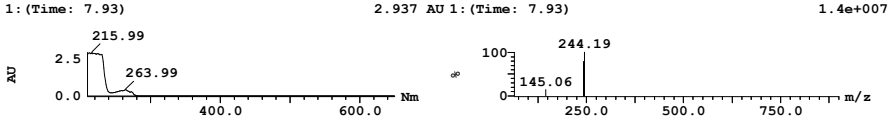
Sample: 2
Date:26-Sep-2006

Vial:3:2,C
Time:13:55:57

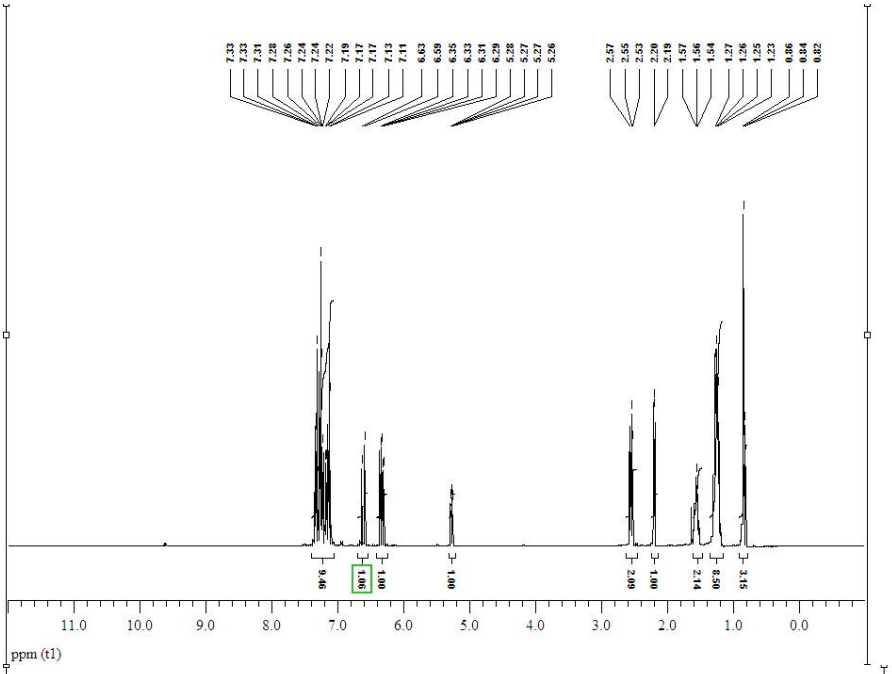
File:LAAH165_2_1

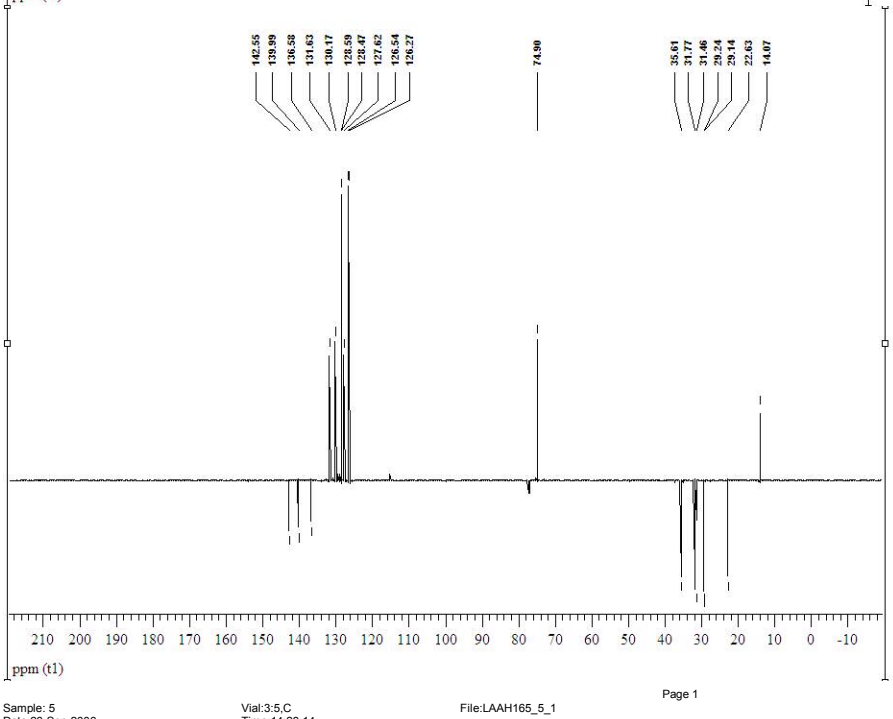


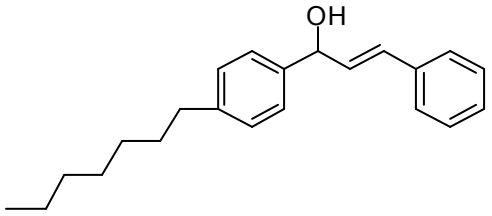
Peak Number	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1	7.93	1e+007	100.00	0.6	3.9e+007	



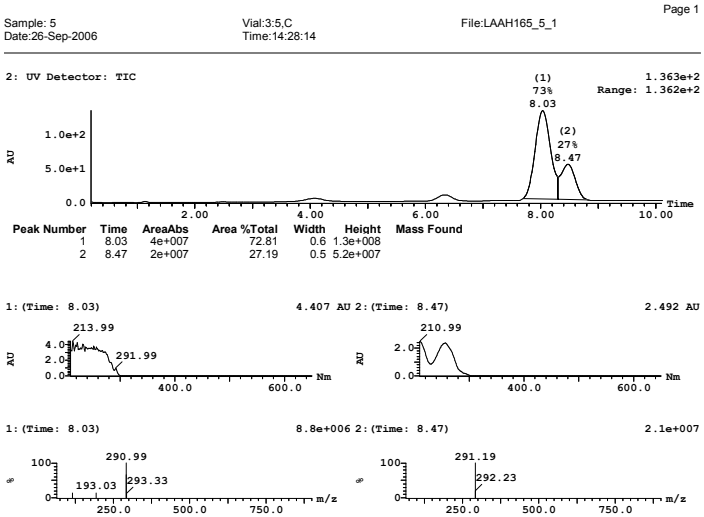
Spectral data 5f



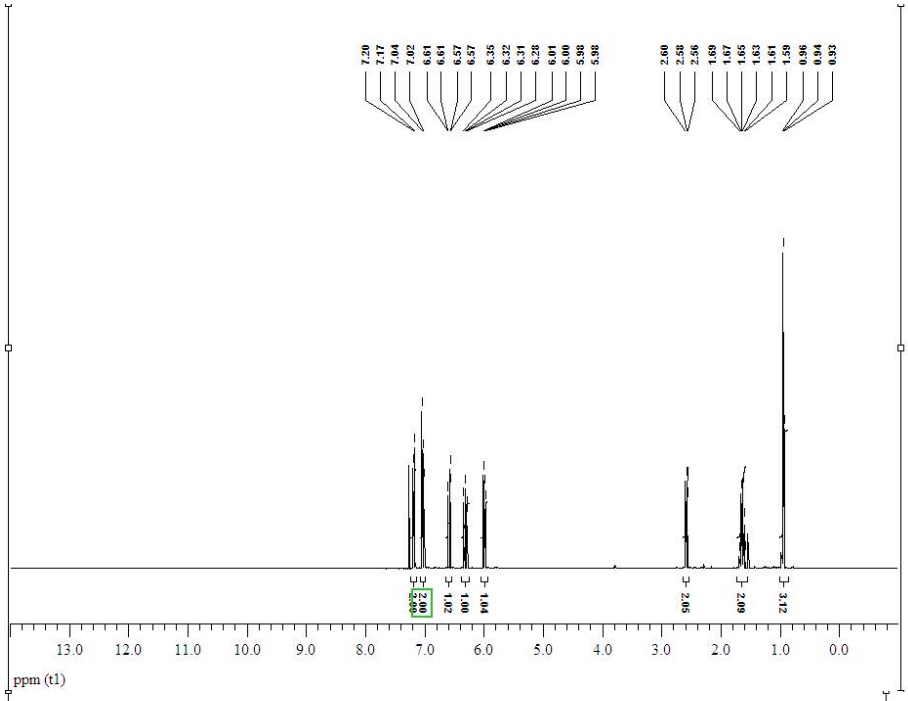


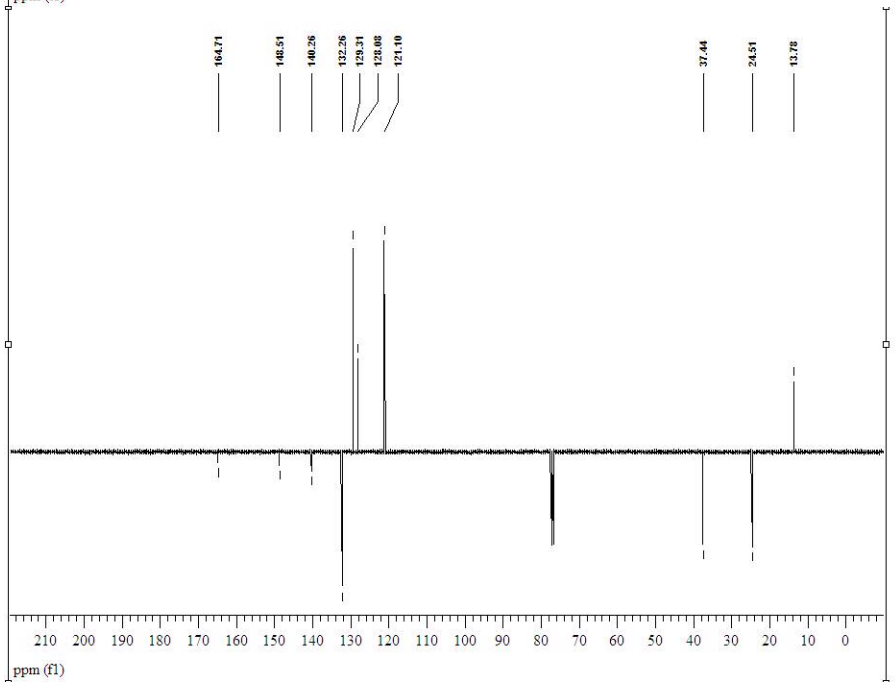


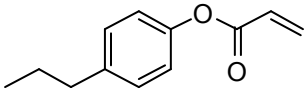
(*E*)-1-(4-heptylphenyl)-3-phenylprop-2-en-1-ol



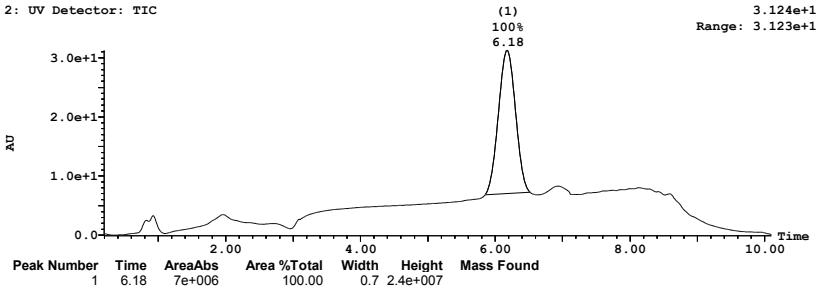
Spectral data 6a

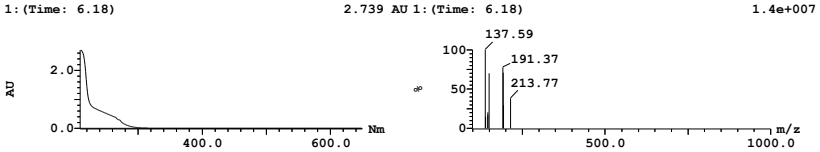




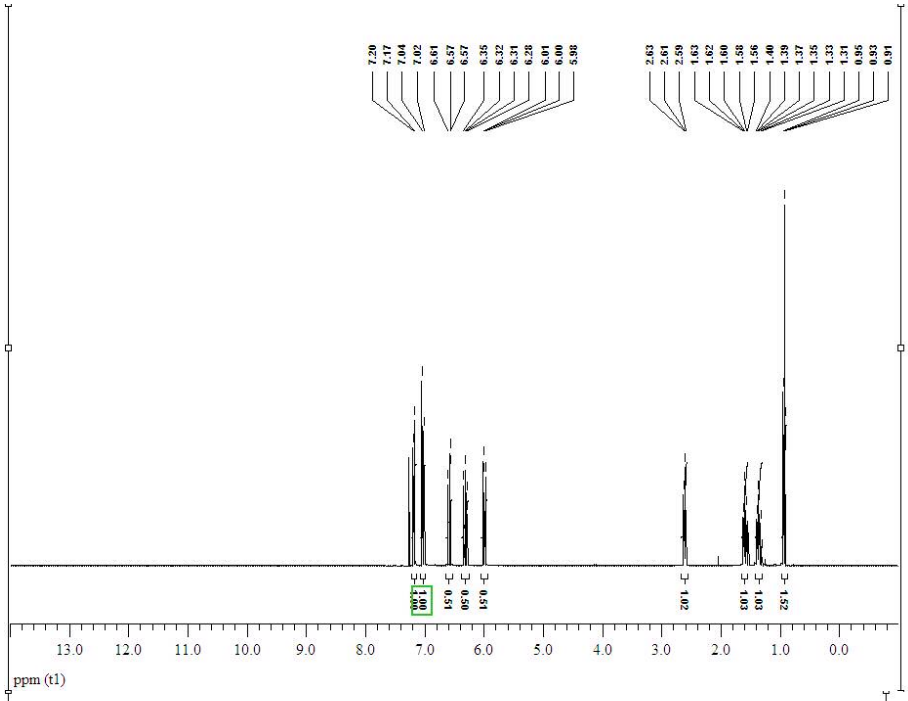


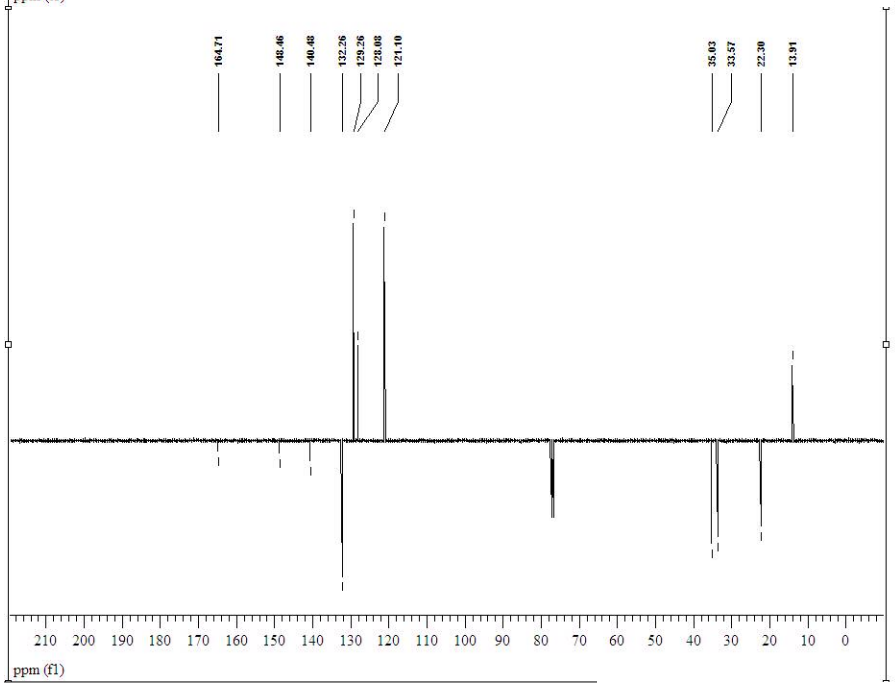
4-propylphenyl acrylate

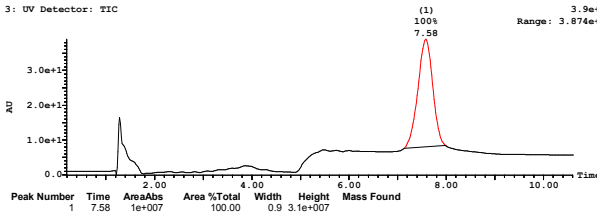


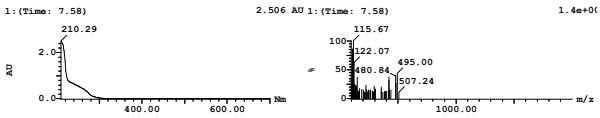


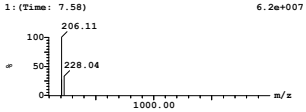
Spectral data 6b

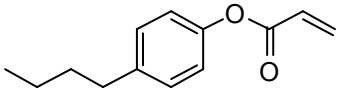






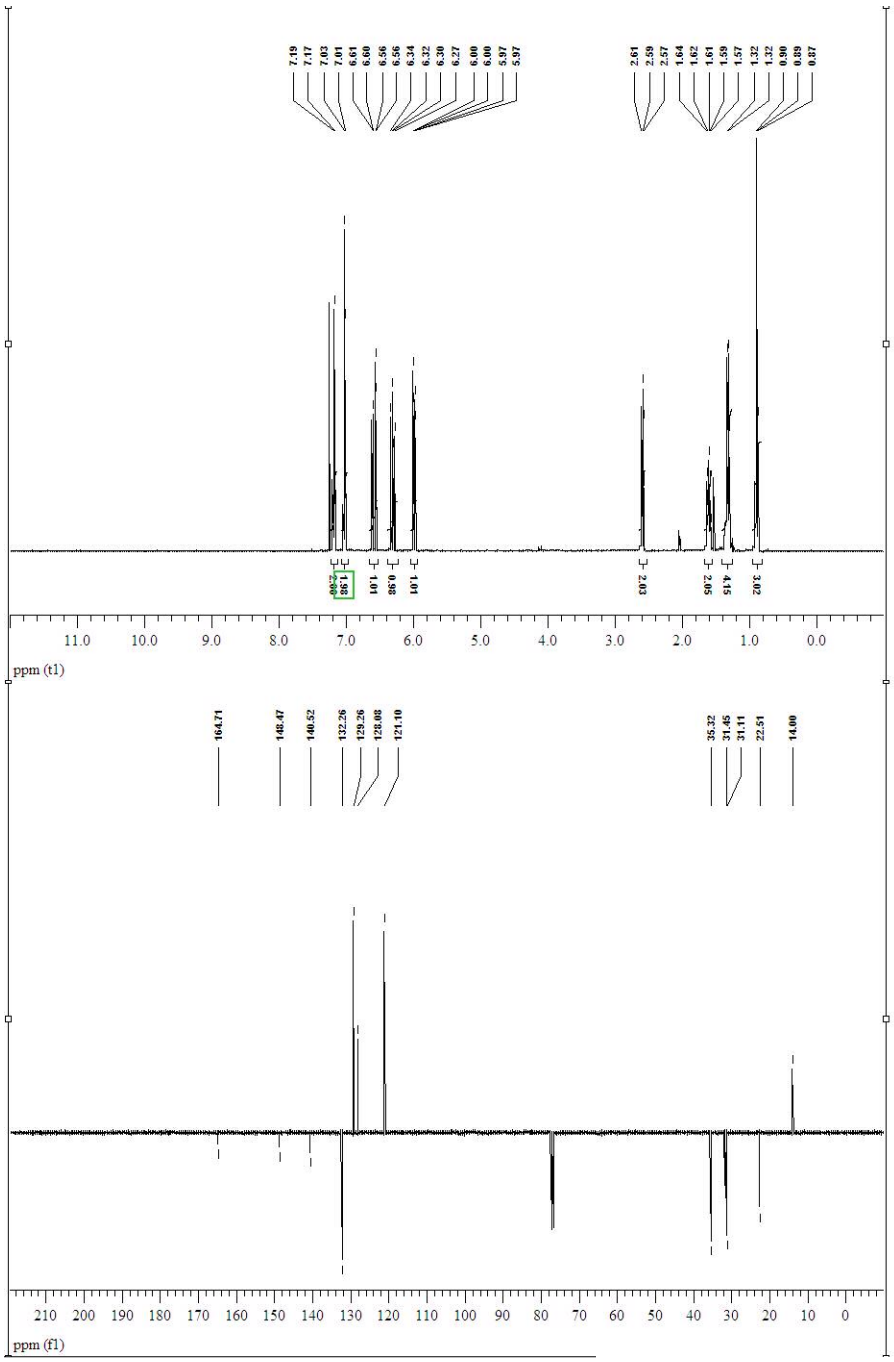


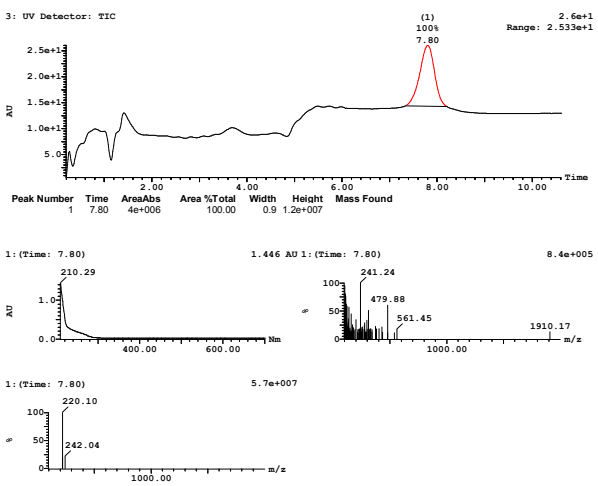


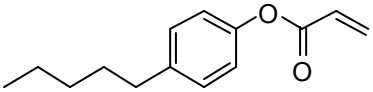


4-butylphenyl acrylate

Spectral data 6c

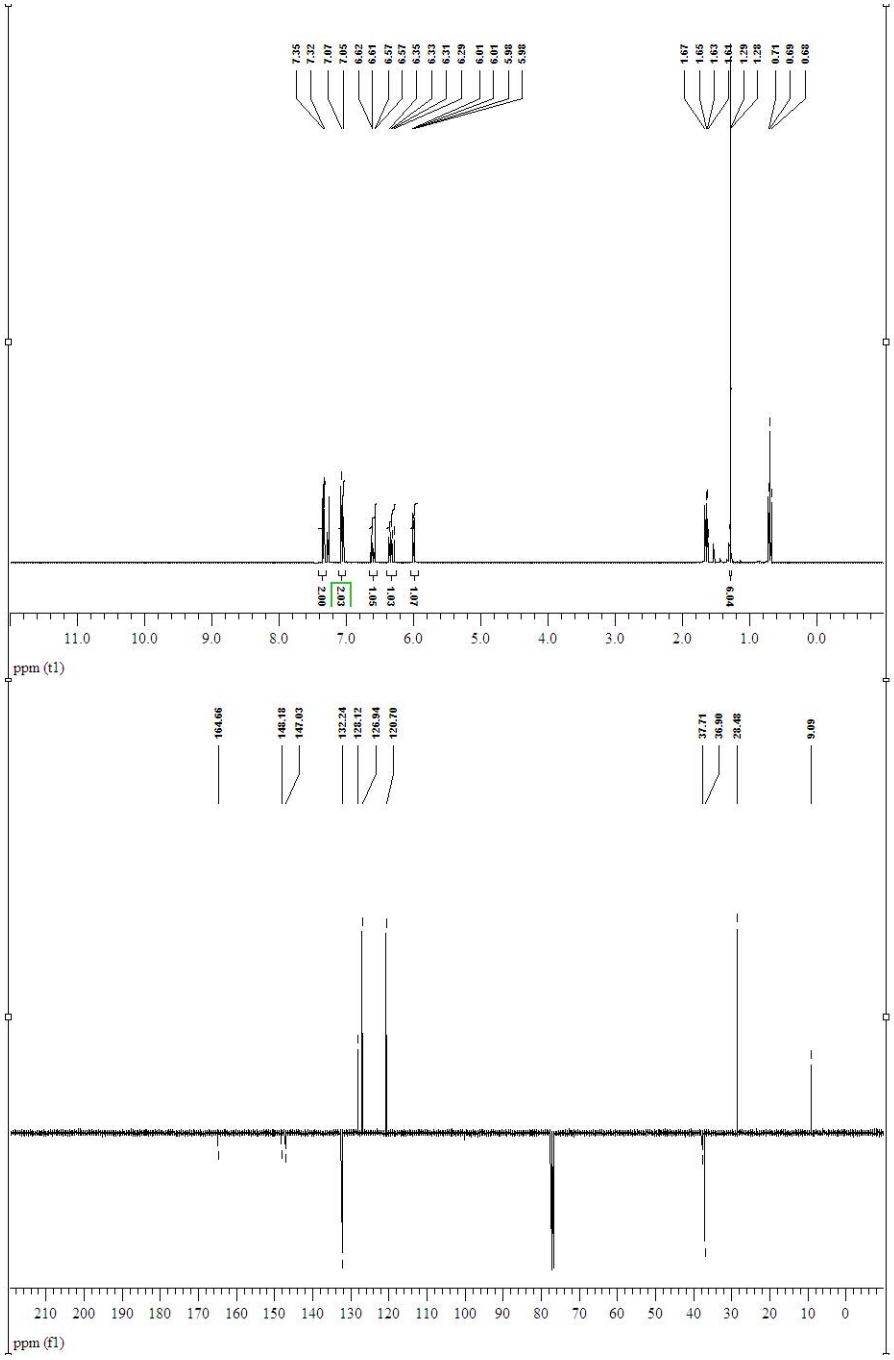


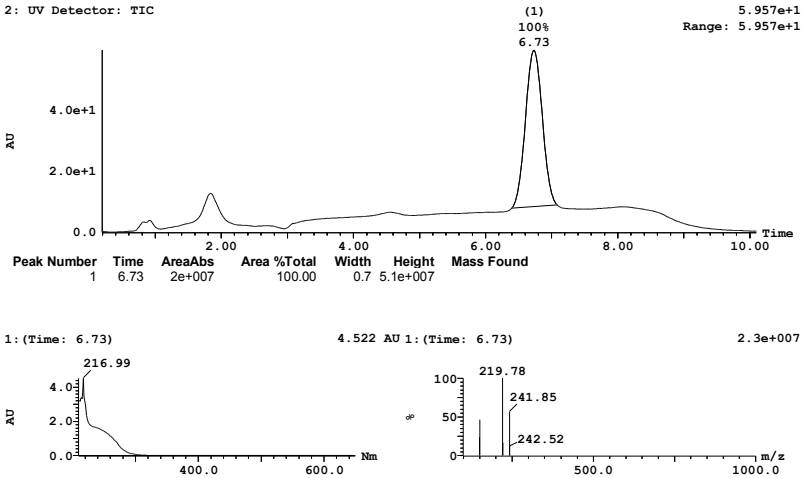


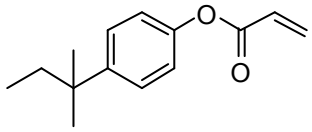


4-pentylphenyl acrylate

Spectral data 6d

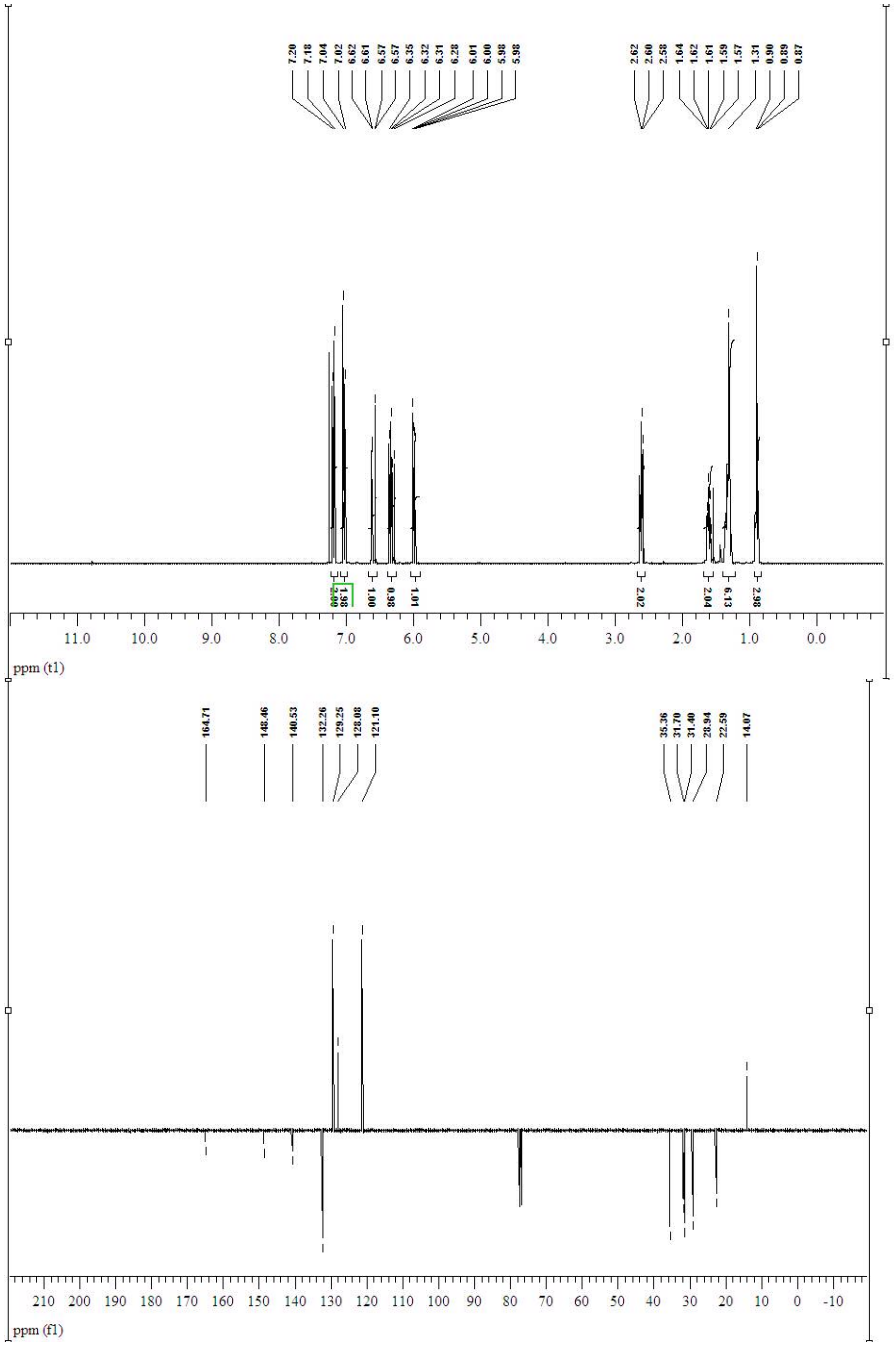


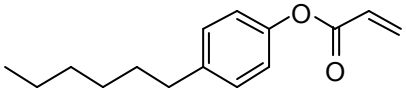




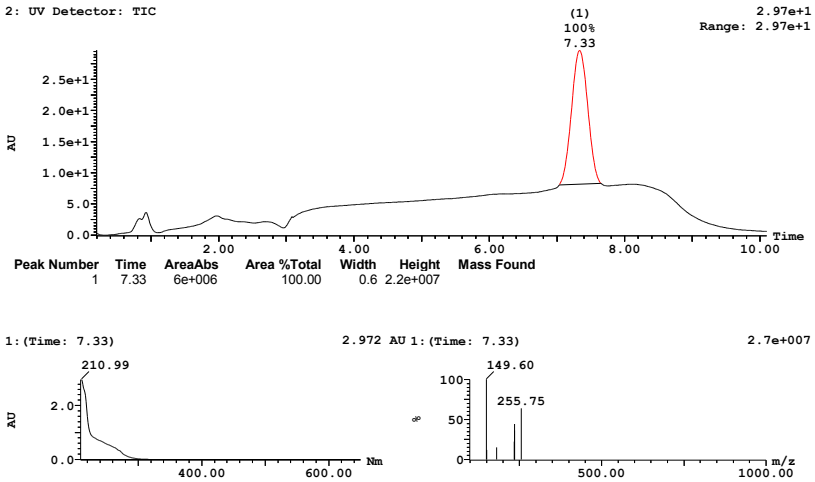
4-*tert*-pentylphenyl acrylate

Spectral data 6e

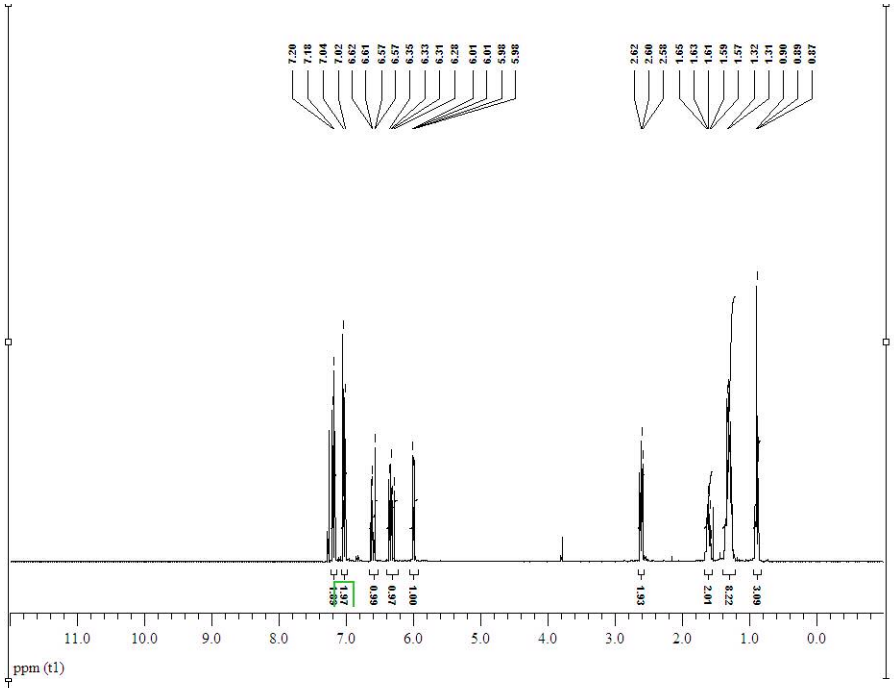


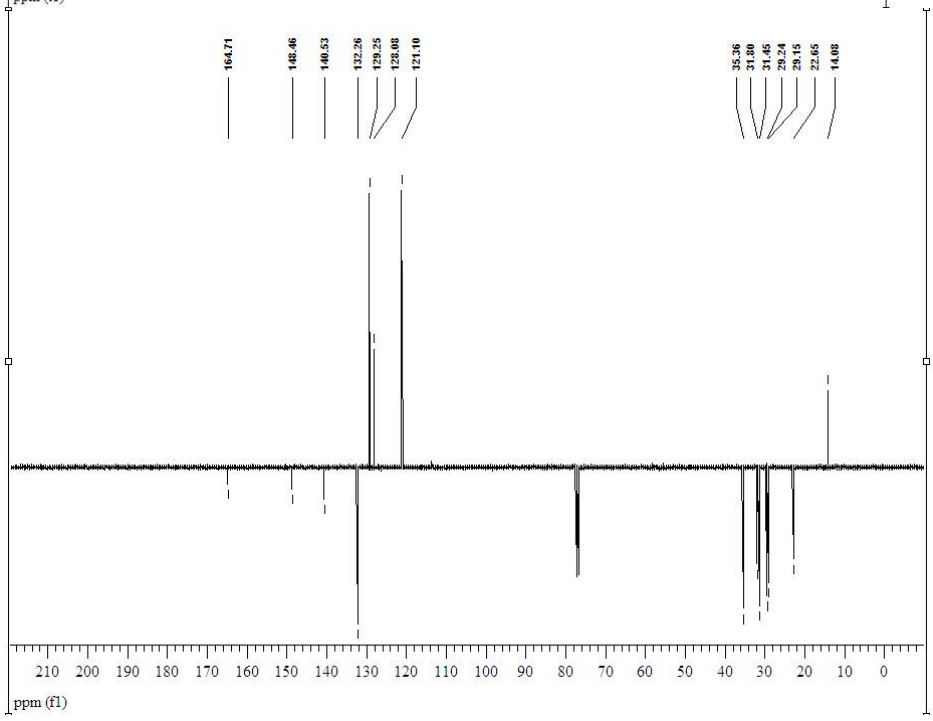


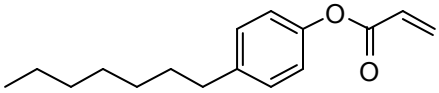
4-hexylphenyl acrylate



Spectral data 6f







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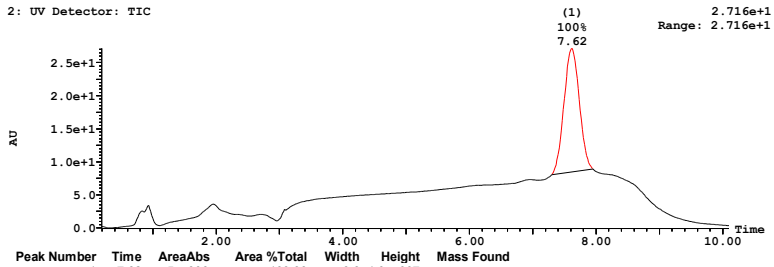
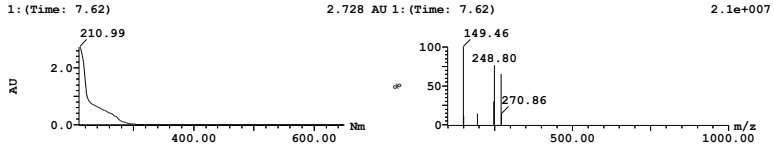
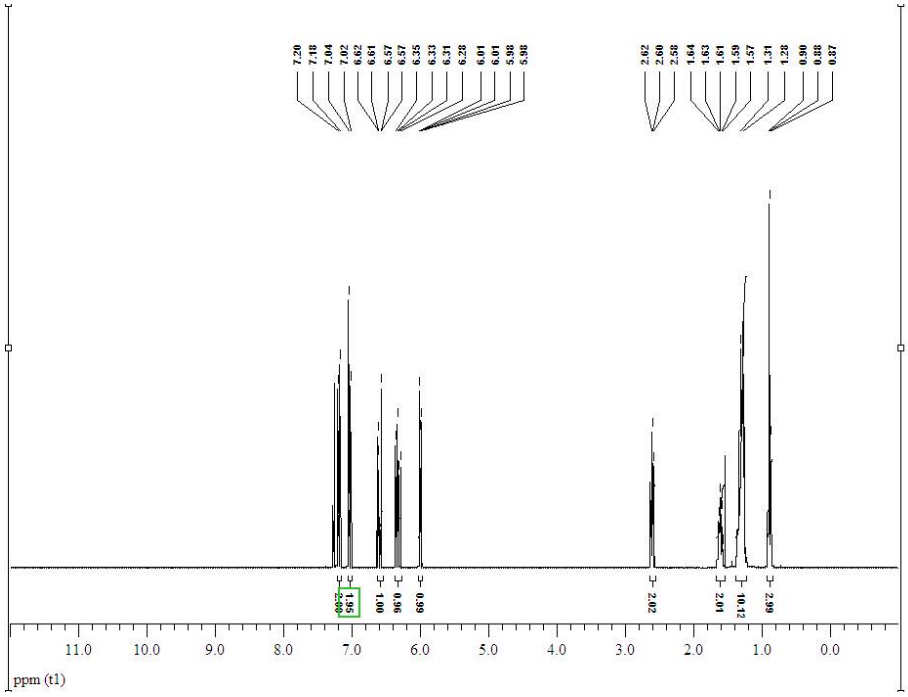
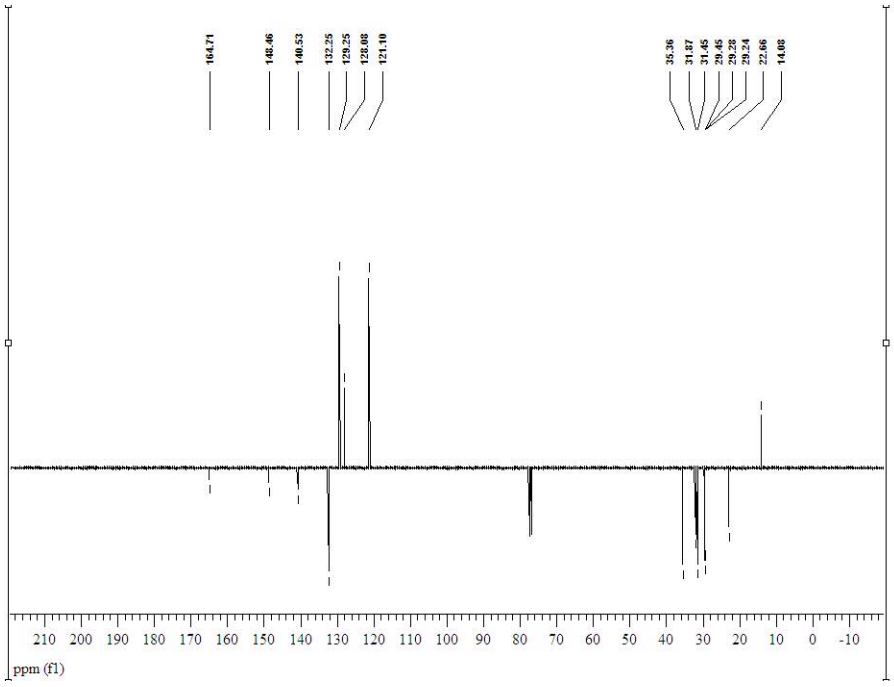
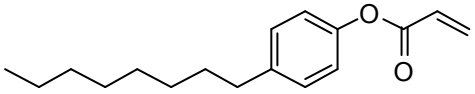




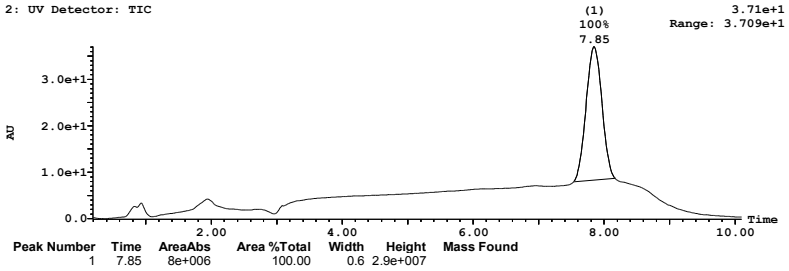
Spectral data 6g

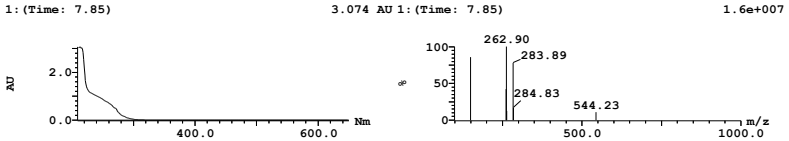




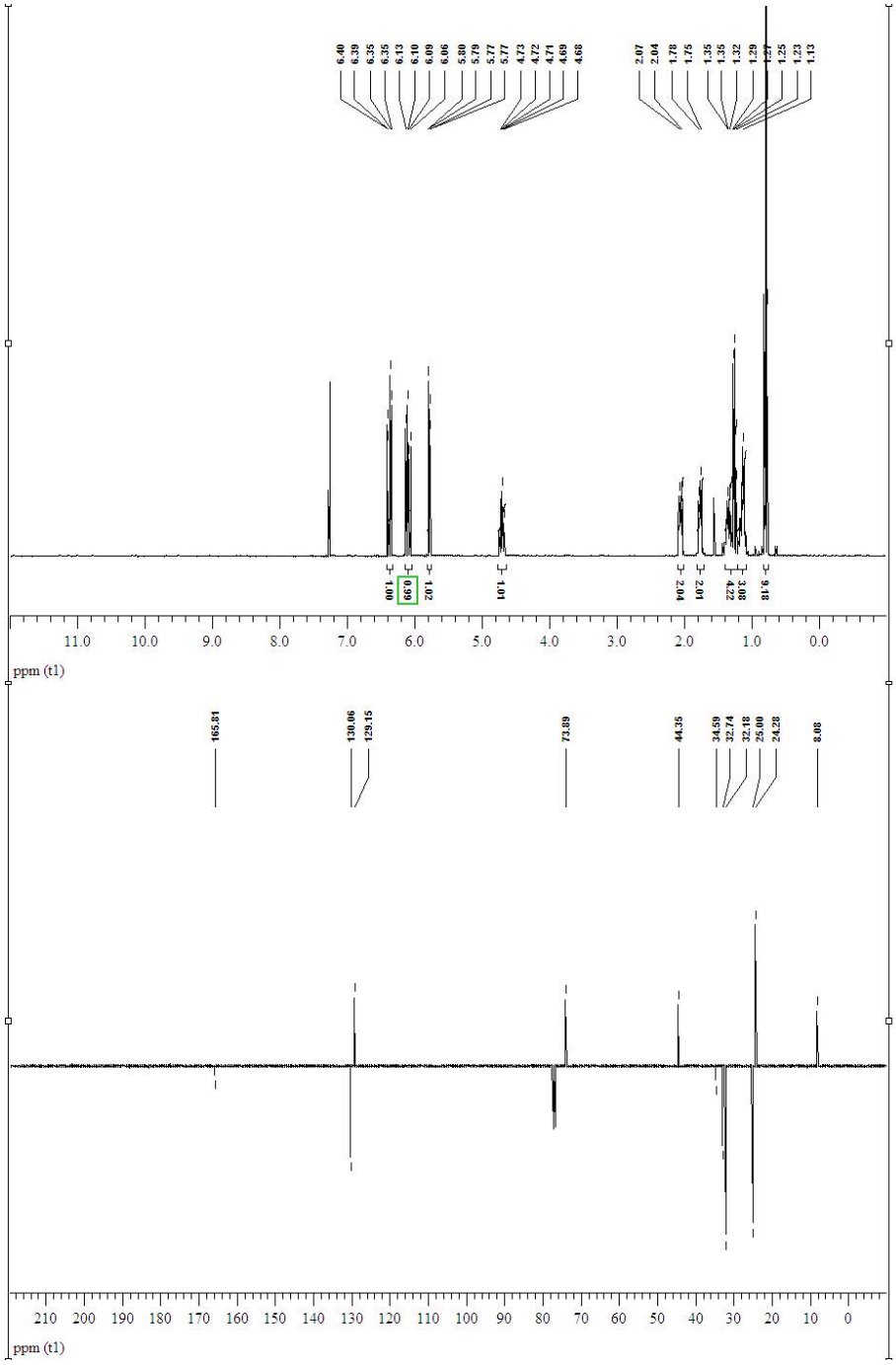


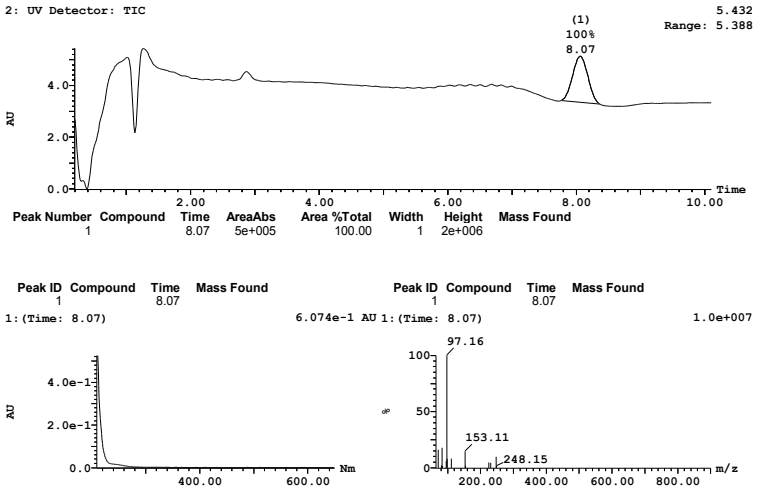
4-octylphenyl acrylate

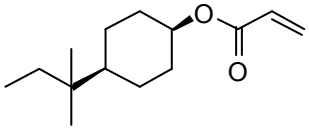




Spectral data 6h

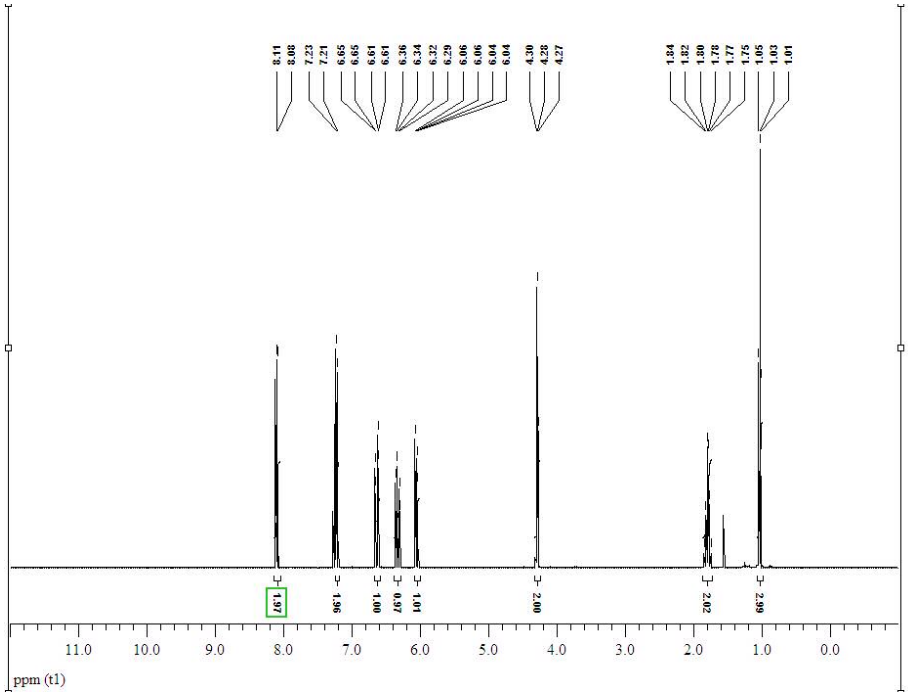


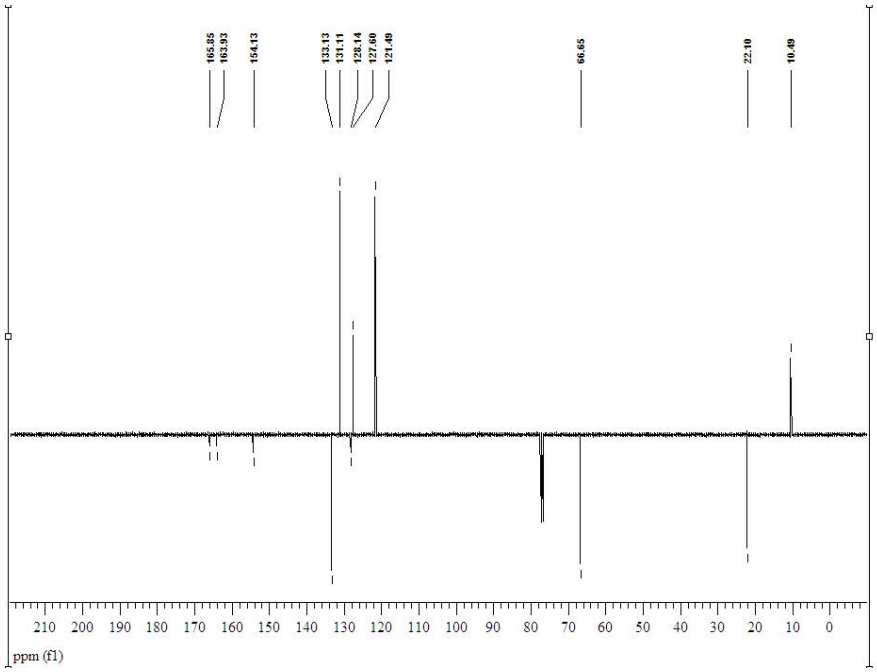


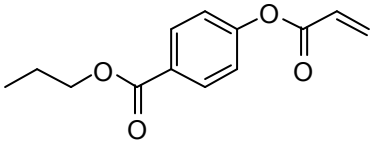


(*trans*)-4-*tert*-pentylcyclohexyl acrylate

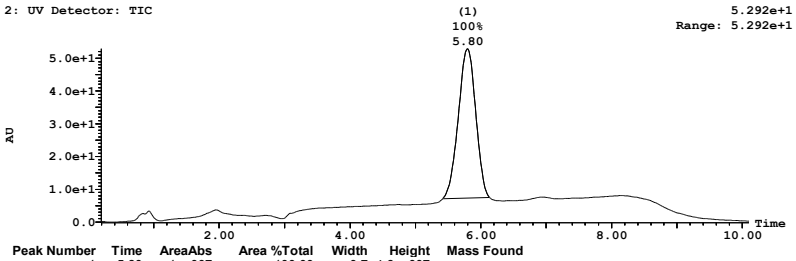
Spectral data 6i

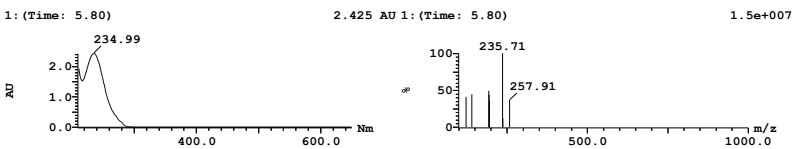




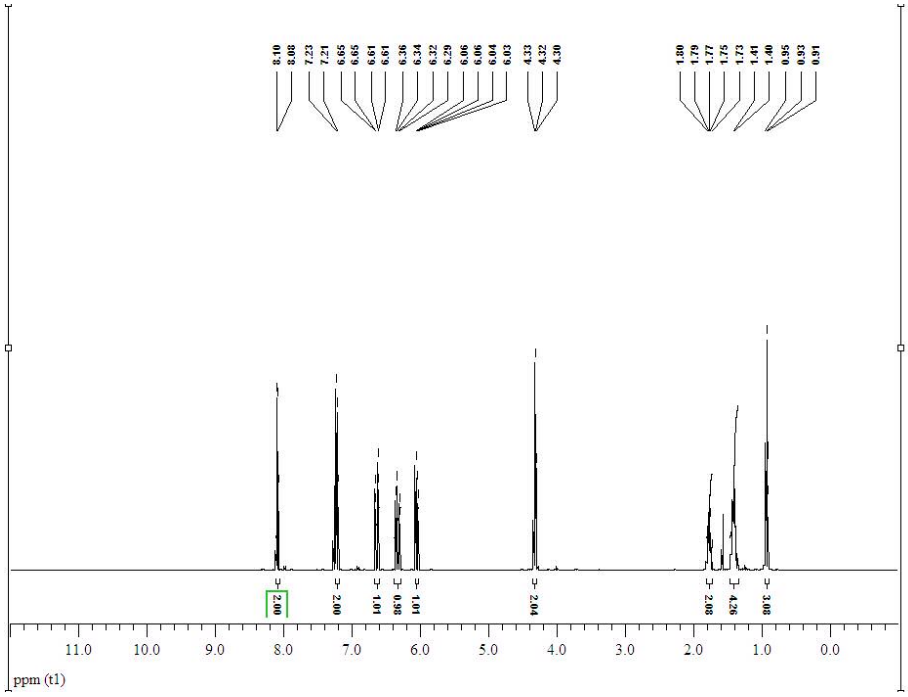


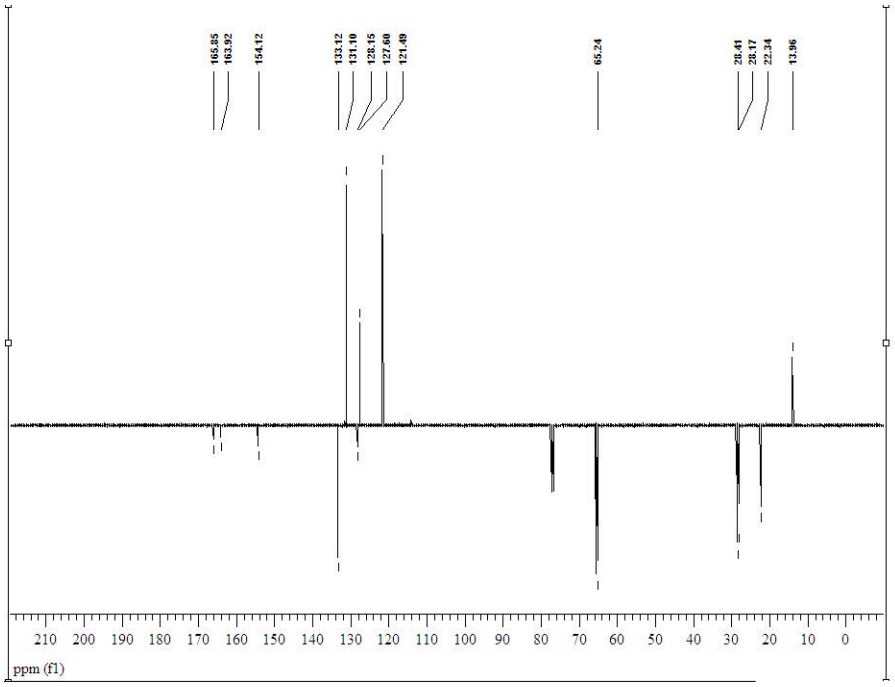
propyl 4-(acryloyloxy)benzoate

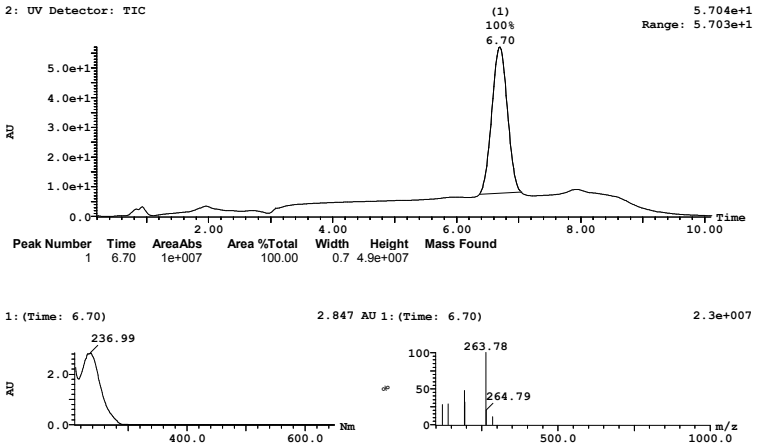


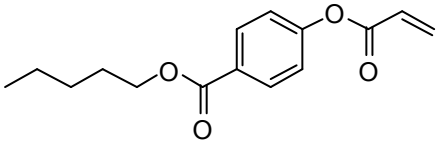


Spectral data 6j



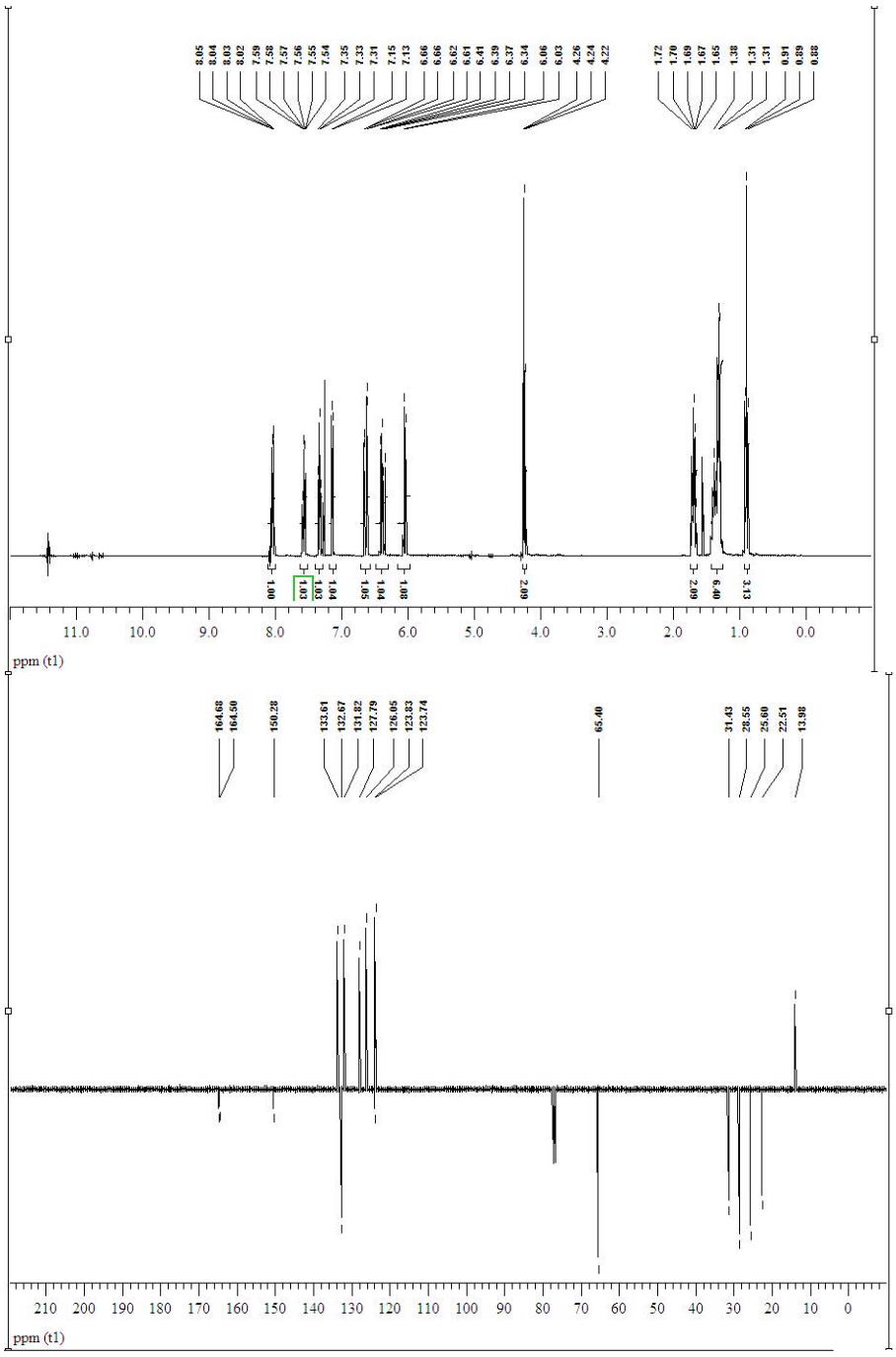


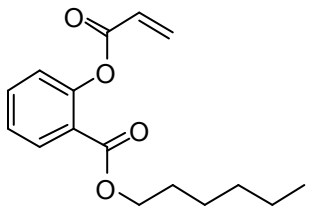




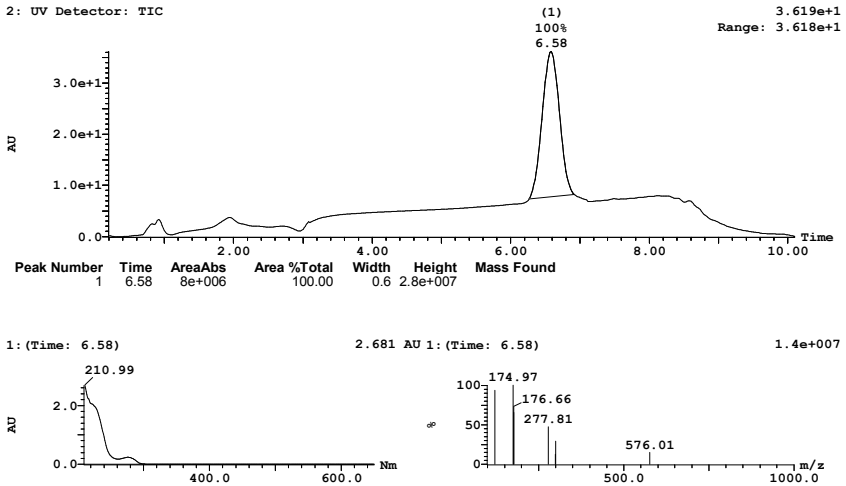
pentyl 4-(acryloyloxy)benzoate

Spectral data 6k

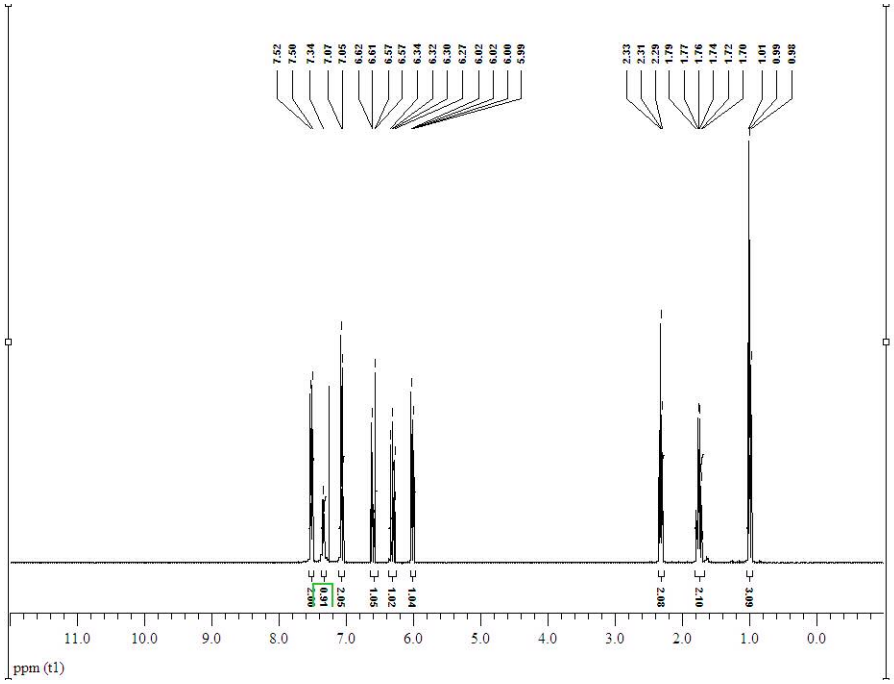


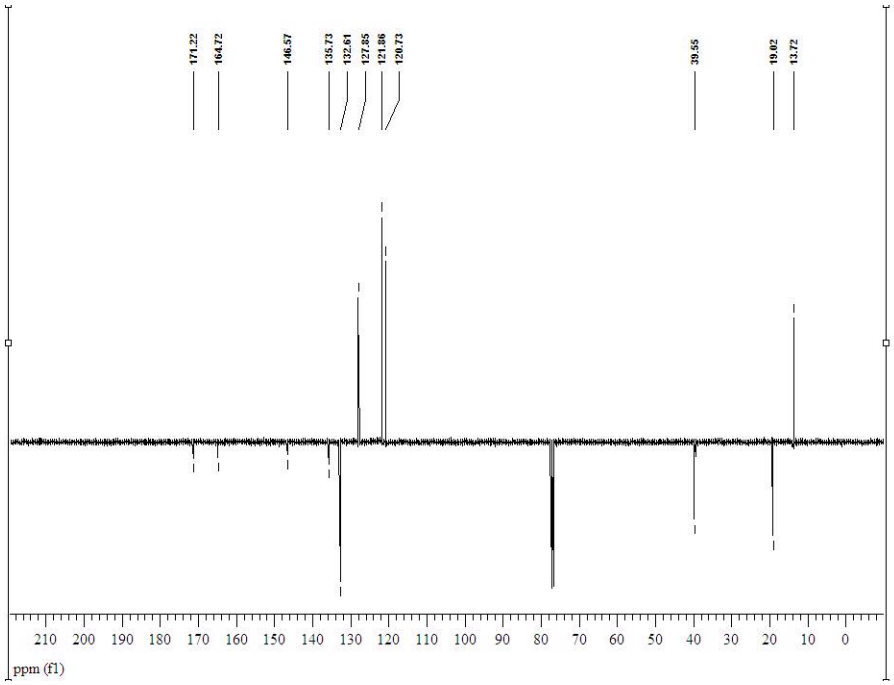


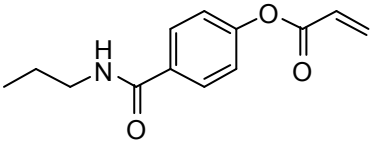
hexyl 2-(acryloyloxy)benzoate



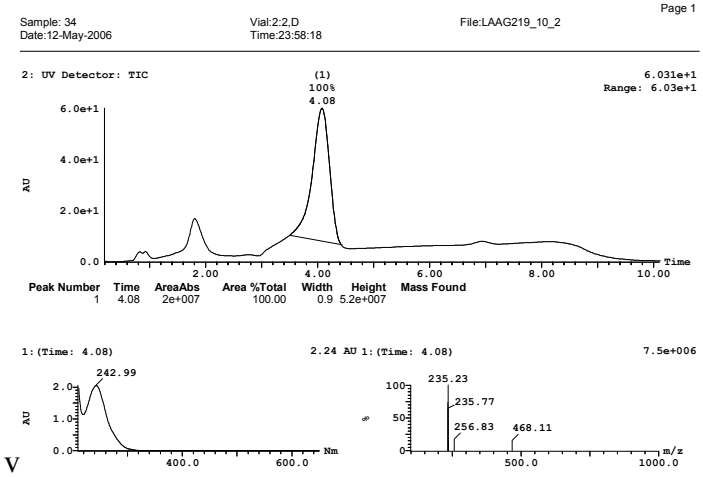
Spectral data 6l





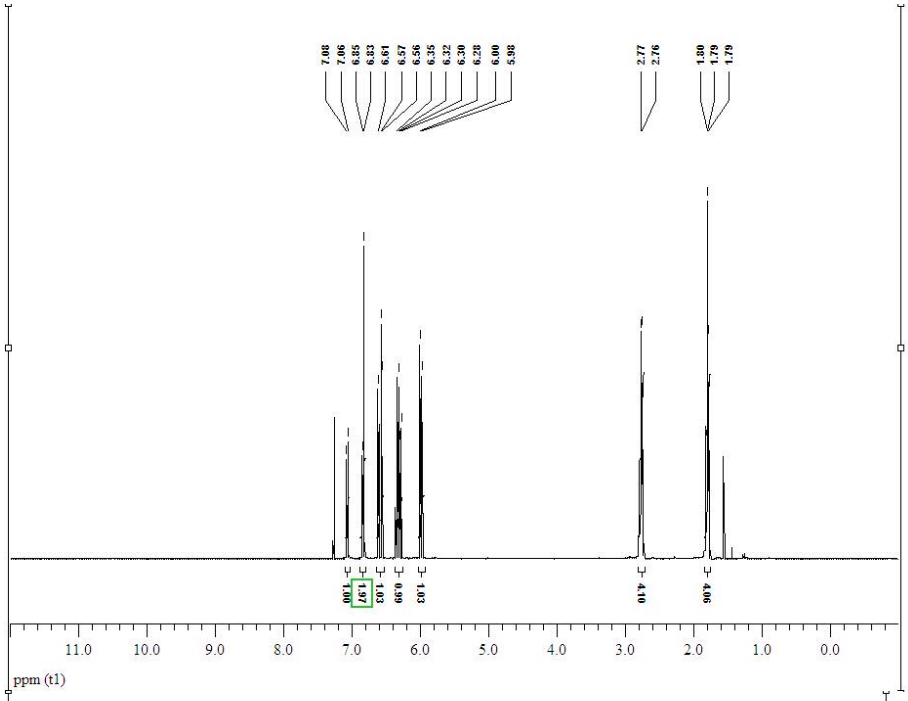


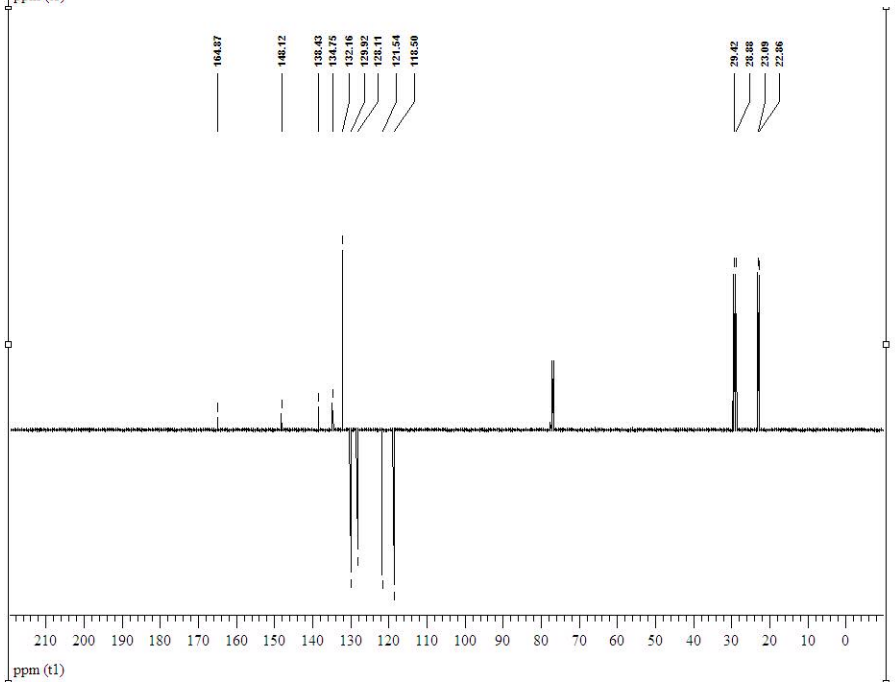
4-(propylcarbamoyl)phenyl acrylate

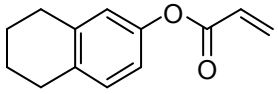


V

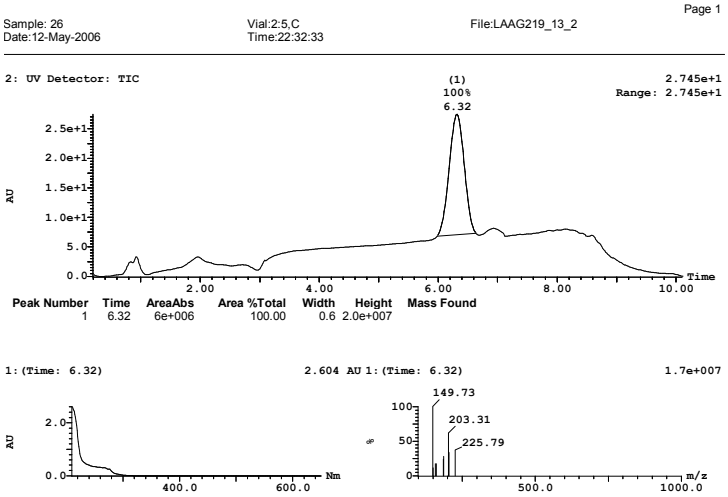
Spectral data 6m



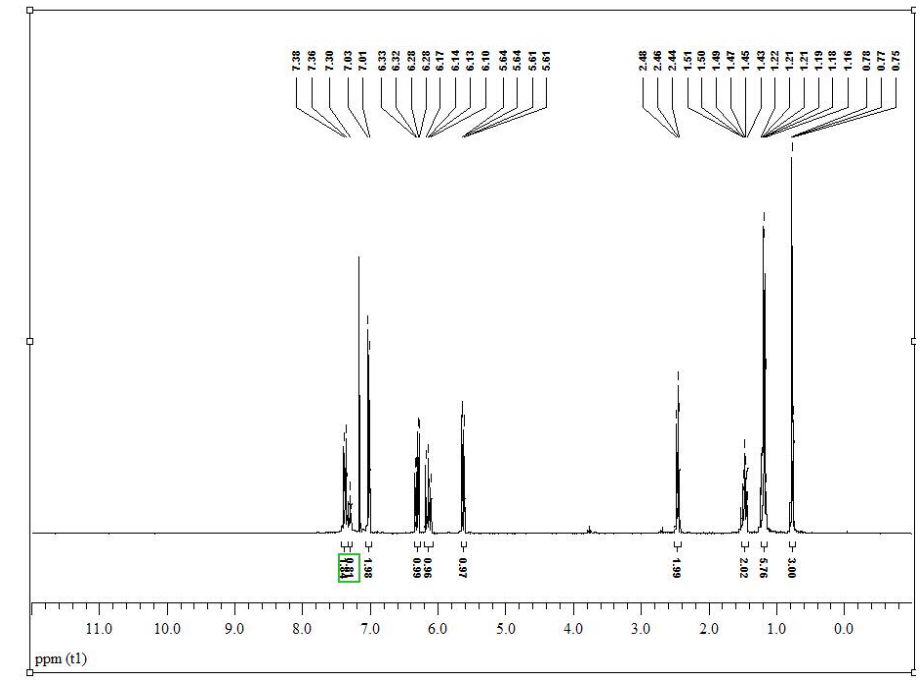


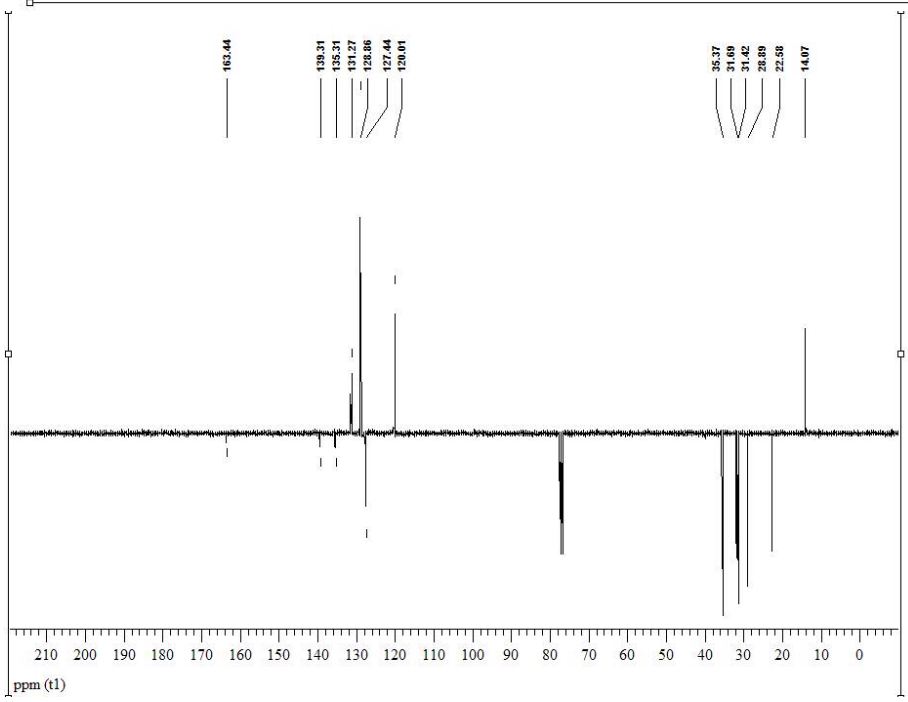


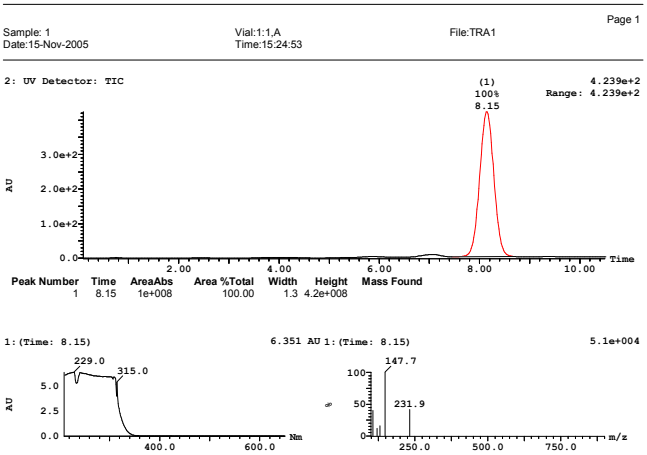
5,6,7,8-tetrahydronaphthalen-2-yl acrylate

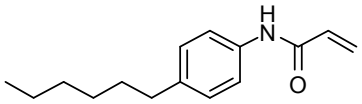


Spectral data 7a



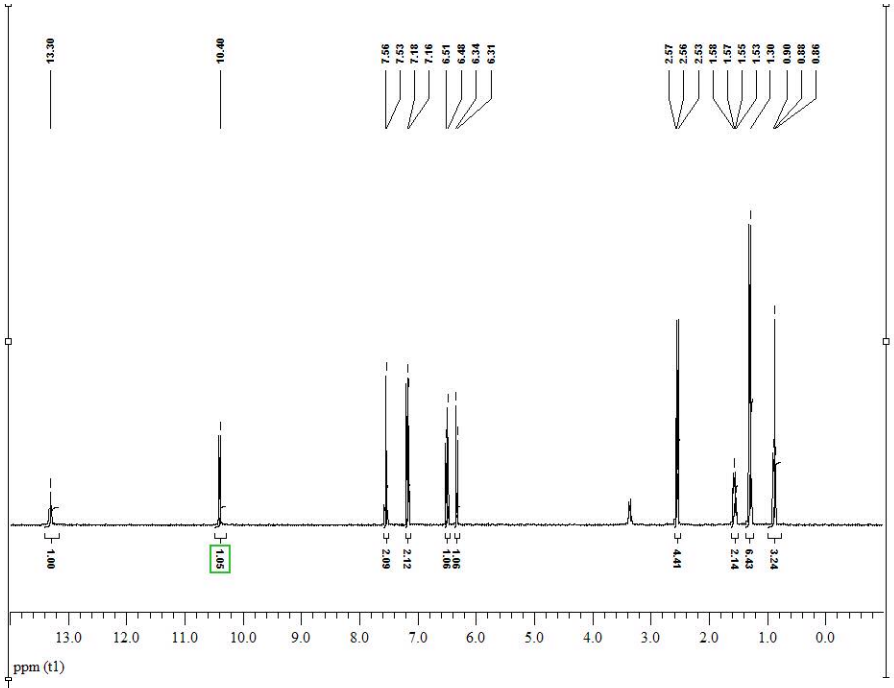


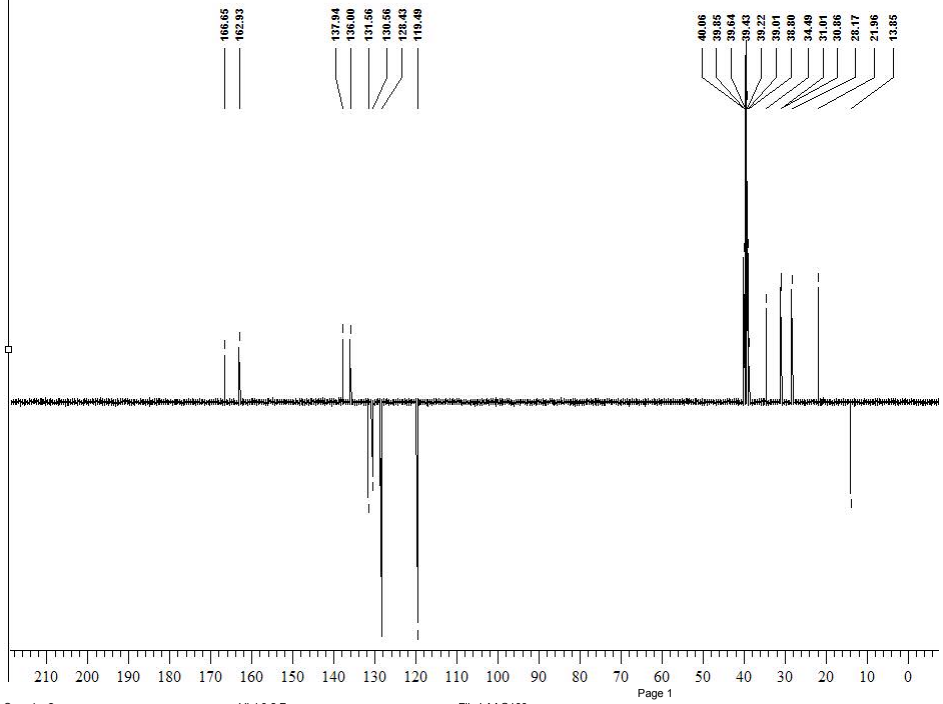




N-(4-hexylphenyl)acrylamide

Spectral data 7b

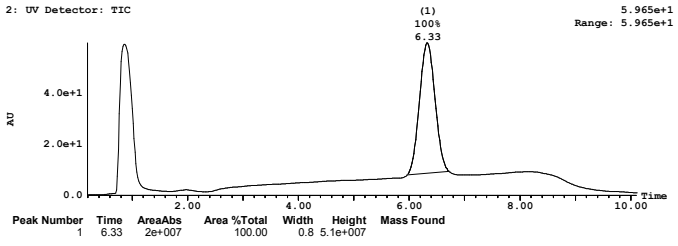


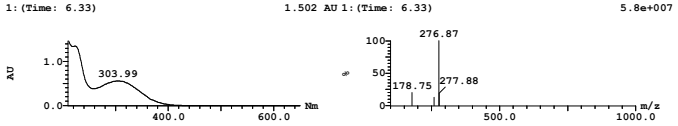


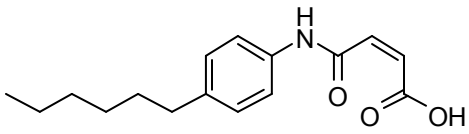
Sample: 2
Date:24-Apr-2006

Vial:3:2,F
Time:17:00:18

File:LAAG133

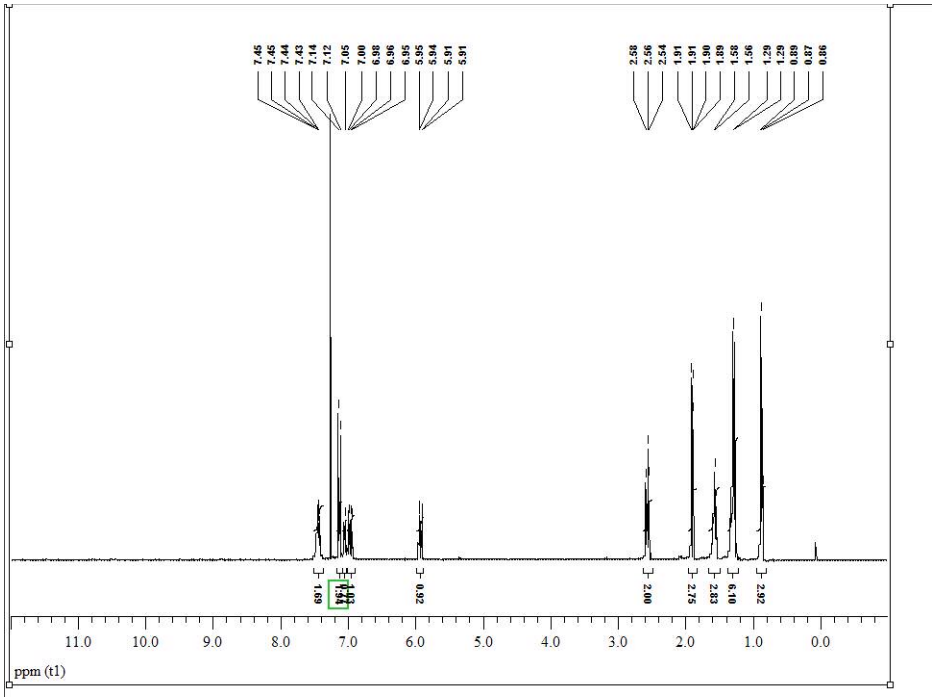


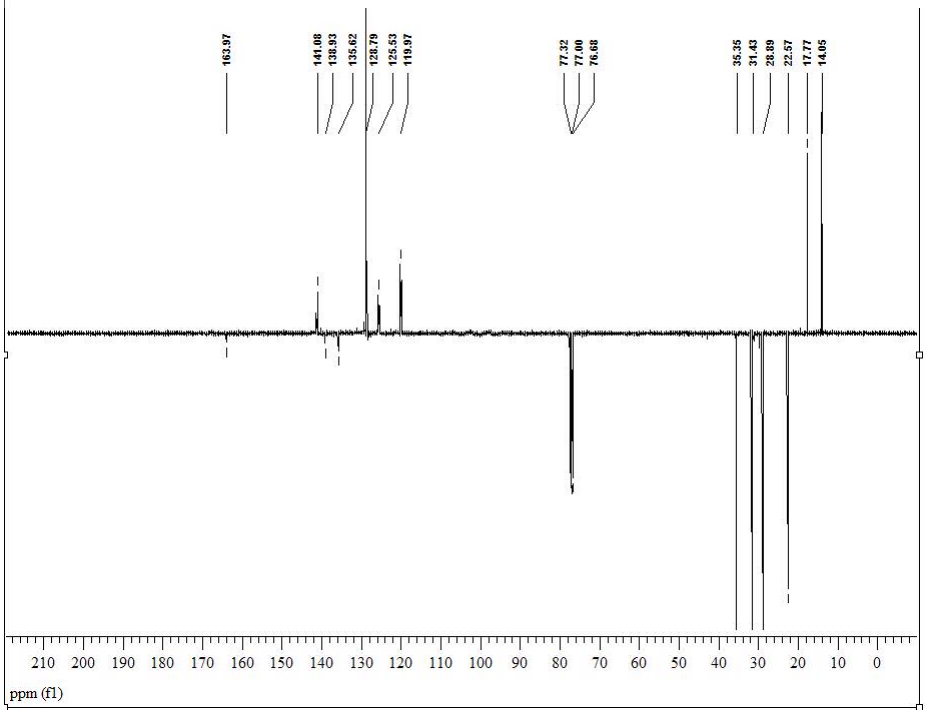


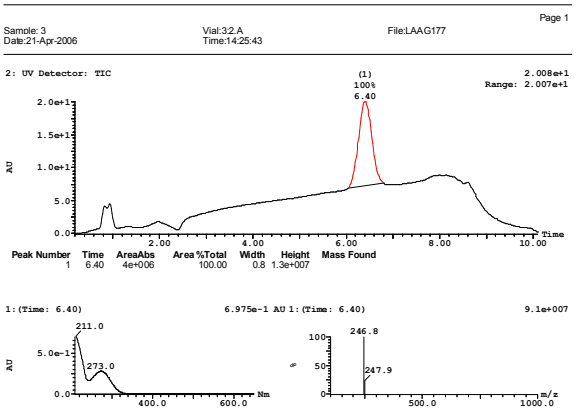


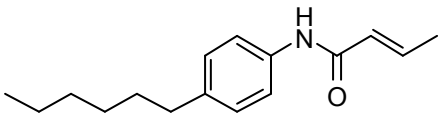
(*Z*)-4-(4-hexylphenylamino)-4-oxobut-2-enoic acid

Spectral data 7c



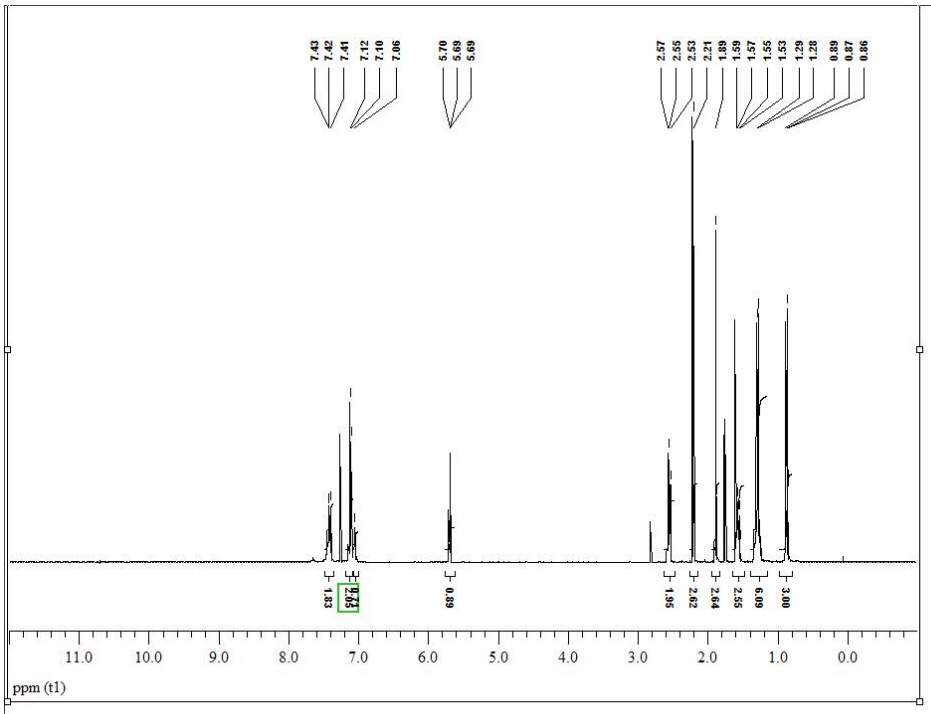


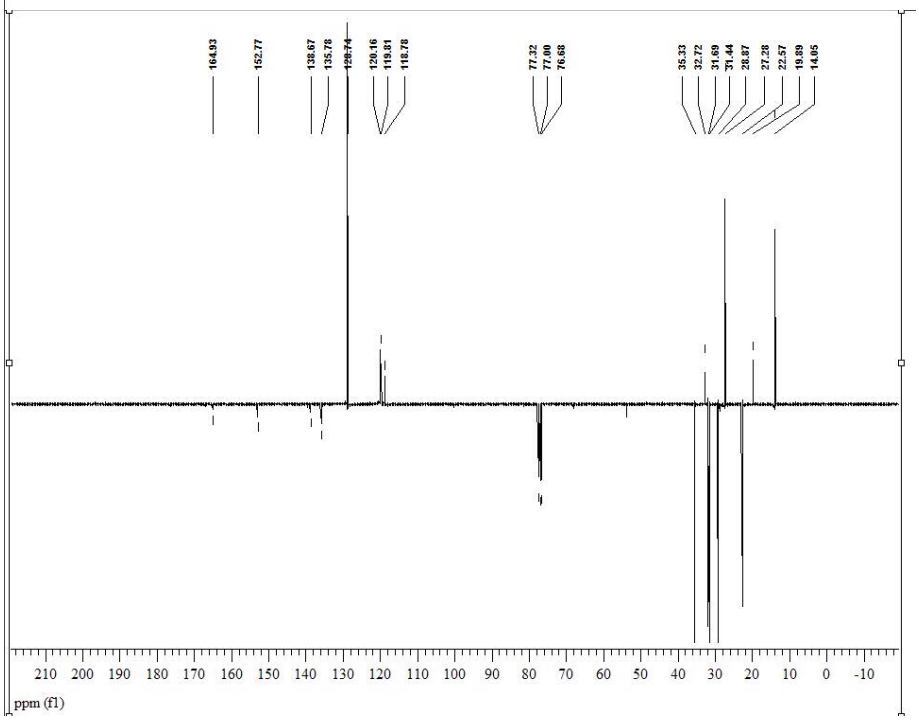


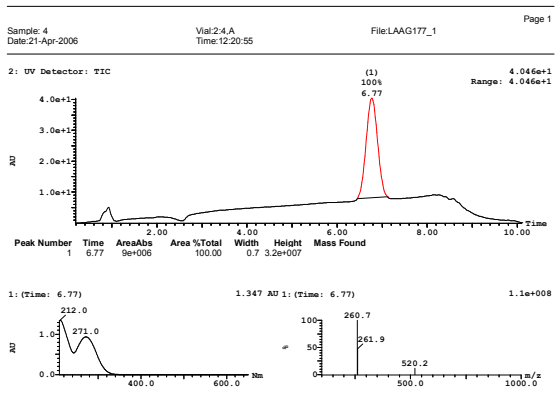


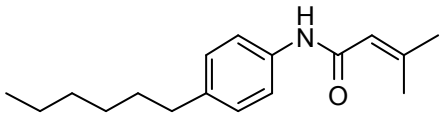
(*E*)-*N*-(4-hexylphenyl)but-2-enamide

Spectral data 7d



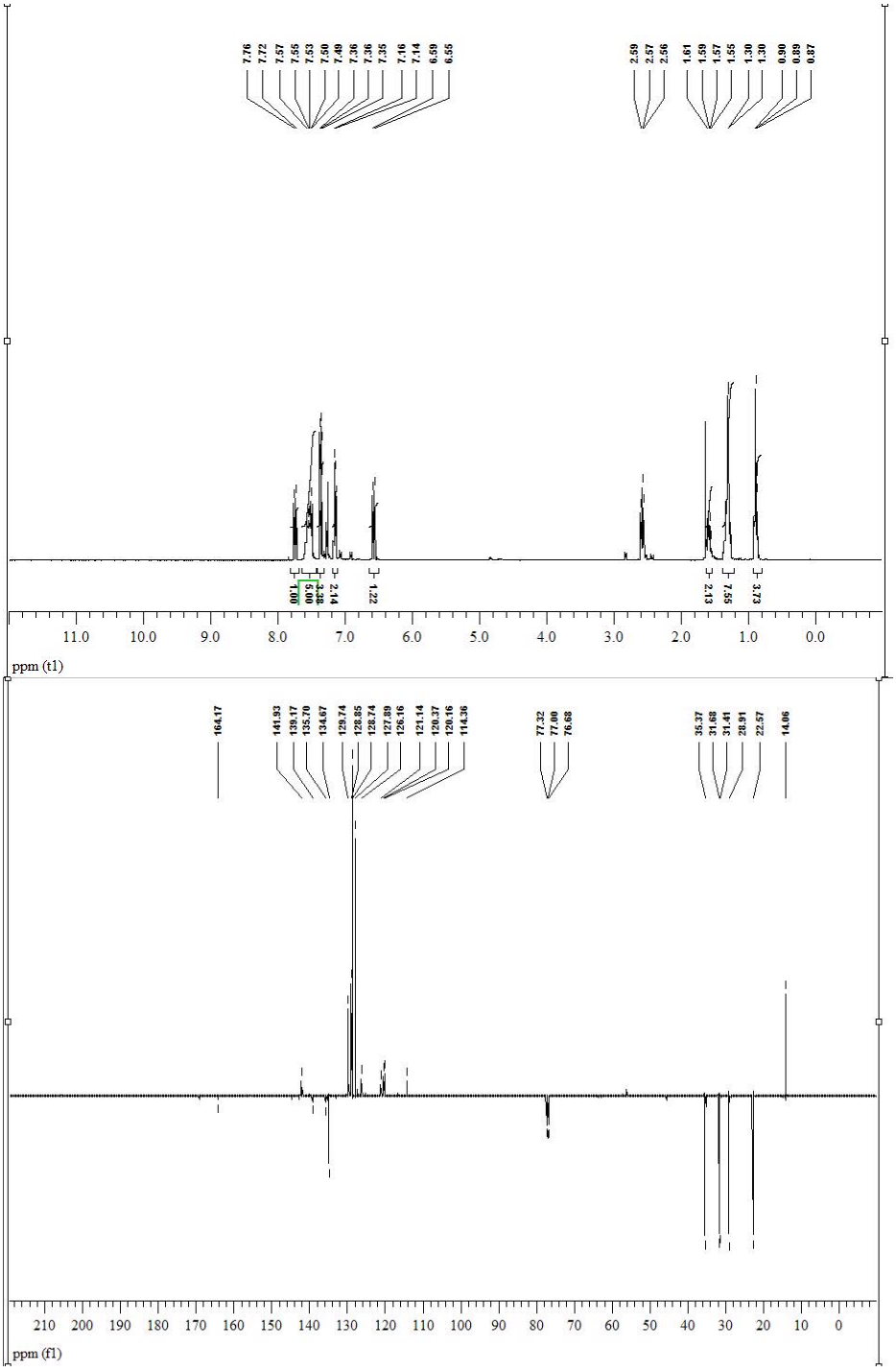


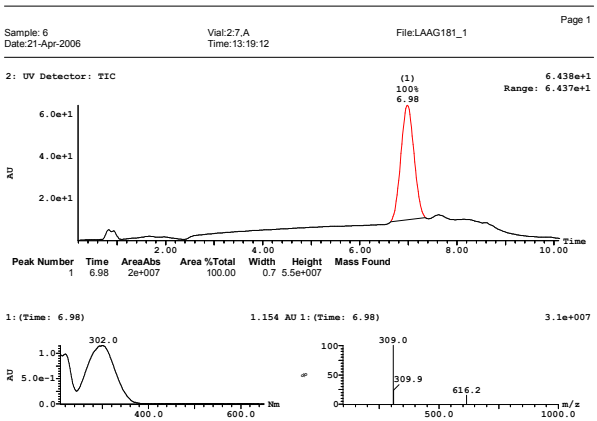


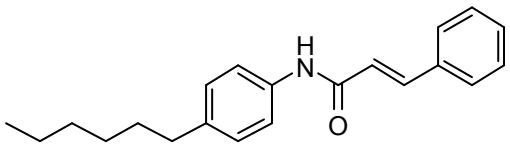


N-(4-hexylphenyl)-3-methylbut-2-enamide

Spectral data 7e

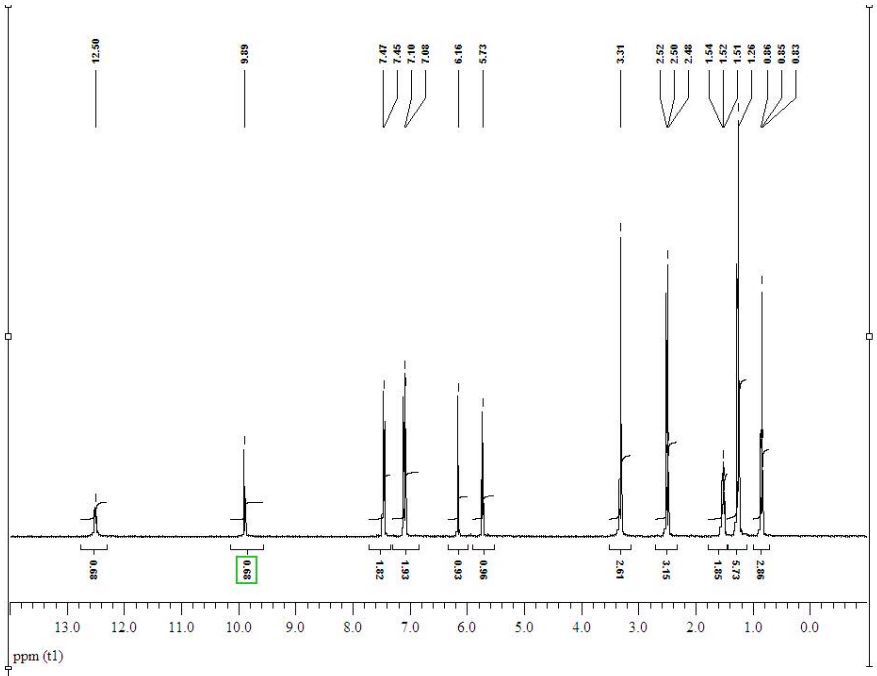


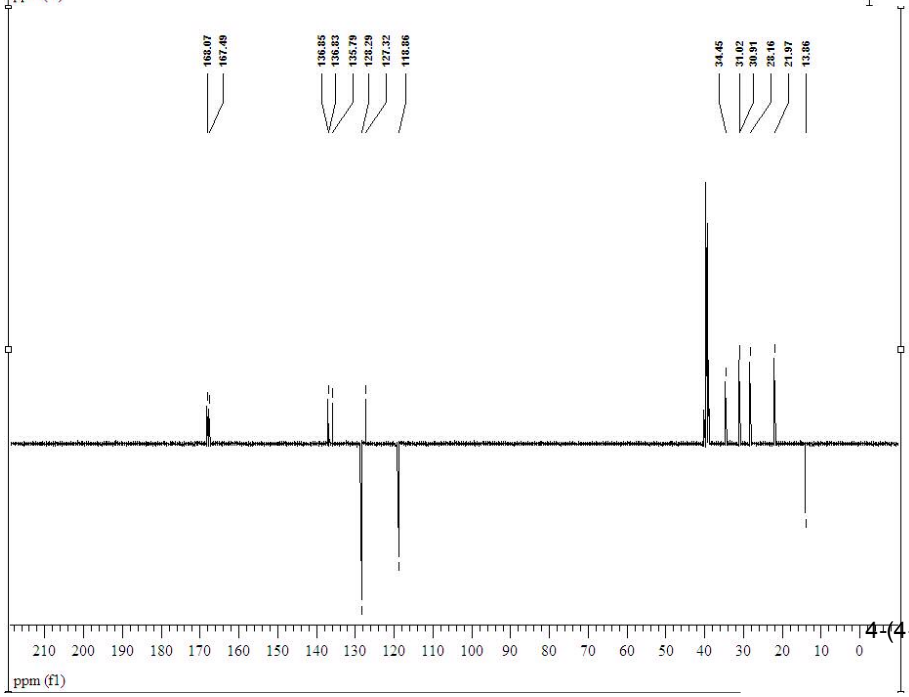


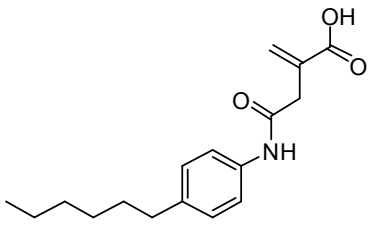


N-(4-hexylphenyl)cinnamamide

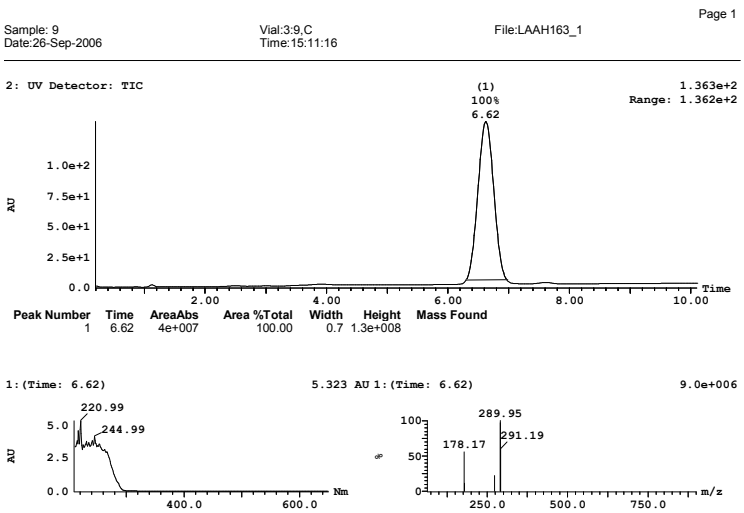
Spectral data 7f



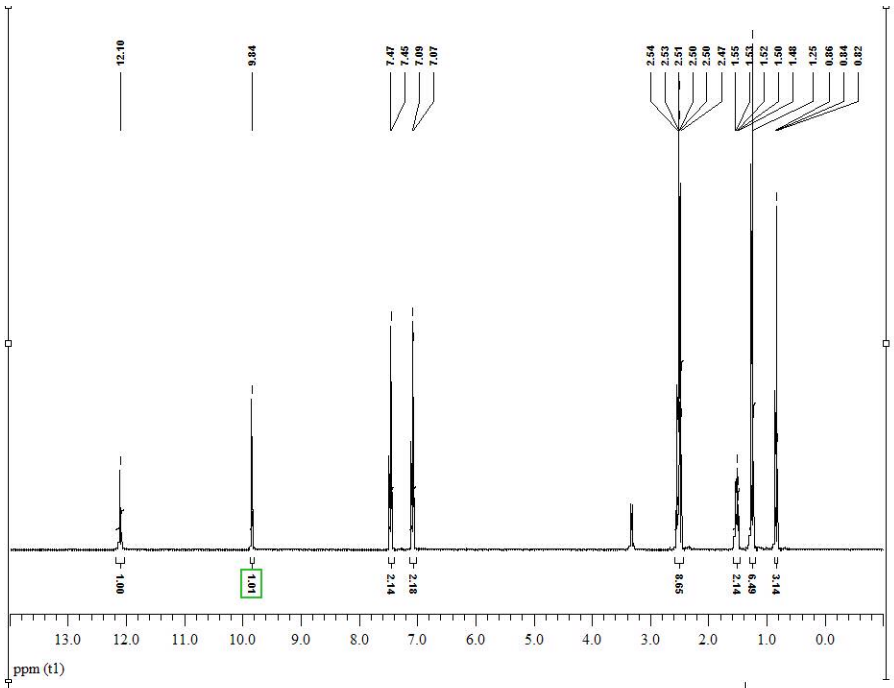


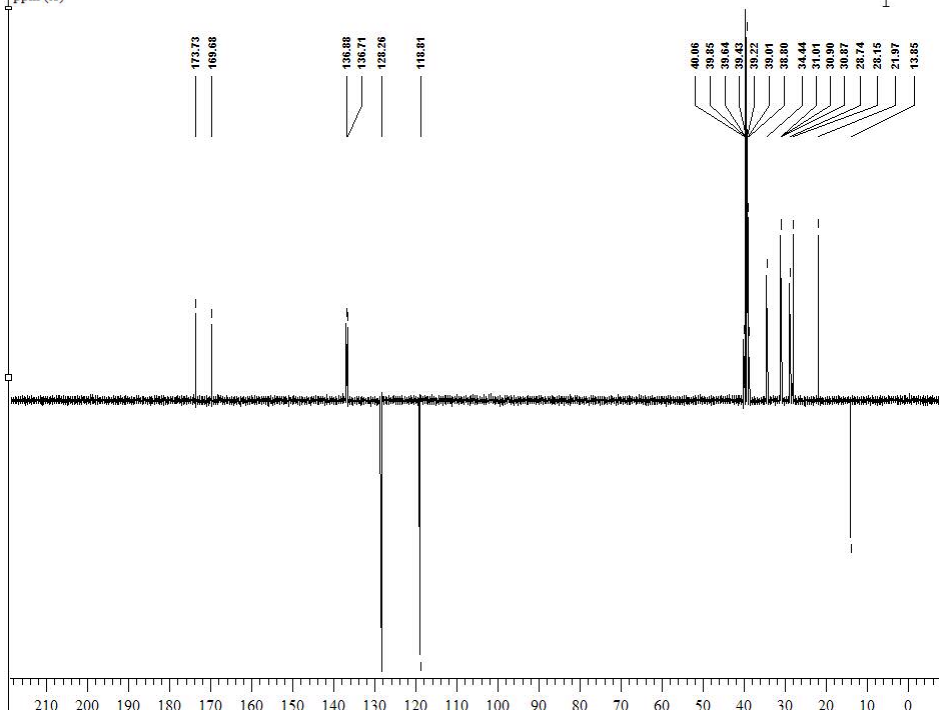


4-(4-hexylphenylamino)-2-methylene-4-oxobutanoic acid



Spectral data 7g



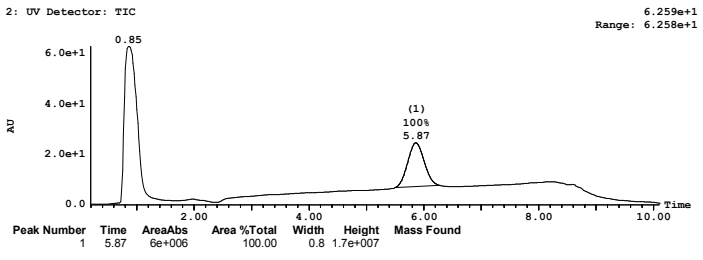


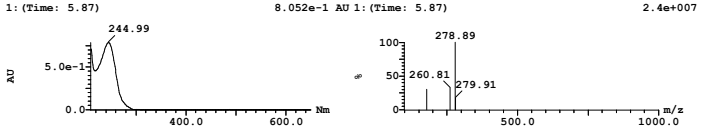
Page 1

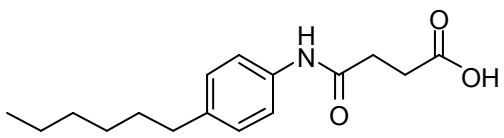
Sample: 3
Date:24-Apr-2006

Vial:3:3,F
Time:17:11:00

File:LAAG135

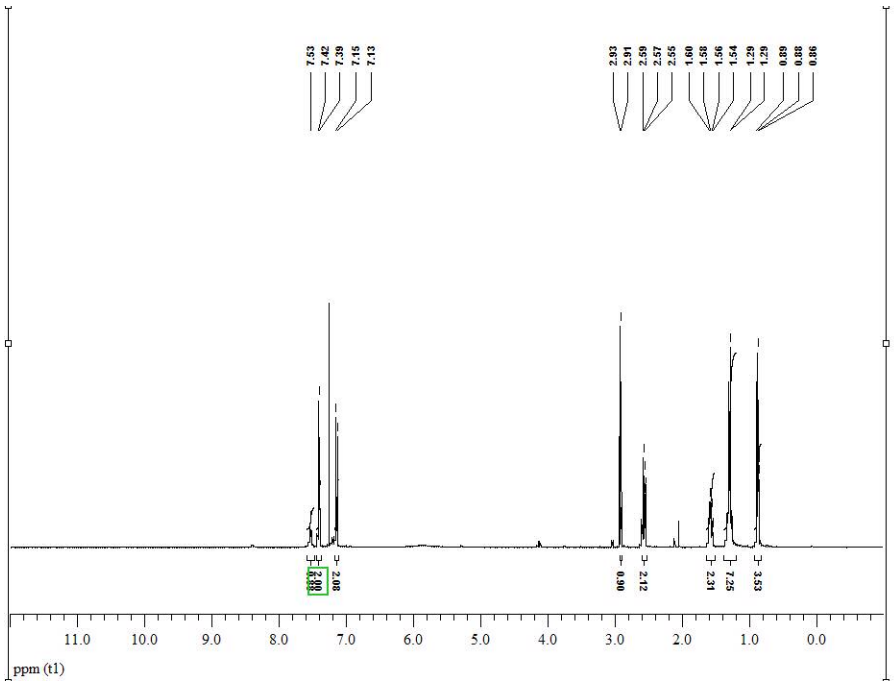


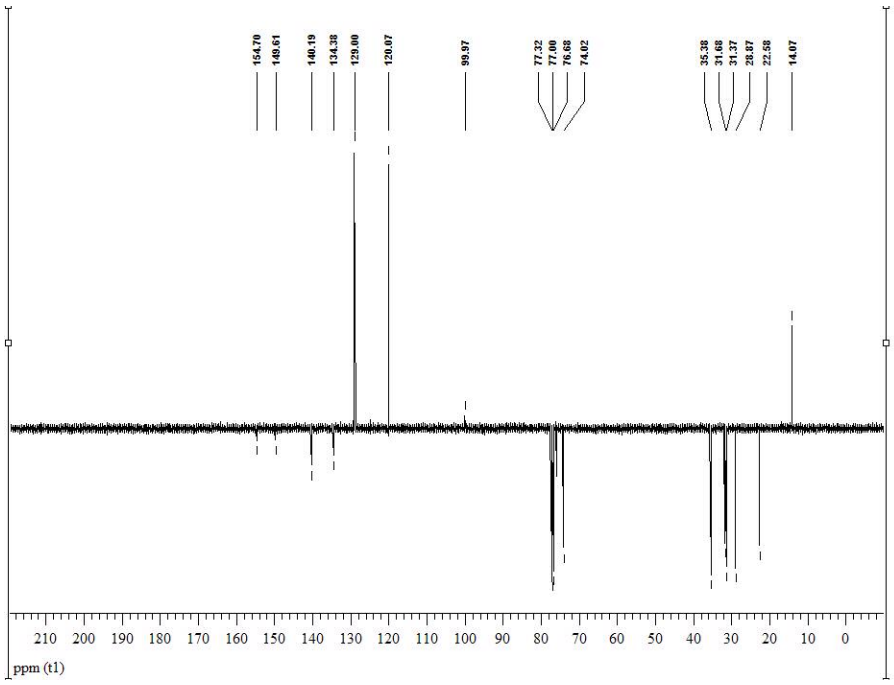


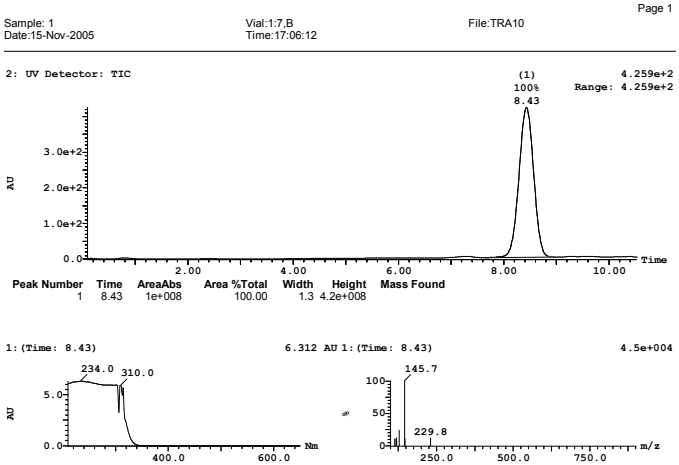


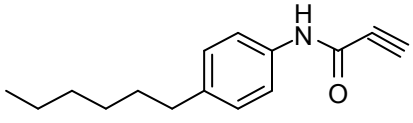
4-(4-hexylphenylamino)-4-oxobutanoic acid

Spectral data 8a



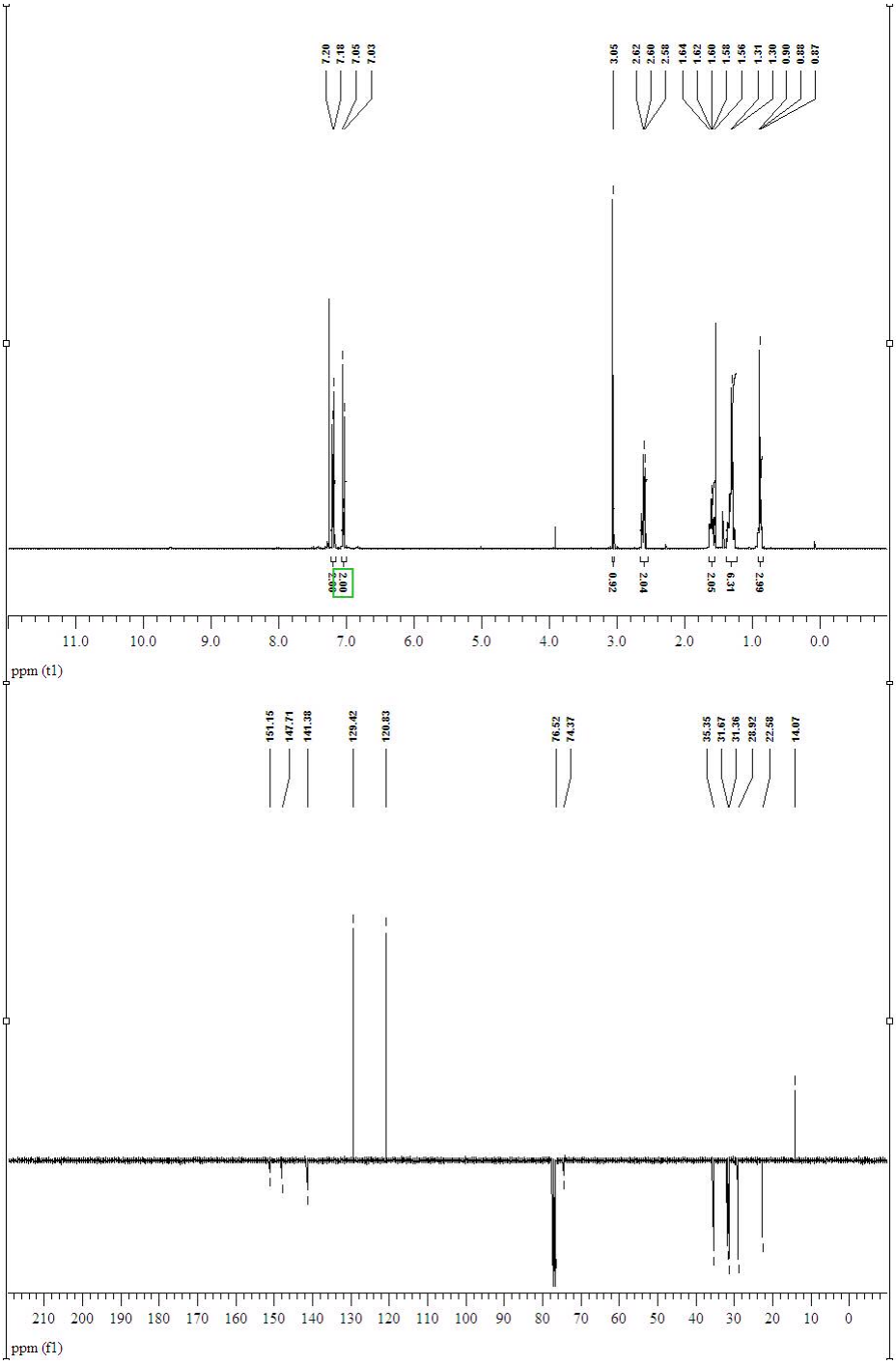


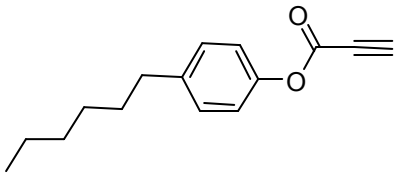




N-(4-hexylphenyl)propiolamide

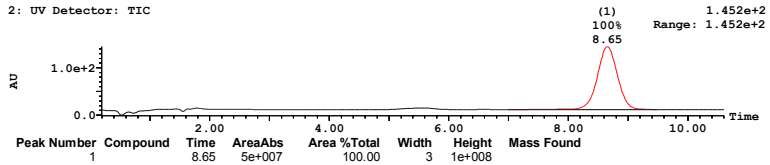
Spectral data 8b





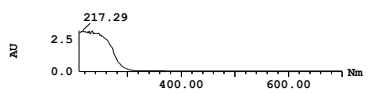
Sample Report:

Sample 2 Vial 1:6,F ID File LAAH215_3 Date 14-Nov-2006 Time 16:30:26 Description

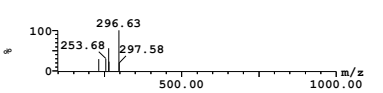


Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1		8.65	5e+007	100.00	3	1e+008	

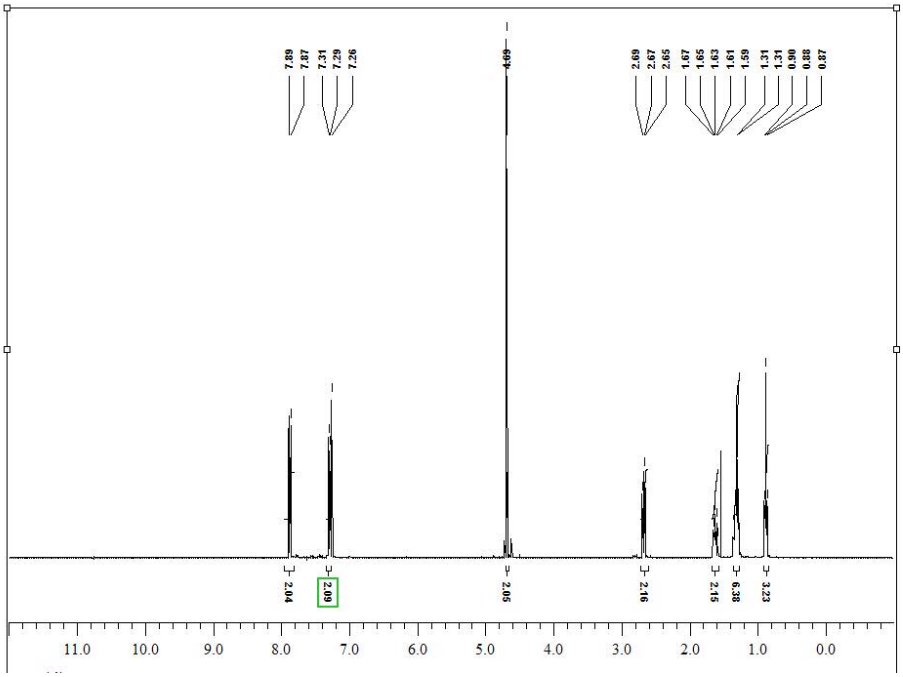
Peak ID	Compound	Time	Mass Found
1		8.65	

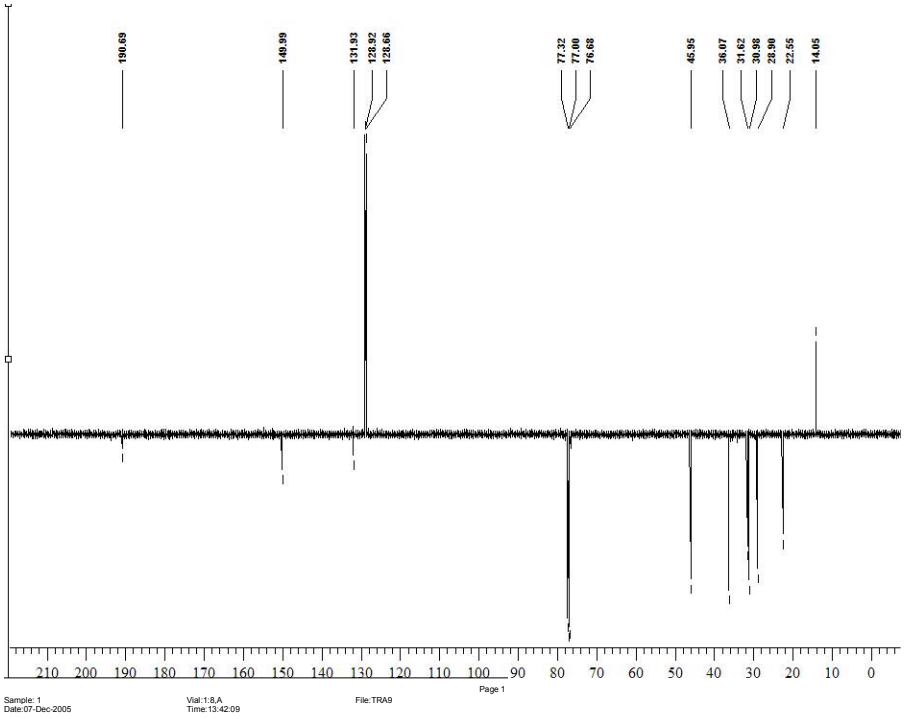


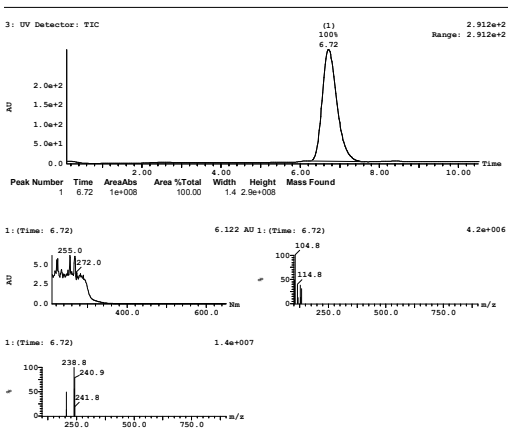
Peak ID	Compound	Time	Mass Found
1		8.65	

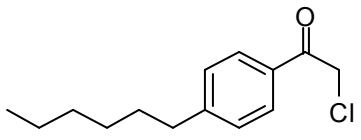


Spectral data 8c



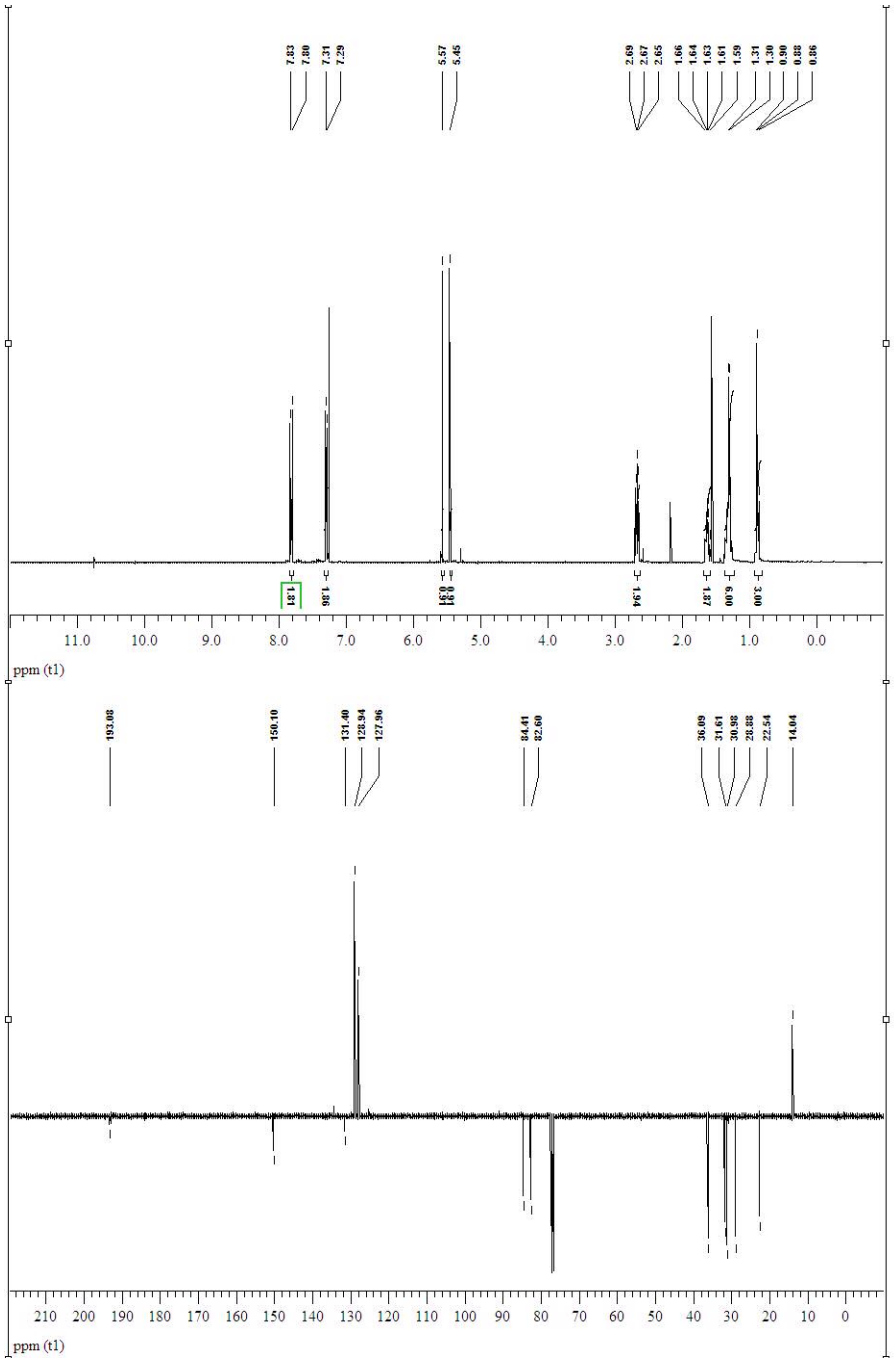


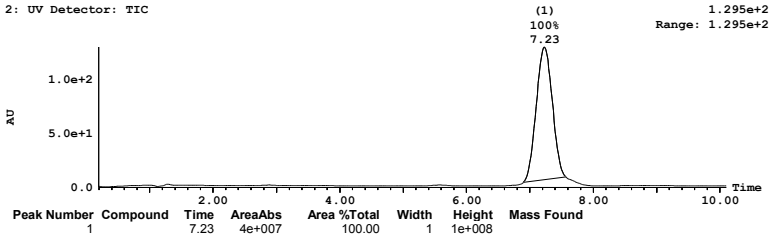


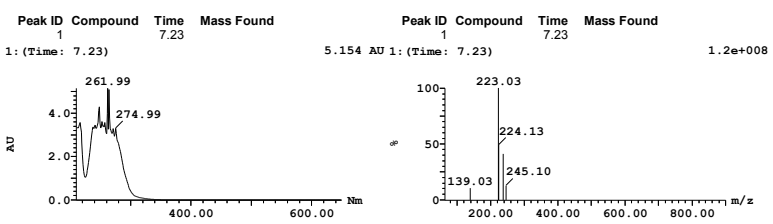


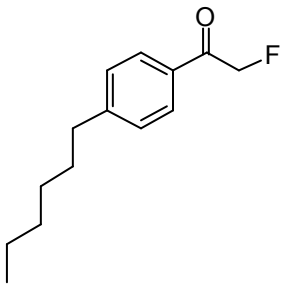
2-chloro-1-(4-hexylphenyl)ethanone

Spectral data 8d



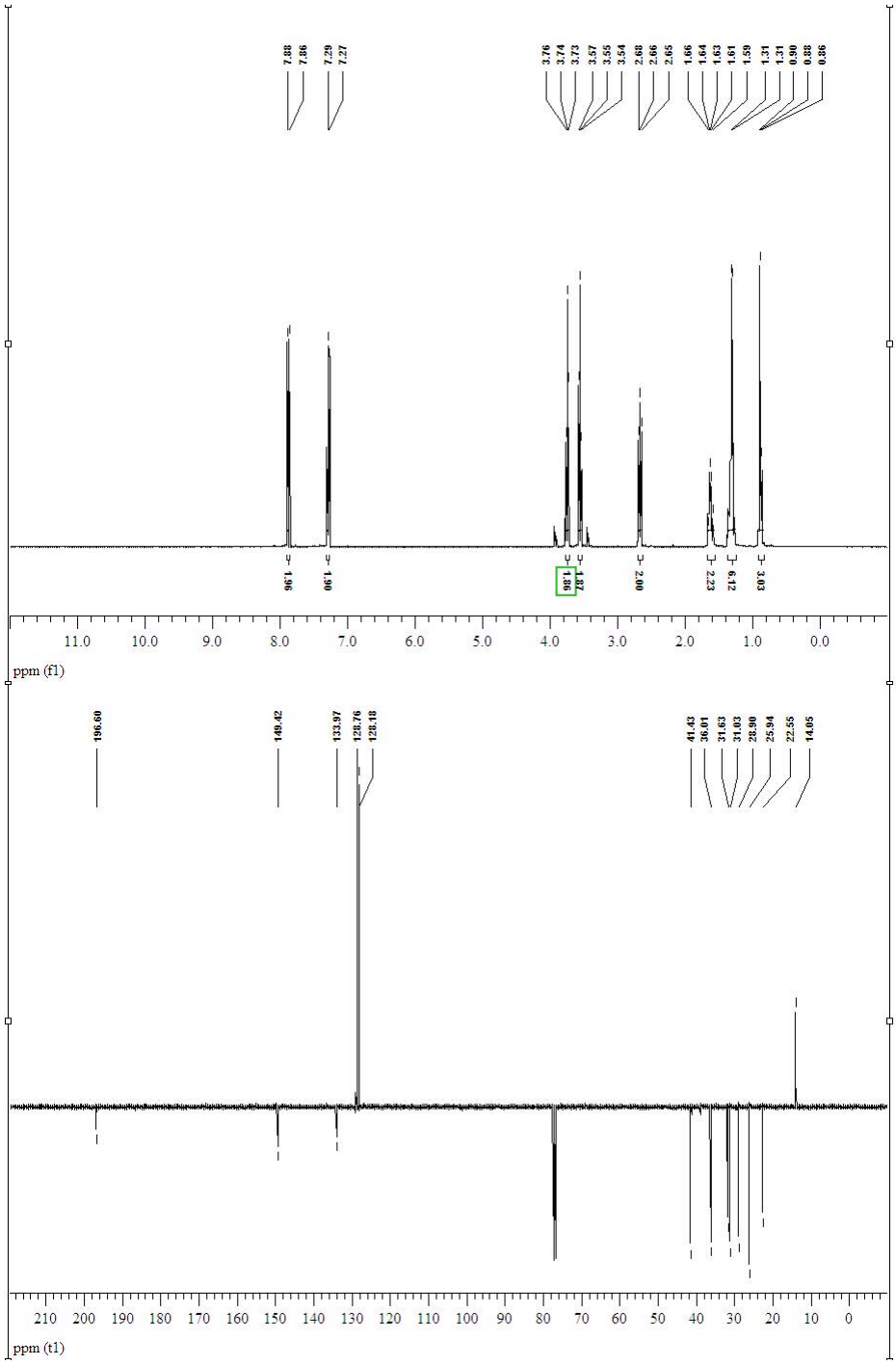


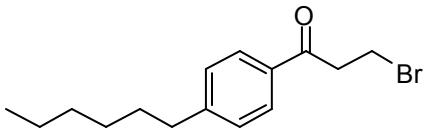




2-fluoro-1-(4-hexylphenyl)ethanone

Spectral data 8e

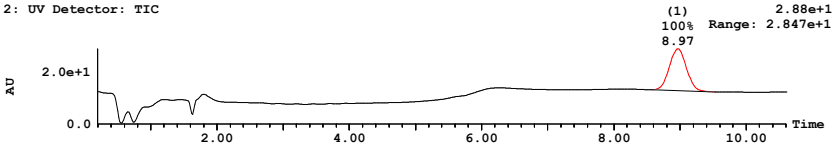




3-bromo-1-(4-hexylphenyl)propan-1-one

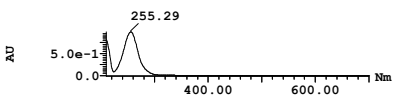
Sample Report:

Sample 2 Vial 1:5,F ID File LAAH195 Date 27-Oct-2006 Time 16:41:47 Description

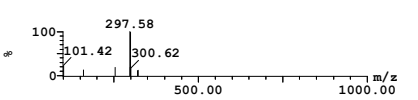


Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1		8.97	5e+006	100.00	1	2e+007	

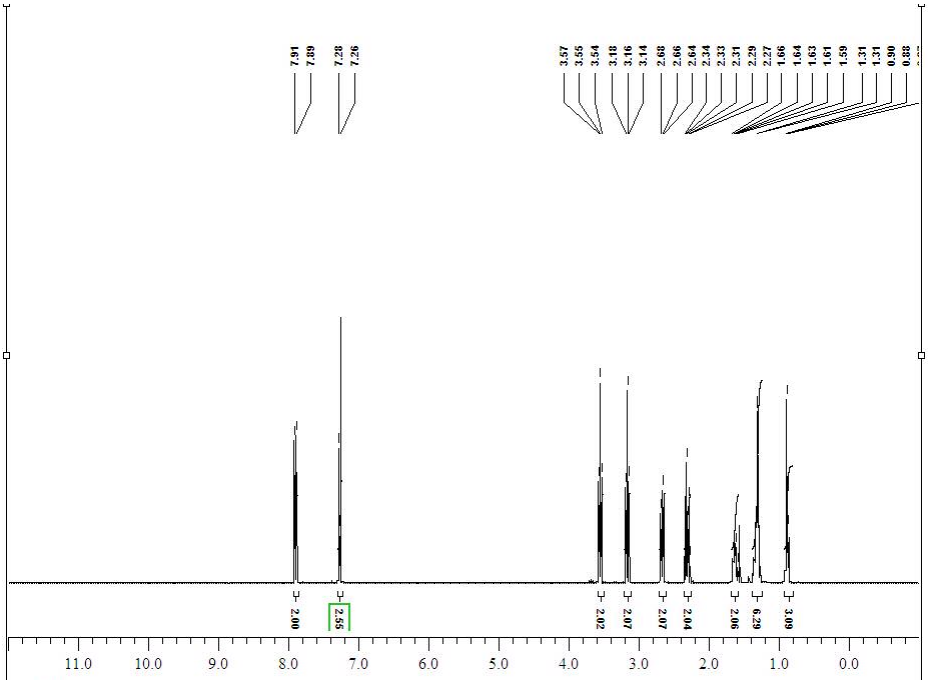
Peak ID	Compound	Time	Mass Found
1		8.97	

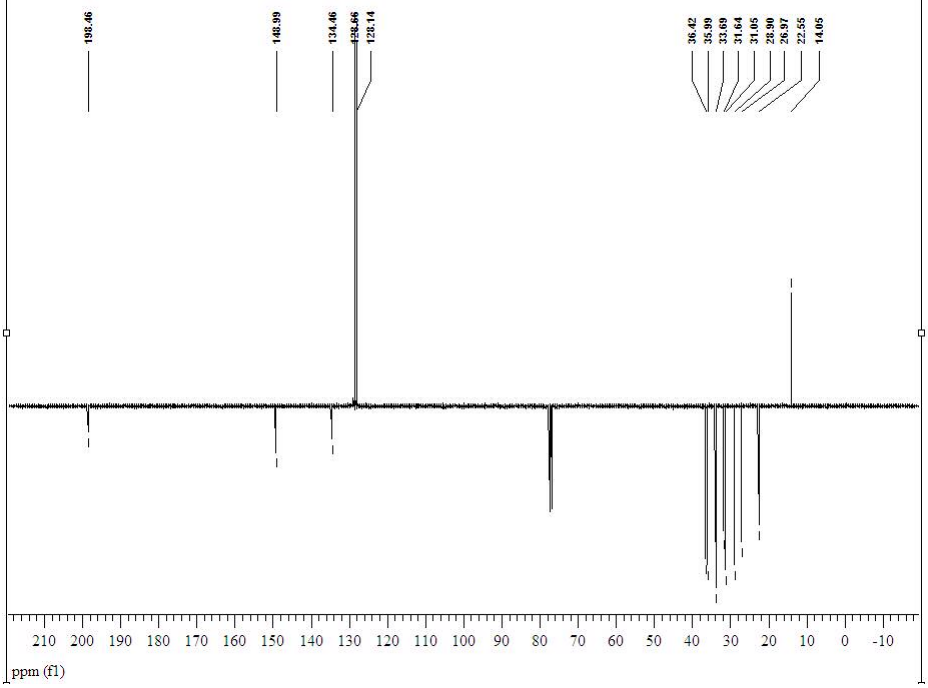


Peak ID	Compound	Time	Mass Found
1		8.97	



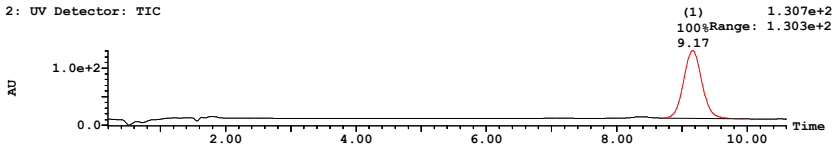
Spectral data 8f





Sample Report:

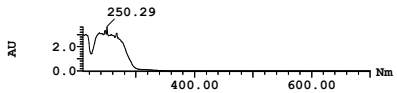
Sample 2 Vial 1:8,F ID File LAAH221 Date 15-Nov-2006 Time 15:53:55 Description



Peak Number	Compound	Time	AreaAbs	Area %Total	Width	Height	Mass Found
1		9.17	4e+007	100.00	1	1e+008	

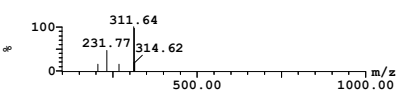
Peak ID	Compound	Time	Mass Found
1		9.17	

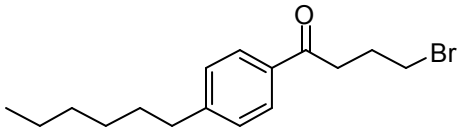
1:(Time: 9.17)



Peak ID	Compound	Time	Mass Found
1		9.17	

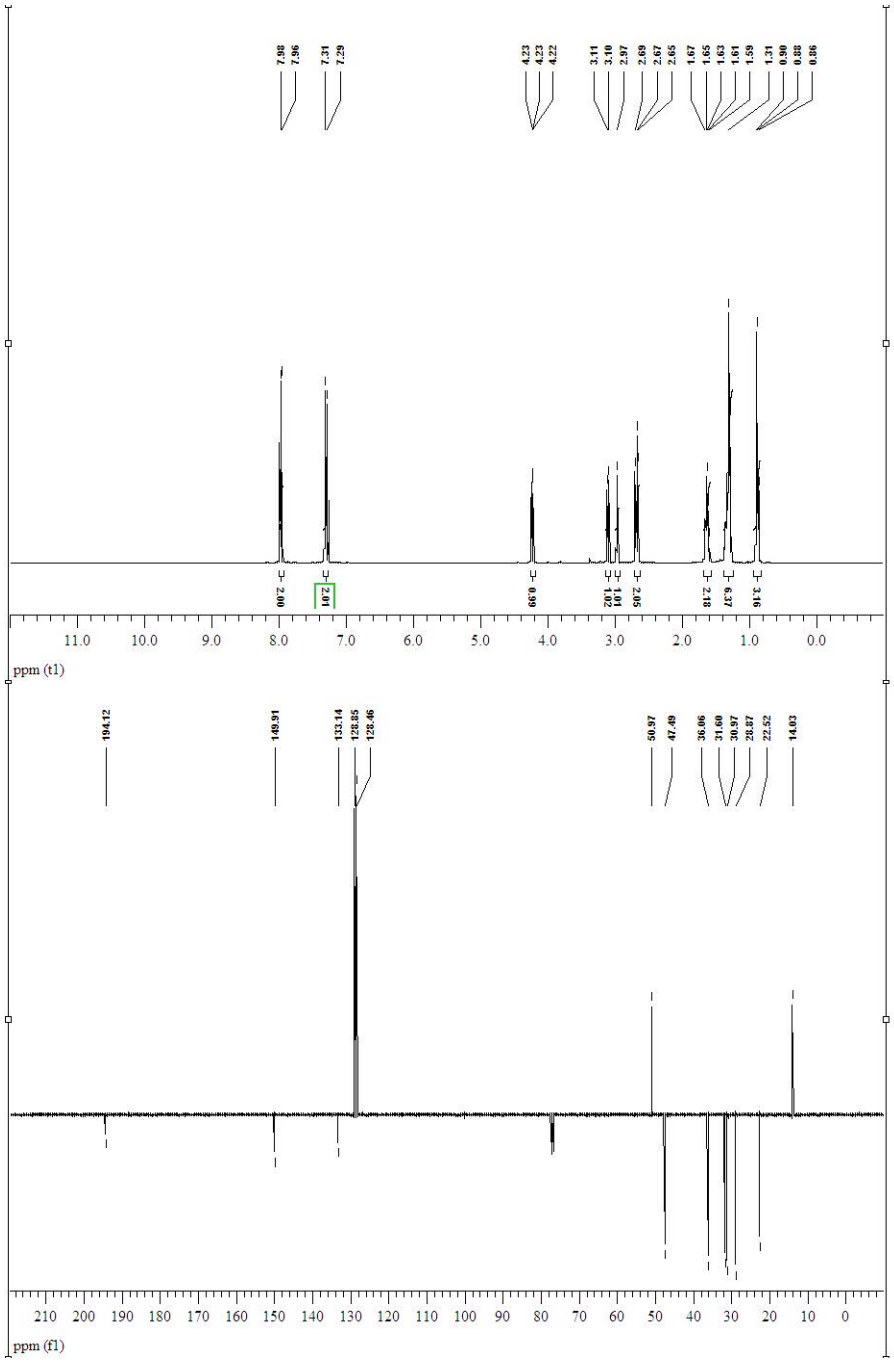
3.608 AU 1:(Time: 9.17) 4.3e+007

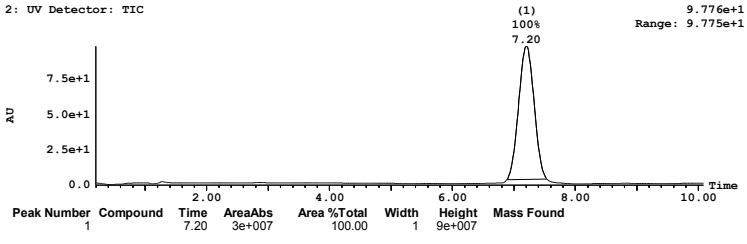


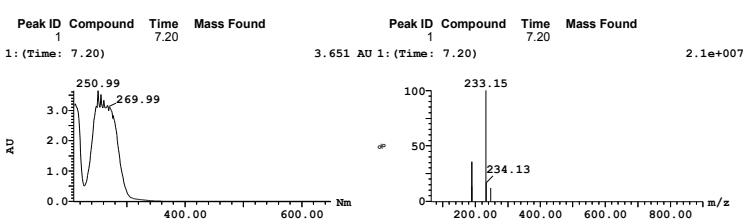


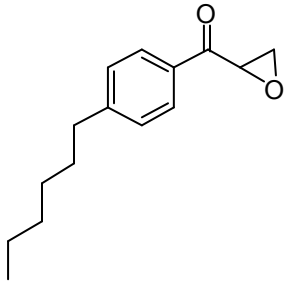
4-bromo-1-(4-hexylphenyl)butan-1-one

Spectral data 8g









(4-hexylphenyl)(oxiran-2-yl)methanone