Supporting Information

An Novel Efficient Method for the Allylation of Carbonyl Compounds and Imines using Triallylaluminum

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General. All reactions were performed in over-dried glassware under nitrogen. The spectrum of ^{1}H and ^{13}C were recorded with Bruker EX 400 NMR.

Material. Aldehydes **1a-1l** , ketones **1m-1y** , aldimine **4h** and ketimine **4q** were purchased from Acros Chemical Co , Aldrich Chemical Co and other commercially available reagent were used without further purification. aldimine **4a-4g** , **4i** , keimine **4j-4p**, **4r** were prepared according to the literature procedures and all the spectra data were consistent with the literature reports.

Experimental Section

(1) The formation of triallylaluminum **2**

A dry 250mL flask fitted with a mechanical stirrer is assembled with vacuum seal, a dropping funnel, and a reflux condenser to which a nitrogen inlet and an oil bubbler are attached. The flask is charged with aluminum granules (2.7g, 0.1mol), mercuric chloride (0.1g), and iodine (0.1g), and then the apparatus is thoroughly flushed with dry nitrogen. Ether (65mL) and allyl bromide (fresh distilled, 10mL) are added successively under dropping funnel. The rest of allyl bromide (25mL) is slowly added at rate sufficient to maintain a gentle reflux. The mixture is stirred under refluxing condition to dissolve the aluminum completely.

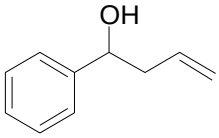
(2) Typical Experimental Procedure for the Allylation Reaction of Carbonyl Compounds: A typical experimental procedure is described for the allylation of benzaldehyde with triallylaluminum. To a stirred solution of benzaldehyde **1a** (1mmol) in ether (3 mL) was added triallylaluminum reagent **2** (0.4 mmol, 0.5M x 0.8 mL) rapidly at -78°C under nitrogen. The mixture was slowly warmed to 0°C during a period of 90 min. and quenched with ice cold dilute HCl at 0°C. The reaction mixture was extracted with Et_2O (3 x 25 mL) and the combined ether layers were dried over anhyd. $MgSO_4$, and evaporated under reduced pressure to obtain quantitative yield of **3a**. The crude product was passed through a small plug of silica to obtain pure **3a** as colorless oil in (98% Y). Similar procedure was adopted for the allylation of ketones except the amount of addition of triallylaluminum and stirred at 20°C during a period of 30 min.

(3) Typical Experimental Procedure for the Allylation Reaction of Imines:

A typical experimental procedure is described for the allylation of *N*-benzylidene aniline with triallylaluminum. To a stirred solution of *N*-benzylidene aniline **4a** (1mmol) in ether (3 mL) was added triallylaluminum reagent **2** (0.6 mmol, 0.5 M x 1.2 mL) rapidly at 20°C under nitrogen. The reaction mixture was stirred for 30 min. at the same temperature and quenched with ice cold dilute HCl. Then, it was extracted with Et_2O (3 x 25 mL) and the combined ether layers were dried over anhyd. $MgSO_4$, and evaporated under reduced pressure to obtain quantitative yield of **5a**. The mixture was passed through a small plug of silica to obtain the pure product **5a** as colorless oil in (98% Y). Similar procedure was adopted for the allylation of ketimines, except the amount of addition of triallylaluminum and stirred at 50°C and the reaction mixture was stirred for 1 h.

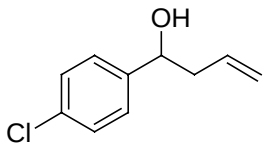
^{1}H and ^{13}C NMR data of 3a-3y

1-Phenyl-3-butene-1-ol (3a)



^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.99 (br, 1H), 2.49-2.57 (m, 2H), 4.75 (t, 1H, *J* = 5.32 Hz), 5.14-5.20 (m, 2H), 5.82-5.84 (m, 1H), 7.24-7.43 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 43.6, 73.2, 118.1, 125.7, 127.4, 128.3, 134.4, 143.8.; M.W. ($C_{10}H_{12}O$) 148; GC-MS (70 eV): 148 (1, M^+), 107 (100), 79 (86), 77 (50).

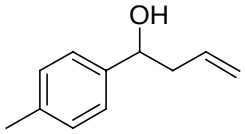
1-(4-chlorophenyl)-3-butene-1-ol (3b)



^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.43-2.48 (m, 2H), 4.65-4.68 (t, 1H, *J* = 7.24 Hz), 5.11-5.15 (m, 2H), 5.70-5.81 (m, 1H), 7.24-7.33 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 43.7, 72.5, 118.6, 127.1, 128.4, 133.0, 133.9, 142.2.; M.W.

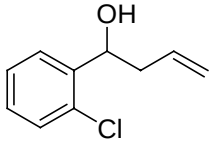
($C_{10}H_{11}ClO$) 182; GC-MS (70 ev): 182 (1, M^+), 141 (100), 113 (20), 77 (76).

1-(4-methylphenyl)-3-butene-1-ol (3c)



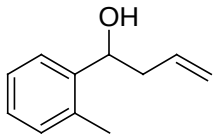
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.01 (br, 1H), 2.33 (s, 3H), 2.48-2.51 (m, 2H), 4.69 (t, 1H, *J* = 6.40 Hz), 5.11-5.17 (m, 2H), 5.75-5.80 (m, 1H), 7.14 (d, 2H, *J* = 7.80 Hz), 7.23 (d, 2H, *J* = 7.76 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.1, 43.8, 73.2 , 118.2, 125.7, 129.1, 134.6, 137.2, 140.9.; M.W. ($C_{11}H_{14}O$) 162; GC-MS (70 ev): 162 (1, M^+), 121 (100), 93 (51), 91 (49), 77 (34), 65 (13).

1-(2-chlorophenyl)-3-butene-1-ol (3d)



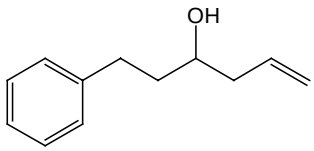
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.31-2.38 (m, 1H), 2.52-2.59 (m, 1H), 5.10-5.15 (m, 3H), 5.76-5.86 (m, 1H), 7.13-7.29(m, 3H), 7.51 (d, 1H, ^3J (H, H) = 7.72 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 41.9, 69.5, 118.5, 126.91, 127.00, 128.3, 129.2, 131.6, 134.1, 141.1.

1-(2-methylphenyl)-3-butene-1-ol (3e)



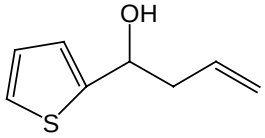
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.29 (s, 9H), 2.39-2.46 (m, 2H), 4.89-4.93 (m, 1H), 5.10-5.16 (m, 2H), 5.78-5.82 (m, 1H), 7.09-7.21 (m, 3H), 7.44 (d, 1H, *J* = 7.56 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 18.9, 42.4, 69.6, 118.0, 125.1, 126.1, 127.1, 130.2, 134.2, 134.6, 141.9.

1-Phenyl-5-hexene-3-ol (3f)



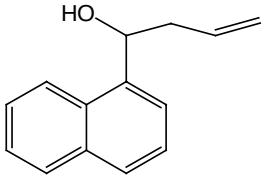
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.61 (br, 1H), 1.62-1.82 (m, 3H), 2.18-2.32 (m, 2H), 2.70-2.83 (m, 2H), 3.62-3.71 (m, 1H), 5.14-5.18 (m, 2H), 5.76-5.90 (m, 1H), 7.20-7.32 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 32.0, 38.4, 42.0, 69.9, 118.18, 125.8, 128.32, 128.36, 134.6, 142.0.; M.W. ($C_{12}H_{16}O$) 176; GC-MS (70 ev): 176 (1, M^+), 135 (21), 117 (29), 91 (100).

1-(2-thienyl)-3-butene-1-ol (3g)



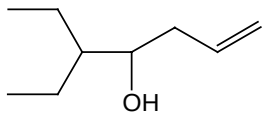
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.56 (dd, 2H, *J* = 7.84, 6.80 Hz), 4.88 (t, 1H, *J* = 6.52 Hz), 5.07-5.13 (m, 2H), 5.73-5.78 (m, 1H), 6.91 (m, 2H), 7.18 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 43.3, 69.2, 118.2, 123.5, 124.3, 126.4, 133.8, 147.7.; M.W. ($C_8H_{10}OS$) 154; GC-MS (70 ev): 154 (5, M^+), 113 (100), 85 (65), 45 (27).

1-(1-Naphthalenyl)-3-buten-1-ol (3h)



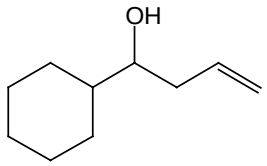
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.30 (br, 1H), 2.60-2.78 (m, 2H), 5.18-5.25 (m, 2H), 5.13 (m, 1H), 5.75-5.98 (m, 1H), 7.49-8.09 (m, 7H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 42.8, 69.9, 118.2, 122.79, 122.92, 125.4, 125.4, 125.9, 127.9, 128.9, 130.2, 133.7, 134.7, 139.4.; M.W. ($C_{14}H_{14}O$) 198; GC-MS (70 ev): 198 (6, M^+), 157 (96), 129 (100), 128 (58), 127 (33).

5-Ethyl-1-hepten-4-ol (3i)



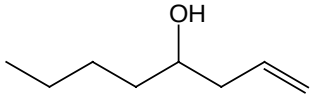
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.96 (t, 6H, *J* = 7.20 Hz), 1.19-1.24 (m, 4H), 1.52 (br, 1H), 2.18-2.34 (m, 2H), 5.07-5.15 (m, 2H), 5.83-5.94 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.9, 22.6, 41.5, 49.1, 76.3, 118.4, 134.2.; M.W. ($C_9H_{18}O$) 142; GC-MS (70 ev): 142 (1, M^+), 99 (44), 71 (100), 69 (60), 55 (18), 43 (64), 41 (56).

1-Cyclohexyl-3-buten-1-ol (3j)



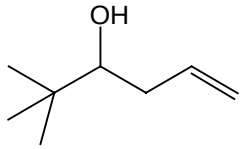
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.07-1.81 (m, 11H), 2.16-2.21 (m, 1H), 2.27-2.32 (m, 1H), 5.06-5.14 (m, 2H), 5.84-5.91 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.5, 26.7, 26.9, 41.1, 45.4, 75.0, 118.3, 134.1.; M.W. ($C_{10}H_{18}O$) 154; GC-MS (70 ev): 154 (1, M^+), 111 (51), 83 (100), 69 (33), 55 (46), 41 (47).

1-Octen-4-ol (3k)



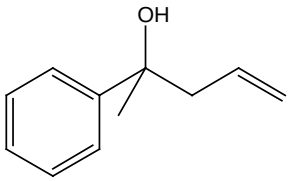
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.89 (t, 3H, *J* = 7.20 Hz), 1.27-1.45 (m, 6H), 2.13-2.25 (m, 2H), 2.47 (s, 1H), 3.59-3.62 (m, 1H), 5.07-5.12 (m, 2H), 5.77-5.84 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.0, 22.7, 27.8, 36.5, 42.0, 70.7, 117.9, 134.9.; M.W. ($C_8H_{16}O$) 154; GC-MS (70 ev): 128 (1, M^+), 85 (100), 69 (19), 57 (65), 41 (34).

2,2-Dimethylhex-5-en-3-ol (3l)



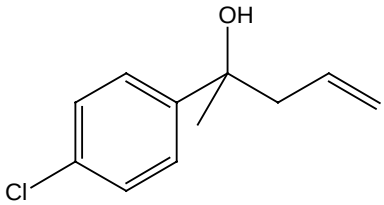
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.91 (s, 9H), 1.94-2.03 (m, 1H), 2.33-2.38 (m, 1H), 3.23-3.27 (m, 1H), 5.11-5.16 (m, 2H), 5.82-5.87 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 25.7, 34.6, 36.5, 78.1, 117.7, 136.6.

2-Phenyl-4-penten-2-ol (3m)



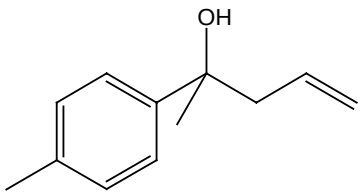
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.56 (s, 3H), 1.86 (br, 1H), 2.49-2.54 (m, 1H), 2.68-2.73 (m, 1H), 5.12-5.17 (m, 2H), 5.62-5.65 (m, 1H), 7.24 (t, 1H, *J* = 7.52 Hz), 7.35 (t, 2H, *J* = 7.40 Hz), 7.45 (d, 2H, *J* = 7.40 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 30.0, 48.4, 73.6, 119.4, 124.7, 126.6, 128.2, 133.7, 147.6. ; M.W. ($C_{11}H_{14}O$) 162; GC-MS (70 ev): 162 (1, M^+), 121 (100), 105 (18), 77 (19), 43 (59).

2-(4-Chlorophenyl)-4-penten-2-ol (3n)



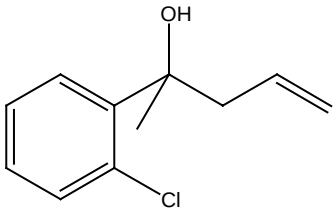
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.53 (s, 3H), 2.27 (br, 1H), 2.45-2.51 (m, 1H), 2.61-2.66 (m, 1H), 5.10-5.14 (m, 2H), 5.57-5.64 (m, 1H), 7.28 (d, 2H, *J* = 8.60 Hz), 7.36 (d, 2H, *J* = 8.60 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 29.7, 48.3, 73.3, 119.6, 126.3, 128.1, 132.3, 133.2, 146.1.; M.W. ($C_{11}H_{13}ClO$) 196; GC-MS (70 ev): 196 (1, M^+), 155 (89), 43 (100).

2-(4-Methylphenyl)-4-penten-2-ol (3o)



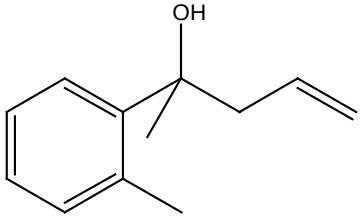
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.55 (s, 3H), 2.05 (br, 1H), 2.36 (s, 3H), 2.50-2.54 (m, 1H), 2.67-2.72 (m, 1H), 5.12-5.17 (m, 2H), 5.60-5.68 (m, 1H), 7.17 (d, 2H, *J* = 8.24 Hz), 7.35 (d, 2H, *J* = 8.24 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.9, 29.9, 48.4, 73.5, 119.2, 124.7, 128.8, 133.8, 136.1, 144.7. ; M.W. ($C_{12}H_{16}O$) 176; GC-MS (70 ev): 176 (1, M^+), 135 (70), 91 (15), 43 (100).

2-(2-Chlorophenyl)-4-penten-2-ol (3p)



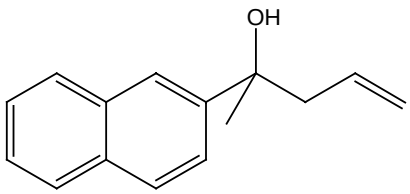
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.72 (s, 3H), 2.66 (dd, 1H, *J* = 14.00, 8.40 Hz), 2.70 (br, 1H), 3.22 (dd, 1H, *J* =14.00, 6.40 Hz), 5.07-5.15 (m, 2H), 5.10-5.14 (m, 2H), 5.52-5.61 (m, 1H), 7.18 (t, 1H, *J* = 7.50 Hz), 7.26 (t, 1H, *J* = 7.60 Hz), 7.36 (d, 1H, *J* = 7.80 Hz), 7.36 (d, 1H, *J* =7.80 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 27.2, 45.1, 74.2, 119.1, 126.7, 127.9, 128.2, 130.7, 131.2, 134.6, 143.6.

2-(2-Methylphenyl)-4-penten-2-ol (3q)



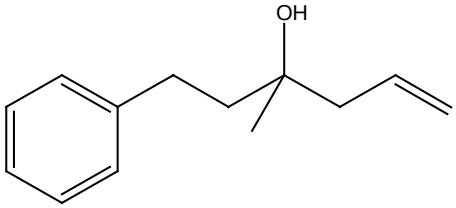
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.57 (s, 3H), 2.17 (br, 1H), 2.54 (dd, 1H, *J* = 13.20, 8.50 Hz), 2.53 (s, 3H), 2.81 (dd, 1H, *J* = 13.90, 6.60 Hz), 5.06-5.12 (m, 2H), 5.59-5.64 (m, 1H), 7.11-7.13 (m, 3H), 7.40 (d, 1H, *J* = 8.20 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 22.3, 28.8, 46.5, 74.7, 119.0, 125.5, 125.9, 126.8, 132.5, 133.9, 135.2, 144.4.

2-(2-Naphthyl)-4-penten-2-ol (3r)



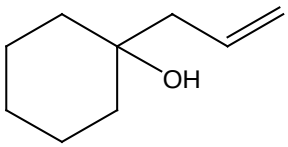
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.66 (s, 3H), 2.15 (br, 1H), 2.59-2.64 (m, 1H), 2.80-2.85 (m, 1H), 5.12-5.16 (m, 2H), 5.16-5.21 (m, 1H), 7.47-7.58 (m, 3H), 7.59-7.84 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 29.9, 48.3, 73.8, 119.6, 123.2, 123.5, 125.7, 126.0, 127.4, 127.9, 128.1, 132.2, 133.1, 133.6, 145.0; M.W. ($C_{15}H_{16}O$) 212; GC-MS (70 ev): 212 (1, M^+), 171 (49), 127 (28), 43 (100).

3-Methyl-1-phenyl-5-hexen-3-ol (3s)



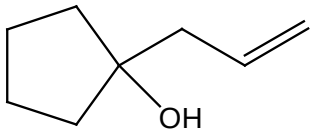
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.29 (s, 3H), 1.71 (br, 1H), 1.79-1.84 (m, 2H), 2.33 (d, 2H, J = 7.44 Hz), 2.72-2.77 (m, 2H), 5.17-5.22 (m, 2H), 5.90-5.97 (m, 1H), 7.21-7.35 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.7, 30.2, 43.6, 46.4, 71.9, 118.7, 125.7, 128.24, 128.32, 133.8, 142.4.; M.W. ($C_{13}H_{18}O$) 190; GC-MS (70 ev): 190(1, M^+), 149 (46), 131 (17) 91 (100), 43 (18).

1-Allylcyclohexanol (3t)



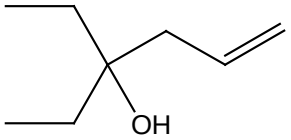
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.26-1.62 (m, 10H), 2.21 (d, 2H, J = 7.52 Hz), 5.09-5.17 (m, 2H), 5.86-5.93 (m, 1H). ^{13}C NMR (100MHz, $CDCl_3$): δ 22.2, 25.8, 37.4, 46.7, 70.9, 118.6, 133.7.; M.W. ($C_9H_{16}O$) 140;GC-MS (70 ev): 140 (1, M^+), 99 (100), 81 (91), 55 (42), 41 (29).

1-Allylcyclopentanol (3u)



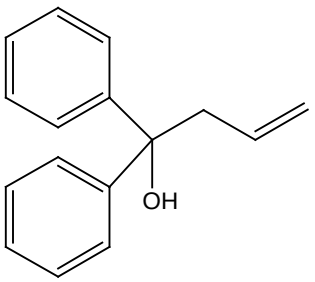
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.56-1.76 (m, 9H), 2.35 (d, 2H, *J* = 7.60 Hz), 5.12-5.16 (m, 2H), 5.85-5.95 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 23.8, 39.3, 45.8, 81.3, 118.4, 134.5.; M.W. ($C_8H_{14}O$) 126; GC-MS (70 ev): 126 (1, M^+), 85 (100), 67 (64), 55 (37), 41 (27).

3-Ethyl-5-hexen-3-ol (3v)



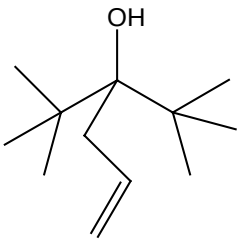
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 0.88 (t, 6H, *J* = 7.52 Hz), 1.48 (q, 4H, *J* = 7.72 Hz), 2.2 (d, 2H, *J* = 7.40 Hz), 5.12-5.15 (m, 2H), 5.81-5.88 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 7.7, 30.9, 42.9, 74.2, 118.4, 134.0.; M.W. ($C_8H_{16}O$) 128;GC-MS (70 ev): 128 (1, M^+), 99 (19), 87 (100), 69 (30), 57 (100), 45 (47), 41 (23).

1,1-Diphenyl-3-buten-1-ol (3w)



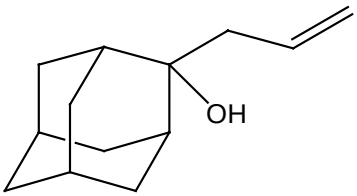
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.55 (br , 1H), 3.04 (d, 2H, *J* = 7.80 Hz), 5.12-5.23 (m, 2H), 5.61-5.66 (m, 1H), 7.17 (t, 2H, *J* = 7.76 Hz), 7.28 (t, 4H, *J* = 7.36 Hz), 7.44 (d, 4H, *J* = 8.20 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 46.6, 76.8, 120.4, 125.9, 126.8, 128.1, 133.4, 146.5.; M.W. ($C_{16}H_{16}O$) 224; GC-MS (70 ev): 224 (1, M^+), 183 (76), 105 (100), 77 (62), 51 (10).

3-*tert*-Butyl-2,2-dimethylhex-5-en-3-ol (3x)

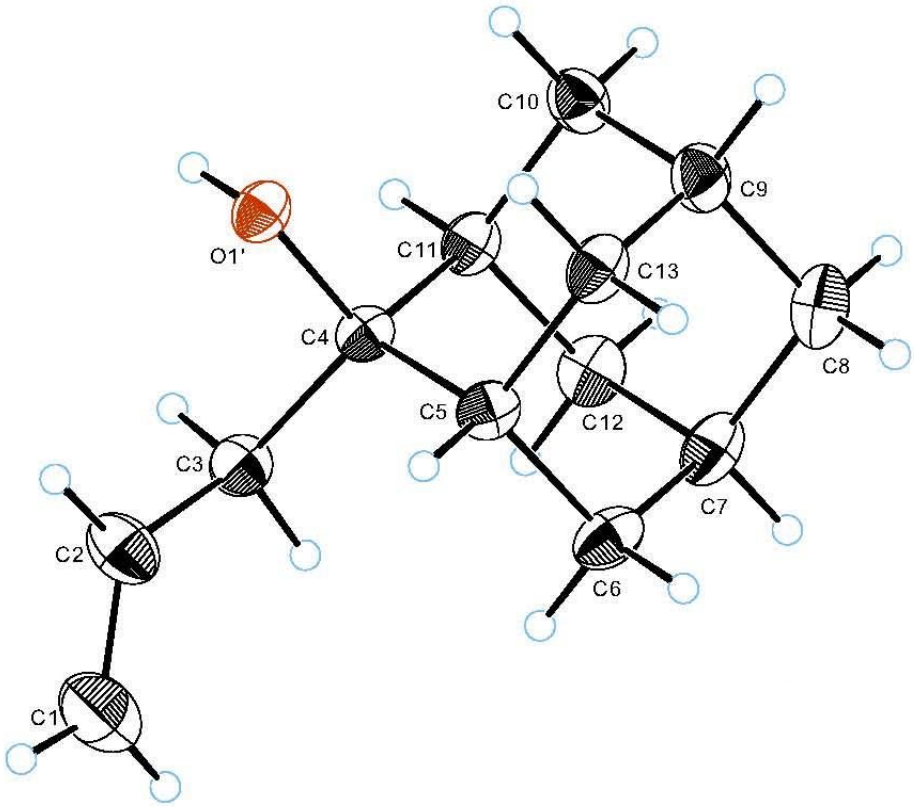


^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.07 (s, 18H), 2.46 (d, 2H, *J* = 7.52 Hz), 5.06-5.15 (m, 2H), 5.89-5.97 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 28.7, 37.9, 42.3, 78.9, 118.5, 137.2.

1-Adamantyl-3-buten-1-ol (3y)

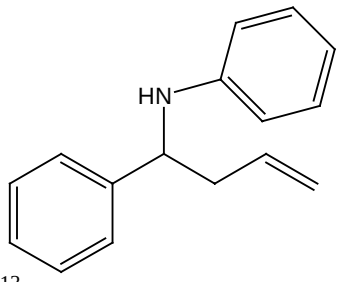


White solid, Mp: 46-48 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.50 (d, 2H, *J* = 12.20 Hz), 1.67-1.88 (m, 11H), 2.17 (d, 2H, *J* = 12.40 Hz), 2.42 (d, 2H, *J* = 7.52 Hz), 5.10-5.16 (m, 2H), 5.84-5.91 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 27.2, 27.3, 32.8, 34.3, 36.9, 38.3, 42.6, 74.4, 118.6, 133.6. IR (neat) ν 3400, 3071, 2904, 2858, 2666, 1638, 1455, 1370, 1356, 1281, 1233, 1183, 1140, 1130, 1099, 1041, 1026, 992, 908, 864, 732 cm^{-1}.; M.W. ($C_{13}H_{20}O$) 192; GC-MS (70 ev): 192 (1, M^+), 151 (100), 133 (12), 107 (14), 91 (18), 79 (14). Elemental analysis calcd for $C_{13}H_{20}O$: C, 81.20; H, 10.48; Found: C: 81.03; H, 10.45.


C10
C9
O1'
C11
C13
C4
C8
C5
C12
C3
C7
C2
C6
C1

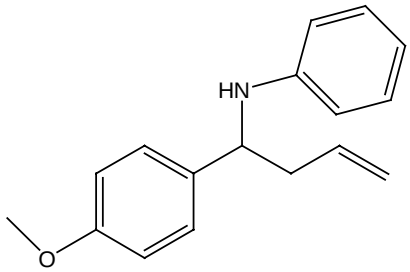
^{1}H and ^{13}C NMR data of 5a-5r

4-(*N*-Phenyl)amino-4-phenyl-1-butene (5a)



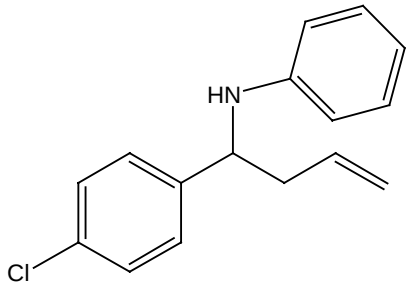
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.60-2.80 (m, 2H), 4.18-4.40 (br, 1H), 4.55 (t, 1H, *J* = 5.40 Hz), 5.29-5.36 (m, 2H), 5.89-5.96 (m, 1H), 6.67-6.69 (d, 2H, *J* = 8.32 Hz), 6.82 (t, 1H, *J* = 7.32 Hz), 7.25 (t, 2H, *J* = 7.88 Hz), 7.37-7.53 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 43.1, 57.1, 113.5, 117.4, 118.2, 126.2, 126.9, 128.5, 129.0, 134.5, 143.4, 147.1.; M.W. ($C_{16}H_{17}N$) 223 ; GC-MS (70 ev): 223 (1, M^+), 196 (54), 91 (100), 65 (10).

4-(*N*-Phenyl)amino-4-(4-methoxyphenyl)-1-butene (5b)



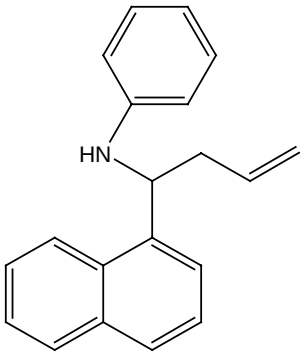
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.47-2.53 (m, 2H), 3.72 (s, 3H), 4.05-4.19 (br, 1H), 4.29 (dd, 1H, *J* = 7.32, 5.92 Hz), 5.09-5.16 (m, 2H), 5.25-5.40 (m, 1H), 6.49 (d, 2H, *J* = 8.40 Hz), 6.63 (t, 1H, *J* = 7.28 Hz), 6.83 (d, 2H, *J* = 8.60 Hz), 7.06 (t, 2H, *J* = 8.52 Hz), 7.25 (d, 2H, *J* = 8.60 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 43.2, 55.1, 56.6, 113.5, 113.9, 117.3, 118.1, 127.3, 128.9, 134.6, 135.3, 147.2, 158.5.; M.W. ($C_{17}H_{19}NO$) 253 ; GC-MS (70 ev): 253 (1, M^+), 212 (100), 104 (24), 77 (28).

4-(*N*-Phenyl)amino-4-(4-chlorophenyl)-1-butene (5c)



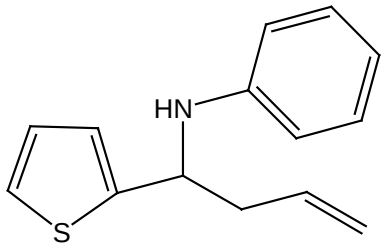
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.57-2.66 (m, 2H), 4.05-4.15 (br, 1H), 4.48 (dd, 1H, *J* = 7.84, 5.20 Hz), 5.27-5.30 (m, 2H), 5.78-5.92 (m, 1H), 6.60 (d, 2H, *J* = 8.40 Hz), 6.86 (t, 1H, *J* = 7.72 Hz), 7.22 (t, 2H, *J* = 7.72 Hz) 7.41 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 43.0, 56.5, 113.4, 117.6, 118.5, 127.6, 128.6, 129.0, 132.4, 134.1, 142.0, 146.9.; M.W. ($C_{16}H_{16}ClN$) 257 ; GC-MS (70 ev): 257 (1, M^+), 216 (100), 104 (20), 77 (35).

4-(*N*-Phenyl)amino-4-(1-naphtyl)-1-butene (5d)



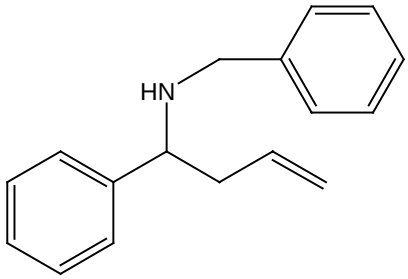
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.46-2.51 (m, 1H), 2.73-2.79 (m, 1H), 4.06-4.22 (br, 1H), 5.09-5.18 (m, 2H), 5.74-5.78 (m, 1H), 6.42 (d, 2H, *J* = 7.80 Hz), 6.60 (t, 1H, *J* = 7.80 Hz), 6.98 (t, 2H, *J* = 7.60 Hz), 7.42 (t, 1H, *J* = 7.60 Hz), 7.42-7.48 (m, 2H), 7.59 (d, 1H, *J* = 7.12 Hz), 7.65 (d, 1H, *J* = 8.20 Hz), 7.80 (d, 1H, *J* = 8.40 Hz), 8.10 (d, 1H, *J* = 8.40 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 41.5, 52.9, 113.3, 117.3, 118.2, 122.2, 123.1, 125.1, 125.7, 126.0, 127.4, 129.0, 129.2, 130.5, 134.1, 134.7, 137.9, 147.0.; M.W. ($C_{20}H_{19}N$) 273 ; GC-MS (70 ev): 273 (1, M^+), 232 (100), 104 (32), 77 (31).

4-(*N*-Phenyl)amino-4-(2'-thienyl)-1-butene (5e)



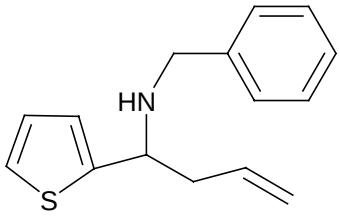
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.70-2.77 (m, 2H), 2.76 (t, 1H, *J* = 6.80 Hz), 4.86 (br, 1H), 5.13-5.20 (m, 2H), 5.76-5.79 (m, 1H), 6.71-7.66 (m, 8H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 42.9, 53.3, 113.5, 117.8, 118.5, 123.3, 123.6, 126.7, 129.0, 133.9, 146.9, 148.5.; M.W. ($C_{14}H_{15}NS$) 229 ; GC-MS (70 ev): 229 (5, M^+), 188 (100), 104 (28) 77 (26).

4-(*N*-Benzyl)amino-4-phenyl-1-butene (5f)



^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.51-2.58 (m, 2H), 3.60 (d, 1H, *J* = 13.32 Hz), 3.78-3.83 (m, 2H), 5.14-5.21 (m, 2H), 5.77-5.87 (m, 1H), 7.21-7.48(m, 10H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 43.0, 51.3, 61.5, 117.5, 126.7, 127.0, 127.2, 128.0, 128.23, 128.30, 135.3, 140.4, 143.6.; M.W. ($C_{17}H_{19}N$) 237 ; GC-MS (70 ev): 237 (1, M^+), 196 (46), 91 (100), 65 (10).

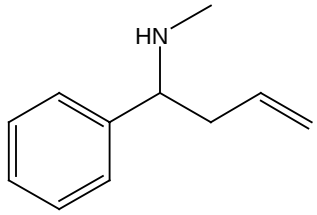
4-(*N*-Benzyl)amino-4-(2-thienyl)-1-butene (5g)



^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.89 (br, 1H), 2.46-2.48 (m, 2H), 3.57(d, 1H, *J* = 13.32 Hz), 3.76 (d, 1H, *J* = 13.32 Hz), 3.97(t, 1H, *J* = 6.72 Hz), 5.02-5.09 (m, 2H), 5.64-5.75 (m, 1H), 6.89-6.92 (m, 2H), 7.17-7.29 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 43.3, 51.1, 56.9, 117.8, 123.9, 124.0, 126.2, 126.8, 128.0, 128.2 134.7, 140.1, 148.8.; M.W. ($C_{15}H_{17}NS$) 243 ;

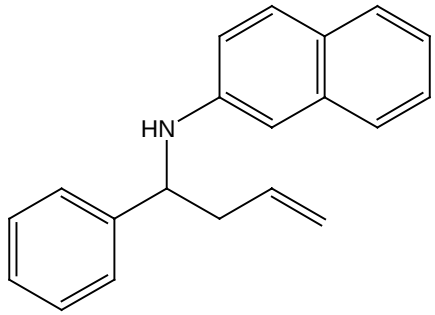
GC-MS (70 ev): 243 (1, M^+), 202 (86), 91 (100).

4-(*N*-Methyl)amino-4-phenyl-1-butene (5h)



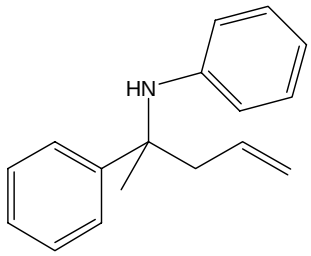
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.91 (br, 1H), 2.28 (s, 3H), 2.42-2.45 (m, 2H), 3.54 (t, 1H, *J* = 6.92 Hz), 5.03-5.11 (m, 2H), 5.68-5.75 (m, 1H), 7.25-7.35 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 34.3, 42.5, 64.6, 117.6, 127.11, 127.22, 128.4, 135.2, 143.0

4-(*N*-1-Naphtyl)amino-4-phenyl-1-butene (5i)



^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.59-2.71 (m, 2H), 4.53 (m, 1H), 5.17-5.29 (m, 2H), 5.74-5.84 (m, 1H), 6.30 (d, 1H, *J* = 6.92 Hz), 7.09-7.43 (m, 9H), 7.71-7.76 (m, 1H), 7.86-7.90 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 43.4, 56.7, 106.1, 117.2, 118.5, 119.6, 123.4, 124.6, 125.5, 126.1, 126.5, 126.9, 128.5, 128.7, 134.2, 134.7, 142.0, 143.1.; M.W. ($C_{20}H_{19}N$) 273 ; GC-MS (70 ev): 273 (8, M^+), 232 (100), 127 (23).

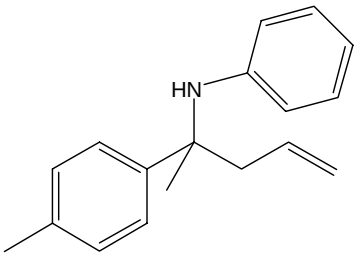
***N*-(1-Methyl-1-phenyl-3-butenyl)aniline (5j)**



^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.85 (s, 3H), 2.70-2.76 (m, 1H), 2.81-2.87 (m, 1H), 5.29-5.34 (m, 2H), 5.86-5.93 (m, 1H), 6.52 (d, 2H, ^3J (H, H) = 8.52 Hz), 6.80 (t, 1H, *J* =

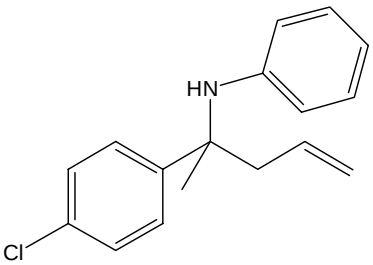
7.20 Hz), 7.18 (t, 2H, J = 7.60 Hz), 7.41 (t, 1H, J = 7.80 Hz), 7.51 (t, 2H, ^3J = 7.60 Hz), 7.67 (t, 2H, J = 8.20 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 25.5, 48.6, 57.4, 115.3, 117.0, 119.2, 125.9, 126.3, 128.3, 128.6, 133.4, 145.7, 146.4.; M.W. ($C_{17}H_{19}N$) 237 ; GC-MS (70 ev): 237 (7, M^+), 196 (100), 118 (16), 77 (57).

_N_-[1-Methyl-1-(4-methylphenyl)-3-butenyl]aniline (5k)



^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.66 (s, 3H), 2.35 (s, 3H), 2.52-2.57 (m, 1H), 2.63-2.68 (m, 1H), 5.12-5.17 (m, 2H), 5.71-5.74 (m, 1H), 6.32 (d, 2H, J = 8.00 Hz), 6.62 (t, 1H, J = 7.32 Hz), 7.01 (t, 2H, J = 7.32 Hz), 7.16 (d, 2H, J = 7.80 Hz), 7.37 (d, 2H, J = 8.12 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.9, 25.6, 48.7, 57.3, 115.4, 117.0, 119.1, 125.9, 128.6, 129.1, 133.6, 135.8, 143.5, 145.9. IR (neat) ν 3411, 3053, 3020, 2976, 2923, 2857, 1638, 1602, 1498, 1454, 1429, 1374, 1306, 1289, 1257, 1185, 1155, 1019, 997, 816, 750, 695, 666 cm^{-1}.; M.W. ($C_{18}H_{21}N$) 251 ; GC-MS (70 ev): 251 (1, M^+), 210 (100), 118 (23), 91 (11), 77 (35). HRMS calcd for $C_{18}H_{21}N$ [M^+] 251.1674, found 251.1673.

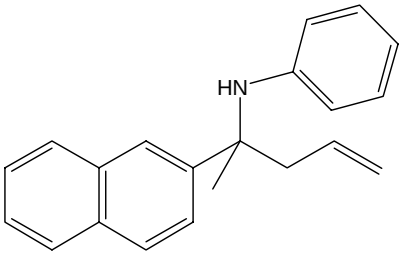
_N_-[1-Methyl-1-(4-chlorophenyl)-3-butenyl]aniline (5l)



^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.80 (s, 3H), 2.64-2.69 (m, 1H), 2.75-2.80 (m, 1H), 4.20 (br, 1H), 5.27-5.33 (m, 1H), 5.81-5.87 (m, 1H), 6.50 (d, 2H, J = 8.12 Hz), 6.81 (t, 1H, J = 7.20 Hz), 7.18 (t, 2H, J = 7.72 Hz), 7.46 (d, 2H, J = 8.40 Hz), 7.58 (d, 2H, J = 8.40 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 25.4, 48.6, 57.3, 115.4, 117.4, 119.5, 127.5, 128.5, 128.7, 132.1, 133.0, 145.0, 145.4. IR (neat) ν 3412, 3076, 3054, 2977, 2927, 2855, 1638, 1602, 1497, 1457, 1428, 1398,, 1375, 1318,

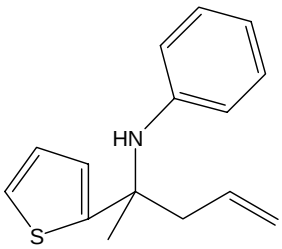
1309, 1289, 1256, 1214, 1181, 1155, 1094, 1012, 997, 921, 877, 831, 750, 695, 666 cm^{-1}.; M.W. ($C_{17}H_{18}ClN$) 271 ; GC-MS (70 ev): 271 (1, M^+), 230 (100), 77 (38). HRMS calcd for $C_{17}H_{18}ClN$ [M^+] 271.1128, found 271.1128.

***N*-(1-Methyl-1-naphtyl -3-butenyl)aniline (5m)**



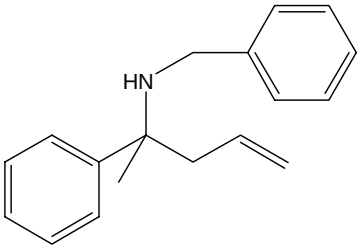
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.73 (s, 3H), 2.62-2.67 (m, 1H), 2.68-2.73 (m, 1H), 4.18 (br, 1H), 5.10-5.17 (m, 2H), 5.64-5.74 (m, 1H), 6.36 (d, 2H, *J* = 7.82 Hz), 6.58 (t, 1H, *J* = 7.82 Hz), 6.94 (t, 2H, *J* = 8.20 Hz), 7.40-7.46 (m, 2H), 7.65-7.83 (m, 4H), 7.86 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 25.5, 48.5, 57.7, 115.5, 117.3, 119.3, 124.3, 124.8, 125.6, 125.8, 127.4, 128.1, 128.2, 128.7, 132.2, 133.38, 133.43, 144.4, 145.8. IR (neat) ν 3408, 3055, 3016, 2976, 2925, 2854, 1710, 1678, 1637, 1602, 1497, 1428, 1376, 1318, 1307, 1272, 1181, 1155, 1129, 996, 916, 857, 820, 749, 694, 666 cm^{-1}.; M.W. ($C_{21}H_{21}N$) 287 ; GC-MS (70 ev): 287 (6, M^+), 246 (100), 118 (20), 77 (16). HRMS calcd for $C_{21}H_{21}N$ [M^+] 287.1674, found 287.1677.

***N*-(1-Methyl-1-thienyl -3-butenyl)aniline (5n)**



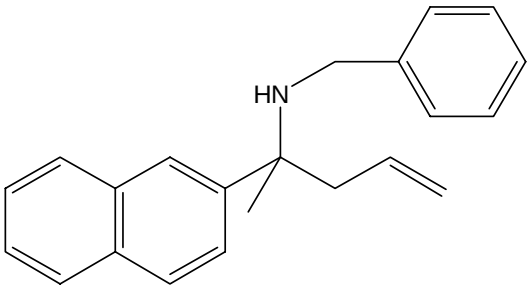
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.67 (s, 3H), 2.58 (dd, 2H, *J* = 13.72, 7.00 Hz), 2.76 (dd, 2H, *J* = 13.72, 7.64 Hz), 5.10-5.16 (m, 2H), 5.68-5.78 (m, 1H), 6.44 (d, 2H, ^3J (H, H) = 7.72 Hz), 6.65 (t, 1H, *J* = 7.40 Hz), 6.68-6.93 (m, 2H), 7.03 (t, 2H, *J* = 8.40 Hz), 7.17-7.19 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.6, 48.9, 56.8, 115.9, 118.0, 119.5, 122.8, 124.4, 126.6, 128.6, 133.0, 145.4, 153.3.; M.W. ($C_{15}H_{17}NS$) 243 ; GC-MS (70 ev): 243 (1, M^+), 202 (100), 151 (36), 118 (33), 77 (43).

***N*-(1-Methyl-1-phenyl -3-butenyl)benzylamine (5o)**



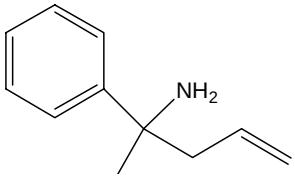
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.51 (s, 3H), 2.54 (m, 2H), 3.44 (d, 1H, *J* = 12.44 Hz), 3.54 (d, 1H, *J* = 12.44 Hz), 5.02-5.08 (m, 2H), 5.60-5.70 (m, 1H), 7.14-7.35 (m, 10H), 7.50 (d, 2H, *J* = 7.60 Hz). ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 25.5, 46.9, 47.3, 58.4, 118.2, 126.3, 126.67, 126.71, 128.10, 128.12, 128.24, 134.1, 141.0, 146.4.; M.W. ($C_{18}H_{21}N$) 251 ; GC-MS (70 ev): 251 (1, M^+), 210 (56), 91 (100).

***N*-(1-Methyl-1-naphtyl -3-butenyl)benzylamine (5p)**



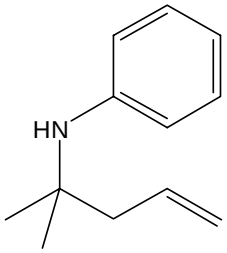
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.61 (s, 3H), 2.63 (m, 2H), 3.43 (d, 1H, *J* = 12.44 Hz), 3.56 (d, 1H, *J* = 12.44 Hz), 5.03-5.11 (m, 2H), 5.64-5.68 (m, 1H), 7.13-7.45 (m, 7H), 7.71-7.87 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 25.4, 47.04, 47.10, 58.5, 118.3, 124.9, 125.0, 125.6, 125.8, 126.7, 127.4, 127.9, 128.03, 128.13, 128.3, 132.2, 133.2, 134.1, 141.1, 144.0. IR (neat) ν 3434, 3059, 3027, 2963, 2924, 2852, 1682, 1638, 1600, 1504, 1495, 1453, 1374, 1275, 1188, 1157, 1129, 1028, 996, 914, 858, 819, 747, 698, 666 cm^{-1}.; M.W. ($C_{22}H_{23}N$) 301 ; GC-MS (70 ev): 301 (1, M^+), 260 (64), 91 (100). HRMS calcd for $C_{22}H_{23}N$ [M^+] 301.1830, found 301.1837.

***N*-(1,1-Diphenyl-3-butenyl)amine (5q)**



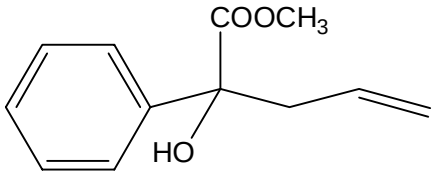
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.01 (d, 2H, *J* = 7.12Hz), 5.05-5.15 (m, 2H), 5.48-5.54 (m, 1H), 7.17 (t, 2H, *J* = 7.20 Hz), 7.26 (t, 4H, *J* = 7.52 Hz), 7.34 (d, 4H,*J* = 7.32 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 47.2, 60.0, 118.9, 126.1, 126.3, 127.9, 133.9, 147.9.; M.W. ($C_{16}H_{17}N$) 223 ; GC-MS (70 ev): 223 (1, M^+), 182 (100), 104 (47), 77 (21).

_N_-(1,1-Dimethyl-3-butenyl)aniline (5r)



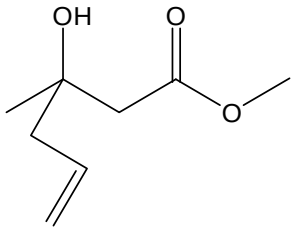
^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.30 (s, 6H), 2.36 (d, 2H, *J* = 7.40 Hz), 5.06-5.11 (m, 2H), 5.06-5.12 (m, 1H), 6.72-6.75 (m, 3H), 7.14 (t, 2H, *J* = 7.80 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 27.9, 46.4, 53.5, 117.4, 118.20, 118.32, 128.9, 134.4, 146.5.; M.W. ($C_{12}H_{17}N$) 175 ; GC-MS (70 ev): 175 (1, M^+), 134 (100), 77 (17).

Methyl 2-hydroxy-2-phenyl-4-pentenoate (8)



^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 2.77-2.81 (m, 1H), 2.96-3.01 (m, 1H), 3.72 (br, 1H), 3.76 (s, 3H), 5.14-5.17 (m, 2H), 5.80-5.82 (m, 1H), 7.27-7.82 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 44.1, 53.2, 78.1, 119.4, 125.5, 127.8, 128.3, 132.3, 141.2, 175.0.; M.W. ($C_{12}H_{14}O_3$) 206 ; GC-MS (70 ev): 206 (1, M^+), 165 (38), 105 (100), 77 (62).

Methyl 3-hydroxy-3-methyl-4-pentenoate (9)



^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 1.21 (s, 3H), 2.27 (d, 1H, *J* = 7.40 Hz), 2.39 (d, 1H, *J* = 15.72 Hz), 2.48 (d, 2H, *J* = 15.72 Hz), 3.68 (s, 3H), 4.95-5.04 (m, 2H), 5.70-5.82 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.7, 44.1, 46.4, 51.5, 70.6, 118.5, 133.5, 173.2.

Known compound citation:

3a: Beilstein Registry Number 2041385
3b: Beilstein Registry Number 2248797
3c: Beilstein Registry Number 2081243
3d: Beilstein Registry Number 2517528
3e: Beilstein Registry Number 2516390
3f: Beilstein Registry Number 1945694
3g: Beilstein Registry Number 111306
3h: Beilstein Registry Number 3251180
3i: Beilstein Registry Number 2233536
3j: Beilstein Registry Number 2432335
3l: Beilstein Registry Number 2036814
3k: Beilstein Registry Number 1700555
3m: Beilstein Registry Number 1363772
3n: Beilstein Registry Number 8679877
3o: Beilstein Registry Number 2517145
3q: Beilstein Registry Number 9323955
3r: Beilstein Registry Number 3248617
3s: Beilstein Registry Number 3236095
3t: Beilstein Registry Number 1561190
3u: Beilstein Registry Number 2038481
3v: Beilstein Registry Number 1742557
3w: Beilstein Registry Number 2097128
3x: Beilstein Registry Number 1750945
5a: Beilstein Registry Number 3265955
5b: Beilstein Registry Number 7481271
5c: Beilstein Registry Number 7478787
5d: Beilstein Registry Number 9333330
5e: Beilstein Registry Number 7807468
5f: Beilstein Registry Number 3608800
5g: Beilstein Registry Number 9764844
5h: Beilstein Registry Number 2828878
5i: Beilstein Registry Number 8773685
5j: Beilstein Registry Number 7807446
5n: Beilstein Registry Number 7477793
5o: Beilstein Registry Number 3609675
5q: Beilstein Registry Number 9621021
5r: Beilstein Registry Number 5497124
8: Beilstein Registry Number 4249285
9: Beilstein Registry Number 6693726

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 4296

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Calculated Reported
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Hall group -P 1 ?
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Mr 192.29 192.29
Dx,g cm-3 1.128 1.128
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Tmin' 0.971
Correction method= 'MULTI-SCAN'
Data completeness= Ratio = 1.00 Theta(max)= 24.99
R(reflections)= 0.0599(4404) wR2(reflections)= 0.1955(7957)
S = 0.993 Npar= 506

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT027_ALERT_3_B _diffrn_reflns_theta_full (too) Low ..... 24.99 Deg.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C33 - C34 .. 7.14 su
PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for C34

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without