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Supporting Information

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Copper-Catalyzed Asymmetric Conjugate Addition of Aryl Aluminum Reagents to Trisubstituted Enones: Construction of Aryl-Substituted Quaternary Chiral Centers

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General. ^{1}H (400 MHz or 300 MHz) and ^{13}C (100 MHz or 75 MHz) NMR spectra were recorded in $CDCl_3$ and chemical shifts are given in ppm relative to residual $CHCl_3$. Evolution of reaction was followed by GC-MS Hewlett Packard (EI mode) HP6890-5973. Optical rotations were measured at 25°C in a 10 cm cell in the stated solvent; $[\alpha]_D$ values are given in 10^{-1} deg cm^2 g^{-1} (concentration c given as g/100 mL). Enantiomeric excesses were determined by chiral-GC (capillary column, 10 psi H_2) or chiral Super Fluid Chromatography (SFC) with an appropriate program using a gradient of methanol. Temperature programs for chiral GC are described as follows: initial temperature (°C)-initial time (min)–temperature gradient (°C/min)–final temperature (°C)-final time (min) or initial temperature (°C)-initial time (min)–temperature gradient (°C/min)– temperature (°C)-time (min)-temperature gradient (°C/min)-final temperature(°C)-final time. Retention times (R_T) are given in min. Programs for chiral SFC are described as follows: initial methanol concentration (%)–initial time (min)–methanol gradient (%/min)–final methanol concentration. Flash chromatographies were performed using silica gel 32-63 μm, 60 Å and a pentane-diethylether mixture as eluent.
All reactions were carried out under inert atmosphere. All solvents were dried on alumina columns and degassed before use. 3-methyl cyclohex-2-en-1-one is commercially available (Acros) and was used without further purification. Diethylaluminum chloride (1 M in hexanes) was purchased from Aldrich and used as received. *n*-Butyllithium (1.6 M in hexanes) was purchased from Acros and used as received. Phenyllithium (2M in dibutylether) was purchased from Acros and used as received. Copper(I)-thiophene-2-carboxylate was purchased from Frontier Scientific and used as received. Phosphoramidite ligands were synthesized according to known procedures.[1]

Typical procedure for product synthesis (2-11): The aryl iodide (1,05 mmol) was dissolved in diethylether (0,5 mL) in a flame-dried flask and the solution was cooled to -55°C before the addition of *n*-BuLi (3.15 mmol, 656 μL, 1.6M in hexanes). The mixture was stirred for 30 min at -55°C. Then, Et_2AlCl (1.05 mmol, 1.05 mL, 1M in hexanes) was added dropwise and stirred between -50 and -20°C for 30 min. In a separate flame-dried two-necked flask, the copper salt (10 mol%), the ligand (11 mol%) and Et_2O (1.5 mL) were stirred thoroughly at room temperature for 30 min. The flask was cooled to -30°C and the aluminium compound including the salts (3 eq) was taken up by a syringe and added to the copper/ligand mixture, which lead to an orange color instantly in most cases. (In the reactions where only the supernatant was employed, the suspension of alane and salts was left without stirring until the salts precipitated.) The mixture was stirred for 5 min before the addition of 3-methyl-2-cyclohexen-1-one (0.35 mmol, 39.6 μL). The reaction generally turned yellow and was stirred for 5 hours at -30°C before it was quenched with 10% HCl (20 mL). Et_2O was added (20 mL) and the layers were separated. The aqueous phase was extracted one more time with Et_2O (20 mL). The combined organic phases were extracted once with NaOH (1M, 20 mL) and once with H_2O (20 mL). The organic layers were combined and dried over $MgSO_4$. The solution was then filtered over silica, and then concentrated in vacuo. The crude was purified

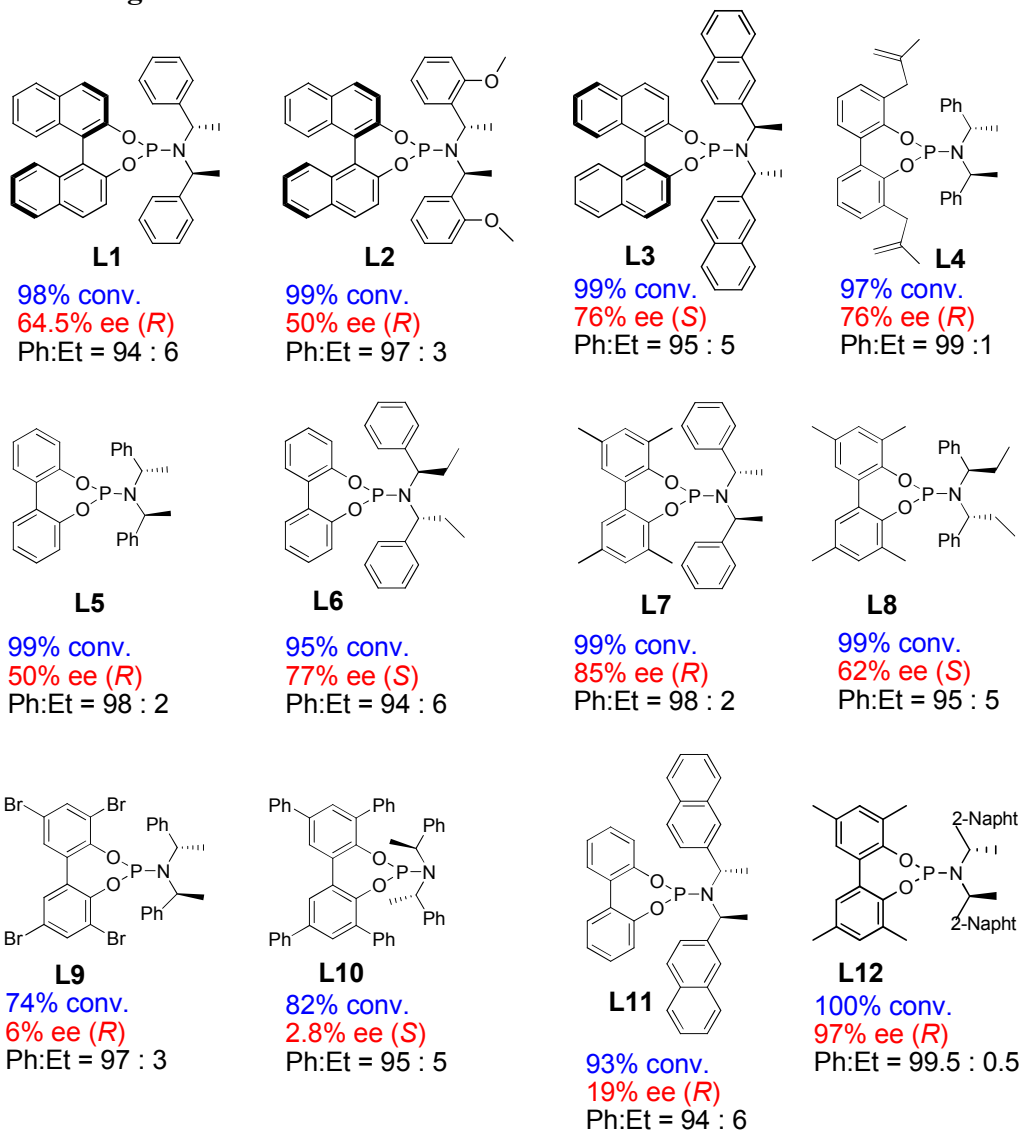
[1] Polet D.; Rosset S.; March S.; Alexakis A. *J. Org. Chem.* **2004**, *69*, 5660-5667.

by flash chromatography on a silica column with pentane:Et_2O 9:1 or 8:2 to give the pure product.

For the synthesis of product **12**, the reaction was left to stir over night. For the synthesis of products **6, 13-16**, the reaction was carried out over night at -10°C.

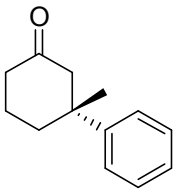
Important note: It is very important to use clean and freshly prepared ligand. Furthermore, it is crucial to keep the reaction mixture below -50°C during the halogen/lithium-exchange step to restrain the formation of LiI.

Ligand screening:



Scheme 1: Results with Ligands Used in Ligand Screening Giving the Conversion, Enantiomeric Excess and the Ratio Between Phenyl and Ethyl Transfer.

Spectral characterization of products

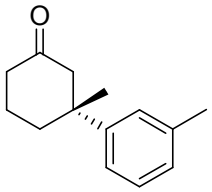


(*R*)-3-phenyl-3-methylcyclohexanone (2):[2, 3]

^{1}H-NMR (300 MHz; $CDCl_3$): δ 7.32 (d, 4H, *J* = 4.20 Hz), 7.23-7.19 (m, 1H) 2.88 (d, 1H, *J* = 14.10 Hz), 2.44 (d, 1H, *J* = 14.10 Hz), 2.31 (t, 2H, *J* = 6.69 Hz), 2.22-2.15 (m, 1H), 1.97-1.81 (m, 2H), 1.73-1.61 (m, 1H), 1.32 (s, 3H).

^{13}C-NMR (75 MHz, $CDCl_3$): δ 211.74, 147.73, 128.81, 126.48, 125.87, 53.37, 43.11, 41.08, 38.24, 30.09, 22.31.

$[\alpha]_D$: -77.1 ($CHCl_3$, *c* = 1.28, ee = 97% *R*. Absolute configuration was assigned in analogy with[3].) Enantiomeric excess was measured by chiral GC (Hydrodex B-3P, 140-30-1-145-0-20-170-3, 50 cm/s, Rt_1 = 20.94 min (*R*), Rt_2 = 21.47 min (*S*)).



(*R*)-3-(3-methylphenyl)-3-methylcyclohexanone (3)

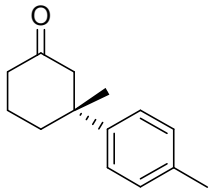
^{1}H-NMR (400 MHz; $CDCl_3$): δ 7.21 (t, 1H, *J* = 7.60 Hz), 7.13-7.11 (m, 2H), 7.03 (d, 1H, *J* = 7.08 Hz), 2.88 (d, 1H, *J* = 14.20 Hz), 2.43 (d, 1H, *J* = 14.20 Hz), 2.35 (s, 3H), 2.31 (t, 2H, *J* = 6.80 Hz), 2.21-2.15 (m, 1H), 1.94-1.83 (m, 2H), 1.73-1.63 (m, 1H), 1.3 (s, 3H).

^{13}C-NMR (100 MHz, $CDCl_3$): δ 211.90, 147.75, 138.29, 128.70, 127.24, 126.64, 122.91, 53.42, 42.98, 41.11, 38.22, 30.02, 22.33, 22.00.

IR (neat): ν = 2954, 1709, 784.

EI-MSHR: $[M]^+$ found 202.1361, calcld. for $C_{14}H_{18}O$: 202.1358.

$[\alpha]_D$: -71.4 ($CHCl_3$, *c* = 1.05, ee = 97% *R*). Enantiomeric excess was measured by chiral GC (Hydrodex B-3P, 140-30-1-150-0-20-170, 50 cm/s, Rt_1 = 28.05 min (*R*), Rt_2 = 28.71 min (*S*)).



(*R*)-3-(4-methylphenyl)-3-methylcyclohexanone (4)[4]

^{1}H-NMR (300 MHz; $CDCl_3$): δ 7.21 (d, 2H, *J* = 8.28 Hz), 7.13 (d, 2H, *J* = 8.19 Hz), 2.87 (d, 1H, *J* = 14.13 Hz), 2.42 (d, 1H, *J* = 14.10 Hz), 2.32-2.29 (m, 5H), 2.21-2.13 (m, 1H), 1.94-1.81 (m, 2H), 1.74-1.60 (m, 1H), 1.31 (s, 3H).

^{13}C-NMR (75 MHz, $CDCl_3$): δ 211.91, 144.79, 136.04, 129.53, 125.80, 53.51, 42.84, 41.13, 38.29, 30.19, 22.37, 21.18.

$[\alpha]_D$: -72.0 ($CHCl_3$, *c* = 1.05, ee = 96% *R*). Enantiomeric excess was measured by chiral GC (Hydrodex B-3P, 140-30-1-170-5, 50cm/s, Rt_1 = 34.06 min (*R*), Rt_2 = 34.42 min (*S*)).

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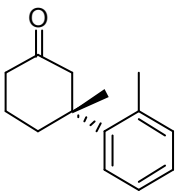
[2] House, H.O.; Lee, T.L. *J. Org. Chem.* **1979**, *44*, 16, 2819-2824.
[3] Lee, K.; Brown, K.; Hird, A. W.; Hoveyda, A. H., *J. Am. Chem. Soc.* **2006**, *128*, 7182-7184.
[4] Beeraiah B.; Srikrishna A. *Indian J. Chem.* **2005**, *44B*, 1641-1643.

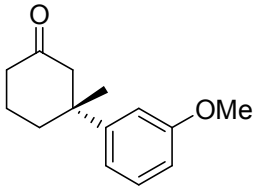


(*R*)-3-(2-methylphenyl)-3-methylcyclohexanone (5)[5]

^{1}H-NMR (400 MHz; $CDCl_3$): δ 7.27-7.24 (m, 1H), 7.17-7.13 (m, 3H), 3.03-2.99 (d, 1H, *J* = 16.00 Hz), 2.55 (s, 3H), 2.52-2.46 (m, 2H), 2.32 (t, 2H, 6.82 Hz), 1.98-1.84 (m, 2H), 1.66-1.57 (m, 1H), 1.43 (s, 3H).

^{13}C-NMR (100 MHz, $CDCl_3$): 212.03, 144.48, 135.90, 133.68, 127.34, 126.79, 126.43, 55.31, 44.41, 41.04, 36.18, 27.60, 23.62, 22.10.

$[\alpha]_D$: -66.3 ($CHCl_3$, *c* = 1.15, ee = 84.6% *R* (lit[6b] $[\alpha]_D^{20}$: +32 ($CHCl_3$, *c* = 0.71, 91% ee, *S*))). Enantiomeric excess was measured by chiral GC (Hydrodex B-3P, 140-30-1-145-0-20-170-3 50 cm/s, Rt_1 = 35.82 (*R*), Rt_2 = 36.26 min (*S*)).

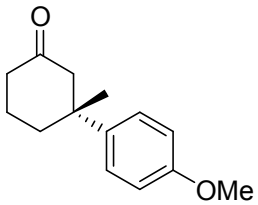


(*R*)-3-(3-methoxyphenyl)-3-methylcyclohexanone (6)[6]

^{1}H-NMR (300 MHz; $CDCl_3$): δ 7.27-7.22 (m, 1H), 7.62-6.86 (m, 2H), 6.77-6.73 (dd, 1H, *J* = 8.19, 2.43 Hz), 3.80 (s, 3H), 2.86 (d, 1H, *J* = 14.1 Hz), 2.42 (d, 1H, *J* = 14.22 Hz), 2.31 (t, 2H, *J* = 6.68 Hz), 2.21-2.13 (m, 1H), 1.94-1.81 (m, 2H), 1.74-1.63 (m, 1H), 1.31 (s, 3H).

^{13}C-NMR (75 MHz, $CDCl_3$): 211.71, 160.02, 149.60, 129.80, 118.37, 112.52, 111.24, 55.50, 53.45, 43.21, 41.12, 38.29, 30.04, 22.67, 22.35, 14.39.

$[\alpha]_D$: -69.0 ($CHCl_3$, *c* = 0.71, ee = 97.8% *R* (lit[6] $[\alpha]^{29}_D$:+10.8° ($CHCl_3$, *c* = 0.7, *S*)). Enantiomeric excess was measured by chiral GC (Hydrodex B-6-TBDM, 120-0-1-170-5, 50 cm/s, Rt_1 = 44.67 min (*R*), Rt_2 = 45.53 min (*S*)).

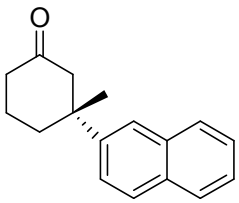


(*R*)-3-(4-methoxyphenyl)-3-methylcyclohexanone (7)[3]

^{1}H-NMR (300 MHz; $CDCl_3$): δ 7.24-7.21 (m, 2H), 6.88-6.84 (m, 2H), 3.78 (s, 3H), 2.85 (d, 1H, *J* = 14.13 Hz), 2.41 (d, 1H, *J* = 14.22 Hz), 2.30 (t, 2H, *J* = 6.68 Hz), 2.20-2.11 (m, 1H), 1.93-1.80 (m, 2H), 1.72-1.59 (m, 1H), 1.30 (s, 3H).

^{13}C-NMR (75 MHz, $CDCl_3$): δ 211.94, 158.11, 139.78, 126.99, 114.11, 55.55, 53.63, 42.62, 41.13, 38.41, 30.43, 22.37.

$[\alpha]_D$: -64.6 ($CHCl_3$, *c* = 1.04, ee = 94% *R* (lit[3] $[\alpha]^{20}_D$:+ 51.71 ($CHCl_3$, *c* = 0.960, ee = 90% *S*)). Enantiomeric excess was measured by chiral GC (Hydrodex B-6-TBDM, 120-0-1-170-5, 50cm/s, Rt_1 = 50.10 min (*R*), Rt_2 = 50.64 min (*S*)).



(*R*)-3-(2-naphthyl)-3-methylcyclohexanone (8)

^{1}H-NMR (400 MHz; $CDCl_3$): δ 7.83-7.79 (m, 3H), 7.71 (s, 1H), 7.50-7.44 (m, 1H), 3.03 (d, 1H, *J* = 14.36 Hz), 2.53 (d, 1H, *J* = 14.12 Hz), 2.35-2.29 (m, 3H), 2.02-1.85 (m, 2H), 1.70-1.60 (m, 1H), 1.41 (s, 3H).

^{13}C-NMR (100 MHz, $CDCl_3$): δ 211.76, 144.94, 133.57, 132.15, 128.59, 128.39, 127.62, 126.43, 126.09, 124.61, 124.39, 53.38, 43.26, 41.12, 38.07, 30.14, 22.31.

EI-MSHR: $[M]^+$ found 238.1357, calcld. for $C_{17}H_{18}O$: 238.1358.

IR (neat): ν = 2956, 1708, 817.

$[\alpha]_D$: -59.6 ($CHCl_3$, *c* = 0.99, ee = 98.7% *R*). Enantiomeric excess was measured by chiral SFC (OD 5%-1-2-15% MeOH, 2 mL/min, 10°C, 200 bar, Rt_1 = 6.66 min (*R*), Rt_2 = 7.05 min (*S*)).

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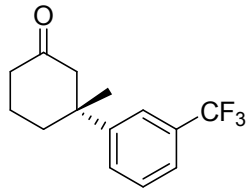
[5] (a) S. Matsuzawa, Y. Horiguchi, E. Makamura, I. Kuwajima *Tetrahedron* **1989**, *45*, 2, 349-362. (b)

[6] Shimizu, M; Kamikubo, T.; Ogasawara K. *Heterocycles* **1997**, *46*, 21-26.



(*R*)-3-(3-trifluoromethylphenyl)-3-methylcyclohexanone (9)

^{1}H-NMR (300 MHz; $CDCl_3$): δ 7.56 (s, 1H), 7.52-7.40 (m, 3H), 2.85 (d, 1H, J = 14.04 Hz), 2.47 (d, 1H, J = 14.10 Hz), 2.35-2-30 (m, 2H), 2.22-2.14 (m, 1H), 2.00-1.85 (m, 2H), 1.74-1.60 (m, 1H), 1.32 (s, 3H).

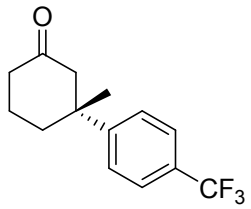
^{13}C-NMR (75 MHz, $CDCl_3$): δ 210.92, 148.87, 131.35, 130.93, 129.34, 126.30, 123.45, 122.57, 53.17, 43.25, 40.98, 37.97, 29.68, 22.27.

^{19}F-NMR (282 MHz, $CDCl_3$): δ 62.45.

IR (neat): ν = 2961, 1713, 1328, 1162, 1119, 1073, 802.

EI-MSHR: $[M]^+$ found 256.1074, calcld. for $C_{14}H_{15}OF_3$: 256.1075.

$[\alpha]_D$: -48.2 ($CHCl_3$, c = 1.09, ee = 94.9% *R*). Enantiomeric excess was measured by chiral GC (Hydrodex-6-B-TBDM, 120-0-1-170-5, 50cm/s, Rt_1 = 26.48 min (*R*), Rt_2 = 27.57 min (*S*)).



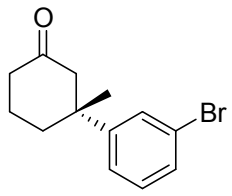
(*R*)-3-(4-trifluoromethylphenyl)-3-methylcyclohexanone (10)[7]

^{1}H-NMR (300 MHz; $CDCl_3$): δ 7.57 (d, 2H, J = 8.19 Hz), 7.43 (d, 2H, J = 8.10 Hz), 2.87 (d, 1H, J = 14.13 Hz), 2.47 (d, 1H, J = 14.13 Hz), 2.32 (t, 2H, J = 6.32 Hz), 2.23-2.17 (m, 1H), 1.98-1.86 (m, 2H), 1.70-1.59 (m, 1H), 1.33 (s, 3H).

^{13}C-NMR (75 MHz, $CDCl_3$): δ 211.05, 151.76, 128.88, 126.41, 125.83 (q, $J_{C,F}$ = 3.20 Hz) , 53.15, 43.43, 41.03, 38.13, 30.15, 22.27.

^{19}F-NMR (282 MHz, $CDCl_3$): δ 62.45.

$[\alpha]_D$: -54.5 ($CHCl_3$, c = 1.09, ee = 98.4% *R* (lit[7] $[\alpha]^{20}_D$:+ 30.3 ($CHCl_3$, c = 1.4, ee = 66% *S*)). Enantiomeric excess was measured by chiral GC (Chirasil DEX-CB, 120-0-1-170-5, 30 cm/s, Rt_1 = 36.02 min (*S*), Rt_2 = 36.28 min (*R*)).



(*R*)-3-(3-bromophenyl)-3-methylcyclohexanone (11)

^{1}H-NMR (300 MHz; $CDCl_3$): 7.46-7.45 (m, 1H), 7.36-7.32 (m, 1H) 7.25-7.18 (m, 2H), 2.82 (d, 1H, J = 14.10 Hz), 2.43 (d, 1H, J = 14.13 Hz), 2.32 (t, 2H, J = 6.60 Hz), 2.19-2.11 (m, 1H), 1.94-1.87 (m, 2H), 1.75-1.63 (m, 1H), 1.30 (s, 3H).

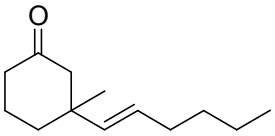
^{13}C-NMR (75 MHz, $CDCl_3$): 211.07, 150.32, 130.43, 129.74, 129.23, 124.67, 123.22, 53.22, 43.20, 41.05, 38.10, 29.84, 22.30.

EI-MSHR: $[M]^+$ found 266.0309, calcld. for $C_{13}H_{15}OBr$: 266.0306.

IR (neat): ν = 2956, 1708, 1072, 783..

$[\alpha]_D$: -61.0 ($CHCl_3$, c = 1.00, ee = 97.4% *R*). Enantiomeric excess was measured by chiral GC (Hydrodex-6-B-TBDM, 120-0-1-170-5, 50 cm/s, Rt_1 = 51.39 min (*R*), Rt_2 = 52.47 min (*S*)).

[7] Vuagnoux-d'Augustin, M.; Alexakis, A. *Chem. Eur. J.* **2007**, *13*, 9647-9662.



(*E*)-3-(hex-1-enyl)-3-methylcyclohexanone (12)

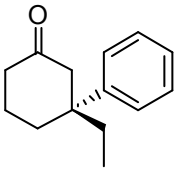
^{1}H-NMR (400 MHz, $CDCl_3$) : 5.34-5.25 (m, 2H), 2.42 (d, 1H, J = 14.0 Hz), 2.27-2.20 (m, 2H), 2.14 (d, 1H, J = 14.0 Hz), 1.97-1.96 (m, 2H), 1.84-1.81 (m, 2H), 1.67-1.58 (m, 2H), 1.28-1.27 (m, 4H), 1.03 (s. 3H), 0.87 (t, 3H, J = 7.1 Hz).

^{13}C-NMR (100 MHz, $CDCl_3$) : 212.1, 137.8, 129.1, 64.4, 52.7, 41.2, 41.1, 37.4, 32.7, 32.0, 28.5, 22.5, 14.3.

EI-MSHR: $[M]^+$ found 194.1669, calcld. for $C_{13}H_{22}O$: 194.1671.

IR (neat): ν = 2955, 2926, 2872, 1713, 1455.

$[\alpha]_D$: -45.2 ($CHCl_3$, c = 0.3, ee = 85.5%). Enantiomeric excess was measured by chiral GC (Hydrodex-6-B-TBDM, 60-0-1-170-5, 50 cm/s, Rt_1 = 67.38 min, Rt_2 = 68.93 min).



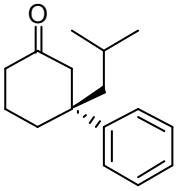
(*R*)-3-phenyl-3-ethylcyclohexanone (13)[3]

^{1}H-NMR (400 MHz, $CDCl_3$) : 7.34-7.25 (m, 4H), 7.21-7.17 (m, 1H), 2.92 (d, 1H, J = 14.1 Hz), 2.42 (d, 1H, J = 14.1 Hz), 2.31-2.28 (m, 2H), 2.21-2.14 (d, 1H) 2.02-1.95 (m, 1H), 1.88-1.72 (m, 2H), 1.69-1.53 (m, 2H), 0.6 (t, 3H, J = 7.4 Hz).

^{13}C-NMR (100 MHz, $CDCl_3$) : 211.9, 145.1, 128.7, 126.8, 126.3, 50.8, 46.7, 41.3, 36.5, 36.0, 21.8, 8.2.

IR (neat): ν = 2955, 2926, 2872, 1713, 1455.

$[\alpha]_D$: -75.8 ($CHCl_3$, c = 1.03, ee = 95% *R* (lit[3] $[\alpha]^{20}_D$:+63.77 ($CHCl_3$, c = 1.00, ee = 94% *S*)). Enantiomeric excess was measured by chiral GC (Chirasil DEX-CB, 135-0-1-160-0-20-170-5, 40 cm/s, Rt_1 = 22.88 min (*S*), Rt_2 = 23.29 min (*R*)).



(*R*)-3-phenyl-3-*iso*butylcyclohexanone (14)

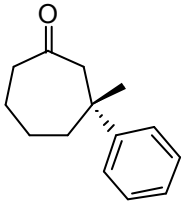
^{1}H-NMR (300 MHz, $CDCl_3$) : 7.33-7.26 (m, 4H), 7.20-7.15 (m, 1H), 2.98 (d, 1H, J = 14.4 Hz), 2.45 (d, 1H, J = 14.4 Hz), 2.27 (t, 2H, J = 6.8 Hz), 2.22-2.13 (m, 1H), 2.01-1.92 (m, 1H), 1.86-1.67 (m, 1H), 1.59-1.52 (m, 3H), 1.46-1.33 (m, 1H), 0.73 (m, 3H, J = 6.6 Hz), 0.54 (m, 3H, J = 6.7 Hz).

^{13}C-NMR (75 MHz, $CDCl_3$) : 212.0 ,145.7, 128.7, 126.9, 126.4, 52.7, 51.9, 46.7, 41.3, 37.9, 25.2, 24.8, 24.4, 21.6.

EI-MSHR: $[M]^+$ found 230.1670, calcld. for $C_{16}H_{22}O$: 230.1671.

IR (neat): ν = 2954, 2868, 1709, 1447.

$[\alpha]_D$: -65.7 ($CHCl_3$, c = 1.03, ee = 98.6% *R*). Enantiomeric excess was measured by chiral GC (Chirasil DEX-CB, 140-30-1-170-5, 40 cm/s, Rt_1 = 33.38 min (*S*), Rt_2 = 34.57 min (*R*)).

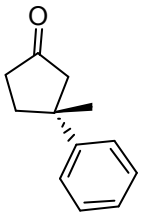


(*R*)-3-phenyl-3-methylcycloheptanone (15)[8], [3]

^{1}H-NMR (400 MHz, $CDCl_3$) : 7.32 (d, 4H, *J* = 4.3 Hz), 7.22-7.17 (m, 1H), 3.21 (d, 1H, *J* = 14.4 Hz), 2.71 (d, 1H, *J* = 14.4 Hz), 2.46-2.36 (m, 2H), 2.22-2.15 (m, 1H), 1.84-1.73 (m, 5H), 1.27 (s, 3H).

^{13}C-NMR (100 MHz, $CDCl_3$) : 214.2, 148.2, 128.9, 126.3, 125.9, 56.0, 44.5, 43.8, 40.1, 32.2, 26.1, 24.2.

$[\alpha]_D$: -83.8 ($CHCl_3$, *c* = 1.03, ee = 96.5% *R* (lit[3] $[\alpha]^{20}_D$:+74.78 ($CHCl_3$, *c* = 1.00, ee = 96% *S*)). Enantiomeric excess was measured by chiral GC (Hydrodex B-3P, 140-30-1-145-0-20-170-3, 50cm/s, Rt_1 = 32.85 min (*R*), Rt_2 = 33.34 min (*S*)).



(*R*)-3-phenyl-3-methylcyclopentanone (16)[9]

^{1}H-NMR (400 MHz, $CDCl_3$) : 7.37-7.29 (m, 4H), 7.26-7.22 (m, 1H), 2.66 (d, 1H, *J* = 17.3 Hz), 2.49 (d, 1H, *J* = 17.3 Hz), 2.44-2.36 (m, 2H), 2.33-2.26 (m, 2H), 1.39 (s, 3H).

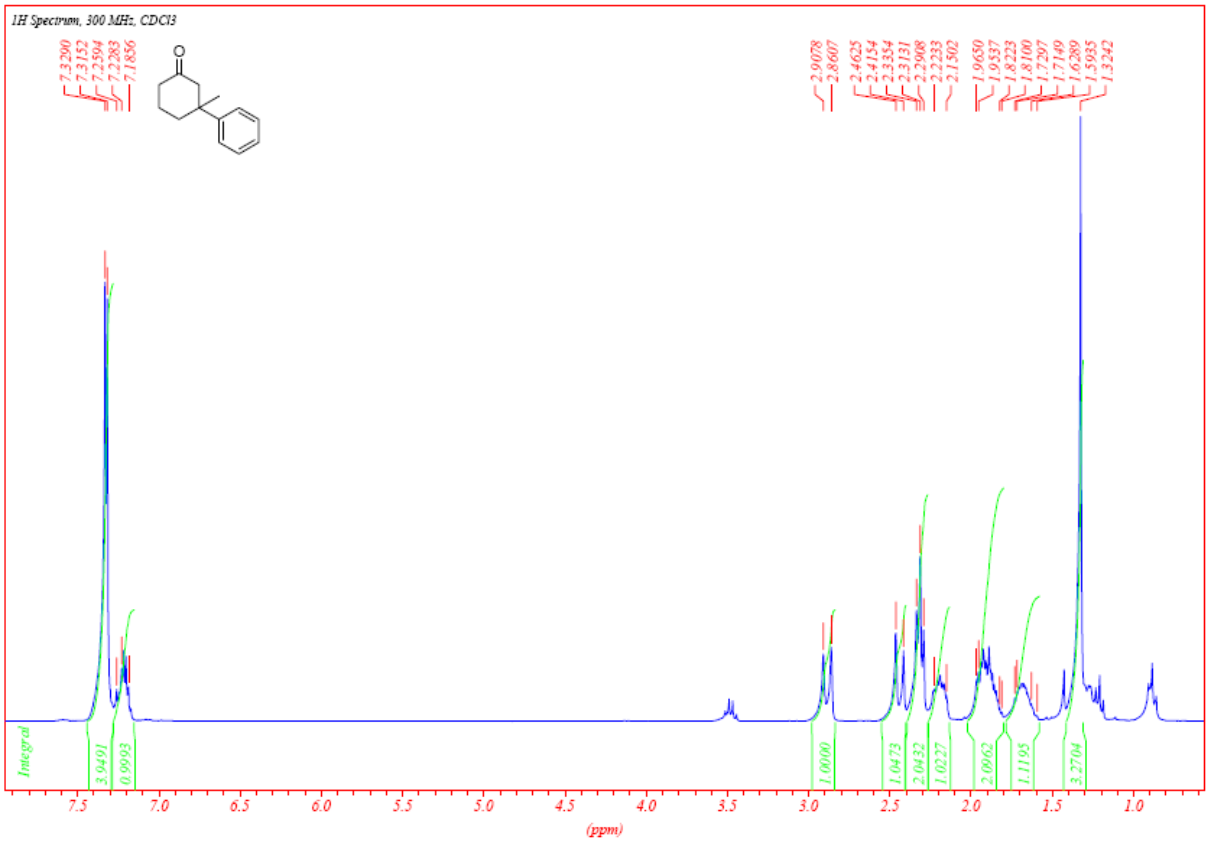
^{13}C-NMR (100 MHz, $CDCl_3$) : 219.0, 148.8, 128.9, 126.6, 125.8, 52.6, 44.1, 37.0, 36.1, 29.7.

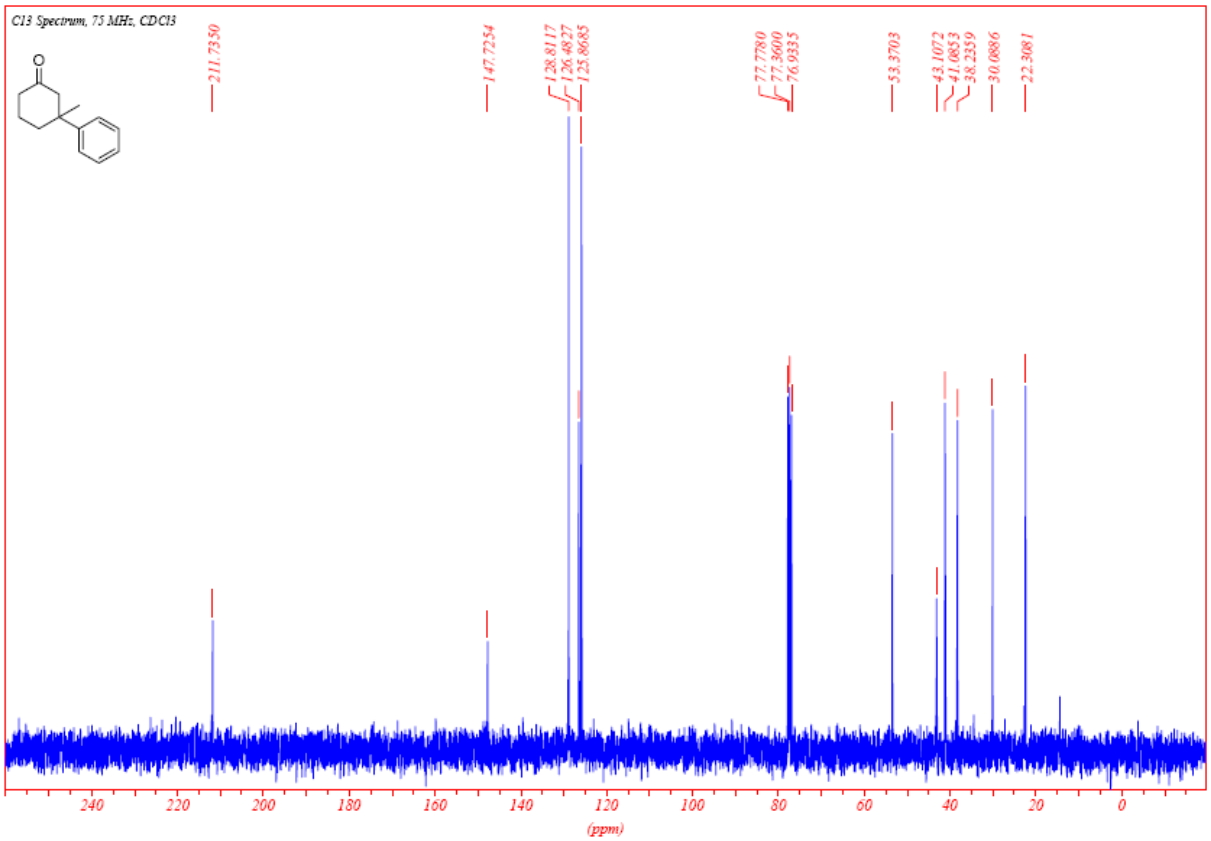
$[\alpha]_D$: +15.7 ($CHCl_3$, *c* = 0.84, ee = 77% *R* (lit[9b] $[\alpha]^{26}_D$:+4.8 ($CHCl_3$, *c* = 1.02, *R*)). Enantiomeric excess was measured by chiral GC (Hydrodex B-3P, 140-30-1-170-5, 50cm/s, Rt_1 = 14.22 min (*R*), Rt_2 = 14.53 min (*S*)).

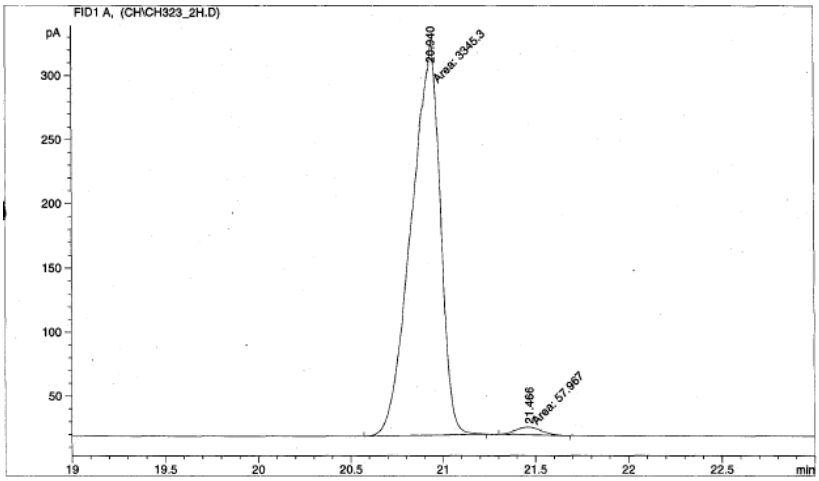
[8] Ushiyama, H.; Hagiwara, H.; Sato, K.; Uda, H. *Chem. Lett.* **1977**, 925-928.

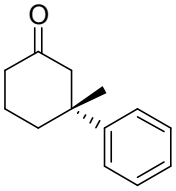
[9] (a) Gadwood, R. C. *J. Org. Chem.* **1983**, *48*, 2098-2101. (b) Gilday, J. P.; Ra, C. S.; Paquette, L. A. *J. Am. Chem. Soc.* **1987** *109*, 6858-6860.

2

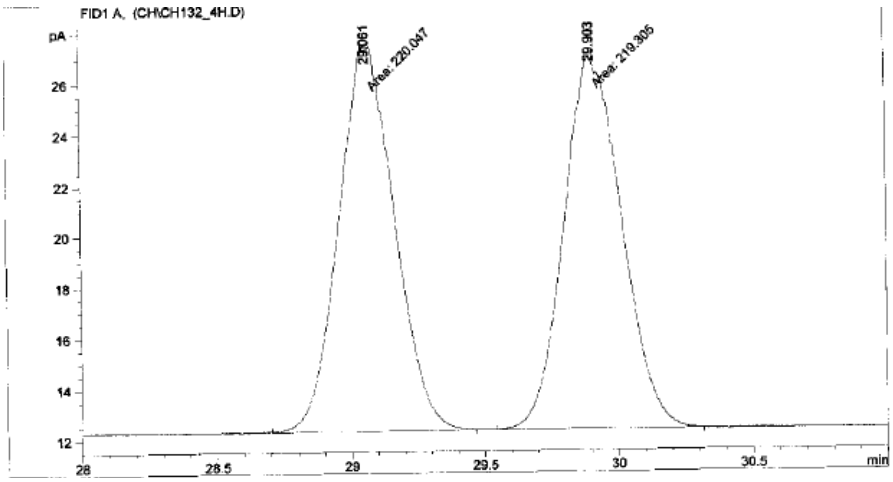

1H Spectrum, 300 MHz, CDCl3
7.3290
7.3152
7.2594
7.2283
7.1856
2.9078
2.8607
2.4625
2.4154
2.3354
2.3131
2.2908
2.2233
2.1502
1.9650
1.9537
1.8223
1.8100
1.7297
1.7149
1.6289
1.5935
1.3242
Integral
3.9491
0.9993
1.0000
1.0473
2.0432
1.0227
2.0062
1.1195
3.2704
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
(ppm)


C13 Spectrum, 75 MHz, CDCl3
211.7350
147.7254
128.8117
126.4827
125.8685
77.7780
77.3600
76.9335
53.3703
43.1072
41.0853
38.2359
30.0886
22.3081
240
220
200
180
160
140
120
100
80
60
40
20
0
(ppm)



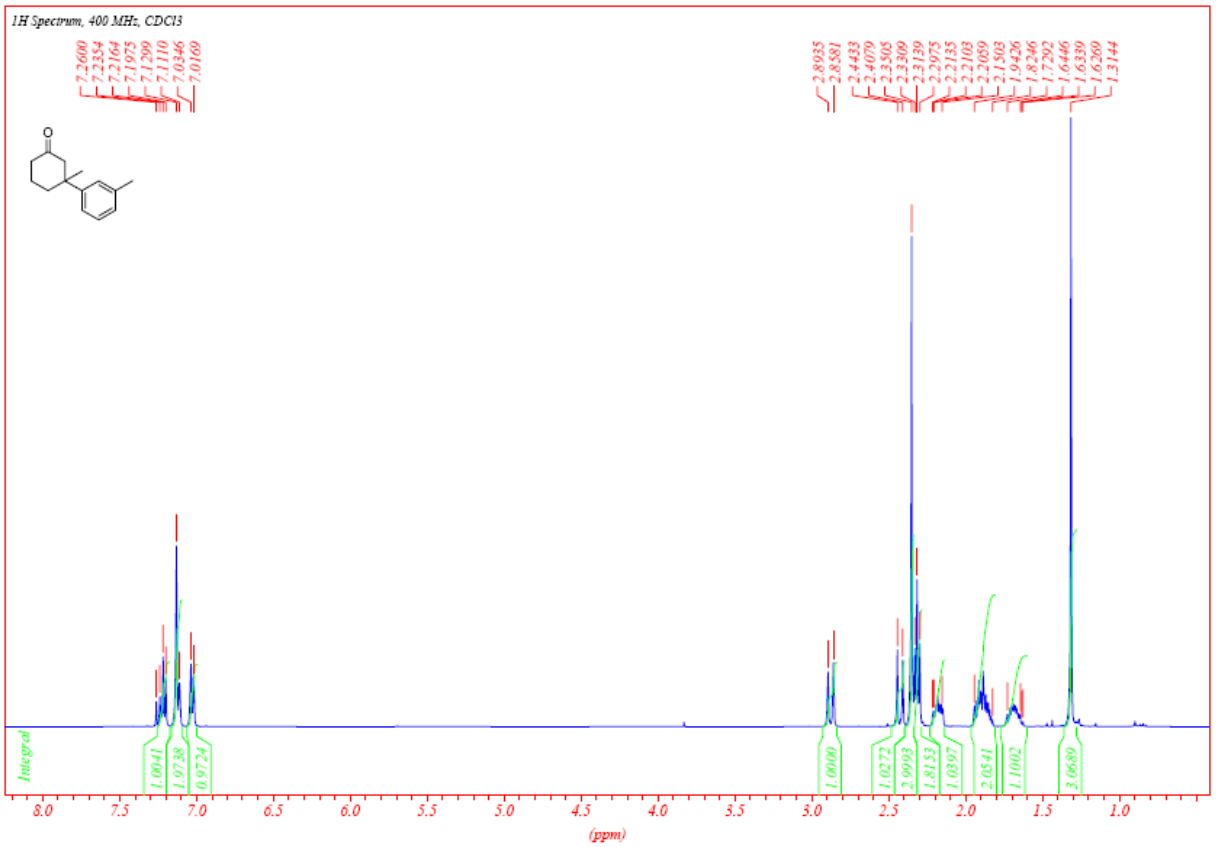


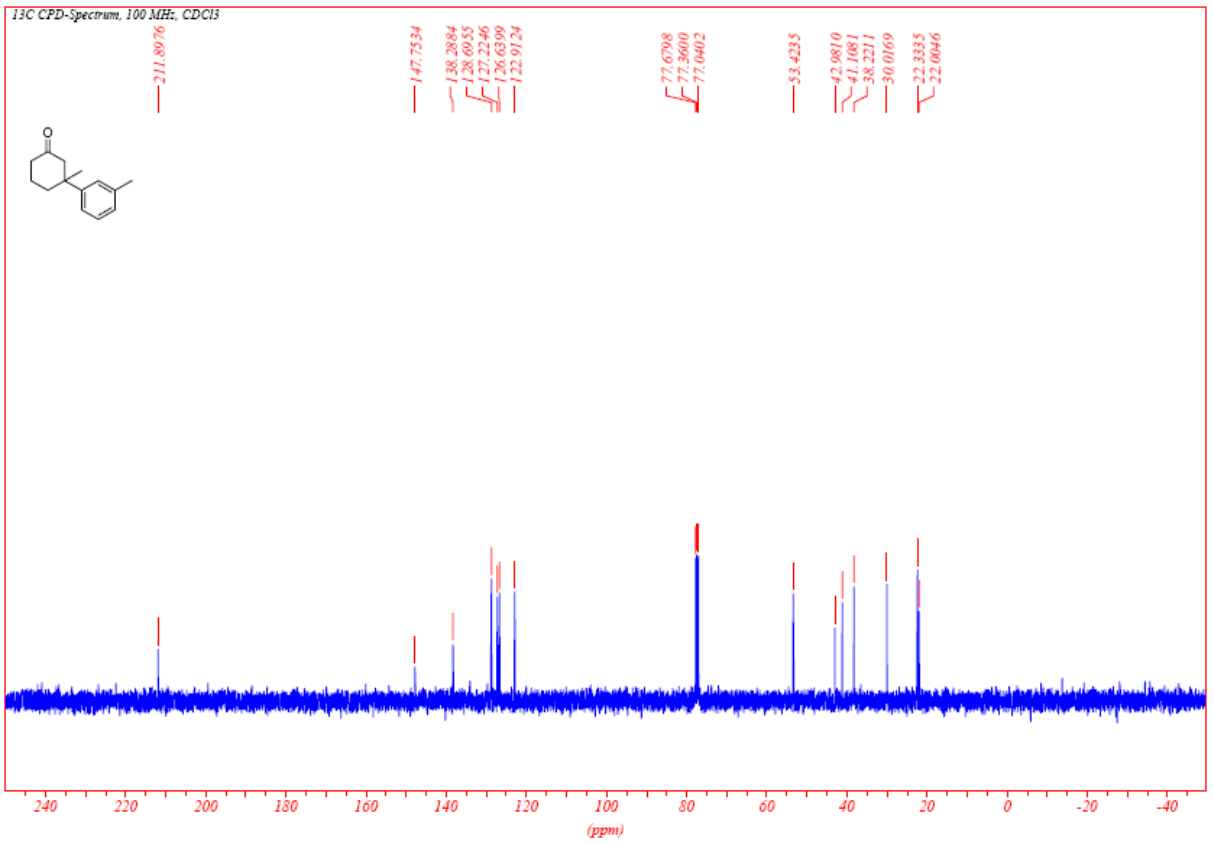
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	20.940	MM	0.1831	3345.30322	304.55820	98.29673
2	21.466	MM	0.1629	57.96696	5.92934	1.70327
Totals :				3403.27019	310.48753	

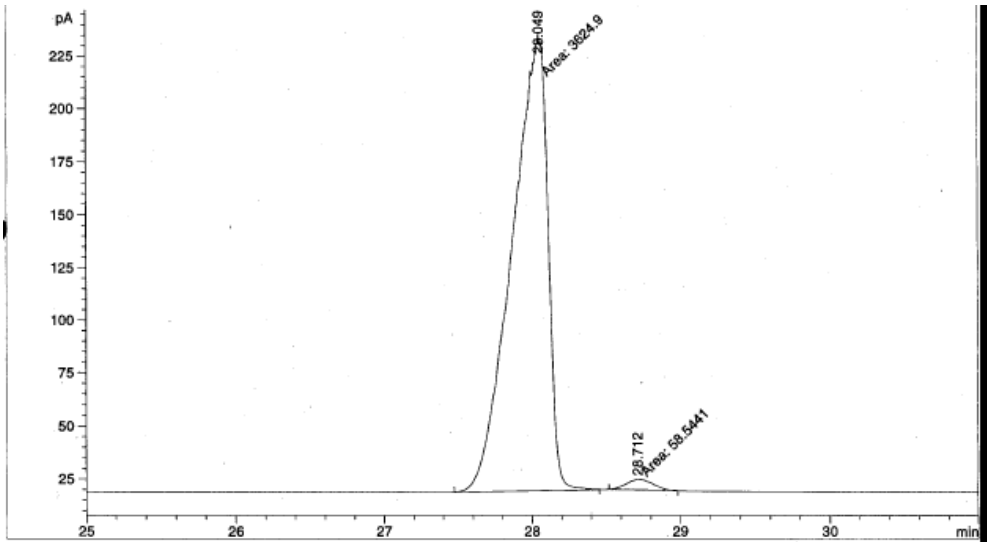


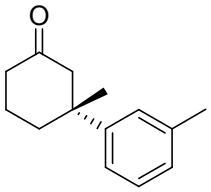
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	29.061	MM	0.2408	220.04674	15.22897	50.08445
2	29.903	MM	0.2494	219.30464	14.65436	49.91555
Totals :				439.35138	29.88332	

3

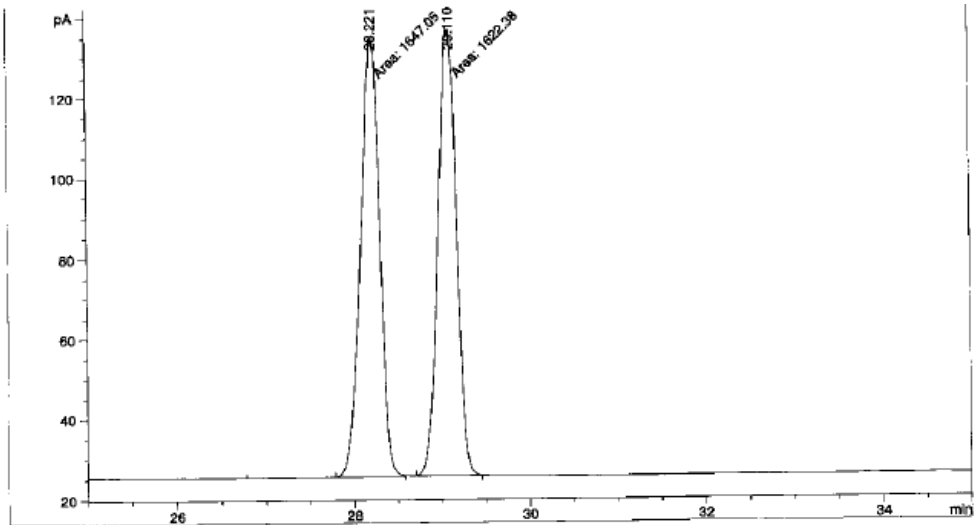

1H Spectrum, 400 MHz, CDCl3
7.2600
7.2354
7.2164
7.1975
7.1299
7.1110
7.0346
7.0169
2.8935
2.8581
2.4433
2.4079
2.3505
2.3309
2.3139
2.2975
2.2135
2.2103
2.2059
2.1503
1.9426
1.8246
1.7292
1.6446
1.6339
1.6260
1.3144
Integral
1.0041
1.9738
0.9724
1.0000
1.0272
2.9993
1.8153
1.0397
2.0541
1.1002
3.0689
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
(ppm)


13C CPD-Spectrum, 100 MHz, CDCl3
211.8976
147.7534
138.2884
128.6955
127.2246
126.6399
122.9124
77.6798
77.3600
77.0402
53.4235
42.0810
41.1081
38.2211
30.0169
23.3335
22.0046
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
-40
(ppm)



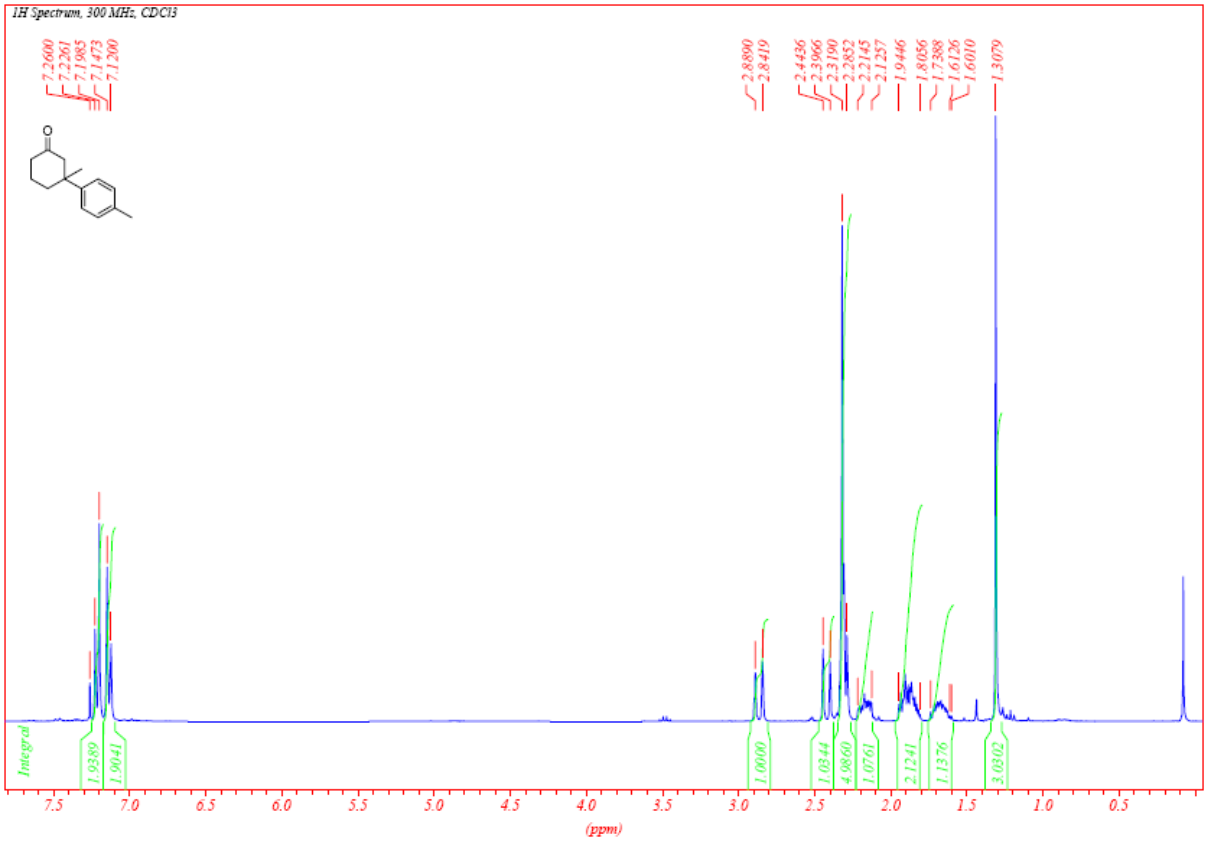


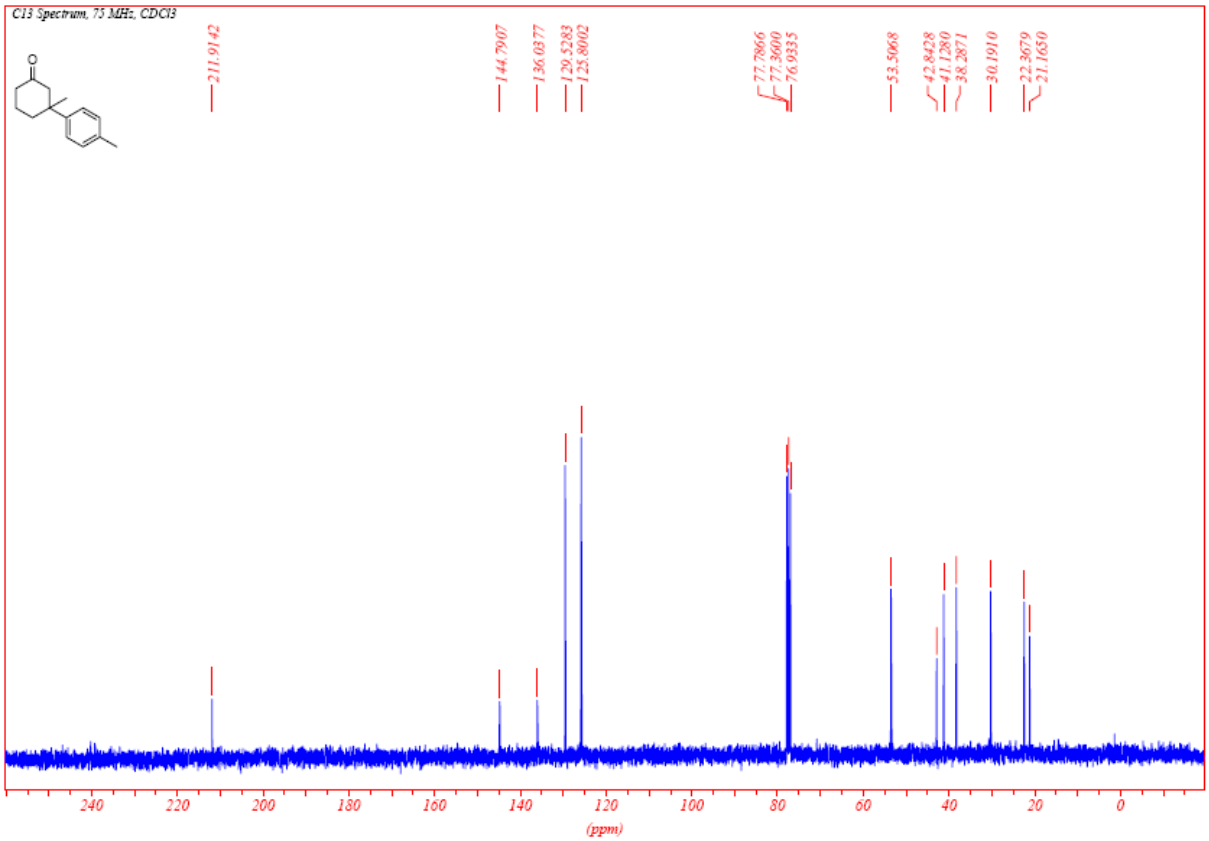
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	28.049	MM	0.2784	3624.89819	217.02956	98.41061
2	28.712	MM	0.2013	58.54412	4.84683	1.58939
Totals :				3683.44231	221.87639	

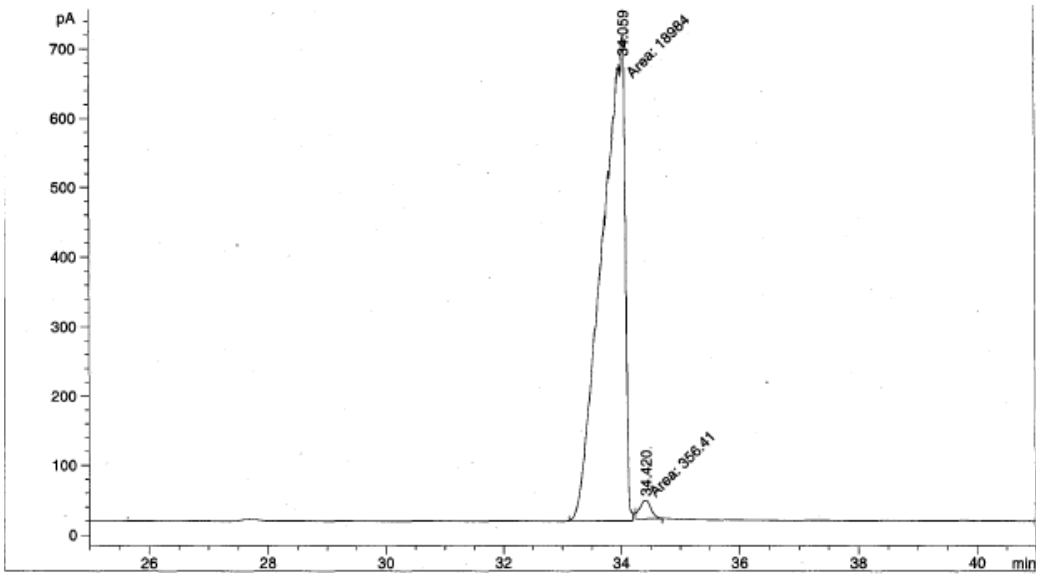


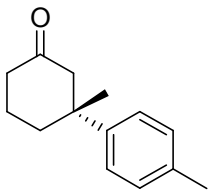
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	28.221	MM	0.2504	1647.04749	109.64384	50.37721
2	29.110	MM	0.2435	1622.38245	111.05584	49.62279
Totals :				3269.42993	220.69968	

4


1H Spectrum, 300 MHz, CDCl3
7.2600
7.2261
7.1985
7.1473
7.1200
2.8890
2.8419
2.4436
2.3966
2.3190
2.2852
2.2145
2.1257
1.9446
1.8056
1.7388
1.6126
1.6010
1.3079
Integral
1.9389
1.9041
1.0000
1.0344
4.9860
1.0761
2.1241
1.1376
3.0302
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)

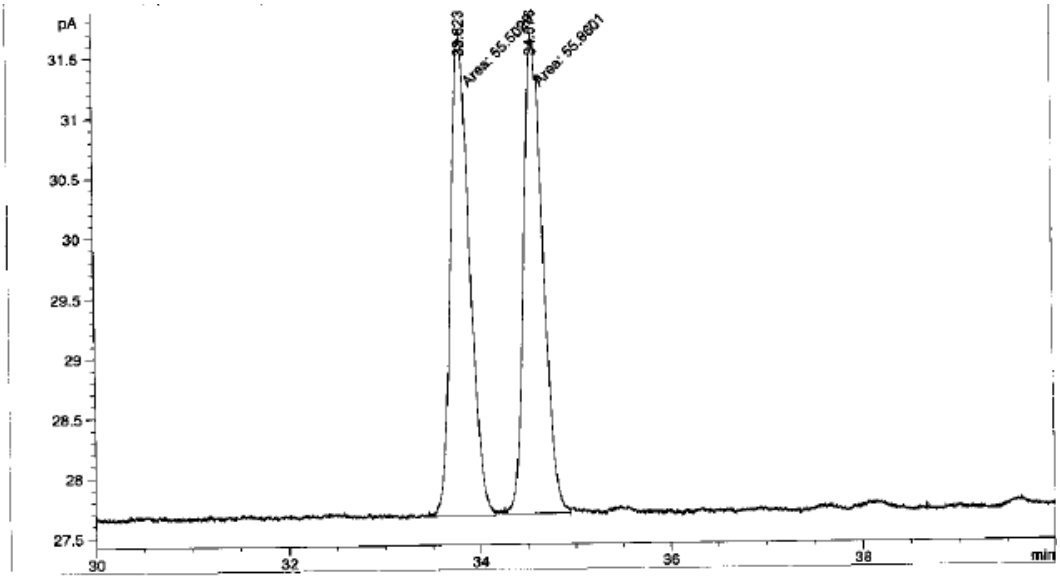

C13 Spectrum, 75 MHz, CDCl3
211.9142
144.7907
136.0377
129.5283
125.8002
77.7866
77.3600
76.9335
53.5068
42.8428
41.1280
38.2871
30.1910
22.3679
21.1650
240
220
200
180
160
140
120
100
80
60
40
20
0
(ppm)





Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Area %	Name
1	23.349		0.0000	0.00000	0.00000	
2	24.031		0.0000	0.00000	0.00000	
3	34.059	MM	0.4508	1.89840e4	98.15717	?
4	34.420	MM	0.2224	356.41046	1.84283	?

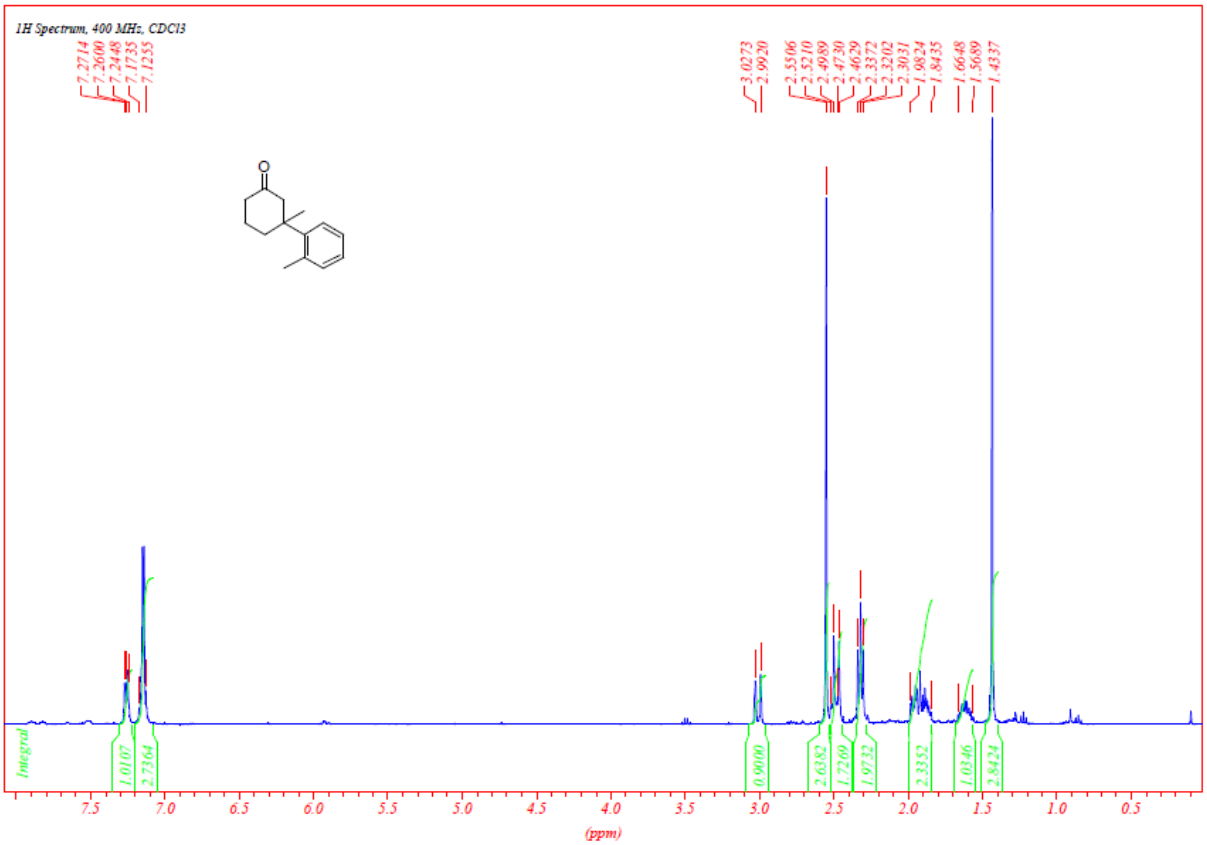
Totals : 1.93404e4

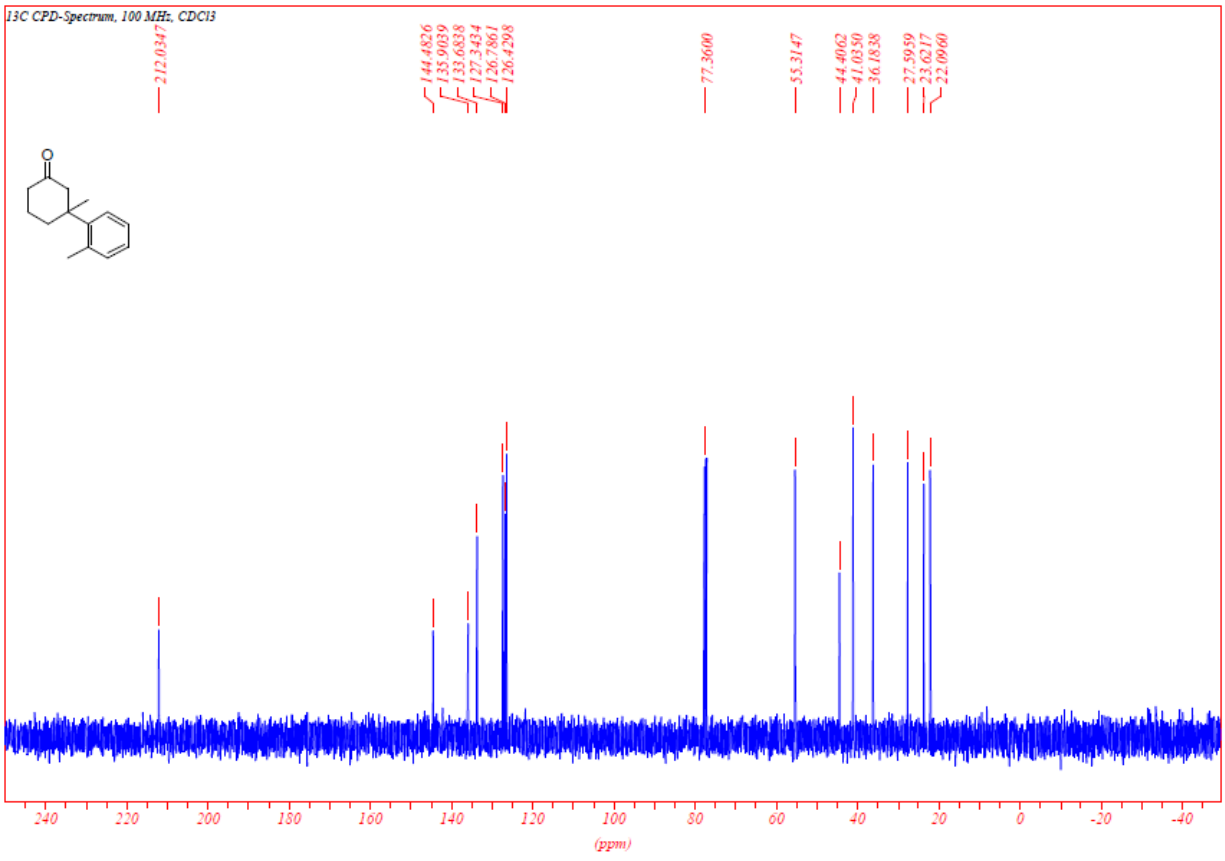


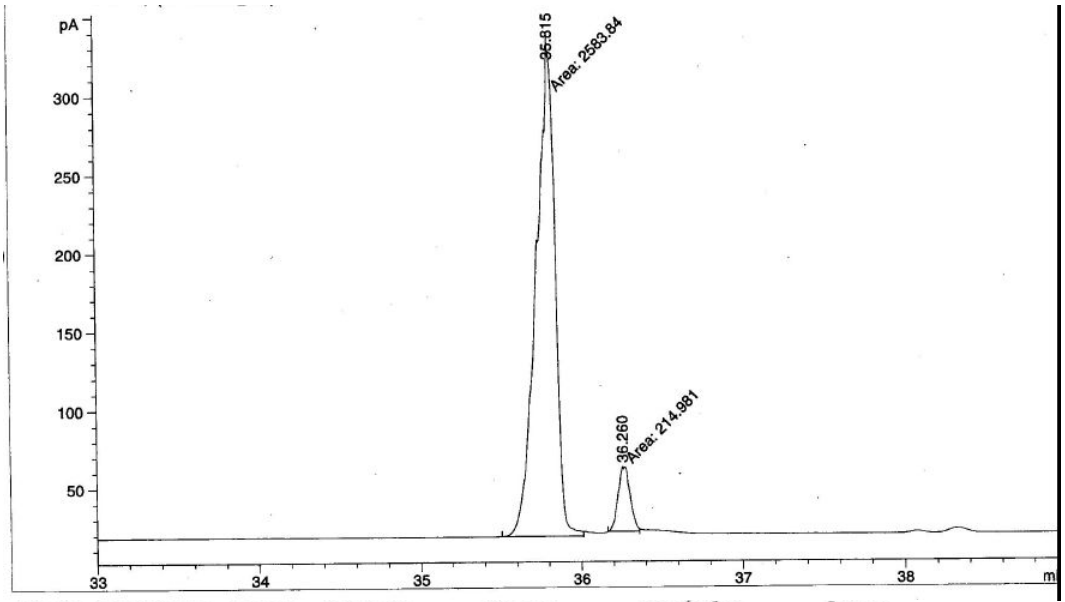
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	33.823	MM	0.2312	55.50247	4.00103	49.83945
2	34.576	MM	0.2338	55.86007	3.98266	50.16055

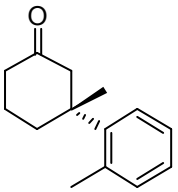
Totals : 111.36254 7.98369

5

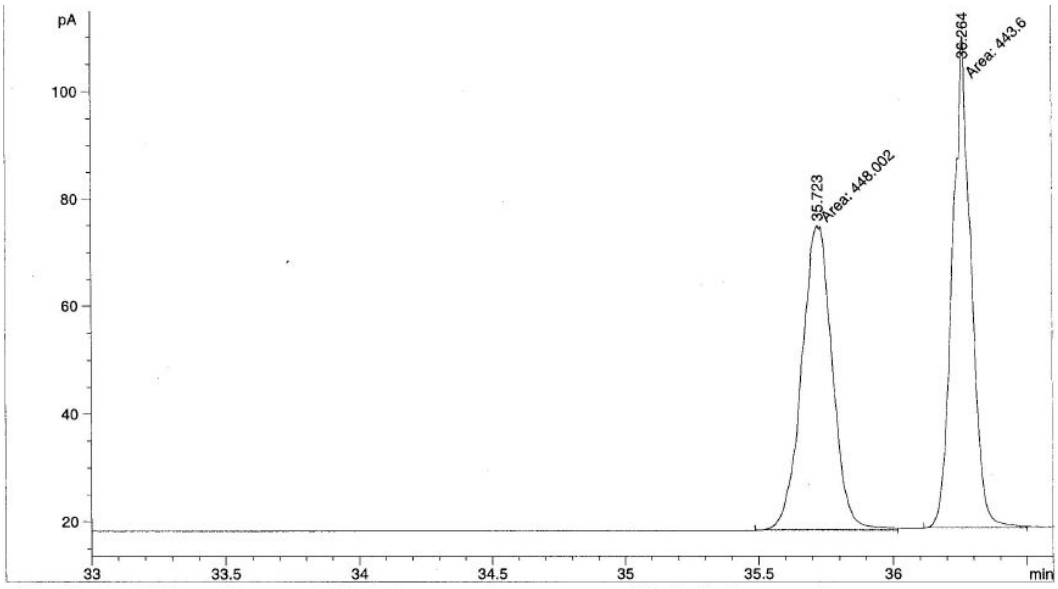

1H Spectrum, 400 MHz, CDCl3
7.2714
7.2600
7.2448
7.1735
7.1255
3.0273
2.9920
2.5506
2.5210
2.4989
2.4730
2.4629
2.3372
2.3202
2.3031
1.9824
1.8435
1.6648
1.5689
1.4437
Integral
1.0107
2.7364
0.9000
2.6382
1.7269
1.9732
2.3352
1.0346
2.8424
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)


13C CPD-Spectrum, 100 MHz, CDCl3
212.0347
144.4826
135.9039
133.6838
127.3434
126.7861
126.4298
77.3600
55.3147
44.4062
41.0350
36.1838
27.5959
23.6217
22.0960
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
-40
(ppm)



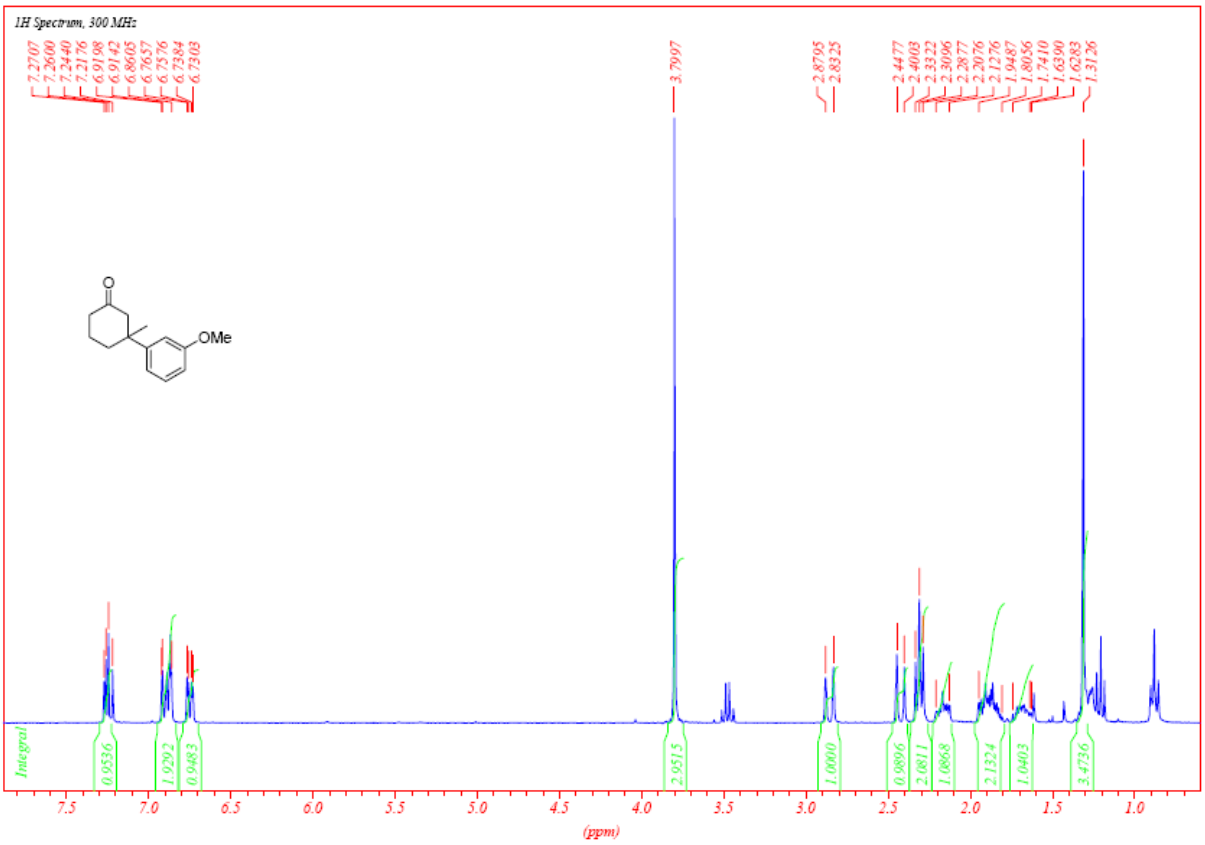


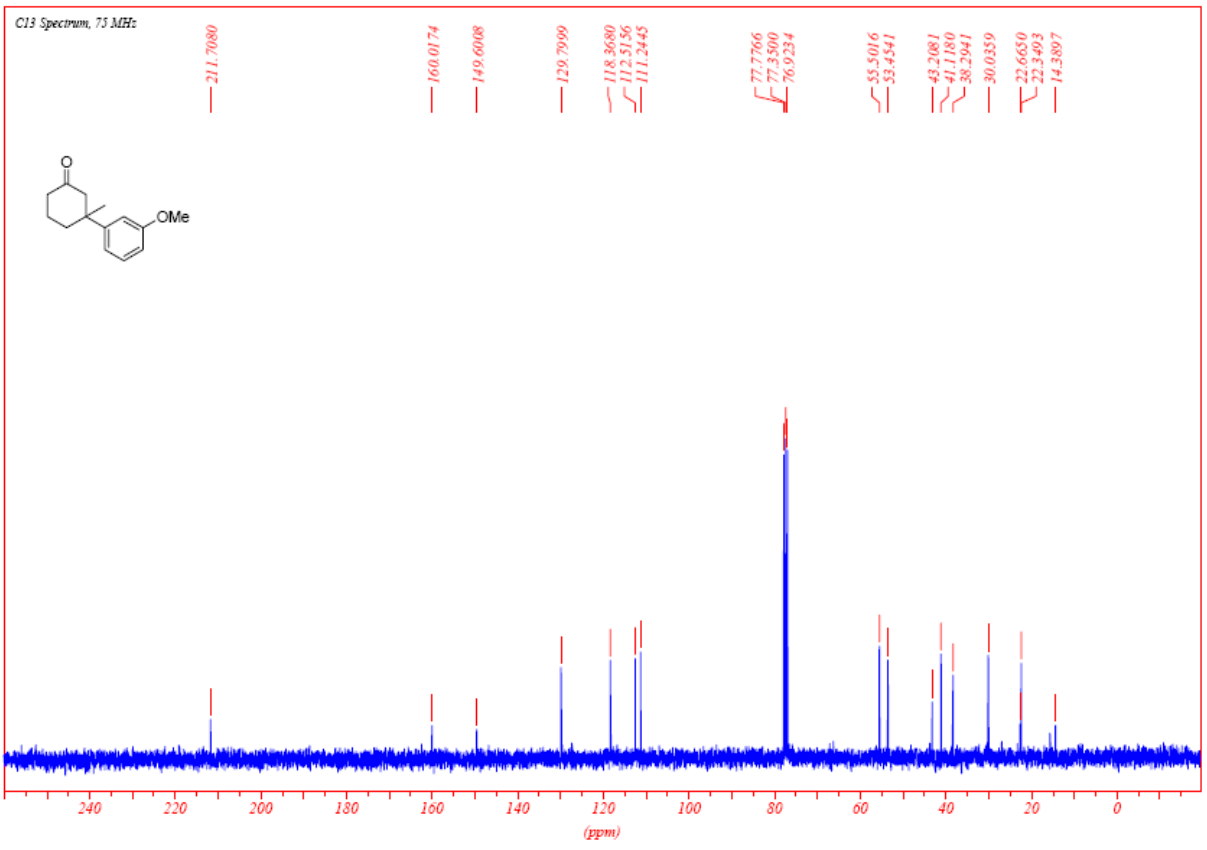
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	35.815	MM	0.1353	2583.84448	318.27676	92.31889
2	36.260	MM	0.0865	214.98090	41.42929	7.68111

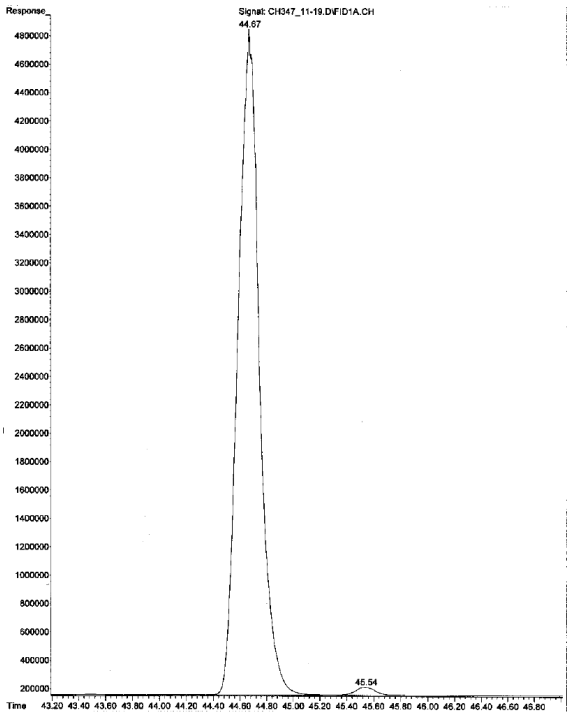


Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	35.723	MM	0.1317	448.00192	56.69716	50.24683
2	36.264	MM	0.0809	443.60046	91.44176	49.75317

6

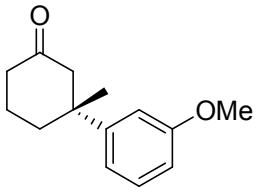

1H Spectrum, 300 MHz
7.2707
7.2600
7.2440
7.2176
6.9198
6.9142
6.8605
6.7657
6.7576
6.7384
6.7303
3.7997
2.8795
2.8325
2.4477
2.4063
2.3522
2.3096
2.2877
2.2076
2.1276
1.9487
1.8056
1.7410
1.6390
1.6283
1.3126
OMe
Integral
0.9536
1.9292
0.9483
2.0515
1.0000
0.8896
2.0811
1.0868
2.1324
1.0403
3.4736
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
(ppm)

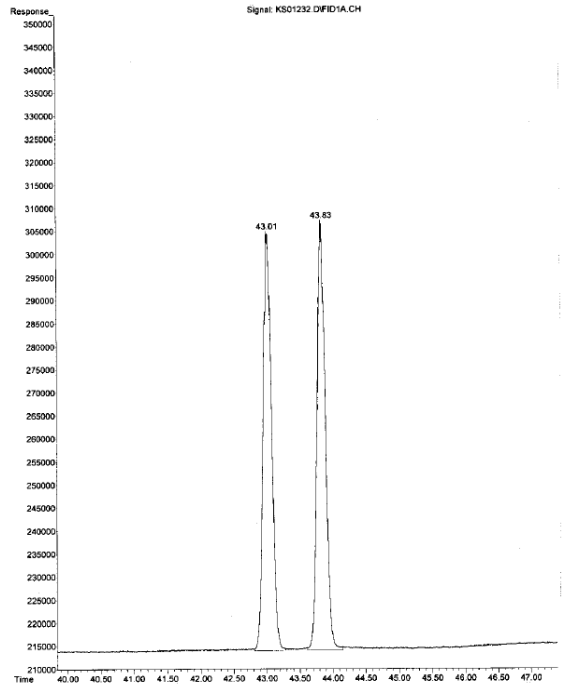

C13 Spectrum, 75 MHz
211.7080
160.0174
149.6008
129.7999
118.3680
112.5156
111.2445
77.7766
77.3500
76.9234
55.5016
53.4541
43.2081
41.1180
38.2941
30.0359
22.6650
22.3493
14.3897
OMe
240
220
200
180
160
140
120
100
80
60
40
20
0
(ppm)



peak #	R.T. min	Start min	End min	PK TY	peak height	peak area	peak % max.	% of total
1	44.668	44.300	45.217	M	4693819	520778551	100.00%	98.913%
2	45.536	45.320	45.779	M	57203	5724350	1.10%	1.087%

Sum of corrected areas: 526502901



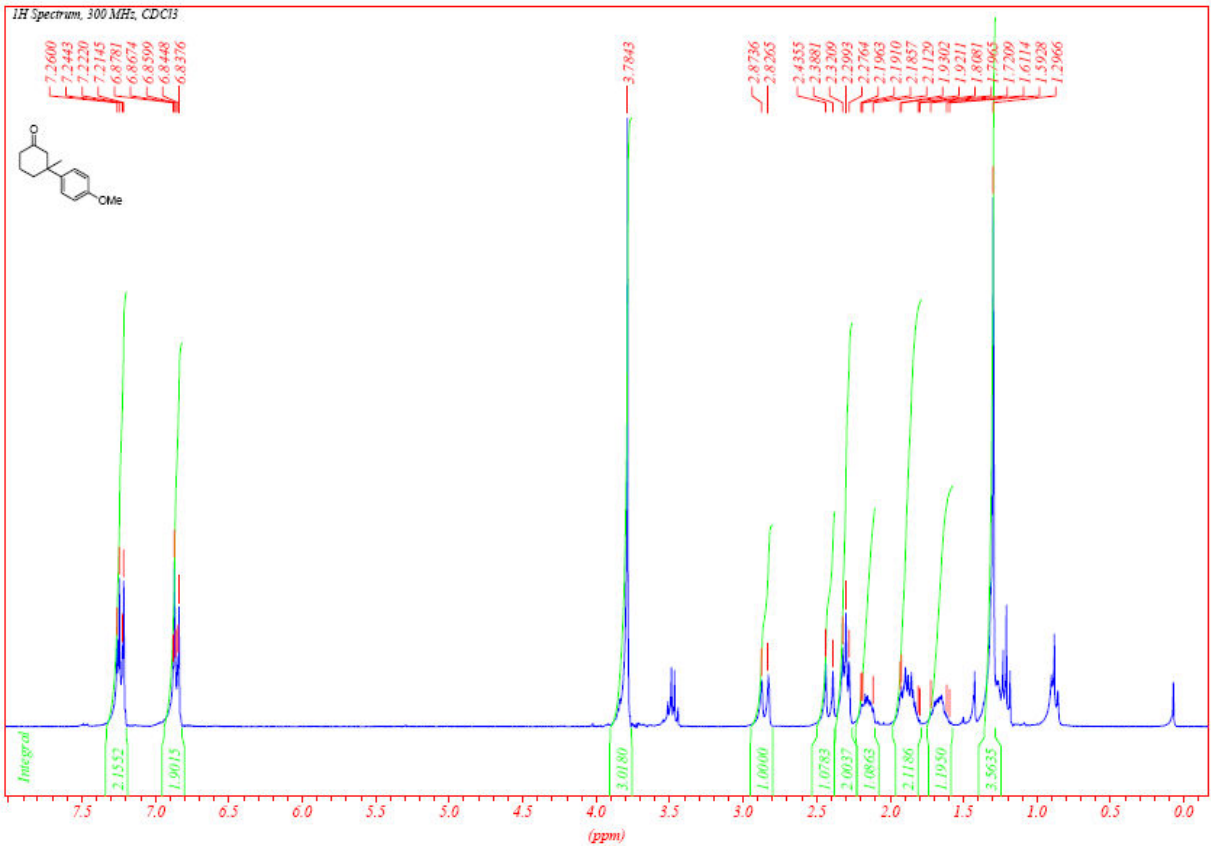


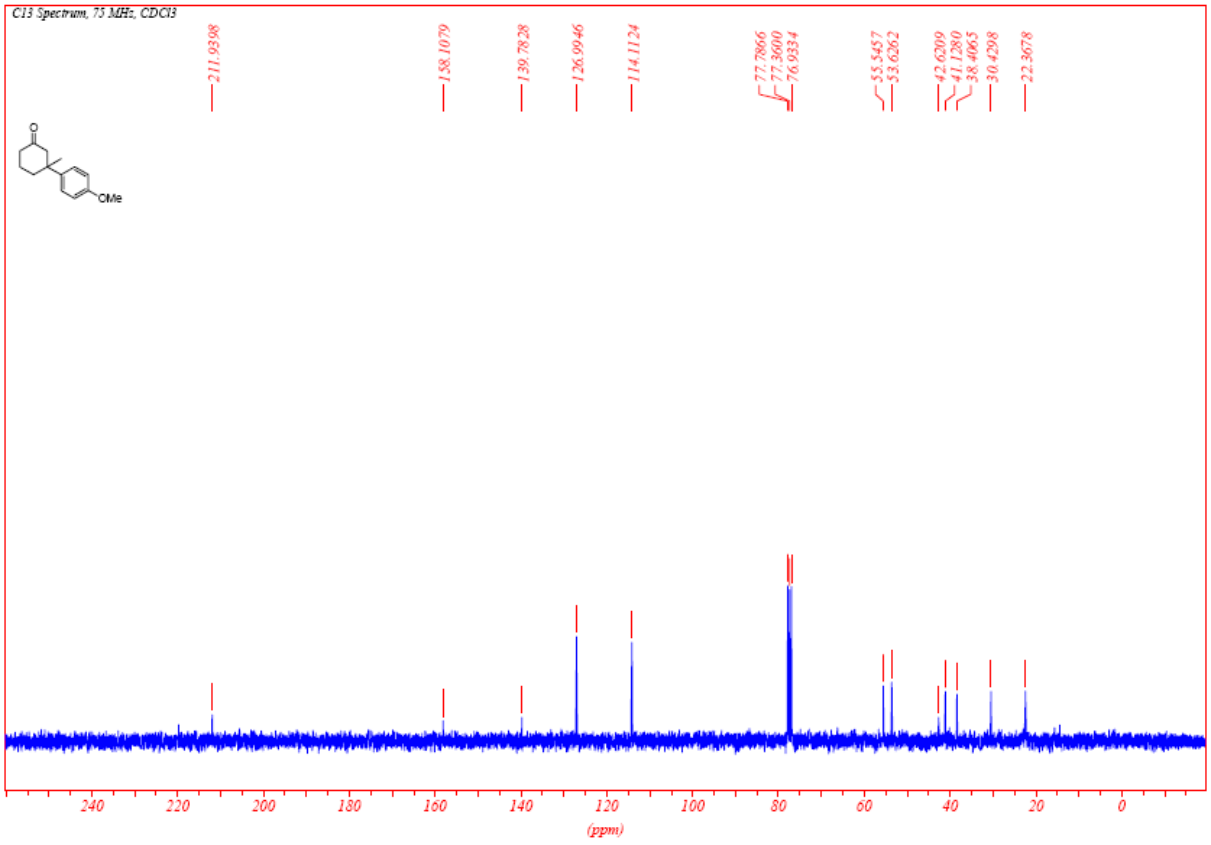
Signal : FID1A.CH

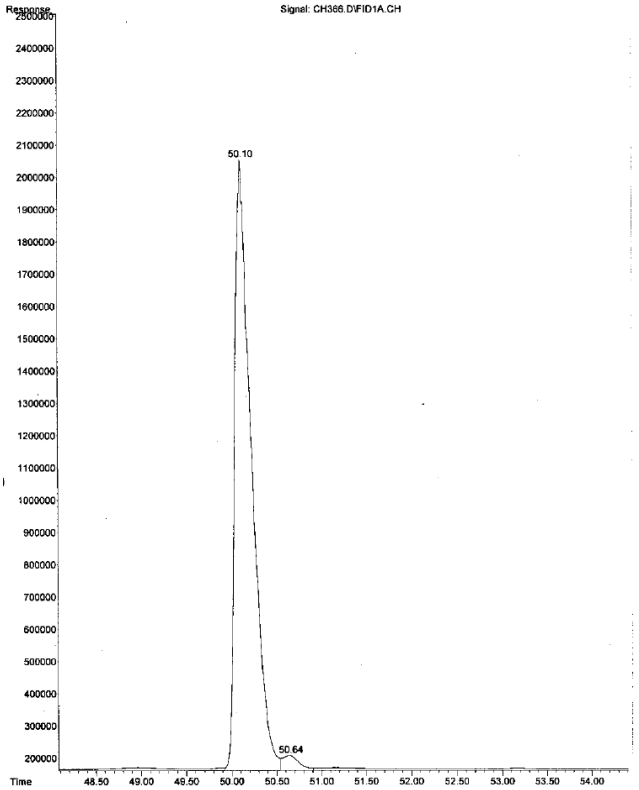
peak #	R.T. min	Start min	End min	PK TY	peak height	peak area	peak % max.	% of total
1	43.006	42.804	43.283	M	90815	8039731	98.56%	49.636%
2	43.832	43.613	44.149	M	93241	8157541	100.00%	50.364%

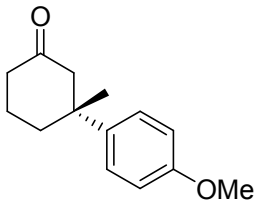
Sum of corrected areas: 16197272

7


1H Spectrum, 300 MHz, CDCl3
7.2600
7.2443
7.2220
7.2145
6.8781
6.8674
6.8599
6.8448
6.8376
3.7843
2.8736
2.8265
2.4355
2.3881
2.3306
2.2993
2.2764
2.1963
2.1910
2.1857
2.1129
1.9802
1.9211
1.8081
1.7965
1.7209
1.6114
1.5928
1.2966
OMe
Integral
2.1552
1.9015
3.0180
1.0000
1.0783
2.0037
1.0863
2.1186
1.1950
3.5635
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

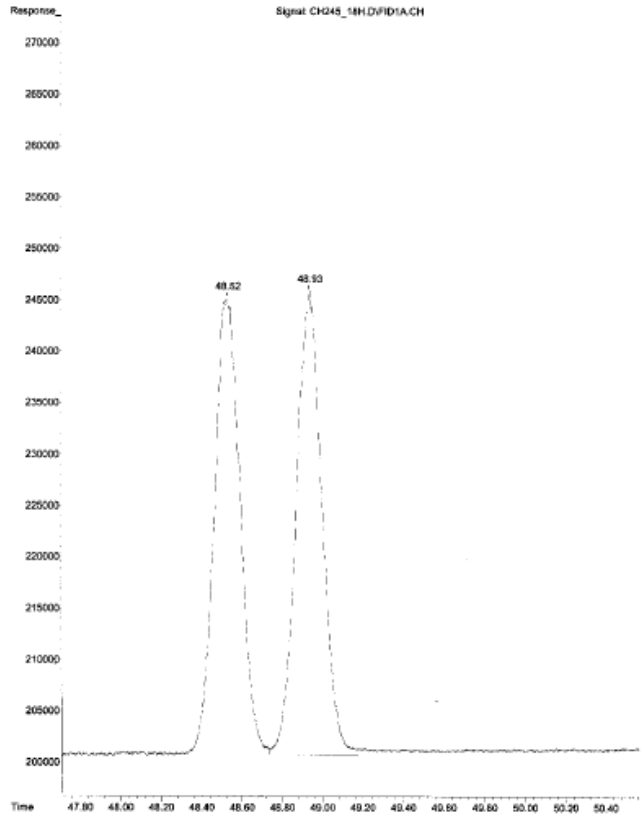

C13 Spectrum, 75 MHz, CDCl3
211.9398
158.1079
139.7828
126.9946
114.1124
77.7866
77.3600
76.9334
55.5457
53.6262
42.6209
41.1280
38.4065
30.4298
22.3678
OMe
240
220
200
180
160
140
120
100
80
60
40
20
0
(ppm)





peak #	R.T. min	Start min	End min	PK TY	peak height	peak area	peak % max.	% of total
1	50.102	49.919	50.536	M	1893975	241884579	100.00%	97.516%
2	50.643	50.536	50.906	M	47348	6161119	2.55%	2.484%

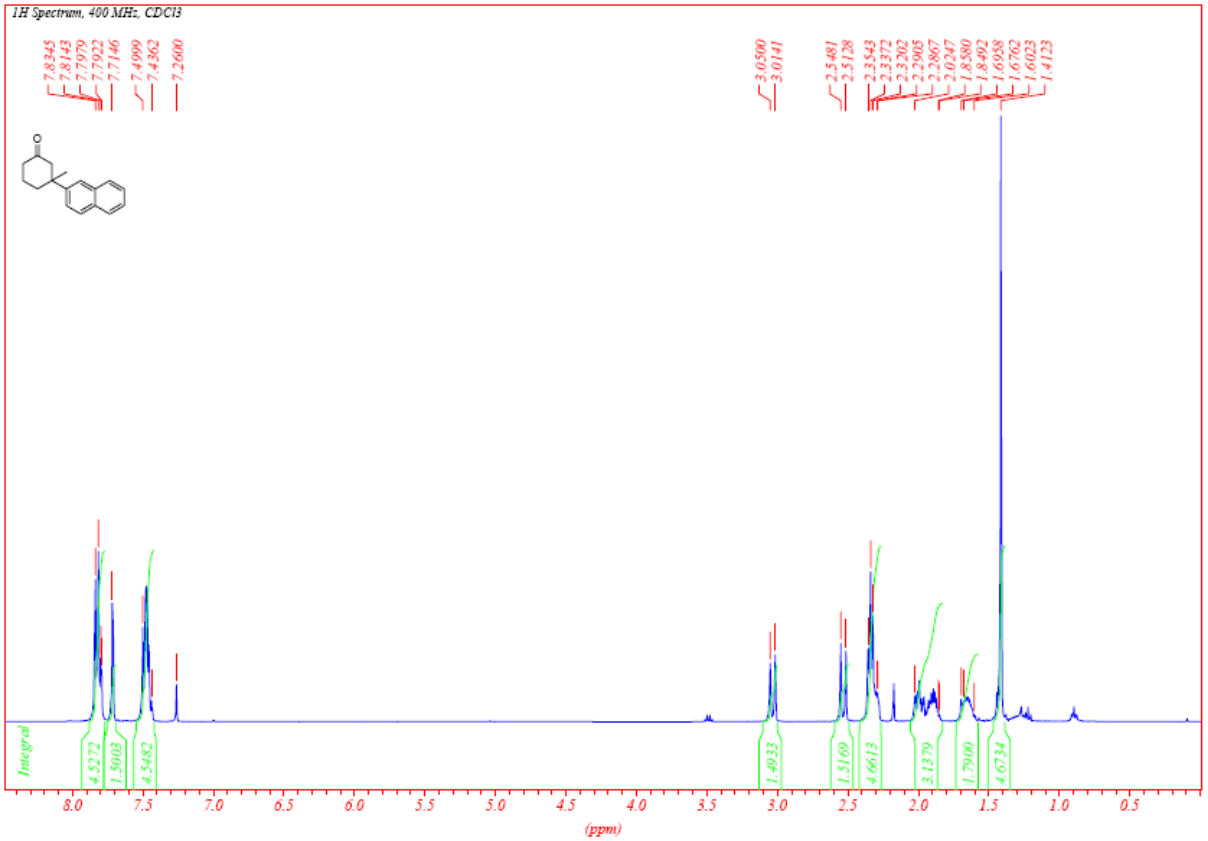
Sum of corrected areas: 248045698

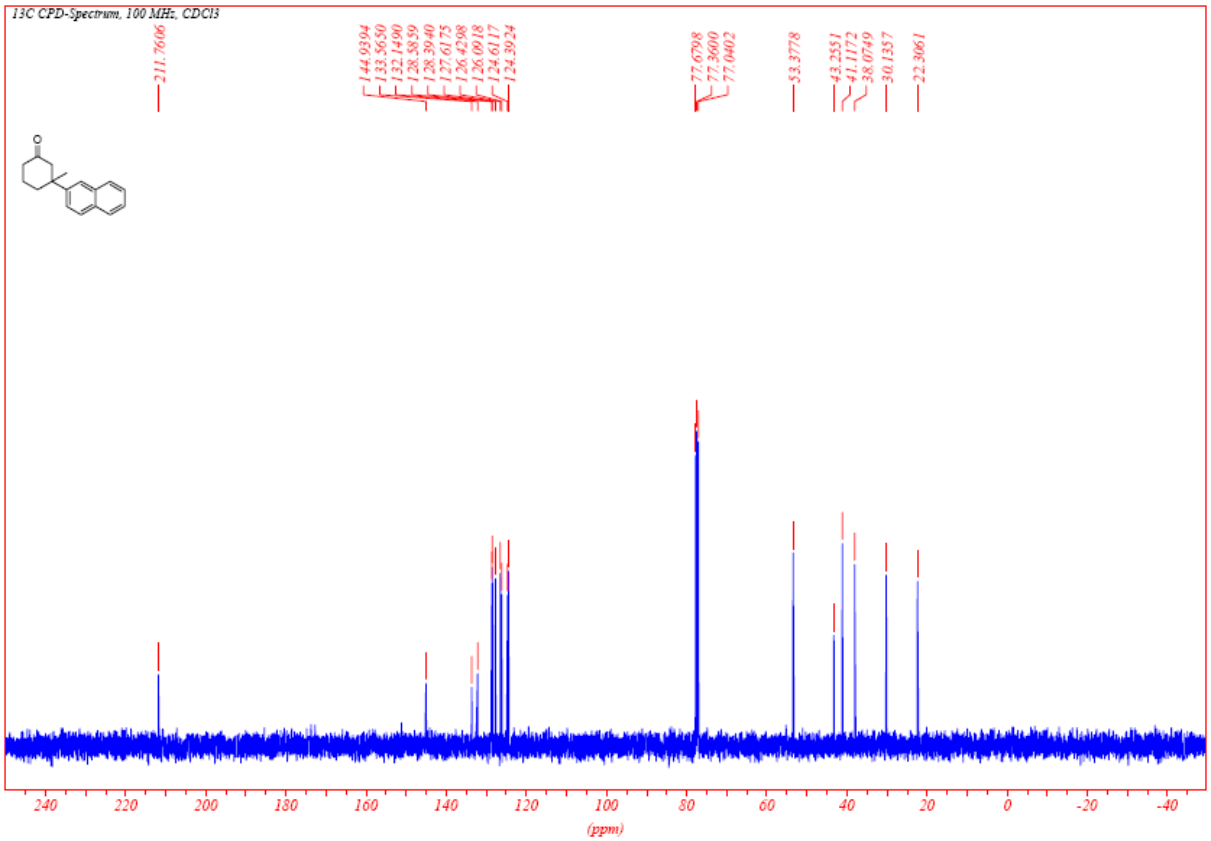


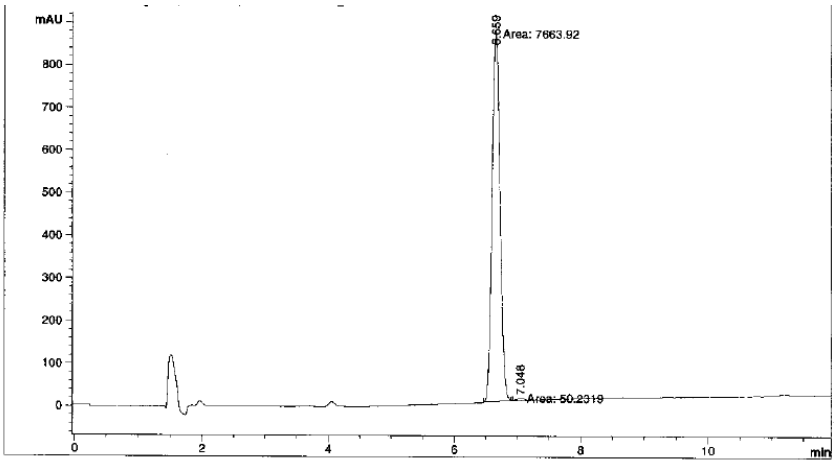
peak #	R.T. min	Start min	End min	PK TY	peak height	peak area	peak % max.	% of total
1	48.524	48.308	48.731	M	45018	3937757	98.60%	49.646%
2	48.932	48.737	49.176	M	45751	3993857	100.00%	50.354%

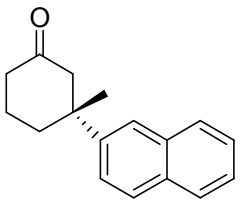
Sum of corrected areas: 7931614

8


1H Spectrum, 400 MHz, CDCl3
7.8345
7.8143
7.7979
7.7922
7.7146
7.4999
7.4362
7.2600
3.0500
3.0141
2.5481
2.5128
2.3543
2.3372
2.3202
2.2905
2.2867
2.0247
1.8580
1.8492
1.6958
1.6762
1.6023
1.4123
Integral
4.5272
1.5003
4.5482
1.4933
1.5169
4.6613
3.1379
1.7900
4.6734
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)


13C CPD-Spectrum, 100 MHz, CDCl3
211.7606
144.9394
133.5650
132.1490
128.5859
128.3940
127.6175
126.4298
126.0918
124.6117
124.3924
77.6798
77.3600
77.0402
53.3778
43.2551
41.1172
38.0749
30.1357
22.3061
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
-40
(ppm)





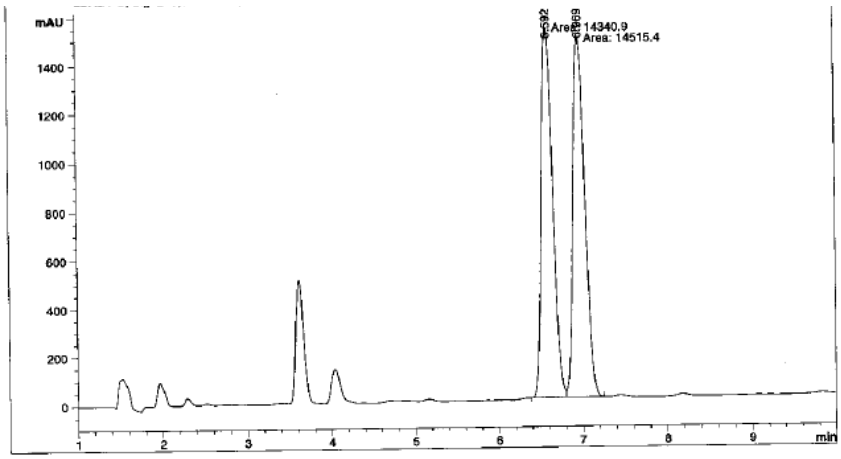
Area Percent Report

Sorted by Signal
Multiplier : 1.000000

Signal 1: LDAD1 C, Sig=210,8 Ref=360,100

Peak #	RT [min]	Type	Width [min]	Area [mAU*sec]	Height [mAU]	Area %
1	6.659	MM	0.148	7663.91992	863.70941	99.3488
2	7.048	MM	0.153	50.23194	5.46509	0.6512

Totals : 7714.15186 869.17450



Area Percent Report

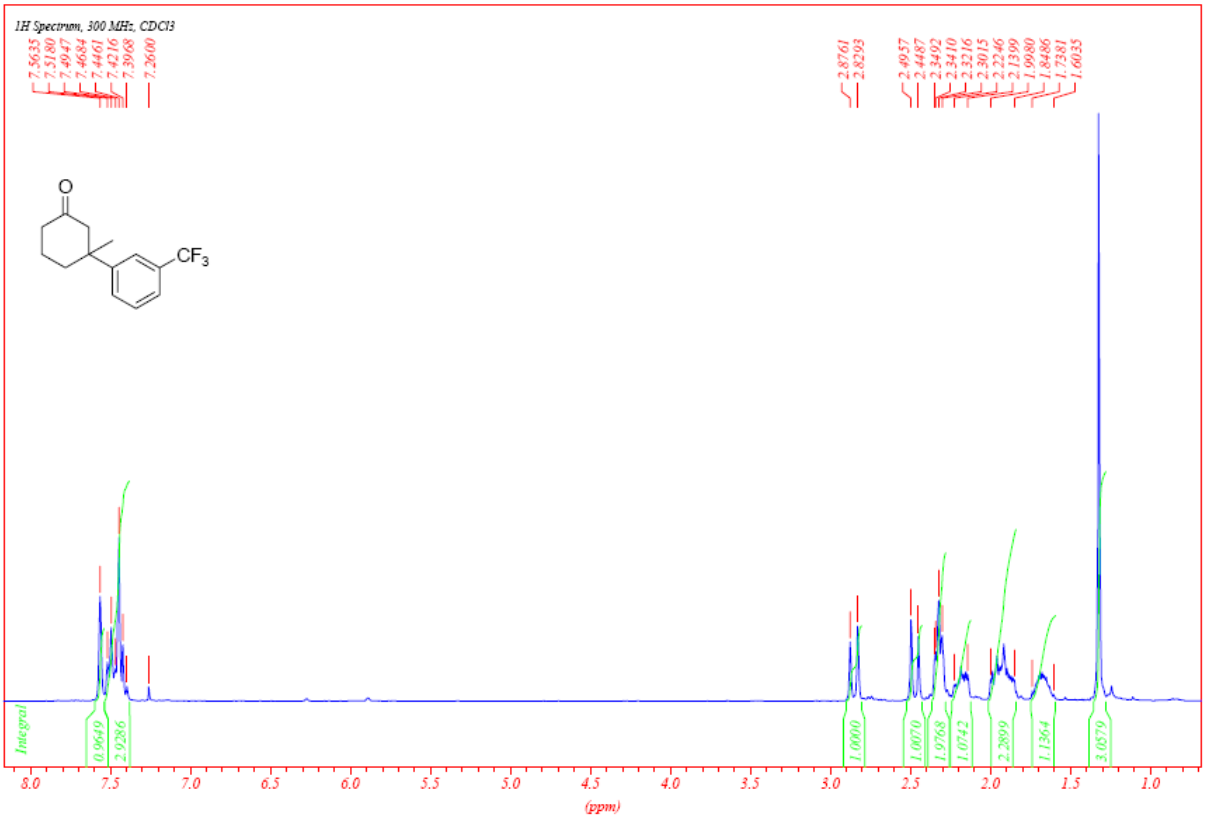
Sorted by Signal
Multiplier : 1.000000

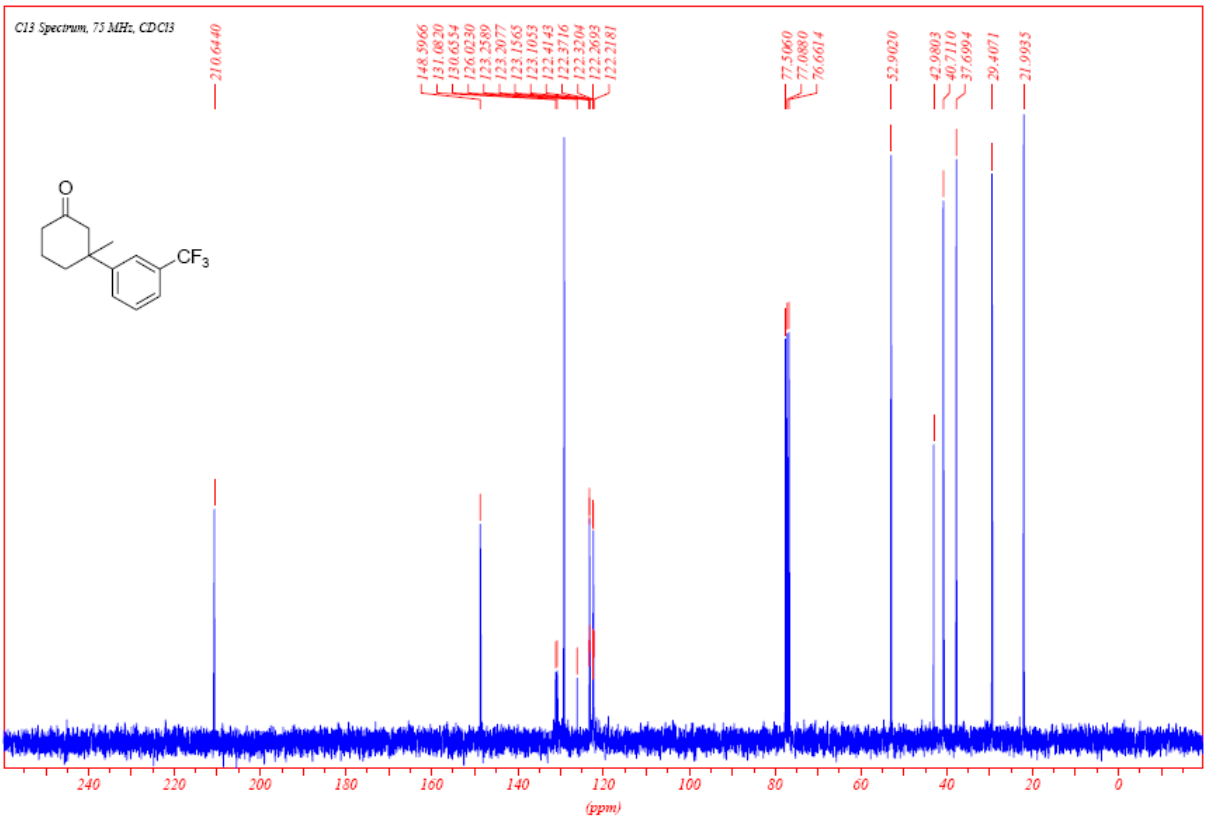
Signal 1: LDAD1 C, Sig=210,8 Ref=360,100

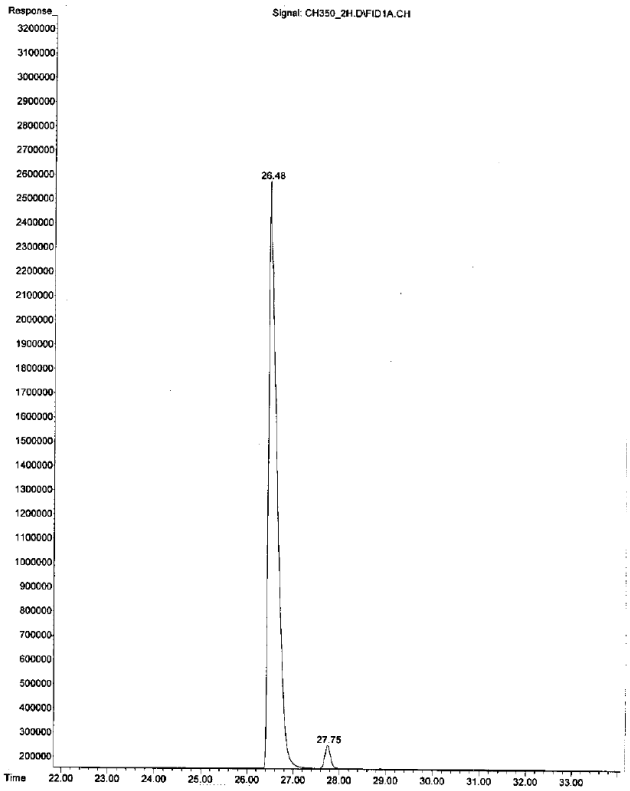
Peak #	RT [min]	Type	Width [min]	Area [mAU*sec]	Height [mAU]	Area %
1	6.592	MM	0.157	14340.86426	1522.11279	49.6976
2	6.969	MM	0.164	14515.38281	1477.75940	50.3024

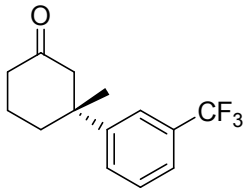
Totals : 28856.24609 2999.87207

9


1H Spectrum, 300 MHz, CDCl3
7.5635
7.5180
7.4947
7.4684
7.4461
7.4216
7.3968
7.2600
2.8761
2.8293
2.4957
2.4487
2.3492
2.3410
2.3216
2.3015
2.2246
2.1399
1.9980
1.8486
1.7381
1.6035
O
CF3
Integral
0.9649
2.9286
1.0000
1.0070
1.9768
1.0742
2.2899
1.1364
3.0579
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
(ppm)

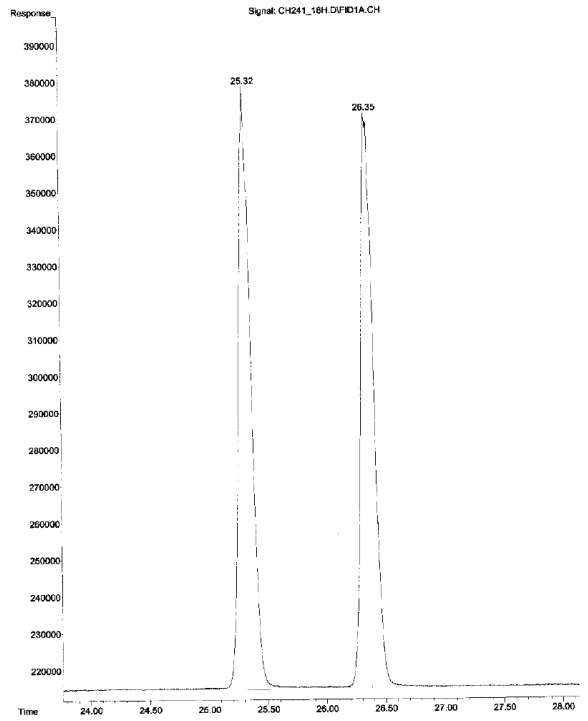

C13 Spectrum, 75 MHz, CDCl3
210.6440
148.3966
131.6820
130.6534
126.6230
123.2589
123.2077
123.1565
123.1053
122.4143
122.3716
122.3204
122.2693
122.2181
77.5060
77.0880
76.6614
52.9020
42.9803
40.7110
37.6994
29.4071
21.9935
O
CF3
240
220
200
180
160
140
120
100
80
60
40
20
0
(ppm)





peak #	R.T. min	Start min	End min	PK TY	peak height	peak area	peak % max.	% of total
1	26.477	26.343	27.494	M	2421843	306106433	100.00%	97.437%
2	27.748	27.567	28.047	M	96249	8050392	2.63%	2.563%

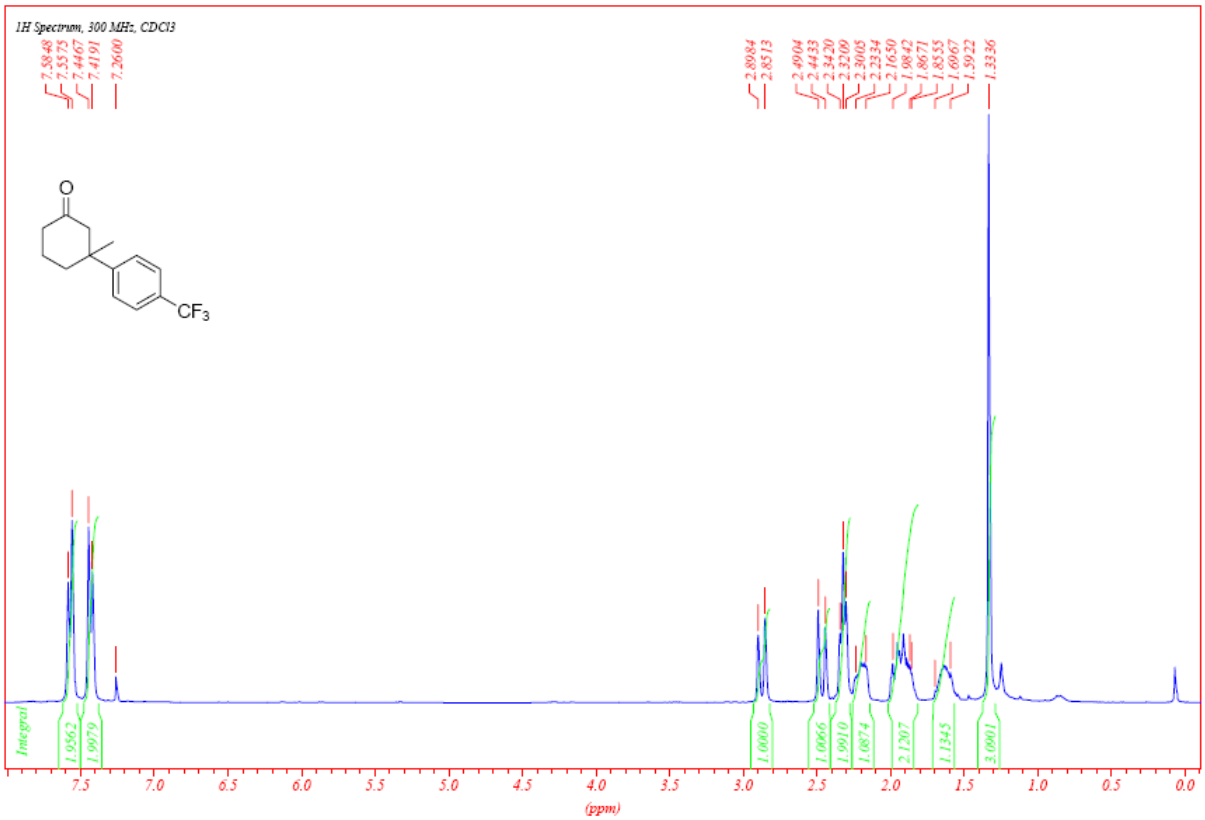
Sum of corrected areas: 314156825

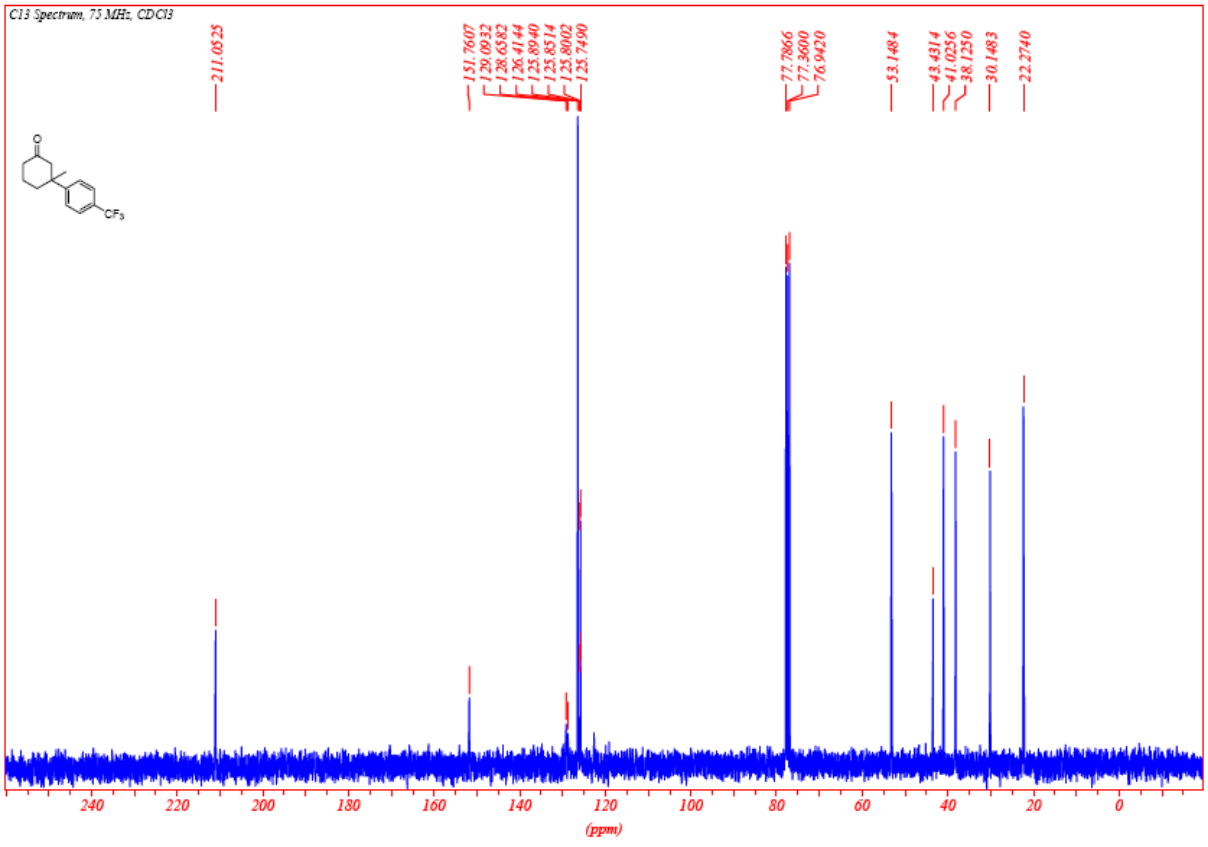


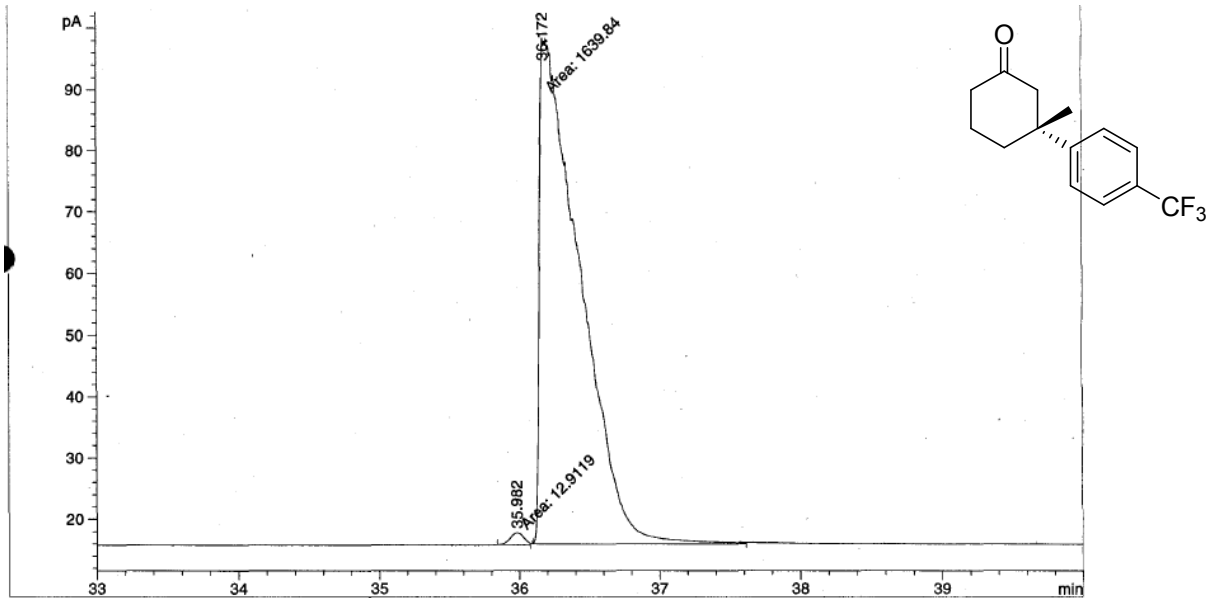
peak #	R.T. min	Start min	End min	PK TY	peak height	peak area	peak % max.	% of total
1	25.317	25.141	25.591	M	164140	11674232	100.00%	50.176%
2	26.346	26.186	26.597	M	156356	11592324	99.30%	49.824%

Sum of corrected areas: 23266556

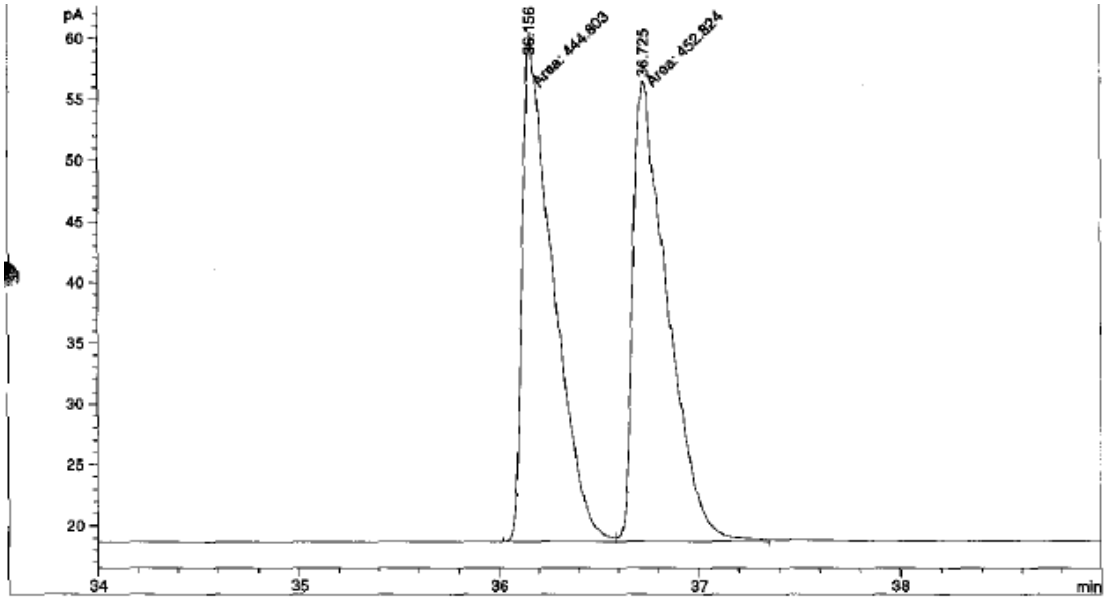
10


1H Spectrum, 300 MHz, CDCl3
7.5848
7.5575
7.4467
7.4191
7.2600
2.8984
2.8513
2.4904
2.4433
2.3420
2.3209
2.3005
2.2534
2.1650
1.9842
1.8671
1.8555
1.6967
1.5922
1.3336
O
CF3
Integral
1.9562
1.9979
1.0000
1.0066
1.9910
1.0874
2.1207
1.1345
3.0601
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)


C13 Spectrum, 75 MHz, CDCl3
211.0525
151.7607
129.0932
128.6582
126.4144
125.8940
125.8514
125.8002
125.7490
77.7866
77.3600
76.9420
53.1484
43.4314
41.0256
38.1250
30.1483
22.2740
O
CF3
240
220
200
180
160
140
120
100
80
60
40
20
0
(ppm)

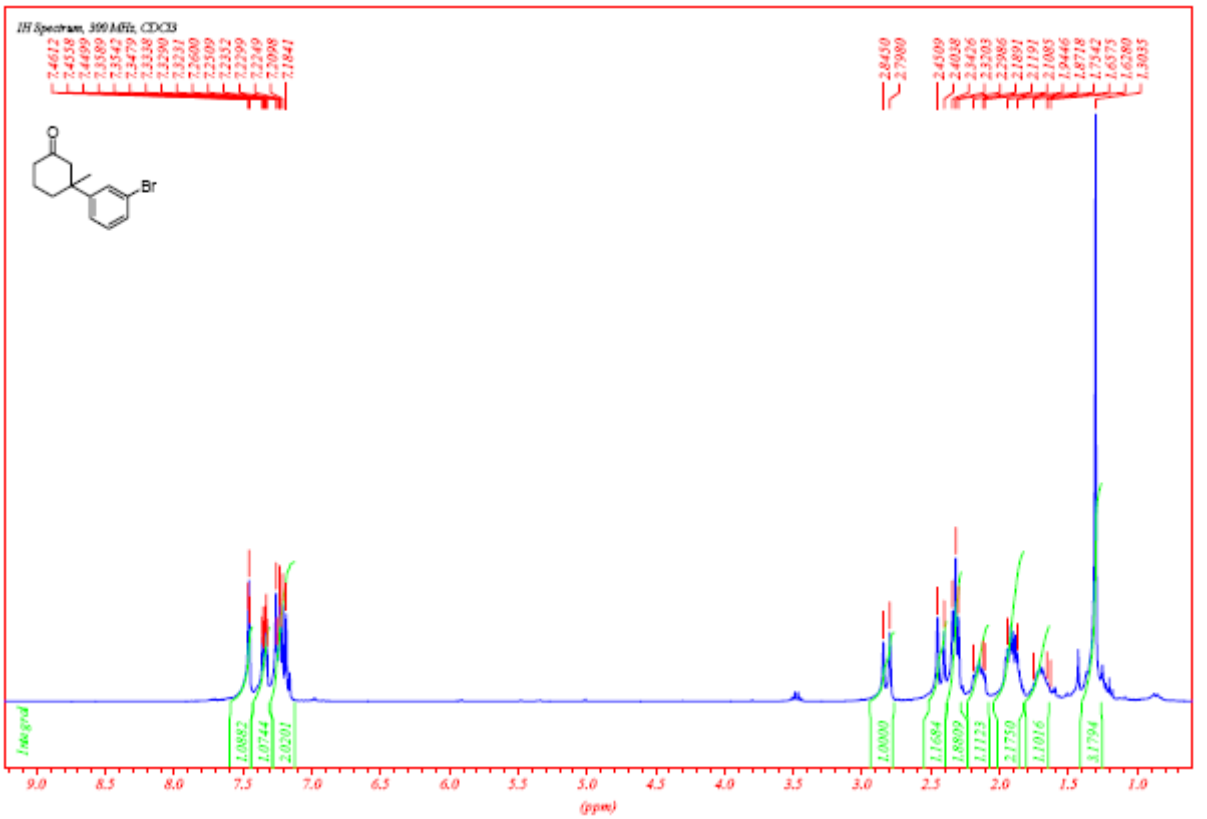


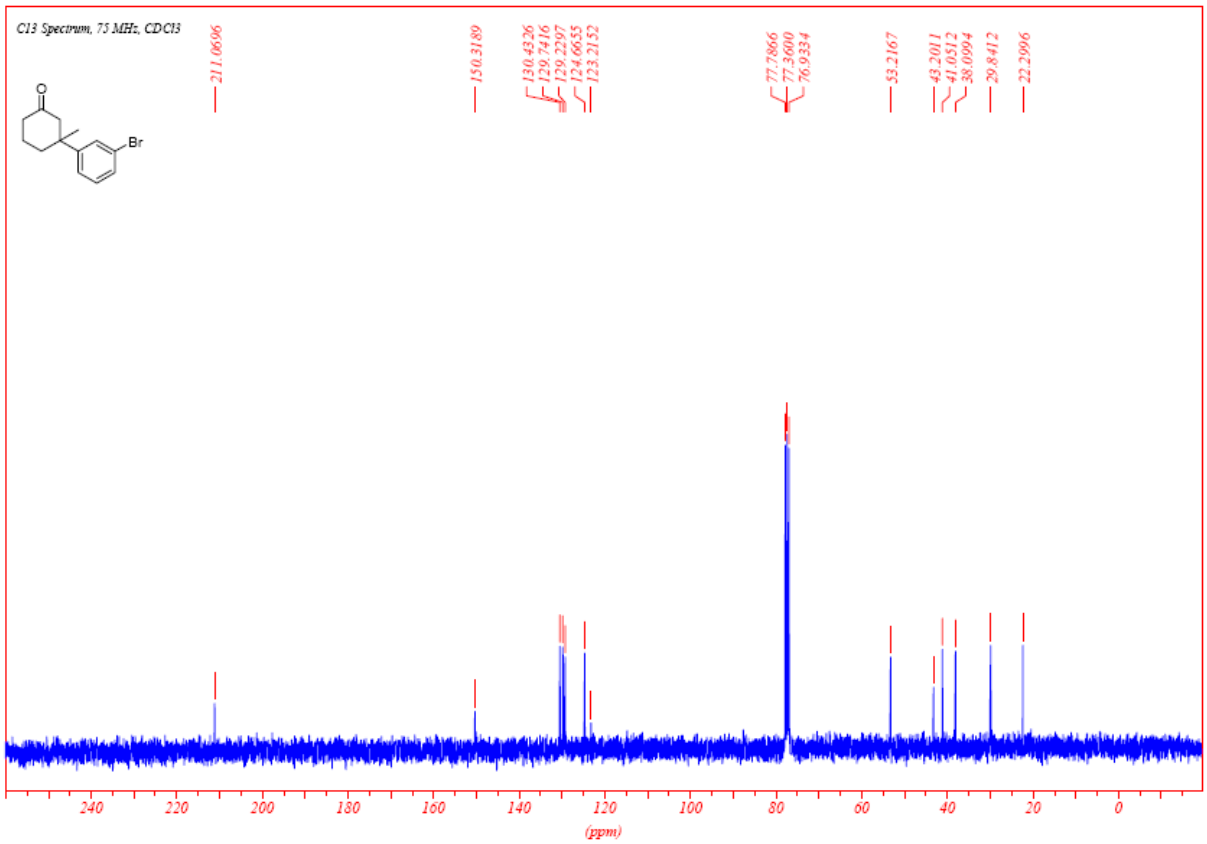
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	35.982	MM	0.1103	12.91188	1.95017	0.78124
2	36.172	MM	0.3306	1639.83777	82.68103	99.21876
Totals :				1652.74965	84.63120	

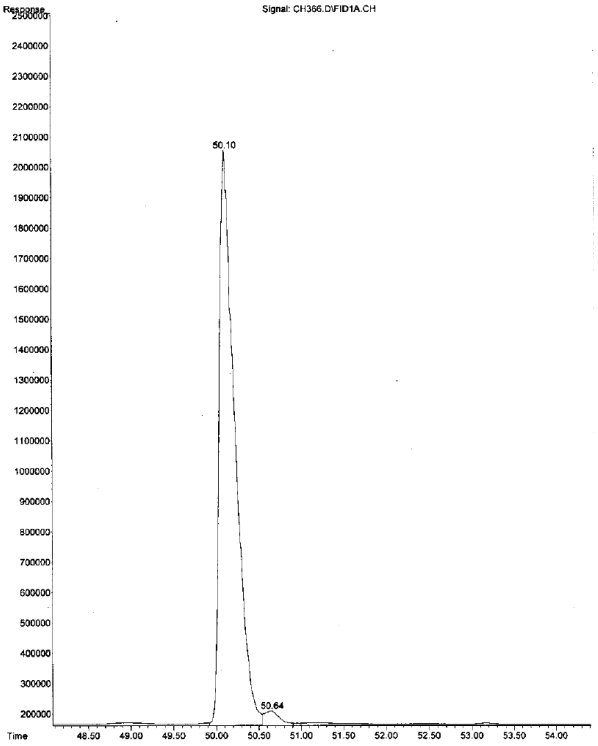


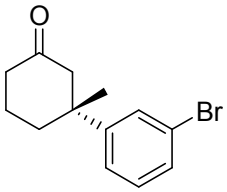
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	36.156	MM	0.1769	444.80341	41.90745	49.55325
2	36.725	MM	0.1998	452.82364	37.78034	50.44675
Totals :				897.62704	79.68779	

11





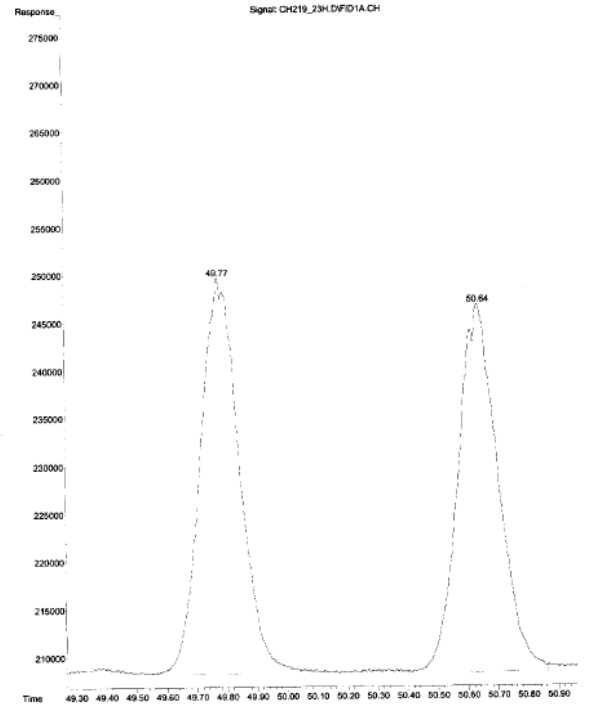




peak #	R.T. min	Start min	End min	PK TY	peak height	peak area	peak % max.	% of total
1	50.102	49.919	50.536	M	1893975	241884579	100.00%	97.516%
2	50.643	50.536	50.906	M	47348	6161119	2.55%	2.484%

Sum of corrected areas: 248045698

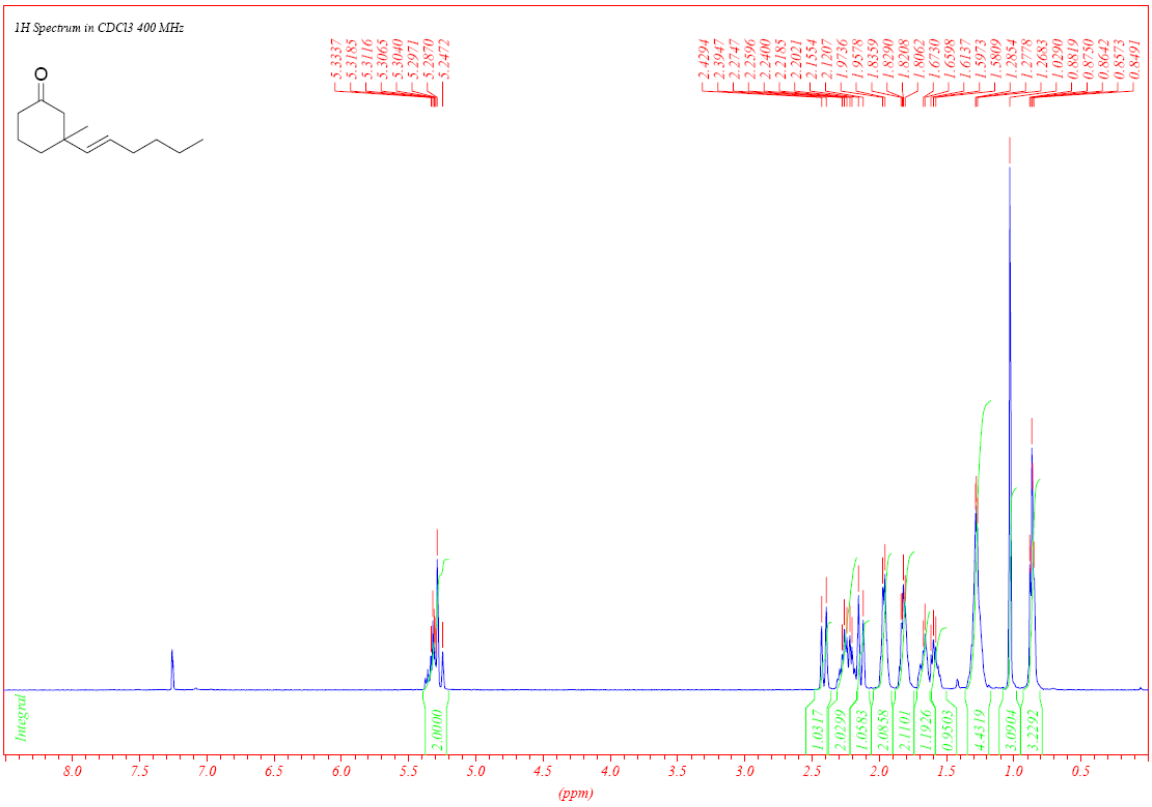
```
File       :C:\MSDChem\2\DATA\CH219_23H.D
Operator   : CH
Acquired   : 11.09.2007 01:28:21 PM using AcqMethod FRONT.M
Instrument :
  GC CHIRAL
Sample Name: CH219_23H
Misc Info  : HYDRODEX-B-6  (120-0-1-170-5) v=50 cm/s
Vial Number: 1
```

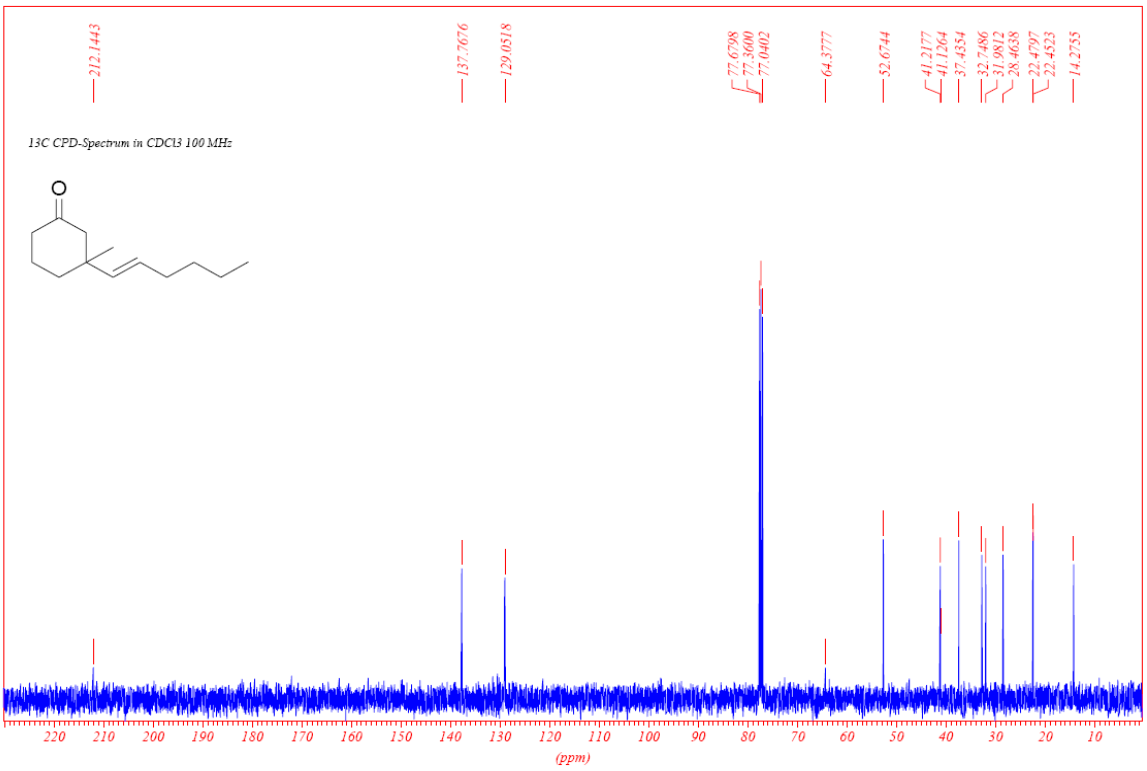


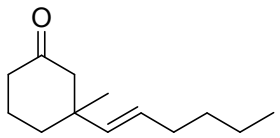
peak #	R.T. min	Start min	End min	PK TY	peak height	peak area	peak % max.	% of total
1	51.389	51.008	52.149	M	3469138	499411376	100.00%	98.841%
2	52.472	52.216	52.722	M	46826	5857496	1.17%	1.159%

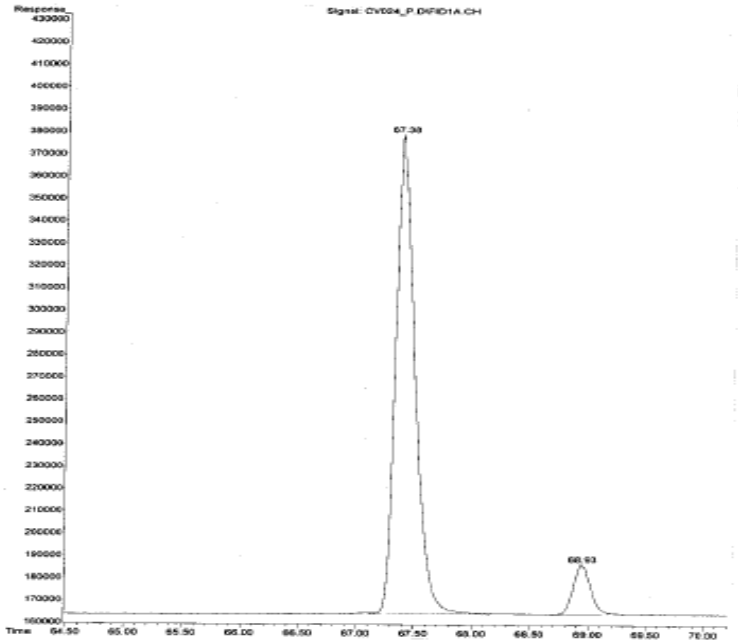
Sum of corrected areas: 505268871

12


1H Spectrum in CDCl3 400 MHz
5.3337
5.3185
5.3116
5.3065
5.3040
5.2971
5.2870
5.2472
2.4294
2.3947
2.2747
2.2596
2.2400
2.2185
2.2021
2.1554
2.1207
1.9736
1.9578
1.8359
1.8290
1.8208
1.8062
1.6730
1.6598
1.6137
1.5973
1.5809
1.2854
1.2778
1.2683
1.0290
0.8819
0.8750
0.8642
0.8573
0.8491
Integral
2.0000
1.0317
2.0299
1.0583
2.0858
2.1101
1.1926
0.9503
4.4319
3.0904
3.2292
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)

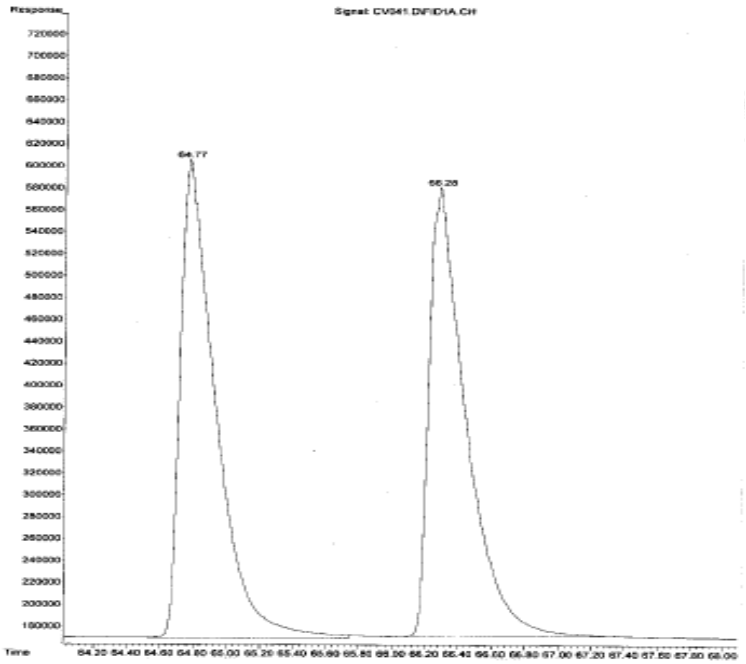

212.1443
137.7676
129.0518
77.6798
77.3600
77.0402
64.3777
52.6744
41.2177
41.1264
37.4354
32.7486
31.9812
28.4638
22.4797
22.4523
14.2755
13C CPD-Spectrum in CDCl3 100 MHz
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)





peak #	R.T. min	Start min	End min	PK TY	peak height	peak area	peak % max.	% of total
1	67.381	67.115	68.182	M	215257	26172175	100.00%	91.738%
2	68.931	68.679	69.264	M	22573	2267091	9.01%	8.262%

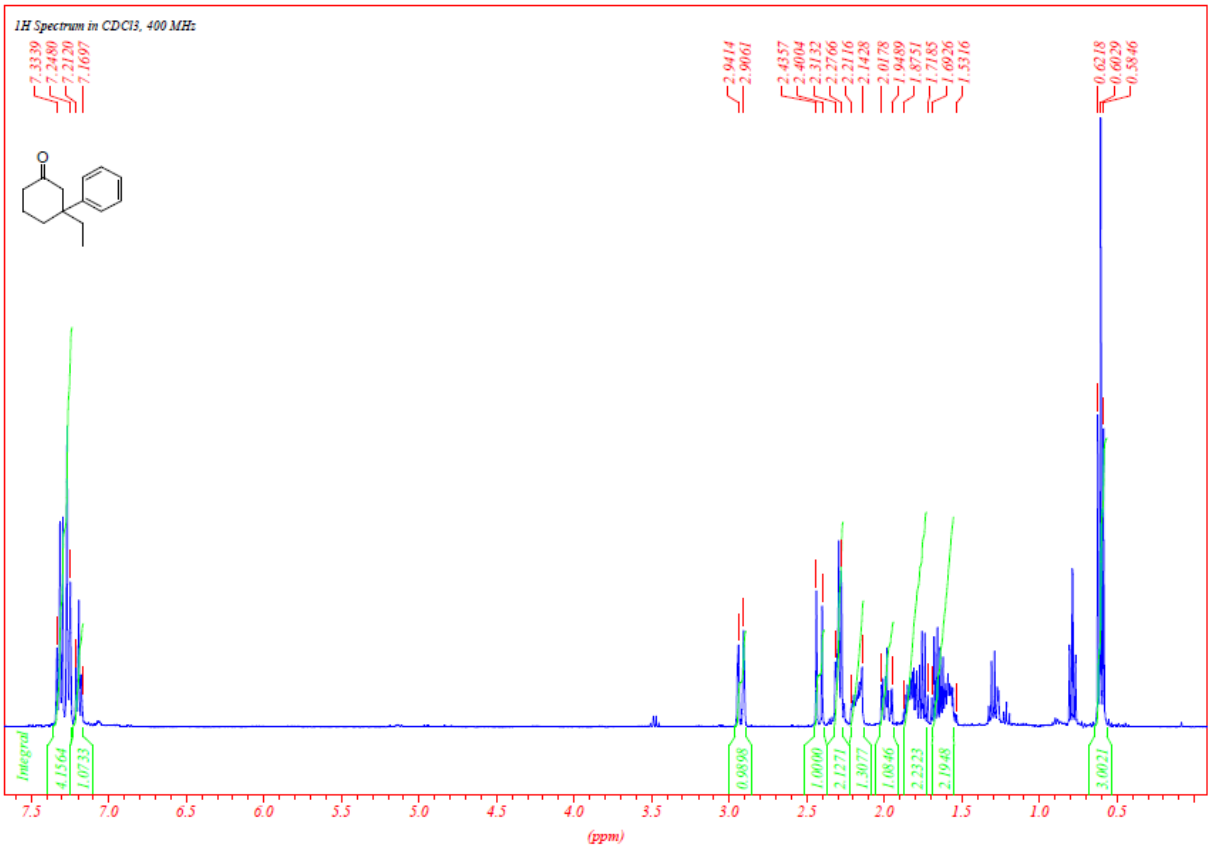
Sum of corrected areas: 27439265

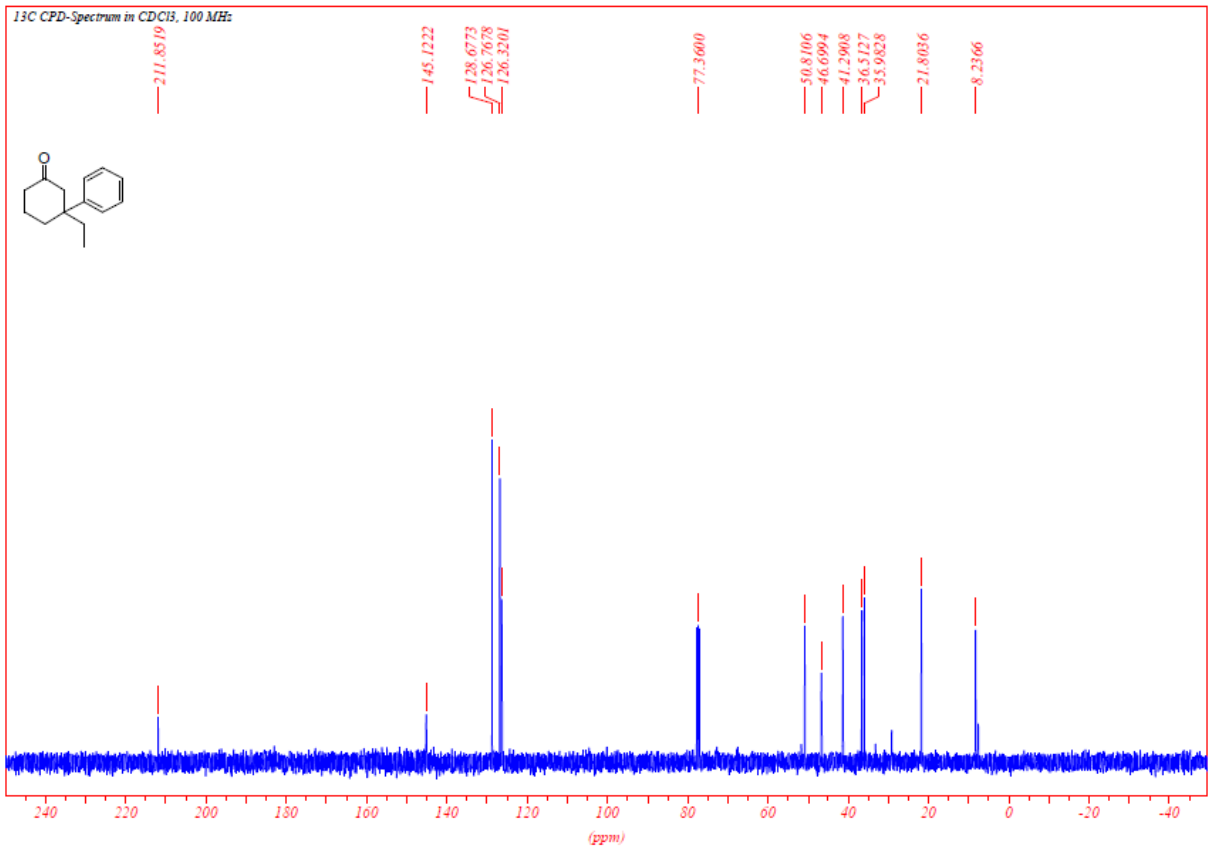


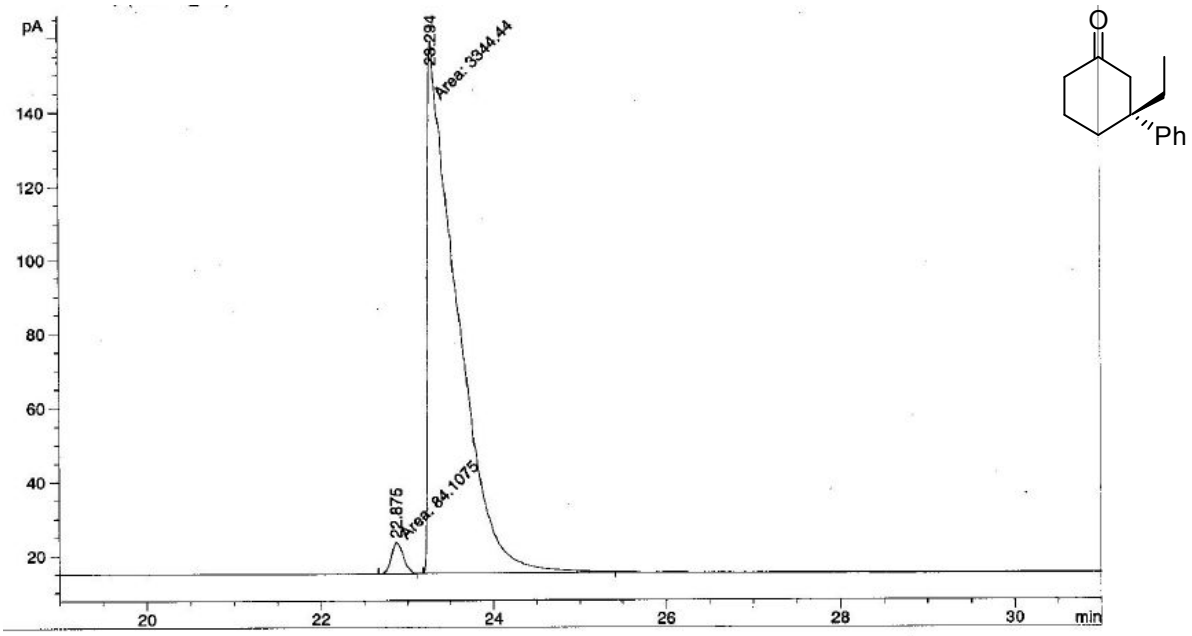
peak #	R.T. min	Start min	End min	PK TY	peak height	peak area	peak % max.	% of total
1	64.767	64.525	65.742	M	436938	64208849	100.00%	50.379%
2	66.281	66.082	67.259	M	410038	63241335	98.49%	49.621%

Sum of corrected areas: 127449985

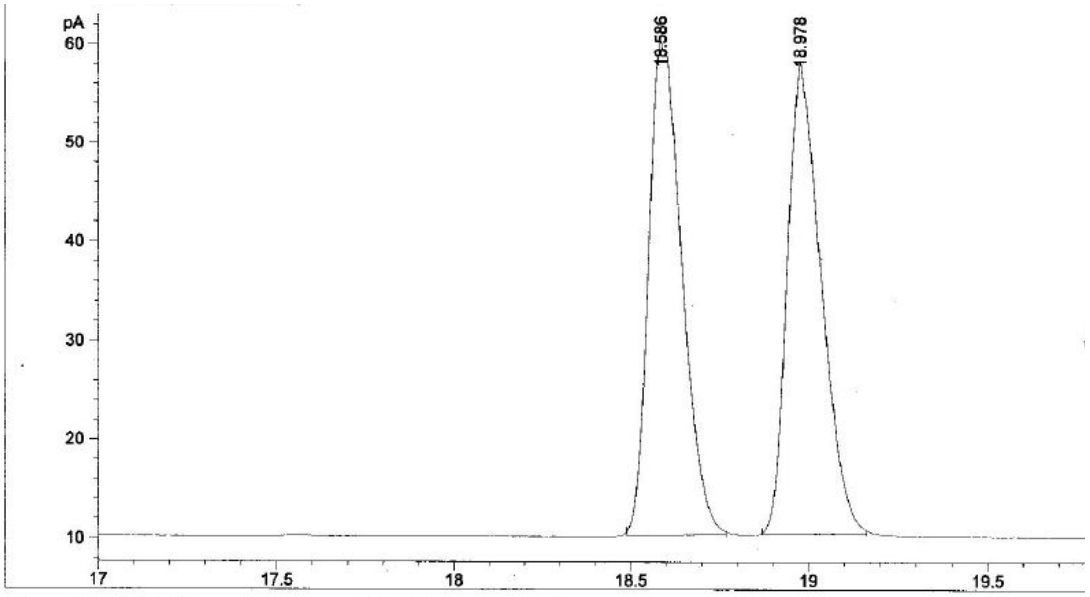
13


1H Spectrum in CDCl3, 400 MHz
7.3339
7.2480
7.2120
7.1697
2.9414
2.9061
2.4357
2.4004
2.3132
2.2766
2.2116
2.1428
2.0178
1.9489
1.8751
1.7185
1.6926
1.5316
0.6218
0.6029
0.5846
Integral
4.1564
1.0733
0.9898
1.0000
2.1271
1.3077
1.0846
2.2322
2.1948
3.0021
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)


13C CPD-Spectrum in CDCl3, 100 MHz
211.8519
145.1222
128.6773
126.7678
126.3201
77.3600
50.8106
46.6994
41.2968
36.5127
35.9828
21.8036
8.2366
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
-40
(ppm)

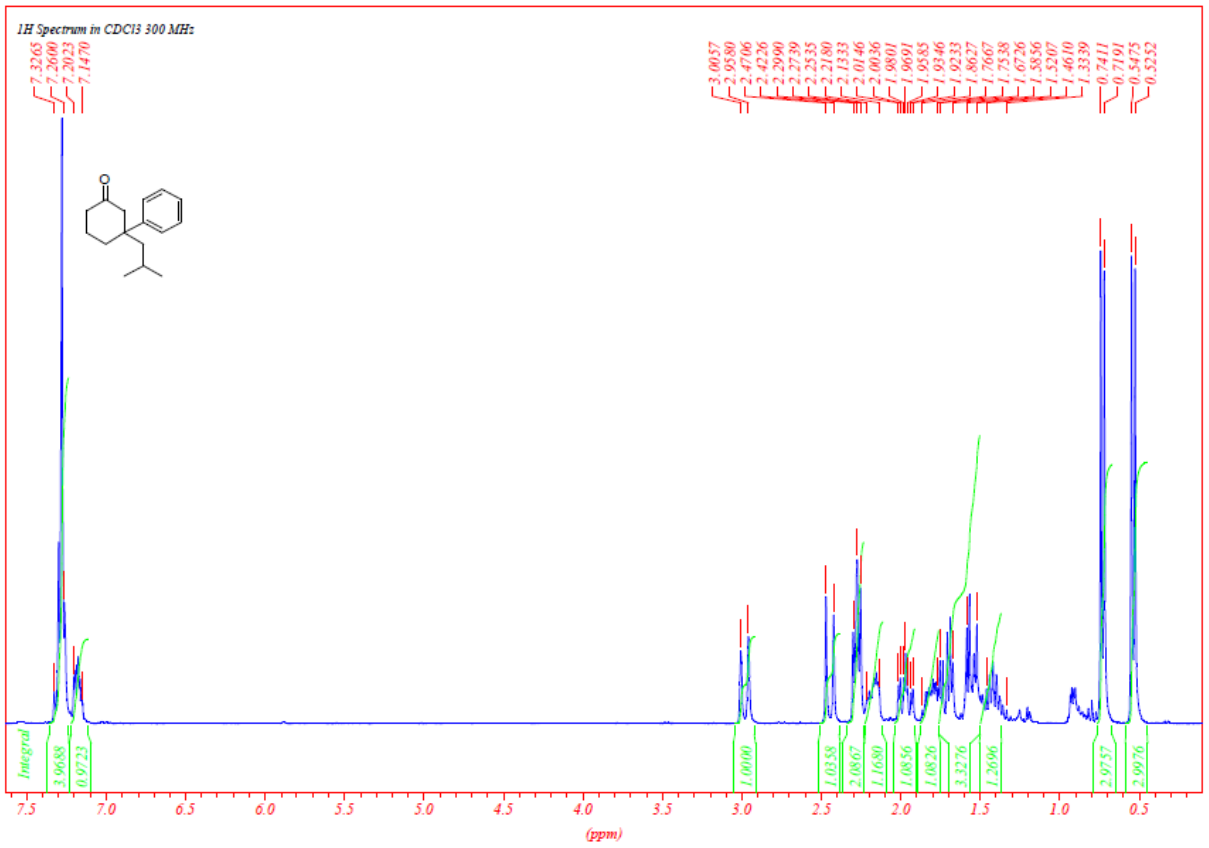


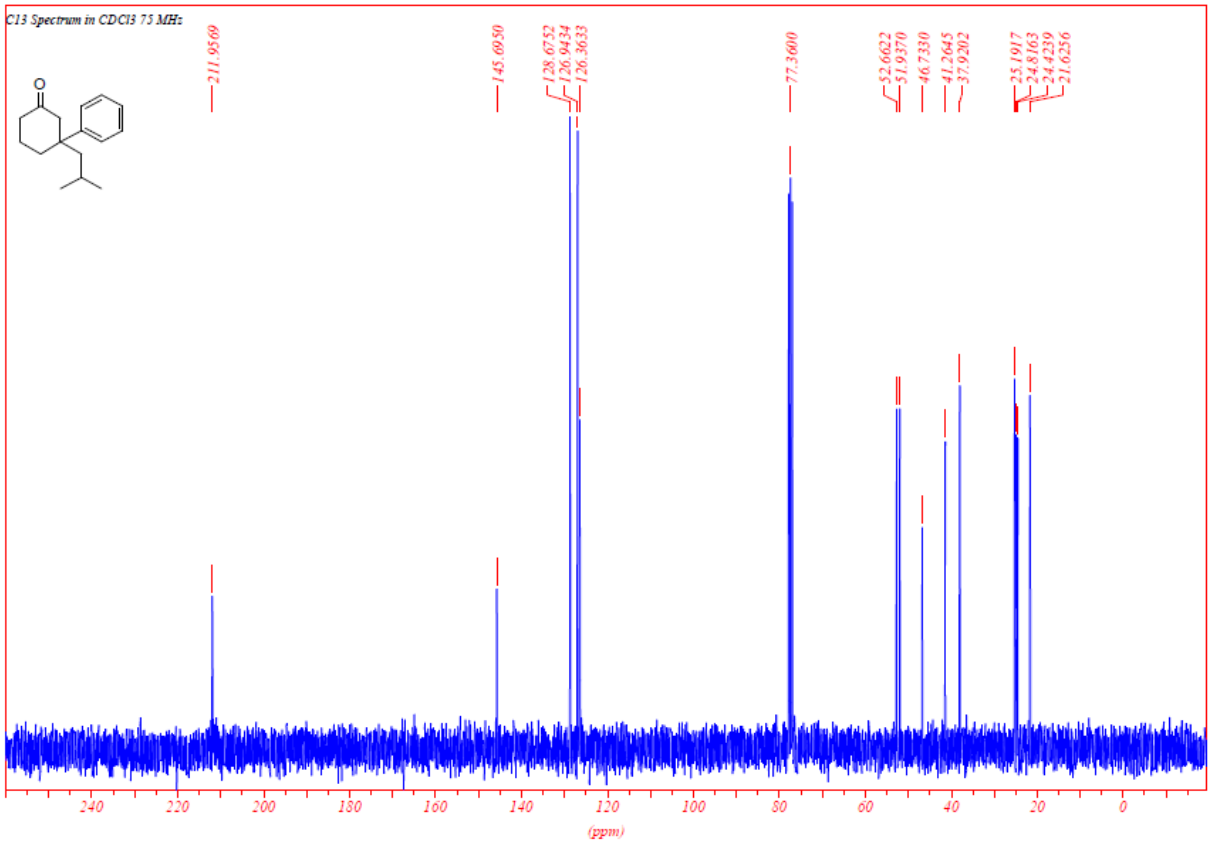
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	22.875	MM	0.1654	84.10752	8.47424	2.45315
2	23.294	MM	0.3879	3344.44141	143.68651	97.54685
Totals :				3428.54893	152.16075	

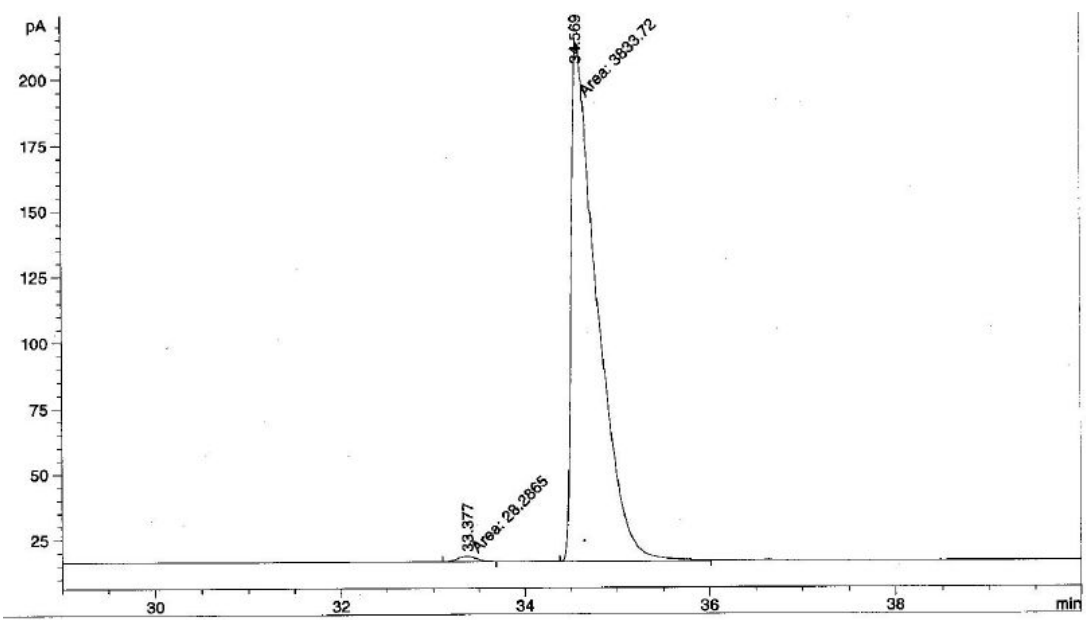


Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	18.586	BB	0.0870	326.48895	50.10294	50.98794
2	18.978	BB	0.0907	313.83694	47.73767	49.01206
Totals :				640.32590	97.84060	

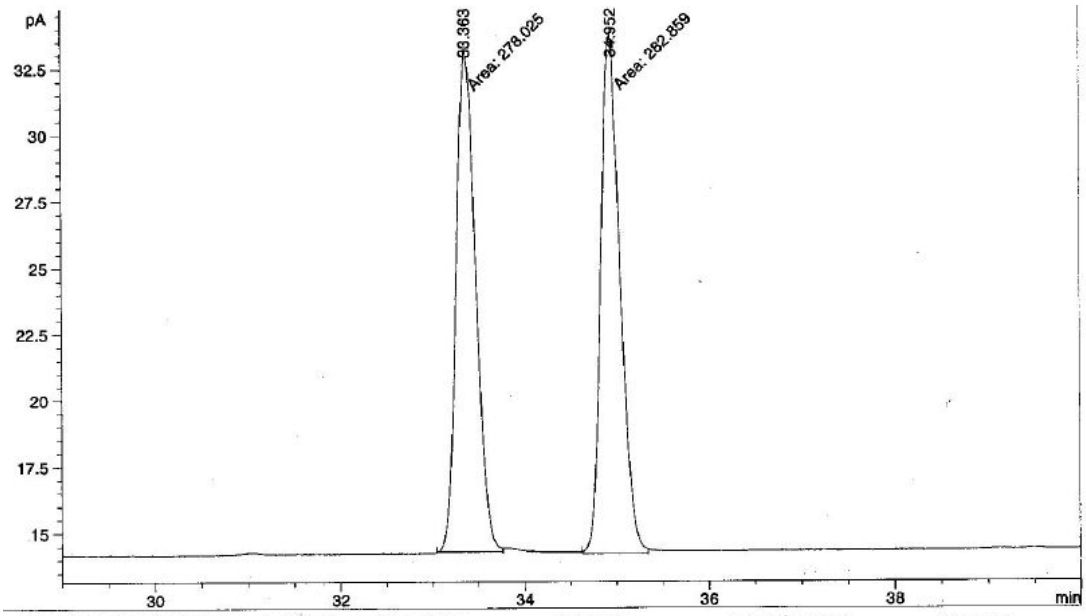
14


1H Spectrum in CDCl3 300 MHz
7.3265
7.2600
7.2023
7.1470
3.0057
2.9580
2.4706
2.4226
2.2990
2.2739
2.2535
2.2180
2.1333
2.0146
2.0036
1.9801
1.9691
1.9585
1.9346
1.9233
1.8627
1.7667
1.7538
1.6726
1.5856
1.5207
1.4610
1.3339
0.7411
0.7191
0.5475
0.5252
Integral
3.9688
0.9723
1.0000
1.0358
2.0867
1.1680
1.0856
1.0826
3.3276
1.2696
2.9757
2.9976
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)


C13 Spectrum in CDCl3 75 MHz
211.9569
145.6950
128.6752
126.9434
126.3633
77.3600
52.6622
51.9370
46.7330
41.2645
37.9202
25.1917
24.8163
24.4239
21.6256
240
220
200
180
160
140
120
100
80
60
40
20
0
(ppm)

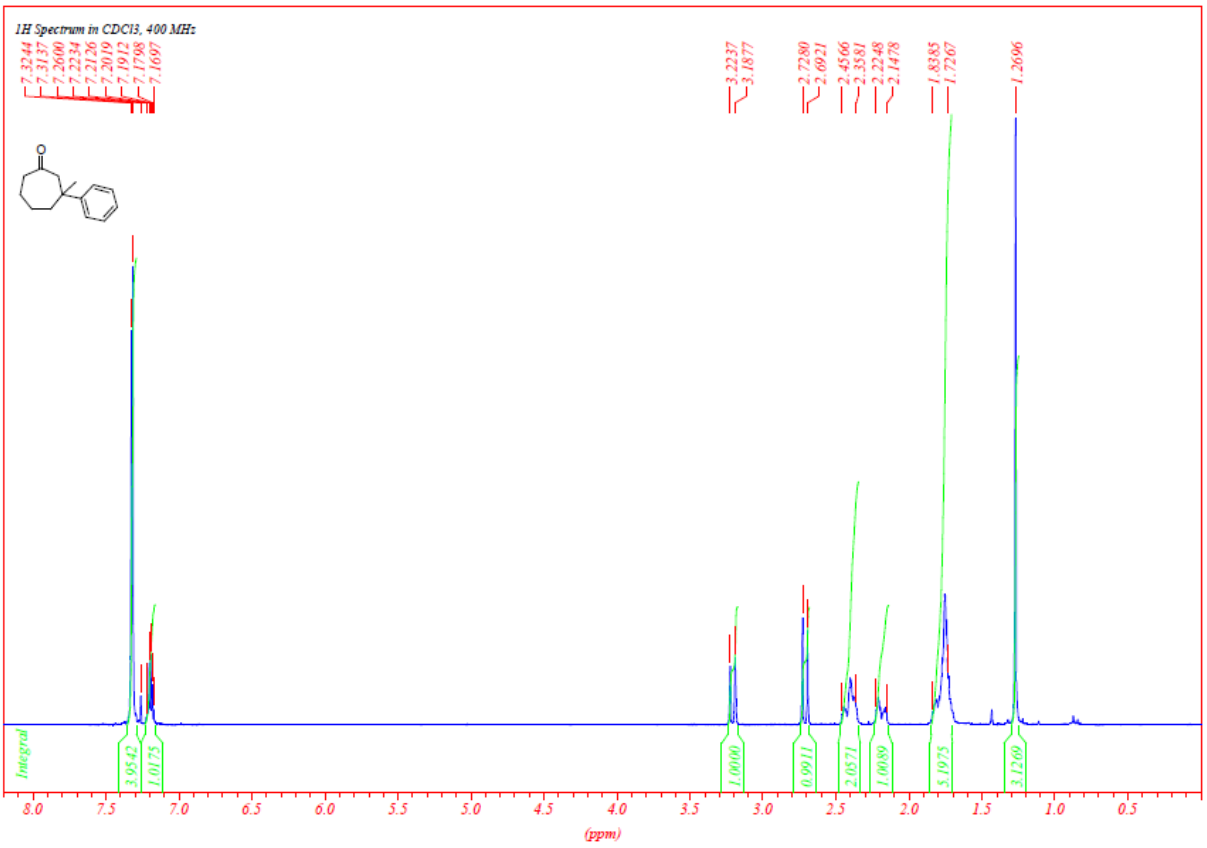


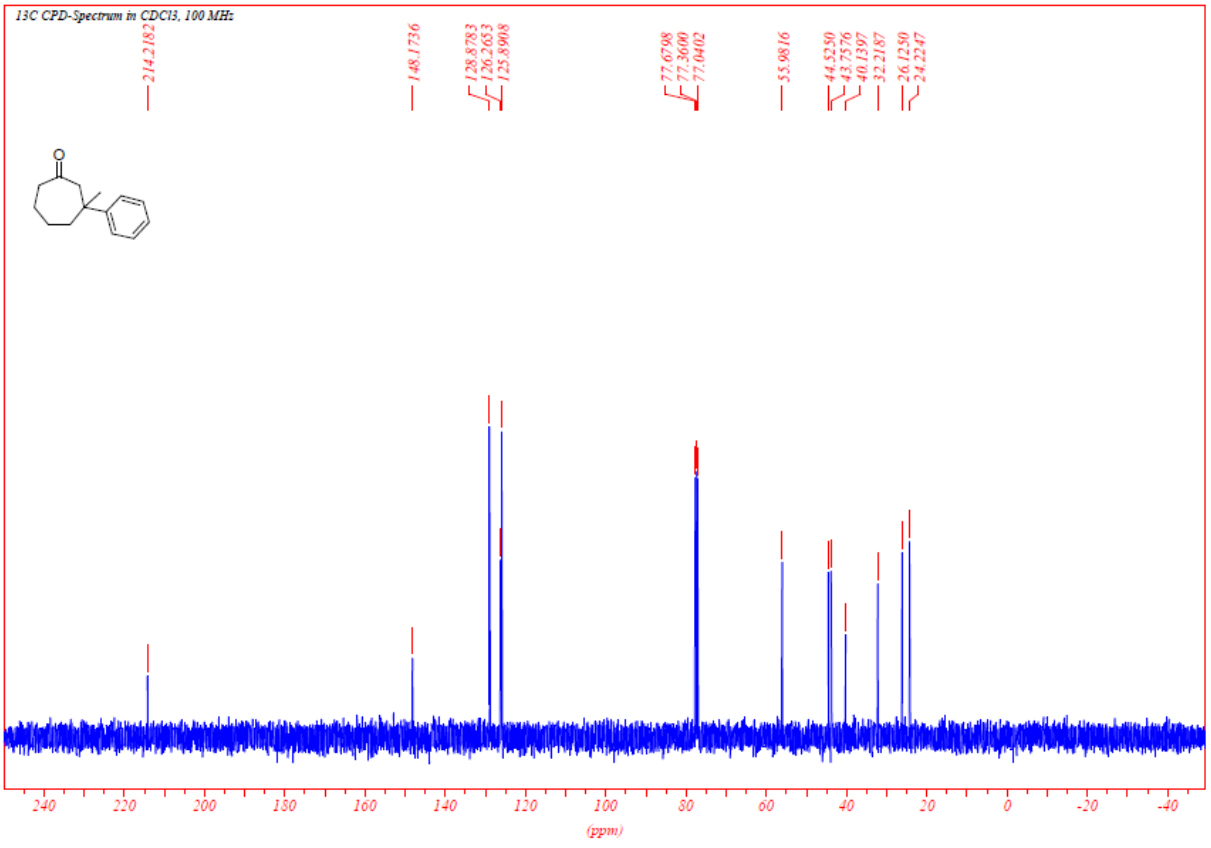
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	33.377	MM	0.2367	28.28653	1.99142	0.73243
2	34.569	MM	0.3223	3833.72339	198.25659	99.26757
Totals :				3862.00992	200.24801	

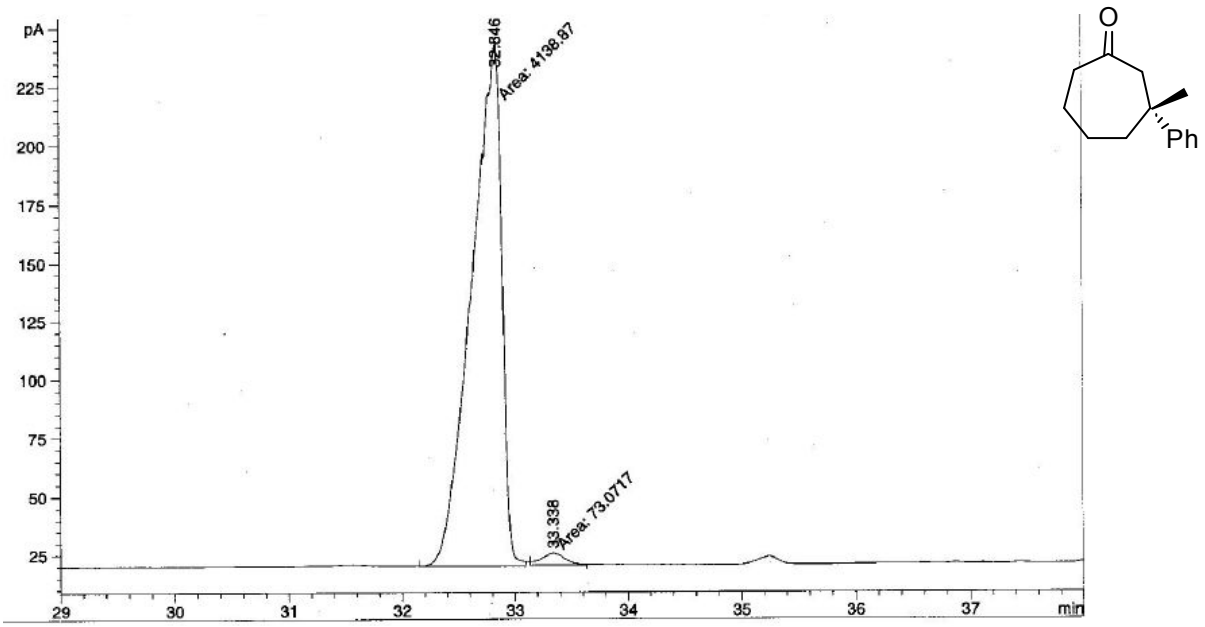


Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	33.363	MM	0.2437	278.02463	19.01638	49.56906
2	34.952	MM	0.2411	282.85883	19.55738	50.43094
Totals :				560.88345	38.57376	

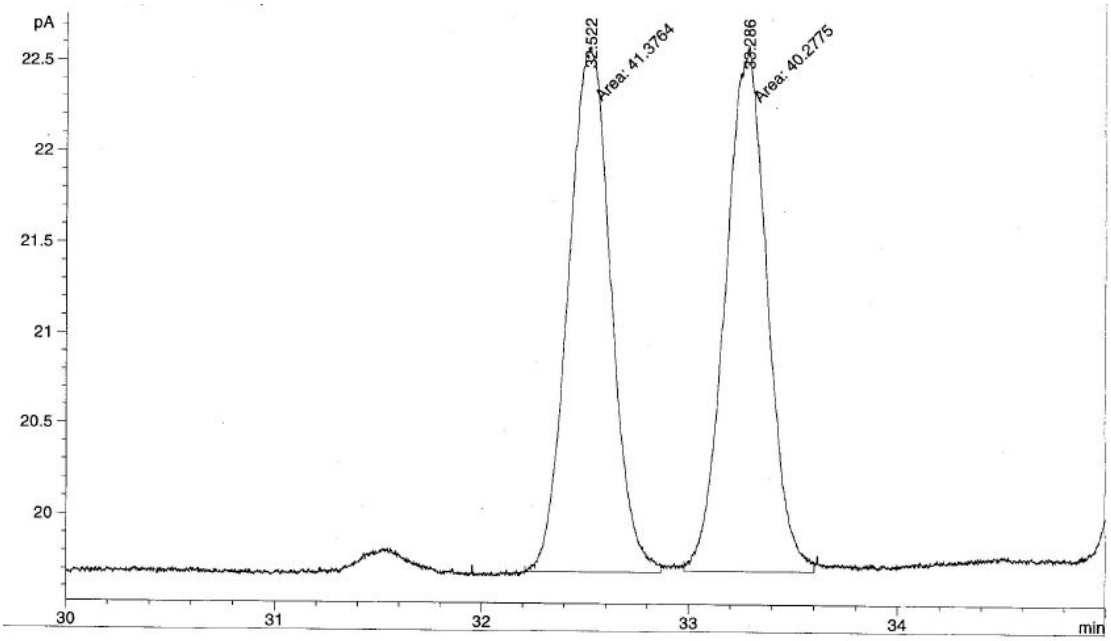
15


1H Spectrum in CDCl3, 400 MHz
7.3244
7.3137
7.2660
7.2234
7.2126
7.2019
7.1912
7.1798
7.1697
3.2237
3.1877
2.7280
2.6921
2.4566
2.3581
2.2248
2.1478
1.8385
1.7267
1.2696
Integral
3.9542
1.0175
1.0000
0.9911
2.0571
1.0089
5.1975
3.1269
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)


13C CPD-Spectrum in CDCl3, 100 MHz
214.2182
148.1736
128.8783
126.2653
125.8968
77.6798
77.3600
77.0402
55.9816
44.5250
43.7576
40.1397
32.2187
26.1250
24.2247
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
-40
(ppm)

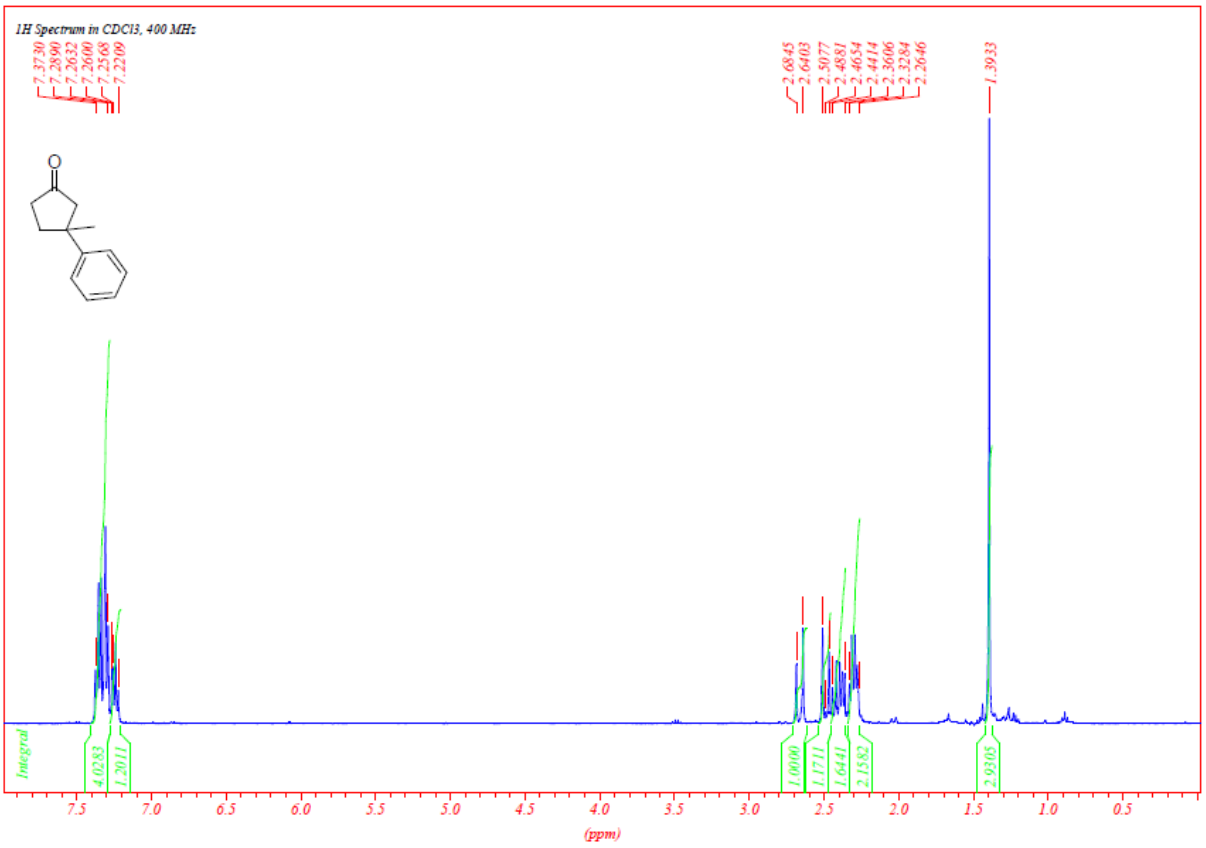


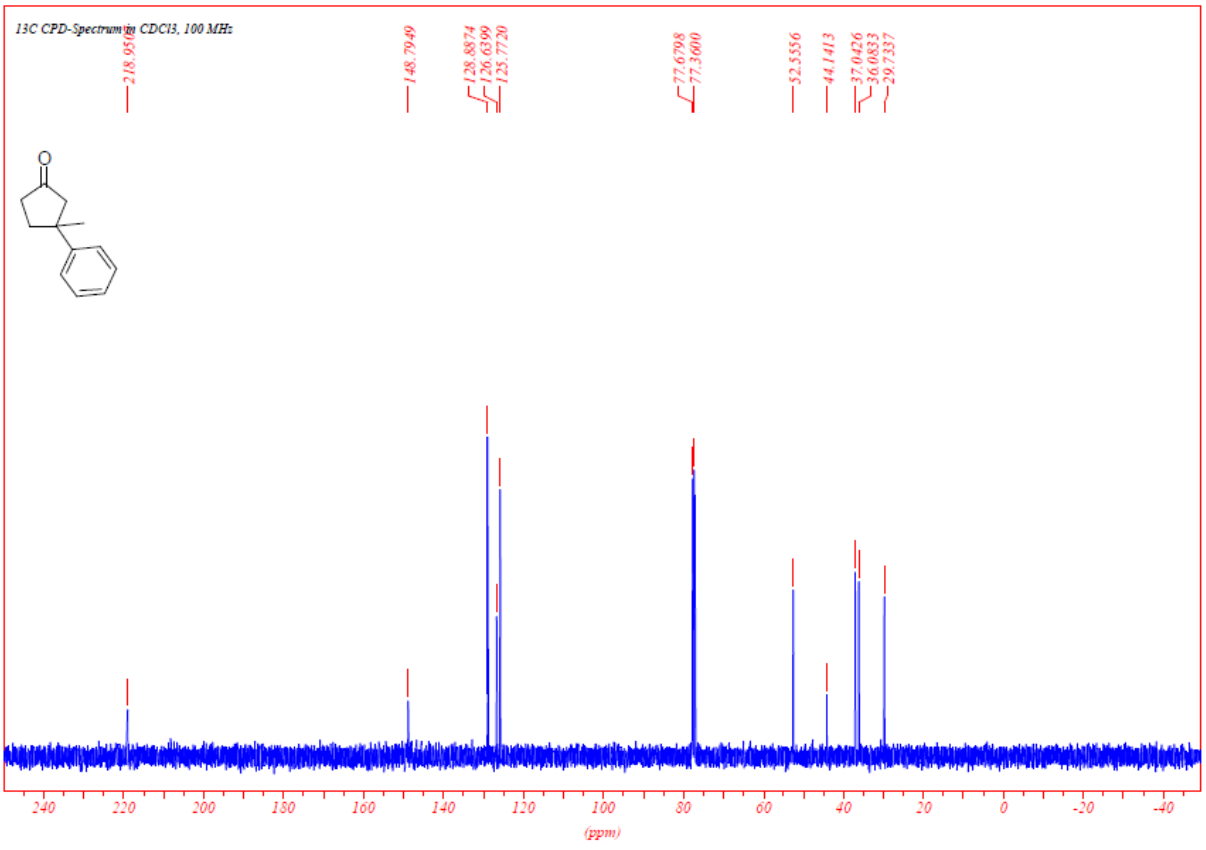
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	32.846	MM	0.3091	4138.87207	223.15489	98.26513
2	33.338	MM	0.2400	73.07167	5.07392	1.73487
Totals :				4211.94374	228.22881	

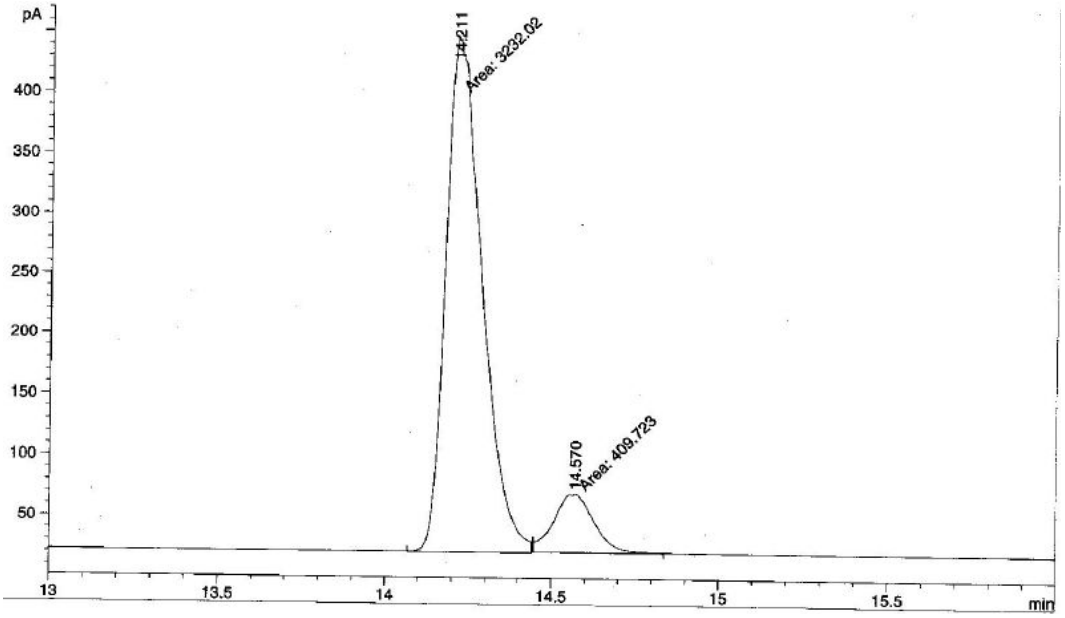


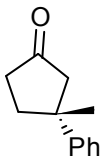
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	32.522	MM	0.2386	41.37643	2.89013	50.67292
2	33.286	MM	0.2314	40.27749	2.90162	49.32708
Totals :				81.65392	5.79175	

16

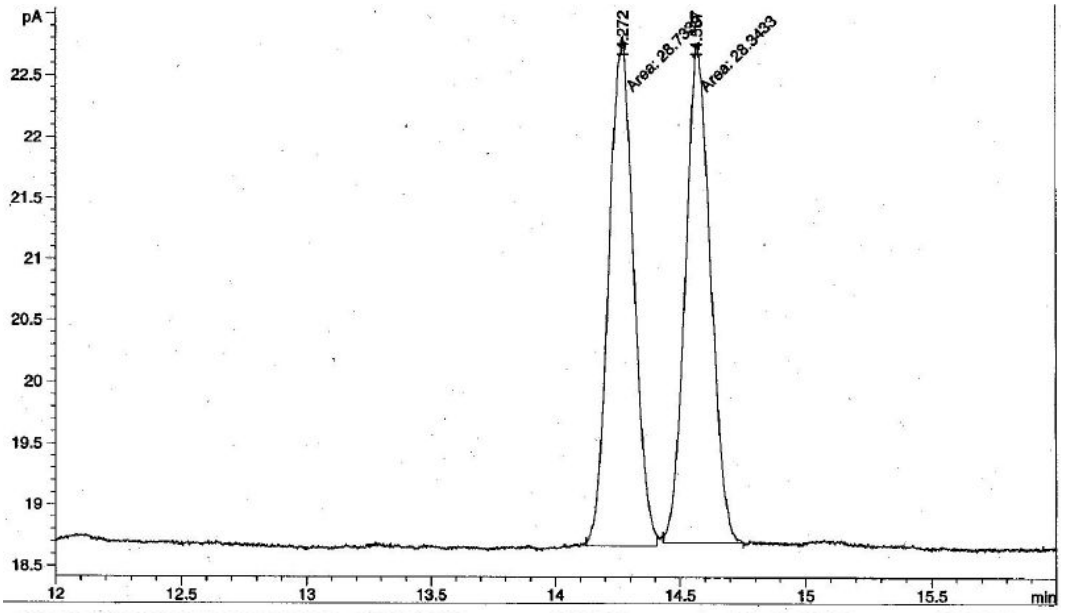

1H Spectrum in CDCl3, 400 MHz
7.3730
7.2690
7.2632
7.2600
7.2568
7.2269
2.6845
2.6403
2.5077
2.4881
2.4654
2.4414
2.3606
2.3284
2.2646
1.3933
Integral
4.0283
1.2011
1.0000
1.1711
1.6441
2.1582
2.9305
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)


13C CPD-Spectrum in CDCl3, 100 MHz
218.9508
148.7949
128.8874
126.6399
125.7720
77.6798
77.3600
52.5556
44.1413
37.0426
36.0833
29.7337
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
-40
(ppm)





Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	14.211	MM	0.1266	3232.02271	425.47849	88.74926
2	14.570	MM	0.1406	409.72330	48.55186	11.25074
Totals :				3641.74600	474.03035	



Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	14.272	MM	0.1152	28.73387	4.15792	50.34213
2	14.567	MM	0.1159	28.34332	4.07697	49.65787
Totals :				57.07718	8.23489	