Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

Bis-salophen palladium complex immobilized on Fe_3O_4@SiO_2 nanoparticles as a highly active and durable phosphine-free catalyst for Heck and copper-free Sonogashira coupling reactions

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Table S1 Elemental analysis results and colours of the compounds

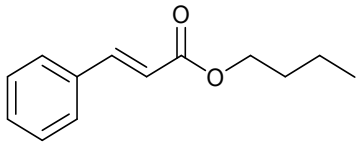
Compounds	Elemental analysis		
	%C	%H	%N
PDBP **1**	77.46 (77.39)[a]	5.75 (5.68)	17.00 (16.92)
Pd-Slp. Ligand **2**	78.49 (78.93)	5.04 (4.86)	9.60 (9.20)
Pd-Slp. Comp. **3**	65.12 (64.99)	3.78 (3.52)	7.22 (7.33)

[a] Theoretically calculated.

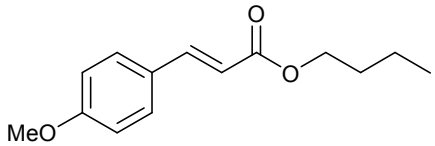
Table S2 BET results for Fe_3O_4, Fe_3O_4@SiO_2 and catalyst **5.**

Entry	Sample	Specific surface area (m^2/g)	Pore volume (cm^3/g)	Average pore radius (nm)
1	Fe_3O_4	478	0.803	1.254
2	Fe_3O_4@SiO_2	453	0.785	1.787
3	Catalyst **5**	372	0.718	1.980

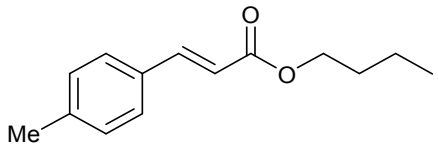
Spectral data of the Heck and Sonogashira coupling products



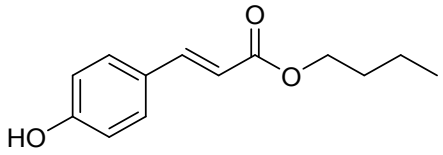
^{1}H-NMR (250 MHz, $CDCl_3$) δ: 0.90 (t, 3H, *J*= 7.5 Hz), 1.37 (m, 2H), 1.65 (m, 2H), 4.17 (t, 2H, *J*= 6.7 Hz), 6.53 (d, 1H, *J*= 16 Hz), 7.60 (d, 2H, *J*= 8.7 Hz), 7.63 (d, 1H, *J*= 16.2 Hz), 8.18 (d, 2H, *J*= 8.7 Hz) ppm; ^{13}C NMR (62.9 MHz, $CDCl_3$) δ: 13.7, 19.1, 30.6, 64.8, 122.5, 124.1, 128.5, 140.5, 141.5, 166.0 ppm.



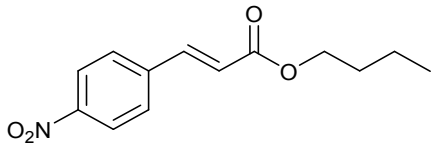
^{1}H NMR (250 MHz, $CDCl_3$) δ: 0.89 (t, 3H, *J*= 7.5 Hz), 1.35 (m, 2H, *J*= 7.5 Hz), 1.61 (quint, 2H, *J*= 5.0 Hz), 3.76 (s, 3H), 4.13 (t, 2H, *J*= 6.7 Hz), 6.24 (d, 1H, *J*= 15.0 Hz), 6.83 (d, 1H, *J*= 5.0 Hz), 7.40 (d, 2H, *J*= 5.0 Hz), 7.56 (d, 1H, *J*= 16.0 Hz) ppm; ^{13}C NMR ($CDCl_3$, 62.9 MHz) δ: 13.7, 19.2, 30.8, 55.3, 64.2, 114.3, 115.8, 129.7, 144.2, 161.3 ppm.



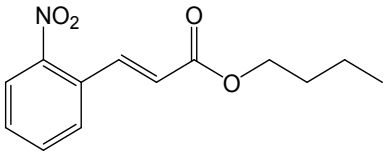
^{1}H-NMR (250 MHz, $CDCl_3$) δ: 0.85 (t, 3H, *J*= 4.7 Hz), 1.32 (m, 2H), 1.56 (m, 2H), 2.24 (s, 3H), 4.09 (t, 2H, *J*= 5.0 Hz), 6.30 (dd, 1H, *J*= 16.0 Hz, *J′*= 5.9 Hz), 7.06 (m, 2H), 7.29 (m, 2H), 7.52 (dd, 1H, *J*= 18.2 Hz, *J′*= 5.5 Hz) ppm; ^{13}C NMR (62.9 MHz, $CDCl_3$) δ: 13.7, 19.2, 21.4, 30.8, 64.2, 117.1, 128.3, 129.5, 131.7, 140.5, 144.5, 167.2 ppm.



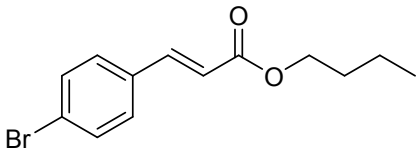
^{1}H-NMR (250 MHz, $CDCl_3$) δ: 0.87 (t, 3H, *J*= 7. 5 Hz), 1.33 (m, 2H), 1.52 (m, 2H), 4.13 (t, 2H, *J*= 7.5 Hz), 6.20 (d, 1H, *J*= 12.5 Hz), 6.80 (d, 3H, *J*=7.5 Hz), 7.32 (d, 2H, *J*=10 Hz), 7.55 (d, 1H, *J*=15 Hz) ppm; ^{13}C NMR (62.9 MHz, $CDCl_3$) δ: 13.7, 19.1, 30.7, 64.7, 116.0 (2C), 126.5, 130.0 (2C), 145.1, 158.6, 168.4 ppm.



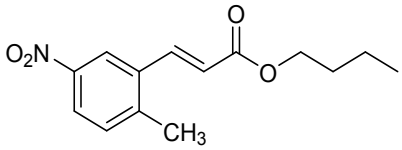
^{1}H-NMR (250 MHz, $CDCl_3$) δ: 0.97 (t, 3H, *J*= 7.2 Hz), 1.45 (m, 2H), 1.67 (m, 2H), 4.23 (t, 2H, *J*= 7.5 Hz), 6.54 (dd, 1H, *J*= 16.0 Hz, *J′*= 6.2 Hz), 7.67 (m, 3H), 8.24 (m, 2H) ppm; ^{13}C NMR (62.9 MHz, $CDCl_3$) δ: 13.7, 19.1, 30.6, 64.9, 122.5, 124.1, 128.6, 140.5, 141.5 ppm.



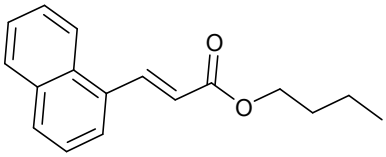
^{1}H-NMR (250 MHz, $CDCl_3$) δ: 0.88 (t, 3H, *J*= 7.5 Hz), 1.35 (m, 2H), 1.62 (m, 2H), 4.14 (t, 2H, *J*= 7.5 Hz), 6.29 (d, 1H, *J*= 17.5 Hz), 7.42-7.57 (m, 2H), 7.94-7.97 (m, 2H), 8.02 (d, 1H, *J*= 17.5 Hz) ppm; ^{13}C NMR (62.9 MHz, $CDCl_3$) δ: 13.9, 19.1, 30.6, 64.7, 123.3, 124.6, 129.2, 130.2, 130.3, 133.5, 139.7, 148.2, 165.9 ppm.



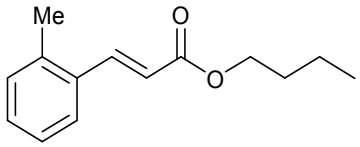
^{1}H-NMR (250 MHz, $CDCl_3$) δ: 0.87 (t, 3H, *J*= 7.5 Hz), 1.34 (m, 2H), 1.60 (m, 2H), 4.12 (t, 2H, *J*= 7.5 Hz), 6.33 (d, 1H, *J*= 17.5 Hz), 7.19-7.30 (m, 2H), 7.40-7.43 (m, 2H), 7.51 (d, 1H, *J*= 17.5 Hz) ppm; ^{13}C NMR (62.9 MHz, $CDCl_3$) δ: 13.7, 19.1, 30.7, 64.5, 111.9, 124.4, 129.3 (2C), 132.0 (2C), 133.3, 143.1, 166.7 ppm.



^{1}H-NMR (250 MHz, $CDCl_3$) δ: 0.88 (t, 3H, *J*= 7.5 Hz), 1.35 (m, 2H), 1.60 (m, 2H), 2.44 (s, 3H), 4.14 (t, 2H, *J*= 7.5 Hz), 6.40 (d, 1H, *J*= 17.5 Hz), 7.29 (d, 1H, *J*=10 Hz), 7.81(d, 1H, *J*= 17.5 Hz) 7.99 (d, 1H, *J*=7.5 Hz), 8.28 (s, 1H) ppm; ^{13}C NMR (62.9 MHz, $CDCl_3$) δ: 13.6, 19.2, 20.1, 31.0, 64.7, 121.1, 122.2, 123.9, 131.6, 134.7, 139.6, 144.4, 146.8, 166.4 ppm.

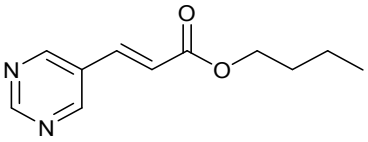


^{1}H-NMR (250 MHz, $CDCl_3$) δ: 0.87 (t, 3H, *J*= 7.2 Hz), 1.37 (m, 2H), 1.65 (m, 2H), 4.17 (t, 2H, *J*= 7.0 Hz), 6.40 (d, 1H, *J*= 14.0 Hz), 7.31-7.42 (m, 3H), 7.58-7.74 (m, 3H), 8.05 (d, 1H, *J*= 8.2 Hz), 8.40 (d, 1H, *J*= 15.7 Hz) ppm; ^{13}C NMR (62.9 MHz, $CDCl_3$) δ: 13.8, 19.2, 30.8, 64.5, 120.9, 123.3, 124.4, 124.9, 125.4, 125.8, 126.2, 126.4, 126.6, 126.8, 128.7, 129.1, 130.4, 131.4, 131.8, 133.6, 141.5, 166.9 ppm.

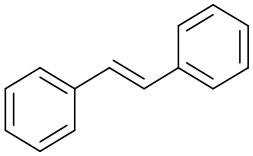


^{1}H-NMR (250 MHz, $CDCl_3$) δ: 0.85 (t, 3H, *J*= 2.5 Hz), 1.32 (m, 2H), 1.57 (m, 2H), 2.30 (s, 3H), 4.11 (t, 2H), 6.27 (dd, 1H, *J*= 15.9 Hz, *J′*= 4.8 Hz), 7.11 (m, 3H), 7.41 (m, 1H), 7.84 (dd, 1H, *J*=

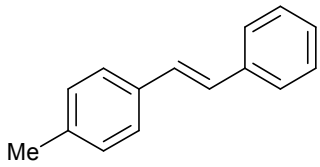
13.7 Hz, *J′*= 4.3 Hz) ppm; ^{13}C NMR (62.9 MHz, $CDCl_3$) *δ*: 13.7, 18.9, 19.7, 30.7, 64.3, 119.2, 126.3, 129.9, 130.7, 133.4, 137.5, 142.2, 167.0 ppm.



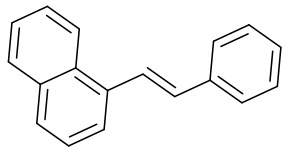
^{1}H NMR (250 MHz, $CDCl_3$) *δ*: 0.90 (t, 3H, *J*= 7.5 Hz), 1.39 (m, 2H), 1.61 (m, 2H), 4.17 (t, 2H, *J*= 5.5 Hz), 6.53 (d, 1H, *J*= 15.0 Hz), 7.52 (d, 1H, *J*= 15.0 Hz), 8.82 (s, 2H), 9.13 (s, 1H) ppm; ^{13}C NMR (62.9 MHz, $CDCl_3$) *δ*: 13.6, 19.1, 30.6, 64.9, 122.4, 137.0, 155.5, 159.1, 165.7 ppm.



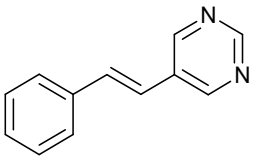
^{1}H-NMR (250 MHz, $CDCl_3$) *δ*: 7.13 (d, 2H), 7.31 (m, 6H), 7.52 (m, 4H) ppm.



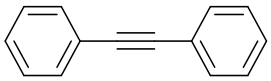
^{1}H-NMR (250 MHz, $CDCl_3$) *δ*: 2.26 (s, 3H), 6.91-7.64 (m, 9H) ppm; ^{13}C NMR (62.9 MHz, $CDCl_3$,) *δ*: 21.3, 126.4, 126.4, 127.4, 127.7, 128.6, 129.4, 134.5, 137.5 ppm.



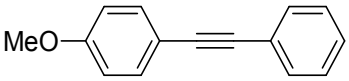
^{1}H-NMR (250 MHz, $CDCl_3$) *δ*: 7.02-8.11 (m, 12H) ppm; ^{13}C NMR (62.9 MHz, $CDCl_3$) *δ*: 123.6, 123.8, 125.7, 125.8, 126.1, 126.7, 127.8, 128.0, 128.6, 128.7, 131.4, 131.7, 133.7, 135.0, 137.6 ppm.



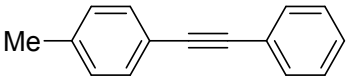
^{1}H-NMR (250 MHz, $CDCl_3$) δ: 6.89 (d, 1H, J= 16.5 Hz), 7.15 (d, 1H, J= 16.5 Hz), 7.25-7.47 (m, 5H), 8.77 (s, 2H), 9.12 (s, 1H) ppm; ^{13}C NMR (62.9 MHz, $CDCl_3$) δ: 121.0, 126.8, 128.8, 128.8, 130.9, 132.8, 135.9, 154.2, 157.1 ppm.



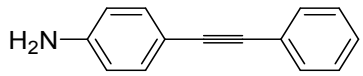
^{1}H-NMR (250 MHz, $CDCl_3$) δ: 7.23-7.28 (m, 6H), 7.43-7.47 (m, 4H) ppm; ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ: 89.5, 123.3, 128.3, 129.2, 131.6 ppm; MS (m/e)= 178 [M^+]; Elemental Analysis: Calcd. C: 94.33, H: 5.67%, Found. C: 94.19, H: 5.81%.



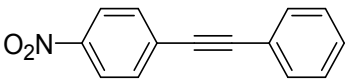
^{1}H-NMR (250 MHz, $CDCl_3$) δ: 3.76 (s, 3H, CH_3), 6.79 (d, 2H, J= 8.2 Hz, Ar-H), 7.21-7.25 (m, 3H, Ar-H), 7.37-7.44 (m, 4H, Ar-H) ppm; ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ: 55.2, 88.0, 89.4, 114.0, 115.3, 123.6, 127.9, 128.3, 131.4, 133.0, 159.6 ppm; MS (m/e)= 208 [M^+]; Elemental Analysis: Calcd. C: 86.50, H: 5.82%, Found. C: 86.62, H: 5.71%.



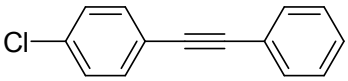
^{1}H-NMR ($CDCl_3$, 250 MHz) δ: 2.22 (s, 3H, CH_3), 7.14 (d, 2H, J= 8.4 Hz, Ar-H), 7.19-7.42 (m, 7H, Ar-H) ppm; ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ: 21.5, 88.7, 89.6, 120.2, 123.5, 128.1, 128.3, 129.1, 131.5, 131.7, 138.4 ppm; MS (m/e)= 192 [M^+]; Elemental Analysis: Calcd. C: 93.70, H: 6.30%, Found. C: 93.54, H: 6.46%.



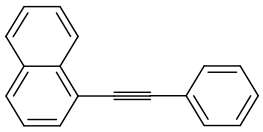
^{1}H-NMR ($CDCl_3$, 250 MHz) δ: 3.62 (s, 2H, NH_2), 6.52 (s, 2H, Ar-H), 7.22-7.40 (m, 7H, Ar-H) ppm; ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ: 87.3, 90.2, 112.5, 114.7, 123.9, 127.7, 128.3, 131.3, 132.9, 146.7 ppm.



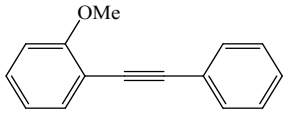
^{1}H-NMR (250 MHz, $CDCl_3$) δ: 7.37-7.41 (m, 3H, Ar-H), 7.54-7.57 (m, 2H, Ar-H), 7.68 (d, 2H, *J*= 12.5 Hz, Ar-H), 8.22 (d, 2H, *J*= 7.5 Hz, Ar-H) ppm; ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ: 87.5, 94.7, 122.0, 123.6, 128.5, 129.2, 130.2, 131.8, 132.2, 146.9 ppm; MS (m/e)= 224 [M^+]; Elemental Analysis: Calcd. C: 75.32, H: 4.07, N: 6.27%, Found. C: 75.46, H: 4.19, N: 6.13%.



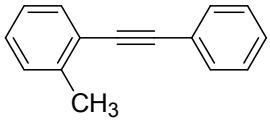
^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.13-7.43 (m, 9H, Ar-H) ppm; ^{13}C NMR (62.9 MHz, $CDCl_3$) δ: 88.2, 90.3, 121.8, 122.9, 128.4, 128.5, 128.7, 131.6, 132.8, 134.2 ppm.



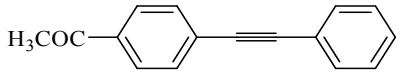
^{1}H-NMR (250 MHz, $CDCl_3$) δ: 7.26-7.74 (m, 11H, Ar-H), 8.36 (d, 1H, *J*= 8.2 Hz, Ar-H); ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ: 87.5, 94.3, 120.9, 123.4, 125.3, 125.6, 126.2, 126.4, 126.8, 128.3, 128.42, 128.47, 128.8, 130.4, 131.7, 133.2, 133.3, 141.1 ppm; MS (m/e)= 228 [M^+]; Elemental Analysis: Calcd. C: 94.69, H: 5.31%, Found. C: 94.45, H: 5.55%.



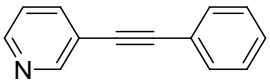
^{1}H NMR (250 MHz, $CDCl_3$) δ: 3.82 (s, 3H, CH_3), 6.87 (d, 2H, *J*= 7.25 Hz, Ar-H), 7.31-7.33 (m, 3H, Ar-H), 7.45-7.53 (m, 4H, Ar-H) ppm; ^{13}C NMR ($CDCl_3$, 62.9 MHz): δ: 55.8, 85.6, 93.3, 110.6, 112.4, 120.4, 123.5, 128.0, 128.1, 129.7, 131.6, 133.5, 159.8 ppm.



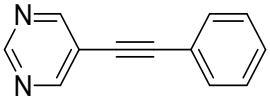
^{1}H NMR (250 MHz, $CDCl_3$) δ: 2.44 (s, 3H, CH_3), 7.14-7.46 (m, 9H, Ar-H) ppm; ^{13}C NMR ($CDCl_3$, 62.9 MHz) δ: 20.7, 86.01, 94.2, 123.0, 125.5, 128.1, 128.30, 128.35, 129.4, 131.5, 131.8, 140.1 ppm; MS (m/e)= 192 [M^+]; Elemental Analysis: Calcd. C: 93.70, H: 6.30%, Found. C: 93.80, H: 6.20%.



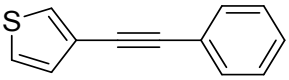
^{1}H-NMR (250 MHz, $CDCl_3$) δ: 2.51 (s, 3H, CH_3), 7.16-7.33 (m, 3H, Ar-H), 7.45-7.54 (m, 4H, Ar-H), 7.86 (d, 2H, J=7.5 Hz, Ar-H) ppm; ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ: 27.0, 88.9, 92.9, 123.0, 128.2, 128.3, 128.8, 129.5, 132.0, 132.2, 136.5, 197.6 ppm.



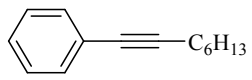
^{1}H-NMR (250 MHz, $CDCl_3$) δ: 7.26-7.29 (m, 4H, Ar-H), 7.44-7.47 (m, 2H, Ar-H), 7.70 (m, 1H, Ar-H), 8.45 (m, 1H, Ar-H), 8.68 (s, 1H, Ar-H) ppm; ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ: 85.9, 92.7, 120.5, 122.4, 123.0, 128.4, 128.8, 131.6, 138.4, 148.4, 152.1 ppm; MS (m/e)= 179 [M^+]; Elemental Analysis: Calcd. C: 87.12, H: 5.07, N: 7.81%, Found. C: 87.23, H: 4.92, N: 7.85%.



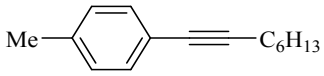
^{1}H-NMR (250 MHz, $CDCl_3$) δ: 7.29-7.48 (m, 5H, Ar-H), 8.77 (s, 2H, Ar-H), 9.06 (s, 1H, Ar-H) ppm; ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ: 82.3, 96.3, 119.9, 121.7, 128.5, 128.7, 129.1, 129.3, 131.7, 139.3, 156.6, 158.5 ppm; MS (m/e)= 180 [M^+]; Elemental Analysis: Calcd. C: 79.98, H: 4.48, N: 15.54%, Found. C: 79.81, H: 4.60, N: 15.59%.



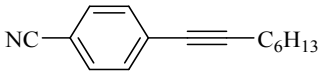
^{1}H-NMR (250 MHz, $CDCl_3$) δ: 7.31-7.42 (m, 5H, Ar-H), 7.59-7.64 (m, 3H, Ar-H) ppm; ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ: 84.7, 89.1, 123.3, 125.5, 127.2, 128.5, 128.7, 129.3, 129.9, 131.7, 132.6 ppm; MS (m/e)= 184 [M^+]; Elemental Analysis: Calcd. C: 78.22, H: 4.39%, Found. C: 78.06, H: 4.49%.



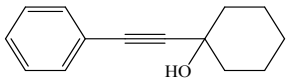
^{1}H-NMR (250 MHz, $CDCl_3$) δ: 0.83 (t, 3H, J= 7.0 Hz, CH_3), 1.20-1.55 (m, 8H, CH_2), 2.31 (t, 2H, J= 7.0 Hz, CH_2), 7.15-7.21 (m, 3H, Ar-H), 7.28-7.33 (m, 2H, Ar-H) ppm;; ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ: 14.0, 19.3, 22.5, 28.5, 28.7, 31.3, 80.5, 90.4, 124.0, 127.4, 128.1, 131.5 ppm.



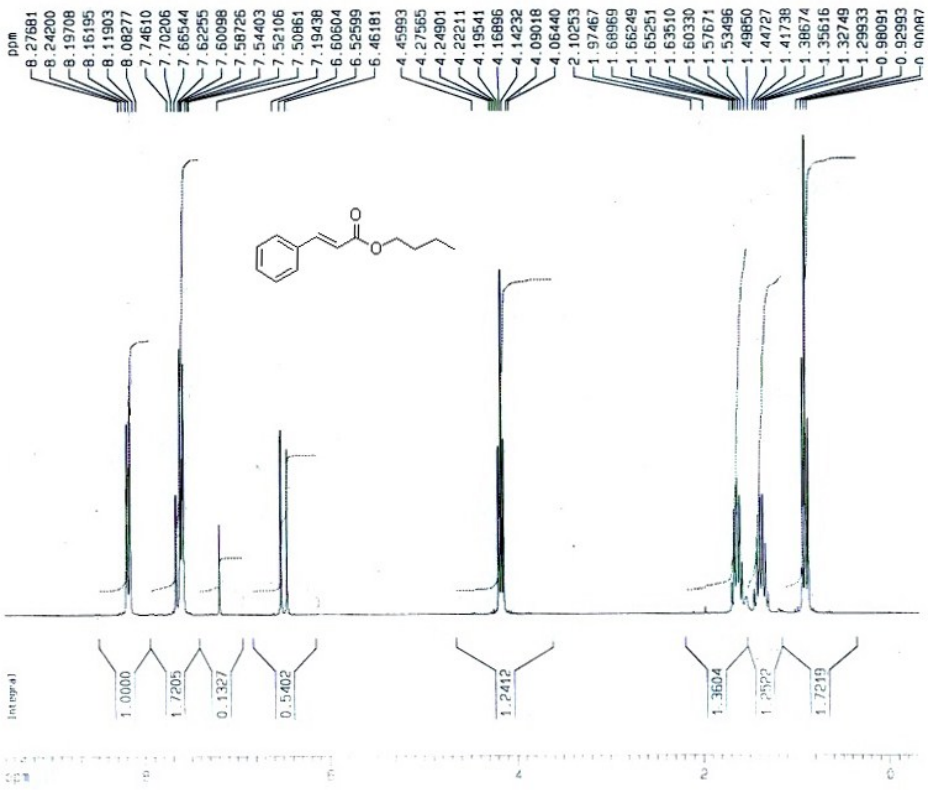
^{1}H-NMR (250 MHz, $CDCl_3$) δ: 0.93 (t, 3H, J= 7.0 Hz, -$CH_2\underline{CH_3}$), 1.31-1.65 (m, 8H, -CH_2), 2.35 (s, 3H, CH_3), 2.41 (t, 2H, J= 7.0 Hz, CH_2), 7.10 (d, 2H, J= 8.5 Hz, Ar-H), 7.31 (d, 2H, J= 8.0 Hz, Ar-H) ppm; ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ: 14.0, 19.4, 21.3, 22.5, 28.6, 28.7, 31.3, 80.5, 89.5, 121.0, 128.8, 131.3, 137.3 ppm.



^{1}H-NMR (250 MHz, $CDCl_3$) δ: 0.89 (t, 3H, J= 7.0 Hz, -$CH_2\underline{CH_3}$), 1.24-1.63 (m, 8H, -CH_2), 2.41 (t, 2H, J= 7.0 Hz, CH_2), 7.42 (d, 2H, J = 8.75 Hz, Ar-H), 7.56 (d, 2H, J= 8.75 Hz, Ar-H) ppm.



^{1}H-NMR (250 MHz, $CDCl_3$) δ: 1.27-1.29 (s, 1H, OH), 1.55-1.77 (m, 7H, -CH_2), 1.98-2.04 (m, 2H, -CH_2), 2.27 (s, 1H, CH_2), 7.26-7.31 (m, 3H, Ar-H), 7.40-7.45 (m, 2H, Ar-H) ppm.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7.60098
7.58726
7.54403
7.52106
7.50861
7.19438
6.60604
6.52599
6.46181
4.45993
4.27565
4.24901
4.22211
4.19541
4.16896
4.14232
4.09018
4.06440
2.10253
1.97467
1.68969
1.66249
1.65251
1.63510
1.60330
1.57671
1.53496
1.49850
1.44727
1.41738
1.38674
1.35616
1.32749
1.29933
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Integral
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1.2412
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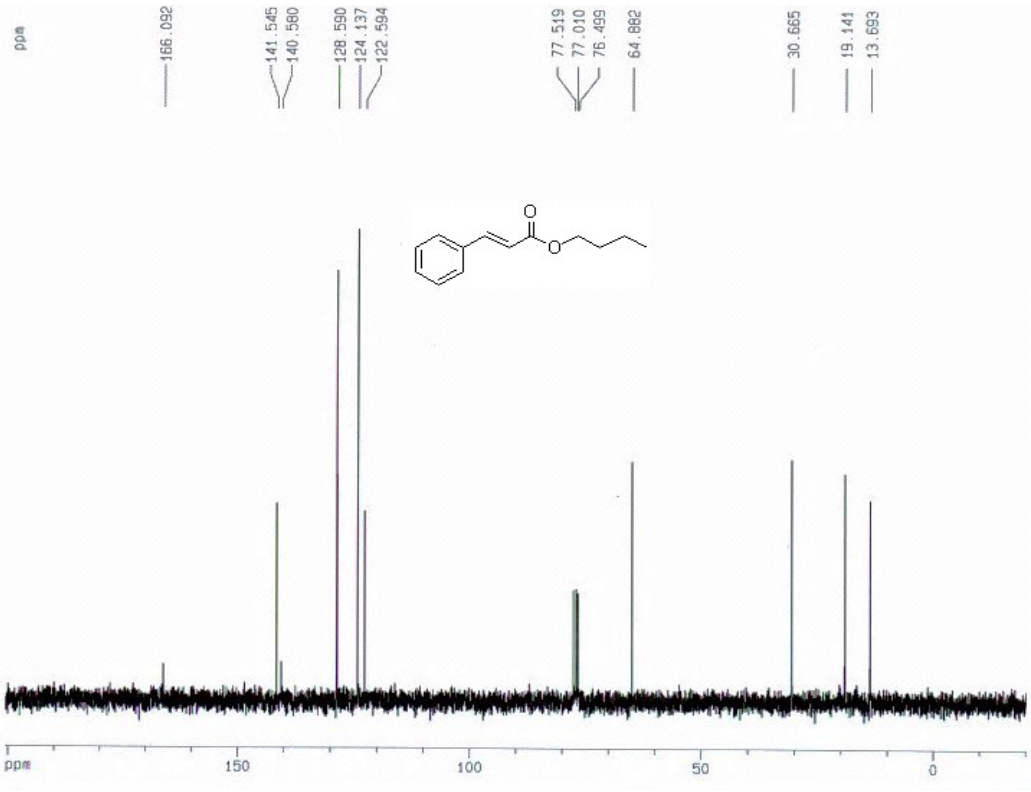
1.3522
1.7219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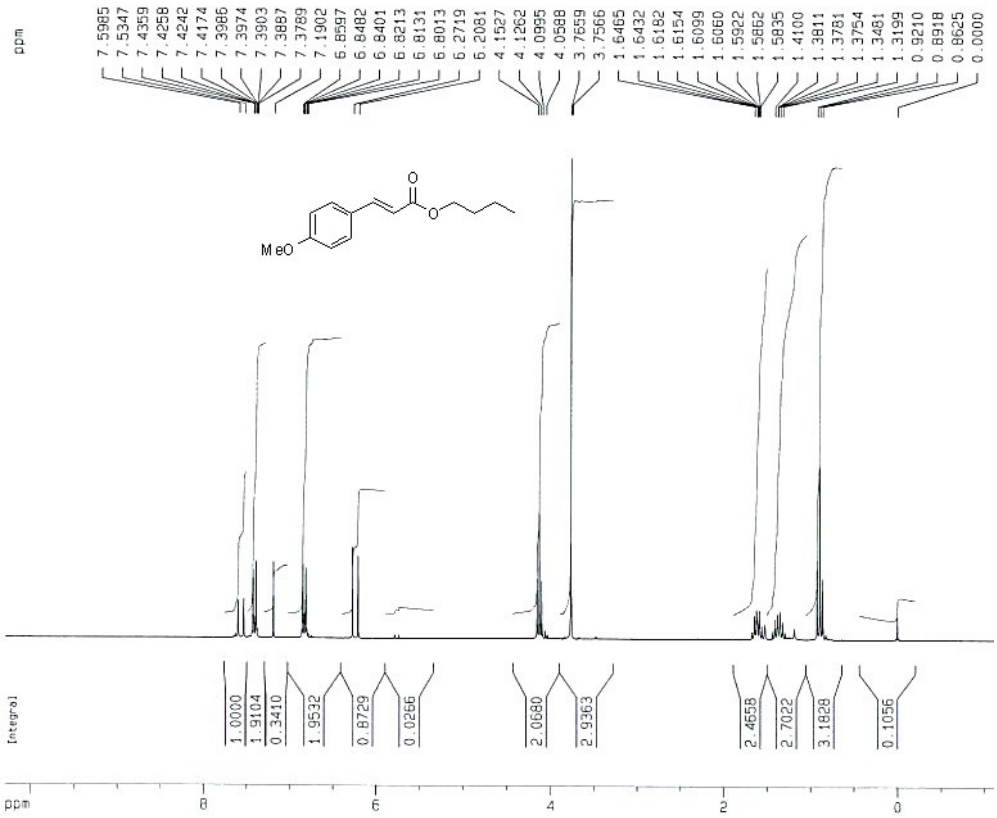
100
50
0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7.3789
7.1902
6.8597
6.8482
6.8401
6.8213
6.8131
6.8013
6.2719
6.2081
4.1527
4.1262
4.0995
4.0588
3.7659
3.7566
1.6465
1.6432
1.6182
1.6154
1.6099
1.6060
1.5922
1.5862
1.5835
1.4100
1.3811
1.3781
1.3754
1.3481
1.3199
0.9210
0.8918
0.8625
0.0000
MeO
Integral
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0.3410
1.9532
0.8729
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2.9363
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2.7022
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0.1056
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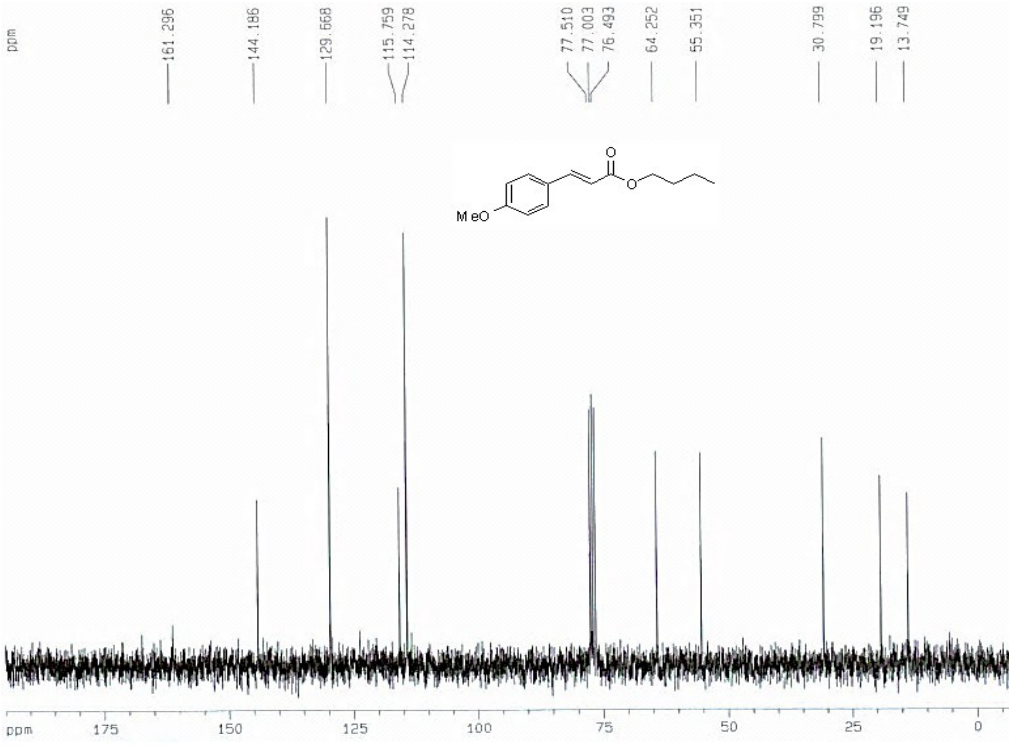
6
4
2
0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19.196
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MeO
ppm
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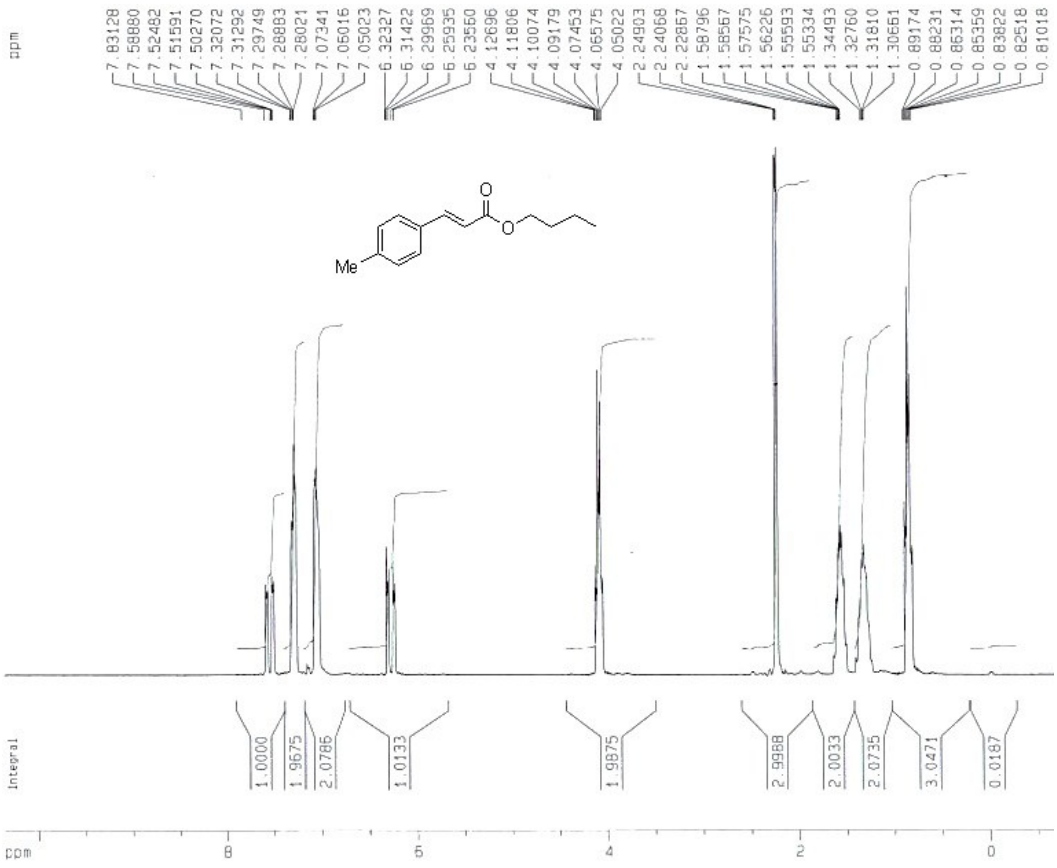
75
50
25
0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7.05023
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6.31422
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6.25935
6.23560
4.12696
4.11806
4.10074
4.09179
4.07453
4.06575
4.05022
2.24903
2.24068
2.22867
1.58796
1.58567
1.57575
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1.55593
1.55334
1.34493
1.32760
1.31810
1.30661
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0.88231
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0.85359
0.83822
0.82518
0.81018
O
O
Me
Integral
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2.0735
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ppm
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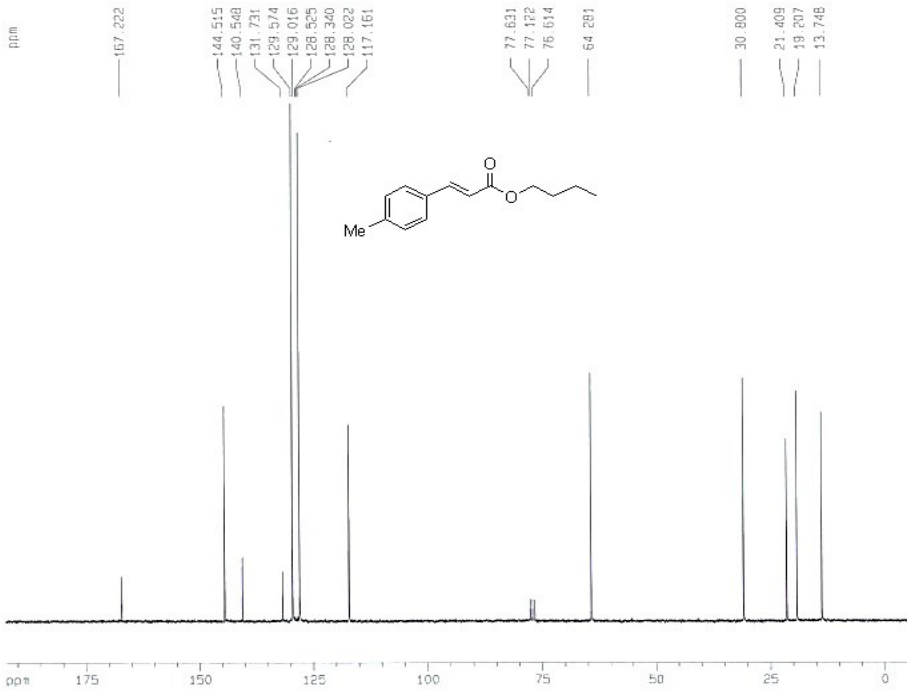
6
4
2
0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128.022
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77.122
76.614
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19.207
13.748
O
O
Me
ppm
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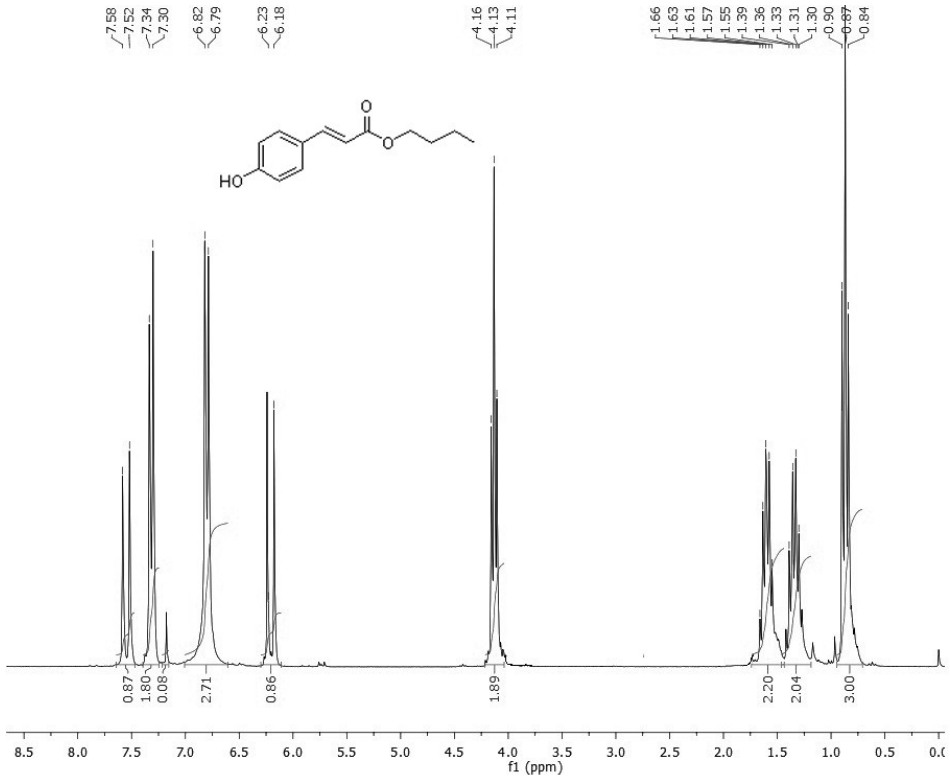
150
125
100
75
50
25
0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7.34
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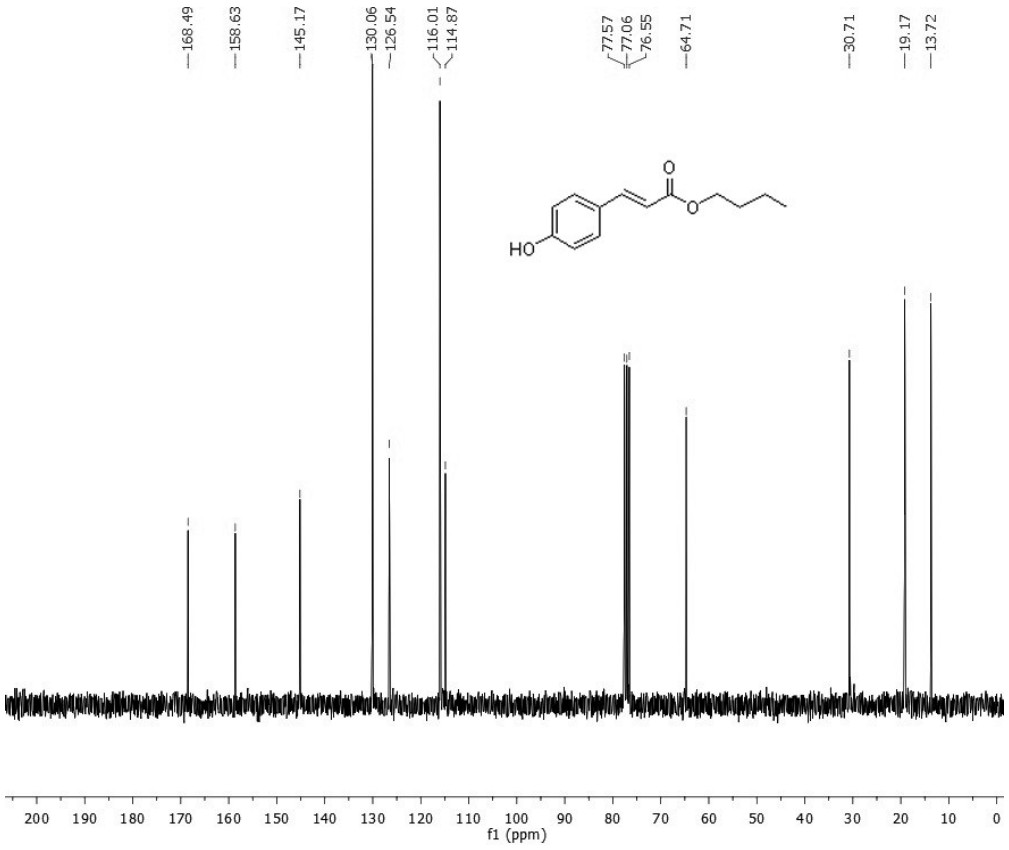
6.82
6.79
6.23
6.18
4.16
4.13
4.11
1.66
1.63
1.61
1.57
1.55
1.39
1.36
1.33
1.31
1.30
0.90
0.87
0.84
HO
O
O
0.87
1.80
0.08
2.71
0.86
1.89
2.20
2.04
3.00
f1 (ppm)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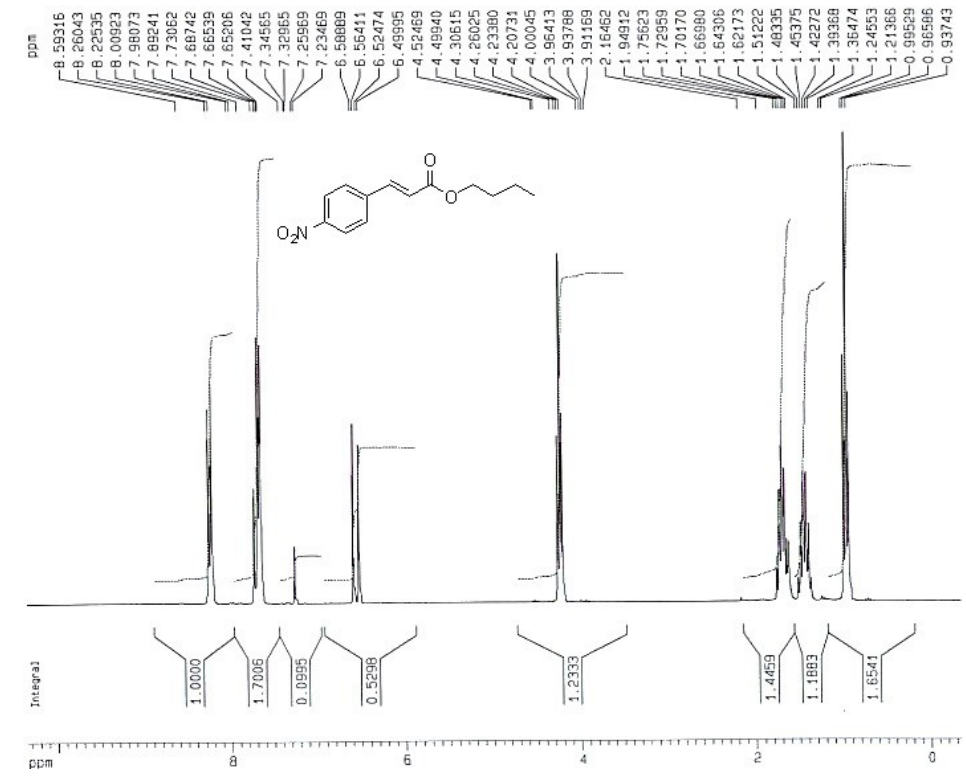
145.17
130.06
126.54
116.01
114.87
77.57
77.06
76.55
64.71
30.71
19.17
13.72
HO
O
O
f1 (ppm)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7.34565
7.32965
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7.23469
6.58869
6.55411
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4.49940
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4.26025
4.23380
4.20731
4.00045
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3.93788
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2.16462
1.94912
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0.96586
0.93743
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O
O
Integral
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0.5298
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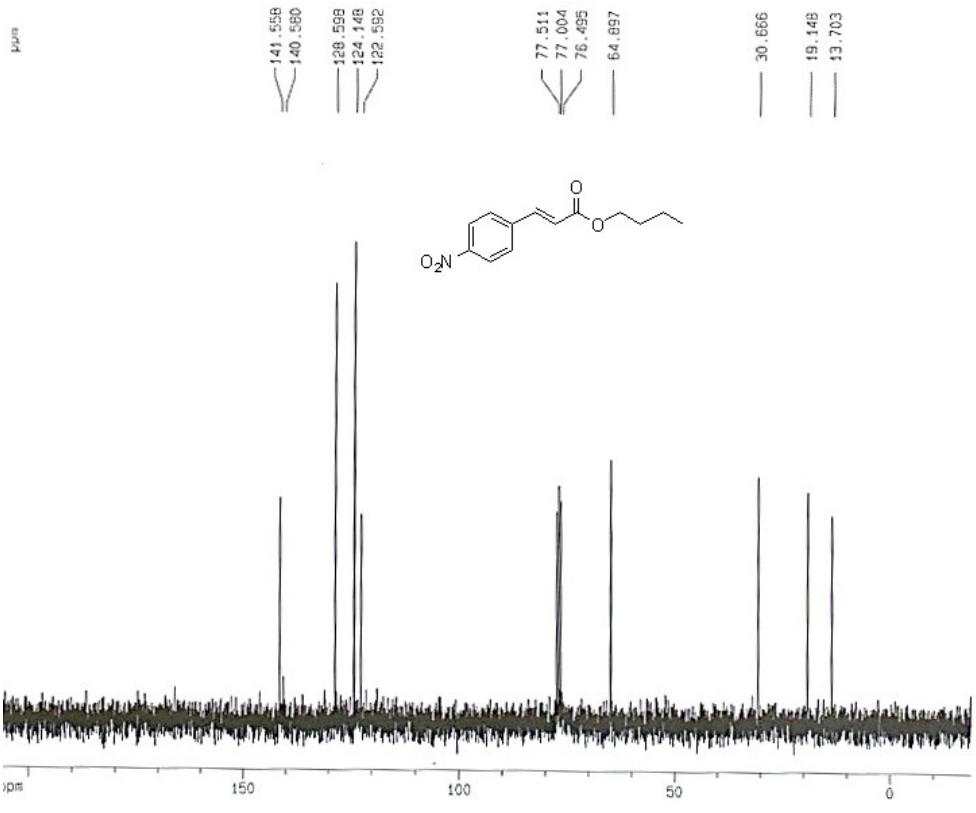
6
4
2
0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O
ppm
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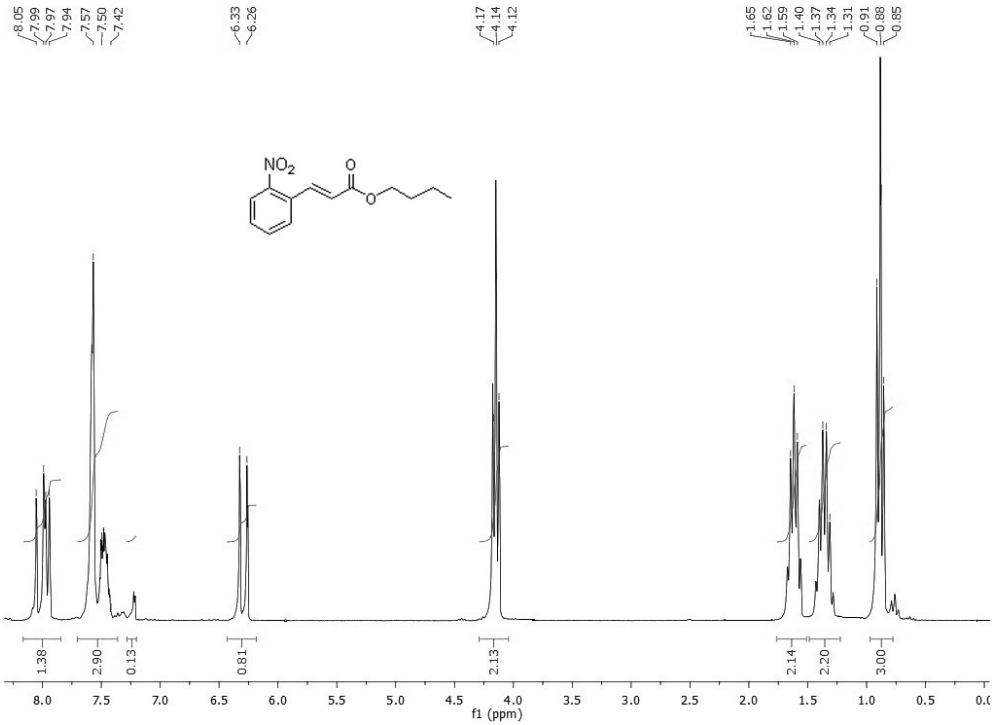
50
0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6.26
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4.14
4.12
1.65
1.62
1.59
1.40
1.37
1.34
1.31
0.91
0.88
0.85
NO2
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O
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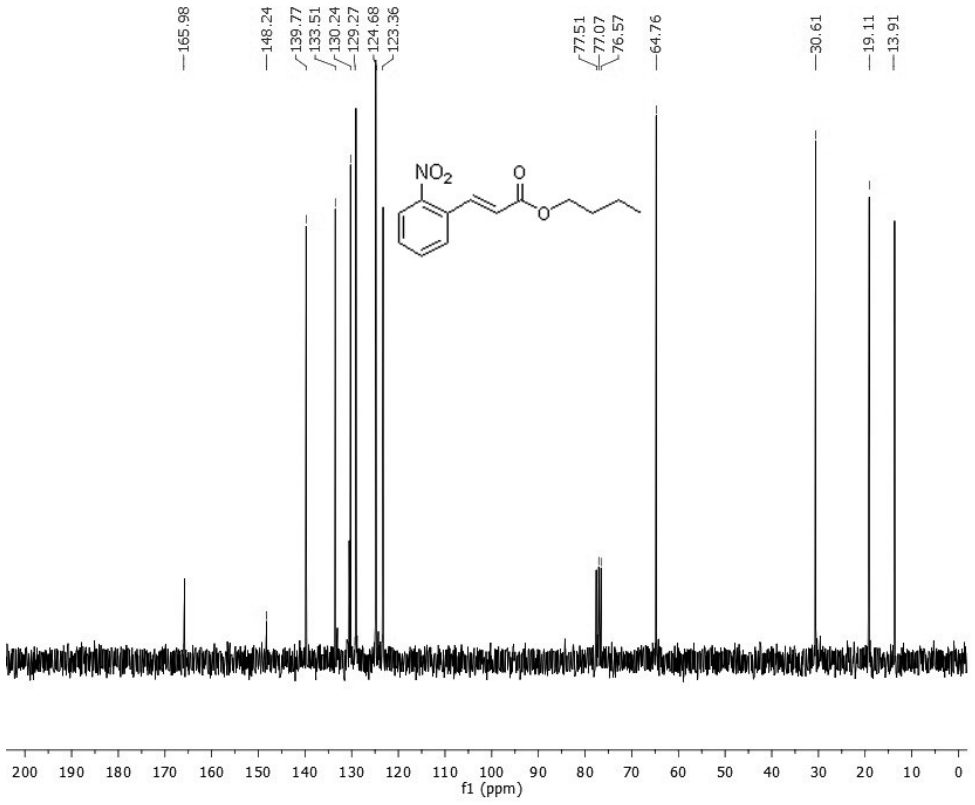
2.90
0.13
0.81
2.13
2.14
2.20
3.00
f1 (ppm)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130.24
129.27
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123.36
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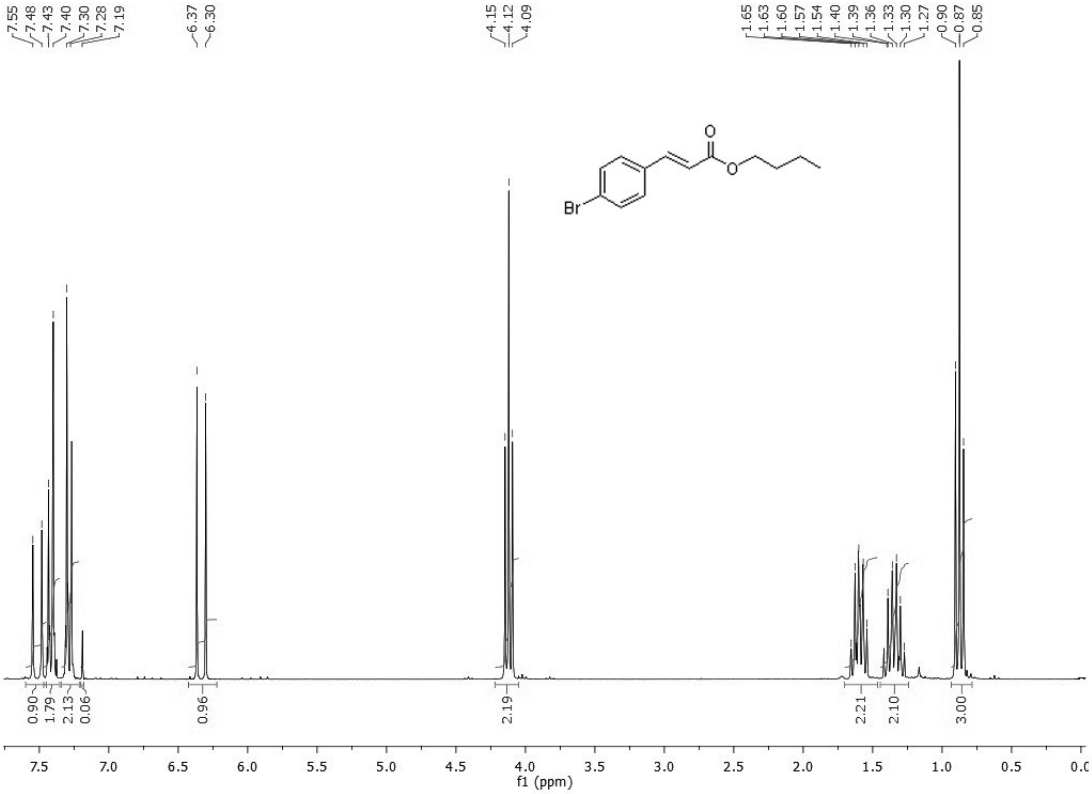
77.07
76.57
64.76
30.61
19.11
13.91
NO2
O
O
f1 (ppm)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6.37
6.30
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4.12
4.09
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1.63
1.60
1.57
1.54
1.40
1.39
1.36
1.33
1.30
1.27
0.90
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0.85
O
O
Br
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2.13
0.06
0.96
2.19
2.21
2.10
3.00
7.5
7.0
6.5
6.0
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4.0
3.5
3.0
2.5
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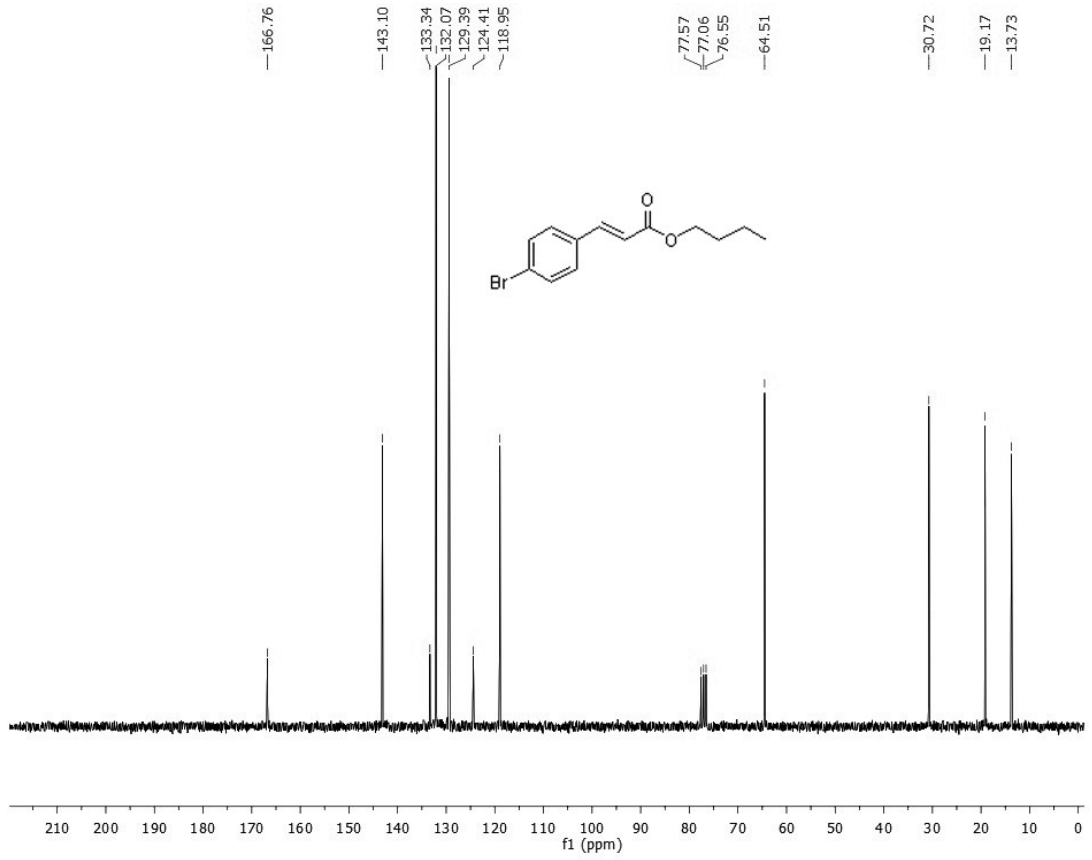
1.5
1.0
0.5
f1 (ppm)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77.57
77.06
76.55
64.51
30.72
19.17
13.73
O
O
Br
210
200
190
180
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130
120
110
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90
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70
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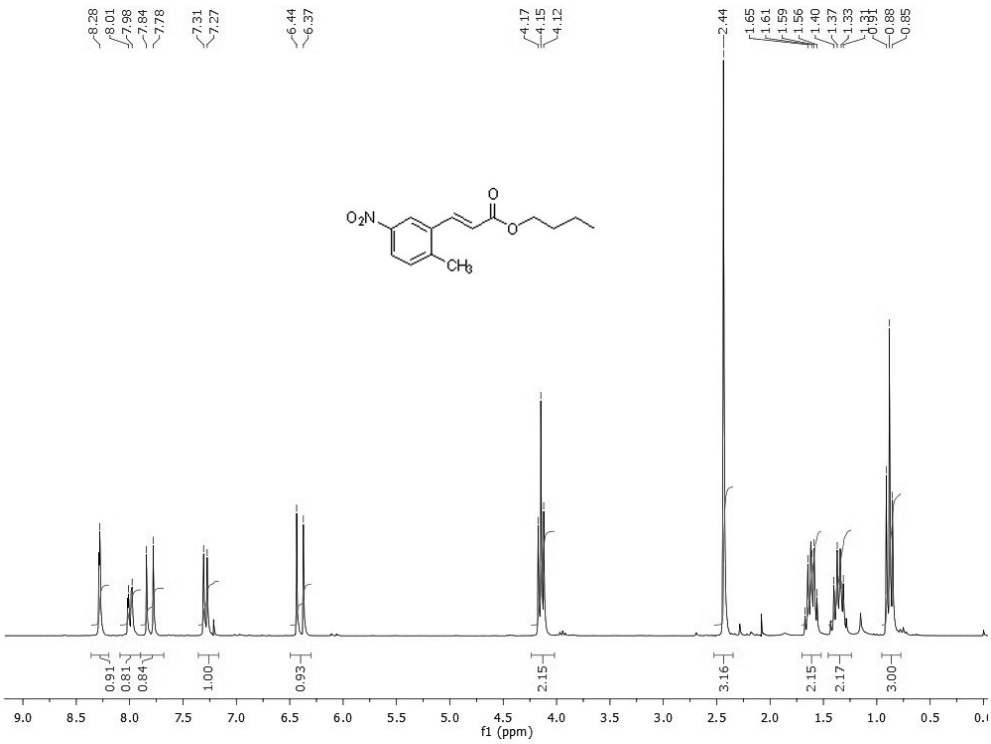
50
40
30
20
10
0
f1 (ppm)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4.15
4.12
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1.61
1.59
1.56
1.40
1.37
1.33
1.31
0.91
0.88
0.85
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O
O
CH3
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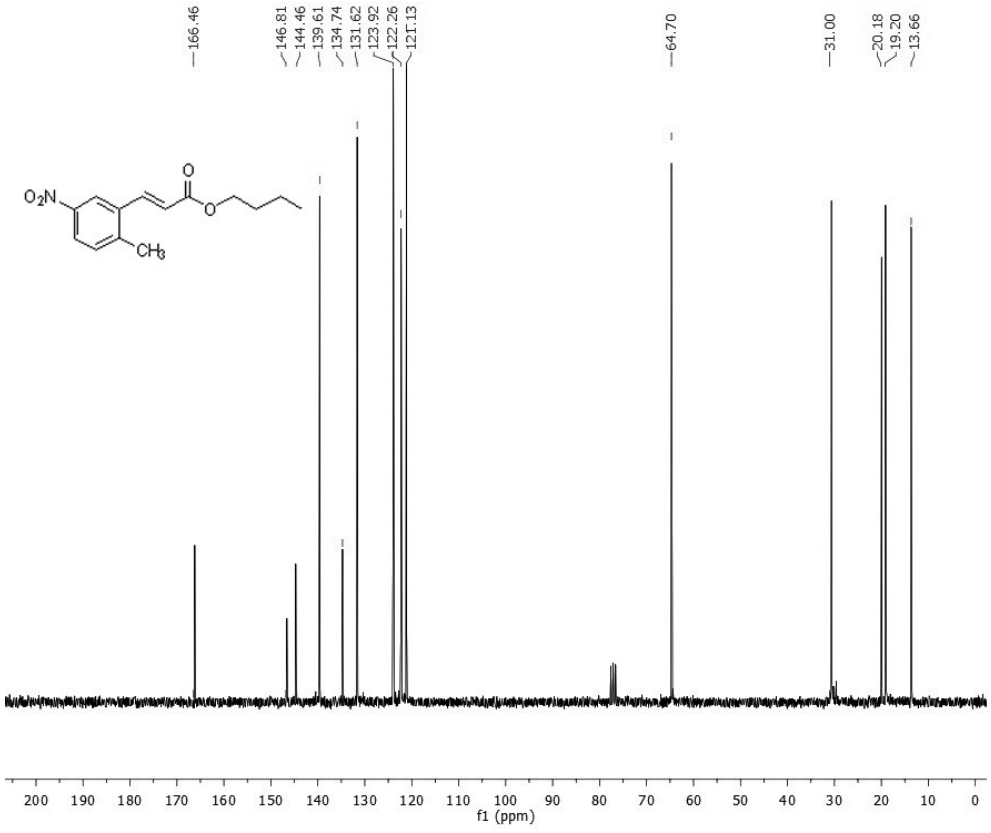
0.84
1.00
0.93
2.15
3.16
2.15
2.17
3.00
f1 (ppm)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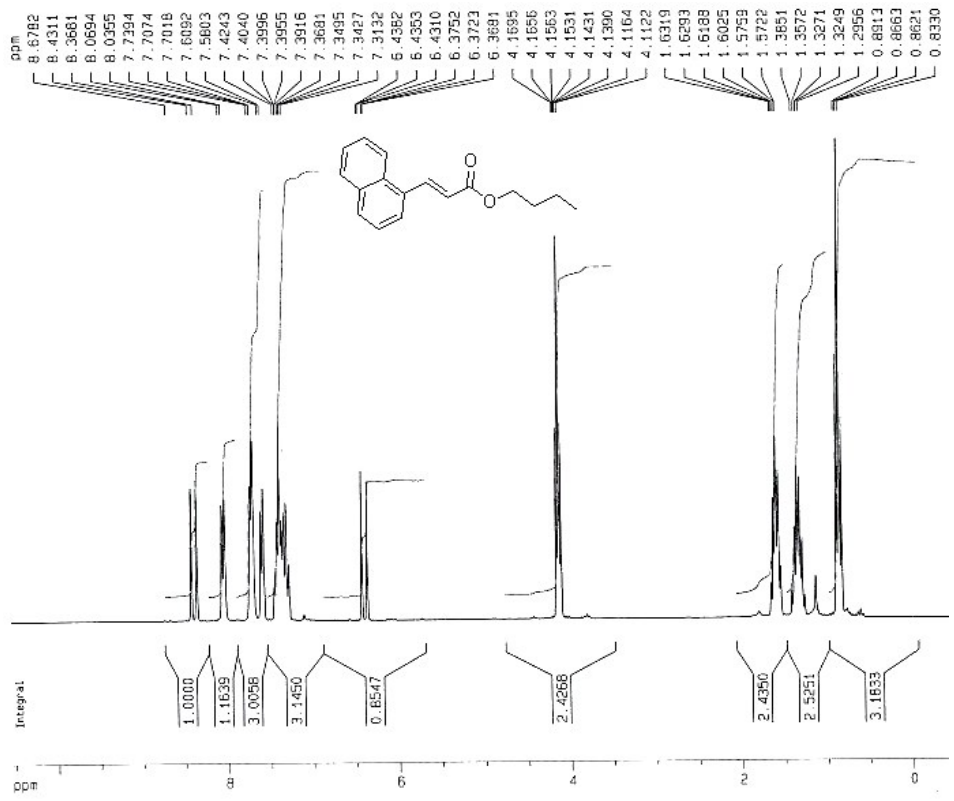
O
O
CH3
f1 (ppm)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6.3723
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1.2956
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0.8621
0.8330
Integral
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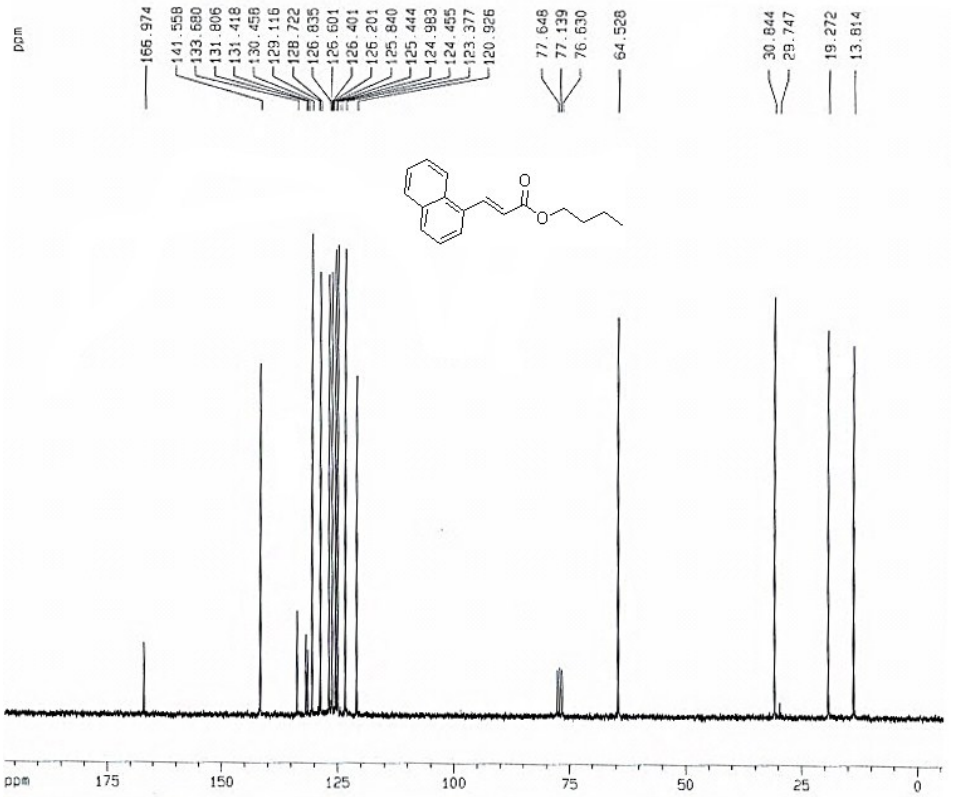
2.5251
3.1833
ppm
8
6
4
2
0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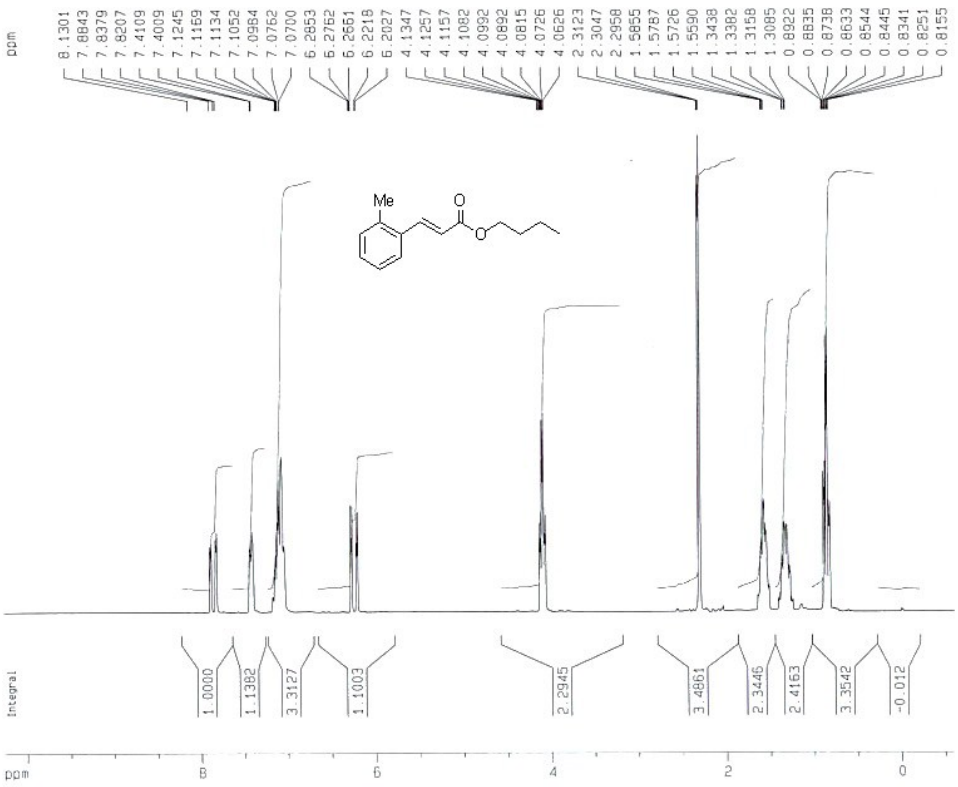
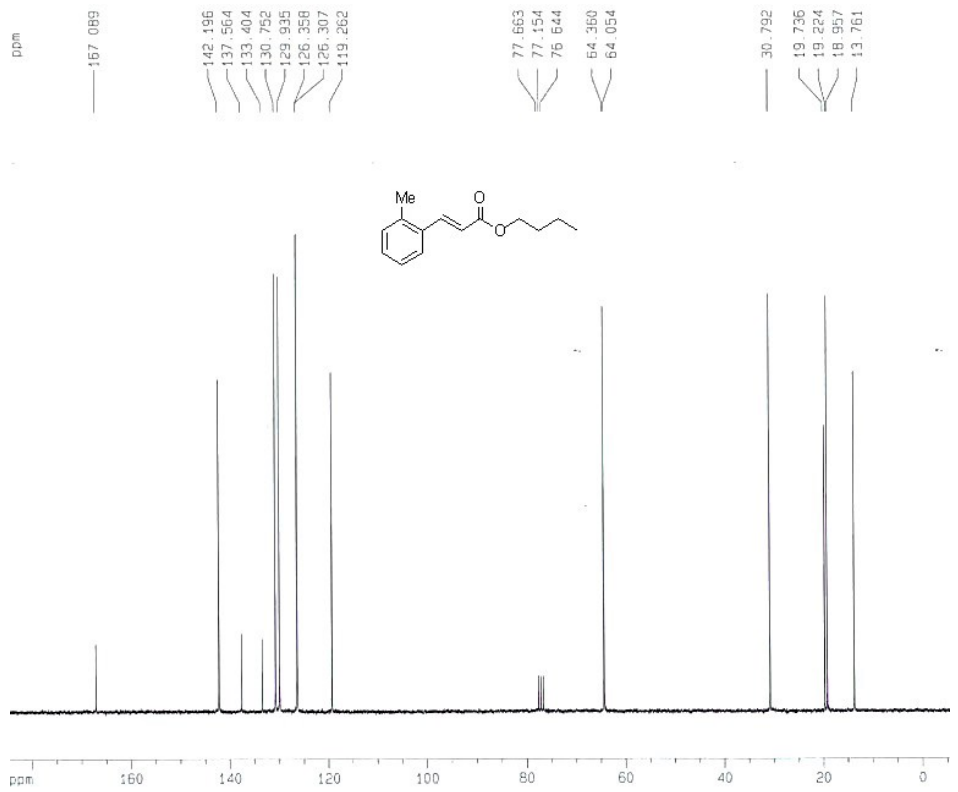
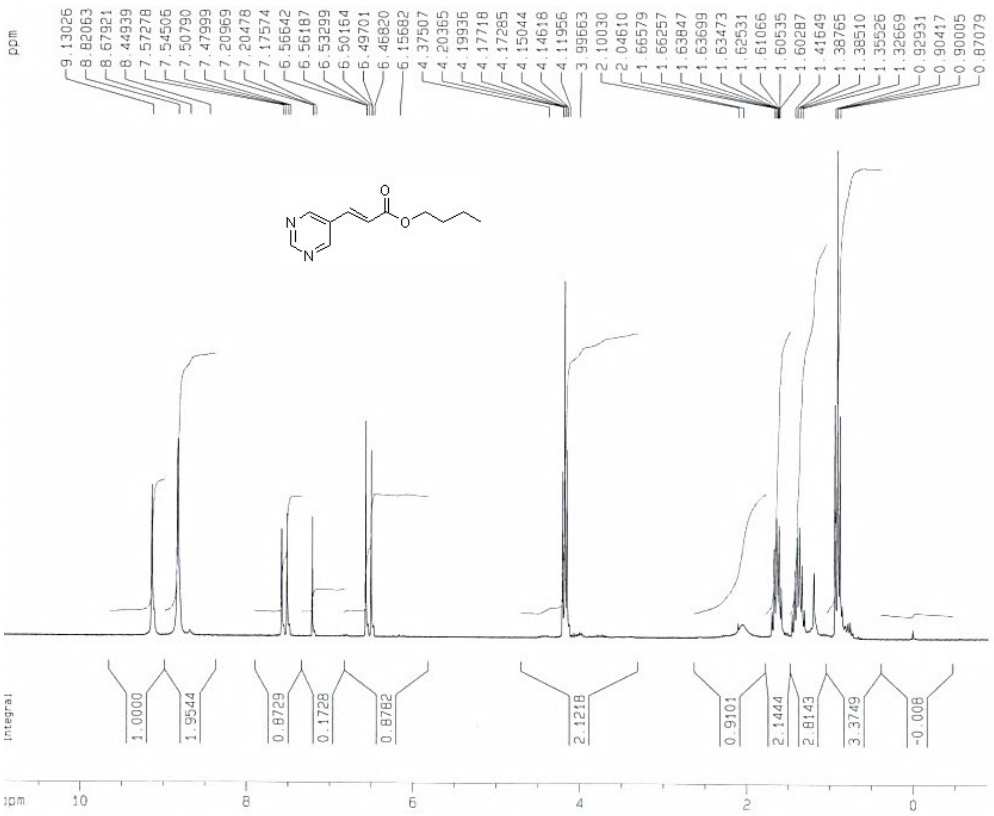
166.974
141.558
133.680
131.806
131.418
130.456
129.116
128.722
126.835
126.601
126.401
126.201
125.840
125.444
124.983
124.455
123.377
120.926
77.648
77.139
76.630
64.528
30.844
29.747
19.272
13.814
ppm
175
150
125
100
75
50
25
0


ppm
8.1301
7.8843
7.8379
7.8207
7.4109
7.4009
7.1245
7.1169
7.1134
7.1052
7.0984
7.0762
7.0700
6.2853
6.2762
6.2651
6.2218
6.2027
4.1347
4.1257
4.1157
4.1082
4.0992
4.0892
4.0815
4.0726
4.0626
2.3123
2.3047
2.2958
1.5855
1.5787
1.5726
1.5590
1.3438
1.3382
1.3158
1.3085
0.8922
0.8835
0.8738
0.8633
0.8544
0.8445
0.8341
0.8251
0.8155
Me
O
O
Integral
1.0000
1.1382
3.3127
1.1003
2.2945
3.4861
2.3446
2.4163
3.3542
-0.012
ppm
8
6
4
2
0


ppm
167.089
142.196
137.564
133.404
130.752
129.935
126.358
126.307
119.262
77.663
77.154
76.644
64.360
64.054
30.792
19.736
19.224
18.957
13.761
Me
O
O
ppm
160
140
120
100
80
60
40
20
0


ppm
9.13026
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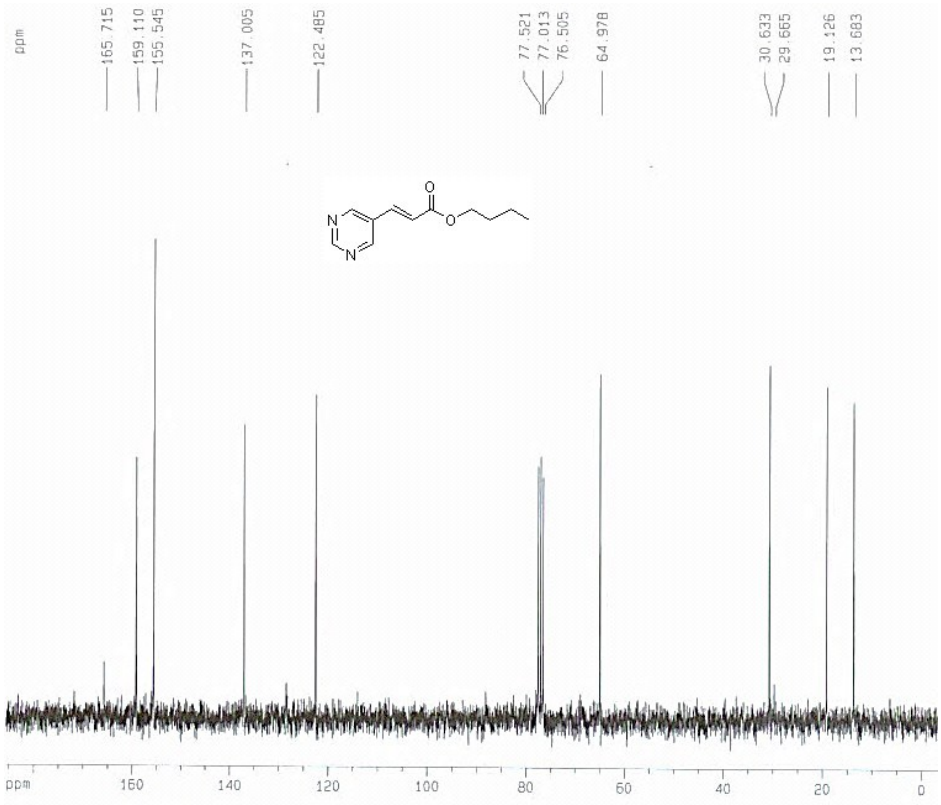
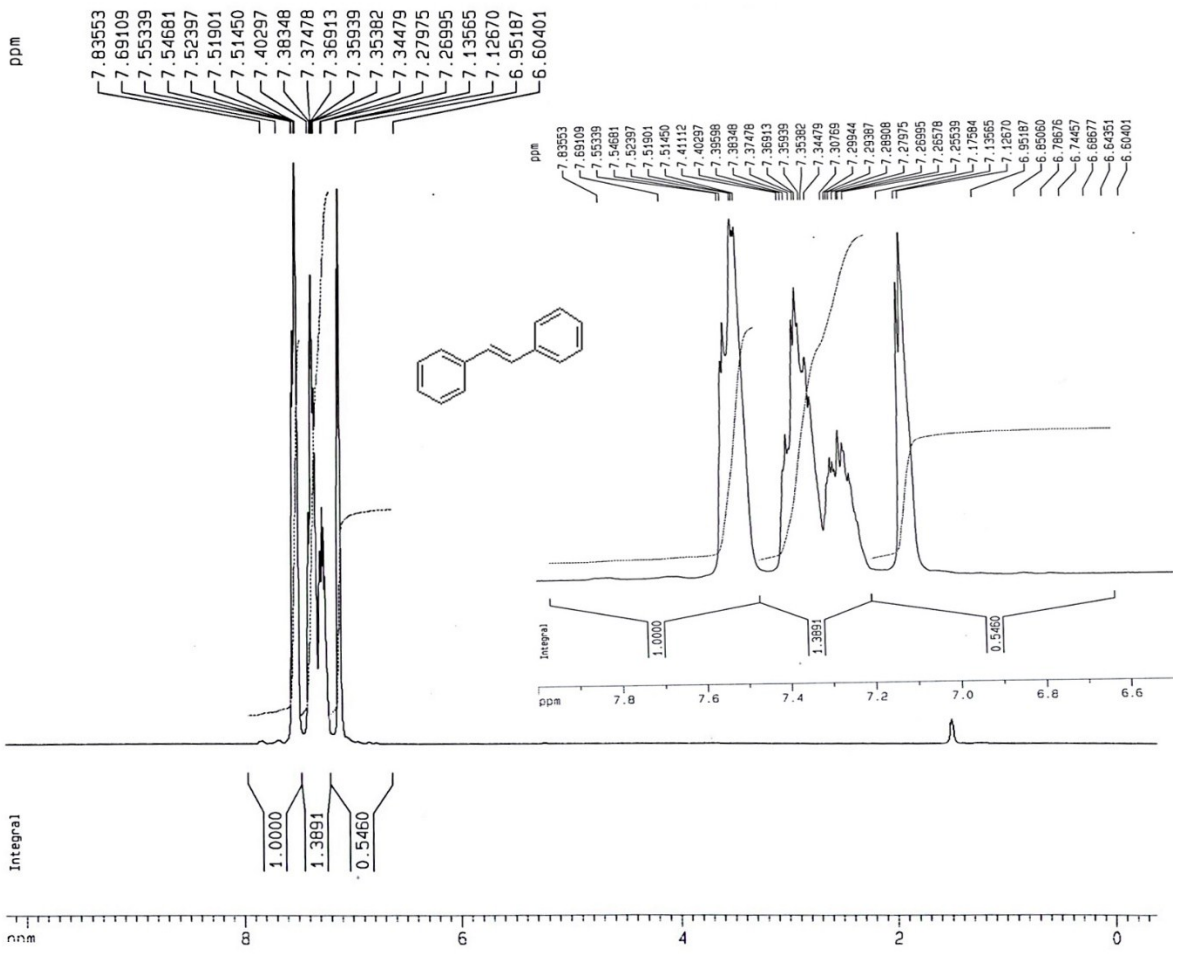
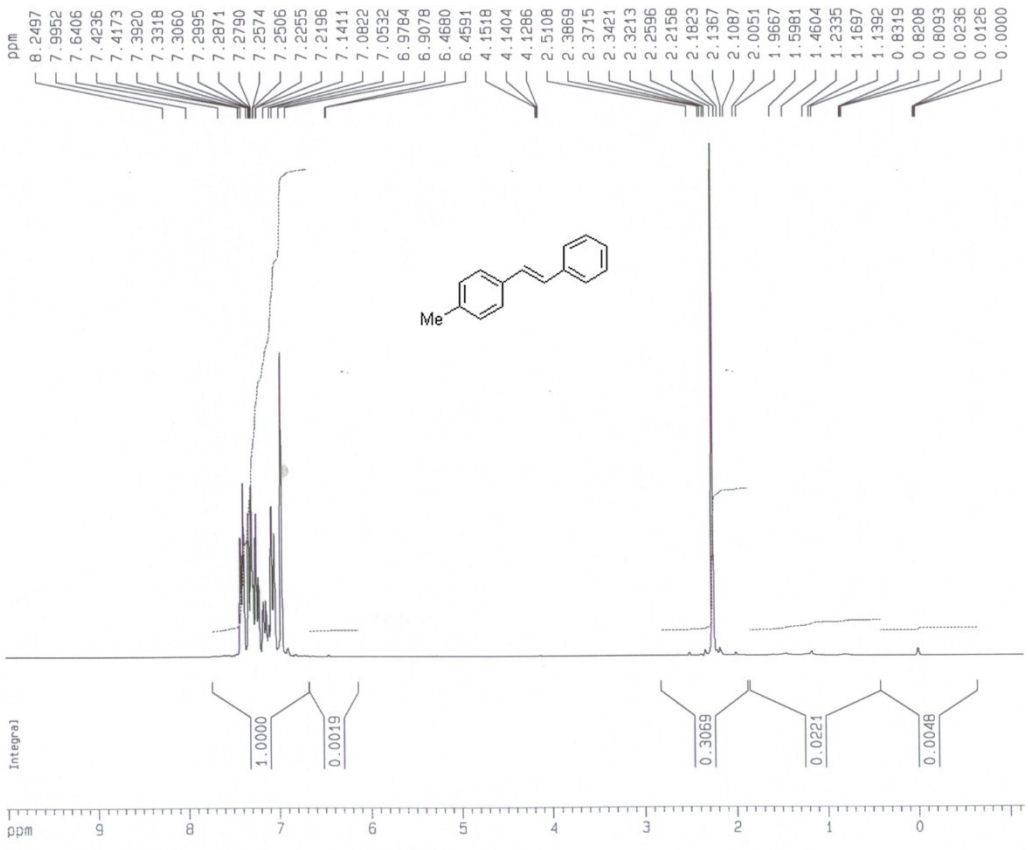
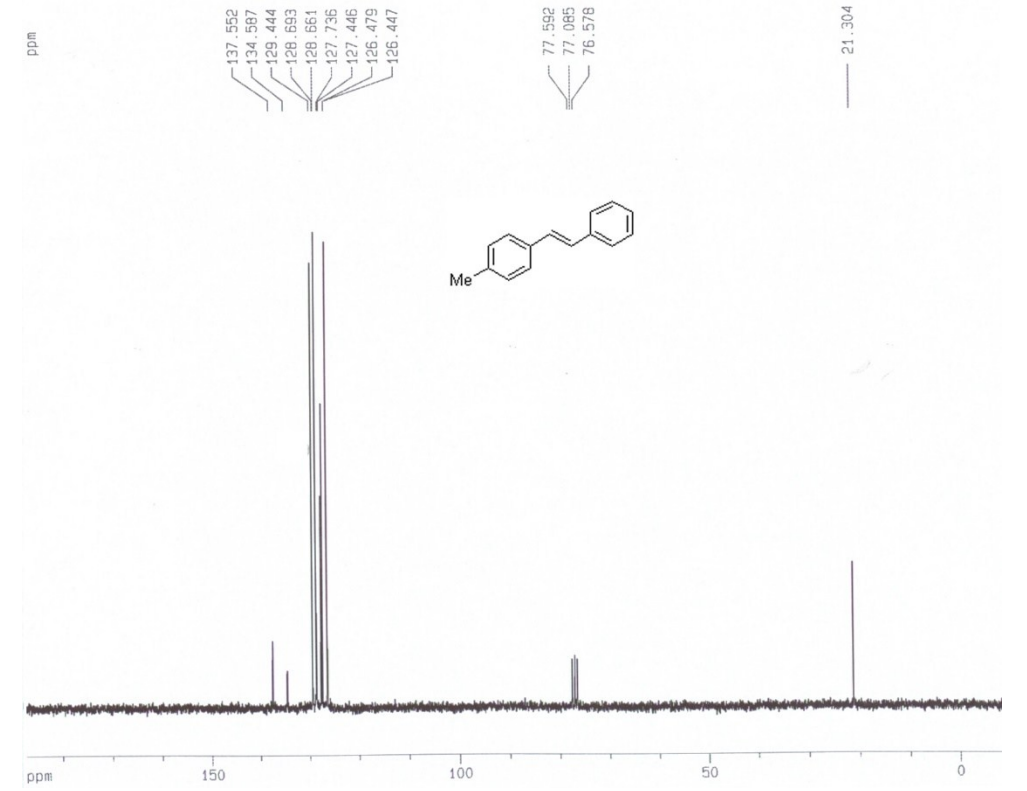
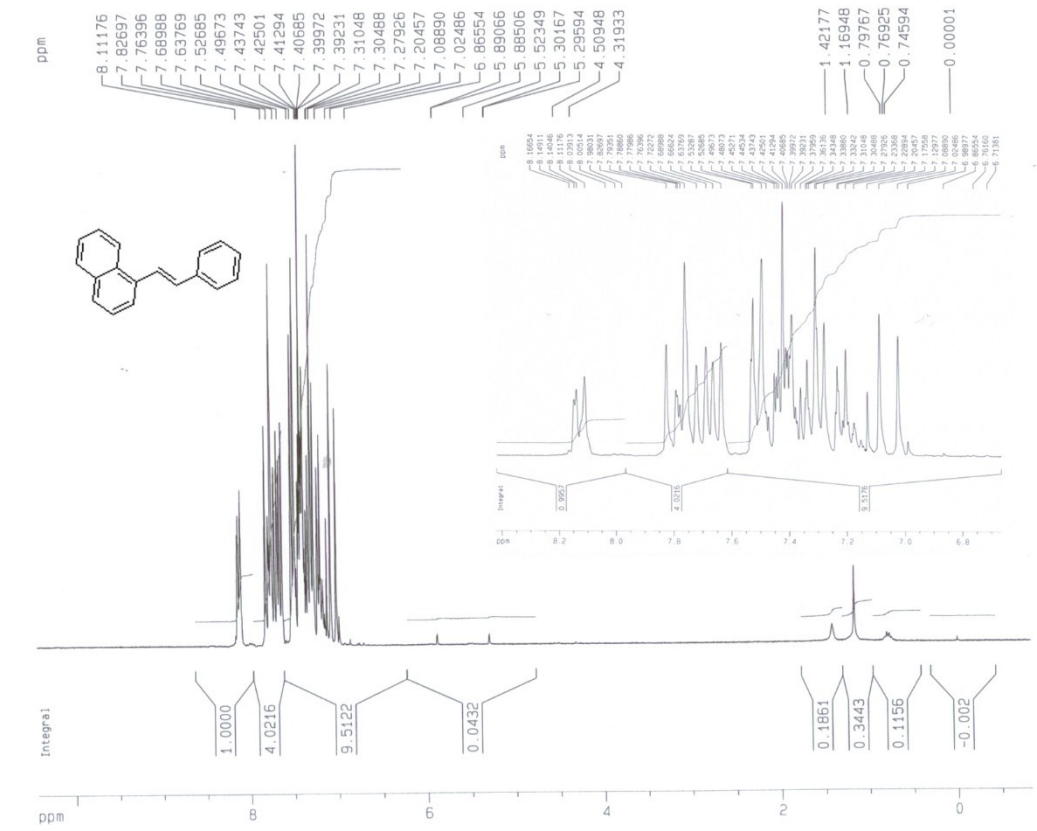
8.67921
8.44939
7.57278
7.54506
7.50790
7.47999
7.20969
7.20478
7.17574
6.56642
6.56187
6.53299
6.50164
6.49701
6.46820
6.15682
4.37507
4.20365
4.19936
4.17718
4.17285
4.15044
4.14618
4.11956
3.99663
2.10030
2.04610
1.66579
1.66257
1.63847
1.63699
1.63473
1.62531
1.61066
1.60535
1.60287
1.41649
1.38765
1.38510
1.35526
1.32669
0.92931
0.90417
0.90005
0.87079
Integral
1.0000
1.9544
0.8729
0.1728
0.8782
2.1218
0.9101
2.1444
2.8143
3.3749
-0.008
ppm
10
8
6
4
2
0

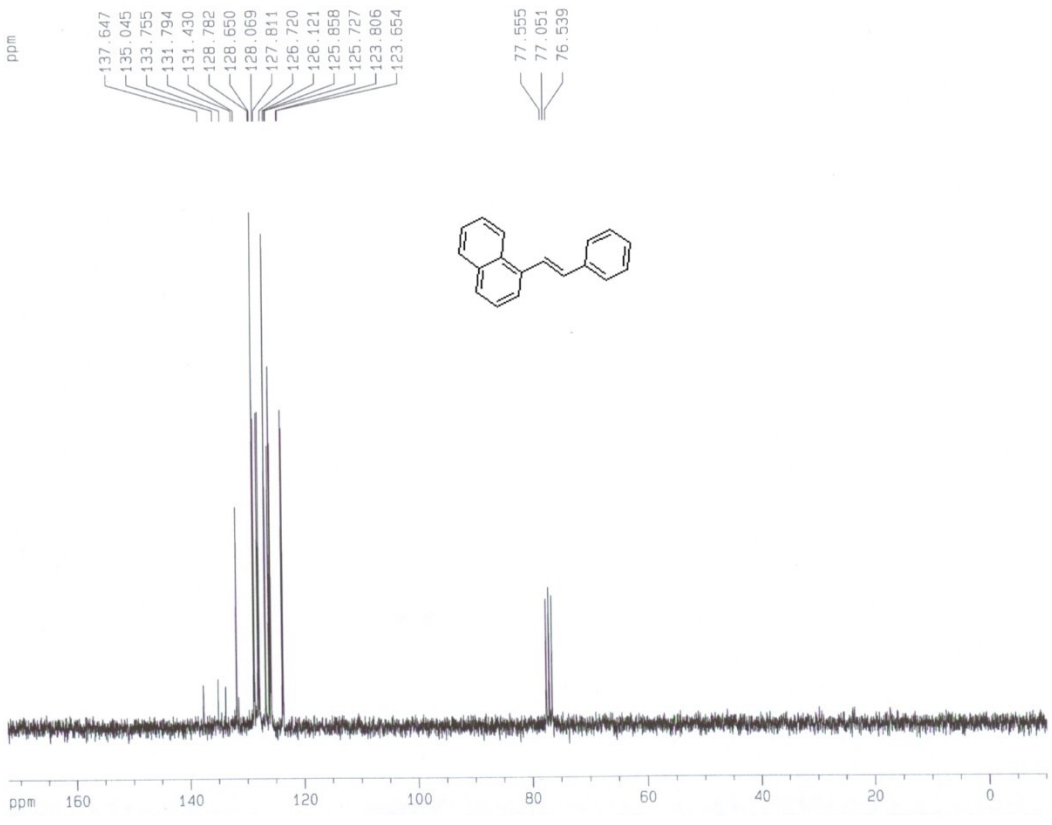

ppm
165.715
159.110
155.545
137.005
122.485
77.521
77.013
76.505
64.978
30.633
29.665
19.126
13.683
ppm
160
140
120
100
80
60
40
20
0

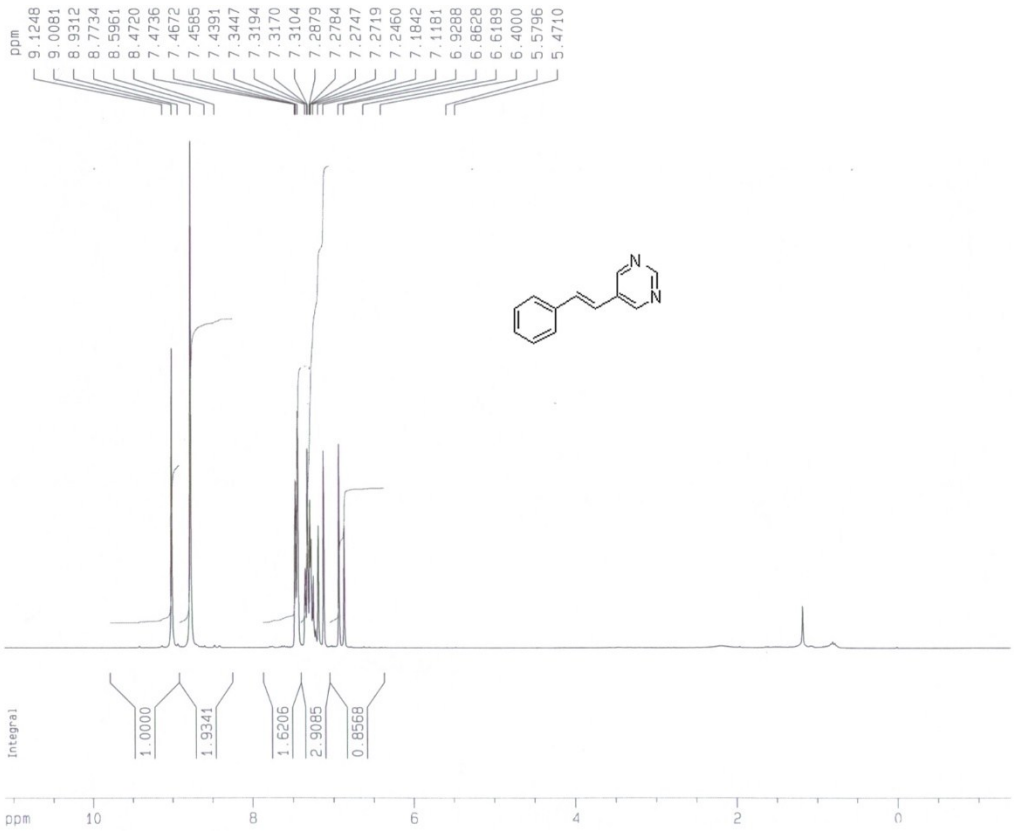

ppm
7.83553
7.69109
7.55339
7.54681
7.52397
7.51901
7.51450
7.40297
7.38348
7.37478
7.36913
7.35939
7.35382
7.34479
7.27975
7.26995
7.13565
7.12670
6.95187
6.60401
Integral
1.0000
1.3891
0.5460
ppm
8
6
4
2
0

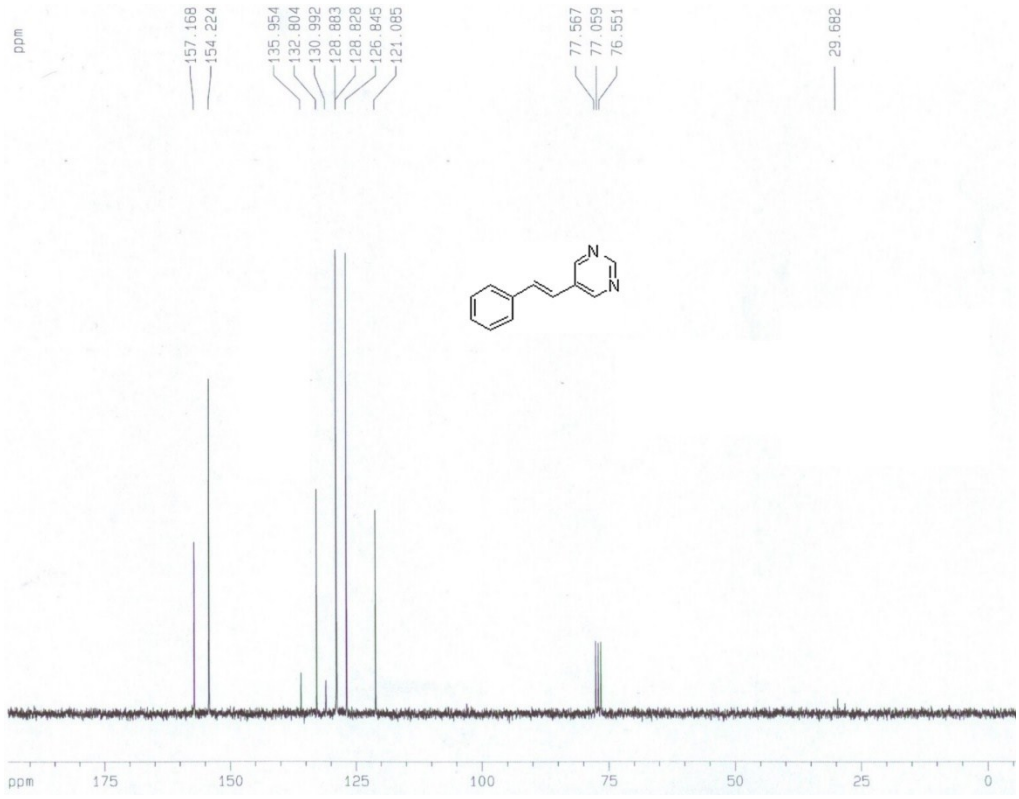

ppm
8.2497
7.9952
7.6406
7.4236
7.4173
7.3920
7.3318
7.3060
7.2995
7.2871
7.2790
7.2574
7.2506
7.2255
7.2196
7.1411
7.0822
7.0532
6.9784
6.9078
6.4680
6.4591
4.1518
4.1404
4.1286
2.5108
2.3869
2.3715
2.3421
2.3213
2.2596
2.2156
2.1823
2.1367
2.1087
2.0051
1.9667
1.5981
1.4604
1.2335
1.1697
1.1392
0.8319
0.8208
0.8093
0.0236
0.0126
0.0000
Me
Integral
1.0000
0.0019
0.3069
0.0221
0.0048
ppm
9
8
7
6
5
4
3
2
1
0

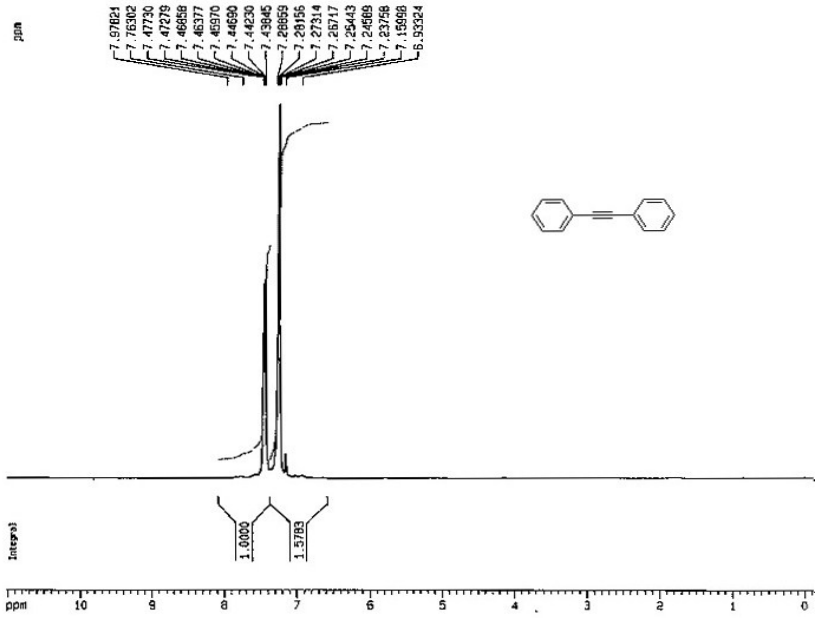

ppm
137.552
134.587
129.444
128.693
128.661
127.736
127.446
126.479
126.447
77.592
77.085
76.578
21.304
Me
ppm
150
100
50
0

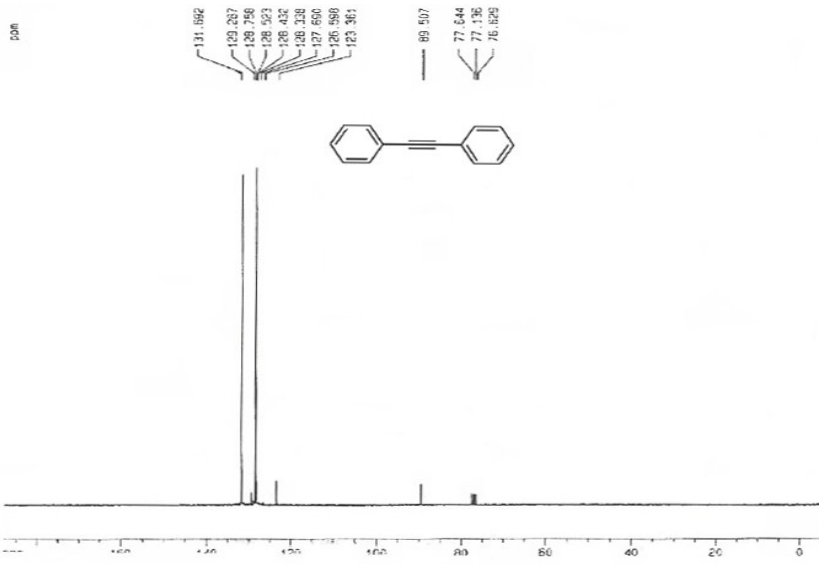

ppm
8.11176
7.82697
7.76396
7.68988
7.63769
7.52685
7.49673
7.43743
7.42501
7.41294
7.40685
7.39972
7.39231
7.31048
7.30488
7.27926
7.20457
7.08890
7.02486
6.86554
5.89066
5.88506
5.52349
5.30167
5.29594
4.50948
4.31933
1.42177
1.16948
0.79767
0.76925
0.74594
0.00001
Integral
1.0000
4.0216
9.5122
0.0432
0.1861
0.3443
0.1156
-0.002
ppm
8
6
4
2
0

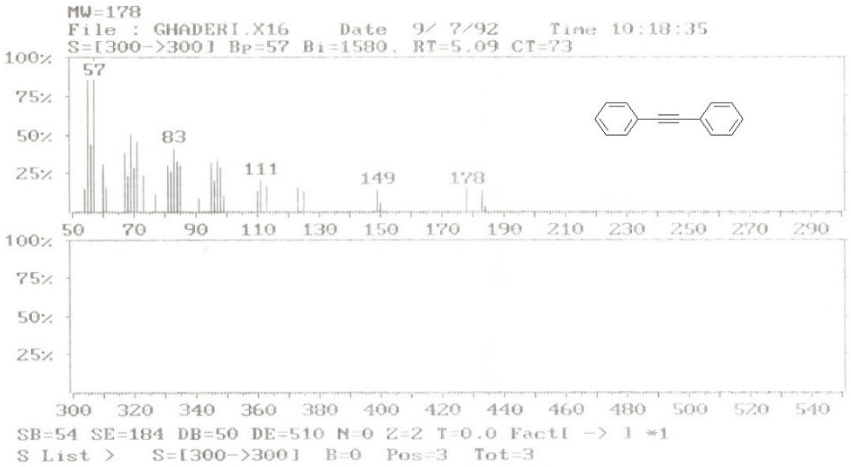

ppm
137.647
135.045
133.755
131.794
131.430
128.782
128.650
128.069
127.811
126.720
126.121
125.858
125.727
123.806
123.654
77.555
77.051
76.539
ppm
160
140
120
100
80
60
40
20
0

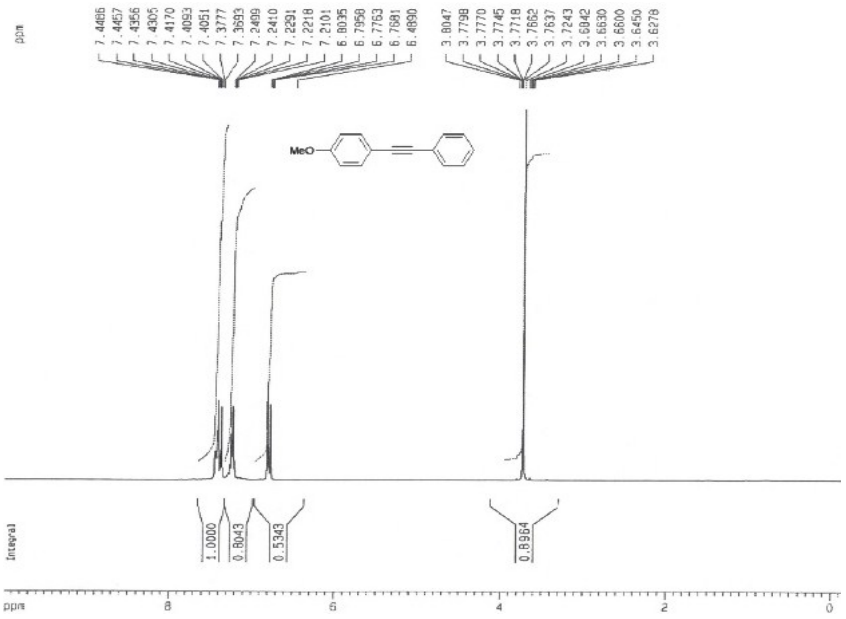

ppm
9.1248
9.0081
8.9312
8.7734
8.5961
8.4720
7.4736
7.4672
7.4585
7.4391
7.3447
7.3194
7.3170
7.3104
7.2879
7.2784
7.2747
7.2719
7.2460
7.1842
7.1181
6.9288
6.8628
6.6189
6.4000
5.5796
5.4710
Integral
1.0000
1.9341
1.6206
2.9085
0.8568
ppm
10
8
6
4
2
0

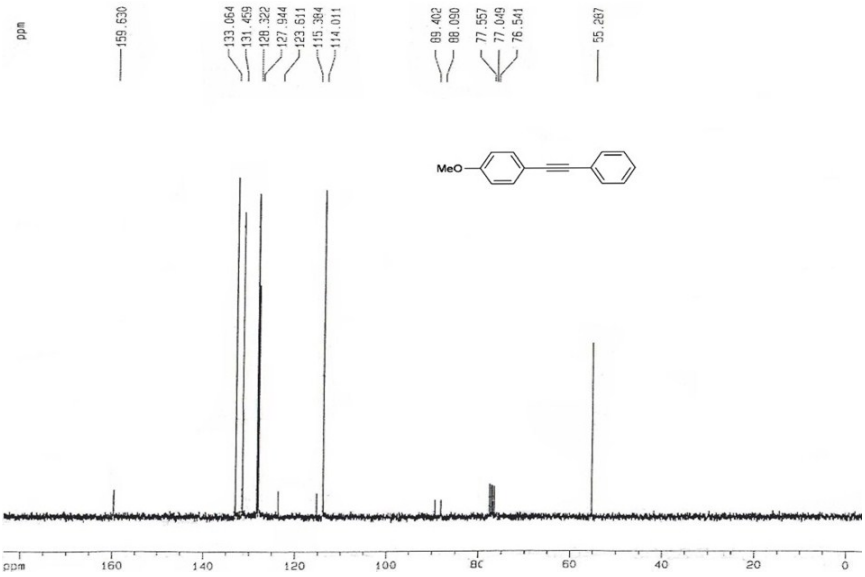

ppm
157.168
154.224
135.954
132.804
130.992
128.883
128.828
126.845
121.085
77.567
77.059
76.551
29.682
ppm
175
150
125
100
75
50
25
0

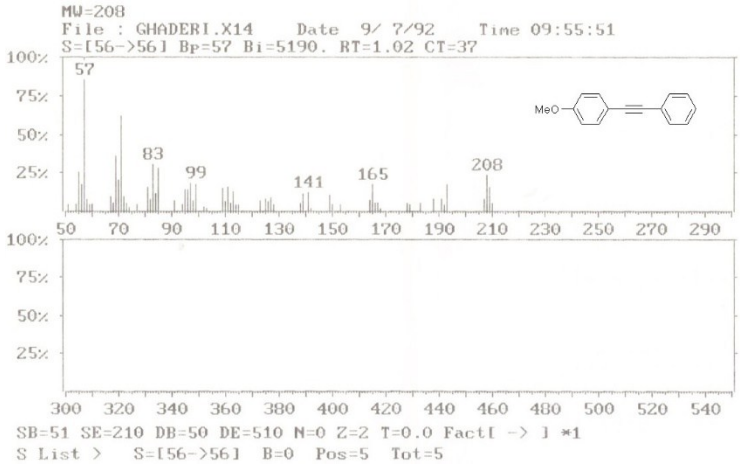

ppm
7.97624
7.76302
7.47730
7.47279
7.46858
7.46377
7.46970
7.44690
7.44230
7.43945
7.28659
7.28156
7.27314
7.26717
7.25443
7.24569
7.23758
7.15998
6.93324
Integral
1.0000
1.5783
ppm
10
9
8
7
6
5
4
3
2
1
0

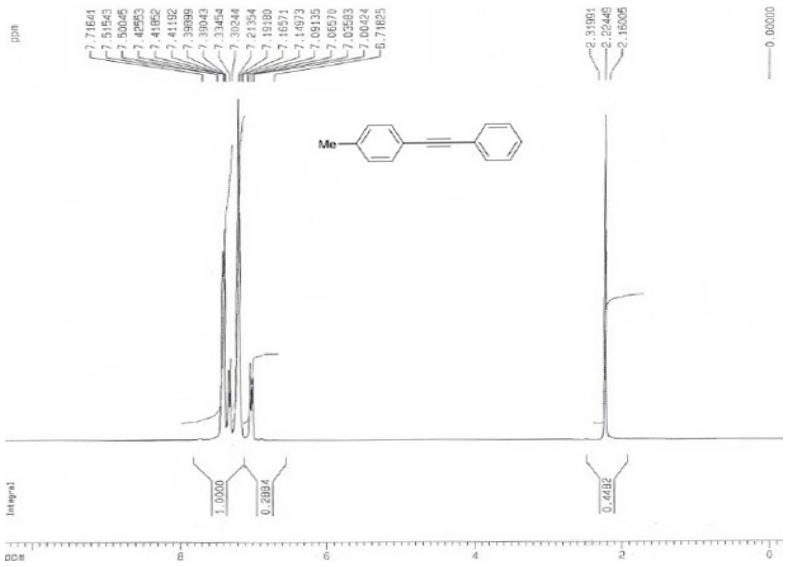

ppm
131.692
129.287
128.756
128.523
128.432
128.328
127.650
126.598
123.361
89.507
77.644
77.138
76.629

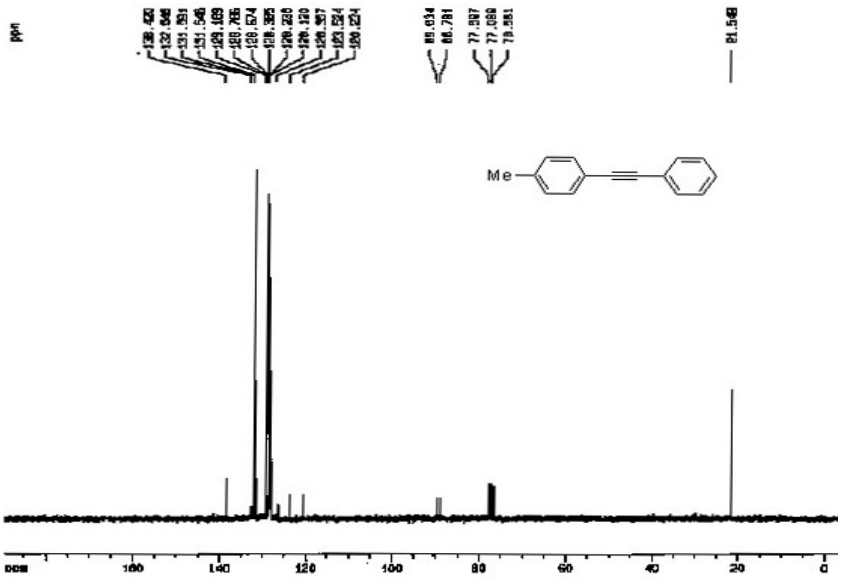

MW=178
File : GHADERI.X16 Date 9/ 7/92 Time 10:18:35
S=[300->300] Bp=57 Bi=1580. RT=5.09 CT=73
100%
75%
50%
25%
57
83
111
149
178
50 70 90 110 130 150 170 190 210 230 250 270 290
100%
75%
50%
25%
300 320 340 360 380 400 420 440 460 480 500 520 540
SB=54 SE=184 DB=50 DE=510 N=0 Z=2 T=0.0 Factl -> 1 *1
S List > S=[300->300] B=0 Pos=3 Tot=3

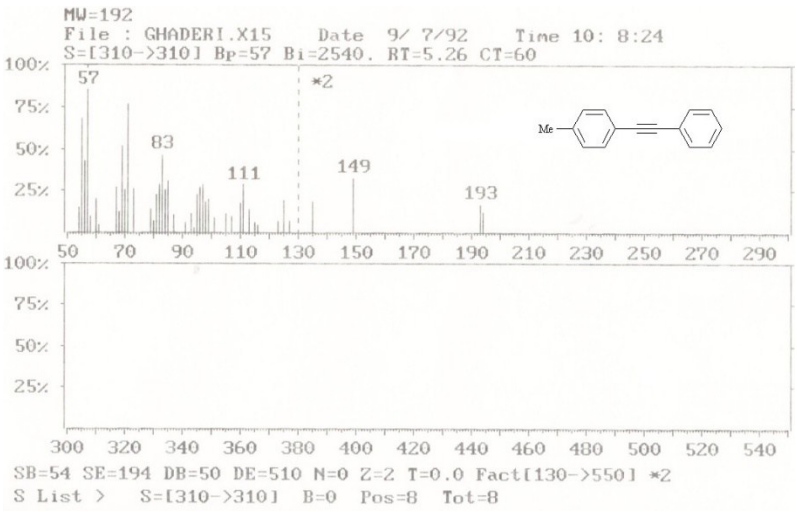

ppm
7.4466
7.4457
7.4356
7.4305
7.4170
7.4093
7.4051
7.3777
7.3693
7.2499
7.2410
7.2291
7.2218
7.2101
6.8035
6.7958
6.7763
6.7681
6.4890
3.8047
3.7798
3.7770
3.7745
3.7718
3.7652
3.7637
3.7243
3.6942
3.6539
3.6500
3.6450
3.6278
MeO
Integral
1.0000
0.8043
0.5343
0.8964
ppm
8
6
4
2
0

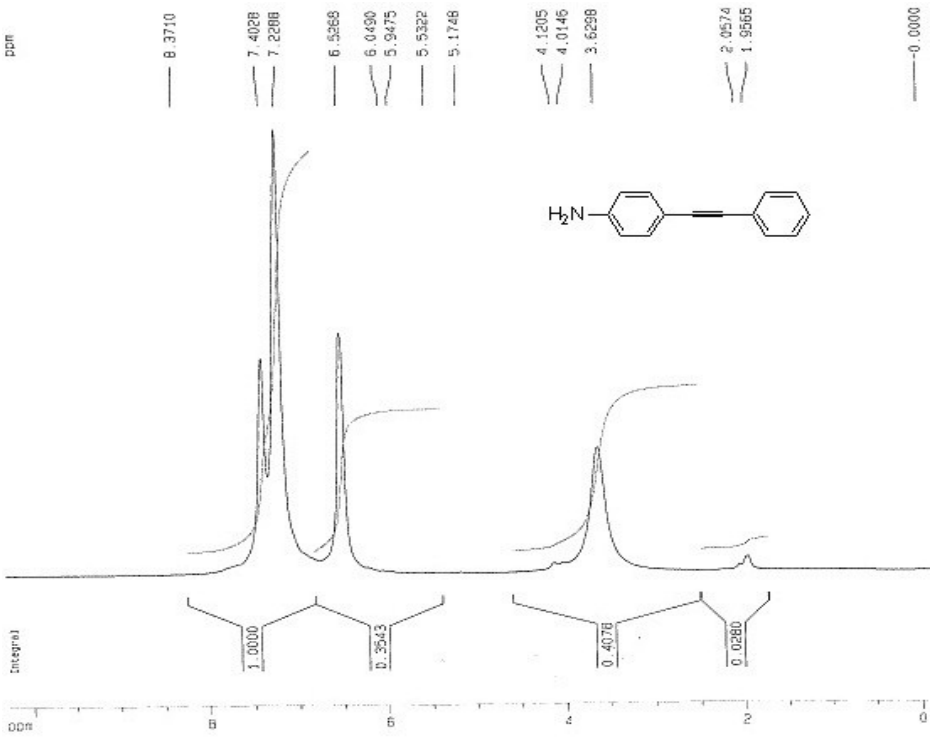

ppm
159.630
133.054
131.459
128.322
127.944
123.611
115.384
114.011
89.402
88.090
77.557
77.049
76.541
55.287
MeO
ppm
160
140
120
100
80
60
40
20
0

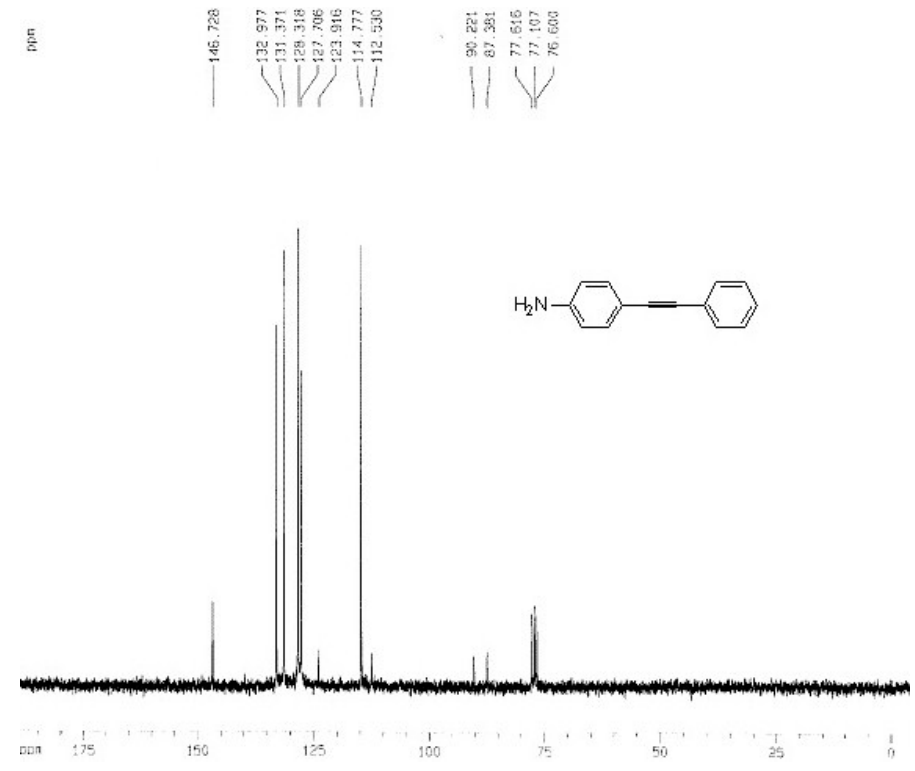

MW=208
File : GHADERI.X14 Date 9/ 7/92 Time 09:55:51
S=[56->56] Bp=57 Bi=5190. RT=1.02 CT=37
100%
75%
50%
25%
57
83
99
141
165
208
MeO
50 70 90 110 130 150 170 190 210 230 250 270 290
300 320 340 360 380 400 420 440 460 480 500 520 540
SB=51 SE=210 DB=50 DE=510 N=0 Z=2 T=0.0 Fact[->] *1
S List > S=[56->56] B=0 Pos=5 Tot=5

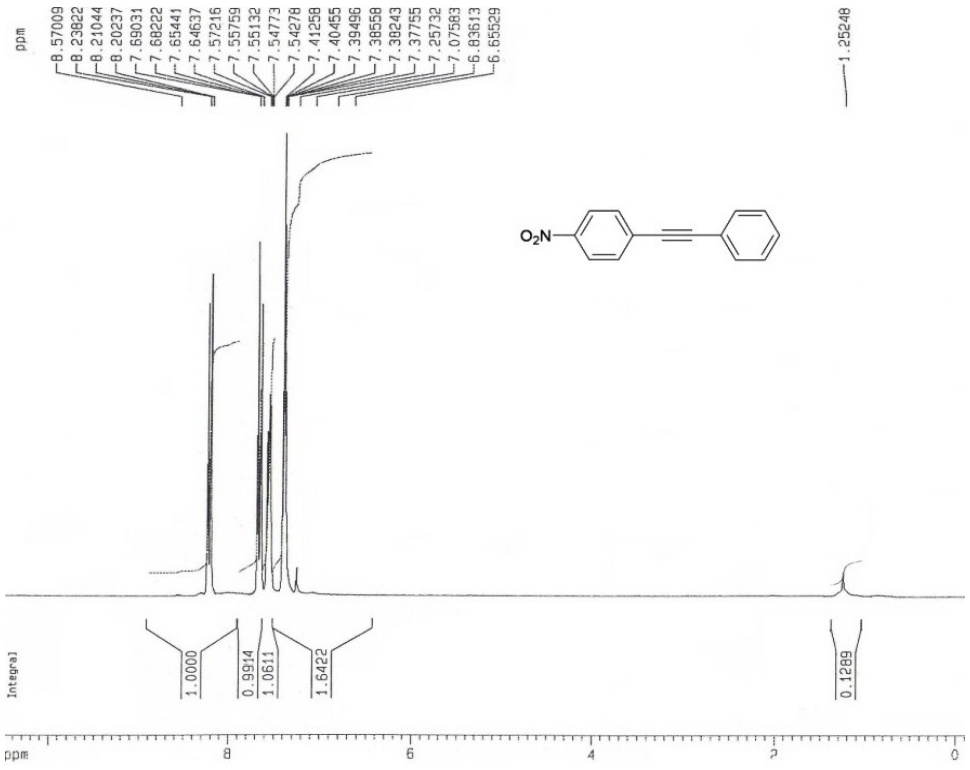

Me
Integral
1.0000
0.2884
0.4482

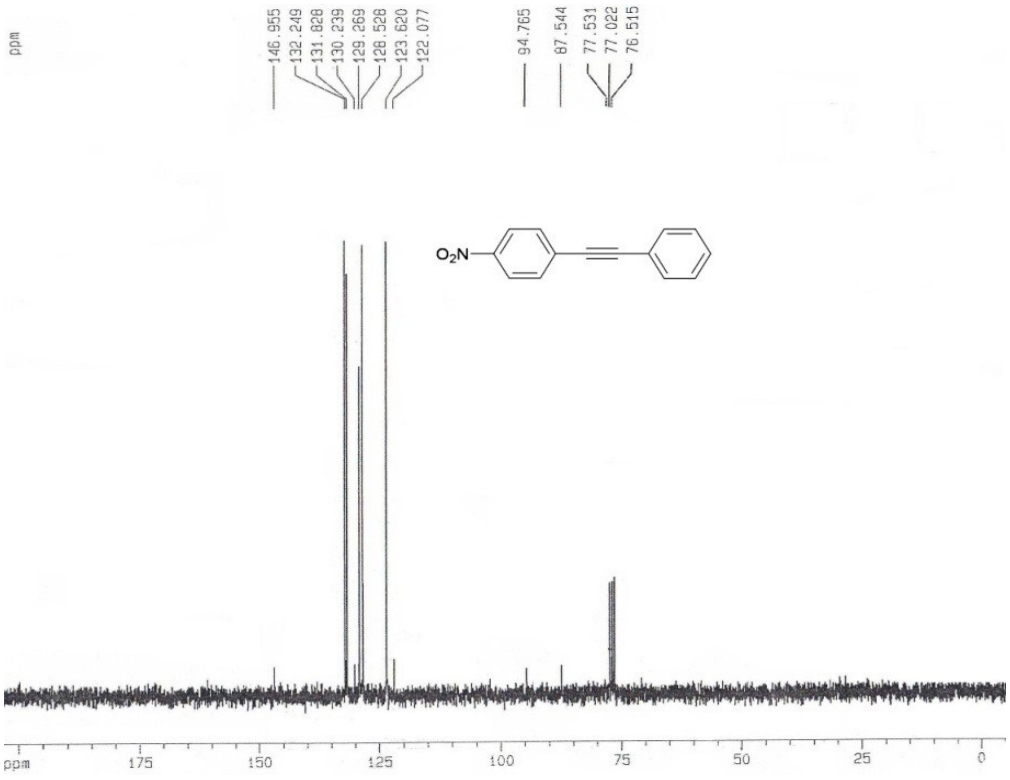

Me

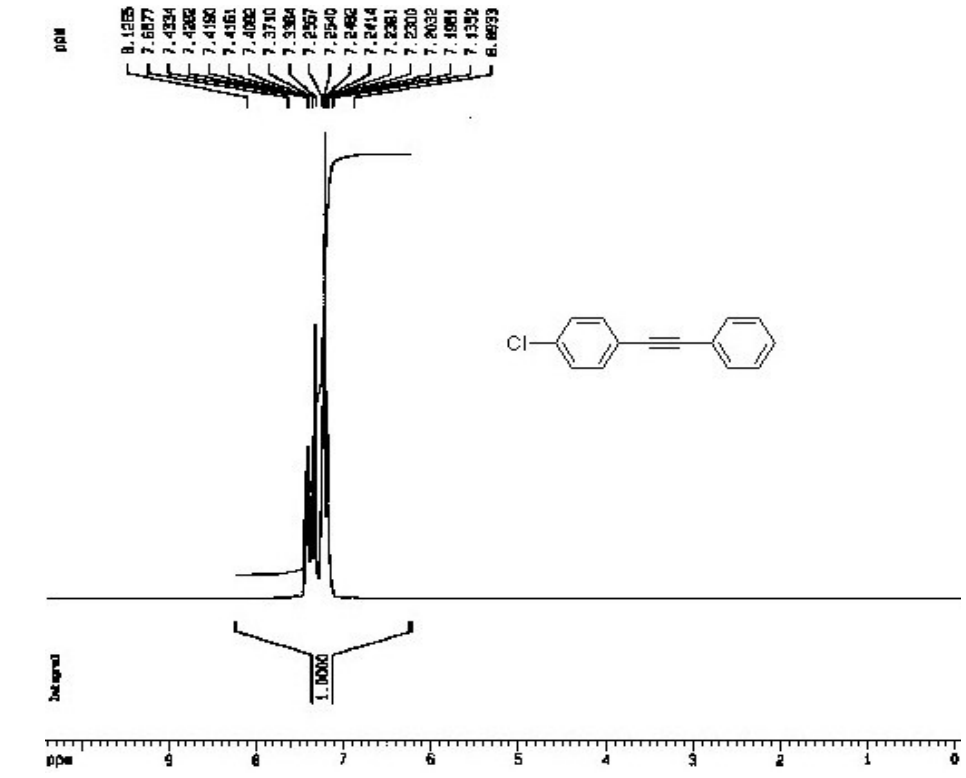

MW=192
File : GHADERI.X15 Date 9/ 7/92 Time 10: 8:24
S=[310->310] Bp=57 Bi=2540. RT=5.26 CT=60
*2
Me
57
83
111
149
193
SB=54 SE=194 DB=50 DE=510 N=0 Z=2 T=0.0 Fact[130->550] *2
S List > S=[310->310] B=0 Pos=8 Tot=8

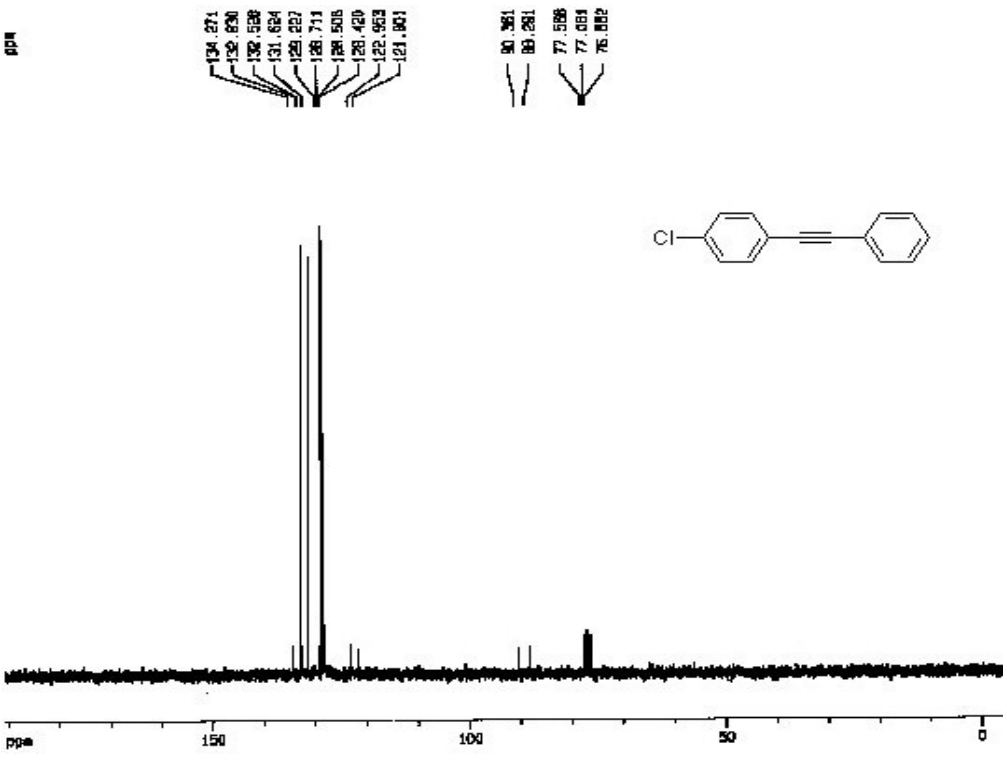

ppm
8.3710
7.4028
7.2286
6.5268
6.0490
5.9475
5.5322
5.1748
4.1205
4.0146
3.6298
2.0574
1.9565
0.0000
H2N
Integral
1.0000
0.3543
0.4076
0.0280
ppm
8
6
4
2
0

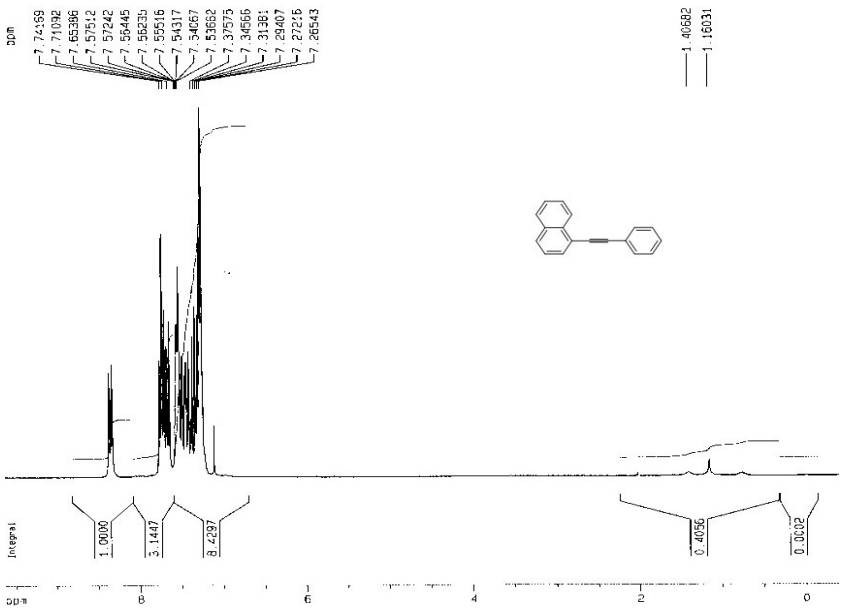

ppm
146.728
132.977
131.371
129.318
127.706
123.916
114.777
112.530
90.221
87.381
77.616
77.107
76.600
H2N
ppm
175
150
125
100
75
50
25
0

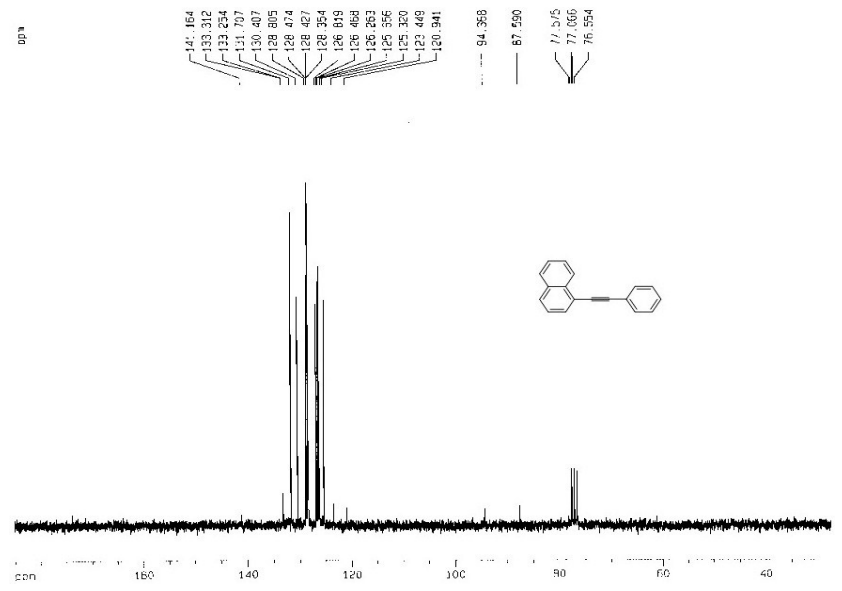

ppm
8.57009
8.23822
8.21044
8.20237
7.69031
7.68222
7.65441
7.64637
7.57216
7.55759
7.55132
7.54773
7.54278
7.41258
7.40455
7.39496
7.38558
7.38243
7.37755
7.25732
7.07583
6.83613
6.65529
1.25248
O2N
Integral
1.0000
0.9914
1.0611
1.6422
0.1269
ppm
8
6
4
2
0

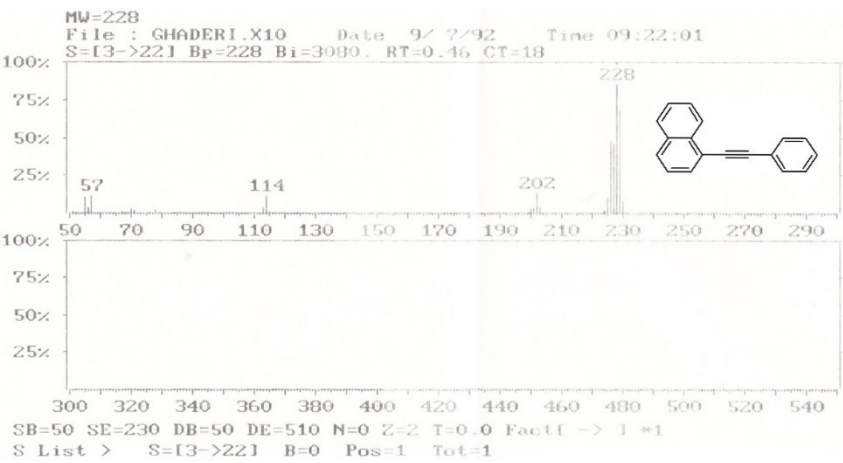

ppm
146.955
132.249
131.828
130.239
129.269
128.528
123.620
122.077
94.765
87.544
77.531
77.022
76.515
O2N
ppm
175
150
125
100
75
50
25
0

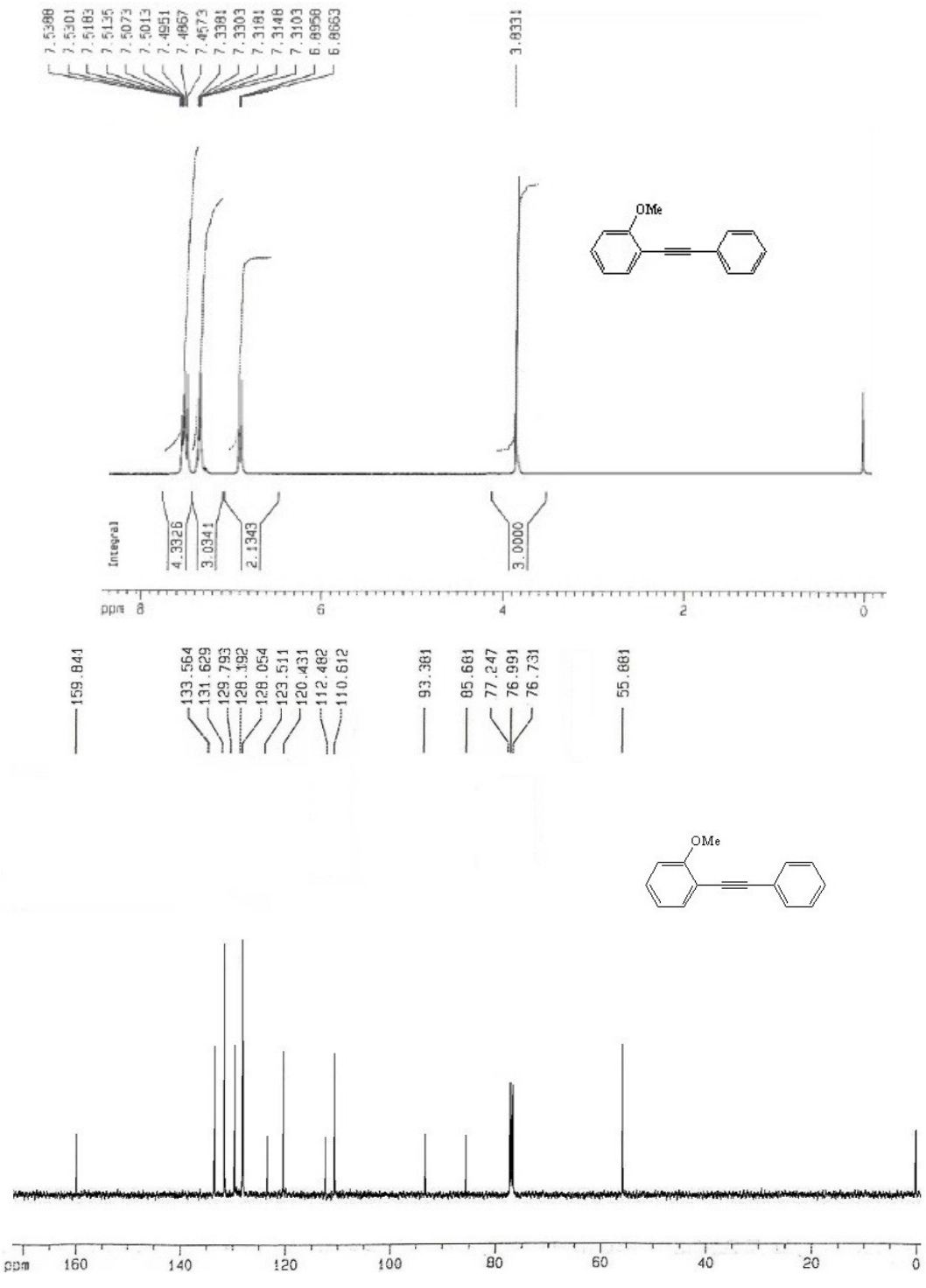

ppm
8.1255
7.6877
7.4334
7.4288
7.4190
7.4161
7.4082
7.3710
7.3384
7.2957
7.2540
7.2462
7.2414
7.2361
7.2300
7.2032
7.1981
7.1332
6.8693
Integral
1.0000
ppm
9
8
7
6
5
4
3
2
1
0
Cl

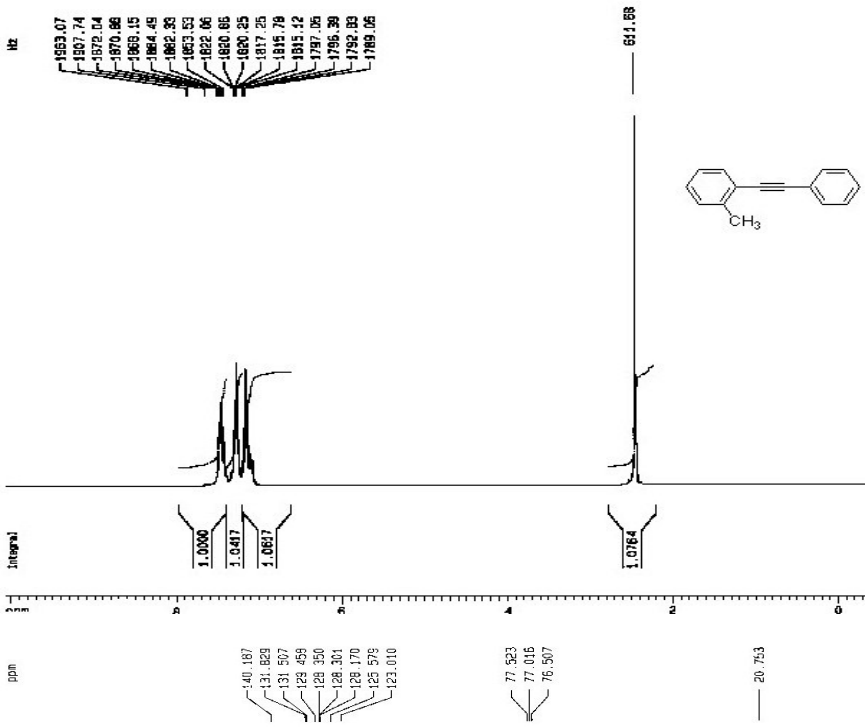

ppm
134.271
132.830
132.538
131.624
129.227
128.711
128.506
128.429
122.953
121.901
90.361
89.291
77.586
77.084
76.582
Cl
ppm
150
100
50
0

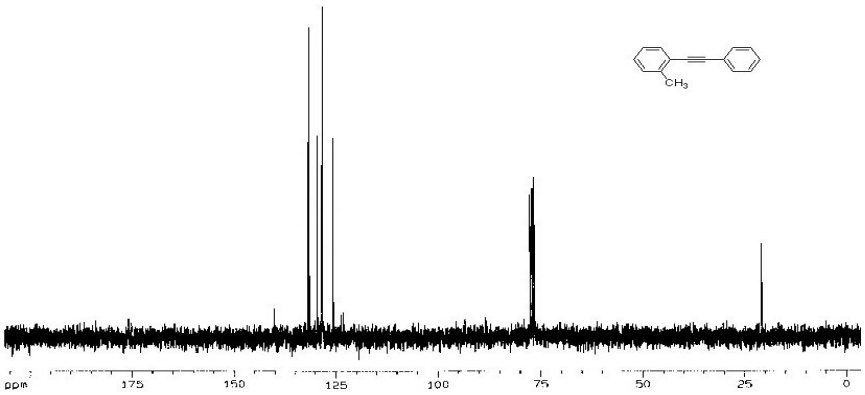

ppm
7.74169
7.71092
7.66396
7.57512
7.57242
7.56445
7.56230
7.55516
7.54317
7.54067
7.53682
7.37575
7.34566
7.31381
7.29407
7.27216
7.26543
1.40682
1.16031
Integral
1.0000
3.1447
8.4297
0.4056
0.0002
ppm
8
6
4
2
0

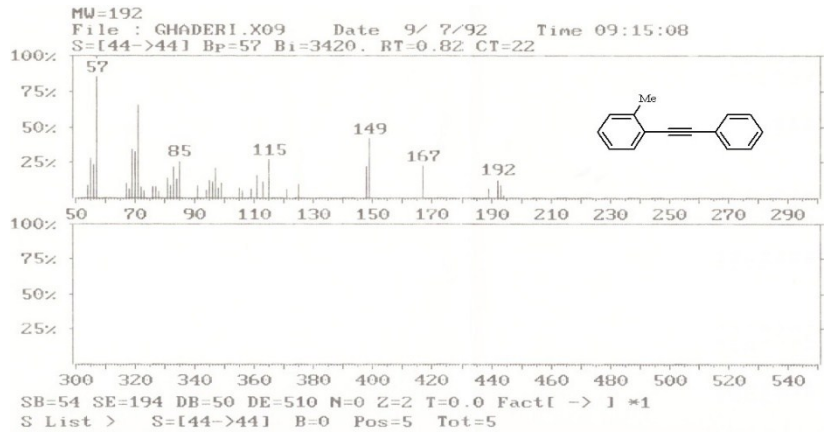

ppm
141.164
133.312
133.234
131.707
130.407
128.805
128.474
128.427
128.354
126.819
126.468
126.263
125.356
125.320
123.449
120.941
94.368
87.590
77.575
77.066
76.554
con
160
140
120
100
80
60
40

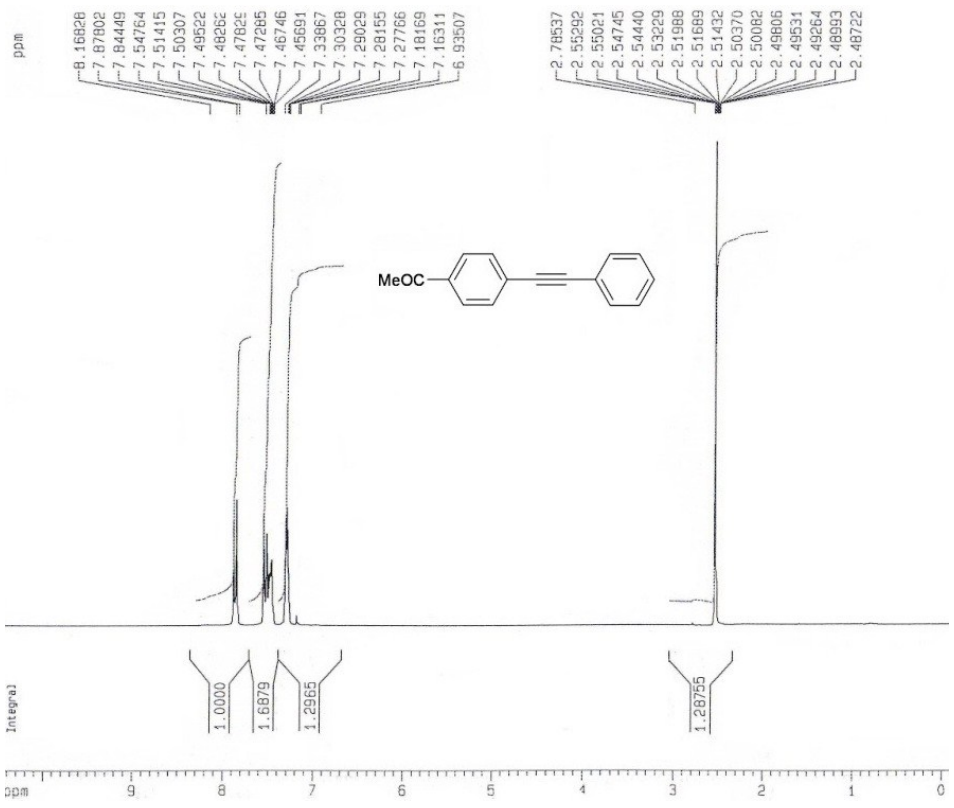

MW=228
File : GHADERI.X10 Date 9/ 7/92 Time 09:22:01
S=[3->22] Bp=228 Bi=3080. RT=0.46 CT=18
100%
75%
50%
25%
228
57
114
202
50 70 90 110 130 150 170 190 210 230 250 270 290
100%
75%
50%
25%
300 320 340 360 380 400 420 440 460 480 500 520 540
SB=50 SE=230 DB=50 DE=510 N=0 Z=2 T=0.0 Fact[->] *1
S List > S=[3->22] B=0 Pos=1 Tot=1

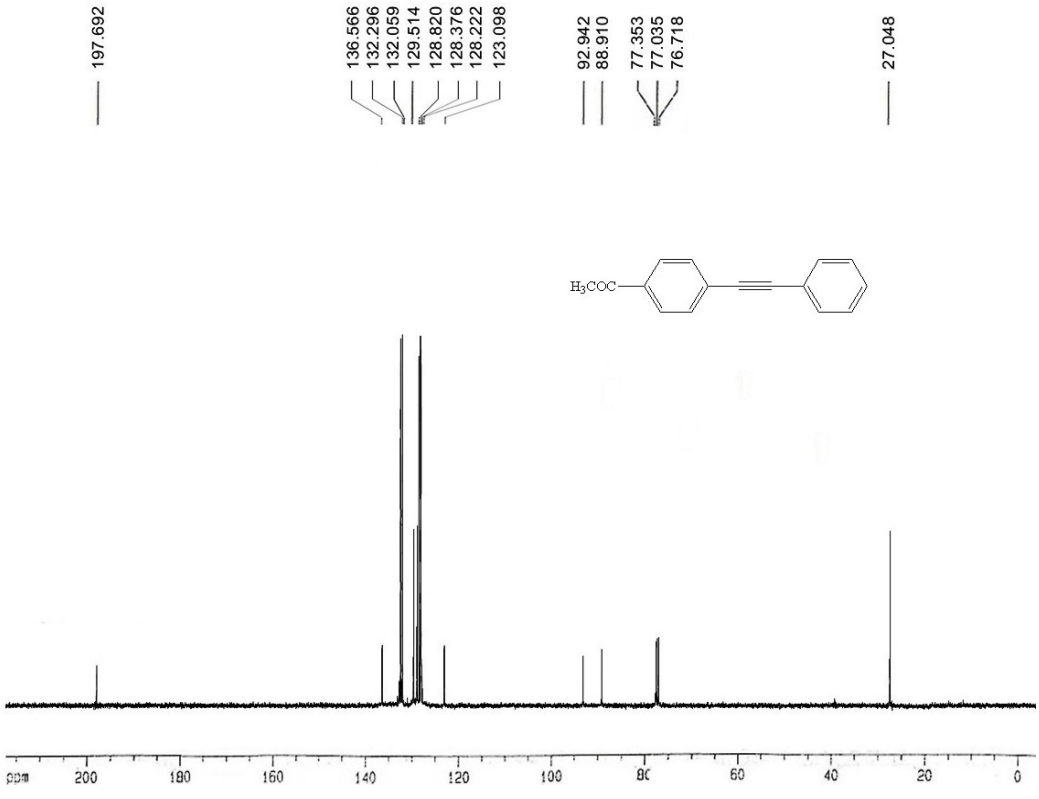

7.5388
7.5301
7.5183
7.5135
7.5073
7.5013
7.4951
7.4867
7.4573
7.3381
7.3303
7.3161
7.3148
7.3103
6.8958
6.8663
3.8331
OMe
Integral
4.3326
3.0341
2.1343
3.0000
ppm
8
6
4
2
0
159.841
133.564
131.629
129.793
128.192
128.054
123.511
120.431
112.482
110.612
93.381
85.681
77.247
76.991
76.731
55.881
OMe
ppm
160
140
120
100
80
60
40
20
0

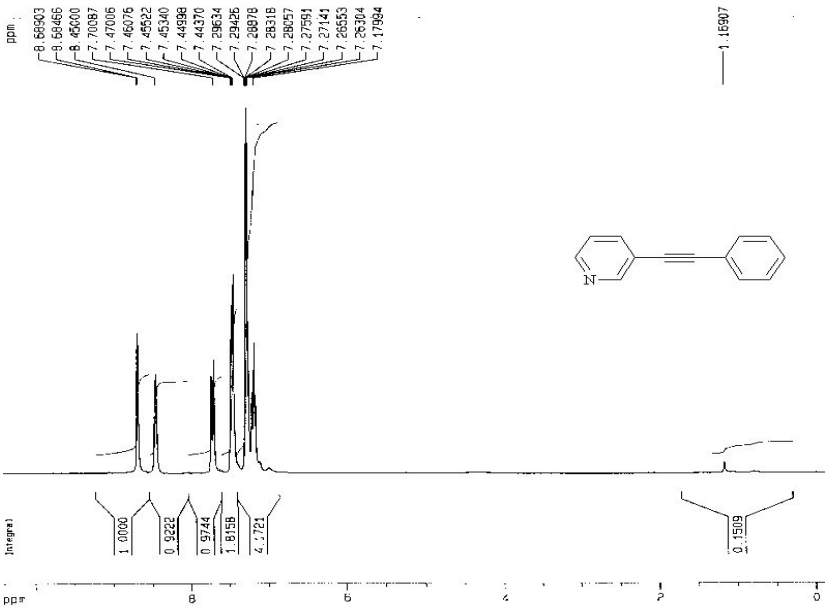

Hz
2611.68
Integral
1.0000
1.0417
1.0617
1.0764
ppm
20.753

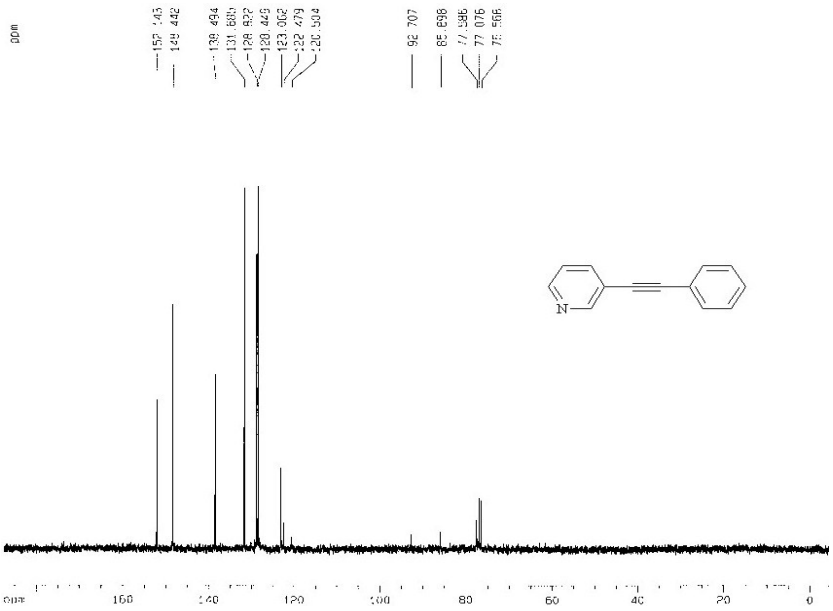

ppm

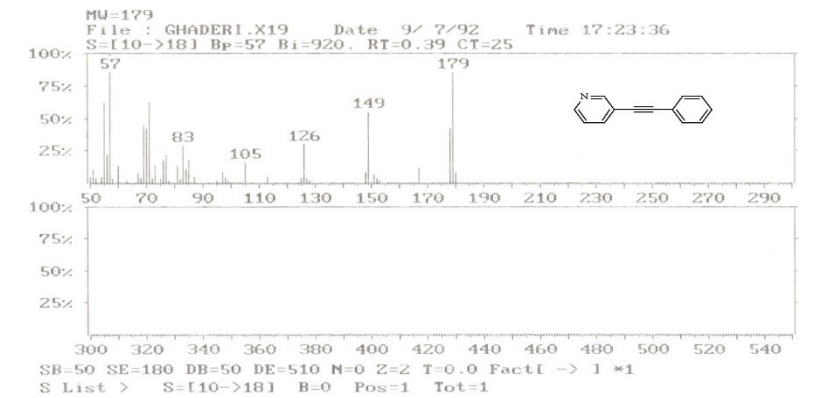

MW=192
File : GHADERI.X09 Date 9/ 7/92 Time 09:15:08
S=[44->44] Bp=57 Bi=3420. RT=0.82 CT=22
100%
75%
50%
25%
57
85
115
149
167
192
Me
SB=54 SE=194 DB=50 DE=510 N=0 Z=2 T=0.0 Fact[->] *1
S List > S=[44->44] B=0 Pos=5 Tot=5


ppm
8.16828
7.87802
7.84449
7.54764
7.51415
7.50307
7.49522
7.48265
7.47825
7.47285
7.46746
7.45691
7.33867
7.30328
7.29029
7.28155
7.27766
7.18169
7.16311
6.93507
2.78537
2.55292
2.55021
2.54745
2.54440
2.53229
2.51988
2.51689
2.51432
2.50370
2.50082
2.49806
2.49531
2.49264
2.48993
2.48722
MeOC
Integral
1.0000
1.6879
1.2965
1.28755
ppm
9
8
7
6
5
4
3
2
1
0

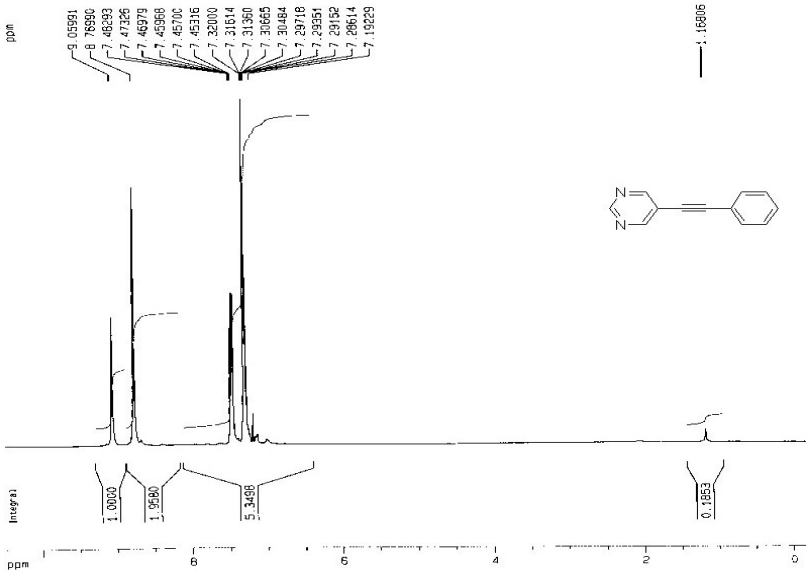

197.692
136.566
132.296
132.059
129.514
128.820
128.376
128.222
123.098
92.942
88.910
77.353
77.035
76.718
27.048
H3COC
ppm
200
180
160
140
120
100
80
60
40
20
0

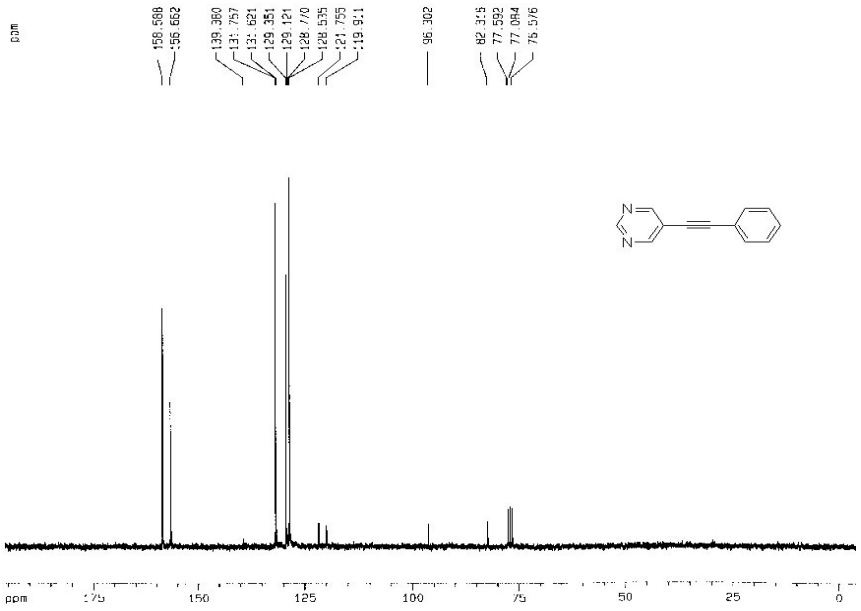


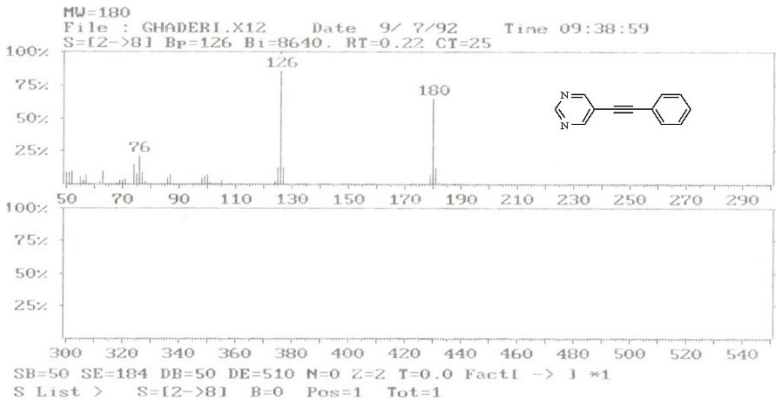


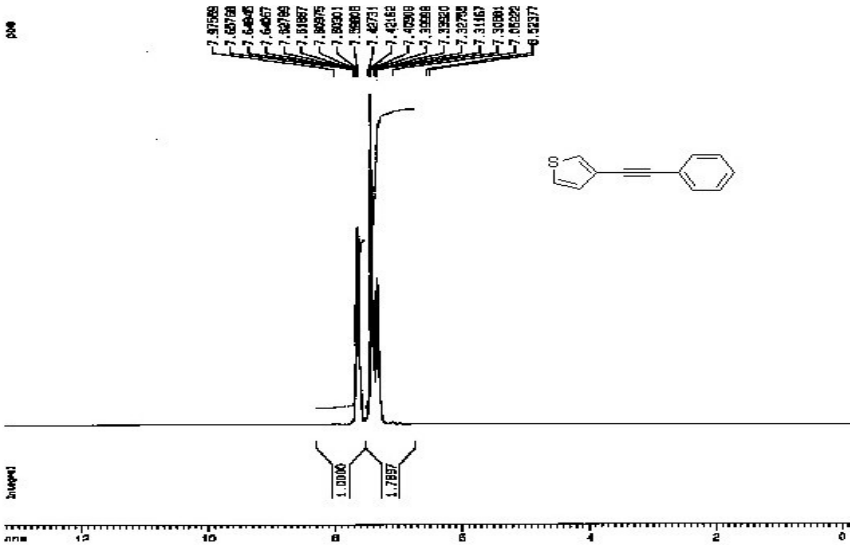


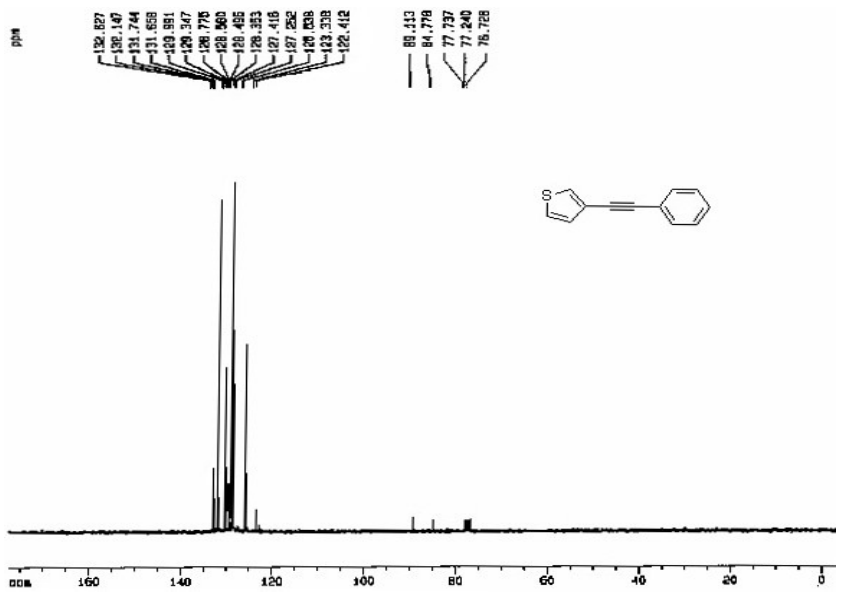
MW=179
File : GHADERI.X19 Date 9/ 7/92 Time 17:23:36
S=[10->18] Bp=57 Bi=920. RT=0.39 CT=25
100%
75%
50%
25%
57
179
149
83
126
105
50 70 90 110 130 150 170 190 210 230 250 270 290
300 320 340 360 380 400 420 440 460 480 500 520 540
SB=50 SE=180 DB=50 DE=510 N=0 Z=2 T=0.0 Fact[->] *1
S List > S=[10->18] B=0 Pos=1 Tot=1

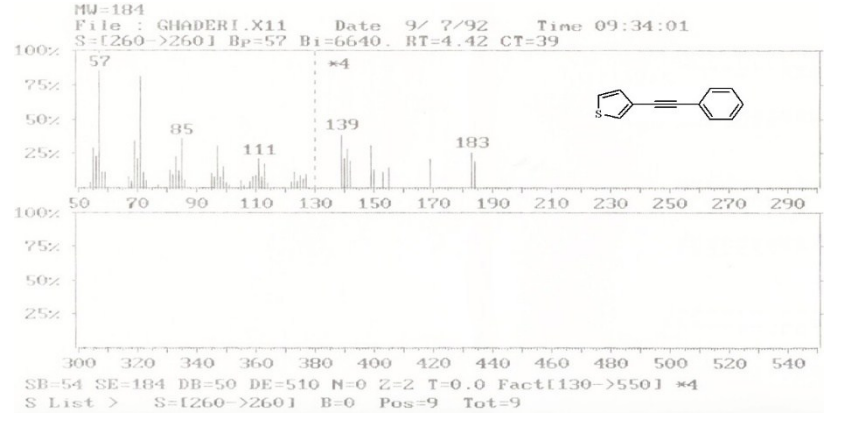

ppm
9.05991
8.76990
8.48293
7.47326
7.46979
7.45968
7.45700
7.45316
7.32000
7.31614
7.31360
7.30665
7.30484
7.29718
7.29351
7.29152
7.28614
7.19229
1.16806
Integral
1.0000
1.0680
5.3498
0.1853
8
6
4
2
0

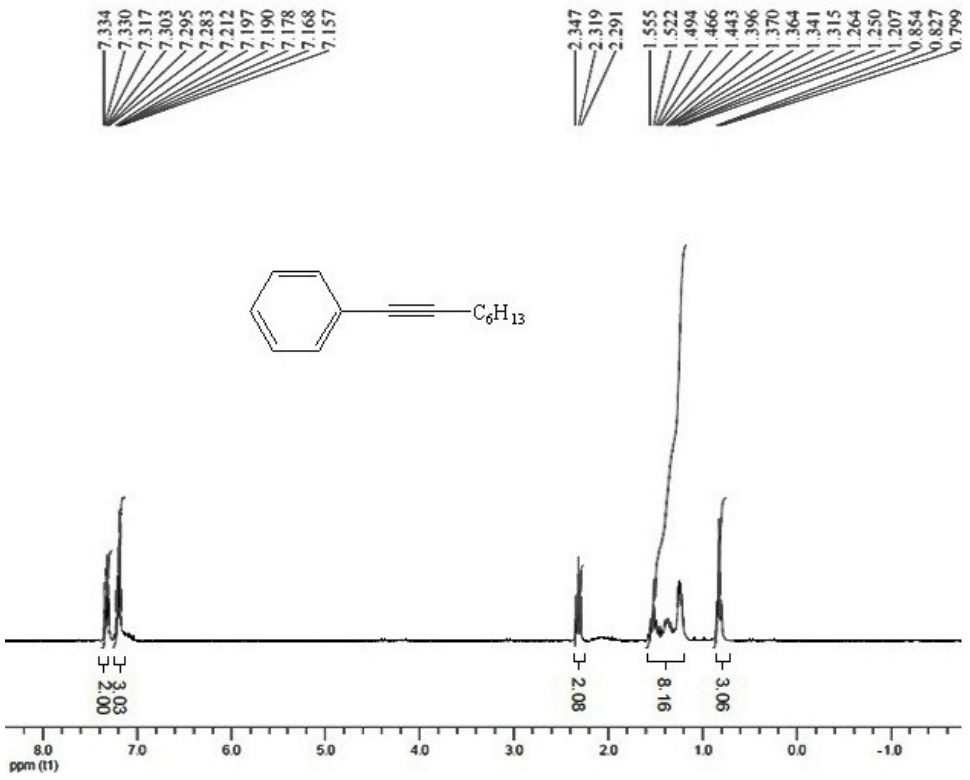

ppm
158.588
156.662
139.360
131.757
131.621
129.351
129.121
128.770
128.535
121.755
119.911
96.302
82.315
77.592
77.084
75.576
175
150
125
100
75
50
25
0

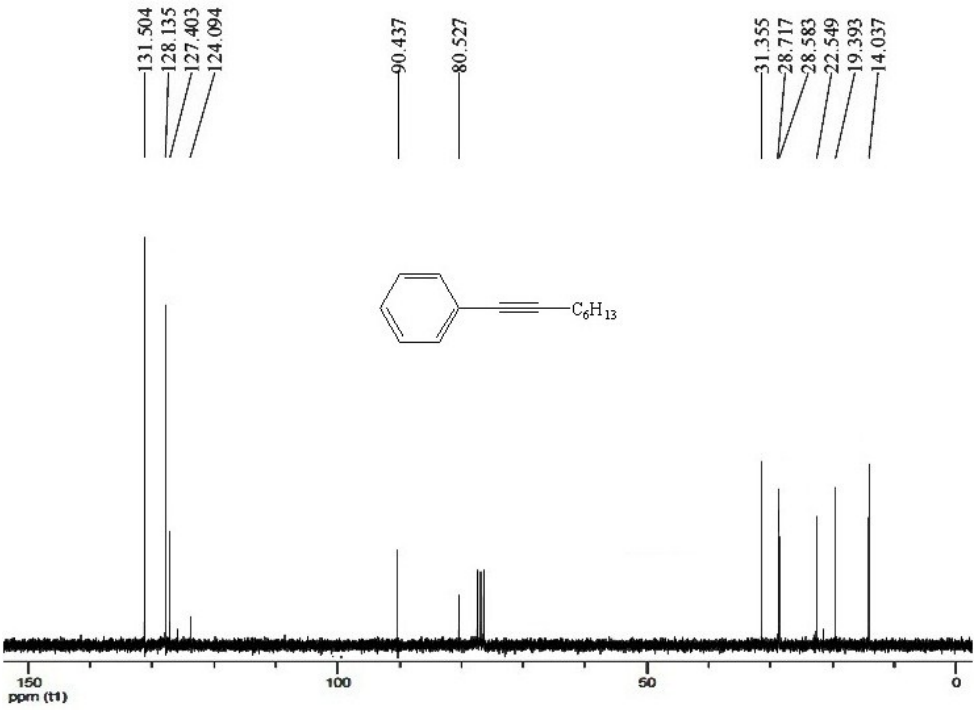

MW=180
File : GHADERI.X12 Date 9/ 7/92 Time 09:38:59
S=[2->8] Bp=126 Bi=8640. RT=0.22 CT=25
100%
75%
50%
25%
126
180
76
50 70 90 110 130 150 170 190 210 230 250 270 290
300 320 340 360 380 400 420 440 460 480 500 520 540
SB=50 SE=184 DB=50 DE=510 N=0 Z=2 T=0.0 Factl -> 1 *1
S List > S=[2->8] B=0 Pos=1 Tot=1

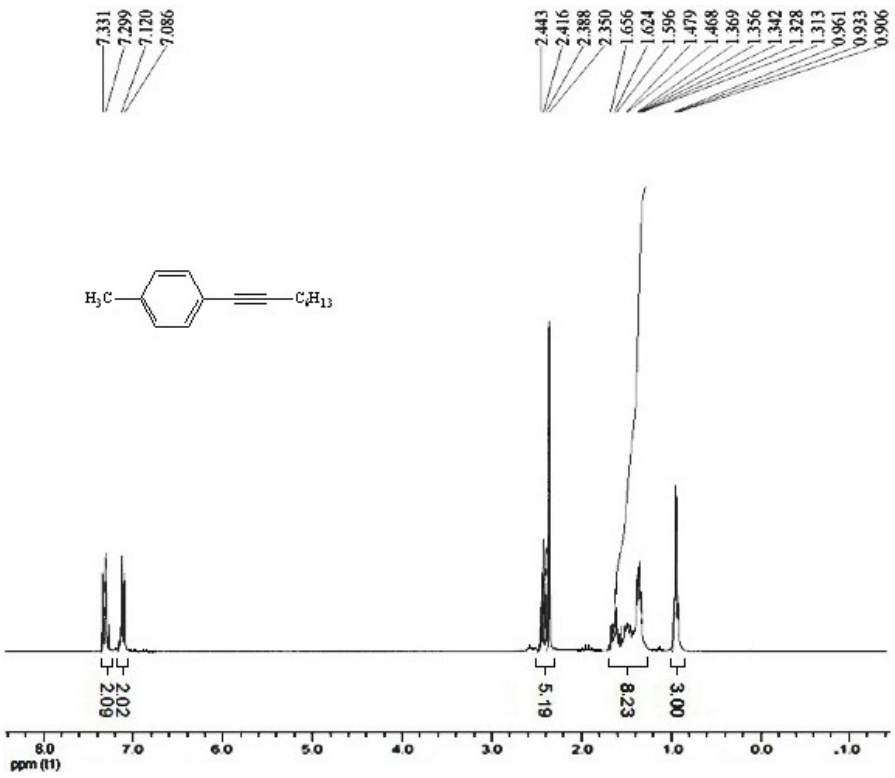


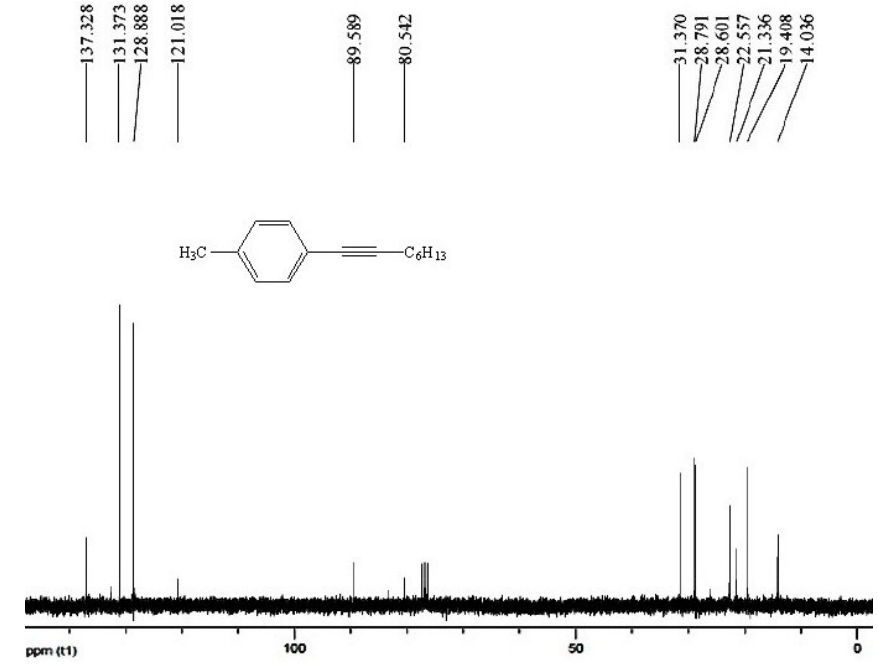


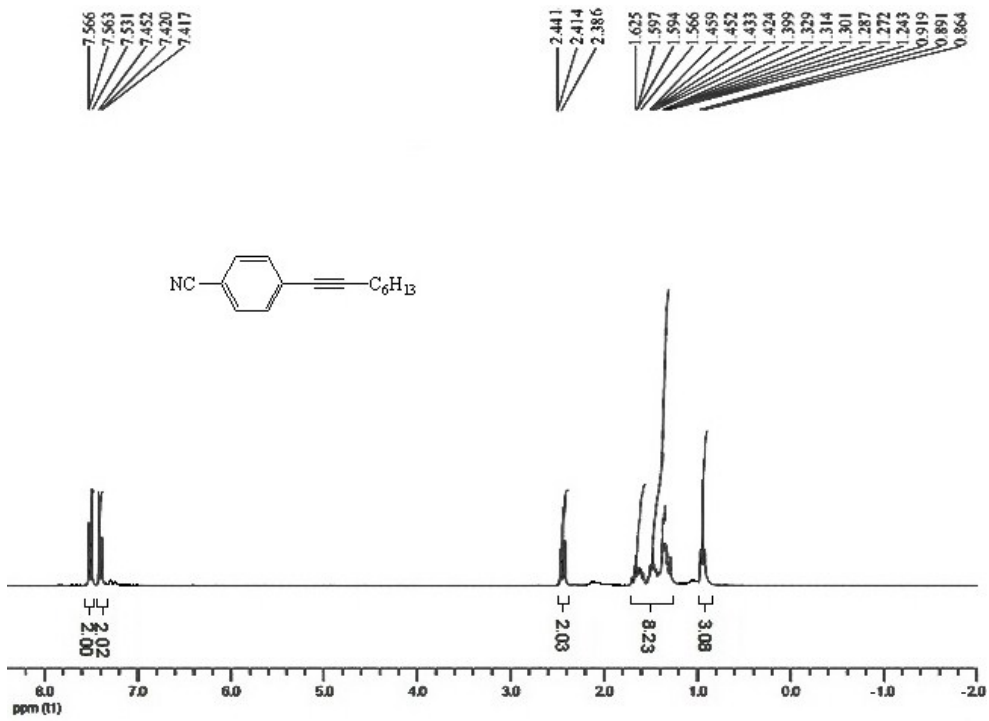

MW=184
File : GHADERI.X11 Date 9/ 7/92 Time 09:34:01
S=[260->260] Bp=57 Bi=6640. RT=4.42 CT=39
100%
75%
50%
25%
57
*4
85
111
139
183
50 70 90 110 130 150 170 190 210 230 250 270 290
300 320 340 360 380 400 420 440 460 480 500 520 540
SB=54 SE=184 DB=50 DE=510 N=0 Z=2 T=0.0 Fact[130->550] *4
S List > S=[260->260] B=0 Pos=9 Tot=9

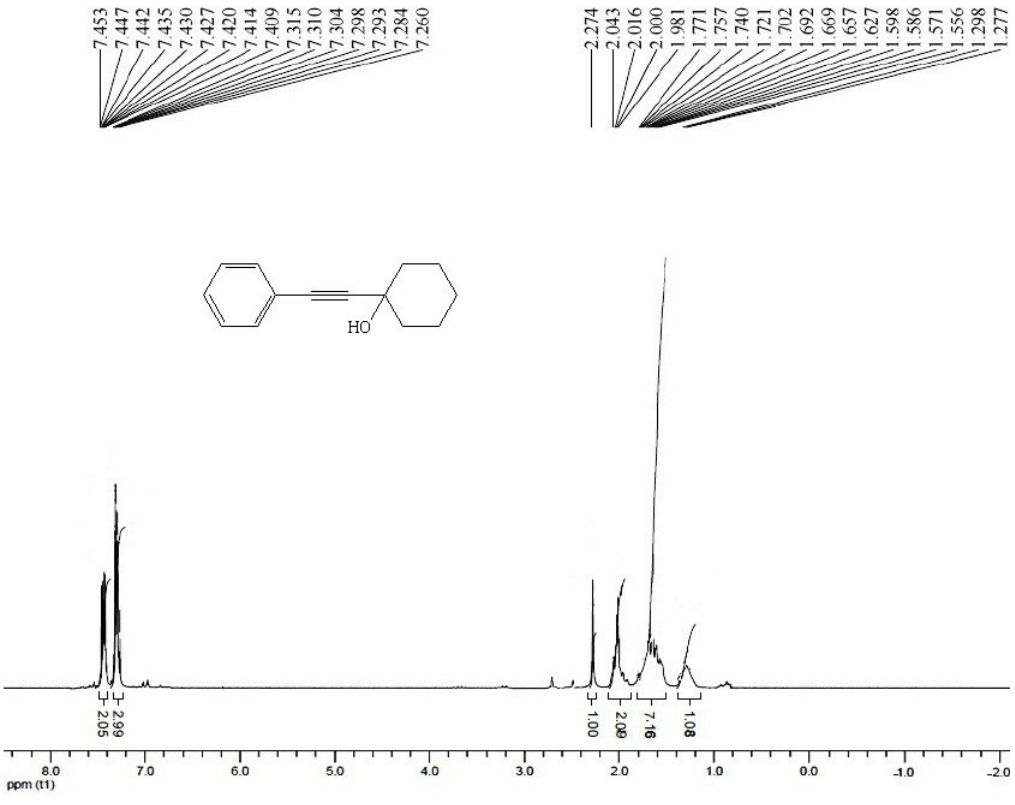

7.334
7.330
7.317
7.303
7.295
7.283
7.212
7.197
7.190
7.178
7.168
7.157
2.347
2.319
2.291
1.555
1.522
1.494
1.466
1.443
1.396
1.370
1.364
1.341
1.315
1.264
1.250
1.207
0.854
0.827
0.799
C_6H_{13}
2.00
3.03
2.08
8.16
3.06
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
ppm (t1)


131.504
128.135
127.403
124.094
90.437
80.527
31.355
28.717
28.583
22.549
19.393
14.037
C_6H_{13}
150
100
50
0
ppm (t1)


7.331
7.299
7.120
7.086
2.443
2.416
2.388
2.350
1.656
1.624
1.596
1.479
1.468
1.369
1.356
1.342
1.328
1.313
0.961
0.933
0.906
H3C
C6H13
2.09
2.02
5.19
8.23
3.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
ppm (t1)


137.328
131.373
128.888
121.018
89.589
80.542
31.370
28.791
28.601
22.557
21.336
19.408
14.036
H3C
C6H13
ppm (t1)
100
50
0


7.566
7.563
7.531
7.452
7.420
7.417
2.441
2.414
2.386
1.625
1.597
1.594
1.566
1.459
1.452
1.433
1.424
1.399
1.329
1.314
1.301
1.287
1.272
1.243
0.919
0.891
0.864
NC
C6H13
2.00
2.02
2.03
8.23
3.08
ppm (t1)


7.453
7.447
7.442
7.435
7.430
7.427
7.420
7.414
7.409
7.315
7.310
7.304
7.298
7.293
7.284
7.260
2.274
2.043
2.016
2.000
1.981
1.771
1.757
1.740
1.721
1.702
1.692
1.669
1.657
1.627
1.598
1.586
1.571
1.556
1.298
1.277
HO
2.05
2.99
1.00
2.09
7.16
1.08
ppm (t1)