Supplementary Information

Rational design and expeditious synthesis of aromatic cyanodienone derivatives assisted by cyanide-halide exchange

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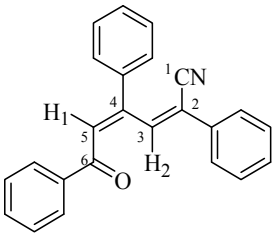
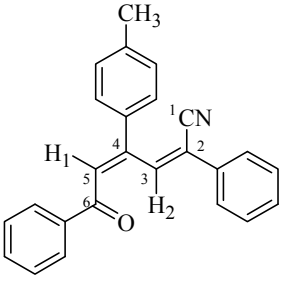
(*2Z,4E)-6-oxo-2,4,6-triphenyl-2,4-hexadienenitrile* (**2A**)

Yield 78%; yellow crystals, m.p.:103-105 ˚C (from EtOH); IR (neat): ν = 2218 (CN), 1645 (CO) cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.33 (s, 1H, H_1), 7.45-8.05 (m, 15H, Ar-H), 8.4 (s, 1H, H_2) ppm; ^{13}CNMR (100MHz, $CDCl_3$): δ = 115.9 (C-2), 119.6 (C-1), 126.2 (C-5), 126.9, 128.8, 129.1, 129.2, 129.4, 129.5, 130.3, 130.6, 133.6 (ArC), 134.1, 138.8, 139.4 (ArC_q), 141.8 (C-3), 151.9 (C-4), 190.6 (C-6), ppm.



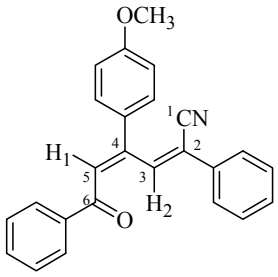
(2Z,4E)-4-(4-methylphenyl)-6-oxo-2,6-diphenyl-2,4-hexadienenitrile(**2B**)

Yield 81%; yellow crystals, m.p.:116-118 ˚C (from EtOH); IR (neat): ν = 2218 (CN), 1644 (CO) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.46 (s, 3H, CH_3), 7.32 (s, 1H, H_1), 7.45-8.04 (m, 14H, Ar-H), 8.37 (s, 1H, H_2) ppm; ^{13}C NMR (100MHz, $CDCl_3$,): δ = 21.5 (CH_3), 115.7 (C-2), 118.9 (C-1), 124.8 (C-5),126.4, 128.4, 128.6, 128.7, 129.0, 129.7, 129.8, 133.1 (ArC), 133.7, 136.1, 138.5, 140.7 (ArC_q) 142.0 (C-3), 151.6 (C-4), 190.2 (C-6), ppm.



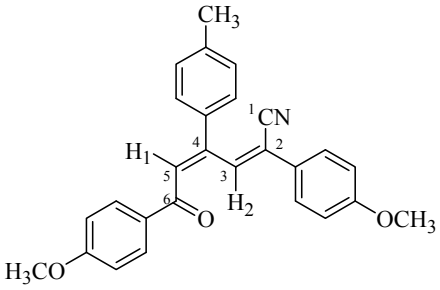
(2Z,4E)-4-(4-methoxyphenyl)-6-oxo-2,6-diphenyl-2,4-hexadienenitrile(**2C**)

Yield 91%; yellow crystals, m.p.:112-114 ˚C (from EtOH); IR (neat): ν = 2218 (CN), 1643 (CO) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.89 (s, 3H, OCH_3), 7.30 (s, 1H, H_1), 7.00-7.02, 7.43-8.03 (m, 14H, Ar-H), 8.35 (s, 1H, H_2) ppm; ^{13}C NMR (100MHz, $CDCl_3$): δ = 55.4 (OCH_3), 114.4 (C-5), 115.2 (C-2), 118.8 (C-1),123.5, 126.4, 128.3, 128.7, 129.0, 129.8, 130.2 (ArC),131.2 (ArC_q),133.0 (ArC), 133.6, 138.6 (ArC_q), 142.5 (C-3), 151.3 (ArC_q)161.5 (C-4), 190.1 (C-6), ppm.



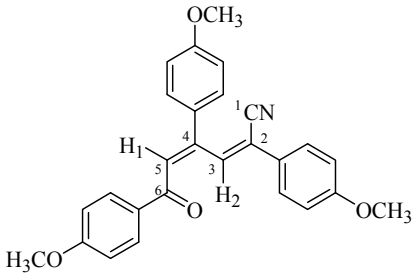
(2Z,4E)-2,6-bis(4-methoxyphenyl)-4-(4-methylphenyl)-6-oxo-2,4-hexadienenitrile(**2D**)

Yield 95%; yellow crystals, m.p.:129-131 ˚C (from EtOH); IR (neat): ν = 2217 (CN), 1638 (CO) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.44 (s, 3H, CH_3), 3.86, 3.89 (s, 6H, OCH_3), 7.25 (s, 1H, H_1), 6.95-6.99, 7.23-7.28, 7.43-8.02 (m, 12H, Ar-H), 8.31 (s, 1H, H_2) ppm; ^{13}C NMR (100MHz, $CDCl_3$): δ = 21.5 (CH_3), 55.4, 55.5 (OCH_3),113.9 (C-5),114.4 (ArC), 115.8 (C-2), 118.3 (C-1), 124.9 (ArC), 126.4 (ArC_q), 127.9, 128.6, 129.6, 130.7 (ArC),131.7, 136.6 (ArC_q), 139.5 (C-3),140.3 (ArC_q), 151.1 (C-4),160.9, 163.5 (ArC_q), 188.7 (C-6) ppm.



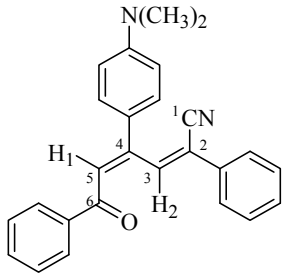
(2Z,4E)-2,4,6-tris(4-methoxyphenyl)-6-oxo-2,4-hexadienenitrile(**2E**)

Yield 93%; yellow crystals, m.p.:131-133 ˚C (from EtOH); IR (neat): ν = 2218 (CN), 1636 (CO) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.87, 3.88, 3.9 (s, 9H, OCH_3), 7.22 (d, *J* = 1.004 Hz, 1H, H_1), 6.95-7.01, 7.49-8.03 (m, 12H, Ar-H), 8.29 (d, *J* = 1.004 Hz, 1H, H_2) ppm; ^{13}C NMR (100MHz, $CDCl_3$): 55.2, 55.3, 55.4 (OCH_3), 113.7 (C-5),113.9, 114.4 (ArC), 115.9 (C-2), 118.2 (C-1), 123.7 (ArC), 126.4 (ArC_q),127.8, 127.9, 129.2, 130.3 (ArC), 141.0 (ArC_q), 150.8 (C-3),157.1, 160.9, 161.2 (ArC_q), 163.4 (C-4), 188.7 (C-6) ppm.



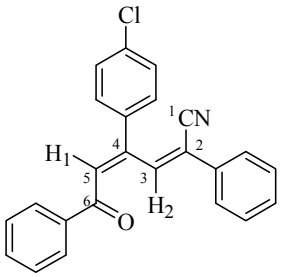
(2Z,4E)-4-[4-(dimethylamino)phenyl]-6-oxo-2,6-diphenyl-2,4-hexadienenitrile (**2F**)

Yield 88%; red crystals, m.p.:174-176 ˚C (from EtOH); IR (neat): ν = 2215 (CN), 1628 (CO) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.07 (s, 6H, $N(CH_3)_2$), 7.30 (d, *J* = 1.009 Hz, 1H, H_1), 6.74-6.76, 7.41-8.03 (m, 14H, Ar-H), 8.32 (d, *J* = 1.009 Hz, 1H, H_2) ppm; ^{13}C NMR (100MHz, $CDCl_3$): δ = 40.1 ($N(CH_3)_2$), 111.9 (C-5), 116.1 (C-2), 118.0 (C-1), 119.8 (ArC),125.7 (ArC_q),126.4, 128.2, 128.6, 129.0, 129.5, 130.0, 132.5 (ArC), 133.8, 139.2 (ArC_q), 144.0 (C-3), 151.9 (ArC_q), 152.2 (C-4), 190.0 (C-6) ppm.



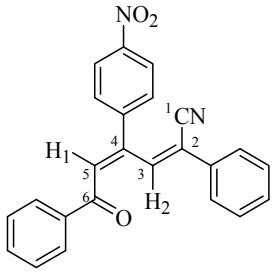
(2Z,4E)-4-(4-chlorophenyl)-6-oxo-2,6-diphenyl-2,4-hexadienenitrile (**2G**)

Yield 70%; yellow crystals, m.p.:109-111 ˚C (from EtOH); IR (neat): ν = 2218 (CN), 1647 (CO) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.29 (s, 1H, H_1), 7.41- 8.03 (m, 14H, Ar-H), 8.35(s, 1H, H_2) ppm; ^{13}C NMR (100MHz, $CDCl_3$): δ = 115.5 (C-2), 119.4 (C-1), 126.0 (C-5), 126.4, 128.4, 128.8, 129.1, 129.3, 129.9 (ArC),130.0 (ArC_q),133.3, 133.4 (ArC),136.4, 137.3, 138.3 (ArC_q), 140.9 (C-3), 150.2 (C-4), 190.0 (C-6) ppm.



(2Z,4E)-4-(4-nitrophenyl)-6-oxo-2,6-diphenyl-2,4-hexadienenitrile(**2H**)

Yield 72%; brown crystals, m.p.:151-153 ˚C (from EtOH); IR (neat): ν = 2218 (CN), 1651 (CO), 1345, 1518 (NO_2) cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.30 (s, 1H, H_1), 7.24, 7.44-8.34 (m, 14H, Ar-H), 8.39 (s, 1H, H_2) ppm; ^{13}C NMR (100MHz, $CDCl_3$): δ = 115.4 (C-2), 120.0 (C-1), 124.2 (C-5), 126.5, 128.3, 128.5, 128.9, 129.2, 129.7, 130.4 (ArC),133.1 (ArC_q),133.7 (ArC),137.9 (ArC_q), 139.4 (C-3), 145.2, 148.5 (ArC_q), 148.8 (C-4), 189.8 (C-6) ppm.



2. IR, ^{1}H NMR and ^{13}CNMR Spectra for New Compounds:

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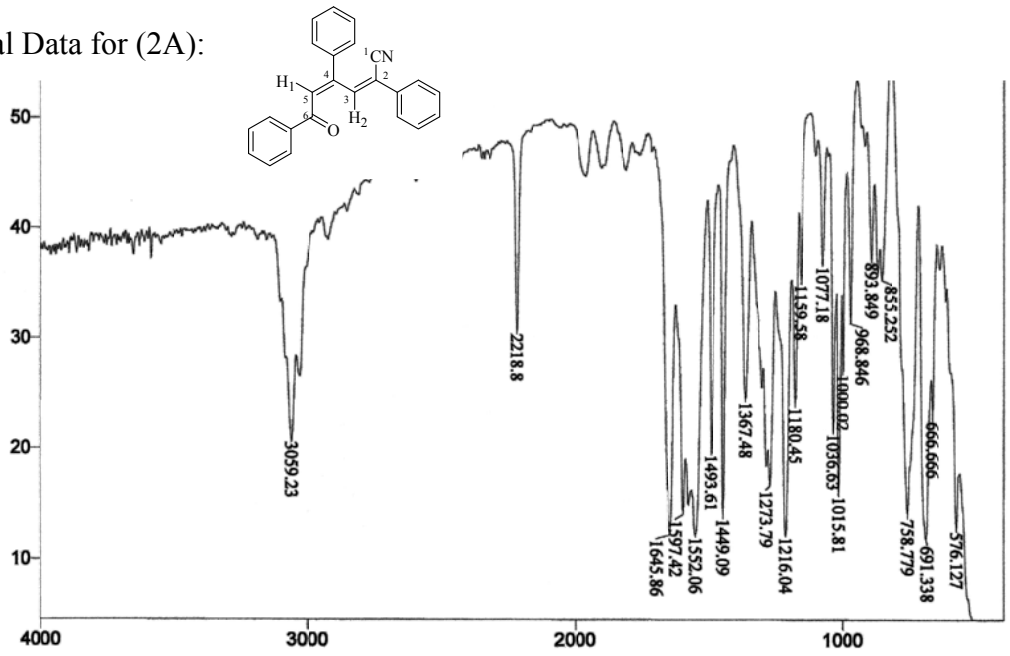

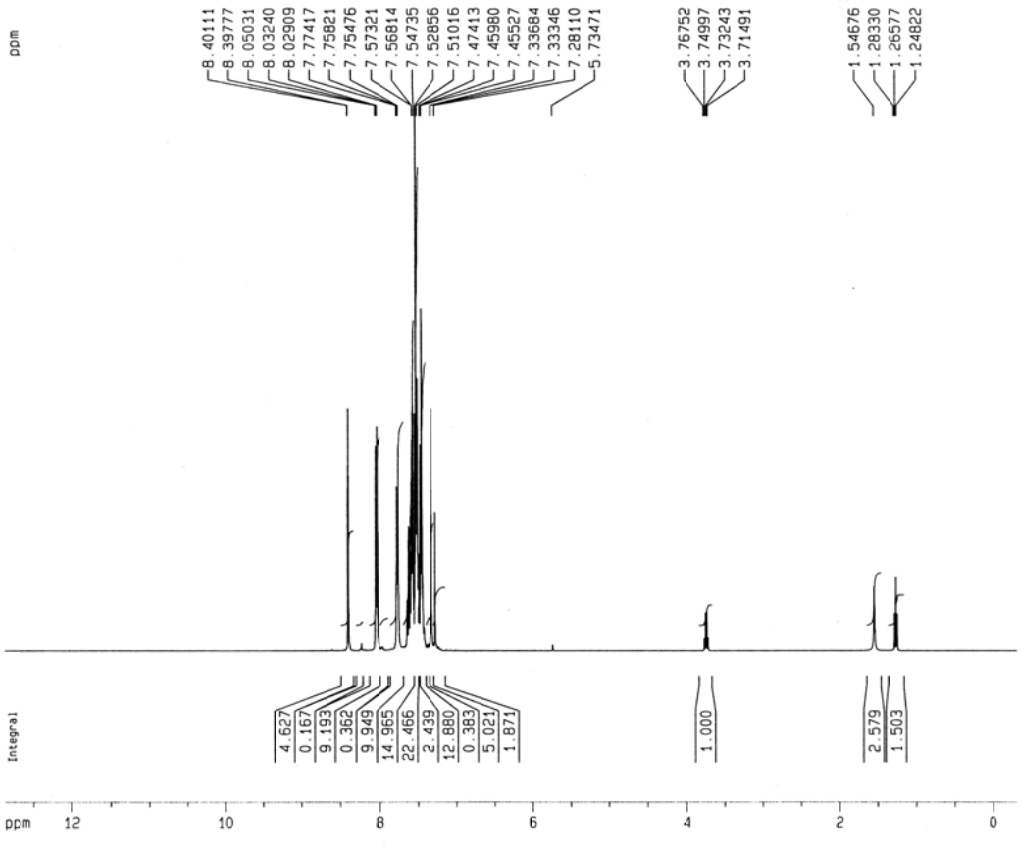

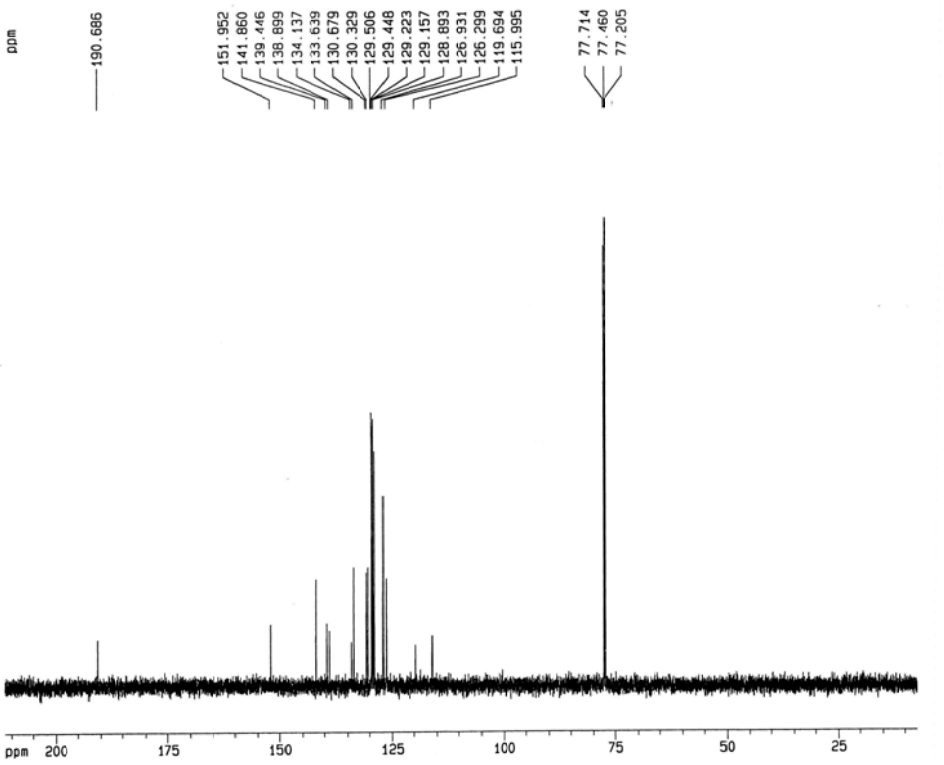

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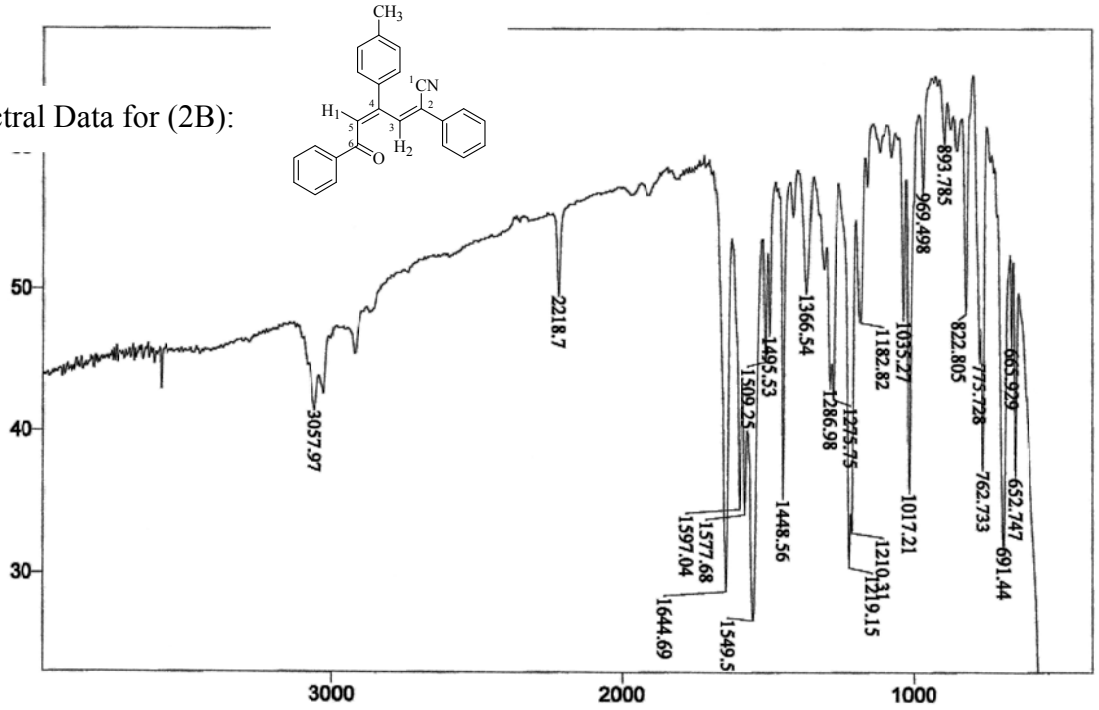

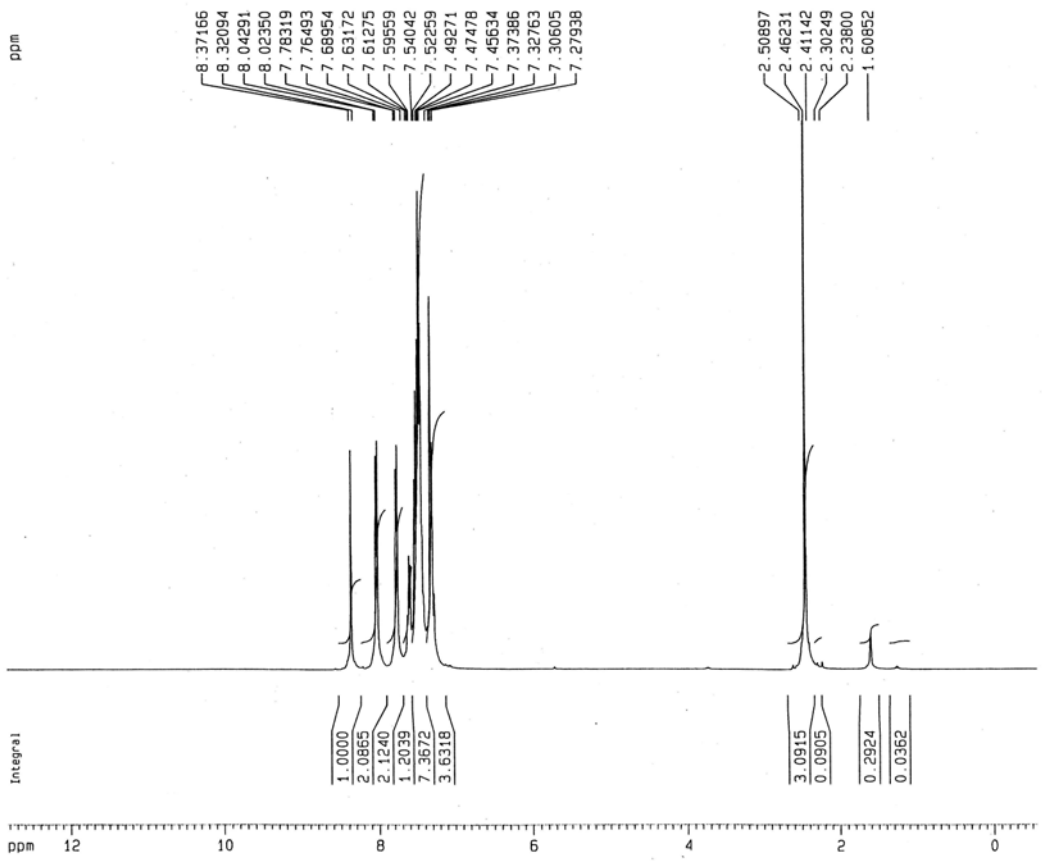
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2.41142
2.30249
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Integral
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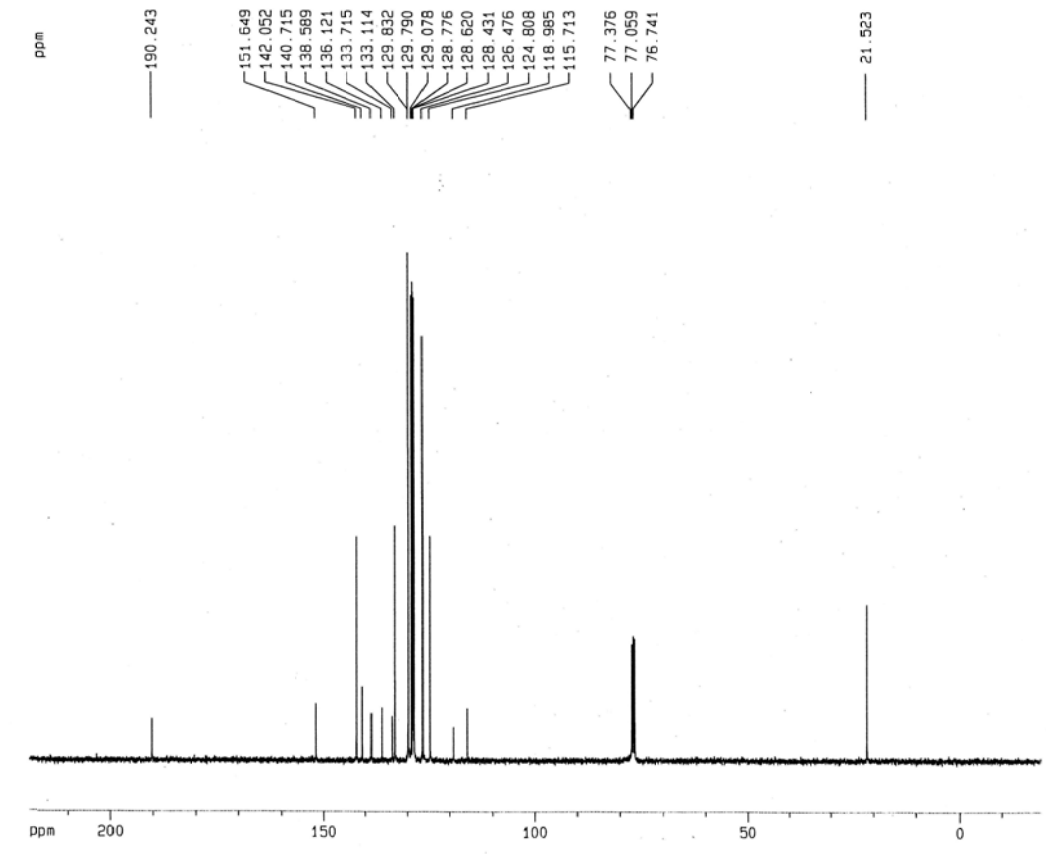
0.2924
0.0362
ppm 12 10 8 6 4 2 0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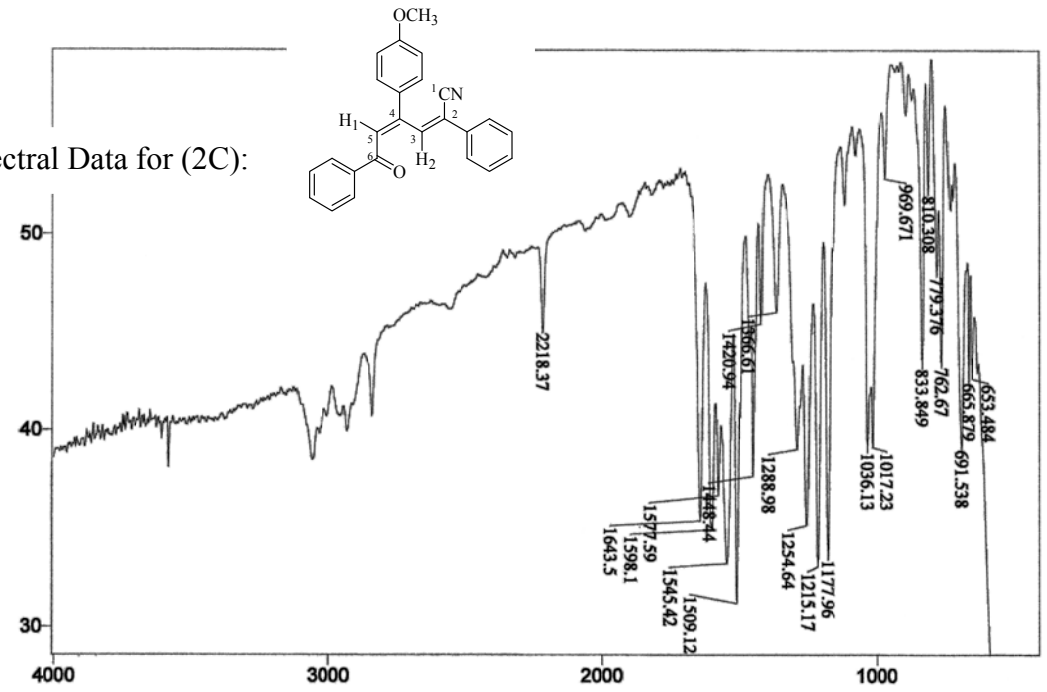

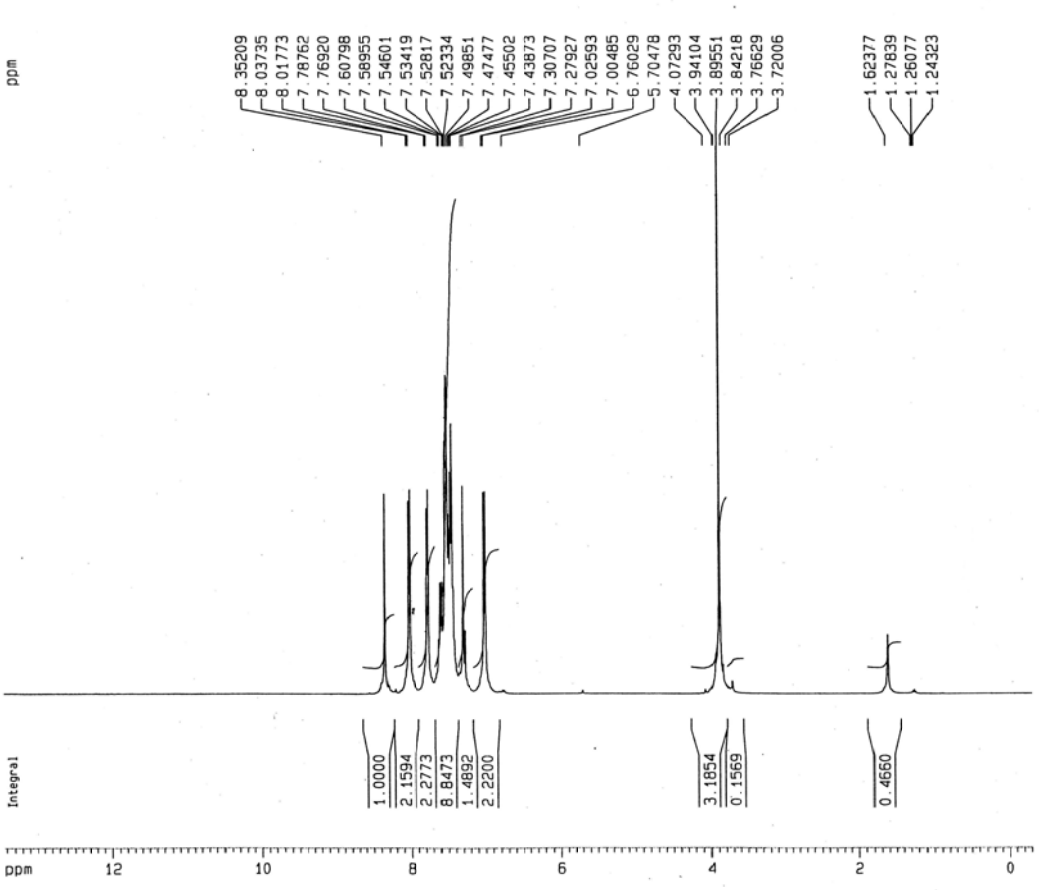

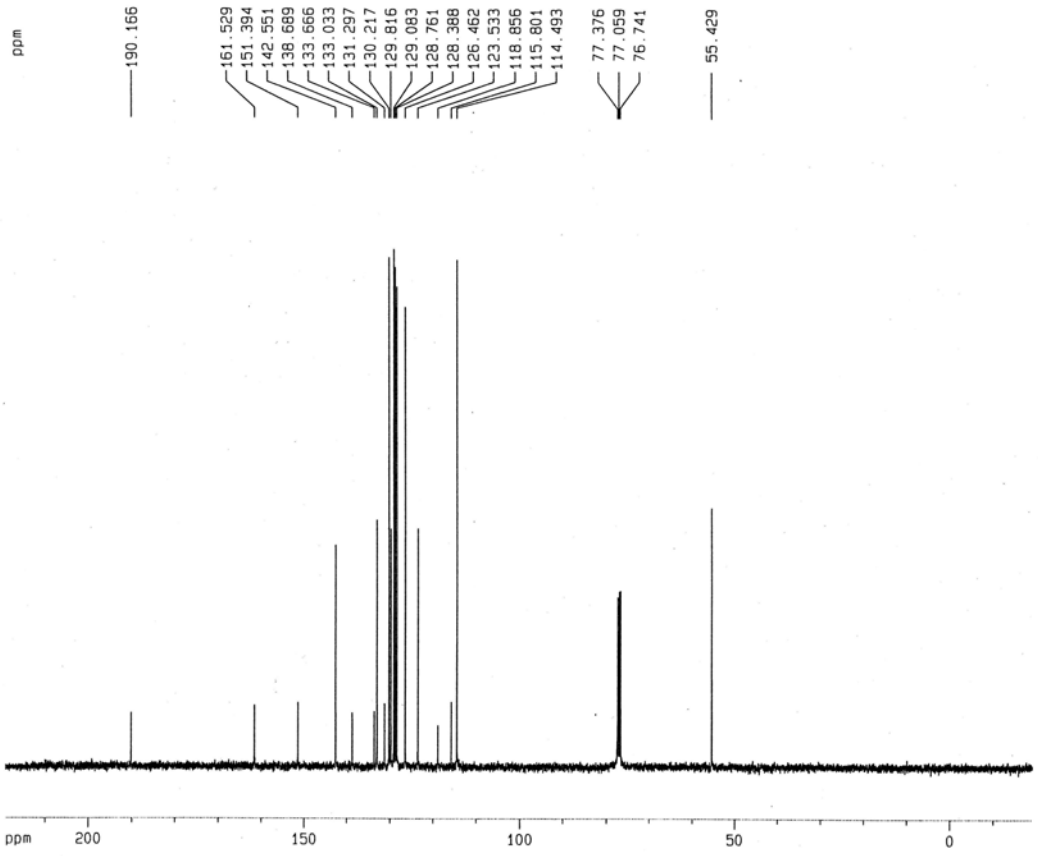

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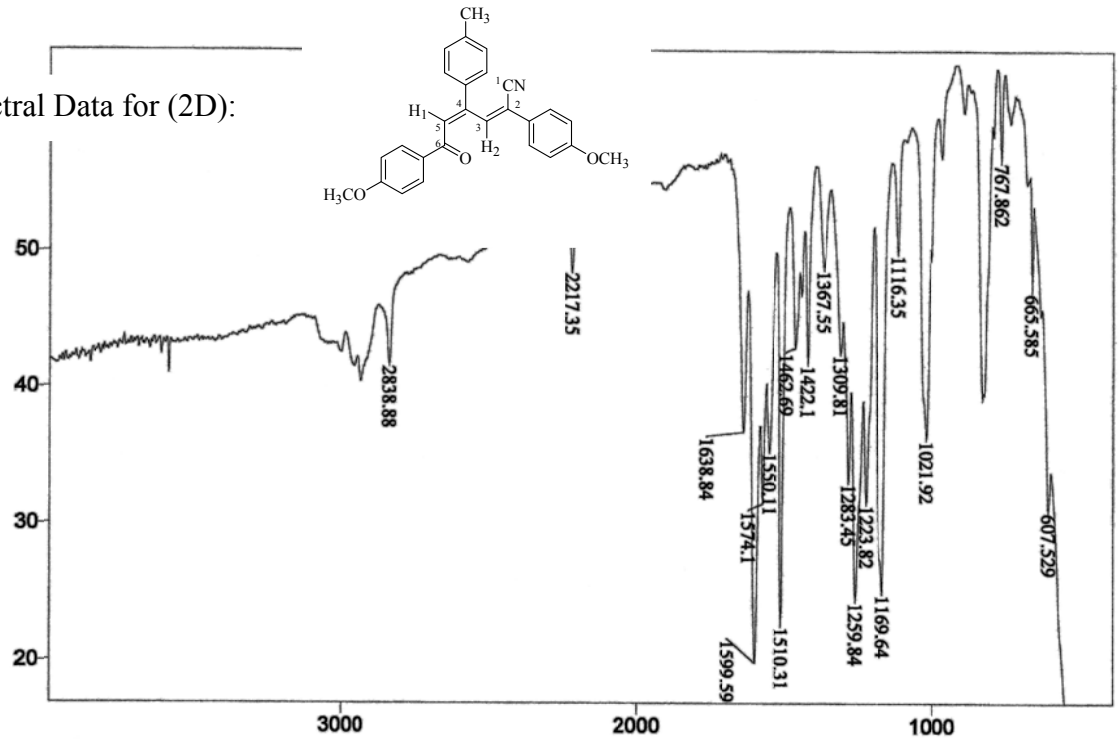

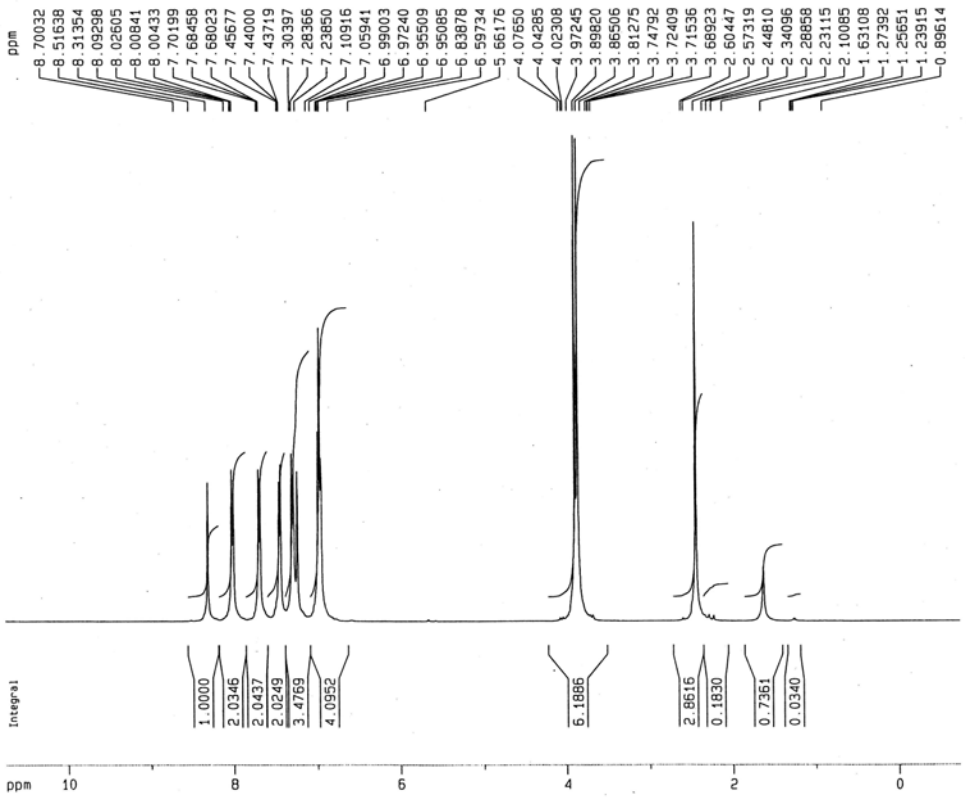
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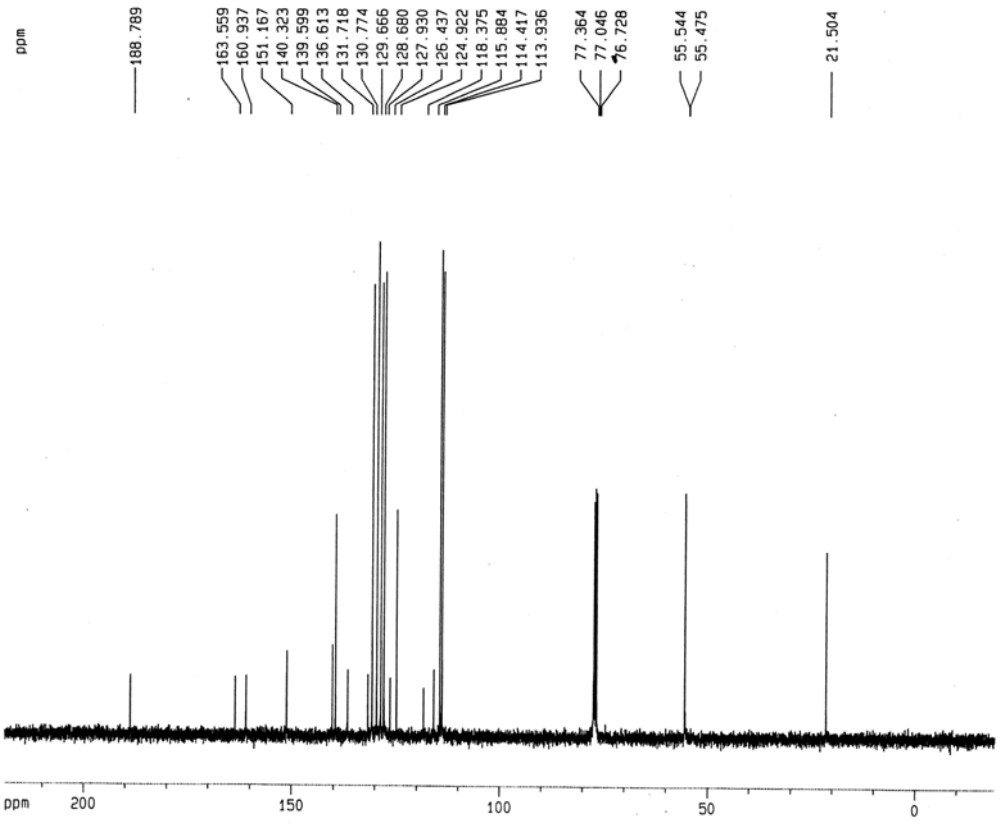
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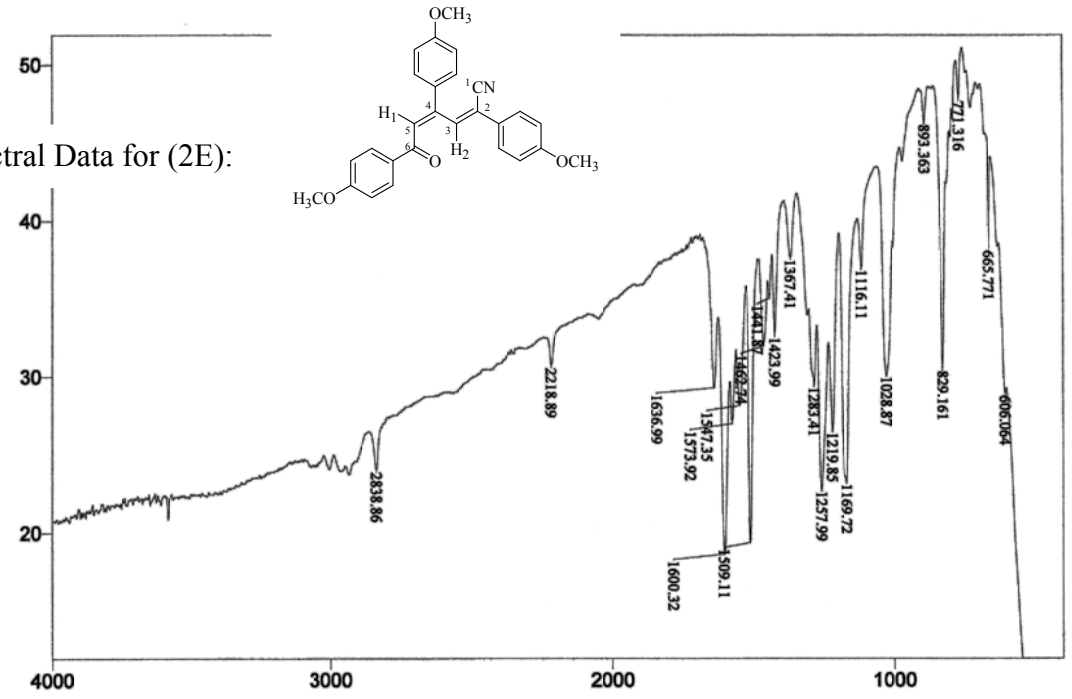

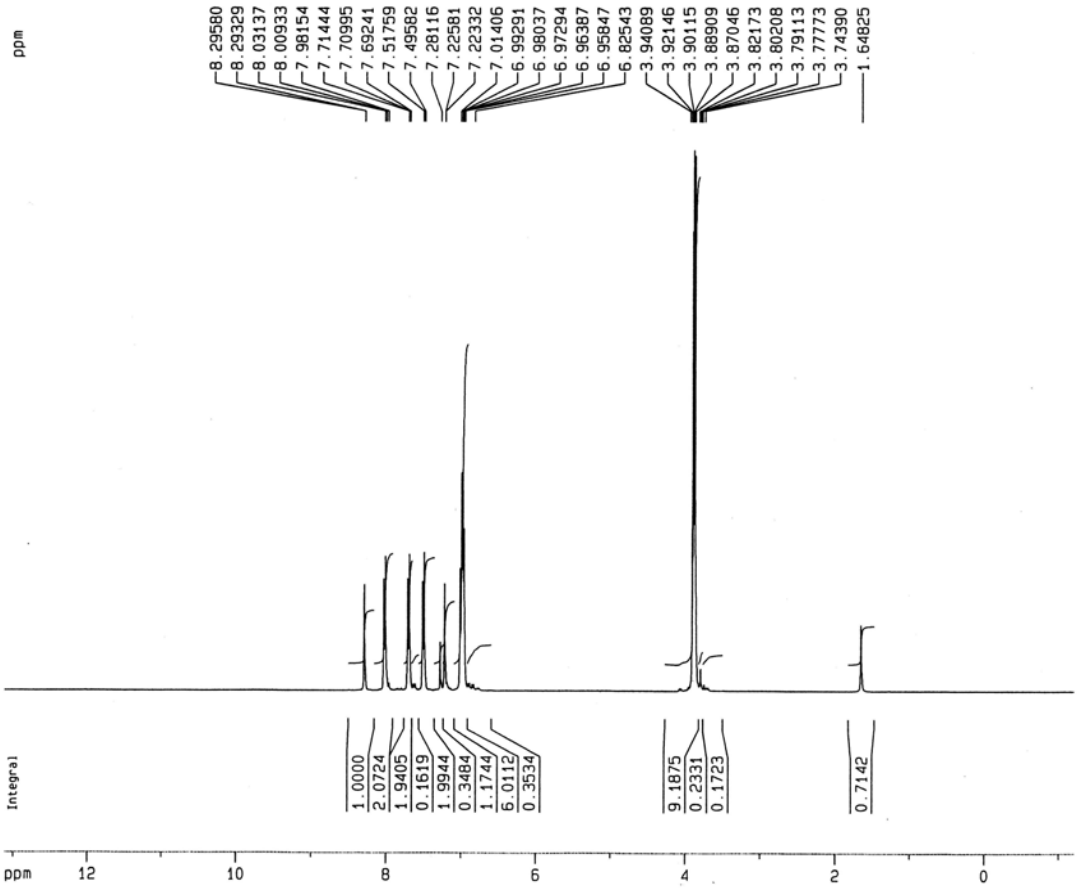

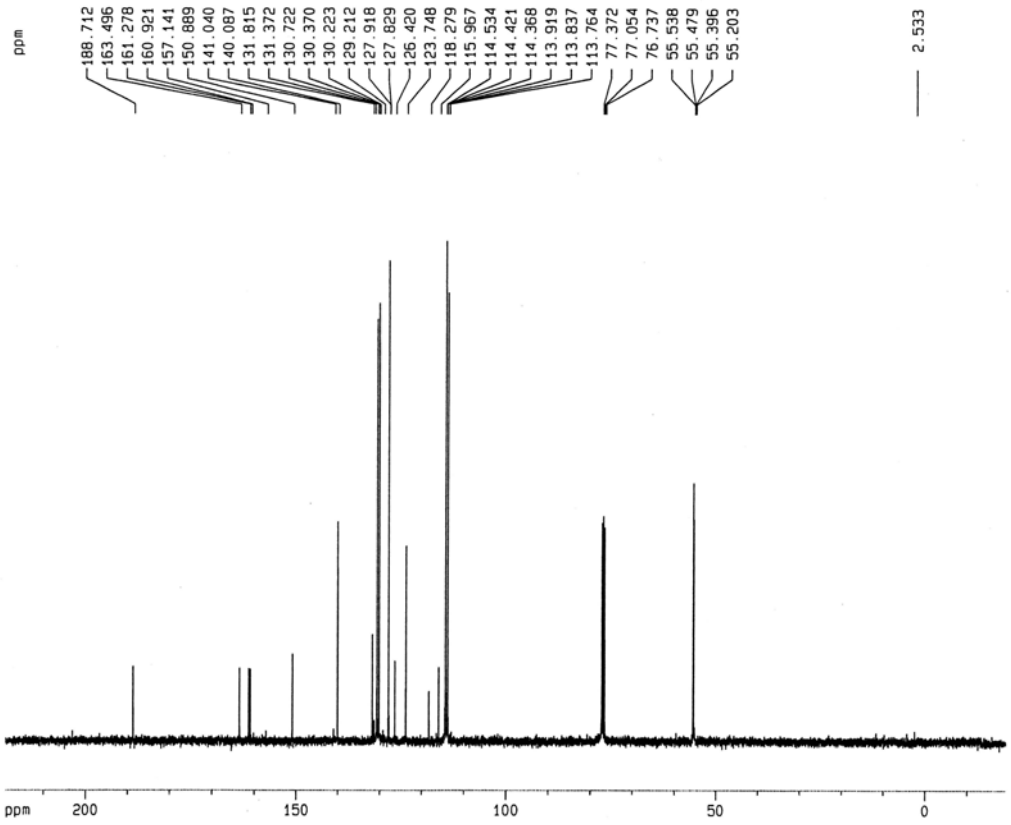

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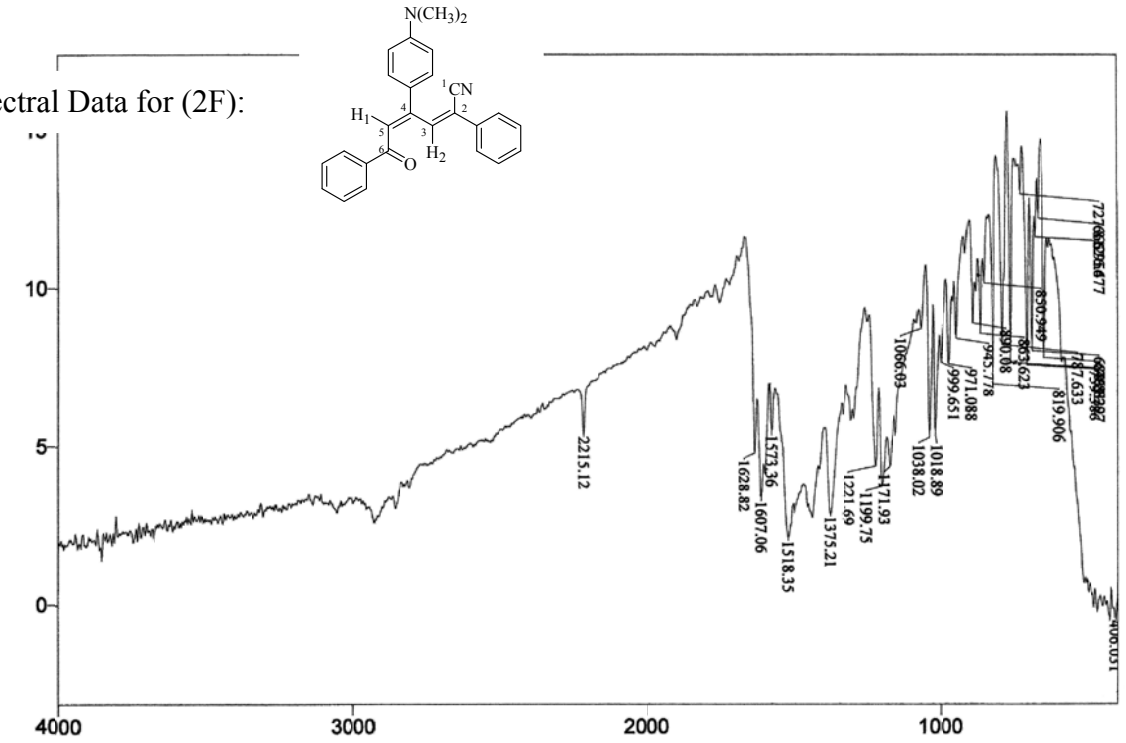

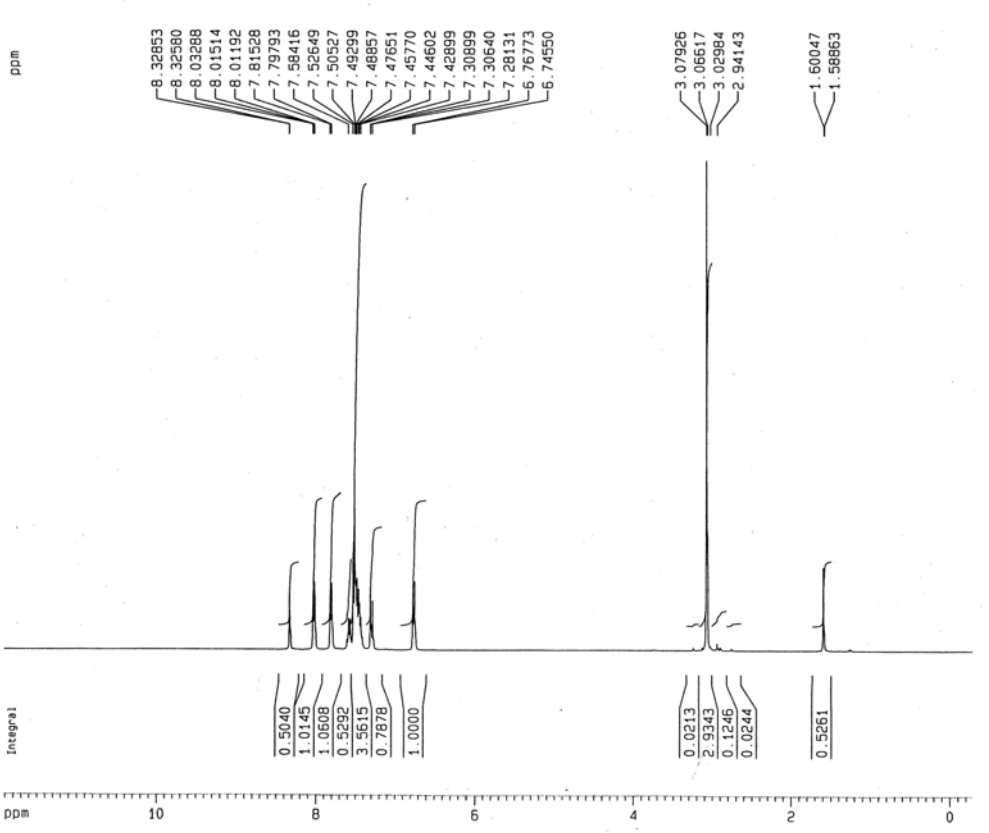
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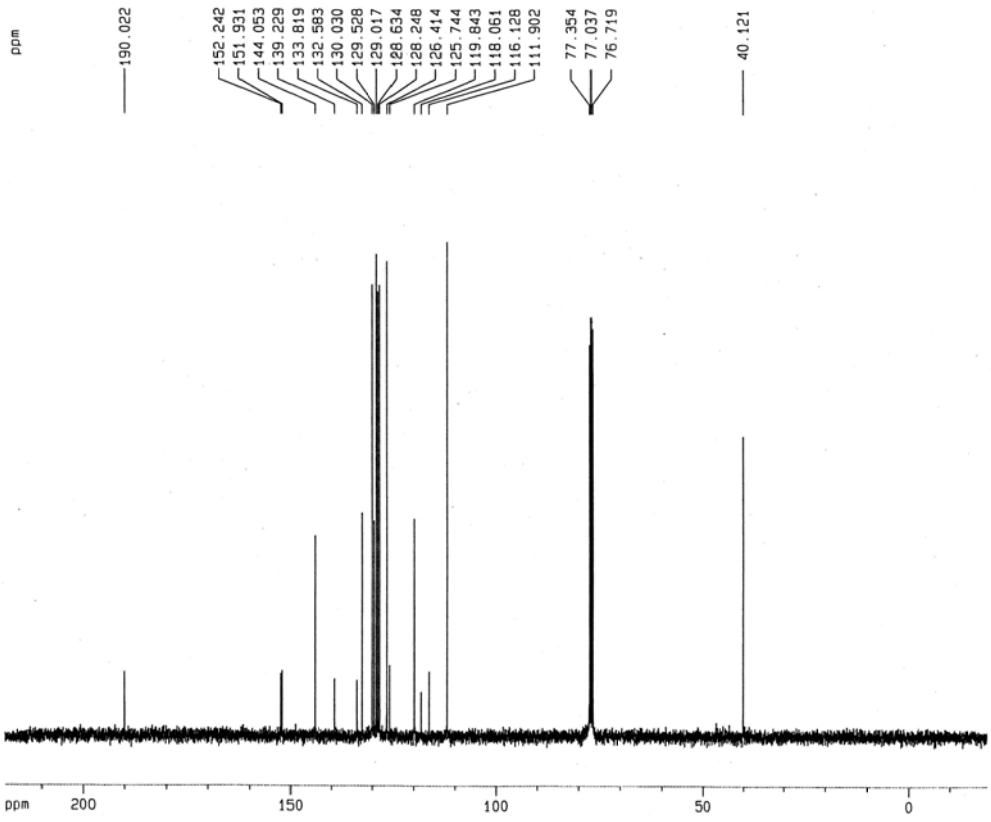
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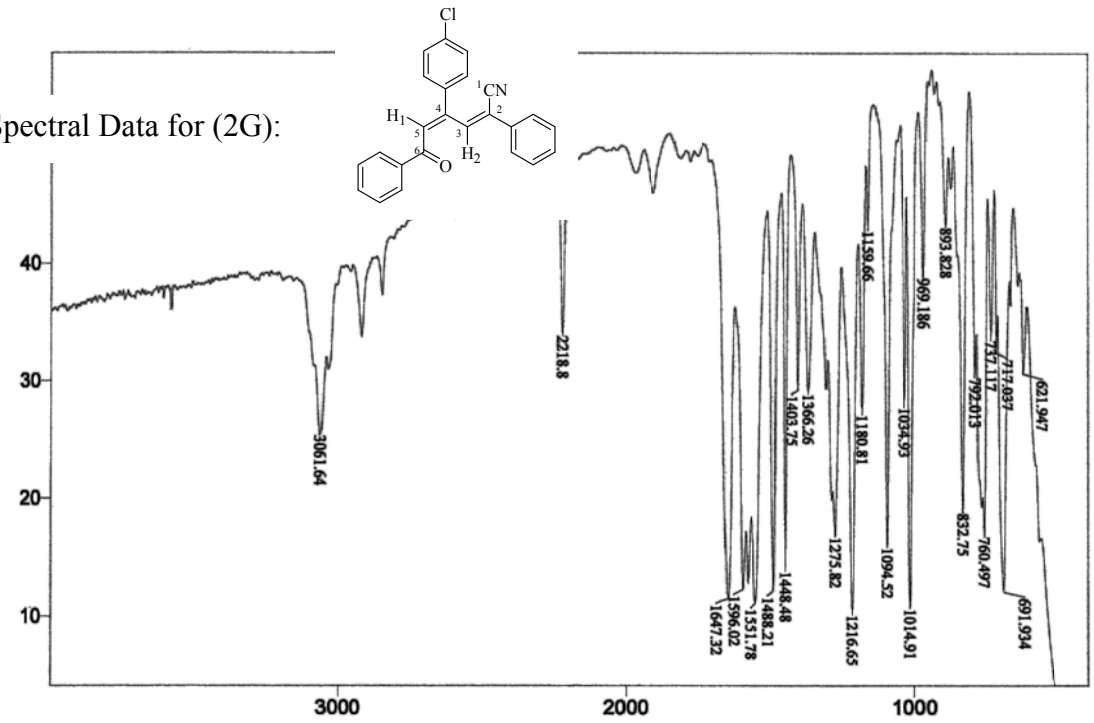

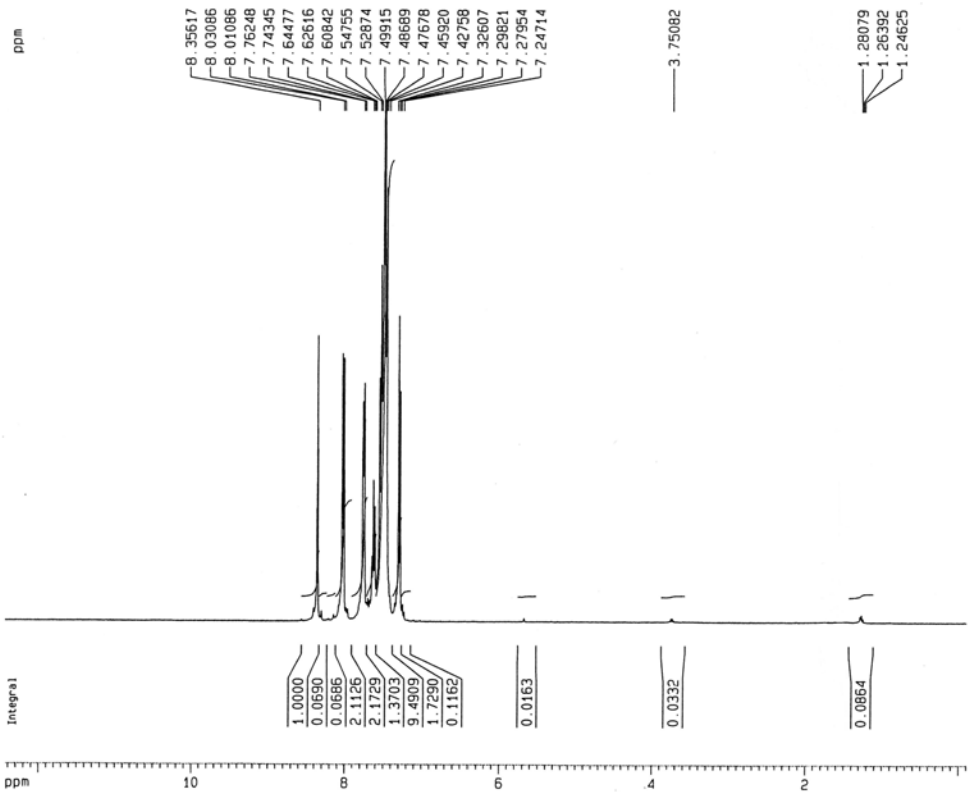

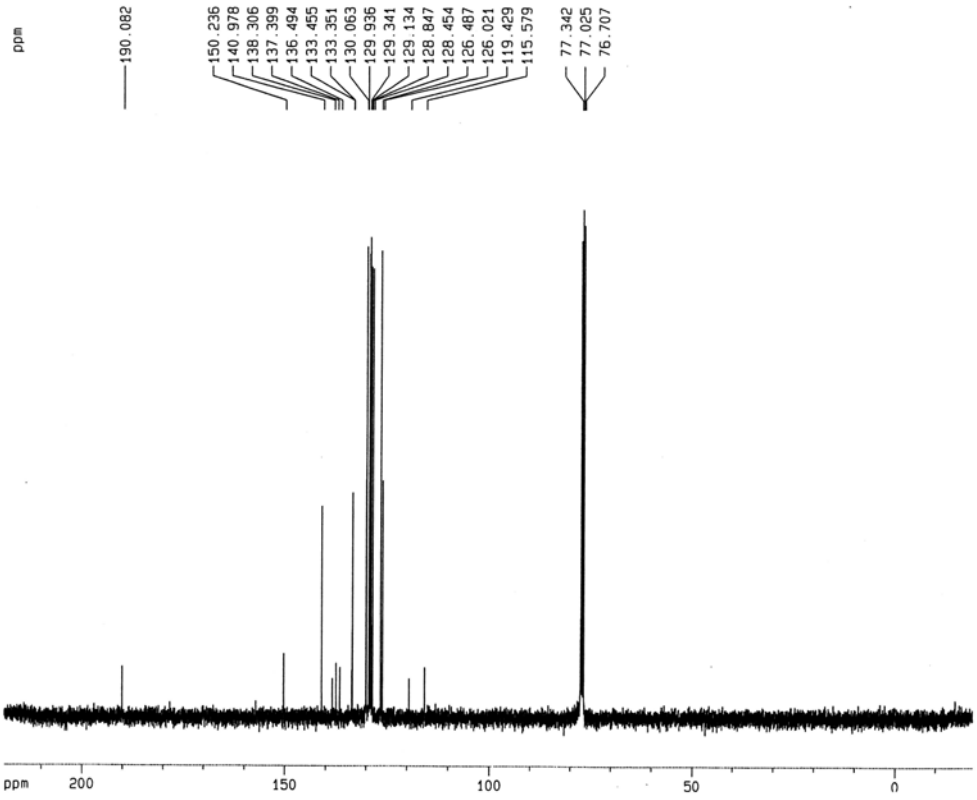

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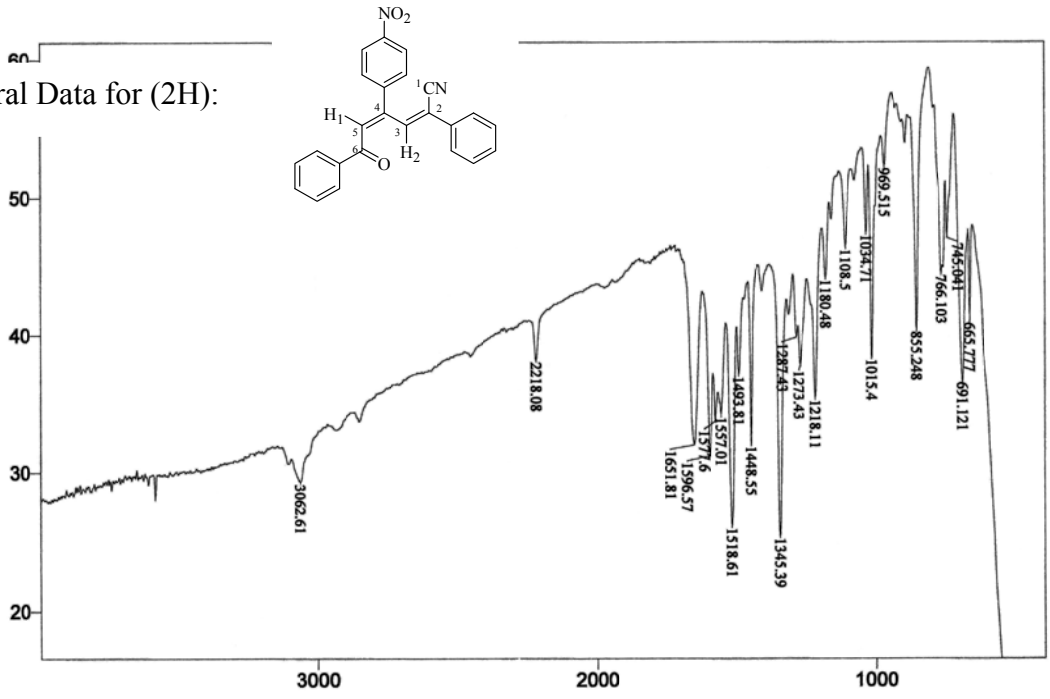

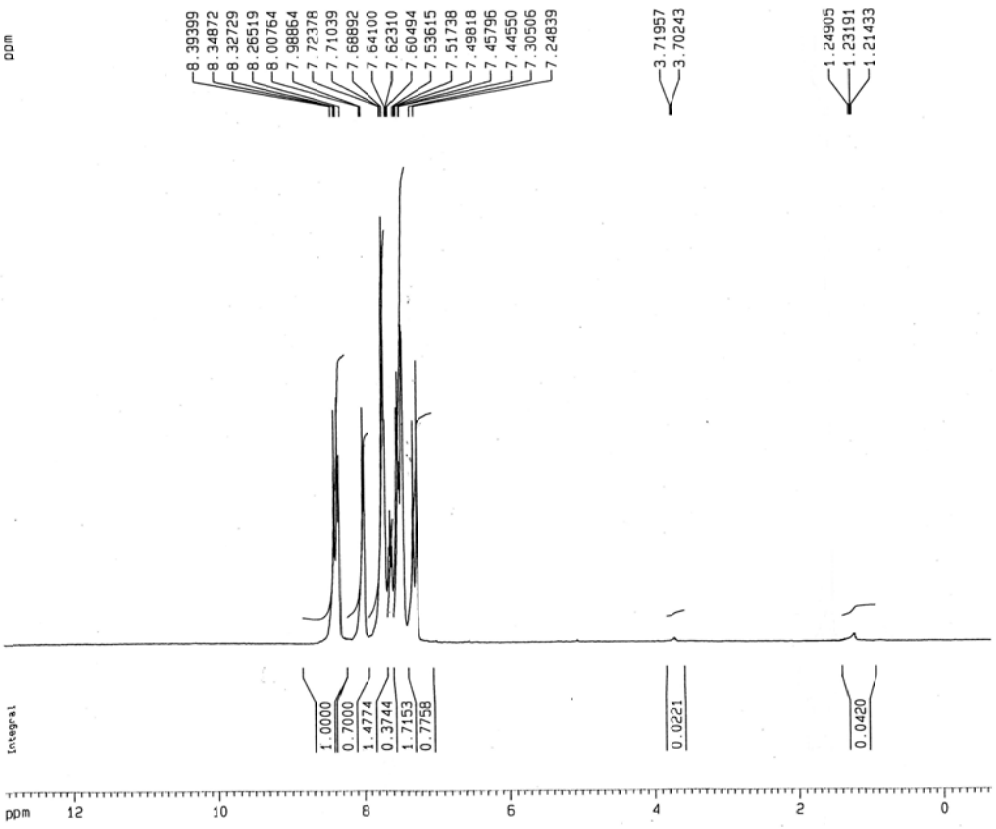
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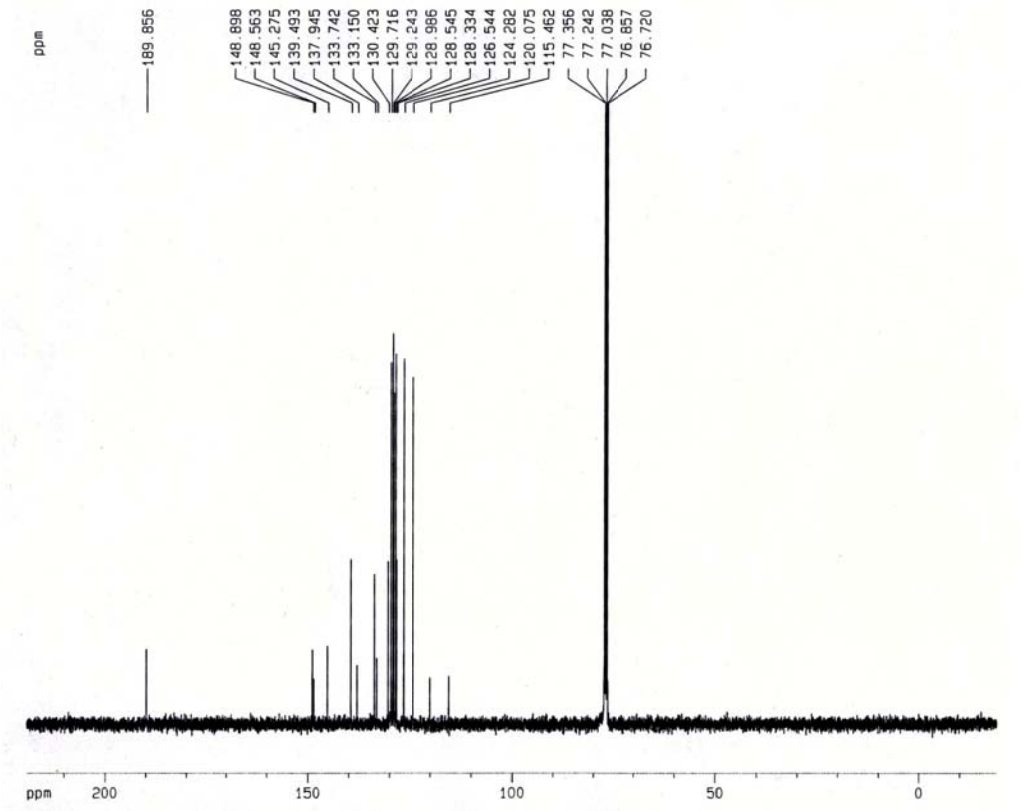
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ppm
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