

Supplementary Information

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

Fatemeh Zeraatpisheh*, Fatemeh Abadast & Maryam Shahmorad

Department of Chemistry, Behbahan Khatam Alanbia University of Technology, Behbahan, Iran

E-mail: fzeraatpisheh@gmail.com

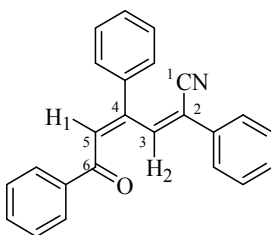
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1. Physical and Spectral Data

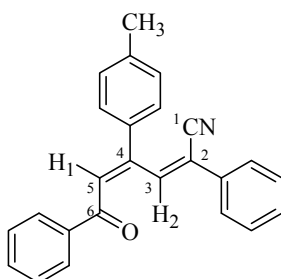
(2Z,4E)-6-oxo-2,4,6-triphenyl-2,4-hexadienenitrile (**2A**)

Yield 78%; yellow crystals, m.p.:103-105 °C (from EtOH); IR (neat): $\nu = 2218$ (CN), 1645 (CO) cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): $\delta = 7.33$ (s, 1H, H₁), 7.45-8.05 (m, 15H, Ar-H), 8.4 (s, 1H, H₂) ppm; ^{13}C NMR (100MHz, CDCl_3): $\delta = 115.9$ (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.



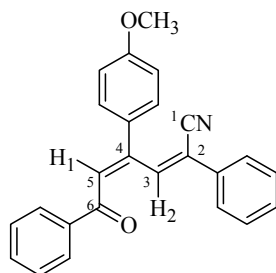
(2Z,4E)-4-(4-methylphenyl)-6-oxo-2,6-diphenyl-2,4-hexadienenitrile (**2B**)

Yield 81%; yellow crystals, m.p.:116-118 °C (from EtOH); IR (neat): $\nu = 2218$ (CN), 1644 (CO) cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): $\delta = 2.46$ (s, 3H, CH₃), 7.32 (s, 1H, H₁), 7.45-8.04 (m, 14H, Ar-H), 8.37 (s, 1H, H₂) ppm; ^{13}C NMR (100MHz, CDCl_3): $\delta = 21.5$ (CH₃), 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.



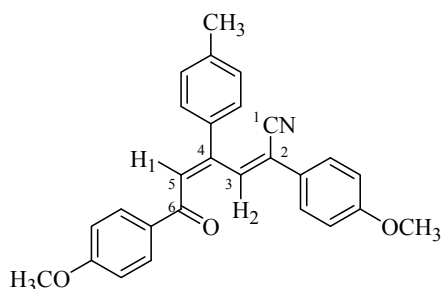
(2Z,4E)-4-(4-methoxyphenyl)-6-oxo-2,6-diphenyl-2,4-hexadienenitrile(**2C**)

Yield 91%; yellow crystals, m.p.:112-114 °C (from EtOH); IR (neat): $\nu = 2218$ (CN), 1643 (CO) cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): $\delta = 3.89$ (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): $\delta = 55.4$ (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.



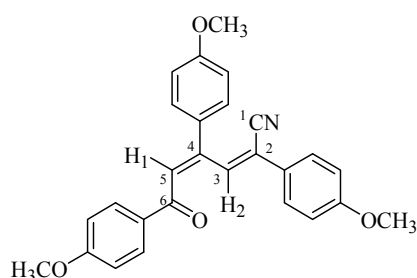
(2Z,4E)-2,6-bis(4-methoxyphenyl)-4-(4-methylphenyl)-6-oxo-2,4-hexadienenitrile(**2D**)

Yield 95%; yellow crystals, m.p.:129-131 °C (from EtOH); IR (neat): $\nu = 2217$ (CN), 1638 (CO) cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): $\delta = 2.44$ (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): $\delta = 21.5$ (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.



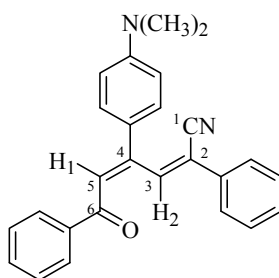
(2Z,4E)-2,4,6-tris(4-methoxyphenyl)-6-oxo-2,4-hexadienenitrile(**2E**)

Yield 93%; yellow crystals, m.p.:131-133 °C (from EtOH); IR (neat): $\nu = 2218$ (CN), 1636 (CO) cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): $\delta = 3.87, 3.88, 3.9$ (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.



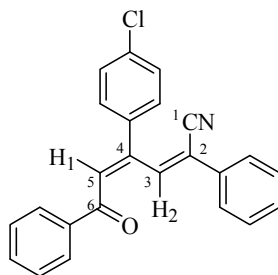
(2Z,4E)-4-[4-(dimethylamino)phenyl]-6-oxo-2,6-diphenyl-2,4-hexadienenitrile (**2F**)

Yield 88%; red crystals, m.p.:174-176 °C (from EtOH); IR (neat): $\nu = 2215$ (CN), 1628 (CO) cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): $\delta = 3.07$ (s, 6H, $\text{N}(\text{CH}_3)_2$), 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): $\delta = 40.1$ ($\text{N}(\text{CH}_3)_2$), 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.



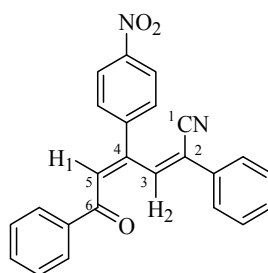
(2Z,4E)-4-(4-chlorophenyl)-6-oxo-2,6-diphenyl-2,4-hexadienenitrile (**2G**)

Yield 70%; yellow crystals, m.p.:109-111 °C (from EtOH); IR (neat): $\nu = 2218$ (CN), 1647 (CO) cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): $\delta = 7.29$ (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): $\delta = 115.5$ (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.



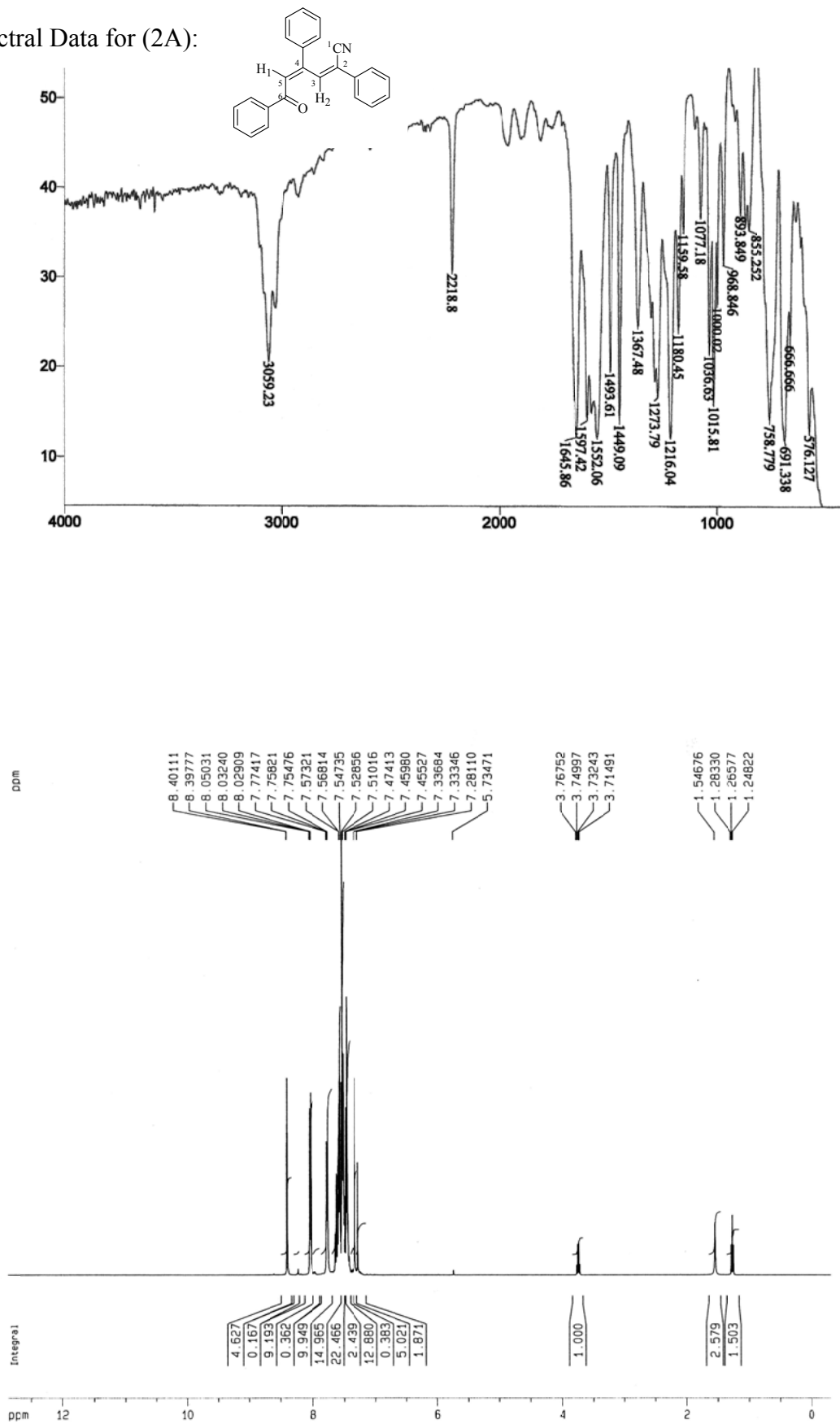
(2Z,4E)-4-(4-nitrophenyl)-6-oxo-2,6-diphenyl-2,4-hexadienenitrile(**2H**)

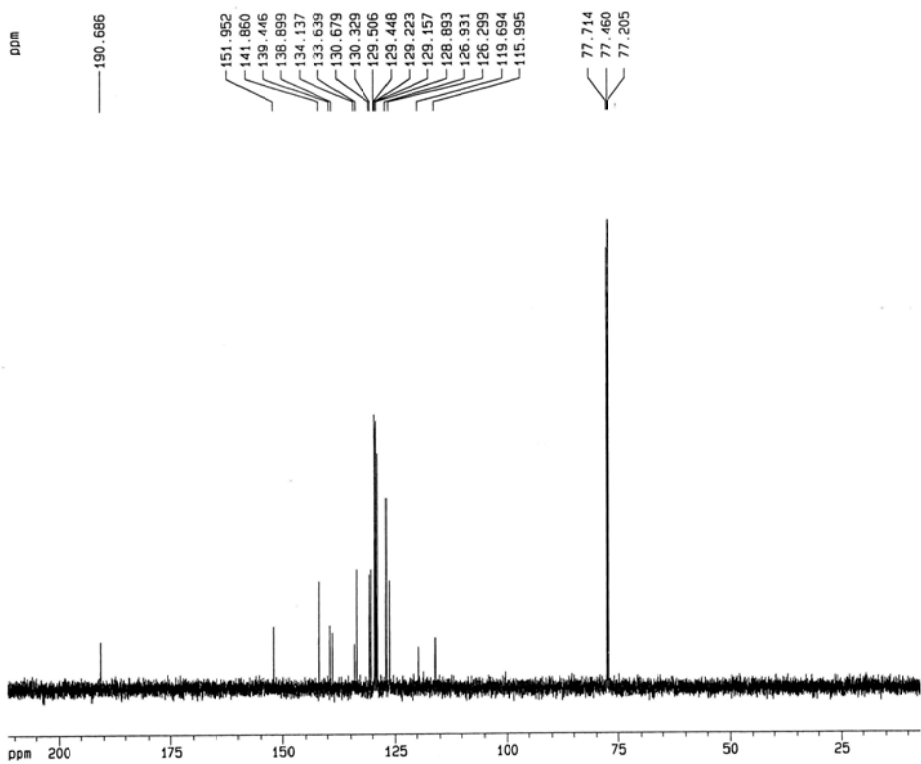
Yield 72%; brown crystals, m.p.:151-153 °C (from EtOH); IR (neat): $\nu = 2218$ (CN), 1651 (CO), 1345 , 1518 (NO_2) cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): $\delta = 7.30$ (s, 1H, H_1), 7.24, 7.44-8.34 (m, 14H, Ar-H), 8.39 (s, 1H, H_2) ppm; ^{13}C NMR (100MHz, CDCl_3): $\delta = 115.4$ (C-2), 120.0 (C-1), 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.



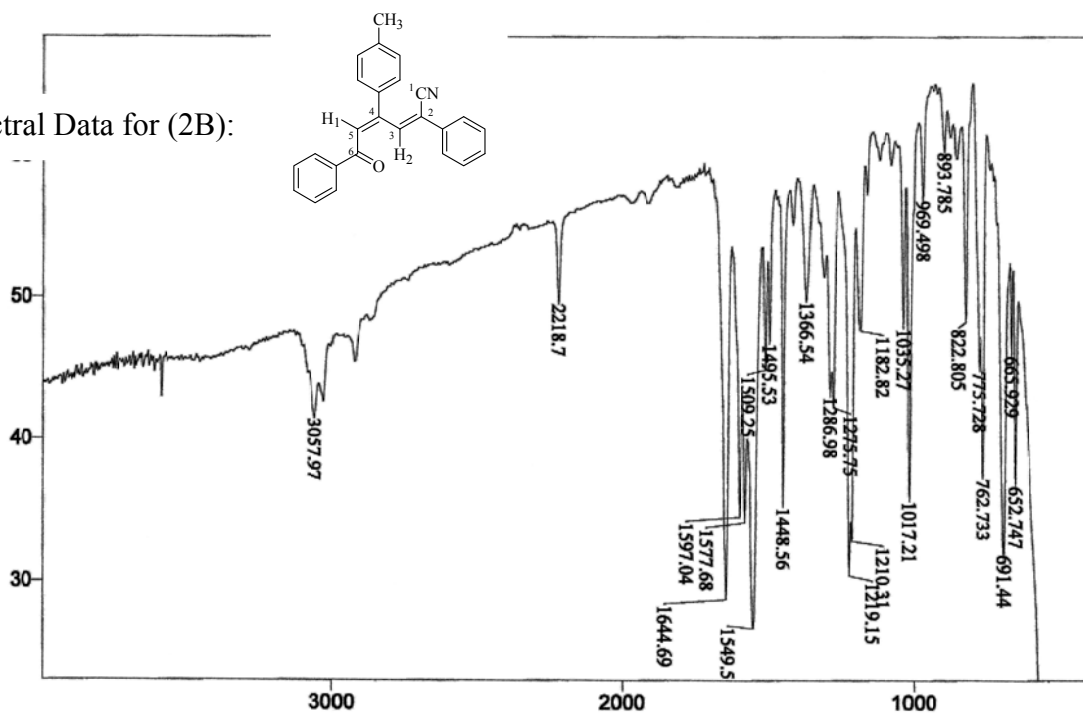
2. IR, ¹H NMR and ¹³CNMR Spectra for New Compounds:

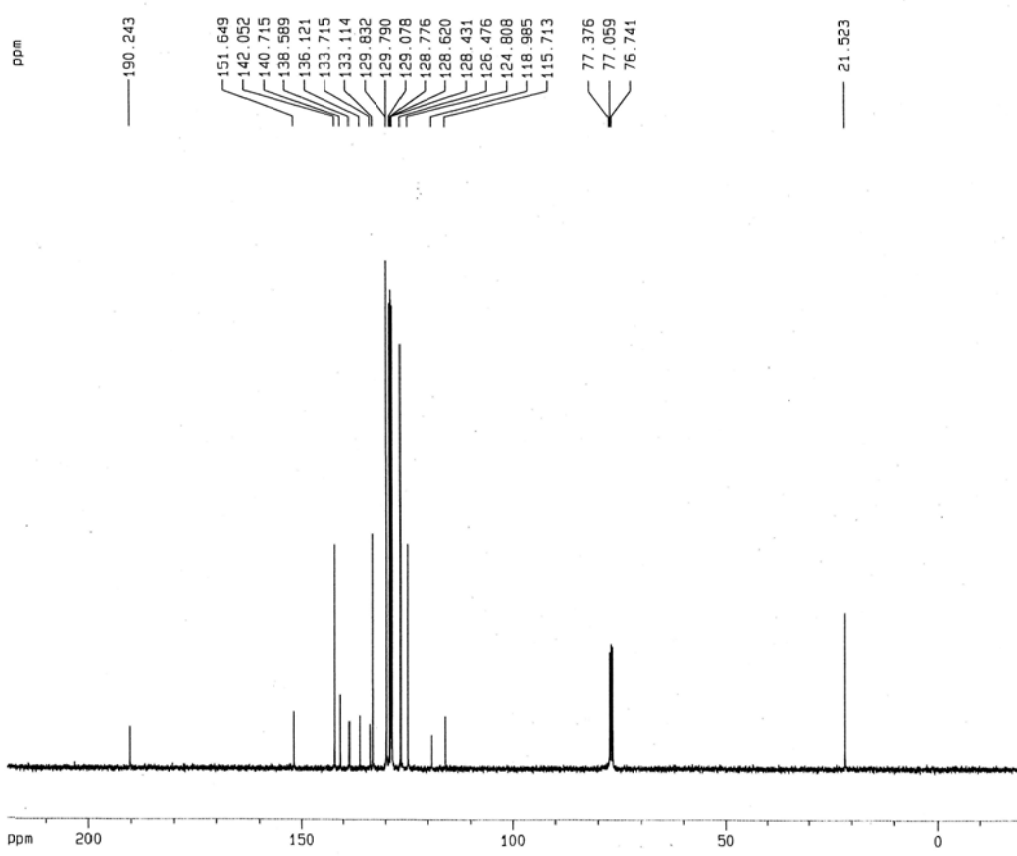
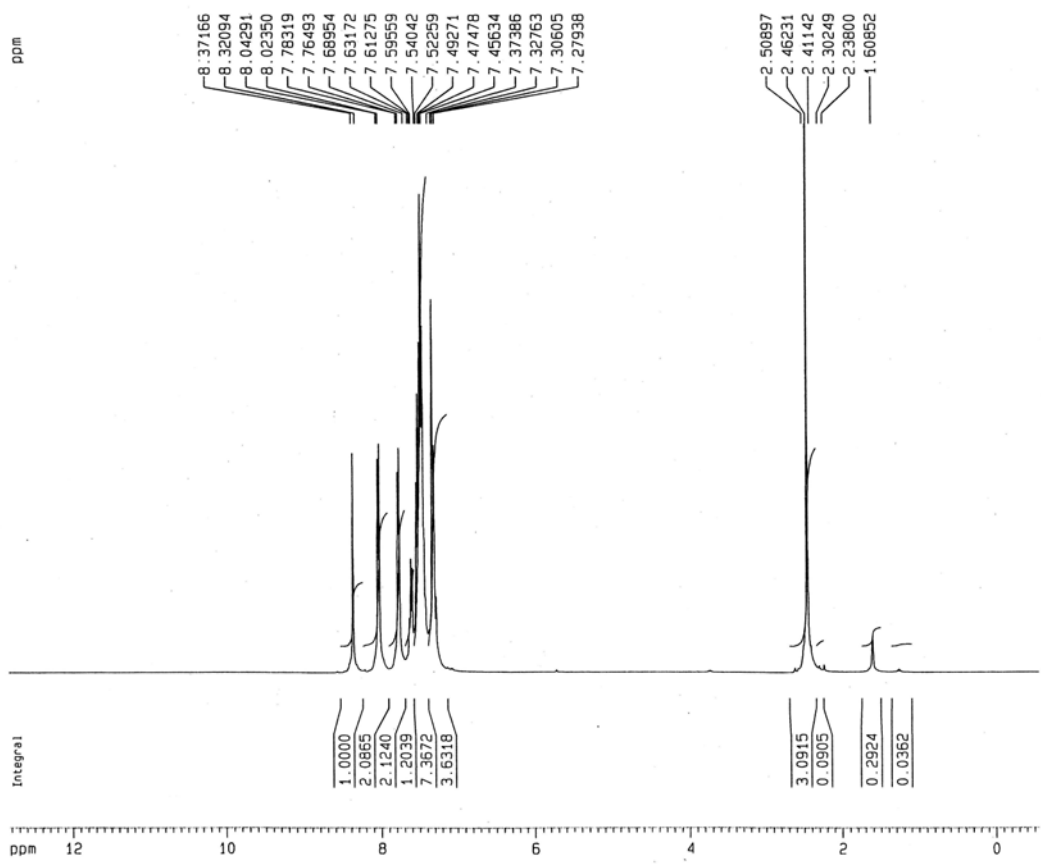
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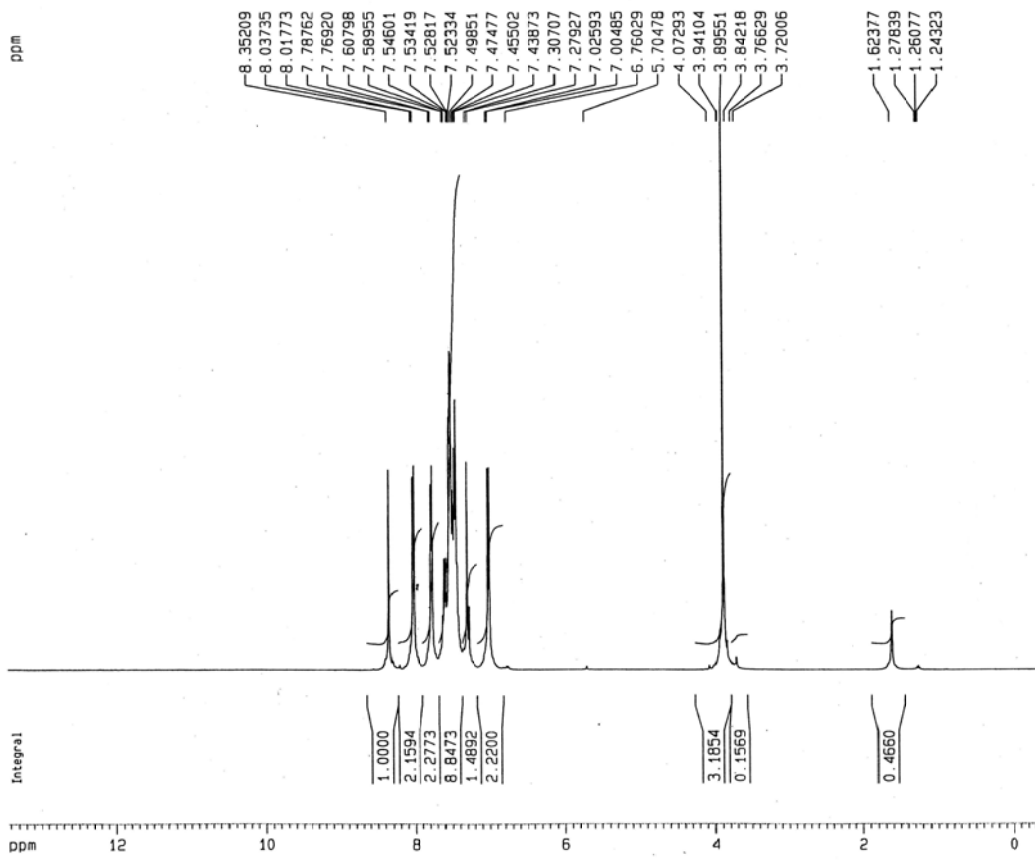
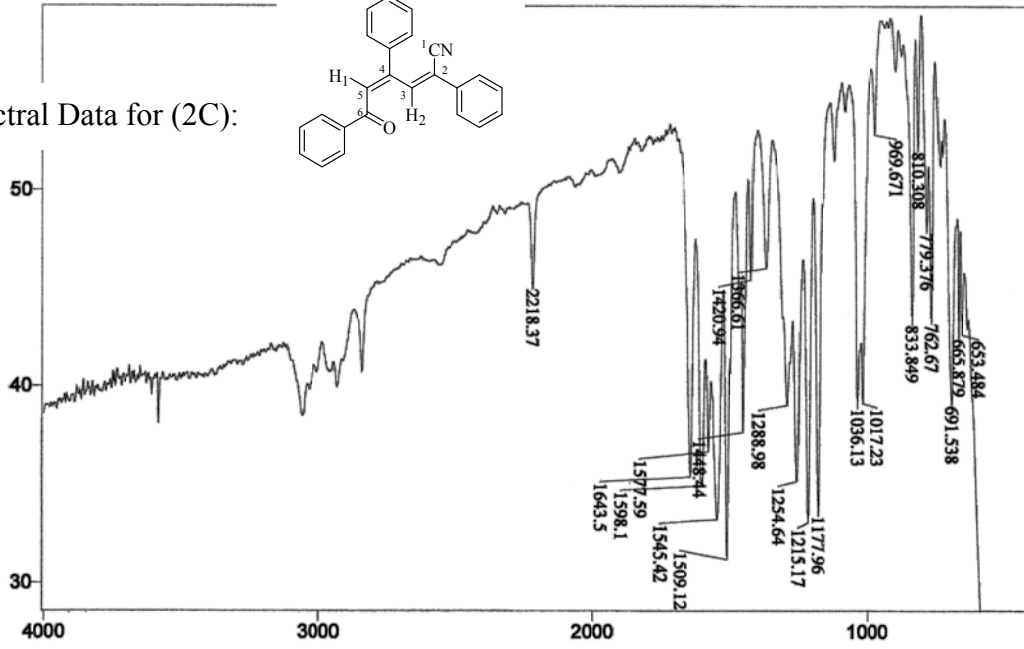
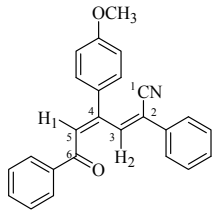


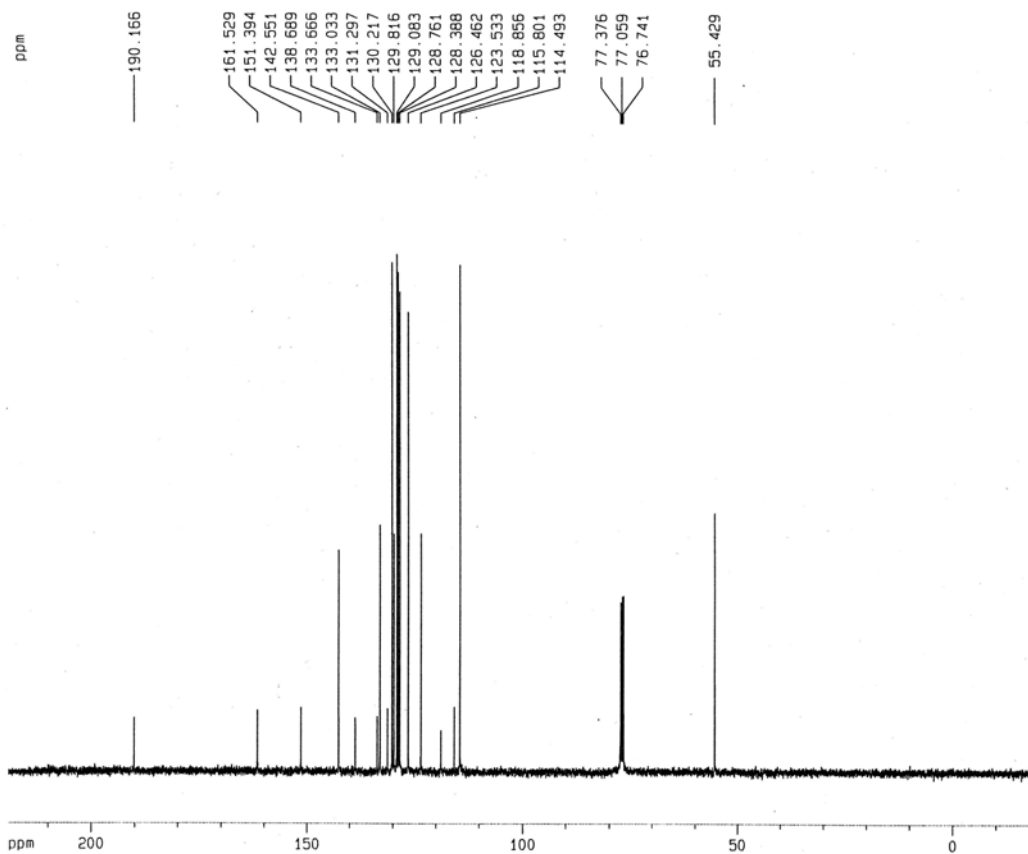
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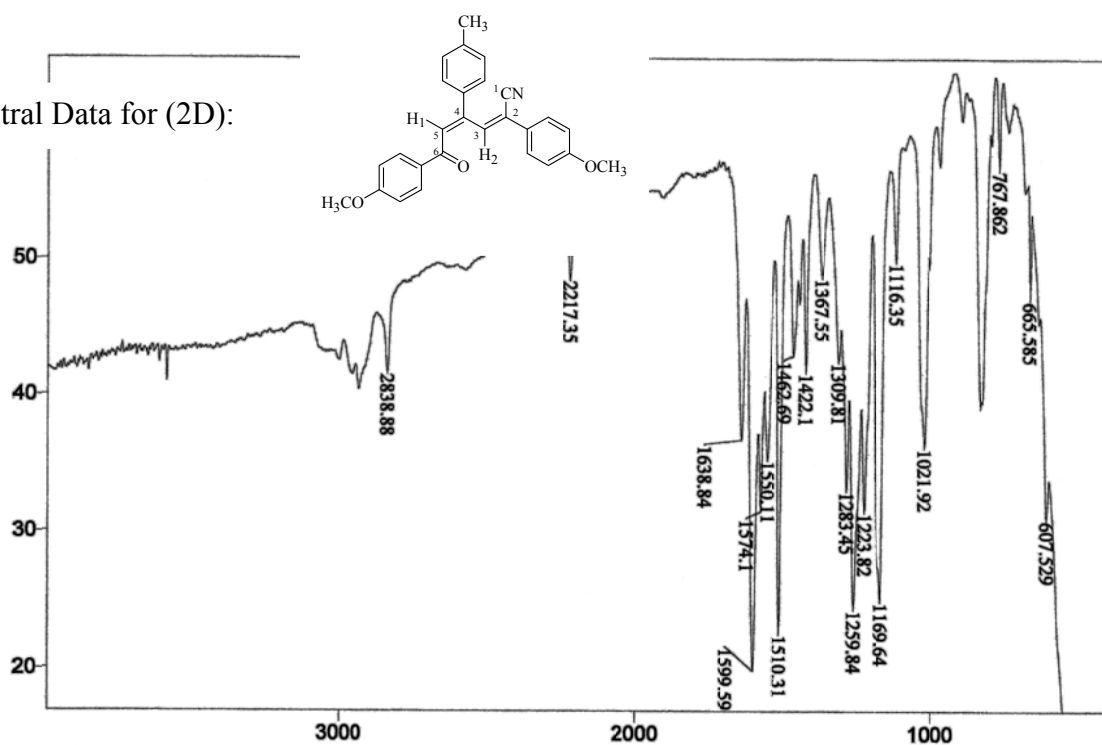


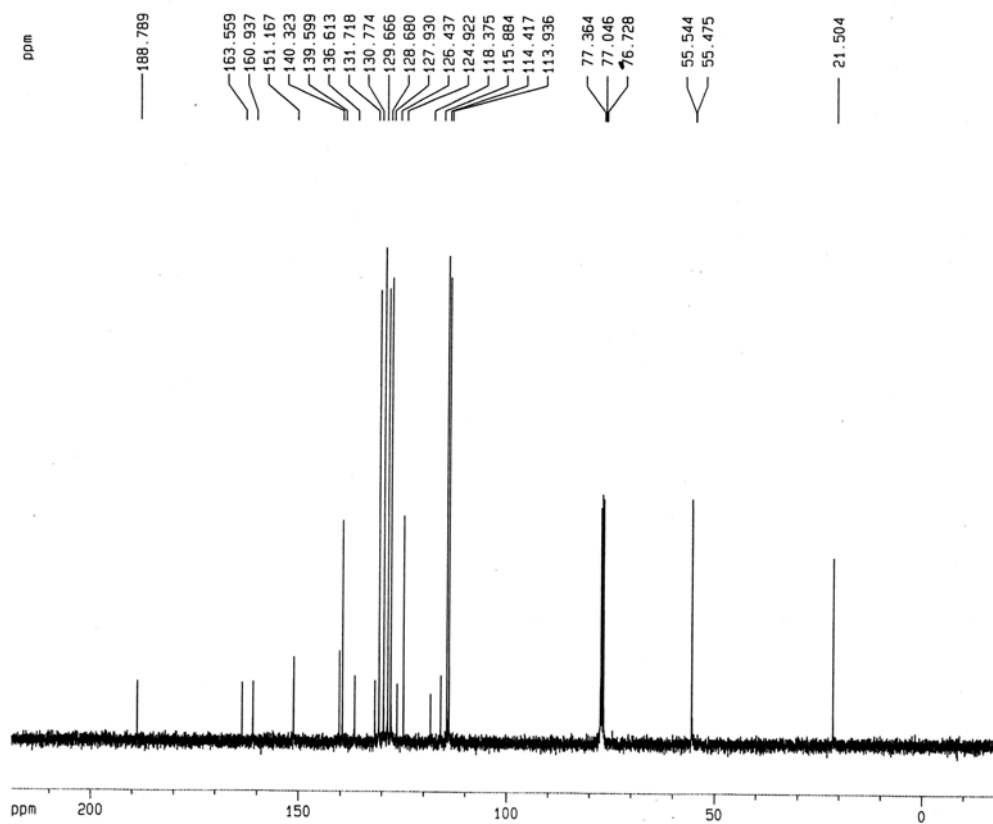
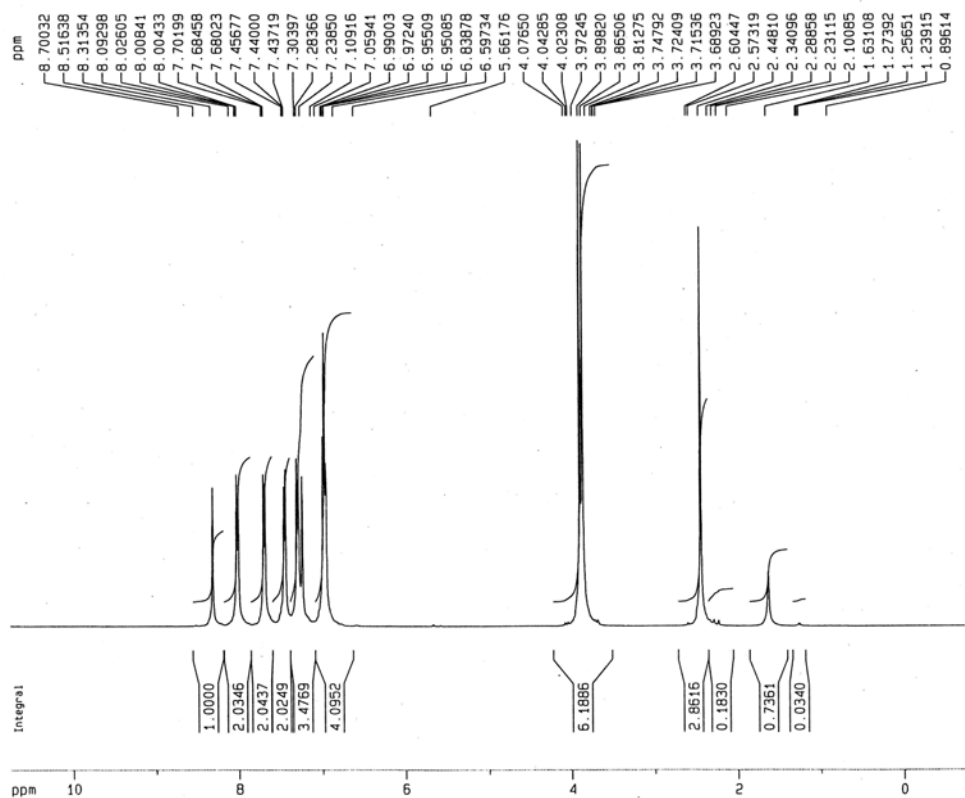
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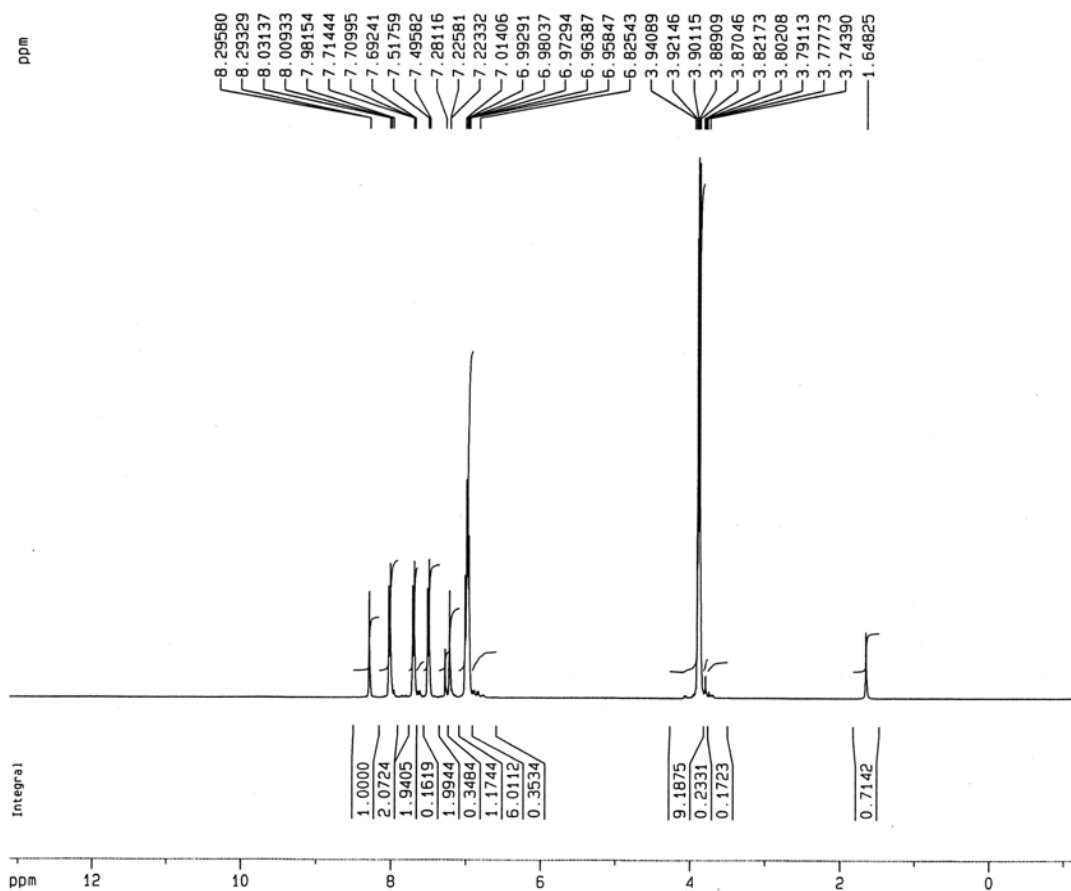
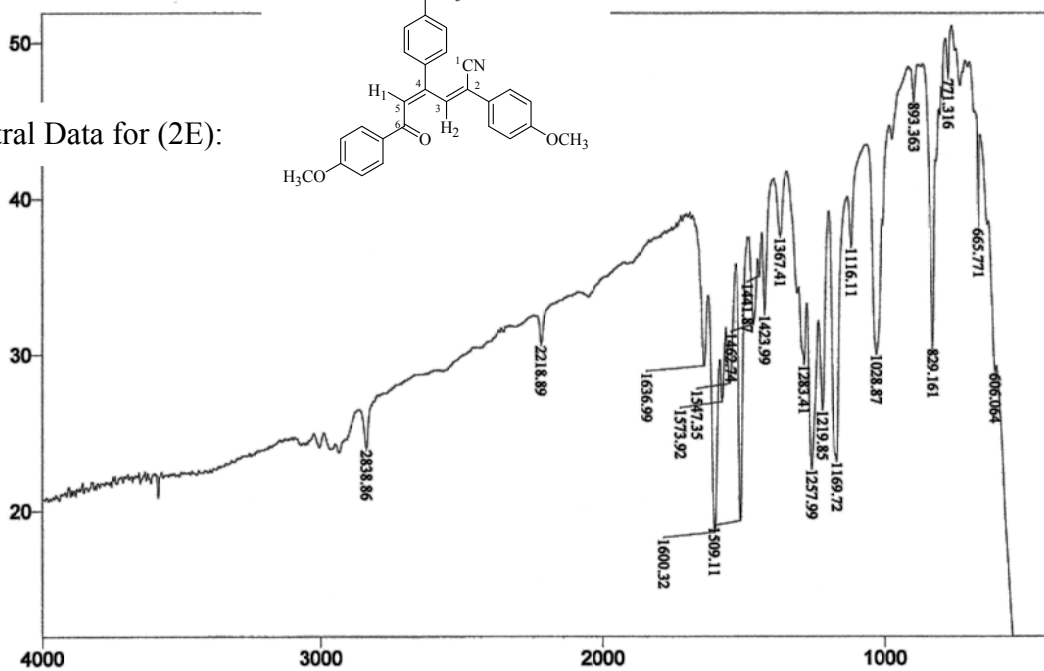
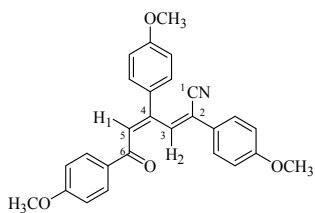


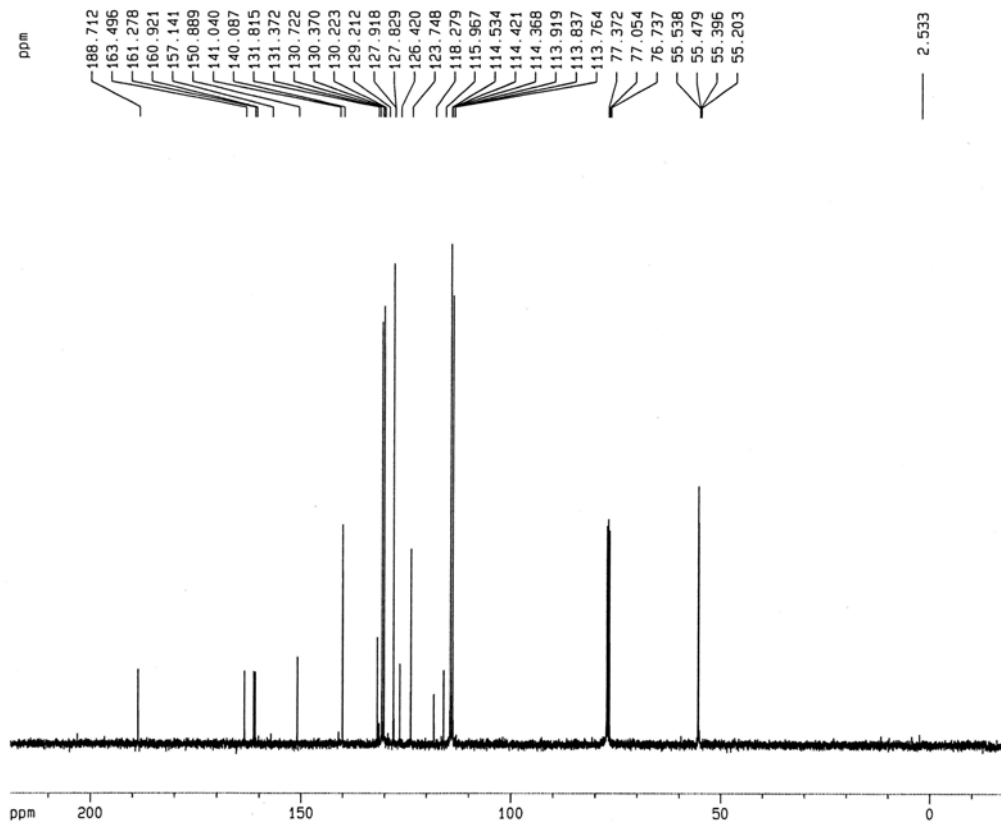
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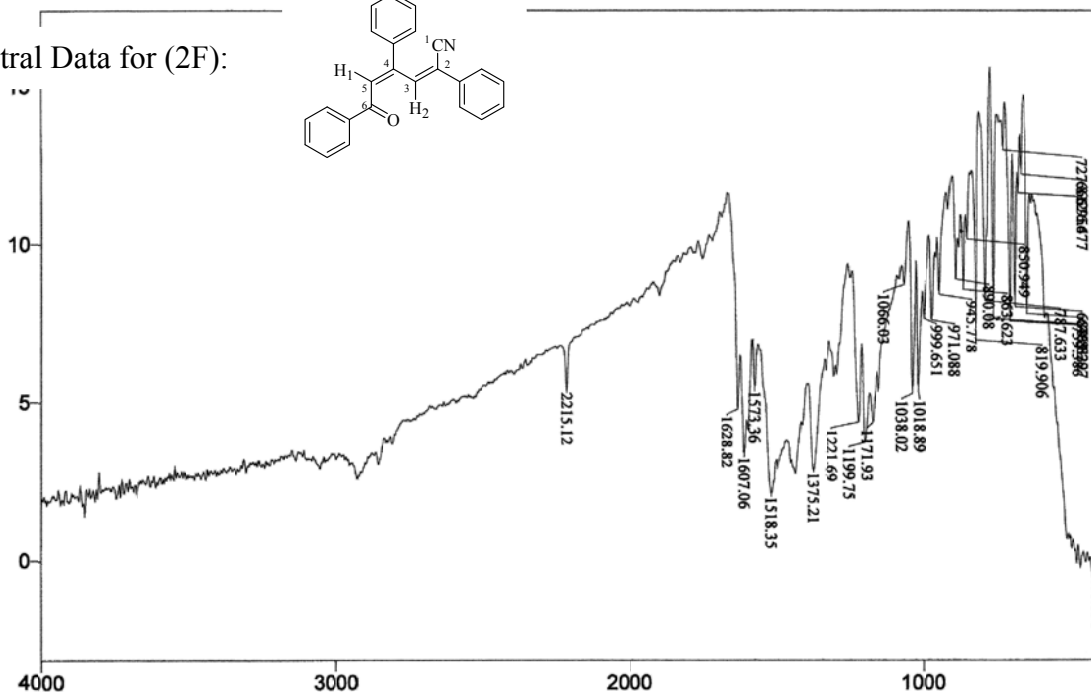
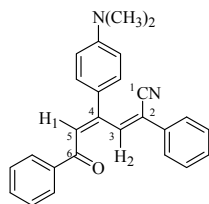


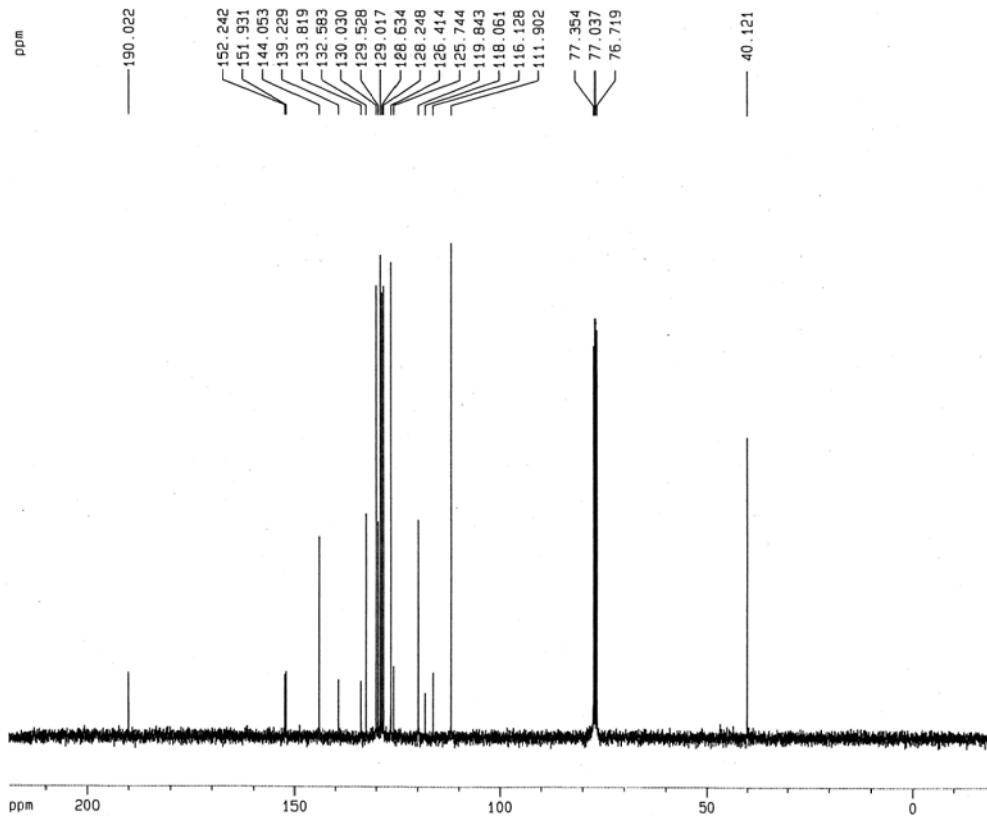
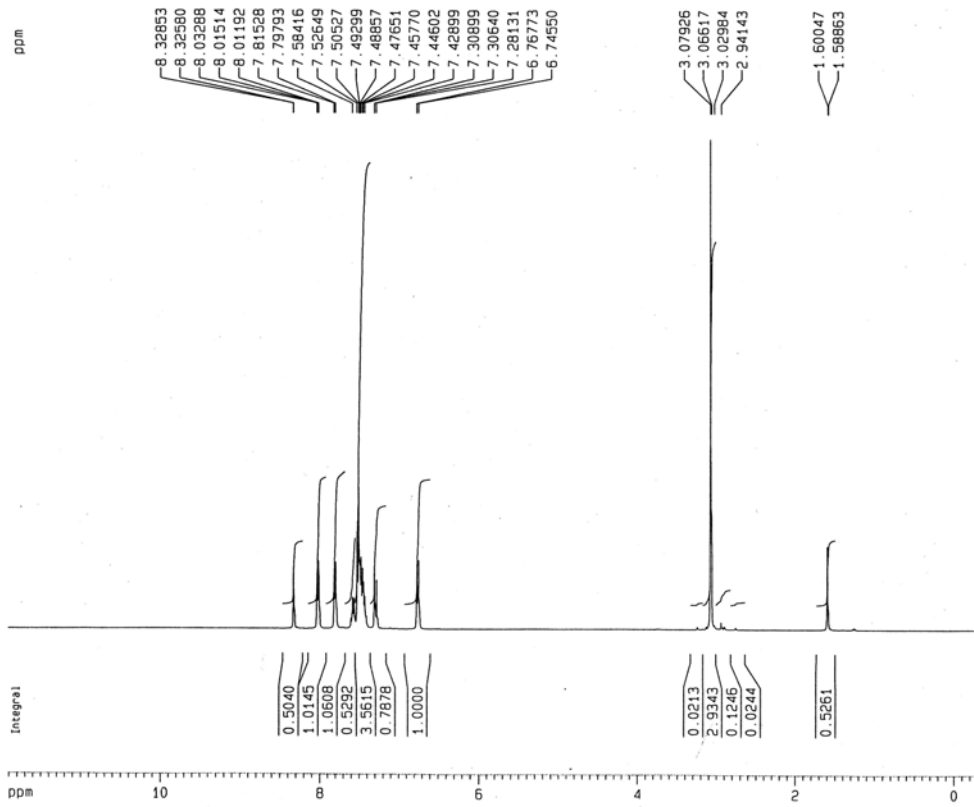
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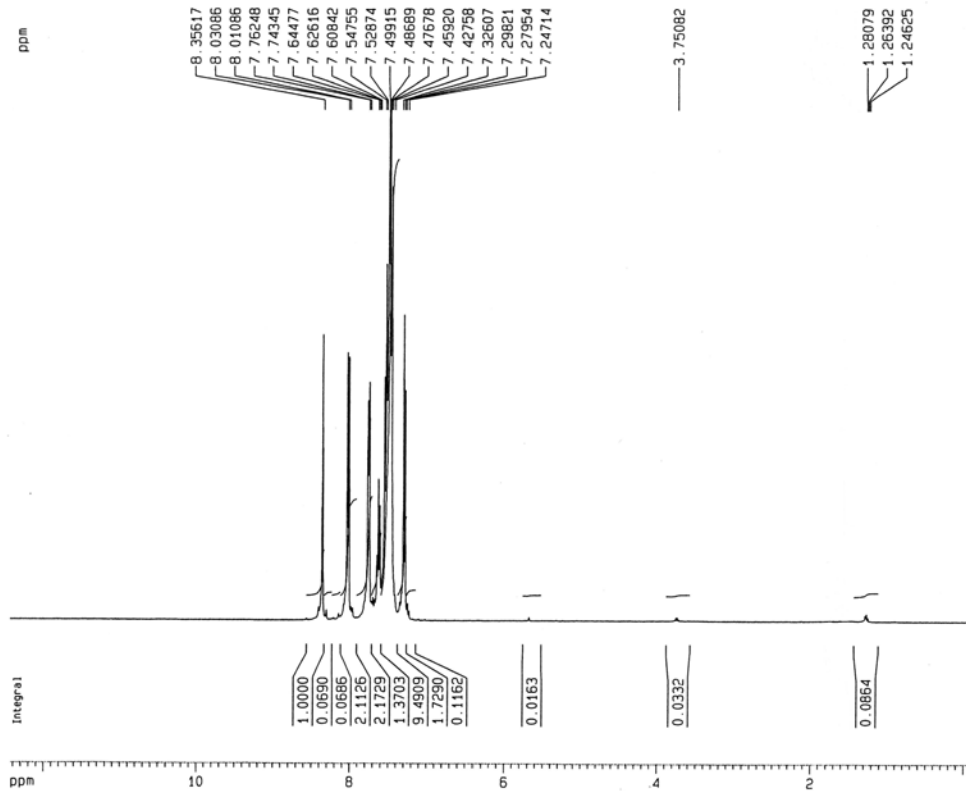
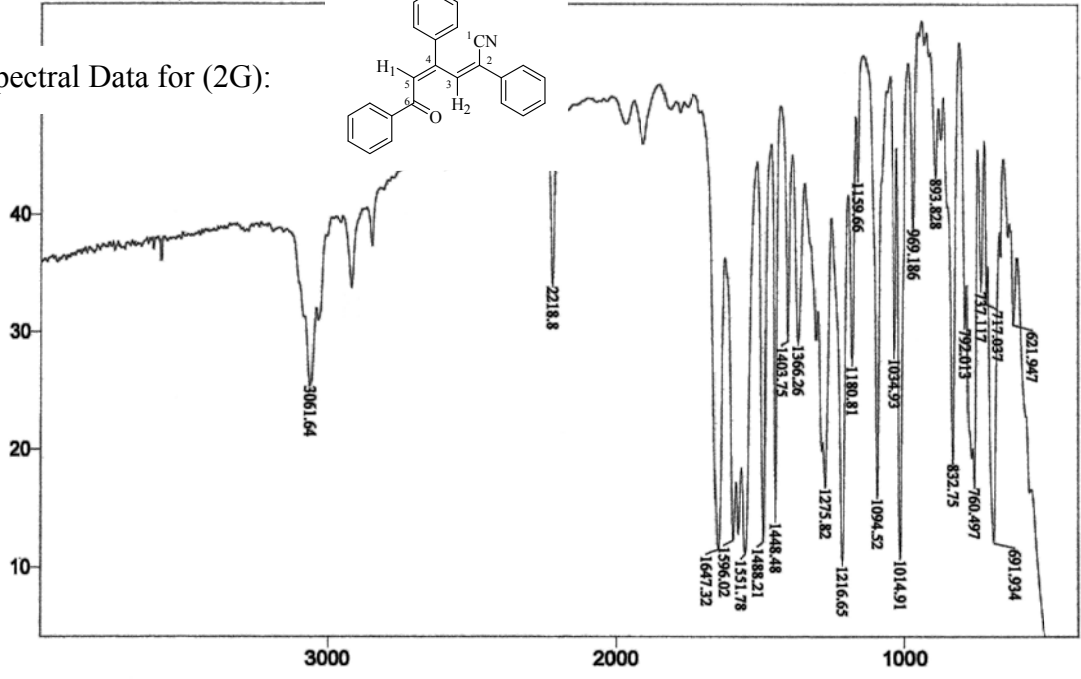
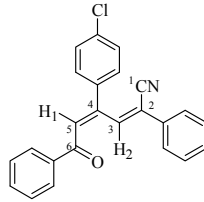


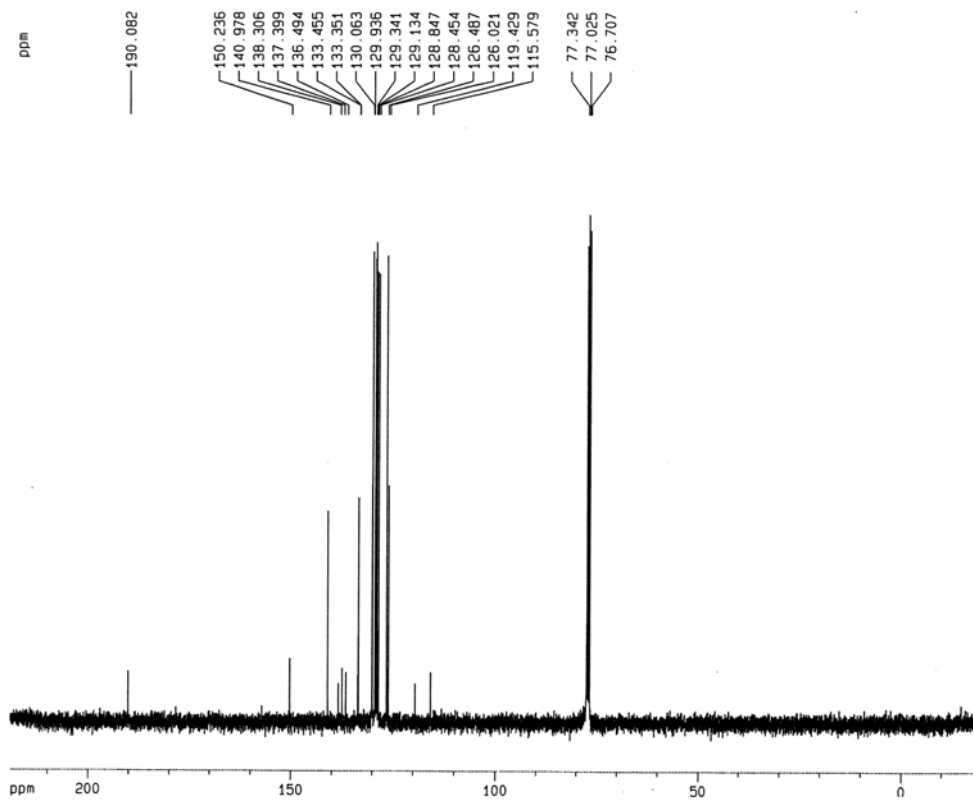
Spectral Data for (2F):





Spectral Data for (2G):





Spectral Data for (2H):

