

**One-pot synthesis of 1H-pyrazolo[1,2-*b*]phthalazine-5,10-dione
derivatives under solvent-free conditions**

Supporting Information

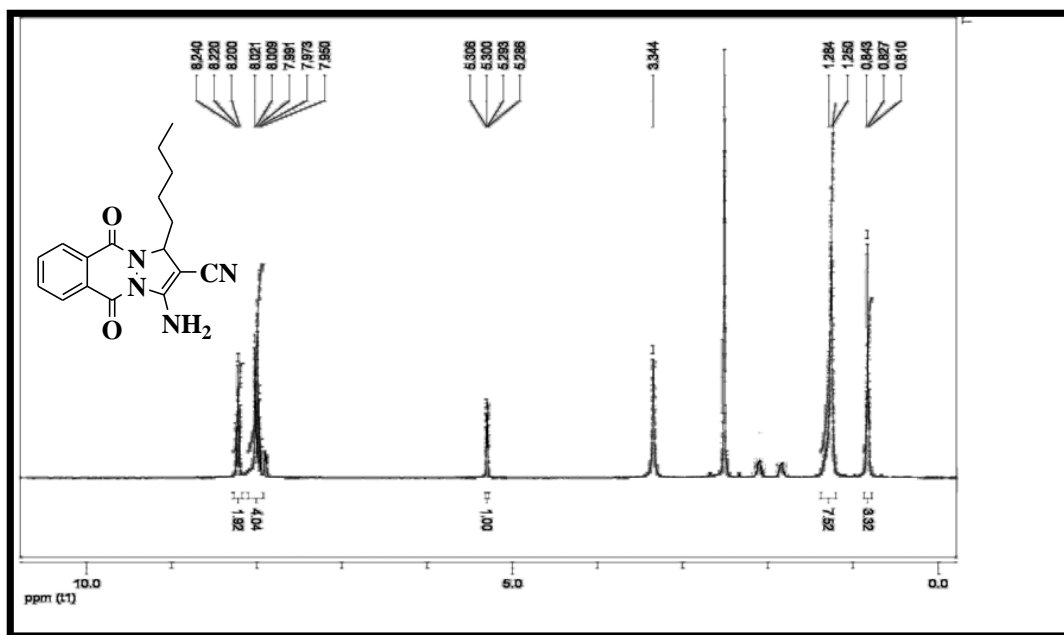
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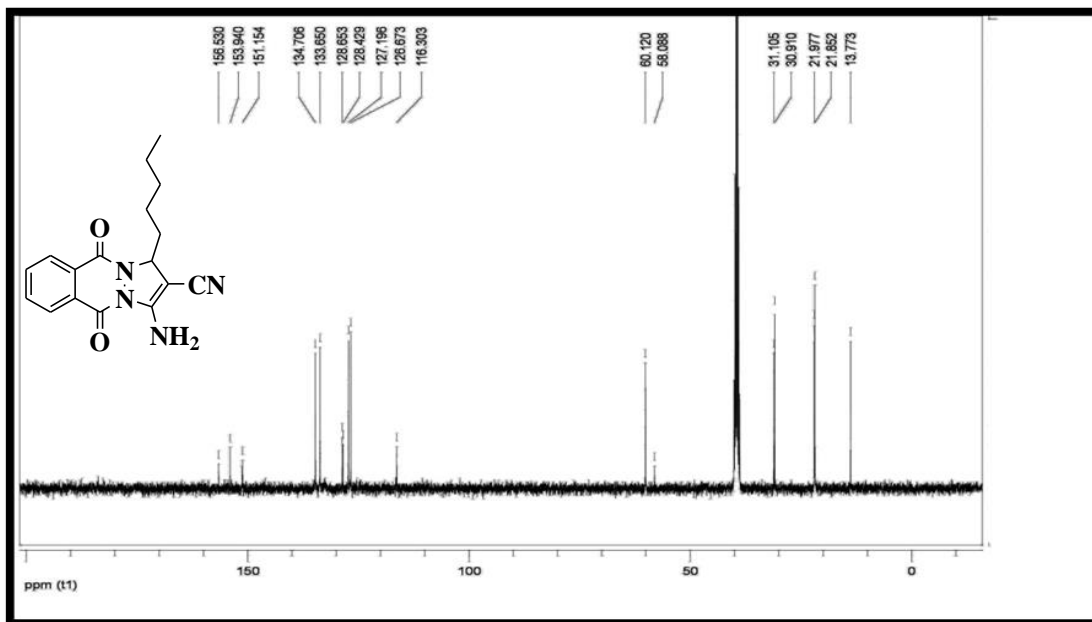
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3-Amino-5,10-dioxo-1-pentyl-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile **11**: ^1H NMR (400 MHz, DMSO- d_6): δ_{H} (ppm) 0.81-0.84(t, CH_3 , 3H), 1.25-1.28 (m, CH_2 , 8H), 5.28-5.30 (m, CH, 1H), 7.95-8.24 (m, 6H, Ar-H and NH_2). ^{13}C NMR (100 MHz, DMSO- d_6): δ_{C} (ppm) 13.7, 21.8, 21.9, 30.9, 31.1, 58.0, 60.1, 116.3, 126.6, 127.1, 128.4, 128.6, 133.6, 134.7, 151.1, 153.9, 156.5

^1H NMR

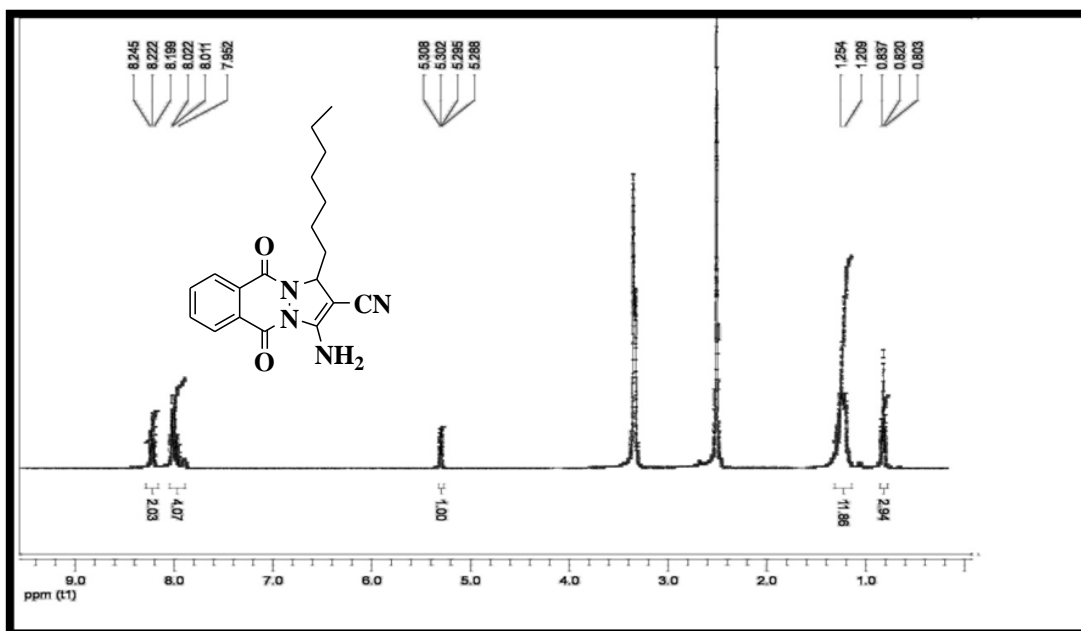


^{13}C NMR

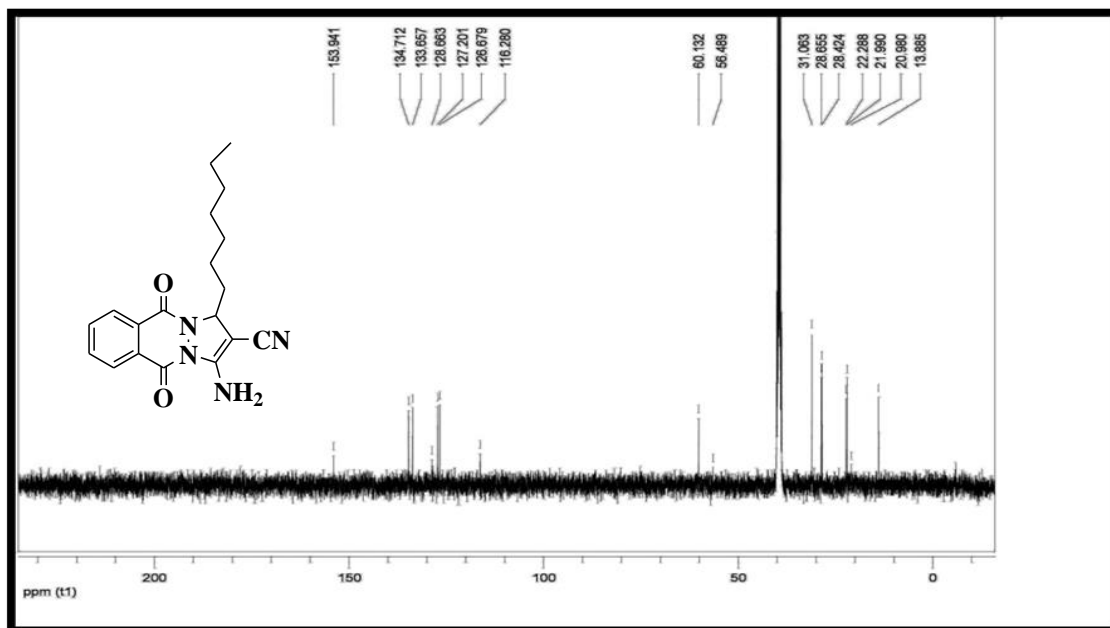


3-Amino-1-heptyl-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile **14**: ^1H NMR (400 MHz, DMSO- d_6): δ_{H} (ppm) 0.80-0.83 (t, CH_3 , 3H), 1.20-1.25 (m, CH_2 , 12H), 5.28-5.30 (q, CH, 1H), 7.95-8.24 (m, Ar-H and NH_2 , 6H). ^{13}C NMR (100 MHz, DMSO- d_6): δ_{C} (ppm) 13.8, 20.9, 21.9, 22.2, 28.4, 28.6, 31.0, 56.4, 60.1, 116.2, 126.6, 127.2, 128.6, 133.6, 134.7, 153.9.

^1H NMR

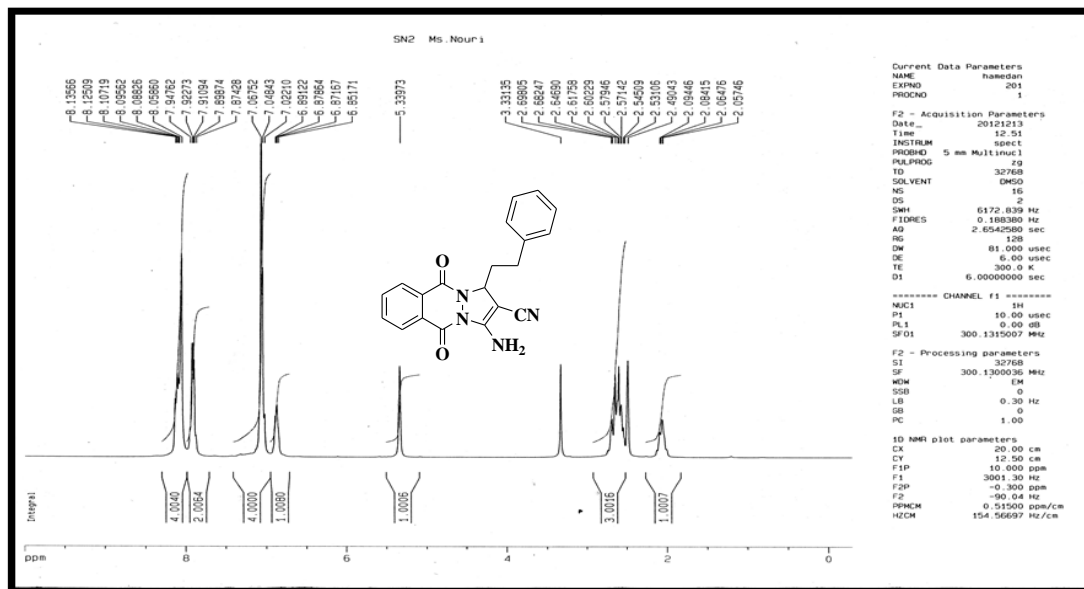


^{13}C NMR

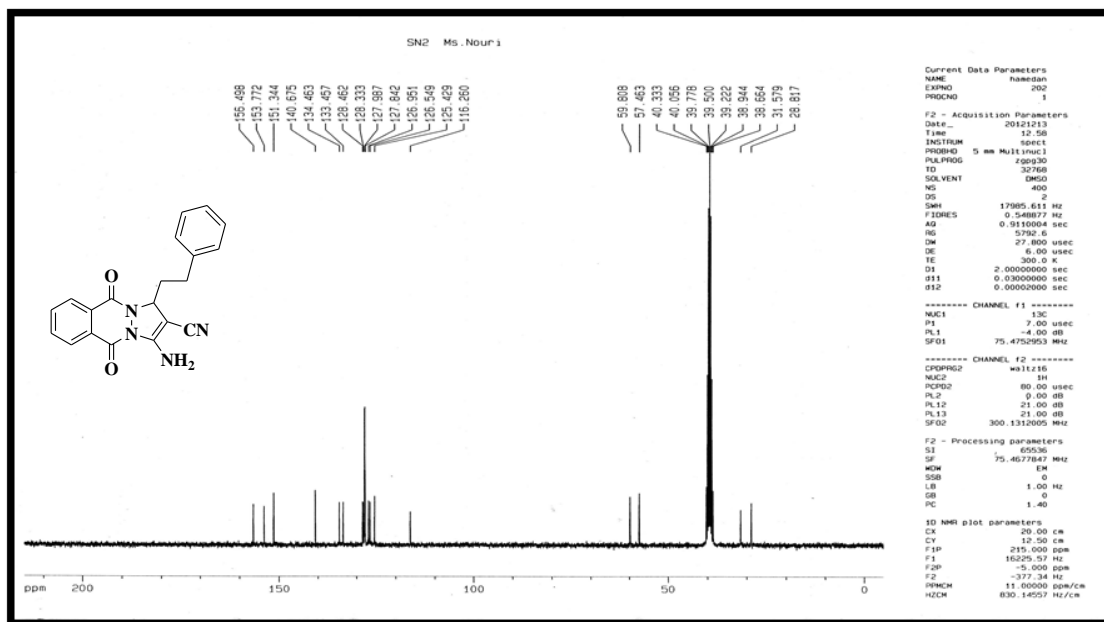


3-Amino-5,10-dioxo-1-phenethyl-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile **12**:
 ^1H NMR (300 MHz, DMSO- d_6): δ_{H} (ppm) 2.05-2.09 (m, 1H), 2.53-2.69 (m, 3H), 5.33 (m, 1H),
 6.85-8.13 (m, 11H). ^{13}C NMR (75 MHz, DMSO- d_6): δ_{C} (ppm) 28.8, 31.5, 57.4, 59.8, 116.2,
 125.4, 126.5, 126.9, 127.8, 127.9, 128.3, 128.4, 133.4, 134.4, 140.6, 151.3, 153.7, 156.4.

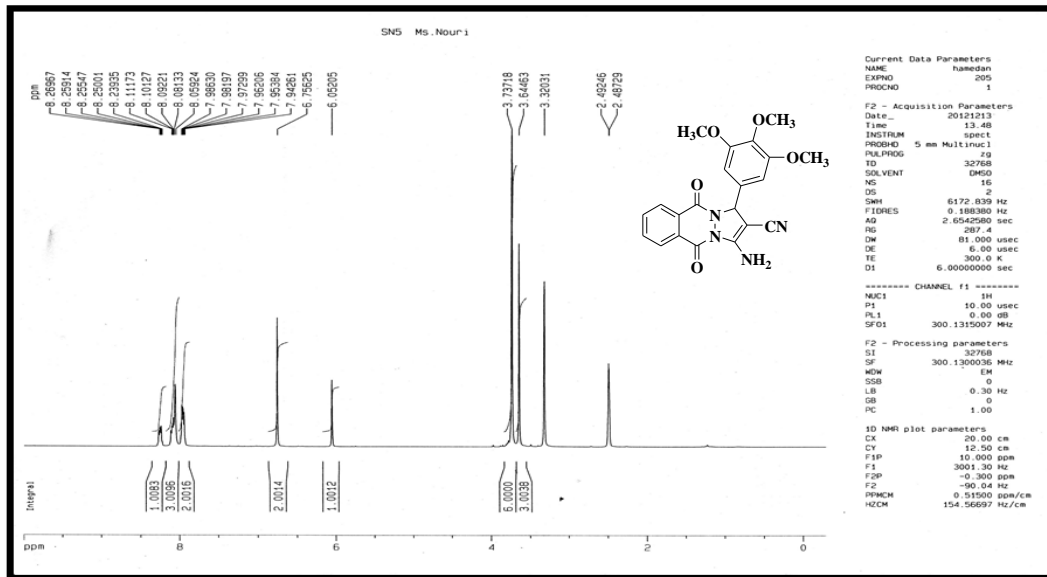
^1H NMR



^{13}C NMR

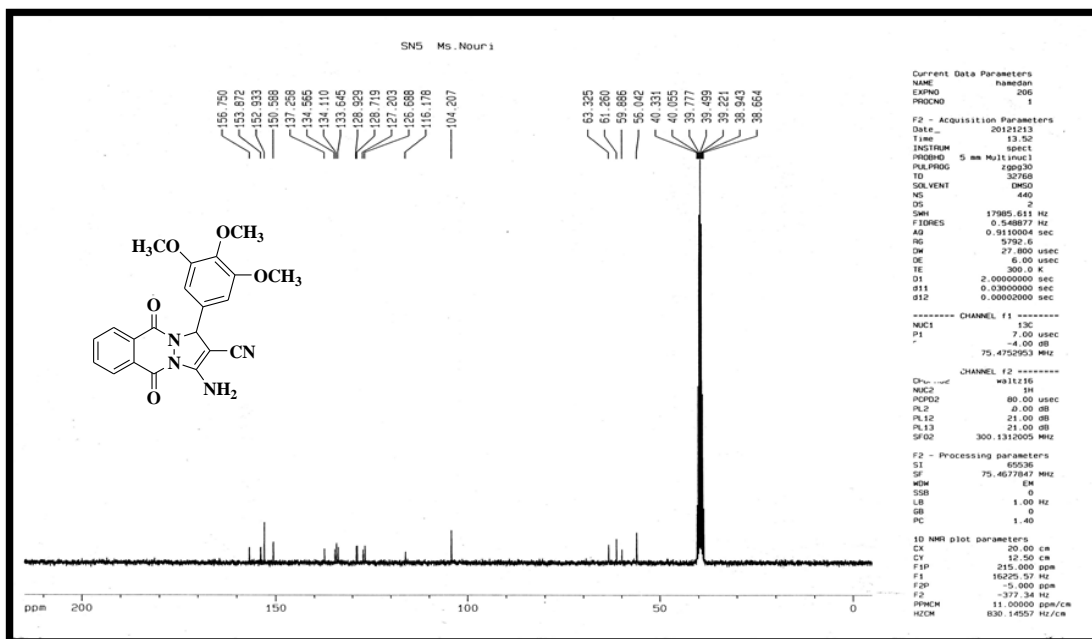


3-Amino-5,10-dioxo-1-(3,4,5-trimethoxyphenyl)-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile **7**: ^1H NMR (300 MHz, DMSO- d_6): δ_{H} (ppm) 3.64-3.73 (m, 9H), 6.05 (s, 1H), 6.75 (s, 2H), 7.94-8.26 (m, 6H). ^{13}C NMR (75 MHz, DMSO- d_6): δ_{C} (ppm) 56.0, 59.8, 61.2, 63.3, 104.2, 116.1, 126.6, 127.2, 128.7, 128.9, 133.6, 134.1, 134.5, 137.2, 150.5, 152.9, 153.8, 156.7.



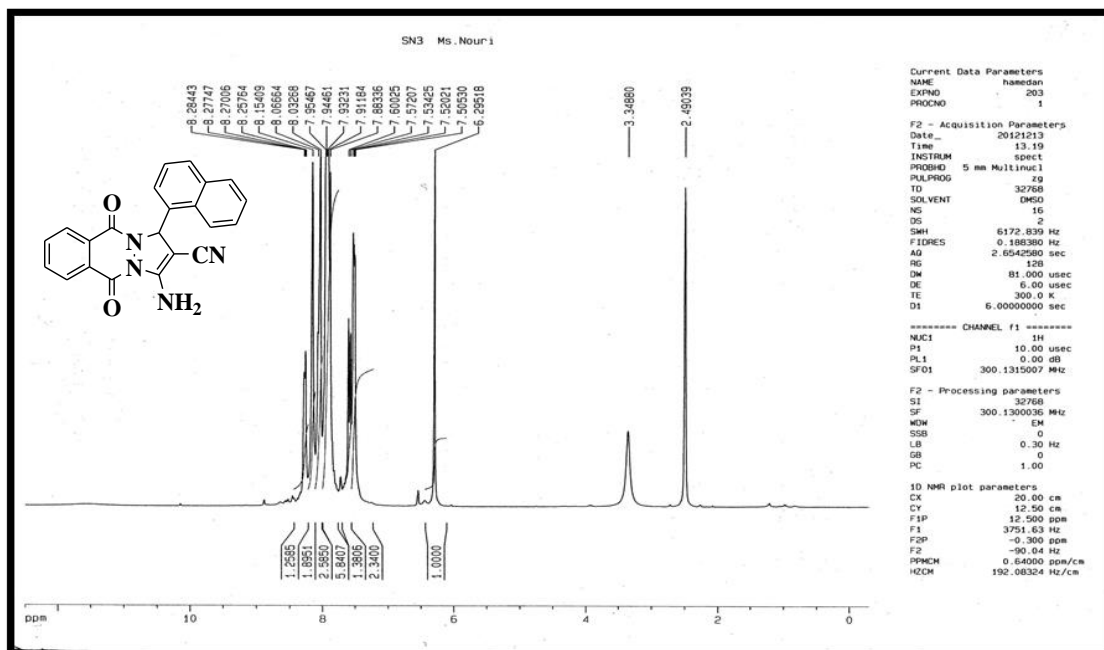
^1H NMR

^{13}C NMR

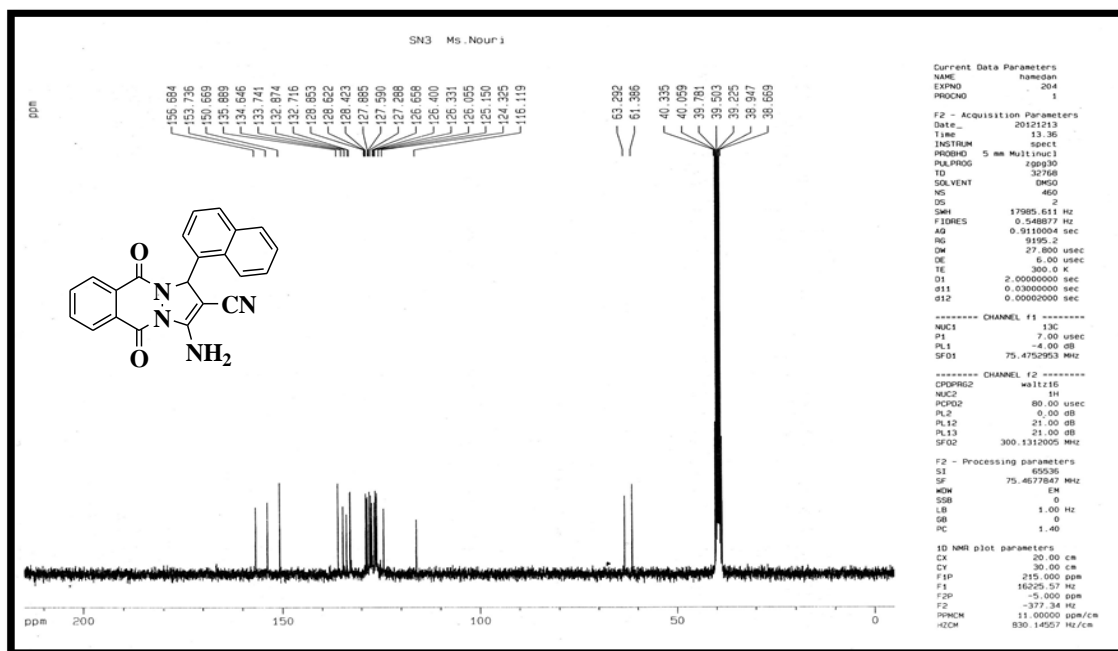


3-Amino-5,10-dioxo-1-(naphthalene-2-yl)-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile **6**: ^1H NMR (300 MHz, DMSO- d_6): δ_{H} (ppm) 6.29 (s, 1H), 7.50-8.28 (m, 13H). ^{13}C NMR (75 MHz, DMSO- d_6): δ_{C} (ppm) 61.3, 63.2, 116.1, 124.3, 125.1, 126.0, 126.3, 126.4, 126.6, 127.2, 127.5, 127.8, 128.4, 128.6, 128.8, 132.7, 132.8, 133.7, 134.6, 135.8, 150.6, 153.7, 156.6

^1H NMR

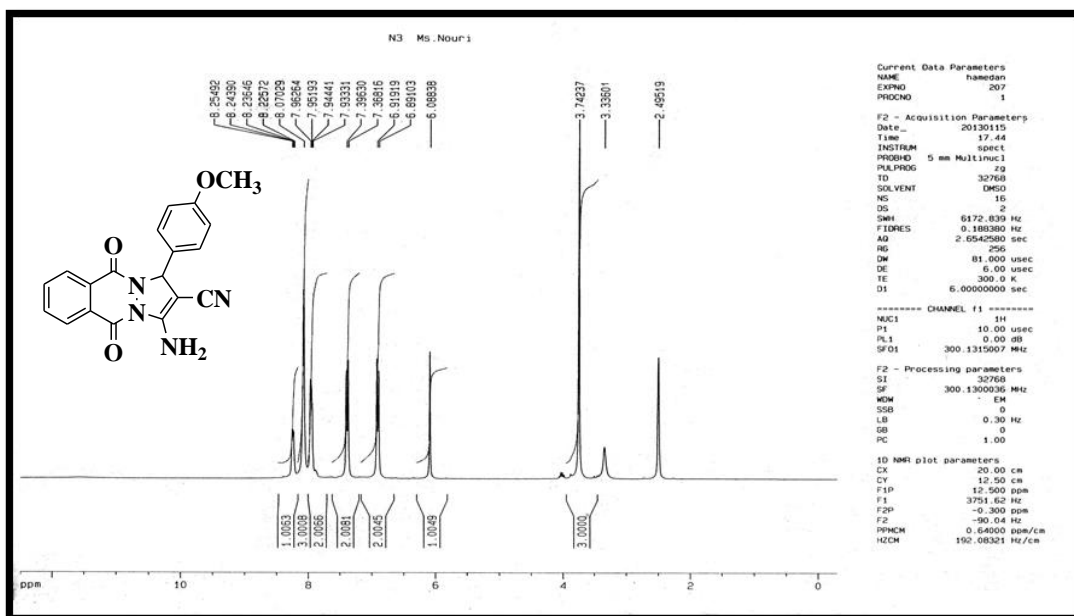


^{13}C NMR

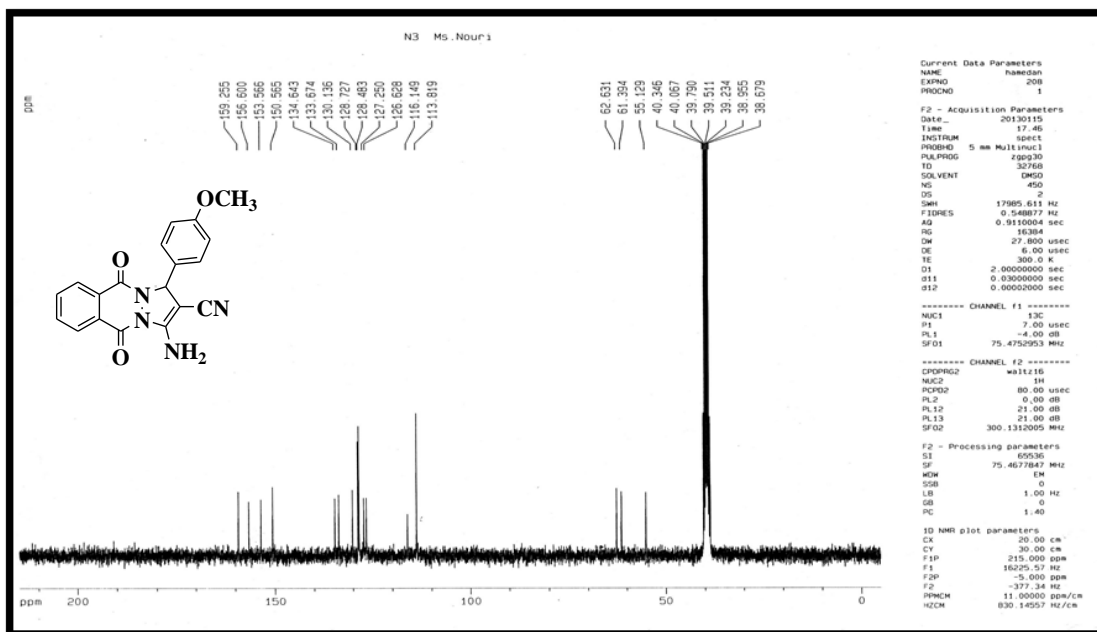


3-Amino-5,10-dioxo-1-(4-methoxyphenyl)-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile **4**: ^1H NMR (300 MHz, DMSO- d_6): δ_{H} (ppm) 3.74 (s, 3H), 6.08 (s, 1H), 6.89- 6.91 (d, 2H), 7.36-7.39 (d, 2H), 7.93-8.25 (m, 6H). ^{13}C NMR (75 MHz, DMSO- d_6): δ_{C} (ppm) 55.1, 61.3, 62.6, 113.8, 116.1, 126.6, 127.2, 128.4, 128.7, 130.1, 133.6, 134.6, 150.5, 153.5, 156.6, 159.2

^1H NMR

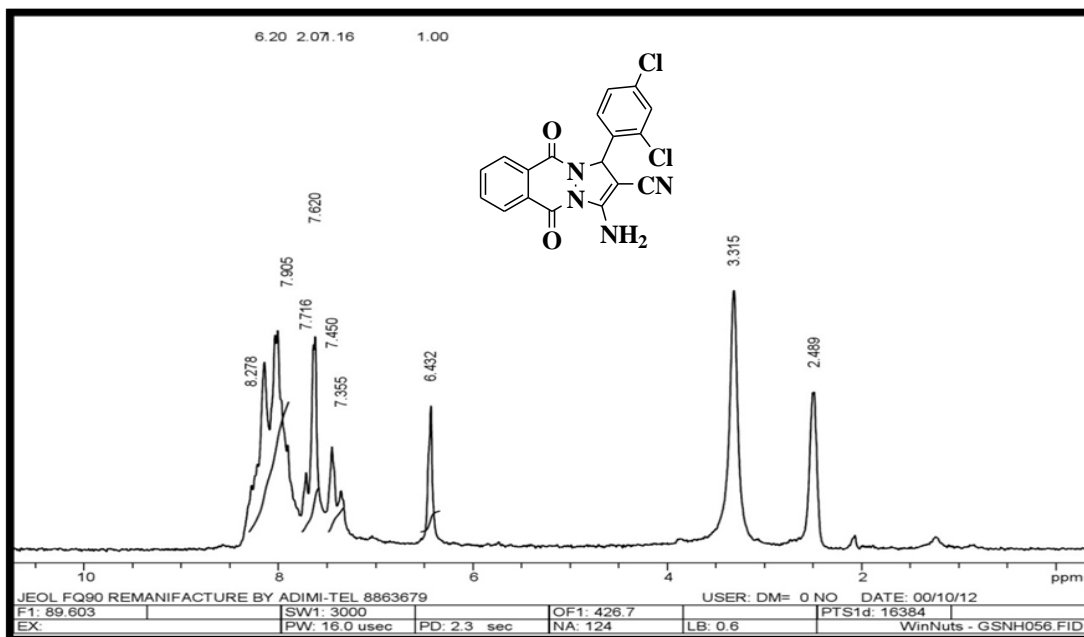


^{13}C NMR

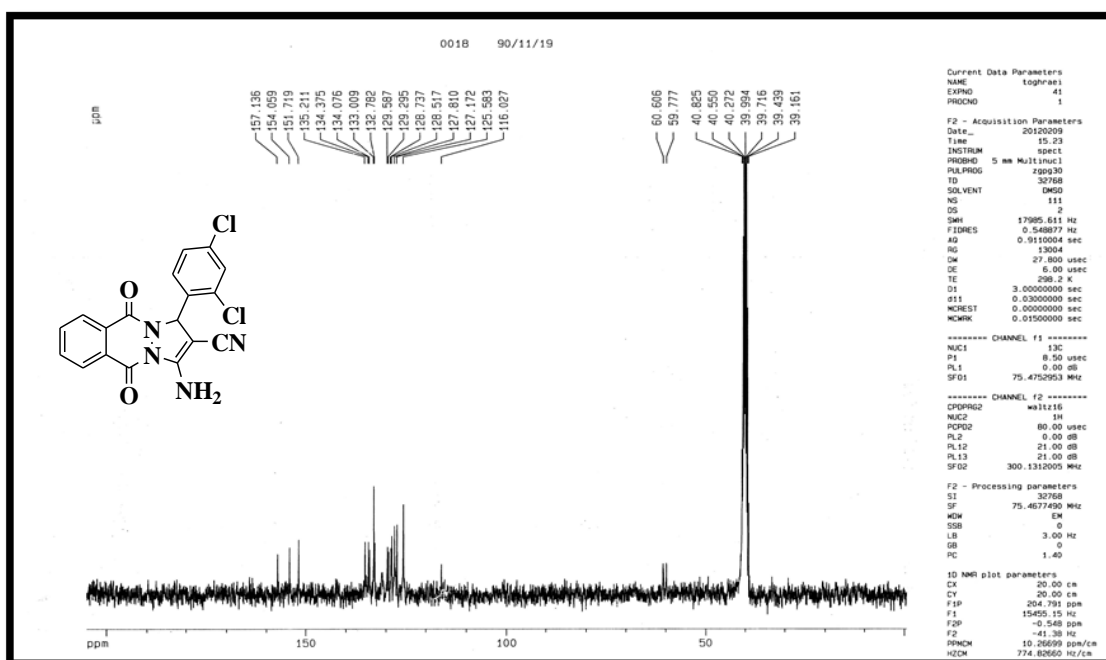


3-Amino-5,10-dioxo-1-(2,4-dichlorophenyl)-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile **10**: ^1H NMR (90 MHz, DMSO- d_6): δ_{H} (ppm) 6.43 (s, 1H), 7.35-8.27 (m, 9H), ^{13}C NMR (75 MHz, DMSO- d_6): δ_{C} (ppm) 59.7, 60.0, 116.0, 125.5, 127.1, 127.8, 128.5, 128.7, 129.2, 129.5, 132.7, 133.0, 134.0, 134.3, 135.2, 151.7, 154.0, 157.1

^1H NMR

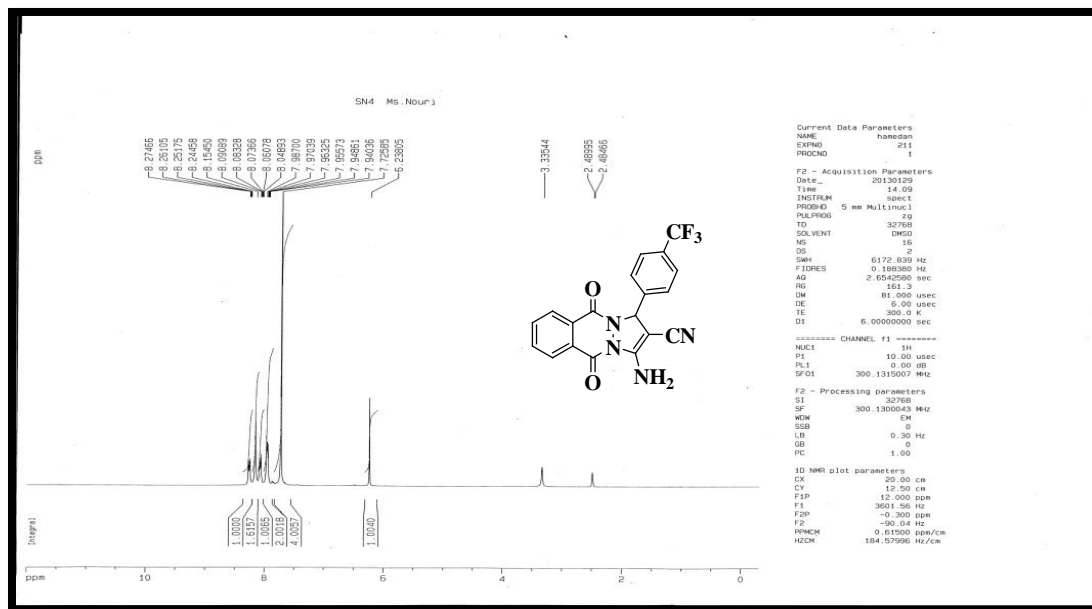


^{13}C NMR

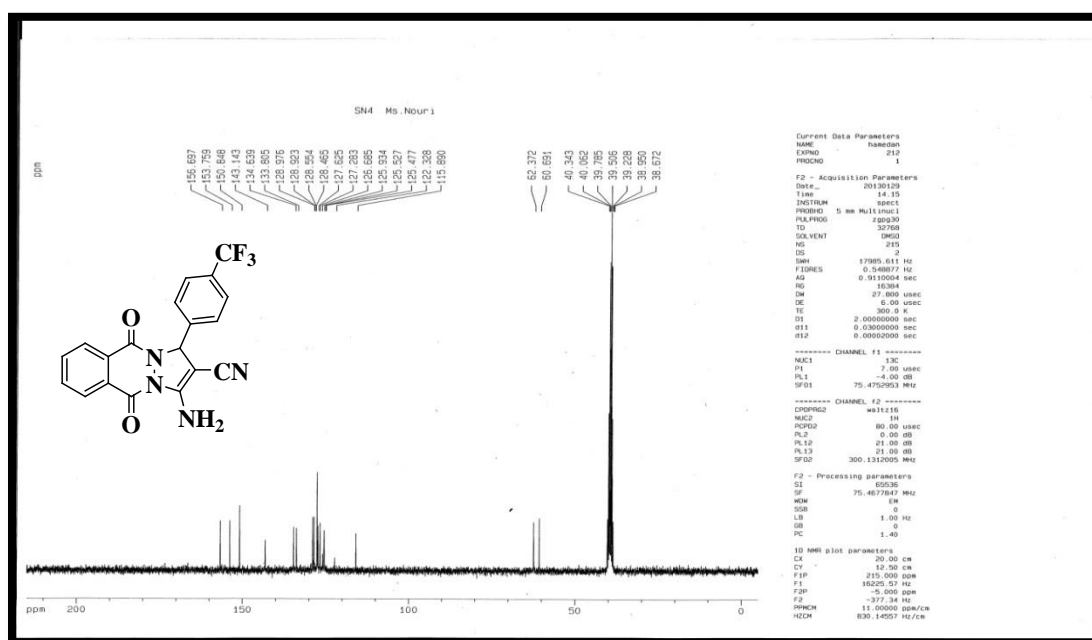


3-Amino-5,10-dioxo-1-(4-trifluoromethylphenyl)-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile **5**: ^1H NMR (300 MHz, DMSO- d_6): δ_{H} (ppm) 6.23 (s, 1H), 7.72-8.27 (m, 10H), ^{13}C NMR (75 MHz, DMSO- d_6): δ_{C} (ppm) 60.6, 62.3, 115.8, 122.3, 125.4, 125.5, 125.9, 126.6, 127.2, 127.6, 128.4, 128.5, 128.9, 129.0, 133.8, 134.6, 143.1, 150.8, 153.7, 156.6

^1H NMR

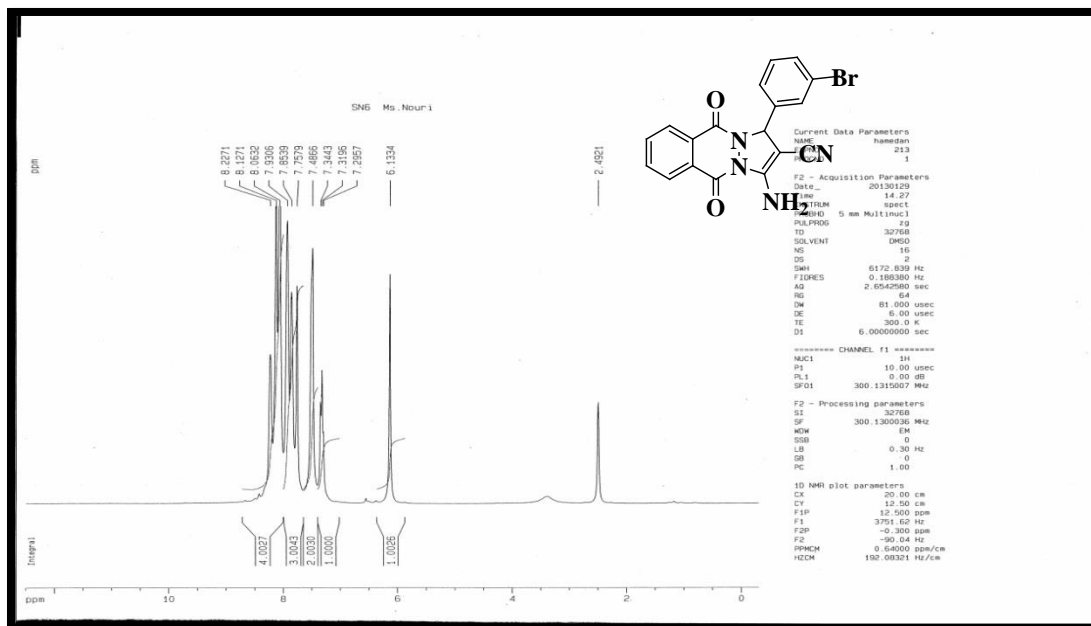


^{13}C NMR

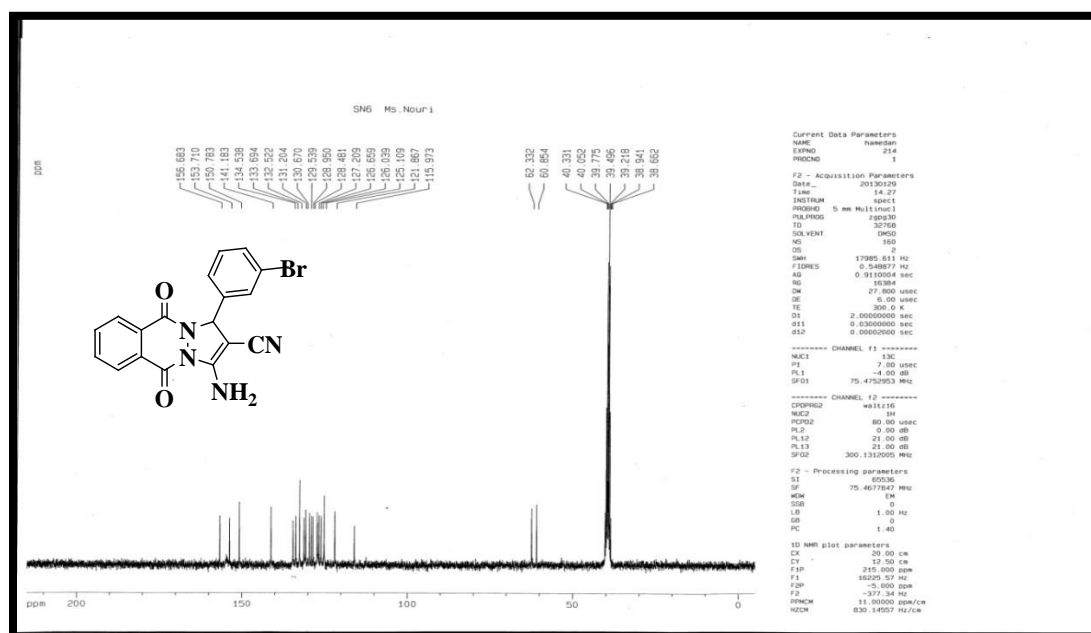


3-Amino-5,10-dioxo-1-(3-bromophenyl)-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile **3**: ^1H NMR (300 MHz, DMSO- d_6): δ_{H} (ppm) 6.13 (s, 1H), 7.29-8.22 (m, 10H), ^{13}C NMR (75 MHz, DMSO- d_6): δ_{C} (ppm) 60.8, 62.3, 115.9, 121.8, 125.1, 126.0, 126.6, 127.2, 128.4, 128.9, 129.5, 130.6, 131.2, 132.5, 133.6, 134.5, 141.1, 150.7, 153.7, 156.6

^1H NMR

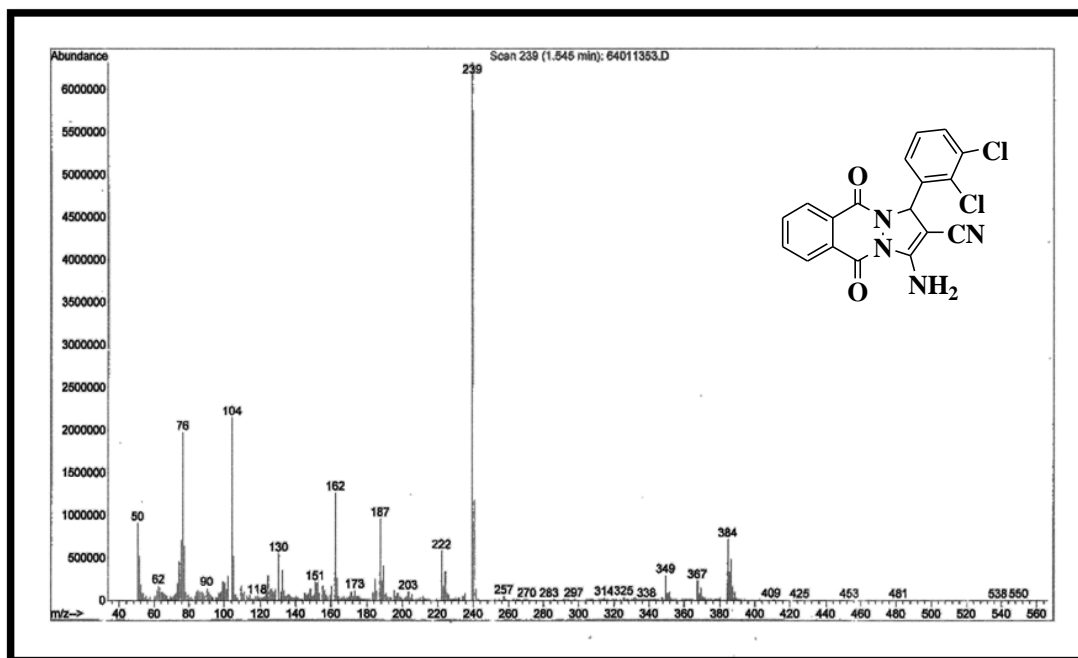
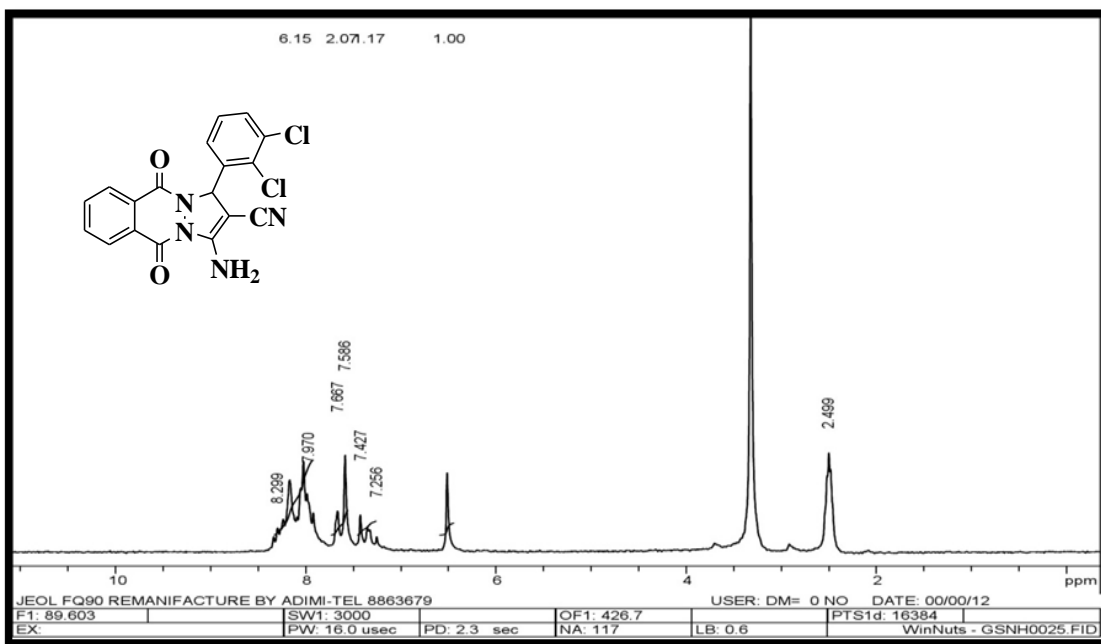


^{13}C NMR



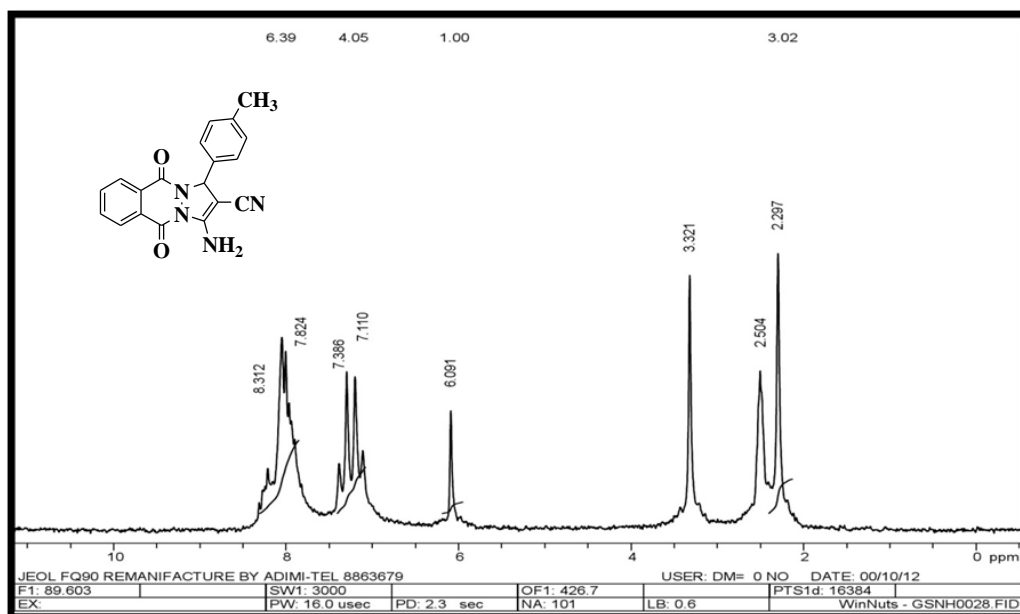
3-Amino-5,10-dioxo-1-(2,3-dichlorophenyl)-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile **9**: ^1H NMR (90 MHz, DMSO- d_6): δ_{H} (ppm) 6.51 (s, 1H), 7.25-8.29 (m, 9H), MS: m/z : 384, 367, 349, 239, 222, 187, 162, 130, 104, 76, 50

^1H NMR

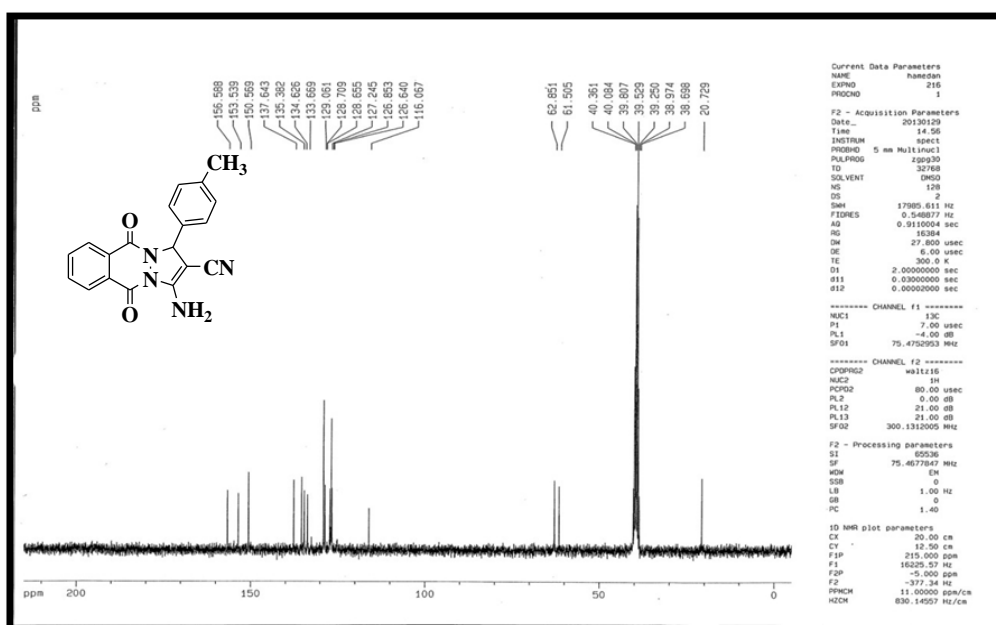


3-Amino-5,10-dioxo-1-(4-methylphenyl)-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile **2**: ^1H NMR (90 MHz, DMSO- d_6): δ_{H} (ppm) 2.29 (s, 3H), 6.09 (s, 1H), 7.11-7.38 (m, 4H), 7.82-8.31 (m, 6H), ^{13}C NMR (75 MHz, DMSO- d_6): δ_{C} (ppm) 20.7, 61.5, 62.8, 116.0, 126.6, 126.8, 127.2, 128.6, 128.7, 129.0, 133.6, 134.6, 135.3, 137.6, 150.5, 153.5, 156.5

^1H NMR

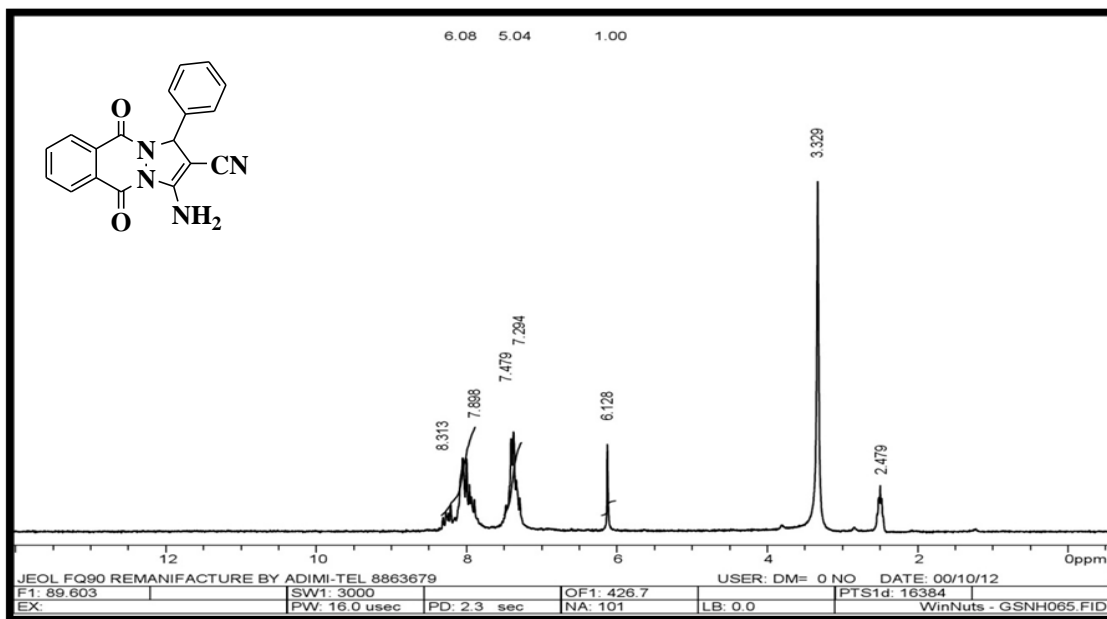


^{13}C NMR



3-Amino-5,10-dioxo-1-phenyl-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile **1**: ^1H NMR (90 MHz, DMSO- d_6): δ_{H} (ppm) 6.12 (s, 1H), 7.29-7.47 (m, 5H), 7.8-8.3 (m, 6H) ^{13}C NMR (75 MHz, DMSO- d_6): δ_{C} (ppm) 61.4, 62.9, 116.0, 126.6, 126.7, 127.2, 128.2, 128.5, 128.6, 128.7, 133.7, 134.6, 138.4, 150.6, 153.6, 156.6

^1H NMR



^{13}C NMR

