

Supporting Information

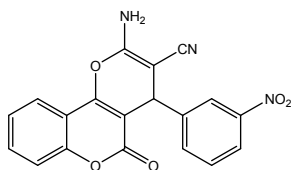
***N*,2-dibromo-6-chloro-3,4-dihydro-2*H*-benzo[*e*][1,2,4] thiadiazine-7-sulfonamide 1,1-dioxide: An efficient and homogeneous catalyst for one-pot synthesis of 4*H*-pyran , pyranopyrazole and pyrazolo[1,2-*b*] phthalazine derivatives under aqueous media**

Ardeshir Khazaei,* Mohammad Ali Zolfigol,* Fatemeh Karimitabar, Iraj Nikokar and Ahmad Reza Moosavi-Zare

Table of Contents

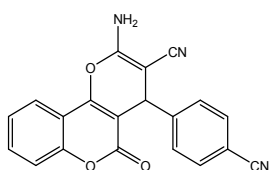
Data of compounds.....	2
NMR, IR and Mass spectra of compounds.....	9

2-Amino-4-(4-nitrophenyl)-5-oxo-4H,5H-pyrano-[3,2-c]chromene-3-carbonitrile (4a).



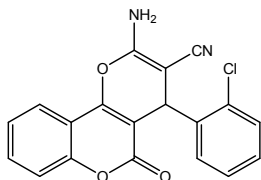
Pale yellow solid, mp = 263–265 °C [lit: (262-264 °C)]. ¹H NMR (400 MHz, DMSO-d₆): δ_{ppm}: 4.747 (1H, s, CH), 7.469-7.490 (1H, d, *J* = 8.4 Hz, HAr), 7.504-7.542 (1H, t, *J* = 7.6 Hz, HAr), 7.590 (2H, br s, NH₂), 7.626-7.665 (1H, t, *J* = 8.0 Hz, HAr), 7.721-7.764 (1H, t, *J* = 8.4 Hz, HAr), 7.820-7.839 (1H, d, *J* = 7.6 Hz, HAr), 7.90-7.940 (1H, d, *J* = 8 Hz, HAr), 8.131-8.153 (2H, d, *J* = 8.8 Hz, HAr) ppm.

2-Amino-4-(4-cyanophenyl)-5-oxo-4H,5H-pyrano-[3,2-c]chromene-3-carbonitrile (4c).



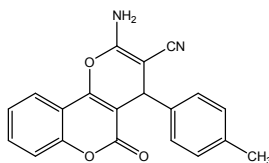
White solid; 286-288 °C (lit:289–290 °C). ¹H NMR (400 MHz, DMSO-d₆): δ_{ppm}: 4.619 (s, 1H, CH), 7.481-7.581 (m, 4H, ArH and NH₂), 7.721-7.749 (d, *J* = 8.4 Hz, 2H, ArH), 7.727-7.770 (t, *J* = 8.8 Hz, 1H, ArH), 7.799-7.856 (m, 2H, ArH), 7.909-7.938 (d, *J* = 8.0 Hz, 1H, ArH) ppm.

2-amino-4-(2-chlorophenyl)-5-oxo-4,5-dihydropyrano[3,2-c]chromene-3-carbonitrile (4e).



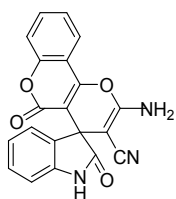
White solid; mp 257–259 °C (lit: 256-258 °C). IR (KBr, cm⁻¹) ν_{max} = 3397, 3282, 3177, 2199, 1708, 1674, 1600, 1380, 1258, 1172, 1061, 754, 521.

2-amino-4-(4-methylphenyl)-5-oxo-4,5-dihydropyrano[3,2-c]chromene-3-carbonitril (4g).



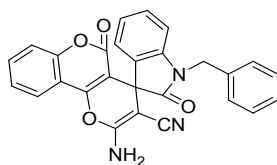
White solid; mp 253-254 °C (lit: 251-252 °C). IR (KBr, cm⁻¹) ν_{max} = 3386, 3292, 3192, 2193, 1714, 1675, 1603, 1375, 1211, 1113, 1056, 755, 508.

Spiro[2-amino-4H-pyran-oxindole] (6a).



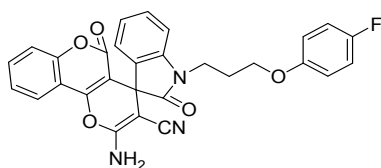
White powder; mp 292-294 °C (lit: 303 °C). IR (KBr) (ν_{\max} , cm^{-1}): 3361, 3297, 3197, 2206, 1734, 11712, 1675, 1360. ^1H NMR (400 MHz, DMSO- d_6) δ_{ppm} : 6.869-6.889 (d, 1H, $J=8$ Hz, ArH), 6.938-6.976 (t, 1H, $J=7.6$ Hz ArH), 7.225-7.241 (d, $J=6.4$ Hz, 2H, ArH), 7.502-7.582 (m, 2H, ArH), 7.707 (s, 2H, NH_2 , D_2O exchangeable), 7.768-7.806 (t, $J=7.2$ Hz, 1H, ArH), 7.954-7.973 (d, $J=7.6$ Hz, 1H, ArH), 10.717 (s, 1H, NH). ^{13}C NMR (400MHz, DMSO- d_6): δ_{ppm} 48.074, 57.494, 101.89, 109.973, 112.929, 117.138, 117.441, 122.524, 123.137, 124.600, 125.482, 129.390, 133.520, 134.140, 142.657, 152.51, 155.542, 158.741, 158.906, 177.615

Spiro[2-amino-4H-pyran-oxindole] (6b).



White powder; mp 278-280 °C (lit: 278-280 °C). IR (KBr) (ν_{\max} , cm^{-1}): 3407, 3342, 3191, 2199, 1708, 1670, 1608, 1354. ^1H NMR (400 MHz, DMSO- d_6) δ_{ppm} : 4.930-5.035 (ABq, 2H, CH_2), 6.803-6.828 (d, $J=8$ Hz, 1H, ArH), 6.990-7.026 (t, $J=7.2$ Hz, 1H, ArH), 7.197-7.348 (m, 5H, ArH), 7.475-7.506 (t, $J=7.2$ Hz, 3H, ArH), 7.549-7.585 (t, $J=7.2$ Hz, 1H, ArH), 7.770-7.790 (br s, 2H, NH_2), 7.965-7.988 (dd, 1H, ArH). ^{13}C NMR (400MHz, DMSO- d_6): δ_{ppm} 43.924, 57.206, 91.466, 101.638, 109.604, 112.939, 116.850, 117.191, 117.507, 123.227, 123.373, 123.660, 124.403, 124.556, 125.542, 127.632, 127.729, 128.855, 129.455, 136.352, 143.233, 152.560, 155.783, 158.841, 159.08, 159.097, 176.359.

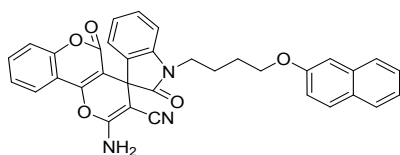
Spiro[2-amino-4H-pyran-oxindole] (6c).



White powder; mp 270-272 °C. IR (KBr) (ν_{\max} , cm^{-1}): 3451, 3452, 3166, 2946, 2880, 2196, 1695, 1673, 1611, 1505, 1466, 1360, 762, 746. ^1H NMR (400 MHz, DMSO- d_6) δ_{ppm} : 2.066-2.128 (m, 2H, CH_2), 3.841-3.976 (m, 2H, $\text{CH}_2\text{-N}$), 4.032-4.048 (d, 2H, $J=6.4$ Hz, $\text{CH}_2\text{-O}$), 6.941-6.971 (m, 2H, ArH), 6.989-7.026 (t, $J=7.6$ Hz, 1H, ArH), 7.101-7.145 (m, 3H, ArH),

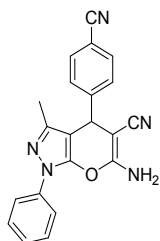
7.268-7.319 (m, 2H, ArH), 7.504-7.524(d, $J=8$ Hz, 1H, ArH), 7.553-7.591 (t, $J=7.6$ Hz, 1H, ArH), 7.771-7.816(m, 3H, NH₂ and ArH, D₂O exchangeable), 7.962-7.980 (d, $J=7.2$ Hz, 1H, ArH). ¹³C NMR (400MHz, DMSO-d₆): δ_{ppm} 27.27, 37.123, 47.616, 57.132, 65.708, 101.669, 108.970, 112.919, 116.127, 116.207, 116.287, 116.354, 117.184, 117.389, 123.186, 124.588, 125.539, 129.577, 132.739, 134.238, 143.346, 152.524, 155.246, 155.694, 155.753, 158.095, 158.825, 158.985, 176.109.

Spiro[2-amino-4H-pyran-oxindole] (6d).



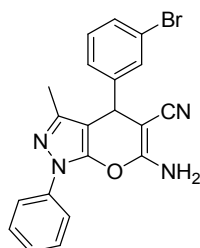
Pale yellow powder; mp 268-270 °C. ¹H NMR (400 MHz, DMSO-d₆) δ_{ppm} : 1.839-1.873 (br s, 4H, CH₂), 3.794-3.824 (t, $J=6$ Hz, 2H, CH₂N), 4.127-4.155 (t, $J=5.6$ Hz, 2H, CH₂O), 7.002-7.039 (t, $J=7.6$ Hz, 1H, ArH), 7.091-7.120 (dd, $J=2.4$ Hz, 1H, ArH), 7.288-7.353 (m, 3H, ArH), 7.430- 7.448 (d, $J=7.2$ Hz, 2H, ArH), 7.467-7.496 (1H, ArH), 7.538-7.576 (t, $J=7.6$ Hz, 1H, ArH), 7.637-7.657 (d, $J=8$ Hz, 2H, ArH), 7.699 (br s, 2H, NH₂, D₂O exchangeable), 7.759-7.822 (m, 4H, ArH), 7.902-7.922(d, $J=8$ Hz, 1H, ArH), 7.958-7.977 (d, $J=7.6$ Hz, 1H, ArH). ¹³C NMR (400MHz, DMSO-d₆): 23.948, 24.188, 26.387, 57.140, 67.391, 67.675, 101.726, 107.150, 117.165, 118.614, 119.225, 123.099, 123.184, 123.812, 123.909, 123.996, 126.120, 126.759, 126.830, 127.107, 127.953, 128.868, 129.571, 129.676, 132.855, 134.793, 146.983, 152.533, 155.664, 156.830, 156.994, 158,744, 176.089

6-Amino-4-(4-cyanophenyl)-3-methyl-1-phenyl-1,4-dihydropyrano[2,3-c]pyrazole-5-carbonitrile (8a).



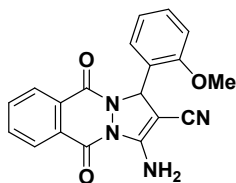
White solid, mp: 198–200 °C (lit: 197–199 °C). ¹H NMR (400 MHz, DMSO-d₆): δ_{ppm} : 1.796 (s, 3H, CH₃), 4.860 (s, 1H, C–H), 7.327-7.378 (m, 2H, ArH), 7.494–7.533 (m, 5H, NH₂ and ArH), 7.790-7.806 (d, $J = 7.6$ Hz, 2H, ArH), 7.844-7.864 (d, $J = 8$ Hz, 2H, ArH) ppm.

6-Amino-4-(3-bromophenyl)-3-methyl-1-phenyl-1,4-dihydropyrano[2,3-c]pyrazole-5-carbonitrile (8i).



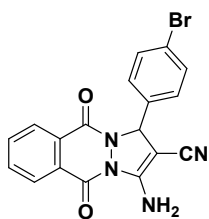
White solid, mp: 166-168 °C (lit: 169-170 °C). ¹HNMR (400 MHz, DMSO-d₆): δ_{ppm}: 2.338 (s, 3H, CH₃), 5.017 (s, 1H, C-H), 7.254-7.291 (m, 3H, ArH), 7.405-7.482 (m, 5H, NH₂ and ArH), 7.706-7.725 (d, *J* = 7.6 Hz, 2H, ArH) ppm.

3-Amino-1-(2-methoxyphenyl)-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile (10f).



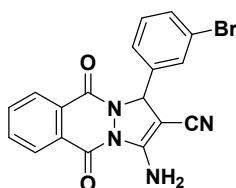
Pale yellow solid; mp 250-252 °C (lit: 248-250 °C). IR (KBr, cm⁻¹)_{ν_{max}} = 3384, 3255, 3191, 2926, 2201, 1681, 1659, 1565, 1382, 1279, 1246, 1112, 694.

3-Amino-1-(4-bromophenyl)-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile (10 g).



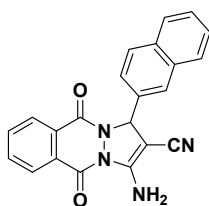
Pale yellow solid; mp 264-266 °C (lit: 263-265°C). IR (KBr, cm⁻¹)_{ν_{max}} = 3373, 3261, 3187, 2198, 1657, 1562, 1378, 1275, 1251, 828, 695.

3-Amino-1-(3-bromophenyl)-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile (10 j).



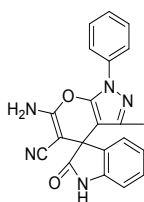
Pale yellow solid; mp 274-276 °C (lit: 271-273°C). IR (KBr, cm⁻¹)_{ν_{max}} = 3364, 3255, 3191, 2192, 1682, 1652, 1594, 1438, 1386, 1278, 1163, 691, 596; ¹H NMR (90 MHz, DMSO-d₆): δ_{ppm}: = 6.13(s,1H), 7.33-8.29(m, 10H, ArH,NH2)

3-amino-1-(naphthalen-2-yl)-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-b] phthalazine - 2-carbonitrile (10 k).



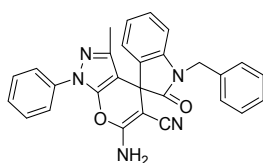
Pale yellow solid; mp 275–277 °C (lit: 276–278°C). IR (KBr, cm^{-1}) ν_{max} = 3368, 3258, 3191, 2191, 1681, 1655, 1567, 1434, 1387, 1267, 1163, 693.

Spiro[pyrano[2,3-c]pyrazole] (11a).



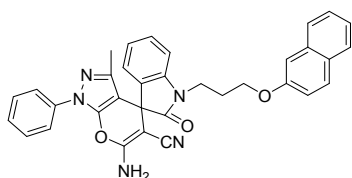
White powder; mp 237-238 °C (lit: 236-237 °C). IR (KBr) (ν_{max} , cm^{-1}): 3410, 3287, 3124, 2202, 1692, 1655, 1526, 1132. ^1H NMR (400 MHz, DMSO- d_6) δ_{ppm} : 1.560(s, 3H, CH_3), 6.955-6.974 (d, $J=7.6$ Hz, 1H, ArH), 7.03-7.067 (t, $J=7.6$ Hz, 1H, ArH), 7.190-7.208 (d, $J=7.2$ Hz, 1H, ArH), 7.286-7.324 (t, $J=7.6$ Hz, 2H, ArH), 7.353-7.390 (t, $J=7.2$ Hz, 1H, ArH), 7.516-7.556 (t, $J=8.4$ Hz, 2H, ArH), 7.612 (s, 2H, NH_2 , D_2O exchangeable), 7.796-7.815 (d, $J = 7.6$ Hz, 2H, ArH) 10.774 (s, 1H, NH). ^{13}C NMR (400MHz, DMSO- d_6): δ_{ppm} 12.17, 48.24, 56.62, 96.82, 110.32, 118.40, 118.43, 120.60, 123.12, 125.38, 127.05, 129.76, 129.94, 132.60, 137.71, 142.07, 144.42, 145.40, 161.46, 161.50, 177.98.

Spiro[pyrano[2,3-c]pyrazole] (11b).



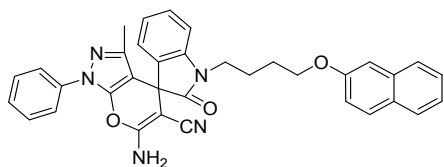
Pale yellow powder; mp 228-230 °C (lit: 232–234°C). IR (KBr) (ν_{max} , cm^{-1}): 3390, 3314, 3191, 2904, 2200, 2208, 1701, 1662, 1396, 746. ^1H NMR (400 MHz, DMSO- d_6) δ_{ppm} : 1.368 (s, 3H, CH_3), 4.943-5.096 (AB-q, 2H, CH_2), 7.094-7.130 (t, $J=7.6$ Hz, 2H, ArH), 7.276-7.399 (m, 6H, ArH), 7.444-7.462 (d, $J=7.2$ Hz, 2H, ArH), 7.523-7.563 (t, $J=7.6$ Hz, 2H, ArH), 7.697 (s, 2H, NH_2 , D_2O exchangeable), 7.801-7.821 (d, $J=8$ Hz, 2H, ArH). ^{13}C NMR (400MHz, DMSO- d_6): δ_{ppm} 12.19, 43.79, 47.98, 56.33, 96.58, 110.00, 118.42, 120.67, 123.93, 125.33, 127.13, 128.08, 129.06, 129.83, 129.95, 131.82, 136.51, 137.67, 142.60, 144.33, 145.46, 161.59, 161.63, 161.67, 176.61.

Spiro[pyrano[2,3-c]pyrazole] (11c).



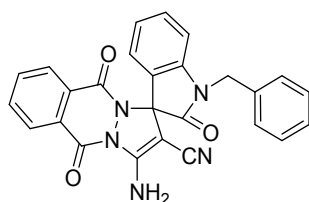
Yellow powder; mp 210-212 °C. IR (KBr) (ν_{\max} , cm^{-1}): 3401, 3380, 3021, 2890, 2870, 2238, 1702, 1691, 1610, 1515, 1450, 1341, 1203, 755. ^1H NMR (400 MHz, DMSO- d_6) δ_{ppm} : 1.516(s, 3H, CH_3), 2.152-2.303 (m, 2H, CH_2), 3.933-4.06 (m, 2H, CH_2N), 4.189-4.213(t, $J=7.6$ Hz, 2H, CH_2O), 7.079-7.135 (t, $J=7.6$ Hz, 1H, ArH), 7.168-7.304 (m, 4H, ArH), 7.344-7.393 (m, 3H, ArH), 7.444-7.480 (t, $J=7.2$ Hz, 1H, ArH), 7.518-7.558 (t, $J=7.6$ Hz, 1H, ArH), 7.697 (s, 2H, NH_2 , D_2O exchangeable), 7.797-7.859(m, 5H, ArH). ^{13}C NMR (400MHz, DMSO- d_6): δ_{ppm} 12.30, 26.94, 37.37, 37.63, 47.87, 56.47, 96.49, 107.23, 101.45, 118.65, 119.23, 120.65, 123.80, 124.06, 126.84, 127.11, 127.16, 127.99, 128.99, 129.76, 129.94, 132.02, 134.71, 137.68, 142.68, 144.34, 145.48, 156.78, 161.46, 161.46, 161.50, 176.33.

Spiro[pyrano[2,3-c]pyrazole] (11d).



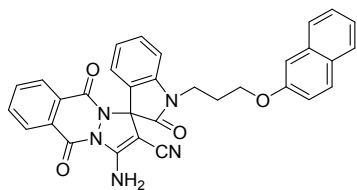
Yellow powder; mp 198-200 °C. IR (KBr) (ν_{\max} , cm^{-1}): 3370, 3329, 3181, 2944, 2875, 2207, 1699, 1662, 1601, 1552, 1467, 1395, 1359, 1219, 751, 652. ^1H NMR (400 MHz, DMSO- d_6) δ_{ppm} : 1.504(s, 3H, CH_3), 1.872-1.196 (m, 4H, CH_2), 3.884-3.896 (t, $J=6$ Hz 2H, CH_2N), 4.148-4.175 (t, $J=6.4$ Hz 2H, CH_2O), 7.112-7.189 (m, 2H, ArH), 7.252-7.285 (t, $J=8$ Hz, 2H, ArH), 7.328-7.345 (m, 4H, ArH), 7.440-7.476(t, $J=7.2$ Hz, 1H, ArH), 7.521-7.61 (t, d, $J=7.2$ Hz, 2H, ArH), 7.663 (s, 2H, NH_2), 7.798-7.837 (t, $J=8.4$ Hz, 1H, ArH, 5H, ArH). ^{13}C NMR (400MHz, DMSO- d_6): δ_{ppm} 12.28, 18.99, 19.04, 24.40, 26.55, 47.87, 56.39, 96.56, 107.16, 109.55, 118.23, 119.20, 120.64, 123.72, 123.97, 125.31, 126.82, 127.13, 127.96, 128.91, 129.73, 129.94, 131.96, 134.79, 137.68, 142.86, 144.31, 145.49, 156.98, 161.49, 161.54, 176.34.

Spiro[indoline-3,1'-pyrazolo[1,2-b]phthalazine] (12b).



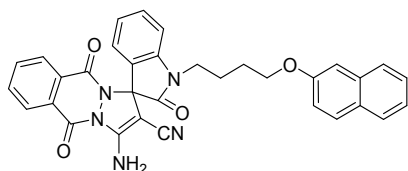
Yellow powder; mp 260-263 °C (lit: 265-266 °C). ^1H NMR (400 MHz, DMSO- d_6) δ_{H} : 4.957(s, 2H, CH_2), 7.062-7.082(d, $J=8$ Hz, 1H, ArH), 7.192-7.231(t, $J=8$ Hz, 1H, ArH), 7.306-7.348(m, 1H, ArH), 7.367-7.441 (m, 4H, ArH), 7.582-7.620 (t, $J=7.6$ Hz, 1H, ArH), 7.892-7.925 (m, 4H, ArH), 7.962-7.981 (d, $J=7.6$ Hz, 1H, ArH), 8.091(br s, 2H, NH_2).

Spiro[indoline-3,1'-pyrazolo[1,2-b]phthalazine] (12c).



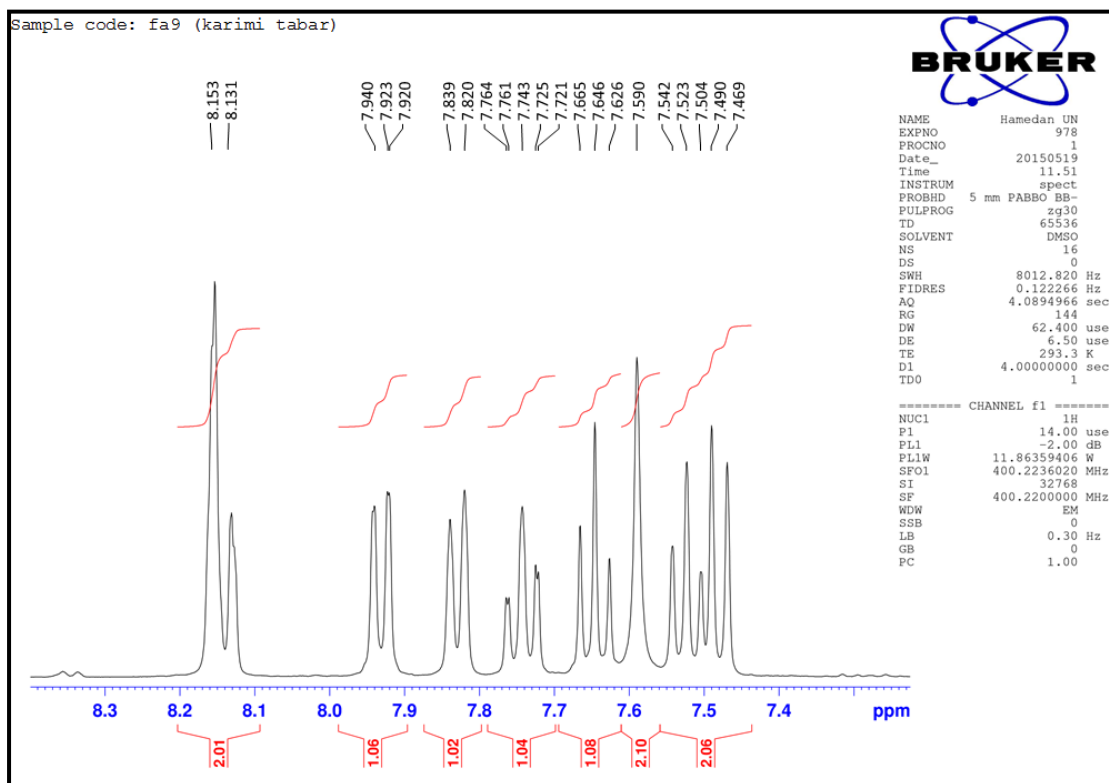
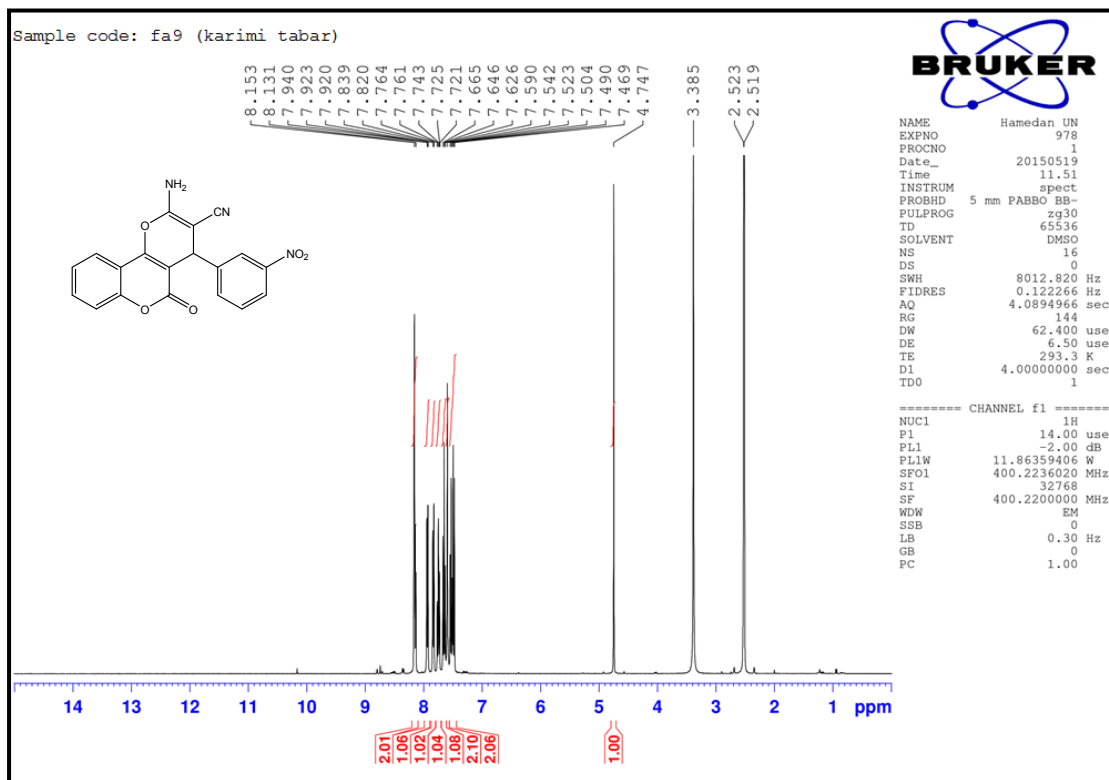
Yellow powder; mp 218-220 °C. IR (KBr) (ν_{\max} , cm⁻¹): 3434, 3434, 3029, 2926, 2870, 2228, 1727, 1661, 1628, 1613, 1597, 1470, 1371, 1259, 1180, 837, 762, 748. ¹H NMR (400 MHz, DMSO-d₆) δ_{ppm} : 2.136- 2.184 (m, 2H, CH₂), 3.917-3.951 (t, $J=6.8$ Hz, 2H, CH₂N), 4.164-4.193 (t, $J=5.6$ Hz, 2H, CH₂O), 7.094- 7.122 (dd, $J=2.4$ Hz, 1H, ArH), 7.170-7.208 (t, $J=7.6$ Hz, 1H, ArH), 7.241-7.261 (m, 2H, ArH), 7.332-7.372 (m, 1H, ArH), 7.439-7.480 (m, 1H, ArH), 7.439-7.480 (m, 1H, ArH), 7.588-7.629 (m, 1H, ArH), 7.762-7.787 (d, $J=8$ Hz 1H, ArH), 7.809-7.884 (m, 2H, ArH), 7.892-7.956 (m, 5H, ArH), 8.090 (br s, 2H, NH₂). ¹³C NMR (400MHz, DMSO-d₆): δ_{ppm} 26.93, 37.37, 37.63, 65.51, 81.50, 107.23, 111.08, 111.91, 113.43, 118.65, 119.06, 123.80, 124.06, 125.58, 126.10, 126.87, 127.11, 127.99, 128.96, 129.74, 133.10, 134.66, 138.11, 147.10, 150.30, 156.64, 163.00.

Spiro[indoline-3,1'-pyrazolo[1,2-*b*]phthalazine] (12d).

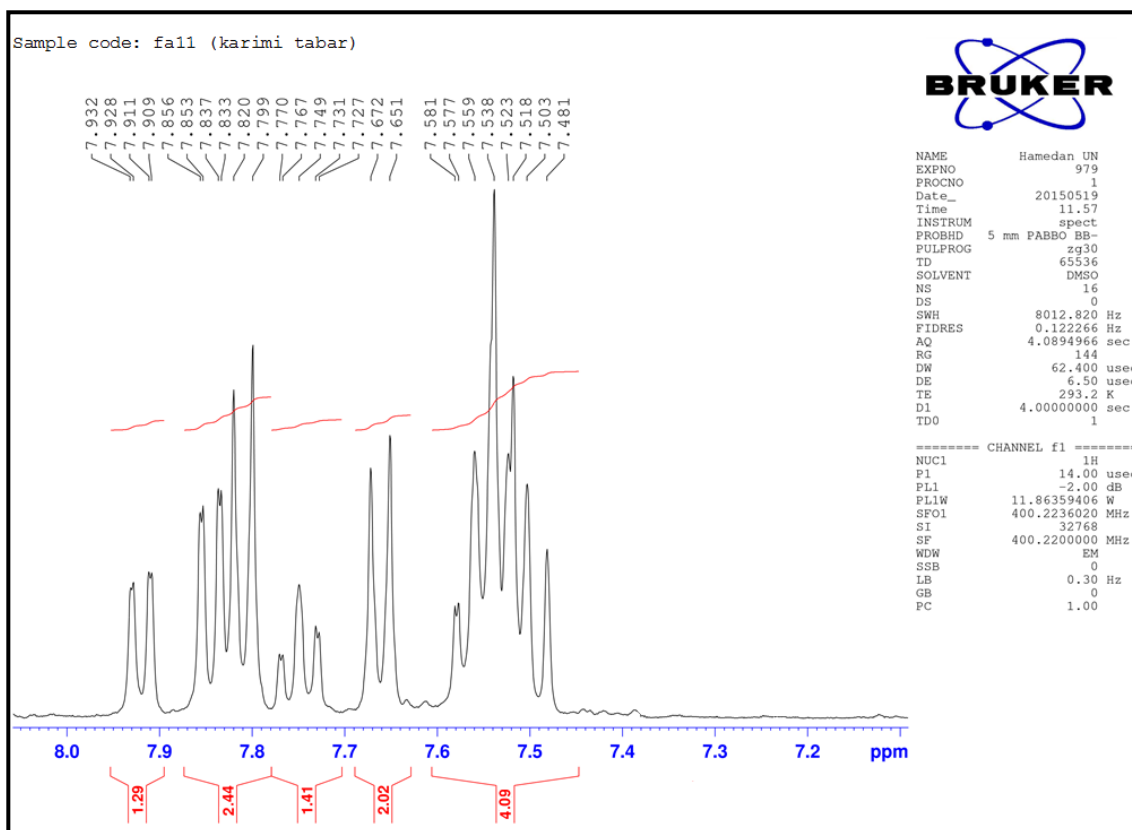
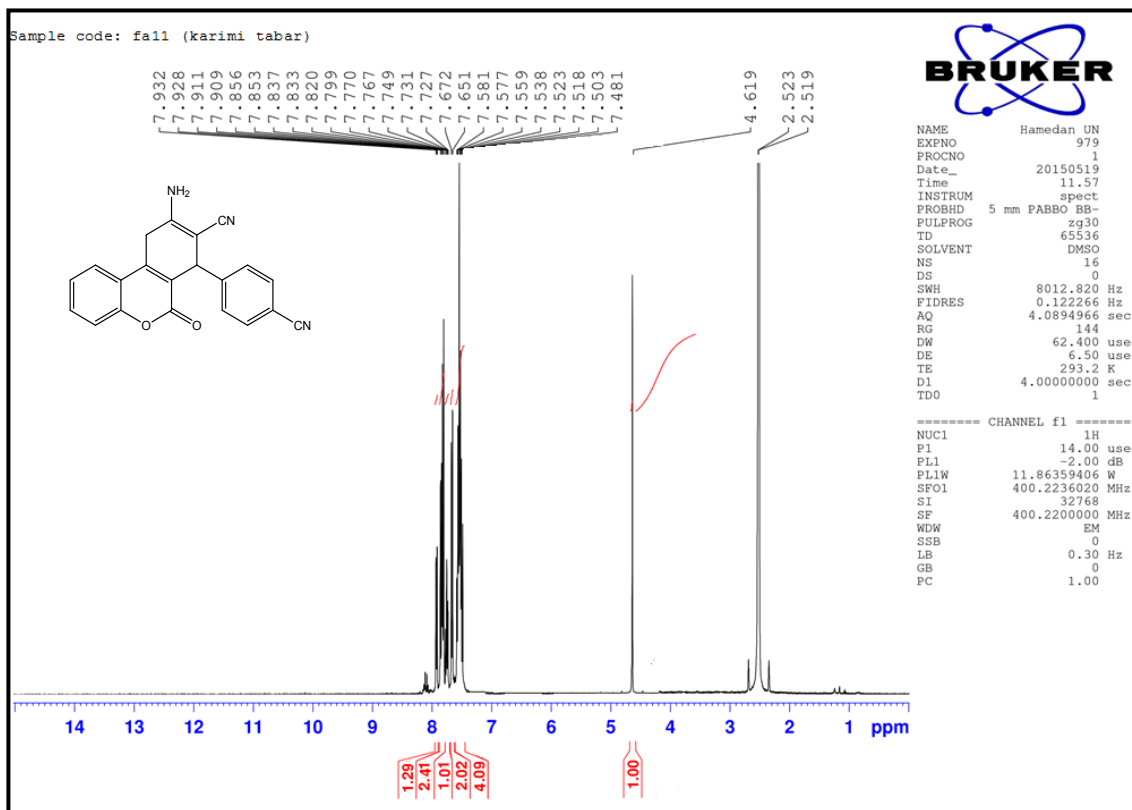


Yellow powder; mp 210-212 °C. IR (KBr) (ν_{\max} , cm⁻¹): 3430, 3401, 3180, 2931, 2870, 2221, 1720, 1668, 1610, 1603, 1590, 1470, 1370, 1240, 1110, 768, 750, 718. ¹H NMR (400 MHz, DMSO-d₆) δ_{ppm} : 1.846 (br s, 4H, 2CH₂), 3.784-3.816 (t, $J=7.6$ Hz, 2H, CH₂N), 4.115-4.147 (t, $J=6.8$ Hz, 2H, CH₂O), 7.098-7.126 (dd, $J=2.4$ Hz, 1H, ArH), 7.188-7.226 (t, $J=7.6$ Hz, 1H, ArH), 7.249-7.268 (d, $J=8$ Hz, 1H, ArH), 7.289-7.298 (d, $J=2$ Hz, 1H, ArH), 7.327-7.363 (t, $J=7.2$ Hz, 1H, ArH), 7.439-7.475 (t, $J=7.2$ Hz, 1H, ArH), 7.645-7.683 (t, $J=7.6$ Hz, 1H, ArH), 7.782-7.831 (m, 3H, ArH), 7.889-7.921 (m, 3H, ArH), 8.089 (br s, 2H, NH₂). ¹³C NMR (400MHz, DMSO-d₆): δ_{ppm} 23.97, 26.40, 37.35, 37.60, 67.39, 81.61, 107.15, 111.13, 111.94, 113.37, 118.59, 119.11, 123.82, 124.01, 125.58, 126.12, 126.84, 127.12, 127.97, 128.88, 129.73, 133.08, 134.73, 138.11, 146.96, 150.10, 156.80, 162.93.

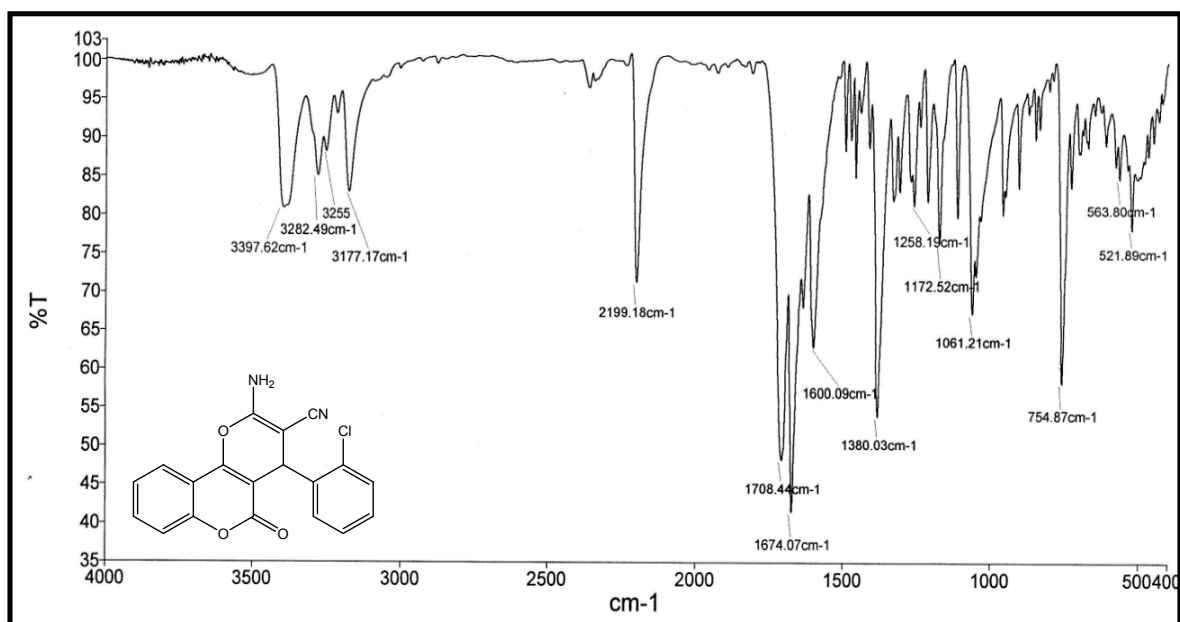
2-Amino-4-(4-nitrophenyl)-5-oxo-4H,5H-pyrano-[3,2-c]chromene-3-carbonitrile (4a).



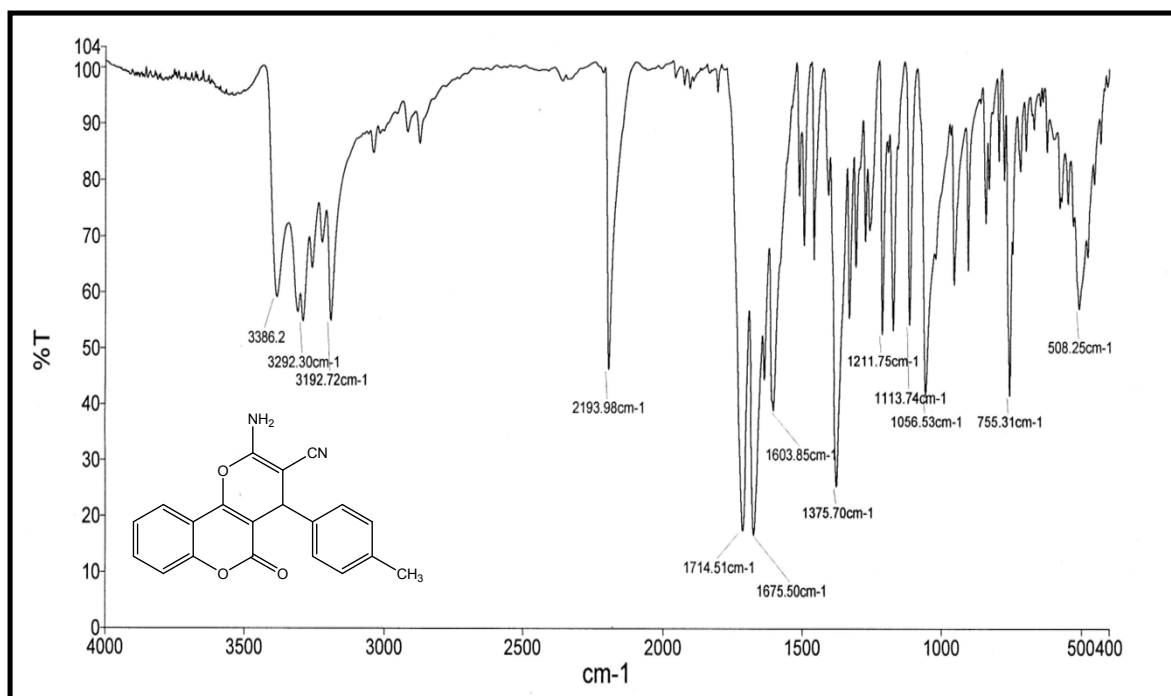
2-Amino-4-(4-cyanophenyl)-5-oxo-4H,5H-pyrano-[3,2-c]chromene-3-carbonitrile (4c).



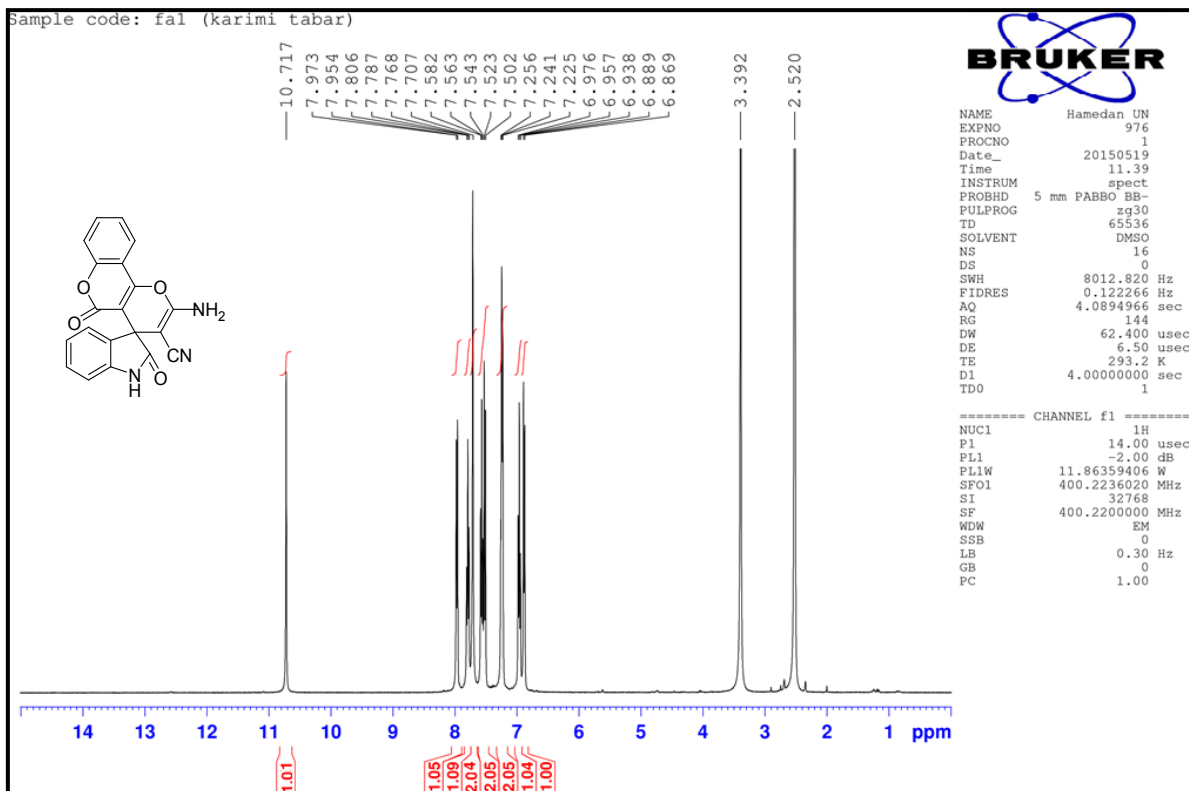
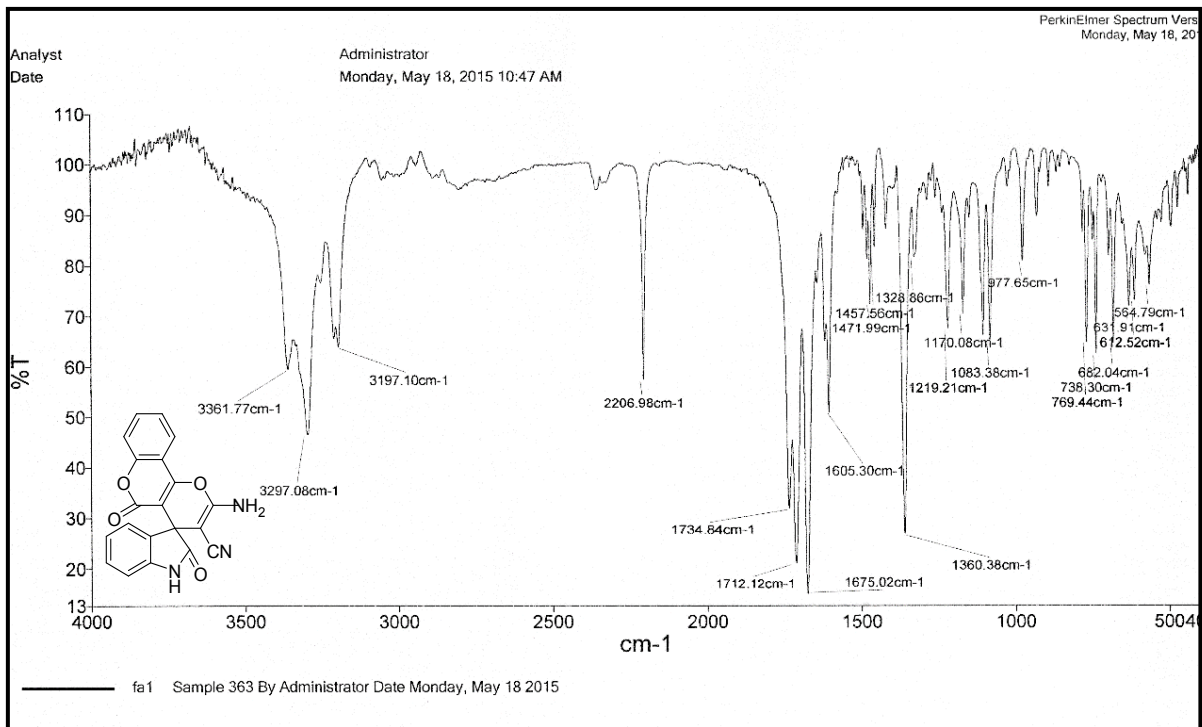
2-amino-4-(2-chlorophenyl)-5-oxo-4,5-dihydropyrano[3,2-c]chromene-3-carbonitrile (4e).



2-amino-4-(4-methylphenyl)-5-oxo-4,5-dihydropyrano[3,2-c]chromene-3-carbonitril (4g).

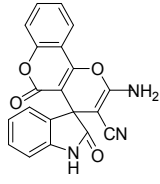


Spiro[2-amino-4H-pyran-oxindole] (6a).



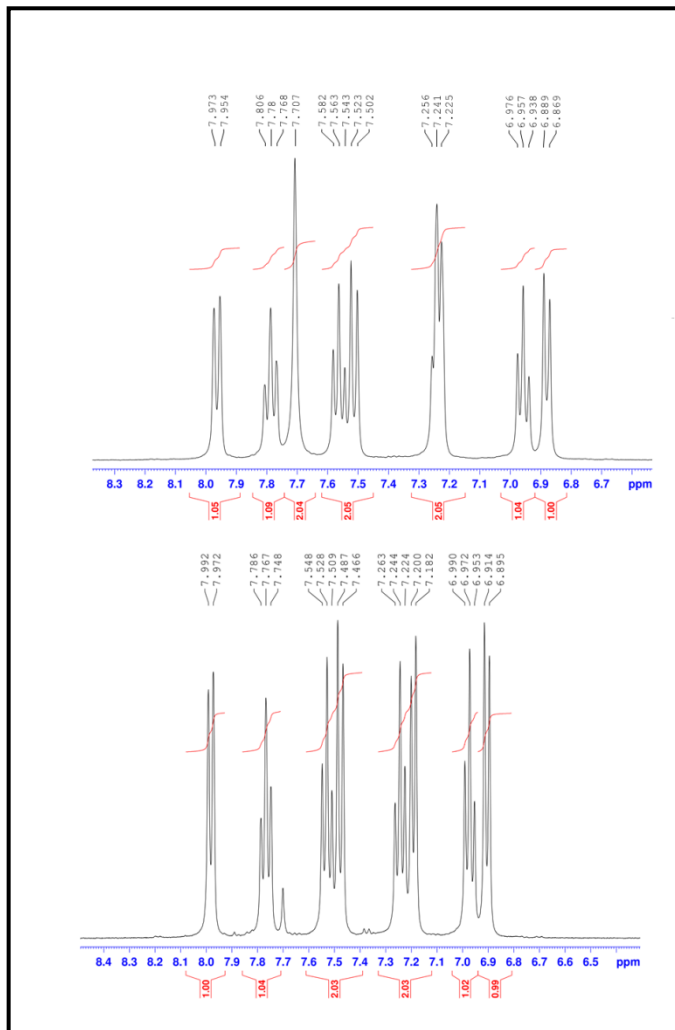
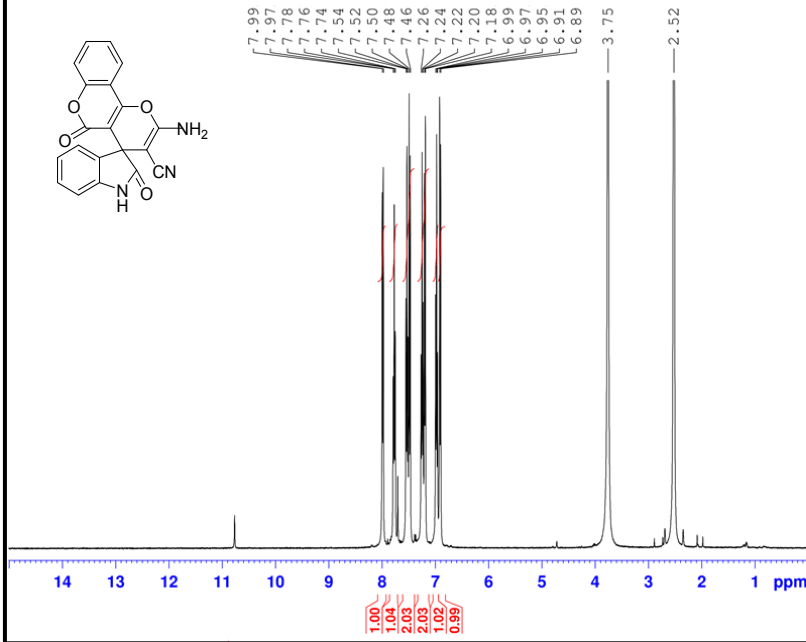
D₂O exchange

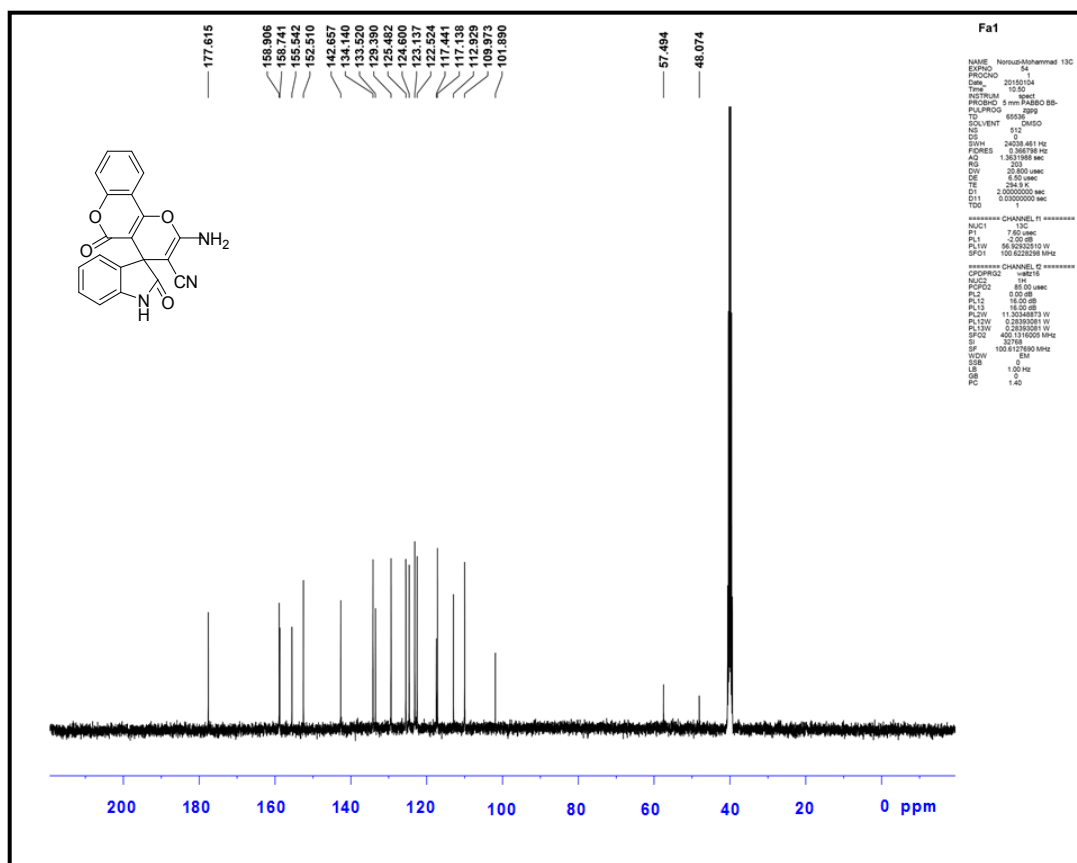
Sample code: fa1+D2O (karimi tabar)



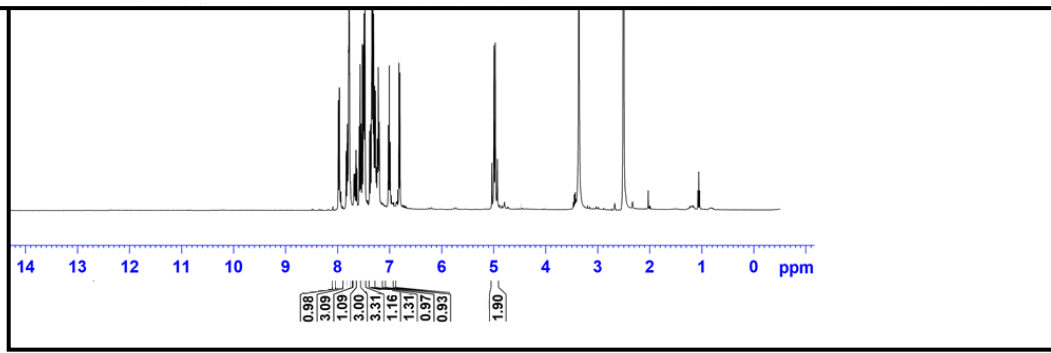
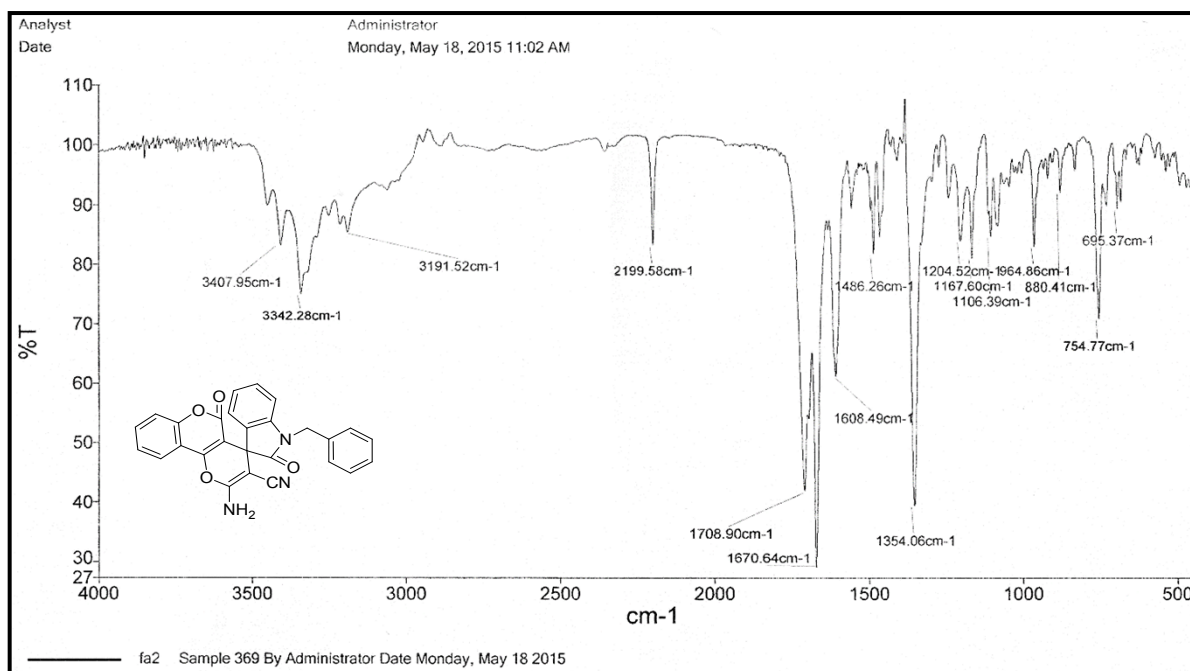
NAME Hamedan_UN
EXPNO 1005
PROCNO 1
Date_ 20150519
Time 15.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 293.7 K
D1 4.0000000 sec
TDO 1

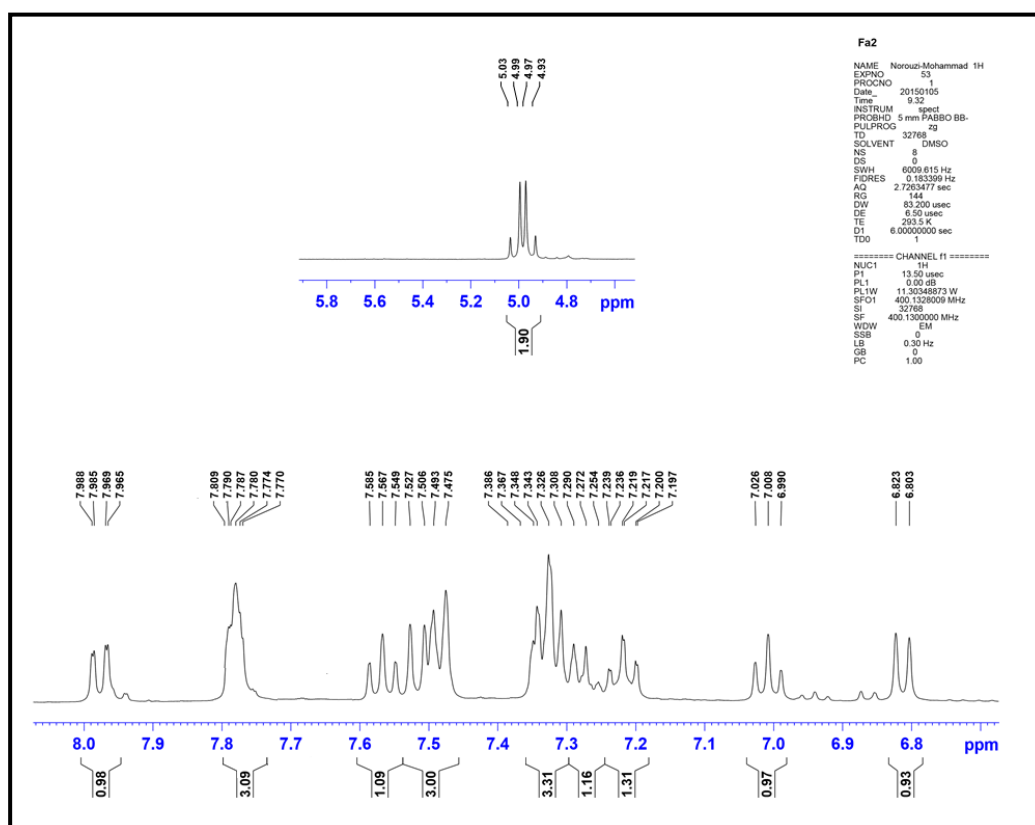
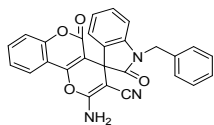
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



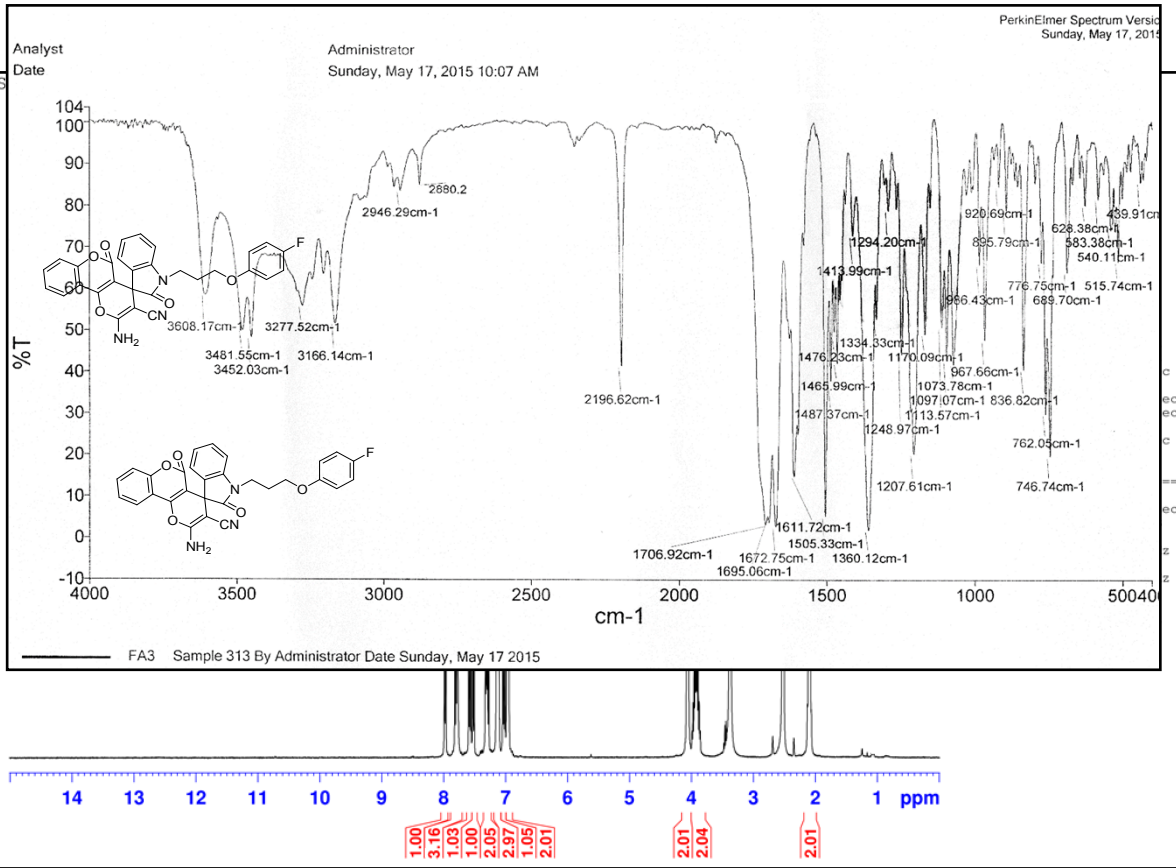


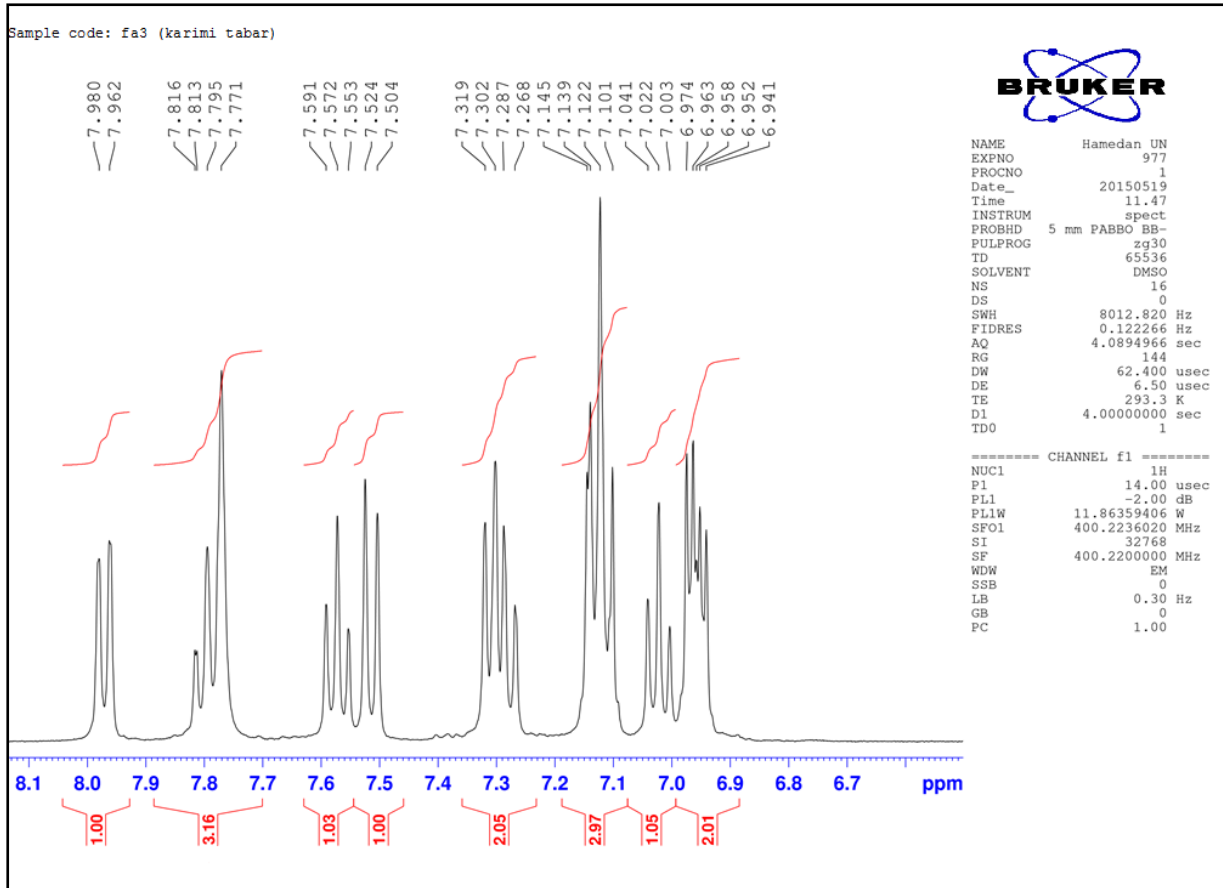
Spiro[2-amino-4H-pyran-oxindole] (6b).



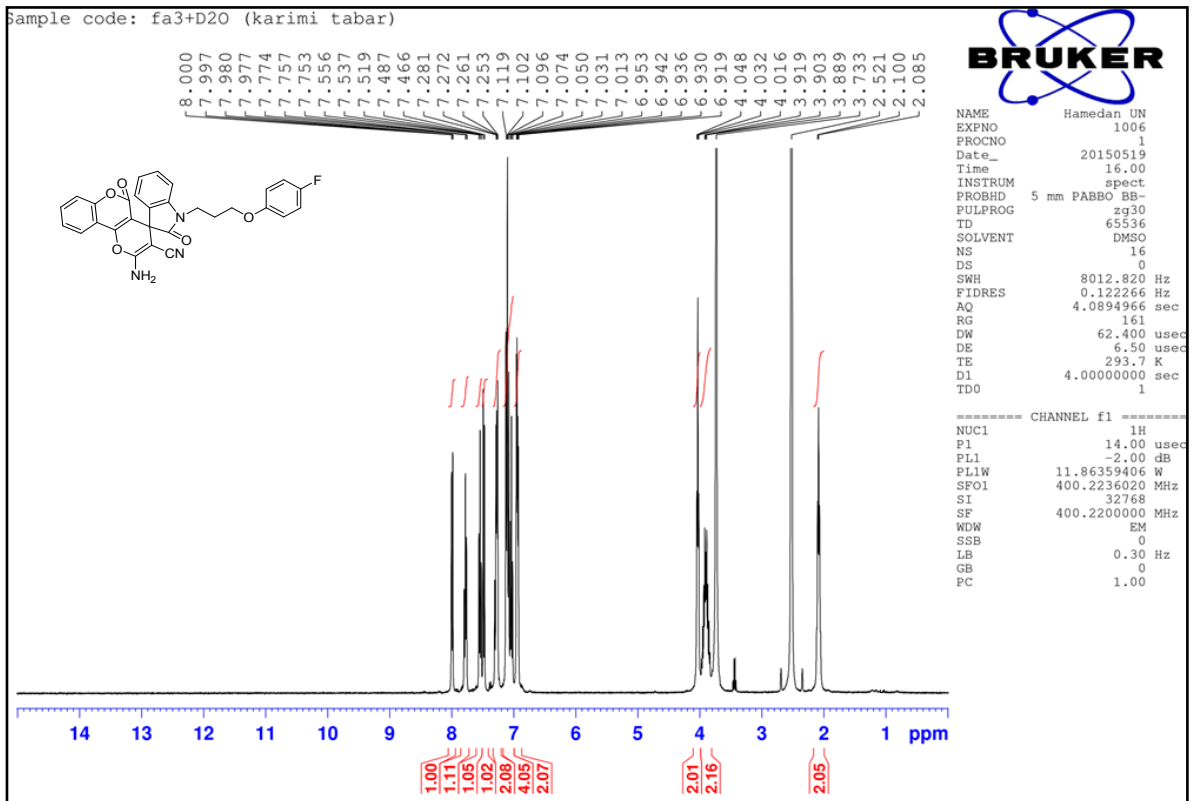


Spiro[2-amino-4H-pyran-oxindole] (6c).

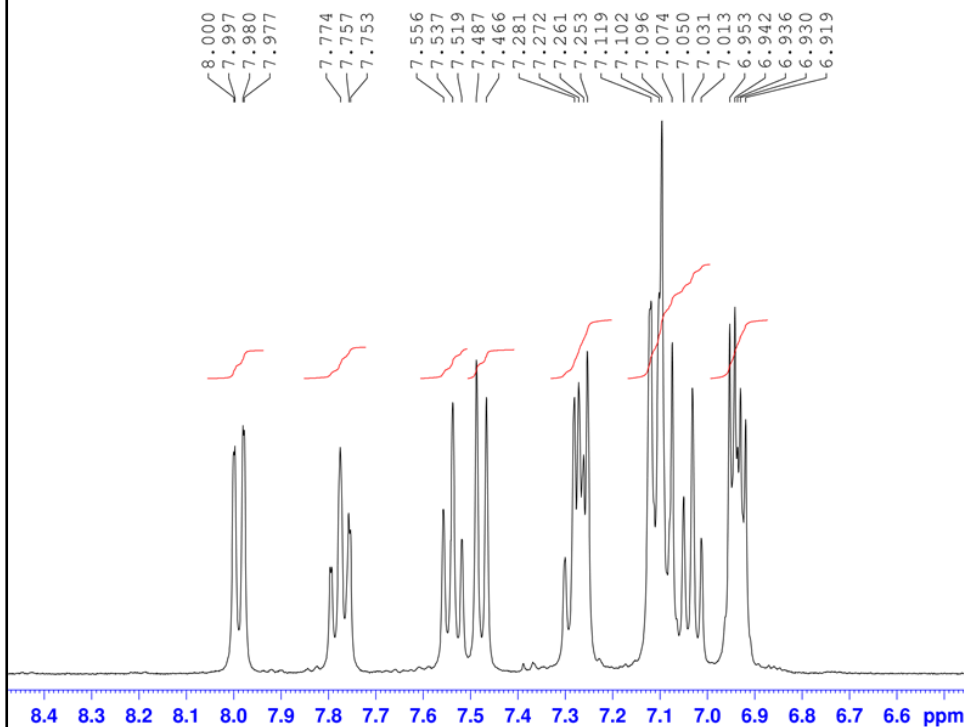




D₂O exchange

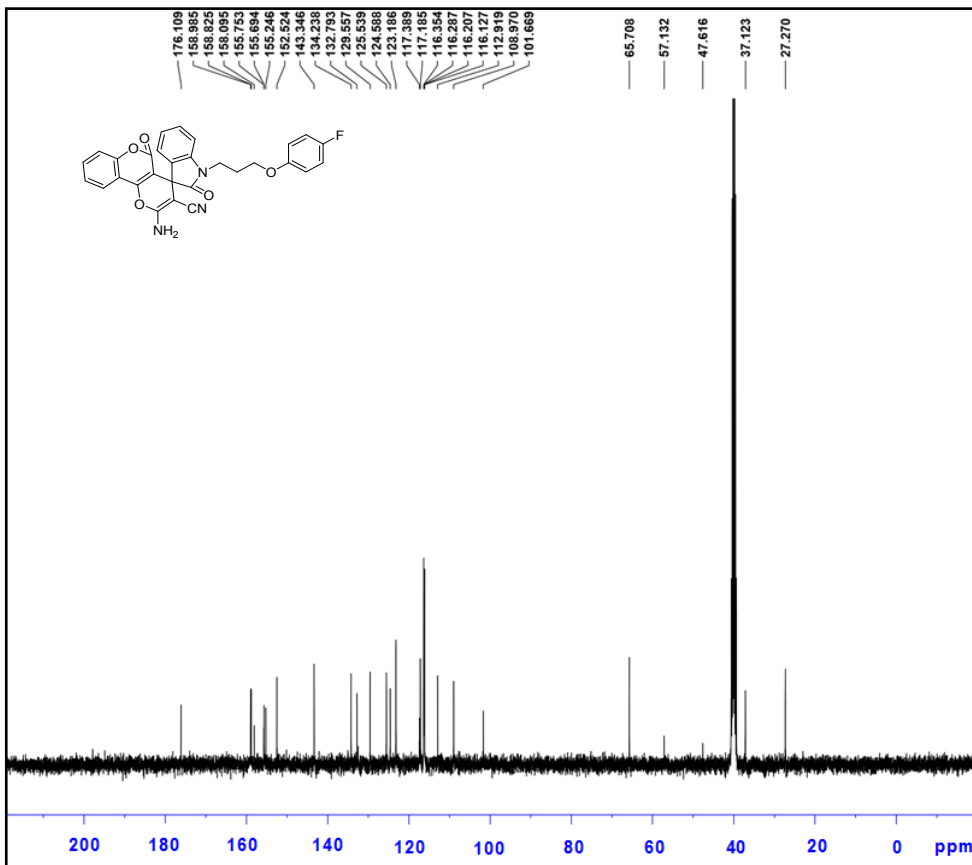


Sample code: fa3+D2O (karimi tabar)



NAME Hamedan UN
EXPNO 1006
PROCNO 1
Date_ 20150519
Time 16.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 293.7 K
D1 4.00000000 sec
TD0 1

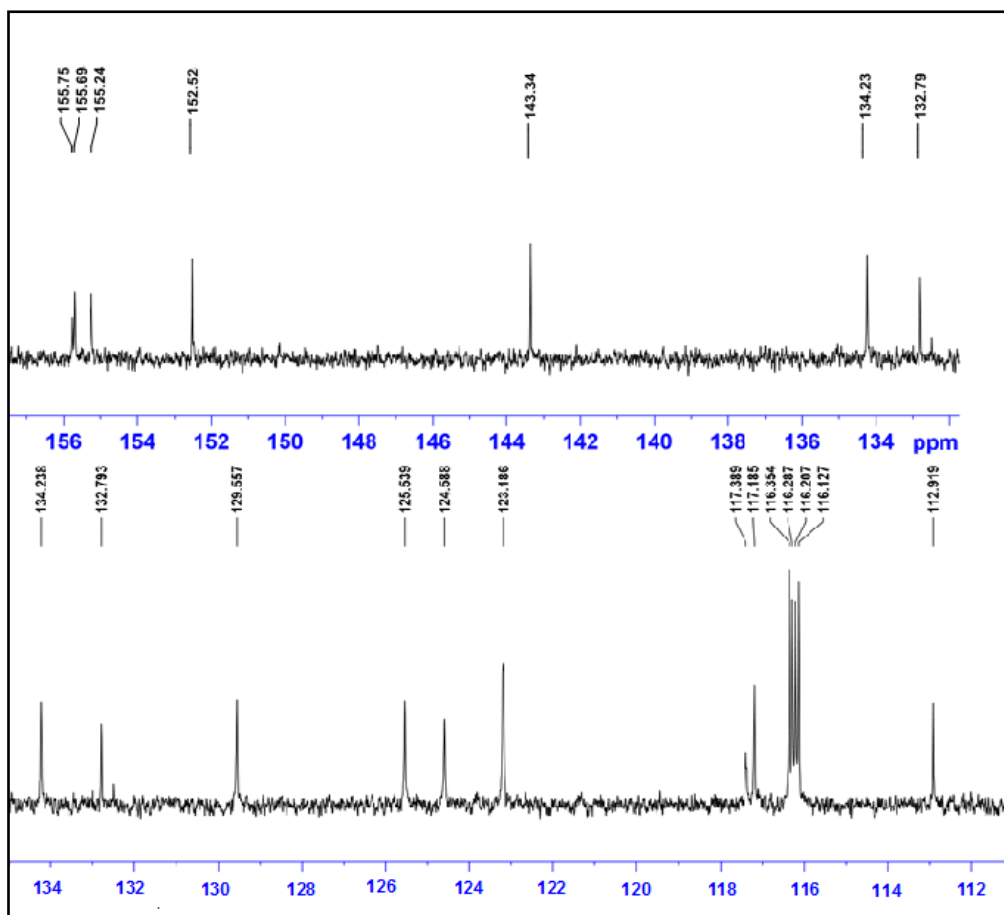
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



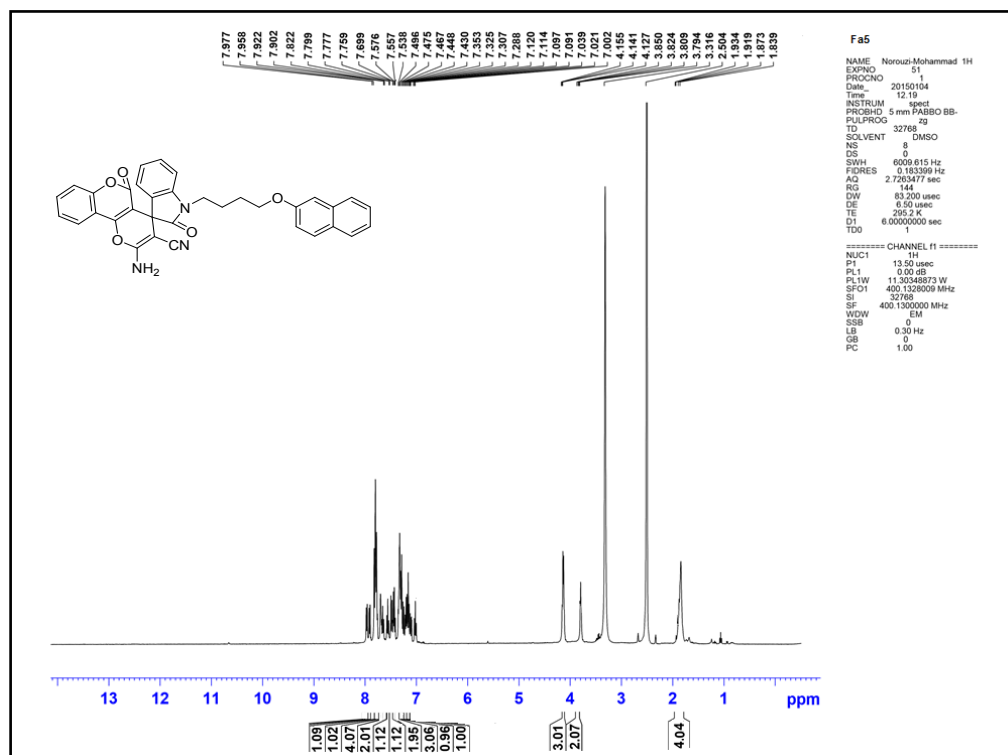
Fa3
NAME NorouziMohammad 13C
EXPNO 5
PROCNO 1
Date_ 20150519
Time 9.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 26000.461 Hz
FIDRES 1.366798 Hz
AQ 1.3531088 sec
RG 203
DW 28.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

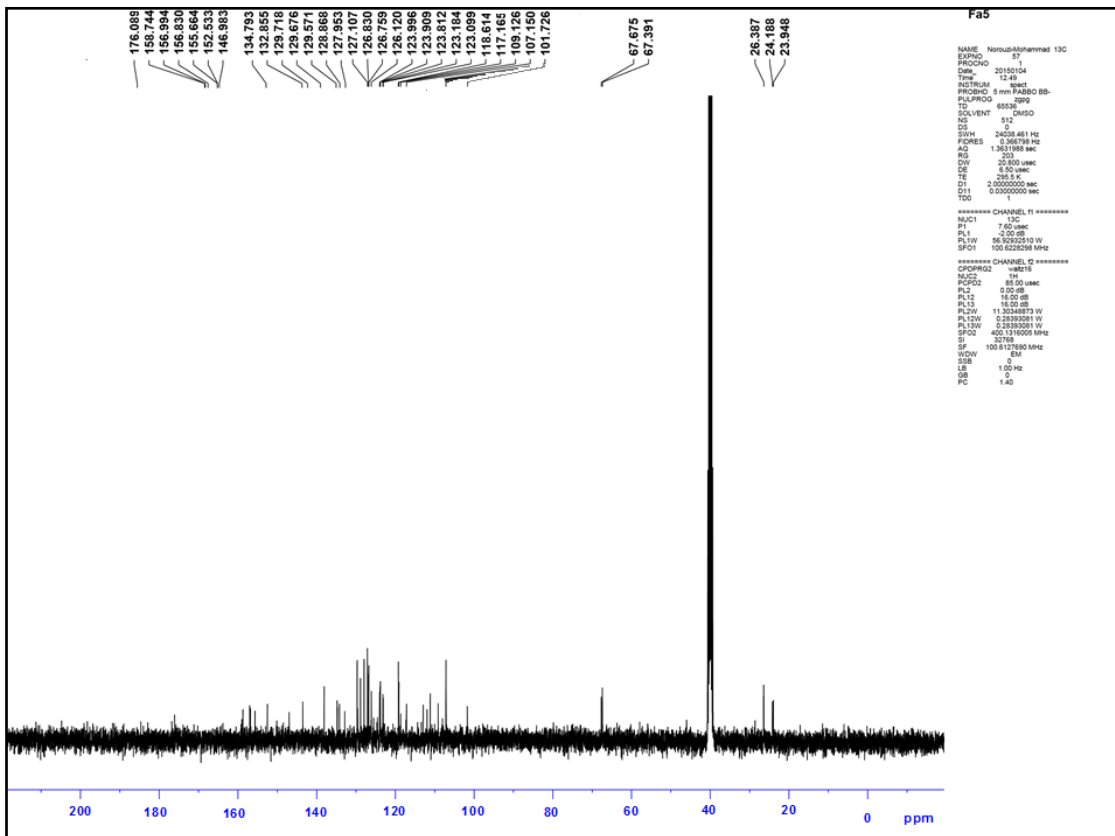
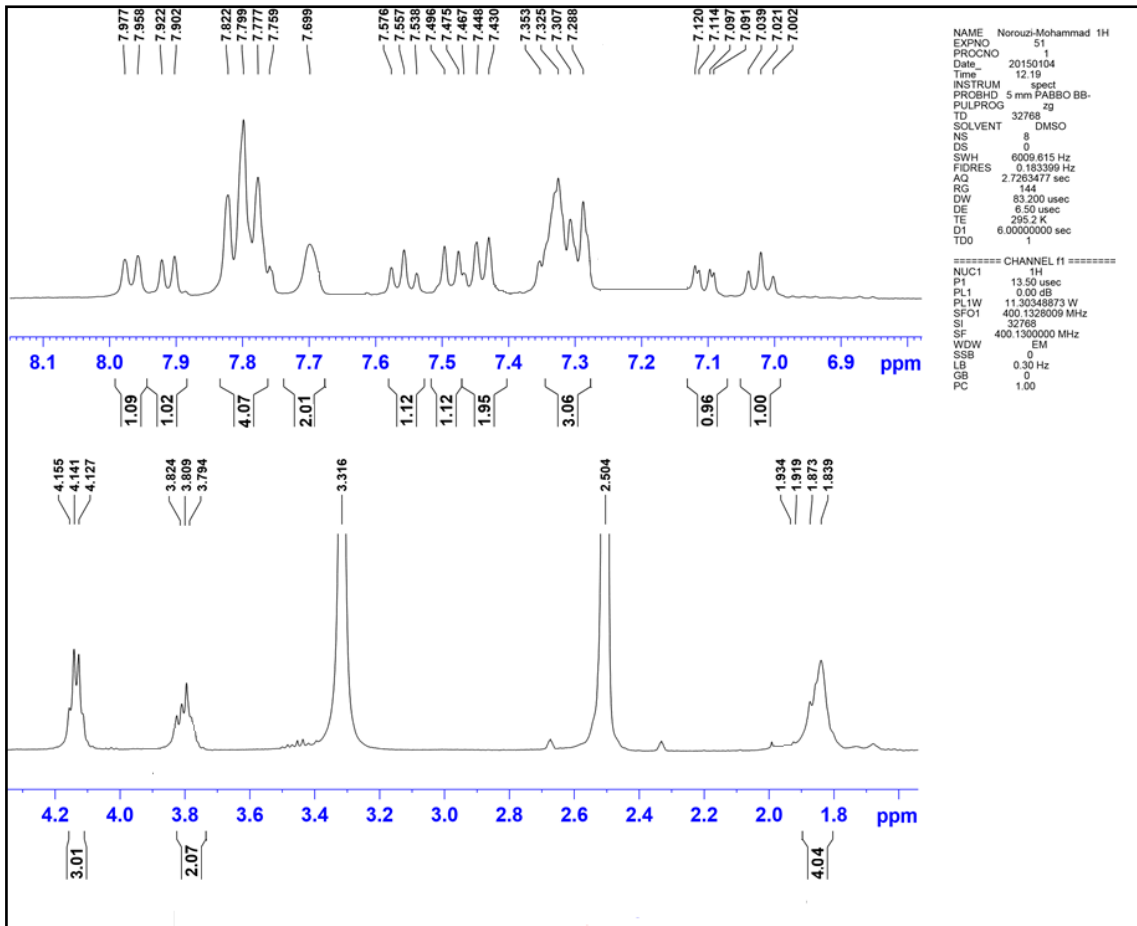
===== CHANNEL f1 =====
NUC1 13C
P1 7.50 usec
PL1 -2.00 dB
PL1W 96.9282510 W
SFO1 100.6282298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 85.00 usec
PL2 0.00 dB
PL21 16.00 dB
PL22 16.00 dB
PL23 16.00 dB
PL2W 11.53348870 W
PL2XW 0.28380081 W
PL2YW 0.28380081 W
SFO2 400.14190000 MHz
SI 32768
SF 100.61723900 MHz
WDW BH
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

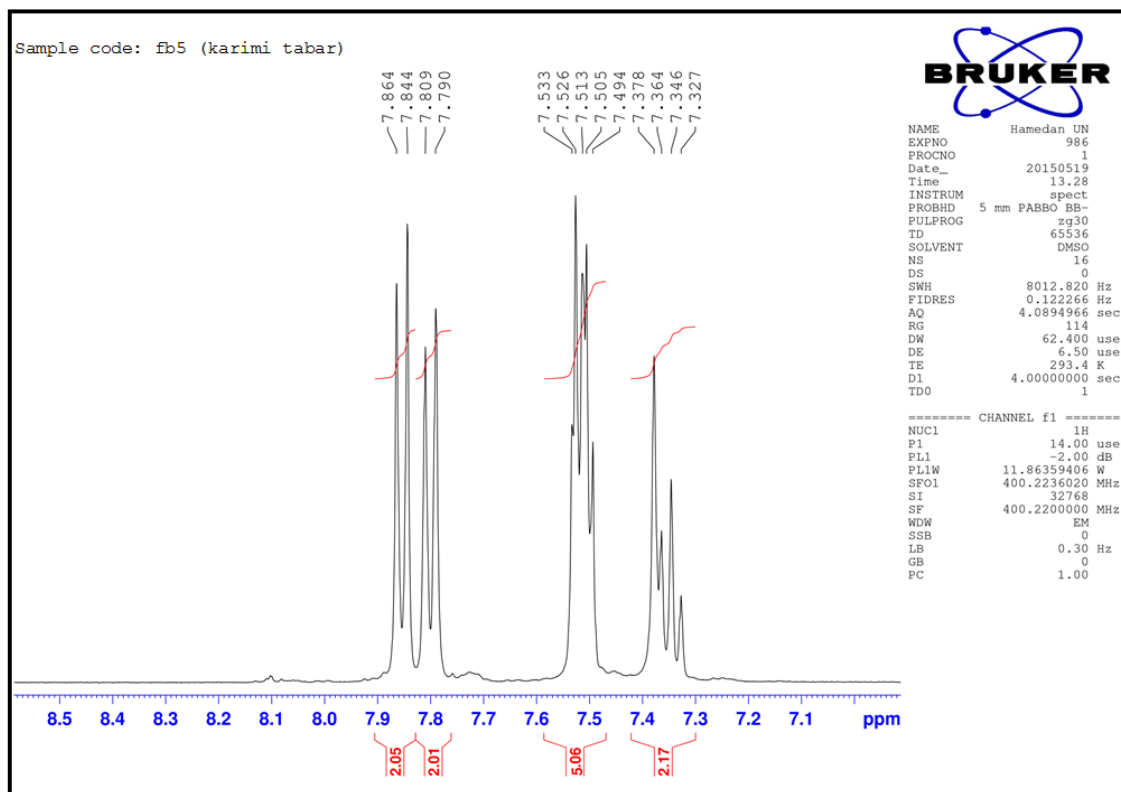
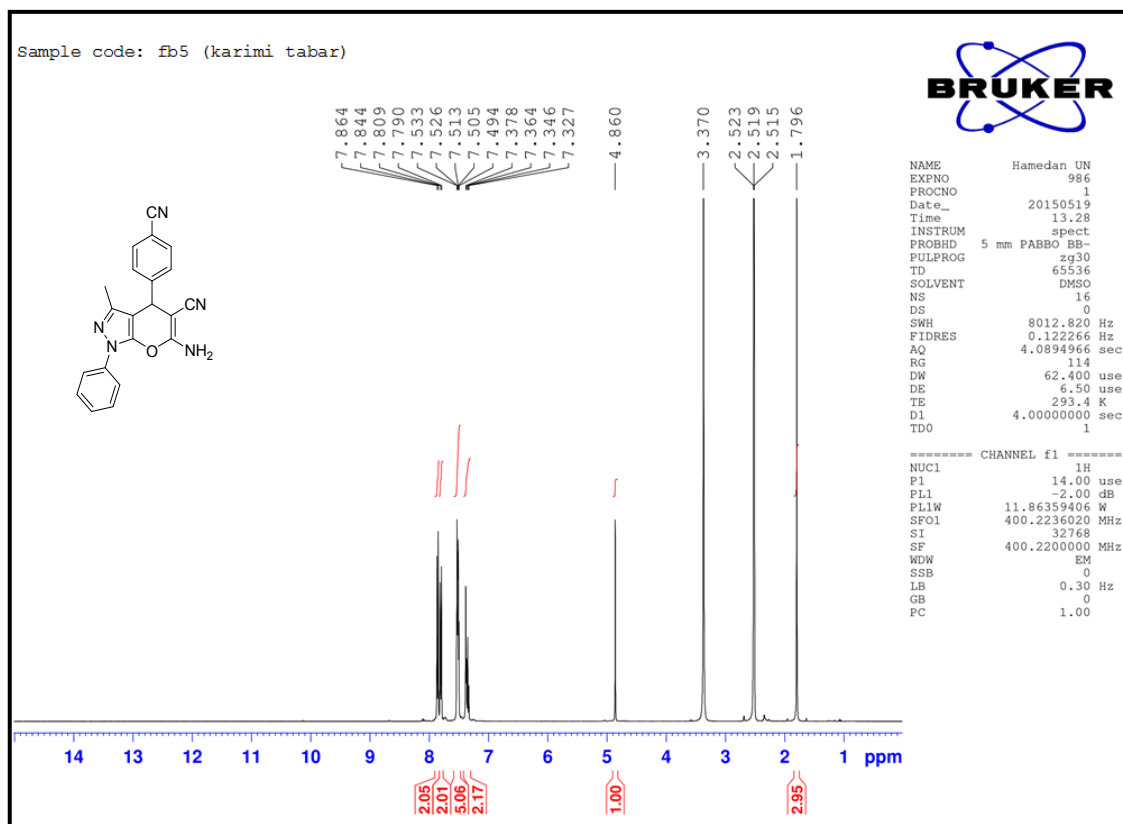


Spiro[2-amino-4H-pyran-oxindole] (6d, Table 4).

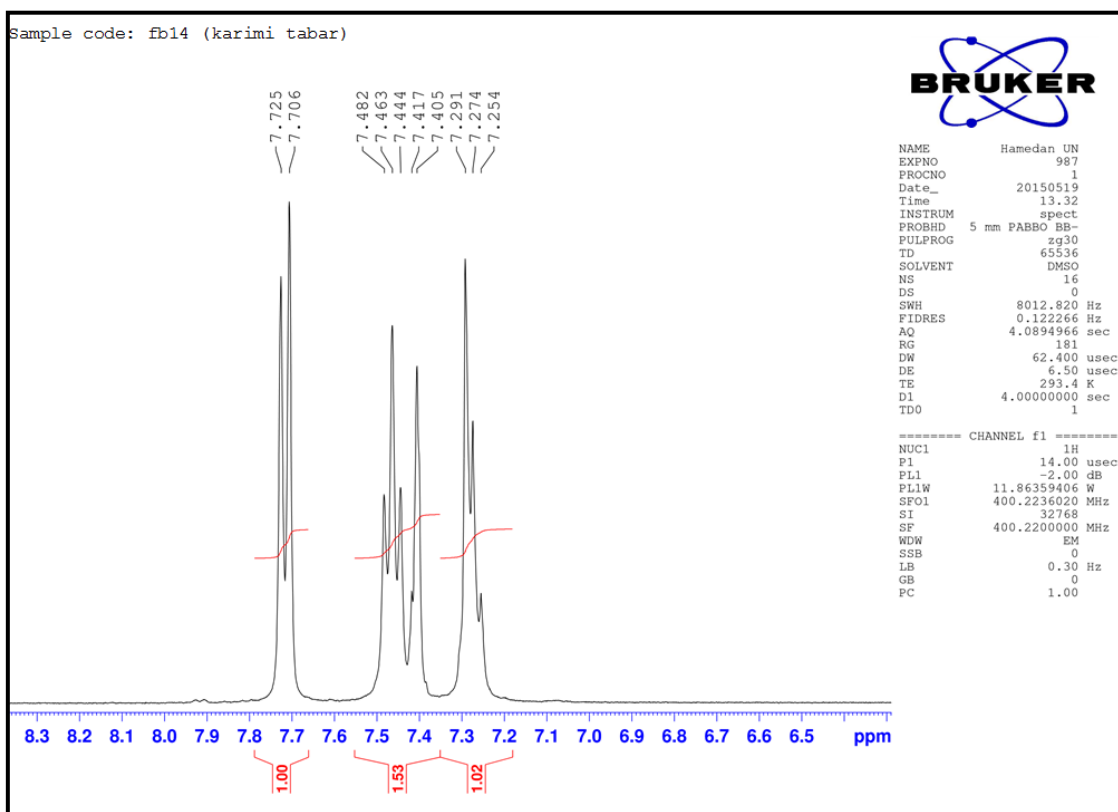
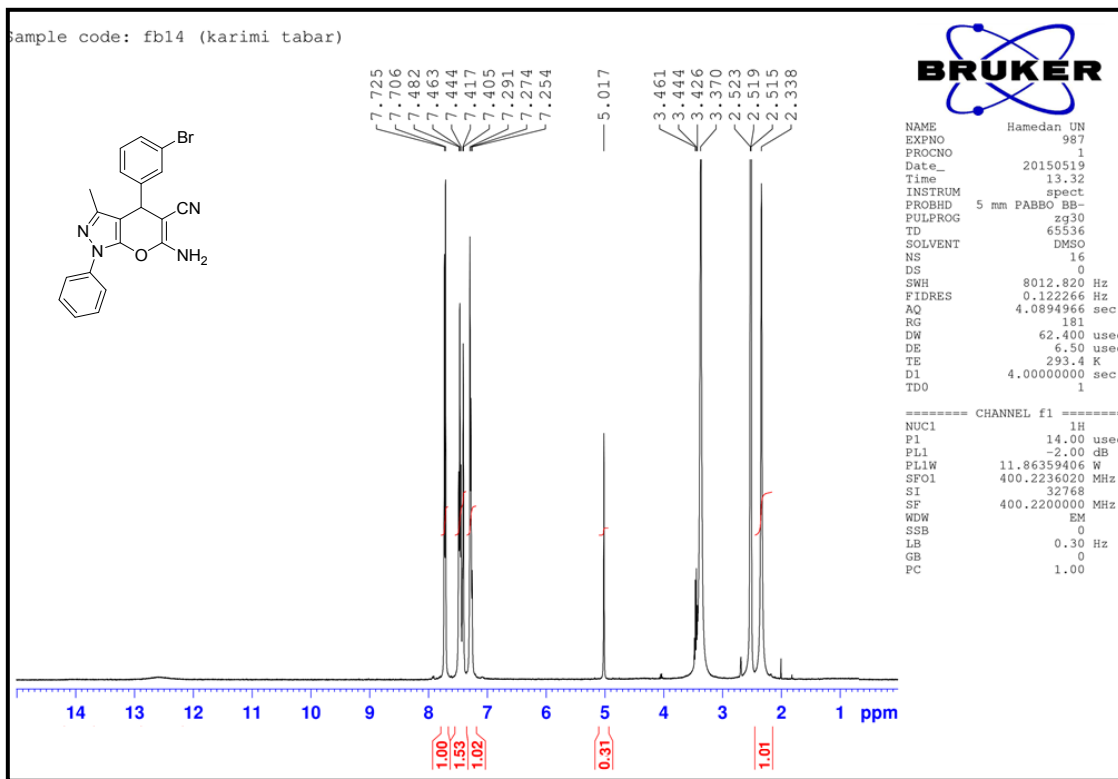




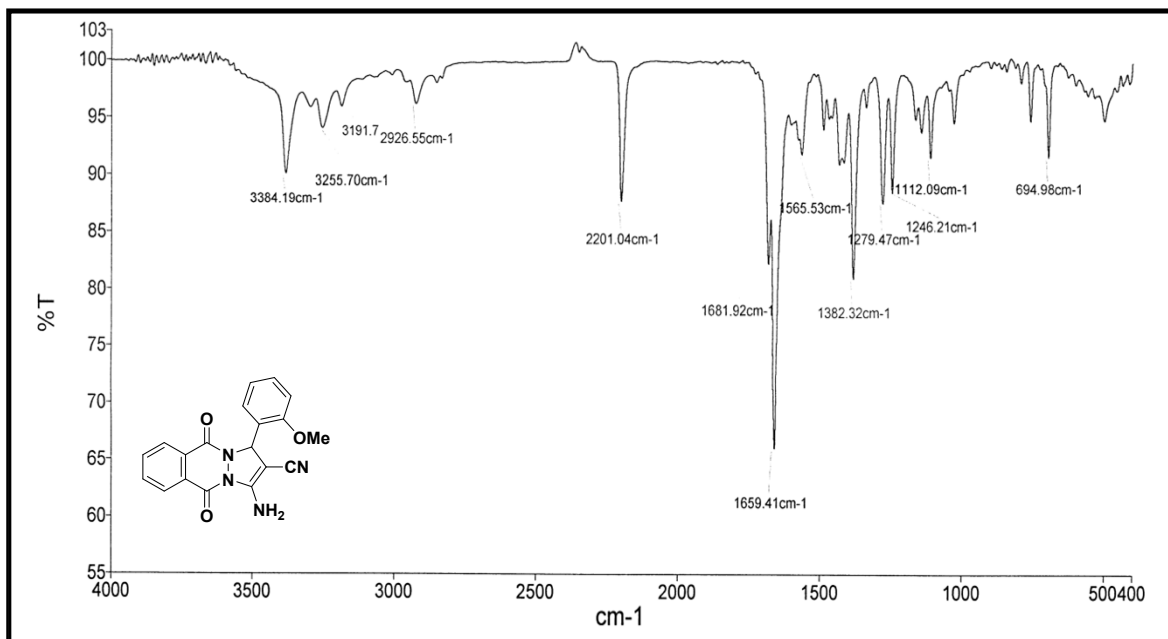
6-Amino-4-(4-cyanophenyl)-3-methyl-1-phenyl-1,4-dihydropyrano[2,3-c]pyrazole-5-carbonitrile (8a).



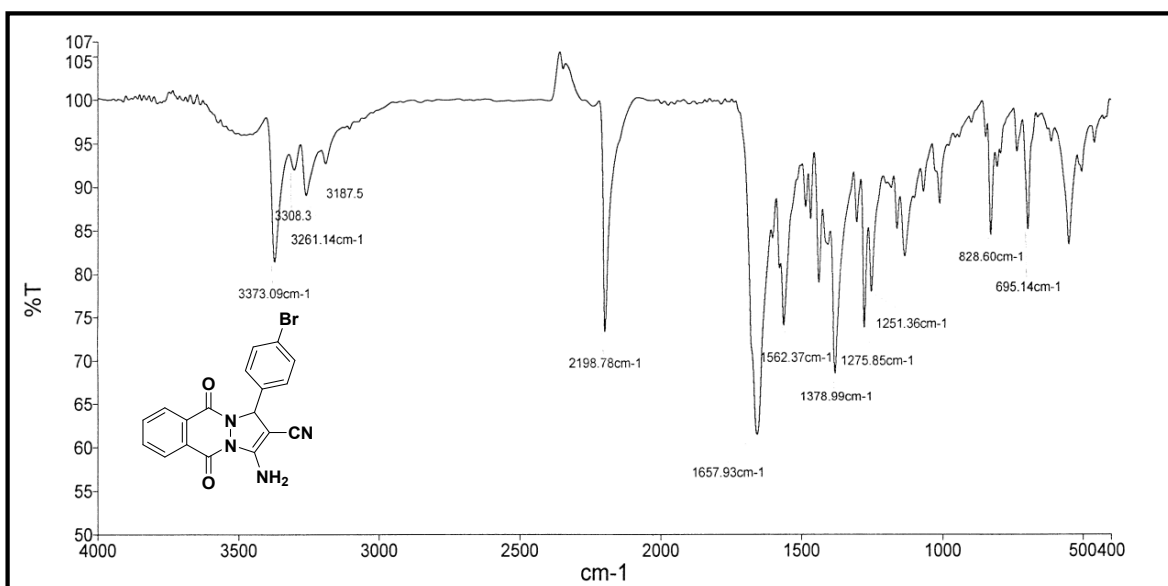
6-Amino-4-(3-bromophenyl)-3-methyl-1-phenyl-1,4-dihydropyran[2,3-c]pyrazole-5-carbonitrile (8i).



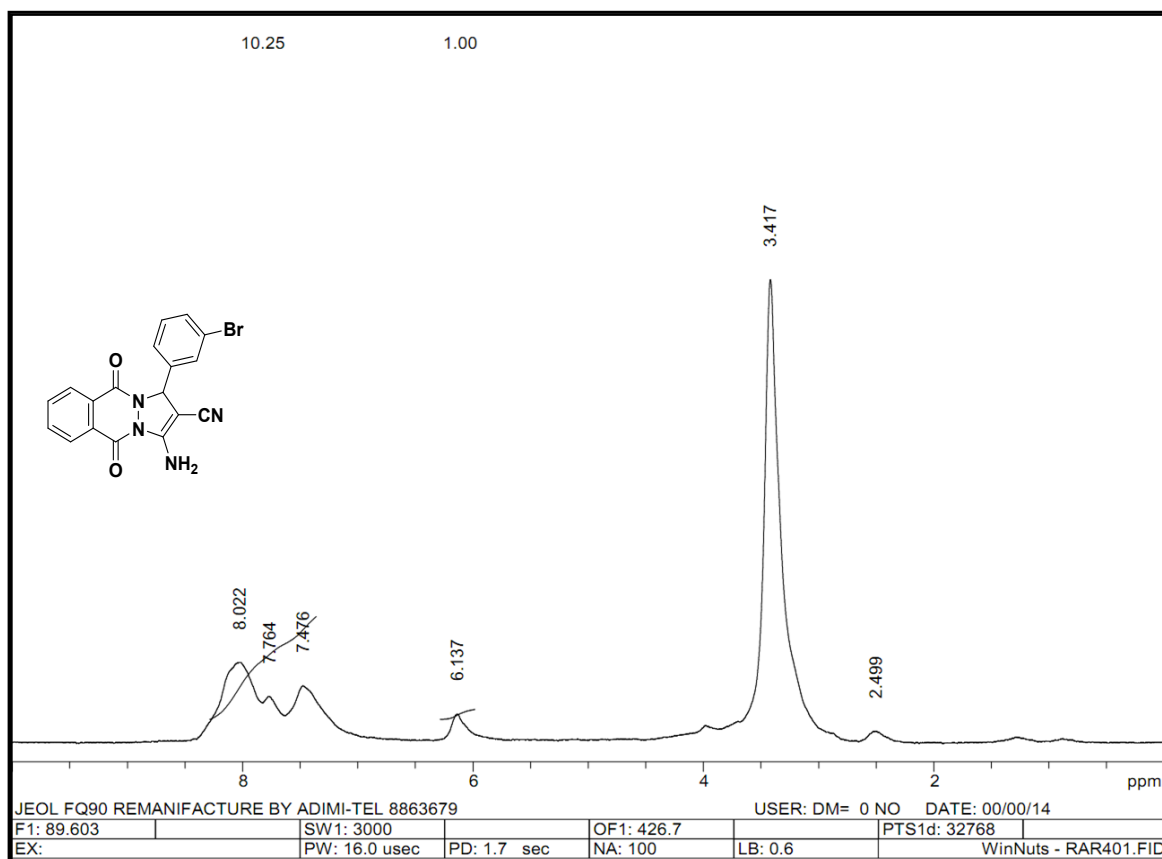
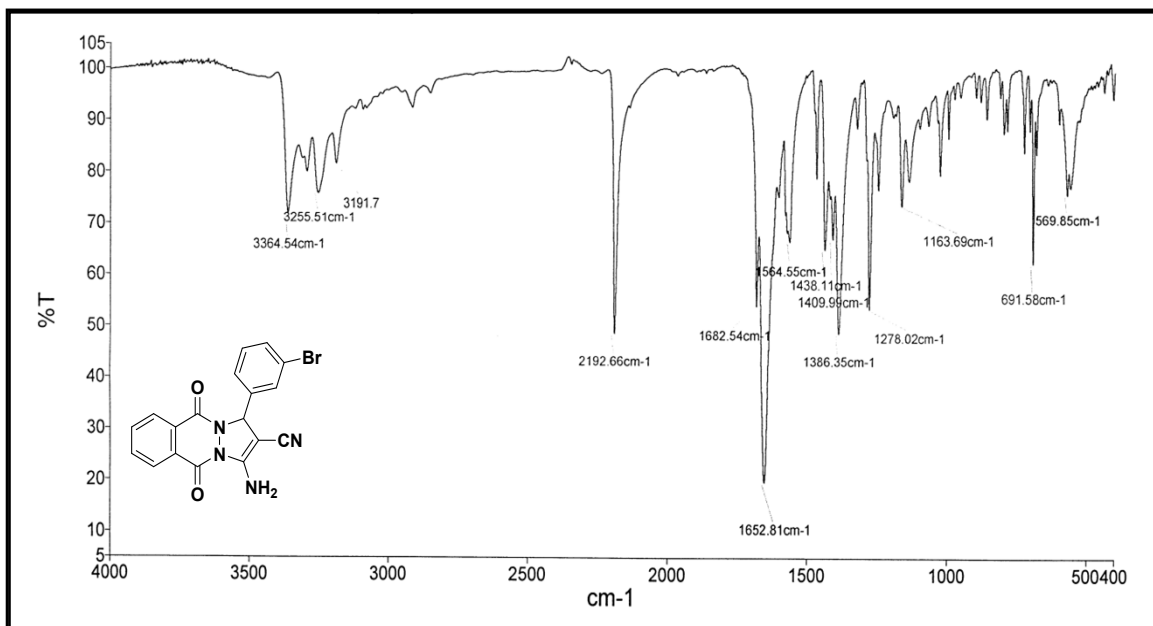
3-Amino-1-(2-methoxyphenyl)-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile (10f).



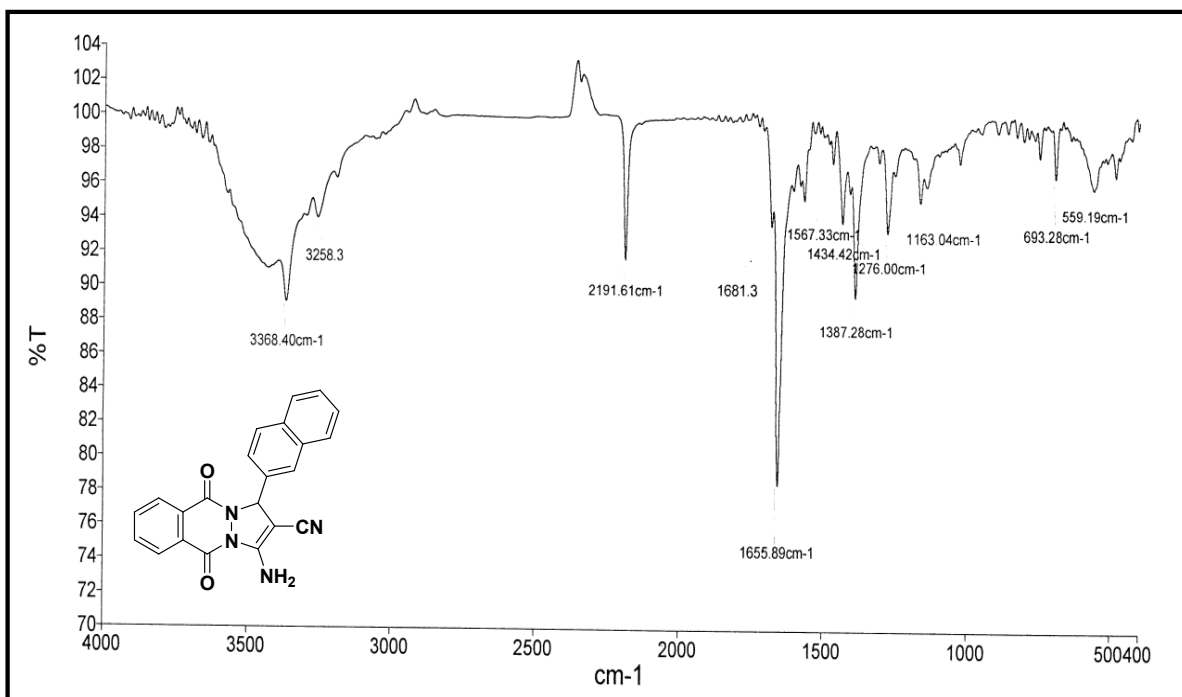
3-Amino-1-(4-bromophenyl)-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile (10g).



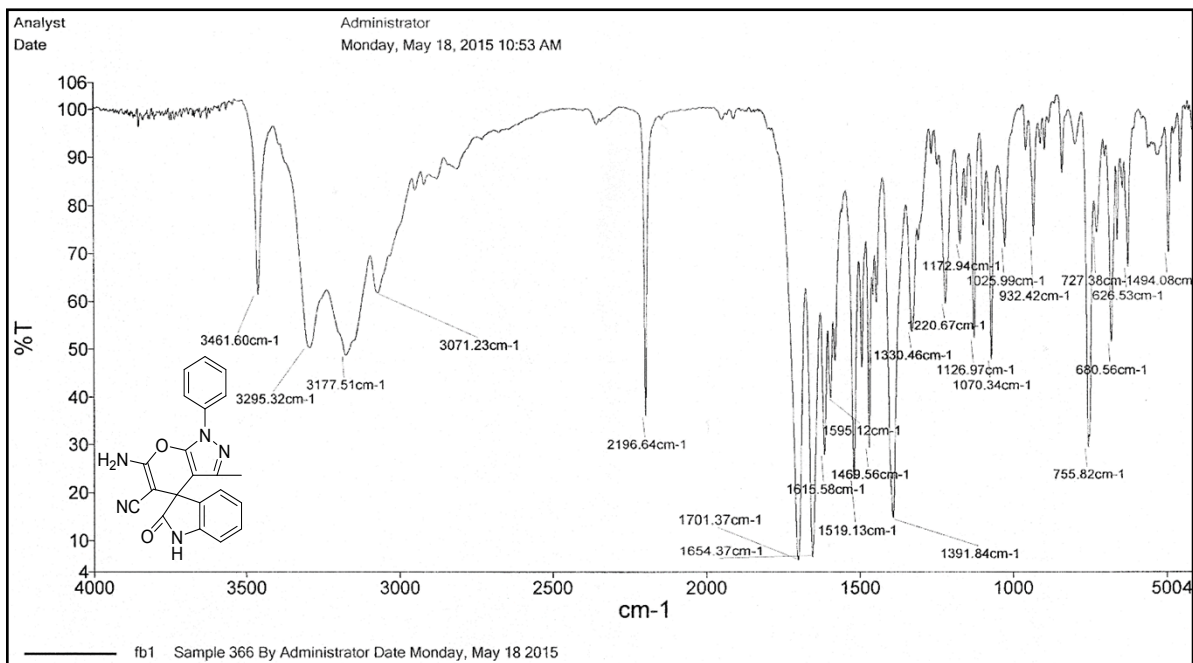
3-Amino-1-(3-bromophenyl)-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile (10 j).



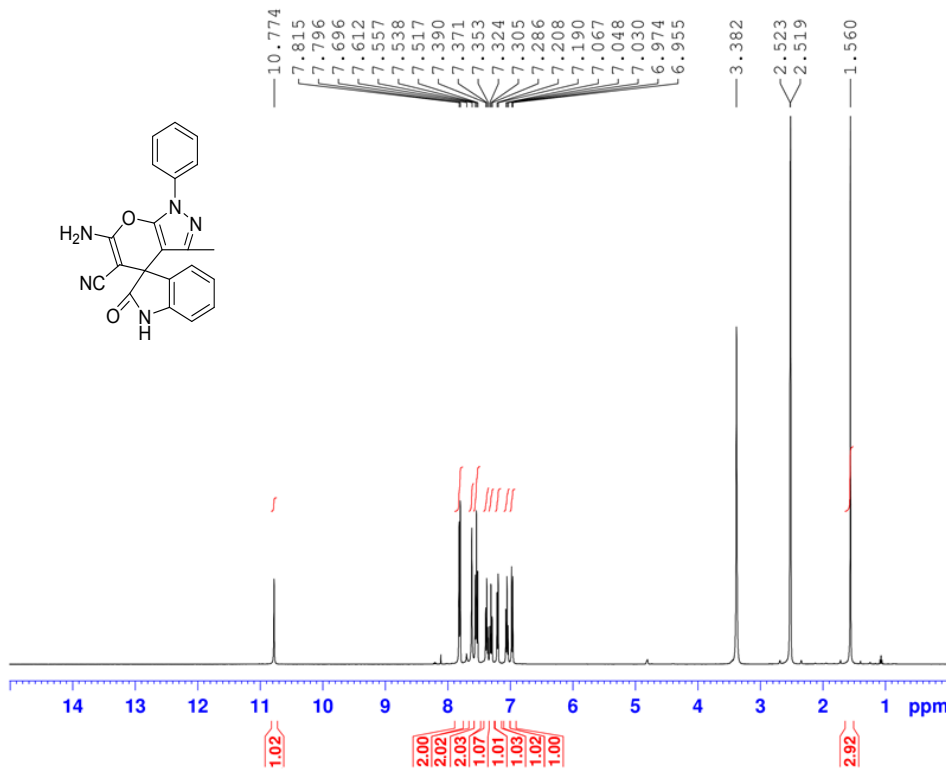
3-amino-1-(naphthalen-2-yl)-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-b] phthalazine - 2-carbonitrile (10k).



Spiro[pyrano[2,3-c]pyrazole] (11a).



Sample code: fbl (karimi tabar)

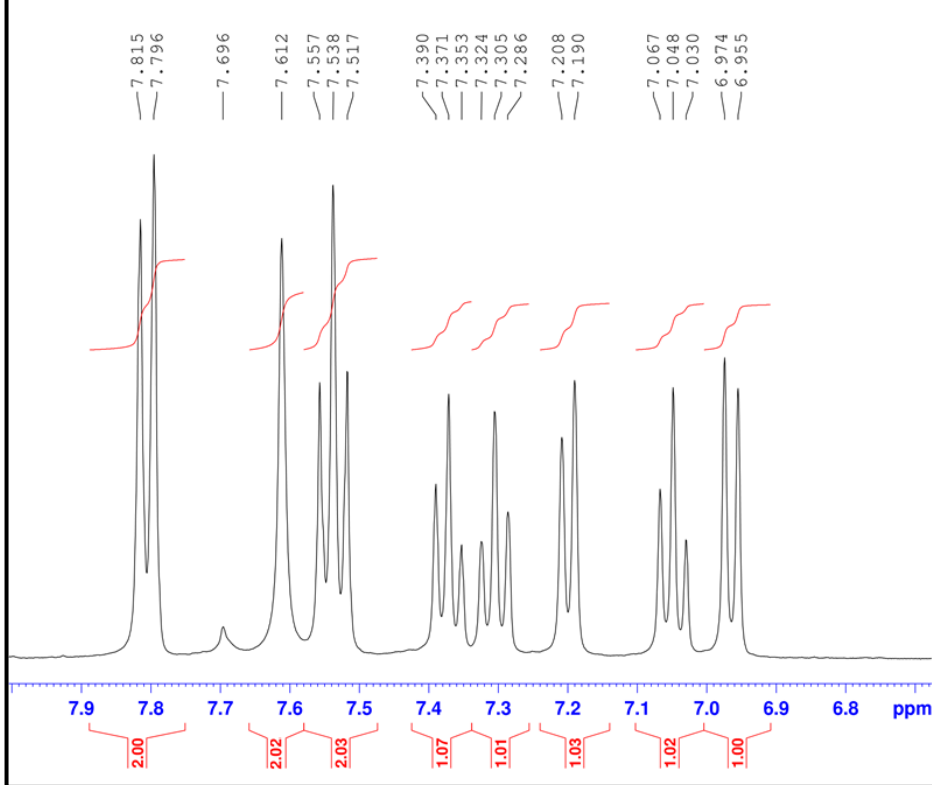


BRUKER

NAME Hamedan UN
EXPNO 982
PROCNO 1
Date_ 20150519
Time 12.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 144
DW 62.400 usec
DE 6.50 usec
TE 293.4 K
D1 4.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Sample code: fbl (karimi tabar)



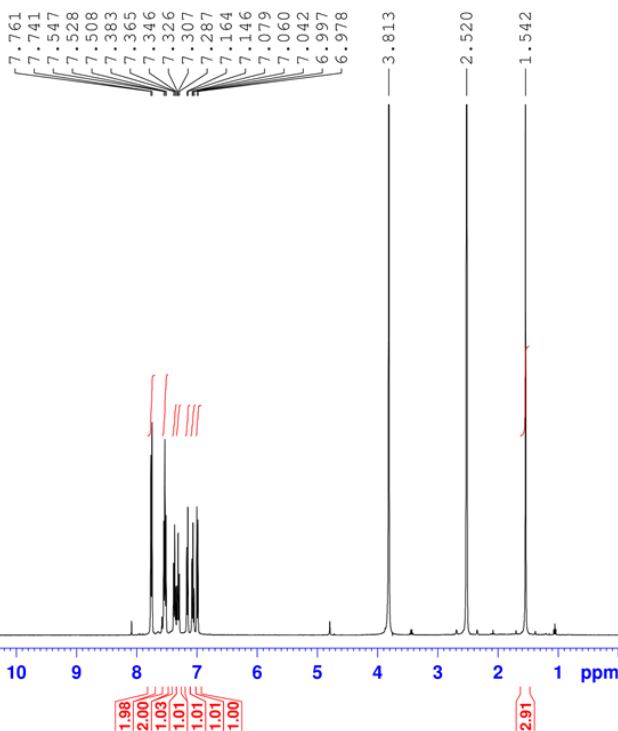
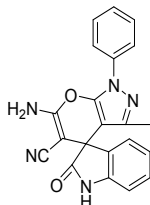
BRUKER

NAME Hamedan UN
EXPNO 982
PROCNO 1
Date_ 20150519
Time 12.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 144
DW 62.400 usec
DE 6.50 usec
TE 293.4 K
D1 4.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

D₂O exchange

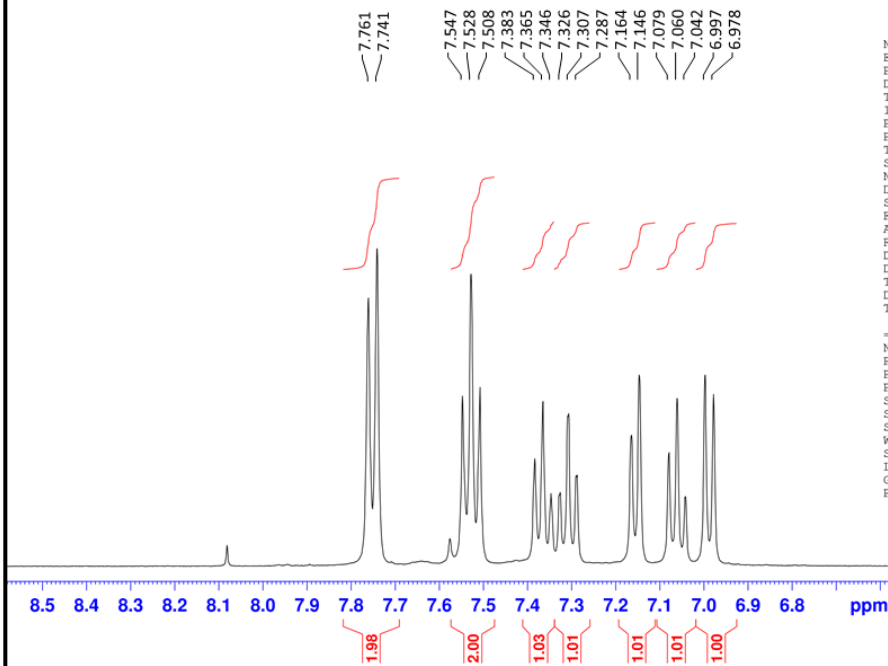
Sample code: fb1+D20 (karimi tabar)



NAME Hamedan UN
 EXPNO 1008
 PROCNO 1
 Date_ 20150519
 Time 16.05
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 161
 DW 62.400 usec
 DE 6.50 usec
 TE 293.6 K
 D1 4.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL1 -2.00 dB
 PL1W 11.86359406 W
 SFO1 400.2236020 MHz
 SI 32768
 SF 400.2200000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

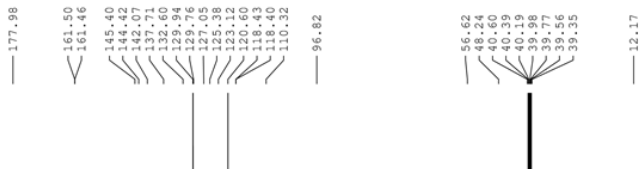
Sample code: fb1+D20 (karimi tabar)



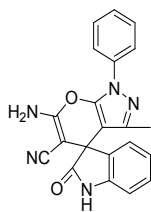
NAME Hamedan UN
 EXPNO 1008
 PROCNO 1
 Date_ 20150519
 Time 16.05
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 161
 DW 62.400 usec
 DE 6.50 usec
 TE 293.6 K
 D1 4.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL1 -2.00 dB
 PL1W 11.86359406 W
 SFO1 400.2236020 MHz
 SI 32768
 SF 400.2200000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

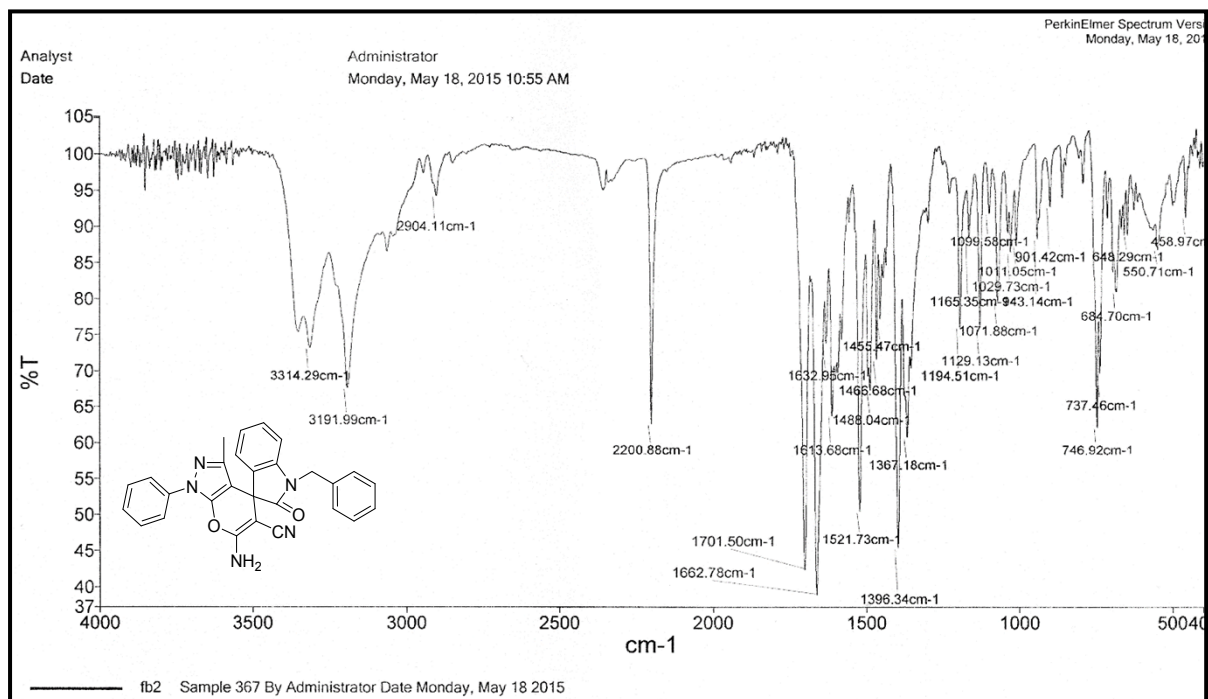
Sample code: FB1 (karimi tabar)

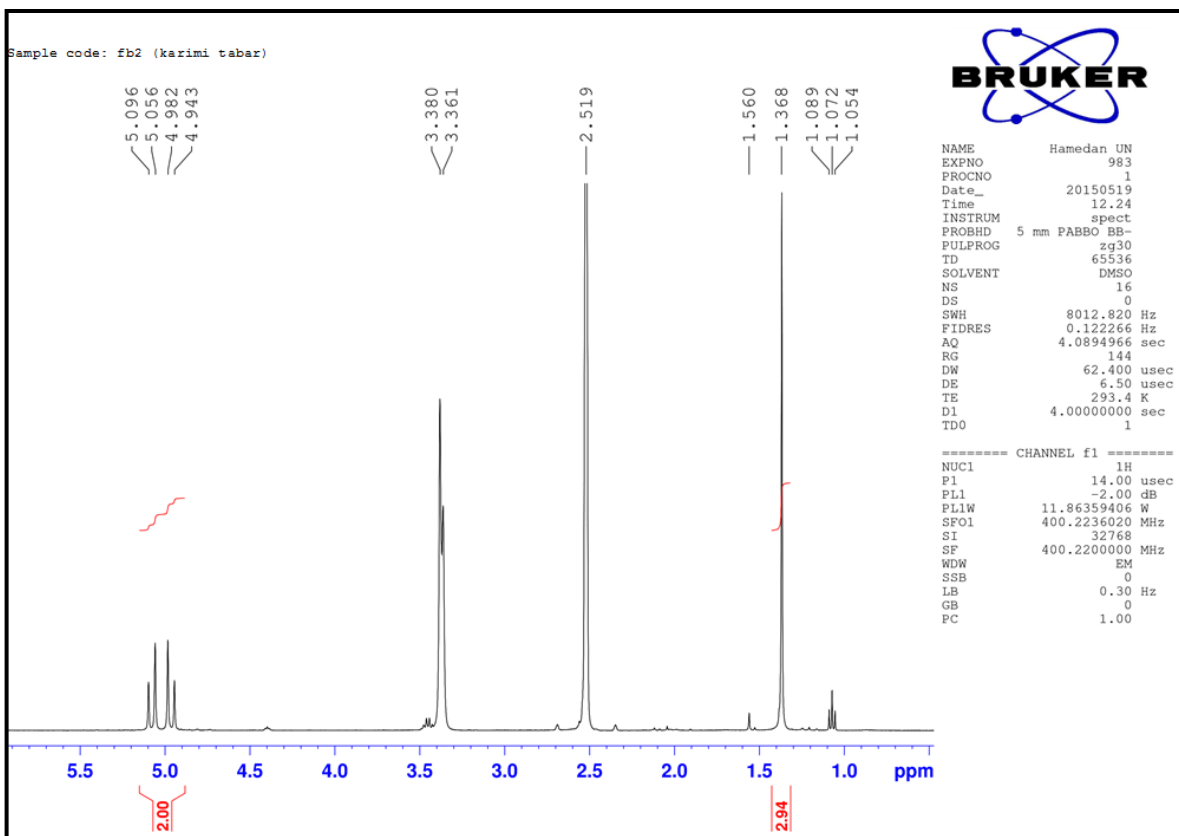
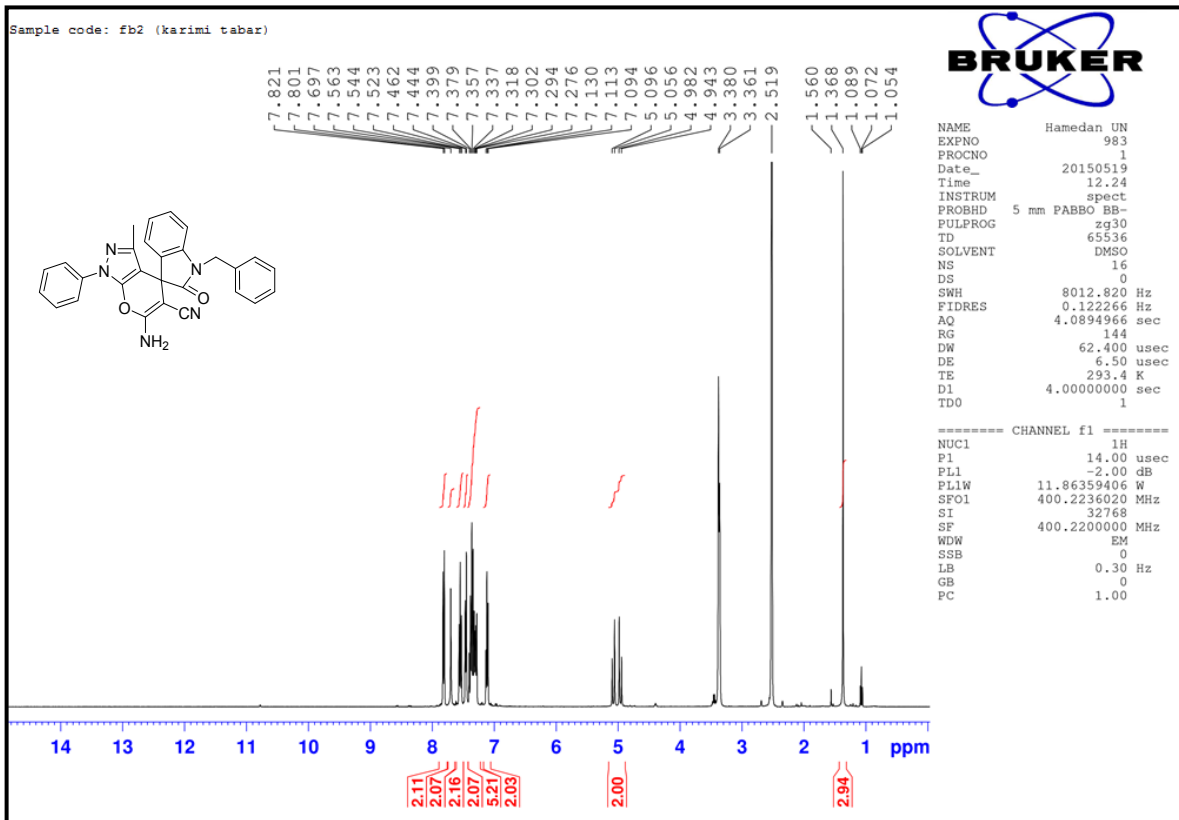


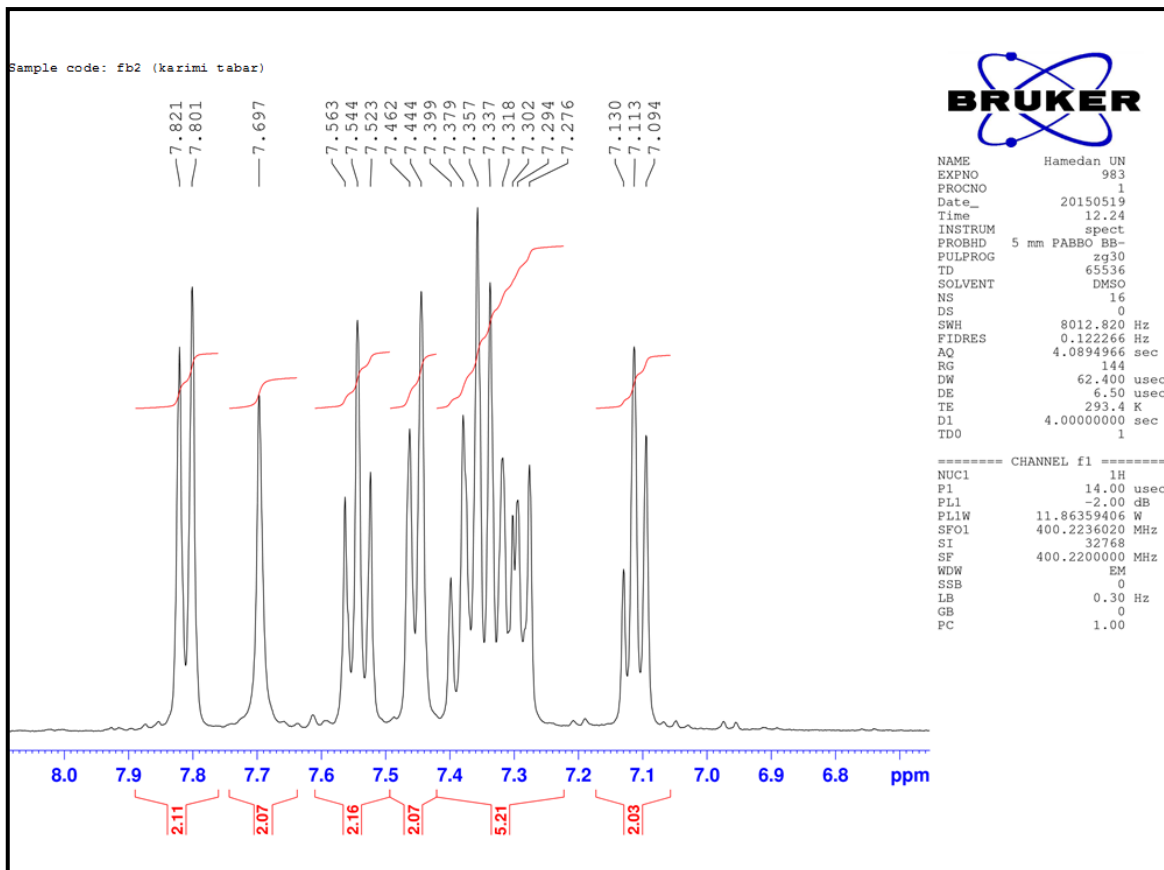
NAME Hamedan UN
 EXPNO 922
 PROCNO 1
 Date_ 20150204
 Time 16.03
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30



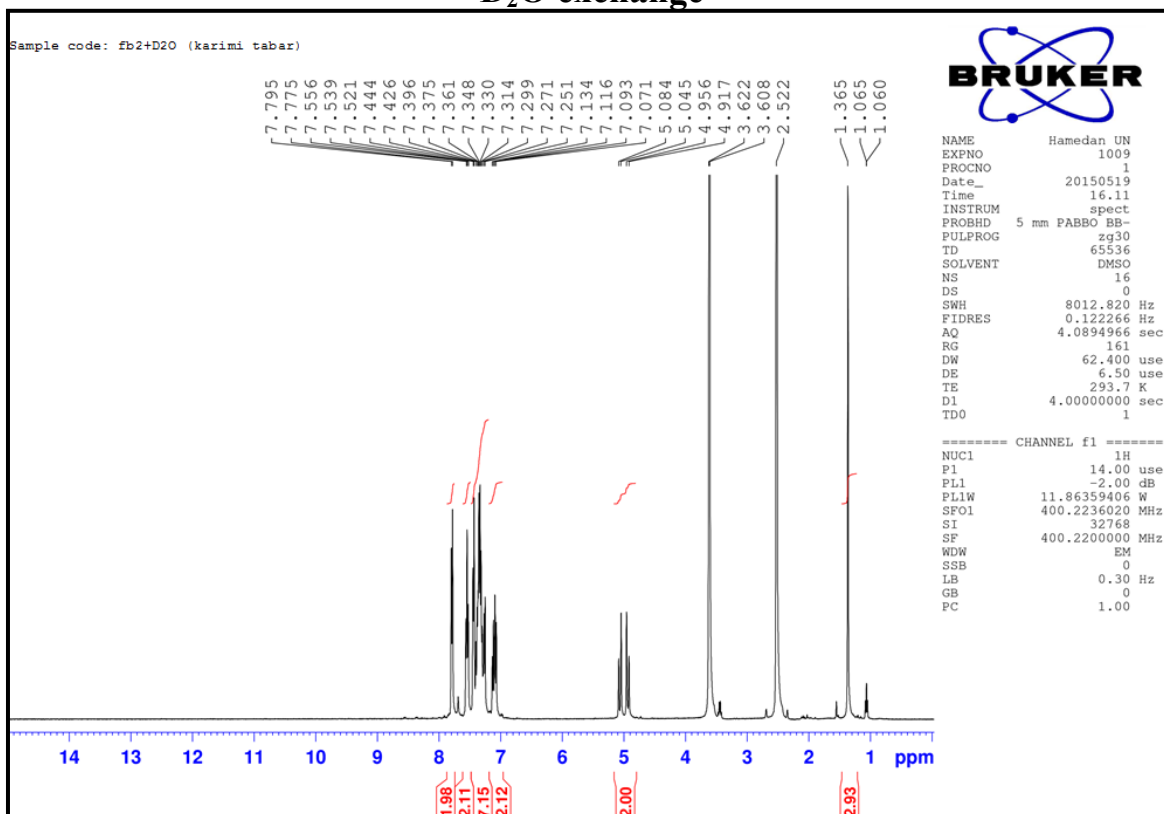
Spiro[pyrano[2,3-c]pyrazole] (11b).



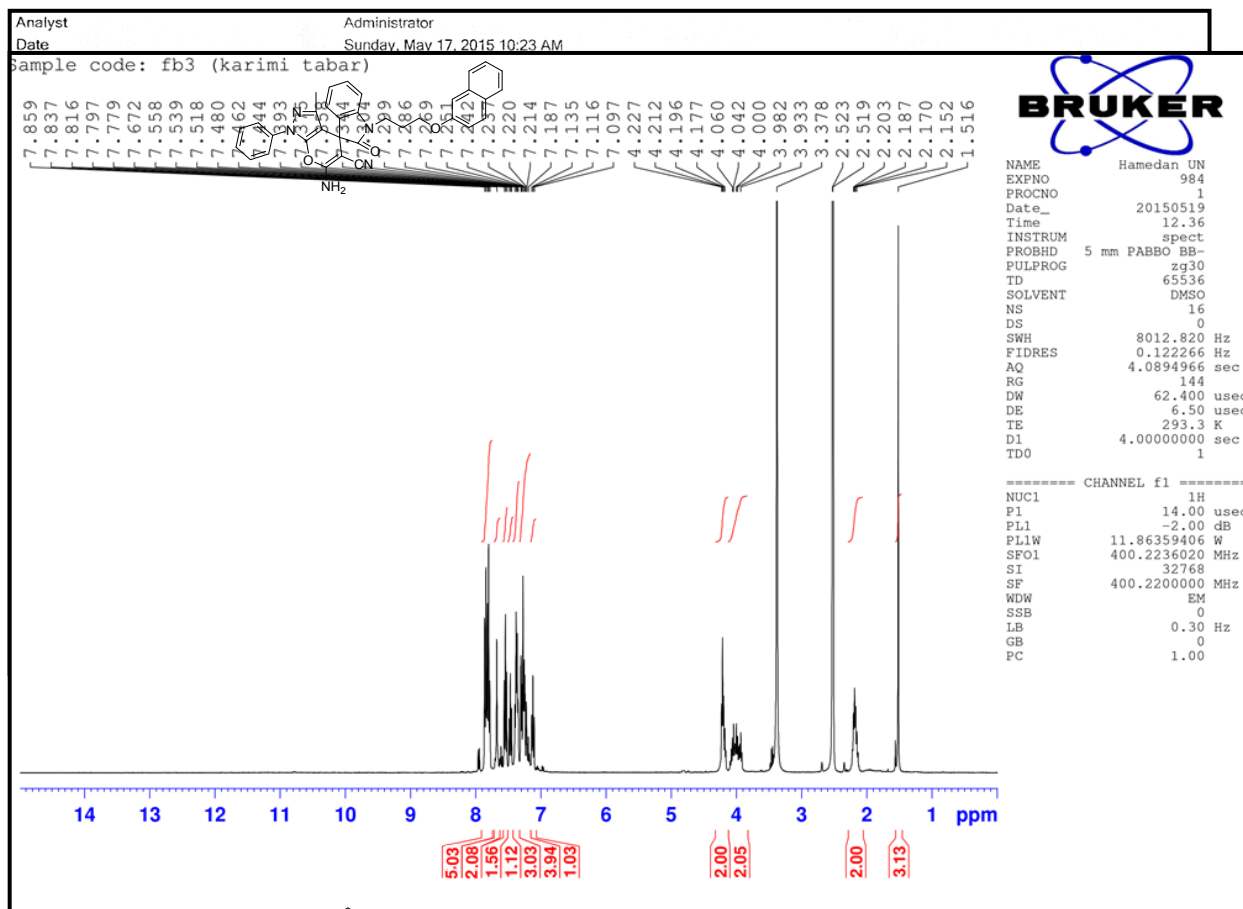




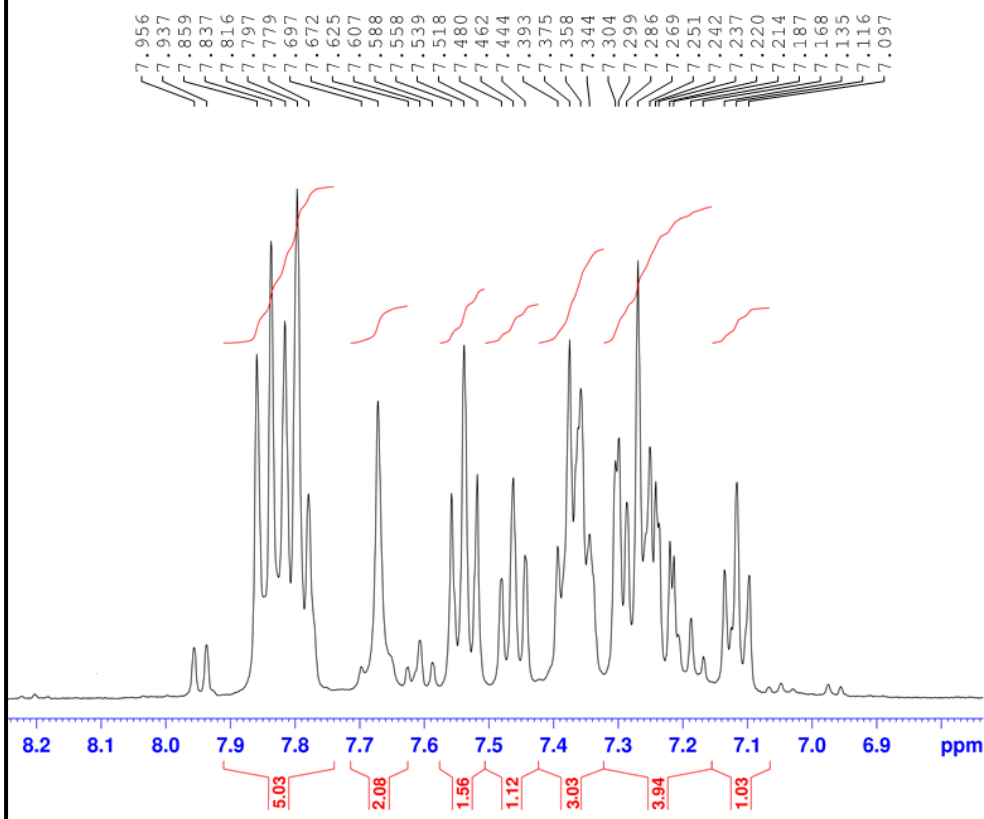
D₂O exchange



Spiro[pyrano[2,3-c]pyrazole] (11c).



Sample code: fb3 (karimi tabar)

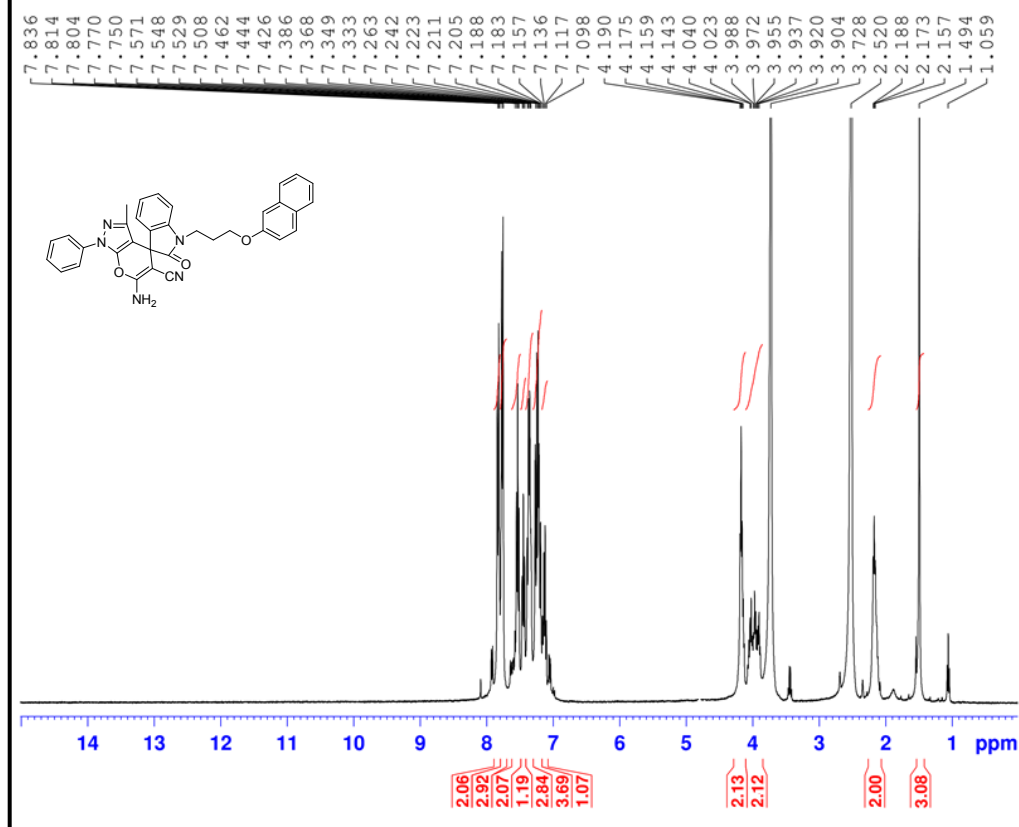


NAME Hamedan UN
EXPNO 984
PROCNO 1
Date_ 20150519
Time 12.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 144
DW 62.400 usec
DE 6.50 usec
TE 293.3 K
D1 4.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

D₂O exchange

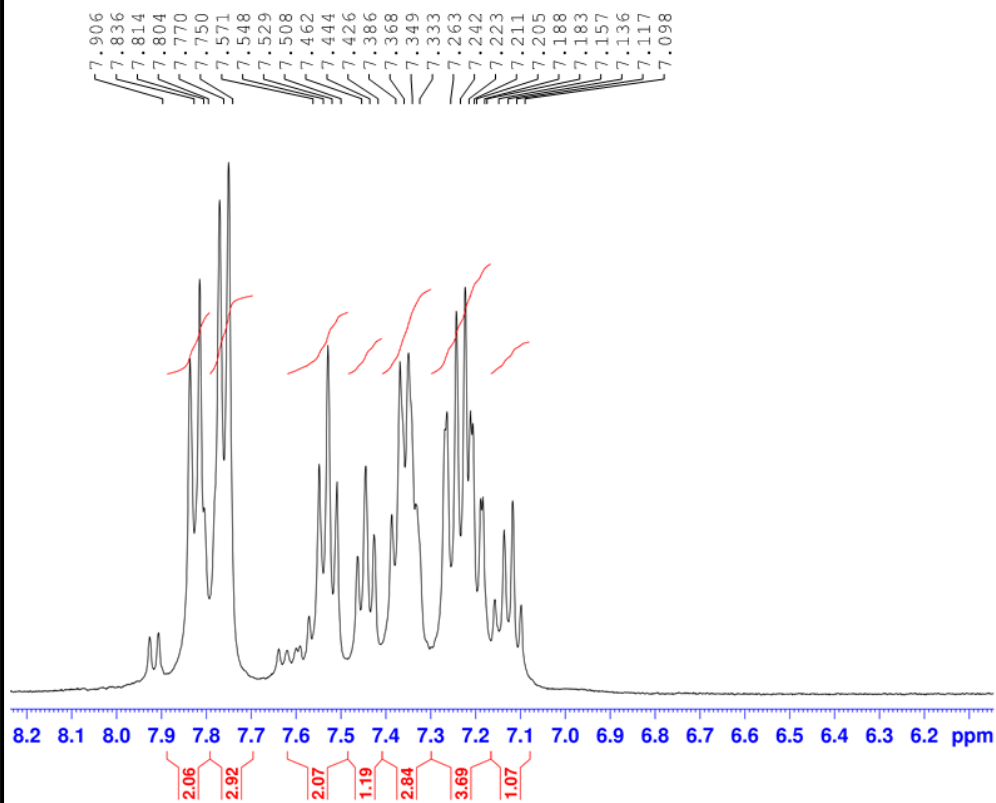
Sample code: fb3+D2O (karimi tabar)



NAME Hamedan UN
EXPNO 1010
PROCNO 1
Date_ 20150519
Time 16.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 293.7 K
D1 4.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PL1W 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Sample code: fb3+D2O (karimi tabar)

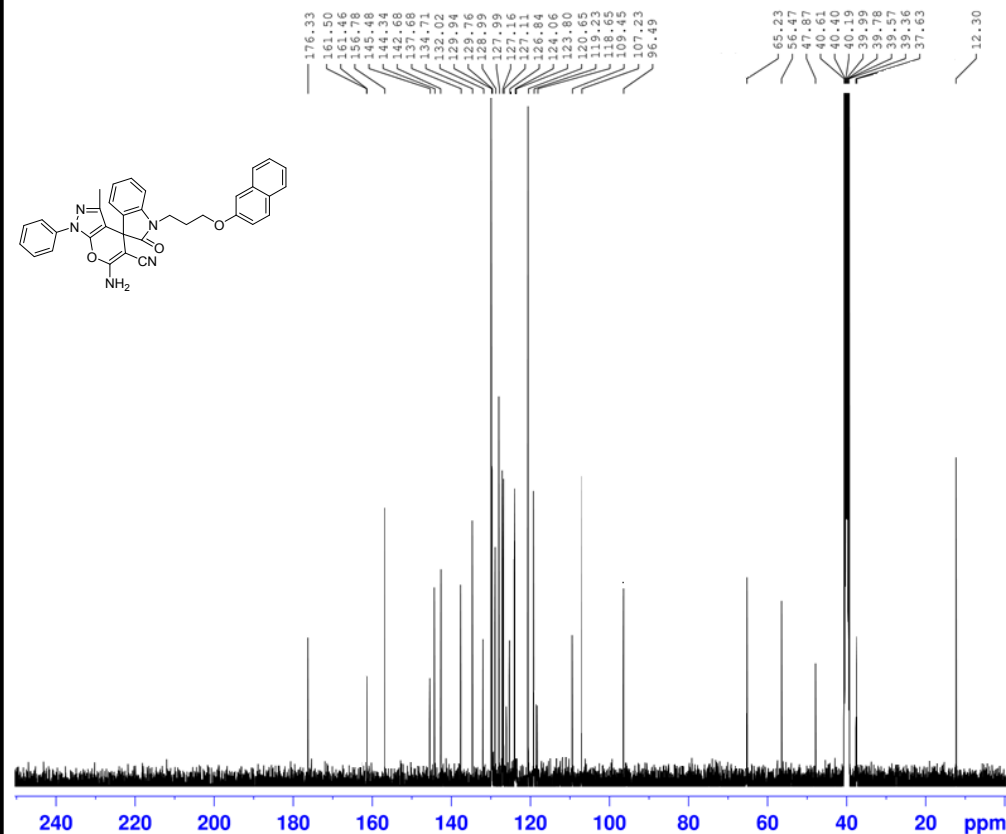


BRUKER

NAME Hamedan UN
 EXPNO 1010
 PROCNO 1
 Date_ 20150519
 Time 16.15
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 161
 DW 62.400 usec
 DE 6.50 usec
 TE 293.7 K
 D1 4.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL1 -2.00 dB
 PL1W 11.86359406 W
 SF01 400.2236020 MHz
 SI 32768
 SF 400.2200000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Sample code:FB3 (karimi tabar)



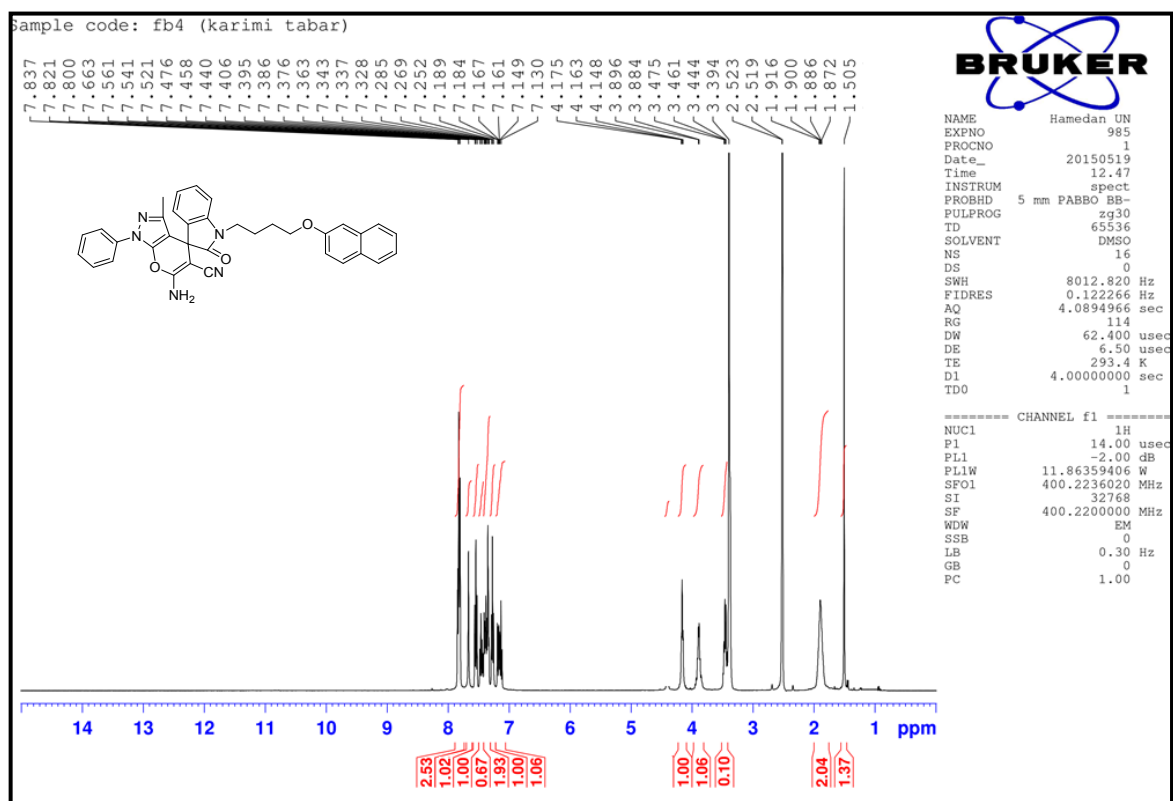
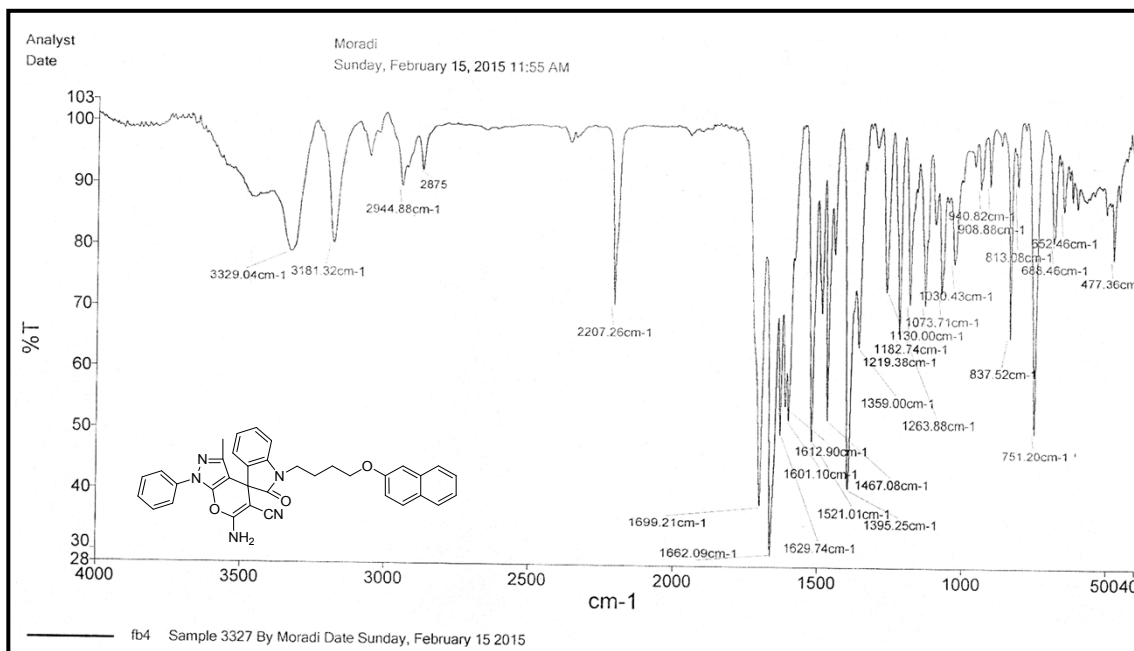
BRUKER

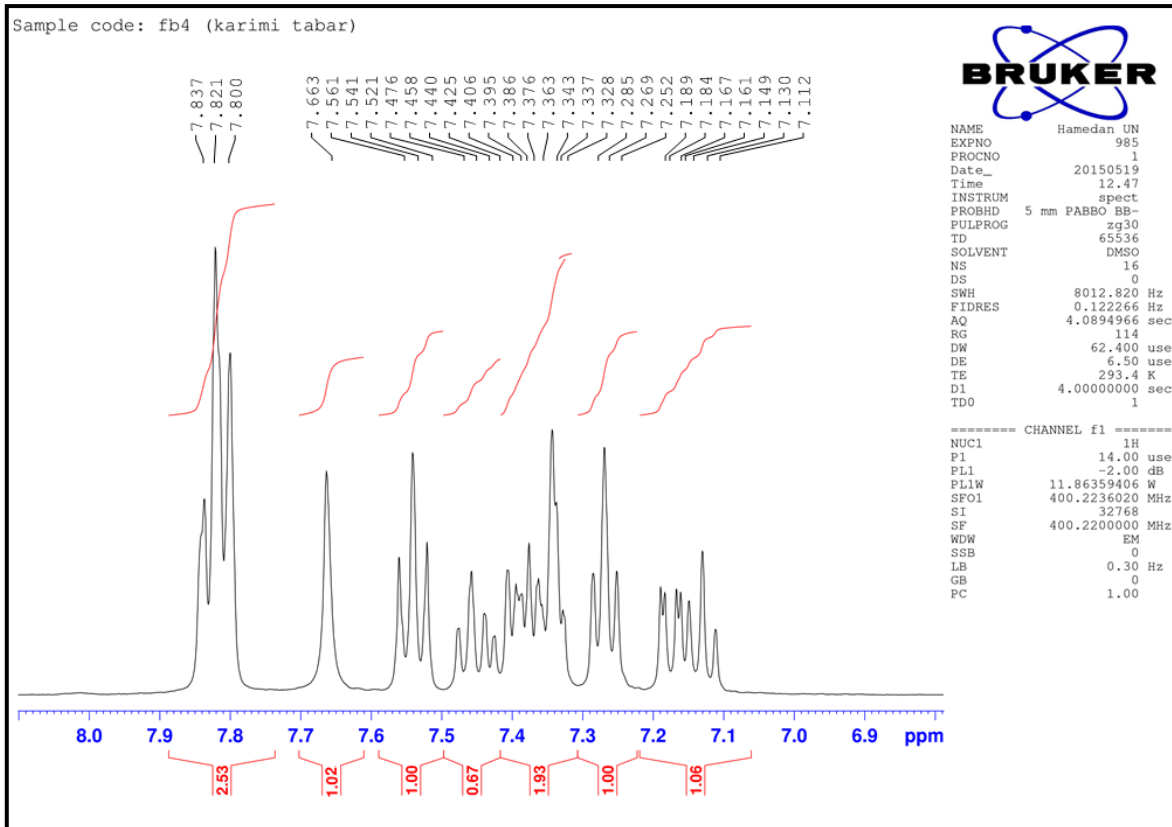
NAME Hamedan UN
 EXPNO 929
 PROCNO 1
 Date_ 20150208
 Time 9.53
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1011
 DS 0
 SWH 25252.525 Hz
 FIDRES 0.385323 Hz
 AQ 1.2976629 sec
 RG 2050
 DW 19.800 usec
 DE 6.50 usec
 TE 296.0 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PL1 -0.90 dB
 PL1W 42.02801895 W
 SF01 100.6479784 MHz

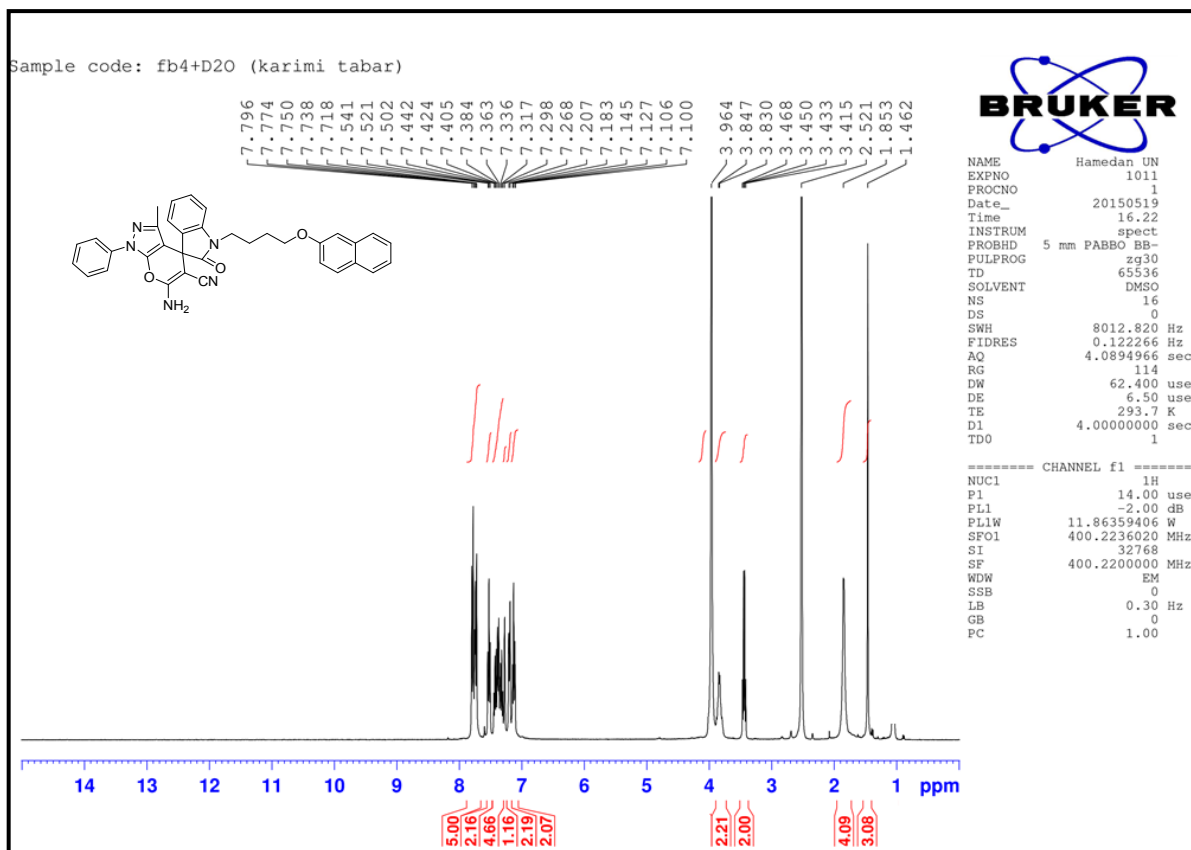
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -2.00 dB
 PLI2 14.16 dB
 PLI3 17.90 dB
 PL2W 11.86359406 W
 PLI2W 0.28722104 W
 PLI3W 0.12139934 W
 SF02 400.2216009 MHz
 SI 32768
 SF 100.6353990 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

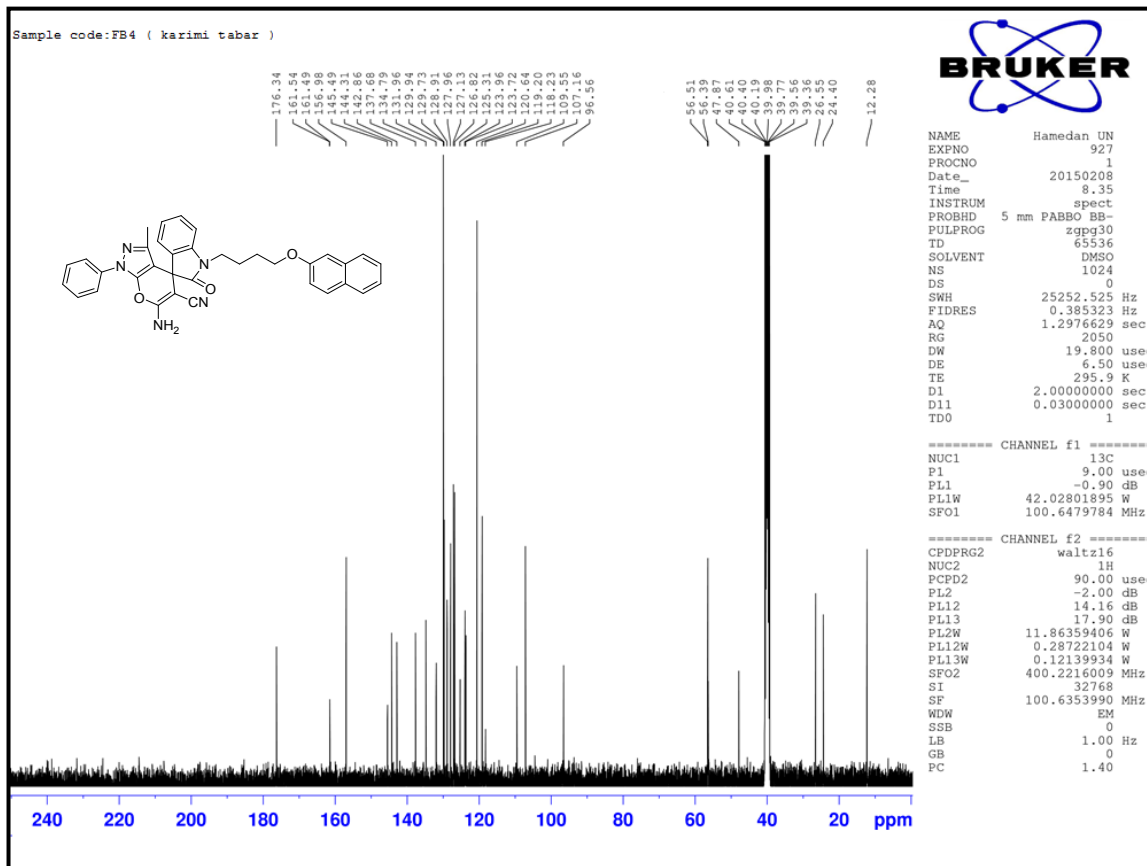
Spiro[pyrano[2,3-c]pyrazole] (11d).



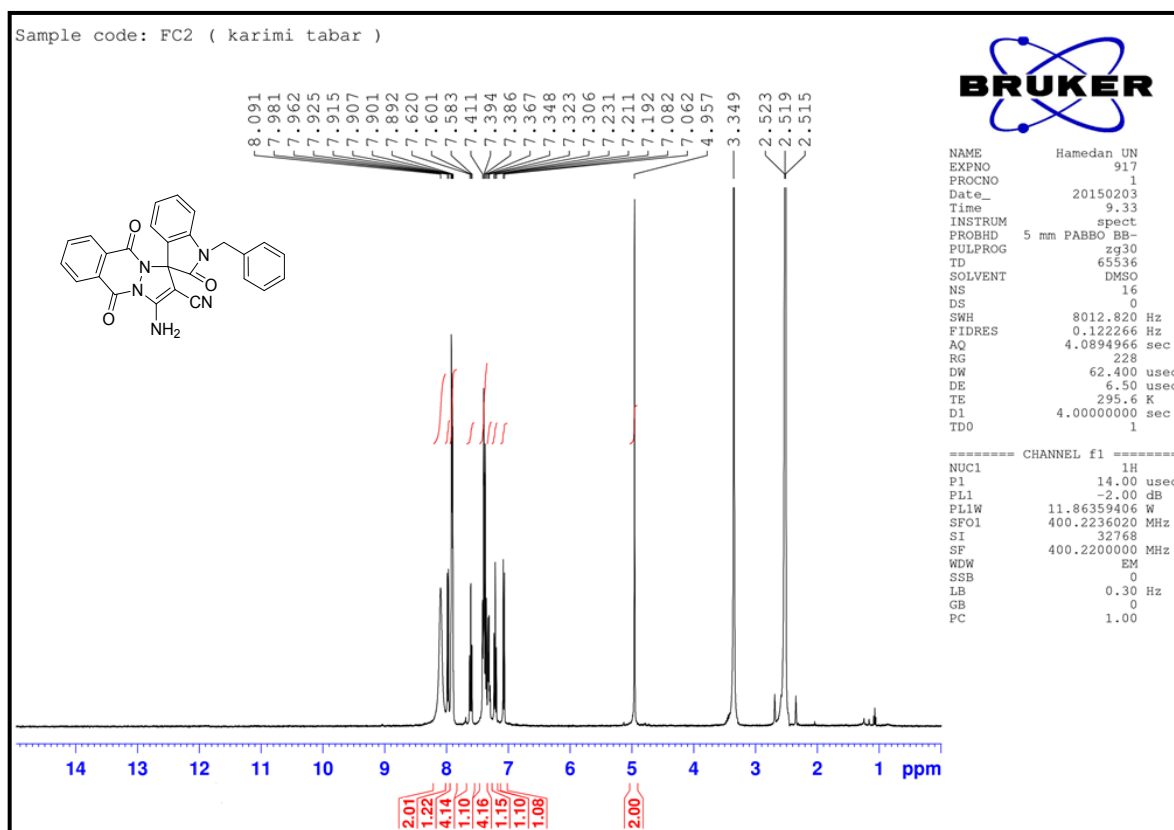


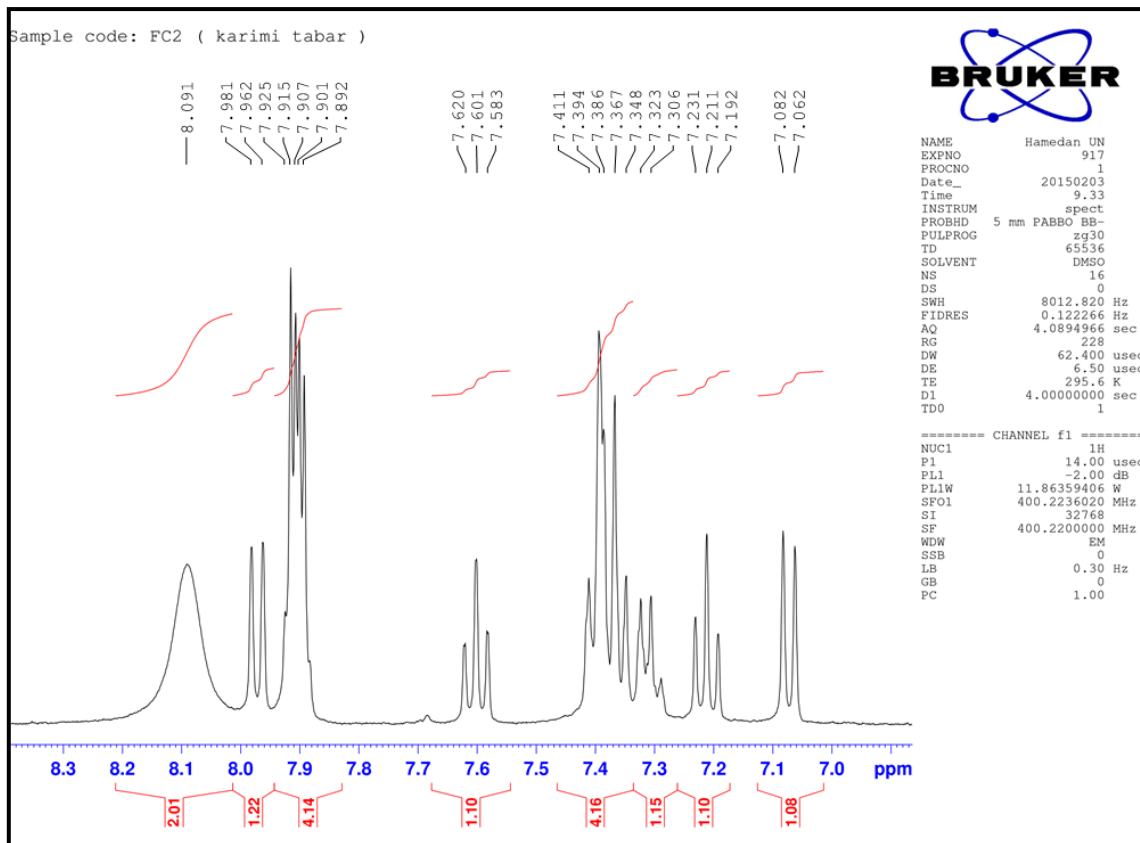
D₂O exchange



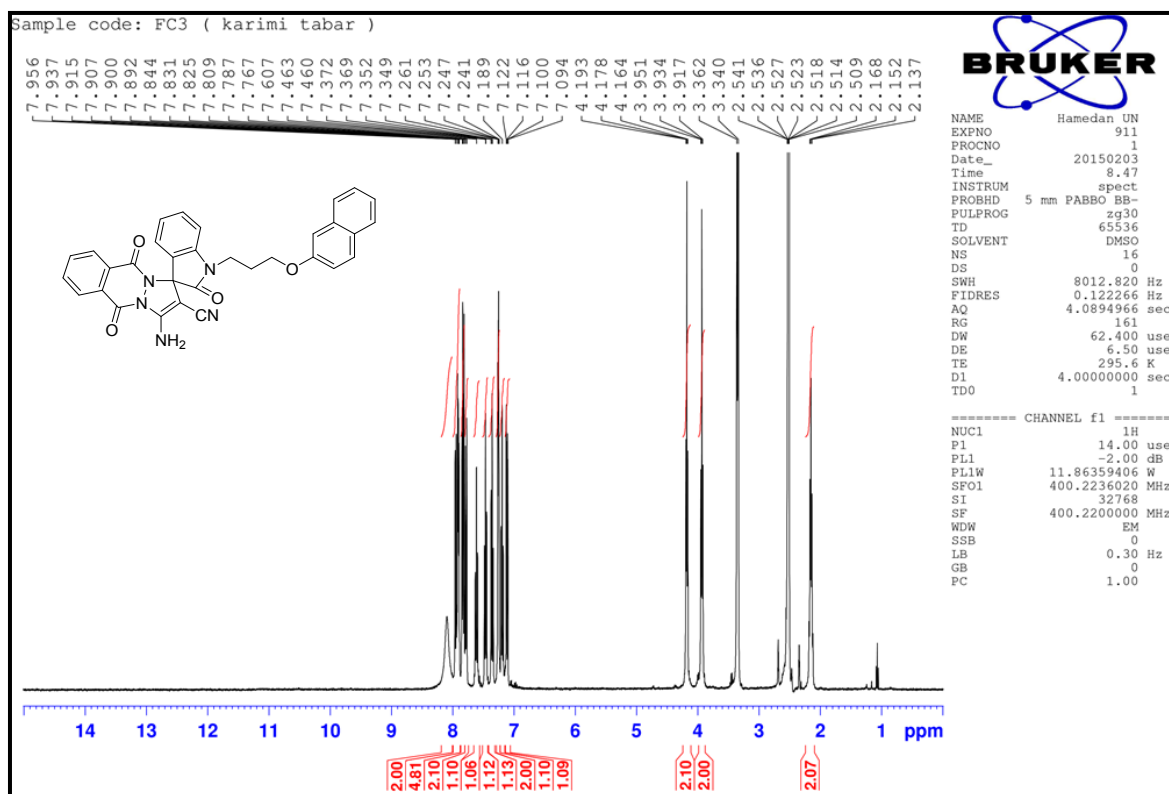


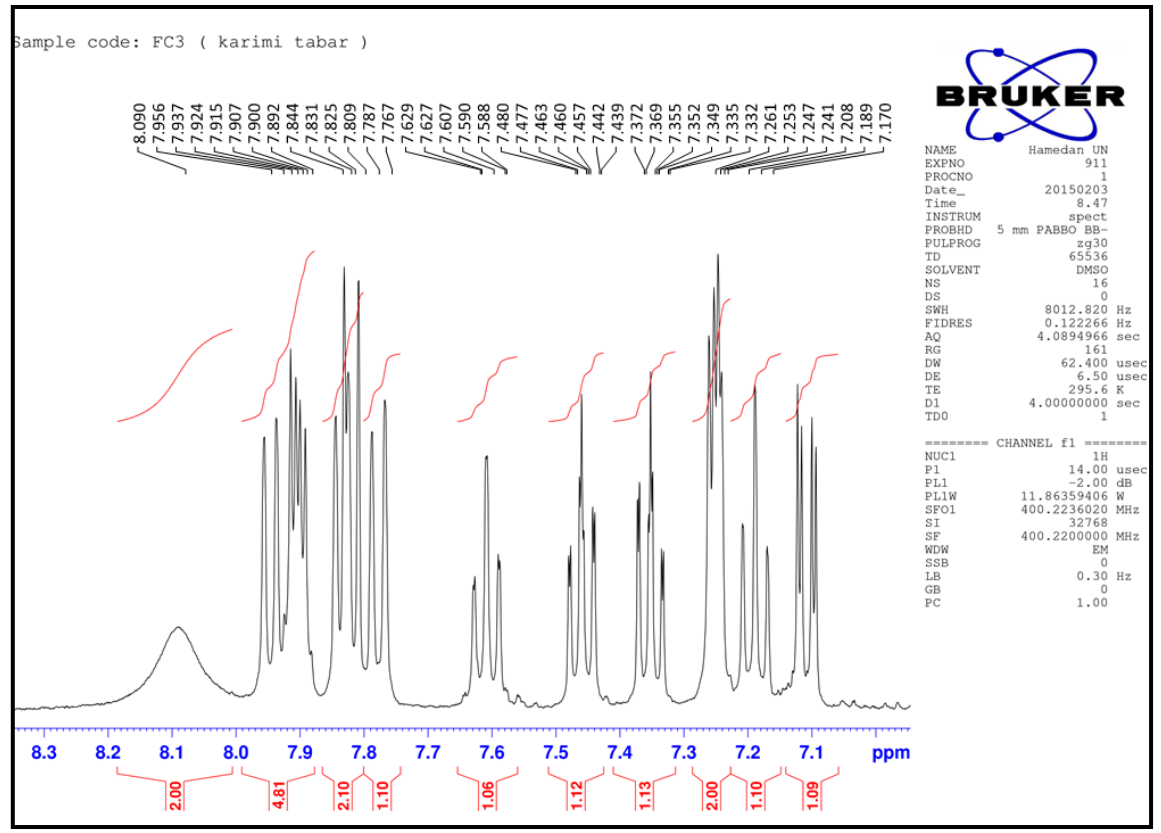
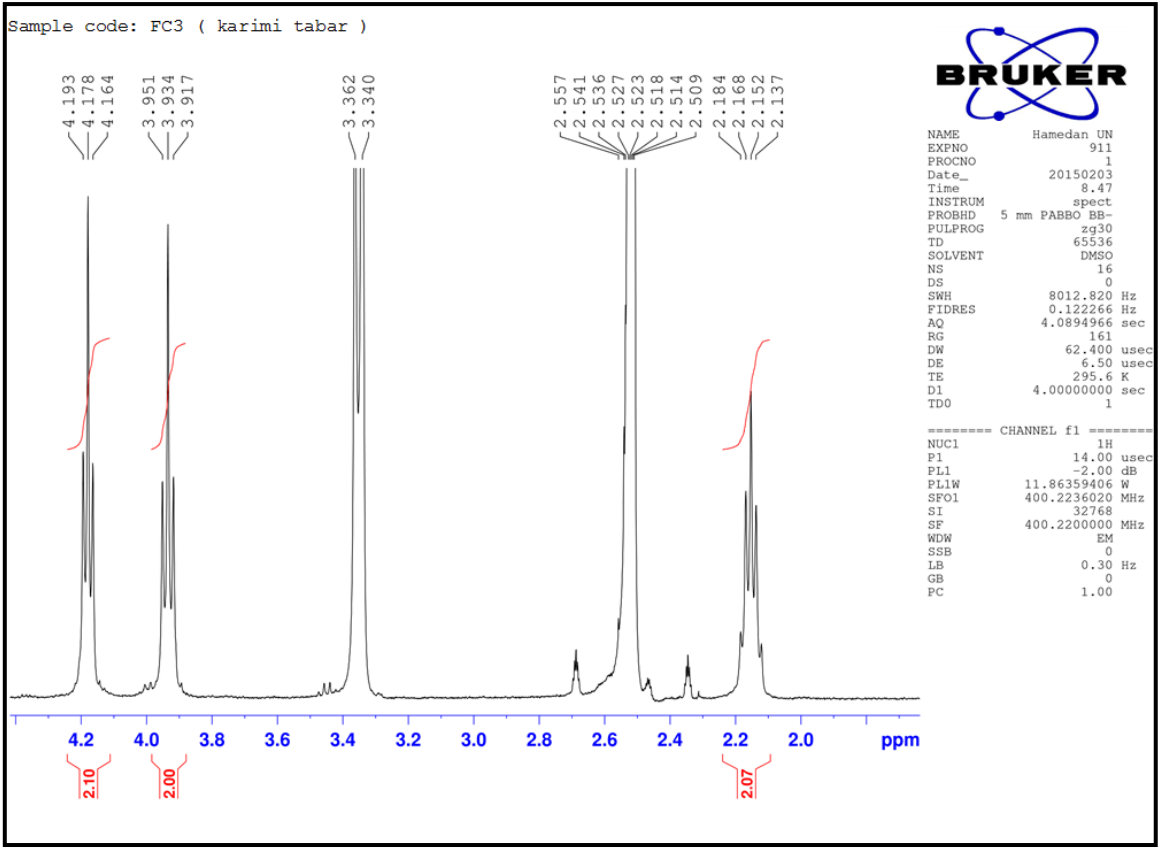
Spiro[indoline-3,1'-pyrazolo[1,2-b]phthalazine] (12b).

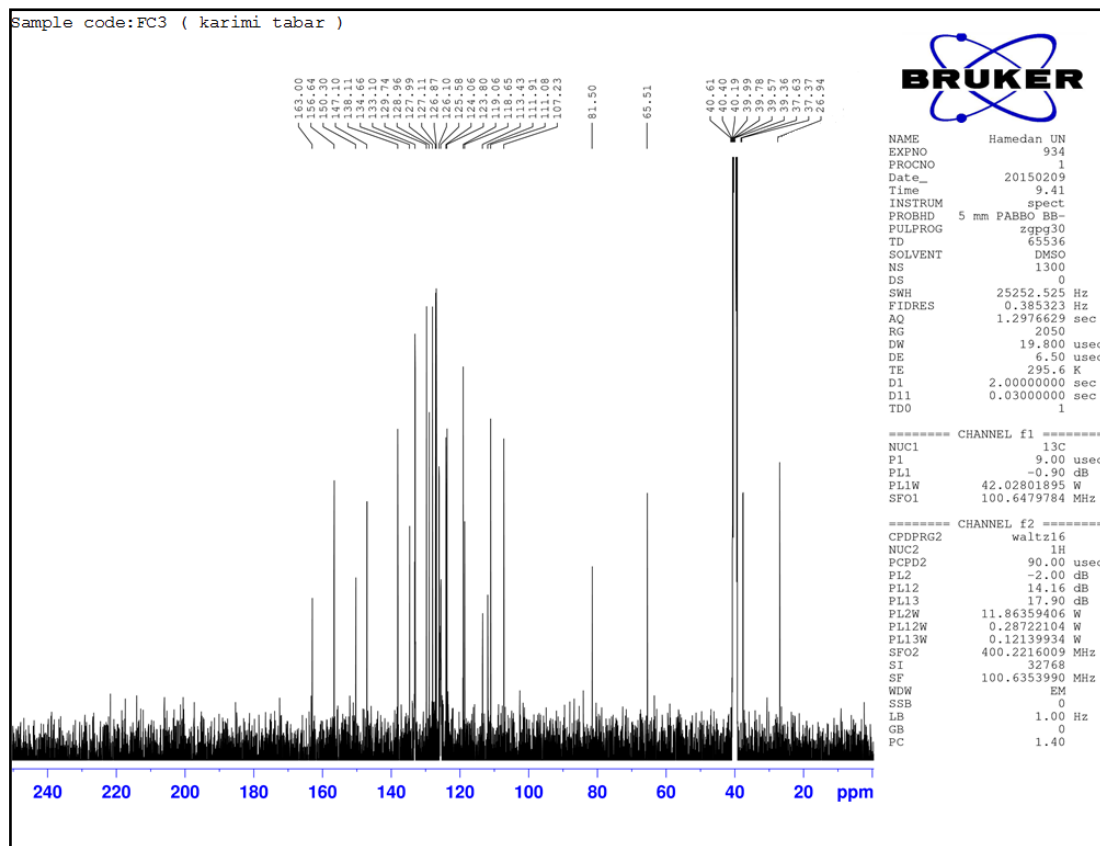




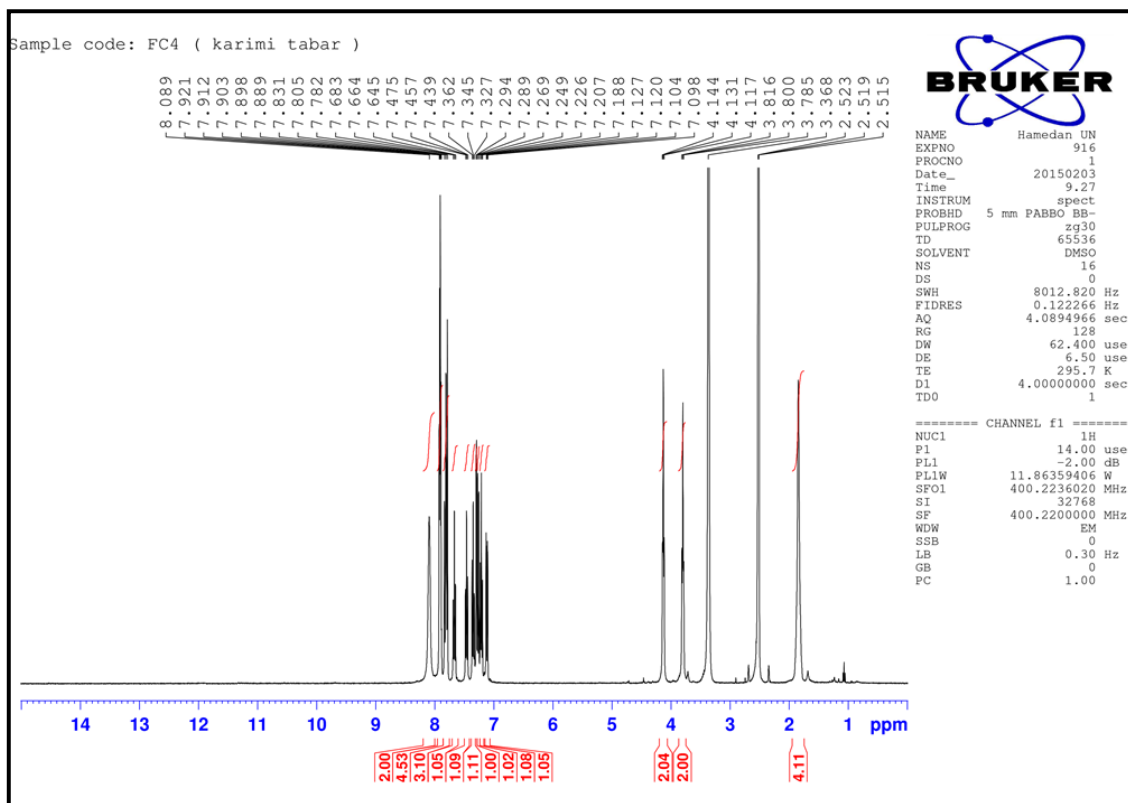
Spiro[indoline-3,1'-pyrazolo[1,2-b]phthalazine] (12c).

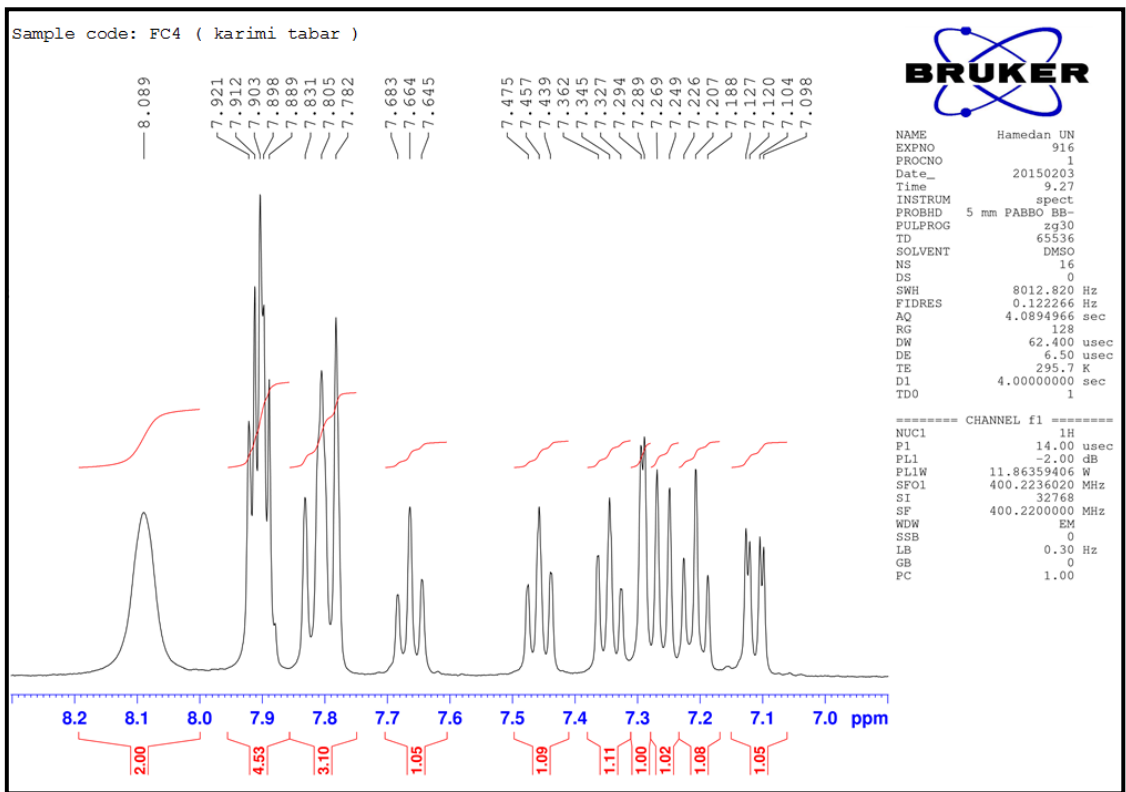
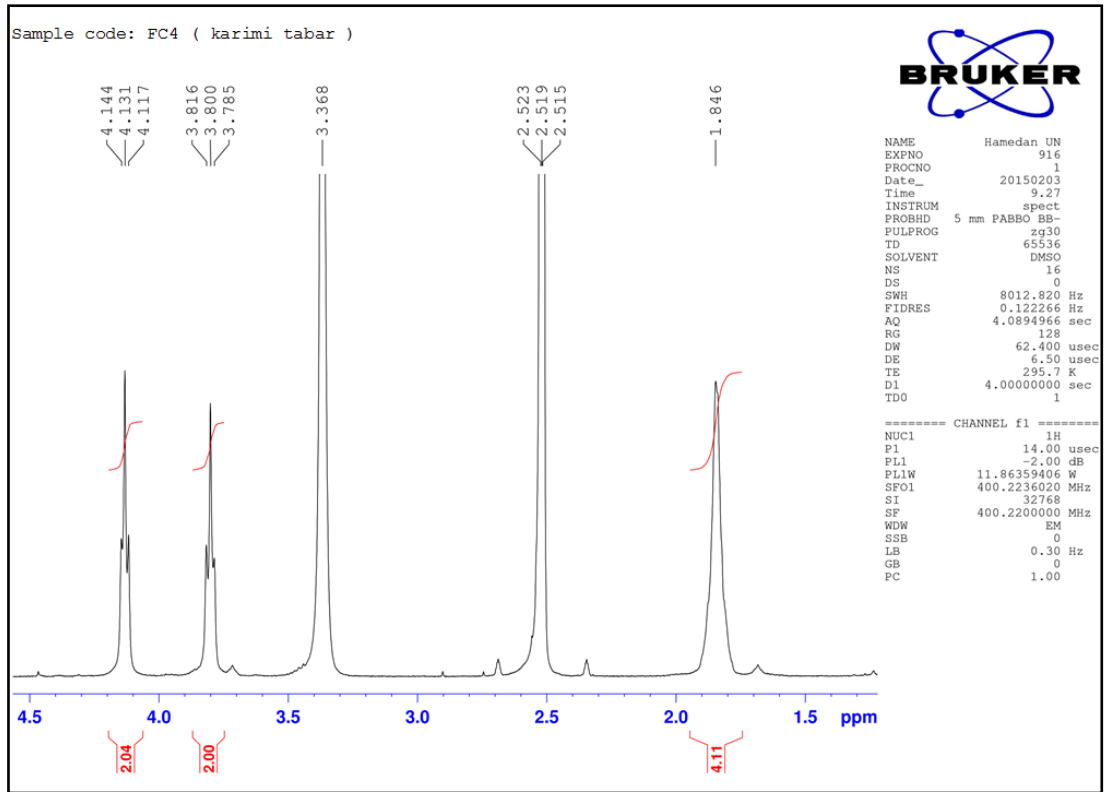




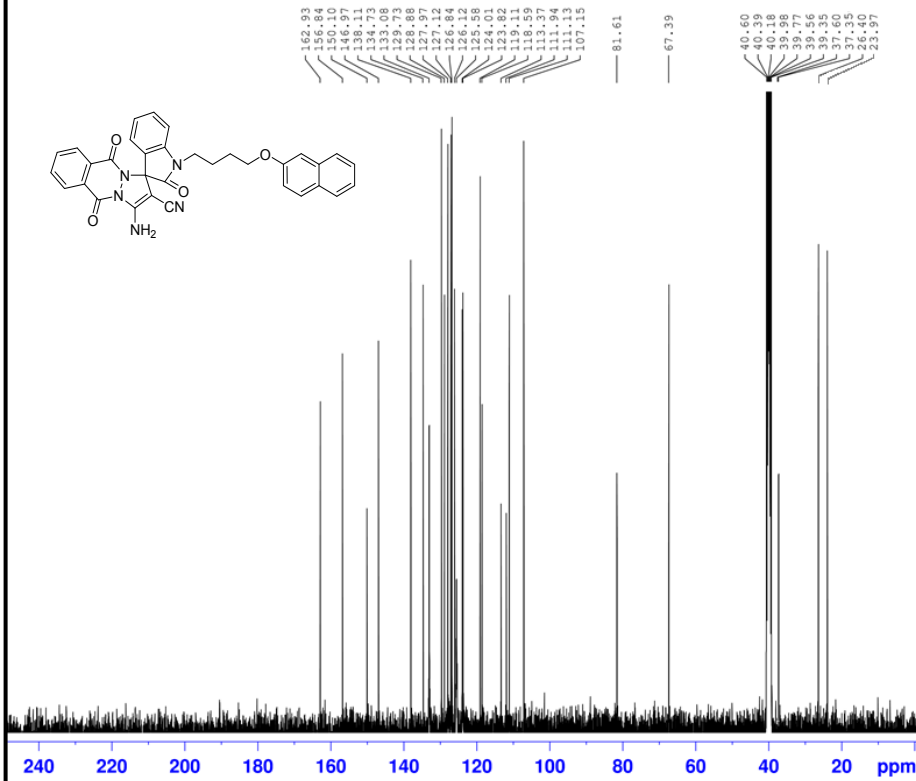


Spiro[indoline-3,1'-pyrazolo[1,2-b]phthalazine] (12d).





Sample code:FC4 (karimi tabar)



NAME Hamedan UN
EXPNO 932
PROCNO 1
Date_ 20150208
Time 14.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 980
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 296.5 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40