Supplementary file

Spectral data of 3,5-dinitrobenzohydrazones:

3,5-dinitrobenzohydrazide (**1**): 1H NMR (400 MHz, DMSO-d6) *δ*H (ppm): 10.52 (s, NH, 1H), 9.02 (d, *J*=2.1 Hz, 2H), 8.93 (m, 1H), 4.78 (s, NH2, 2H). 13C NMR (100 MHz, DMSO-d6) *δ*C: 161.9 (C=O), 148.6, 136.0, 127.6, 120.6.

(*E*)-N'-benzylidene-3,5-dinitrobenzohydrazide (**2**): C14H10N4O5; MW (g/mol): 314.26; White solid;  yield: 64.3%; m.p.: 274°C; IR (ATR)  ν (cm-1): 1662 (C=O), 3178 (N-H), 1627 (N=C), 1530 and 1341 (-NO2). 1H NMR (DMSO-d6, 400 MHz) *δ*H (ppm): 9.10 (s, 2H), 9.00 (m, 1H), 8.48 (s, 1H), 7.78 (s, 2H), 7.49 (m, 3H). 13C NMR (100 MHz, DMSO-d6) *δ*C: 160.0 (C=O), 148.5, 143.0, 135.5, 131.0, 129.4, 127.8, 123.3, 120.8.

(*E*)-3,5-dinitro-N'-(2-nitrobenzylidene)benzohydrazide (**3**): C14H9N5O7; MW (g/mol): 359.25; yellowish solid; yield: 83.5%; m.p.: 276°C ; IR (ATR)  ν (cm-1): 1679 (C=O), 3179 (N-H), 1626 (C=N), 1526 and 1343 (-NO2). 1H NMR (DMSO-d6, 400MHz) *δ*H (ppm): 12.69 (s, 1H, NH), 9.13 (s, 2H), 9.00 (s, 1H), 8.90 (s, 1H), 8.15 (m, 2H), 7.85 (m, 1H), 7.73 (m, 1H). 13C NMR (100 MHz, DMSO-d6) *δ*C: 159.7 (C=O), 148.8, 148.6, 145.4, 136.0, 134.3, 131.6, 128.8, 128.5, 128.4, 125.2, 121.9.

(*E*)-3,5-dinitro-N'-(4-nitrobenzylidene)benzohydrazide (**4**): C14H9N5O7; MW (g/mol): 359.25; yellowish solid; yield: 95.4%; m.p.: 243°C; IR (ATR)  ν (cm-1): 1665 (C=O), 3225 (N-H), 1589 (N=C), 1513 and 1342 (-NO2). 1H NMR (DMSO-d6, 400MHz) *δ*H (ppm): 12.70 (s, 1H, NH), 9.14 (s, 2H), 9.02 (t, *J*=2.1 Hz, 1H), 8.61 (s, 1H), 8.34 (d, *J*=8.8 Hz), 8.05 (d, *J*=8.8 Hz, 2H). 13C NMR (100 MHz, DMSO-d6) *δ*C: 159.9 (C=O), 148.6, 148.6, 147.6, 140.6, 136.1, 128.8, 128.5, 124.6, 122.0.

(*E*)-3,5-dinitro-N'-(4-fluorobenzylidene)benzohydrazide (**5**): C14H9N4O5F; MW (g/mol): 332.25; yellowish solid; yield: 68.9%; m.p.: 233-234oC; IR (ATR)  ν (cm-1): 1667 (C=O), 3176 (N-H), 1628 (N=C), 1536 and 1343 (-NO2), 1230 (C-F). 1H NMR (400 MHz, DMSO-d6) *δ*H (ppm): 12.44 (s, NH, 1H), 9.08 (m, 2H), 8.99 (m, 1H), 8.46 (s, 1H), 7.83 (m, 2H), 7.31 (m, 2H). 13C NMR (100 MHz, DMSO-d6) *δ*C: 163.8 (d, *J=*252.0 Hz), 160.3 (C=O), 148.6, 139.8, 136.0, 129.9 (d, *J=*3.7 Hz), 128.9 (d, *J=*8.8 Hz), 128.0, 121.8, 116.2 (d, *J*=21.9 Hz).

(*E*)-N'-(4-chlorobenzylidene)-3,5-dinitrobenzohydrazide (**6**): C14H9N4O5Cl; MW (g/mol): 348.70; yield: 90.7%; White solid, mp: 275oC; IR (ATR)  ν (cm-1): 1650 (C=O), 3194 (N-H), 1614 (N=C), 1530 and 1344 (-NO2), 1088 (C-Cl). 1H NMR (DMSO-d6, 400MHz) *δ*H (ppm): 12.49 (s, 1H, N-H), 9.13 (s, 2H), 9.01 (t, *J*=2.1 Hz, 8.50 (s, 1H,), 7.81 (d, *J* =8.3 Hz), 7.56 (d, *J*=8.3 Hz). 13C NMR (100 MHz, DMSO-d6) *δ*C (ppm): 159.6, 148.8, 148.7, 136.3, 135.5, 133.3, 129.5, 129.5, 128.4, 121.8.

(*E*)-3,5-dinitro-N'-(3-methoxy-4-hydroxybenzylidene)benzohydrazide (**7**): C15H12N4O7;MW (g/mol): 360.28; yellowish solid; yield: 54.1%; m.p.: 326°C with degradation; IR (ATR)  ν (cm-1): 1678 (C=O), 3220 (N-H), 1625 (N=C), 1531 and 1342 (-NO2), 3340 (O-H), 1273 δ(C-O-C). 1H NMR (400 MHz, DMSO-d6) *δ*H (ppm): 11.70 (s, NH, 1H), 9.00 (m, 2H), 8.95 (m, 1H), 7.61 (s, 1H), 7.15 (d, *J=*1,5 Hz, 1H), 7,06 (dd, *J*=1.8 and 8.4 Hz), 6.94 (d, *J*=8.4 Hz), 3.82 (s, 3H). 13C NMR (100 MHz, DMSO-d6) *δ*C: 160.3 (C=O), 148.7, 148.4, 143.4, 137.2, 127.6, 125.9, 122.9, 121.6, 120.6, 114.8, 107.7, 56.0.

(*E*)-3,5-dinitro-N'-(4-methoxybenzylidene)benzohydrazide (**8**): C15H12N4O6; MW (g/mol): 344.28; yellowish solid; yield: 71.4%; m.p.: 243°C; IR (ATR)  ν (cm-1): 1665 (C=O), 3216 (N-H), 1629 (N=C), 1538 and 1343 (-NO2), 1288 δ (C-O-C). 1H NMR (400 MHz, DMSO-d6) *δ*H (ppm): 11.34 (s, NH, 1H), 9.06 (m, 2H), 9.00 (m, 1H), 7.85 (d, *J*=8.1 Hz, 2H), 7.62 (s, 1H), 7.02 (d, *J*=8.1 Hz, 2H), 3.82 (s, 3H). 13C NMR (100 MHz, DMSO-d6) *δ*C: 160.3 (C=O), 158.6, 148.4, 147.9, 137.2, 130.4, 128.7, 127.8, 121.4, 114.2, 55.8.

(*E*)-N'-(2-hydroxybenzylidene)-3,5-dinitrobenzohydrazide (**9**): C14H10N4O6; MW (g/mol): 330.25; yellow solid, yield: 71.0%; m.p. 256°C; IR (ATR) ν (cm-1): 1691 (C=O), 3102 (N-H), 1616 (N=C), 1532 and 1348 (-NO2), 3336 (OH). 1H NMR (DMSO-d6, 400MHz) *δ*H (ppm): 12.59 (s, 1H), 9.14 (d, *J*=2.2 Hz), 8.99 (m, 1H), 8.72 (s, 1H), 7.63 (m, 1H), 7.33 (m, 1H), 6.94 (m, 2H). 13C NMR (100 MHz, DMSO-d6) *δ*C 159.2, 157.8, 149.5, 148.6, 135.9, 133.0, 132.4, 128.3, 121.8, 119.9, 119.1, 116.8.

 (*E*)-N'-(furan-2-ylmethylene)-3,5-dinitrobenzohydrazide (**10**): C12H8N4O6; MW (g/mol): 304.22; White solid; yield: 67.4%; m.p. 246°C with degradation; IR (ATR)  ν (cm-1): 1651 (C=O), 3173 (N-H), 1630 (N=C), 1533 and 1343 (-NO2), 1290 (C-O-C). 1H NMR (DMSO-d6, 400MHz) *δ*H (ppm): 12.37 (s, 1H, N-H), 9.11 (s, 2H), 9.01 (s, 1H), 8.38 (s, 1H), 7.92 (m, 1H), 7.04 (m, 1H), 6.69 (m, 1H). 13C NMR (100 MHz, DMSO-d6): *δ*C 159.4 (C=O), 149.4, 148.7, 146.2, 139.7, 136.3, 128.3, 121.6, 115.3, 112.8.

(*E*)-3,5-dinitro-N'-(thiophen-2-ylmethylene)benzohydrazide (**11**): C12H8N4O5S; MW(g/mol): 320.29; White solid; yield: 62.1%; IR (ATR)  ν (cm-1): 1652 (C=O), 3177 (N-H), 1627 (N=C), 1530 and 1339 (-NO2), 836 (C-S-C). 1H NMR (DMSO-d6, 400MHz) *δ*H (ppm): 12.38 (s, 1H, N-H), 9.11 (s, 2H), 9.01 (s, 1H), 8.71 (s, 1H), 7.75 (m, 1H), 7.57 (m, 1H), 7.19 (m, 1H). 13C NMR (100 MHz, DMSO-d6): *δ*C 159.3 (C=O), 148.7, 145.1, 139.0, 136.4, 132.4, 130.2, 128.5, 128.3, 121.7.

(*E*)-3,5-dinitro-N'-[1-(4-methoxyphenyl)ethylidene]benzohydrazide (**12**): C15H12N4O5; MW(g/mol): 328.28; White solid; Yield: 64.1%; IR (ATR)  ν (cm-1): 1657 (C=O), 3177 (N-H), 1627 (N=C), 1528 and 1344 (-NO2), 2969 (CHsp3). 1H NMR (DMSO-d6, 400MHz): *δ*H (ppm): 11.39 (s, 1H, N-H), 9.08 (s, 2H), 9.01 (m), 7.90 (s, 1H), 7.80 (m, 1H), 7.48 (m, 2H), 7.37 (s, 1H), 2.40 (s, 3H). 13C NMR (100 MHz, DMSO-d6): *δ*C 160.5 (C=O), 158.4, 148.4, 138.1, 137.1, 130.5, 130.3, 128.9, 127.1, 121.4, 15.6.

(*E*)-3,5-dinitro-N'-(4-methoxy-fluorobenzylidene)benzohydrazide (**13**): C16H14N4O6; MW (g/mol): 358.31; yellowish solid; yield: 66.5%; IR (ATR)  ν (cm-1): 1670 (C=O), 3246 (N-H), 1623 (N=C), 1533 and 1343 (-NO2), 2846 (C-H)sp3, 1253 δ(C-O-C).

(*E*)-N’-cyclohexylidene-3,5-dinitrobenzohydrazide (**14**): C13H14N4O5; MW (g/mol): 306.28; yellowish solid; yield: 46.3%; IR (ATR)  ν (cm-1): 1657 (C=O), 3177 (N-H), 1629 (N=C), 1528 and 1344 (-NO2), 2877 (C-H)sp3.

Ethyl-(2*E)-*2-[2-(3,5-dinitrobenzoyl)hydrazinylidene]propanoate (**15**): C11H10N4O7; MW (g/mol): 310.22; yellowish solid; yield: 52.6%; (ATR)  ν (cm-1): 1668 (C=O), 3239 (N-H), 1626 (N=C), 1538 and 1342 (-NO2), 1727 (C=O)ester.1H NMR (400 MHz, DMSO-d6) *δ*H (ppm): 11.46 (s, NH, 1H), 9.01 (d, *J*=2.1 Hz, 2H), 8.95 (m, 1H), 4.20 (m, 2H), 2.20 (s, 1H), 1.13 (t, 3H). 13C NMR (100 MHz, DMSO-d6) *δ*C: 164.8 (C=O), 161.9 (C=O), 148.3, 147.9, 136.3, 129.2, 121.9, 61.8, 14.4, 13.0.

(*E*)-3,5-dinitro-N'-(2-oxo-1,2-dihydro-3*H*-indol-3-ylidene)benzohydrazide (**16**): C15H9N5O6; MW (g/mol): 355.27; yellowish solid; yield: 61.1%; IR (ATR)  ν (cm-1): 1670 (C=O), 3177 (N-H), 1604 (N=C), 1546 and 1342 (-NO2), 2882 (C-H)sp3, 1743 (C=O)amide. 1H NMR (400 MHz, DMSO-d6) *δ*H (ppm): 14.10 (s, NH, 1H), 11.41 (s, NH, 1H), 9.14 (m, 2H), 9.04 (m, 1H), 7.60 (m, 1H), 7.42 (m, 1H), 7.11 (m, 1H), 6.96 (m, 1H). 13C NMR (100 MHz, DMSO-d6): *δ*C 163.5 (C=O), 160.6 (C=O), 148.8, 143.3, 135.5, 132.8, 128.0, 123.4, 122.4, 119.9, 111.9.

(*E*)-1-(3,5-dinitrophenyl)-2-(1,7,7-trimethylbicyclo[2.2.1]heptan-2-ylidene)hydrazine (**17**): C17H20N4O5; W.M (g/mol): 360.37; White solid; yield: 41.8%; IR (ATR)  ν (cm-1): 1643 (C=O), 3172 (N-H), 1624 (N=C), 1536 and 1342 (-NO2), 2955 and 2872 (C-H). 1H NMR (400 MHz, DMSO-d6) *δ*H (ppm): 10.86 (s, NH, 1H), 9.00 (m, 2H), 8.95 (m, 1H), 2.51 (m), 2.15 (m), 1.97 (m), 1.22-1.36 (m), 1.00 (s, 3H), 0.92 (s, 3H), 0.77 (s, 3H). 13C NMR (100 MHz, DMSO-d6) *δ*C: 176.9 (C=N), 159.9 (C=O), 148.4, 137.3, 128.4, 121.3, 53.4, 48.1, 43.7, 35.6, 32.7, 27.2, 19.8, 18.9, 11.8.