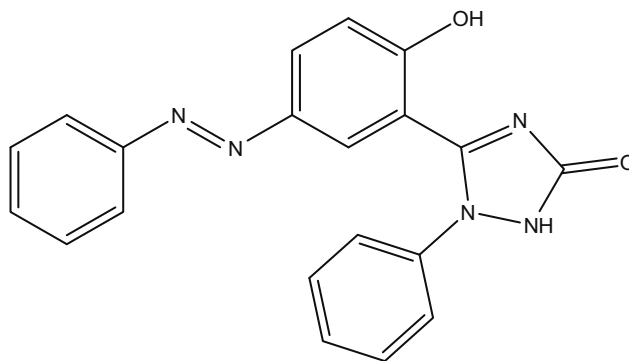


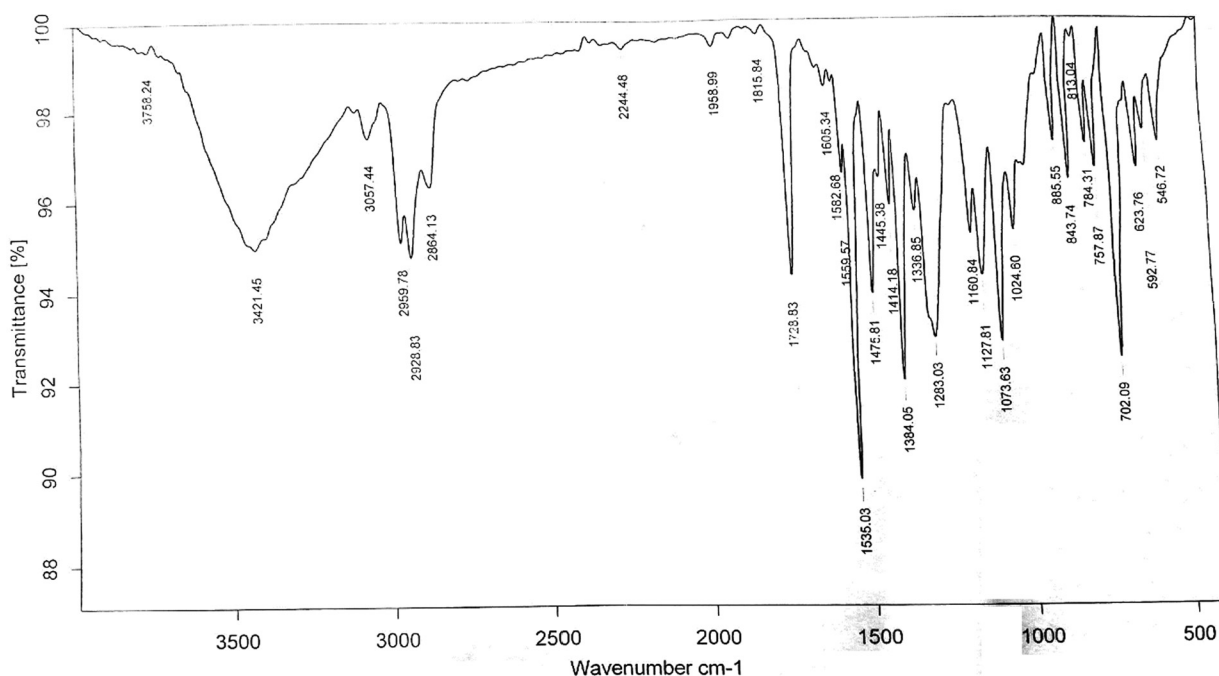
Supplementary material

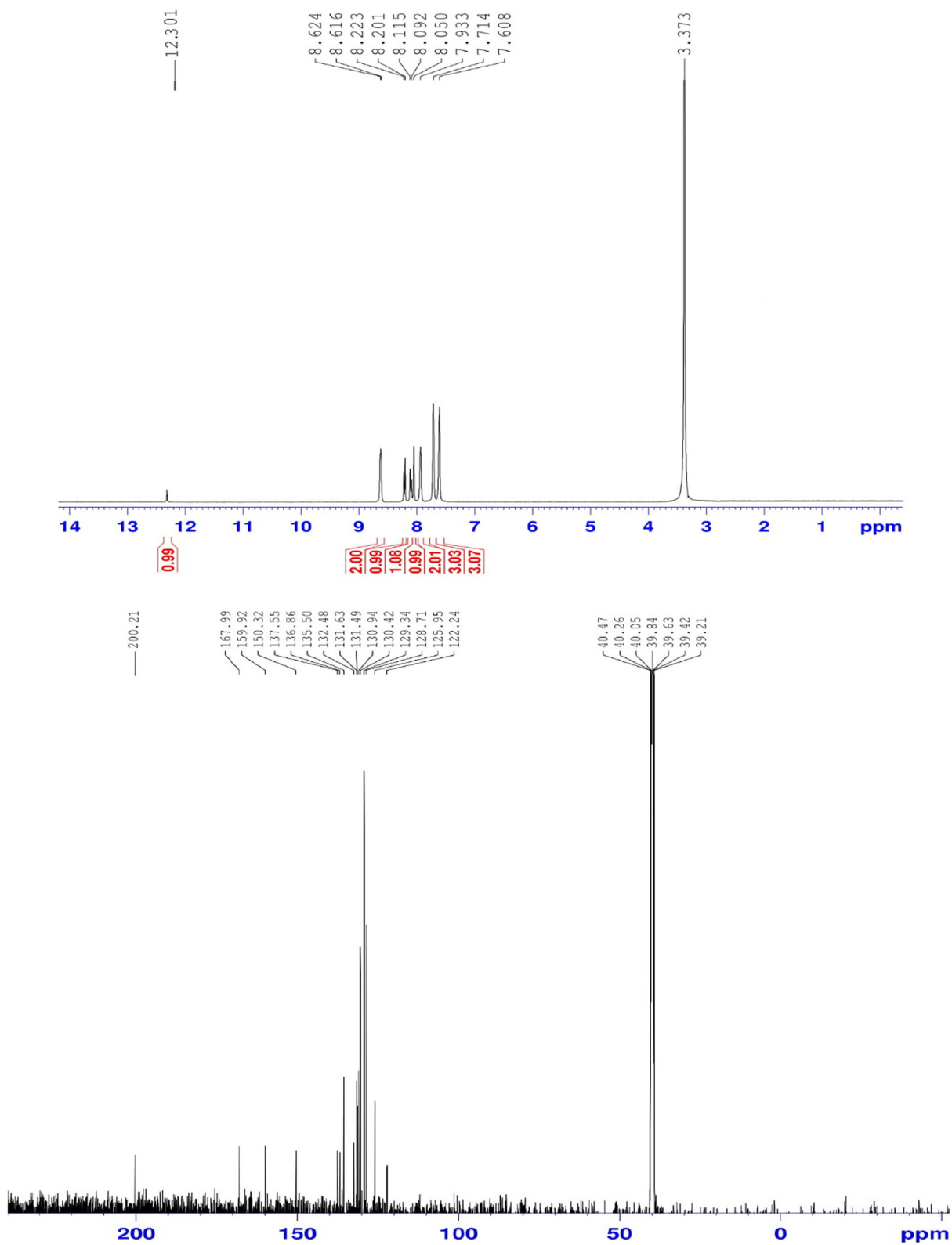


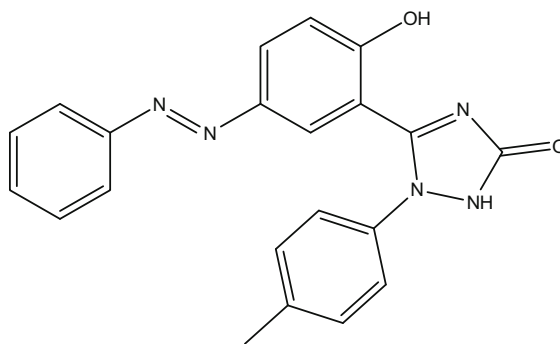
5a

5-(2-hydroxy-5-(phenyldiazenyl)phenyl)-1-phenyl-1H-1,2,4-triazol-3(2H)-one (5a)

White solid, m.p. 231–233°C; FT-IR (KBr) (ν_{max} cm⁻¹): 3421 (O–H), 3057 (CH-Ar), 2981 (CH-Aliphatic), 1738 (C=O), 1582, and 1535 (C=C, Ar); ¹H NMR (400 MHz, DMSO-*d*₆) δ : 12.30 (s, 1H, OH), 8.63 (t, *J* = 2.8 Hz, 2H), 8.21 (d, *J* = 8.2 Hz, 1H), 8.11 (d, *J* = 8.2 Hz, 1H), 8.04 (s, 1H), 7.94 (d, *J* = 2.8 Hz, 2H), 7.72 (s, 3H), 7.57–7.63 (m, 3H) ppm; ¹³C NMR (100 Hz, DMSO-*d*₆) δ : 200.2, 168.1, 160.0, 150.3, 137.6, 136.8, 135.5, 132.5, 131.6, 131.4, 131.0, 130.3, 129.3, 128.8, 126.0, 122.2 ppm. HRMS (*m/z* 357.12). Anal. Calc. for C₂₀H₁₅N₅O₂: C, 67.22; H, 4.23; N, 19.60. Found: C, 67.20; H, 4.22; N, 19.63.

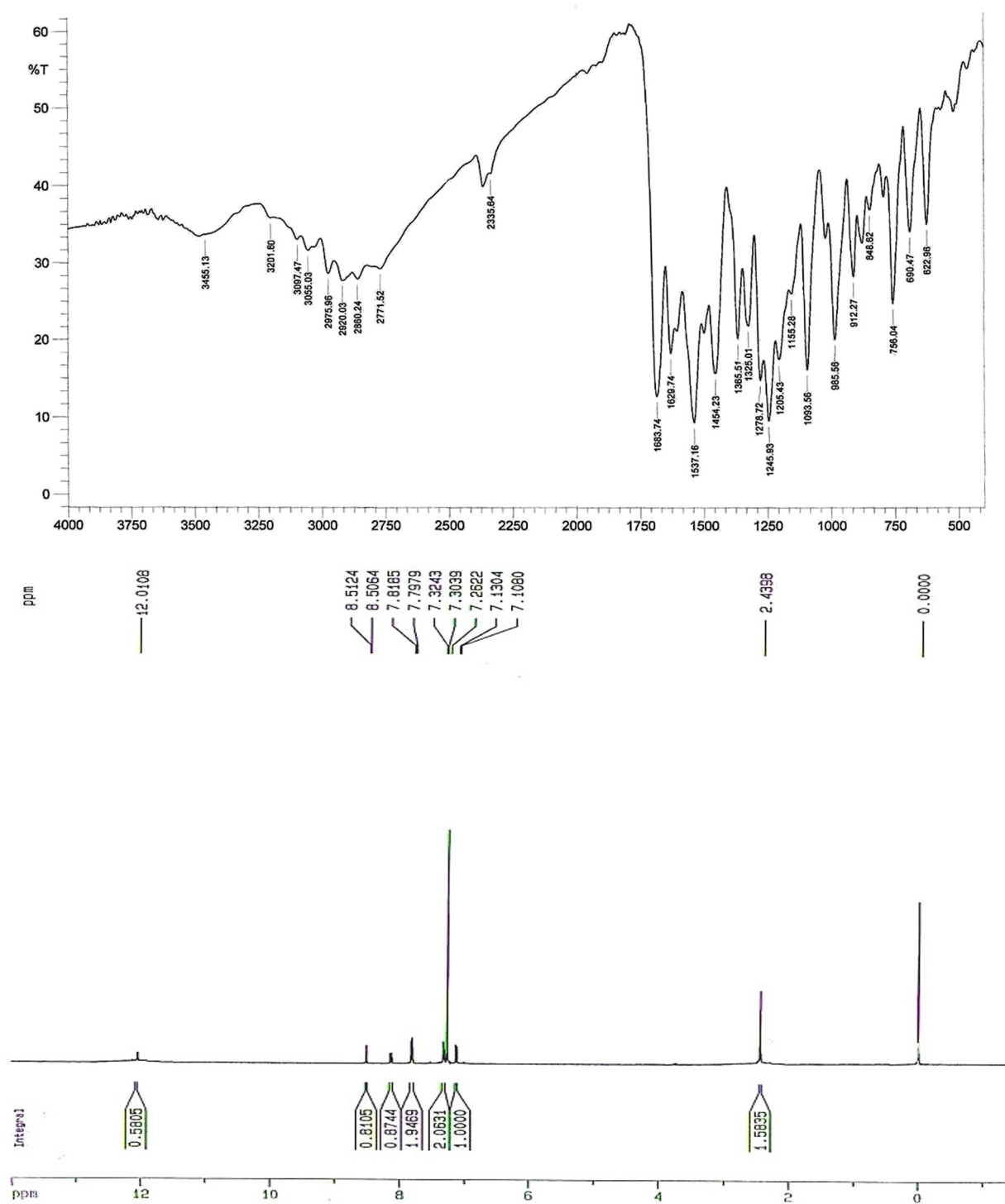


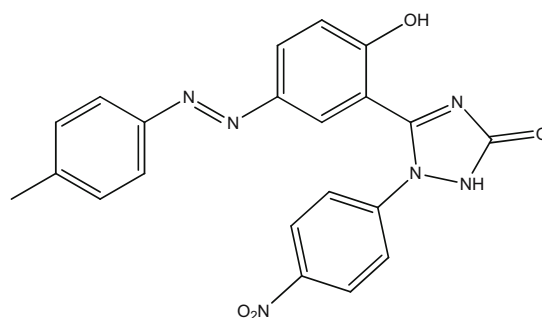
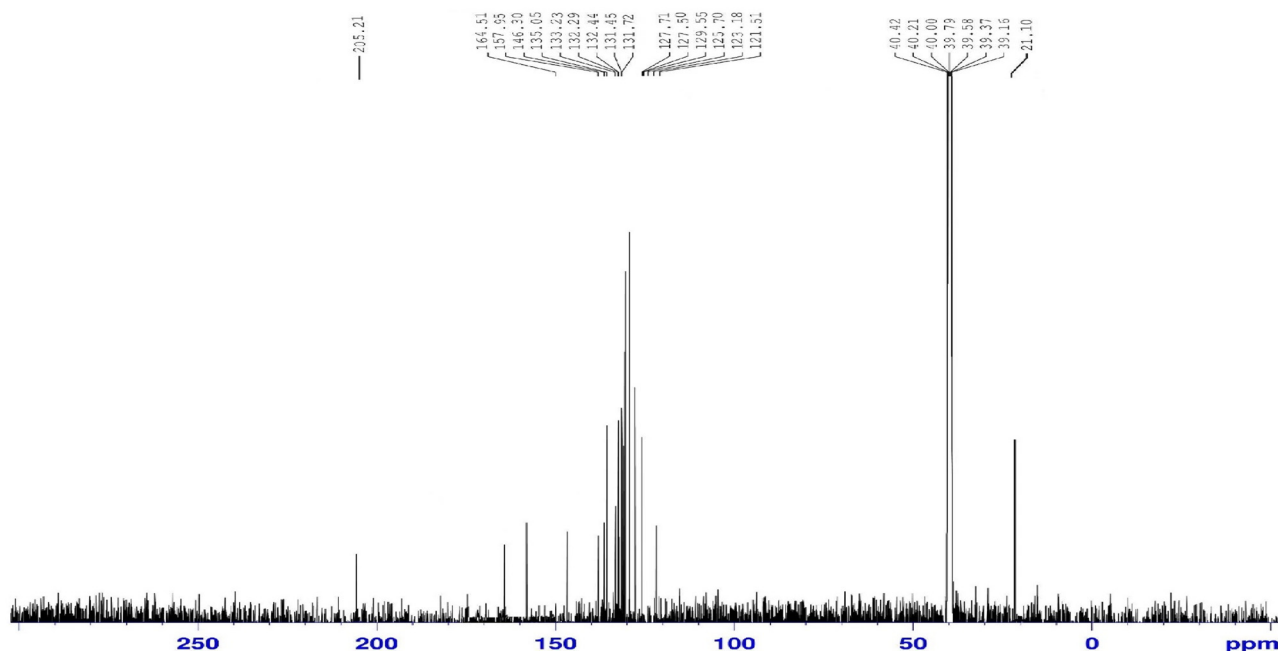


**5b**

5-(2-hydroxy-5-(phenyldiazenyl)phenyl)-1-(p-tolyl)-1H-1,2,4-triazol-3(2H)-one (5b)

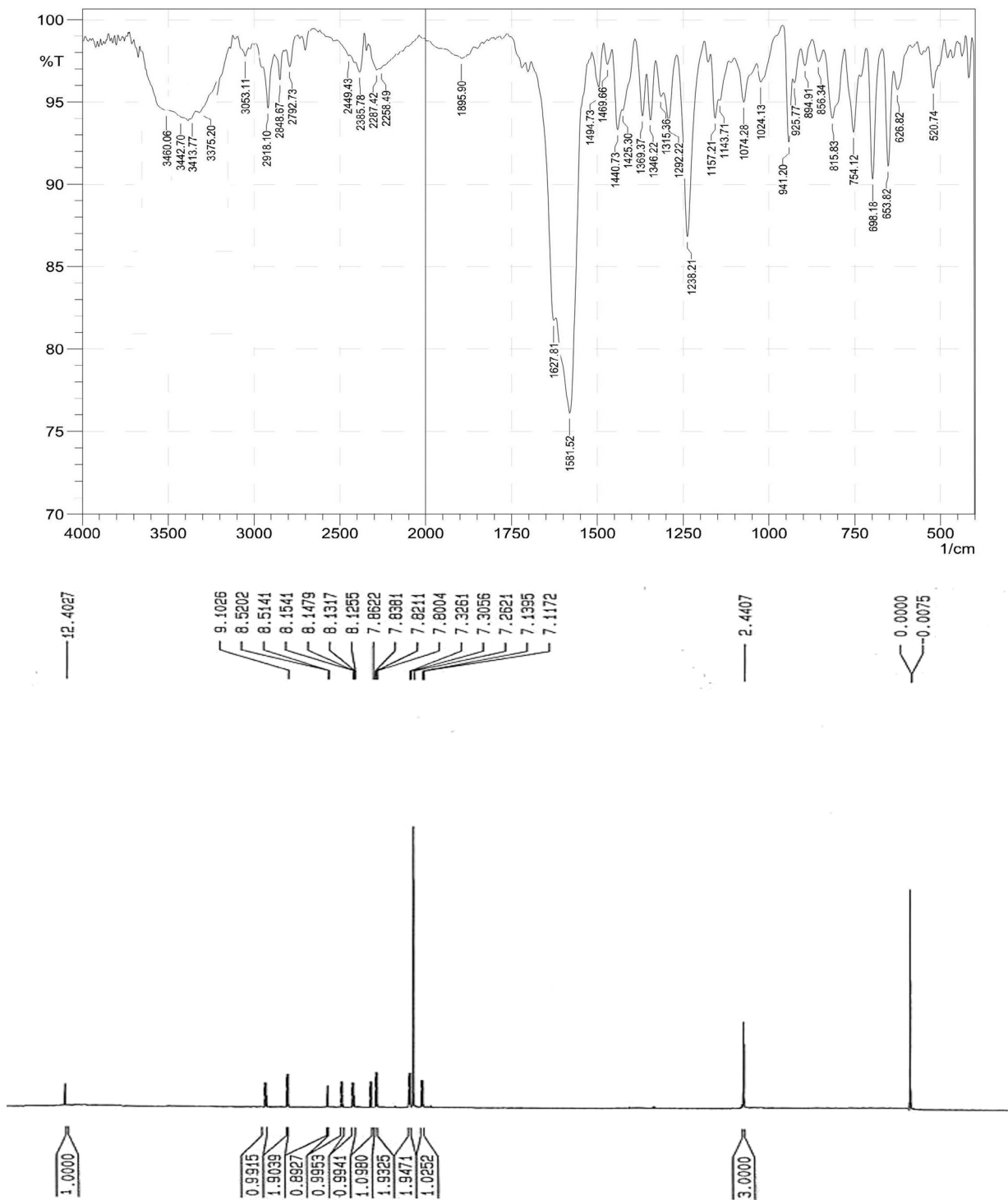
White solid, m.p. 206–208°C; FT-IR (KBr) (ν_{max} cm^{-1}): 3041 (CH-Ar), 2985 (CH-Aliphatic), 1635 (C=O), 1573, and 1554 (C=C, Ar); ^1H NMR (400 MHz, CDCl_3) δ : 12.01 (s, 1H, OH), 8.51 (d, $J = 2.2$ Hz, 1H), 8.32 (d, $J = 8.2$ Hz, 1H), 7.80 (d, $J = 8.2$ Hz, 4H), 7.30 (d, $J = 7.8$ Hz, 4H), 7.11 (d, $J = 8.2$ Hz, 2H), 2.44 (s, 3H, CH_3) ppm; ^{13}C NMR (100 Hz, $\text{DMSO}-d_6$) δ : 201.1, 165.7, 159.3, 157.2, 146.1, 136.0, 133.6, 133.3, 131.9, 131.0, 129.4, 129.6, 129.1, 125.2, 123.5, 121.4, 21.1 (CH_3) ppm. HRMS (m/z 371.14). Anal. Calc. for $\text{C}_{21}\text{H}_{17}\text{N}_5\text{O}_2$: C, 67.91; H, 4.61; N, 18.86. Found: C, 67.90; H, 4.63; N, 18.88.

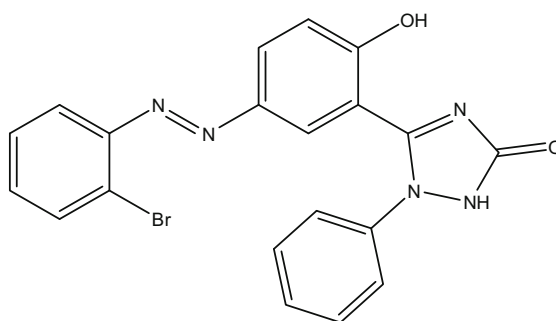
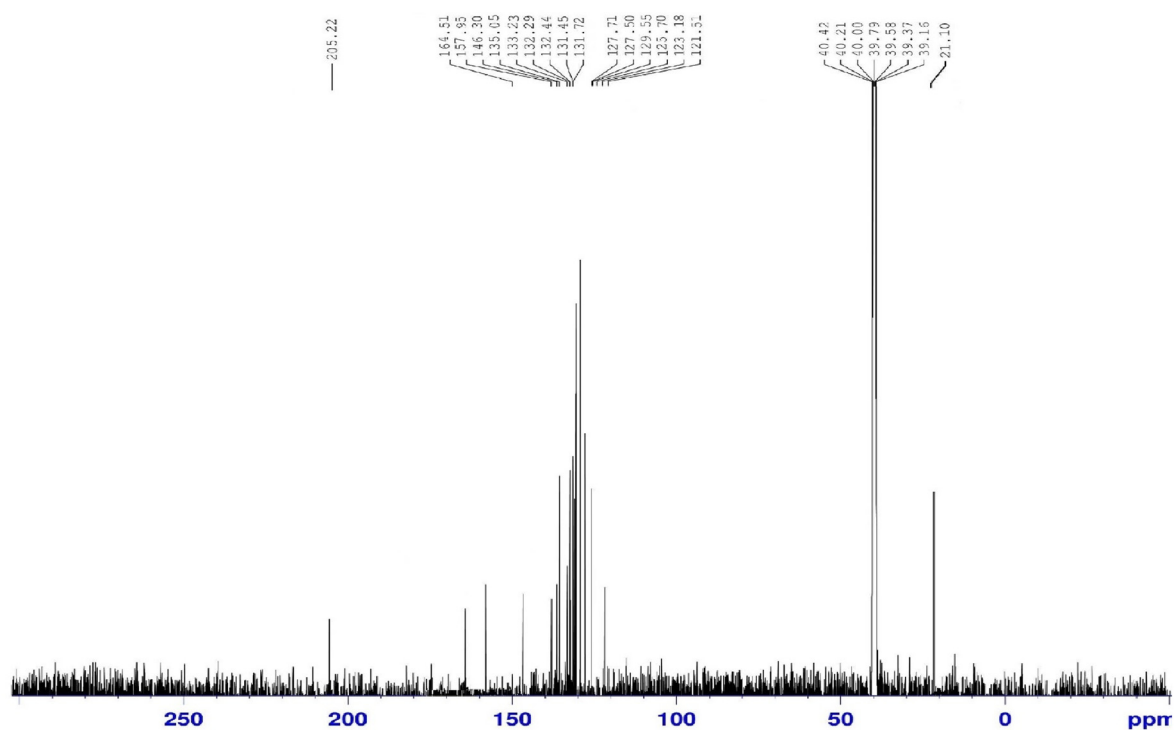


**5c**

5-(2-hydroxy-5-((2-nitrophenyl)diazenyl)phenyl)-1-(p-tolyl)-1H-1,2,4-triazol-3(2H)-one (5c)

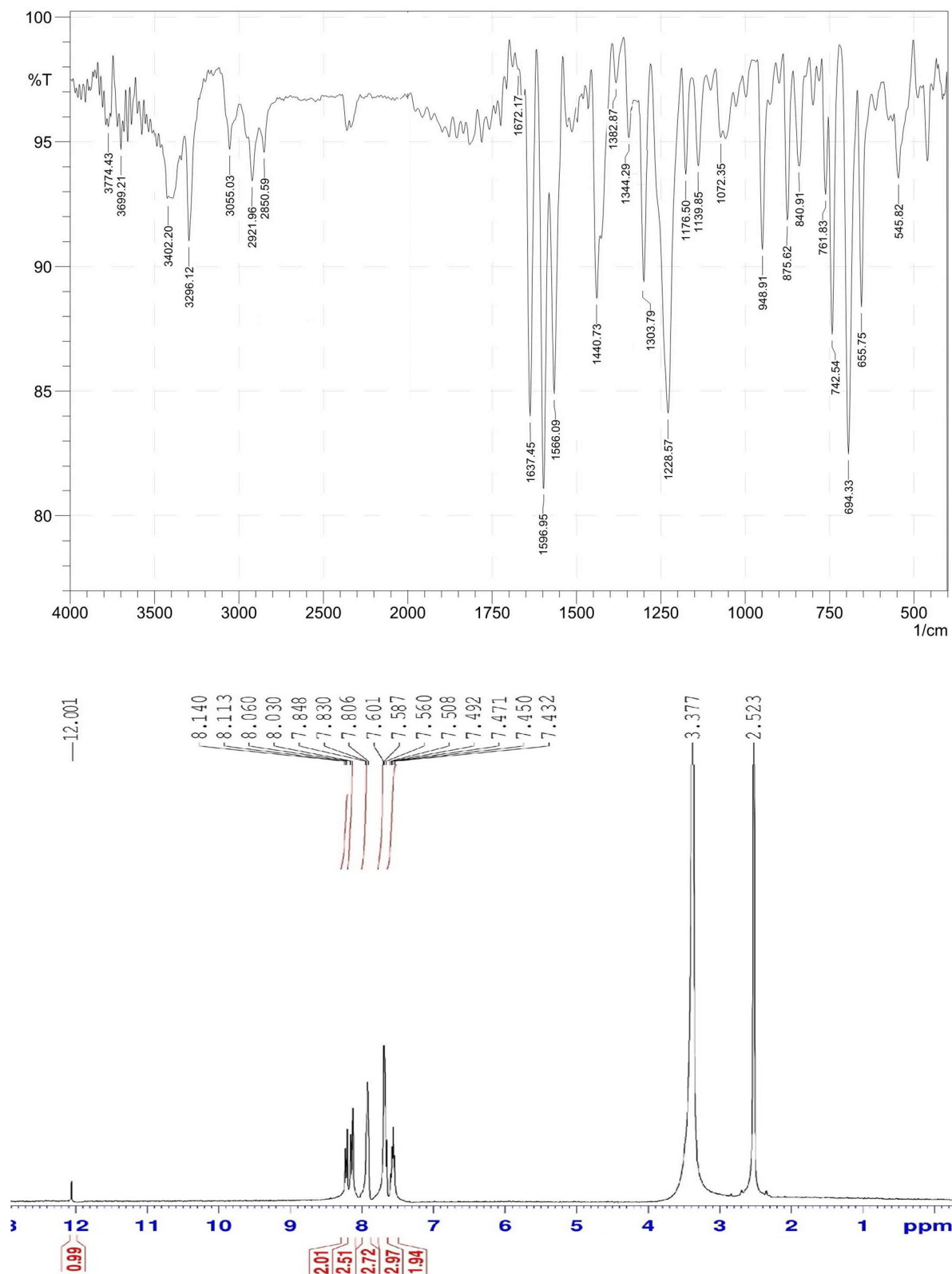
Off-white solid, m.p. 212–214°C; FT-IR (KBr) ($\nu_{\max}$ cm⁻¹): 3027 (CH-Ar), 2963 (CH-Aliphatic), 1605 (C=O), 1581, and 1556 (C=C, Ar), 1351 (NO₂); ¹H NMR (400 MHz, CDCl₃) δ : 12.40 (s, 1H, OH), 9.11 (s, 1H), 8.50 (d, J = 2.6 Hz, 2H), 8.30 (d, J = 2.8 Hz, 1H), 8.31 (d, J = 7.8 Hz, 1H), 8.06 (d, J = 7.8 Hz, 1H), 7.82 (d, J = 8.2 Hz, 1H), 7.80 (d, J = 8.2 Hz, 2H), 7.33 (d, J = 8.2 Hz, 2H), 7.11 (d, J = 8.2 Hz, 1H), 2.45 (s, 3H, CH₃) ppm; ¹³C NMR (100 Hz, DMSO-*d*₆) δ : 201.2, 164.3, 157.2, 149.4, 138.4, 135.7, 133.8, 133.6, 131.2, 131.1, 128.1, 127.1, 125.3, 123.4, 121.4, 21.2 (CH₃) ppm. HRMS (m/z 416.12). Anal. Calc. for C₂₁H₁₆N₆O₄: C, 60.57; H, 3.87; N, 20.18. Found: C, 60.59; H, 3.85; N, 20.16.

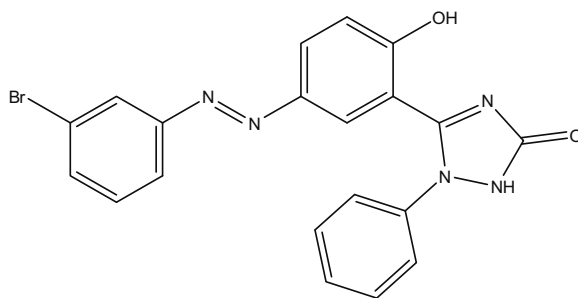
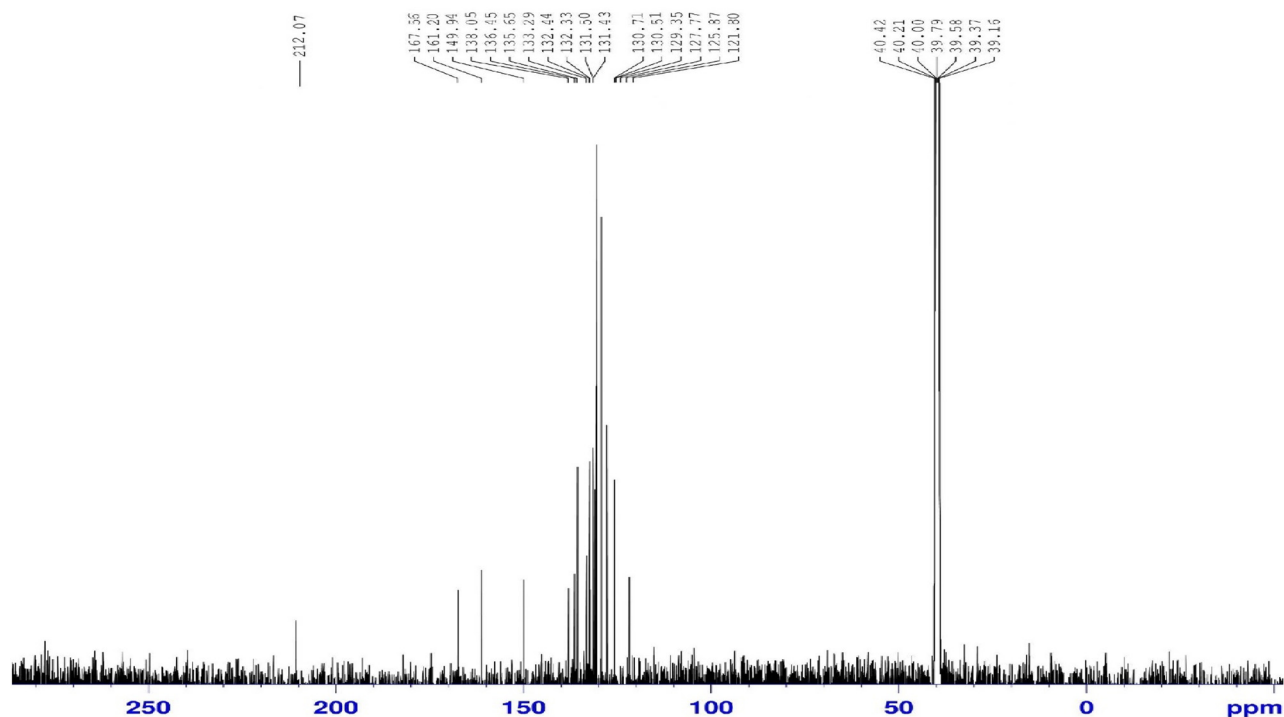


**5d**

5-(5-((2-bromophenyl)diazenyl)-2-hydroxyphenyl)-1-phenyl-1H-1,2,4-triazol-3(2H)-one (5d)

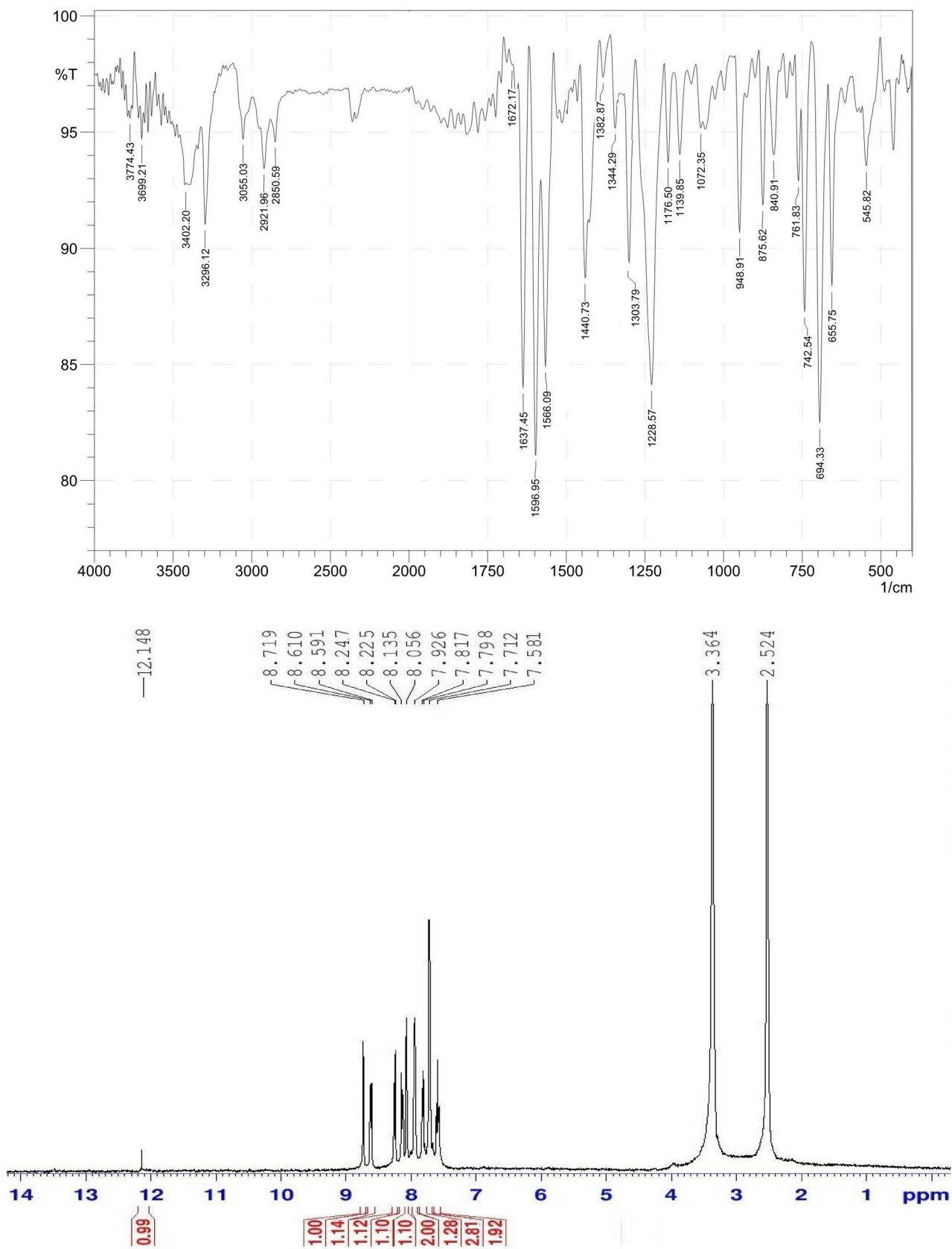
White solid, m.p. 221–223°C; FT-IR (KBr) ($\nu_{\max}$ cm^{-1}): 3402 (O–H), 3055 (CH–Ar), 2922 (CH–Aliphatic), 1638 (C=O), 1566, and 1520 (C=C, Ar), 1228 (C–O); ^1H NMR (400 MHz, DMSO- d_6) δ : 12.01 (s, 1H, OH), 8.15 (d, J = 8.2 Hz, 2H), 8.07–8.03 (m, 3H), 7.82 (s, br., 3H), 7.53–7.62 (m, 3H), 7.42–7.50 (m, 2H) ppm; ^{13}C NMR (100 Hz, DMSO- d_6) δ : 211.3, 164.5, 163.1, 152.2, 148.3, 142.4, 138.3, 134.9, 133.3, 133.0, 131.8, 131.6, 130.5, 129.6, 129.1, 127.0, 125.4, 121.9 ppm. HRMS (m/z 435.03). Anal. Calc. for $\text{C}_{20}\text{H}_{14}\text{BrN}_5\text{O}_2$: C, 55.06; H, 3.23; N, 16.05. Found: C, 55.09; H, 3.26; N, 16.02.

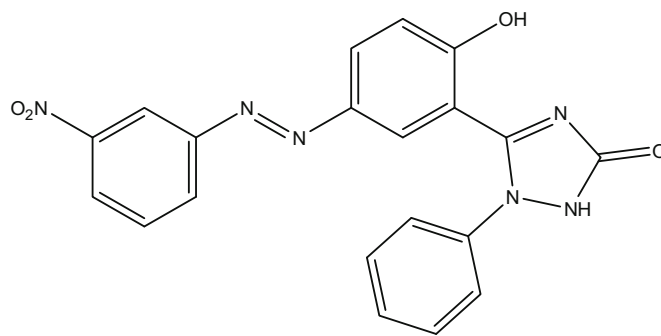
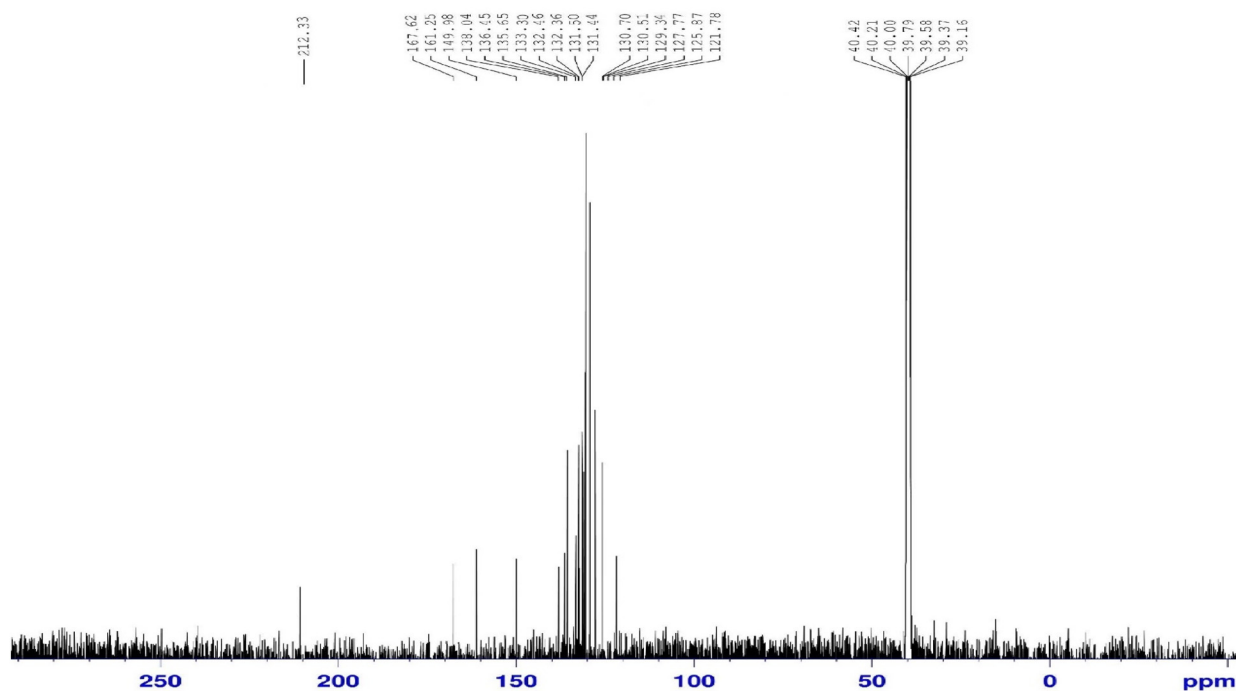


**5e**

5-((3-bromophenyl)diazenyl)-2-hydroxyphenyl-1-phenyl-1H-1,2,4-triazol-3(2H)-one (5e**)**

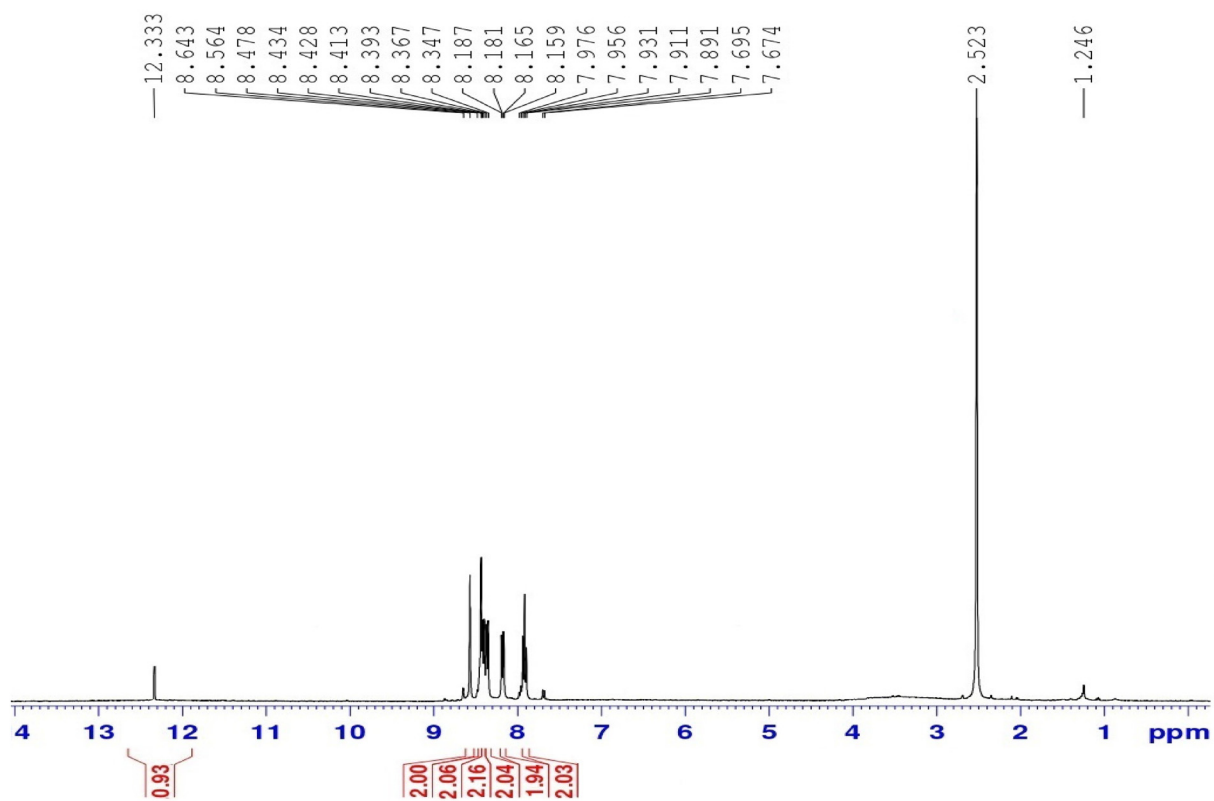
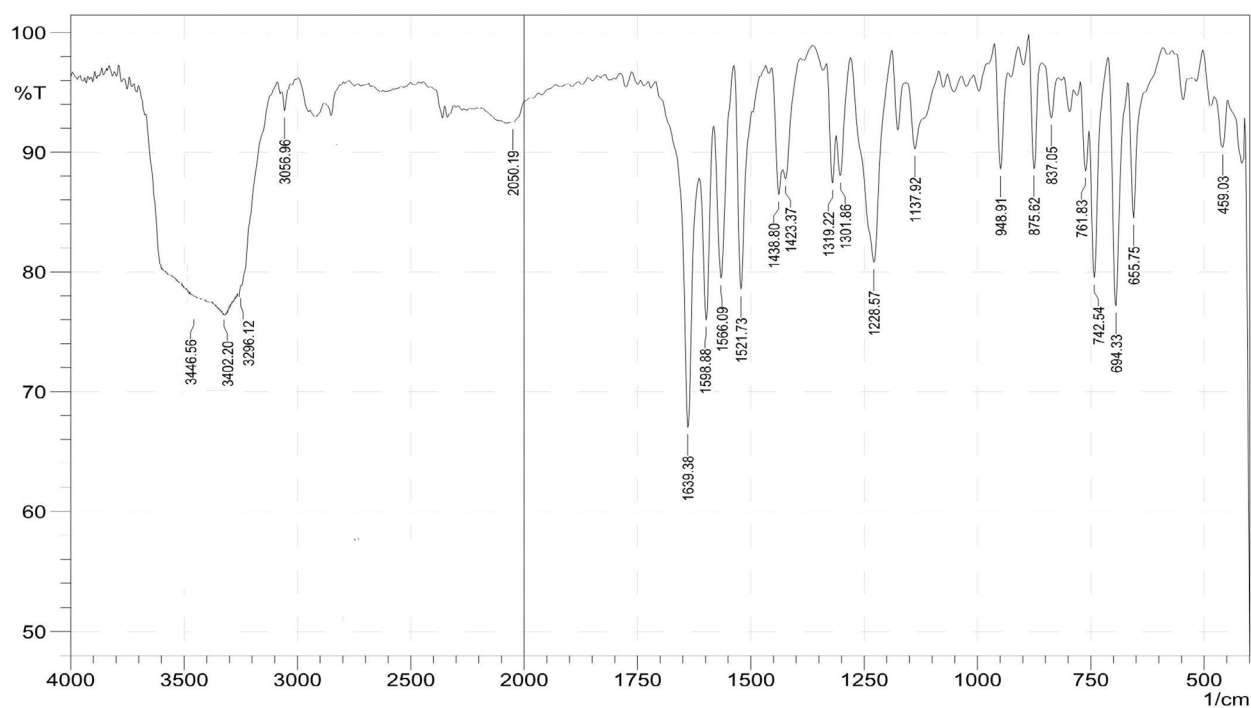
White solid, m.p. 219–221°C; FT-IR (KBr) ($\nu_{\max}$ cm⁻¹): 3402 (O–H), 3056 (CH–Ar), 1637 (C=O), 1596, and 1566 (C=C, Ar), 949 (C–Br); ¹H NMR (400 MHz, DMSO-*d*₆) δ : 12.15 (s, 1H, OH), 8.72 (s, 1H), 8.62 (d, *J* = 7.8 Hz, 1H), 8.22 (d, *J* = 8.2 Hz, 1H), 8.14 (d, *J* = 8.2 Hz, 1H), 8.05 (d, *J* = 7.8 Hz, 1H), 7.92 (s, 2H), 7.78–7.82 (m, 1H), 7.72 (d, *J* = 7.8 Hz, 2H), 7.59 (t, *J* = 7.8 Hz, 2H) ppm; ¹³C NMR (100 Hz, DMSO-*d*₆) δ : 212.4, 163.9, 161.4, 149.2, 138.7, 136.8, 135.6, 133.3, 133.5, 132.1, 131.5, 131.4, 130.7, 130.4, 129.7, 128.4, 125.2, 121.5 ppm. HRMS (*m/z* 435.03). Anal. Calc. for C₂₀H₁₄BrN₅O₂: C, 55.06; H, 3.23; N, 16.05. Found: C, 55.03; H, 3.25; N, 16.03.

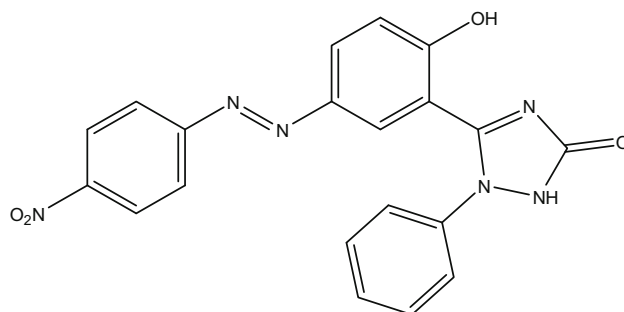
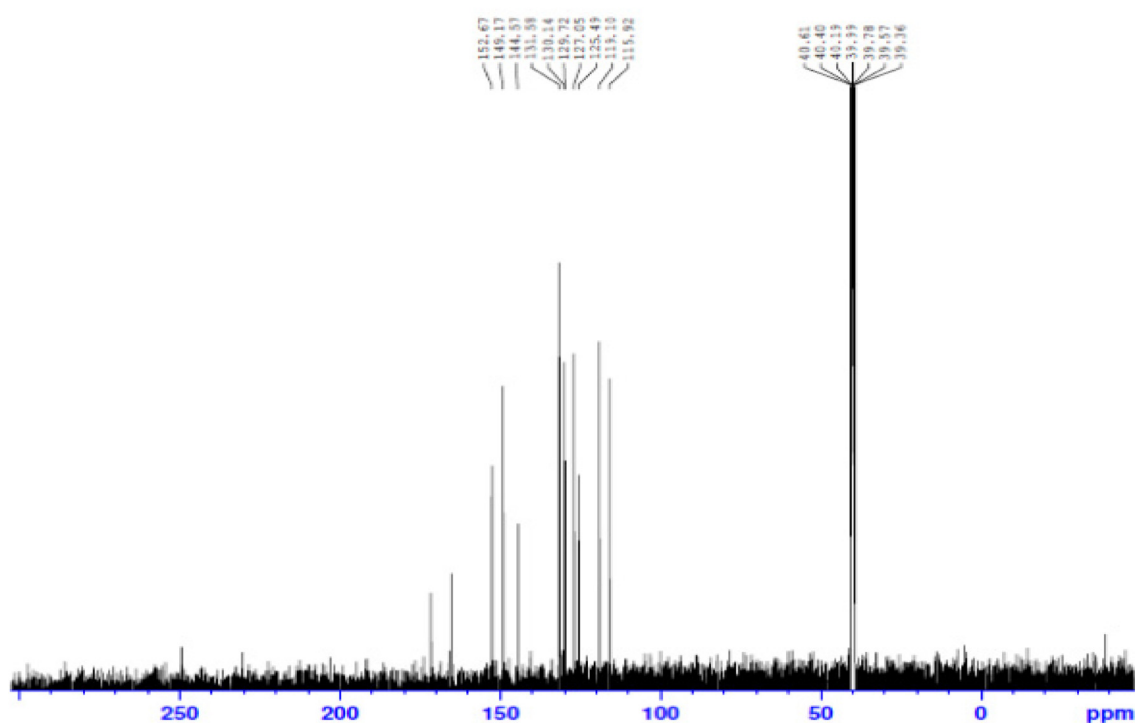


**5f**

5-(2-hydroxy-5-((3-nitrophenyl)diazenyl)phenyl)-1-phenyl-1H-1,2,4-triazol-3(2H)-one (5f)

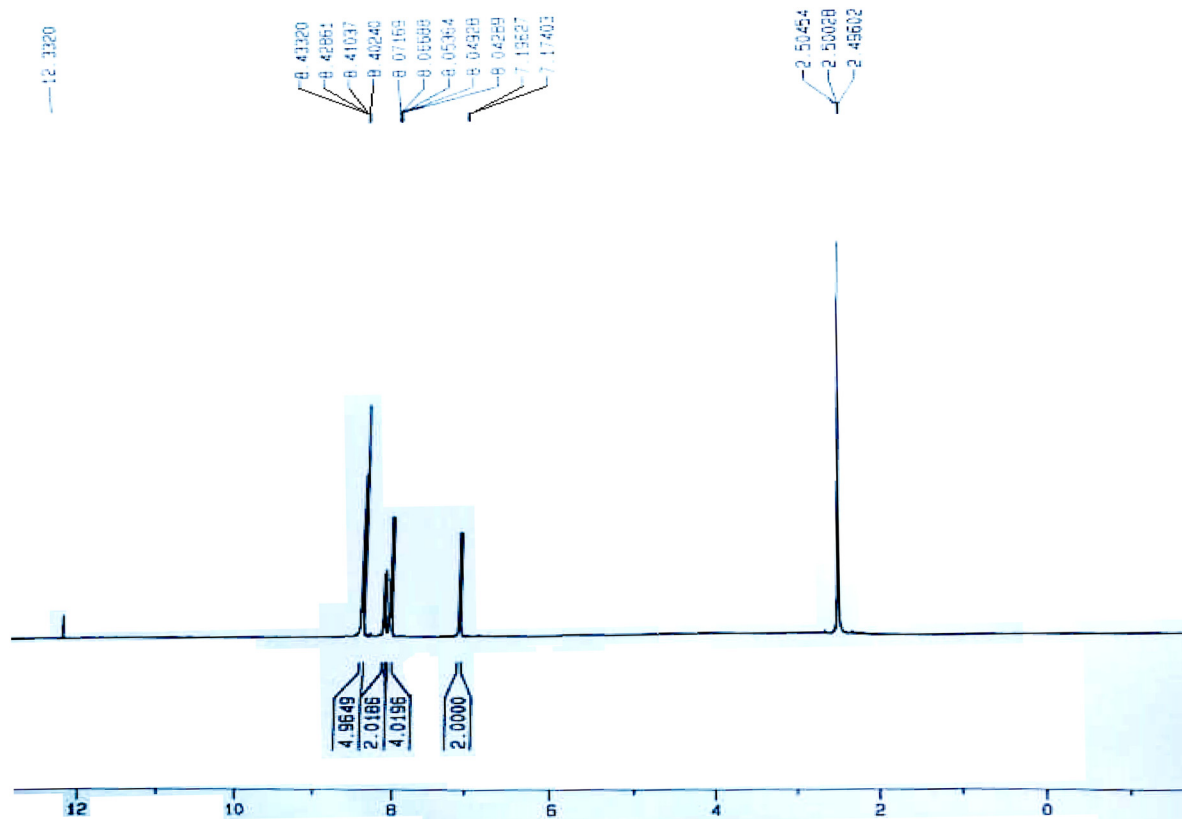
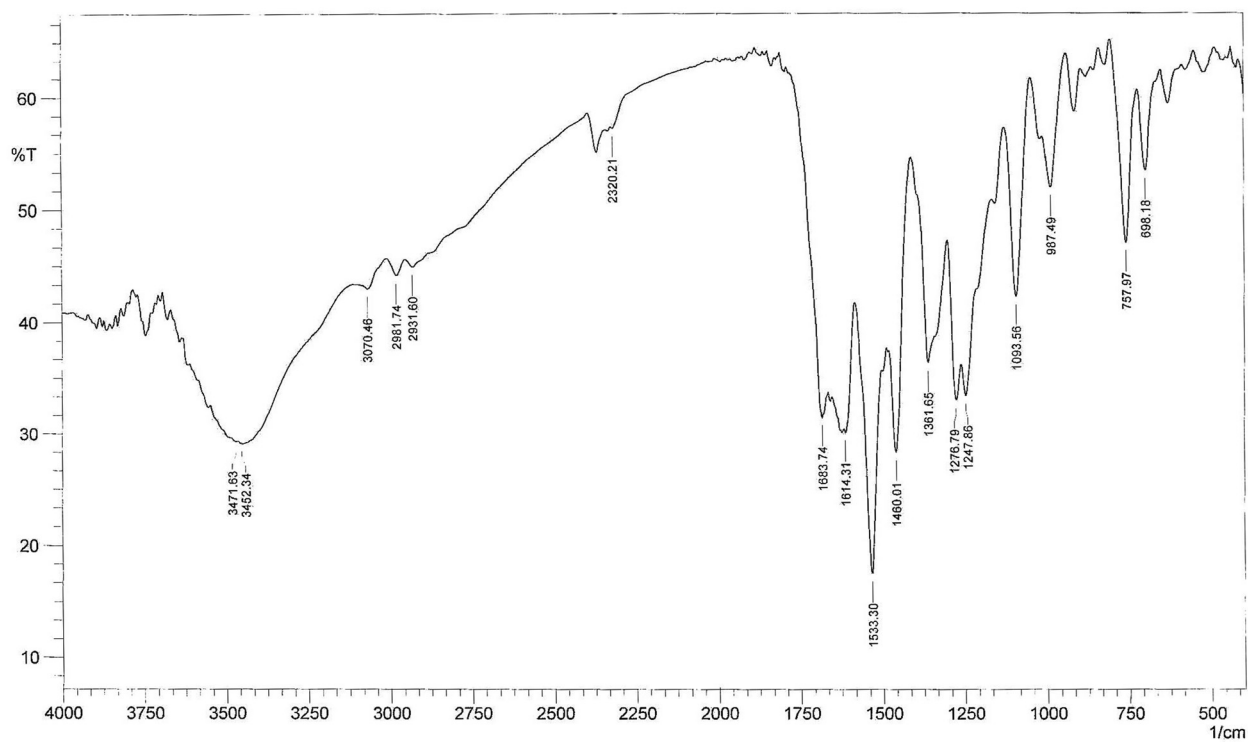
Off-white solid, m.p. 232–234°C; FT-IR (KBr) ($\nu_{\max}$ cm⁻¹): 3402 (O–H), 3068 (CH-Ar), 1639 (C=O), 1596, and 1568 (C=C, Ar), 1531, and 1319 (NO₂); ¹H NMR (400 MHz, DMSO-*d*₆) δ : 12.33 (s, 1H, OH), 8.64 (s, 2H), 8.34–8.48 (m, 6H), 7.92 (d, *J* = 8.4 Hz, 2H), 7.67 (t, *J* = 8.2 Hz, 2H) ppm; ¹³C NMR (100 Hz, DMSO-*d*₆) δ : 197.4, 167.4, 161.7, 149.4, 147.4, 145.2, 133.2, 131.3, 130.6, 129.4, 129.0, 119.4, 115.2 ppm. HRMS (*m/z* 402.11). Anal. Calc. for C₂₀H₁₄N₆O₄: C, 59.70; H, 3.51; N, 20.89. Found: C, 59.68; H, 3.49; N, 20.91.

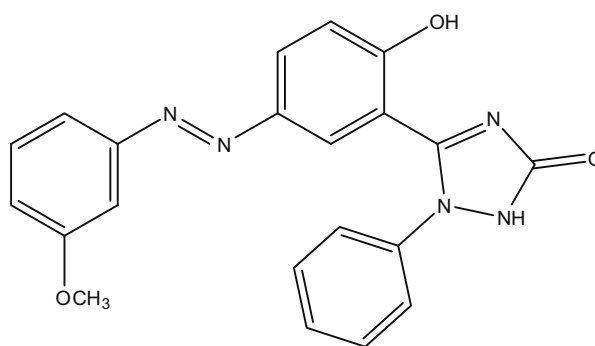
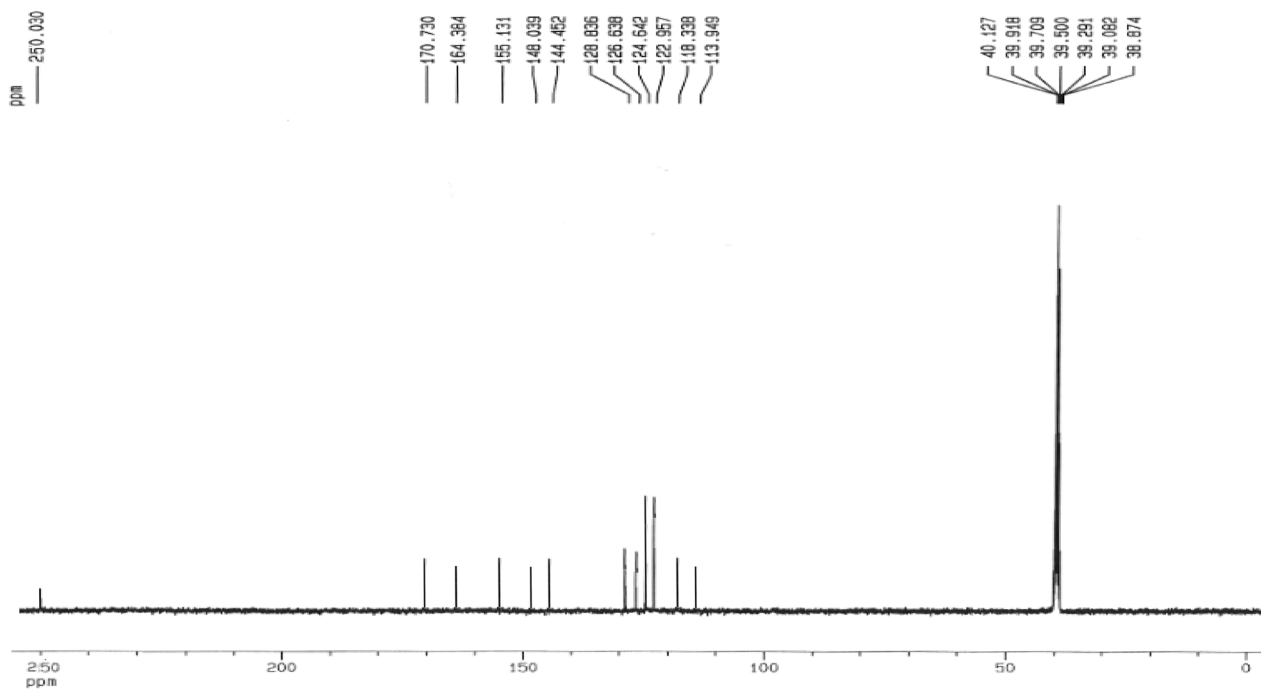


**5g**

5-(2-hydroxy-5-((4-nitrophenyl)diazenyl)phenyl)-1-phenyl-1H-1,2,4-triazol-3(2H)-one (5g)

Off-white solid, m.p. 231–233°C; FT-IR (KBr) ($\nu_{\max}$ cm⁻¹): 3372 (O–H), 3070 (CH-Ar), 1663 (C=O), 1614, and 1561 (C=C, Ar), 1533, and 1361 (NO₂); ¹H NMR (400 MHz, DMSO-*d*₆) δ : 12.33 (s, 1H, OH), 8.40–8.44 (m, 5H), 8.07 (d, *J* = 8.2 Hz, 2H), 8.04–8.06 (m, 4H), 7.20 (t, *J* = 7.8 Hz, 2H) ppm; ¹³C NMR (100 Hz, DMSO-*d*₆) δ : 205.3, 170.7, 155.4, 148.3, 144.4, 128.4, 126.8, 124.6, 122.0, 121.2, 118.4, 113.9 ppm. HRMS (*m/z* 402.11). Anal. Calc. for C₂₀H₁₄N₆O₄: C, 59.70; H, 3.51; N, 20.89. Found: C, 59.72; H, 3.48; N, 20.91.



**5h**

5-(2-hydroxy-5-((4-methoxyphenyl)diazenyl)phenyl)-1-phenyl-1H-1,2,4-triazol-3(2H)-one (5h)

White solid, m.p. 211–213°C; FT-IR (KBr) ($\nu_{\max}$ cm^{-1}): 3422 (O–H), 3029 (CH–Ar), 2926 (CH–Aliphatic), 1729 (C=O), 1534, and 1475 (C=C, Ar), 1284 (C–O); ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ : 12.22 (s, 1H, OH), 8.50 (d, J = 8.2 Hz, 2H), 8.18 (d, J = 7.8 Hz, 1H), 8.07 (t, J = 8.2 Hz, 1H), 7.72 (s, br., 2H), 7.42 (s, br., 4H), 7.40 (d, J = 7.8 Hz, 2H), 3.71 (s, 3H, OCH_3) ppm; ^{13}C NMR (100 Hz, $\text{DMSO}-d_6$) δ : 202.2, 150.4, 141.8, 135.7, 132.5, 131.3, 130.7, 130.3, 129.7, 129.2, 128.5, 125.9, 59.1 ppm. HRMS (m/z 387.13). Anal. Calc. for $\text{C}_{21}\text{H}_{17}\text{N}_5\text{O}_3$: C, 65.11; H, 4.42; N, 18.08. Found: C, 65.09; H, 4.45; N, 18.10.

