

Supplementary Information

Quinoline-bearing 1,6-dihydropyrimidine azo dye derivatives:
Synthesis, antimicrobial activity, molecular docking, ADMET,
and dye fastness studies

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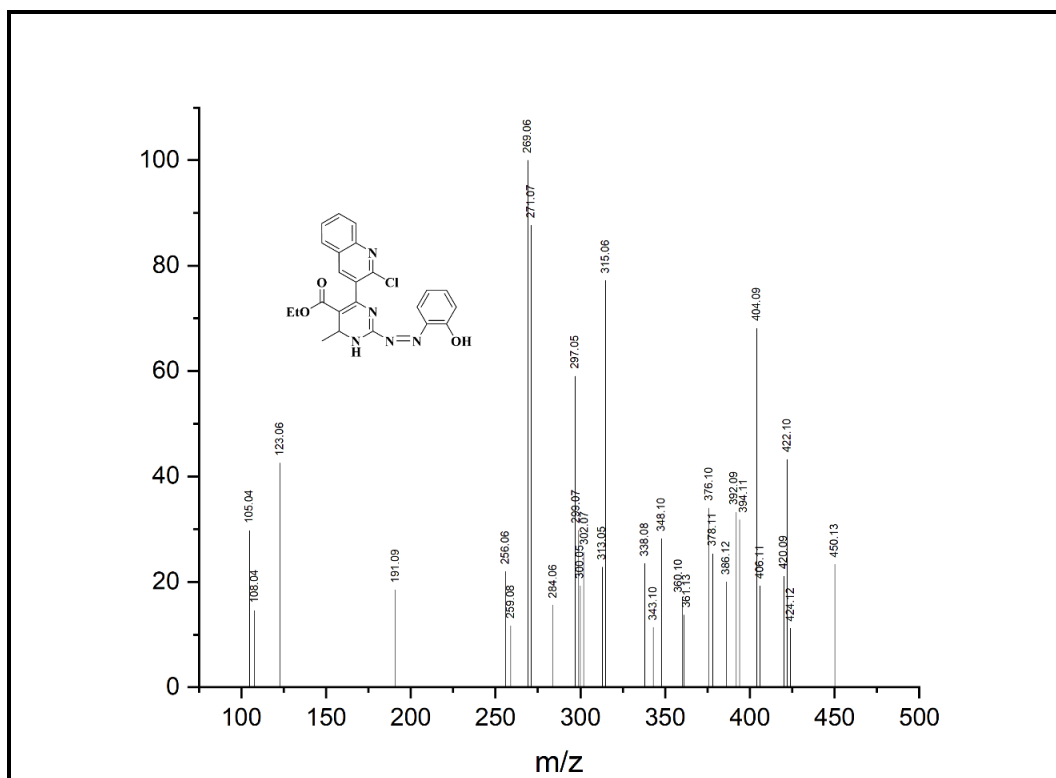


Fig. 1 — MS of compound **3a**

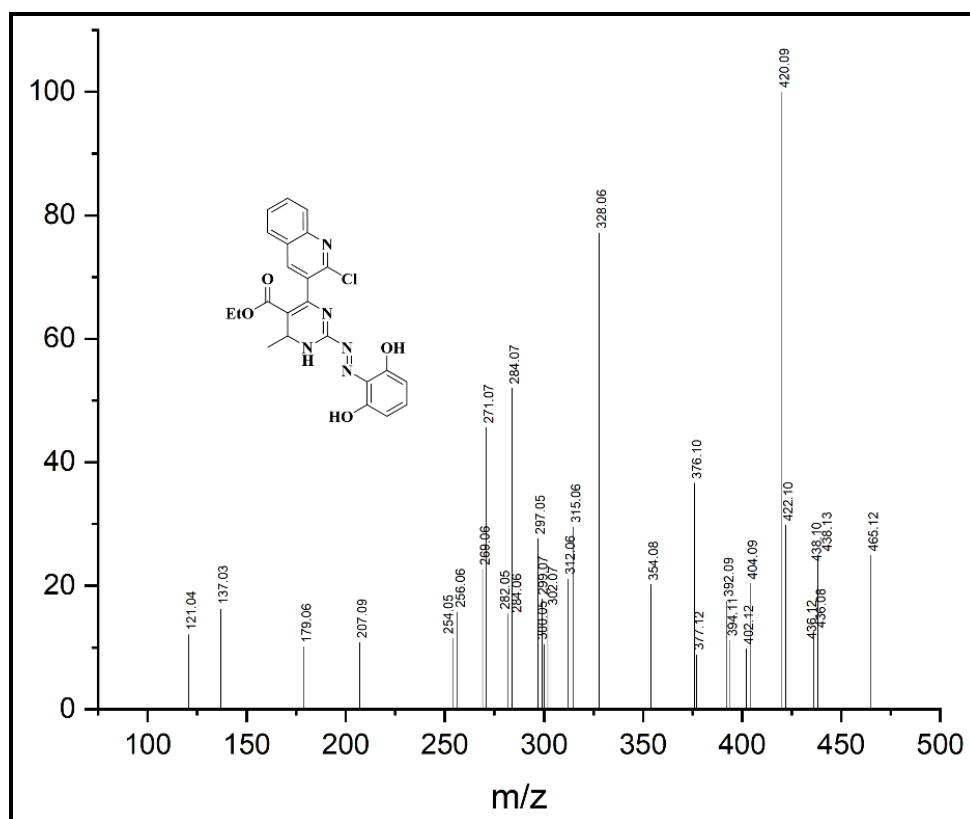


Fig. 2 — MS of compound **3d**

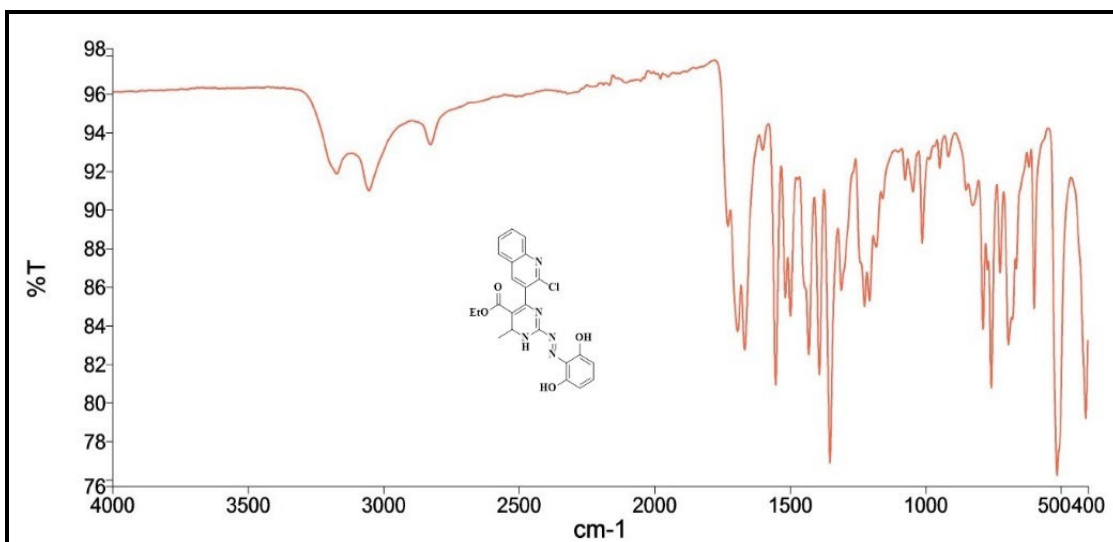


Fig. 3 — FTIR spectrum of compound **3d**

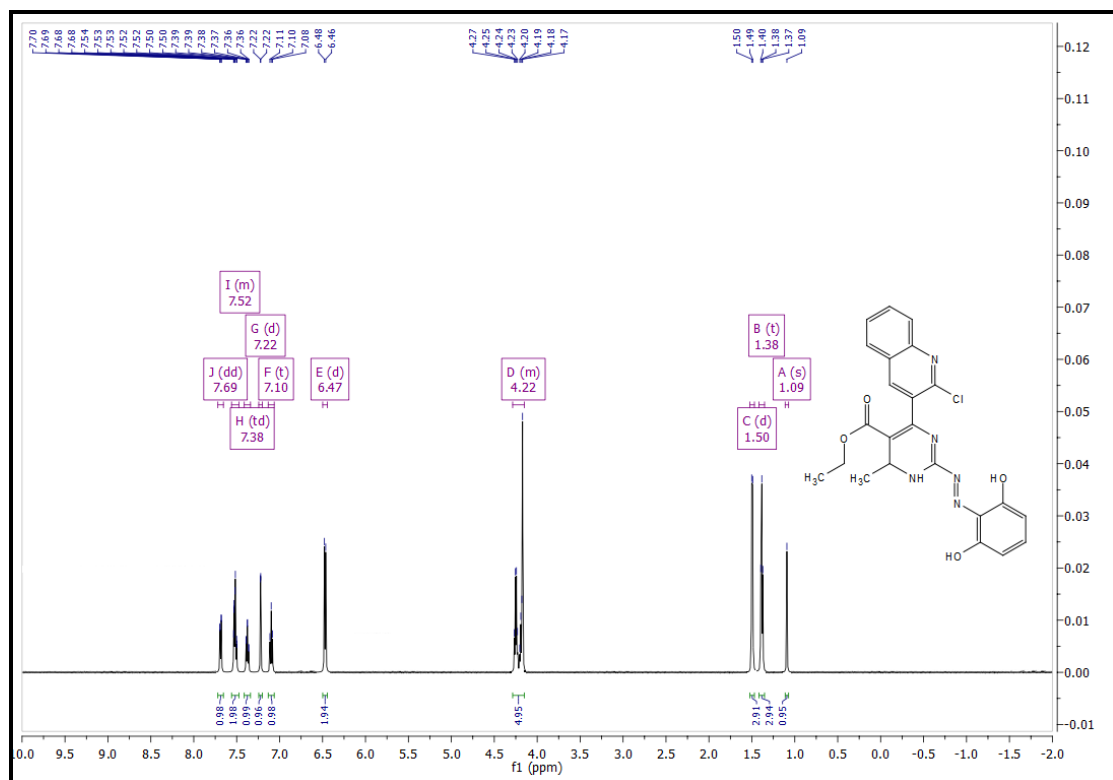


Fig. 4 — ¹H NMR of compound **3d**

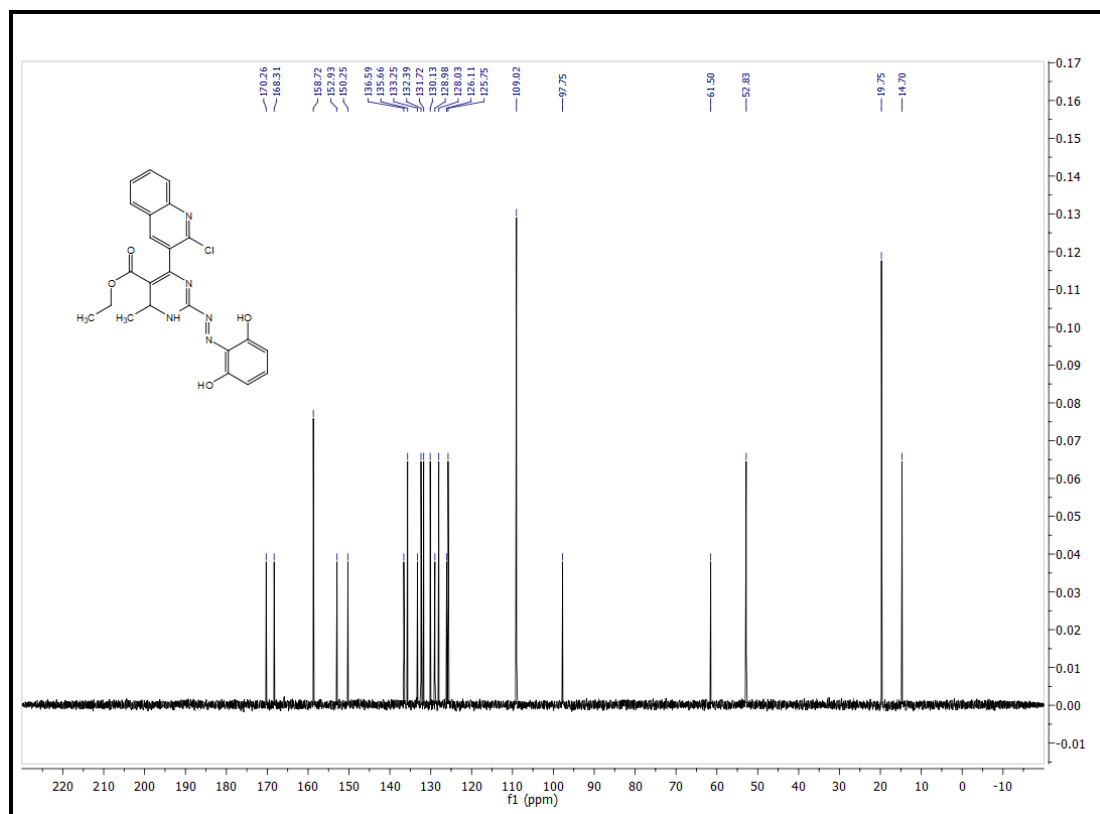


Fig. 5 — ^{13}C NMR of compound 3d

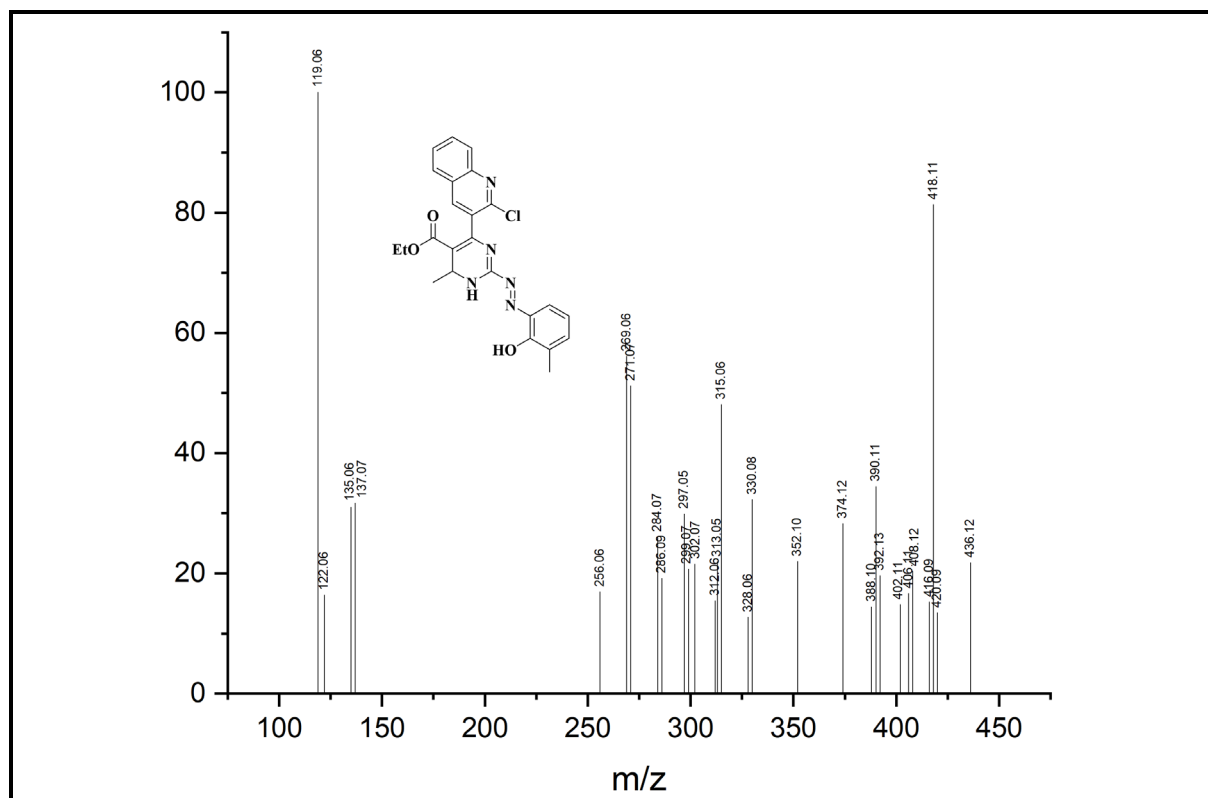


Fig. 6 — MS of compound 3e

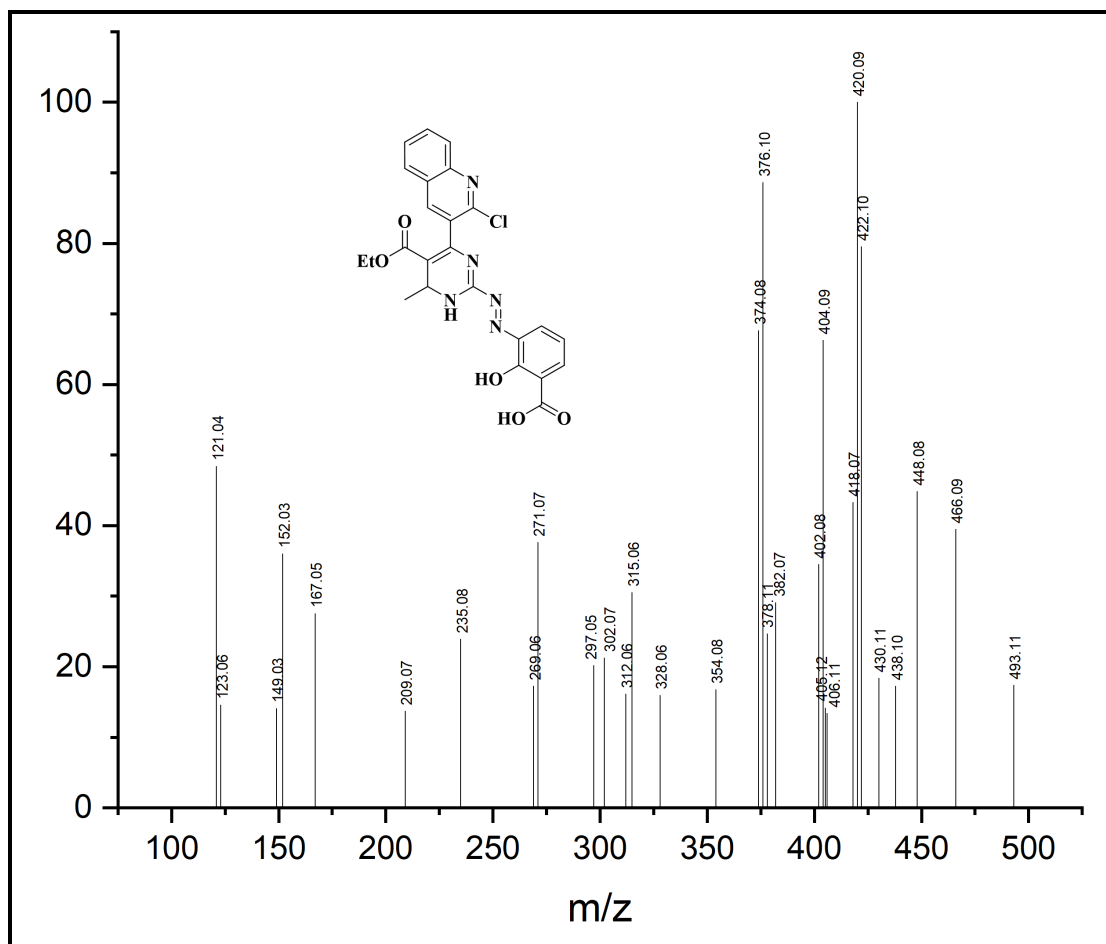


Fig. 7 — MS of compound **3h**

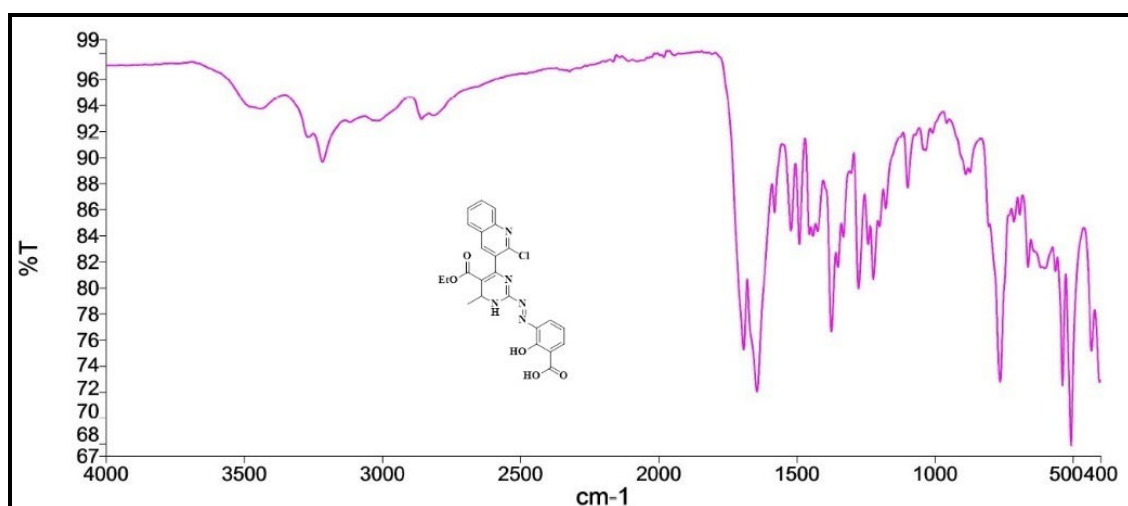


Fig. 8 — FTIR spectrum of compound **3h**

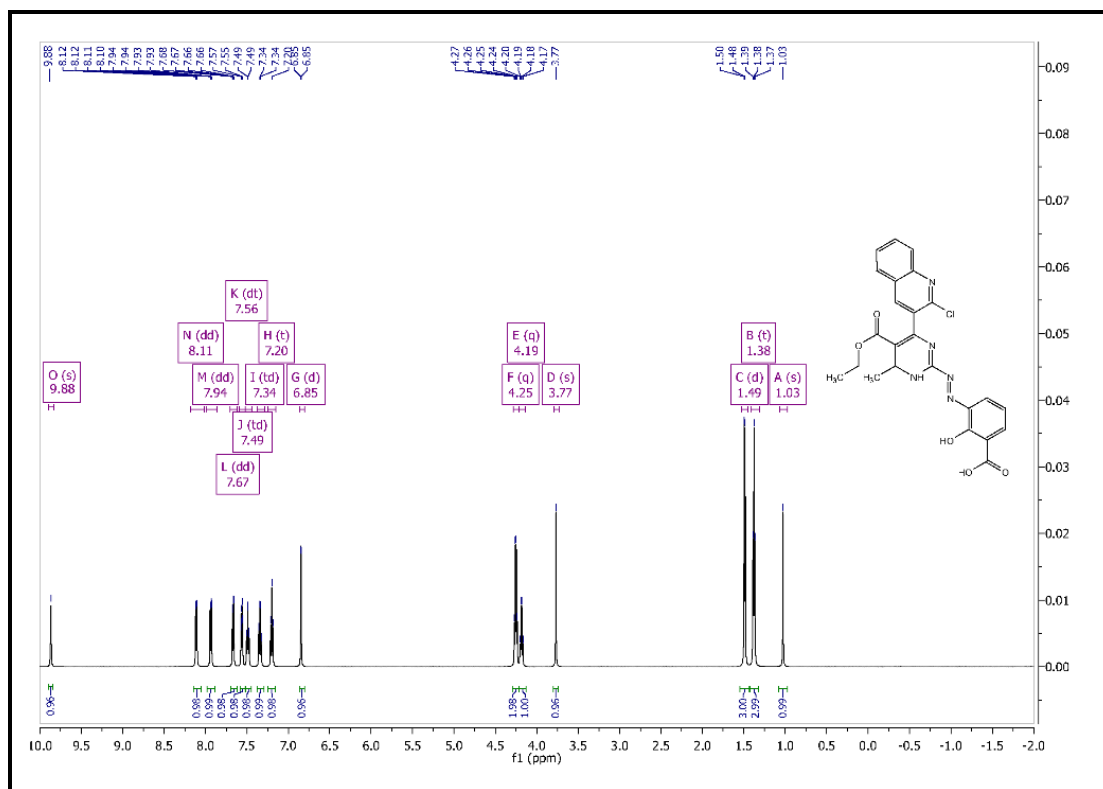


Fig. 9 — ^1H NMR of compound 3h

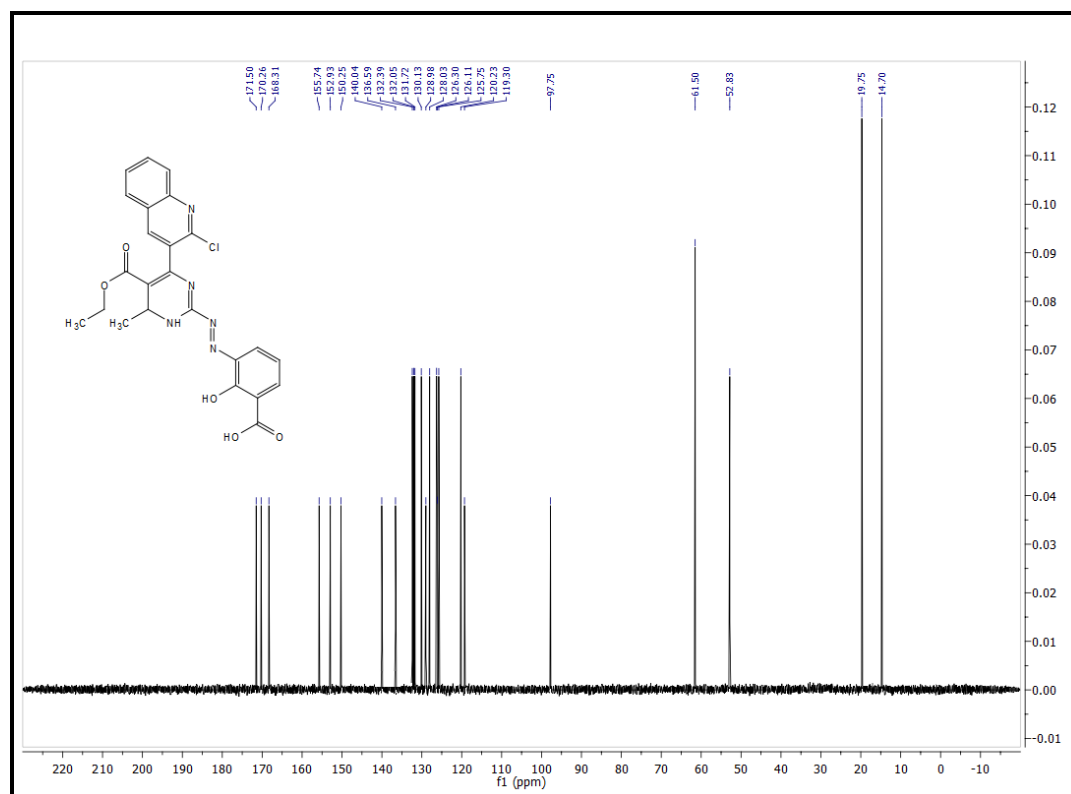


Fig. 10 — ^{13}C NMR of compound 3h

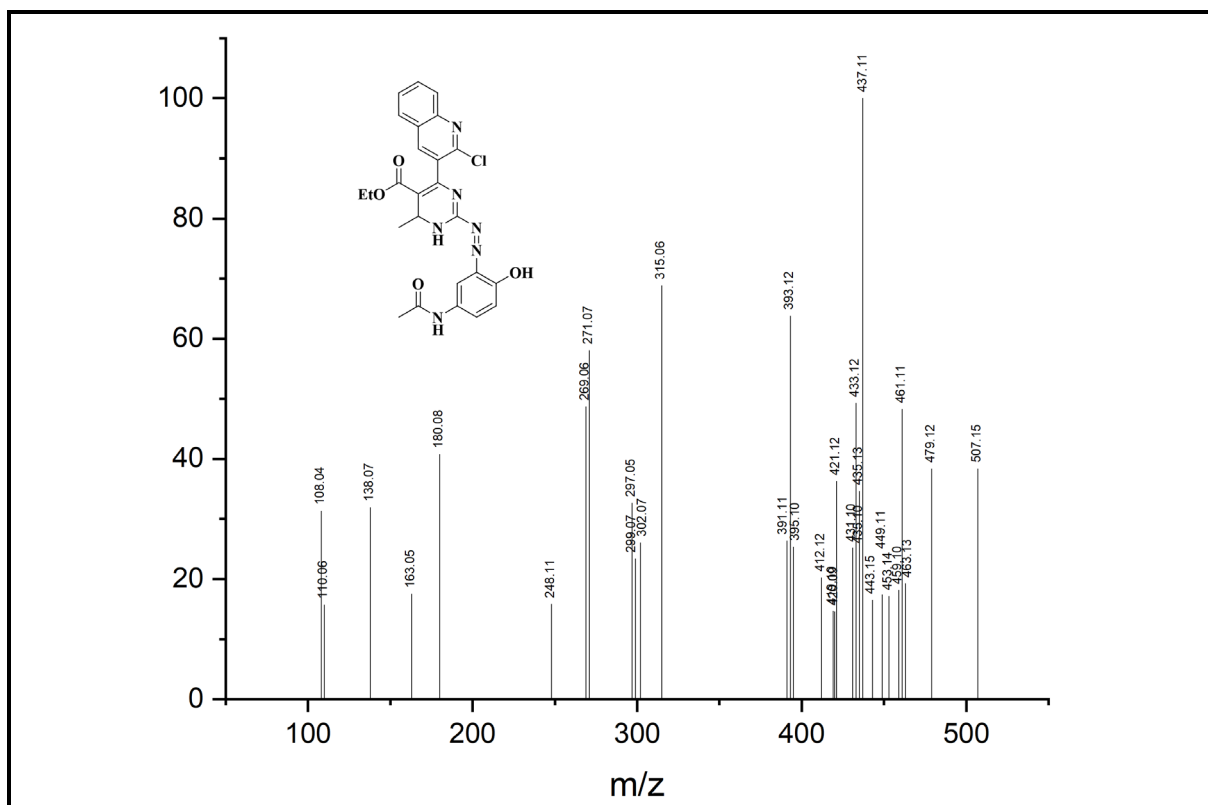


Fig. 11 — MS of compound **3i**

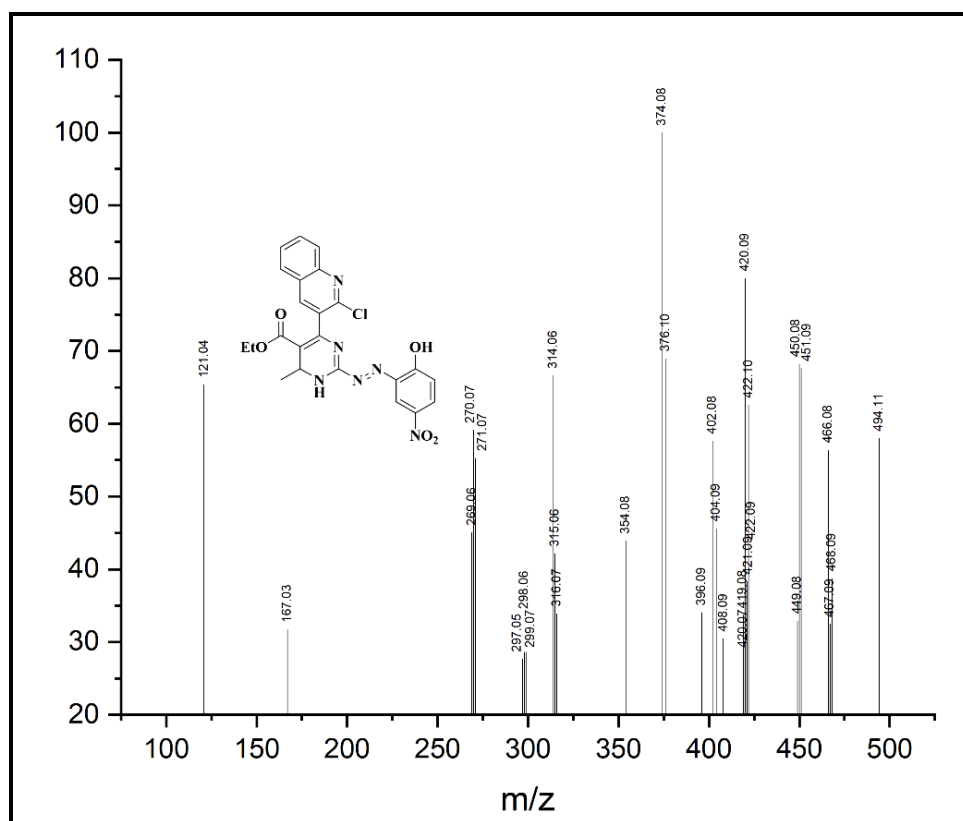


Fig. 12 — MS of compound **3o**

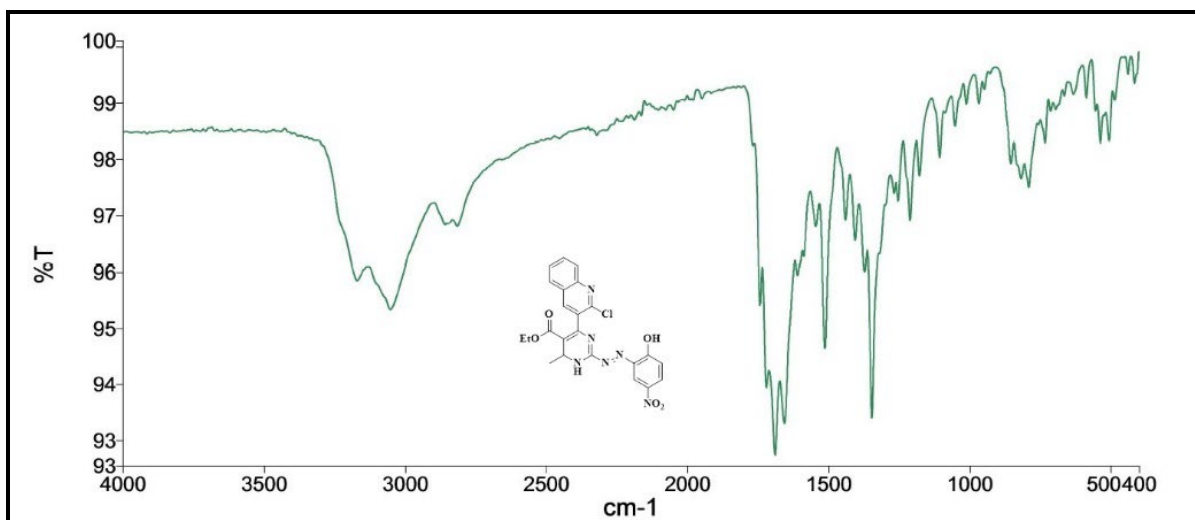


Fig. 13 — FTIR spectrum of compound **3o**

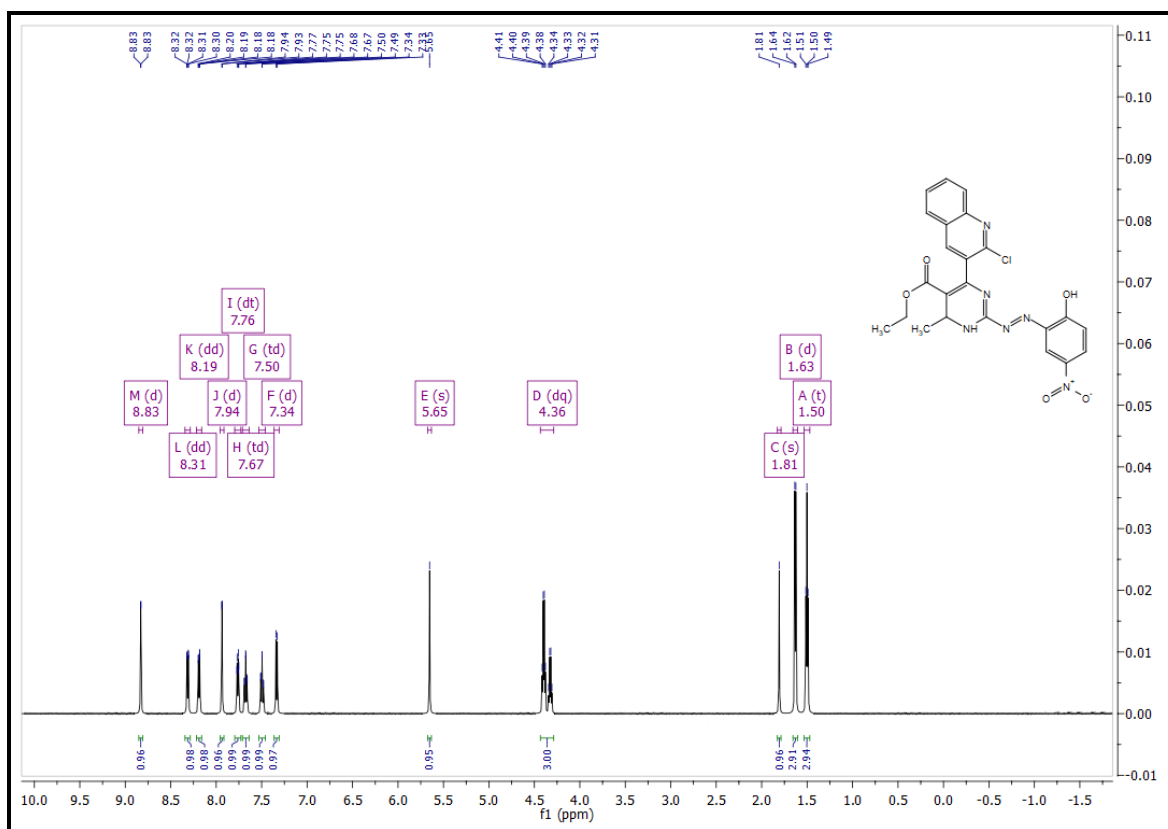


Fig. 14 — ^1H NMR of compound **3o**

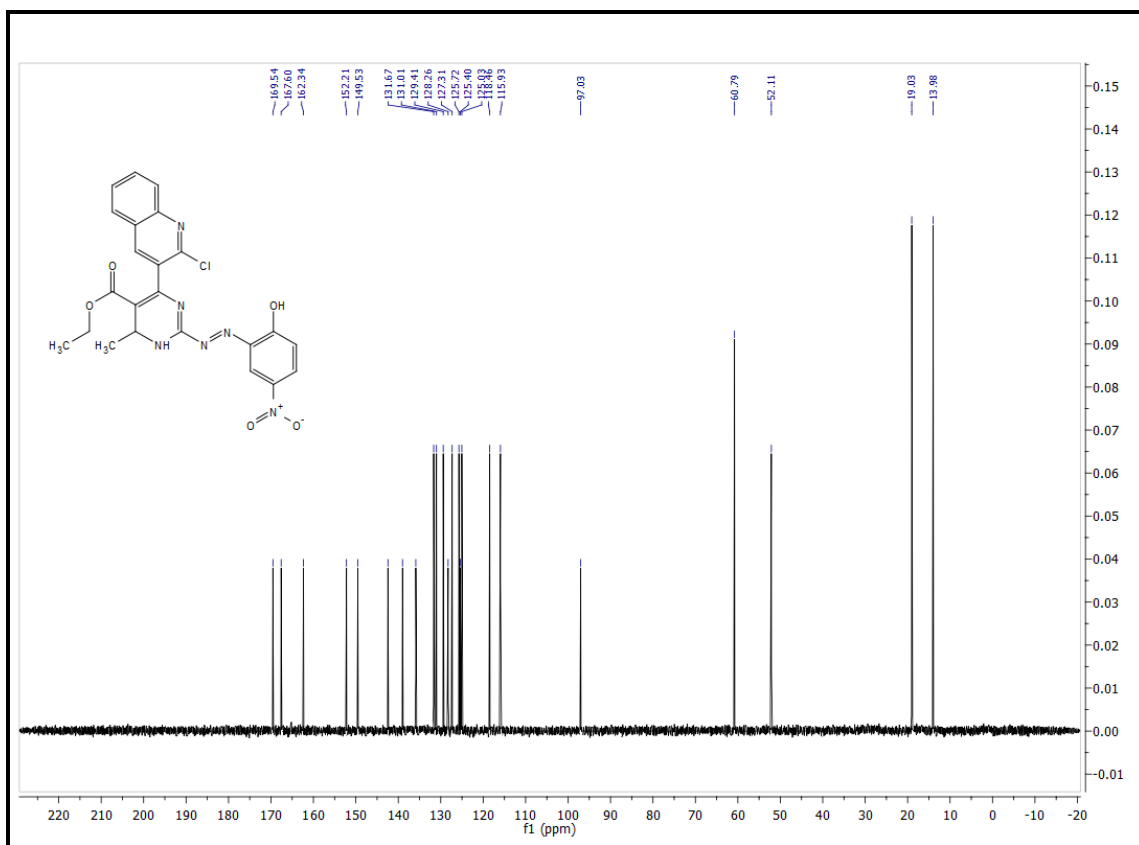


Fig. 15 — ^{13}C NMR of compound **3o**

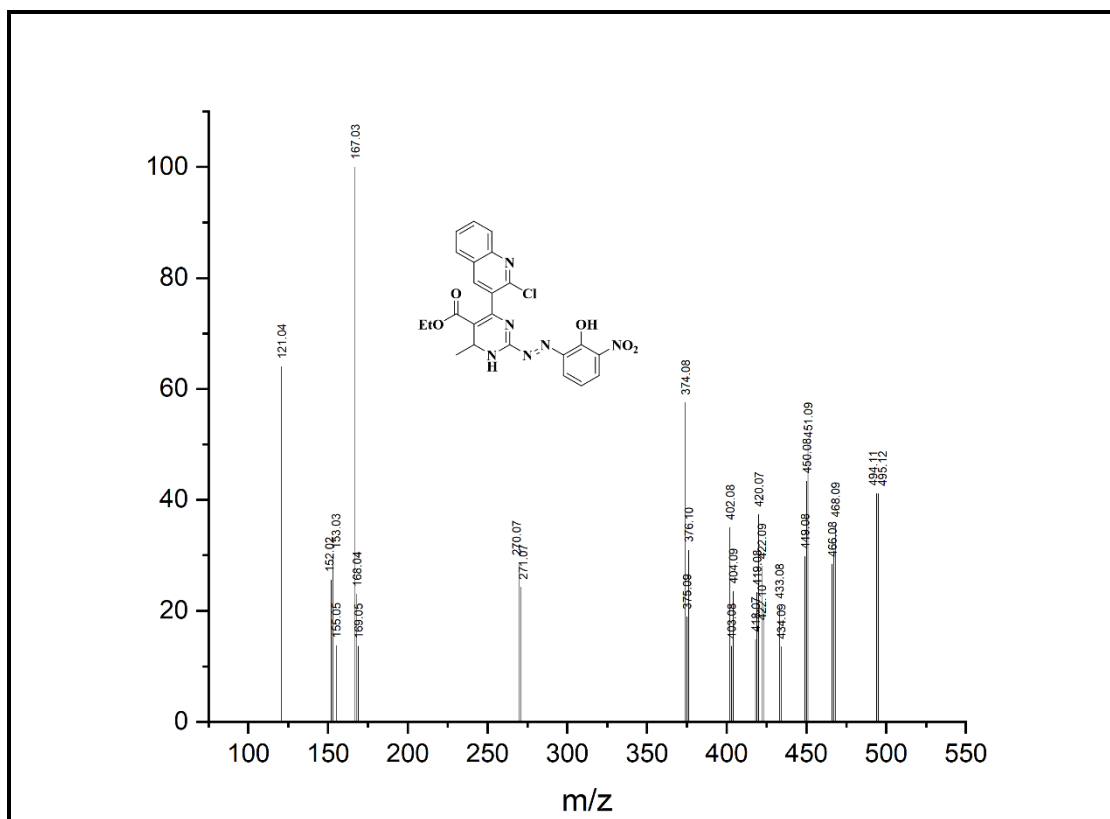


Fig. 16 — MS of compound **3p**

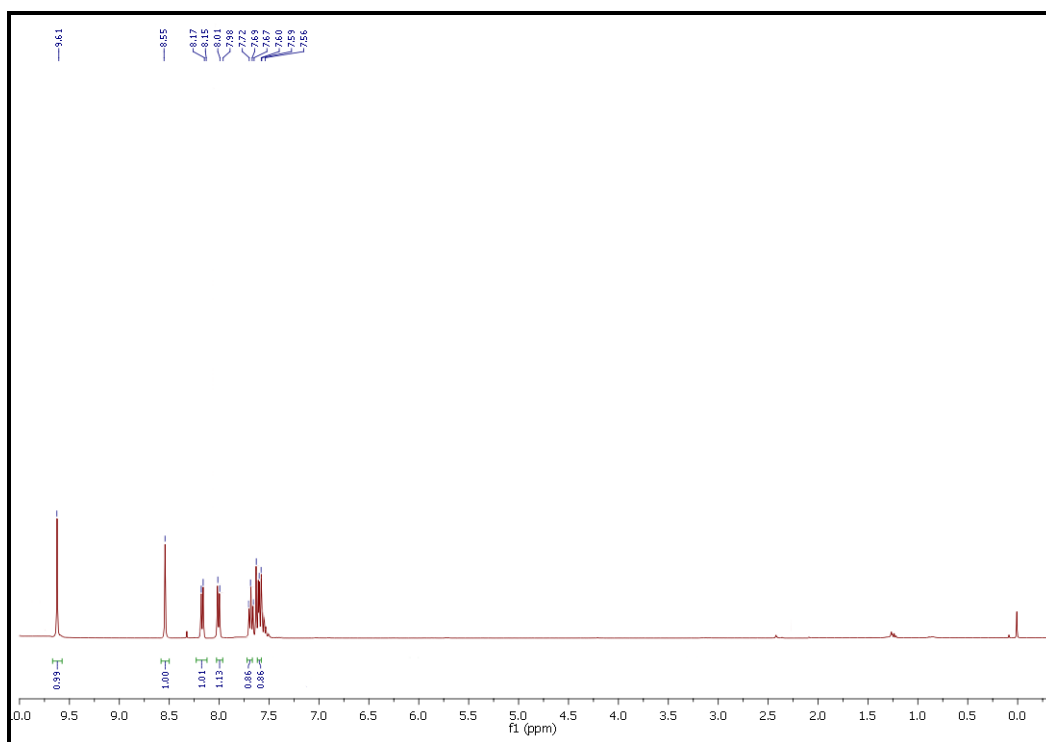
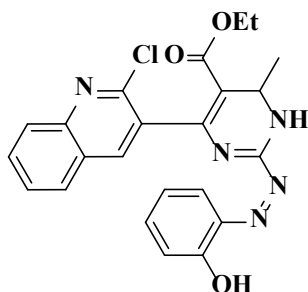


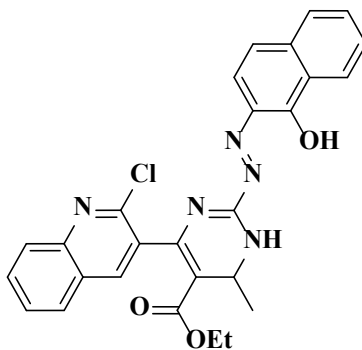
Fig. 17 — ^1H NMR of compound 1

Ethyl-4-(2-chloroquinolin-3-yl)-2-((2-hydroxyphenyl)diazenyl)-6-methyl-1,6-dihydropyrimidine-5-carboxylate (3a)



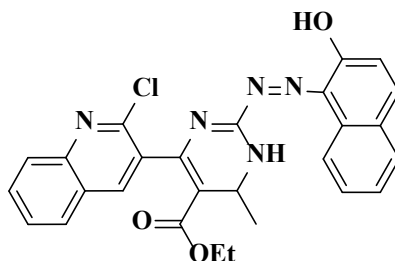
Light yellow solid, yield 79%, m.p. 174-176°C. IR_{vmax} cm⁻¹: 3375 (2° N-H), 3255 (OH), 2689 (C-H), 1625 (C=N), 1408 (C=C), 1223 (C-N), 1012 (C-O), 745 (Ar-Cl). ¹H NMR (500 MHz, DMSO-*d*₆, δ ppm): 6.93-8.04 (m, 9H, Ar-H), 5.01 (s, 1H, OH), 4.26 (q, *J* = 6.0 Hz, 2H, CH₂), 4.19 (m, 1H, CH), 1.64 (d, 1H, NH), 1.53 (d, *J* = 6.0 Hz, 3H, CH₃), 1.39 (t, *J* = 6.0 Hz, 3H, CH₃); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ ppm): 168.3 (C=O), 158.3 (C-OH), 152.9, 150.2 (C-Cl), 149.2, 139.9, 136.6, 132.4, 130.1, 126.1, 125.7, 121.1, 117.1, 97.7, 61.5, 52.8 (C-CH₃), 19.7, 14.7. MS (*m/z*): 450.13 (M⁺). Anal. Calcd for C₂₃H₂₀ClN₅O₃: C 61.40, H 4.48, N 15.57; Found C 61.53, H 4.56, N 15.46%.

Ethyl-4-(2-chloroquinolin-3-yl)-2-((1-hydroxynaphthalen-2-yl)diazenyl)-6-methyl-1,6-dihydropyrimidine-5-carboxylate (3b)



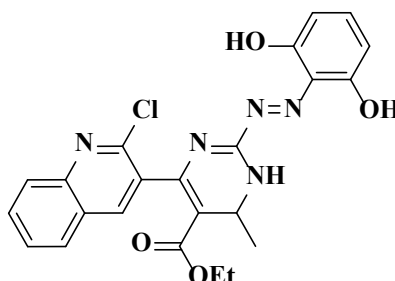
Light brown solid, yield 76%, m.p. 188-190°C. IR_{vmax} cm⁻¹: 3225 (2° N-H), 3180 (OH), 2689 (C-H), 1609 (C=N), 1417 (C=C), 1208 (C-N), 1021 (C-O), 743 (Ar-Cl). ¹H NMR (500 MHz, DMSO-*d*₆, δ ppm): 7.32-8.00 (m, 11H, Ar-H), 7.03 (s, 1H, OH), 4.24 (q, *J* = 6.0 Hz, 2H, CH₂), 4.19 (m, 1H, CH), 1.50 (d, *J* = 6.10 Hz, 3H, CH₃), 1.39 (t, *J* = 6.0 Hz, 3H, CH₃), 1.17 (d, 1H, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ ppm): 170.3, 168.3 (C=O), 152.9, 151.3 (C-OH), 150.2 (C-Cl), 136.6, 132.4, 130.1, 128.7, 126.1, 125.7, 122.3, 97.7, 61.5, 52.8 (C-CH₃), 19.7, 14.7. MS (*m/z*): 499.14 (M⁺). Anal. Calcd for C₂₇H₂₂ClN₅O₃: C 64.87, H 4.44, N 14.01; Found C 64.75, H 4.54, N 14.11%.

Ethyl 4-(2-chloroquinolin-3-yl)-2-((2-hydroxynaphthalen-1-yl)diazenyl)-6-methyl-1,6-dihydropyrimidine-5-carboxylate (3c)



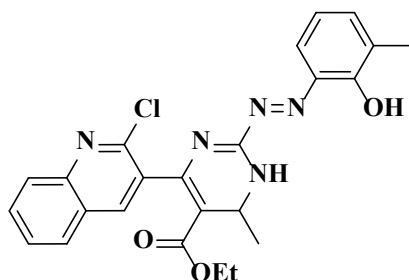
Light brown solid, yield 79%, m.p. 185-187°C. IR ν_{max} cm⁻¹: 3250 (2° N-H), 3205 (OH), 2656 (C-H), 1603 (C=N), 1407 (C=C), 1257 (C-N), 1011 (C-O), 745 (Ar-Cl). ¹H NMR(500 MHz, DMSO-*d*₆, δ ppm): 7.31-8.07 (m, 11H, Ar-H), 4.24 (q, *J* = 6.0 Hz, 2H, CH₂), 4.19 (m, 1H, CH), 1.80 (s, 1H, OH), 1.67 (d, 1H, NH), 1.50 (d, *J* = 6.0 Hz, 3H, CH₃), 1.32 (t, *J* = 6.0 Hz, 3H, CH₃); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ ppm): 168.3 (C=O), 156.1 (C-OH), 152.9, 150.2 (C-Cl), 149.2, 136.6, 132.4, 130.1, 126.1, 120.1, 97.7, 61.5, 52.8 (C-CH₃), 19.7, 14.7. MS (*m/z*): 499.14 (M⁺). Anal. Calcd for C₂₇H₂₂ClN₅O₃: C 64.87, H 4.44, N 14.01; Found C 64.76, H 4.56, N 14.13%.

Ethyl 4-(2-chloroquinolin-3-yl)-2-((2,6-dihydroxyphenyl)diazenyl)-6-methyl-1,6-dihydropyrimidine-5-carboxylate (3d)



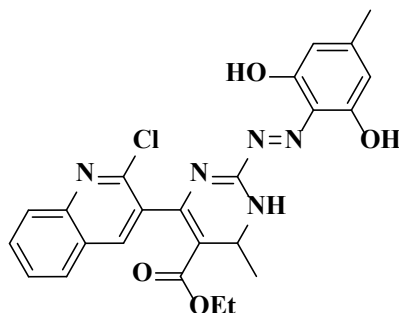
Light yellow solid, yield 72%, m.p. 180-182°C. IR ν_{max} cm⁻¹: 3290 (2° N-H), 3235 (OH), 2750 (C-H), 1620 (C=N), 1417 (C=C), 1218 (C-N), 1015 (C-O), 745 (Ar-Cl). ¹H NMR(500 MHz, DMSO-*d*₆, δ ppm): 6.47-7.69 (m, 8H, Ar-H), 4.25 (q, *J* = 6.0 Hz, 2H, CH₂), 4.19 (m, 1H, CH), 4.17 (m, 2H, OH), 1.50 (d, *J* = 6.10 Hz, 3H, CH₃), 1.38 (t, *J* = 6.0 Hz, 3H, CH₃), 1.09 (d, 1H, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ ppm): 170.3, 168.3 (C=O), 158.7 (C-OH), 158.7 (C-OH), 152.9, 150.2 (C-Cl), 136.6, 132.4, 131.7, 130.1, 126.1, 109.1, 97.7, 61.5, 52.8 (C-CH₃), 19.7, 14.7. MS (*m/z*): 465.12 (M⁺). Anal. Calcd for C₂₃H₂₀ClN₅O₄: C 59.30, H 4.33, N 15.03; Found C 59.39, H 4.24, N 15.12%.

Ethyl 4-(2-chloroquinolin-3-yl)-2-((2-hydroxy-3-methylphenyl)diazenyl)-6-methyl-1,6-dihydropyrimidine-5-carboxylate (3e)



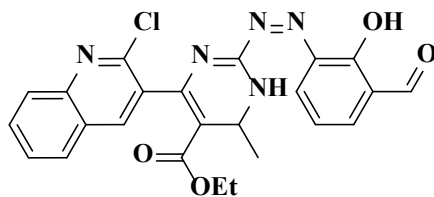
Light brown solid, yield 78%, m.p. 172-174°C. IR ν_{max} cm⁻¹: 3380 (2° N-H), 3145 (OH), 2609 (C-H), 1615 (C=N), 1402 (C=C), 1250 (C-N), 1008 (C-O), 745 (Ar-Cl). ¹H NMR(500 MHz, DMSO-*d*₆, δ ppm): 6.94-7.66 (m, 8H, Ar-H), 4.25 (q, *J* = 6.0 Hz, 2H, CH₂), 4.24 (s, 1H, OH), 4.19 (m, 1H, CH), 2.32 (s, 3H, CH₃), 1.50 (d, *J* = 6.0 Hz, 3H, CH₃), 1.38 (t, *J* = 6.0 Hz, 3H, CH₃), 1.10 (d, 1H, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ ppm): 170.3, 168.3 (C=O), 152.9, 150.8 (C-OH), 150.2 (C-Cl), 138.2, 136.6, 133.9, 132.4, 130.1, 126.1, 110.7, 97.7, 61.5, 52.8 (C-CH₃), 19.7, 14.7. MS (*m/z*): 463.14 (M⁺). Anal. Calcd for C₂₄H₂₂ClN₅O₃: C 62.14, H 4.78, N 15.10; Found C 62.18, H 4.67, N 15.22%.

Ethyl 4-(2-chloroquinolin-3-yl)-2-((2,6-dihydroxy-4-methylphenyl)diazenyl)-6-methyl-1,6-dihydropyrimidine-5-carboxylate (3f)



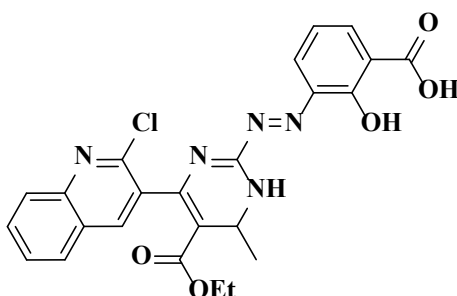
Gray white solid, yield 73%, m.p. 176-178°C. IR ν_{max} cm⁻¹: 3305 (2° N-H), 3255 (OH), 3170 (OH), 2780 (C-H), 1609 (C=N), 1412 (C=C), 1210 (C-N), 1011 (C-O), 745 (Ar-Cl). ¹H NMR(500 MHz, DMSO-*d*₆, δ ppm): 6.40-7.66 (m, 7H, Ar-H), 4.25 (q, *J* = 6.0 Hz, 2H, CH₂), 4.19 (m, 1H, CH), 4.18 (m, 2H, OH), 2.35 (s, 3H, CH₃), 1.49 (d, *J* = 6.10 Hz, 3H, CH₃), 1.38 (t, *J*=6.0 Hz, 3H, CH₃), 1.01 (d, 1H, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ ppm): 170.3, 168.3 (C=O), 157.8 (C-OH), 152.9, 150.2 (C-Cl), 145.3, 136.6, 132.4, 131.7, 130.1, 126.1, 110.7, 97.7, 61.5, 52.8 (C-CH₃), 21.8, 19.7, 14.7. MS (*m/z*): 479.14 (M⁺). Anal. Calcd for C₂₄H₂₂ClN₅O₄: C 60.06, H 4.62, N 14.59; Found C 60.15, H 4.53, N 14.68%.

Ethyl-4-(2-chloroquinolin-3-yl)-2-((3-formyl-2-hydroxyphenyl)diazenyl)-6-methyl-1,6-dihydropyrimidine-5-carboxylate (3g)



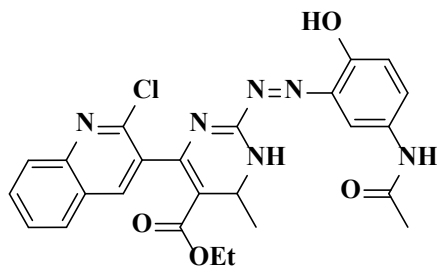
Light yellow solid, yield 83%, m.p. 180-182°C. IR ν_{max} cm $^{-1}$: 3350 (2° N-H), 3102 (OH), 2715 (C-H), 1720 (CO), 1609 (C=N), 1412 (C=C), 1210 (C-N), 1011 (C-O), 745 (Ar-Cl). ^1H NMR(500 MHz, DMSO- d_6 , δ ppm): 10.11 (s, 1H, CHO), 10.04 (s, 1H, OH), 7.20-8.04 (m, 8H, Ar-H), 4.25 (q, J = 5.90 Hz, 2H, CH $_2$), 4.19 (m, 1H, CH), 1.69 (d, 1H, NH), 1.53 (d, J = 6 Hz, 3H, CH $_3$), 1.39 (t, J = 5.90 Hz, 3H, CH $_3$); ^{13}C -NMR (100 MHz, DMSO- d_6 , δ ppm): 192.3 (CHO), 168.3 (C=O), 160.6 (C-OH), 152.9, 150.2 (C-Cl), 149.2, 136.6, 136.1, 132.4, 131.7, 130.0, 126.1, 121.4, 97.7, 61.5, 52.8 (C-CH $_3$), 19.7, 14.7. MS (m/z): 477.12 (M^+). Anal. Calcd for C $_{24}$ H $_{20}$ ClN $_5$ O $_4$: C 60.32, H 4.22, N 14.65; Found C 60.38, H 4.13 N 14.68%.

3-((4-(2-chloroquinolin-3-yl)-5-(ethoxycarbonyl)-6-methyl-1,6-dihydropyrimidin-2-yl)diazenyl)-2-hydroxybenzoic acid (3h)



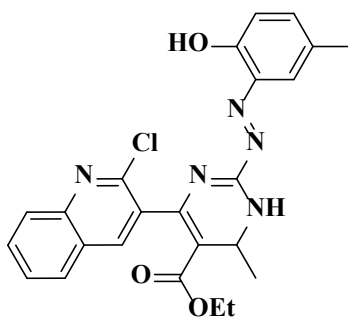
Light Brown solid, yield 69%, m.p. 198-200°C. IR ν_{max} cm $^{-1}$: 3242 (2° N-H), 3240 (OH), 2645 (C-H), 1780 (C=O), 1618 (C=N), 1390 (C=C), 1225 (C-N), 1018 (C-O), 745 (Ar-Cl). ^1H NMR(500 MHz, DMSO- d_6 , δ ppm): 10.11(s, 1H, COOH), 6.83-8.11 (m, 8H, Ar-H), 4.25 (q, J = 6.0 Hz, 2H, CH $_2$), 4.19 (m, 1H, CH), 3.77 (s, 1H, OH), 1.49 (d, J = 6.10 Hz, 3H, CH $_3$), 1.38 (t, J = 6.0 Hz, 3H, CH $_3$), 1.02 (d, 1H, NH); ^{13}C -NMR (100 MHz, DMSO- d_6 , δ ppm): 171.51 (COOH), 170.26, 168.3 (C=O), 155.74 (C-OH), 152.9, 150.2 (C-Cl), 140.2, 136.6, 132.4, 131.1, 130.0, 126.1, 120.2, 97.7, 61.5, 52.8 (C-CH $_3$), 19.7, 14.7. MS (m/z): 493.12 (M^+). Anal. Calcd for C $_{24}$ H $_{20}$ ClN $_5$ O $_5$: C 58.36, H 4.08, N 14.18; Found C 58.24, H 4.18, N 14.26%.

Ethyl 2-((5-acetamido-2-hydroxyphenyl)diazenyl)-4-(2-chloroquinolin-3-yl)-6-methyl-1,6-dihydropyrimidine-5-carboxylate (3i)



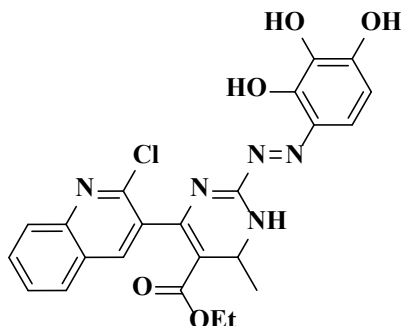
Brown solid, yield 75%, m.p. 206-208°C. IR v_{max} cm $^{-1}$: 3280 (2° N-H), 3145 (OH), 2735 (C-H), 1820 (CO), 1602 (C=N), 1340 (C=C), 1245 (C-N), 1016 (C-O), 745 (Ar-Cl). ^1H NMR(500 MHz, DMSO- d_6 , δ ppm): 8.97 (s, 1H, OH), 7.02-7.99 (m, 8H, Ar-H), 6.27 (s, 1H, NH), 4.25 (q, J = 6.0 Hz, 2H, CH $_2$), 4.19 (m, 1H, CH), 2.22 (s, 3H, CH $_3$), 1.50 (d, J = 6.10 Hz, 3H, CH $_3$), 1.37 (t, J = 6.0 Hz, 3H, CH $_3$), 1.18 (d, 1H, NH); ^{13}C -NMR (100 MHz, DMSO- d_6 , δ ppm): 170.4 (CONH), 170.3, 168.3 (C=O), 155.74 (C-OH), 152.9, 150.2 (C-Cl), 140.2, 136.6, 132.4, 131.1, 130.0, 126.1, 120.2, 97.7, 61.5, 52.8 (C-CH $_3$), 23.8 (CH $_3$ -CO), 19.7, 14.7. MS (m/z): 506.15 (M^+). Anal. Calcd for C $_{25}$ H $_{23}$ ClN $_6$ O $_4$: C 59.23, H 4.57, N 16.58; Found C 59.17, H 4.63, N 16.50%.

Ethyl 4-(2-chloroquinolin-3-yl)-2-((2-hydroxy-5-methylphenyl)diazenyl)-6-methyl-1,6-dihydropyrimidine-5-carboxylate (3j)



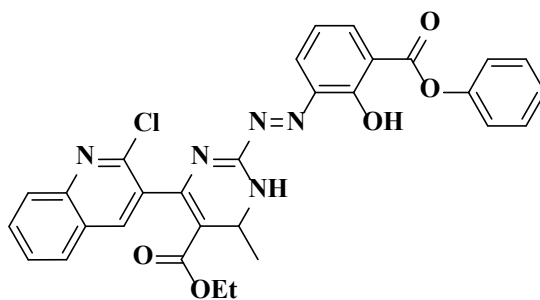
Light brown solid, yield 78%, m.p. 176-178°C. IR v_{max} cm $^{-1}$: 3230 (2° N-H), 3180 (OH), 2685 (C-H), 1826 (CO), 1625 (C=N), 1356 (C=C), 1236 (C-N), 1046 (C-O), 745 (Ar-Cl). ^1H NMR(500 MHz, DMSO- d_6 , δ ppm): 6.86-7.99 (m, 8H, Ar-H), 4.41 (s, 1H, OH), 4.25 (q, J = 6.0 Hz, 2H, CH $_2$), 4.19 (m, 1H, CH), 2.32 (s, 3H, CH $_3$), 1.49 (d, J = 6.10 Hz, 3H, CH $_3$), 1.37 (t, J = 6.0 Hz, 3H, CH $_3$), 1.09 (d, 1H, NH); ^{13}C -NMR (100 MHz, DMSO- d_6 , δ ppm): 170.3, 168.3 (C=O), 152.9, 152.3 (C-OH), 150.2 (C-Cl), 139.8, 136.6, 132.4, 131.1, 130.0, 126.1, 124.6, 97.7, 61.5, 52.8 (C-CH $_3$), 21.2 (C-CH $_3$), 19.7, 14.7. MS (m/z): 463.14 (M^+). Anal. Calcd for C $_{24}$ H $_{22}$ ClN $_5$ O $_3$: C 62.14, H 4.78, N 15.10; Found C 62.22, H 4.66, N 15.23%.

Ethyl-4-(2-chloroquinolin-3-yl)-6-methyl-2-((2,3,4-trihydroxyphenyl)diazenyl)-1,6-dihydropyrimidine-5-carboxylate (3k)



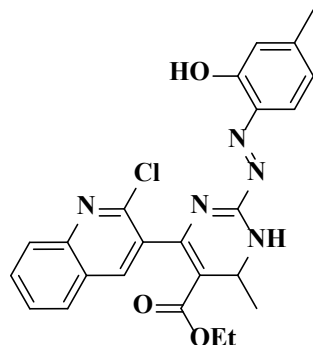
Brown solid, yield 78%, m.p. 190-192 °C. IR v_{max} cm⁻¹: 3250 (OH), 3186 (2° N-H), 2785 (C-H), 1865 (CO), 1601 (C=N), 1310 (C=C), 1202 (C-N), 1015 (C-O), 745 (Ar-Cl). ¹H NMR(500 MHz, DMSO-*d*₆, δ ppm): 8.88 (s, 1H, OH), 6.34-7.66 (m, 7H, Ar-H), 4.25 (q, *J* = 6.0 Hz, 2H, CH₂), 4.19 (m, 1H, CH), 3.16 (s, 1H, OH), 2.46 (s, 1H, OH), 1.49 (d, *J* = 6.10 Hz, 3H, CH₃), 1.39 (t, *J* = 6.0 Hz, 3H, CH₃), 1.02 (d, 1H, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ ppm): 170.3, 168.3 (C=O), 152.9, 152.3 (C-OH), 150.2 (C-Cl), 140.4 (C-OH), 136.6, 133.1 (C-OH), 132.4, 131.1, 130.0, 126.1, 125.6, 97.7, 61.5, 52.8 (C-CH₃), 19.7, 14.7. MS (*m/z*): 481.12 (M⁺). Anal. Calcd for C₂₃H₂₀ClN₅O₅: C 57.33, H 4.18, N 14.53; Found C 57.45, H 4.07, N 14.64%.

Ethyl-4-(2-chloroquinolin-3-yl)-2-((2-hydroxy-3-(phenoxy-carbonyl)phenyl)diazenyl)-6-methyl-1,6-dihydropyrimidine-5-carboxylate (3l)



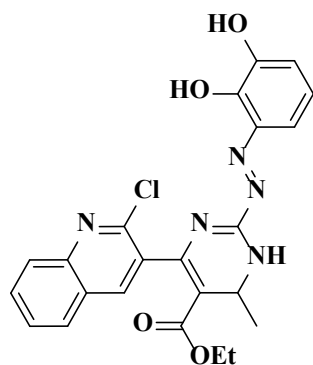
Yellow solid, yield 66%, m.p. 194-196°C. IR v_{max} cm⁻¹: 3075 (OH), 2915 (2° N-H), 2765 (C-H), 1836 (CO), 1605 (C=N), 1313 (C=C), 1256 (C-N), 1021 (C-O), 745 (Ar-Cl). ¹H NMR(500 MHz, DMSO-*d*₆, δ ppm): 7.07-7.96 (m, 7H, Ar-H), 4.25 (q, *J* = 6.0 Hz, 2H, CH₂), 4.19 (m, 1H, CH), 3.67 (s, 1H, OH), 1.50 (d, *J* = 6.10 Hz, 3H, CH₃), 1.37 (t, *J* = 6.0 Hz, 3H, CH₃), 1.22 (d, 1H, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ ppm): 170.3, 169.7, 168.3 (C=O), 158.6 (C-OH), 152.9, 150.2 (C-Cl), 140.7, 136.6, 132.4, 131.1, 130.0, 126.1, 125.6, 97.7, 61.5, 52.8 (C-CH₃), 19.7, 14.7. MS (*m/z*): 579.15 (M⁺). Anal. Calcd for C₃₀H₂₄ClN₅O₅: C 63.22, H 4.24, N 12.29; Found C 63.33, H 4.16, N 12.41%.

Ethyl-4-(2-chloroquinolin-3-yl)-2-((2-hydroxy-4-methylphenyl)diazenyl)-6-methyl-1,6-dihydropyrimidine-5-carboxylate (3m)



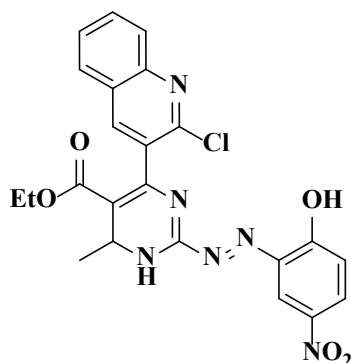
Brown solid, yield 82%, m.p. 176-178°C. IR_{vmax}cm⁻¹: 3125 (OH), 2975 (2° N-H), 2705 (C-H), 1820 (CO), 1619 (C=N), 1346 (C=C), 1237 (C-N), 1005 (C-O), 745 (Ar-Cl). ¹H NMR(500 MHz, DMSO-*d*₆, δ ppm): 6.83-7.99 (m, 8H, Ar-H), 4.59 (s, 1H, OH), 4.25 (q, *J* = 6.0 Hz, 2H, CH₂), 4.19 (m, 1H, CH), 2.35 (s, 3H, CH₃), 1.49 (d, *J* = 6.10 Hz, 3H, CH₃), 1.37 (t, *J* = 6.0 Hz, 3H, CH₃), 1.10 (d, 1H, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ ppm): 170.3, 168.3 (C=O), 153.2 (C-OH), 152.9, 150.2 (C-Cl), 142.8, 136.6, 132.4, 131.1, 130.0, 126.1, 123.1, 97.7, 61.5, 52.8 (C-CH₃), 21.2 (C-CH₃), 19.7, 14.7. MS (*m/z*): 463.14 (M⁺). Anal. Calcd for C₂₄H₂₂ClN₅O₃: C 62.14, H 4.78, N 15.10; Found C 62.27, H 4.63, N 15.23%.

Ethyl-4-(2-chloroquinolin-3-yl)-2-((2,3-dihydroxyphenyl)diazenyl)-6-methyl-1,6-dihydropyrimidine-5-carboxylate (3n)



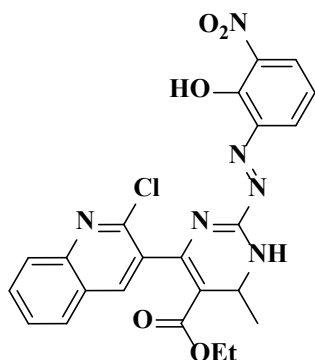
Light brown solid, yield 77%, m.p. 182-184°C. IR_{vmax}cm⁻¹: 3188 (OH), 2977 (2° N-H), 2715 (C-H), 1829 (CO), 1625 (C=N), 1356 (C=C), 1228 (C-N), 1016 (C-O), 745 (Ar-Cl). ¹H NMR(500 MHz, DMSO-*d*₆, δ ppm): 6.75-8.01 (m, 8H, Ar-H), 4.25 (q, *J* = 6.0 Hz, 2H, CH₂), 4.19 (m, 1H, CH), 3.79 (s, 1H, OH), 1.49 (d, *J* = 6.1 Hz, 3H, CH₃), 1.39 (t, *J* = 6.0 Hz, 3H, CH₃), 1.01 (d, 1H, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ ppm): 170.3, 168.3 (C=O), 152.9, 150.2 (C-Cl), 146.6 (C-OH), 145.8, 136.6, 132.4, 131.7, 130.1, 126.1, 110.7, 97.7, 61.5, 52.8 (C-CH₃), 19.7, 14.7. MS (*m/z*): 465.12 (M⁺). Anal. Calcd for C₂₃H₂₀ClN₅O₄: C 59.30, H 4.33, N 15.03; Found C 59.42, H 4.25, N 15.11%

Ethyl-4-(2-chloroquinolin-3-yl)-2-((2-hydroxy-5-nitrophenyl)diazenyl)-6-methyl-1,6-dihydropyrimidine-5-carboxylate (3o)



Light brown solid, yield 70%, m.p. 204-206°C. IR v_{max} cm⁻¹: 3295 (OH), 2967 (2° N-H), 2659 (C-H), 1856 (CO), 1617 (C=N), 1339 (C=C), 1237 (C-N), 1009 (C-O), 745 (Ar-Cl). ¹H NMR(500 MHz, DMSO-*d*₆, δ ppm): 6.20-8.69 (m, 8H, Ar-H), 5.51 (s, 1H, OH), 4.26 (q, *J* = 5.90 Hz, 2H, CH₂), 4.19 (m, 1H, CH), 1.67 (d, 1H, NH), 1.49 (d, *J* = 6.0 Hz, 3H, CH₃), 1.36 (t, *J* = 5.90 Hz, 3H, CH₃); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ ppm): 170.3, 168.3 (C=O), 163.1 (C-OH), 152.9, 150.2 (C-Cl), 143.2, 139.7 (NO₂), 136.6, 132.4, 131.7, 130.1, 126.1, 116.6, 97.7, 61.5, 52.8 (C-CH₃), 19.7, 14.7. MS (*m/z*): 494.11 (M⁺). Anal. Calcd for C₂₃H₁₉ClN₆O₅: C 55.82, H 3.87, N 16.98; Found C 55.97, H 3.95, N 16.85%.

Ethyl-4-(2-chloroquinolin-3-yl)-2-((2-hydroxy-3-nitrophenyl)diazenyl)-6-methyl-1,6-dihydropyrimidine-5-carboxylate (3p)



Brown solid, yield 68%, m.p. 186-188°C. IR v_{max} cm⁻¹: 3285 (OH), 2947 (2° N-H), 2689 (C-H), 1866 (CO), 1616 (C=N), 1319 (C=C), 1217 (C-N), 1026 (C-O), 745 (Ar-Cl). ¹H NMR(500 MHz, DMSO-*d*₆, δ ppm): 7.26-8.14 (m, 8H, Ar-H), 5.43 (s, 1H, OH), 4.23 (q, *J* = 5.90 Hz, 2H, CH₂), 4.19 (m, 1H, CH), 1.49 (d, *J* = 6.0 Hz, 3H, CH₃), 1.36 (t, *J* = 5.90 Hz, 3H, CH₃), 0.96 (d, 1H, NH); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ ppm): 170.3, 168.3 (C=O), 152.9, 150.2 (C-Cl), 147.0 (C-OH), 142.1, 136.6, 134.4 (NO₂), 132.4, 131.7, 130.1, 126.1, 120.7, 97.7, 61.5, 52.8 (C-CH₃), 19.7, 14.7. MS (*m/z*): 494.11 (M⁺). Anal. Calcd for C₂₃H₁₉ClN₆O₅: C 55.82, H 3.87, N 16.98; Found C 55.96, H 3.95, N 16.84%.

Results of docking studies
























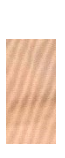












Compounds **3a-p** were also evaluated for *in-silico* docking studies using different targets of bacteria and fungi namely, Dehydrosqualene synthase, Glucosamine-6-phosphate synthase, DNA gyrase, **Squalene epoxidase** and Alpha-beta Tubulin. Promising results were not obtained against these enzymes. Compounds with their total score values are given in Table S1.

Table S1 — Results of docking studies

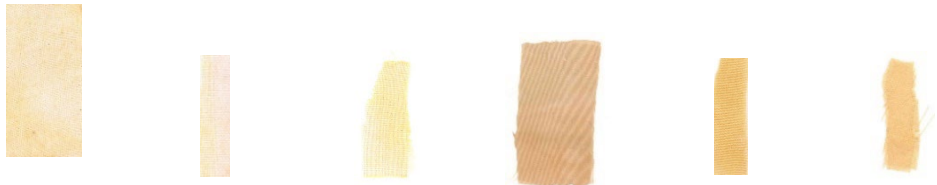
Compound	Total Score*				
	(Dehydrosqualene synthase, <i>S. aureus</i> , PDB ID: 3ACX)	(Glucosamine-6-phosphate synthase, <i>E. coli</i> , PDB ID: 2VF5)	(DNA gyrase, <i>S. aureus</i> , PDB ID: 2XCT)	(Squalene epoxidase , <i>Aspergillus fumigatus</i> , PDB ID: 7CP6)	(Alpha-beta tubulin, Bos taurus: PDB ID: 1JFF)
3a	5.10	5.05	6.10	4.86	5.12
3b	5.41	4.82	6.11	4.84	5.26
3c	6.01	5.41	5.84	4.63	5.24
3d	5.84	5.30	5.72	4.21	5.17
3e	5.21	5.84	6.06	4.10	4.56
3f	5.61	4.56	6.61	4.86	4.76
3g	5.56	4.61	5.41	5.04	4.04
3h	6.44	4.20	5.20	5.10	4.14
3i	6.25	5.12	5.72	5.34	4.16
3j	5.68	5.14	6.06	5.16	4.24
3k	5.40	5.74	6.20	4.00	4.51
3l	5.84	6.08	6.00	4.04	4.46
3m	5.41	4.51	6.05	4.10	5.47
3n	4.82	5.40	6.36	5.14	4.70
3o	5.14	6.10	6.17	3.13	4.29
3p	5.06	6.04	6.16	4.00	4.40
Ampicillin	6.89	7.56	7.23	---	---
Chloramphenicol	6.76	7.34	6.90	---	---
Fluconazole	---	---	---	7.10	6.99

*Total score is expressed in $-\log_{10}(K_d)$ units to represent binding affinities

Table S2 — Scanned pictures of dyed fabrics of compounds **3a-p**

Compound	Dyes applied to cotton fabric	Colour Fastness	Rubbing Fastness	Dyes applied to silk fabric	Colour Fastness	Rubbing Fastness
3a						
3b						
3c						
3d						
3e						
3f						

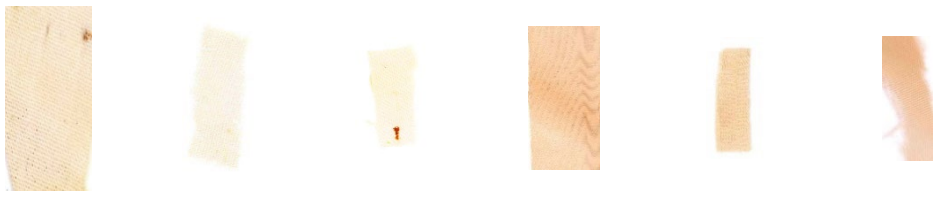
3g



3h



3i



3j



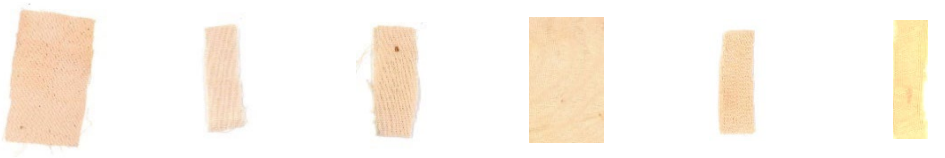
3k



3l



3m



3n



3o



3p

