

Supporting Information

Copper Catalyst Supported Modified Magnetic Chitosan for the Synthesis of Novel 2-Arylthio-2,3-dihydroquinazolin-4(1H)-one Derivatives via Chan-Lam Coupling

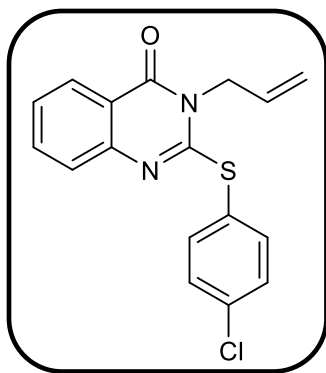
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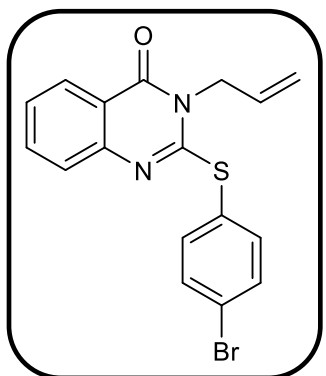
³ *Stem Cells Technology Research Center, Shiraz University of Medical Sciences, Shiraz, Iran.*

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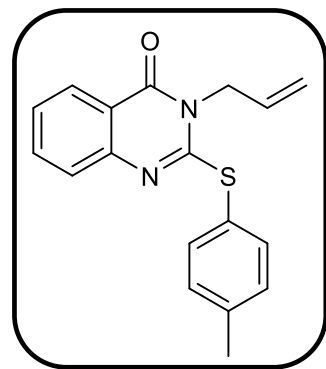
3-allyl-2-((4-chlorophenyl)thio)quinazolin-4(3H)-one (4a)

White solid; m.p. 157-159 °C; ^1H NMR (400 MHz, DMSO- d_6) δ 7.70 (dd, J = 7.8, 1.6 Hz, 1H), 7.39 – 7.25 (m, 4H), 7.16 (d, J = 8.8 Hz, 2H), 6.88 (td, J = 8.0, 1.3 Hz, 1H), 5.89 (ddt, J = 17.2, 10.4, 5.3 Hz, 1H), 5.18 (dd, J = 17.2, 1.6 Hz, 1H), 5.09 (dd, J = 10.3, 1.7 Hz, 1H), 3.94 – 3.81 (m, 2H); ^{13}C NMR (101 MHz, DMSO) δ 168.42, 143.51, 140.70, 135.13, 131.86, 129.34, 129.14, 128.82, 124.73, 120.47, 119.48, 118.78, 115.53, 115.25, 41.30; MS (70 eV): m/z = 328 (M^+).



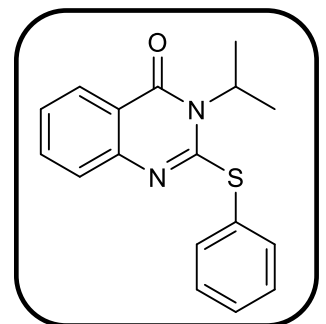
3-allyl-2-((4-bromophenyl)thio)quinazolin-4(3H)-one (4b)

White solid; m.p. 136-139 °C; ^1H NMR (400 MHz, DMSO- d_6) δ 7.69 (dd, J = 7.8, 1.5 Hz, 1H), 7.43 (d, J = 8.7 Hz, 2H), 7.37 – 7.33 (m, 1H), 7.30 (dd, J = 8.4, 1.3 Hz, 1H), 7.11 (d, J = 8.8 Hz, 2H), 6.95 – 6.80 (m, 1H), 5.88 (ddt, J = 17.2, 10.3, 5.3 Hz, 1H), 5.18 (dd, J = 17.2, 1.8 Hz, 1H), 5.09 (dd, J = 10.2, 1.6 Hz, 1H), 3.98 – 3.81 (m, 2H); ^{13}C NMR (101 MHz, DMSO) δ 168.40, 143.31, 141.17, 135.12, 132.29, 132.00, 131.84, 128.83, 120.73, 119.68, 118.91, 115.70, 115.26, 112.38, 41.30; MS (70 eV): m/z = 371 (M^+).



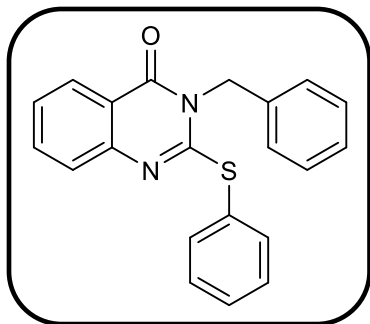
3-allyl-2-(p-tolylthio)quinazolin-4(3H)-one (4c)

White solid; m.p. 166-168 °C; ^1H NMR (400 MHz, DMSO- d_6) δ 7.69 (dd, J = 8.0, 1.6 Hz, 1H), 7.29 (ddd, J = 8.5, 7.1, 1.5 Hz, 1H), 7.20 (dd, J = 8.5, 1.2 Hz, 1H), 7.12 (d, J = 8.5 Hz, 2H), 7.05 (d, J = 8.4 Hz, 2H), 6.78 (td, J = 7.7, 1.2 Hz, 1H), 5.90 (ddt, J = 17.3, 10.4, 5.2 Hz, 1H), 5.19 (dd, J = 17.2, 1.8 Hz, 1H), 5.09 (dd, J = 10.3, 1.7 Hz, 1H), 3.90 (ddd, J = 5.6, 3.7, 1.7 Hz, 2H), 2.26 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ 168.69, 145.10, 138.64, 135.24, 131.89, 131.08, 129.82, 129.78, 128.71, 120.29, 117.68, 117.37, 115.18, 114.16, 41.28, 20.34; MS (70 eV): m/z = 308 (M^+).



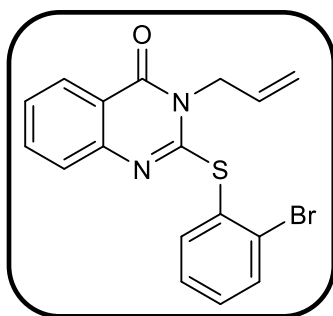
3-isopropyl-2-(phenylthio)quinazolin-4(3H)-one (4d)

White solid; m.p. 161-161 °C; ^1H NMR (400 MHz, DMSO- d_6) δ 8.03 (dd, J = 8.0, 1.6 Hz, 1H), 7.69 – 7.61 (m, 3H), 7.57 – 7.49 (m, 3H), 7.43 – 7.37 (m, 1H), 7.11 (dd, J = 8.3, 1.1 Hz, 1H), 4.80 (s, 1H), 1.65 (d, J = 6.6 Hz, 6H); ^{13}C NMR (101 MHz, DMSO) δ 161.10, 156.27, 146.14, 135.76, 134.40, 129.88, 129.32, 127.96, 126.06, 126.00, 125.69, 120.12, 52.64, 19.22; MS (70 eV): m/z = 296 (M^+).



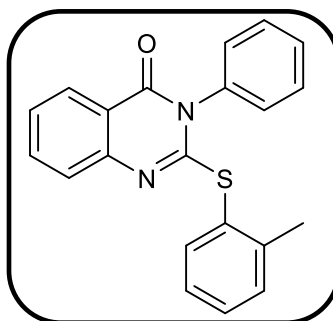
3-benzyl-2-(phenylthio)quinazolin-4(3H)-one (4e)

White solid; m.p. 194-197 °C; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 8.11 (dd, $J = 8.0, 1.5$ Hz, 1H), 7.72 (ddd, $J = 8.6, 7.2, 1.6$ Hz, 1H), 7.60 (dd, $J = 7.8, 1.8$ Hz, 2H), 7.54 – 7.43 (m, 4H), 7.41 – 7.28 (m, 5H), 7.23 – 7.18 (m, 1H), 5.47 (s, 2H); ^{13}C NMR (101 MHz, DMSO) δ 161.00, 156.65, 146.73, 135.74, 135.52, 134.82, 129.93, 129.35, 128.68, 127.45, 126.72, 126.57, 126.30, 126.11, 118.91, 47.15; MS (70 eV): $m/z = 344$ (M^+).



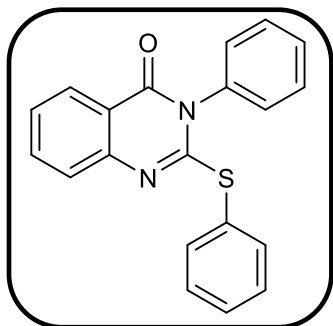
3-allyl-2-((2-bromophenyl)thio)quinazolin-4(3H)-one (4f)

White solid; m.p. 144-146 °C; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 8.08 (dd, $J = 8.0, 1.5$ Hz, 1H), 7.86 (ddd, $J = 7.6, 1.7$ Hz, 1H), 7.81 (dd, $J = 7.4, 1.9$ Hz, 1H), 7.72 – 7.66 (m, 1H), 7.55 – 7.41 (m, 3H), 7.16 (dd, $J = 8.2, 1.0$ Hz, 1H), 6.04 (ddt, $J = 17.3, 10.2, 5.0$ Hz, 1H), 5.35 – 5.15 (m, 2H), 4.86 (dd, $J = 4.2, 2.5$ Hz, 2H); ^{13}C NMR (101 MHz, DMSO) δ 160.39, 155.02, 146.72, 138.05, 134.75, 133.58, 132.09, 131.42, 130.06, 129.02, 128.67, 126.47, 126.36, 126.16, 118.89, 117.50, 46.27; MS (70 eV): $m/z = 373$ (M^+).



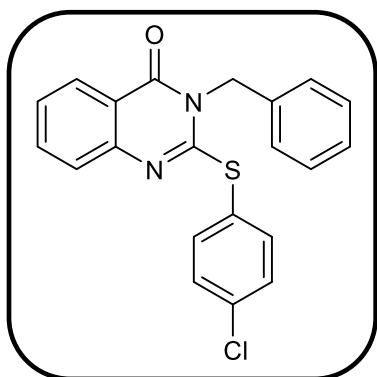
3-phenyl-2-(o-tolylthio)quinazolin-4(3H)-one (4g)

White solid; m.p. 151-153 °C; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 8.07 (dd, $J = 7.9, 1.5$ Hz, 1H), 7.72 (ddd, $J = 8.6, 7.1, 1.6$ Hz, 1H), 7.66 – 7.57 (m, 5H), 7.50 (dd, $J = 7.6, 1.2$ Hz, 1H), 7.47 – 7.38 (m, 3H), 7.28 (td, $J = 7.1, 2.4$ Hz, 1H), 7.21 (dd, $J = 8.2, 1.1$ Hz, 1H), 2.34 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ 160.86, 156.20, 147.20, 142.80, 136.53, 136.25, 134.78, 130.64, 130.48, 129.92, 129.56, 129.40, 127.54, 126.70, 126.50, 126.12, 126.04, 119.66, 20.40; MS (70 eV): $m/z = 344$ (M^+).



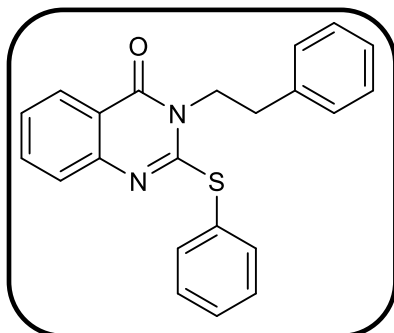
3-phenyl-2-(phenylthio)quinazolin-4(3H)-one (4h)

White solid; m.p. 149-152 °C; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 8.08 (dd, $J = 7.8, 1.6$ Hz, 1H), 7.74 (ddd, $J = 8.5, 7.2, 1.6$ Hz, 1H), 7.65 – 7.55 (m, 7H), 7.52 – 7.43 (m, 4H), 7.25 (dd, $J = 8.1, 1.2$ Hz, 1H); ^{13}C NMR (101 MHz, DMSO) δ 160.83, 156.87, 147.13, 136.02, 135.38, 134.80, 129.96, 129.73, 129.52, 129.20, 128.18, 126.51, 126.12, 119.70; MS (70 eV): $m/z = 330$ (M^+).



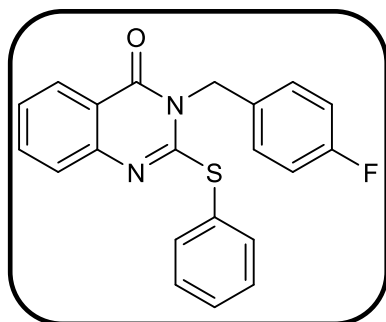
3-benzyl-2-((4-chlorophenyl)thio)quinazolin-4(3H)-one (4i)

White solid; m.p. 172-174 °C; ^1H NMR (400 MHz, DMSO- d_6) δ 8.12 (dd, J = 8.1, 1.6 Hz, 1H), 7.73 (td, J = 8.6, 1.6 Hz, 1H), 7.63 (d, J = 8.6 Hz, 2H), 7.57 (d, J = 8.6 Hz, 2H), 7.48 (td, J = 8.2, 1.1 Hz, 1H), 7.40 – 7.30 (m, 5H), 7.27 – 7.24 (m, 1H), 5.45 (s, 2H); ^{13}C NMR (101 MHz, DMSO) δ 160.97, 156.26, 146.67, 137.28, 135.64, 134.96, 134.86, 129.37, 128.69, 127.48, 126.73, 126.58, 126.51, 126.41, 126.18, 118.94, 47.18; MS (70 eV): m/z = 378 (M^+).



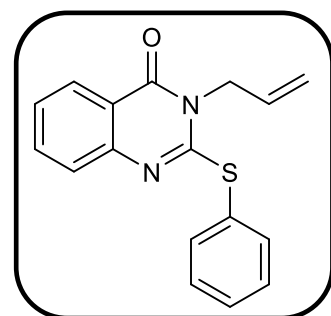
3-phenethyl-2-(phenylthio)quinazolin-4(3H)-one (4j)

White solid; m.p. 188-189 °C; ^1H NMR (400 MHz, DMSO- d_6) δ 8.09 (dd, J = 8.0, 1.6 Hz, 1H), 7.70 (ddd, J = 8.4, 7.2, 1.7 Hz, 1H), 7.66 – 7.60 (m, 2H), 7.57 – 7.51 (m, 3H), 7.45 (t, J = 7.5 Hz, 1H), 7.40 – 7.26 (m, 5H), 7.18 (d, J = 8.1 Hz, 1H), 4.36 (t, J = 8.0 Hz, 2H), 3.11 (t, J = 8.0 Hz, 2H); ^{13}C NMR (101 MHz, DMSO) δ 160.54, 156.11, 146.64, 137.79, 135.66, 134.62, 129.95, 129.35, 128.79, 128.63, 127.30, 126.70, 126.36, 126.16, 126.04, 118.97, 45.84, 33.53; MS (70 eV): m/z = 358 (M^+).



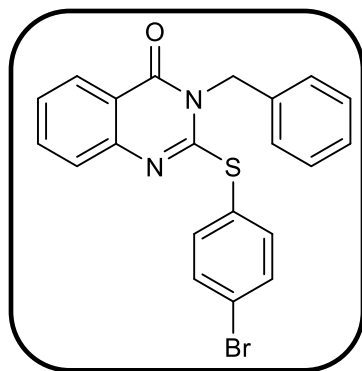
3-(4-fluorobenzyl)-2-(phenylthio)quinazolin-4(3H)-one (4k)

White solid; m.p. 165-167 °C; ^1H NMR (400 MHz, DMSO- d_6) δ 8.11 (dd, J = 8.0, 1.5 Hz, 1H), 7.72 (ddd, J = 8.4, 7.1, 1.6 Hz, 1H), 7.61 (dd, J = 7.8, 1.9 Hz, 2H), 7.56 – 7.38 (m, 6H), 7.27 – 7.16 (m, 3H), 5.44 (s, 2H); ^{13}C NMR (101 MHz, DMSO) δ 162.66 (d, $^1J_{\text{CF}}$ = 242 Hz), 161.02, 156.48, 146.71, 135.53, 134.84, 131.97 (d, $^4J_{\text{CF}}$ = 3 Hz), 129.95, 129.36, 129.11 (d, $^3J_{\text{CF}}$ = 8 Hz), 127.36, 126.56, 126.31, 126.11, 118.93, 115.58 (d, $^2J_{\text{CF}}$ = 21 Hz), 46.54; MS (70 eV): m/z = 362 (M^+).



3-allyl-2-(phenylthio)quinazolin-4(3H)-one (4l)

White solid; m.p. 146-148 °C; ^1H NMR (400 MHz, DMSO- d_6) δ 8.08 (dd, J = 8.0, 1.6 Hz, 1H), 7.70 (ddd, J = 8.4, 7.1, 1.6 Hz, 1H), 7.67 – 7.61 (m, 2H), 7.56 – 7.49 (m, 3H), 7.44 (td, J = 7.6, 7.1, 1.2 Hz, 1H), 7.19 (dd, J = 8.3, 1.0 Hz, 1H), 6.03 (ddt, J = 17.2, 10.2, 5.0 Hz, 1H), 5.28 (dd, J = 10.5, 1.4 Hz, 1H), 5.21 (dd, J = 17.2, 1.4 Hz, 1H), 4.87 – 4.75 (m, 2H); ^{13}C NMR (101 MHz, DMSO) δ 160.44, 156.40, 146.70, 135.56, 134.67, 131.61, 129.91, 129.36, 127.48, 126.44, 126.18, 126.05, 118.89, 117.41, 46.07; MS (70 eV): m/z = 294 (M^+).

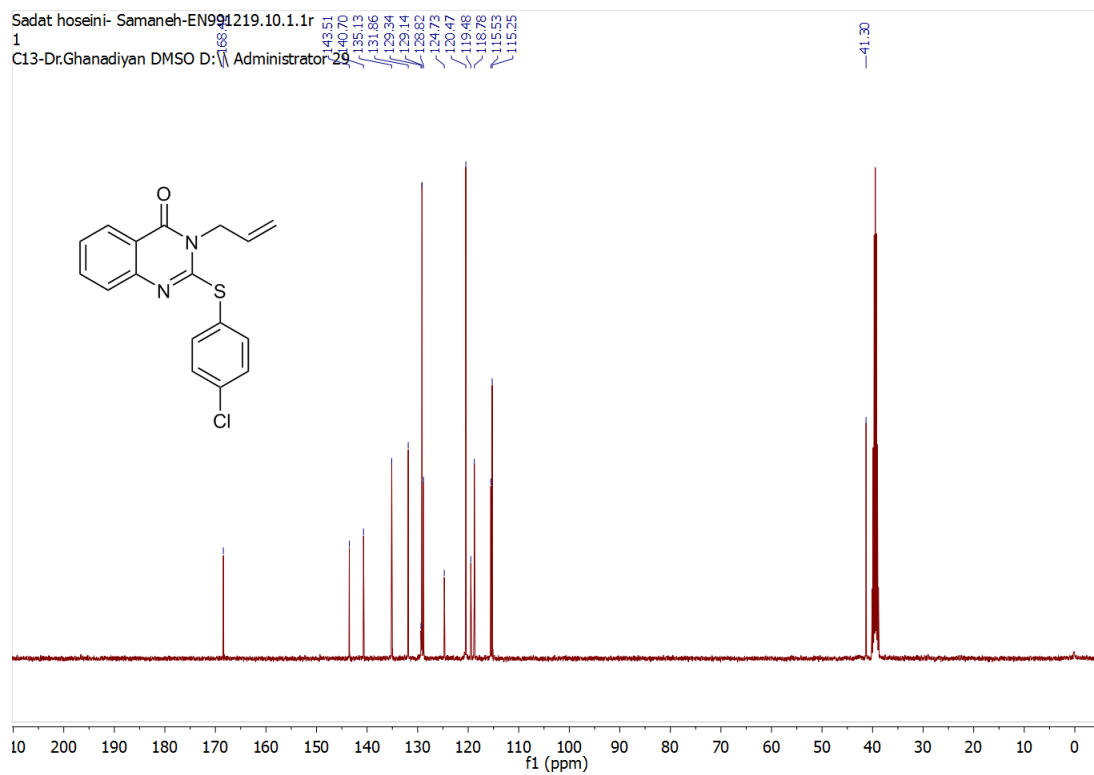
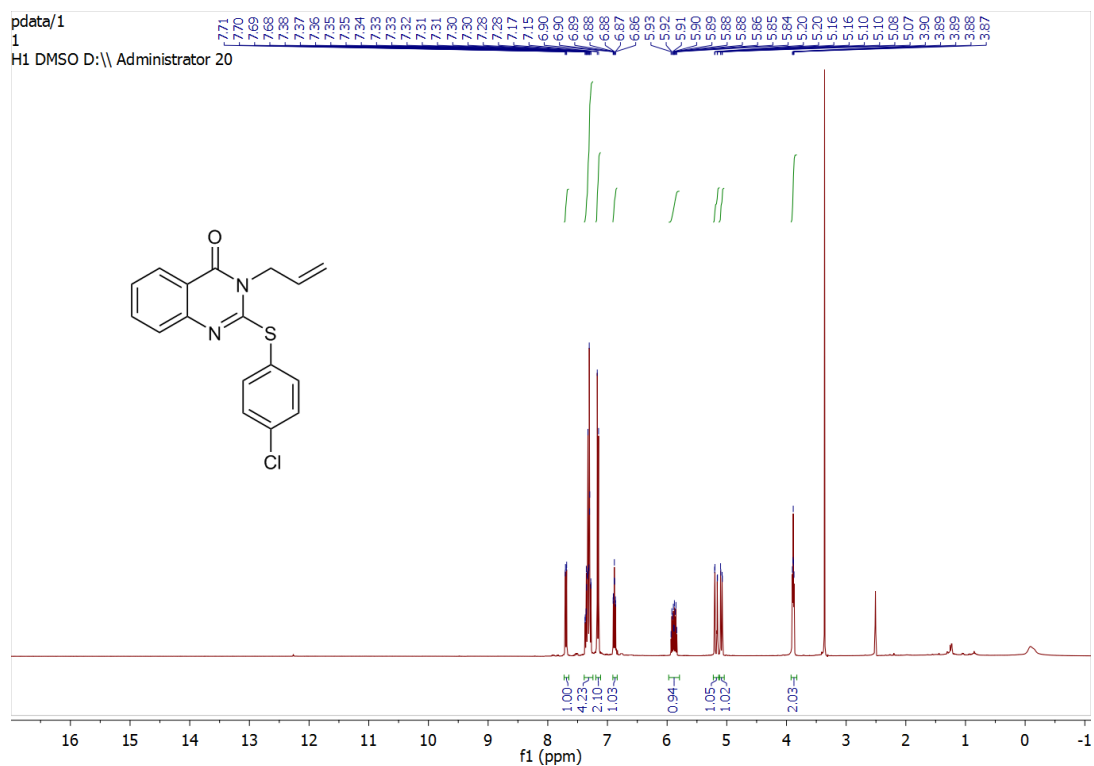


3-benzyl-2-((4-bromophenyl)thio)quinazolin-4(3*H*)-one (4m)

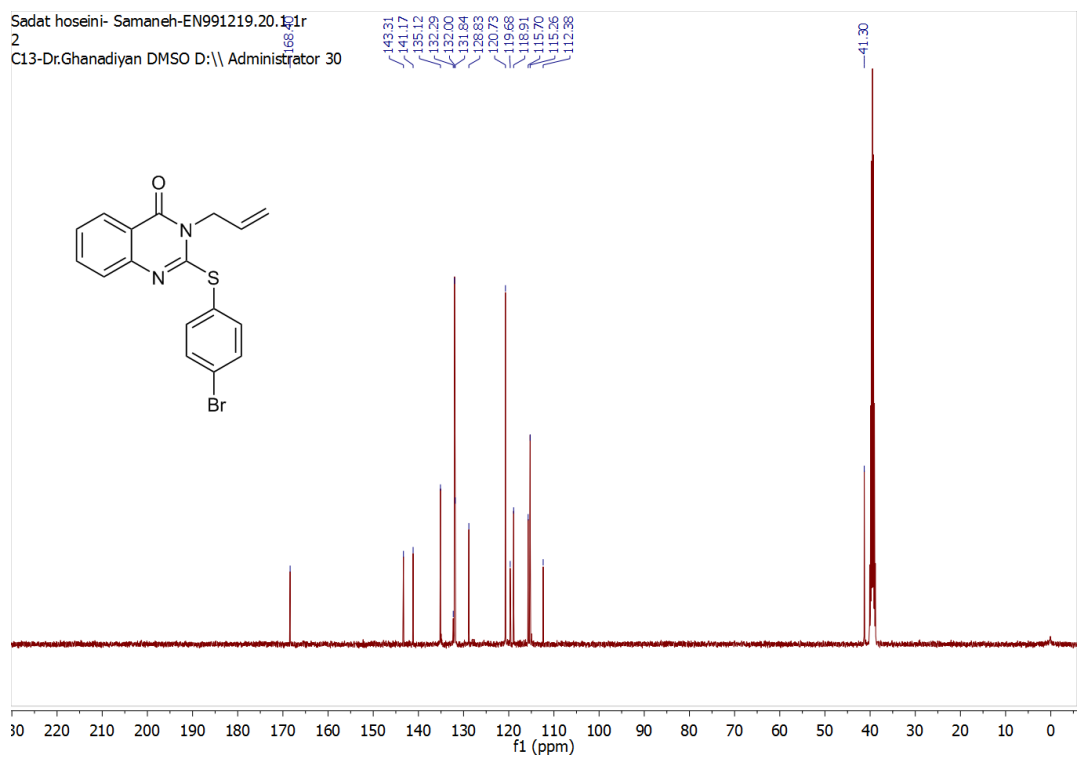
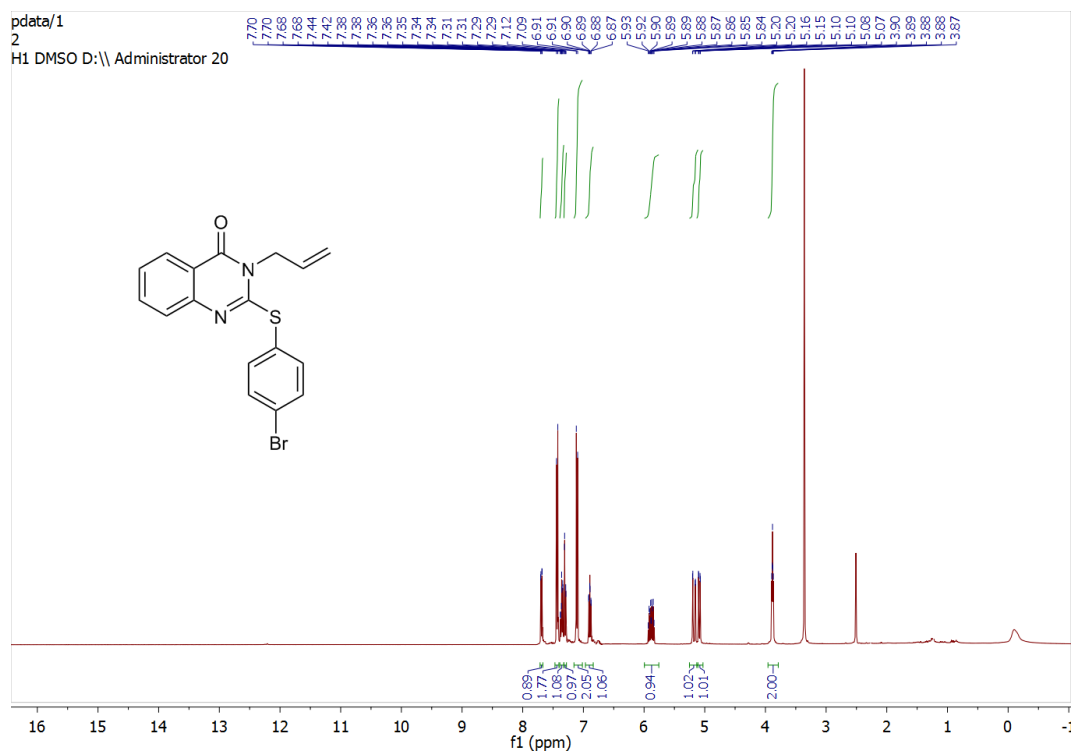
White solid; m.p. 154-156 °C; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.12 (dd, $J = 8.0$, 1.6 Hz, 1H), 7.77 – 7.67 (m, 3H), 7.55 (d, $J = 8.4$ Hz, 2H), 7.50 – 7.45 (m, 1H), 7.42 – 7.29 (m, 5H), 7.26 (dd, $J = 8.2$, 1.0 Hz, 1H), 5.45 (s, 2H); ^{13}C NMR (101 MHz, DMSO) δ 160.97, 156.13, 146.66, 137.44, 135.64, 134.86, 132.29, 128.69, 127.48, 127.03, 126.72, 126.57, 126.41, 126.19, 123.71, 118.94, 47.19; MS (70 eV): $m/z = 422$ (M^+).

Spectral data of the products

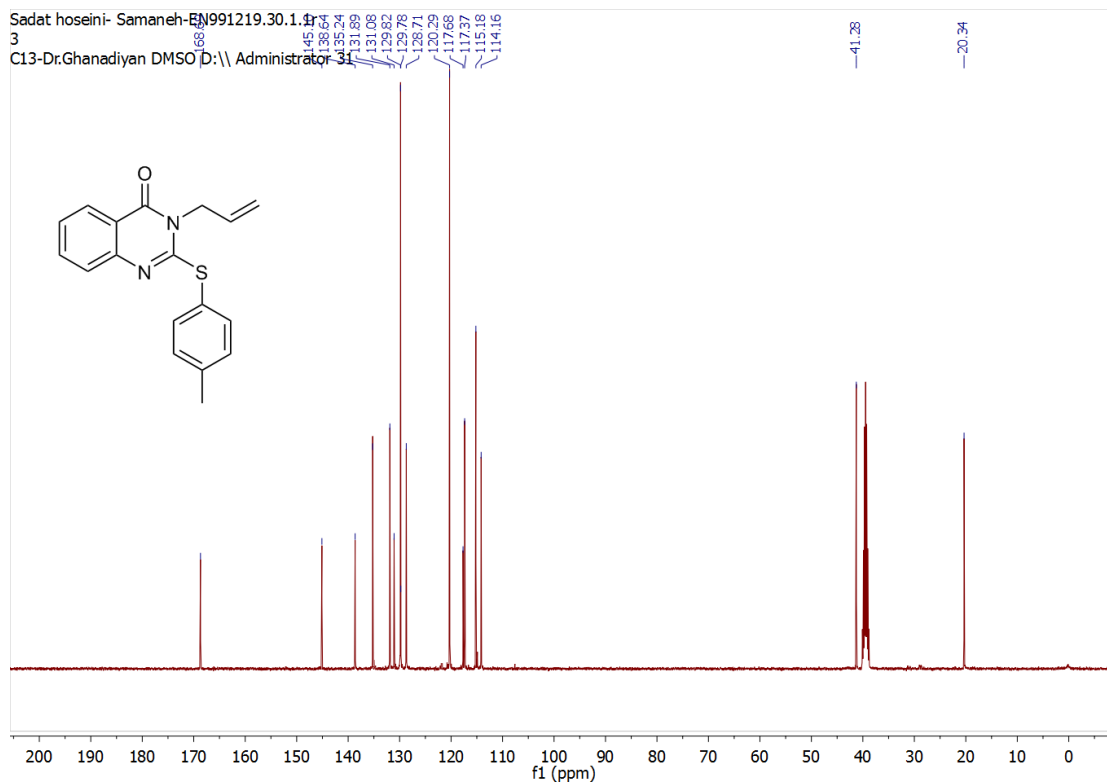
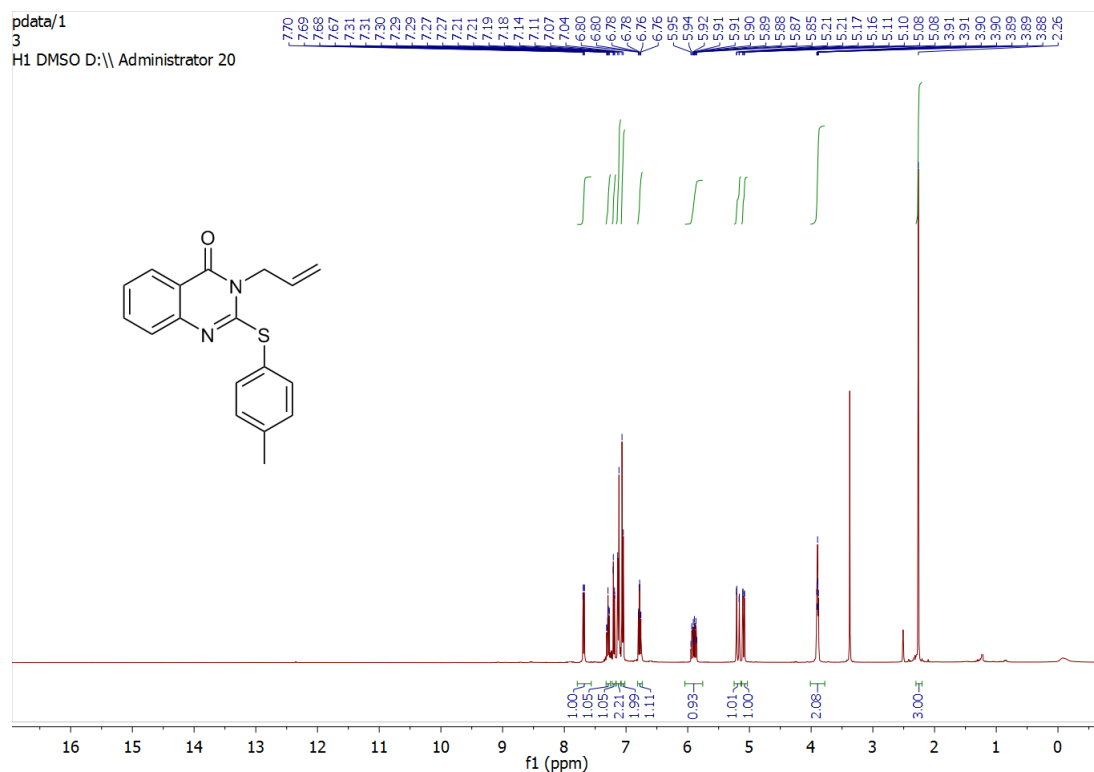
3-allyl-2-((4-chlorophenyl)thio)quinazolin-4(3H)-one (4a)



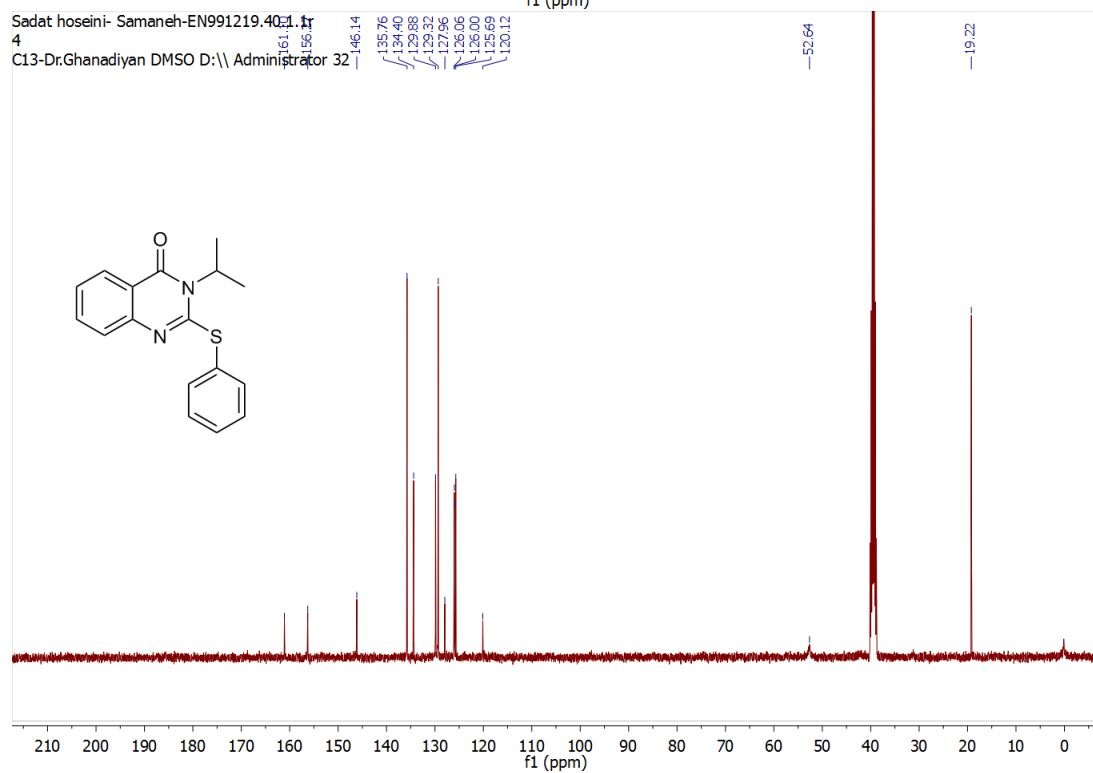
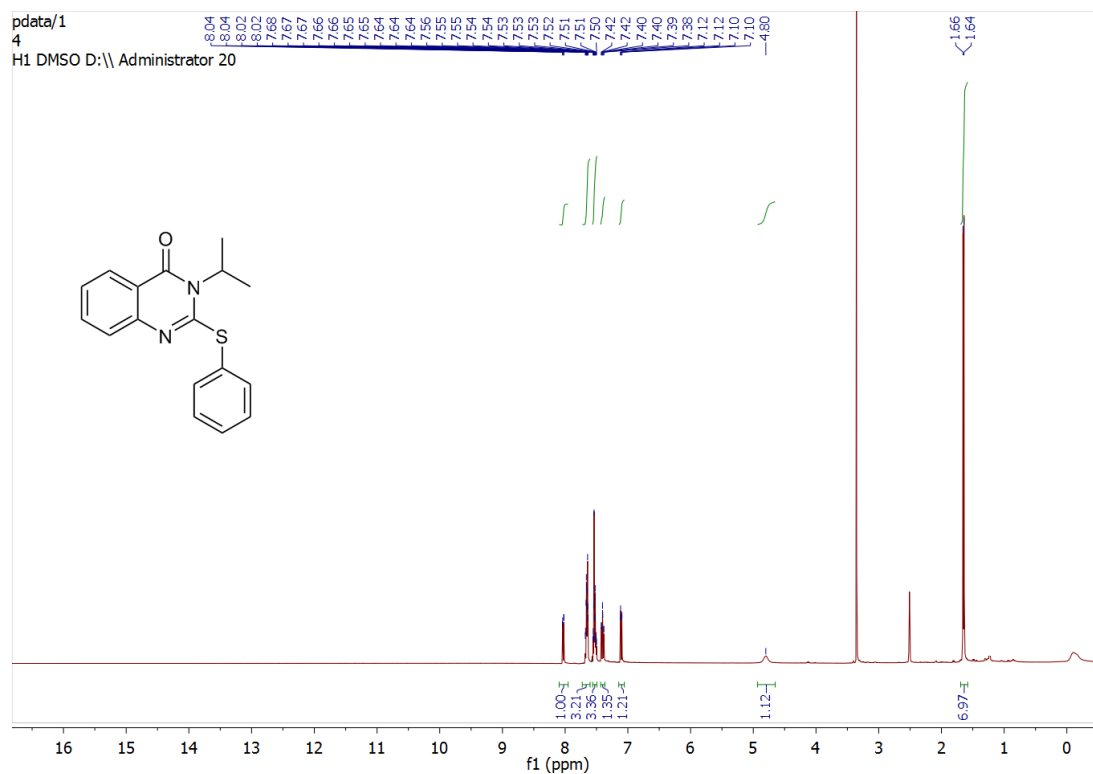
3-allyl-2-((4-bromophenyl)thio)quinazolin-4(3H)-one (4b)



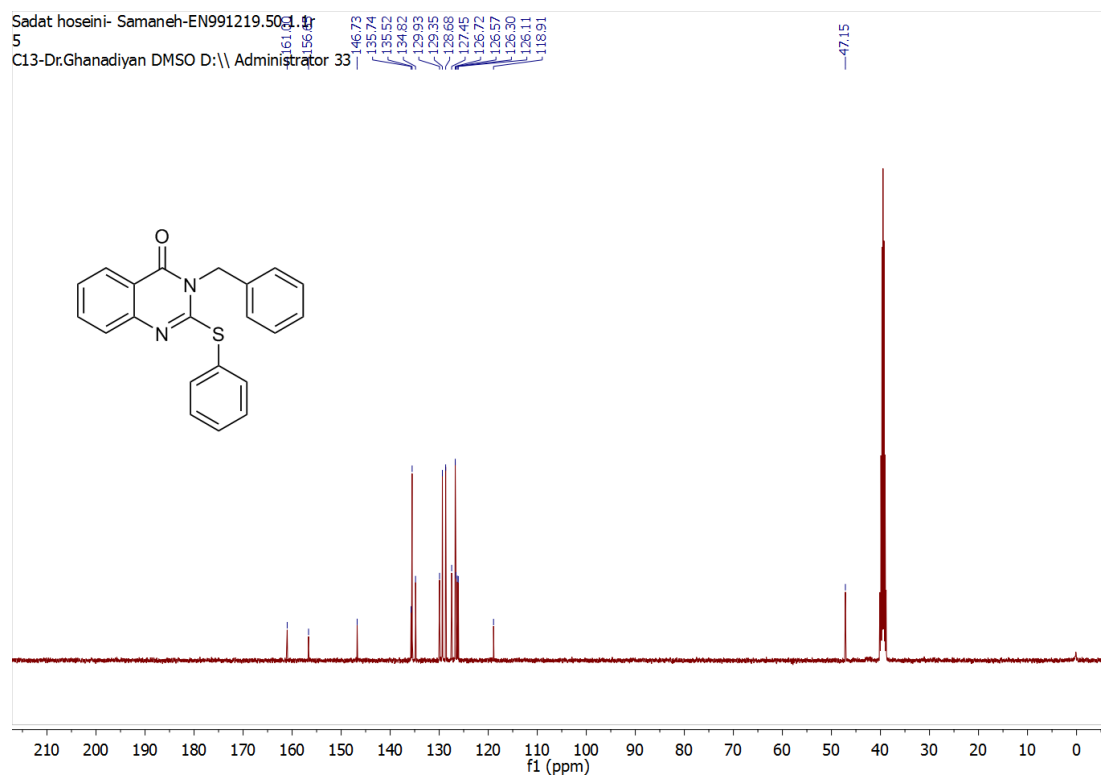
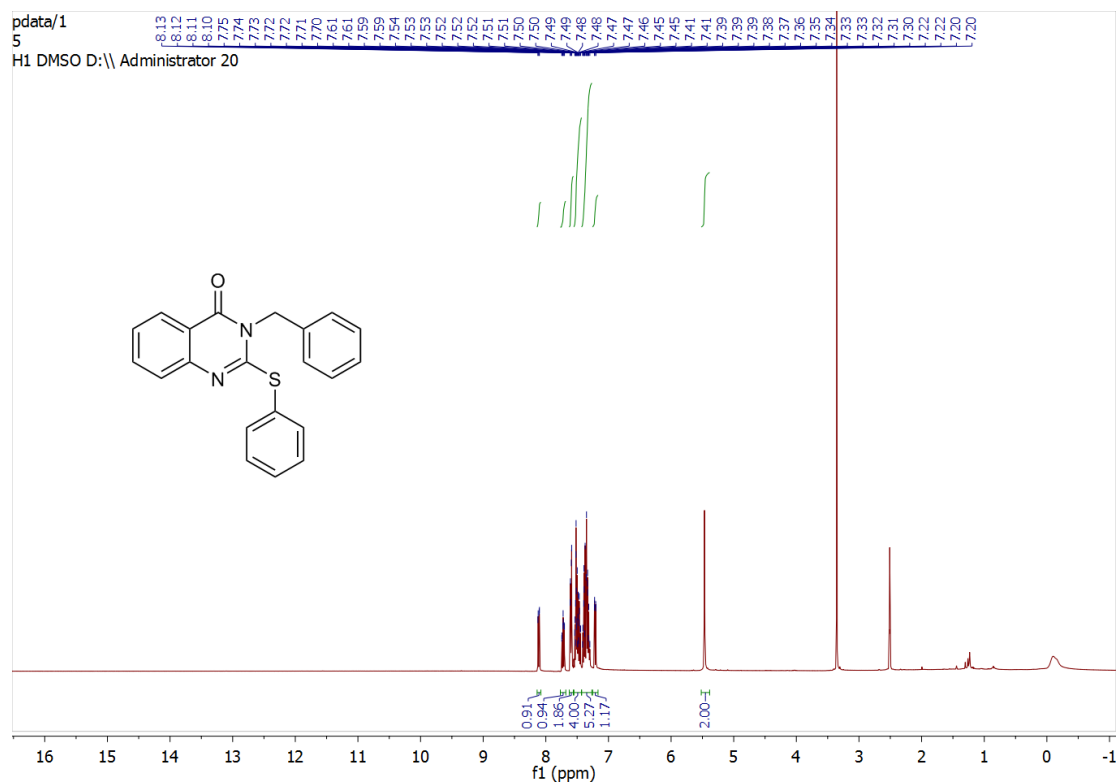
3-allyl-2-(*p*-tolylthio)quinazolin-4(3*H*)-one (4c)



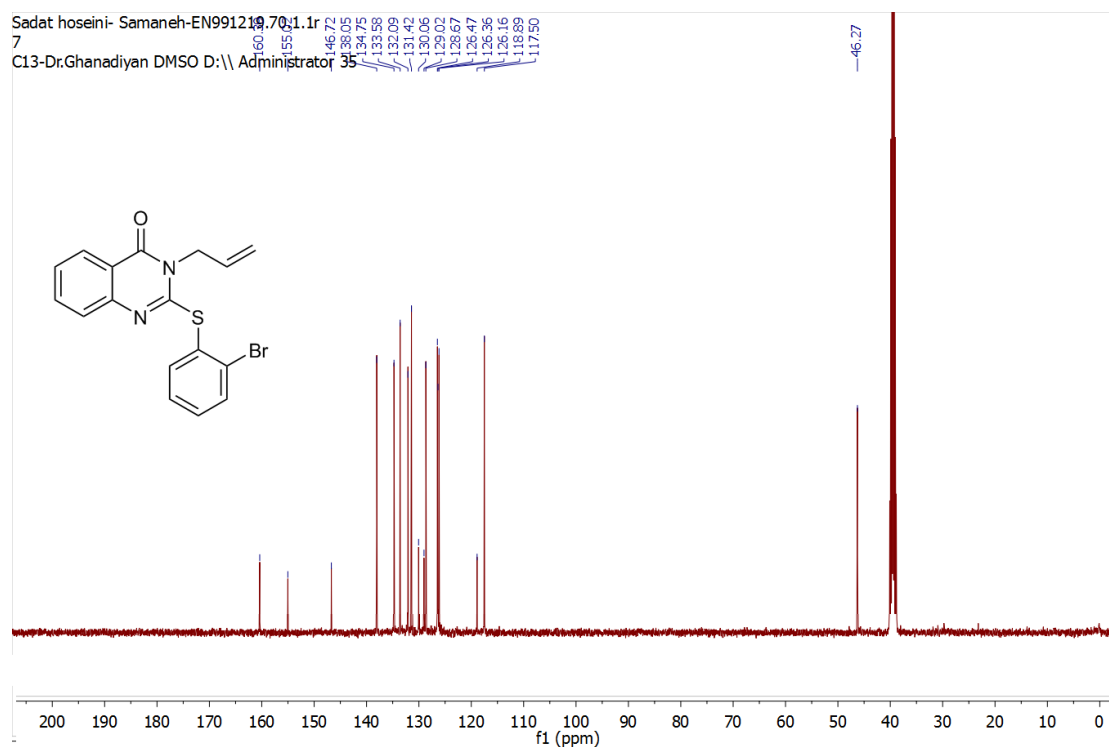
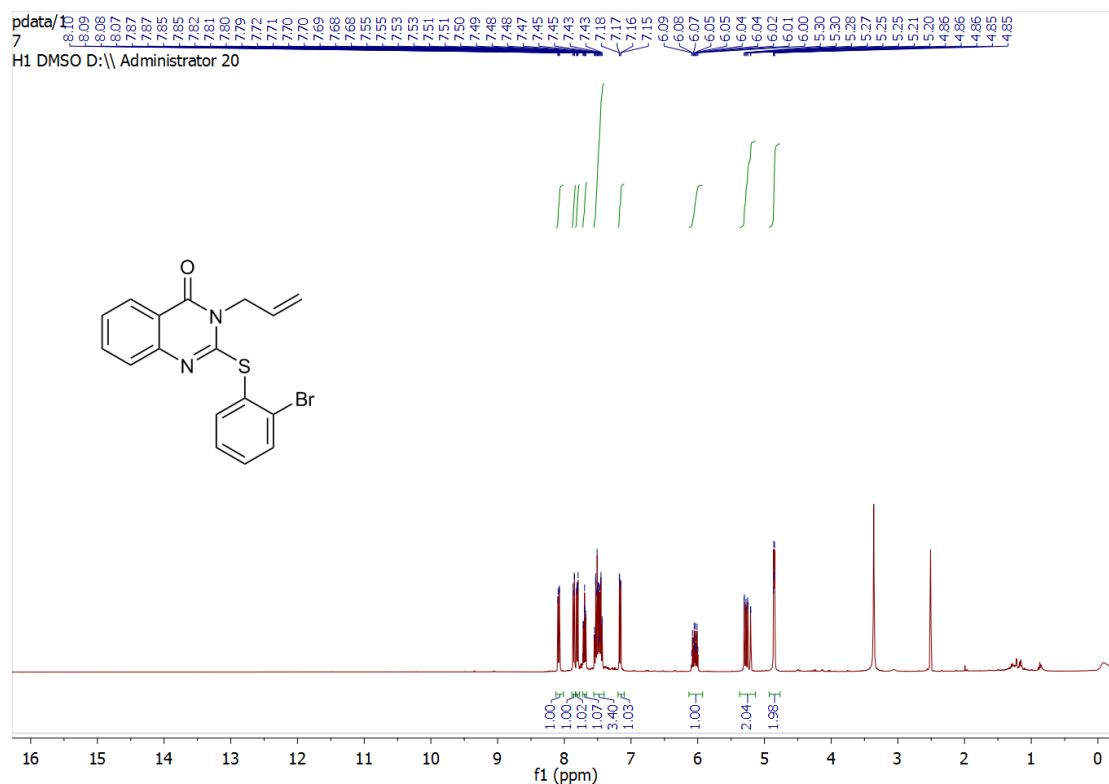
3-isopropyl-2-(phenylthio)quinazolin-4(3H)-one (4d)



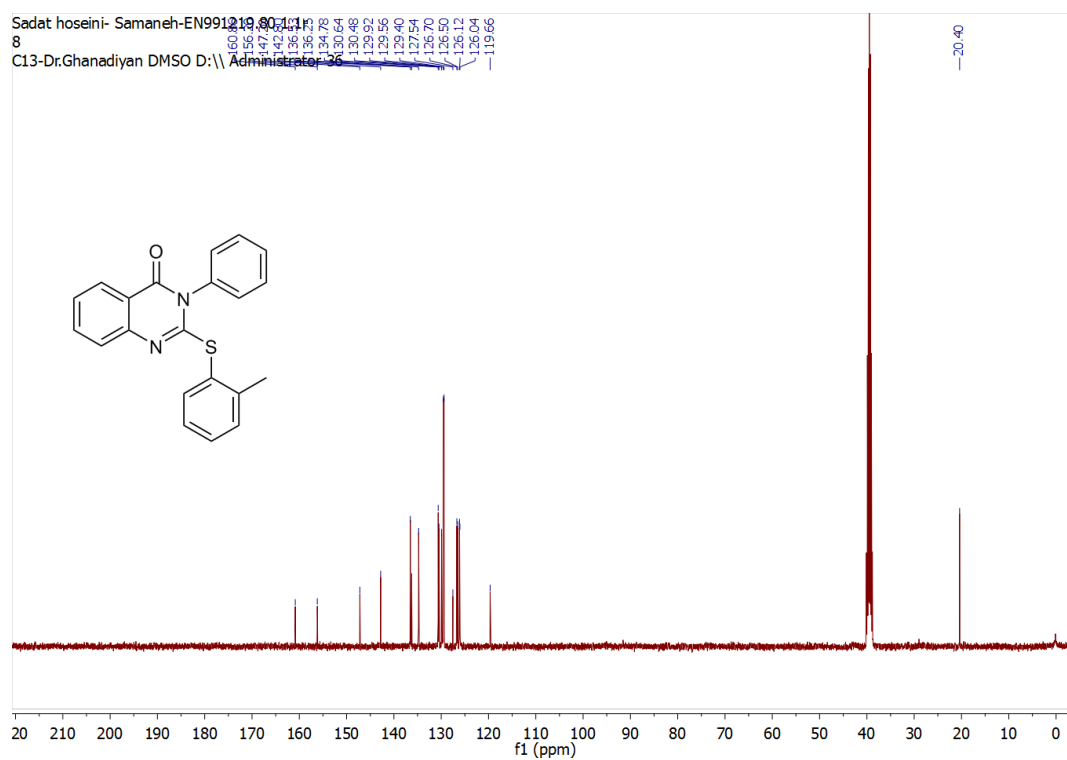
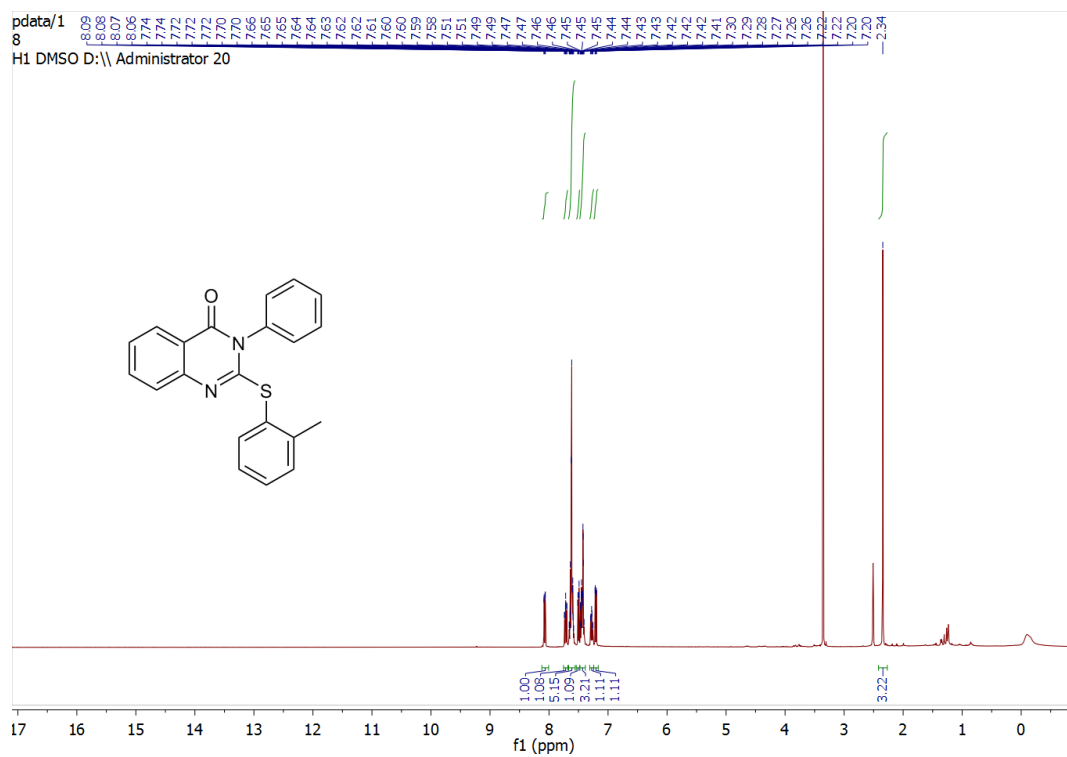
3-benzyl-2-(phenylthio)quinazolin-4(3H)-one (4e)



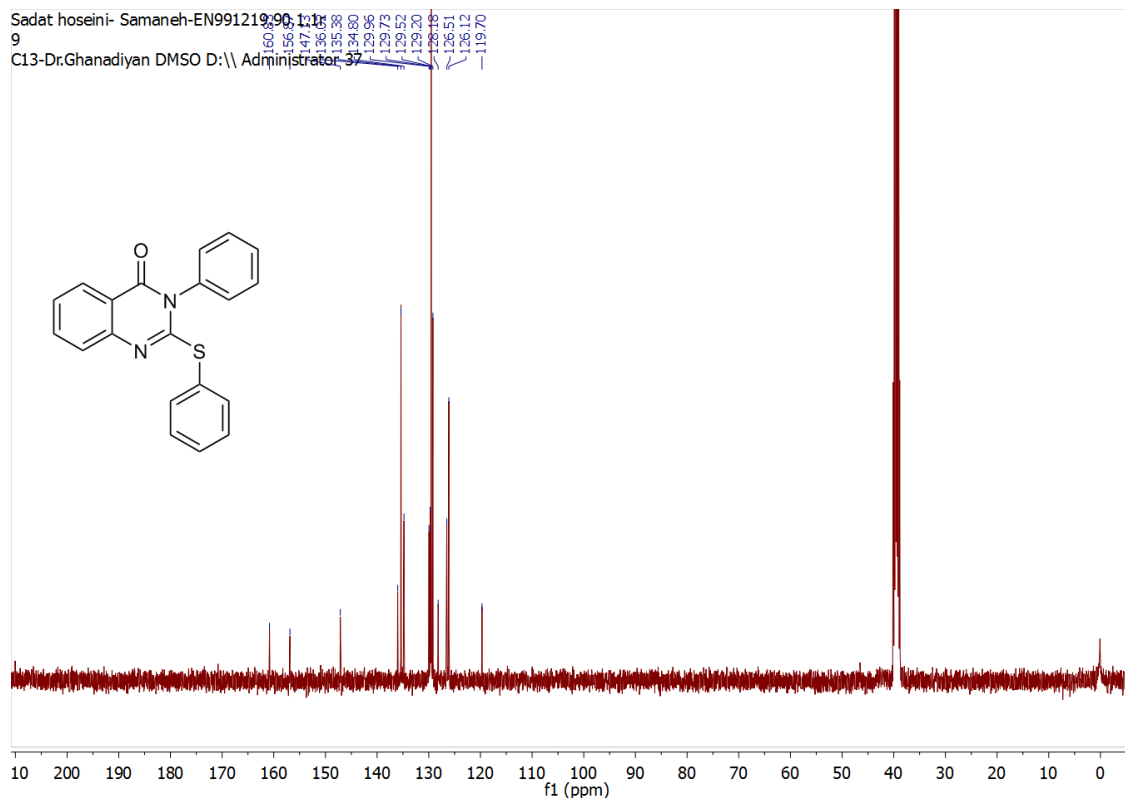
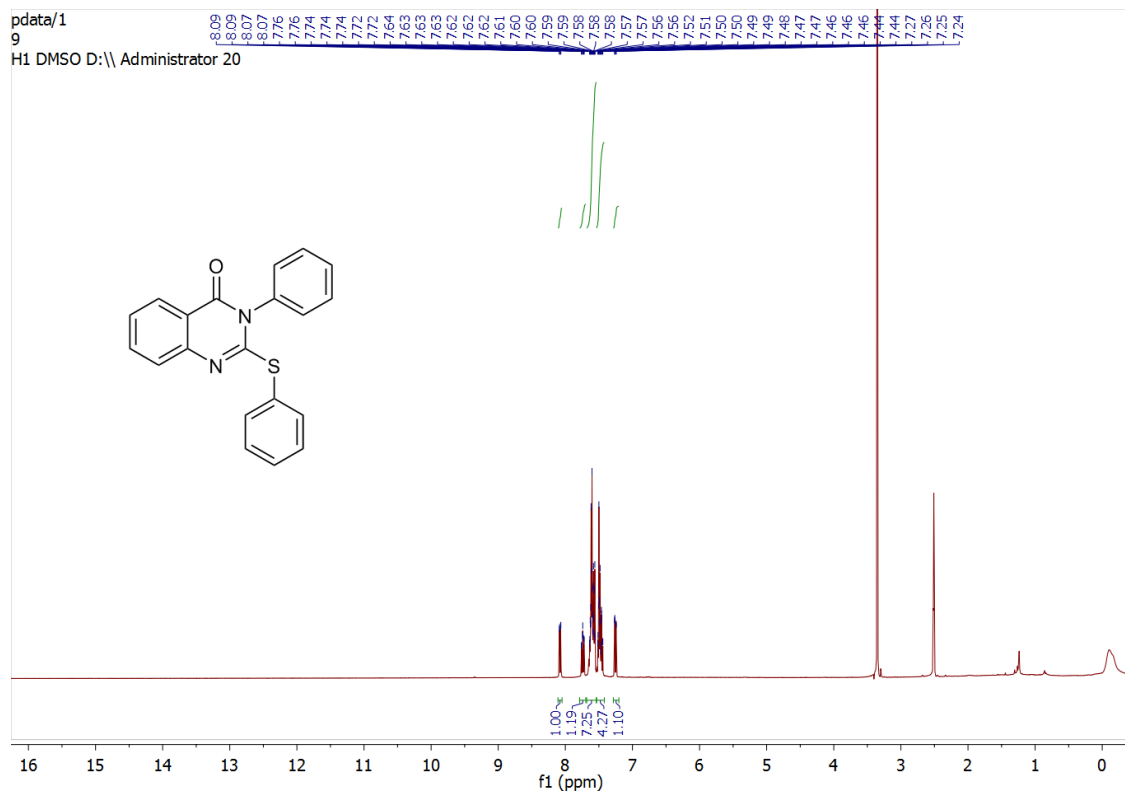
3-allyl-2-((2-bromophenyl)thio)quinazolin-4(3H)-one (4f)



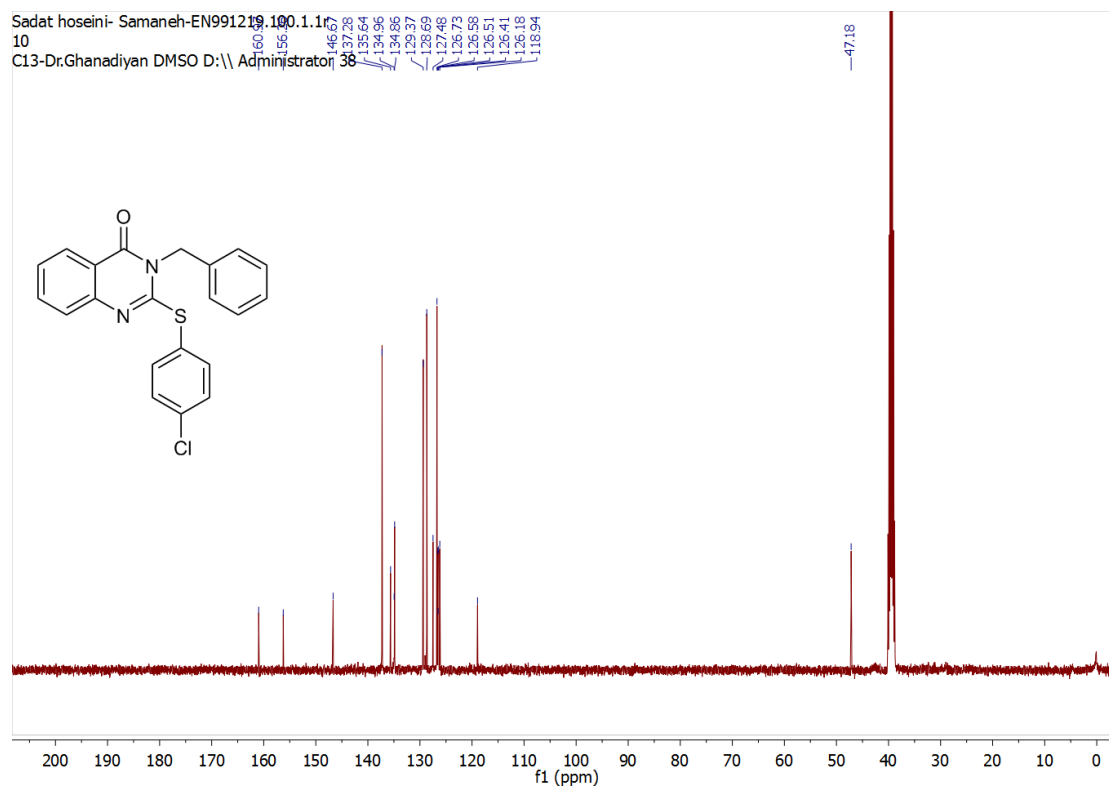
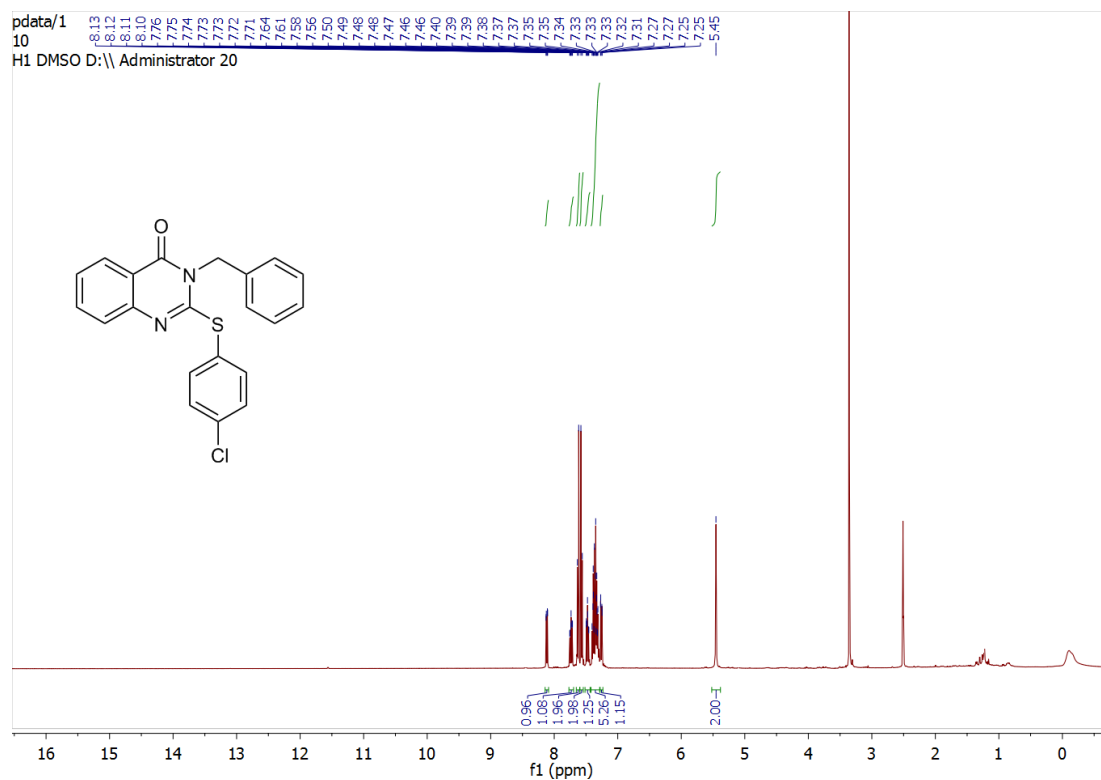
3-phenyl-2-(*o*-tolylthio)quinazolin-4(3*H*)-one (4g)



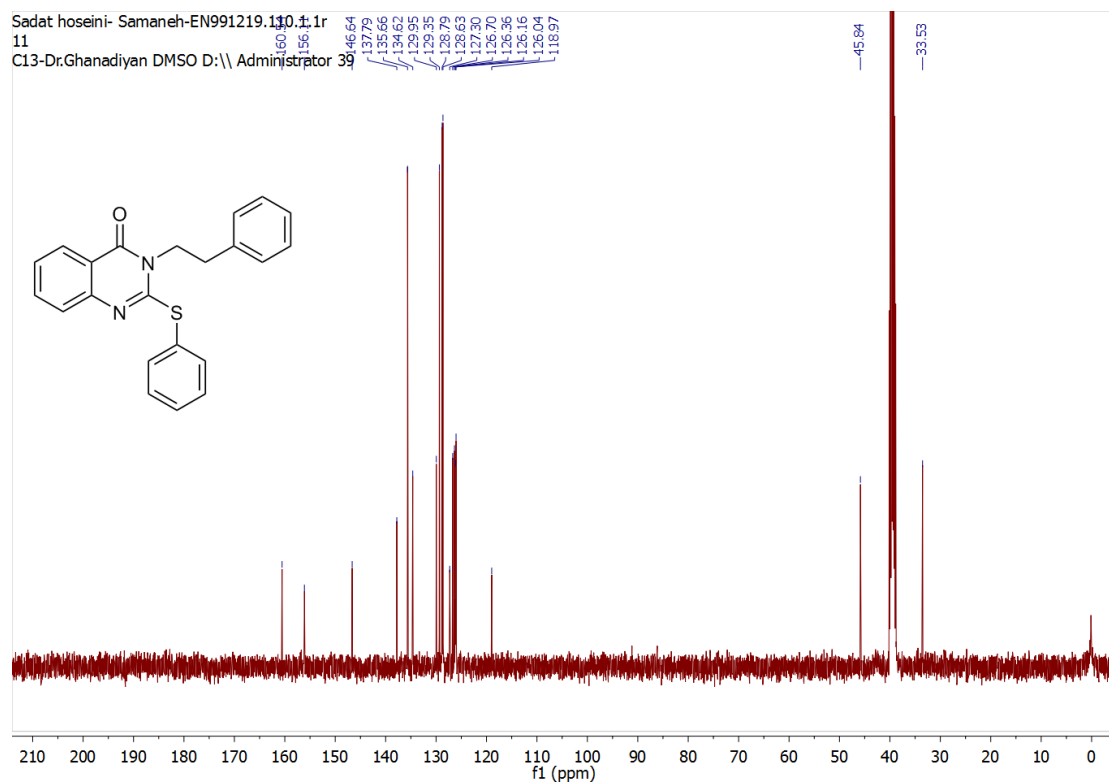
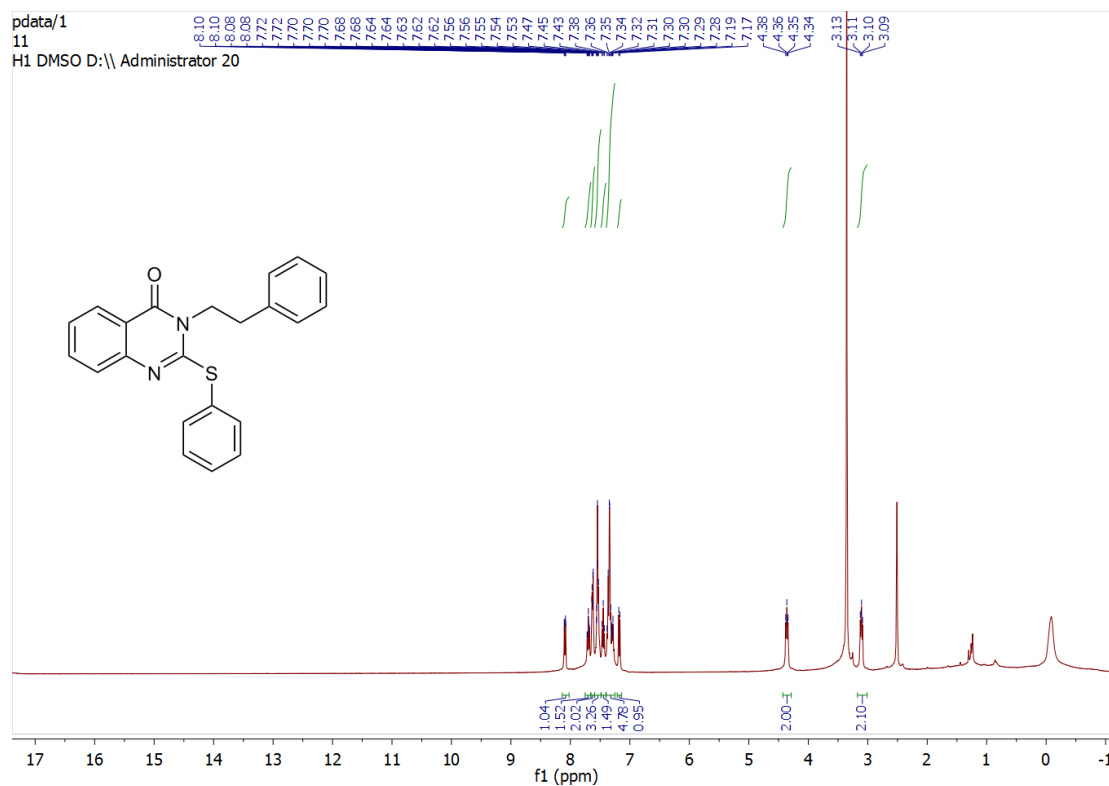
3-phenyl-2-(phenylthio)quinazolin-4(3*H*)-one (4h)



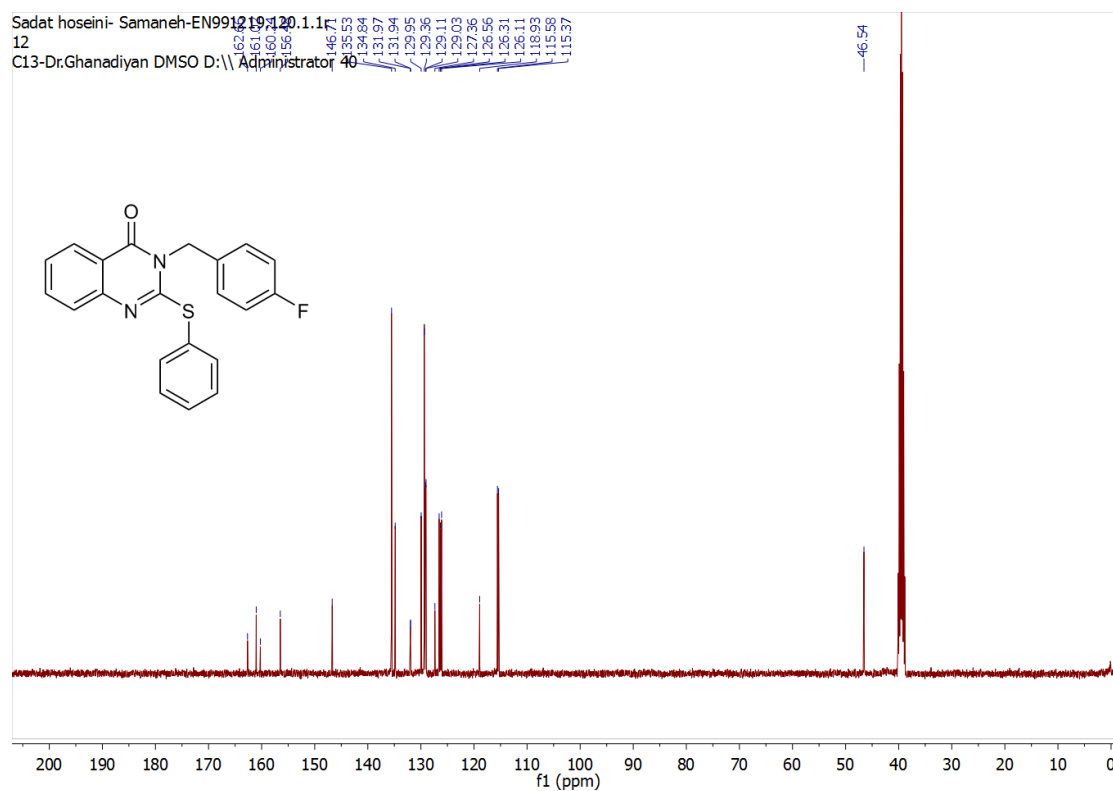
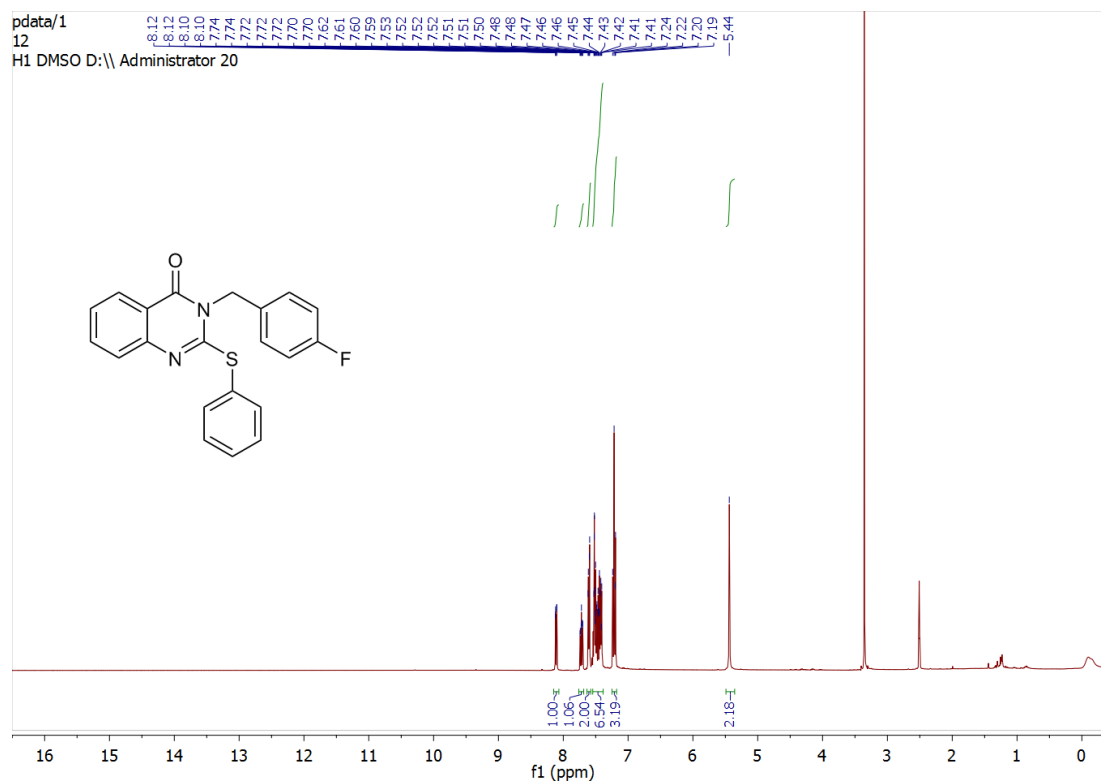
3-benzyl-2-((4-chlorophenyl)thio)quinazolin-4(3H)-one (4i)



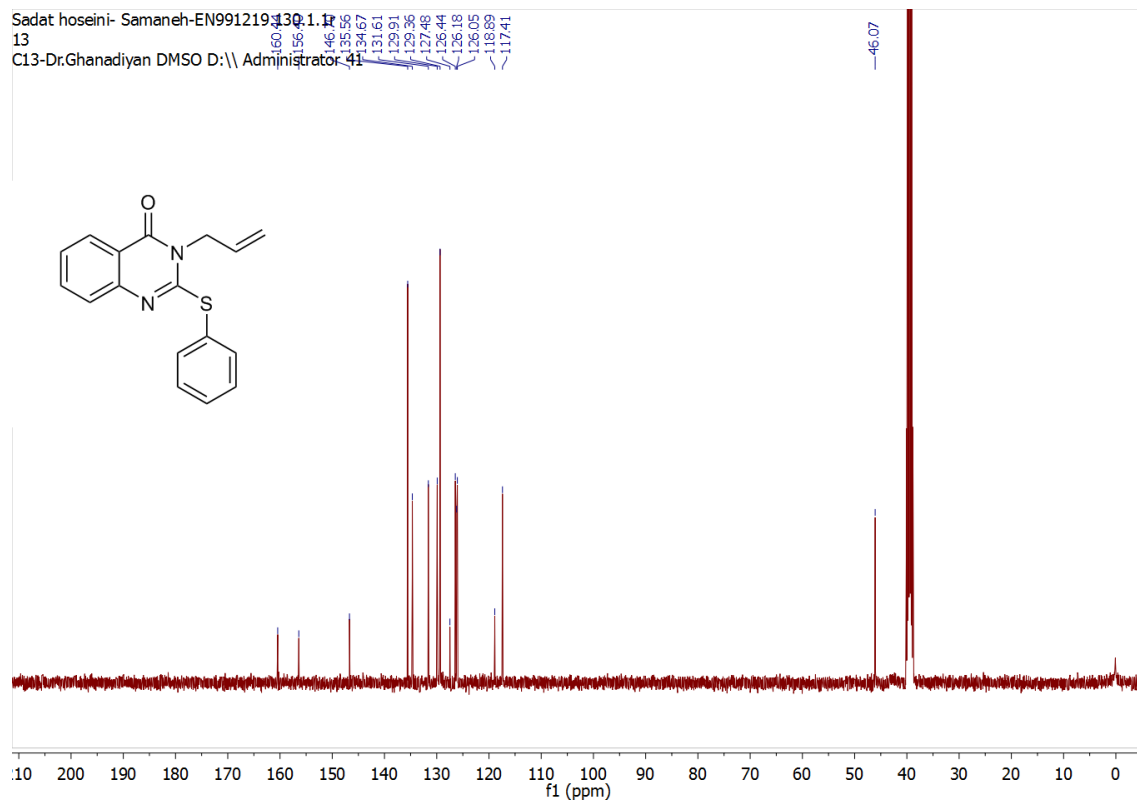
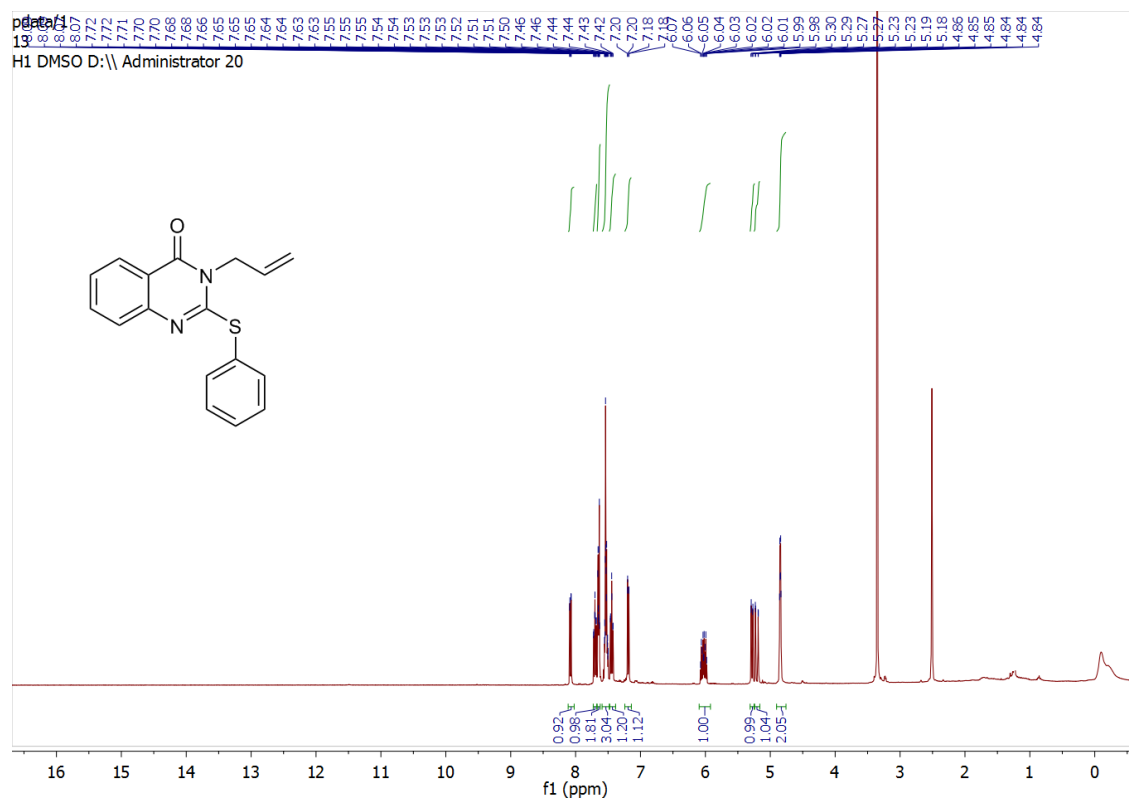
3-phenethyl-2-(phenylthio)quinazolin-4(3H)-one (4j)



3-(4-fluorobenzyl)-2-(phenylthio)quinazolin-4(3H)-one (4k)



3-allyl-2-(phenylthio)quinazolin-4(3H)-one (4l)



3-benzyl-2-((4-bromophenyl)thio)quinazolin-4(3H)-one (4m)

