Synthesis, In Vitro Analysis and Molecular Docking Study of Novel Benzoxazole-Based Oxazole Derivatives for the Treatment of Alzheimer’s Disease

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### 3.3. Spectral Analysis

### 3.2.1. (E)-2-((2-(4-methoxyphenyl)-2-(2-(4-(2-nitrophenyl)oxazol-2-yl)hydrazono) ethyl)thio)benzo[d]oxazole (1)

Yield: 65%, 1H-NMR (500 MHz, DMSO-*d6*): *δ*10.31 (s, 1H, NH), 8.00 (dd, *J*(6’’,5’’) = 6.8Hz, *J*(6’’,4’’) = 1.7Hz, 1H, H-6’’), 7.97 (d, *J*(3’’,4’’) = 7.4Hz, 1H, H-3’’), 7.88 (d, *J*(2’, 3’/ 6’, 5’) = 8.0 Hz, 2H, H-2’/H-6’), 7.84-7.69 (m, 2H, H-4’’/H-5’’), 7.54 (s, 1H, oxazole-H), 7.50 (dd, *J*(7,6) = 6.6Hz, *J*(7,5) = 1.2Hz, 1H, H-7), 7.45 (dd, *J*(4,5) = 7.0Hz, *J*(4,6) = 1.5Hz, 1H, H-4), 7.20-7.14 (m, 2H, H-5/H-6), 7.02 (d, *J*(3’, 2’/ 5’, 6’) = 9.0 Hz, 2H, H-3’/H-5’), 3.78 (s, 3H, -OCH3), 3.62 (s, 2H, -SCH2); 13C-NMR (125 MHz, DMSO-*d6*): *δ* 162.6, 156.0, 154.7, 151.0, 149.7, 149.1, 140.6, 139.2, 139.0, 135.6, 132.9, 129.9, 128.4, 128.4, 126.0, 125.5, 124.7, 123.9, 122.9, 118.2, 114.1, 114.1, 109.7, 55.5, 36.6; Elem. Anal. C, 59.85; H, 3.80; N, 13.95; O, 15.93; S, 6.35; HREI-MS: (m/z) [M + H]+ calcd for C25H20N5O5S 502.1180, found 502.1175.

### 3.2.2. (E)-2-((2-(4-methoxyphenyl)-2-(2-(4-(4-nitrophenyl)oxazol-2-yl)hydrazono) ethyl)thio)benzo[d]oxazole (2)

Yield: 62%, 1H-NMR (500 MHz, DMSO-*d6*): *δ*10.33 (s, 1H, NH), 8.23 (d, *J*(3’’, 2’’/ 5’’, 6’’) = 7.2 Hz, 2H, H-3’’/H-5’’), 7.94 (d, *J*(2’’, 3’’/ 6’’, 5’’) = 8.9Hz, 2H, H-2’’/H-6’’), 7.86 (d, *J*(2’, 3’/ 6’, 5’) = 8.2 Hz, 2H, H-2’/H-6’), 7.56 (s, 1H, oxazole-H), 7.52 (dd, *J*(7,6) = 6.7Hz, *J*(7,5) = 1.3Hz, 1H, H-7), 7.47 (dd, *J*(4,5) = 7.6Hz, *J*(4,6) = 1.6Hz, 1H, H-4), 7.22-7.16 (m, 2H, H-5/H-6), 7.00 (d, *J*(3’, 2’/ 5’, 6’) = 8.8 Hz, 2H, H-3’/H-5’), 3.76 (s, 3H, -OCH3), 3.64 (s, 2H, -SCH2); 13C-NMR (125 MHz, DMSO-*d6*): *δ* 162.9, 155.8, 154.5, 150.8, 149.5, 148.3, 140.4, 139.0, 138.8, 137.3, 128.7, 128.7, 127.2, 127.2, 126.3, 125.3, 125.3, 123.7, 122.7, 118.0, 114.4, 114.4, 109.5, 55.8, 36.4; Elem. Anal. C, 59.85; H, 3.81; N, 13.94; O, 15.92; S, 6.37;HREI-MS: (m/z) [M + H]+ calcd for C25H20N5O5S 502.1180, found 502.1175.

### 3.2.3. (E)-2-((2-(2-(4-(3-nitrophenyl)oxazol-2-yl)hydrazono)-2-(p-tolyl)ethyl)thio) benzo[d]oxazole (3)

Yield: 65%, 1H-NMR (500 MHz, DMSO-*d6*): *δ*10.35 (s, 1H, NH), 8.57 (t, *J* (2’’/4’’,6’’) = 9.0Hz, 1H, H-2’’), 8.29 (d, *J* (4’’,5’’) = 8.8Hz, 1H, H-4’’), 8.20 (dt, *J*(6’’,5’’) = 7.2Hz, *J*(6’’/2’’,4’’) = 2.0Hz, 1H, H-6’’), 7.81-7.68 (m, 1H, H-5’’), 7.67 (d, *J*(2’, 3’/ 6’, 5’) = 8.4Hz, 2H, H-2’/H-6’), 7.58 (s, 1H, oxazole-H), 7.54 (dd, *J*(7,6) = 6.9Hz, *J*(7,5) = 1.8Hz, 1H, H-7), 7.49 (dd, *J*(4,5) = 7.9Hz, *J*(4,6) = 1.3Hz, 1H, H-4), 7.27 (d, *J*(3’, 2’/ 5’, 6’) = 7.9 Hz, 2H, H-3’/H-5’), 7.24-7.18 (m, 2H, H-5/H-6), 3.66 (s, 2H, -SCH2), 2.38 (s, 3H, -CH3); 13C-NMR (125 MHz, DMSO-*d6*): *δ* 156.1, 154.8, 151.1, 149.8, 148.9, 140.7, 140.3, 139.3, 139.1, 134.4, 134.1, 131.1, 130.6, 128.7, 128.7, 126.4, 126.4, 124.4, 124.0, 123.2, 123.0, 118.3, 109.8, 36.7, 19.9; Elem. Anal. C, 61.83; H, 3.92; N, 14.40; O, 13.15; S, 6.59;HREI-MS: (m/z) [M + H]+ calcd for C25H20N5O4S 486.1231, found 486.1226.

### 3.2.4. (E)-2-((2-(p-tolyl)-2-(2-(4-(p-tolyl)oxazol-2-yl)hydrazono)ethyl)thio)benzo[d]oxazole (4)

Yield: 71%, 1H-NMR (500 MHz, DMSO-*d6*): *δ*10.32 (s, 1H, NH), 7.67 (d, *J*(2’’, 3’’/ 6’’, 5’’) = 8.4Hz, 2H, H-2’’/H-6’’), 7.65 (d, *J*(2’, 3’/ 6’, 5’) = 8.6Hz, 2H, H-2’/H-6’), 7.55 (s, 1H, oxazole-H), 7.51 (dd, *J*(7,6) = 6.5Hz, *J*(7,5) = 1.9Hz, 1H, H-7), 7.46 (dd, *J*(4,5) = 7.7Hz, *J*(4,6) = 1.8Hz, 1H, H-4), 7.28 (d, *J*(3’’, 2’’/ 5’’, 6’’) = 7.9 Hz, 2H, H-3’’/H-5’’), 7.25 (d, *J*(3’, 2’/ 5’, 6’) = 8.0 Hz, 2H, H-3’/H-5’), 7.21-7.15 (m, 2H, H-5/H-6), 3.63 (s, 2H, -SCH2), 2.38 (s, 3H, -CH3), 2.36 (s, 3H, -CH3);13C-NMR (125 MHz, DMSO-*d6*): *δ* 155.9, 154.6, 150.9, 149.6, 140.5, 140.1, 139.1, 138.9, 132.2, 130.4, 130.0, 130.0, 128.5, 128.5, 128.2, 126.4, 126.4, 126.2, 126.2, 123.8, 122.8, 118.1, 109.6, 36.6, 21.8, 19.7; Elem. Anal. C, 68.70; H, 4.86; N, 12.30; O, 7.01; S, 7.04; HREI-MS: (m/z) [M + H]+ calcd for C26H23N4O2S 455.1537, found 455.1532.

### 3.2.5. (E)-2-((2-(2-(4-(3-methoxyphenyl)oxazol-2-yl)hydrazono)-2-(p-tolyl)ethyl)thio) benzo[d]oxazole (5)

Yield: 63%, 1H-NMR (500 MHz, DMSO-*d6*): *δ*10.36 (s, 1H, NH), 7.66 (d, *J*(2’, 3’/ 6’, 5’) = 8.8Hz, 2H, H-2’/H-6’), 7.59 (s, 1H, oxazole-H), 7.53 (dd, *J*(7,6) = 6.8Hz, *J*(7,5) = 1.4Hz, 1H, H-7), 7.49 (dt, *J*(6’’,5’’) = 7.5Hz, *J*(6’’/2’’,4’’) = 2.2Hz, 1H, H-6’’), 7.46 (dd, *J*(4,5) = 7.5Hz, *J*(4,6) = 1.4Hz, 1H, H-4), 7.41-7.28 (m, 1H, H-5’’), 7.31 (t, *J* (2’’/4’’,6’’) = 6.4Hz, 1H, H-2’’), 7.28 (d, *J*(3’, 2’/ 5’, 6’) = 7.6 Hz, 2H, H-3’/H-5’), 7.25-7.19 (m, 2H, H-5/H-6), 7.01 (d, *J* (4’’,5’’) = 8.6Hz, 1H, H-4’’), 3.78 (s, 3H, -OCH3), 3.67 (s, 2H, -SCH2), 2.37 (s, 3H, -CH3); 13C-NMR (125 MHz, DMSO-*d6*): *δ* 161.6, 155.5, 154.2, 150.5, 149.2, 140.2, 140.0, 138.7, 138.5, 134.5, 130.7, 130.5, 128.6, 128.6, 126.3, 126.3, 123.4, 122.4, 120.3, 117.7, 114.8, 114.1, 109.2, 56.3, 36.2, 19.8; Elem. Anal. C, 66.37; H, 4.71; N, 11.91; O, 10.20; S, 6.81;HREI-MS: (m/z) [M + H]+ calcd for C26H23N4O3S 471.1485, found 471.1480.

### 3.2.6. (E)-2-((2-(2-(4-(3,4-dichlorophenyl)oxazol-2-yl)hydrazono)-2-(p-tolyl)ethyl) thio)benzo[d]oxazole (6)

Yield: 66%, 1H-NMR (500 MHz, DMSO-*d6*): *δ*10.34 (s, 1H, NH), 7.88 (d, *J*(2’’, 6’’) = 7.2Hz, 1H, H-2’’), 7.83 (dd, *J*(6’’, 5’’) = 7.4Hz, *J*(6’’,2’’) = 2.4Hz, 1H, H-6’’), 7.64 (d, *J*(2’, 3’/ 6’, 5’) = 8.5Hz, 2H, H-2’/H-6’), 7.57 (s, 1H, oxazole-H), 7.54 (dd, *J*(7,6) = 8.0Hz, *J*(7,5) = 2.2Hz, 1H, H-7), 7.51 (d, *J*(5’’, 6’’) = 7.5Hz, 1H, H-5’’), 7.48 (dd, *J*(4,5) = 8.4Hz, *J*(4,6) = 1.7Hz, 1H, H-4), 7.25 (d, *J*(3’, 2’/ 5’, 6’) = 7.5 Hz, 2H, H-3’/H-5’), 7.23-7.17 (m, 2H, H-5/H-6), 3.65 (s, 2H, -SCH2), 2.35 (s, 3H, -CH3); 13C-NMR (125 MHz, DMSO-*d6*): *δ* 155.7, 154.4, 153.7, 150.7, 149.4, 140.5, 140.3, 138.9, 138.7, 133.0, 132.8, 131.0, 130.8, 129.1, 128.9, 128.9, 127.3, 126.8, 126.8, 123.6, 122.6, 117.9, 109.4, 36.4, 21.1; Elem. Anal. C 59.83, H 3.78, N 13.93, O 15.91, S 6.34;HREI-MS: (m/z) [M + H]+ calcd for C25H19Cl2N4O2S 509.0601, found 509.0595.

### 3.2.7. (E)-2-((2-(2-(4-(4-bromophenyl)oxazol-2-yl)hydrazono)-2-(p-tolyl)ethyl)thio) benzo[d]oxazole (7)

Yield: 61%, 1H-NMR (500 MHz, DMSO-*d6*): *δ*10.38 (s, 1H, NH), 7.75 (d, *J*(2’’, 3’’/ 6’’, 5’’) = 6.8Hz, 2H, H-2’’/H-6’’), 7.67 (d, *J*(2’, 3’/ 6’, 5’) = 8.6Hz, 2H, H-2’/H-6’), 7.61 (s, 1H, oxazole-H), 7.57 (dd, *J*(7,6) = 8.4Hz, *J*(7,5) = 2.6Hz, 1H, H-7), 7.52 (d, *J*(3’’, 2’’/ 5’’, 6’’) = 7.3 Hz, 2H, H-3’’/H-5’’), 7.48 (dd, *J*(4,5) = 8.6Hz, *J*(4,6) = 2.0Hz, 1H, H-4), 7.27-7.21 (m, 2H, H-5/H-6), 7.18 (d, *J*(3’, 2’/ 5’, 6’) = 6.9 Hz, 2H, H-3’/H-5’), 3.69 (s, 2H, -SCH2), 2.38 (s, 3H, -CH3); 13C-NMR (125 MHz, DMSO-*d6*): *δ* 156.2, 154.9, 151.2, 149.9, 140.9, 140.6, 139.4, 139.2, 132.6, 132.6, 131.2, 130.2, 129.3, 129.3, 128.8, 128.8, 127.2, 127.2, 124.1, 123.6, 123.1, 118.4, 109.9, 36.8, 21.5; Elem. Anal. C, 57.80; H, 3.67; Br, 15.36; N, 10.75; O, 6.14; S, 6.15;HREI-MS: (m/z) [M + H]+ calcd for C25H20BrN4O2S 519.0485, found 519.0480.

### 3.2.8. (E)-2-((2-(2-(4-(2-methoxyphenyl)oxazol-2-yl)hydrazono)-2-(p-tolyl)ethyl)thio) benzo[d]oxazole (8)

Yield: 63%, 1H-NMR (500 MHz, DMSO-*d6*): *δ*10.39 (s, 1H, NH), 8.40 (dd, *J*(6’’, 5’’) = 7.5Hz, *J*(6’’,4’’) = 1.8Hz, 1H, H-6’’), 7.66 (d, *J*(2’, 3’/ 6’, 5’) = 8.7Hz, 2H, H-2’/H-6’), 7.62 (s, 1H, oxazole-H), 7.58 (dd, *J*(7,6) = 8.2Hz, *J*(7,5) = 2.4Hz, 1H, H-7), 7.53 (dd, *J*(4,5) = 8.0Hz, *J*(4,6) = 2.2Hz, 1H, H-4), 7.46-7.37 (m, 2H, H-4’’/H-5’’), 7.28-7.22 (m, 2H, H-5/H-6), 7.20 (d, *J*(3’, 2’/ 5’, 6’) = 7.4 Hz, 2H, H-3’/H-5’), 7.12 (d, *J*(3’’,4’’) = 7.2Hz, 1H, H-3’’), 3.76 (s, 3H, -OCH3), 3.70 (s, 2H, -SCH2), 2.37 (s, 3H, -CH3); 13C-NMR (125 MHz, DMSO-*d6*): *δ* 157.6, 156.4, 155.1, 151.4, 150.1, 141.0, 140.8, 139.6, 139.4, 131.4, 131.1, 130.0, 129.2, 129.2, 121.8, 127.1, 127.1, 124.3, 123.3, 119.2, 118.6, 111.4, 110.1, 56.4, 37.0, 21.4; Elem. Anal. C, 66.35; H, 4.70; N, 11.90; O, 10.19; S, 6.80;HREI-MS: (m/z) [M + H]+ calcd for C26H23N4O3S 471.1485, found 471.1480.

### 3.2.9. (E)-4-(2-(2-(2-(benzo[d]oxazol-2-ylthio)-1-(p-tolyl)ethylidene)hydrazinyl) oxazol-4-yl)phenol (9)

Yield: 67%, 1H-NMR (500 MHz, DMSO-*d6*): *δ*13.25 (s, 1H, NH), 9.80 (s, 1H, -OH), 8.40 (s, 1H, oxazole-H), 7.70 (d, *J*(2’’, 3’’/ 6’’, 5’’) = 8.0 Hz, 2H, H-3’’/H-5’’), 7.61 (d, *J*(3’’, 2’’/ 5’’, 6’’) = 8.8 Hz, 2H, H-2’’/H-6’’), 7.53 (d, *J*(2’, 3’/ 6’, 5’) = 8.4 Hz, 2H, H-2’/H-6’), 7.39 (d, *J*(3’, 2’/ 5’, 6’) = 8.0 Hz, 2H, H-3’/H-5’), 7.44-7.41 (m, 2H, H-4/H-7), 7.40 (m, 2H, H-5/H-6), 1.45 (s, 2H, -SCH2), 1.23 (s, 3H, -CH3); 13C-NMR (125 MHz, DMSO-*d6*): *δ* 198.2, 196.1, 191.2, 167.3, 146.3, 135.1, 134.9, 133.6, 133.5, 133.3, 133.1, 132.8, 132.0, 131.0, 130.8, 130.6, 130.5, 129.3, 129.2, 129.0, 128.6, 128.5, 128.4, 88.7, 52.5; Elem. Anal. C, 65.76; H, 4.41; N, 12.25; O, 10.50; S, 7.01;HREI-MS: (m/z) [M + H]+ calcd for C25H21N4O3S 457.1329, found 457.1324.

### 3.2.10. (E)-2-((2-(2-(4-(3-nitrophenyl)oxazol-2-yl)hydrazono)-2-phenylethyl)thio) benzo[d]oxazole (10)

Yield: 69%, 1H-NMR (500 MHz, DMSO-*d6*): *δ*10.40 (s, 1H, NH), 8.55 (t, *J* (2’’/4’’,6’’) = 8.8Hz, 1H, H-2’’), 8.27 (d, *J* (4’’,5’’) = 8.2Hz, 1H, H-4’’), 8.18 (dt, *J*(6’’,5’’) = 7.5Hz, *J*(6’’/2’’,4’’) = 2.2Hz, 1H, H-6’’), 7.82 (d, *J*(2’, 3’/ 6’, 5’) = 9.0Hz, 2H, H-2’/H-6’), 7.79-7.69 (m, 1H, H-5’’), 7.63 (s, 1H, oxazole-H), 7.59 (dd, *J*(7,6) = 7.6Hz, *J*(7,5) = 1.6Hz, 1H, H-7), 7.54 (dd, *J*(4,5) = 6.7Hz, *J*(4,6) = 2.6Hz, 1H, H-4), 7.50-7.45 (m, 3H, H-3’/H-4’/H-5’), 7.29-7.23 (m, 2H, H-5/H-6), 3.71 (s, 2H, -SCH2);13C-NMR (125 MHz, DMSO-*d6*): *δ* 156.3, 155.0, 151.3, 150.0, 148.8, 140.9, 139.5, 139.3, 134.6, 134.3, 134.0, 131.3, 131.0, 129.1, 129.1, 128.5, 128.5, 124.5, 124.2, 123.3, 123.0, 118.5, 110.0, 36.9; Elem. Anal. C, 61.12; H, 3.61; N, 14.83; O, 13.56; S, 6.77;HREI-MS: (m/z) [M + H]+ calcd for C24H18N5O4S 472.1074, found 472.1069.

### 3.2.11. (E)-2-((2-(4-chlorophenyl)-2-(2-(4-(3-nitrophenyl)oxazol-2-yl)hydrazono)ethyl) thio)benzo[d]oxazole (11)

Yield: 62%, 1H-NMR (500 MHz, DMSO-*d6*): *δ*10.36 (s, 1H, NH), 8.53 (t, *J* (2’’/4’’,6’’) = 8.0Hz, 1H, H-2’’), 8.25 (d, *J* (4’’,5’’) = 7.8Hz, 1H, H-4’’), 8.16 (dt, *J*(6’’,5’’) = 7.7Hz, *J*(6’’/2’’,4’’) = 2.4Hz, 1H, H-6’’), 7.95 (d, *J*(2’, 3’/ 6’, 5’) = 7.6Hz, 2H, H-2’/H-6’), 7.77-7.64 (m, 1H, H-5’’), 7.59 (s, 1H, oxazole-H), 7.53 (dd, *J*(7,6) = 9.0Hz, *J*(7,5) = 1.7Hz, 1H, H-7), 7.49 (d, *J*(3’, 2’/ 5’, 6’) = 7.9 Hz, 2H, H-3’/H-5’), 7.45 (dd, *J*(4,5) = 8.8Hz, *J*(4,6) = 2.1Hz, 1H, H-4), 7.25-7.19 (m, 2H, H-5/H-6), 3.67 (s, 2H, -SCH2); 13C-NMR (125 MHz, DMSO-*d6*): *δ* 165.2, 155.8, 152.1, 150.8, 148.7, 141.7, 140.4, 140.1, 137.1, 134.2, 133.9, 132.6, 130.9, 129.4, 129.4, 128.7, 128.7, 125.0, 124.6, 124.0, 123.0, 119.3, 110.8, 37.7; Elem. Anal. C, 56.96; H, 3.16; Cl, 7.00; N, 13.82; O, 12.64; S, 6.31;HREI-MS: (m/z) [M + H]+ calcd for C24H17ClN5O4S 506.0685, found 506.0680.

### 3.2.12. (E)-2-((2-([1,1'-biphenyl]-4-yl)-2-(2-(4-(3-nitrophenyl)oxazol-2-yl)hydrazono) ethyl)thio)benzo [d] oxazole (12)

Yield: 67%, 1H-NMR (500 MHz, DMSO-*d6*): *δ*10.34 (s, 1H, NH), 8.56 (t, *J* (2’’/4’’,6’’) = 9.2Hz, 1H, H-2’’), 8.29 (d, *J* (4’’,5’’) = 8.9Hz, 1H, H-4’’), 8.26 (d, *J*(2’, 3’/ 6’, 5’) = 9.0Hz, 2H, H-2’/H-6’), 8.19 (dt, *J*(6’’,5’’) = 7.0Hz, *J*(6’’/2’’,4’’) = 1.8Hz, 1H, H-6’’), 7.85 (d, *J*(3’, 2’/ 5’, 6’) = 8.8 Hz, 2H, H-3’/H-5’), 7.80-7.72 (m, 1H, H-5’’), 7.69-7.60 (m, 5H, ph-H), 7.57 (s, 1H, oxazole-H), 7.53 (dd, *J*(7,6) = 7.9Hz, *J*(7,5) = 2.8Hz, 1H, H-7), 7.48 (dd, *J*(4,5) = 6.8Hz, *J*(4,6) = 1.5Hz, 1H, H-4), 7.23-7.17 (m, 2H, H-5/H-6), 3.65 (s, 2H, -SCH2); 13C-NMR (125 MHz, DMSO-*d6*): *δ* 156.5, 155.2, 151.5, 150.2, 148.2, 143.4, 141.5, 141.1, 139.7, 139.5, 134.1, 133.8, 133.2, 130.8, 130.0, 130.0, 129.5, 129.5, 128.3, 128.3, 128.2, 128.2, 127.9, 124.4, 124.1, 123.4, 122.9, 118.7, 110.2, 37.1; Elem. Anal. C, 65.77; H, 3.86; N, 12.75; O, 11.67; S, 5.83;HREI-MS: (m/z) [M + H]+ calcd for C30H22N5O4S 548.1387, found 548.1382.

### 3.2.13. (E)-2-((2-(2-(4-(4-chlorophenyl)oxazol-2-yl)hydrazono)-2-(p-tolyl)ethyl)thio) benzo[d]oxazole (13)

Yield: 68%, 1H-NMR (500 MHz, DMSO-*d6*): *δ* 11.69 (s, 1H, NH), 8.40 (d, *J*(3’’, 2’’/ 5’’, 6’’) = 7.2 Hz, 2H, H-3’’/H-5’’), 8.17 (d, *J*(2’’, 3’’/ 6’’, 5’’) = 8.2 Hz, 2H, H-2’’/H-6’’), 7.81 (s, 1H, oxazole-H), 7.91 (d, *J*(2’, 3’/ 6’, 5’) = 7.9 Hz, 2H, H-2’/H-6’), 7.86 (d, *J*(3’, 2’/ 5’, 6’) = 8.2 Hz, 2H, H-3’/H-5’), 7.78 (m, 2H, H-4/H-7), 7.46 (m, 2H, H-5/H-6), 4.01 (s, 2H, -SCH2), 3.91 (s, 3H, -CH3); 13C-NMR (125 MHz, DMSO-*d6*): *δ* 191.7, 171.9, 169.8, 165.4, 162.9, 148.2, 148.0, 147.8, 146.0, 135.3, 135.2, 134.9, 134.0, 132.4, 130.7, 130.5, 128.8, 128.5, 128.3, 128.0, 127.3, 125.6, 123.6, 39.9, 21.0; Elem. Anal. C, 63.21; H, 4.02; Cl, 7.43; N, 11.77; O, 6.72; S, 6.73;HREI-MS: (m/z) [M + H]+ calcd for C25H20ClN4O2S 475.0990, found 475.0985.

### 3.2.14. (E)-2-((2-(2-(4-phenyloxazol-2-yl)hydrazono)-2-(p-tolyl)ethyl)thio)benzo[d]oxazole (14)

Yield: 59%, 1H-NMR (500 MHz, DMSO-*d6*): *δ*10.40 (s, 1H, NH), 7.81 (d, *J*(2’’, 3’’/ 6’’, 5’’) = 9.0Hz, 2H, H-2’’/H-6’’), 7.66 (d, *J*(2’, 3’/ 6’, 5’) = 9.0Hz, 2H, H-2’/H-6’), 7.62 (s, 1H, oxazole-H), 7.59 (dd, *J*(7,6) = 7.3Hz, *J*(7,5) = 1.9Hz, 1H, H-7), 7.54 (dd, *J*(4,5) = 7.7Hz, *J*(4,6) = 2.7Hz, 1H, H-4), 7.50-7.45 (m, 3H, H-3’’/H-4’’/H-5’’), 7.29-7.23 (m, 2H, H-5/H-6), 7.21 (d, *J*(3’, 2’/ 5’, 6’) = 8.2 Hz, 2H, H-3’/H-5’), 3.71 (s, 2H, -SCH2), 2.35 (s, 3H, -CH3); 13C-NMR (125 MHz, DMSO-*d6*): *δ* 156.1, 154.8, 151.1, 149.8, 140.7, 139.3, 139.1, 140.7, 134.0, 131.3, 131.0, 129.1, 129.1, 128.8, 128.8, 128.2, 128.2, 127.0, 127.0, 124.0, 123.0, 118.3, 109.8, 36.7, 21.3; Elem. Anal. C, 68.15; H, 4.56; N, 12.70; O, 7.25; S, 7.26;HREI-MS: (m/z) [M + H]+ calcd for C25H21N4O2S 441.1380, found 441.1375.

### 3.2.15. (E)-2-((2-(2-(4-(2,4-dichlorophenyl)oxazol-2-yl)hydrazono)-2-(p-tolyl)ethyl) thio)benzo[d]oxazole (15)

Yield: 70%, 1H-NMR (500 MHz, DMSO-*d6*): *δ*9.54 (s, 1H, NH), 8.44 (s, 1H, H-3’’), 8.40 (d, *J*(5’’,6’’) = 7.5 Hz, 1H, H-5’’), 8.29 (d, *J*(6’’, 5’’) = 7.3 Hz, 1H, H-6’’), 7.78 (s, 1H, oxazole-H), 7.68 (d, *J*(2’, 3’/ 6’, 5’) = 8.2 Hz, 2H, H-2’/H-6’), 7.49 (d, *J*(3’, 2’/ 5’, 6’) = 7.9 Hz, 2H, H-3’/H-5’), 7.31 (m, 2H, H-4/H-7), 7.11 (m, 2H, H-5/H-6), 3.90 (s, 2H, -SCH2), 1.23 (s, 3H, -CH3); 13C-NMR (125 MHz, DMSO-*d6*): *δ* 179.6, 161.5, 157.6, 148.6, 148.0, 146.1, 143.6, 135.3, 133.6, 133.4, 131.7, 130.5, 130.4, 130.2, 128.0, 127.8, 127.7, 127.4, 127.3, 124.3, 124.1, 120.1, 119.7, 64.0, 24.3; Elem. Anal. C, 58.94; H, 3.54; Cl, 13.91; N, 11.04; O, 6.25; S, 6.28; HREI-MS: (m/z) [M + H]+ calcd for C25H19Cl2N4O2S 509.0601, found 509.0596.

### 3.2.16. (E)-2-((2-([1,1'-biphenyl]-4-yl)-2-(2-(4-(3-methoxyphenyl)oxazol-2-yl) hydrazono)ethyl)thio)benzo[d]oxazole (16)

Yield: 65%, 1H-NMR (500 MHz, DMSO-*d6*): *δ*10.31 (s, 1H, NH), 8.26 (d, *J*(2’, 3’/ 6’, 5’) = 8.7Hz, 2H, H-2’/H-6’), 7.81 (d, *J*(3’, 2’/ 5’, 6’) = 8.4 Hz, 2H, H-3’/H-5’), 7.71-7.61 (m, 5H, ph-H), 7.54 (s, 1H, oxazole-H), 7.50 (dd, *J*(7,6) = 6.6Hz, *J*(7,5) = 1.2Hz, 1H, H-7), 7.48 (dt, *J*(6’’,5’’) = 7.6Hz, *J*(6’’/2’’,4’’) = 2.4Hz, 1H, H-6’’), 7.45 (dd, *J*(4,5) = 7.0Hz, *J*(4,6) = 1.5Hz, 1H, H-4), 7.40-7.27 (m, 1H, H-5’’), 7.25 (t, *J* (2’’/4’’,6’’) = 6.6Hz, 1H, H-2’’), 7.20-7.14 (m, 2H, H-5/H-6), 7.00 (d, *J* (4’’,5’’) = 8.5Hz, 1H, H-4’’), 3.77 (s, 3H, -OCH3),3.62 (s, 2H, -SCH2); 13C-NMR (125 MHz, DMSO-*d6*): *δ* 161.3, 155.9, 154.6, 150.9, 149.6, 143.3, 141.0, 140.5, 139.1, 138.9, 133.1, 129.9, 129.9, 129.4, 129.4, 128.4, 128.4, 128.0, 128.0, 127.8, 123.8, 122.8, 118.1, 109.6, 36.6, 134.2, 130.4, 120.0, 114.5, 113.8, 56.0; Elem. Anal. C, 69.90; H, 4.52; N, 10.51; O, 9.00; S, 6.04;HREI-MS: (m/z) [M + H]+ calcd for C31H25N4O3S 533.1642, found 533.1637.

### 3.2.17. (E)-2-((2-(2-(4-(2-nitrophenyl)oxazol-2-yl)hydrazono)-2-phenylethyl)thio) benzo[d]oxazole (17)

Yield: 69%, 1H-NMR (500 MHz, DMSO-*d6*): *δ*10.36 (s, 1H, NH), 7.99 (dd, *J*(6’’,5’’) = 7.0Hz, *J*(6’’,4’’) = 1.7Hz, 1H, H-6’’), 7.96 (d, *J*(3’’,4’’) = 7.8Hz, 1H, H-3’’), 7.85 (d, *J*(2’, 3’/ 6’, 5’) = 8.5Hz, 2H, H-2’/H-6’), 7.81-7.68 (m, 2H, H-4’’/H-5’’), 7.59 (s, 1H, oxazole-H), 7.53 (dd, *J*(7,6) = 9.0Hz, *J*(7,5) = 1.7Hz, 1H, H-7), 7.49 (dd, *J*(4,5) = 8.8Hz, *J*(4,6) = 2.1Hz, 1H, H-4), 7.41-7.34 (m, 3H, H-3’/H-4’/H-5’), 7.25-7.19 (m, 2H, H-5/H-6), 3.67 (s, 2H, -SCH2); 13C-NMR (125 MHz, DMSO-*d6*): *δ* 156.7, 155.4, 151.7, 150.4, 149.0, 141.3, 139.9, 139.7, 133.7, 135.5, 133.0, 132.8, 129.8, 128.5, 128.5, 127.9, 127.9, 125.4, 124.9, 124.6, 123.6, 118.9, 110.4, 37.3; Elem. Anal. C, 61.13; H, 3.61; N, 14.83; O, 13.55; S, 6.83; HREI-MS: (m/z) [M + H]+ calcd for C24H18N5O4S 472.1074, found 472.1069.

### 3.2.18. (E)-2-((2-(4-chlorophenyl)-2-(2-(4-(2-nitrophenyl)oxazol-2-yl)hydrazono)ethyl) thio)benzo [d] oxazole (18)

Yield: 72%, 1H-NMR (500 MHz, DMSO-*d6*): *δ* 10.38 (s, 1H, NH), 7.97 (dd, *J*(6’’,5’’) = 7.2Hz, *J*(6’’,4’’) = 1.7Hz, 1H, H-6’’), 7.94 (d, *J*(3’’,4’’) = 7.9Hz, 1H, H-3’’), 7.89 (d, *J*(2’, 3’/ 6’, 5’) = 7.8Hz, 2H, H-2’/H-6’), 7.83-7.66 (m, 2H, H-4’’/H-5’’), 7.61 (s, 1H, oxazole-H), 7.57 (dd, *J*(7,6) = 8.4Hz, *J*(7,5) = 2.6Hz, 1H, H-7), 7.52 (dd, *J*(4,5) = 8.6Hz, *J*(4,6) = 2.0Hz, 1H, H-4), 7.47 (d, *J*(3’, 2’/ 5’, 6’) = 8.2 Hz, 2H, H-3’/H-5’), 7.27-7.21 (m, 2H, H-5/H-6), 3.69 (s, 2H, -SCH2);13C-NMR (125 MHz, DMSO-*d6*): *δ* 155.7, 154.4, 150.7, 149.4, 148.5, 140.3, 138.9, 138.7, 136.1, 135.0, 132.3, 131.6, 129.3, 128.4, 128.4, 127.7, 127.7, 124.9, 124.1, 123.6, 122.6, 117.9, 109.4, 36.4; Elem. Anal. C, 56.96; H, 3.17; Cl, 7.04; N, 13.82; O, 12.64; S, 6.32;HREI-MS: (m/z) [M + H]+ calcd for C24H17ClN5O4S 506.0685, found 506.0680.

### 3.2.19. (E)-2-((2-(4-chlorophenyl)-2-(2-(4-(3-methoxyphenyl)oxazol-2-yl)hydrazono) ethyl)thio)benzo [d] oxazole (19)

Yield: 66%, 1H-NMR (500 MHz, DMSO-*d6*): *δ*10.34 (s, 1H, NH), 7.92 (d, *J*(2’, 3’/ 6’, 5’) = 8.0Hz, 2H, H-2’/H-6’), 7.57 (s, 1H, oxazole-H), 7.53 (dd, *J*(7,6) = 8.0Hz, *J*(7,5) = 2.2Hz, 1H, H-7), 7.48 (dd, *J*(4,5) = 8.4Hz, *J*(4,6) = 1.7Hz, 1H, H-4), 7.46 (d, *J*(3’, 2’/ 5’, 6’) = 6.6 Hz, 2H, H-3’/H-5’), 7.43 (dt, *J*(6’’,5’’) = 7.5Hz, *J*(6’’/2’’,4’’) = 2.2Hz, 1H, H-6’’), 7.39-7.30 (m, 1H, H-5’’), 7.27 (t, *J* (2’’/4’’,6’’) = 6.4Hz, 1H, H-2’’), 7.23-7.17 (m, 2H, H-5/H-6), 6.99 (d, *J* (4’’,5’’) = 8.6Hz, 1H, H-4’’), -SCH2), 3.76 (s, 3H, -OCH3), 3.65 (s, 2H); 13C-NMR (125 MHz, DMSO-*d6*): *δ* 160.8, 155.8, 154.5, 150.8, 149.5, 140.4, 139.0, 138.8, 136.2, 133.7, 131.9, 129.9, 128.7, 128.7, 128.0, 128.0, 123.7, 122.7, 119.5, 118.0, 114.0, 113.3, 109.5, 55.5, 36.4; Elem. Anal. C, 61.15; H, 3.93; Cl, 7.24; N, 11.40; O, 9.77; S, 6.51; HREI-MS: (m/z) [M + H]+ calcd for C25H20ClN4O3S 491.0940, found 491.0935.