

SUPPORTING INFORMATION

2-(5-bromo-1*H*-benzimidazol-2-yl)phenol (**HL**₁): Beige solid. Yield: 0.468 g (81%), m.p: 278 °C. Anal. calcd. for C₁₃H₉BrN₂O (%): C, 54.00; H, 3.14; N, 9.69; Found (%): C, 54.18; H, 3.27; N, 9.57. MW: 289.13 g/mol. ESI-MS (m/z, %): 289.3 (100, M⁺), 291.3 (73.6, [M+2H]⁺). FT-IR (ATR, cm⁻¹): 3333 s ν(OH), 3222 m ν(NH), 3061 m ν(CH_{arom}), 1634 m ν(C=N), 1599 m ν(C=C), 1585 m, 1487 s, 1462 m, 1382 s, 1259 s ν(C-O), 1198 m, 1134 m, 804 m, 737 s δ(CH_{arom}), 686 m, 595 m ν(C-Br), 566 m, 511 m, 468 m, 433 m. ¹H-NMR (DMSO-d₆) δ_H, ppm: 13.29 s,br (1H, NH), 12.73 s (1H, OH), 8.05 dd (1H, J=7.8, 1.5, H3'), 7.85 s (1H, H4), 7.61 d (1H, J=8.3, H7), 7.40 m (2H, H6+H5'), 7.05 d (1H, J=8.3, H6'), 7.02 t (1H, J=8.3, 6.8, H4'). Fluorescence spectra (λ_{max} / nm): 454 s, 407 sh.

2-(5-bromo-1*H*-benzimidazol-2-yl)-6'-chlorophenol (**HL**₂): Beige solid. Yield: 0.544 g (84%), m.p: 299 °C. Anal. calcd. for C₁₃H₈BrClN₂O (%): C, 48.25; H, 2.49; N, 8.66; Found (%): C, 48.31; H, 2.29; N, 8.62. MW: 323.57 g/mol. ESI-MS (m/z, %): 325.7 (100, [M+2H]⁺), 323.8 (70.6, M⁺). FT-IR (ATR, cm⁻¹): 3334 m ν(NH+OH), 3072 m ν(CH_{arom}), 1673 m ν(C=O), 1634 m ν(C=N), 1588 m ν(C=C), 1461 s, 1382 s, 1304 m, 1264 s ν(C-O), 1196 m, 1162 m, 1107 m, 919 m, 788 s δ(CH_{arom}), 753 m, 741 m, 713 m ν(C-Cl), 684 m, 616 m, 588 m ν(C-Br), 558 m, 428 m. ¹H-NMR (DMSO-d₆) δ_H, ppm: 13.75 s,br (1H, NH), 13.47 s,br (1H, OH), 8.00 dd (1H, J=7.7, 1.4, H3'), 7.88 s,br (1H, H4), 7.62 s,br (1H, H6), 7.55 dd (1H, J=8.0, 1.4, H5'), 7.43 d (1H, J=8.5, H7), 7.04 t (1H, J=8.0, 8.0, H4'). Fluorescence spectra (λ_{max}/nm): 464 s.

2-(5-bromo-1*H*-benzimidazol-2-yl)-4'-chlorophenol (**HL**₃): Beige solid. Yield: 0.590 g (91%), m.p: 307 °C. Anal. calcd. for C₁₃H₈BrClN₂O (%): C, 48.25; H, 2.49; N, 8.66; Found (%): C, 48.31; H, 2.29; N, 8.62. MW: 323.57 g/mol. ESI-MS (m/z, %): 320.2 (100, [M-2H]⁺), 321.0 (50.1, [M-3H]⁺), 321.8 (41.9, [M-2H]⁺). FT-IR (ATR, cm⁻¹): 3344 m ν(NH+OH), 3085 w ν(CH_{arom}), 1628 m ν(C=N), 1581 m ν(C=C), 1487 s, 1381 s, 1280 m, 1254 s ν(C-O), 1104 m, 1048 m, 974 m, 813 s δ(CH_{arom}), 721 m ν(C-Cl), 698 m, 686 m, 652 m, 585 m ν(C-Br), 569 m, 547 m, 418 m. ¹H-NMR (DMSO-d₆) δ_H, ppm, Isomer A: 13.35 s (1H, NH+OH), 7.94 s,br (1/2H, H4), 7.67 s,br (1/2H, H6), 7.07 d (1H, J=8.8, H7); Isomer B: 13.30 s (1H, NH), 12.81 s (1H, OH), 7.81 s,br (1/2H, H7), 7.59 s,br (1/2H, H5), 7.07 d (1H, J=8.8, H4); Isomer A+B: 8.15 d (1H, J=2.4, H3'), 7.41 dd (2H, J=8.8, 2.9, H5'+H6'). Fluorescence spectra (λ_{max}/nm): 468 m.

2-(5-bromo-1*H*-benzimidazol-2-yl)-6'-methylphenol (**HL**₄): Beige solid. Yield: 0.582 g (96%), m.p: 147 °C. Anal. calcd. for C₁₄H₁₁BrN₂O (%): C, 54.47; H, 3.66; N, 9.24; Found (%): C, 54.61; H, 3.77; N, 9.07. MW: 303.15 g/mol. ESI-MS (m/z, %): 305.2 (100, [M+2H]⁺), 303.3 (99.8, M⁺). FT-IR (ATR, cm⁻¹): 3332 m ν(OH+NH), 3060 m ν(CH_{arom}), 2925 m ν(CH_{aliph}), 1615 m ν(C=N), 1604 m ν(C=C), 1474 s, 1422 m, 1379 m, 1307 m, 1257 s ν(C-O), 1222 m, 1086 m, 1047 m, 1017 m, 921 m, 841 m, 785 s δ(CH_{arom}), 751 s, 640 m, 590 m ν(C-Br), 558 m, 519 m, 481 m, 428 m. ¹H-NMR (DMSO-d₆) δ_H, ppm: 13.08 s,br (2H, NH+OH), 8.86

s (1H, H4), 7.45 d (1H, J=7.4, H6), 7.34 t (1H, J=7.3, 7.6, H4'), 6.95 d (1H, J=7.5, H7), 6.88 d (1H, J=7.5, H3'), 6.75 dd (1H, J=8.4, 2.2, H5'), 2.23 s (3H, CH₃). Fluorescence spectra (λ_{max} /nm): 470 s.

2-(5-bromo-1*H*-benzimidazol-2-yl)-4'-methylphenol (**HL₅**): Light brown solid. Yield: 0.552 g (91%), m.p: 176 °C. Anal. calcd. for C₁₄H₁₁BrN₂O (%): C, 54.47; H, 3.66; N, 9.24; Found (%): C, 54.72; H, 3.75; N, 9.35. MW: 303.15 g/mol. ESI-MS (m/z, %): 303.3 (100, M⁺), 305.3 (86.7, [M+2H]⁺). FT-IR (ATR, cm⁻¹): 3328 m v(OH+NH), 3050 w v(CH_{arom}), 2922 w v(CH_{aliph}), 1615 m v(C=N), 1582 m v(C=C), 1506 m, 1463 m, 1384 m, 1254 m v(C-O), 1133 m, 1048 m, 923 m, 806 s δ (CH_{arom}), 704 m, 587 m (C-Br), 548 m, 470 m. ¹H-NMR (DMSO-d₆) δ_{H} , ppm: 13.24 s (1H, NH, isomer B), 13.19 s (1H, OH, isomer B), 12.45 s (2H, NH+OH, isomer A), 7.91 s,br (1/2H, H4, isomer A), 7.88 d (1H, J=1.5, H3'), 7.76 s,br (1/2H, H7, isomer B), 7.66 d (1/2H, J=7.9, H7, isomer A), 7.56 d (1/2H, J=8.2, H4, isomer B), 7.41 t (2H, J=8.3, 1.6, H6+H5, isomer A+B), 7.21 dd (1H, J=8.3, 1.6, H5'), 6.95 d (1H, J=8.3, H6'), 2.32 s (3H, CH₃). Fluorescence spectra (λ_{max} /nm): 474 s.

2-(5-bromo-1*H*-benzimidazol-2-yl)-6'-hydroxyphenol (**HL₆**): Dirty white solid. Yield: 0.451 g (74%), m.p: 218 °C. Anal. calcd. for C₁₃H₉BrN₂O₂ (%): C, 51.17; H, 2.97; N, 9.18; Found (%): C, 51.08; H, 3.07; N, 9.11. MW: 305.13 g/mol. ESI-MS (m/z, %): 305.4 (100, M⁺), 307.4 (59.8, [M+2H]⁺). FT-IR (ATR, cm⁻¹): 3398 m v(OH), 3308 m v(NH), 3060 m v(CH_{arom}), 1612 m v(C=N), 1582 m v(C=C), 1461 m, 1363 m, 1273 s v(C-O), 1244 m v(C-O), 1193 m, 1071 m, 854 m, 793 s δ (CH_{arom}), 736 s, 634 m, 563 m v(C-Br), 508 m, 469 m. ¹H-NMR (DMSO-d₆) δ_{H} , ppm: 13.26 s,br (1H, NH), 12.87 s,br (1H, OH1'), 9.25 s (1H, OH3'), 7.87 s,br (1H, H4), 7.63 d,br (1H, J=7.3, H7), 7.50 dd (1H, J=8.3, 1.5, H6), 7.42 dd (1H, J=8.8, 8.3, 1.9, 1.5, H3'), 6.94 dd (1H, J=7.8, 1.0, H5'), 6.85 t (1H, J=7.8, 7.8, H4'). Fluorescence spectra (λ_{max} /nm): 490 m.

2-(5-bromo-1*H*-benzimidazol-2-yl)-5'-hydroxyphenol (**HL₇**): Dirty white solid. Yield: 0.495 g (81%), m.p: 285 °C. Anal. calcd. for C₁₃H₉BrN₂O₂ (%): C, 51.17; H, 2.97; N, 9.18; Found (%): C, 51.32; H, 3.15; N, 9.09. MW: 305.13 g/mol. ESI-MS (m/z, %): 305.3 (100, M⁺), 307.3 (93.3, [M+2H]⁺). FT-IR (ATR, cm⁻¹): 3342 m,br v(OH), 3189 m,br v(NH), 3079 m v(CH_{arom}), 1635 m v(C=N), 1614 m v(C=C), 1579 m, 1464 m, 1322 m, 1263 m v(C-O), 1246 m v(C-O), 1169 s, 1049 m, 917 m, 848 m, 797 s δ (CH_{arom}), 746 m, 633 m, 559 m v(C-Br), 457 m. ¹H-NMR (DMSO-d₆) δ_{H} , ppm: 12.98 s,br (1H, NH), 10.29 s (1H, OH1'), 10.05 s (1H, OH5'), 8.06 dd (1H, J=8.6, 2.9, H6), 7.84 d (1H, J=8.6, H7), 7.77 d,br (1H, J=1.6, H7), 7.53 d (1H, J=8.5, H3'), 7.35 dd (1H, J=8.5, 1.9, H4'), 6.41 d (1H, J=2.1, H6'). Fluorescence spectra (λ_{max} /nm): 442 s.

2-(5-bromo-1*H*-benzimidazol-2-yl)-4'-hydroxyphenol (**HL₈**): Dark beige solid. Yield: 0.476 g (78%), m.p: 249 °C. Anal. calcd. for C₁₃H₉BrN₂O₂ (%): C, 51.17; H, 2.97; N, 9.18; Found (%): C, 51.25; H, 3.11; N, 9.03. MW: 305.13 g/mol. ESI-MS (m/z, %): 306.3 (100, [M+H]⁺), 307.1 (81.5, [M+2H]⁺). FT-IR (ATR, cm⁻¹): 3361 m v(OH), 3277 m v(NH), 3066 m v(CH_{arom}), 1614 m v(C=N), 1585 m v(C=C), 1569 m, 1488 m, 1268 m v(C-O), 1233 m v(C-O), 1195 m, 1154 m, 958 m, 905 m, 818 m, 786 s δ (CH_{arom}), 635 m, 600 m, 579 m

$\nu(\text{C-Br})$, 479 m, 442 m. $^1\text{H-NMR}$ (DMSO-d_6) δ_{H} , ppm: 13.09 s,br (1H, NH), 12.03 s,br (1H, OH1'), 9.13 s (1H, OH4'), 7.83 s (1H, H4), 7.60 d (1H, $J=8.5$, H7), 7.45 d (1H, $J=2.6$, H3'), 7.39 dd (1H, $J=8.5$, 1.9, H6), 6.87 m (2H, H5'+H6'). Fluorescence spectra ($\lambda_{\text{max}}/\text{nm}$): 511 m.

2-(5-bromo-1*H*-benzimidazol-2-yl)-6'-methoxyphenol (**HL₉**): Light khaki solid. Yield: 0.562 g (88%), m.p: 297 °C. Anal. calcd. for $\text{C}_{14}\text{H}_{11}\text{BrN}_2\text{O}_2$ (%): C, 52.69; H, 3.47; N, 8.78; Found (%): C, 52.80; H, 3.56; N, 8.67. MW: 319.15 g/mol. ESI-MS (m/z , %): 319.6 (100, M^+), 317.9 (76.7, $[\text{M}-2\text{H}]^+$). FT-IR (ATR, cm^{-1}): 3298 m,br $\nu(\text{NH}+\text{OH})$, 3069 m $\nu(\text{CH}_{\text{arom}})$, 2938 w $\nu(\text{CH}_{\text{aliph}})$, 1628 m $\nu(\text{C}=\text{N})$, 1591 m $\nu(\text{C}=\text{C})$, 1479 m, 1423 m, 1383 m, 1254 s $\nu(\text{C}-\text{OH})$, 1183 m $\nu(\text{C}-\text{OCH}_3)$, 1064 m, 920 m, 784 m $\delta(\text{C}-\text{H})$, 734 m, 605 m, 587 m $\nu(\text{C}-\text{Br})$, 512 m, 427 m. $^1\text{H-NMR}$ (DMSO-d_6) δ_{H} , ppm: 13.06 s,br (2H, NH+OH), 7.86 s,br (1H, H4), 7.62 dd (2H, $J=8.0$, 1.3, H6+H7), 7.41 dd (1H, $J=8.6$, 1.8, H3'), 7.10 dd (1H, $J=8.0$, 1.3, H5'), 6.96 t (1H, $J=8.0$, 8.0, H4'), 3.88 s (3H, OCH_3). Fluorescence spectra ($\lambda_{\text{max}}/\text{nm}$): 482 m.

2-(5-bromo-1*H*-benzimidazol-2-yl)-5'-methoxyphenol (**HL₁₀**): Cream colored solid. Yield: 0.523 g (82%), m.p: 285 °C. Anal. calcd. for $\text{C}_{14}\text{H}_{11}\text{BrN}_2\text{O}_2$ (%): C, 52.69; H, 3.47; N, 8.78; Found (%): C, 52.76; H, 3.19; N, 8.78. MW: 319.15 g/mol. ESI-MS (m/z , %): 319.3 (100, M^+), 321.2 (77.6, $[\text{M}+2\text{H}]^+$). FT-IR (ATR, cm^{-1}): 3334 m $\nu(\text{NH}+\text{OH})$, 3059 w $\nu(\text{CH}_{\text{arom}})$, 2932 w $\nu(\text{CH}_{\text{aliph}})$, 1632 m $\nu(\text{C}=\text{N})$, 1605 s $\nu(\text{C}=\text{C})$, 1490 m, 1442 m, 1395 s, 1268 m $\nu(\text{C}-\text{OH})$, 1201 m $\nu(\text{C}-\text{OCH}_3)$, 1167 m, 1136 m, 1032 m, 953 m, 817 m, 789 m $\delta(\text{C}-\text{H})$, 721 m, 578 m $\nu(\text{C}-\text{Br})$, 522 m. $^1\text{H-NMR}$ (DMSO-d_6) δ_{H} , ppm: 13.02 s,br (2H, NH+OH), 7.93 d (1H, $J=8.8$, H5'), 7.78 s,br (1H, H4), 7.54 d (1H, $J=8.3$, H6), 7.35 dd (1H, $J=8.3$, 2.0, H7), 6.62 dd (1H, $J=8.8$, 2.4, H6'), 6.58 d (1H, $J=2.4$, H3'), 3.80 s (3H, OCH_3). Fluorescence spectra ($\lambda_{\text{max}}/\text{nm}$): 444 m.

2-(5-bromo-1*H*-benzimidazol-2-yl)-4'-methoxyphenol (**HL₁₁**): Beige solid. Yield: 0.582 g (92%), m.p: 254 °C. Anal. calcd. for $\text{C}_{14}\text{H}_{11}\text{BrN}_2\text{O}_2$ (%): C, 52.69; H, 3.47; N, 8.78; Found (%): C, 52.91; H, 3.60; N, 8.67. MW: 319.15 g/mol. ESI-MS (m/z , %): 319.5 (100, M^+), 321.2 (73.5, $[\text{M}+2\text{H}]^+$). FT-IR (ATR, cm^{-1}): 3314 m $\nu(\text{NH}+\text{OH})$, 3080 w $\nu(\text{CH}_{\text{arom}})$, 2983 m $\nu(\text{CH}_{\text{aliph}})$, 1618 m $\nu(\text{C}=\text{N})$, 1597 s $\nu(\text{C}=\text{C})$, 1527 m, 1498 m, 1456 m, 1384 m, 1271 m $\nu(\text{C}-\text{OH})$, 1213 m $\nu(\text{C}-\text{OCH}_3)$, 1171 m, 1040 m, 853 m, 800 s $\delta(\text{C}-\text{H})$, 757 m, 686 m, 587 m $\nu(\text{C}-\text{Br})$, 478 m, 414 m. $^1\text{H-NMR}$ (DMSO-d_6) δ_{H} , ppm: 13.20 s,br (1H, NH), 12.20 s,br (1H, OH), 7.68 s,br (1H, H4), 7.64 d (1H, $J=2.9$, H3'), 7.61 d,br (1H, $J=7.00$, H7), 7.40 dd (1H, $J=8.5$, 1.5, H6), 7.01 dd (1H, $J=9.0$, 3.0, H5'), 6.97 d (1H, $J=9.0$, H6'), 3.80 s (3H, OCH_3). Fluorescence spectra ($\lambda_{\text{max}}/\text{nm}$): 506 m.

2-(5-bromo-1*H*-benzimidazol-2-yl)-4'-fluorophenol (**HL₁₂**): Beige solid. Yield: 0.559 g (91%), m.p: 298 °C. Anal. calcd. for $\text{C}_{13}\text{H}_8\text{BrFN}_2\text{O}$ (%): C, 50.84; H, 2.63; N, 9.12; Found (%): C, 50.97; H, 2.77; N, 9.04. MW: 307.12 g/mol. ESI-MS (m/z , %): 307.4 (100, M^+), 309.4 (96.7, $[\text{M}+2\text{H}]^+$). FT-IR (ATR, cm^{-1}): 3228 m $\nu(\text{NH}+\text{OH})$, 3068 w $\nu(\text{CH}_{\text{arom}})$, 1633 m $\nu(\text{C}=\text{N})$, 1604 m $\nu(\text{C}=\text{C})$, 1583 m, 1498 s, 1438 m, 1382 m, 1270 m

$\nu(\text{C-O})$, 1253 m, 1194 m, 1122 m, 1049 m, 986 m, 907 m, 808 s $\delta(\text{C-H})$, 775 s, 753 m, 725 m, 690 m, 676 m, 591 m $\nu(\text{C-Br})$, 557 m, 497 m, 474 m, 464 m, 429 m. $^1\text{H-NMR}$ (DMSO-d_6) δ_{H} , ppm: 13.24 s,br (1H, NH), 12.51 s,br (1H, OH), 7.90 dd (1H, $J=2.9, 9.8$, H6), 7.86 s,br (1H, H4), 7.63 d (1H, $J=7.8$, H7), 7.41 dd (1H, $J=8.8, 1.5$, H3'), 7.25 td (1H, $J=8.3, 7.8, 2.9$, H5'), 7.06 dd (1H, $J=8.8, 4.9$, H6'). Fluorescence spectra ($\lambda_{\text{max}}/\text{nm}$): 472 s.

2-(5-bromo-1*H*-benzimidazol-2-yl)-4'-bromophenol (**HL₁₃**): Light khaki solid. Yield: 0.626 g (85%), m.p: 122 °C. Anal. calcd. for $\text{C}_{13}\text{H}_8\text{Br}_2\text{N}_2\text{O}$ (%): C, 42.43; H, 2.19; N, 7.61; Found (%): C, 42.58; H, 2.25; N, 7.55. MW: 368.02 g/mol. ESI-MS (m/z , %): 369.2 (100, $[\text{M}+\text{H}]^+$), 371.2 (71.9, $[\text{M}+3\text{H}]^+$). FT-IR (ATR, cm^{-1}): 3394 m $\nu(\text{OH})$, 3351 m $\nu(\text{NH})$, 3066 m $\nu(\text{CH}_{\text{arom}})$, 1612 s $\nu(\text{C=N})$, 1573 m $\nu(\text{C=C})$, 1533 m, 1472 s, 1352 m, 1276 s $\nu(\text{C-O})$, 1182 m, 1119 m, 918 m, 807 s $\delta(\text{CH}_{\text{arom}})$, 712 m, 687 w, 670 w, 630 m, 590 m $\nu(\text{C-Br}_{\text{bz}})$, 552 m $\nu(\text{C-Br}_{\text{ph}})$, 500 m, 439 m. $^1\text{H-NMR}$ (DMSO-d_6) δ_{H} , ppm: (Isomer A and B, 50%) 13.35 s (1/2H, NH, Isomer A), 13.31 s (1/2H, NH, Isomer B), 12.82 s (1H, OH), 8.28 d (1H, $J=2.0$, H4+H7, Isomer A+B), 7.95 s,br (1/2H, H6, Isomer A), 7.80 s,br (1/2H, H5, Isomer B), 7.67 s,br (1/2H, H7, Isomer A), 7.58 s,br (1/2H, H4, Isomer B), 7.53 dd (1H, $J=8.8, 2.4$, H5'), 7.42 d,br (1H, $J=2.4$, H3'), 7.02 d (1H, $J=8.8$, H6'). Fluorescence spectra ($\lambda_{\text{max}}/\text{nm}$): 468 s.

2-(5-bromo-1*H*-benzimidazol-2-yl)-4'-nitrophenol (**HL₁₄**): Light brown solid. Yield: 0.615 g (92%), m.p: 145 °C. Anal. calcd. for $\text{C}_{13}\text{H}_8\text{BrN}_3\text{O}_3$ (%): C, 46.73; H, 2.41; N, 12.58; Found (%): C, 46.89; H, 2.56; N, 12.43. MW: 334.12 g/mol. ESI-MS (m/z , %): 331.3 (100, $[\text{M}-2\text{H}]^+$), 328.8 (81.1, $[\text{M}-5\text{H}]^+$), 329.6 (80.1, $[\text{M}-4\text{H}]^+$). FT-IR (ATR, cm^{-1}): 3482 m $\nu(\text{OH})$, 3377 m $\nu(\text{NH})$, 3065 m $\nu(\text{CH}_{\text{arom}})$, 1617 m $\nu(\text{C=N})$, 1585 m $\nu(\text{C=C})$, 1480 m $\nu(\text{NO}_2)$, 1334 s $\nu(\text{NO}_2)$, 1286 m $\nu(\text{C-O})$, 1182 m, 1098 m, 862 m, 791 m $\delta(\text{CH}_{\text{arom}})$, 693 m, 643 m, 588 m $\nu(\text{C-Br})$, 548 m, 484 m. $^1\text{H-NMR}$ (DMSO-d_6) δ_{H} , ppm: 11.21 s,br (2H, NH+OH), 9.12 d (1H, $J=2.7$ Hz, H4), 8.27 dd (1H, $J=9.2, 2.7$, H6), 7.97 d (1H, $J=3.0$, H3'), 7.69 d (1H, $J=9.6$, H6'), 7.46 dd (1H, $J=8.7, 1.8$, H5'), 7.25 d (1H, $J=9.3$, H7). Fluorescence spectra ($\lambda_{\text{max}}/\text{nm}$): 475 m,br.

2-(5-bromo-1*H*-benzimidazol-2-yl)-4',6'-dichlorophenol (**HL₁₅**): Beige solid. Yield: 0.551 g (77%), m.p: 297 °C. Anal. calcd. for $\text{C}_{13}\text{H}_7\text{BrCl}_2\text{N}_2\text{O}$ (%): C, 43.61; H, 1.97; N, 7.82; Found (%): C, 43.47; H, 2.06; N, 7.70. MW: 358.02 g/mol. MS (ESI), m/z : 359.2 (100%, $[\text{M}+\text{H}]^+$), 357.2 (60.0%, $[\text{M}-\text{H}]^+$). FT-IR (ATR, cm^{-1}): 3370 m $\nu(\text{OH}+\text{NH})$, 3076 m $\nu(\text{CH}_{\text{arom}})$, 1725 w $\nu(\text{C=O})$, 1630 w $\nu(\text{C=N})$, 1602 w $\nu(\text{C=C})$, 1578 m, 1453 m, 1367 m, 1305 m, 1254 m $\nu(\text{C-O})$, 1187 m, 1048 m, 986 m, 922 m, 852 m, 799 s $\delta(\text{CH}_{\text{arom}})$, 764 m, 724 m $\nu(\text{C-Cl})$, 705 m $\nu(\text{C-Cl})$, 687 m, 615 m, 590 s $\nu(\text{C-Br})$, 577 m, 517 m, 507 m, 432 m. $^1\text{H-NMR}$ (DMSO-d_6) δ_{H} , ppm: 14.00 s,br (1H, NH), 13.72 s,br (1H, OH), 8.15 d (1H, $J=2.3$, H4), 7.94 s,br (1H, H5'), 7.72 d (1H, $J=2.7$, H6), 7.68 d,br (1H, $J=2.0$, H3'), 7.48 dd (1H, $J=8.6, 1.5$, H7). Fluorescence spectra ($\lambda_{\text{max}}/\text{nm}$): 471 s.

2-(5-bromo-1*H*-benzimidazol-2-yl)-4',6'-dibromophenol (**HL₁₆**): Beige solid. Yield: 0.760 g (85%), m.p: 266 °C. Anal. calcd. for C₁₃H₇Br₃N₂O (%): C, 34.94; H, 1.58; N, 6.27; Found (%): C, 35.05; H, 1.66; N, 6.19. MW: 446.92 g/mol. ESI-MS (m/z, %): 449.2 (100, [M+2H]⁺), 447.2 (95, M⁺). FT-IR (ATR, cm⁻¹): 3386 m ν(NH+OH), 3075 m ν(CH_{arom}), 1718 w ν(C=O), 1626 w ν(C=N), 1578 m ν(C=C), 1514 m, 1444 m, 1359 m, 1254 m ν(C-O), 1176 m, 1048 m, 922 m, 858 m, 798 s δ(CH_{arom}), 737 m, 702 m, 681 m, 606 m, 588 m ν(C-Br), 575 m ν(C-Br), 558 s ν(C-Br), 541 m, 505 m, 430 m. ¹H-NMR (DMSO-d₆) δ_H, ppm: 14.04 s,br (1H, NH), 13.64 s,br (1H, OH), 8.23 d (1H, J=2.3, H4), 7.91 s,br (1H, H5'), 7.84 d (1H, J=2.3, H6), 7.56 d,br (1H, J=2.0, H3'), 7.41 dd (1H, J=8.4, 1.3, H7). Fluorescence spectra (λ_{max}/nm): 417 sh, 470 s.

2-(5-bromo-1*H*-benzimidazol-2-yl)-4',6'-diiodophenol (**HL₁₇**): Light khaki solid. Yield: 0.449 g (83%), m.p: 235 °C. Anal. calcd. for C₁₃H₇BrI₂N₂O (%): C, 28.87; H, 1.30; N, 5.18; Found (%): C, 28.72; H, 1.20; N, 5.09. MW: 540.92 g/mol. ESI-MS (m/z, %): 541.2 (100, M⁺), 543.2 (91.4, [M+2H]⁺). FT-IR (ATR, cm⁻¹): 3329 m ν(NH+OH), 3062 m ν(CH_{arom}), 1739 w ν(C=O), 1654 w ν(C=N), 1624 m ν(C=C), 1581 m, 1437 s, 1373 m, 1257 s ν(C-O), 1185 m, 1091 m, 974 m, 920 m, 859 m, 807 m δ(CH_{arom}), 722 m, 660 s, 603 w, 591 m ν(C-Br), 567 m, 547 sh, ν(C-I), 502 m, 425 m. ¹H-NMR (DMSO-d₆) δ_H, ppm: 13.62 s,br (2H, NH+OH), 8.39 d (1H, J=2.0, H5'), 8.12 d (1H, J=2.0, H3'), 7.48 dd (1H, J=7.5, 2.0, H6), 7.63 d (1H, J=2.1, H4), 7.45 d (1H, J=7.4, H7). Fluorescence spectra (λ_{max}/nm): 480 s.

2-(5-bromo-1*H*-benzimidazol-2-yl)-4'-chloro-6'-methoxyphenol (**HL₁₈**): Dirty white solid. Yield: 0.622 g (88%), m.p: 271 °C. Anal. calcd. for C₁₄H₁₀BrClN₂O₂ (%): C, 47.55; H, 2.85; N, 7.92; Found (%): C, 47.49; H, 2.79; N, 7.88. MW: 353.60 g/mol. ESI-MS (m/z, %): 355.5 (100, [M+2H]⁺), 352.4 (74.7, [M-H]⁺). FT-IR (ATR, cm⁻¹): 3299 m ν(NH+OH), 3082 m,br ν(CH_{arom}), 2928 w ν(CH_{aliph}), 1661 w ν(C=N), 1632 w ν(C=C), 1584 m, 1487 s, 1461 m, 1403 m, 1249 s ν(C-O), 1231 sh ν(C-OCH₃), 1184 m, 1047 m, 987 m, 922 m, 894 m, 798 s δ(CH_{arom}), 730 m, 715 m ν(C-Cl), 684 m, 663 m, 645 m, 578 m ν(C-Br), 515 m, 427 m. ¹H-NMR (DMSO-d₆) δ_H, ppm: 13.17 s,br (2H, NH+OH), 7.88 s,br (1H, H4), 7.73 d (1H, J=2.3, H3'), 7.63 d (1H, J=8.0, H6), 7.43 dd (1H, J=1.6, 8.5, H7), 7.14 d (1H, J=2.2, H5'), 3.86 s (3H, OCH₃). Fluorescence spectra (λ_{max}/nm): 477 s.

2-(5-bromo-1*H*-benzimidazol-2-yl)-4'-bromo-6'-methoxyphenol (**HL₁₉**): Beige solid. Yield: 0.573 g (72%), m.p: 236 °C. Anal. calcd. for C₁₄H₁₀Br₂N₂O₂ (%): C, 42.24; H, 2.53; N, 7.04; Found (%): C, 42.38; H, 2.66; N, 6.97. MW: 398.05 g/mol. ESI-MS (m/z, %): 399.1 (100, [M+H]⁺), 397.1 (56.0, [M-H]⁺). FT-IR (ATR, cm⁻¹): 3308 m ν(NH+OH), 3072 w ν(CH_{arom}), 2970 m ν(CH_{aliph}), 1661 w ν(C=N), 1630 w ν(C=C), 1583 m, 1488 m, 1402 m, 1246 s ν(C-O), 1231 m ν(C-OCH₃), 1177 m, 1046 m, 987 m, 923 m, 831 m, 797 s δ(CH_{arom}), 713 m, 687 m, 656 m, 641 m, 593 m ν(C-Br_{bz}), 575 m ν(C-Br_{ph}), 539 m, 512 m, 426 m. ¹H-NMR (DMSO-d₆) δ_H, ppm; Isomer A (50%): 13.40 s (1H, NH), 13.36 s (1H, OH), 7.96 s,br (1/2H, H4), 7.87 s,br (1H, H5'), 7.69 dd,br (1/2H, J=8.2, 1.8, H6), 7.57 d (1/2H, J=8.4, H7), 7.24 d (1H, J=2.2, H3'), 3.86 s (3H,

OCH₃); Isomer B (50%): 12.98 s (2H, NH+OH), 7.79 s,br (1/2H, H7), 7.87 s (1H, H5'), 7.44 d (1/2H, J=8.7, H4), 7.41 d (1/2H, J=8.7, H5), 7.24 d (1H, J=2.2, H3'), 3.86 s (3H, OCH₃). Fluorescence spectra ($\lambda_{\text{max}}/\text{nm}$): 478 s.

2-(5-bromo-1*H*-benzimidazol-2-yl)-6'-fluoro-4'-bromophenol (**HL₂₀**): Beige solid. Yield: 0.656 g (85%), m.p: 314 °C. Anal. calcd. for C₁₃H₇Br₂FN₂O (%): C, 40.45; H, 1.83; N, 7.26; Found (%): C, 40.51; H, 1.87; N, 7.20. MW: 386.01 g/mol. ESI-MS (m/z, %): 387.2 (100, [M+H]⁺), 385.2 (45.1, [M-H]⁺). FT-IR (ATR, cm⁻¹): 3329 m v(NH+OH), 3075 m v(CH_{arom}), 1723 m v(C=O), 1627 m v(C=N), 1581 m v(C=C), 1488 m, 1380 m, 1263 s v(C-O), 1163 m, 1049 m, 915 m, 850 m, 796 m δ (CH_{arom}), 708 m, 623 m, 591 m v(C-Br_{bz}), 565 m v(C-Br_{ph}), 540 m, 515 m, 492 m, 433 m. ¹H-NMR (DMSO-d₆) δ_{H} , ppm: 13.48 s,br (2H, NH+OH), 8.11 d (1H, J=2.0, H4), 7.90 s,br (1H, H6), 7.67 d (1H, J=2.3, H3'), 7.65 d (1H, J=2.3, H5'), 7.44 dd (1H, J=8.8, 1.8, H7). Fluorescence spectra ($\lambda_{\text{max}}/\text{nm}$): 463 s.

2-(5-bromo-1*H*-benzimidazol-2-yl)-6'-bromo-4'-chlorophenol (**HL₂₁**): Light yellow solid. Yield: 0.572 g (71%), m.p: 280 °C. Anal. calcd. for C₁₃H₇Br₂ClN₂O (%): C, 38.80; H, 1.75; N, 6.96; Found (%): C, 38.91; H, 1.81; N, 6.89. MW: 402.47 g/mol. ESI-MS (m/z, %): 403.3 (100, [M+H]⁺), 405.3 (70.3, [M+2H]⁺), 401.3 (56.7, [M-H]⁺). FT-IR (ATR, cm⁻¹): 3381 m v(NH+OH), 3072 m v(CH_{arom}), 1733 w v(C=O), 1625 w v(C=N), 1602 w v(C=C), 1581 m, 1447 m, 1367 m, 1252 m v(C-O), 1179 m, 1049 m, 928 s, 856 m, 799 s δ (CH_{arom}), 722 m, 704 m v(C-Cl), 687 m, 609 m, 591 m v(C-Br_{bz}), 561 s v(C-Br_{ph}), 550 m, 505 m, 430 m. ¹H-NMR (DMSO-d₆) δ_{H} , ppm: 13.70 s,br (2H, NH+OH), 8.20 d (1H, J=2.44, H4), 7.95 s,br (1H, H3'), 7.83 dd (1H, J=2.44, 5.37, 7.81, H6), 7.67 s,br (1H, H5'), 7.47 dd (1H, J=8.3, 1.46, H7). Fluorescence spectra ($\lambda_{\text{max}}/\text{nm}$): 471 s.

2-(5-bromo-1*H*-benzimidazol-2-yl)-6'-chloro-4'-fluorophenol (**HL₂₂**): Beige solid. Yield: 0.581 g (85%), m.p: 259 °C. Anal. calcd. for C₁₃H₇BrClFN₂O (%): C, 45.71; H, 2.07; N, 8.20; Found (%): C, 45.60; H, 2.01; N, 8.15. MW: 341.56 g/mol. ESI-MS (m/z, %): 343.2 (100, [M+2H]⁺), 341.2 (77.0, M⁺). FT-IR (ATR, cm⁻¹): 3345 m v(NH+OH), 3083 m v(CH_{arom}), 1725 m v(C=O), 1633 w v(C=N), 1608 w v(C=C), 1526 m, 1476 s, 1375 m, 1260 m v(C-O), 1211 m, 1079 m, 1003 m, 919 m, 845 m, 789 s δ (CH_{arom}), 705 m v(C-Cl), 688 m, 636 sh, 628 m, 612 m, 590 m v(C-Br), 512 m, 432 m. ¹H-NMR (DMSO-d₆) δ_{H} , ppm: 13.68 s,br (1H, NH), 13.62 s,br (1H, OH), 7.97 s,br (1H, J=1.5, H4), 7.91 dd (1H, J=9.3, 2.9, H6), 7.68 d (1H, J=2.9, H5'), 7.60 dd (1H, J=8.3, 2.9, H7), 7.47 s,br (1H, H3'). Fluorescence spectra ($\lambda_{\text{max}}/\text{nm}$): 485 s.

2-(5-bromo-1*H*-benzimidazol-2-yl)-4'-chloro-6'-iodophenol (**HL₂₃**): Beige solid. Yield: 0.701 g (78%), m.p: 129 °C. Anal. calcd. for C₁₃H₇BrClIN₂O (%): C, 34.74; H, 1.57; N, 6.23; Found (%): C, 35.06; H, 1.48; N, 6.05. MW: 449.50 g/mol. ESI-MS (m/z, %): 451.2 (43.5, [M+2H]⁺), 449.2 (36.0, M⁺). FT-IR (ATR, cm⁻¹): 3360 m v(NH+OH), 3073 m v(CH_{arom}), 1654 m v(C=N), 1627 w v(C=C), 1605 w, 1580 m, 1488 m, 1453 m,

1384 m, 1255 m $\nu(\text{C-O})$, 1051 m, 979 m, 922 m, 866 m, 802 s $\delta(\text{CH}_{\text{arom}})$, 711 m $\nu(\text{C-Cl})$, 666 m, 651 m, 591 m $\nu(\text{C-Br})$, 575 m, 551 m $\nu(\text{C-I})$, 502 m, 427 m. $^1\text{H-NMR}$ (DMSO-d_6) δ_{H} , ppm: 13.76 s,br (2H, NH+OH), 8.18 d (1H, $J=2.5$, H5'), 7.93 d (1H, $J=2.5$, H3'), 7.64 d (1H, $J=8.5$, H7), 7.46 dd (1H, $J=8.6$, 2.0, H6), 7.43 d (1H, $J=2.0$, H4). Fluorescence spectra ($\lambda_{\text{max}}/\text{nm}$): 474 s.

2-(5-bromo-1*H*-benzimidazol-2-yl)-4',6'-dibromo-5'-methoxyphenol (**HL₂₄**): Beige solid. Yield: 0.608 g (85%), m.p: 187 °C. Anal. calcd. for $\text{C}_{14}\text{H}_9\text{Br}_3\text{N}_2\text{O}_2$ (%): C, 35.26; H, 1.90; N, 5.87; Found (%): C, 35.38; H, 1.97; N, 5.79. MW: 476.95 g/mol. ESI-MS (m/z , %): 477.1 (100, M^+), 479.0 (95, $[\text{M}+2\text{H}]^+$). FT-IR (ATR, cm^{-1}): 3172 m,br $\nu(\text{NH+OH})$, 3076 m $\nu(\text{CH}_{\text{arom}})$, 2841 m $\nu(\text{CH}_{\text{aliph}})$, 1721 m $\nu(\text{C=O})$, 1610 w $\nu(\text{C=N})$, 1590 w $\nu(\text{C=C})$, 1461 m, 1397 m, 1265 m $\nu(\text{C-O})$, 1228 m $\nu(\text{C-OCH}_3)$, 1213 m, 1150 m, 1051 m, 919 m, 805 m $\delta(\text{CH}_{\text{arom}})$, 732 m, 695 m, 587 m $\nu(\text{C-Br}_{\text{bz}})$, 547 m $\nu(\text{C-Br}_{\text{ph}})$, 494 m, 427 m. $^1\text{H-NMR}$ (DMSO-d_6) δ_{H} , ppm: 13.69 s,br (2H, NH+OH), 8.41 s (1H, H4), 7.92 s,br (1H, H3'), 7.67 dd,br (1H, $J=3.1$, 9.0, H6), 7.47 dd (1H, $J=8.6$, 1.7, H7), 3.87 s (3H, OCH_3). Fluorescence spectra ($\lambda_{\text{max}}/\text{nm}$): 463 s.

4-(5-bromo-1*H*-benzimidazol-2-yl)benzene-1',2',3'-triol (**HL₂₅**): Light yellow solid. Yield: 0.488 g (76%), m.p: 189 °C. Anal. calcd. for $\text{C}_{13}\text{H}_9\text{BrN}_2\text{O}_3$ (%): C, 48.62; H, 2.82; N, 8.72; Found (%): C, 48.75; H, 2.95; N, 8.61. MW: 321.13 g/mol. ESI-MS (m/z , %): 317.3 (100, $[\text{M-4H}]^+$), 319.7 (26, $[\text{M+H}]^+$). FT-IR (ATR, cm^{-1}): 3465 m $\nu(\text{NH+OH})$, 3281 m $\nu(\text{OH})$, 3074 m $\nu(\text{CH}_{\text{arom}})$, 2960 m, 1723 m $\nu(\text{C=O})$, 1629 w $\nu(\text{C=N})$, 1611 m $\nu(\text{C=C})$, 1455 m, 1364 m, 1283 sh $\nu(\text{C-O})$, 1260 s $\nu(\text{C-O})$, 1233 m $\nu(\text{C-O})$, 1161 s, 1070 m, 980 m, 850 m, 802 m $\delta(\text{CH}_{\text{arom}})$, 743 m, 692 m, 606 m, 582 m $\nu(\text{C-Br})$, 555 m, 533 m, 504 m, 465 m. $^1\text{H-NMR}$ (DMSO-d_6) δ_{H} , ppm: 12.95 s,br (2H, NH+OH1'), 9.50 s (1H, OH5'), 8.52 s (1H, OH6'), 7.77 s (1H, H4), 7.54 d (1H, $J=8.4$, H6), 7.36 d (1H, $J=8.5$, H7), 7.34 d (1H, $J=8.6$, H3'), 6.47 d (1H, $J=8.7$, H4'). Fluorescence spectra ($\lambda_{\text{max}}/\text{nm}$): 477 m.

Antibacterial Activity Determination

The samples were diluted with DMSO (100%) at 700 $\mu\text{g/mL}$, 600 $\mu\text{g/mL}$, 500 $\mu\text{g/mL}$, 250 $\mu\text{g/mL}$, 125 $\mu\text{g/mL}$ concentrations. The used microorganisms were two Gram-positive (*Bacillus subtilis* ATCC 6633 and *Enterococcus faecalis* ATCC 29212) and two Gram-negative (*Escherichia coli* ATCC25922 and *Salmonella typhimurium* ATCC14028) bacteria. The studied bacteria were diluted with Mueller Hinton Broth (MHB) containing 10^6 cfu/mL. DMSO and Ciprofloxacin were used negative control and positive control, respectively. Mueller Hinton Agar (MHA) was used as the medium. Antibacterial activity was evaluated by disc diffusion method described by Karaçelik *et al.* [39]. Each bacterial solution was separately spreaded on MHA medium in sterile conditions. Then, 6mm standard discs were individually impregnated with 10 μL of each concentration of tested compounds and were and placed on MHA. The prepared experimental setups were incubated at 37 °C and after 24 h the diameters of the transparent inhibition zone around the standard discs, on which the compounds were impregnated, were measured and recorded. Each experiment was

performed in triplicate. The results of disc diffusion method were confirmed by the micro broth dilutions technique strictly following the National Committee for Clinical Laboratory Standards (NCCLS) recommendations [40]. The bacterial cultures were adjusted to a turbidity equivalent to a 0.5 McFarland standard (corresponds to 10^8 cfu/mL) diluted in broth media to give a final concentration of 5×10^5 cfu/mL for bacteria. All the concentrations of the compounds were tested against all the bacteria on the plate. Then, the plates were covered, placed in plastic bags to prevent evaporation and incubated at 36 °C for 18–20 h. The minimum inhibitory concentrations (MIC) were defined as the lowest concentration of compound giving complete inhibition of visible growth. Antibacterial effects of the solvents were investigated against test microorganisms. The experiments were performed in triplicate.