**Supplementary material**

**Quantum chemical calculations, Hirshfeld surface analysis, and molecular docking studies of antibacterial (*E*)-*N*′-((1*H*-Indol-3-yl)methylene)-4-bromobenzohydrazide**

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| **Table S1.** Optimized geometrical parameters of (*E*)-*N*′-((1*H*-Indol-3-yl)methylene)-4-bromobenzohydrazide calculated at the Becke, 3-parameter, Lee-Yang-Parr functional and Coulomb-attenuating method (CAM-B3LYP) with the 6-311++G(d,p) basis set. | | | | | | | | | | | | | | |
| Bond Lengths (Å) | | | |  | Bond Angles (º) | | | |  | Dihedral Angles (º) | | | | |
| Parameters | Exp. [9] | B3LYP | CAM-B3LYP |  | Parameters | Exp. [9] | B3LYP | CAM-B3LYP |  | Parameters |  | Exp. [9] | B3LYP | CAM-B3LYP |
| Br1-C3 | 1.887(1) | 1.916 | 1.900 |  | H1N1-N1-N2 | 116.6(1) | 119.206 | 119.226 |  | H1N1-N1-N2-C8 |  | 31(1) | 2.848 | 3.439 |
| C1-C2 | 1.388(2) | 1.390 | 1.385 |  | H1N1-N1-C7 | 124.8(1) | 119.160 | 119.403 |  | C7-N1-N2-C8 |  | -157.5(1) | 173.864 | 173.676 |
| C2-C3 | 1.389(2) | 1.393 | 1.387 |  | N2-N1-C7 | 117.92(9) | 121.029 | 120.653 |  | H1N1-N1-C7-O1 |  | 172(2) | 168.901 | 168.449 |
| C3-C4 | 1.387(2) | 1.391 | 1.385 |  | N1-N2-C8 | 113.46(9) | 116.692 | 116.783 |  | H1N1-N1-C7-C6 |  | -7(2) | -10.436 | -10.886 |
| C4-C5 | 1.393(2) | 1.393 | 1.388 |  | H1N3-N3-C10 | 123.5(1) | 125.100 | 125.219 |  | N2-N1-C7-O1 |  | 1.79(2) | -2.118 | -1.771 |
| C5-C6 | 1.398(2) | 1.399 | 1.392 |  | H1N3-N3-C11 | 127.0(1) | 125.439 | 125.506 |  | N2-N1-C7-C6 |  | -177.31(9) | 178.544 | 178.893 |
| C6-C7 | 1.492(2) | 1.505 | 1.501 |  | C10-N3-C11 | 109.20(9) | 109.462 | 109.274 |  | N1-N2-C8-C9 |  | -179.59(1) | 179.464 | 179.517 |
| O1-C7 | 1.248(1) | 1.215 | 1.209 |  | C2-C1-C6 | 120.8(1) | 120.881 | 120.737 |  | H1N3-N3-C10-C9 |  | -175(1) | 179.908 | 179.942 |
| N1-C7 | 1.339(1) | 1.382 | 1.374 |  | C1-C2-C3 | 119.2(1) | 119.102 | 119.155 |  | C11-N3-C10-C9 |  | -0.7(1) | 0.032 | 0.033 |
| N1-H1N1 | 0.84(2) | 1.016 | 1.014 |  | Br1-C3-C2 | 118.88(9) | 119.450 | 119.475 |  | H1N3-N3-C11-C12 |  | -7(2) | 0.043 | 0.013 |
| N1-N2 | 1.400(1) | 1.363 | 1.361 |  | Br1-C3-C4 | 119.88(8) | 119.348 | 119.385 |  | H1N3-N3-C11-C16 |  | 174(1) | -179.900 | -179.922 |
| N2-C8 | 1.292(1) | 1.284 | 1.274 |  | C2-C3-C4 | 121.2(1) | 121.201 | 121.138 |  | C10-N3-C11-C12 |  | 179.3(1) | 179.918 | 179.922 |
| C8-H8 | 0.930 | 1.100 | 1.098 |  | C3-C4-C5 | 119.1(1) | 119.056 | 119.123 |  | C10-N3-C11-C16 |  | -0.2(1) | -0.024 | -0.013 |
| C8-C9 | 1.435(2) | 1.441 | 1.443 |  | C4-C5-C6 | 120.6(1) | 120.816 | 120.664 |  | C6-C1-C2-C3 |  | -0.0(2) | -0.931 | -0.884 |
| C9-C10 | 1.384(2) | 1.381 | 1.370 |  | C1-C6-C5 | 119.1(1) | 118.926 | 119.166 |  | C2-C1-C6-C5 |  | 1.5(2) | 1.569 | 1.531 |
| N3-C10 | 1.360(2) | 1.372 | 1.367 |  | C1-C6-C7 | 117.0(1) | 117.349 | 117.286 |  | C2-C1-C6-C7 |  | -177.5(1) | 179.391 | 179.541 |
| N3-H1N3 | 0.93 | 1.006 | 1.005 |  | C5-C6-C7 | 123.9(1) | 123.687 | 123.516 |  | C1-C2-C3-Br1 |  | 178.31(10) | -179.777 | -179.815 |
| N3-C11 | 1.388(2) | 1.387 | 1.382 |  | O1-C7-N1 | 121.9(1) | 123.655 | 123.746 |  | C1-C2-C3-C4 |  | -1.7(2) | -0.307 | -0.317 |
| C16-C11 | 1.413(2) | 1.416 | 1.407 |  | O1-C7-C6 | 120.1(1) | 122.186 | 122.015 |  | Br1-C3-C4-C5 |  | -178.26(8) | -179.659 | -179.660 |
| C11-C12 | 1.397(2) | 1.395 | 1.392 |  | N1-C7-C6 | 117.98(9) | 114.156 | 114.236 |  | C2-C3-C4-C5 |  | 1.7(2) | 0.871 | 0.841 |
| C12-C13 | 1.386(2) | 1.389 | 1.381 |  | N2-C8-C9 | 122.2(1) | 122.108 | 121.907 |  | C4-C5-C6-C1 |  | -1.5(2) | -0.990 | -0.994 |
| C13-C14 | 1.405(2) | 1.408 | 1.404 |  | C8-C9-C10 | 124.1(1) | 124.467 | 124.742 |  | C4-C5-C6-C7 |  | 177.5(1) | -178.665 | -178.873 |
| C14-C15 | 1.385(2) | 1.388 | 1.381 |  | C8-C9-C16 | 129.5(1) | 128.940 | 128.583 |  | C1-C6-C7-O1 |  | -19.2(2) | -27.618 | -27.495 |
| C15-C16 | 1.401(2) | 1.403 | 1.399 |  | C10-C9-C16 | 106.44(9) | 106.593 | 106.675 |  | C1-C6-C7-N1 |  | 159.9(1) | 151.731 | 151.854 |
| C1-H1 | 0.930 | 1.083 | 1.083 |  | N3-C10-C9 | 110.0(1) | 109.727 | 109.794 |  | C5-C6-C7-O1 |  | 161.8(1) | 150.092 | 150.421 |
| C2-H2 | 0.930 | 1.082 | 1.082 |  | N3-C11-C12 | 129.9(1) | 130.116 | 130.070 |  | C5-C6-C7-N1 |  | -19.1(2) | -30.560 | -30.231 |
| C4-H4 | 0.931 | 1.082 | 1.082 |  | N3-C11-C16 | 107.73(9) | 107.422 | 107.542 |  | N2-C8-C9-C10 |  | -174.9(1) | -179.564 | -179.370 |
| C5-H5 | 0.929 | 1.084 | 1.084 |  | C12-C11-C16 | 122.3(1) | 122.462 | 122.387 |  | N2-C8-C9-C16 |  | 6.4(2) | 0.423 | 0.614 |
| C10-H10 | 0.930 | 1.079 | 1.079 |  | C11-C12-C13 | 117.2(1) | 117.209 | 117.204 |  | C8-C9-C10-N3 |  | -177.6(1) | 179.964 | 179.948 |
| C12-H12 | 0.930 | 1.084 | 1.084 |  | C12-C13-C14 | 121.3(1) | 121.227 | 121.271 |  | C16-C9-C10-N3 |  | 1.3(1) | -0.025 | -0.039 |
| C13-H13 | 0.929 | 1.084 | 1.083 |  | C13-C14-C15 | 121.2(1) | 121.397 | 121.353 |  | C8-C9-C16-C11 |  | 177.4(1) | -179.978 | -179.956 |
| C14-H14 | 0.930 | 1.084 | 1.083 |  | C14-C15-C16 | 118.6(1) | 118.482 | 118.424 |  | C8-C9-C16-C15 |  | -2.1(2) | 0.161 | 0.175 |
| C15-H15 | 0.930 | 1.082 | 1.082 |  | C9-C16-C11 | 106.58(9) | 106.797 | 106.715 |  | N3-C11-C12-C13 |  | 179.6(1) | -179.924 | -179.913 |
|  |  |  |  |  | C9-C16-C15 | 134.1(1) | 133.980 | 133.924 |  | N3-C11-C16-C9 |  | 1.0(1) | 0.008 | -0.010 |
|  |  |  |  |  | C11-C16-C15 | 119.3(1) | 119.222 |  |  | N3-C11-C16-C15 |  | -179.4(1) | 179.893 | 179.882 |
| *R*2 |  | 0.9817 | 0.9815 |  |  |  | 0.9671 | 0.9684 |  |  |  |  | - | - |

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| **Table S2.** Comparison of the experimental and theoretical vibrational frequencies (cm-1) by the Becke, 3-parameter, Lee-Yang-Parr functional (B3LYP) and Coulomb-attenuating method (CAM-B3LYP) with the 6-311++G(d,p) basis set. | | | | | | | | | | | | | | |
|  |  | Expt.a | Theoretical | | | |  |  |  | Expt.a | Theoretical | | | |
|  |  |  | B3LYP | | CAM-B3LYP | |  |  |  |  | B3LYP | | CAM-B3LYP | |
| ν | Assignments (%PEDb) |  | Unscaled | Scaled | Unscaled | Scaled |  | ν | Assignments (%PEDb) |  | Unscaled | Scaled | Unscaled | Scaled |
| 1 | ν(NH)ind(100) | 3346 | 3667 | 3374 | 3699 | 3491 |  | 45 | τ(HCCC)ind(82) |  | 994 | 952 | 1022 | 965 |
| 2 | ν(NH)bhydr(100) | 3195 | 3505 | 3225 | 3556 | 3357 |  | 46 | τ(HCCC)ph(78) |  | 992 | 950 | 1017 | 960 |
| 3 | νs(CH)ind(99) | 3088 | 3244 | 3082 | 3260 | 3077 |  | 47 | τ(HCCC)ph(60), τ(CCCC)ph(24) |  | 966 | 925 | 992 | 936 |
| 4 | νs(CH)ind(94) |  | 3210 | 3050 | 3230 | 3049 |  | 48 | τ(HCCC)ind(82) |  | 954 | 914 | 983 | 928 |
| 5 | νs(CH)ph(96) |  | 3208 | 3048 | 3229 | 3048 |  | 49 | γ(HCNN)bhydr(87) |  | 949 | 909 | 976 | 921 |
| 6 | νs(CH)ph(91) |  | 3203 | 3043 | 3224 | 3043 |  | 50 | σ(O=CN)bhydr(23), σ(NNC)bhydr(11) |  | 922 | 883 | 934 | 882 |
| 7 | νas(CH)ph(100) |  | 3190 | 3031 | 3211 | 3031 |  | 51 | σ(CCC)ind(34), σ(CNC)ind(27) |  | 886 | 849 | 904 | 853 |
| 8 | νs(CH)ind(97) |  | 3188 | 3029 | 3199 | 3020 |  | 52 | ω(HCCC)ind(81) |  | 863 | 827 | 877 | 828 |
| 9 | νas(CH)ind(94) |  | 3175 | 3016 | 3195 | 3016 |  | 53 | γ(ONCC)bhydr(10), ω(HCCC)ph(57) |  | 859 | 823 | 859 | 811 |
| 10 | νas(CH)ph(94) |  | 3172 | 3013 | 3188 | 3009 |  | 54 | ω(HCCC)ph(73) |  | 838 | 803 | 841 | 794 |
| 11 | νas(CH)ind(99) | 2963 | 3163 | 3005 | - | - |  | 55 | σ(NCC)ind(29), σ(CC=N) bhydr(13) |  | 805 | 771 | - | - |
| 12 | ν(CH)bhydr(100) |  | 2992 | 2842 | 3028 | 2858 |  | 56 | γ(HCCC)ind(90) |  | 798 | 764 | 814 | 768 |
| 13 | ν(C=O)(84) | 1619 | 1750 | 1677 | 1795 | 1694 |  | 57 | ν(CC)ind(32), σ(CNC)ind(13) |  | 769 | 737 | 793 | 749 |
| 14 | ν(N=C)bhydr(63), ν(C8C9)(12) | 1601 | 1669 | 1599 | 1738 | 1640 |  | 58 | τ(CCNC)ind(23), τ(CCCC)ind(23) |  | 767 | 735 | 781 | 737 |
| 15 | σ(CCN)bhydr(15), ν(CC)ind(37) |  | 1657 | 1587 | 1669 | 1575 |  | 59 | γ(ONCC)bhydr(46), ω(HCCC)ph(25) |  | 758 | 726 | 769 | 726 |
| 16 | ν(CC)ph(40) |  | 1624 | 1556 | 1653 | 1560 |  | 60 | ω(HCCC)ind(84) |  | 751 | 719 | - | - |
| 17 | ν(CC)ind(37), σ(CCC)ind(23), σ(CCN)bhydr(11) |  | 1613 | 1545 | 1644 | 1552 |  | 61 | ν(BrC)ph(21), σ(CCC)ph(39) |  | 724 | 694 | 738 | 697 |
| 18 | ν(CC)ph(48), σ(CCC)ph(14) | 1534 | 1602 | 1535 | 1615 | 1524 |  | 62 | τ(CCCC)ph(58) |  | 697 | 668 | 715 | 675 |
| 19 | σ(HNN)bhydr(15), ν(CC)ind(30) |  | 1579 | 1513 | - | - |  | 63 | σ(CCN)ind(12), σ(CCC)ph(32) |  | 643 | 616 | 652 | 615 |
| 20 | ν(CC)ind(14), ν(NC)bhydr(11), σ(HNN)bhydr(48) |  | 1543 | 1478 | 1571 | 1483 |  | 64 | σ(CCN)ind(22) |  | 640 | 613 | 648 | 612 |
| 21 | ν(CC)ind(30) |  | 1523 | 1459 | 1548 | 1461 |  | 65 | ω(CCCC)ind(22), ω(CNCC)ind(42) |  | 627 | 601 | 645 | 609 |
| 22 | σ(HCC)ph(62) |  | 1516 | 1452 | 1534 | 1448 |  | 66 | ω(CNCC)ind(49) |  | 580 | 556 | 598 | 564 |
| 23 | σ(CCN)ind(11) |  | 1480 | 1418 | 1507 | 1422 |  | 67 | σ(CCC)ind(33) |  | 558 | 535 | 565 | 533 |
| 24 | σ(NCC)ind(15), σ(HNC)ind(30) |  | 1444 | 1383 | 1471 | 1388 |  | 68 | σ(NCC)bhydr(18) |  | 535 | 513 | 544 | 513 |
| 25 | σ(HCC)ph(23), ν(CC)ph(36) |  | 1417 | 1357 | 1444 | 1363 |  | 69 | γ(HNN=C)bhydr(76) |  | 499 | 478 | 499 | 471 |
| 26 | ν(C8C9)(11) |  | 1390 | 1332 | 1408 | 1329 |  | 70 | ω(CCCC)ph(12), ω(BrCCC)(17) |  | 454 | 435 | 463 | 437 |
| 27 | δ(HC=N)bhydr(42) |  | 1383 | 1325 | 1399 | 1321 |  | 71 | ν(C6C7)(17) |  | 451 | 432 | 459 | 433 |
| 28 | ν(CC)ind(50) |  | 1363 | 1306 | 1367 | 1290 |  | 72 | γ(HNCC)ind(44) |  | 436 | 418 | 450 | 425 |
| 29 | δ(HCC)ph(73), ν(CC)ph(11) |  | 1326 | 1270 | 1363 | 1287 |  | 73 | ω(HCCC)ind(10), ω(CNCC)ind(25), ω (CCCC)ind(40) |  | 431 | 413 | 440 | 415 |
| 30 | ν(CC)ph(82) |  | 1318 | 1263 | 1336 | 1261 |  | 74 | τ(CCCC)ph(75) |  | 417 | 399 | 424 | 400 |
| 31 | ν(NC)ind(28), δ(HCC)ind(11), δ(HC=N)bhydr(18) |  | 1309 | 1254 | 1327 | 1253 |  | 75 | γ(HNCC)ind(45) |  | 373 | 357 | 391 | 369 |
| 32 | δ(HCC)ind(31), ν(NC)ind(11) |  | 1274 | 1220 | 1315 | 1241 |  | 76 | σ(CC=N) bhydr(12) |  | 367 | 352 | 373 | 352 |
| 33 | ν(NC)bhydr(15),ν(C6C7)bhydr(26),σ(HNN)bhydr(14) |  | 1255 | 1202 | 1282 | 1210 |  | 77 | σ(C7C6C5)(13), σ(BrCC)(15) |  | 319 | 306 | 319 | 301 |
| 34 | ν(NC)ind(17), σ(HNC)ind(15), σ(HCC)ind(14) |  | 1239 | 1187 | 1258 | 1187 |  | 78 | σ(BrCC)(31) |  | 264 | 253 | 265 | 250 |
| 35 | δ(HCC)ph(74) |  | 1201 | 1151 | 1212 | 1144 |  | 79 | τ(C10C9C8N)(18), τ(CCCC)ind(13), γ(BrCCC)(17) |  | 238 | 228 | 238 | 225 |
| 36 | δ(HCC)ind(58) |  | 1179 | 1129 | 1187 | 1120 |  | 80 | ω(CCNC)ind(20), τ(CCCC)ind(21) |  | 233 | 223 | 203 | 192 |
| 37 | ν(NN)bhydr(16) |  | 1165 | 1116 | 1183 | 1117 |  | 81 | σ(C10C9C8)(19), σ(NNC)bhydr(15) |  | 200 | 192 | - | - |
| 38 | ν(NN)bhydr(16), σ(HCC)ind(23) |  | 1152 | 1104 | 1165 | 1100 |  | 82 | τ(CNNC)bhydr(10), τ(C10C9C8N)(10) |  | 193 | 185 | 193 | 182 |
| 39 | σ(HCC)ph(56), ν(CC)ph(26) |  | 1131 | 1083 | 1141 | 1077 |  | 83 | σ(C7C6C5)(15), σ(BrCC)(24) |  | 175 | 168 | 175 | 165 |
| 40 | σ(HCC)ind(23), ν(NC)ind(33), σ(HNC)ind(23) |  | 1120 | 1073 | 1129 | 1066 |  | 84 | τ(CNNC)bhydr(18), τ(C10C9C8N)(11) |  | 124 | 119 | 124 | 117 |
| 41 | σ(CCC)ind(25) |  | 1109 | 1062 | 1123 | 1060 |  | 85 | τ(C10C9C8N)(15) |  | 85 | 81 | 94 | 89 |
| 42 | ν(CC)ph(44) |  | 1084 | 1038 | 1111 | 1049 |  | 86 | σ(C10C9C8)(12), σ(C9C8N)(11) |  | 58 | 56 | 72 | 68 |
| 43 | ν(NC)bhydr(18), ν(NN)bhydr(24) |  | 1068 | 1023 | 1092 | 1031 |  | 87 | τ(CNNC)bhydr(23) |  | 32 | 31 | 31 | 29 |
| 44 | σ(HCC)ind(23), σ(CCN)ind(20) |  | 1030 | 987 | 1049 | 990 |  | 88 | τ(NC7C6C1)(25) |  | 25 | 24 | 25 | 24 |
| 45 | σ(CCC)ph(83) |  | 1025 | 982 | 1039 | 981 |  | 89 | γ(NNC7C6)bhydr(42) |  | 17 | 16 | 17 | 16 |
| a Taken from Ref. [9]; b Potential Energy Distribution (PED) ≤ 10% are not shown; ν, stretching; β, in-plane bending; γ, out-of-plane bending; ω , wagging; τ, twisting; σ, scissoring; δ, rocking; s, simetric; as, antisimetric; ph, phenyl; bhydr, benzohydrazide linkage; ind, indole. | | | | | | | | | | | | | | |

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