**New thieno[2,3-*b*]pyridine-based compounds: Synthesis, molecular modelling, antibacterial and antifungal activities**

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**Table S1**. The DFT dihedral angle data of the investigated compounds.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **4** |  | **5** |  | **6** |
| **Dihedral** | **(°)** | **Dihedral** | **(°)** | **Dihedral** | **(°)** |
| N(16)-C(17)-N(18)-H(33) | 172.3 | C(19)-C(20)-S(21)-C(17) | 0.0 | C(25)-C(26)-C(27)-C(22) | 0.0 |
| N(16)-C(17)-N(18)-H(34) | -16.0 | N(18)-C(19)-C(20)-S(21) | 0.0 | C(24)-C(25)-C(26)-C(27) | 0.0 |
| S(19)-C(17)-N(18)-H(33) | -4.0 | C(22)-C(19)-C(20)-S(21) | -180.0 | C(23)-C(24)-C(25)-C(26) | 0.0 |
| S(19)-C(17)-N(18)-H(34) | 167.7 | C(17)-N(18)-C(19)-C(20) | 0.0 | C(22)-C(23)-C(24)-C(25) | 0.0 |
| N(14)-N(16)-C(17)-N(18) | -178.0 | C(17)-N(18)-C(19)-C(22) | -180.0 | C(19)-C(22)-C(27)-C(26) | 179.9 |
| N(14)-N(16)-C(17)-S(19) | -1.9 | N(16)-C(17)-S(21)-C(20) | -180.0 | C(23)-C(22)-C(27)-C(26) | -0.1 |
| H(32)-N(16)-C(17)-N(18) | -24.3 | N(18)-C(17)-S(21)-C(20) | 0.0 | C(19)-C(22)-C(23)-C(24) | -179.9 |
| H(32)-N(16)-C(17)-S(19) | 151.8 | N(16)-C(17)-N(18)-C(19) | 180.0 | C(27)-C(22)-C(23)-C(24) | 0.1 |
| C(13)-N(14)-N(16)-C(17) | -54.8 | S(21)-C(17)-N(18)-C(19) | 0.0 | C(19)-C(20)-S(21)-C(17) | 0.0 |
| C(13)-N(14)-N(16)-H(32) | 150.3 | N(14)-N(16)-C(17)-N(18) | 179.2 | N(18)-C(19)-C(22)-C(23) | -0.7 |
| C(8)-C(13)-N(14)-N(16) | 177.8 | N(14)-N(16)-C(17)-S(21) | -0.8 | N(18)-C(19)-C(22)-C(27) | 179.2 |
| C(15)-C(13)-N(14)-N(16) | -8.4 | H(35)-N(16)-C(17)-N(18) | 0.5 | C(20)-C(19)-C(22)-C(23) | 179.2 |
| C(5)-C(9)-N(12)-H(27) | -0.3 | H(35)-N(16)-C(17)-S(21) | -179.5 | C(20)-C(19)-C(22)-C(27) | -0.8 |
| C(5)-C(9)-N(12)-H(28) | -170.0 | C(13)-N(14)-N(16)-C(17) | 177.9 | N(18)-C(19)-C(20)-S(21) | 0.0 |
| C(8)-C(9)-N(12)-H(27) | 177.8 | C(13)-N(14)-N(16)-H(35) | -3.5 | C(22)-C(19)-C(20)-S(21) | -179.9 |
| C(8)-C(9)-N(12)-H(28) | 8.1 | C(8)-C(13)-N(14)-N(16) | -177.5 | C(17)-N(18)-C(19)-C(20) | 0.0 |
| S(7)-C(8)-C(13)-N(14) | 6.7 | C(15)-C(13)-N(14)-N(16) | -2.5 | C(17)-N(18)-C(19)-C(22) | 180.0 |
| S(7)-C(8)-C(13)-C(15) | -167.3 | C(5)-C(9)-N(12)-H(30) | 5.8 | N(16)-C(17)-S(21)-C(20) | -179.9 |
| C(9)-C(8)-C(13)-N(14) | -172.6 | C(5)-C(9)-N(12)-H(31) | -158.1 | N(18)-C(17)-S(21)-C(20) | 0.0 |
| C(9)-C(8)-C(13)-C(15) | 13.4 | C(8)-C(9)-N(12)-H(30) | -176.8 | N(16)-C(17)-N(18)-C(19) | 179.9 |
| S(7)-C(8)-C(9)-C(5) | 3.4 | C(8)-C(9)-N(12)-H(31) | 19.3 | S(21)-C(17)-N(18)-C(19) | 0.0 |
| S(7)-C(8)-C(9)-N(12) | -174.9 | S(7)-C(8)-C(13)-N(14) | 14.6 | N(14)-N(16)-C(17)-N(18) | 179.1 |
| C(13)-C(8)-C(9)-C(5) | -177.3 | S(7)-C(8)-C(13)-C(15) | -160.4 | N(14)-N(16)-C(17)-S(21) | -1.0 |
| C(13)-C(8)-C(9)-N(12) | 4.5 | C(9)-C(8)-C(13)-N(14) | -165.7 | H(40)-N(16)-C(17)-N(18) | 0.5 |
| C(4)-S(7)-C(8)-C(9) | -2.8 | C(9)-C(8)-C(13)-C(15) | 19.3 | H(40)-N(16)-C(17)-S(21) | -179.5 |
| C(4)-S(7)-C(8)-C(13) | 177.8 | S(7)-C(8)-C(9)-C(5) | 4.1 | C(13)-N(14)-N(16)-C(17) | 177.9 |
| C(4)-C(5)-C(9)-C(8) | -2.2 | S(7)-C(8)-C(9)-N(12) | -173.6 | C(13)-N(14)-N(16)-H(40) | -3.7 |
| C(4)-C(5)-C(9)-N(12) | 176.1 | C(13)-C(8)-C(9)-C(5) | -175.6 | C(8)-C(13)-N(14)-N(16) | -177.6 |
| C(6)-C(5)-C(9)-C(8) | 178.0 | C(13)-C(8)-C(9)-N(12) | 6.8 | C(15)-C(13)-N(14)-N(16) | -2.5 |
| C(6)-C(5)-C(9)-N(12) | -3.7 | C(4)-S(7)-C(8)-C(9) | -3.3 | C(5)-C(9)-N(12)-H(35) | 5.7 |
| C(4)-C(5)-C(6)-C(1) | -0.2 | C(4)-S(7)-C(8)-C(13) | 176.4 | C(5)-C(9)-N(12)-H(36) | -158.7 |
| C(4)-C(5)-C(6)-C(11) | 179.4 | C(4)-C(5)-C(9)-C(8) | -2.8 | C(8)-C(9)-N(12)-H(35) | -176.9 |
| C(9)-C(5)-C(6)-C(1) | 179.6 | C(4)-C(5)-C(9)-N(12) | 174.9 | C(8)-C(9)-N(12)-H(36) | 18.8 |
| C(9)-C(5)-C(6)-C(11) | -0.8 | C(6)-C(5)-C(9)-C(8) | 178.1 | S(7)-C(8)-C(13)-N(14) | 14.4 |
| N(3)-C(4)-S(7)-C(8) | -178.8 | C(6)-C(5)-C(9)-N(12) | -4.2 | S(7)-C(8)-C(13)-C(15) | -160.7 |
| C(5)-C(4)-S(7)-C(8) | 1.5 | C(4)-C(5)-C(6)-C(1) | 0.2 | C(9)-C(8)-C(13)-N(14) | -165.9 |
| N(3)-C(4)-C(5)-C(6) | 0.2 | C(4)-C(5)-C(6)-C(11) | 179.8 | C(9)-C(8)-C(13)-C(15) | 19.0 |
| N(3)-C(4)-C(5)-C(9) | -179.6 | C(9)-C(5)-C(6)-C(1) | 179.3 | S(7)-C(8)-C(9)-C(5) | 4.1 |
| S(7)-C(4)-C(5)-C(6) | 179.9 | C(9)-C(5)-C(6)-C(11) | -1.1 | S(7)-C(8)-C(9)-N(12) | -173.6 |
| S(7)-C(4)-C(5)-C(9) | 0.0 | N(3)-C(4)-S(7)-C(8) | -179.0 | C(13)-C(8)-C(9)-C(5) | -175.7 |
| C(2)-N(3)-C(4)-C(5) | 0.0 | C(5)-C(4)-S(7)-C(8) | 1.7 | C(13)-C(8)-C(9)-N(12) | 6.7 |
| C(2)-N(3)-C(4)-S(7) | -179.6 | N(3)-C(4)-C(5)-C(6) | 0.1 | C(4)-S(7)-C(8)-C(9) | -3.3 |
| C(1)-C(2)-N(3)-C(4) | -0.2 | N(3)-C(4)-C(5)-C(9) | -179.1 | C(4)-S(7)-C(8)-C(13) | 176.5 |
| C(10)-C(2)-N(3)-C(4) | 179.8 | S(7)-C(4)-C(5)-C(6) | 179.5 | C(4)-C(5)-C(9)-C(8) | -2.7 |
| C(2)-C(1)-C(6)-C(5) | 0.0 | S(7)-C(4)-C(5)-C(9) | 0.2 | C(4)-C(5)-C(9)-N(12) | 175.0 |
| C(2)-C(1)-C(6)-C(11) | -179.6 | C(2)-N(3)-C(4)-C(5) | -0.3 | C(6)-C(5)-C(9)-C(8) | 178.2 |
| C(6)-C(1)-C(2)-N(3) | 0.2 | C(2)-N(3)-C(4)-S(7) | -179.6 | C(6)-C(5)-C(9)-N(12) | -4.1 |
| C(6)-C(1)-C(2)-C(10) | -179.8 | C(1)-C(2)-N(3)-C(4) | 0.2 | C(4)-C(5)-C(6)-C(1) | 0.2 |
|  |  | C(10)-C(2)-N(3)-C(4) | -179.7 | C(4)-C(5)-C(6)-C(11) | 179.9 |
|  |  | C(2)-C(1)-C(6)-C(5) | -0.3 | C(9)-C(5)-C(6)-C(1) | 179.3 |
|  |  | C(2)-C(1)-C(6)-C(11) | -180.0 | C(9)-C(5)-C(6)-C(11) | -1.1 |
|  |  | C(6)-C(1)-C(2)-N(3) | 0.1 | N(3)-C(4)-S(7)-C(8) | -179.0 |
|  |  | C(6)-C(1)-C(2)-C(10) | 180.0 | C(5)-C(4)-S(7)-C(8) | 1.7 |
|  |  |  |  | N(3)-C(4)-C(5)-C(6) | 0.1 |
|  |  |  |  | N(3)-C(4)-C(5)-C(9) | -179.1 |
|  |  |  |  | S(7)-C(4)-C(5)-C(6) | 179.4 |
|  |  |  |  | S(7)-C(4)-C(5)-C(9) | 0.2 |
|  |  |  |  | C(2)-N(3)-C(4)-C(5) | -0.3 |
|  |  |  |  | C(2)-N(3)-C(4)-S(7) | -179.6 |
|  |  |  |  | C(1)-C(2)-N(3)-C(4) | 0.2 |
|  |  |  |  | C(10)-C(2)-N(3)-C(4) | -179.7 |
|  |  |  |  | C(2)-C(1)-C(6)-C(5) | -0.3 |
|  |  |  |  | C(2)-C(1)-C(6)-C(11) | -180.0 |
|  |  |  |  | C(6)-C(1)-C(2)-N(3) | 0.1 |
|  |  |  |  | C(6)-C(1)-C(2)-C(10) | 180.0 |
|  | **7** |  | 8 |  | 9 |
| **Dihedral** | **(°)** | **Dihedral** | **(°)** | **Dihedral** | **(°)** |
| C(19)-C(20)-S(21)-C(17) | 0.1 | C(27)-C(28)-C(29)-C(24) | 0.1 | C(27)-C(28)-C(29)-C(24) | 0.0 |
| N(18)-C(19)-C(20)-S(21) | -0.1 | C(26)-C(27)-C(28)-C(29) | -0.3 | C(26)-C(27)-O(30)-C(31) | 179.8 |
| O(22)-C(19)-C(20)-S(21) | 179.9 | C(30)-C(27)-C(28)-C(29) | 179.2 | C(28)-C(27)-O(30)-C(31) | -0.2 |
| C(17)-N(18)-C(19)-C(20) | 0.1 | C(25)-C(26)-C(27)-C(28) | 0.3 | C(26)-C(27)-C(28)-C(29) | 0.0 |
| C(17)-N(18)-C(19)-O(22) | -179.9 | C(25)-C(26)-C(27)-C(30) | -179.2 | O(30)-C(27)-C(28)-C(29) | 180.0 |
| N(16)-C(17)-S(21)-C(20) | 180.0 | C(24)-C(25)-C(26)-C(27) | -0.1 | C(25)-C(26)-C(27)-C(28) | 0.1 |
| N(18)-C(17)-S(21)-C(20) | -0.1 | C(23)-C(24)-C(29)-C(28) | -179.9 | C(25)-C(26)-C(27)-O(30) | -179.9 |
| N(16)-C(17)-N(18)-C(19) | 180.0 | C(25)-C(24)-C(29)-C(28) | 0.1 | C(24)-C(25)-C(26)-C(27) | 0.0 |
| S(21)-C(17)-N(18)-C(19) | 0.0 | C(23)-C(24)-C(25)-C(26) | 179.9 | C(23)-C(24)-C(29)-C(28) | -179.8 |
| N(14)-N(16)-C(17)-N(18) | -179.3 | C(29)-C(24)-C(25)-C(26) | -0.1 | C(25)-C(24)-C(29)-C(28) | 0.1 |
| N(14)-N(16)-C(17)-S(21) | 0.6 | C(20)-C(23)-C(24)-C(25) | -179.5 | C(23)-C(24)-C(25)-C(26) | 179.8 |
| H(35)-N(16)-C(17)-N(18) | -0.8 | C(20)-C(23)-C(24)-C(29) | 0.5 | C(29)-C(24)-C(25)-C(26) | 0.0 |
| H(35)-N(16)-C(17)-S(21) | 179.1 | C(19)-C(20)-C(23)-C(24) | 179.9 | C(20)-C(23)-C(24)-C(25) | -179.9 |
| C(13)-N(14)-N(16)-C(17) | -177.3 | S(21)-C(20)-C(23)-C(24) | 0.0 | C(20)-C(23)-C(24)-C(29) | -0.1 |
| C(13)-N(14)-N(16)-H(35) | 4.4 | C(19)-C(20)-S(21)-C(17) | -0.1 | C(19)-C(20)-C(23)-C(24) | 179.7 |
| C(8)-C(13)-N(14)-N(16) | 178.5 | C(23)-C(20)-S(21)-C(17) | 179.9 | S(21)-C(20)-C(23)-C(24) | -0.2 |
| C(15)-C(13)-N(14)-N(16) | 2.5 | N(18)-C(19)-C(20)-S(21) | 0.1 | C(19)-C(20)-S(21)-C(17) | -0.2 |
| C(5)-C(9)-N(12)-H(30) | -4.8 | N(18)-C(19)-C(20)-C(23) | -179.9 | C(23)-C(20)-S(21)-C(17) | 179.7 |
| C(5)-C(9)-N(12)-H(31) | 162.9 | O(22)-C(19)-C(20)-S(21) | -179.9 | N(18)-C(19)-C(20)-S(21) | 0.2 |
| C(8)-C(9)-N(12)-H(30) | 177.6 | O(22)-C(19)-C(20)-C(23) | 0.1 | N(18)-C(19)-C(20)-C(23) | -179.7 |
| C(8)-C(9)-N(12)-H(31) | -14.7 | C(17)-N(18)-C(19)-C(20) | 0.0 | O(22)-C(19)-C(20)-S(21) | -179.8 |
| S(7)-C(8)-C(13)-N(14) | -12.0 | C(17)-N(18)-C(19)-O(22) | 179.9 | O(22)-C(19)-C(20)-C(23) | 0.3 |
| S(7)-C(8)-C(13)-C(15) | 164.0 | N(16)-C(17)-S(21)-C(20) | -180.0 | C(17)-N(18)-C(19)-C(20) | -0.1 |
| C(9)-C(8)-C(13)-N(14) | 168.2 | N(18)-C(17)-S(21)-C(20) | 0.0 | C(17)-N(18)-C(19)-O(22) | 179.9 |
| C(9)-C(8)-C(13)-C(15) | -15.8 | N(16)-C(17)-N(18)-C(19) | -180.0 | N(16)-C(17)-S(21)-C(20) | -179.7 |
| S(7)-C(8)-C(9)-C(5) | -3.8 | S(21)-C(17)-N(18)-C(19) | 0.0 | N(18)-C(17)-S(21)-C(20) | 0.1 |
| S(7)-C(8)-C(9)-N(12) | 174.1 | N(14)-N(16)-C(17)-N(18) | 179.1 | N(16)-C(17)-N(18)-C(19) | 179.9 |
| C(13)-C(8)-C(9)-C(5) | 176.0 | N(14)-N(16)-C(17)-S(21) | -0.9 | S(21)-C(17)-N(18)-C(19) | 0.0 |
| C(13)-C(8)-C(9)-N(12) | -6.2 | H(43)-N(16)-C(17)-N(18) | 0.7 | N(14)-N(16)-C(17)-N(18) | 178.9 |
| C(4)-S(7)-C(8)-C(9) | 3.1 | H(43)-N(16)-C(17)-S(21) | -179.3 | N(14)-N(16)-C(17)-S(21) | -1.2 |
| C(4)-S(7)-C(8)-C(13) | -176.7 | C(13)-N(14)-N(16)-C(17) | 177.3 | H(44)-N(16)-C(17)-N(18) | 0.6 |
| C(4)-C(5)-C(9)-C(8) | 2.5 | C(13)-N(14)-N(16)-H(43) | -4.4 | H(44)-N(16)-C(17)-S(21) | -179.6 |
| C(4)-C(5)-C(9)-N(12) | -175.4 | C(8)-C(13)-N(14)-N(16) | -178.7 | C(13)-N(14)-N(16)-C(17) | 176.4 |
| C(6)-C(5)-C(9)-C(8) | -178.3 | C(15)-C(13)-N(14)-N(16) | -2.8 | C(13)-N(14)-N(16)-H(44) | -5.3 |
| C(6)-C(5)-C(9)-N(12) | 3.8 | C(5)-C(9)-N(12)-H(38) | 4.8 | C(8)-C(13)-N(14)-N(16) | -179.0 |
| C(4)-C(5)-C(6)-C(1) | -0.2 | C(5)-C(9)-N(12)-H(39) | -162.5 | C(15)-C(13)-N(14)-N(16) | -2.9 |
| C(4)-C(5)-C(6)-C(11) | -179.9 | C(8)-C(9)-N(12)-H(38) | -177.7 | C(5)-C(9)-N(12)-H(39) | 4.3 |
| C(9)-C(5)-C(6)-C(1) | -179.4 | C(8)-C(9)-N(12)-H(39) | 15.0 | C(5)-C(9)-N(12)-H(40) | -163.8 |
| C(9)-C(5)-C(6)-C(11) | 0.9 | S(7)-C(8)-C(13)-N(14) | 12.0 | C(8)-C(9)-N(12)-H(39) | -178.1 |
| N(3)-C(4)-S(7)-C(8) | 178.8 | S(7)-C(8)-C(13)-C(15) | -164.0 | C(8)-C(9)-N(12)-H(40) | 13.9 |
| C(5)-C(4)-S(7)-C(8) | -1.7 | C(9)-C(8)-C(13)-N(14) | -168.0 | S(7)-C(8)-C(13)-N(14) | 11.0 |
| N(3)-C(4)-C(5)-C(6) | 0.1 | C(9)-C(8)-C(13)-C(15) | 16.0 | S(7)-C(8)-C(13)-C(15) | -165.2 |
| N(3)-C(4)-C(5)-C(9) | 179.4 | S(7)-C(8)-C(9)-C(5) | 3.9 | C(9)-C(8)-C(13)-N(14) | -169.0 |
| S(7)-C(4)-C(5)-C(6) | -179.4 | S(7)-C(8)-C(9)-N(12) | -173.7 | C(9)-C(8)-C(13)-C(15) | 14.8 |
| S(7)-C(4)-C(5)-C(9) | -0.1 | C(13)-C(8)-C(9)-C(5) | -176.0 | S(7)-C(8)-C(9)-C(5) | 3.7 |
| C(2)-N(3)-C(4)-C(5) | 0.2 | C(13)-C(8)-C(9)-N(12) | 6.3 | S(7)-C(8)-C(9)-N(12) | -174.1 |
| C(2)-N(3)-C(4)-S(7) | 179.6 | C(4)-S(7)-C(8)-C(9) | -3.2 | C(13)-C(8)-C(9)-C(5) | -176.3 |
| C(1)-C(2)-N(3)-C(4) | -0.2 | C(4)-S(7)-C(8)-C(13) | 176.8 | C(13)-C(8)-C(9)-N(12) | 5.9 |
| C(10)-C(2)-N(3)-C(4) | 179.7 | C(4)-C(5)-C(9)-C(8) | -2.7 | C(4)-S(7)-C(8)-C(9) | -3.0 |
| C(2)-C(1)-C(6)-C(5) | 0.2 | C(4)-C(5)-C(9)-N(12) | 175.1 | C(4)-S(7)-C(8)-C(13) | 177.0 |
| C(2)-C(1)-C(6)-C(11) | 179.9 | C(6)-C(5)-C(9)-C(8) | 178.1 | C(4)-C(5)-C(9)-C(8) | -2.6 |
| C(6)-C(1)-C(2)-N(3) | 0.0 | C(6)-C(5)-C(9)-N(12) | -4.1 | C(4)-C(5)-C(9)-N(12) | 175.3 |
| C(6)-C(1)-C(2)-C(10) | -179.9 | C(4)-C(5)-C(6)-C(1) | 0.2 | C(6)-C(5)-C(9)-C(8) | 178.0 |
|  |  | C(4)-C(5)-C(6)-C(11) | 179.9 | C(6)-C(5)-C(9)-N(12) | -4.1 |
|  |  | C(9)-C(5)-C(6)-C(1) | 179.4 | C(4)-C(5)-C(6)-C(1) | 0.1 |
|  |  | C(9)-C(5)-C(6)-C(11) | -0.9 | C(4)-C(5)-C(6)-C(11) | 179.7 |
|  |  | N(3)-C(4)-S(7)-C(8) | -178.8 | C(9)-C(5)-C(6)-C(1) | 179.5 |
|  |  | C(5)-C(4)-S(7)-C(8) | 1.6 | C(9)-C(5)-C(6)-C(11) | -0.9 |
|  |  | N(3)-C(4)-C(5)-C(6) | 0.0 | N(3)-C(4)-S(7)-C(8) | -178.9 |
|  |  | N(3)-C(4)-C(5)-C(9) | -179.3 | C(5)-C(4)-S(7)-C(8) | 1.5 |
|  |  | S(7)-C(4)-C(5)-C(6) | 179.6 | N(3)-C(4)-C(5)-C(6) | 0.1 |
|  |  | S(7)-C(4)-C(5)-C(9) | 0.2 | N(3)-C(4)-C(5)-C(9) | -179.4 |
|  |  | C(2)-N(3)-C(4)-C(5) | -0.2 | S(7)-C(4)-C(5)-C(6) | 179.7 |
|  |  | C(2)-N(3)-C(4)-S(7) | -179.7 | S(7)-C(4)-C(5)-C(9) | 0.2 |
|  |  | C(1)-C(2)-N(3)-C(4) | 0.2 | C(2)-N(3)-C(4)-C(5) | -0.2 |
|  |  | C(10)-C(2)-N(3)-C(4) | -179.7 | C(2)-N(3)-C(4)-S(7) | -179.8 |
|  |  | C(2)-C(1)-C(6)-C(5) | -0.2 | C(1)-C(2)-N(3)-C(4) | 0.1 |
|  |  | C(2)-C(1)-C(6)-C(11) | -179.9 | C(10)-C(2)-N(3)-C(4) | -179.7 |
|  |  | C(6)-C(1)-C(2)-N(3) | 0.1 | C(2)-C(1)-C(6)-C(5) | -0.2 |
|  |  | C(6)-C(1)-C(2)-C(10) | 179.9 | C(2)-C(1)-C(6)-C(11) | -179.8 |
|  |  |  |  | C(6)-C(1)-C(2)-N(3) | 0.1 |
|  |  |  |  | C(6)-C(1)-C(2)-C(10) | 179.9 |
|  | **10** |  |  |  |  |
| **Dihedral** | **(°)** |  |  |  |  |
| C(27)-C(28)-C(29)-C(24) | 0.0 |  |  |  |  |
| C(26)-C(27)-C(28)-C(29) | 0.0 |  |  |  |  |
| Cl(30)-C(27)-C(28)-C(29) | 180.0 |  |  |  |  |
| C(25)-C(26)-C(27)-C(28) | 0.0 |  |  |  |  |
| C(25)-C(26)-C(27)-Cl(30) | -180.0 |  |  |  |  |
| C(24)-C(25)-C(26)-C(27) | 0.0 |  |  |  |  |
| C(23)-C(24)-C(29)-C(28) | -179.9 |  |  |  |  |
| C(25)-C(24)-C(29)-C(28) | 0.0 |  |  |  |  |
| C(23)-C(24)-C(25)-C(26) | 179.9 |  |  |  |  |
| C(29)-C(24)-C(25)-C(26) | 0.0 |  |  |  |  |
| C(20)-C(23)-C(24)-C(25) | -179.7 |  |  |  |  |
| C(20)-C(23)-C(24)-C(29) | 0.2 |  |  |  |  |
| C(19)-C(20)-C(23)-C(24) | 179.9 |  |  |  |  |
| S(21)-C(20)-C(23)-C(24) | -0.1 |  |  |  |  |
| C(19)-C(20)-S(21)-C(17) | -0.2 |  |  |  |  |
| C(23)-C(20)-S(21)-C(17) | 179.7 |  |  |  |  |
| N(18)-C(19)-C(20)-S(21) | 0.2 |  |  |  |  |
| N(18)-C(19)-C(20)-C(23) | -179.7 |  |  |  |  |
| O(22)-C(19)-C(20)-S(21) | -179.8 |  |  |  |  |
| O(22)-C(19)-C(20)-C(23) | 0.3 |  |  |  |  |
| C(17)-N(18)-C(19)-C(20) | -0.1 |  |  |  |  |
| C(17)-N(18)-C(19)-O(22) | 179.9 |  |  |  |  |
| N(16)-C(17)-S(21)-C(20) | -179.8 |  |  |  |  |
| N(18)-C(17)-S(21)-C(20) | 0.2 |  |  |  |  |
| N(16)-C(17)-N(18)-C(19) | 179.9 |  |  |  |  |
| S(21)-C(17)-N(18)-C(19) | 0.0 |  |  |  |  |
| N(14)-N(16)-C(17)-N(18) | 179.0 |  |  |  |  |
| N(14)-N(16)-C(17)-S(21) | -1.1 |  |  |  |  |
| H(43)-N(16)-C(17)-N(18) | 0.6 |  |  |  |  |
| H(43)-N(16)-C(17)-S(21) | -179.5 |  |  |  |  |
| C(13)-N(14)-N(16)-C(17) | 176.4 |  |  |  |  |
| C(13)-N(14)-N(16)-H(43) | -5.3 |  |  |  |  |
| C(8)-C(13)-N(14)-N(16) | -179.0 |  |  |  |  |
| C(15)-C(13)-N(14)-N(16) | -2.8 |  |  |  |  |
| C(5)-C(9)-N(12)-H(38) | 4.2 |  |  |  |  |
| C(5)-C(9)-N(12)-H(39) | -164.2 |  |  |  |  |
| C(8)-C(9)-N(12)-H(38) | -178.2 |  |  |  |  |
| C(8)-C(9)-N(12)-H(39) | 13.5 |  |  |  |  |
| S(7)-C(8)-C(13)-N(14) | 10.7 |  |  |  |  |
| S(7)-C(8)-C(13)-C(15) | -165.5 |  |  |  |  |
| C(9)-C(8)-C(13)-N(14) | -169.4 |  |  |  |  |
| C(9)-C(8)-C(13)-C(15) | 14.4 |  |  |  |  |
| S(7)-C(8)-C(9)-C(5) | 3.8 |  |  |  |  |
| S(7)-C(8)-C(9)-N(12) | -174.1 |  |  |  |  |
| C(13)-C(8)-C(9)-C(5) | -176.1 |  |  |  |  |
| C(13)-C(8)-C(9)-N(12) | 6.0 |  |  |  |  |
| C(4)-S(7)-C(8)-C(9) | -3.0 |  |  |  |  |
| C(4)-S(7)-C(8)-C(13) | 176.9 |  |  |  |  |
| C(4)-C(5)-C(9)-C(8) | -2.6 |  |  |  |  |
| C(4)-C(5)-C(9)-N(12) | 175.4 |  |  |  |  |
| C(6)-C(5)-C(9)-C(8) | 178.0 |  |  |  |  |
| C(6)-C(5)-C(9)-N(12) | -4.1 |  |  |  |  |
| C(4)-C(5)-C(6)-C(1) | 0.1 |  |  |  |  |
| C(4)-C(5)-C(6)-C(11) | 179.7 |  |  |  |  |
| C(9)-C(5)-C(6)-C(1) | 179.5 |  |  |  |  |
| C(9)-C(5)-C(6)-C(11) | -0.9 |  |  |  |  |
| N(3)-C(4)-S(7)-C(8) | -178.8 |  |  |  |  |
| C(5)-C(4)-S(7)-C(8) | 1.5 |  |  |  |  |
| N(3)-C(4)-C(5)-C(6) | 0.1 |  |  |  |  |
| N(3)-C(4)-C(5)-C(9) | -179.4 |  |  |  |  |
| S(7)-C(4)-C(5)-C(6) | 179.7 |  |  |  |  |
| S(7)-C(4)-C(5)-C(9) | 0.2 |  |  |  |  |
| C(2)-N(3)-C(4)-C(5) | -0.2 |  |  |  |  |
| C(2)-N(3)-C(4)-S(7) | -179.8 |  |  |  |  |
| C(1)-C(2)-N(3)-C(4) | 0.1 |  |  |  |  |
| C(10)-C(2)-N(3)-C(4) | -179.7 |  |  |  |  |
| C(2)-C(1)-C(6)-C(5) | -0.2 |  |  |  |  |
| C(2)-C(1)-C(6)-C(11) | -179.8 |  |  |  |  |
| C(6)-C(1)-C(2)-N(3) | 0.1 |  |  |  |  |
| C(6)-C(1)-C(2)-C(10) | 179.9 |  |  |  |  |

**Table S2**. The DFT bond length data of the investigated compounds.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **4** |  |  | **5** |  |  | **6** |  |
| **Bond** | **Å** | **Std.** | **Bond** | **Å** | **Std.** | **Bond** | **Å** | **Std.** |
| N(18)-H(34) | 1.02 | 1.01 | C(20)-S(21) | 1.80 | 1.66 | C(26)-C(27) | 1.40 | 1.42 |
| N(18)-H(33) | 1.02 | 1.01 | C(19)-C(22) | 1.49 | 1.50 | C(25)-C(26) | 1.41 | 1.42 |
| C(17)-S(19) | 1.72 | 1.58 | C(19)-C(20) | 1.38 | 1.42 | C(24)-C(25) | 1.40 | 1.42 |
| C(17)-N(18) | 1.37 | 1.37 | N(18)-C(19) | 1.39 | 1.36 | C(23)-C(24) | 1.40 | 1.42 |
| N(16)-H(32) | 1.03 | 1.01 | C(17)-S(21) | 1.82 | 1.66 | C(22)-C(27) | 1.41 | 1.42 |
| N(16)-C(17) | 1.38 | 1.37 | C(17)-N(18) | 1.31 | 1.36 | C(22)-C(23) | 1.41 | 1.42 |
| N(14)-N(16) | 1.38 | 1.43 | N(16)-H(35) | 1.03 | 1.05 | C(20)-S(21) | 1.80 | 1.66 |
| C(13)-C(15) | 1.49 | 1.50 | N(16)-C(17) | 1.37 | 1.46 | C(19)-C(22) | 1.46 | 1.50 |
| C(13)-N(14) | 1.33 | 1.26 | N(14)-N(16) | 1.36 | 1.43 | C(19)-C(20) | 1.38 | 1.42 |
| N(12)-H(28) | 1.02 | 1.05 | C(13)-C(15) | 1.50 | 1.50 | N(18)-C(19) | 1.39 | 1.36 |
| N(12)-H(27) | 1.02 | 1.05 | C(13)-N(14) | 1.32 | 1.26 | C(17)-S(21) | 1.82 | 1.66 |
| C(9)-N(12) | 1.38 | 1.46 | N(12)-H(31) | 1.02 | 1.05 | C(17)-N(18) | 1.31 | 1.36 |
| C(8)-C(13) | 1.43 | 1.50 | N(12)-H(30) | 1.02 | 1.05 | N(16)-H(40) | 1.03 | 1.05 |
| C(8)-C(9) | 1.40 | 1.42 | C(9)-N(12) | 1.39 | 1.46 | N(16)-C(17) | 1.37 | 1.46 |
| S(7)-C(8) | 1.82 | 1.66 | C(8)-C(13) | 1.44 | 1.50 | N(14)-N(16) | 1.36 | 1.43 |
| C(6)-C(11) | 1.50 | 1.50 | C(8)-C(9) | 1.40 | 1.42 | C(13)-C(15) | 1.50 | 1.50 |
| C(5)-C(9) | 1.45 | 1.42 | S(7)-C(8) | 1.82 | 1.66 | C(13)-N(14) | 1.32 | 1.26 |
| C(5)-C(6) | 1.42 | 1.42 | C(6)-C(11) | 1.50 | 1.50 | N(12)-H(36) | 1.02 | 1.05 |
| C(4)-S(7) | 1.80 | 1.66 | C(5)-C(9) | 1.45 | 1.42 | N(12)-H(35) | 1.02 | 1.05 |
| C(4)-C(5) | 1.43 | 1.42 | C(5)-C(6) | 1.42 | 1.42 | C(9)-N(12) | 1.38 | 1.46 |
| N(3)-C(4) | 1.33 | 1.36 | C(4)-S(7) | 1.80 | 1.66 | C(8)-C(13) | 1.44 | 1.50 |
| C(2)-C(10) | 1.49 | 1.50 | C(4)-C(5) | 1.43 | 1.42 | C(8)-C(9) | 1.40 | 1.42 |
| C(2)-N(3) | 1.35 | 1.36 | N(3)-C(4) | 1.33 | 1.36 | S(7)-C(8) | 1.82 | 1.66 |
| C(1)-C(6) | 1.40 | 1.42 | C(2)-C(10) | 1.49 | 1.50 | C(6)-C(11) | 1.50 | 1.50 |
| C(1)-C(2) | 1.41 | 1.42 | C(2)-N(3) | 1.35 | 1.36 | C(5)-C(9) | 1.45 | 1.42 |
| RSMD | 6.02E-02 |  | C(1)-C(6) | 1.40 | 1.42 | C(5)-C(6) | 1.42 | 1.42 |
|  |  |  | C(1)-C(2) | 1.41 | 1.42 | C(4)-S(7) | 1.80 | 1.66 |
|  |  |  | RSMD | 6.93E-02 |  | C(4)-C(5) | 1.43 | 1.42 |
|  |  |  |  |  |  | N(3)-C(4) | 1.33 | 1.36 |
|  |  |  |  |  |  | C(2)-C(10) | 1.49 | 1.50 |
|  |  |  |  |  |  | C(2)-N(3) | 1.35 | 1.36 |
|  |  |  |  |  |  | C(1)-C(6) | 1.40 | 1.42 |
|  |  |  |  |  |  | C(1)-C(2) | 1.41 | 1.42 |
|  |  |  |  |  |  | RSMD | 6.34E-02 |  |
|  | **7** |  |  | **8** |  |  | **9** |  |
| **Bond** | **Å** | **Std.** | **Bond** | **Å** | **Std.** | **Bond** | **Å** | **Std.** |
| C(20)-S(21) | 1.88 | 1.86 | C(28)-C(29) | 1.39 | 1.42 | O(30)-C(31) | 1.44 | 1.40 |
| C(19)-O(22) | 1.24 | 1.21 | C(27)-C(30) | 1.50 | 1.50 | C(28)-C(29) | 1.40 | 1.42 |
| C(19)-C(20) | 1.54 | 1.51 | C(27)-C(28) | 1.41 | 1.42 | C(27)-O(30) | 1.37 | 1.36 |
| N(18)-C(19) | 1.39 | 1.43 | C(26)-C(27) | 1.41 | 1.42 | C(27)-C(28) | 1.41 | 1.42 |
| C(17)-S(21) | 1.83 | 1.86 | C(25)-C(26) | 1.40 | 1.42 | C(26)-C(27) | 1.41 | 1.42 |
| C(17)-N(18) | 1.31 | 1.26 | C(24)-C(29) | 1.42 | 1.42 | C(25)-C(26) | 1.39 | 1.42 |
| N(16)-H(35) | 1.03 | 1.05 | C(24)-C(25) | 1.42 | 1.42 | C(24)-C(29) | 1.41 | 1.42 |
| N(16)-C(17) | 1.35 | 1.46 | C(23)-C(24) | 1.44 | 1.50 | C(24)-C(25) | 1.42 | 1.42 |
| N(14)-N(16) | 1.36 | 1.43 | C(20)-C(23) | 1.36 | 1.34 | C(23)-C(24) | 1.44 | 1.50 |
| C(13)-C(15) | 1.50 | 1.50 | C(20)-S(21) | 1.82 | 1.86 | C(20)-C(23) | 1.36 | 1.34 |
| C(13)-N(14) | 1.32 | 1.26 | C(19)-O(22) | 1.25 | 1.21 | C(20)-S(21) | 1.82 | 1.86 |
| N(12)-H(31) | 1.02 | 1.05 | C(19)-C(20) | 1.50 | 1.52 | C(19)-O(22) | 1.25 | 1.21 |
| N(12)-H(30) | 1.02 | 1.05 | N(18)-C(19) | 1.40 | 1.43 | C(19)-C(20) | 1.50 | 1.52 |
| C(9)-N(12) | 1.38 | 1.46 | C(17)-S(21) | 1.84 | 1.86 | N(18)-C(19) | 1.41 | 1.43 |
| C(8)-C(13) | 1.43 | 1.50 | C(17)-N(18) | 1.31 | 1.26 | C(17)-S(21) | 1.84 | 1.86 |
| C(8)-C(9) | 1.40 | 1.42 | N(16)-H(43) | 1.03 | 1.05 | C(17)-N(18) | 1.31 | 1.26 |
| S(7)-C(8) | 1.82 | 1.66 | N(16)-C(17) | 1.36 | 1.46 | N(16)-H(44) | 1.03 | 1.05 |
| C(6)-C(11) | 1.50 | 1.50 | N(14)-N(16) | 1.36 | 1.43 | N(16)-C(17) | 1.36 | 1.46 |
| C(5)-C(9) | 1.45 | 1.42 | C(13)-C(15) | 1.50 | 1.50 | N(14)-N(16) | 1.36 | 1.43 |
| C(5)-C(6) | 1.42 | 1.42 | C(13)-N(14) | 1.32 | 1.26 | C(13)-C(15) | 1.50 | 1.50 |
| C(4)-S(7) | 1.80 | 1.66 | N(12)-H(39) | 1.02 | 1.05 | C(13)-N(14) | 1.32 | 1.26 |
| C(4)-C(5) | 1.42 | 1.42 | N(12)-H(38) | 1.02 | 1.05 | N(12)-H(40) | 1.02 | 1.05 |
| N(3)-C(4) | 1.34 | 1.36 | C(9)-N(12) | 1.38 | 1.46 | N(12)-H(39) | 1.02 | 1.05 |
| C(2)-C(10) | 1.49 | 1.50 | C(8)-C(13) | 1.43 | 1.50 | C(9)-N(12) | 1.38 | 1.46 |
| C(2)-N(3) | 1.35 | 1.36 | C(8)-C(9) | 1.40 | 1.42 | C(8)-C(13) | 1.43 | 1.50 |
| C(1)-C(6) | 1.40 | 1.42 | S(7)-C(8) | 1.82 | 1.66 | C(8)-C(9) | 1.40 | 1.42 |
| C(1)-C(2) | 1.42 | 1.42 | C(6)-C(11) | 1.50 | 1.50 | S(7)-C(8) | 1.82 | 1.66 |
| RSMD | 5.73E-02 |  | C(5)-C(9) | 1.45 | 1.42 | C(6)-C(11) | 1.50 | 1.50 |
|  |  |  | C(5)-C(6) | 1.42 | 1.42 | C(5)-C(9) | 1.45 | 1.42 |
|  |  |  | C(4)-S(7) | 1.80 | 1.66 | C(5)-C(6) | 1.42 | 1.42 |
|  |  |  | C(4)-C(5) | 1.43 | 1.42 | C(4)-S(7) | 1.80 | 1.66 |
|  |  |  | N(3)-C(4) | 1.33 | 1.36 | C(4)-C(5) | 1.42 | 1.42 |
|  |  |  | C(2)-C(10) | 1.49 | 1.50 | N(3)-C(4) | 1.34 | 1.36 |
|  |  |  | C(2)-N(3) | 1.35 | 1.36 | C(2)-C(10) | 1.49 | 1.50 |
|  |  |  | C(1)-C(6) | 1.40 | 1.42 | C(2)-N(3) | 1.35 | 1.36 |
|  |  |  | C(1)-C(2) | 1.41 | 1.42 | C(1)-C(6) | 1.40 | 1.42 |
|  |  |  | RSMD | 5.09E-02 |  | C(1)-C(2) | 1.41 | 1.42 |
|  |  |  |  |  |  | RSMD | 5.07E-02 |  |
|  | **10** |  |  |  |  |  |  |  |
| **Bond** | **Å** | **Std.** |  |  |  |  |  |  |
| C(28)-C(29) | 1.40 | 1.42 |  |  |  |  |  |  |
| C(27)-Cl(30) | 1.80 | 1.72 |  |  |  |  |  |  |
| C(27)-C(28) | 1.40 | 1.42 |  |  |  |  |  |  |
| C(26)-C(27) | 1.40 | 1.42 |  |  |  |  |  |  |
| C(25)-C(26) | 1.40 | 1.42 |  |  |  |  |  |  |
| C(24)-C(29) | 1.42 | 1.42 |  |  |  |  |  |  |
| C(24)-C(25) | 1.42 | 1.42 |  |  |  |  |  |  |
| C(23)-C(24) | 1.45 | 1.50 |  |  |  |  |  |  |
| C(20)-C(23) | 1.36 | 1.34 |  |  |  |  |  |  |
| C(20)-S(21) | 1.82 | 1.86 |  |  |  |  |  |  |
| C(19)-O(22) | 1.25 | 1.21 |  |  |  |  |  |  |
| C(19)-C(20) | 1.51 | 1.52 |  |  |  |  |  |  |
| N(18)-C(19) | 1.40 | 1.43 |  |  |  |  |  |  |
| C(17)-S(21) | 1.84 | 1.86 |  |  |  |  |  |  |
| C(17)-N(18) | 1.31 | 1.26 |  |  |  |  |  |  |
| N(16)-H(43) | 1.03 | 1.05 |  |  |  |  |  |  |
| N(16)-C(17) | 1.35 | 1.46 |  |  |  |  |  |  |
| N(14)-N(16) | 1.36 | 1.43 |  |  |  |  |  |  |
| C(13)-C(15) | 1.50 | 1.50 |  |  |  |  |  |  |
| C(13)-N(14) | 1.32 | 1.26 |  |  |  |  |  |  |
| N(12)-H(39) | 1.02 | 1.05 |  |  |  |  |  |  |
| N(12)-H(38) | 1.02 | 1.05 |  |  |  |  |  |  |
| C(9)-N(12) | 1.38 | 1.46 |  |  |  |  |  |  |
| C(8)-C(13) | 1.43 | 1.50 |  |  |  |  |  |  |
| C(8)-C(9) | 1.40 | 1.42 |  |  |  |  |  |  |
| S(7)-C(8) | 1.82 | 1.66 |  |  |  |  |  |  |
| C(6)-C(11) | 1.50 | 1.50 |  |  |  |  |  |  |
| C(5)-C(9) | 1.45 | 1.42 |  |  |  |  |  |  |
| C(5)-C(6) | 1.42 | 1.42 |  |  |  |  |  |  |
| C(4)-S(7) | 1.80 | 1.66 |  |  |  |  |  |  |
| C(4)-C(5) | 1.42 | 1.42 |  |  |  |  |  |  |
| N(3)-C(4) | 1.34 | 1.36 |  |  |  |  |  |  |
| C(2)-C(10) | 1.49 | 1.50 |  |  |  |  |  |  |
| C(2)-N(3) | 1.35 | 1.36 |  |  |  |  |  |  |
| C(1)-C(6) | 1.40 | 1.42 |  |  |  |  |  |  |
| C(1)-C(2) | 1.41 | 1.42 |  |  |  |  |  |  |
| RSMD | 5.27E-02 |  |  |  |  |  |  |  |

**Table S3.** The DFT bond angle data of the investigated compounds.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **4** |  |  | **5** |  |  | **6** |  |
| **Angle** | **(°)** | **Std.** | **Angle** | **(°)** | **Std.** | **Angle** | **(°)** | **Std.** |
| H(34)-N(18)-H(33) | 119.7 | 118.8 | C(20)-S(21)-C(17) | 85.8 | 98.5 | C(26)-C(27)-C(22) | 120.7 | 120.0 |
| H(34)-N(18)-C(17) | 122.9 | 118.8 | S(21)-C(20)-C(19) | 111.8 | 115.0 | C(27)-C(26)-C(25) | 120.2 | 120.0 |
| H(33)-N(18)-C(17) | 116.9 | 118.8 | C(22)-C(19)-C(20) | 126.0 | 121.4 | C(26)-C(25)-C(24) | 119.6 | 120.0 |
| S(19)-C(17)-N(18) | 121.1 | 124.3 | C(22)-C(19)-N(18) | 119.1 | 115.1 | C(25)-C(24)-C(23) | 120.2 | 120.0 |
| S(19)-C(17)-N(16) | 125.9 | 124.3 | C(20)-C(19)-N(18) | 114.9 | 120.0 | C(24)-C(23)-C(22) | 120.7 | 120.0 |
| N(18)-C(17)-N(16) | 112.8 | 120.0 | C(19)-N(18)-C(17) | 111.9 | 115.0 | C(27)-C(22)-C(23) | 118.7 | 120.0 |
| H(32)-N(16)-C(17) | 116.3 | 117.4 | S(21)-C(17)-N(18) | 115.7 | 126.0 | C(27)-C(22)-C(19) | 122.3 | 120.0 |
| H(32)-N(16)-N(14) | 110.8 | 107.0 | S(21)-C(17)-N(16) | 120.4 | 120.0 | C(23)-C(22)-C(19) | 118.9 | 120.0 |
| C(17)-N(16)-N(14) | 128.3 | 120.0 | N(18)-C(17)-N(16) | 124.0 | 126.0 | C(20)-S(21)-C(17) | 85.9 | 98.5 |
| N(16)-N(14)-C(13) | 119.5 | 120.0 | H(35)-N(16)-C(17) | 116.7 | 118.0 | S(21)-C(20)-C(19) | 111.9 | 113.0 |
| C(15)-C(13)-N(14) | 124.8 | 115.1 | H(35)-N(16)-N(14) | 124.0 | 113.0 | C(22)-C(19)-C(20) | 126.2 | 120.0 |
| C(15)-C(13)-C(8) | 120.8 | 121.4 | C(17)-N(16)-N(14) | 119.3 | 124.0 | C(22)-C(19)-N(18) | 119.2 | 120.0 |
| N(14)-C(13)-C(8) | 114.1 | 120.0 | N(16)-N(14)-C(13) | 119.2 | 115.0 | C(20)-C(19)-N(18) | 114.6 | 120.0 |
| H(28)-N(12)-H(27) | 118.9 | 118.8 | C(15)-C(13)-N(14) | 122.1 | 115.1 | C(19)-N(18)-C(17) | 112.0 | 115.0 |
| H(28)-N(12)-C(9) | 120.3 | 120.0 | C(15)-C(13)-C(8) | 121.8 | 121.4 | S(21)-C(17)-N(18) | 115.6 | 126.0 |
| H(27)-N(12)-C(9) | 120.0 | 120.0 | N(14)-C(13)-C(8) | 115.9 | 120.0 | S(21)-C(17)-N(16) | 119.9 | 120.0 |
| N(12)-C(9)-C(8) | 125.0 | 120.0 | H(31)-N(12)-H(30) | 118.2 | 118.8 | N(18)-C(17)-N(16) | 124.5 | 126.0 |
| N(12)-C(9)-C(5) | 122.4 | 120.0 | H(31)-N(12)-C(9) | 120.3 | 120.0 | H(40)-N(16)-C(17) | 117.0 | 118.0 |
| C(8)-C(9)-C(5) | 112.6 | 120.0 | H(30)-N(12)-C(9) | 119.6 | 120.0 | H(40)-N(16)-N(14) | 124.0 | 113.0 |
| C(13)-C(8)-C(9) | 129.5 | 120.0 | N(12)-C(9)-C(8) | 124.5 | 120.0 | C(17)-N(16)-N(14) | 118.9 | 124.0 |
| C(13)-C(8)-S(7) | 117.3 | 119.0 | N(12)-C(9)-C(5) | 122.6 | 120.0 | N(16)-N(14)-C(13) | 119.3 | 115.0 |
| C(9)-C(8)-S(7) | 113.2 | 119.0 | C(8)-C(9)-C(5) | 112.9 | 120.0 | C(15)-C(13)-N(14) | 122.2 | 115.1 |
| C(8)-S(7)-C(4) | 88.8 | 98.5 | C(13)-C(8)-C(9) | 129.6 | 120.0 | C(15)-C(13)-C(8) | 121.8 | 121.4 |
| C(11)-C(6)-C(5) | 123.4 | 121.4 | C(13)-C(8)-S(7) | 117.5 | 119.0 | N(14)-C(13)-C(8) | 115.9 | 120.0 |
| C(11)-C(6)-C(1) | 119.4 | 121.4 | C(9)-C(8)-S(7) | 113.0 | 119.0 | H(36)-N(12)-H(35) | 118.2 | 118.8 |
| C(5)-C(6)-C(1) | 117.2 | 120.0 | C(8)-S(7)-C(4) | 89.0 | 98.5 | H(36)-N(12)-C(9) | 120.4 | 120.0 |
| C(9)-C(5)-C(6) | 130.7 | 120.0 | C(11)-C(6)-C(5) | 123.3 | 121.4 | H(35)-N(12)-C(9) | 119.6 | 120.0 |
| C(9)-C(5)-C(4) | 112.5 | 120.0 | C(11)-C(6)-C(1) | 119.5 | 121.4 | N(12)-C(9)-C(8) | 124.6 | 120.0 |
| C(6)-C(5)-C(4) | 116.8 | 120.0 | C(5)-C(6)-C(1) | 117.3 | 120.0 | N(12)-C(9)-C(5) | 122.5 | 120.0 |
| S(7)-C(4)-C(5) | 112.7 | 119.0 | C(9)-C(5)-C(6) | 130.8 | 120.0 | C(8)-C(9)-C(5) | 112.8 | 120.0 |
| S(7)-C(4)-N(3) | 121.7 | 126.0 | C(9)-C(5)-C(4) | 112.6 | 120.0 | C(13)-C(8)-C(9) | 129.6 | 120.0 |
| C(5)-C(4)-N(3) | 125.6 | 120.0 | C(6)-C(5)-C(4) | 116.6 | 120.0 | C(13)-C(8)-S(7) | 117.4 | 119.0 |
| C(4)-N(3)-C(2) | 117.7 | 115.0 | S(7)-C(4)-C(5) | 112.4 | 119.0 | C(9)-C(8)-S(7) | 113.0 | 119.0 |
| C(10)-C(2)-N(3) | 116.8 | 115.1 | S(7)-C(4)-N(3) | 121.8 | 126.0 | C(8)-S(7)-C(4) | 89.0 | 98.5 |
| C(10)-C(2)-C(1) | 122.1 | 121.4 | C(5)-C(4)-N(3) | 125.8 | 120.0 | C(11)-C(6)-C(5) | 123.3 | 121.4 |
| N(3)-C(2)-C(1) | 121.1 | 120.0 | C(4)-N(3)-C(2) | 117.7 | 115.0 | C(11)-C(6)-C(1) | 119.5 | 121.4 |
| C(6)-C(1)-C(2) | 121.7 | 120.0 | C(10)-C(2)-N(3) | 116.9 | 115.1 | C(5)-C(6)-C(1) | 117.3 | 120.0 |
| RSMD | 4.94E+00 | max | C(10)-C(2)-C(1) | 122.2 | 121.4 | C(9)-C(5)-C(6) | 130.8 | 120.0 |
|  |  | min | N(3)-C(2)-C(1) | 121.0 | 120.0 | C(9)-C(5)-C(4) | 112.6 | 120.0 |
|  |  |  | C(6)-C(1)-C(2) | 121.7 | 120.0 | C(6)-C(5)-C(4) | 116.6 | 120.0 |
|  |  |  | RSMD | 5.46E+00 | max | S(7)-C(4)-C(5) | 112.4 | 119.0 |
|  |  |  |  |  | min | S(7)-C(4)-N(3) | 121.8 | 126.0 |
|  |  |  |  |  |  | C(5)-C(4)-N(3) | 125.8 | 120.0 |
|  |  |  |  |  |  | C(4)-N(3)-C(2) | 117.7 | 115.0 |
|  |  |  |  |  |  | C(10)-C(2)-N(3) | 116.9 | 115.1 |
|  |  |  |  |  |  | C(10)-C(2)-C(1) | 122.2 | 121.4 |
|  |  |  |  |  |  | N(3)-C(2)-C(1) | 121.0 | 120.0 |
|  |  |  |  |  |  | C(6)-C(1)-C(2) | 121.7 | 120.0 |
|  |  |  |  |  |  | RSMD | 5.00E+00 |  |
|  | **7** |  |  | **8** |  |  | **9** |  |
| **Angle** | **(°)** | **Std.** | **Angle** | **(°)** | **Std.** | **Angle** | **(°)** | **Std.** |
| C(20)-S(21)-C(17) | 85.8 | 98.5 | C(28)-C(29)-C(24) | 120.8 | 120.0 | C(31)-O(30)-C(27) | 117.5 | 110.8 |
| S(21)-C(20)-C(19) | 108.4 | 111.0 | C(29)-C(28)-C(27) | 121.4 | 120.0 | C(28)-C(29)-C(24) | 121.4 | 120.0 |
| O(22)-C(19)-C(20) | 121.1 | 122.5 | C(30)-C(27)-C(28) | 120.7 | 121.4 | C(29)-C(28)-C(27) | 119.8 | 120.0 |
| O(22)-C(19)-N(18) | 125.8 | 124.3 | C(30)-C(27)-C(26) | 121.3 | 121.4 | O(30)-C(27)-C(28) | 123.9 | 124.3 |
| C(20)-C(19)-N(18) | 113.2 | 116.5 | C(28)-C(27)-C(26) | 117.9 | 120.0 | O(30)-C(27)-C(26) | 116.2 | 124.3 |
| C(19)-N(18)-C(17) | 113.0 | 115.0 | C(27)-C(26)-C(25) | 121.0 | 120.0 | C(28)-C(27)-C(26) | 119.9 | 120.0 |
| S(21)-C(17)-N(18) | 119.6 | 126.0 | C(26)-C(25)-C(24) | 121.3 | 120.0 | C(27)-C(26)-C(25) | 119.8 | 120.0 |
| S(21)-C(17)-N(16) | 118.2 | 120.0 | C(29)-C(24)-C(25) | 117.6 | 120.0 | C(26)-C(25)-C(24) | 121.5 | 120.0 |
| N(18)-C(17)-N(16) | 122.2 | 126.0 | C(29)-C(24)-C(23) | 124.6 | 120.0 | C(29)-C(24)-C(25) | 117.6 | 120.0 |
| H(35)-N(16)-C(17) | 116.7 | 118.0 | C(25)-C(24)-C(23) | 117.7 | 120.0 | C(29)-C(24)-C(23) | 124.5 | 120.0 |
| H(35)-N(16)-N(14) | 124.1 | 113.0 | C(24)-C(23)-C(20) | 131.0 | 120.0 | C(25)-C(24)-C(23) | 117.9 | 120.0 |
| C(17)-N(16)-N(14) | 119.2 | 124.0 | C(20)-S(21)-C(17) | 85.2 | 98.5 | C(24)-C(23)-C(20) | 131.0 | 120.0 |
| N(16)-N(14)-C(13) | 119.2 | 115.0 | C(23)-C(20)-S(21) | 129.0 | 119.0 | C(20)-S(21)-C(17) | 85.3 | 98.5 |
| C(15)-C(13)-N(14) | 123.0 | 115.1 | C(23)-C(20)-C(19) | 119.8 | 117.6 | C(23)-C(20)-S(21) | 128.7 | 119.0 |
| C(15)-C(13)-C(8) | 121.5 | 121.4 | S(21)-C(20)-C(19) | 111.2 | 113.0 | C(23)-C(20)-C(19) | 120.0 | 117.6 |
| N(14)-C(13)-C(8) | 115.5 | 120.0 | O(22)-C(19)-C(20) | 123.0 | 123.0 | S(21)-C(20)-C(19) | 111.2 | 113.0 |
| H(31)-N(12)-H(30) | 118.3 | 118.8 | O(22)-C(19)-N(18) | 124.8 | 124.3 | O(22)-C(19)-C(20) | 123.1 | 123.0 |
| H(31)-N(12)-C(9) | 120.9 | 120.0 | C(20)-C(19)-N(18) | 112.1 | 122.0 | O(22)-C(19)-N(18) | 124.7 | 124.3 |
| H(30)-N(12)-C(9) | 119.7 | 120.0 | C(19)-N(18)-C(17) | 112.6 | 115.0 | C(20)-C(19)-N(18) | 112.1 | 122.0 |
| N(12)-C(9)-C(8) | 125.0 | 120.0 | S(21)-C(17)-N(18) | 118.8 | 126.0 | C(19)-N(18)-C(17) | 112.6 | 115.0 |
| N(12)-C(9)-C(5) | 122.3 | 120.0 | S(21)-C(17)-N(16) | 117.9 | 117.0 | S(21)-C(17)-N(18) | 118.8 | 126.0 |
| C(8)-C(9)-C(5) | 112.7 | 120.0 | N(18)-C(17)-N(16) | 123.3 | 126.0 | S(21)-C(17)-N(16) | 117.8 | 117.0 |
| C(13)-C(8)-C(9) | 129.7 | 120.0 | H(43)-N(16)-C(17) | 116.5 | 118.0 | N(18)-C(17)-N(16) | 123.5 | 126.0 |
| C(13)-C(8)-S(7) | 117.2 | 119.0 | H(43)-N(16)-N(14) | 124.0 | 113.0 | H(44)-N(16)-C(17) | 116.6 | 118.0 |
| C(9)-C(8)-S(7) | 113.1 | 119.0 | C(17)-N(16)-N(14) | 119.4 | 124.0 | H(44)-N(16)-N(14) | 124.2 | 113.0 |
| C(8)-S(7)-C(4) | 88.9 | 98.5 | N(16)-N(14)-C(13) | 119.2 | 115.0 | C(17)-N(16)-N(14) | 119.2 | 124.0 |
| C(11)-C(6)-C(5) | 123.3 | 121.4 | C(15)-C(13)-N(14) | 122.8 | 115.1 | N(16)-N(14)-C(13) | 119.6 | 115.0 |
| C(11)-C(6)-C(1) | 119.6 | 121.4 | C(15)-C(13)-C(8) | 121.6 | 121.4 | C(15)-C(13)-N(14) | 123.0 | 115.1 |
| C(5)-C(6)-C(1) | 117.1 | 120.0 | N(14)-C(13)-C(8) | 115.5 | 120.0 | C(15)-C(13)-C(8) | 121.5 | 121.4 |
| C(9)-C(5)-C(6) | 130.8 | 120.0 | H(39)-N(12)-H(38) | 118.3 | 118.8 | N(14)-C(13)-C(8) | 115.4 | 120.0 |
| C(9)-C(5)-C(4) | 112.5 | 120.0 | H(39)-N(12)-C(9) | 120.8 | 120.0 | H(40)-N(12)-H(39) | 118.3 | 118.8 |
| C(6)-C(5)-C(4) | 116.7 | 120.0 | H(38)-N(12)-C(9) | 119.7 | 120.0 | H(40)-N(12)-C(9) | 120.9 | 120.0 |
| S(7)-C(4)-C(5) | 112.7 | 119.0 | N(12)-C(9)-C(8) | 125.0 | 120.0 | H(39)-N(12)-C(9) | 119.7 | 120.0 |
| S(7)-C(4)-N(3) | 121.6 | 126.0 | N(12)-C(9)-C(5) | 122.3 | 120.0 | N(12)-C(9)-C(8) | 125.0 | 120.0 |
| C(5)-C(4)-N(3) | 125.7 | 120.0 | C(8)-C(9)-C(5) | 112.7 | 120.0 | N(12)-C(9)-C(5) | 122.2 | 120.0 |
| C(4)-N(3)-C(2) | 117.6 | 115.0 | C(13)-C(8)-C(9) | 129.7 | 120.0 | C(8)-C(9)-C(5) | 112.7 | 120.0 |
| C(10)-C(2)-N(3) | 117.7 | 115.1 | C(13)-C(8)-S(7) | 117.3 | 119.0 | C(13)-C(8)-C(9) | 129.9 | 120.0 |
| C(10)-C(2)-C(1) | 121.3 | 121.4 | C(9)-C(8)-S(7) | 113.1 | 119.0 | C(13)-C(8)-S(7) | 117.1 | 119.0 |
| N(3)-C(2)-C(1) | 121.0 | 120.0 | C(8)-S(7)-C(4) | 88.9 | 98.5 | C(9)-C(8)-S(7) | 113.0 | 119.0 |
| C(6)-C(1)-C(2) | 121.8 | 120.0 | C(11)-C(6)-C(5) | 123.4 | 121.4 | C(8)-S(7)-C(4) | 88.9 | 98.5 |
| RSMD | 5.27E+00 |  | C(11)-C(6)-C(1) | 119.4 | 121.4 | C(11)-C(6)-C(5) | 123.3 | 121.4 |
|  |  |  | C(5)-C(6)-C(1) | 117.2 | 120.0 | C(11)-C(6)-C(1) | 119.6 | 121.4 |
|  |  |  | C(9)-C(5)-C(6) | 130.8 | 120.0 | C(5)-C(6)-C(1) | 117.2 | 120.0 |
|  |  |  | C(9)-C(5)-C(4) | 112.6 | 120.0 | C(9)-C(5)-C(6) | 130.8 | 120.0 |
|  |  |  | C(6)-C(5)-C(4) | 116.7 | 120.0 | C(9)-C(5)-C(4) | 112.6 | 120.0 |
|  |  |  | S(7)-C(4)-C(5) | 112.6 | 119.0 | C(6)-C(5)-C(4) | 116.7 | 120.0 |
|  |  |  | S(7)-C(4)-N(3) | 121.7 | 126.0 | S(7)-C(4)-C(5) | 112.7 | 119.0 |
|  |  |  | C(5)-C(4)-N(3) | 125.7 | 120.0 | S(7)-C(4)-N(3) | 121.5 | 126.0 |
|  |  |  | C(4)-N(3)-C(2) | 117.7 | 115.0 | C(5)-C(4)-N(3) | 125.8 | 120.0 |
|  |  |  | C(10)-C(2)-N(3) | 116.8 | 115.1 | C(4)-N(3)-C(2) | 117.6 | 115.0 |
|  |  |  | C(10)-C(2)-C(1) | 122.2 | 121.4 | C(10)-C(2)-N(3) | 117.7 | 115.1 |
|  |  |  | N(3)-C(2)-C(1) | 121.0 | 120.0 | C(10)-C(2)-C(1) | 121.3 | 121.4 |
|  |  |  | C(6)-C(1)-C(2) | 121.7 | 120.0 | N(3)-C(2)-C(1) | 121.0 | 120.0 |
|  |  |  | RSMD | 5.25E+00 |  | C(6)-C(1)-C(2) | 121.8 | 120.0 |
|  |  |  |  |  |  | RSMD | 5.42E+00 |  |
|  | **7** |  |  |  |  |  |  |  |
| **Angle** | **(°)** | **Std.** |  |  |  |  |  |  |
| C(28)-C(29)-C(24) | 120.9 | 120.0 |  |  |  |  |  |  |
| C(29)-C(28)-C(27) | 119.5 | 120.0 |  |  |  |  |  |  |
| Cl(30)-C(27)-C(28) | 119.4 | 118.8 |  |  |  |  |  |  |
| Cl(30)-C(27)-C(26) | 119.5 | 118.8 |  |  |  |  |  |  |
| C(28)-C(27)-C(26) | 121.1 | 120.0 |  |  |  |  |  |  |
| C(27)-C(26)-C(25) | 119.0 | 120.0 |  |  |  |  |  |  |
| C(26)-C(25)-C(24) | 121.4 | 120.0 |  |  |  |  |  |  |
| C(29)-C(24)-C(25) | 118.1 | 120.0 |  |  |  |  |  |  |
| C(29)-C(24)-C(23) | 124.3 | 120.0 |  |  |  |  |  |  |
| C(25)-C(24)-C(23) | 117.7 | 120.0 |  |  |  |  |  |  |
| C(24)-C(23)-C(20) | 130.8 | 120.0 |  |  |  |  |  |  |
| C(20)-S(21)-C(17) | 85.3 | 98.5 |  |  |  |  |  |  |
| C(23)-C(20)-S(21) | 129.1 | 119.0 |  |  |  |  |  |  |
| C(23)-C(20)-C(19) | 119.6 | 117.6 |  |  |  |  |  |  |
| S(21)-C(20)-C(19) | 111.2 | 113.0 |  |  |  |  |  |  |
| O(22)-C(19)-C(20) | 122.8 | 123.0 |  |  |  |  |  |  |
| O(22)-C(19)-N(18) | 125.0 | 124.3 |  |  |  |  |  |  |
| C(20)-C(19)-N(18) | 112.1 | 122.0 |  |  |  |  |  |  |
| C(19)-N(18)-C(17) | 112.6 | 115.0 |  |  |  |  |  |  |
| S(21)-C(17)-N(18) | 118.8 | 126.0 |  |  |  |  |  |  |
| S(21)-C(17)-N(16) | 117.6 | 117.0 |  |  |  |  |  |  |
| N(18)-C(17)-N(16) | 123.7 | 126.0 |  |  |  |  |  |  |
| H(43)-N(16)-C(17) | 116.7 | 118.0 |  |  |  |  |  |  |
| H(43)-N(16)-N(14) | 124.2 | 113.0 |  |  |  |  |  |  |
| C(17)-N(16)-N(14) | 119.2 | 124.0 |  |  |  |  |  |  |
| N(16)-N(14)-C(13) | 119.5 | 115.0 |  |  |  |  |  |  |
| C(15)-C(13)-N(14) | 123.0 | 115.1 |  |  |  |  |  |  |
| C(15)-C(13)-C(8) | 121.5 | 121.4 |  |  |  |  |  |  |
| N(14)-C(13)-C(8) | 115.3 | 120.0 |  |  |  |  |  |  |
| H(39)-N(12)-H(38) | 118.3 | 118.8 |  |  |  |  |  |  |
| H(39)-N(12)-C(9) | 121.0 | 120.0 |  |  |  |  |  |  |
| H(38)-N(12)-C(9) | 119.7 | 120.0 |  |  |  |  |  |  |
| N(12)-C(9)-C(8) | 125.1 | 120.0 |  |  |  |  |  |  |
| N(12)-C(9)-C(5) | 122.2 | 120.0 |  |  |  |  |  |  |
| C(8)-C(9)-C(5) | 112.7 | 120.0 |  |  |  |  |  |  |
| C(13)-C(8)-C(9) | 129.9 | 120.0 |  |  |  |  |  |  |
| C(13)-C(8)-S(7) | 117.1 | 119.0 |  |  |  |  |  |  |
| C(9)-C(8)-S(7) | 113.0 | 119.0 |  |  |  |  |  |  |
| C(8)-S(7)-C(4) | 88.9 | 98.5 |  |  |  |  |  |  |
| C(11)-C(6)-C(5) | 123.3 | 121.4 |  |  |  |  |  |  |
| C(11)-C(6)-C(1) | 119.6 | 121.4 |  |  |  |  |  |  |
| C(5)-C(6)-C(1) | 117.1 | 120.0 |  |  |  |  |  |  |
| C(9)-C(5)-C(6) | 130.8 | 120.0 |  |  |  |  |  |  |
| C(9)-C(5)-C(4) | 112.6 | 120.0 |  |  |  |  |  |  |
| C(6)-C(5)-C(4) | 116.7 | 120.0 |  |  |  |  |  |  |
| S(7)-C(4)-C(5) | 112.7 | 119.0 |  |  |  |  |  |  |
| S(7)-C(4)-N(3) | 121.5 | 126.0 |  |  |  |  |  |  |
| C(5)-C(4)-N(3) | 125.8 | 120.0 |  |  |  |  |  |  |
| C(4)-N(3)-C(2) | 117.6 | 115.0 |  |  |  |  |  |  |
| C(10)-C(2)-N(3) | 117.7 | 115.1 |  |  |  |  |  |  |
| C(10)-C(2)-C(1) | 121.3 | 121.4 |  |  |  |  |  |  |
| N(3)-C(2)-C(1) | 121.0 | 120.0 |  |  |  |  |  |  |
| C(6)-C(1)-C(2) | 121.8 | 120.0 |  |  |  |  |  |  |
| RSMD | 5.28E+00 |  |  |  |  |  |  |  |

**Antibacterial activity**

***Minimum inhibitory concentration testing***

Minimum inhibitory concentration (MIC) values of the synthesized derivatives were specified using agar dilution bacterial cultures were grown in nutrient broth medium at 30°C. After 16 h of growth, each microorganism, at a concentration of 108cells/mL, was inoculated on the surface of Mueller–Hinton agar plates using sterile cotton swab. Subsequently, uniform size filter paper disks (6 mm in diameter) were impregnated by equal volume (10 μL) from the specific concentration of dissolved compounds and carefully placed on surface of each inoculated plate. The plates were incubated in the upright position at 36°C for 24 h. After incubation, the diameters of the growth inhibition zones formed around the disc were measured with transparent ruler in millimetre, averaged and the mean values were recorded

**Molecular docking**

|  |  |  |
| --- | --- | --- |
| C:\Users\Dream\Desktop\Gentamicin\2d.png | C:\Users\Dream\Desktop\Gentamicin\3d.png | C:\Users\Dream\Desktop\Gentamicin\sm.png |
| 2D | 3D | Surface Map |

Figure S1: Binding interactions between **Gentamicin** and 1AJ6 amino-acids

|  |  |  |
| --- | --- | --- |
|  |  |  |
| 2D | 3D | Surface Map |

Figure S2: Binding interactions between derivative **3** and 1AJ6 amino-acids

|  |  |  |
| --- | --- | --- |
|  |  |  |
| 2D | 3D | Surface Map |

Figure S3: Binding interactions between derivative **4** and 1AJ6 amino-acids

|  |  |  |
| --- | --- | --- |
|  |  |  |
| 2D | 3D | Surface Map |

Figure S4: Binding interactions between derivative **6** and 1AJ6 amino-acids

|  |  |  |
| --- | --- | --- |
|  |  |  |
| 2D | 3D | Surface Map |

Figure S5: Binding interactions between derivative **7** and 1AJ6 amino-acids

|  |  |  |
| --- | --- | --- |
|  |  |  |
| 2D | 3D | Surface Map |

Figure S6: Binding interactions between derivative **10** and 1AJ6 amino-acids