Supporting Information

**Synthesis, molecular modelling and docking studies of new thieno[2,3-*b*:4,5-*b*'] dipyridine compounds as antimicrobial agents**

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**DFT studies**

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

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **2** |  | **3** |  | **4** |
| C(13)-C(14)-N(17)-H(30) | 180.0 | C(13)-C(17)-N(19)-H(33) | 178.7 | C(13)-C(14)-N(15)-C(9) | 1.5 |
| C(13)-C(14)-N(17)-H(31) | 0.0 | C(13)-C(17)-N(19)-H(34) | 6.5 | C(18)-C(14)-N(15)-C(9) | -179.2 |
| N(15)-C(14)-N(17)-H(30) | 0.0 | O(20)-C(17)-N(19)-H(33) | 0.9 | C(12)-C(13)-C(17)-C(19) | 39.1 |
| N(15)-C(14)-N(17)-H(31) | 180.0 | O(20)-C(17)-N(19)-H(34) | -171.3 | C(12)-C(13)-C(17)-O(20) | -145.1 |
| C(13)-C(14)-N(15)-C(9) | 0.0 | C(13)-C(14)-N(18)-H(31) | 178.1 | C(14)-C(13)-C(17)-C(19) | -140.2 |
| N(17)-C(14)-N(15)-C(9) | 180.0 | C(13)-C(14)-N(18)-H(32) | -4.9 | C(14)-C(13)-C(17)-O(20) | 35.6 |
| C(12)-C(13)-C(18)-N(19) | 180.0 | N(15)-C(14)-N(18)-H(31) | -1.8 | C(12)-C(13)-C(14)-N(15) | -2.1 |
| C(14)-C(13)-C(18)-N(19) | 0.0 | N(15)-C(14)-N(18)-H(32) | 175.2 | C(12)-C(13)-C(14)-C(18) | 178.6 |
| C(12)-C(13)-C(14)-N(15) | 0.0 | C(13)-C(14)-N(15)-C(9) | 2.7 | C(17)-C(13)-C(14)-N(15) | 177.1 |
| C(12)-C(13)-C(14)-N(17) | -180.0 | N(18)-C(14)-N(15)-C(9) | -177.4 | C(17)-C(13)-C(14)-C(18) | -2.2 |
| C(18)-C(13)-C(14)-N(15) | 180.0 | C(12)-C(13)-C(17)-N(19) | 20.5 | C(8)-C(12)-C(13)-C(14) | 1.2 |
| C(18)-C(13)-C(14)-N(17) | 0.0 | C(12)-C(13)-C(17)-O(20) | -161.9 | C(8)-C(12)-C(13)-C(17) | -178.0 |
| C(8)-C(12)-C(13)-C(14) | 0.0 | C(14)-C(13)-C(17)-N(19) | -157.8 | C(16)-C(12)-C(13)-C(14) | -176.2 |
| C(8)-C(12)-C(13)-C(18) | 180.0 | C(14)-C(13)-C(17)-O(20) | 19.8 | C(16)-C(12)-C(13)-C(17) | 4.6 |
| C(16)-C(12)-C(13)-C(14) | 180.0 | C(12)-C(13)-C(14)-N(15) | -5.6 | C(5)-C(9)-N(15)-C(14) | 178.9 |
| C(16)-C(12)-C(13)-C(18) | 0.0 | C(12)-C(13)-C(14)-N(18) | 174.5 | C(8)-C(9)-N(15)-C(14) | 0.0 |
| C(5)-C(9)-N(15)-C(14) | 180.0 | C(17)-C(13)-C(14)-N(15) | 172.8 | S(7)-C(8)-C(12)-C(13) | -179.8 |
| C(8)-C(9)-N(15)-C(14) | 0.0 | C(17)-C(13)-C(14)-N(18) | -7.1 | S(7)-C(8)-C(12)-C(16) | -2.2 |
| S(7)-C(8)-C(12)-C(13) | 180.0 | C(8)-C(12)-C(13)-C(14) | 3.9 | C(9)-C(8)-C(12)-C(13) | 0.3 |
| S(7)-C(8)-C(12)-C(16) | 0.0 | C(8)-C(12)-C(13)-C(17) | -174.4 | C(9)-C(8)-C(12)-C(16) | 177.8 |
| C(9)-C(8)-C(12)-C(13) | 0.0 | C(16)-C(12)-C(13)-C(14) | -173.6 | S(7)-C(8)-C(9)-C(5) | 0.1 |
| C(9)-C(8)-C(12)-C(16) | 180.0 | C(16)-C(12)-C(13)-C(17) | 8.2 | S(7)-C(8)-C(9)-N(15) | 179.1 |
| S(7)-C(8)-C(9)-C(5) | 0.0 | C(5)-C(9)-N(15)-C(14) | 179.8 | C(12)-C(8)-C(9)-C(5) | -179.9 |
| S(7)-C(8)-C(9)-N(15) | 180.0 | C(8)-C(9)-N(15)-C(14) | 1.7 | C(12)-C(8)-C(9)-N(15) | -0.9 |
| C(12)-C(8)-C(9)-C(5) | 180.0 | S(7)-C(8)-C(12)-C(13) | 178.9 | C(4)-S(7)-C(8)-C(9) | 0.0 |
| C(12)-C(8)-C(9)-N(15) | 0.0 | S(7)-C(8)-C(12)-C(16) | -3.4 | C(4)-S(7)-C(8)-C(12) | -179.9 |
| C(4)-S(7)-C(8)-C(9) | 0.0 | C(9)-C(8)-C(12)-C(13) | 0.1 | C(4)-C(5)-C(9)-C(8) | -0.2 |
| C(4)-S(7)-C(8)-C(12) | -180.0 | C(9)-C(8)-C(12)-C(16) | 177.8 | C(4)-C(5)-C(9)-N(15) | -179.2 |
| C(4)-C(5)-C(9)-C(8) | 0.0 | S(7)-C(8)-C(9)-C(5) | -0.4 | C(6)-C(5)-C(9)-C(8) | 179.8 |
| C(4)-C(5)-C(9)-N(15) | 180.0 | S(7)-C(8)-C(9)-N(15) | 177.9 | C(6)-C(5)-C(9)-N(15) | 0.8 |
| C(6)-C(5)-C(9)-C(8) | 180.0 | C(12)-C(8)-C(9)-C(5) | 178.5 | C(4)-C(5)-C(6)-C(1) | -0.3 |
| C(6)-C(5)-C(9)-N(15) | 0.0 | C(12)-C(8)-C(9)-N(15) | -3.2 | C(4)-C(5)-C(6)-C(11) | 179.7 |
| C(4)-C(5)-C(6)-C(1) | 0.0 | C(4)-S(7)-C(8)-C(9) | 0.3 | C(9)-C(5)-C(6)-C(1) | 179.7 |
| C(4)-C(5)-C(6)-C(11) | -180.0 | C(4)-S(7)-C(8)-C(12) | -178.5 | C(9)-C(5)-C(6)-C(11) | -0.3 |
| C(9)-C(5)-C(6)-C(1) | 180.0 | C(4)-C(5)-C(9)-C(8) | 0.2 | N(3)-C(4)-S(7)-C(8) | 179.7 |
| C(9)-C(5)-C(6)-C(11) | 0.0 | C(4)-C(5)-C(9)-N(15) | -178.0 | C(5)-C(4)-S(7)-C(8) | -0.2 |
| N(3)-C(4)-S(7)-C(8) | -179.993 | C(6)-C(5)-C(9)-C(8) | 179.8 | N(3)-C(4)-C(5)-C(6) | 0.4 |
| C(5)-C(4)-S(7)-C(8) | -0.006 | C(6)-C(5)-C(9)-N(15) | 1.6 | N(3)-C(4)-C(5)-C(9) | -179.6 |
| N(3)-C(4)-C(5)-C(6) | -0.01 | C(4)-C(5)-C(6)-C(1) | -0.2 | S(7)-C(4)-C(5)-C(6) | -179.8 |
| N(3)-C(4)-C(5)-C(9) | 179.993 | C(4)-C(5)-C(6)-C(11) | 179.9 | S(7)-C(4)-C(5)-C(9) | 0.3 |
| S(7)-C(4)-C(5)-C(6) | -179.997 | C(9)-C(5)-C(6)-C(1) | -179.8 | C(2)-N(3)-C(4)-C(5) | -0.2 |
| S(7)-C(4)-C(5)-C(9) | 0.007 | C(9)-C(5)-C(6)-C(11) | 0.3 | C(2)-N(3)-C(4)-S(7) | 179.9 |
| C(2)-N(3)-C(4)-C(5) | 0.01 | N(3)-C(4)-S(7)-C(8) | 179.8 | C(1)-C(2)-N(3)-C(4) | 0.0 |
| C(2)-N(3)-C(4)-S(7) | 179.996 | C(5)-C(4)-S(7)-C(8) | -0.2 | C(10)-C(2)-N(3)-C(4) | -180.0 |
| C(1)-C(2)-N(3)-C(4) | -0.005 | N(3)-C(4)-C(5)-C(6) | 0.4 | C(2)-C(1)-C(6)-C(5) | 0.1 |
| C(10)-C(2)-N(3)-C(4) | 179.995 | N(3)-C(4)-C(5)-C(9) | -179.9 | C(2)-C(1)-C(6)-C(11) | -179.9 |
| C(2)-C(1)-C(6)-C(5) | 0 | S(7)-C(4)-C(5)-C(6) | -179.7 | C(6)-C(1)-C(2)-N(3) | 0.1 |
| C(2)-C(1)-C(6)-C(11) | 180 | S(7)-C(4)-C(5)-C(9) | 0.0 | C(6)-C(1)-C(2)-C(10) | 180.0 |
| C(6)-C(1)-C(2)-N(3) | 0 | C(2)-N(3)-C(4)-C(5) | -0.267 |  |  |
| C(6)-C(1)-C(2)-C(10) | 180 | C(2)-N(3)-C(4)-S(7) | 179.807 |  |  |
|  |  | C(1)-C(2)-N(3)-C(4) | -0.036 |  |  |
|  |  | C(10)-C(2)-N(3)-C(4) | -179.993 |  |  |
|  |  | C(2)-C(1)-C(6)-C(5) | -0.039 |  |  |
|  |  | C(2)-C(1)-C(6)-C(11) | 179.833 |  |  |
|  |  | C(6)-C(1)-C(2)-N(3) | 0.185 |  |  |
|  |  | C(6)-C(1)-C(2)-C(10) | -179.86 |  |  |
|  | **5** |  | **6** |  | **8** |
| C(17)-O(19)-C(21)-C(22) | -179.9 | C(13)-C(14)-N(15)-C(9) | 0.0 | C(17)-O(18)-C(20)-C(21) | -179.9 |
| C(13)-C(17)-O(19)-C(21) | 180.0 | C(12)-C(13)-C(14)-N(15) | 0.0 | C(13)-C(17)-O(18)-C(20) | 180.0 |
| O(20)-C(17)-O(19)-C(21) | 0.0 | C(8)-C(12)-O(16)-H(26) | -180.0 | O(19)-C(17)-O(18)-C(20) | 0.0 |
| C(13)-C(14)-N(15)-C(9) | 0.0 | C(13)-C(12)-O(16)-H(26) | 0.0 | C(13)-C(14)-N(15)-C(9) | 0.0 |
| C(18)-C(14)-N(15)-C(9) | -180.0 | C(8)-C(12)-C(13)-C(14) | 0.0 | C(12)-C(13)-C(17)-O(18) | 0.0 |
| C(12)-C(13)-C(17)-O(19) | 0.2 | O(16)-C(12)-C(13)-C(14) | -180.0 | C(12)-C(13)-C(17)-O(19) | -180.0 |
| C(12)-C(13)-C(17)-O(20) | -179.9 | C(5)-C(9)-N(15)-C(14) | 180.0 | C(14)-C(13)-C(17)-O(18) | -180.0 |
| C(14)-C(13)-C(17)-O(19) | -179.8 | C(8)-C(9)-N(15)-C(14) | 0.0 | C(14)-C(13)-C(17)-O(19) | 0.0 |
| C(14)-C(13)-C(17)-O(20) | 0.1 | S(7)-C(8)-C(12)-C(13) | -180.0 | C(12)-C(13)-C(14)-N(15) | 0.0 |
| C(12)-C(13)-C(14)-N(15) | 0.0 | S(7)-C(8)-C(12)-O(16) | 0.0 | C(17)-C(13)-C(14)-N(15) | 180.0 |
| C(12)-C(13)-C(14)-C(18) | 180.0 | C(9)-C(8)-C(12)-C(13) | 0.0 | C(8)-C(12)-O(16)-H(30) | -180.0 |
| C(17)-C(13)-C(14)-N(15) | 180.0 | C(9)-C(8)-C(12)-O(16) | 180.0 | C(13)-C(12)-O(16)-H(30) | 0.0 |
| C(17)-C(13)-C(14)-C(18) | 0.0 | S(7)-C(8)-C(9)-C(5) | 0.0 | C(8)-C(12)-C(13)-C(14) | 0.0 |
| C(8)-C(12)-C(13)-C(14) | 0.0 | S(7)-C(8)-C(9)-N(15) | 180.0 | C(8)-C(12)-C(13)-C(17) | -180.0 |
| C(8)-C(12)-C(13)-C(17) | -180.0 | C(12)-C(8)-C(9)-C(5) | -180.0 | O(16)-C(12)-C(13)-C(14) | -180.0 |
| C(16)-C(12)-C(13)-C(14) | -180.0 | C(12)-C(8)-C(9)-N(15) | 0.0 | O(16)-C(12)-C(13)-C(17) | 0.0 |
| C(16)-C(12)-C(13)-C(17) | 0.0 | C(4)-S(7)-C(8)-C(9) | 0.0 | C(5)-C(9)-N(15)-C(14) | -180.0 |
| C(5)-C(9)-N(15)-C(14) | 180.0 | C(4)-S(7)-C(8)-C(12) | 180.0 | C(8)-C(9)-N(15)-C(14) | 0.0 |
| C(8)-C(9)-N(15)-C(14) | 0.0 | C(4)-C(5)-C(9)-C(8) | 0.0 | S(7)-C(8)-C(12)-C(13) | -180.0 |
| S(7)-C(8)-C(12)-C(13) | -180.0 | C(4)-C(5)-C(9)-N(15) | -180.0 | S(7)-C(8)-C(12)-O(16) | 0.0 |
| S(7)-C(8)-C(12)-C(16) | 0.0 | C(6)-C(5)-C(9)-C(8) | -180.0 | C(9)-C(8)-C(12)-C(13) | 0.0 |
| C(9)-C(8)-C(12)-C(13) | 0.0 | C(6)-C(5)-C(9)-N(15) | 0.0 | C(9)-C(8)-C(12)-O(16) | 180.0 |
| C(9)-C(8)-C(12)-C(16) | 180.0 | C(4)-C(5)-C(6)-C(1) | 0.0 | S(7)-C(8)-C(9)-C(5) | 0.0 |
| S(7)-C(8)-C(9)-C(5) | 0.0 | C(4)-C(5)-C(6)-C(11) | -180.0 | S(7)-C(8)-C(9)-N(15) | 180.0 |
| S(7)-C(8)-C(9)-N(15) | 180.0 | C(9)-C(5)-C(6)-C(1) | 180.0 | C(12)-C(8)-C(9)-C(5) | 180.0 |
| C(12)-C(8)-C(9)-C(5) | 180.0 | C(9)-C(5)-C(6)-C(11) | 0.0 | C(12)-C(8)-C(9)-N(15) | 0.0 |
| C(12)-C(8)-C(9)-N(15) | 0.0 | N(3)-C(4)-S(7)-C(8) | 180.0 | C(4)-S(7)-C(8)-C(9) | 0.0 |
| C(4)-S(7)-C(8)-C(9) | 0.0 | C(5)-C(4)-S(7)-C(8) | 0.0 | C(4)-S(7)-C(8)-C(12) | -180.0 |
| C(4)-S(7)-C(8)-C(12) | -180.0 | N(3)-C(4)-C(5)-C(6) | 0.0 | C(4)-C(5)-C(9)-C(8) | 0.0 |
| C(4)-C(5)-C(9)-C(8) | 0.0 | N(3)-C(4)-C(5)-C(9) | -180.0 | C(4)-C(5)-C(9)-N(15) | -180.0 |
| C(4)-C(5)-C(9)-N(15) | -180.0 | S(7)-C(4)-C(5)-C(6) | 180.0 | C(6)-C(5)-C(9)-C(8) | -180.0 |
| C(6)-C(5)-C(9)-C(8) | -180.0 | S(7)-C(4)-C(5)-C(9) | 0.0 | C(6)-C(5)-C(9)-N(15) | 0.0 |
| C(6)-C(5)-C(9)-N(15) | 0.0 | C(2)-N(3)-C(4)-C(5) | 0.0 | C(4)-C(5)-C(6)-C(1) | 0.0 |
| C(4)-C(5)-C(6)-C(1) | 0.0 | C(2)-N(3)-C(4)-S(7) | -180.0 | C(4)-C(5)-C(6)-C(11) | -180.0 |
| C(4)-C(5)-C(6)-C(11) | -180.0 | C(1)-C(2)-N(3)-C(4) | 0.0 | C(9)-C(5)-C(6)-C(1) | 180.0 |
| C(9)-C(5)-C(6)-C(1) | 180.0 | C(10)-C(2)-N(3)-C(4) | -179.9 | C(9)-C(5)-C(6)-C(11) | 0.0 |
| C(9)-C(5)-C(6)-C(11) | 0.0 | C(2)-C(1)-C(6)-C(5) | 0.0 | N(3)-C(4)-S(7)-C(8) | 180.0 |
| N(3)-C(4)-S(7)-C(8) | 180.0 | C(2)-C(1)-C(6)-C(11) | -180.0 | C(5)-C(4)-S(7)-C(8) | 0.0 |
| C(5)-C(4)-S(7)-C(8) | 0.0 | C(6)-C(1)-C(2)-N(3) | 0.0 | N(3)-C(4)-C(5)-C(6) | 0.0 |
| N(3)-C(4)-C(5)-C(6) | 0.0 | C(6)-C(1)-C(2)-C(10) | 179.9 | N(3)-C(4)-C(5)-C(9) | -180.0 |
| N(3)-C(4)-C(5)-C(9) | -180.0 |  |  | S(7)-C(4)-C(5)-C(6) | 180.0 |
| S(7)-C(4)-C(5)-C(6) | 180.0 |  |  | S(7)-C(4)-C(5)-C(9) | 0.0 |
| S(7)-C(4)-C(5)-C(9) | 0.0 |  |  | C(2)-N(3)-C(4)-C(5) | 0.0 |
| C(2)-N(3)-C(4)-C(5) | 0.0 |  |  | C(2)-N(3)-C(4)-S(7) | -180.0 |
| C(2)-N(3)-C(4)-S(7) | -180.0 |  |  | C(1)-C(2)-N(3)-C(4) | 0.0 |
| C(1)-C(2)-N(3)-C(4) | 0.0 |  |  | C(10)-C(2)-N(3)-C(4) | -180.0 |
| C(10)-C(2)-N(3)-C(4) | -180.0 |  |  | C(2)-C(1)-C(6)-C(5) | 0.0 |
| C(2)-C(1)-C(6)-C(5) | 0.0 |  |  | C(2)-C(1)-C(6)-C(11) | -180.0 |
| C(2)-C(1)-C(6)-C(11) | 180.0 |  |  | C(6)-C(1)-C(2)-N(3) | 0.0 |
| C(6)-C(1)-C(2)-N(3) | 0.0 |  |  | C(6)-C(1)-C(2)-C(10) | 180.0 |
| C(6)-C(1)-C(2)-C(10) | 180.0 |  |  |  |  |

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

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **2** |  |  | **3** |  |  | **4** |  |
| **Angle** | **(°)** | **Std.** | **Angle** | **(°)** | **Std.** | **Angle** | **(°)** | **Std.** |
| N(19)-C(18)-C(13) | 176.395 | 180 | H(34)-N(19)-H(33) | 119.655 | 119 | O(20)-C(17)-C(19) | 118.992 | 123 |
| H(31)-N(17)-H(30) | 120.167 | 119 | H(34)-N(19)-C(17) | 123.415 | 120 | O(20)-C(17)-C(13) | 120.446 | 123 |
| H(31)-N(17)-C(14) | 121.752 | 120 | H(33)-N(19)-C(17) | 116.47 | 120 | C(19)-C(17)-C(13) | 120.43 | 115 |
| H(30)-N(17)-C(14) | 118.081 | 120 | H(32)-N(18)-H(31) | 124.958 | 119 | C(14)-N(15)-C(9) | 119.224 | 115 |
| C(14)-N(15)-C(9) | 118.34 | 115 | H(32)-N(18)-C(14) | 117.248 | 119 | C(18)-C(14)-N(15) | 115.378 | 115 |
| N(17)-C(14)-N(15) | 117.421 | 126 | H(31)-N(18)-C(14) | 117.72 | 119 | C(18)-C(14)-C(13) | 123.067 | 121 |
| N(17)-C(14)-C(13) | 120.583 | 120 | O(20)-C(17)-N(19) | 118.099 | 123 | N(15)-C(14)-C(13) | 121.551 | 120 |
| N(15)-C(14)-C(13) | 121.996 | 120 | O(20)-C(17)-C(13) | 122.116 | 123 | C(17)-C(13)-C(14) | 118.495 | 118 |
| C(18)-C(13)-C(14) | 118.414 | 120 | N(19)-C(17)-C(13) | 119.746 | 113 | C(17)-C(13)-C(12) | 121.597 | 118 |
| C(18)-C(13)-C(12) | 121.566 | 120 | C(14)-N(15)-C(9) | 118.614 | 115 | C(14)-C(13)-C(12) | 119.904 | 120 |
| C(14)-C(13)-C(12) | 120.02 | 120 | N(18)-C(14)-N(15) | 116.242 | 126 | C(16)-C(12)-C(13) | 124.607 | 121 |
| C(16)-C(12)-C(13) | 122.09 | 121 | N(18)-C(14)-C(13) | 121.344 | 120 | C(16)-C(12)-C(8) | 118.871 | 121 |
| C(16)-C(12)-C(8) | 121.546 | 121 | N(15)-C(14)-C(13) | 122.414 | 120 | C(13)-C(12)-C(8) | 116.47 | 120 |
| C(13)-C(12)-C(8) | 116.365 | 120 | C(17)-C(13)-C(14) | 117.602 | 118 | N(15)-C(9)-C(8) | 121.541 | 120 |
| N(15)-C(9)-C(8) | 122.147 | 120 | C(17)-C(13)-C(12) | 124.095 | 118 | N(15)-C(9)-C(5) | 125.206 | 120 |
| N(15)-C(9)-C(5) | 125.055 | 120 | C(14)-C(13)-C(12) | 118.283 | 120 | C(8)-C(9)-C(5) | 113.245 | 120 |
| C(8)-C(9)-C(5) | 112.798 | 120 | C(16)-C(12)-C(13) | 124.785 | 121 | C(12)-C(8)-C(9) | 121.279 | 120 |
| C(12)-C(8)-C(9) | 121.133 | 120 | C(16)-C(12)-C(8) | 117.907 | 121 | C(12)-C(8)-S(7) | 125.862 | 119 |
| C(12)-C(8)-S(7) | 125.655 | 119 | C(13)-C(12)-C(8) | 117.262 | 120 | C(9)-C(8)-S(7) | 112.86 | 119 |
| C(9)-C(8)-S(7) | 113.212 | 119 | N(15)-C(9)-C(8) | 121.83 | 120 | C(8)-S(7)-C(4) | 88.672 | 98.5 |
| C(8)-S(7)-C(4) | 88.52 | 98.5 | N(15)-C(9)-C(5) | 125.115 | 120 | C(11)-C(6)-C(5) | 121.709 | 121 |
| C(11)-C(6)-C(5) | 121.759 | 121 | C(8)-C(9)-C(5) | 113.031 | 120 | C(11)-C(6)-C(1) | 121.676 | 121 |
| C(11)-C(6)-C(1) | 121.508 | 121 | C(12)-C(8)-C(9) | 121.359 | 120 | C(5)-C(6)-C(1) | 116.615 | 120 |
| C(5)-C(6)-C(1) | 116.733 | 120 | C(12)-C(8)-S(7) | 125.827 | 119 | C(9)-C(5)-C(6) | 129.927 | 120 |
| C(9)-C(5)-C(6) | 129.924 | 120 | C(9)-C(8)-S(7) | 112.804 | 119 | C(9)-C(5)-C(4) | 112.694 | 120 |
| C(9)-C(5)-C(4) | 112.754 | 120 | C(8)-S(7)-C(4) | 88.638 | 98.5 | C(6)-C(5)-C(4) | 117.379 | 120 |
| C(6)-C(5)-C(4) | 117.323 | 120 | C(11)-C(6)-C(5) | 121.715 | 121 | S(7)-C(4)-C(5) | 112.528 | 119 |
| S(7)-C(4)-C(5) | 112.716 | 119 | C(11)-C(6)-C(1) | 121.555 | 121 | S(7)-C(4)-N(3) | 121.545 | 126 |
| S(7)-C(4)-N(3) | 121.488 | 126 | C(5)-C(6)-C(1) | 116.729 | 120 | C(5)-C(4)-N(3) | 125.927 | 120 |
| C(5)-C(4)-N(3) | 125.796 | 120 | C(9)-C(5)-C(6) | 129.813 | 120 | C(4)-N(3)-C(2) | 117.241 | 115 |
| C(4)-N(3)-C(2) | 117.368 | 115 | C(9)-C(5)-C(4) | 112.807 | 120 | C(10)-C(2)-N(3) | 116.661 | 115 |
| C(10)-C(2)-N(3) | 116.684 | 115 | C(6)-C(5)-C(4) | 117.378 | 120 | C(10)-C(2)-C(1) | 122.358 | 121 |
| C(10)-C(2)-C(1) | 122.348 | 121 | S(7)-C(4)-C(5) | 112.718 | 119 | N(3)-C(2)-C(1) | 120.98 | 120 |
| N(3)-C(2)-C(1) | 120.968 | 120 | S(7)-C(4)-N(3) | 121.484 | 126 | C(6)-C(1)-C(2) | 121.857 | 120 |
| C(6)-C(1)-C(2) | 121.812 | 120 | C(5)-C(4)-N(3) | 125.798 | 120 | RSMD | 2.14E+01 |  |
| RSMD | 3.56E+01 |  | C(4)-N(3)-C(2) | 117.315 | 115 |  |  |  |
|  |  |  | C(10)-C(2)-N(3) | 116.643 | 115 |  |  |  |
|  |  |  | C(10)-C(2)-C(1) | 122.348 | 121 |  |  |  |
|  |  |  | N(3)-C(2)-C(1) | 121.008 | 120 |  |  |  |
|  |  |  | C(6)-C(1)-C(2) | 121.769 | 120 |  |  |  |
|  |  |  | RSMD | 4.24E+01 | max |  |  |  |
|  | **5** |  |  | **6** |  |  | **8** |  |
| **Angle** | **(°)** | **Std.** | **Angle** | **(°)** | **Std.** | **Angle** | **(°)** | **Std.** |
| C(22)-C(21)-O(19) | 106.959 | 107 | H(26)-O(16)-C(12) | 113.325 | 108 | C(21)-C(20)-O(18) | 107.288 | 107 |
| C(21)-O(19)-C(17) | 115.301 | 110 | C(14)-N(15)-C(9) | 117.341 | 115 | C(20)-O(18)-C(17) | 116.48 | 110 |
| O(20)-C(17)-O(19) | 120.077 | 122 | N(15)-C(14)-C(13) | 123.63 | 124 | O(19)-C(17)-O(18) | 120.53 | 122 |
| O(20)-C(17)-C(13) | 125.633 | 123 | C(14)-C(13)-C(12) | 119.219 | 120 | O(19)-C(17)-C(13) | 127.221 | 123 |
| O(19)-C(17)-C(13) | 114.291 | 124 | O(16)-C(12)-C(13) | 124.595 | 124 | O(18)-C(17)-C(13) | 112.249 | 124 |
| C(14)-N(15)-C(9) | 119.294 | 115 | O(16)-C(12)-C(8) | 117.6 | 124 | H(30)-O(16)-C(12) | 108.685 | 108 |
| C(18)-C(14)-N(15) | 114.404 | 115 | C(13)-C(12)-C(8) | 117.804 | 120 | C(14)-N(15)-C(9) | 117.274 | 115 |
| C(18)-C(14)-C(13) | 123.933 | 121 | N(15)-C(9)-C(8) | 122.268 | 120 | N(15)-C(14)-C(13) | 124.051 | 124 |
| N(15)-C(14)-C(13) | 121.663 | 120 | N(15)-C(9)-C(5) | 125.463 | 120 | C(17)-C(13)-C(14) | 117.903 | 118 |
| C(17)-C(13)-C(14) | 117.629 | 118 | C(8)-C(9)-C(5) | 112.27 | 120 | C(17)-C(13)-C(12) | 123.208 | 118 |
| C(17)-C(13)-C(12) | 122.617 | 118 | C(12)-C(8)-C(9) | 119.738 | 120 | C(14)-C(13)-C(12) | 118.889 | 120 |
| C(14)-C(13)-C(12) | 119.754 | 120 | C(12)-C(8)-S(7) | 126.292 | 119 | O(16)-C(12)-C(13) | 123.924 | 124 |
| C(16)-C(12)-C(13) | 125.46 | 121 | C(9)-C(8)-S(7) | 113.97 | 119 | O(16)-C(12)-C(8) | 119.122 | 124 |
| C(16)-C(12)-C(8) | 118.421 | 121 | C(8)-S(7)-C(4) | 88.221 | 98.5 | C(13)-C(12)-C(8) | 116.954 | 120 |
| C(13)-C(12)-C(8) | 116.119 | 120 | C(11)-C(6)-C(5) | 121.603 | 121 | N(15)-C(9)-C(8) | 122.361 | 120 |
| N(15)-C(9)-C(8) | 121.549 | 120 | C(11)-C(6)-C(1) | 121.81 | 121 | N(15)-C(9)-C(5) | 125.233 | 120 |
| N(15)-C(9)-C(5) | 124.927 | 120 | C(5)-C(6)-C(1) | 116.587 | 120 | C(8)-C(9)-C(5) | 112.406 | 120 |
| C(8)-C(9)-C(5) | 113.524 | 120 | C(9)-C(5)-C(6) | 129.814 | 120 | C(12)-C(8)-C(9) | 120.471 | 120 |
| C(12)-C(8)-C(9) | 121.621 | 120 | C(9)-C(5)-C(4) | 112.725 | 120 | C(12)-C(8)-S(7) | 125.539 | 119 |
| C(12)-C(8)-S(7) | 125.941 | 119 | C(6)-C(5)-C(4) | 117.462 | 120 | C(9)-C(8)-S(7) | 113.99 | 119 |
| C(9)-C(8)-S(7) | 112.438 | 119 | S(7)-C(4)-C(5) | 112.815 | 119 | C(8)-S(7)-C(4) | 88.201 | 98.5 |
| C(8)-S(7)-C(4) | 88.809 | 98.5 | S(7)-C(4)-N(3) | 121.34 | 126 | C(11)-C(6)-C(5) | 121.729 | 121 |
| C(11)-C(6)-C(5) | 121.716 | 121 | C(5)-C(4)-N(3) | 125.845 | 120 | C(11)-C(6)-C(1) | 121.792 | 121 |
| C(11)-C(6)-C(1) | 121.782 | 121 | C(4)-N(3)-C(2) | 117.22 | 115 | C(5)-C(6)-C(1) | 116.479 | 120 |
| C(5)-C(6)-C(1) | 116.502 | 120 | C(10)-C(2)-N(3) | 117.251 | 115 | C(9)-C(5)-C(6) | 129.872 | 120 |
| C(9)-C(5)-C(6) | 129.859 | 120 | C(10)-C(2)-C(1) | 121.753 | 121 | C(9)-C(5)-C(4) | 112.613 | 120 |
| C(9)-C(5)-C(4) | 112.604 | 120 | N(3)-C(2)-C(1) | 120.996 | 120 | C(6)-C(5)-C(4) | 117.516 | 120 |
| C(6)-C(5)-C(4) | 117.536 | 120 | C(6)-C(1)-C(2) | 121.89 | 120 | S(7)-C(4)-C(5) | 112.791 | 119 |
| S(7)-C(4)-C(5) | 112.625 | 119 | RSMD | 3.26E+01 |  | S(7)-C(4)-N(3) | 121.396 | 126 |
| S(7)-C(4)-N(3) | 121.53 | 126 |  |  |  | C(5)-C(4)-N(3) | 125.814 | 120 |
| C(5)-C(4)-N(3) | 125.845 | 120 |  |  |  | C(4)-N(3)-C(2) | 117.167 | 115 |
| C(4)-N(3)-C(2) | 117.139 | 115 |  |  |  | C(10)-C(2)-N(3) | 117.251 | 115 |
| C(10)-C(2)-N(3) | 117.227 | 115 |  |  |  | C(10)-C(2)-C(1) | 121.686 | 121 |
| C(10)-C(2)-C(1) | 121.691 | 121 |  |  |  | N(3)-C(2)-C(1) | 121.064 | 120 |
| N(3)-C(2)-C(1) | 121.082 | 120 |  |  |  | C(6)-C(1)-C(2) | 121.961 | 120 |
| C(6)-C(1)-C(2) | 121.895 | 120 |  |  |  | RSMD | 2.12E+01 |  |
| RSMD | 2.08E+01 |  |  |  |  |  |  |  |

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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **2** |  |  | **3** | |  |  | **4** |  |
| **Bond** | **Å** | **Std.** | **Bond** | **Å** | | **Std.** | **Bond** | **Å** | **Std.** |
| C(18)-N(19) | 1.18 | 1.16 | N(19)-H(34) | 1.01 | | 1.01 | C(17)-O(20) | 1.25 | 1.21 |
| N(17)-H(31) | 1.02 | 1.05 | N(19)-H(33) | 1.02 | | 1.01 | C(17)-C(19) | 1.50 | 1.51 |
| N(17)-H(30) | 1.02 | 1.05 | N(18)-H(32) | 1.03 | | 1.05 | C(14)-C(18) | 1.49 | 1.50 |
| C(14)-N(17) | 1.35 | 1.46 | N(18)-H(31) | 1.02 | | 1.05 | C(14)-N(15) | 1.34 | 1.36 |
| C(14)-N(15) | 1.34 | 1.36 | C(17)-O(20) | 1.27 | | 1.21 | C(13)-C(17) | 1.47 | 1.52 |
| C(13)-C(18) | 1.40 | 1.47 | C(17)-N(19) | 1.36 | | 1.37 | C(13)-C(14) | 1.42 | 1.42 |
| C(13)-C(14) | 1.43 | 1.42 | C(14)-N(18) | 1.35 | | 1.46 | C(12)-C(16) | 1.49 | 1.50 |
| C(12)-C(16) | 1.48 | 1.50 | C(14)-N(15) | 1.35 | | 1.36 | C(12)-C(13) | 1.41 | 1.42 |
| C(12)-C(13) | 1.40 | 1.42 | C(13)-C(17) | 1.46 | | 1.52 | C(9)-N(15) | 1.35 | 1.36 |
| C(9)-N(15) | 1.35 | 1.36 | C(13)-C(14) | 1.44 | | 1.42 | C(8)-C(12) | 1.39 | 1.42 |
| C(8)-C(12) | 1.39 | 1.42 | C(12)-C(16) | 1.49 | | 1.50 | C(8)-C(9) | 1.40 | 1.42 |
| C(8)-C(9) | 1.41 | 1.42 | C(12)-C(13) | 1.41 | | 1.42 | S(7)-C(8) | 1.80 | 1.66 |
| S(7)-C(8) | 1.80 | 1.66 | C(9)-N(15) | 1.34 | | 1.36 | C(6)-C(11) | 1.48 | 1.50 |
| C(6)-C(11) | 1.48 | 1.50 | C(8)-C(12) | 1.39 | | 1.42 | C(5)-C(9) | 1.43 | 1.42 |
| C(5)-C(9) | 1.43 | 1.42 | C(8)-C(9) | 1.41 | | 1.42 | C(5)-C(6) | 1.41 | 1.42 |
| C(5)-C(6) | 1.41 | 1.42 | S(7)-C(8) | 1.81 | | 1.66 | C(4)-S(7) | 1.82 | 1.66 |
| C(4)-S(7) | 1.82 | 1.66 | C(6)-C(11) | 1.48 | | 1.50 | C(4)-C(5) | 1.40 | 1.42 |
| C(4)-C(5) | 1.41 | 1.42 | C(5)-C(9) | 1.44 | | 1.42 | N(3)-C(4) | 1.32 | 1.36 |
| N(3)-C(4) | 1.32 | 1.36 | C(5)-C(6) | 1.40 | | 1.42 | C(2)-C(10) | 1.48 | 1.50 |
| C(2)-C(10) | 1.48 | 1.50 | C(4)-S(7) | 1.82 | | 1.66 | C(2)-N(3) | 1.35 | 1.36 |
| C(2)-N(3) | 1.35 | 1.36 | C(4)-C(5) | 1.41 | | 1.42 | C(1)-C(6) | 1.39 | 1.42 |
| C(1)-C(6) | 1.39 | 1.42 | N(3)-C(4) | 1.32 | | 1.36 | C(1)-C(2) | 1.40 | 1.42 |
| C(1)-C(2) | 1.40 | 1.42 | C(2)-C(10) | 1.48 | | 1.50 | RSMD | 5.02E-02 |  |
| RSMD | 5.49E-02 |  | C(2)-N(3) | 1.35 | | 1.36 |  |  |  |
|  |  |  | C(1)-C(6) | 1.39 | | 1.42 |  |  |  |
|  |  |  | C(1)-C(2) | 1.40 | | 1.42 |  |  |  |
|  |  |  | RSMD | 5.36E-02 | |  |  |  |  |
|  | **5** |  |  | **6** | |  |  | **8** |  |
| **Bond** | **Å** | **Std.** | **Bond** | **Å** | | **Std.** | **Bond** | **Å** | **Std.** |
| C(21)-C(22) | 1.50 | 1.51 | O(16)-H(26) | | 0.98 | 0.97 | C(20)-C(21) | 1.50 | 1.51 |
| O(19)-C(21) | 1.46 | 1.39 | C(14)-N(15) | | 1.34 | 1.36 | O(18)-C(20) | 1.46 | 1.39 |
| C(17)-O(20) | 1.24 | 1.21 | C(13)-C(14) | | 1.39 | 1.42 | C(17)-O(19) | 1.23 | 1.21 |
| C(17)-O(19) | 1.37 | 1.34 | C(12)-O(16) | | 1.37 | 1.36 | C(17)-O(18) | 1.40 | 1.34 |
| C(14)-C(18) | 1.49 | 1.50 | C(12)-C(13) | | 1.39 | 1.42 | O(16)-H(30) | 1.02 | 0.97 |
| C(14)-N(15) | 1.34 | 1.36 | C(9)-N(15) | | 1.35 | 1.36 | C(14)-N(15) | 1.33 | 1.36 |
| C(13)-C(17) | 1.46 | 1.52 | C(8)-C(12) | | 1.39 | 1.42 | C(13)-C(17) | 1.45 | 1.52 |
| C(13)-C(14) | 1.43 | 1.42 | C(8)-C(9) | | 1.41 | 1.42 | C(13)-C(14) | 1.41 | 1.42 |
| C(12)-C(16) | 1.49 | 1.50 | S(7)-C(8) | | 1.79 | 1.66 | C(12)-O(16) | 1.35 | 1.36 |
| C(12)-C(13) | 1.42 | 1.42 | C(6)-C(11) | | 1.48 | 1.50 | C(12)-C(13) | 1.41 | 1.42 |
| C(9)-N(15) | 1.34 | 1.36 | C(5)-C(9) | | 1.44 | 1.42 | C(9)-N(15) | 1.36 | 1.36 |
| C(8)-C(12) | 1.39 | 1.42 | C(5)-C(6) | | 1.41 | 1.42 | C(8)-C(12) | 1.39 | 1.42 |
| C(8)-C(9) | 1.40 | 1.42 | C(4)-S(7) | | 1.82 | 1.66 | C(8)-C(9) | 1.40 | 1.42 |
| S(7)-C(8) | 1.80 | 1.66 | C(4)-C(5) | | 1.40 | 1.42 | S(7)-C(8) | 1.78 | 1.66 |
| C(6)-C(11) | 1.48 | 1.50 | N(3)-C(4) | | 1.32 | 1.36 | C(6)-C(11) | 1.48 | 1.50 |
| C(5)-C(9) | 1.43 | 1.42 | C(2)-C(10) | | 1.49 | 1.50 | C(5)-C(9) | 1.43 | 1.42 |
| C(5)-C(6) | 1.41 | 1.42 | C(2)-N(3) | | 1.35 | 1.36 | C(5)-C(6) | 1.41 | 1.42 |
| C(4)-S(7) | 1.82 | 1.66 | C(1)-C(6) | | 1.39 | 1.42 | C(4)-S(7) | 1.82 | 1.66 |
| C(4)-C(5) | 1.40 | 1.42 | C(1)-C(2) | | 1.40 | 1.42 | C(4)-C(5) | 1.40 | 1.42 |
| N(3)-C(4) | 1.32 | 1.36 | RSMD | | 5.12E-02 | max | N(3)-C(4) | 1.32 | 1.36 |
| C(2)-C(10) | 1.48 | 1.50 |  | |  | min | C(2)-C(10) | 1.48 | 1.50 |
| C(2)-N(3) | 1.35 | 1.36 |  | |  |  | C(2)-N(3) | 1.35 | 1.36 |
| C(1)-C(6) | 1.39 | 1.42 |  | |  |  | C(1)-C(6) | 1.39 | 1.42 |
| C(1)-C(2) | 1.40 | 1.42 |  | |  |  | C(1)-C(2) | 1.40 | 1.42 |
| RSMD | 5.06E-02 | max |  | |  |  | RSMD | 5.16E-02 | max |

**Antibacterial activity**

*Minimum inhibitory concentration (MIC)*

Minimal inhibition concentration (MIC) values of thieno[2,3-b:4,5-b'] dipyridine hybrids were identified 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. Then, 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 translucent ruler in millimeter, averaged and the mean values were documented.

**Molecular docking Studies**

|  |  |
| --- | --- |
|  |  |
| **2D** | **3D** |

**Figure S1.** Docking interactions over analogue **2** with 1AJ6.

|  |  |
| --- | --- |
|  |  |
| **2D** | **3D** |

**Figure S2.** Docking interactions over analogue **3** with 1AJ6.

|  |  |
| --- | --- |
|  |  |
| **2D** | **3D** |

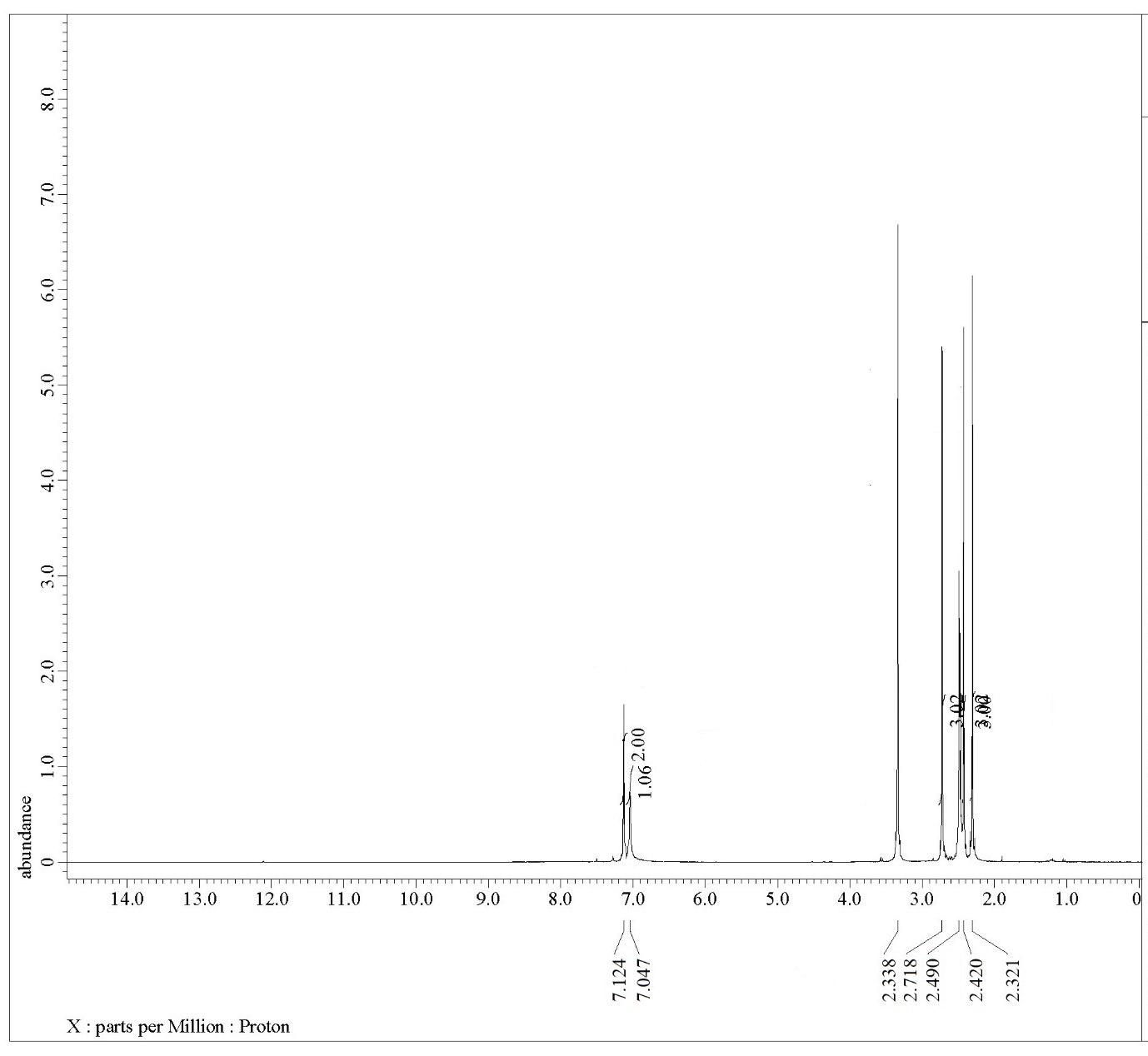
**Figure S3.** Docking interactions over analogue **4** with 1AJ6.

|  |  |
| --- | --- |
|  |  |
| **2D** | **3D** |

**Figure S4.** Docking interactions over analogue **6** with 1AJ6.

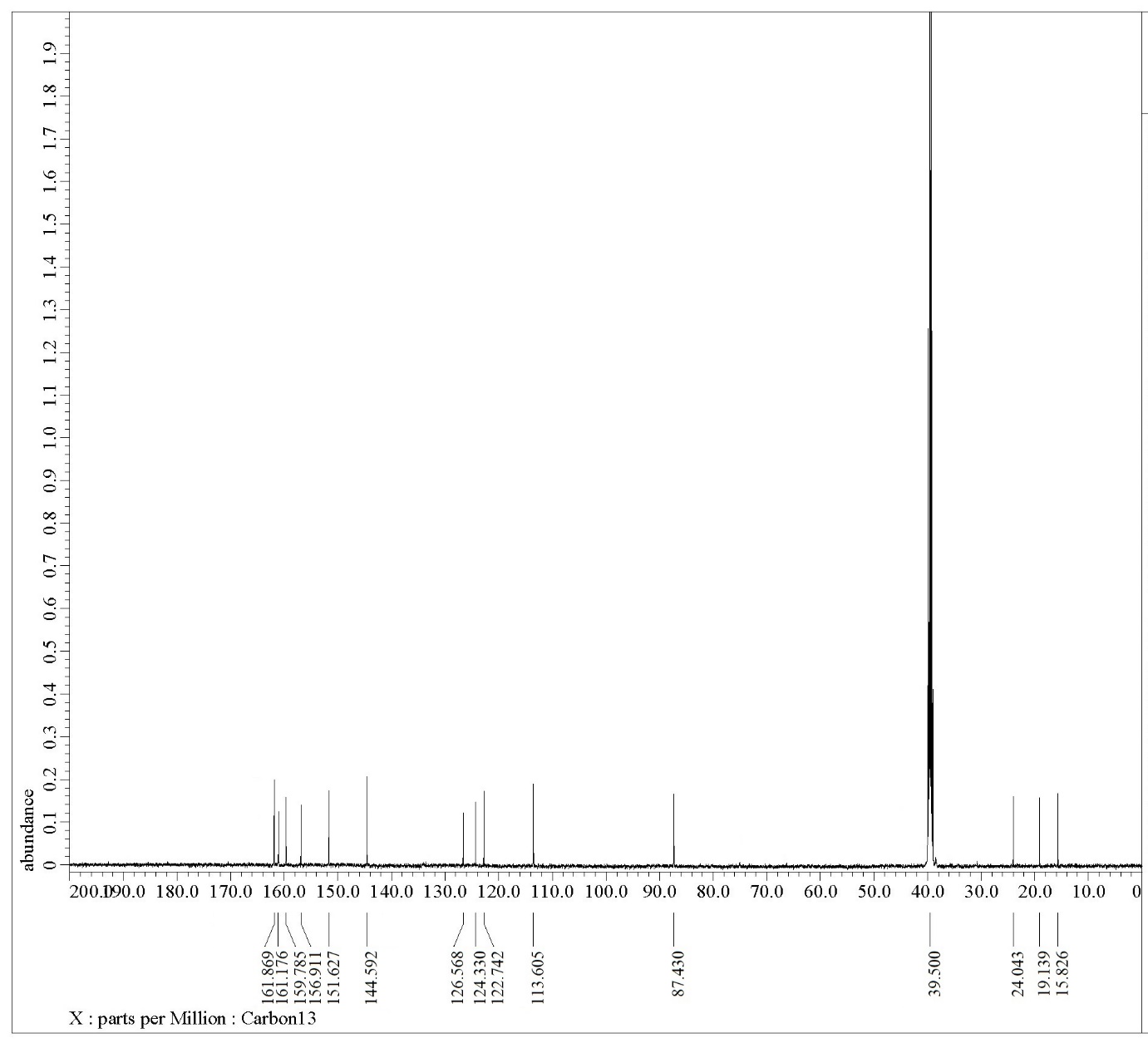
|  |  |
| --- | --- |
| **C:\Users\Dream\Desktop\Ampicilin\2d.png** | **C:\Users\Dream\Desktop\Ampicilin\3d.png** |
| **2D** | **3D** |

**Figure S5.** Docking interactions over ampicillinwith 1AJ6.



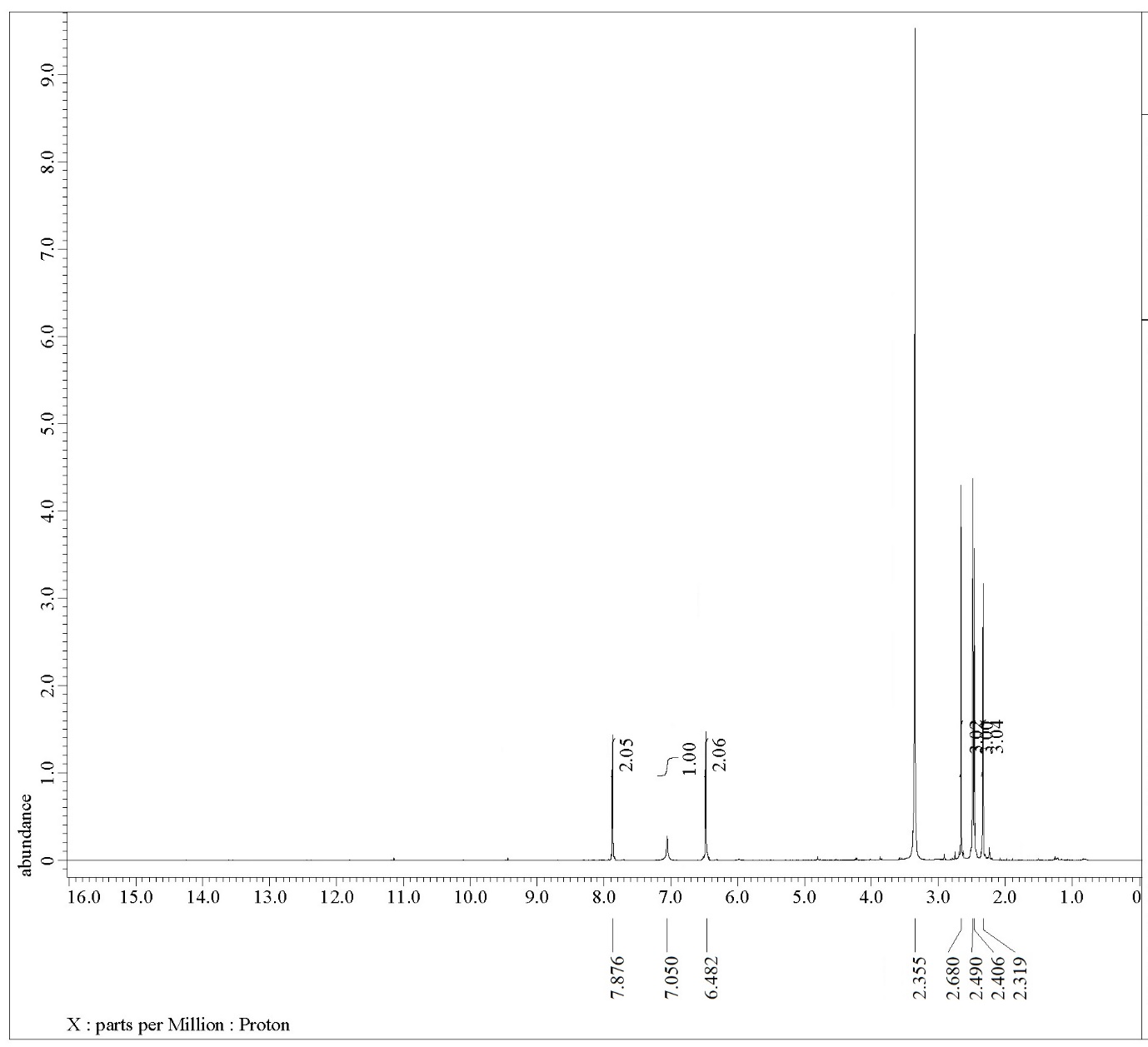


**Figure S6.** 1H NMR spectrum of compound **2**.



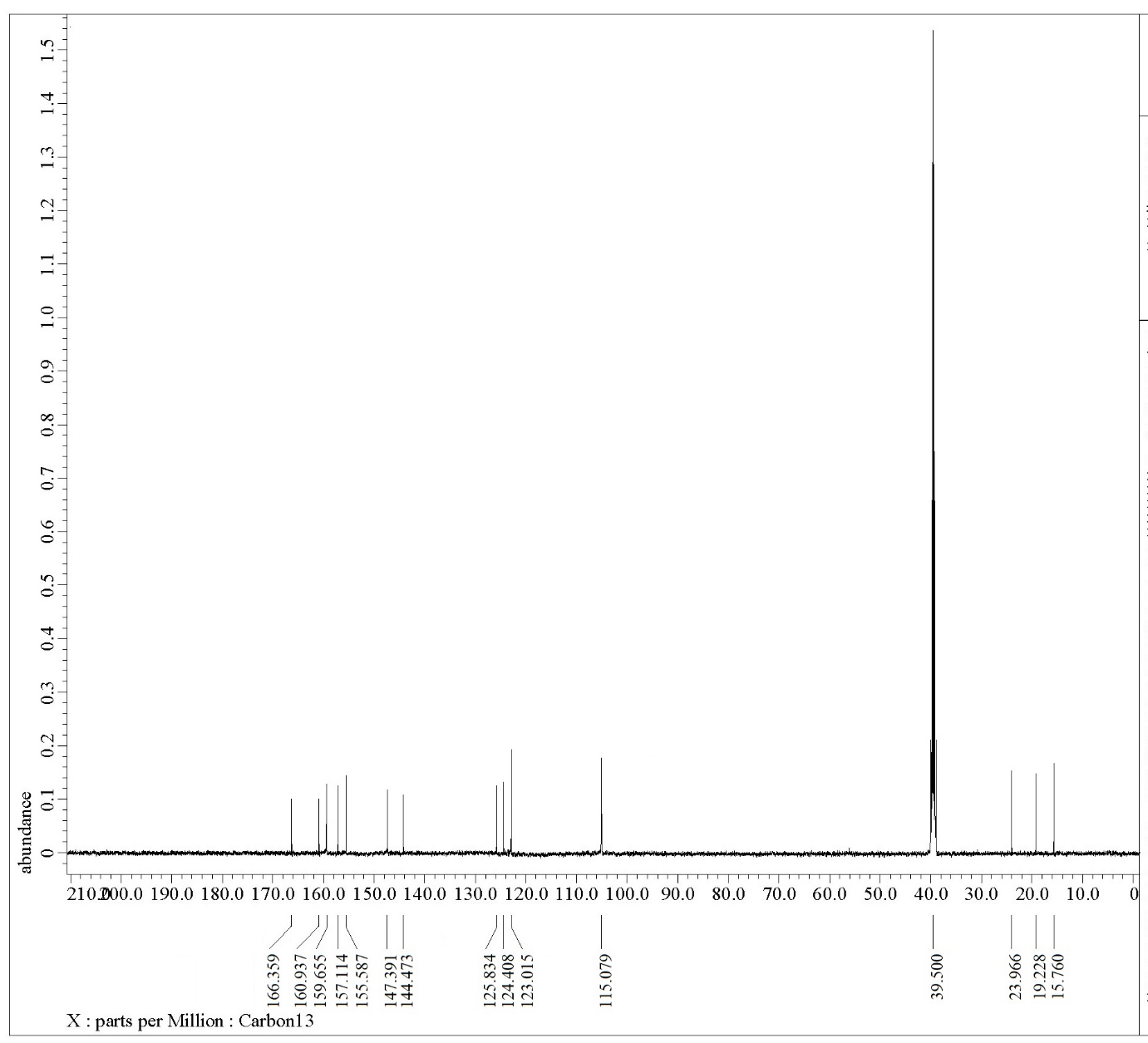


**Figure S7.** 13C NMR spectrum of compound **2**.



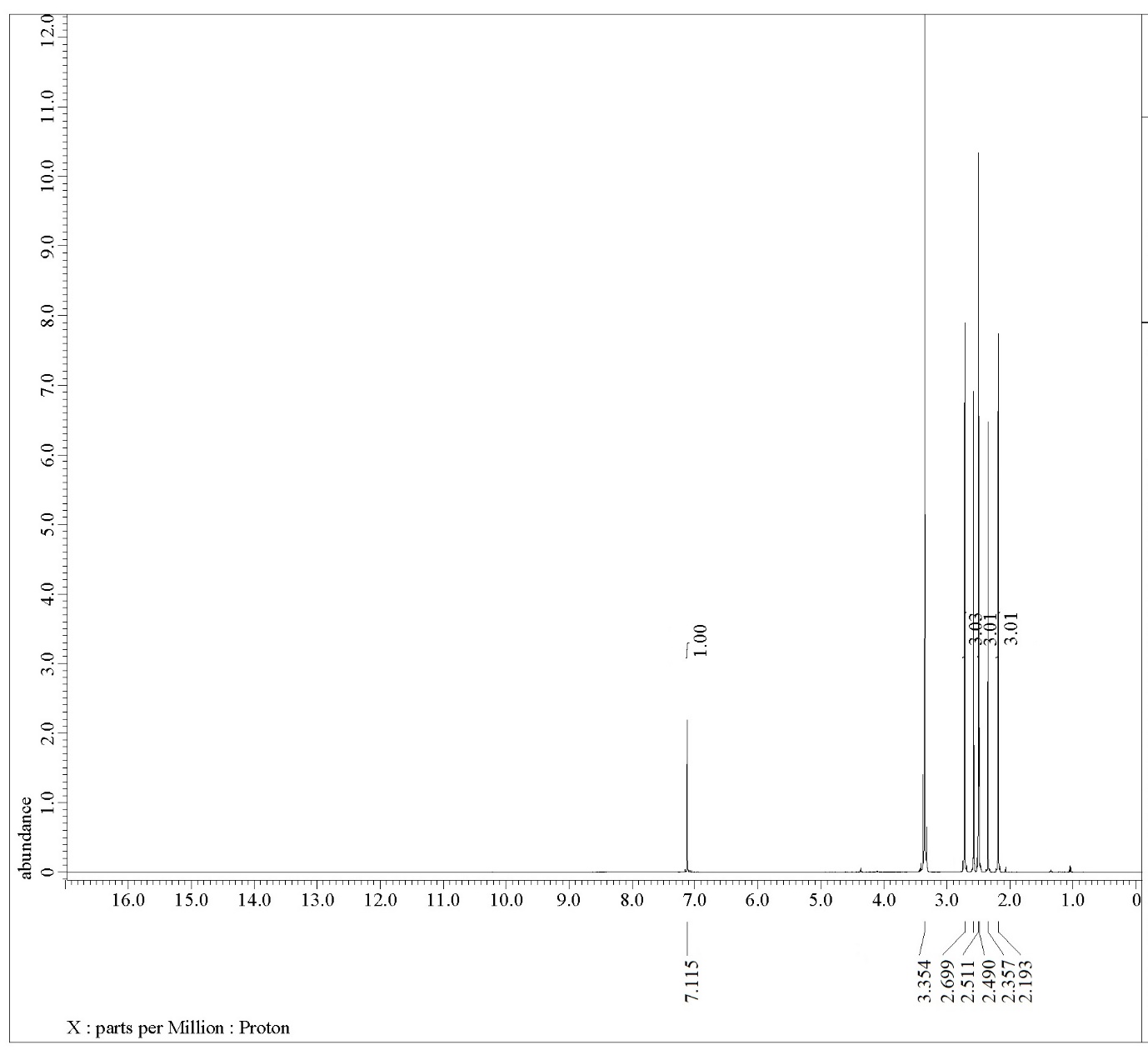


**Figure S8.** 1H NMR spectrum of compound **3**.



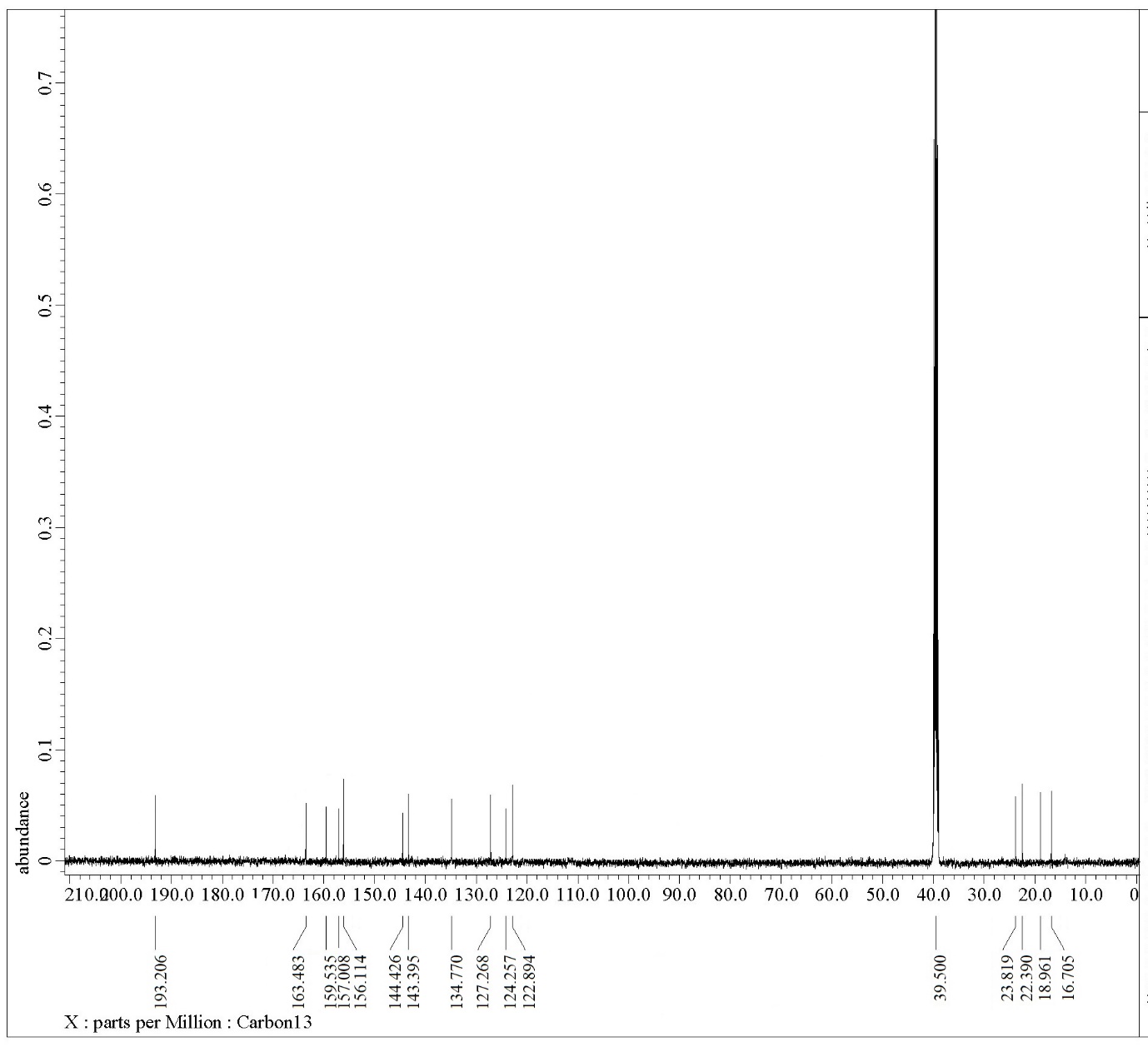


**Figure S9.** 13C NMR spectrum of compound **3**.



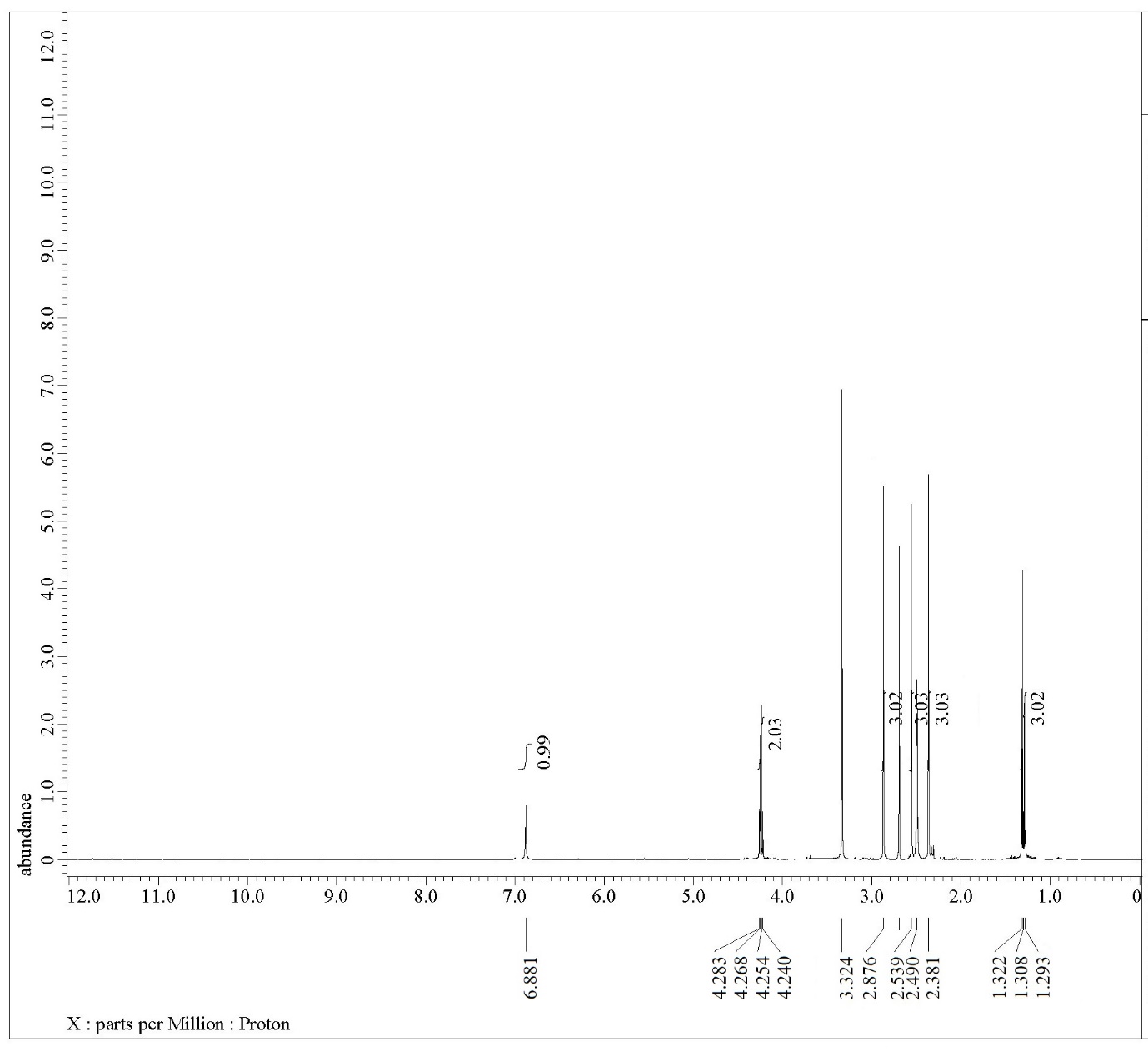


**Figure S10.** 1H NMR spectrum of compound **4**.



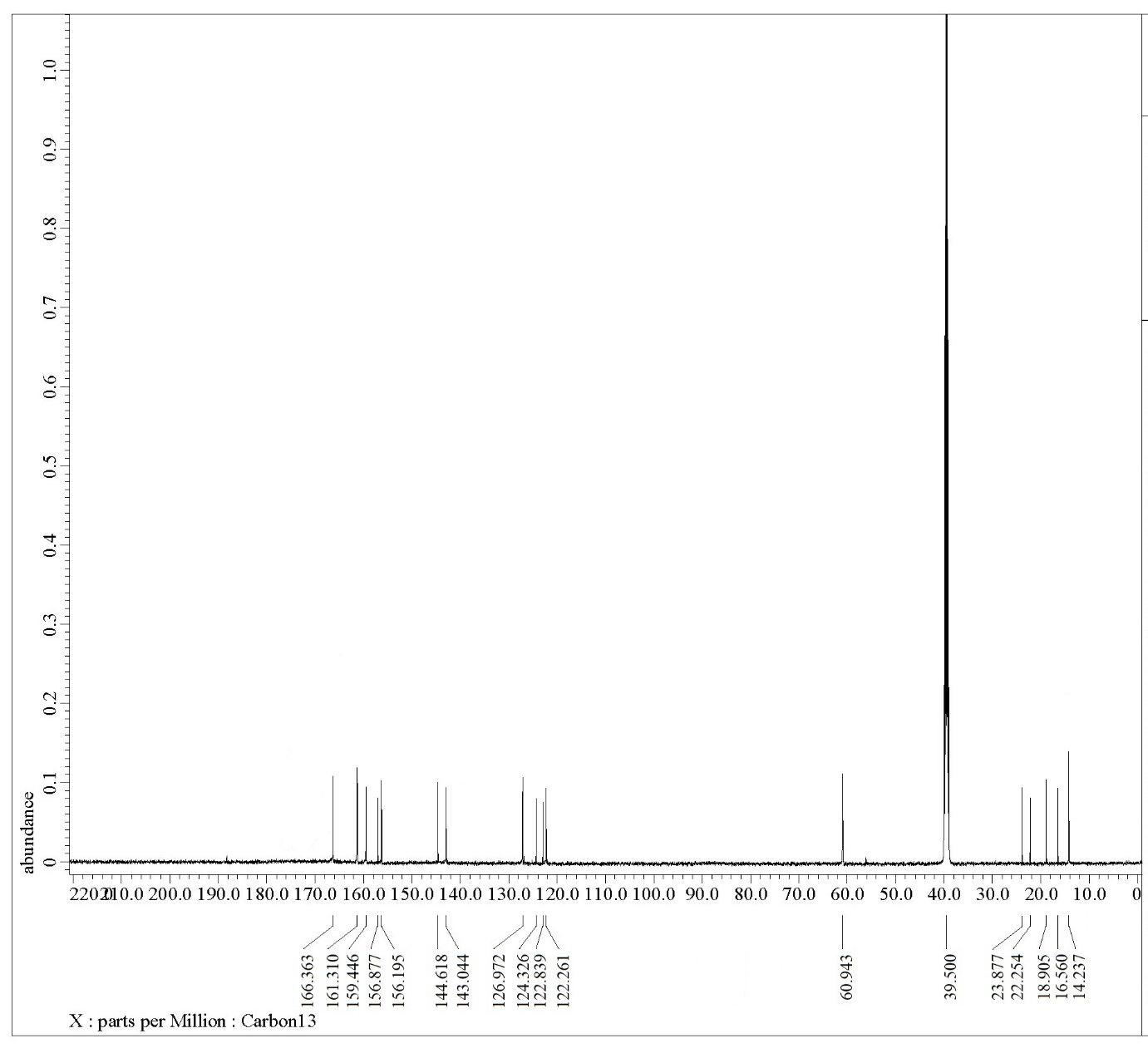


**Figure S11.** 13C NMR spectrum of compound **4**.



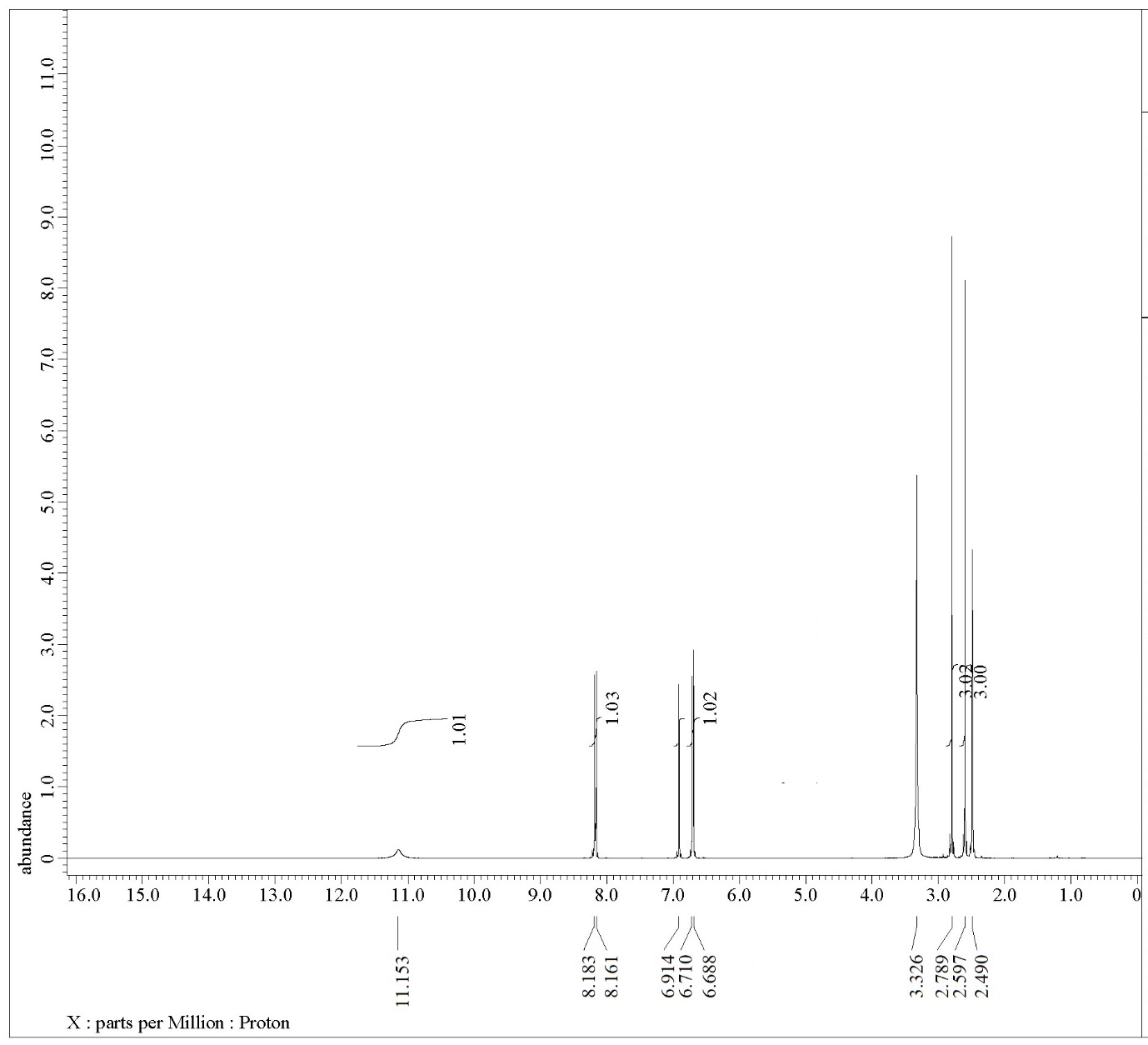


**Figure S12.** 1H NMR spectrum of compound **5**.



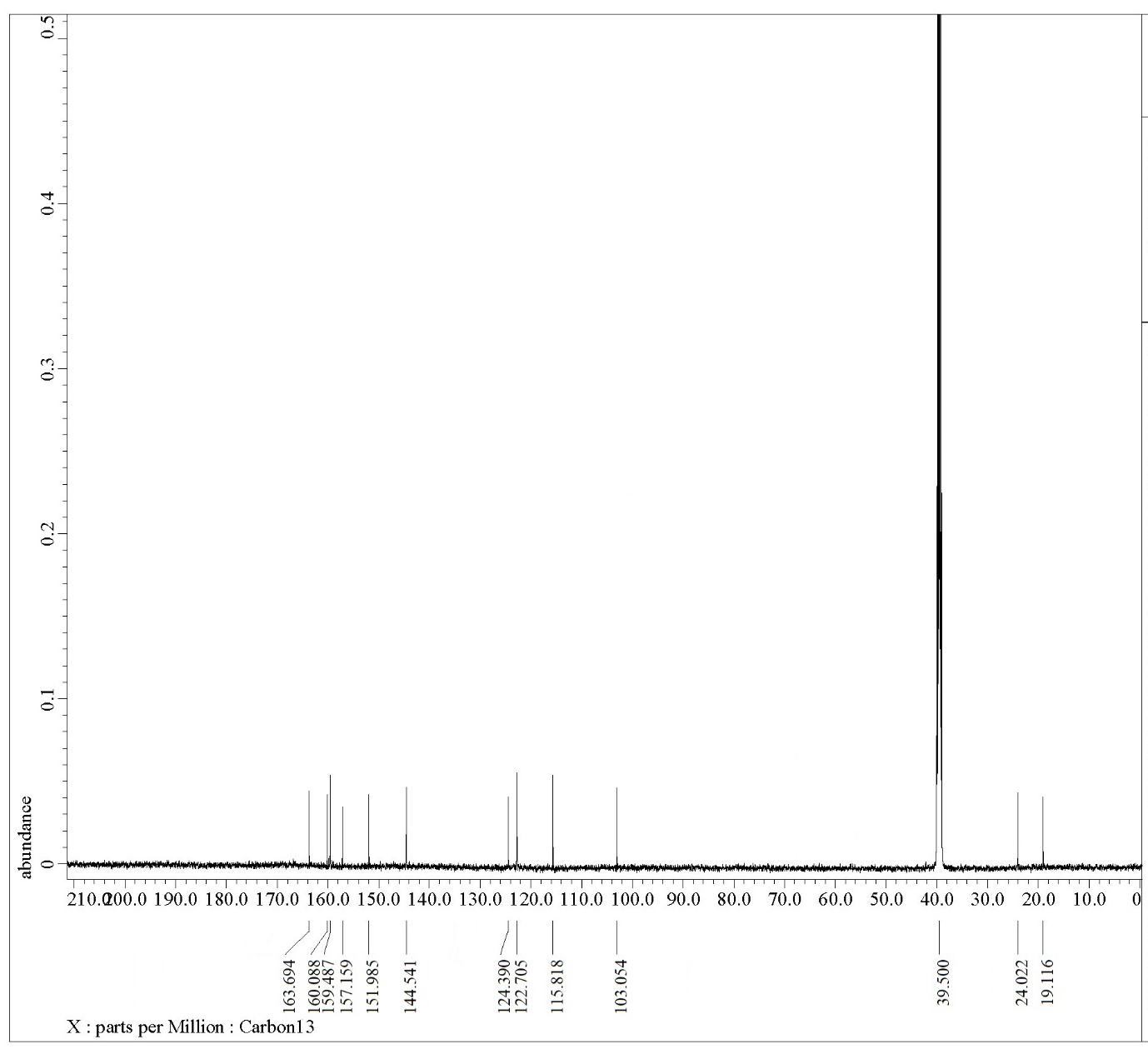


**Figure S13.** 13C NMR spectrum of compound **5**.



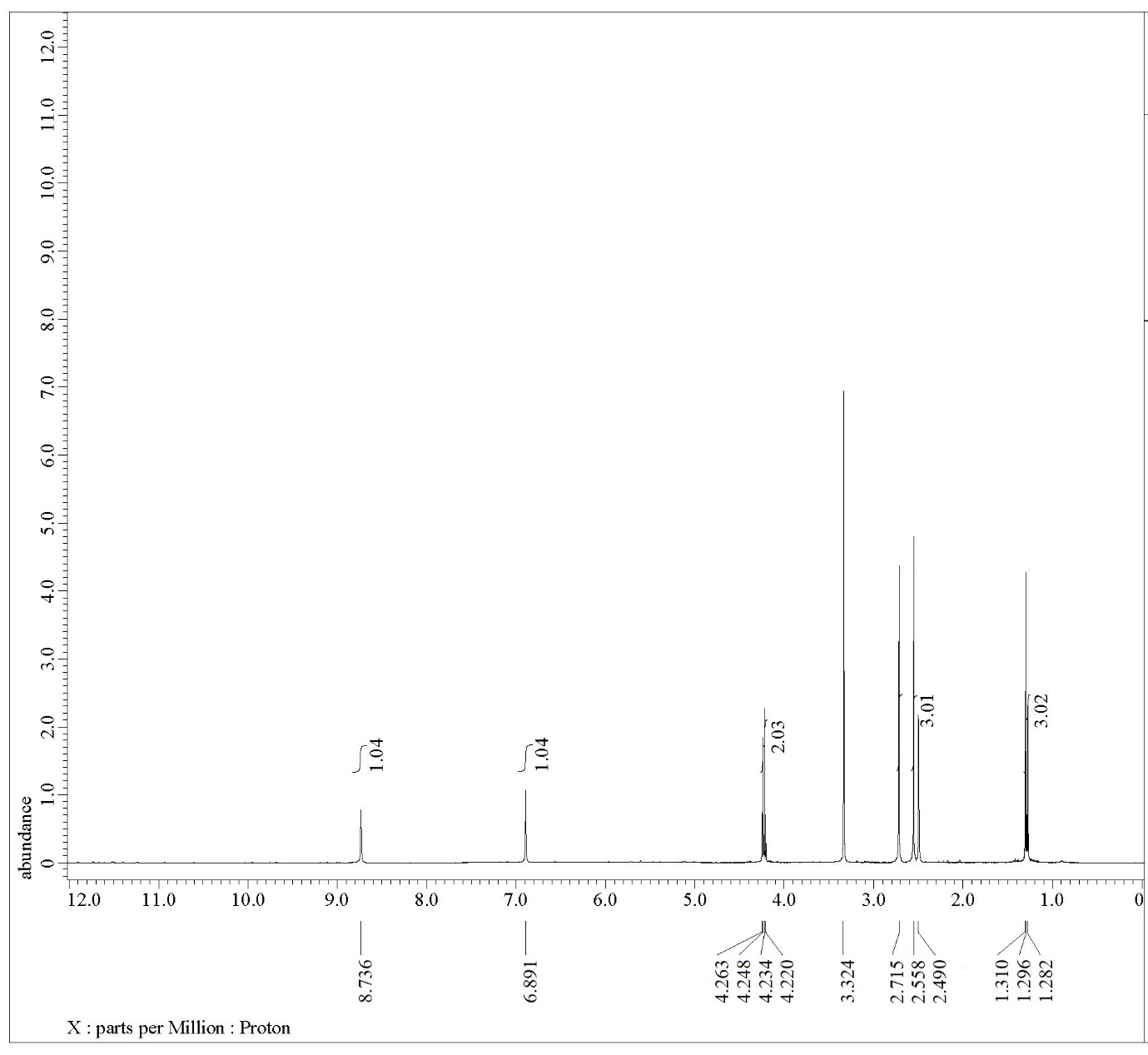


**Figure S14.** 1H NMR spectrum of compound **6**.



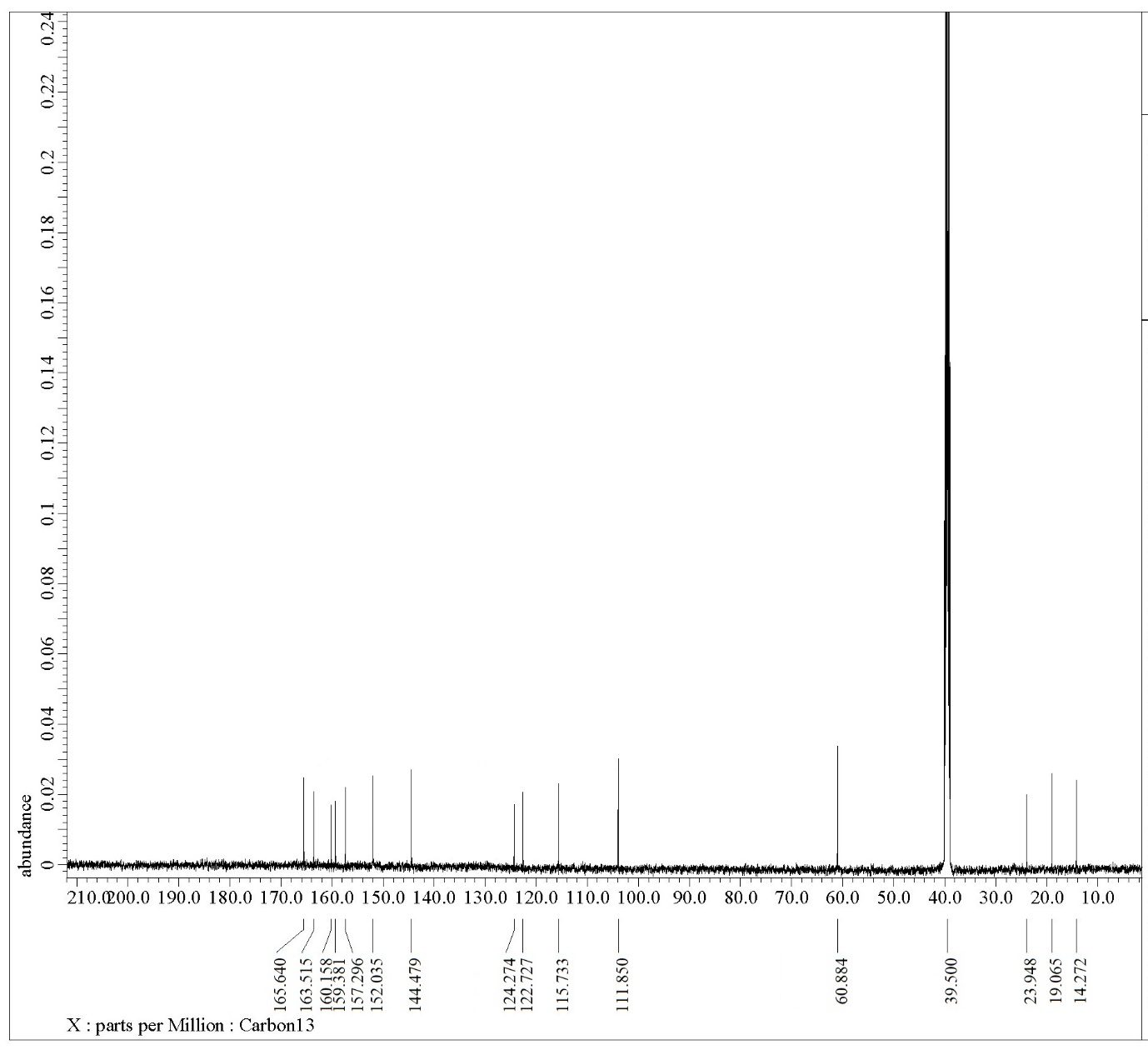


**Figure S15.** 13C NMR spectrum of compound **6**.





**Figure S16.** 1H NMR spectrum of compound **8**.





**Figure S17.** 13C NMR spectrum of compound **8**.