# Supplementary Materials

**Figure S1.** Numbering compound **1–4** according to Spartan program.

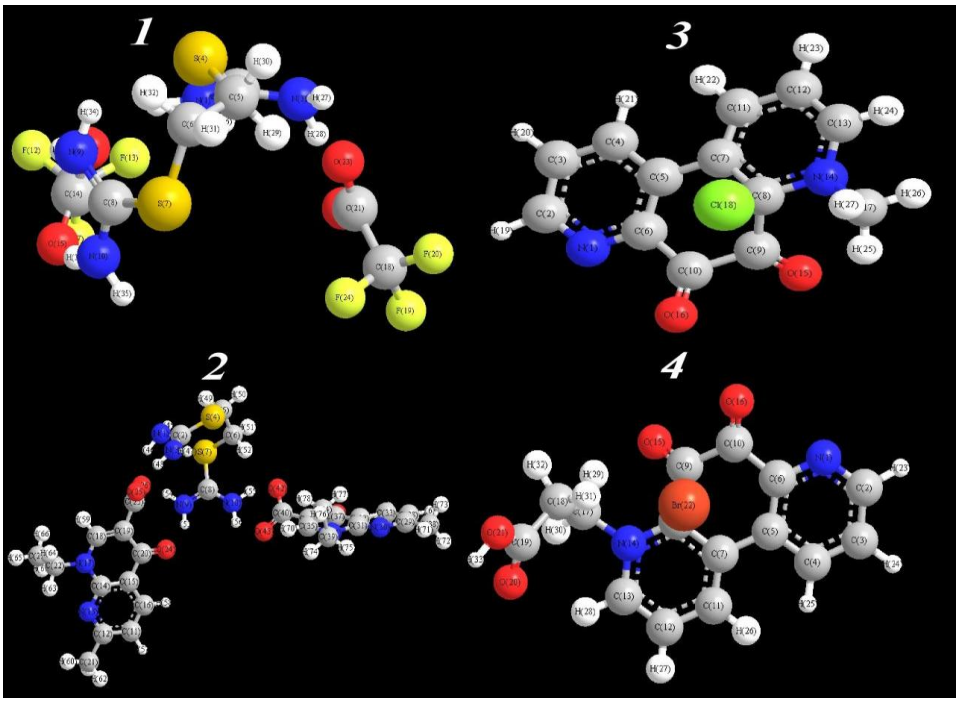


**Table S1.** Optimized geometrical parameters at Semi-empirical PM3.

| **Bond Length Compound 1** | |
|---|---|
| **Atom NO.** | **Length** |
| C(8)-N(9) | 1.2600 |
| N(1)-H(11) | 1.0220 |
| N(9)-H(12) | 1.0220 |
| N(3)-H(28) | 1.0500 |
| C(6)-H(31) | 1.1130 |
| C(6)-H(32) | 1.1130 |
| N(1)-C(2) | 1.2600 |
| N(10)-H(35) | 1.0500 |
| N(10)-H(36) | 1.0500 |
| C(8)-N(10) | 1.2660 |
| N(3)-H(27) | 1.0500 |
| C(8)-S(7) | 1.8150 |
| S(7)-C(6) | 1.8150 |
| C(6)-C(5) | 1.5230 |
| C(5)-S(4) | 1.8150 |
| C(2)-S(4) | 1.8150 |
| C(2)-N(3) | 1.2660 |
| C(5)-H(29) | 1.1130 |
| C(5)-H(30) | 1.1130 |

**Table S1.** *Cont*.

| **Bond Angle of Compound 1** | |
|---|---|
| **Atom NO.** | **Angle** |
| H(36)-N(10)-H(35) | 120.0000 |
| H(36)-N(10)-C(8) | 120.0000 |
| H(35)-N(10)-C(8) | 120.0000 |
| H(12)-N(9)-C(8) | 120.0000 |
| N(9)-C(8)-N(10) | 120.0000 |
| N(10)-C(8)-S(7) | 120.0000 |
| C(8)-S(7)-C(6) | 120.0000 |
| H(32)-C(6)-H(31) | 109.5200 |
| H(32)-C(6)-S(7) | 109.4618 |
| H(32)-C(6)-C(5) | 109.4618 |
| H(31)-C(6)-S(7) | 109.4418 |
| H(31)-C(6)-C(5) | 109.4418 |
| S(7)-C(6)-C(5) | 109.5000 |
| H(30)-C(5)-H(29) | 109.5200 |
| H(30)-C(5)-C(6) | 109.4618 |
| H(30)-C(5)-S(4) | 109.4618 |
| H(29)-C(5)-C(6) | 109.4418 |
| H(29)-C(5)-S(4) | 109.4418 |
| C(6)-C(5)-S(4) | 109.5000 |
| C(5)-S(4)-C(2) | 120.0000 |
| H(28)-N(3)-H(27) | 120.0000 |
| H(28)-N(3)-C(2) | 120.0000 |
| H(27)-N(3)-C(2) | 120.0000 |
| N(1)-C(2)-S(4) | 120.0000 |
| N(1)-C(2)-N(3) | 120.0000 |
| S(4)-C(2)-N(3) | 120.0000 |
| H(11)-N(1)-C(2) | 120.0000 |
| **Bond Length Compound 2** | |
| **Atom NO.** | **Length** |
| N(1)-H(46) | 1.0450 |
| N(9)-H(53) | 1.0450 |
| N(9)-H(54) | 1.0450 |
| C(5)-H(50) | 1.1130 |
| N(10)-H(55) | 1.0500 |
| N(3)-H(48) | 1.0500 |
| C(6)-H(52) | 1.1130 |
| N(10)-H(56) | 1.0500 |
| C(6)-H(51) | 1.1130 |
| N(3)-H(47) | 1.0500 |
| C(5)-H(49) | 1.1130 |
| C(8)-N(10) | 1.2660 |
| C(8)-N(9) | 1.3000 |
| C(8)-S(7) | 1.8150 |
| S(7)-C(6) | 1.8150 |
| C(6)-C(5) | 1.5230 |
| C(5)-S(4) | 1.8150 |
| C(2)-S(4) | 1.8150 |
| C(2)-N(3) | 1.2660 |
| N(1)-C(2) | 1.3000 |
| N(1)-H(45) | 1.0450 |
| N(10)-H(55) | 1.0500 |

**Table S1.** *Cont*.

| **Bond Length Compound 2** | |
|---|---|
| **Atom NO.** | **Angle** |
| H(56)-N(10)-H(55) | 120.0000 |
| H(54)-N(9)-H(53) | 120.0000 |
| H(54)-N(9)-C(8) | 120.0000 |
| H(53)-N(9)-C(8) | 120.0000 |
| N(10)-C(8)-N(9) | 120.0000 |
| N(10)-C(8)-S(7) | 120.0000 |
| N(9)-C(8)-S(7) | 120.0000 |
| C(8)-S(7)-C(6) | 120.0000 |
| H(52)-C(6)-H(51) | 109.5200 |
| H(52)-C(6)-S(7) | 109.4618 |
| H(52)-C(6)-C(5) | 109.4618 |
| H(51)-C(6)-S(7) | 109.4418 |
| H(51)-C(6)-C(5) | 109.4418 |
| S(7)-C(6)-C(5) | 109.5000 |
| H(50)-C(5)-H(49) | 109.5200 |
| H(50)-C(5)-C(6) | 109.4618 |
| H(50)-C(5)-S(4) | 109.4618 |
| H(49)-C(5)-C(6) | 109.4418 |
| H(49)-C(5)-S(4) | 109.4418 |
| C(6)-C(5)-S(4) | 109.5000 |
| C(5)-S(4)-C(2) | 120.0000 |
| H(48)-N(3)-H(47) | 120.0000 |
| H(48)-N(3)-C(2) | 120.0000 |
| H(47)-N(3)-C(2) | 120.0000 |
| S(4)-C(2)-N(3) | 120.0000 |
| S(4)-C(2)-N(1) | 120.0000 |
| N(3)-C(2)-N(1) | 120.0000 |
| H(46)-N(1)-C(2) | 120.0000 |

**Table S2.** Optimized geometrical parameters at Semi-empirical PM3.

| **Bond Angle Compound 3** | |
|---|---|
| **Atom NO.** | **Length** |
| C(17)-H(27) | 1.1130 |
| C(17)-H(26) | 1.1130 |
| C(17)-H(25) | 1.1130 |
| C(13)-H(24) | 1.1000 |
| C(12)-H(23) | 1.1000 |
| C(11)-H(22) | 1.1000 |
| C(4)-H(21) | 1.1130 |
| C(3)-H(20) | 1.1130 |
| N(14)-C(17) | 1.5000 |
| C(10)-O(16) | 1.2080 |
| C(9)-O(15) | 1.2080 |
| C(8)-N(14) | 1.3000 |
| C(13)-N(14) | 1.3000 |
| C(12)-C(13) | 1.2808 |
| C(11)-C(12) | 1.3370 |
| C(7)-C(11) | 1.3370 |
| C(6)-C(10) | 1.3340 |
| C(9)-C(10) | 0.9982 |
| C(8)-C(9) | 1.3510 |

**Table S2.** *Cont*.

| | |
|---|---|
| C(7)-C(8) | 1.3370 |
| C(5)-C(7) | 1.3510 |
| N(1)-C(6) | 1.2600 |
| C(5)-C(6) | 1.3340 |
| C(4)-C(5) | 1.3340 |
| C(3)-C(4) | 1.3340 |
| C(2)-C(3) | 1.3401 |
| N(1)-C(2) | 1.2600 |
| C(2)-H(19) | 1.1130 |
| **Atom NO.** | **Angle** |
| H(27)-C(17)-H(26) | 108.6875 |
| H(27)-C(17)-H(25) | 108.2739 |
| H(27)-C(17)-N(14) | 111.7726 |
| H(26)-C(17)-H(25) | 108.0021 |
| H(26)-C(17)-N(14) | 110.0573 |
| H(25)-C(17)-N(14) | 109.9497 |
| C(17)-N(14)-C(8) | 116.6403 |
| C(17)-N(14)-C(13) | 116.7590 |
| C(8)-N(14)-C(13) | 119.3899 |
| H(24)-C(13)-N(14) | 116.1095 |
| H(24)-C(13)-C(12) | 122.0577 |
| N(14)-C(13)-C(12) | 121.7105 |
| H(23)-C(12)-C(13) | 120.9198 |
| H(23)-C(12)-C(11) | 119.0337 |
| C(13)-C(12)-C(11) | 120.0460 |
| H(22)-C(11)-C(12) | 118.8720 |
| H(22)-C(11)-C(7) | 119.8991 |
| C(12)-C(11)-C(7) | 121.2288 |
| O(16)-C(10)-C(6) | 125.4733 |
| O(16)-C(10)-C(9) | 122.1893 |
| C(6)-C(10)-C(9) | 112.3316 |
| O(15)-C(9)-C(10) | 122.9536 |
| O(15)-C(9)-C(8) | 124.7456 |
| C(10)-C(9)-C(8) | 112.2116 |
| N(14)-C(8)-C(9) | 114.2709 |
| N(14)-C(8)-C(7) | 114.3835 |
| C(9)-C(8)-C(7) | 108.9343 |
| C(11)-C(7)-C(8) | 120.8081 |
| C(11)-C(7)-C(5) | 121.3055 |
| C(8)-C(7)-C(5) | 117.8746 |
| C(10)-C(6)-N(1) | 117.8675 |
| C(10)-C(6)-C(5) | 120.7624 |
| N(1)-C(6)-C(5) | 121.3700 |
| C(7)-C(5)-C(6) | 121.7371 |
| C(7)-C(5)-C(4) | 120.3182 |
| C(6)-C(5)-C(4) | 117.9413 |
| H(21)-C(4)-C(5) | 119.0083 |
| H(21)-C(4)-C(3) | 120.9373 |
| C(5)-C(4)-C(3) | 120.0526 |
| H(20)-C(3)-C(4) | 120.6453 |
| H(20)-C(3)-C(2) | 120.2420 |
| C(4)-C(3)-C(2) | 119.1127 |
| C(3)-C(2)-N(1) | 121.3102 |
| C(3)-C(2)-H(19) | 122.8296 |
| N(1)-C(2)-H(19) | 115.8602 |
| C(6)-N(1)-C(2) | 120.2124 |

**Table S2.** *Cont*.

| **Bond Angle Compound 4** | |
|---|---|
| **Atom NO.** | **Length** |
| O(21)-H(33) | 0.9720 |
| C(18)-H(32) | 1.1130 |
| C(18)-H(31) | 1.1130 |
| C(17)-H(30) | 1.1130 |
| C(17)-H(29) | 1.1130 |
| C(13)-H(28) | 1.1000 |
| C(12)-H(27) | 1.1000 |
| C(11)-H(26) | 1.1000 |
| C(4)-H(25) | 1.1130 |
| C(3)-H(24) | 1.1130 |
| C(19)-O(21) | 1.3380 |
| C(19)-O(20) | 1.2080 |
| C(18)-C(19) | 1.5090 |
| C(17)-C(18) | 1.5230 |
| N(14)-C(17) | 1.5000 |
| C(10)-O(16) | 1.2080 |
| C(9)-O(15) | 1.2080 |
| C(8)-N(14) | 1.3000 |
| C(13)-N(14) | 1.3000 |
| C(12)-C(13) | 1.2808 |
| C(11)-C(12) | 1.3370 |
| C(7)-C(11) | 1.3370 |
| C(6)-C(10) | 1.3340 |
| C(9)-C(10) | 0.9982 |
| C(8)-C(9) | 1.3510 |
| C(7)-C(8) | 1.3370 |
| C(5)-C(7) | 1.3510 |
| N(1)-C(6) | 1.2600 |
| C(5)-C(6) | 1.3340 |
| C(4)-C(5) | 1.3340 |
| C(3)-C(4) | 1.3340 |
| **Atom NO.** | **Angle** |
| H(33)-O(21)-C(19) | 120.0000 |
| O(21)-C(19)-O(20) | 120.0000 |
| O(21)-C(19)-C(18) | 120.0000 |
| O(20)-C(19)-C(18) | 120.0000 |
| H(32)-C(18)-H(31) | 109.5200 |
| H(32)-C(18)-C(19) | 109.4618 |
| H(32)-C(18)-C(17) | 109.4618 |
| H(31)-C(18)-C(19) | 109.4418 |
| H(31)-C(18)-C(17) | 109.4418 |
| C(19)-C(18)-C(17) | 109.5000 |
| H(30)-C(17)-H(29) | 109.5200 |
| H(30)-C(17)-C(18) | 109.4618 |
| H(30)-C(17)-N(14) | 109.4618 |
| H(29)-C(17)-C(18) | 109.4418 |
| H(29)-C(17)-N(14) | 109.4418 |
| C(18)-C(17)-N(14) | 109.5000 |
| C(17)-N(14)-C(8) | 122.5000 |
| C(17)-N(14)-C(13) | 122.5000 |
| C(8)-N(14)-C(13) | 115.0000 |
| H(28)-C(13)-N(14) | 115.2101 |
| H(28)-C(13)-C(12) | 115.2101 |
| N(14)-C(13)-C(12) | 129.5797 |
| H(27)-C(12)-C(13) | 123.9736 |

**Table S2.** *Cont*.

| **Bond Angle Compound 4** | |
|---|---|
| **Atom NO.** | **Angle** |
| H(27)-C(12)-C(11) | 123.9736 |
| C(13)-C(12)-C(11) | 112.0528 |
| H(26)-C(11)-C(12) | 120.0000 |
| H(26)-C(11)-C(7) | 120.0000 |
| C(12)-C(11)-C(7) | 120.0000 |
| O(16)-C(10)-C(6) | 117.7209 |
| O(16)-C(10)-C(9) | 117.7209 |
| C(6)-C(10)-C(9) | 124.5581 |
| O(15)-C(9)-C(10) | 117.3837 |
| C(10)-C(9)-C(8) | 125.2326 |
| N(14)-C(8)-C(9) | 122.3986 |
| N(14)-C(8)-C(7) | 119.9987 |
| C(9)-C(8)-C(7) | 117.6000 |
| C(11)-C(7)-C(8) | 119.9987 |
| C(11)-C(7)-C(5) | 122.3986 |
| C(8)-C(7)-C(5) | 117.6000 |
| C(10)-C(6)-N(1) | 119.9988 |
| C(10)-C(6)-C(5) | 119.9988 |
| N(1)-C(6)-C(5) | 120.0000 |
| C(7)-C(5)-C(6) | 115.0000 |
| C(7)-C(5)-C(4) | 124.9984 |
| C(6)-C(5)-C(4) | 119.9986 |
| H(25)-C(4)-C(5) | 120.0000 |
| H(25)-C(4)-C(3) | 120.0000 |
| C(5)-C(4)-C(3) | 120.0000 |
| H(24)-C(3)-C(4) | 122.7435 |
| H(24)-C(3)-C(2) | 122.7435 |
| C(4)-C(3)-C(2) | 114.5130 |
| C(3)-C(2)-N(1) | 125.4884 |
| C(3)-C(2)-H(23) | 117.2558 |
| N(1)-C(2)-H(23) | 117.2558 |
| C(6)-N(1)-C(2) | 120.0000 |
| C(10)-C(9)-C(8) | 125.2326 |
| N(14)-C(8)-C(9) | 122.3986 |
| N(14)-C(8)-C(7) | 119.9987 |
| C(9)-C(8)-C(7) | 117.6000 |
| C(11)-C(7)-C(8) | 119.9987 |
| C(11)-C(7)-C(5) | 122.3986 |
| C(8)-C(7)-C(5) | 117.6000 |
| C(10)-C(6)-N(1) | 119.9988 |
| C(10)-C(6)-C(5) | 119.9988 |

**Table 3:** Optimized geometrical parameters at Semi-empirical PM3.

| **Bond Angle Compound 3** | |
|---|---|
| **Atom NO.** | **Angle** |
| H(27)-C(17)-H(26) | 108.6875 |
| H(27)-C(17)-H(25) | 108.2739 |
| H(27)-C(17)-N(14) | 111.7726 |
| H(26)-C(17)-H(25) | 108.0021 |
| H(26)-C(17)-N(14) | 110.0573 |
| H(25)-C(17)-N(14) | 109.9497 |
| C(17)-N(14)-C(8) | 116.6404 |
| C(17)-N(14)-C(13) | 116.7589 |
| C(8)-N(14)-C(13) | 119.3900 |
| H(24)-C(13)-N(14) | 116.1097 |
| H(24)-C(13)-C(12) | 122.0576 |
| N(14)-C(13)-C(12) | 121.7104 |
| H(23)-C(12)-C(13) | 120.9199 |
| H(23)-C(12)-C(11) | 119.0337 |
| C(13)-C(12)-C(11) | 120.0460 |
| H(22)-C(11)-C(12) | 118.8720 |
| H(22)-C(11)-C(7) | 119.8991 |
| C(12)-C(11)-C(7) | 121.2287 |
| O(16)-C(10)-C(6) | 125.4731 |
| O(16)-C(10)-C(9) | 122.1894 |
| C(6)-C(10)-C(9) | 112.3317 |
| O(15)-C(9)-C(10) | 122.9536 |
| O(15)-C(9)-C(8) | 124.7456 |
| C(10)-C(9)-C(8) | 112.2116 |
| N(14)-C(8)-C(9) | 114.2709 |
| N(14)-C(8)-C(7) | 114.3835 |
| C(9)-C(8)-C(7) | 108.9344 |
| C(11)-C(7)-C(8) | 120.8082 |
| C(11)-C(7)-C(5) | 121.3054 |
| C(8)-C(7)-C(5) | 117.8746 |
| C(10)-C(6)-N(1) | 117.8675 |
| C(10)-C(6)-C(5) | 120.7624 |
| N(1)-C(6)-C(5) | 121.3701 |
| C(7)-C(5)-C(6) | 121.7371 |
| C(7)-C(5)-C(4) | 120.3182 |
| C(6)-C(5)-C(4) | 117.9414 |
| H(21)-C(4)-C(5) | 119.0084 |
| H(21)-C(4)-C(3) | 120.9372 |
| C(5)-C(4)-C(3) | 120.0526 |
| H(20)-C(3)-C(4) | 120.6454 |
| H(20)-C(3)-C(2) | 120.2420 |
| C(4)-C(3)-C(2) | 119.1126 |
| C(3)-C(2)-N(1) | 121.3102 |
| C(3)-C(2)-H(19) | 122.8295 |
| N(1)-C(2)-H(19) | 115.8602 |
| C(6)-N(1)-C(2) | 120.2123 |
| **Bond Length Compound 4** | |
| **Atom NO.** | **Length** |
| O(21)-H(33) | 0.6962 |
| C(18)-H(32) | 0.8117 |
| C(18)-H(31) | 0.8146 |
| C(17)-H(30) | 0.8114 |
| C(17)-H(29) | 0.8214 |
| C(13)-H(28) | 0.8057 |
| C(12)-H(27) | 0.8002 |
| C(11)-H(26) | 0.8053 |
| C(4)-H(25) | 0.8048 |
| C(3)-H(24) | 0.8003 |
| C(19)-O(21) | 0.9880 |
| C(19)-O(20) | 0.8923 |
| C(18)-C(19) | 1.1003 |
| C(17)-C(18) | 1.1146 |
| N(14)-C(17) | 1.0907 |
| C(10)-O(16) | 0.8824 |
| C(9)-O(15) | 0.8868 |
| C(8)-N(14) | 1.0393 |
| C(13)-N(14) | 1.0224 |
| C(12)-C(13) | 0.9964 |
| C(11)-C(12) | 1.0372 |
| C(7)-C(11) | 1.0002 |
| C(6)-C(10) | 1.0915 |
| C(9)-C(10) | 1.1163 |
| C(8)-C(9) | 1.1111 |
| C(7)-C(8) | 1.0679 |
| C(5)-C(7) | 1.0694 |
| N(1)-C(6) | 0.9925 |
| C(5)-C(6) | 1.0287 |
| C(3)-C(4) | 1.0137 |
| C(2)-C(3) | 1.0217 |
| N(1)-C(2) | 0.9850 |
| C(2)-H(23) | 0.8016 |
| C(3)-C(4) | 1.0137 |
| C(2)-C(3) | 1.0217 |
| **Bond Angle Compound 4** | |
| **Atom NO.** | **Angle** |
| H(33)-O(21)-C(19) | 110.0108 |
| O(21)-C(19)-O(20) | 115.5647 |
| O(21)-C(19)-C(18) | 114.5818 |
| O(20)-C(19)-C(18) | 129.8508 |
| H(32)-C(18)-H(31) | 105.2707 |
| H(32)-C(18)-C(19) | 108.0297 |
| H(32)-C(18)-C(17) | 108.5042 |
| H(31)-C(18)-C(19) | 109.0665 |
| C(19)-C(18)-C(17) | 114.0063 |
| H(30)-C(17)-H(29) | 106.3883 |
| H(30)-C(17)-C(18) | 110.8188 |
| H(30)-C(17)-N(14) | 108.5227 |
| H(29)-C(17)-C(18) | 109.7412 |
| H(29)-C(17)-N(14) | 106.9103 |
| C(18)-C(17)-N(14) | 114.1067 |
| C(17)-N(14)-C(8) | 121.0768 |
| C(17)-N(14)-C(13) | 118.4438 |
| C(8)-N(14)-C(13) | 120.4637 |
| H(28)-C(13)-N(14) | 116.8745 |
| H(28)-C(13)-C(12) | 122.0970 |
| N(14)-C(13)-C(12) | 121.0267 |
| H(27)-C(12)-C(13) | 120.4104 |
| H(27)-C(12)-C(11) | 119.5763 |
| C(13)-C(12)-C(11) | 120.0062 |
| H(26)-C(11)-C(12) | 119.2355 |
| H(26)-C(11)-C(7) | 119.9201 |
| C(12)-C(11)-C(7) | 120.8388 |
| O(16)-C(10)-C(6) | 125.4064 |
| O(16)-C(10)-C(9) | 121.9937 |
| C(6)-C(10)-C(9) | 112.5716 |
| O(15)-C(9)-C(10) | 123.5655 |
| O(15)-C(9)-C(8) | 123.1647 |
| C(10)-C(9)-C(8) | 113.2683 |
| N(14)-C(8)-C(9) | 119.8678 |
| N(14)-C(8)-C(7) | 116.8189 |
| C(9)-C(8)-C(7) | 114.7215 |
| C(11)-C(7)-C(8) | 119.8925 |
| C(11)-C(7)-C(5) | 121.0527 |
| C(8)-C(7)-C(5) | 119.0292 |
| C(10)-C(6)-N(1) | 117.6133 |
| C(10)-C(6)-C(5) | 120.9745 |
| N(1)-C(6)-C(5) | 121.4119 |

**Table S3.** *Cont.*

| **Dihedral Angle compound 1** | | **Dihedral Angle compound 2** | | **Dihedral Angle Compound 3** | | | |
|---|---|---|---|---|---|---|---|
| **Atom NO.** | **Angle** | **Atom NO.** | **Angle** | **Atom NO.** | **Length** | **Atom NO.** | **Angle** |
| S(7)-C(8)-N(9)-H(12) | -180.0000 | S(7)-C(8)-N(10)-H(55) | 15.4935 | C(13)-N(14)-C(17)-H(25) | 0.0000 | H(22)-C(11)-C(12)-H(23) | -19.4628 |
| N(10)-C(8)-N(9)-H(12) | 0.0000 | S(7)-C(8)-N(10)-H(56) | 162.1500 | C(13)-N(14)-C(17)-H(26) | 119.9636 | C(5)-C(7)-C(11)-C(12) | -170.1146 |
| H(11)-N(1)-C(2)-N(3) | 180.0000 | N(9)-C(8)-N(10)-H(55) | -175.0315 | C(13)-N(14)-C(17)-H(27) | -120.0004 | C(5)-C(7)-C(11)-H(22) | 9.8854 |
| H(11)-N(1)-C(2)-S(4) | 0.0000 | N(9)-C(8)-N(10)-H(56) | -28.3750 | C(8)-N(14)-C(17)-H(25) | -180.0000 | C(8)-C(7)-C(11)-C(12) | 10.5008 |
| N(9)-C(8)-N(10)-H(35) | 0.0000 | S(7)-C(8)-N(9)-H(53) | -168.9361 | C(8)-N(14)-C(17)-H(26) | -60.0364 | C(8)-C(7)-C(11)-H(22) | -169.4992 |
| N(9)-C(8)-N(10)-H(36) | 180.0000 | S(7)-C(8)-N(9)-H(54) | -25.6468 | C(8)-N(14)-C(17)-H(27) | 59.9996 | C(5)-C(6)-C(10)-C(9) | 1.1644 |
| N(9)-C(8)-S(7)-C(6) | -180.0000 | N(10)-C(8)-N(9)-H(53) | 21.1393 | C(7)-C(8)-N(14)-C(13) | 0.0000 | C(5)-C(6)-C(10)-O(16) | -178.8356 |
| N(1)-C(2)-S(4)-C(5) | 180.0000 | N(10)-C(8)-N(9)-H(54) | 164.4286 | C(7)-C(8)-N(14)-C(17) | -180.0000 | N(1)-C(6)-C(10)-C(9) | -179.4085 |
| N(1)-C(2)-N(3)-H(27) | 180.0000 | N(9)-C(8)-S(7)-C(6) | 143.6087 | C(9)-C(8)-N(14)-C(13) | -179.3846 | N(1)-C(6)-C(10)-O(16) | 0.5915 |
| N(1)-C(2)-N(3)-H(28) | 0.0000 | N(10)-C(8)-S(7)-C(6) | -46.6352 | C(9)-C(8)-N(14)-C(17) | 0.6154 | C(8)-C(9)-C(10)-C(6) | -0.4563 |
| S(7)-C(8)-N(9)-H(12) | -180.0000 | C(8)-S(7)-C(6)-C(5) | -128.8875 | C(12)-C(13)-N(14)-C(8) | -12.3429 | C(8)-C(9)-C(10)-O(16) | 179.5437 |
| N(10)-C(8)-N(9)-H(12) | 0.0000 | C(8)-S(7)-C(6)-H(51) | 112.0360 | C(12)-C(13)-N(14)-C(17) | 167.6571 | O(15)-C(9)-C(10)-C(6) | 179.5437 |
| H(11)-N(1)-C(2)-N(3) | 180.0000 | C(8)-S(7)-C(6)-H(52) | -2.6672 | H(24)-C(13)-N(14)-C(8) | 167.6571 | O(15)-C(9)-C(10)-O(16) | -0.4563 |
| H(11)-N(1)-C(2)-S(4) | 0.0000 | S(7)-C(6)-C(5)-S(4) | 93.1725 | H(24)-C(13)-N(14)-C(17) | -12.3429 | C(7)-C(8)-C(9)-C(10) | -0.1282 |
| N(9)-C(8)-N(10)-H(35) | 0.0000 | S(7)-C(6)-C(5)-H(49) | -36.5051 | C(11)-C(12)-C(13)-N(14) | 21.8423 | C(7)-C(8)-C(9)-O(15) | 179.8718 |
| N(9)-C(8)-N(10)-H(36) | 180.0000 | S(7)-C(6)-C(5)-H(50) | -152.8072 | C(11)-C(12)-C(13)-H(24) | -158.1577 | N(14)-C(8)-C(9)-C(10) | 179.2704 |
| N(9)-C(8)-S(7)-C(6) | -180.0000 | H(51)-C(6)-C(5)-S(4) | -149.1217 | H(23)-C(12)-C(13)-N(14) | -158.1577 | N(14)-C(8)-C(9)-O(15) | -0.7296 |
| N(1)-C(2)-S(4)-C(5) | 180.0000 | H(51)-C(6)-C(5)-H(49) | 81.2008 | H(23)-C(12)-C(13)-H(24) | 21.8423 | C(5)-C(7)-C(8)-C(9) | 0.0000 |
| N(1)-C(2)-N(3)-H(27) | 180.0000 | H(51)-C(6)-C(5)-H(50) | -35.1013 | C(7)-C(11)-C(12)-C(13) | -19.4628 | C(5)-C(7)-C(8)-N(14) | -179.4137 |
| | | H(52)-C(6)-C(5)-S(4) | -33.9025 | C(7)-C(11)-C(12)-H(23) | 160.5372 | C(11)-C(7)-C(8)-C(9) | 179.4137 |
| | | H(52)-C(6)-C(5)-H(49) | -163.5801 | H(22)-C(11)-C(12)-C(13) | 160.5372 | C(11)-C(7)-C(8)-N(14) | 0.0000 |
| | | H(52)-C(6)-C(5)-H(50) | 80.1178 | H(22)-C(11)-C(12)-H(23) | -19.4628 | C(4)-C(5)-C(7)-C(8) | 180.0000 |
| | | C(6)-C(5)-S(4)-C(2) | -74.9738 | C(5)-C(7)-C(11)-C(12) | -170.1146 | C(4)-C(5)-C(7)-C(11) | 0.6014 |
| | | H(49)-C(5)-S(4)-C(2) | 54.3888 | C(5)-C(7)-C(11)-H(22) | 9.8854 | C(6)-C(5)-C(7)-C(8) | 0.6339 |
| | | H(50)-C(5)-S(4)-C(2) | 166.6753 | C(8)-C(7)-C(11)-C(12) | 10.5008 | C(6)-C(5)-C(7)-C(11) | -178.7648 |
| | | N(1)-C(2)-S(4)-C(5) | -26.5328 | C(8)-C(7)-C(11)-H(22) | -169.4992 | C(2)-N(1)-C(6)-C(5) | 0.0000 |
| | | N(3)-C(2)-S(4)-C(5) | 160.8413 | C(5)-C(6)-C(10)-C(9) | 1.1644 | C(2)-N(1)-C(6)-C(10) | -179.4271 |
| | | N(1)-C(2)-N(3)-H(47) | -179.5590 | C(5)-C(6)-C(10)-O(16) | -178.8356 | C(4)-C(5)-C(6)-N(1) | 0.0000 |
| | | N(1)-C(2)-N(3)-H(48) | 19.5150 | N(1)-C(6)-C(10)-C(9) | -179.4085 | C(4)-C(5)-C(6)-C(10) | 179.4271 |

**Table S3.** *Cont.*

| **Dihedral bond Angle Compound 3** | | **Dihedral bond Angle Compound 4** | | | |
|---|---|---|---|---|---|
| **Atom NO.** | **Angle** | **Atom NO.** | **Length** | **Atom NO.** | **Angle** |
| C(4)-C(5)-C(6)-C(10) | 179.4271 | C(18)-C(19)-O(21)-H(33) | -179.5907 | H(28)-C(13)-N(14)-C(17) | -6.5402 |
| C(7)-C(5)-C(6)-N(1) | 179.4004 | O(20)-C(19)-O(21)-H(33) | 0.9584 | C(11)-C(12)-C(13)-N(14) | -1.6490 |
| C(7)-C(5)-C(6)-C(10) | -1.1725 | C(17)-C(18)-C(19)-O(20) | 2.3757 | C(11)-C(12)-C(13)-H(28) | 177.8604 |
| C(3)-C(4)-C(5)-C(6) | 0.0000 | C(17)-C(18)-C(19)-O(21) | -176.9791 | H(27)-C(12)-C(13)-N(14) | 179.3246 |
| C(3)-C(4)-C(5)-C(7) | -179.3366 | H(31)-C(18)-C(19)-O(20) | -123.0124 | H(27)-C(12)-C(13)-H(28) | -1.1660 |
| H(21)-C(4)-C(5)-C(6) | -180.0000 | H(31)-C(18)-C(19)-O(21) | 57.6328 | C(7)-C(11)-C(12)-C(13) | 2.6349 |
| H(21)-C(4)-C(5)-C(7) | 0.6634 | H(32)-C(18)-C(19)-O(20) | 123.0615 | C(7)-C(11)-C(12)-H(27) | -178.3306 |
| C(2)-C(3)-C(4)-C(5) | 0.0000 | H(32)-C(18)-C(19)-O(21) | -56.2932 | H(26)-C(11)-C(12)-C(13) | -176.5004 |
| C(2)-C(3)-C(4)-H(21) | -180.0000 | N(14)-C(17)-C(18)-C(19) | -86.5880 | H(26)-C(11)-C(12)-H(27) | 2.5341 |
| H(20)-C(3)-C(4)-C(5) | 180.0000 | N(14)-C(17)-C(18)-H(31) | 37.4816 | C(5)-C(7)-C(11)-C(12) | -178.3764 |
| H(20)-C(3)-C(4)-H(21) | 0.0000 | N(14)-C(17)-C(18)-H(32) | 152.9915 | C(5)-C(7)-C(11)-H(26) | 0.7530 |
| H(19)-C(2)-C(3)-C(4) | 180.0000 | H(29)-C(17)-C(18)-C(19) | 153.4688 | C(8)-C(7)-C(11)-C(12) | 3.4831 |
| H(19)-C(2)-C(3)-H(20) | 0.0000 | H(29)-C(17)-C(18)-H(31) | -82.4616 | C(8)-C(7)-C(11)-H(26) | -177.3875 |
| N(1)-C(2)-C(3)-C(4) | 0.0000 | H(29)-C(17)-C(18)-H(32) | 33.0483 | C(5)-C(6)-C(10)-C(9) | -23.5325 |
| N(1)-C(2)-C(3)-H(20) | 180.0000 | H(30)-C(17)-C(18)-C(19) | 36.2651 | C(5)-C(6)-C(10)-O(16) | 158.3764 |
| C(6)-N(1)-C(2)-H(19) | 180.0000 | H(30)-C(17)-C(18)-H(31) | 160.3347 | N(1)-C(6)-C(10)-C(9) | 156.6744 |
| C(6)-N(1)-C(2)-C(3) | 0.0000 | H(30)-C(17)-C(18)-H(32) | -84.1554 | N(1)-C(6)-C(10)-O(16) | -21.4166 |
| C(4)-C(5)-C(6)-C(10) | 179.4271 | C(13)-N(14)-C(17)-C(18) | 89.3960 | C(8)-C(9)-C(10)-C(6) | 45.8336 |
| C(7)-C(5)-C(6)-N(1) | 179.4004 | C(13)-N(14)-C(17)-H(29) | -149.0834 | C(8)-C(9)-C(10)-O(16) | -136.0009 |
| C(7)-C(5)-C(6)-C(10) | -1.1725 | C(13)-N(14)-C(17)-H(30) | -34.6985 | O(15)-C(9)-C(10)-C(6) | -133.7282 |
| C(3)-C(4)-C(5)-C(6) | 0.0000 | C(8)-N(14)-C(17)-C(18) | -92.0428 | O(15)-C(9)-C(10)-O(16) | 44.4373 |
| C(3)-C(4)-C(5)-C(7) | -179.3366 | C(8)-N(14)-C(17)-H(29) | 29.4778 | C(7)-C(8)-C(9)-C(10) | -46.6721 |
| | | C(8)-N(14)-C(17)-H(30) | 143.8627 | C(7)-C(8)-C(9)-O(15) | 132.8917 |
| | | C(7)-C(8)-N(14)-C(13) | 11.2453 | N(14)-C(8)-C(9)-C(10) | 166.4854 |
| | | C(7)-C(8)-N(14)-C(17) | -167.2869 | N(14)-C(8)-C(9)-O(15) | -13.9508 |
| | | C(9)-C(8)-N(14)-C(13) | 157.4177 | C(5)-C(7)-C(8)-C(9) | 23.7117 |
| | | C(9)-C(8)-N(14)-C(17) | -21.1145 | C(5)-C(7)-C(8)-N(14) | 171.6075 |
| | | C(12)-C(13)-N(14)-C(8) | -5.5765 | C(11)-C(7)-C(8)-C(9) | -158.1101 |
| | | C(12)-C(13)-N(14)-C(17) | 172.9938 | C(11)-C(7)-C(8)-N(14) | -10.2144 |
| | | H(28)-C(13)-N(14)-C(8) | 174.8894 | H(28)-C(13)-N(14)-C(17) | -6.5402 |

**Table 4.** Mulliken q(M) and neutral charges q(n) for **1, 2, 3** and **4** at Semi-empirical PM3.

| Atom No. q(M) q(n) | Atom No. q(M) q(n) | Atom No. q(M) q(n) |
|---|---|---|
| **1 and 2** | C3 : -0.085 -0.085 | C1 : +0.461 -0.074 |
| | C4 : -0.011 -0.011 | C2 : -0.432 -0.113 |
| N0 : -0.529 +0.141 | C5 : -0.111 -0.111 | C3 : +0.252 -0.085 |
| C1 : +0.086 -0.306 | C6 : -0.118 -0.118 | C4 : -0.372 -0.011 |
| N2 : -0.508 +0.151 | C7 : +0.031 +0.031 | C5 : +0.486 -0.111 |
| S3 : -0.266 -0.071 | C8 : +0.258 +0.258 | C6 : -0.063 -0.118 |
| C4 : -0.010 -0.204 | C9 : +0.314 +0.314 | C7 : -0.080 +0.031 |
| C5 : -0.010 -0.204 | C10 : +0.003 +0.003 | C8 : +0.558 +0.258 |
| S6 : -0.266 -0.071 | C11 : -0.188 -0.188 | C9 : +0.206 +0.314 |
| C7 : +0.086 -0.306 | C12 : -0.108 -0.108 | C10 : +0.021 +0.003 |
| N8 : -0.529 +0.141 | N13 : +0.236 +0.236 | C11 : -0.249 -0.188 |
| N9 : -0.508 +0.151 | O14 : -0.267 -0.267 | C12 : -0.116 -0.108 |
| H1 : +0.274 +0.059 | O15 : -0.212 -0.212 | N13 : +0.413 +0.236 |
| H2 : +0.313 +0.014 | C16 : -0.136 -0.136 | O14 : -0.444 -0.267 |
| H3 : +0.277 +0.066 | C17 : -0.130 -0.130 | H1 : +0.027 +0.126 |
| H4 : +0.302 +0.013 | C18 : +0.388 +0.388 | H2 : +0.145 +0.117 |
| H5 : +0.076 +0.061 | O19 : -0.419 -0.419 | H3 : +0.061 +0.117 |
| H6 : -0.014 +0.076 | O20 : -0.295 -0.295 | H4 : +0.121 +0.118 |
| H7 : -0.014 +0.076 | H1 : +0.126 +0.126 | H5 : +0.140 +0.130 |
| H8 : +0.076 +0.061 | H2 : +0.117 +0.117 | H6 : +0.177 +0.160 |
| H9 : +0.313 +0.014 | H3 : +0.117 +0.117 | H7 : +0.242 +0.130 |
| H10 : +0.274 +0.059 | H5 : +0.130 +0.130 | H8 : +0.187 +0.091 |
| H11 : +0.277 +0.066 | H7 : +0.130 +0.130 | H9 : +0.154 +0.128 |
| H12 : +0.302 +0.013 | H8 : +0.091 +0.091 | H10 : +0.166 +0.098 |
| **3** | H9 : +0.128 +0.128 | H11 : +0.417 +0.230 |
| | H10 :+0.098 +0.098 | |
| C1 : -0.074 -0.074 | H11 :+0.230 +0.230 | |
| C2 : -0.113 -0.113 | **4** | |
| N1 : -0.002 -0.002 | | |