**Supplementary Information**

New bioactive Cu(I) thiourea derivatives with triphenylphosphine; Synthesis, structure and molecular docking studies

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Table S1. Bond lengths and angles for **3**.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Bond lengths** | | |  | **Bond angles** | | | |
| Cu1-P1 | | 2.2765(6) |  | P1-Cu1-P2 | | | 120.90(2) |
| Cu1-P2 | | 2.2965(6) |  | P1-Cu1-Cl1 | | | 106.56(2) |
| Cu1-Cl1 | | 2.3325(6) |  | P2-Cu1-Cl1 | | | 115.95(3) |
| Cu1-S1 | | 2.4468(7) |  | P1-Cu1-S1 | | | 105.51(2) |
| Cl2-C39 | | 1.731(3) |  | P2-Cu1-S1 | | | 102.96(2) |
| S1-C37 | | 1.685(2) |  | Cl1-Cu1-S1 | | | 102.83(2) |
| P1-C19 | | 1.818(2) |  | C37-S1-Cu1 | | | 107.46(8) |
| P1-C25 | | 1.829(3) |  | C19-P1-C25 | | | 102.16(11) |
| P1-C31 | | 1.833(2) |  | C19-P1-C31 | | | 101.71(11) |
| P2 | C1B | 1.805(3) |  | C25 | P1 | C31 | 103.59(11) |
| P2 | C13 | 1.829(3) |  | C19 | P1 | Cu1 | 117.75(8) |
| P2 | C7 | 1.831(2) |  | C17 | C16 | C15 | 119.5(3) |
| P2 | C1A | 1.879(3) |  | C16 | C17 | C18 | 120.8(3) |