

SUPPORTING INFORMATION

Partial conversion of thioamide into nitrile in a copper(II) complex of 2,6-diacetylpyridine bis(thiosemicarbazone), a drug prototype for Alzheimer's Disease

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Geometric parameters (Å, °)			
C1—C2	1.383(4)	C8—S1	1.736(3)
C1—C6	1.481(4)	C8—N4	1.341(3)
C2—C3	1.378(5)	C9—C10	1.527(4)
C3—C4	1.357(5)	C9—N5	1.293(4)
C4—C5	1.405(4)	N5—N6	1.391(3)
C1—N1	1.346(4)	N6—C11	1.336(4)
C5—N1	1.353(4)	C11—N7	1.144(4)
C5—C9	1.472(5)	Cu1—N6	1.904(2)
C6—C7	1.472(4)	Cu1—N1	1.970(2)
C6—N2	1.290(3)	Cu1—N2	1.938(2)
N2—N3	1.371(3)	Cu1—S1	2.2379(7)
C8—N3	1.321(3)		
N1—C1—C2	121.7(3)	N6—Cu1—N2	174.12(9)
N1—C1—C6	115.2(2)	N6—Cu1—N1	91.77(10)
C2—C1—C6	123.0(3)	N2—Cu1—N1	82.44(9)
C3—C2—C1	118.3(3)	N6—Cu1—S1	100.83(8)
C4—C3—C2	119.9(3)	N2—Cu1—S1	84.97(6)
C3—C4—C5	120.8(3)	N1—Cu1—S1	167.35(8)
C3—C4—C5	119.70	C8—S1—Cu1	94.65(8)
N1—C5—C4	118.4(3)	C1—N1—C5	120.8(2)

N1—C5—C9	119.9(3)	C1—N1—Cu1	112.17(17)
C4—C5—C9	121.6(3)	C5—N1—Cu1	127.0(2)
N2—C6—C7	123.9(3)	C6—N2—N3	120.0(2)
N2—C6—C1	113.7(2)	C6—N2—Cu1	116.32(18)
C7—C6—C1	122.4(3)	N3—N2—Cu1	123.61(16)
N3—C8—N4	117.6(2)	C8—N3—N2	111.0(2)
N3—C8—S1	125.73(19)	C9—N5—N6	120.4(3)
N4—C8—S1	116.65(19)	C11—N6—N5	109.6(2)
N5—C9—C5	130.8(3)	C11—N6—Cu1	120.33(18)
N5—C9—C10	112.0(3)	N5—N6—Cu1	130.0(2)
N7—C11—N6	176.4(3)		

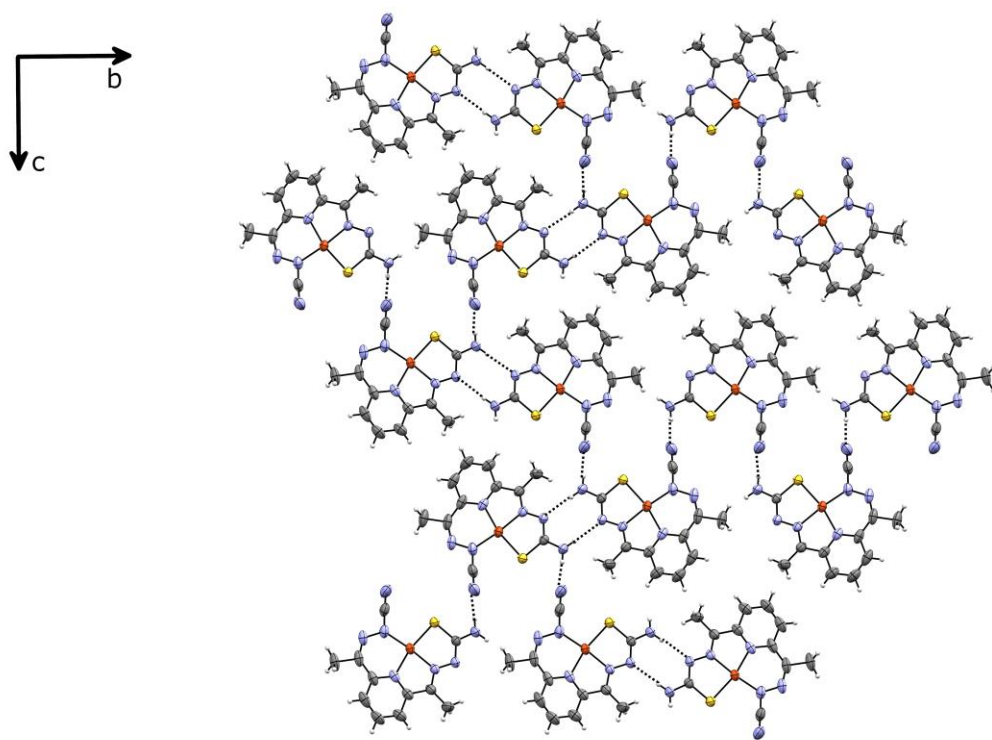


Figure S1. Crystal packing for the structure of CuDAPTn.