Supporting Information for the article "Synthesis, Structural Studies and Anticancer Properties of The [CuBr(PPh3)2(4,6-dimethyl-2-thiopyrimidine-κS]"

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Keywords: Copper(I) – thiopyrimidine – Phosphine - Protein binding – Anticancer properties.

Table S1 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for $C_{42}H_{38}BrCuN_2P_2S$. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Br1	3844.5(2)	6655.2(2)	5203.5(2)	20.97(3)
Cu1	2735.6(2)	6989.1(2)	6125.9(2)	14.39(3)
S1	791.7(3)	6207.5(2)	6159.9(2)	16.85(5)
P1	2148.5(3)	8217.0(2)	5993.6(2)	13.88(5)
P2	4259.1(3)	6504.4(2)	6955.0(2)	12.36(5)
N1	1824.2(11)	5274.9(6)	5414.8(5)	17.22(17)
N2	387.9(12)	4737.8(6)	6037.8(5)	19.60(18)
C1	761.9(13)	8378.8(6)	5318.2(6)	17.8(2)
C2	-489.6(14)	7977.3(7)	5288.1(7)	24.1(2)
C3	-1611.2(16)	8091.9(8)	4801.1(8)	33.0(3)
C4	-1484(2)	8591.3(10)	4332.9(8)	41.0(4)
C5	-254(2)	8980.1(11)	4355.4(8)	41.4(4)
C6	873.6(17)	8881.1(9)	4848.4(7)	29.8(3)
C7	3545.7(13)	8872.3(6)	5894.2(6)	17.19(19)
C10	5780.2(16)	9817.4(9)	5778.3(8)	30.7(3)
C13	1435.9(13)	8686.2(6)	6604.6(5)	16.73(19)
C14	248.4(14)	9143.9(7)	6490.1(6)	21.0(2)
C15	-175.6(17)	9525.5(8)	6976.8(7)	28.6(3)
C16	579.1(19)	9460.1(9)	7575.1(7)	32.7(3)
C17	1756.7(19)	9005.9(10)	7689.7(7)	32.7(3)
C18	2183.9(16)	8614.5(8)	7211.7(6)	25.2(2)
C19	6101.6(12)	6749.6(6)	7038.1(6)	16.13(18)
C20	6407.4(13)	7449.0(7)	6816.7(7)	23.0(2)
C21	7790.3(15)	7689.2(8)	6877.4(8)	29.1(3)
C22	8873.3(14)	7231.2(9)	7157.5(8)	30.1(3)
C23	8579.2(14)	6528.8(9)	7375.4(8)	29.6(3)
C24	7200.0(13)	6287.1(7)	7317.0(7)	22.4(2)
C25	3856.4(11)	6718.7(6)	7714.0(5)	14.24(17)
C26	2462.4(13)	6646.9(8)	7789.0(6)	22.2(2)
C27	2088.2(15)	6819.5(9)	8351.1(7)	27.2(3)
C28	3085.6(15)	7080.3(8)	8842.9(6)	24.1(2)
C29	4461.2(14)	7165.1(8)	8770.7(6)	22.3(2)
C30	4850.2(12)	6980.3(7)	8211.3(6)	17.77(19)
C31	4262.5(11)	5480.5(6)	6932.6(5)	15.37(18)
C32	4770.0(15)	5131.1(7)	6451.9(6)	23.7(2)
C37	1026.8(12)	5346.3(6)	5859.9(5)	15.55(18)
C38	579.6(14)	4075.9(7)	5781.3(6)	21.2(2)
C39	1391.4(14)	3992.2(7)	5324.2(6)	20.6(2)
C40	2019.3(13)	4616.5(7)	5138.2(6)	18.4(2)
C41	-141(2)	3411.4(8)	6000.6(8)	35.0(4)
C42	2866.7(16)	4619.9(8)	4640.0(7)	26.3(3)
C8	4552(9)	8644(5)	5554(4)	22.1(9)
C9	5660(8)	9118(4)	5490(4)	25.8(8)
C11	4825(8)	10040(4)	6116(4)	29.6(9)
C12	3691(9)	9584(4)	6176(4)	26.4(10)
C33	4646(16)	4331(5)	6421(6)	29.7(11)
C34	4157(9)	3922(4)	6868(4)	30.0(9)

Table S1 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for $C_{42}H_{38}BrCuN_2P_2S$. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
C35	3783(8)	4274(3)	7355(4)	30.8(8)
C36	3822(10)	5059(5)	7398(4)	28.0(10)
C8A	4694(10)	8599(6)	5659(5)	22.0(10)
C9A	5804(9)	9073(4)	5618(4)	25.6(9)
C11A	4607(8)	10102(4)	5993(4)	27.5(9)
C12A	3513(10)	9620(5)	6056(5)	24.9(10)
C33A	4752(13)	4374(4)	6354(5)	25.7(8)
C34A	4079(7)	3932(4)	6714(3)	29.7(8)
C35A	3469(7)	4254(3)	7178(3)	32.3(8)
C36A	3578(8)	5025(4)	7289(3)	26.8(9)

Table S2 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $C_{42}H_{38}BrCuN_2P_2S$. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br1	28.87(6)	17.54(5)	18.87(6)	0.91(4)	10.49(5)	0.58(4)
Cu1	15.81(6)	12.71(5)	14.07(6)	0.33(4)	1.39(4)	1.31(4)
S1	15.61(11)	17.13(11)	17.86(12)	-4.71(9)	3.33(9)	-1.01(9)
P1	14.93(12)	12.40(11)	14.12(12)	-0.16(9)	2.29(9)	1.01(9)
P2	10.99(11)	12.75(11)	13.24(11)	0.80(9)	2.09(9)	0.12(8)
N1	17.9(4)	16.2(4)	18.4(4)	-2.1(3)	5.8(3)	-0.7(3)
N2	24.2(5)	17.9(4)	17.0(4)	-1.7(3)	5.0(4)	-3.2(4)
C1	20.5(5)	16.5(4)	15.1(5)	-2.6(4)	0.4(4)	5.4(4)
C2	22.2(6)	17.6(5)	28.6(6)	-3.8(5)	-4.4(5)	2.1(4)
C3	25.7(6)	23.6(6)	42.6(9)	-8.5(6)	-11.8(6)	6.1(5)
C4	41.1(9)	38.1(8)	33.7(8)	-4.1(7)	-18.1(7)	14.1(7)
C5	49.3(10)	44.2(10)	25.7(7)	11.8(7)	-5.2(7)	11.0(8)
C6	32.1(7)	33.9(7)	22.1(6)	9.0(5)	1.9(5)	4.8(6)
C7	19.3(5)	14.4(4)	17.9(5)	1.6(4)	3.7(4)	0.2(3)
C10	28.7(6)	29.2(6)	35.2(7)	4.3(6)	8.4(6)	-10.5(5)
C13	19.9(5)	14.7(4)	16.2(5)	-2.2(4)	5.2(4)	-2.8(4)
C14	22.4(5)	19.7(5)	22.6(6)	-3.1(4)	8.3(4)	1.3(4)
C15	32.4(7)	24.1(6)	34.1(7)	-7.0(5)	18.4(6)	-0.6(5)
C16	45.3(9)	30.6(7)	28.2(7)	-11.5(6)	22.0(7)	-10.7(6)
C17	43.3(9)	37.7(8)	17.9(6)	-7.3(5)	7.8(6)	-9.8(6)
C18	29.4(6)	28.5(6)	17.4(5)	-2.4(5)	3.5(5)	-3.1(5)
C19	12.9(4)	16.8(4)	19.2(5)	-0.3(4)	4.5(4)	-0.9(3)
C20	18.2(5)	18.0(5)	33.8(7)	2.8(5)	7.9(5)	-1.8(4)
C21	22.3(6)	21.0(6)	46.7(9)	-1.8(6)	13.7(6)	-6.9(4)
C22	16.0(5)	29.1(6)	46.8(9)	-7.9(6)	10.4(6)	-6.2(5)
C23	12.5(5)	29.9(7)	45.1(9)	-1.2(6)	2.6(5)	0.4(4)
C24	13.9(5)	22.0(5)	30.3(6)	2.8(5)	2.0(4)	0.2(4)
C25	14.0(4)	14.8(4)	13.7(4)	0.1(3)	2.0(3)	0.6(3)
C26	14.5(5)	35.9(7)	16.6(5)	-5.6(5)	3.6(4)	-1.2(4)
C27	18.8(5)	43.6(8)	20.6(6)	-6.7(5)	7.0(5)	-1.0(5)
C28	27.3(6)	28.0(6)	17.3(5)	-4.3(5)	5.4(5)	1.1(5)
C29	25.1(6)	24.1(5)	16.1(5)	-4.7(4)	0.4(4)	-1.8(4)
C30	16.7(5)	18.1(5)	17.6(5)	-1.1(4)	1.0(4)	-2.0(4)
C31	13.4(4)	13.9(4)	18.2(5)	1.5(4)	1.6(4)	0.7(3)
C32	31.3(6)	18.9(5)	21.1(6)	-0.9(4)	5.6(5)	5.5(4)
C37	15.7(4)	17.0(4)	13.3(4)	-1.2(3)	1.2(3)	-0.1(3)
C38	25.7(6)	18.4(5)	19.2(5)	-2.1(4)	3.4(4)	-3.5(4)
C39	23.8(5)	17.6(5)	19.8(5)	-4.0(4)	2.7(4)	0.2(4)
C40	17.0(5)	19.6(5)	18.4(5)	-3.4(4)	3.0(4)	1.4(4)
C41	51.5(10)	20.8(6)	37.4(8)	-4.4(6)	20.2(7)	-11.1(6)
C42	26.6(6)	26.4(6)	29.4(7)	-6.2(5)	14.3(5)	1.5(5)
C8	26.7(16)	18.8(14)	23(2)	4.0(14)	10.2(15)	1.5(12)
C9	26.8(16)	27.3(13)	26.4(19)	8.1(14)	13.0(15)	0.0(11)
C11	33.9(18)	21.0(14)	33(2)	-2.6(14)	5.5(15)	-9.6(12)
C12	30(2)	18.2(13)	32(2)	-5.5(15)	10.5(17)	-5.3(12)
C33	36(2)	19.2(16)	32(3)	-6.5(16)	0.9(17)	8.3(15)
C34	39.4(15)	13.4(11)	36(2)	0.9(16)	3.2(17)	-0.2(11)

Table S2 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $C_{42}H_{38}BrCuN_2P_2S$. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C35	41.0(19)	16.4(11)	36(2)	5.1(14)	9.8(15)	-3.7(13)
C36	37(2)	16.1(14)	34(2)	5.1(16)	14.9(18)	-3.0(15)
C8A	26.4(18)	18.0(14)	24(2)	4.0(16)	10.7(17)	1.1(13)
C9A	25.1(16)	26.7(14)	27(2)	9.0(15)	9.8(16)	0.3(12)
C11A	29.9(18)	18.5(13)	35(2)	-1.6(15)	9.6(16)	-6.1(12)
C12A	26.9(19)	16.6(13)	33(3)	-2.7(16)	11.2(18)	-4.1(13)
C33A	33.3(17)	18.0(13)	25.6(19)	-0.7(11)	5.3(12)	6.2(11)
C34A	39.5(13)	14.4(10)	34(2)	-1.9(14)	3.1(15)	3.2(9)
C35A	40.5(17)	18.7(10)	39(2)	4.0(13)	10.1(14)	-5.9(12)
C36A	33(2)	17.1(11)	35(2)	0.1(13)	17.1(16)	-4.3(13)

Table S3 Atomic Occupancy for $C_{42}H_{38}BrCuN_2P_2S$.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
H10	0.53(2)	H10A	0.47(2)	H32	0.46(2)
H32A	0.54(2)	C8	0.53(2)	H8	0.53(2)
C9	0.53(2)	H9	0.53(2)	C11	0.53(2)
H11	0.53(2)	C12	0.53(2)	H12	0.53(2)
C33	0.46(2)	H33	0.46(2)	C34	0.46(2)
H34	0.46(2)	C35	0.46(2)	H35	0.46(2)
C36	0.46(2)	H36	0.46(2)	C8A	0.47(2)
H8A	0.47(2)	C9A	0.47(2)	H9A	0.47(2)
C11A	0.47(2)	H11A	0.47(2)	C12A	0.47(2)
H12A	0.47(2)	C33A	0.54(2)	H33A	0.54(2)
C34A	0.54(2)	H34A	0.54(2)	C35A	0.54(2)
H35A	0.54(2)	C36A	0.54(2)	H36A	0.54(2)

Table S4 Bond Lengths for $C_{42}H_{38}BrCuN_2P_2S$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	Cu1	2.5412(2)	C16	C17	1.384(3)
Cu1	S1	2.3576(3)	C17	C18	1.389(2)
Cu1	P1	2.2641(3)	C19	C20	1.3894(17)
Cu1	P2	2.2849(3)	C19	C24	1.3932(17)
S1	C37	1.7017(12)	C20	C21	1.3910(18)
P1	C1	1.8258(12)	C21	C22	1.379(2)
P1	C7	1.8337(12)	C22	C23	1.388(2)
P1	C13	1.8265(12)	C23	C24	1.3889(18)
P2	C19	1.8163(11)	C25	C26	1.4001(16)
P2	C25	1.8253(12)	C25	C30	1.3923(16)
P2	C31	1.8237(11)	C26	C27	1.3873(18)
N1	C37	1.3648(15)	C27	C28	1.386(2)
N1	C40	1.3506(15)	C28	C29	1.383(2)
N2	C37	1.3433(15)	C29	C30	1.3930(18)
N2	C38	1.3348(16)	C31	C32	1.3949(17)
C1	C2	1.4004(19)	C31	C36	1.400(8)
C1	C6	1.3859(19)	C31	C36A	1.382(7)
C2	C3	1.3880(19)	C32	C33	1.430(9)
C3	C4	1.383(3)	C32	C33A	1.364(8)
C4	C5	1.373(3)	C38	C39	1.3986(18)
C5	C6	1.396(2)	C38	C41	1.5003(19)
C7	C8	1.399(8)	C39	C40	1.3674(18)
C7	C12	1.406(7)	C40	C42	1.4902(18)
C7	C8A	1.402(9)	C8	C9	1.394(7)
C7	C12A	1.381(8)	C11	C12	1.393(7)
C10	C9	1.392(7)	C33	C34	1.379(8)
C10	C11	1.354(7)	C34	C35	1.347(7)
C10	C9A	1.373(8)	C35	C36	1.401(8)
C10	C11A	1.408(7)	C8A	C9A	1.385(8)
C13	C14	1.3948(17)	C11A	C12A	1.392(7)
C13	C18	1.3976(18)	C33A	C34A	1.369(7)
C14	C15	1.3943(18)	C34A	C35A	1.396(6)
C15	C16	1.382(2)	C35A	C36A	1.396(6)

Table S5 Bond Angles for $C_{42}H_{38}BrCuN_2P_2S$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
S1	Cu1	Br1	110.564(9)	C24	C19	P2	123.94(9)
P1	Cu1	Br1	104.957(10)	C19	C20	C21	120.61(13)
P1	Cu1	S1	113.000(12)	C22	C21	C20	120.02(13)
P1	Cu1	P2	125.153(12)	C21	C22	C23	119.81(12)
P2	Cu1	Br1	103.851(10)	C22	C23	C24	120.37(13)
P2	Cu1	S1	98.723(12)	C23	C24	C19	120.05(12)
C37	S1	Cu1	110.61(4)	C26	C25	P2	118.00(9)
C1	P1	Cu1	112.65(4)	C30	C25	P2	123.36(9)
C1	P1	C7	104.47(6)	C30	C25	C26	118.58(11)
C1	P1	C13	101.62(6)	C27	C26	C25	120.56(12)
C7	P1	Cu1	117.13(4)	C28	C27	C26	120.38(13)
C13	P1	Cu1	117.95(4)	C29	C28	C27	119.53(12)
C13	P1	C7	100.92(5)	C28	C29	C30	120.43(12)
C19	P2	Cu1	117.65(4)	C25	C30	C29	120.50(11)
C19	P2	C25	103.71(5)	C32	C31	P2	117.97(9)
C19	P2	C31	103.66(5)	C32	C31	C36	121.0(4)
C25	P2	Cu1	115.51(4)	C36	C31	P2	120.9(4)
C31	P2	Cu1	111.12(4)	C36A	C31	P2	124.6(3)
C31	P2	C25	103.62(5)	C36A	C31	C32	116.5(3)
C40	N1	C37	123.45(11)	C31	C32	C33	116.2(5)
C38	N2	C37	118.66(11)	C33A	C32	C31	124.3(4)
C2	C1	P1	117.12(10)	N1	C37	S1	119.89(9)
C6	C1	P1	123.84(11)	N2	C37	S1	120.68(9)
C6	C1	C2	119.03(12)	N2	C37	N1	119.38(10)
C3	C2	C1	120.45(14)	N2	C38	C39	122.74(12)
C4	C3	C2	119.98(16)	N2	C38	C41	116.70(12)
C5	C4	C3	119.88(14)	C39	C38	C41	120.55(12)
C4	C5	C6	120.78(16)	C40	C39	C38	118.23(11)
C1	C6	C5	119.86(16)	N1	C40	C39	117.52(11)
C8	C7	P1	119.2(4)	N1	C40	C42	118.16(11)
C8	C7	C12	118.4(5)	C39	C40	C42	124.30(11)
C12	C7	P1	122.4(4)	C9	C8	C7	120.6(6)
C8A	C7	P1	118.8(4)	C10	C9	C8	119.6(5)
C12A	C7	P1	122.0(4)	C10	C11	C12	121.2(5)
C12A	C7	C8A	119.2(6)	C11	C12	C7	119.9(6)
C11	C10	C9	120.3(4)	C34	C33	C32	122.0(8)
C9A	C10	C11A	119.2(5)	C35	C34	C33	120.1(7)
C14	C13	P1	123.43(10)	C34	C35	C36	120.6(5)
C14	C13	C18	119.09(12)	C31	C36	C35	119.6(6)
C18	C13	P1	117.35(10)	C9A	C8A	C7	119.8(7)
C15	C14	C13	120.10(13)	C10	C9A	C8A	121.3(6)
C16	C15	C14	120.55(14)	C12A	C11A	C10	119.5(6)
C15	C16	C17	119.44(13)	C7	C12A	C11A	120.9(7)
C16	C17	C18	120.78(15)	C32	C33A	C34A	118.1(7)
C17	C18	C13	120.04(14)	C33A	C34A	C35A	120.1(6)
C20	C19	P2	116.91(9)	C34A	C35A	C36A	120.2(4)
C20	C19	C24	119.14(11)	C31	C36A	C35A	120.5(5)

Table S6 Torsion Angles for $C_{42}H_{38}BrCuN_2P_2S$.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Cu1	S1	C37	N1	-28.88(10)	C14	C15	C16	C17	-0.6(2)
Cu1	S1	C37	N2	153.89(9)	C15	C16	C17	C18	-0.2(2)
Cu1	P1	C1	C2	55.30(10)	C16	C17	C18	C13	1.1(2)
Cu1	P1	C1	C6	-126.02(11)	C18	C13	C14	C15	0.31(19)
Cu1	P1	C7	C8	37.3(4)	C19	P2	C25	C26	174.90(10)
Cu1	P1	C7	C12	-139.2(5)	C19	P2	C25	C30	-2.18(11)
Cu1	P1	C7	C8A	25.2(5)	C19	P2	C31	C32	-61.36(11)
Cu1	P1	C7	C12A	-153.3(5)	C19	P2	C31	C36	116.1(4)
Cu1	P1	C13	C14	-133.58(9)	C19	P2	C31	C36A	130.6(4)
Cu1	P1	C13	C18	50.57(11)	C19	C20	C21	C22	0.2(2)
Cu1	P2	C19	C20	30.77(12)	C20	C19	C24	C23	0.5(2)
Cu1	P2	C19	C24	-150.43(10)	C20	C21	C22	C23	0.4(2)
Cu1	P2	C25	C26	44.68(11)	C21	C22	C23	C24	-0.5(3)
Cu1	P2	C25	C30	-132.40(9)	C22	C23	C24	C19	0.0(2)
Cu1	P2	C31	C32	65.93(10)	C24	C19	C20	C21	-0.6(2)
Cu1	P2	C31	C36	-116.6(4)	C25	P2	C19	C20	-98.16(11)
Cu1	P2	C31	C36A	-102.1(4)	C25	P2	C19	C24	80.64(12)
P1	C1	C2	C3	177.48(11)	C25	P2	C31	C32	-169.41(10)
P1	C1	C6	C5	-178.61(13)	C25	P2	C31	C36	8.1(4)
P1	C7	C8	C9	-177.5(3)	C25	P2	C31	C36A	22.6(4)
P1	C7	C12	C11	175.9(3)	C25	C26	C27	C28	1.3(2)
P1	C7	C8A	C9A	-175.9(4)	C26	C25	C30	C29	0.08(18)
P1	C7	C12A	C11A	178.1(4)	C26	C27	C28	C29	-0.3(2)
P1	C13	C14	C15	-175.47(10)	C27	C28	C29	C30	-0.9(2)
P1	C13	C18	C17	174.94(11)	C28	C29	C30	C25	1.0(2)
P2	C19	C20	C21	178.24(12)	C30	C25	C26	C27	-1.2(2)
P2	C19	C24	C23	-178.28(12)	C31	P2	C19	C20	153.86(10)
P2	C25	C26	C27	-178.45(12)	C31	P2	C19	C24	-27.34(12)
P2	C25	C30	C29	177.14(10)	C31	P2	C25	C26	-77.08(11)
P2	C31	C32	C33	-174.9(7)	C31	P2	C25	C30	105.84(10)
P2	C31	C32	C33A	-175.6(7)	C31	C32	C33	C34	-5.1(16)
P2	C31	C36	C35	177.4(4)	C31	C32	C33A	C34A	6.3(13)
P2	C31	C36A	C35A	170.7(3)	C32	C31	C36	C35	-5.2(8)
N2	C38	C39	C40	0.5(2)	C32	C31	C36A	C35A	2.5(6)
C1	P1	C7	C8	-88.1(4)	C32	C33	C34	C35	-0.2(17)
C1	P1	C7	C12	95.5(5)	C32	C33A	C34A	C35A	-1.8(13)
C1	P1	C7	C8A	-100.2(5)	C37	N1	C40	C39	-0.80(18)
C1	P1	C7	C12A	81.3(5)	C37	N1	C40	C42	177.52(12)
C1	P1	C13	C14	-9.92(12)	C37	N2	C38	C39	-1.5(2)
C1	P1	C13	C18	174.23(10)	C37	N2	C38	C41	179.26(13)
C1	C2	C3	C4	1.7(2)	C38	N2	C37	S1	178.67(10)
C2	C1	C6	C5	0.1(2)	C38	N2	C37	N1	1.43(17)
C2	C3	C4	C5	-0.9(3)	C38	C39	C40	N1	0.69(18)
C3	C4	C5	C6	-0.3(3)	C38	C39	C40	C42	-177.52(13)
C4	C5	C6	C1	0.8(3)	C40	N1	C37	S1	-177.54(10)
C6	C1	C2	C3	-1.3(2)	C40	N1	C37	N2	-0.27(18)

Table S6 Torsion Angles for $C_{42}H_{38}BrCuN_2P_2S$.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C7	P1	C1	C2	-176.54(9)	C41	C38	C39	C40	179.63(14)
C7	P1	C1	C6	2.15(13)	C8	C7	C12	C11	-0.6(7)
C7	P1	C13	C14	97.51(11)	C9	C10	C11	C12	-1.2(6)
C7	P1	C13	C18	-78.34(11)	C11	C10	C9	C8	-0.3(6)
C7	C8	C9	C10	1.3(6)	C12	C7	C8	C9	-0.9(7)
C7	C8A	C9A	C10	-2.7(8)	C33	C34	C35	C36	3.0(12)
C10	C11	C12	C7	1.6(7)	C34	C35	C36	C31	-0.4(9)
C10	C11A	C12A	C7	-1.9(7)	C36	C31	C32	C33	7.6(9)
C13	P1	C1	C2	-71.89(10)	C8A	C7	C12A	C11A	-0.4(8)
C13	P1	C1	C6	106.80(12)	C9A	C10	C11A	C12A	1.9(6)
C13	P1	C7	C8	166.8(4)	C11A	C10	C9A	C8A	0.4(6)
C13	P1	C7	C12	-9.7(5)	C12A	C7	C8A	C9A	2.7(8)
C13	P1	C7	C8A	154.7(5)	C33A	C34A	C35A	C36A	-1.9(9)
C13	P1	C7	C12A	-23.9(5)	C34A	C35A	C36A	C31	1.5(7)
C13	C14	C15	C16	0.5(2)	C36A	C31	C32	C33A	-6.6(8)
C14	C13	C18	C17	-1.1(2)					

Table S7 Hydrogen Bonds for $C_{42}H_{38}BrCuN_2P_2S$.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N1	H1	Br1	0.80(2)	2.45(2)	3.233(1)	168.9(17)
C32	H32A	Br1	0.95	3.13	3.841(2)	132.9
C42	H42C	Br1*	0.87(2)	3.03(2)	3.879(2)	164(2)
C8	H8	Br1	0.95	2.76	3.661(9)	158.4

Symmetry operator: 1-*x*,1-*y*,1-*z*