

Supplementary Information For:

**Evaluation of H₂CHXdedpa, H₂dedpa- and H₂CHXdedpa-*N,N'*-
propyl-2-NI Ligands for ⁶⁴Cu(II) Radiopharmaceuticals**

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X-ray structural data for [Cu(dedpa-*N,N'*-propyl-2-NI)]

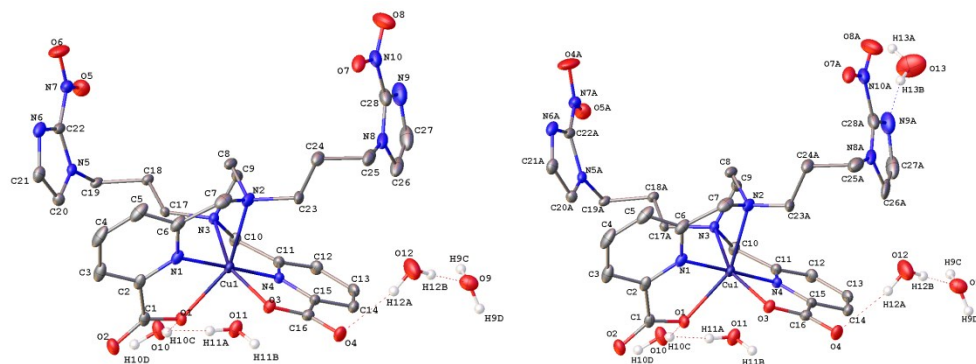


Figure S1. ORTEP of [Cu(dedpa-*N,N'*-propyl-2-NI)]]. Hydrogen atoms omitted for clarity. Ellipsoids drawn with 50% probability.

Crystal Data

Empirical Formula	C ₂₈ H _{38.4} N ₁₀ O _{12.2} Cu
Formula Weight	773.66
Crystal Colour, Habit	blue, blade
Crystal Dimensions	0.03 x 0.09 x 0.25 mm
Crystal System	orthorhombic
Lattice Type	Primitive
Lattice Parameters	a = 13.1713(14) Å b = 15.936(2) Å c = 31.481(3) Å α = 90° β = 90° γ = 90° V 6607.8(12) Å ³
Space Group	<i>P bca</i> (#61)
Z value	8
D _{calc}	1.555 g/cm ³
F ₀₀₀	3223.00
μ(Mo-Kα)	7.41 cm ⁻¹

Bond lengths [Å] and angles [deg] for [Cu(C₂₈H₃₀N₁₀O₈)]·4.2H₂O

Cu (1) – O (1)	2.2128 (12)
Cu (1) – O (3)	2.0741 (11)

Cu(1)-N(1)	1.9664(13)
Cu(1)-N(2)	2.3173(14)
Cu(1)-N(3)	2.2562(13)
Cu(1)-N(4)	1.9263(13)
O(1)-C(1)	1.2685(19)
O(2)-C(1)	1.244(2)
O(3)-C(16)	1.2723(19)
O(4)-C(16)	1.2431(19)
O(9)-H(9C)	0.85(3)
O(9)-H(9D)	0.77(3)
O(10)-H(10C)	0.81(3)
O(10)-H(10D)	0.81(3)
O(11)-H(11A)	0.80(3)
O(11)-H(11B)	0.77(3)
O(12)-H(12A)	0.81(3)
O(12)-H(12B)	0.84(3)
N(1)-C(2)	1.347(2)
N(1)-C(6)	1.344(2)
N(2)-C(7)	1.474(2)
N(2)-C(8)	1.477(2)
N(2)-C(23)	1.508(4)
N(2)-C(23A)	1.33(2)
N(3)-C(9)	1.482(2)
N(3)-C(10)	1.483(2)
N(3)-C(17)	1.471(10)
N(3)-C(17A)	1.56(5)
N(4)-C(11)	1.3374(19)
N(4)-C(15)	1.345(2)
C(1)-C(2)	1.521(2)
C(2)-C(3)	1.389(2)
C(3)-H(3)	0.9500
C(3)-C(4)	1.393(3)
C(4)-H(4)	0.9500
C(4)-C(5)	1.381(3)
C(5)-H(5)	0.9500
C(5)-C(6)	1.394(3)
C(6)-C(7)	1.512(3)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(8)-C(9)	1.518(2)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(10)-C(11)	1.511(2)
C(11)-C(12)	1.390(2)
C(12)-H(12)	0.9500
C(12)-C(13)	1.386(2)
C(13)-H(13)	0.9500
C(13)-C(14)	1.396(2)

C (14) -H (14)	0.9500
C (14) -C (15)	1.386 (2)
C (15) -C (16)	1.522 (2)
C (17) -H (17A)	0.9900
C (17) -H (17B)	0.9900
C (17) -C (18)	1.532 (3)
C (18) -H (18A)	0.9900
C (18) -H (18B)	0.9900
C (18) -C (19)	1.529 (3)
O (5) -N (7)	1.227 (3)
O (6) -N (7)	1.236 (3)
N (5) -C (20)	1.368 (3)
N (5) -C (22)	1.361 (5)
N (5) -C (19)	1.485 (3)
N (6) -C (21)	1.356 (3)
N (6) -C (22)	1.320 (3)
N (7) -C (22)	1.440 (3)
C (19A) -H (19A)	0.9900
C (19A) -H (19B)	0.9900
C (19A) -N (5A)	1.478 (9)
C (19A) -C (18A)	1.530 (9)
C (20) -H (20)	0.9500
C (20) -C (21)	1.369 (4)
C (21) -H (21)	0.9500
C (23) -H (23A)	0.9900
C (23) -H (23B)	0.9900
C (23) -C (24)	1.509 (6)
C (23A) -H (23C)	0.9900
C (23A) -H (23D)	0.9900
C (23A) -C (24A)	1.62 (3)
C (24) -H (24A)	0.9900
C (24) -H (24B)	0.9900
C (24) -C (25)	1.530 (4)
C (24A) -H (24C)	0.9900
C (24A) -H (24D)	0.9900
C (24A) -C (25A)	1.50 (2)
C (25) -H (25A)	0.9900
C (25) -H (25B)	0.9900
C (25) -N (8)	1.467 (4)
C (25A) -H (25C)	0.9900
C (25A) -H (25D)	0.9900
C (25A) -N (8A)	1.442 (17)
O (7) -N (10)	1.227 (5)
O (8) -N (10)	1.229 (4)
N (8) -C (26)	1.372 (4)
N (8) -C (28)	1.369 (4)
N (9) -C (27)	1.369 (4)
N (9) -C (28)	1.329 (4)
N (10) -C (28)	1.421 (6)
C (26) -H (26)	0.9500
C (26) -C (27)	1.372 (5)
C (27) -H (27)	0.9500

O (7A) -N (10A)	1.20 (3)
O (8A) -N (10A)	1.20 (2)
N (8A) -C (26A)	1.405 (17)
N (8A) -C (28A)	1.335 (18)
N (9A) -C (27A)	1.39 (3)
N (9A) -C (28A)	1.310 (9)
N (10A) -C (28A)	1.54 (3)
C (26A) -H (26A)	0.9500
C (26A) -C (27A)	1.38 (2)
C (27A) -H (27A)	0.9500
O (13) -H (13A)	0.8496
O (13) -H (13B)	0.8505
N (7A) -O (5A)	1.16 (2)
N (7A) -C (22A)	1.44 (2)
N (7A) -O (4A)	1.287 (17)
C (22A) -N (6A)	1.285 (16)
C (22A) -N (5A)	1.43 (3)
N (6A) -C (21A)	1.320 (16)
C (21A) -H (21A)	0.9500
C (21A) -C (20A)	1.44 (2)
C (19) -H (19C)	0.9900
C (19) -H (19D)	0.9900
C (20A) -H (20A)	0.9500
C (20A) -N (5A)	1.275 (19)
C (18A) -H (18C)	0.9900
C (18A) -H (18D)	0.9900
C (18A) -C (17A)	1.532 (9)
C (17A) -H (17C)	0.9900
C (17A) -H (17D)	0.9900
O (1) -Cu (1) -N (2)	153.81 (5)
O (1) -Cu (1) -N (3)	94.14 (4)
O (3) -Cu (1) -O (1)	100.39 (4)
O (3) -Cu (1) -N (2)	94.22 (5)
O (3) -Cu (1) -N (3)	156.44 (5)
N (1) -Cu (1) -O (1)	78.14 (5)
N (1) -Cu (1) -O (3)	99.90 (5)
N (1) -Cu (1) -N (2)	78.01 (6)
N (1) -Cu (1) -N (3)	101.18 (5)
N (3) -Cu (1) -N (2)	80.04 (5)
N (4) -Cu (1) -O (1)	100.52 (5)
N (4) -Cu (1) -O (3)	80.72 (5)
N (4) -Cu (1) -N (1)	178.59 (6)
N (4) -Cu (1) -N (2)	103.22 (6)
N (4) -Cu (1) -N (3)	78.45 (5)
C (1) -O (1) -Cu (1)	112.61 (10)
C (16) -O (3) -Cu (1)	113.56 (10)
H (9C) -O (9) -H (9D)	107 (2)
H (10C) -O (10) -H (10D)	106 (2)
H (11A) -O (11) -H (11B)	110 (2)
H (12A) -O (12) -H (12B)	106 (3)
C (2) -N (1) -Cu (1)	118.27 (11)

C(6)-N(1)-Cu(1)	120.47(12)
C(6)-N(1)-C(2)	120.88(15)
C(7)-N(2)-Cu(1)	103.68(10)
C(7)-N(2)-C(8)	110.88(13)
C(7)-N(2)-C(23)	114.90(19)
C(8)-N(2)-Cu(1)	105.71(10)
C(8)-N(2)-C(23)	112.2(2)
C(23)-N(2)-Cu(1)	108.7(2)
C(23A)-N(2)-Cu(1)	109.9(11)
C(23A)-N(2)-C(7)	103.2(9)
C(23A)-N(2)-C(8)	122.1(10)
C(9)-N(3)-Cu(1)	105.59(9)
C(9)-N(3)-C(10)	110.53(13)
C(9)-N(3)-C(17A)	118.8(14)
C(10)-N(3)-Cu(1)	103.66(9)
C(10)-N(3)-C(17A)	110.7(17)
C(17)-N(3)-Cu(1)	111.7(3)
C(17)-N(3)-C(9)	112.1(3)
C(17)-N(3)-C(10)	112.8(4)
C(17A)-N(3)-Cu(1)	106.3(13)
C(11)-N(4)-Cu(1)	121.44(11)
C(11)-N(4)-C(15)	121.59(14)
C(15)-N(4)-Cu(1)	116.88(10)
O(1)-C(1)-C(2)	115.68(14)
O(2)-C(1)-O(1)	126.41(16)
O(2)-C(1)-C(2)	117.91(14)
N(1)-C(2)-C(1)	114.69(14)
N(1)-C(2)-C(3)	121.35(16)
C(3)-C(2)-C(1)	123.95(16)
C(2)-C(3)-H(3)	120.9
C(2)-C(3)-C(4)	118.15(18)
C(4)-C(3)-H(3)	120.9
C(3)-C(4)-H(4)	120.0
C(5)-C(4)-C(3)	119.98(17)
C(5)-C(4)-H(4)	120.0
C(4)-C(5)-H(5)	120.3
C(4)-C(5)-C(6)	119.32(18)
C(6)-C(5)-H(5)	120.3
N(1)-C(6)-C(5)	120.25(17)
N(1)-C(6)-C(7)	115.59(15)
C(5)-C(6)-C(7)	124.15(16)
N(2)-C(7)-C(6)	109.92(13)
N(2)-C(7)-H(7A)	109.7
N(2)-C(7)-H(7B)	109.7
C(6)-C(7)-H(7A)	109.7
C(6)-C(7)-H(7B)	109.7
H(7A)-C(7)-H(7B)	108.2
N(2)-C(8)-H(8A)	109.4
N(2)-C(8)-H(8B)	109.4
N(2)-C(8)-C(9)	110.95(13)
H(8A)-C(8)-H(8B)	108.0
C(9)-C(8)-H(8A)	109.4

C (9) -C (8) -H (8B)	109.4
N (3) -C (9) -C (8)	112.05 (13)
N (3) -C (9) -H (9A)	109.2
N (3) -C (9) -H (9B)	109.2
C (8) -C (9) -H (9A)	109.2
C (8) -C (9) -H (9B)	109.2
H (9A) -C (9) -H (9B)	107.9
N (3) -C (10) -H (10A)	109.7
N (3) -C (10) -H (10B)	109.7
N (3) -C (10) -C (11)	109.66 (13)
H (10A) -C (10) -H (10B)	108.2
C (11) -C (10) -H (10A)	109.7
C (11) -C (10) -H (10B)	109.7
N (4) -C (11) -C (10)	114.27 (13)
N (4) -C (11) -C (12)	120.20 (14)
C (12) -C (11) -C (10)	125.52 (14)
C (11) -C (12) -H (12)	120.6
C (13) -C (12) -C (11)	118.86 (14)
C (13) -C (12) -H (12)	120.6
C (12) -C (13) -H (13)	119.8
C (12) -C (13) -C (14)	120.43 (15)
C (14) -C (13) -H (13)	119.8
C (13) -C (14) -H (14)	121.2
C (15) -C (14) -C (13)	117.66 (15)
C (15) -C (14) -H (14)	121.2
N (4) -C (15) -C (14)	121.25 (14)
N (4) -C (15) -C (16)	113.17 (13)
C (14) -C (15) -C (16)	125.57 (14)
O (3) -C (16) -C (15)	115.15 (13)
O (4) -C (16) -O (3)	126.88 (15)
O (4) -C (16) -C (15)	117.97 (14)
N (3) -C (17) -H (17A)	107.5
N (3) -C (17) -H (17B)	107.5
N (3) -C (17) -C (18)	119.4 (6)
H (17A) -C (17) -H (17B)	107.0
C (18) -C (17) -H (17A)	107.5
C (18) -C (17) -H (17B)	107.5
C (17) -C (18) -H (18A)	109.2
C (17) -C (18) -H (18B)	109.2
H (18A) -C (18) -H (18B)	107.9
C (19) -C (18) -C (17)	111.8 (8)
C (19) -C (18) -H (18A)	109.2
C (19) -C (18) -H (18B)	109.3
C (20) -N (5) -C (19)	124.6 (4)
C (22) -N (5) -C (20)	104.1 (3)
C (22) -N (5) -C (19)	131.1 (3)
C (22) -N (6) -C (21)	103.55 (19)
O (5) -N (7) -O (6)	124.5 (2)
O (5) -N (7) -C (22)	118.61 (19)
O (6) -N (7) -C (22)	116.9 (2)
H (19A) -C (19A) -H (19B)	108.4
N (5A) -C (19A) -H (19A)	110.0

N(5A)-C(19A)-H(19B)	110.0
N(5A)-C(19A)-C(18A)	109(3)
C(18A)-C(19A)-H(19A)	110.0
C(18A)-C(19A)-H(19B)	110.0
N(5)-C(20)-H(20)	126.5
N(5)-C(20)-C(21)	107.1(3)
C(21)-C(20)-H(20)	126.5
N(6)-C(21)-C(20)	110.9(2)
N(6)-C(21)-H(21)	124.6
C(20)-C(21)-H(21)	124.6
N(5)-C(22)-N(7)	123.9(2)
N(6)-C(22)-N(5)	114.4(2)
N(6)-C(22)-N(7)	121.7(2)
N(2)-C(23)-H(23A)	108.0
N(2)-C(23)-H(23B)	108.0
N(2)-C(23)-C(24)	117.0(3)
H(23A)-C(23)-H(23B)	107.3
C(24)-C(23)-H(23A)	108.0
C(24)-C(23)-H(23B)	108.0
N(2)-C(23A)-H(23C)	107.7
N(2)-C(23A)-H(23D)	107.7
N(2)-C(23A)-C(24A)	118.4(17)
H(23C)-C(23A)-H(23D)	107.1
C(24A)-C(23A)-H(23C)	107.7
C(24A)-C(23A)-H(23D)	107.7
C(23)-C(24)-H(24A)	109.7
C(23)-C(24)-H(24B)	109.7
C(23)-C(24)-C(25)	109.6(2)
H(24A)-C(24)-H(24B)	108.2
C(25)-C(24)-H(24A)	109.7
C(25)-C(24)-H(24B)	109.7
C(23A)-C(24A)-H(24C)	109.4
C(23A)-C(24A)-H(24D)	109.4
H(24C)-C(24A)-H(24D)	108.0
C(25A)-C(24A)-C(23A)	111.0(13)
C(25A)-C(24A)-H(24C)	109.4
C(25A)-C(24A)-H(24D)	109.4
C(24)-C(25)-H(25A)	109.3
C(24)-C(25)-H(25B)	109.3
H(25A)-C(25)-H(25B)	108.0
N(8)-C(25)-C(24)	111.5(2)
N(8)-C(25)-H(25A)	109.3
N(8)-C(25)-H(25B)	109.3
C(24A)-C(25A)-H(25C)	109.7
C(24A)-C(25A)-H(25D)	109.7
H(25C)-C(25A)-H(25D)	108.2
N(8A)-C(25A)-C(24A)	109.9(13)
N(8A)-C(25A)-H(25C)	109.7
N(8A)-C(25A)-H(25D)	109.7
C(26)-N(8)-C(25)	125.1(3)
C(28)-N(8)-C(25)	130.4(2)
C(28)-N(8)-C(26)	104.4(3)

C (28) -N (9) -C (27)	102.8 (3)
O (7) -N (10) -O (8)	122.4 (6)
O (7) -N (10) -C (28)	119.3 (5)
O (8) -N (10) -C (28)	118.4 (4)
N (8) -C (26) -H (26)	126.6
C (27) -C (26) -N (8)	106.7 (3)
C (27) -C (26) -H (26)	126.6
N (9) -C (27) -C (26)	111.5 (3)
N (9) -C (27) -H (27)	124.2
C (26) -C (27) -H (27)	124.2
N (8) -C (28) -N (10)	123.3 (3)
N (9) -C (28) -N (8)	114.6 (2)
N (9) -C (28) -N (10)	122.1 (3)
C (26A) -N (8A) -C (25A)	124.2 (14)
C (28A) -N (8A) -C (25A)	132.0 (12)
C (28A) -N (8A) -C (26A)	103.8 (14)
C (28A) -N (9A) -C (27A)	98.9 (14)
O (7A) -N (10A) -C (28A)	117 (3)
O (8A) -N (10A) -O (7A)	129 (3)
O (8A) -N (10A) -C (28A)	114 (3)
N (8A) -C (26A) -H (26A)	128.1
C (27A) -C (26A) -N (8A)	103.9 (16)
C (27A) -C (26A) -H (26A)	128.1
N (9A) -C (27A) -H (27A)	123.1
C (26A) -C (27A) -N (9A)	113.7 (17)
C (26A) -C (27A) -H (27A)	123.1
N (8A) -C (28A) -N (10A)	122.0 (14)
N (9A) -C (28A) -N (8A)	119.2 (14)
N (9A) -C (28A) -N (10A)	118.5 (16)
H (13A) -O (13) -H (13B)	109.5
O (5A) -N (7A) -C (22A)	125.0 (14)
O (5A) -N (7A) -O (4A)	125.6 (16)
O (4A) -N (7A) -C (22A)	109.5 (16)
N (6A) -C (22A) -N (7A)	130.1 (13)
N (6A) -C (22A) -N (5A)	111.1 (13)
N (5A) -C (22A) -N (7A)	118.6 (14)
C (22A) -N (6A) -C (21A)	108.5 (11)
N (6A) -C (21A) -H (21A)	126.8
N (6A) -C (21A) -C (20A)	106.3 (12)
C (20A) -C (21A) -H (21A)	126.8
C (18) -C (19) -H (19C)	109.0
C (18) -C (19) -H (19D)	109.0
N (5) -C (19) -C (18)	113.0 (6)
N (5) -C (19) -H (19C)	109.0
N (5) -C (19) -H (19D)	109.0
H (19C) -C (19) -H (19D)	107.8
C (21A) -C (20A) -H (20A)	125.1
N (5A) -C (20A) -C (21A)	109.7 (16)
N (5A) -C (20A) -H (20A)	125.1
C (22A) -N (5A) -C (19A)	136 (2)
C (20A) -N (5A) -C (19A)	119 (3)
C (20A) -N (5A) -C (22A)	104.3 (17)

C (19A) - C (18A) - H (18C)	110.5
C (19A) - C (18A) - H (18D)	110.5
C (19A) - C (18A) - C (17A)	106 (4)
H (18C) - C (18A) - H (18D)	108.7
C (17A) - C (18A) - H (18C)	110.5
C (17A) - C (18A) - H (18D)	110.5
N (3) - C (17A) - H (17C)	110.3
N (3) - C (17A) - H (17D)	110.3
C (18A) - C (17A) - N (3)	107 (3)
C (18A) - C (17A) - H (17C)	110.3
C (18A) - C (17A) - H (17D)	110.3
H (17C) - C (17A) - H (17D)	108.6

X-ray structural data for [Cu(CHXdedpa-*N,N'*-propyl-2-NI)]

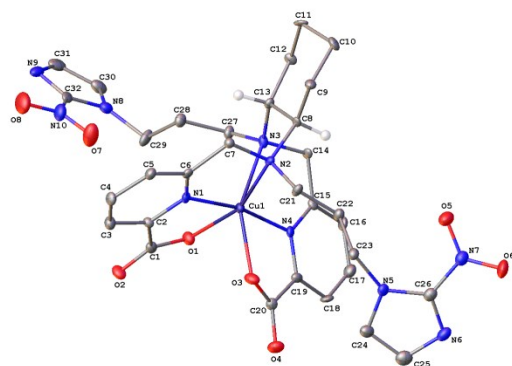


Figure S2. ORTEP of [Cu(CHXdedpa-*N,N'*-propyl-2-NI)]. Hydrogen atoms omitted for clarity. Ellipsoids drawn with 50% probability.

Crystal Data

Empirical Formula	C ₃₂ H ₃₇ N ₁₀ O ₈ Cu
Formula Weight	753.25
Crystal Colour, Habit	green, irregular
Crystal Dimensions	0.09 x 0.10 x 0.18 mm
Crystal System	tetragonal
Lattice Type	primitive
Lattice Parameters	a = 8.344(1) Å b = 8.344 Å c = 44.637(6) Å

	$\alpha = 90^\circ$
	$\beta = 90^\circ$
	$\gamma = 90^\circ$
	$V = 3107.5(8) \text{ \AA}^3$
Space Group	$P 4_1$ (#76)
Z value	4
D _{calc}	1.610 g/cm ³
F ₀₀₀	1568.00
$\mu(\text{MoK}\alpha)$	7.76 cm ⁻¹

Bond lengths [$\text{\AA}$] and angles [deg] for $[\text{Cu}(\text{C}_{32}\text{H}_{36}\text{N}_{10}\text{O}_8)]$

C (1) – C (2)	1.513 (7)
C (1) – O (1)	1.282 (5)
C (1) – O (2)	1.236 (6)
C (2) – C (3)	1.375 (6)
C (2) – N (1)	1.340 (6)
C (3) – H (3)	0.9500
C (3) – C (4)	1.406 (7)
C (4) – H (4)	0.9500
C (4) – C (5)	1.384 (7)
C (5) – H (5)	0.9500
C (5) – C (6)	1.390 (6)
C (6) – C (7)	1.496 (6)
C (6) – N (1)	1.336 (6)
C (7) – H (7A)	0.9900
C (7) – H (7B)	0.9900
C (7) – N (2)	1.489 (5)
C (8) – H (8)	1.0000
C (8) – C (9)	1.525 (6)
C (8) – C (13)	1.536 (6)
C (8) – N (2)	1.497 (5)
C (9) – H (9A)	0.9900
C (9) – H (9B)	0.9900
C (9) – C (10)	1.524 (7)
C (10) – H (10A)	0.9900
C (10) – H (10B)	0.9900
C (10) – C (11)	1.519 (6)
C (11) – H (11A)	0.9900
C (11) – H (11B)	0.9900
C (11) – C (12)	1.521 (6)
C (12) – H (12A)	0.9900
C (12) – H (12B)	0.9900
C (12) – C (13)	1.535 (6)
C (13) – H (13)	1.0000
C (13) – N (3)	1.497 (6)
C (14) – H (14A)	0.9900

C (14) -H (14B)	0.9900
C (14) -C (15)	1.481 (6)
C (14) -N (3)	1.479 (6)
C (15) -C (16)	1.389 (6)
C (15) -N (4)	1.341 (6)
C (16) -H (16)	0.9500
C (16) -C (17)	1.387 (7)
C (17) -H (17)	0.9500
C (17) -C (18)	1.388 (7)
C (18) -H (18)	0.9500
C (18) -C (19)	1.383 (6)
C (19) -C (20)	1.526 (7)
C (19) -N (4)	1.342 (6)
C (20) -O (3)	1.259 (6)
C (20) -O (4)	1.247 (6)
C (21) -H (21A)	0.9900
C (21) -H (21B)	0.9900
C (21) -C (22)	1.532 (6)
C (21) -N (2)	1.483 (5)
C (22) -H (22A)	0.9900
C (22) -H (22B)	0.9900
C (22) -C (23)	1.533 (7)
C (23) -H (23A)	0.9900
C (23) -H (23B)	0.9900
C (23) -N (5)	1.485 (6)
C (24) -H (24)	0.9500
C (24) -C (25)	1.370 (7)
C (24) -N (5)	1.362 (6)
C (25) -H (25)	0.9500
C (25) -N (6)	1.368 (7)
C (26) -N (5)	1.369 (6)
C (26) -N (6)	1.295 (6)
C (26) -N (7)	1.432 (6)
C (27) -H (27A)	0.9900
C (27) -H (27B)	0.9900
C (27) -C (28)	1.529 (6)
C (27) -N (3)	1.476 (6)
C (28) -H (28A)	0.9900
C (28) -H (28B)	0.9900
C (28) -C (29)	1.536 (7)
C (29) -H (29A)	0.9900
C (29) -H (29B)	0.9900
C (29) -N (8)	1.464 (6)
C (30) -H (30)	0.9500
C (30) -C (31)	1.361 (7)
C (30) -N (8)	1.373 (6)
C (31) -H (31)	0.9500
C (31) -N (9)	1.369 (7)
C (32) -N (8)	1.363 (6)
C (32) -N (9)	1.317 (6)
C (32) -N (10)	1.437 (7)
N (1) -Cu (1)	1.937 (4)

N(2)-Cu(1)	2.311(4)
N(3)-Cu(1)	2.342(4)
N(4)-Cu(1)	1.968(4)
N(6)-H(6)	0.8800
N(7)-O(5)	1.237(5)
N(7)-O(6)	1.230(5)
N(10)-O(7)	1.220(6)
N(10)-O(8)	1.231(5)
O(1)-Cu(1)	2.110(3)
O(3)-Cu(1)	2.230(3)
O(1)-C(1)-C(2)	113.8(4)
O(2)-C(1)-C(2)	119.2(4)
O(2)-C(1)-O(1)	127.0(5)
C(3)-C(2)-C(1)	124.1(4)
N(1)-C(2)-C(1)	115.2(4)
N(1)-C(2)-C(3)	120.6(4)
C(2)-C(3)-H(3)	120.4
C(2)-C(3)-C(4)	119.2(4)
C(4)-C(3)-H(3)	120.4
C(3)-C(4)-H(4)	120.7
C(5)-C(4)-C(3)	118.6(4)
C(5)-C(4)-H(4)	120.7
C(4)-C(5)-H(5)	120.2
C(4)-C(5)-C(6)	119.6(5)
C(6)-C(5)-H(5)	120.2
C(5)-C(6)-C(7)	123.3(5)
N(1)-C(6)-C(5)	120.1(4)
N(1)-C(6)-C(7)	116.4(4)
C(6)-C(7)-H(7A)	109.3
C(6)-C(7)-H(7B)	109.3
H(7A)-C(7)-H(7B)	108.0
N(2)-C(7)-C(6)	111.6(4)
N(2)-C(7)-H(7A)	109.3
N(2)-C(7)-H(7B)	109.3
C(9)-C(8)-H(8)	106.9
C(9)-C(8)-C(13)	113.8(4)
C(13)-C(8)-H(8)	106.9
N(2)-C(8)-H(8)	106.9
N(2)-C(8)-C(9)	113.4(4)
N(2)-C(8)-C(13)	108.5(3)
C(8)-C(9)-H(9A)	109.4
C(8)-C(9)-H(9B)	109.4
H(9A)-C(9)-H(9B)	108.0
C(10)-C(9)-C(8)	111.1(4)
C(10)-C(9)-H(9A)	109.4
C(10)-C(9)-H(9B)	109.4
C(9)-C(10)-H(10A)	109.8
C(9)-C(10)-H(10B)	109.8
H(10A)-C(10)-H(10B)	108.2
C(11)-C(10)-C(9)	109.4(4)
C(11)-C(10)-H(10A)	109.8

C(11)-C(10)-H(10B)	109.8
C(10)-C(11)-H(11A)	109.8
C(10)-C(11)-H(11B)	109.8
C(10)-C(11)-C(12)	109.4(4)
H(11A)-C(11)-H(11B)	108.2
C(12)-C(11)-H(11A)	109.8
C(12)-C(11)-H(11B)	109.8
C(11)-C(12)-H(12A)	109.3
C(11)-C(12)-H(12B)	109.3
C(11)-C(12)-C(13)	111.6(4)
H(12A)-C(12)-H(12B)	108.0
C(13)-C(12)-H(12A)	109.3
C(13)-C(12)-H(12B)	109.3
C(8)-C(13)-H(13)	107.0
C(12)-C(13)-C(8)	112.8(4)
C(12)-C(13)-H(13)	107.0
N(3)-C(13)-C(8)	108.9(3)
N(3)-C(13)-C(12)	113.7(3)
N(3)-C(13)-H(13)	107.0
H(14A)-C(14)-H(14B)	107.9
C(15)-C(14)-H(14A)	109.2
C(15)-C(14)-H(14B)	109.2
N(3)-C(14)-H(14A)	109.2
N(3)-C(14)-H(14B)	109.2
N(3)-C(14)-C(15)	112.2(4)
C(16)-C(15)-C(14)	122.4(4)
N(4)-C(15)-C(14)	117.0(4)
N(4)-C(15)-C(16)	120.5(4)
C(15)-C(16)-H(16)	120.5
C(17)-C(16)-C(15)	119.1(5)
C(17)-C(16)-H(16)	120.5
C(16)-C(17)-H(17)	120.2
C(18)-C(17)-C(16)	119.5(4)
C(18)-C(17)-H(17)	120.2
C(17)-C(18)-H(18)	120.6
C(19)-C(18)-C(17)	118.8(4)
C(19)-C(18)-H(18)	120.6
C(18)-C(19)-C(20)	123.4(4)
N(4)-C(19)-C(18)	121.0(4)
N(4)-C(19)-C(20)	115.3(4)
O(3)-C(20)-C(19)	115.1(4)
O(4)-C(20)-C(19)	116.8(4)
O(4)-C(20)-O(3)	128.0(4)
H(21A)-C(21)-H(21B)	107.5
C(22)-C(21)-H(21A)	108.5
C(22)-C(21)-H(21B)	108.5
N(2)-C(21)-H(21A)	108.5
N(2)-C(21)-H(21B)	108.5
N(2)-C(21)-C(22)	115.1(4)
C(21)-C(22)-H(22A)	110.3
C(21)-C(22)-H(22B)	110.3
C(21)-C(22)-C(23)	107.0(4)

H (22A) -C (22) -H (22B)	108.6
C (23) -C (22) -H (22A)	110.3
C (23) -C (22) -H (22B)	110.3
C (22) -C (23) -H (23A)	108.8
C (22) -C (23) -H (23B)	108.8
H (23A) -C (23) -H (23B)	107.7
N (5) -C (23) -C (22)	114.0 (4)
N (5) -C (23) -H (23A)	108.8
N (5) -C (23) -H (23B)	108.8
C (25) -C (24) -H (24)	126.1
N (5) -C (24) -H (24)	126.1
N (5) -C (24) -C (25)	107.8 (4)
C (24) -C (25) -H (25)	125.2
N (6) -C (25) -C (24)	109.5 (5)
N (6) -C (25) -H (25)	125.2
N (5) -C (26) -N (7)	123.1 (4)
N (6) -C (26) -N (5)	114.6 (4)
N (6) -C (26) -N (7)	122.2 (4)
H (27A) -C (27) -H (27B)	107.5
C (28) -C (27) -H (27A)	108.5
C (28) -C (27) -H (27B)	108.5
N (3) -C (27) -H (27A)	108.5
N (3) -C (27) -H (27B)	108.5
N (3) -C (27) -C (28)	115.1 (4)
C (27) -C (28) -H (28A)	110.3
C (27) -C (28) -H (28B)	110.3
C (27) -C (28) -C (29)	107.3 (4)
H (28A) -C (28) -H (28B)	108.5
C (29) -C (28) -H (28A)	110.3
C (29) -C (28) -H (28B)	110.3
C (28) -C (29) -H (29A)	108.3
C (28) -C (29) -H (29B)	108.3
H (29A) -C (29) -H (29B)	107.4
N (8) -C (29) -C (28)	116.0 (4)
N (8) -C (29) -H (29A)	108.3
N (8) -C (29) -H (29B)	108.3
C (31) -C (30) -H (30)	126.3
C (31) -C (30) -N (8)	107.5 (5)
N (8) -C (30) -H (30)	126.3
C (30) -C (31) -H (31)	124.8
C (30) -C (31) -N (9)	110.5 (5)
N (9) -C (31) -H (31)	124.8
N (8) -C (32) -N (10)	123.1 (4)
N (9) -C (32) -N (8)	114.4 (5)
N (9) -C (32) -N (10)	122.6 (4)
C (2) -N (1) -Cu (1)	115.2 (3)
C (6) -N (1) -C (2)	121.7 (4)
C (6) -N (1) -Cu (1)	122.3 (3)
C (7) -N (2) -C (8)	111.4 (3)
C (7) -N (2) -Cu (1)	106.4 (3)
C (8) -N (2) -Cu (1)	110.0 (3)
C (21) -N (2) -C (7)	107.2 (3)

C (21) -N (2) -C (8)	113.7 (3)
C (21) -N (2) -Cu (1)	107.8 (3)
C (13) -N (3) -Cu (1)	108.0 (2)
C (14) -N (3) -C (13)	112.3 (4)
C (14) -N (3) -Cu (1)	106.5 (3)
C (27) -N (3) -C (13)	115.2 (3)
C (27) -N (3) -C (14)	106.6 (3)
C (27) -N (3) -Cu (1)	107.8 (3)
C (15) -N (4) -C (19)	121.0 (4)
C (15) -N (4) -Cu (1)	122.2 (3)
C (19) -N (4) -Cu (1)	116.2 (3)
C (24) -N (5) -C (23)	123.4 (4)
C (24) -N (5) -C (26)	103.7 (4)
C (26) -N (5) -C (23)	132.0 (4)
C (25) -N (6) -H (6)	127.8
C (26) -N (6) -C (25)	104.4 (4)
C (26) -N (6) -H (6)	127.8
O (5) -N (7) -C (26)	118.1 (4)
O (6) -N (7) -C (26)	117.9 (4)
O (6) -N (7) -O (5)	124.0 (4)
C (30) -N (8) -C (29)	122.9 (4)
C (32) -N (8) -C (29)	132.8 (4)
C (32) -N (8) -C (30)	104.0 (4)
C (32) -N (9) -C (31)	103.7 (4)
O (7) -N (10) -C (32)	118.3 (4)
O (7) -N (10) -O (8)	124.2 (5)
O (8) -N (10) -C (32)	117.5 (4)
C (1) -O (1) -Cu (1)	112.1 (3)
C (20) -O (3) -Cu (1)	110.2 (3)
N (1) -Cu (1) -N (2)	78.49 (14)
N (1) -Cu (1) -N (3)	112.92 (14)
N (1) -Cu (1) -N (4)	168.42 (16)
N (1) -Cu (1) -O (1)	79.95 (14)
N (1) -Cu (1) -O (3)	93.11 (14)
N (2) -Cu (1) -N (3)	76.32 (11)
N (4) -Cu (1) -N (2)	110.03 (14)
N (4) -Cu (1) -N (3)	77.39 (15)
N (4) -Cu (1) -O (1)	92.49 (14)
N (4) -Cu (1) -O (3)	77.62 (14)
O (1) -Cu (1) -N (2)	156.93 (12)
O (1) -Cu (1) -N (3)	104.98 (13)
O (1) -Cu (1) -O (3)	86.81 (12)
O (3) -Cu (1) -N (2)	102.42 (12)
O (3) -Cu (1) -N (3)	152.74 (13)

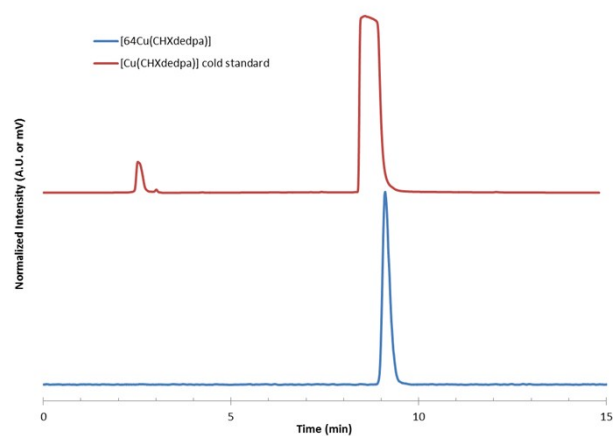


Figure S3. HPLC radio-chromatogram of [$^{64}\text{Cu}(\text{CHXdedpa})$] (blue line, bottom) and corresponding UV-Vis chromatogram of [$^{\text{nat}}\text{Cu}(\text{CHXdedpa})$] (red line, top).

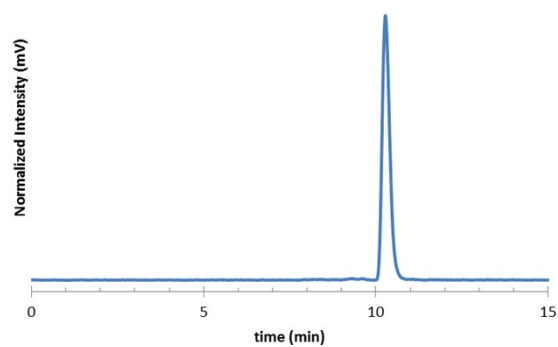


Figure S4. HPLC radio-chromatogram of [$^{64}\text{Cu}(\text{dedpa-}N,N'\text{-propyl-2-NI})$].