

Electronic Supplementary Information

Highly Selective Cu²⁺ Detection with a Naphthalimide-Functionalised Pillar[5]arene Fluorescent Chemosensor

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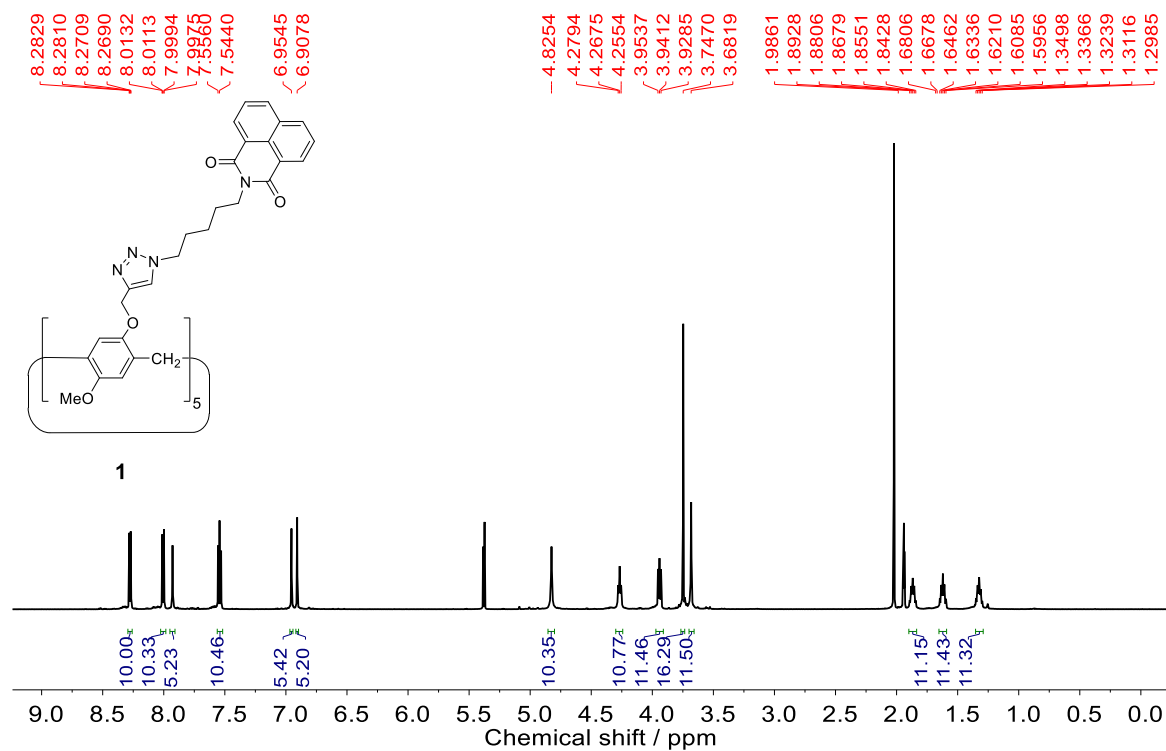


Fig. S1 ¹H NMR (600 MHz, CD₂Cl₂/CD₃CN, ν/ν = 1:1) spectrum of compound 1.

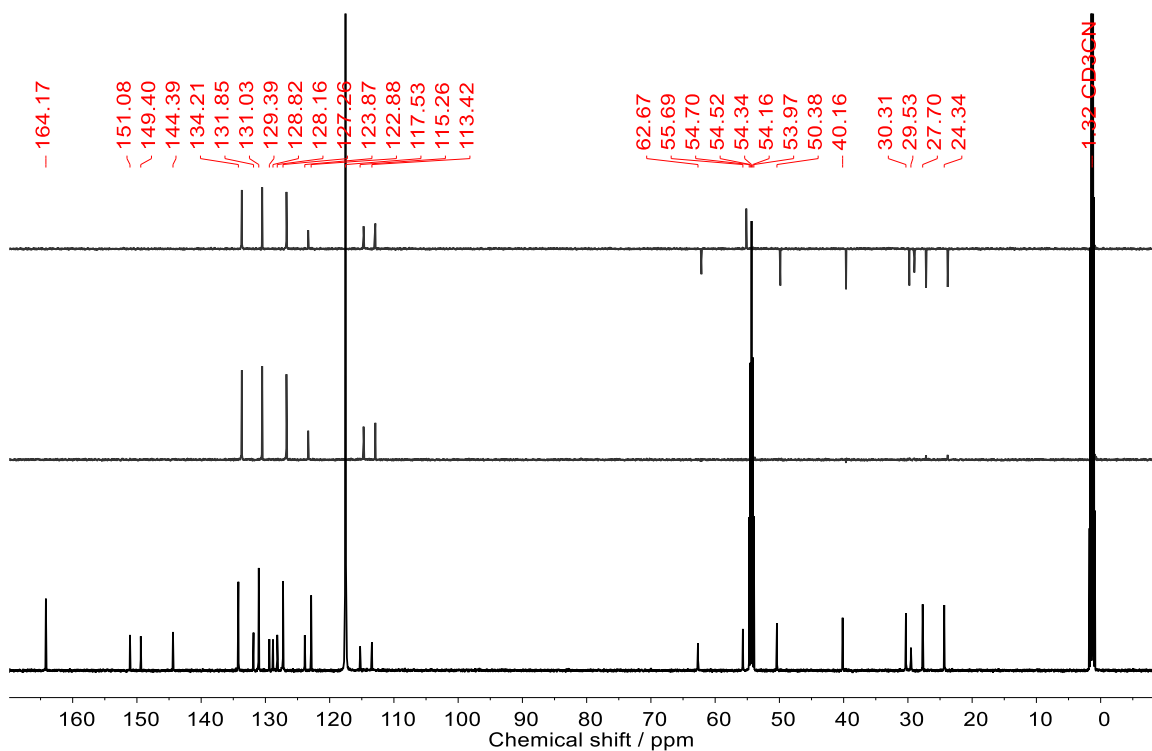


Fig. S2 ¹³C NMR and DEPT spectra (151 MHz, CD₂Cl₂/CD₃CN, ν/ν = 1:1) of compound 1.

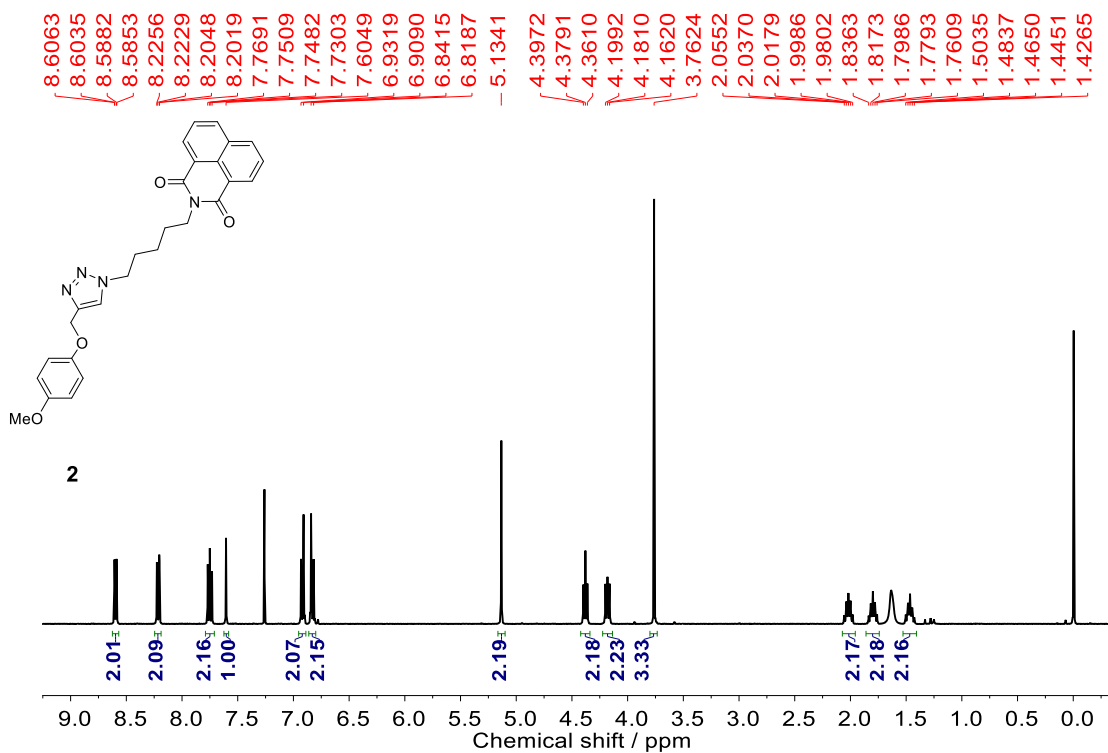


Fig. S3 ^1H NMR (400 MHz, CDCl_3) spectrum of compound 2.

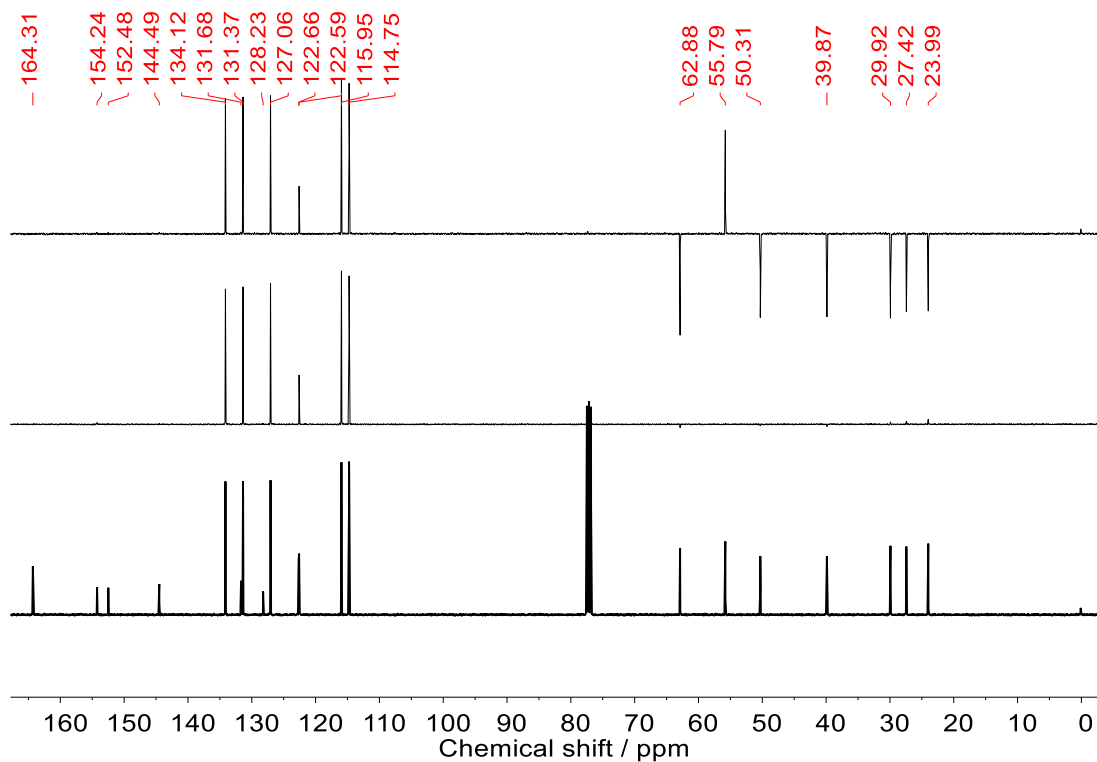


Fig. S4 ^{13}C NMR and DEPT spectra (101 MHz, CDCl_3) of compound 2.

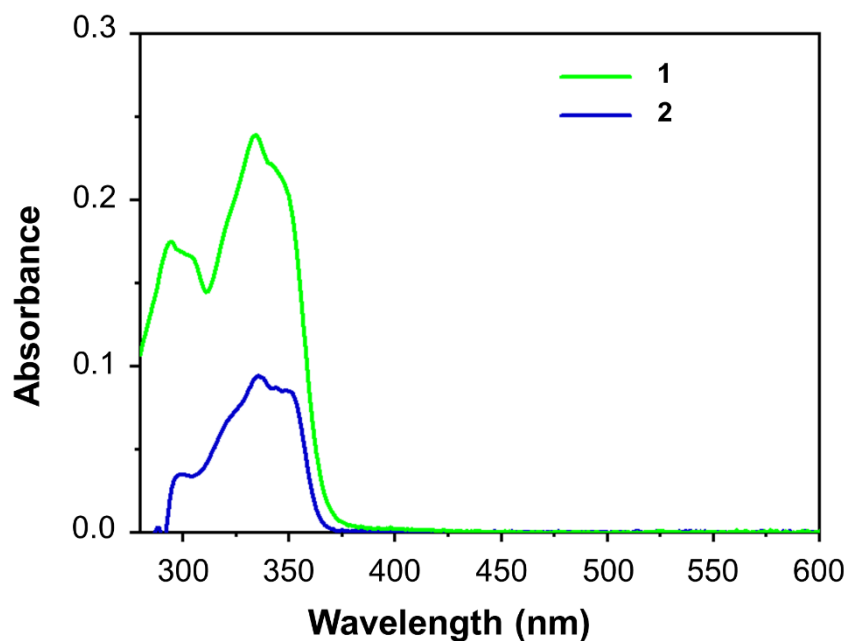


Fig. S5 UV-vis spectra of ligands (5 μM) **1** and **2** in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{CN}$ (v/v , 1:1) co-solvent at 298 K.

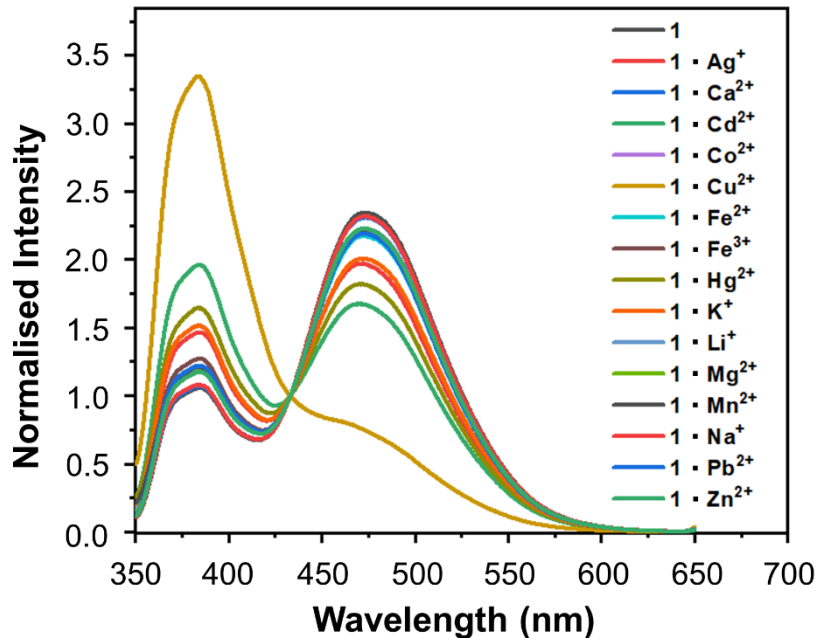


Fig. S6 Fluorescence spectra of ligand **1** (5 μM) in the absence and presence of 5 equiv. of 15 metal perchlorates (Ag^+ , Ca^{2+} , Cd^{2+} , Co^{2+} , Cu^{2+} , Fe^{2+} , Fe^{3+} , Hg^{2+} , K^+ , Li^+ , Mg^{2+} , Mn^{2+} , Na^+ , Pb^{2+} and Zn^{2+}) in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{CN}$ (v/v , 1:1) co-solvent at 298 K (excitation wavelength = 333 nm).

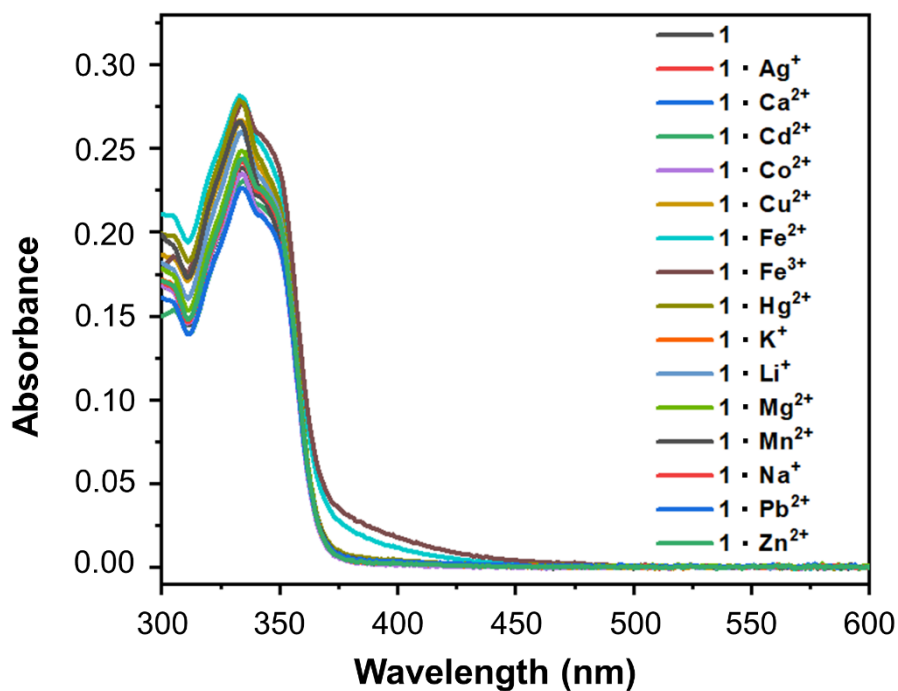


Fig. S7 UV-vis spectra of ligand **1** (5 μM) in the absence and presence of 5 equiv. of 15 metal perchlorates (Ag^+ , Ca^{2+} , Cd^{2+} , Co^{2+} , Cu^{2+} , Fe^{2+} , Fe^{3+} , Hg^{2+} , K^+ , Li^+ , Mg^{2+} , Mn^{2+} , Na^+ , Pb^{2+} and Zn^{2+}) in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{CN}$ (v/v , 1:1) cosolvent at 298 K.

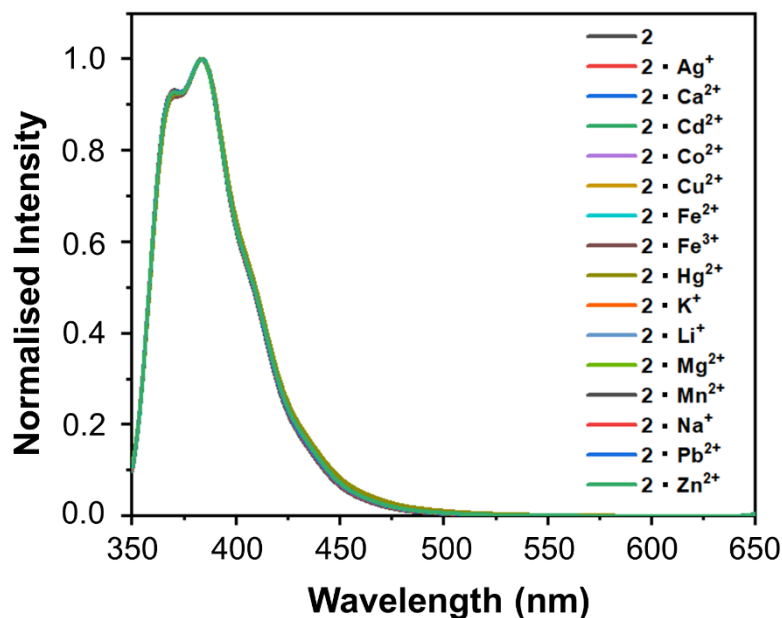


Fig. S8 Fluorescence spectra of ligand **2** (5 μM) in the absence and presence of 5 equiv. of 15 metal perchlorates (Ag^+ , Ca^{2+} , Cd^{2+} , Co^{2+} , Cu^{2+} , Fe^{2+} , Fe^{3+} , Hg^{2+} , K^+ , Li^+ , Mg^{2+} , Mn^{2+} , Na^+ , Pb^{2+} and Zn^{2+}) in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{CN}$ (v/v , 1:1) co-solvent at 298 K (excitation wavelength = 333 nm).

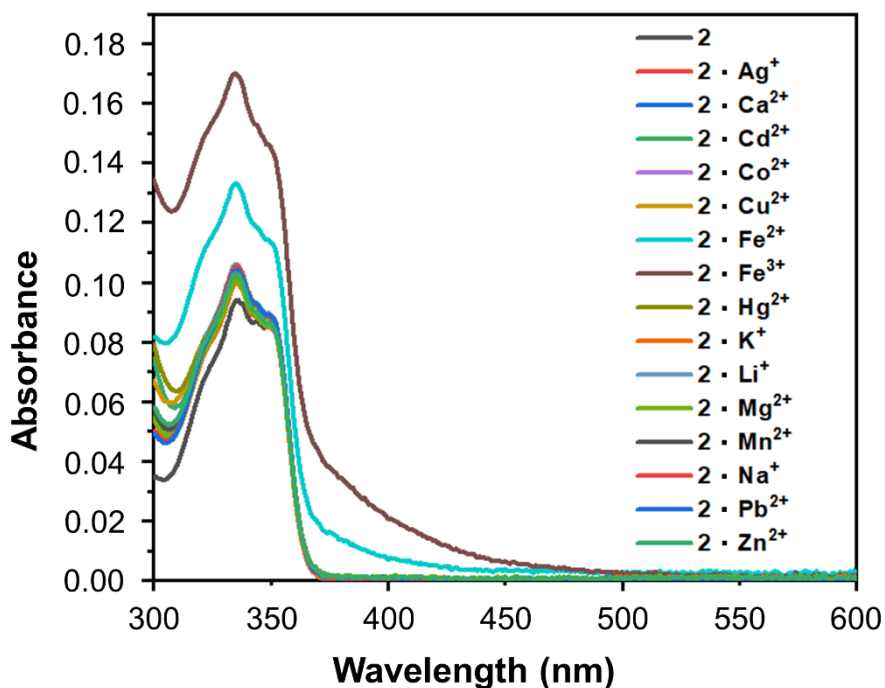


Fig. S9 UV-vis spectra of ligand **2** (5 μM) in the absence and presence of 5 equiv. of 15 metal perchlorates (Ag^+ , Ca^{2+} , Cd^{2+} , Co^{2+} , Cu^{2+} , Fe^{2+} , Fe^{3+} , Hg^{2+} , K^+ , Li^+ , Mg^{2+} , Mn^{2+} , Na^+ , Pb^{2+} and Zn^{2+}) in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{CN}$ (v/v , 1:1) co-solvent at 298 K.

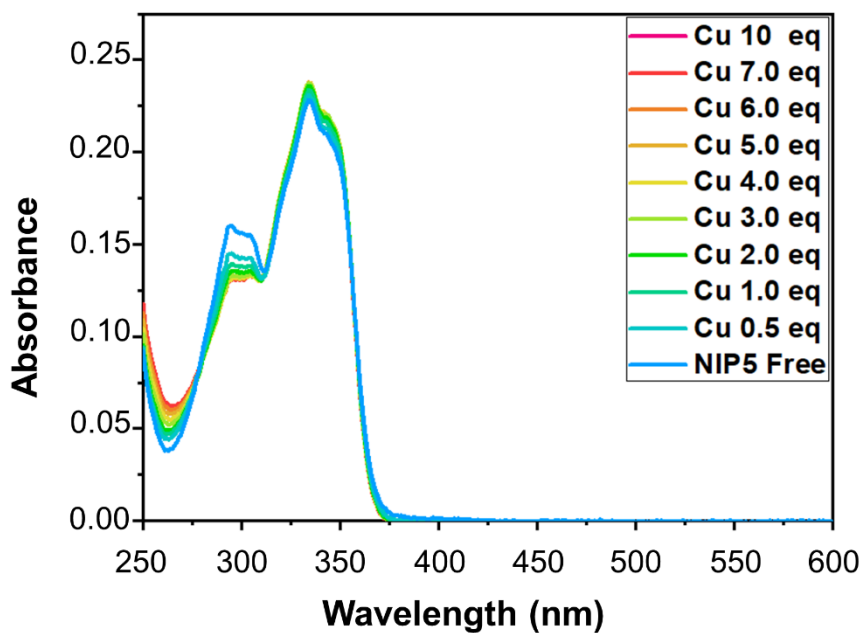


Fig. S10 UV-vis spectra upon the addition of various amount of $\text{Cu}(\text{ClO}_4)_2$ to ligand **1** (5 μM) in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{CN}$ (v/v , 1:1) co-solvent at 298 K.

● **Nonlinear least-square curve-fitting plot**

$$I/I_0 = 1 + \frac{I_{\text{lim}}/I_0 - 1}{2} \left[1 + \frac{C_M}{C_H} + \frac{1}{K_a C_H} - \sqrt{\left(1 + \frac{C_M}{C_H} + \frac{1}{K_a C_H} \right)^2 - 4 \frac{C_M}{C_H}} \right]$$

where I is fluorescent intensity of **1** in presence of Cu^{2+} ion, I_0 is fluorescent intensity of **1** without Cu^{2+} ion, I_{lim} is fluorescent intensity reaching a limitation by adding excessive Cu^{2+} ion, C_M is the concentration of Cu^{2+} ion added and C_H is the concentration of **1**. By allowing I_{lim}/I_0 and $1/K_a C_H$ to be floating parameters (P1 and P2), the K_a value was obtained by a nonlinear least-squares analysis of I/I_0 versus $[\text{Cu}^{2+}]/[\mathbf{1}]$.

References for nonlinear least-square curve-fitting plot

1. L. Fang, W.-H. Chan, Y.-B. He, D. W. J. Kwong and A. W. M. Lee, *J. Org. Chem.* 2005, **70**, 7640–7646.
2. B. Valeur, J. Pouget and J. Bousson, *Journal of Physical Chemistry*, 1992, **96**, 6545–6549.

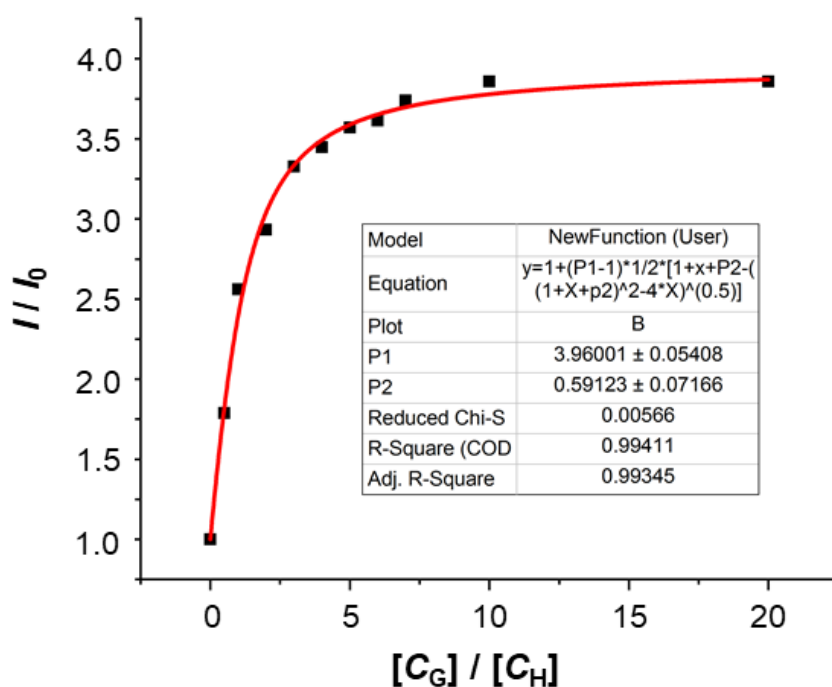


Fig. S11 Binding constant of ligand **1** (5 μM) with $\text{Cu}(\text{ClO}_4)_2$ in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{CN}$ (v/v, 1:1) co-solvent at 298 K by nonlinear least-square curve-fitting plot.

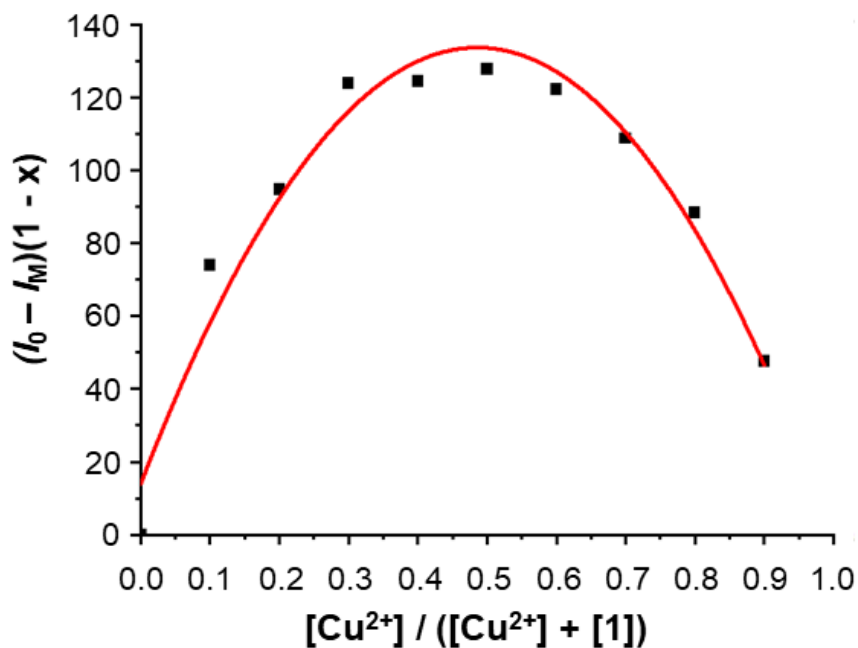


Fig. S12 Job plot of ligand **1** (5 μM) with $\text{Cu}(\text{ClO}_4)_2$ in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{CN}$ (v/v , 1:1) co-solvent at 298 K.

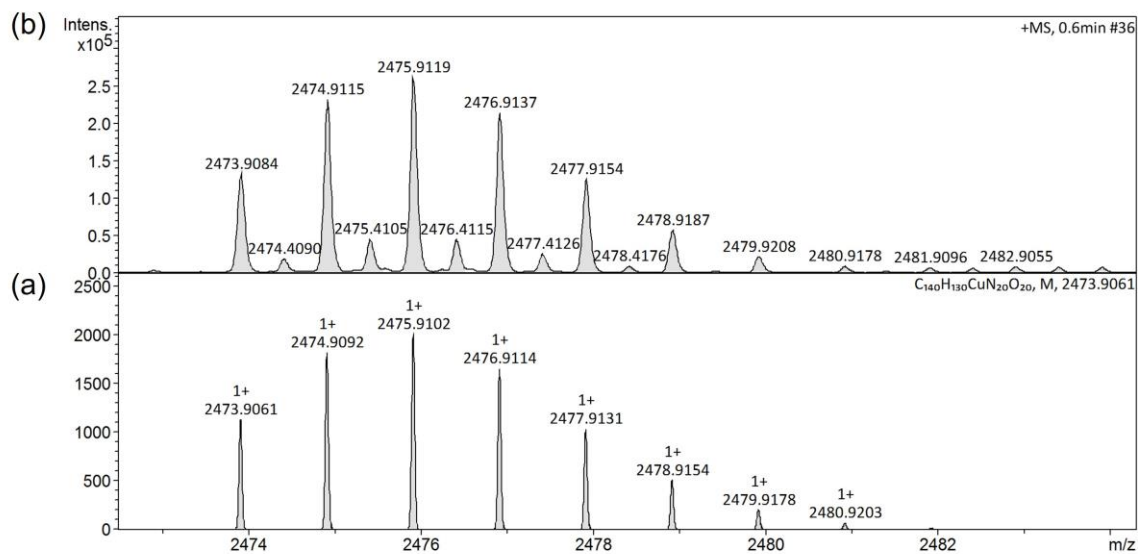


Fig. S13 The ESI-HRMS spectra of the complex $1 \cdot \text{Cu}^{2+}$, where is the (a) calculated $\text{C}_{140}\text{H}_{130}\text{CuN}_{20}\text{O}_{20}$ m/z 2473.9061, (b) found m/z 2473.9084.

● **The limit of Detection (LOD)**

$$\text{LOD} = 3 \times \text{standard deviation/slope}$$

References for LOD.

1. G. L. Long and J. D. Winefordner, *Analytical Chemistry*, 1983, **55**, 712A–724A.
2. V. Thomsen, D. Schatzlein and D. Mercurio, *Spectroscopy*, 2003, **18**, 112–114.
3. H. J. Kim, J. H. Lee and J.-I. Hong, *Tetrahedron*, 2011, **52**, 4944–4946.

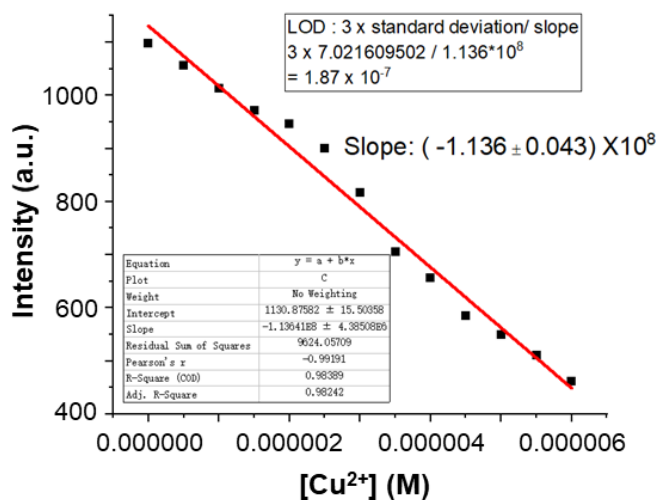


Fig. S14 The limit of detection (LOD) of ligand **1** (5 μM) with $\text{Cu}(\text{ClO}_4)_2$ in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{CN}$ (v/v, 1:1) co-solvent at 298 K was determined to be $3 \times 7.021 / (1.136 \pm 0.043 \times 10^8) \text{ M} = 1.854 \pm 0.070 \times 10^{-7} \text{ M} = 185 \pm 7 \text{ nM}$

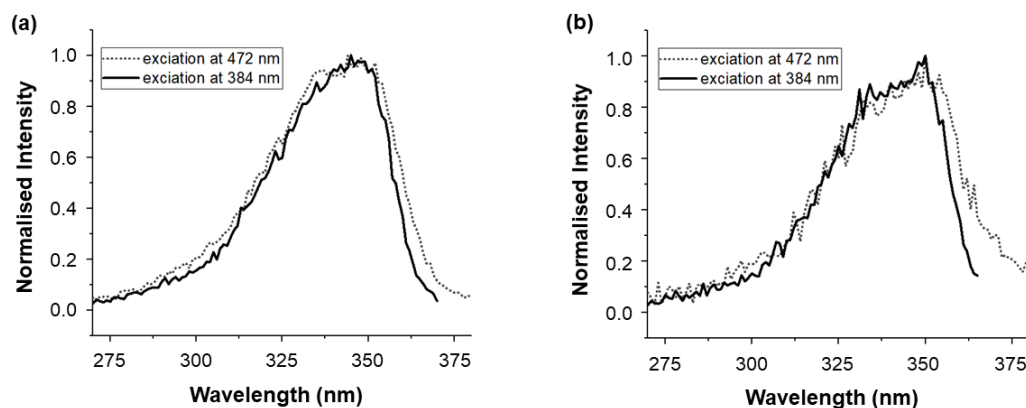


Fig. S15 Normalised excitation spectra of (a) **1** (5 μM) and (b) complex **1**· Cu^{2+} , monitored at 384 nm (solid line) and around 472 nm (dashed line) in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{CN}$ (v/v, 1:1) co-solvent at 298 K (Complex **1**· Cu^{2+} was formed with ligand **1** (5 μM) upon the addition of 10 equiv of Cu^{2+}).

Quantum yields (Φ_F)

The relative fluorescent quantum yields (Φ_F) of (9,10-diphenylanthracene, DPA) and ligand **1** in CH₂Cl₂/CH₃CN (v/v, 1:1) at 298 K were determined using DPA as a standard (Φ_F of DPA in cyclohexane = 0.93 was used) based on eqn 1. $\Phi_F = (F/F_o) \times (A_o/A) \times (n/n_o)^2 \times \Phi_F^o$ (eqn 1), where A and A_o are the absorbance of the sample and the standard at the excitation wavelength, respectively; F and F_o are the integrated fluorescence emissions of the sample and the standard, respectively; and n and n_o are solvent refractive indexes of the sample and the standard, respectively. The results are summarised in Tables S1 and S2. references for quantum yields (Φ_F): (a) A. M. Brouwer, Standards for photoluminescence quantum yield measurements in solution (IUPAC Technical Report), *Pure Appl. Chem.*, 2011, **83**, 2213–2228; (b) W. R. Dawson and M. W. Windsor, Fluorescence yields of aromatic compounds, *J. Phys. Chem.*, 1968, **72**, 3251–3260; (c) N. J. Turro, Modern molecular photochemistry, Benjamin Cummings, Menlo Park, 1978.

Table S1 The data for the quantum yield measurement of DPA in cyclohexane or CH₂Cl₂/CH₃CN (v/v, 1:1) at 298 K (excitation wavelength = 333 nm).

	$A_{(333\text{ nm})}$	$F_{(345-600\text{ nm})}$	F/F_o	A_o/A	Quantum yield, Φ_F
DPA ¹	0.038	685446	1.00	1.00	0.93
DPA	0.055	965413	1.41	0.69	0.90

¹ The data of DPA was measured in cyclohexane.

Table S2 The data for the quantum yield measurement of ligand **1** and complex **1**·Cu²⁺ in CH₂Cl₂/CH₃CN (v/v, 1:1) at 298 K using DPA as the standard (excitation wavelength = 333 nm).

	$A_{(333\text{ nm})}$	$F_{(345-600\text{ nm})}$	F/F_o	A_o/A	Quantum yield, Φ_F
1	0.210	519691	0.54	0.26	0.13
1 ·Cu ²⁺	0.227	483804	0.50	0.24	0.11
DPA	0.055	965413	1.00	1.00	0.90

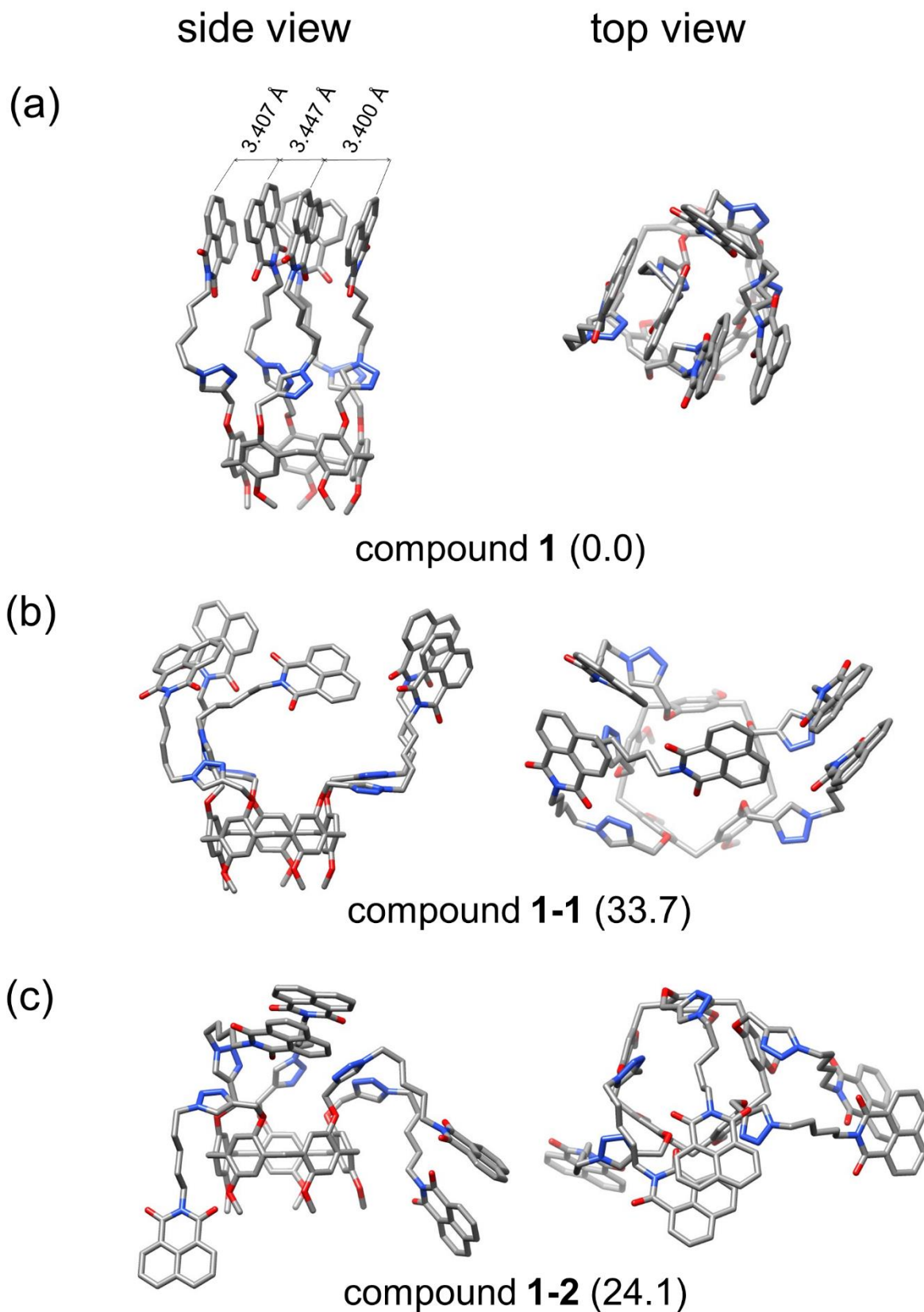


Fig. S16 DFT optimised structures of **1** with different conformations and their relative energies were given in the brackets (kcal mol^{-1}). Hydrogens are omitted for clarity.

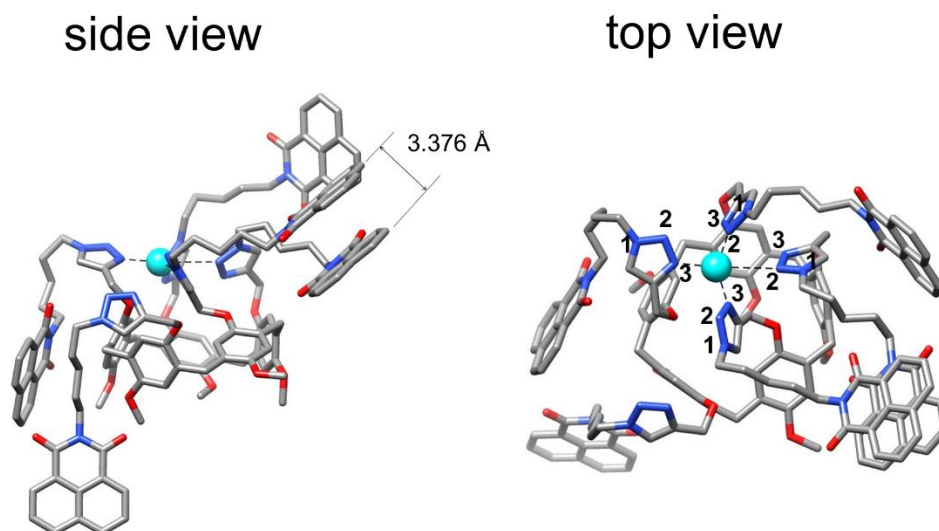


Fig. S17 DFT optimised structures of complex **1**·Cu²⁺. Hydrogens are omitted for clarity.

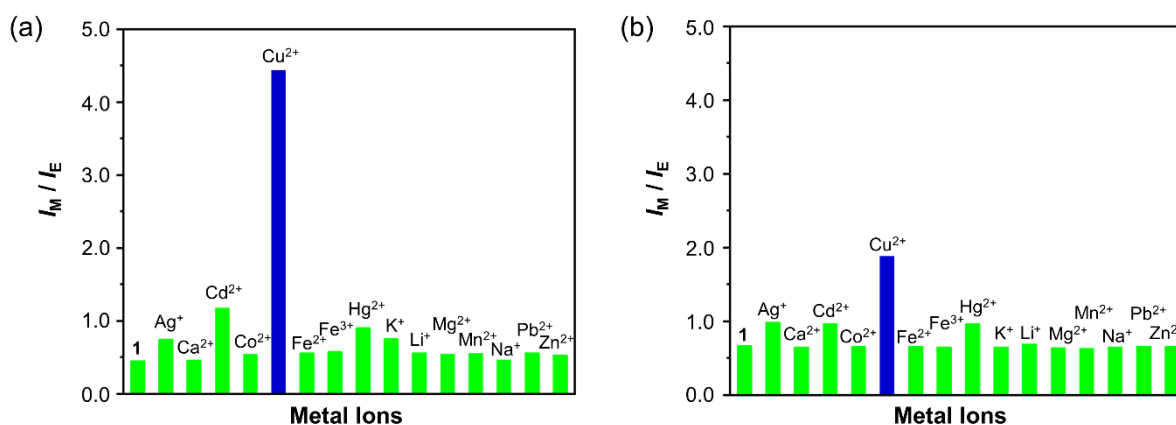


Fig. S18 The ratio of fluorescence intensity (I_M/I_E) of **1** (5 μ M) in the presence of 5 equiv. of 15 metal perchlorates in (a) CH₂Cl₂/CH₃CN (v/v, 1:1) and (b) H₂O/MeOH/CHCl₃ (v/v, 1:7:2) at 298 K (excitation wavelength = 333 nm).

Table S3 Dynamic light scattering (DLS) analysis for ligand **1** (5 μM) in various co-solvents, both in the absence and presence of Cu^{2+} (10 equiv.)

ligand 1 (NIP[5]) Solvent group	Average size (nm)	Average St Dev (nm)	Test 1 size (nm)	St Dev (nm)	PDI	Test 2 size (nm)	St Dev (nm)	PDI	Test 3 size (nm)	St Dev (nm)	PDI
$\text{CH}_2\text{Cl}_2/\text{CH}_3\text{CN}$ (v/v, 1:1)	206.0	67.2	175.0	58.8	0.135	208.9	62.9	0.081	234.0	79.8	0.134
$\text{CH}_2\text{Cl}_2/\text{CH}_3\text{CN}$ (v/v, 1:1) + Cu^{2+}	192.2	65.0	190.6	64.2	0.115	195.0	63.7	0.106	191.0	67.1	0.196
$\text{H}_2\text{O}/\text{MeOH}/\text{CHCl}_3$ (v/v, 1:7:2)	390.6	112.1	380.3	104.5	0.065	392.4	112.5	0.074	399.0	119.3	0.087
$\text{H}_2\text{O}/\text{MeOH}/\text{CHCl}_3$ (v/v, 1:7:2) + Cu^{2+}	1007.7	403.8	254.5	0.112	1095	560.6	0.205	1095.0	396.3	0.224	254.5

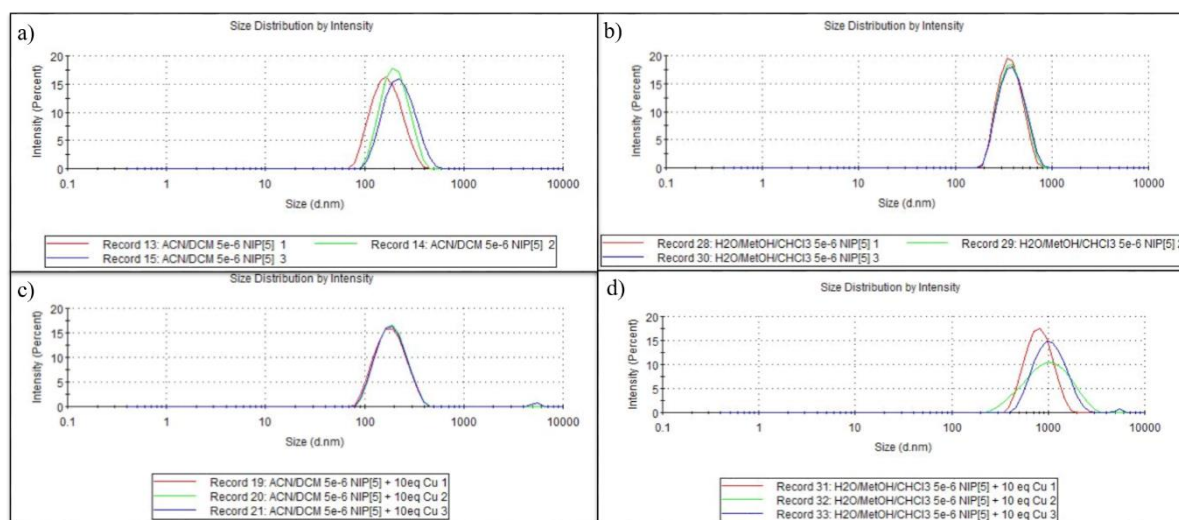


Fig. S19 Dynamic light scattering (DLS) analysis for ligand **1** (5 μM) in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{CN}$ (v/v, 1:1) and $\text{H}_2\text{O}/\text{MeOH}/\text{CHCl}_3$ (v/v, 1:7:2) in the absence (a) and (b) and presence of Cu^{2+} (10 equiv.) (c) and (d).

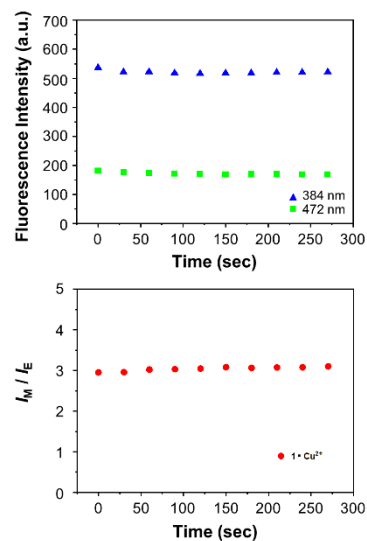
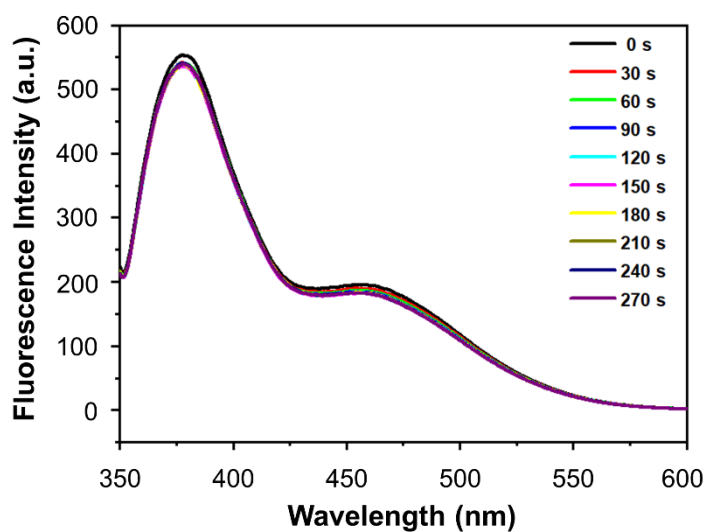


Fig. S20 The response times of ligand **1** (5 μM) in the presence of 5 equiv. of Cu²⁺ in CH₂Cl₂/CH₃CN (v/v, 1:1) at 298 K (excitation wavelength = 333 nm).

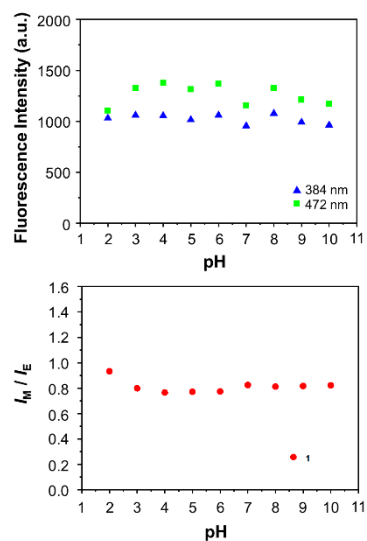
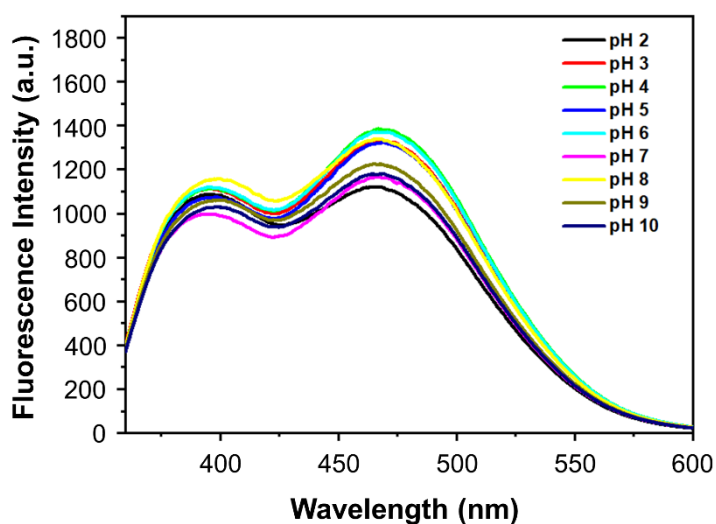


Fig. S21 The influence of pH on the alterations in the fluorescence characteristics was investigated for ligand **1** (5 μM) in H₂O/MeOH/CHCl₃ (v/v, 1:7:2) at 298 K (excitation wavelength = 333 nm).

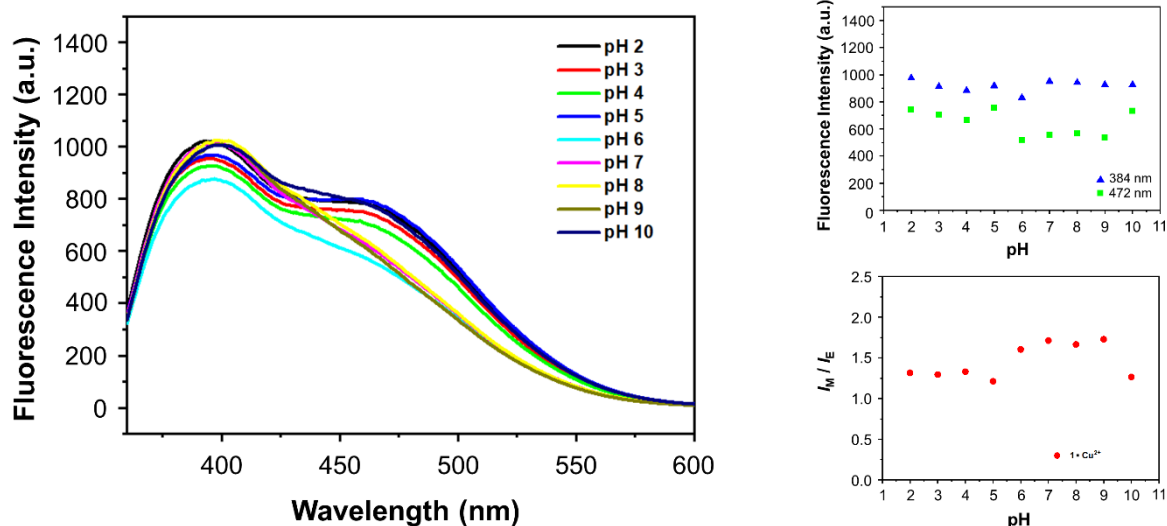


Fig. S22 The influence of pH on the alterations in the fluorescence characteristics was investigated for ligand **1** (5 μ M) in the presence of 5 equiv. of Cu²⁺ in H₂O/MeOH/CHCl₃ (v/v, 1:7:2) at 298 K (excitation wavelength = 333 nm).

Table S4. Cartesian-coordinates for optimised structures.

compound 1				C	4.83200000	-1.32760000	4.07480000
C	7.17940000	3.27050000	2.33720000	C	4.45750000	3.54780000	-2.42390000
C	4.70090000	-2.57490000	3.43320000	C	5.89210000	4.93080000	0.87210000
C	6.64690000	-1.32240000	-3.83410000	H	6.81460000	5.51900000	0.88550000
C	6.88110000	-4.24180000	-0.03640000	H	5.07780000	5.62430000	1.09910000
C	4.78670000	2.36260000	3.52070000	C	7.21050000	-1.34030000	3.79740000
C	5.48090000	-3.82180000	-1.99070000	C	5.74370000	-4.37060000	0.78240000
C	5.88150000	-3.23160000	3.02110000	C	6.13350000	0.67580000	4.92540000
C	4.32770000	-3.91780000	-1.18040000	H	7.08470000	0.76450000	5.45820000
C	4.19340000	-1.29680000	-4.02650000	H	5.34390000	0.75210000	5.67920000
C	5.71750000	4.32210000	-0.51610000	C	6.63250000	0.05790000	-4.04330000
C	6.02420000	1.81350000	3.91910000	C	4.80510000	3.39980000	2.56810000
C	5.44250000	-2.05450000	-3.81470000	C	5.86910000	-4.56550000	2.28430000
C	4.21400000	0.05630000	-4.15680000	H	6.79260000	-5.10640000	2.50810000
C	5.58640000	3.04120000	-3.04940000	H	5.04420000	-5.19370000	2.63350000
C	4.46670000	4.17420000	-1.15800000	C	5.41000000	-3.53910000	-3.49080000
C	6.74070000	-3.99740000	-1.40400000	H	6.24960000	-4.04000000	-3.98390000
C	7.20190000	2.28020000	3.32030000	H	4.49270000	-3.97220000	-3.90280000
C	6.82230000	3.21530000	-2.39080000	C	6.87450000	3.85430000	-1.15430000

C	6.05140000	-0.68970000	4.26380000	H	3.27680000	0.56540000	-4.24170000
C	4.50000000	-4.21180000	0.18430000	H	3.35140000	-3.77110000	-1.59290000
C	5.48940000	2.28220000	-4.36340000	H	3.73840000	-3.01050000	3.26360000
H	6.35610000	2.52780000	-4.98620000	H	3.86520000	2.00290000	3.92880000
H	4.60280000	2.62200000	-4.90760000	H	3.56310000	4.52280000	-0.70310000
C	7.11880000	-2.60110000	3.20790000	O	2.99080000	-1.97650000	-4.03310000
C	5.95870000	3.86080000	1.95060000	O	-7.15130000	-4.88380000	-2.18650000
C	5.43150000	0.76730000	-4.18130000	O	-6.23000000	-0.48790000	-2.87540000
H	7.85800000	-4.33150000	0.39100000	N	0.42220000	-2.88050000	-5.51990000
H	8.16450000	-0.86580000	3.89570000	N	-0.36140000	-3.92420000	-5.66250000
H	8.09230000	3.58320000	1.87490000	N	-0.55770000	-4.44760000	-4.44200000
H	7.72260000	2.85500000	-2.84300000	N	-6.70910000	-2.66870000	-2.46640000
H	7.57850000	-1.82790000	-3.68750000	C	1.62140000	-1.63380000	-3.74090000
O	7.89100000	-3.88120000	-2.24550000	H	1.38200000	-0.81210000	-4.19730000
O	8.28590000	-3.27080000	2.72400000	H	1.51150000	-1.49750000	-2.78680000
O	8.43350000	1.66930000	3.71360000	C	0.73760000	-2.74630000	-4.20020000
O	8.11980000	4.01690000	-0.47060000	C	0.11080000	-3.74370000	-3.49750000
O	7.85370000	0.80100000	-4.07960000	H	0.13830000	-3.90080000	-2.58140000
C	8.91670000	-0.04900000	-4.51840000	C	-1.40670000	-5.62740000	-4.26780000
H	9.64970000	0.53450000	-5.03530000	H	-1.20730000	-6.04350000	-3.41460000
H	9.36900000	-0.52070000	-3.67120000	H	-1.21230000	-6.26920000	-4.96860000
H	8.52680000	-0.79670000	-5.17710000	C	-2.89220000	-5.25720000	-4.31650000
C	8.98080000	-4.60390000	-1.66670000	H	-3.41870000	-6.06770000	-4.23390000
H	9.63890000	-4.93770000	-2.44150000	H	-3.08770000	-4.86380000	-5.18110000
H	9.51550000	-3.96540000	-0.99500000	C	-3.32010000	-4.27760000	-3.22080000
H	8.60330000	-5.44950000	-1.13060000	H	-2.80640000	-3.45860000	-3.29950000
C	9.42770000	-2.83810000	3.46830000	H	-3.13970000	-4.66580000	-2.35030000
H	10.15360000	-3.62360000	3.49670000	C	-4.81080000	-3.95840000	-3.33850000
H	9.85340000	-1.97570000	2.99930000	H	-5.32000000	-4.77500000	-3.21730000
H	9.13030000	-2.59110000	4.46610000	H	-4.99330000	-3.62260000	-4.23010000
C	9.52840000	2.48280000	3.28420000	C	-5.27020000	-2.93290000	-2.31990000
H	10.35290000	2.35340000	3.95370000	H	-5.09060000	-3.26190000	-1.42530000
H	9.82190000	2.19350000	2.29680000	H	-4.77500000	-2.10830000	-2.44440000
H	9.22950000	3.51020000	3.28080000	C	-7.58330000	-3.75560000	-2.38290000
C	9.16740000	4.20630000	-1.42540000	C	-9.02500000	-3.46850000	-2.54240000
H	9.90150000	4.87210000	-1.02210000	C	-9.45100000	-2.15600000	-2.88660000
H	9.62360000	3.26390000	-1.64600000	C	-8.51680000	-1.10710000	-3.01830000
H	8.76100000	4.62460000	-2.32250000	C	-7.08270000	-1.34690000	-2.78920000

C	-9.95020000	-4.47250000	-2.36860000	C	-4.52300000	-2.10770000	3.56790000
H	-9.66520000	-5.32960000	-2.14790000	H	-4.19210000	-1.34790000	4.07200000
C	-10.82620000	-1.90060000	-3.08550000	H	-4.16290000	-2.05460000	2.66880000
C	-11.75900000	-2.95230000	-2.88470000	C	-6.59710000	-0.80710000	3.37460000
H	-12.66810000	-2.79230000	-2.99770000	C	-8.07480000	-0.78020000	3.33080000
C	-11.32300000	-4.21220000	-2.52210000	C	-8.81090000	-1.97770000	3.54720000
H	-11.94120000	-4.89190000	-2.37880000	C	-8.14570000	-3.20630000	3.74300000
C	-8.94240000	0.16690000	-3.38500000	C	-6.67570000	-3.27610000	3.71420000
H	-8.32450000	0.85770000	-3.46270000	C	-8.73500000	0.40370000	3.09220000
C	-11.22940000	-0.57900000	-3.47060000	H	-8.24830000	1.18410000	2.95580000
H	-12.13020000	-0.39260000	-3.60840000	C	-10.22290000	-1.93510000	3.55280000
C	-10.29660000	0.41050000	-3.63680000	C	-10.87670000	-0.70240000	3.28890000
H	-10.56700000	1.25410000	-3.92040000	H	-11.80580000	-0.66520000	3.27470000
O	3.25950000	-4.20200000	0.89560000	C	-10.13960000	0.44210000	3.05280000
O	-5.91440000	0.20570000	3.29560000	H	-10.57500000	1.24240000	2.86690000
O	-6.04300000	-4.30070000	3.86450000	C	-8.87620000	-4.36690000	3.98370000
N	0.67420000	-5.65120000	1.81290000	H	-8.43440000	-5.17640000	4.10410000
N	0.02750000	-5.99390000	2.90280000	C	-10.94450000	-3.14740000	3.81210000
N	0.05520000	-4.93950000	3.73330000	H	-11.87450000	-3.13830000	3.82220000
N	-5.99130000	-2.05870000	3.51280000	C	-10.27290000	-4.31850000	4.04500000
C	1.90260000	-3.71660000	0.86140000	H	-10.75120000	-5.09040000	4.24620000
H	1.50000000	-3.92160000	0.00300000	O	3.56780000	-0.77500000	4.45070000
H	1.89310000	-2.75410000	0.98200000	O	-5.64360000	4.64640000	6.08540000
C	1.12800000	-4.37340000	1.95590000	O	-5.50690000	0.11040000	6.31690000
C	0.73290000	-3.90420000	3.18280000	N	1.75790000	0.03970000	6.83520000
H	0.89360000	-3.06620000	3.55240000	N	1.36140000	1.09960000	7.50080000
C	-0.59850000	-5.00750000	5.04140000	N	1.06640000	2.05090000	6.60060000
H	-0.24150000	-4.31180000	5.61550000	N	-5.61160000	2.37130000	6.14240000
H	-0.40650000	-5.86490000	5.45230000	C	2.12870000	-0.70750000	4.49830000
C	-2.11510000	-4.83300000	4.91650000	H	1.76560000	-1.57140000	4.74880000
H	-2.51300000	-4.92010000	5.79690000	H	1.78010000	-0.47060000	3.62460000
H	-2.46670000	-5.54580000	4.36070000	C	1.72730000	0.32270000	5.50180000
C	-2.53410000	-3.48810000	4.31710000	C	1.28070000	1.60930000	5.33830000
H	-2.14950000	-3.39410000	3.43160000	H	1.15370000	2.07290000	4.54220000
H	-2.19740000	-2.76710000	4.87170000	C	0.58000000	3.36080000	7.03700000
C	-4.05730000	-3.39290000	4.22480000	H	0.70210000	4.00370000	6.32100000
H	-4.43250000	-3.44590000	5.11770000	H	1.09920000	3.65820000	7.80050000
H	-4.39150000	-4.14780000	3.71550000	C	-0.90170000	3.30550000	7.42160000

H	-1.17490000	4.18080000	7.73810000	H	1.80140000	3.23440000	1.76330000
H	-1.01110000	2.67850000	8.15330000	C	1.66030000	5.26580000	1.66690000
C	-1.82220000	2.88740000	6.27210000	C	1.30420000	5.54270000	0.37150000
H	-1.56410000	2.00830000	5.95360000	H	1.26300000	4.95430000	-0.34750000
H	-1.72960000	3.51470000	5.53810000	C	0.58810000	7.71240000	-0.73490000
C	-3.27880000	2.85500000	6.73560000	H	0.79980000	7.27350000	-1.57360000
H	-3.54250000	3.74620000	7.01350000	H	1.06760000	8.55510000	-0.70660000
H	-3.35350000	2.26850000	7.50460000	C	-0.91810000	7.98310000	-0.67030000
C	-4.22530000	2.37410000	5.65260000	H	-1.16080000	8.57290000	-1.40120000
H	-4.15590000	2.95620000	4.87980000	H	-1.11740000	8.44280000	0.16000000
H	-3.97620000	1.47730000	5.37960000	C	-1.77630000	6.71810000	-0.75190000
C	-6.23880000	3.60550000	6.33120000	H	-1.54880000	6.12430000	-0.01940000
C	-7.62930000	3.57970000	6.83330000	H	-1.59360000	6.25550000	-1.58470000
C	-8.22170000	2.34350000	7.21200000	C	-3.26210000	7.07190000	-0.67940000
C	-7.51830000	1.13040000	7.05670000	H	-3.49150000	7.63160000	-1.43770000
C	-6.16110000	1.11820000	6.48690000	H	-3.42700000	7.58230000	0.12880000
C	-8.34320000	4.75120000	6.94360000	C	-4.15470000	5.84580000	-0.68130000
H	-7.94900000	5.55680000	6.69850000	H	-3.99500000	5.33010000	-1.48720000
C	-9.53320000	2.33240000	7.73710000	H	-3.94040000	5.28800000	0.08260000
C	-10.25100000	3.55450000	7.82530000	C	-6.52600000	5.22110000	-0.54770000
H	-11.12060000	3.55740000	8.15500000	C	-7.94380000	5.63760000	-0.49820000
C	-9.66430000	4.73910000	7.42390000	C	-8.28330000	7.01070000	-0.64660000
H	-10.14590000	5.53310000	7.47170000	C	-7.27740000	7.99080000	-0.77980000
C	-8.09700000	-0.07040000	7.45890000	C	-5.85480000	7.61370000	-0.75450000
H	-7.63340000	-0.86890000	7.34720000	C	-8.93200000	4.69630000	-0.31990000
C	-10.09620000	1.07900000	8.14920000	H	-8.70400000	3.79960000	-0.22780000
H	-10.95740000	1.05240000	8.49950000	C	-9.64270000	7.39510000	-0.64760000
C	-9.37380000	-0.07890000	8.03030000	C	-10.63980000	6.40410000	-0.44670000
H	-9.73650000	-0.88000000	8.33320000	H	-11.53720000	6.64740000	-0.43000000
O	3.50320000	3.98460000	2.47870000	C	-10.28350000	5.08020000	-0.27580000
O	-6.18030000	4.04720000	-0.52630000	H	-10.94150000	4.43930000	-0.13080000
O	-4.94180000	8.40690000	-0.85290000	C	-7.62250000	9.32840000	-0.95450000
N	1.57740000	6.41560000	2.39520000	H	-6.95640000	9.97260000	-1.03360000
N	1.19770000	7.39080000	1.60260000	C	-9.96350000	8.78020000	-0.83820000
N	1.02590000	6.86810000	0.37810000	H	-10.85310000	9.05180000	-0.84420000
N	-5.57040000	6.23800000	-0.62180000	C	-8.96830000	9.70560000	-1.01140000
C	2.07100000	3.98510000	2.31530000	H	-9.19010000	10.59510000	-1.16880000
H	1.63990000	3.89980000	3.18010000	O	3.19610000	3.22630000	-3.01590000

O	-6.87710000	1.52890000	-6.73540000	H	-11.30070000	2.54070000	-8.28070000
O	-5.11160000	5.69010000	-6.27140000	C	-7.38730000	6.95650000	-7.39540000
N	1.67080000	4.06130000	-5.58530000	H	-6.67670000	7.50810000	-7.15920000
N	1.18290000	3.55410000	-6.69360000	C	-9.61710000	6.71990000	-8.27070000
N	0.56100000	2.40910000	-6.37050000	H	-10.38770000	7.10610000	-8.62050000
N	-6.02940000	3.62110000	-6.44460000	C	-8.53730000	7.50760000	-7.97020000
C	1.79980000	3.55470000	-3.15960000	H	-8.56930000	8.41950000	-8.15060000
H	1.66310000	4.49920000	-2.98580000				
H	1.27380000	3.04670000	-2.52220000				
C	1.36810000	3.22630000	-4.55070000				
C	0.65190000	2.16440000	-5.04150000				
H	0.30700000	1.44120000	-4.56940000				
C	-0.10110000	1.60750000	-7.40100000				
H	-0.22830000	0.70370000	-7.07260000				
H	0.46470000	1.56500000	-8.18780000				
C	-1.45910000	2.20350000	-7.78420000				
H	-1.84740000	1.66590000	-8.49210000				
H	-1.32020000	3.09760000	-8.13340000				
C	-2.45090000	2.27720000	-6.62050000				
H	-2.07680000	2.82100000	-5.90970000				
H	-2.60650000	1.38610000	-6.27020000				
C	-3.77660000	2.88280000	-7.08270000				
H	-4.16510000	2.31180000	-7.76380000				
H	-3.60620000	3.75020000	-7.48220000				
C	-4.77020000	3.04680000	-5.94870000				
H	-4.94530000	2.18280000	-5.54390000				
H	-4.39380000	3.62840000	-5.26980000				
C	-7.04350000	2.73820000	-6.82490000				
C	-8.29770000	3.33710000	-7.32950000				
C	-8.38300000	4.74380000	-7.52060000				
C	-7.30350000	5.58410000	-7.17590000				
C	-6.07100000	5.02310000	-6.59890000				
C	-9.37510000	2.53260000	-7.62350000				
H	-9.31170000	1.61320000	-7.50060000				
C	-9.56740000	5.30350000	-8.04940000				
C	-10.66790000	4.45080000	-8.32940000				
H	-11.45810000	4.80980000	-8.66330000				
C	-10.57080000	3.09050000	-8.10810000				
				compound 1-1			
				C	7.17936131	3.27054934	2.33719439
				C	4.70089531	-2.57487866	3.43316439
				C	6.64693231	-1.32236066	-3.83411261
				C	6.88114331	-4.24179366	-0.03636861
				C	4.78667831	2.36255034	3.52074439
				C	5.48086231	-3.82179866	-1.99072361
				C	5.88145931	-3.23155666	3.02108739
				C	4.32771031	-3.91780366	-1.18044761
				C	4.19344561	-1.29684097	-4.02648105
				C	5.71747031	4.32212434	-0.51606661
				C	6.02422031	1.81351734	3.91911639
				C	5.44251731	-2.05453266	-3.81466261
				C	4.21402931	0.05625134	-4.15684461
				C	5.58644231	3.04123834	-3.04936161
				C	4.46666131	4.17417634	-1.15798961
				C	6.74065431	-3.99742166	-1.40401361
				C	7.20185731	2.28024934	3.32029939
				C	6.82228731	3.21530734	-2.39077861
				C	4.83201331	-1.32760566	4.07475739
				C	4.45745631	3.54777734	-2.42389261
				C	5.89210531	4.93081434	0.87212839
				H	6.81458731	5.51899334	0.88545739
				H	5.07780031	5.62428534	1.09913439
				C	7.21054031	-1.34032666	3.79740839
				C	5.74373331	-4.37057966	0.78243339
				C	6.13350931	0.67584034	4.92537839
				H	7.08471231	0.76452034	5.45816839
				H	5.34394131	0.75211934	5.67922339
				C	6.63246131	0.05793634	-4.04332361

C	4.80510231	3.39977434	2.56810339	C	9.52837384	2.48278508	3.28419662
C	5.86908131	-4.56545366	2.28429339	H	10.35294436	2.35338251	3.95370273
H	6.79262431	-5.10638866	2.50807939	H	9.82189018	2.19346198	2.29675533
H	5.04419331	-5.19373466	2.63351339	H	9.22952701	3.51019889	3.28081649
C	5.41003931	-3.53912566	-3.49077361	C	9.16742700	4.20628298	-1.42537422
H	6.24962431	-4.04000866	-3.98388361	H	9.90150913	4.87213234	-1.02205293
H	4.49265831	-3.97221966	-3.90276261	H	9.62358288	3.26386821	-1.64600108
C	6.87447031	3.85429534	-1.15434361	H	8.76104589	4.62455554	-2.32248204
C	6.05135631	-0.68967266	4.26382539	H	3.27675144	0.56537635	-4.24170871
C	4.50003931	-4.21184866	0.18429239	H	3.35136428	-3.77108873	-1.59290750
C	5.48944631	2.28222834	-4.36336261	H	3.73840794	-3.01049238	3.26358037
H	6.35607631	2.52778534	-4.98619861	H	3.86523954	2.00287658	3.92877060
H	4.60283531	2.62200734	-4.90761061	H	3.56309074	4.52276912	-0.70307941
C	7.11875231	-2.60113566	3.20787939	O	2.99078496	-1.97653532	-4.03310292
C	5.95869531	3.86076534	1.95064139	O	-1.63841007	-3.70199079	-13.53666259
C	5.43145131	0.76725234	-4.18133861	O	-4.00335691	-1.53890019	-10.31551353
H	7.85796529	-4.33153987	0.39102399	N	2.63184580	-0.67030654	-6.82421001
H	8.16450913	-0.86579342	3.89570225	N	2.96401602	-0.84245130	-8.08263771
H	8.09229276	3.58317817	1.87489646	N	2.79030911	-2.14255528	-8.36866918
H	7.72262859	2.85504630	-2.84299268	N	-2.86717396	-2.67190354	-11.92124187
H	7.57853394	-1.82786758	-3.68754810	C	1.82202973	-1.97773968	-4.87689467
O	7.89101426	-3.88118333	-2.24547700	H	1.24993360	-1.22804709	-4.64980235
O	8.28592118	-3.27079402	2.72396356	H	1.32007475	-2.79718643	-4.74460435
O	8.43350115	1.66930436	3.71361822	C	2.25608326	-1.87235496	-6.30167287
O	8.11984208	4.01689861	-0.47059707	C	2.34917933	-2.82438283	-7.28475496
O	7.85372386	0.80097067	-4.07962472	H	2.15378265	-3.73139284	-7.22162528
C	8.91672752	-0.04896736	-4.51840549	C	3.06893893	-2.65070117	-9.71295933
H	9.64972515	0.53452879	-5.03526786	H	3.18487936	-3.61299111	-9.67500940
H	9.36902437	-0.52073990	-3.67119936	H	3.89502180	-2.26052865	-10.03892588
H	8.52682701	-0.79665833	-5.17706761	C	1.93184798	-2.31488651	-10.68267618
C	8.98077506	-4.60392725	-1.66671743	H	2.17038895	-2.63557983	-11.56654866
H	9.63892952	-4.93769758	-2.44152714	H	1.83861097	-1.35082298	-10.73259480
H	9.51552896	-3.96540043	-0.99498700	C	0.58328783	-2.92083519	-10.28567744
H	8.60328176	-5.44947793	-1.13058047	H	0.32966856	-2.59913356	-9.40642209
C	9.42765400	-2.83806840	3.46833894	H	0.66168783	-3.88677964	-10.24378535
H	10.15363334	-3.62359518	3.49665262	C	-0.49578870	-2.53947054	-11.29958861
H	9.85335324	-1.97571505	2.99926874	H	-0.25616775	-2.90002063	-12.16762061
H	9.13027861	-2.59110738	4.46607545	H	-0.53016440	-1.57315745	-11.37705056

C	-1.86875838	-3.05403052	-10.91191529	H	-0.67339459	-8.42113881	-4.06343288
H	-1.84198771	-4.02040087	-10.83230623	H	-0.78095074	-6.86421327	-3.92000918
H	-2.12125174	-2.68615268	-10.05071373	C	-1.48406995	-7.85463284	-2.25711949
C	-2.63817020	-3.05931376	-13.24408396	H	-1.36931511	-7.11282566	-1.64274332
C	-3.65008756	-2.65643094	-14.24404530	H	-1.26263659	-8.67395870	-1.78741471
C	-4.72629965	-1.80984629	-13.85978917	C	-2.93908701	-7.91061800	-2.72365145
C	-4.87503374	-1.39803168	-12.51868600	H	-3.05600513	-8.67873936	-3.30435264
C	-3.92635392	-1.84708220	-11.48668710	H	-3.13700851	-7.11351991	-3.23979554
C	-3.54310378	-3.09140636	-15.54546688	C	-3.91846896	-8.00894151	-1.56985259
H	-2.83480739	-3.64118745	-15.79157051	H	-3.72635833	-8.80418026	-1.04868590
C	-5.66166247	-1.38911750	-14.83134078	H	-3.81698911	-7.23648095	-0.99213150
C	-5.53457113	-1.86594192	-16.16289950	C	-6.27465852	-8.60950498	-1.22528407
H	-6.15318989	-1.60807057	-16.80765057	C	-7.65522431	-8.67084475	-1.75110678
C	-4.49674513	-2.71104131	-16.50556762	C	-7.91508568	-8.30472794	-3.10055903
H	-4.42856192	-3.03010195	-17.37637739	C	-6.87891779	-7.82397463	-3.92851024
C	-5.91534354	-0.54494999	-12.15997500	C	-5.50955681	-7.67897855	-3.40842546
H	-6.01492393	-0.28235858	-11.27332398	C	-8.68324659	-9.09202986	-0.93862875
C	-6.71634053	-0.50375786	-14.42956764	H	-8.50634351	-9.33422656	-0.05854006
H	-7.34012021	-0.21419226	-15.05583146	C	-9.22823203	-8.41277028	-3.61026714
C	-6.81096664	-0.08192345	-13.12960970	C	-10.27131524	-8.83596775	-2.74456299
H	-7.47853699	0.51939303	-12.88901100	H	-11.14238964	-8.89620049	-3.06470695
O	3.25951119	-4.20202850	0.89555433	C	-9.99887705	-9.15860908	-1.42912495
O	-5.97465829	-9.00571265	-0.10672443	H	-10.68976266	-9.42139458	-0.86487400
O	-4.57674435	-7.26230211	-4.06324970	C	-7.13924101	-7.49696584	-5.25665311
N	1.53934028	-4.42455873	-1.67676798	H	-6.45527508	-7.17250063	-5.79696176
N	1.30788430	-5.23470200	-2.68359823	C	-9.45997403	-8.07559840	-4.98512709
N	1.20803245	-6.47666690	-2.18378702	H	-10.31751506	-8.14284492	-5.33904374
N	-5.29991047	-8.07092260	-2.06922475	C	-8.42667258	-7.65516975	-5.78031067
C	1.85206285	-4.49287448	0.78387382	H	-8.58305555	-7.47282662	-6.67887327
H	1.33945116	-3.67140391	0.84148672	O	3.61175166	-0.70240216	4.48093727
H	1.57708978	-5.07693931	1.50789773	O	-2.89393490	-7.63008997	9.78054662
C	1.60004278	-5.15805082	-0.52895809	O	-4.49107550	-4.80129275	6.60331764
C	1.38431397	-6.47623601	-0.84092479	N	2.16593438	-3.53596233	3.93233655
H	1.36359750	-7.20397046	-0.26230075	N	2.15878765	-4.79800440	4.29401304
C	0.93786433	-7.61276024	-3.06654629	N	2.29887869	-4.83313059	5.62870369
H	1.19042722	-8.43505488	-2.61829656	N	-3.72524999	-6.17652856	8.23892444
H	1.47545337	-7.53030544	-3.86972805	C	2.36775481	-1.27398563	4.93231177
C	-0.54308239	-7.67957505	-3.45181335	H	1.65255838	-1.03098901	4.32374741

H	2.14864976	-0.93376041	5.81389687	O	-4.55816419	6.66544738	7.85349295
C	2.32466467	-2.76234117	5.04385710	O	-1.60231339	5.18456596	10.97081105
C	2.40656252	-3.58342215	6.13957291	N	2.86223981	3.14448374	5.23309277
H	2.51185687	-3.33806931	7.03038570	N	3.05840968	3.45881397	6.49258673
C	2.31662762	-6.11248256	6.33997460	N	2.89931656	4.78721282	6.60351153
H	2.71491215	-5.98773778	7.21558437	N	-3.09579946	5.85853665	9.39974939
H	2.86265314	-6.74572311	5.84827934	C	2.31959008	4.22655021	3.06701708
C	0.90316097	-6.67986890	6.50209456	H	1.75053406	3.46746806	2.86484532
H	0.96139188	-7.54140704	6.94406485	H	1.86421790	5.03481965	2.78366355
H	0.52163990	-6.82363115	5.62210730	C	2.58883346	4.28313363	4.53460272
C	-0.03600304	-5.77626502	7.30513081	C	2.60523535	5.34373145	5.40427943
H	-0.10960752	-4.91410597	6.86676019	H	2.44970409	6.24063994	5.21402289
H	0.33023336	-5.63475703	8.19214637	C	3.04445582	5.44647000	7.90246395
C	-1.42253845	-6.41040654	7.42021820	H	3.19727300	6.39460956	7.76621941
H	-1.34711852	-7.25222296	7.89619203	H	3.81517203	5.08053932	8.36397556
H	-1.75891179	-6.59990920	6.53033915	C	1.79574247	5.25345493	8.76823427
C	-2.41339009	-5.51948779	8.14450068	H	1.94567111	5.67242118	9.63018856
H	-2.08332270	-5.32542277	9.03574710	H	1.66408391	4.30450179	8.91909010
H	-2.50465492	-4.68069715	7.66611157	C	0.52148505	5.83622654	8.15175916
C	-3.85119581	-7.25801843	9.11468576	H	0.35603278	5.41713397	7.29275299
C	-5.17643415	-7.90974180	9.18689347	H	0.63758151	6.78832393	8.00690626
C	-6.21269544	-7.50553491	8.30068237	C	-0.67609836	5.60204706	9.07307072
C	-6.01035943	-6.44545296	7.39208056	H	-0.52195276	6.05865644	9.91487898
C	-4.72625043	-5.72705004	7.35179565	H	-0.75243179	4.65289879	9.25809445
C	-5.40149365	-8.91246958	10.10244387	C	-1.97881175	6.09574460	8.47364696
H	-4.71869333	-9.17531462	10.67620882	H	-1.90979131	7.04485530	8.28562846
C	-7.46073443	-8.16622353	8.34213177	H	-2.14675548	5.63295401	7.63795868
C	-7.66894348	-9.18687129	9.30726882	C	-4.38186924	6.19581005	8.96996828
H	-8.49145450	-9.61833600	9.35422148	C	-5.48901104	5.95769768	9.92062780
C	-6.65600043	-9.54220048	10.17697268	C	-5.20364262	5.52185935	11.24395716
H	-6.80485459	-10.20179420	10.81535880	C	-3.87740752	5.25425795	11.64365804
C	-7.02207737	-6.07830186	6.50873845	C	-2.76265554	5.40813461	10.69481055
H	-6.88777282	-5.37349729	5.91693330	C	-6.79112510	6.16849447	9.52767619
C	-8.47826945	-7.76855762	7.41255475	H	-6.97104631	6.45764015	8.66249807
H	-9.30546812	-8.19374319	7.42329225	C	-6.26300194	5.34379839	12.16149787
C	-8.23980085	-6.76668776	6.50912873	C	-7.59732607	5.55433765	11.72353132
H	-8.89527523	-6.54163905	5.88878543	H	-8.30392042	5.42535206	12.31427479
O	3.57405547	4.09943361	2.36835213	C	-7.85131765	5.94970970	10.42435216

H	-8.72867129	6.07187253	10.14135901	C	-3.31261718	10.66256783	-9.07586026
C	-3.60712985	4.85693000	12.95046594	C	-2.30630260	9.75287411	-8.50450238
H	-2.73242499	4.67343174	13.20783788	C	-1.46766352	12.09888846	-11.96308849
C	-5.94868545	4.94170188	13.50207710	H	-0.62580753	12.05308511	-12.35512238
H	-6.63276211	4.82181776	14.12080373	C	-4.00144196	12.28914933	-10.76316267
C	-4.64767922	4.73305071	13.87709246	C	-3.70558806	13.01560048	-11.94692850
H	-4.45406582	4.50639663	14.75814931	H	-4.35272308	13.56533936	-12.32626236
O	3.12646951	3.32813001	-2.89837043	C	-2.46139827	12.90989141	-12.53812610
O	0.47222239	10.50446538	-10.64755672	H	-2.28018445	13.37795313	-13.32096585
O	-2.50169731	9.04922270	-7.53535394	C	-4.56191803	10.76078478	-8.46901003
N	1.90433092	6.22139143	-2.87538303	H	-4.75770938	10.23984881	-7.72381743
N	2.21921416	7.47439817	-3.10869357	C	-5.27491675	12.37286407	-10.10827112
N	2.94614509	7.50146055	-4.23700979	H	-5.93651347	12.92783298	-10.45389376
N	-1.04468862	9.73302153	-9.13614021	C	-5.52315466	11.64083032	-8.97721251
C	2.24635386	3.96378280	-3.84669353	H	-6.34039635	11.73009214	-8.54216340
H	1.32276212	3.77494776	-3.61816889				
H	2.41774610	3.62069969	-4.73768803		compound 1-2		
C	2.44577510	5.44353014	-3.85565492	C	1.20547200	-5.21117300	5.12329900
C	3.11307187	6.25432523	-4.73815176	C	-2.52172700	-1.23409900	2.61518900
H	3.57481558	6.00475262	-5.50583570	C	3.16509900	-3.03822700	-1.96139000
C	3.44201440	8.77129709	-4.77048109	C	-1.60528000	-2.46231800	-1.38931200
H	4.17139865	8.59820835	-5.38604848	C	0.06319200	-3.03967100	6.41945600
H	3.78446930	9.31351219	-4.04272487	C	0.37907500	-1.25965100	-2.09096600
C	2.33545335	9.54008170	-5.49889783	C	-3.08519000	-2.02378900	1.61366400
H	2.69373347	10.38811666	-5.80459142	C	-0.00787700	-0.19215400	-1.27666300
H	1.62133586	9.72950003	-4.87059821	C	3.54882500	-0.79229500	-1.19404400
C	1.75067245	8.79064614	-6.69880362	C	4.20305000	-4.19094600	4.51341400
H	1.38032454	7.94427106	-6.40317498	C	-0.76345600	-3.90326700	5.70853700
H	2.45470065	8.60575178	-7.33998111	C	2.84096200	-1.67463900	-2.01495000
C	0.65526164	9.62109853	-7.36834450	C	4.58190700	-1.26257000	-0.38086800
H	1.04151602	10.44744293	-7.69827875	C	5.34774900	-3.45564500	2.01600600
H	-0.01757818	9.84909509	-6.70785442	C	4.66673600	-2.90030600	4.27085600
C	-0.00897553	8.89099201	-8.51979652	C	-0.41835200	-2.41396100	-2.12429300
H	0.65832261	8.65941374	-9.18463529	C	-0.17114800	-5.00230800	5.05723200
H	-0.40995270	8.06992644	-8.19449083	C	4.92083600	-4.76925200	2.25953300
C	-0.67670424	10.52617072	-10.22606794	C	-2.27256600	-1.73253900	3.89325700
C	-1.73151101	11.37204170	-10.82448163	C	5.18270000	-2.50885400	3.03127600
C	-3.01413912	11.44093768	-10.21398243	C	3.54639300	-4.54686700	5.83832800

H	3.75323500	-5.59551800	6.07539100	C	-0.711171400	-4.64607600	-2.93803000
H	3.98122800	-3.93312700	6.63160800	H	-0.16766700	-5.33309600	-3.59118200
C	-3.17082900	-3.85568900	3.21561000	H	-0.80055000	-5.09049600	-1.93617900
C	-1.99363800	-1.39411700	-0.57698600	H	-1.72121600	-4.48820400	-3.34422000
C	-2.25094900	-3.63580300	5.57530900	C	-4.44193600	-5.40315900	1.21909100
H	-2.81472100	-4.56325400	5.72287100	H	-4.87603300	-5.78660400	0.29325300
H	-2.55034600	-2.94065700	6.36613000	H	-3.63209200	-6.07075100	1.54615500
C	4.16488800	-3.50994700	-1.10867800	H	-5.22538700	-5.36551000	1.98482300
C	1.44593500	-3.23554900	6.47167900	C	-0.48184000	-6.81214500	3.52565500
C	-3.28440800	-1.46462000	0.21586900	H	-1.32542600	-7.26997200	3.00212600
H	-3.99283700	-2.08792400	-0.33050900	H	0.20606100	-6.37012000	2.79128000
H	-3.71503300	-0.46130800	0.29265600	H	0.05398500	-7.58892700	4.09029400
C	1.68167200	-1.19118500	-2.86645100	C	3.90555200	-7.35738700	2.69762500
H	1.61081800	-1.80379400	-3.76947900	H	3.44918100	-8.26302700	3.10410700
H	1.85459500	-0.15716000	-3.17768000	H	3.33845400	-7.02648500	1.81561800
C	4.33024600	-5.13069800	3.47118500	H	4.93756000	-7.57998300	2.39183000
C	-2.59384600	-3.05732200	4.21287700	H	5.12883700	-0.55913500	0.23274400
C	-1.16229700	-0.26508200	-0.49574800	H	0.62624600	0.68566000	-1.25588600
C	5.95421200	-3.08857200	0.67416900	H	-2.25161200	-0.21066900	2.39300700
H	6.48086800	-3.95922900	0.27441000	H	-0.34459700	-2.17124600	6.92339500
H	6.68817600	-2.29010500	0.81670800	H	4.63297400	-2.16650700	5.06736000
C	-3.40942400	-3.35577500	1.93197600	O	3.16966700	0.54066100	-1.10630600
C	2.04040900	-4.32428600	5.82186100	O	9.62525500	-6.23495300	-2.30517400
C	4.90403600	-2.61437300	-0.31169400	O	5.66005800	-4.97216000	-4.18708100
H	-2.24546100	-3.33745900	-1.41023900	N	5.96252300	1.68101000	-0.52023000
H	-3.39274700	-4.88773000	3.45688200	N	7.23614400	1.40584400	-0.58554400
H	1.66832900	-6.05080300	4.62077300	N	7.48958000	0.94308100	-1.83149200
H	5.03020500	-5.48717000	1.45623800	N	7.59169600	-5.65222500	-3.17307100
H	2.58814600	-3.71841000	-2.57489700	C	3.89314200	1.48037100	-1.91945300
O	0.04019900	-3.44947800	-2.91487300	H	3.51151500	2.45643100	-1.61536800
O	-3.95362100	-4.10726100	0.91127800	H	3.66342800	1.31903100	-2.98290300
O	-1.03579200	-5.82782700	4.37576400	C	5.37264400	1.39889100	-1.71950000
O	3.86040400	-6.39798100	3.73645900	C	6.35102600	0.92353700	-2.56751300
O	4.49860700	-4.83932900	-0.98539500	H	6.31414300	0.56617400	-3.58442500
C	3.72180900	-5.78902800	-1.69982900	C	8.84192100	0.53012900	-2.20254200
H	4.12802700	-6.76733200	-1.43001200	H	9.38589600	0.43805500	-1.25892600
H	2.66413700	-5.73941300	-1.40618500	H	9.30828600	1.33246700	-2.78642600
H	3.81315900	-5.64496200	-2.78204400	C	8.86072400	-0.78694400	-2.98522100

H	9.90932500	-1.00727100	-3.22462300	H	-0.77313800	1.78843300	1.88055000
H	8.35599800	-0.64641100	-3.95102600	C	-1.34298200	3.07045500	0.27167100
C	8.23320700	-1.97317900	-2.24355600	C	-2.43917200	3.74698800	0.77146700
H	7.19619200	-1.73982300	-1.97023000	H	-3.04887500	3.57944900	1.64877300
H	8.77106200	-2.13980700	-1.29953700	C	-3.74509300	5.70314100	-0.16100800
C	8.25823500	-3.25123500	-3.08983300	H	-3.59528900	6.26361200	-1.08764700
H	9.29252900	-3.52296100	-3.33698600	H	-3.60889300	6.38467800	0.68386100
H	7.72508700	-3.07966300	-4.03358800	C	-5.13038700	5.04238100	-0.14726900
C	7.59331600	-4.42074100	-2.36282600	H	-5.87591600	5.83095900	-0.31763200
H	8.12426200	-4.64981400	-1.43804800	H	-5.33401000	4.63576200	0.85278400
H	6.55540400	-4.19118400	-2.13179900	C	-5.28464400	3.92441800	-1.18736500
C	8.69115100	-6.51690500	-3.04437100	H	-4.64008400	3.08504000	-0.89468800
C	8.64838400	-7.77342400	-3.83386200	H	-4.91116600	4.26321500	-2.16334200
C	7.56211500	-8.03320700	-4.70661800	C	-6.73448100	3.43686400	-1.32204600
C	6.50887800	-7.09436300	-4.84355100	H	-7.32237000	4.15446700	-1.90913600
C	6.52981200	-5.82888700	-4.06887000	H	-7.20327500	3.36543800	-0.33554800
C	9.67775500	-8.69031900	-3.71216100	C	-6.78411800	2.06007200	-1.99173100
H	10.49723800	-8.46330500	-3.03818100	H	-6.26275800	2.07838300	-2.94829300
C	7.53196200	-9.24650900	-5.45935800	H	-6.30548300	1.31565300	-1.34831700
C	8.60307500	-10.16599700	-5.30585500	C	-8.53420200	1.42407900	-3.61643000
H	8.58512300	-11.09207300	-5.87519900	C	-9.84962000	0.77944200	-3.86875000
C	9.65221200	-9.89242800	-4.45102200	C	-10.64762700	0.32526000	-2.79048100
H	10.46584800	-10.60348100	-4.34315400	C	-10.20687200	0.49611600	-1.45619200
C	5.45651500	-7.34931900	-5.70547500	C	-8.90742100	1.15497600	-1.18141300
H	4.66872600	-6.60852700	-5.79552900	C	-10.27605700	0.59677900	-5.17241900
C	6.43338700	-9.47734800	-6.32882100	H	-9.64204400	0.94851000	-5.97950500
H	6.40418200	-10.39993600	-6.90335800	C	-11.88901900	-0.32991900	-3.04998900
C	5.41878900	-8.54838600	-6.44848300	C	-12.29810900	-0.49502300	-4.39936300
H	4.58546900	-8.73606100	-7.11906700	H	-13.24276300	-0.99288400	-4.60368300
O	-1.59083600	0.71003400	0.36964700	C	-11.50812900	-0.04090600	-5.43681000
O	-7.81869900	1.81297700	-4.52889900	H	-11.83044100	-0.17422200	-6.46541900
O	-8.49932900	1.33216000	-0.03677900	C	-10.97421300	0.02630300	-0.40585800
N	-0.96225700	3.67033000	-0.89245800	H	-10.61484700	0.16947800	0.60756500
N	-1.76652800	4.67270600	-1.13811200	C	-12.64755300	-0.80630800	-1.94866900
N	-2.66886600	4.72334400	-0.13273200	H	-13.58822100	-1.31636900	-2.14038200
N	-8.14805200	1.57234800	-2.27336700	C	-12.19703800	-0.63378700	-0.65567100
C	-0.75240200	1.80107000	0.78583400	H	-12.78321200	-1.00603100	0.17925400
H	0.28144500	1.68143500	0.45487500	O	-1.64435300	-0.91689200	4.82106200

O	-7.92589500	-1.44291500	-2.18640200	H	-11.22358800	-3.34343000	-5.23810800
O	-7.62672400	-4.60094400	1.10790000	C	-9.58927100	-6.24447800	-0.09512200
N	-2.94425800	1.83105000	4.02788500	H	-9.14644200	-6.56755800	0.84130700
N	-3.94561000	2.32873600	3.34953000	C	-11.12707900	-6.59426100	-1.93447600
N	-5.05095300	1.61920400	3.66660800	H	-11.88488700	-7.19350200	-2.43336700
N	-7.74477400	-3.04237400	-0.55861400	C	-10.57466800	-7.01945600	-0.74222000
C	-2.50538200	-0.08397100	5.61627200	H	-10.89664700	-7.95598300	-0.29662100
H	-1.83042800	0.50245800	6.23972200	O	2.23039600	-2.34341000	7.19267100
H	-3.13285300	-0.70545500	6.27172700	O	3.40146900	6.86356600	1.82986900
C	-3.39417600	0.79438500	4.79580600	O	-1.15137300	6.70324400	1.46375400
C	-4.74627400	0.65561800	4.56628400	N	0.52988700	0.03004700	7.40661100
H	-5.46991500	-0.04887100	4.94333700	N	-0.01021400	1.22272800	7.33252300
C	-6.34661400	1.93646100	3.06715100	N	0.79233500	1.98624500	6.55734800
H	-6.12792000	2.50789300	2.16058100	N	1.12521200	6.79244200	1.65188500
H	-6.90026900	2.58834200	3.75345400	C	2.59060500	-1.16148200	6.48378900
C	-7.16130300	0.68612200	2.72821100	H	2.64128400	-1.38310700	5.41108300
H	-8.10366500	1.03340700	2.29405500	H	3.60405100	-0.90002500	6.81467000
H	-7.41690400	0.14267400	3.64839400	C	1.68273600	0.02257000	6.68627000
C	-6.46723000	-0.24779500	1.73052000	C	1.86935600	1.27899400	6.14015500
H	-5.55338700	-0.67209900	2.16460600	H	2.66333800	1.68293300	5.52446000
H	-6.15867700	0.34755500	0.86171500	C	0.44264600	3.38079000	6.30206300
C	-7.39789600	-1.36676500	1.25229400	H	1.26549600	4.00842700	6.66573100
H	-8.31000000	-0.91410000	0.85064000	H	-0.43242800	3.56922500	6.92873400
H	-7.68620000	-2.01768200	2.08668300	C	0.13339400	3.71215500	4.83521300
C	-6.75040200	-2.21537700	0.15370500	H	-0.27959300	4.72891700	4.85226800
H	-6.29186300	-1.57431600	-0.59817700	H	-0.67257600	3.06211900	4.47337900
H	-5.99218700	-2.88471000	0.55868000	C	1.35119800	3.65566500	3.89153100
C	-8.28266300	-2.53261100	-1.74795700	H	1.56639100	2.61393800	3.62940300
C	-9.29483100	-3.36598400	-2.44041500	H	2.24970800	4.01849500	4.41166100
C	-9.72179600	-4.59162000	-1.86962600	C	1.18067600	4.46804500	2.59586700
C	-9.16667100	-5.04793500	-0.64812400	H	0.28963000	4.14667400	2.04588100
C	-8.13012200	-4.24582600	0.04824300	H	2.04563700	4.29826300	1.94414400
C	-9.82950400	-2.93450400	-3.64146200	C	1.06867700	5.97187700	2.87649100
H	-9.48633200	-1.99631200	-4.06170700	H	0.12442300	6.21338200	3.36338200
C	-10.71697600	-5.37332900	-2.53129500	H	1.89575500	6.29691100	3.51028800
C	-11.24921200	-4.89491200	-3.75841500	C	2.39385200	7.20476100	1.22015000
H	-12.00727600	-5.48595500	-4.26674800	C	2.44673400	8.08649000	0.02924200
C	-10.81095400	-3.70439900	-4.30132900	C	1.25149900	8.46824600	-0.62849500

C	-0.00371700	7.99824900	-0.16919200	H	4.91567900	5.92712600	0.32194800
C	-0.08406500	7.11553700	1.02153200	C	5.85640600	5.14949200	-1.45306000
C	3.66853500	8.55863700	-0.42017100	H	6.79957600	5.27827200	-1.98361000
H	4.56826700	8.25885300	0.10395000	H	5.61394000	4.08792100	-1.41259400
C	1.31351900	9.33680600	-1.76034400	C	5.18537000	6.75776700	-3.21531900
C	2.58372700	9.79104900	-2.19994300	C	4.10500000	7.29984700	-4.07810400
H	2.63848400	10.42653200	-3.07959500	C	2.76153500	6.89362800	-3.88322200
C	3.73591100	9.40980700	-1.54273800	C	2.42848700	5.96810600	-2.86357600
H	4.70474500	9.74483700	-1.89961200	C	3.48789400	5.40404400	-2.00301700
C	-1.16544000	8.38723500	-0.81238200	C	4.41714700	8.22928900	-5.05525900
H	-2.11352200	8.02544600	-0.43398100	H	5.45362500	8.52683200	-5.17614400
C	0.10156600	9.70479900	-2.39936500	C	1.72787800	7.44294100	-4.70002500
H	0.14609600	10.35718000	-3.26775500	C	2.08441000	8.39308300	-5.69140100
C	-1.11193600	9.24268900	-1.93144500	H	1.30164800	8.81724200	-6.31624500
H	-2.03335300	9.53277200	-2.42795700	C	3.40071500	8.77820100	-5.86463000
O	5.56982400	-1.19240500	2.82878900	H	3.65882200	9.50604400	-6.62857900
O	6.35077000	7.12565300	-3.31349200	C	1.11224400	5.59182600	-2.65753800
O	3.25052800	4.61952900	-1.08844700	H	0.87016100	4.87628300	-1.87843200
N	4.48176900	1.88435800	4.25294400	C	0.38791800	7.03281200	-4.46412700
N	5.13364100	3.01240400	4.36891000	H	-0.40302500	7.45471200	-5.07981800
N	6.15606500	2.97129000	3.48961500	C	0.08728200	6.12945000	-3.46537000
N	4.81030600	5.78757900	-2.27581400	H	-0.93510200	5.83139500	-3.26177300
C	4.50654500	-0.22264300	2.93012200	H	8.03111300	3.74621300	3.07164700
H	3.78430000	-0.50851200	3.70077500				
H	3.96871100	-0.18275200	1.97452500				
C	5.06695200	1.11360400	3.29100200	complex 1·Cu ²⁺			
C	6.14902300	1.80855700	2.78940000	C	1.53095400	3.32122400	3.02952500
H	6.86582300	1.58208100	2.01627400	C	-3.28679100	1.88699100	-1.36716200
C	7.04960300	4.12452100	3.37628100	C	-2.83222900	-2.85302900	3.55051100
H	7.13775700	4.53880600	4.38376700	C	-5.70284800	-1.57363200	0.43199000
C	6.53617000	5.18179200	2.39056300	C	-0.42812800	2.01523000	1.56891700
H	7.16785400	6.07448400	2.50008100	C	-4.12558200	-3.34131400	0.98077500
H	5.51943100	5.47452100	2.67900700	C	-4.39006500	1.36189300	-0.69809600
C	6.54740600	4.69755900	0.93848900	C	-3.29852500	-2.86173400	-0.03226200
H	5.97511300	3.76735000	0.86094500	C	-1.81159500	-5.02774200	3.46598500
H	7.57615100	4.44990400	0.63427100	C	2.28280200	0.11461400	4.35254100
C	5.92640900	5.71067900	-0.02732100	C	-0.56537900	3.37972500	1.78503400
H	6.48576800	6.65654700	-0.02593600	C	-2.76765400	-4.11528300	2.96748300
				C	-0.94458900	-4.66175300	4.49899400

C	0.85487900	-1.93478800	5.69104900	O	-5.79775200	1.33097900	1.18380700
C	2.55969500	-1.21499200	4.08995100	O	0.28859400	5.38505000	2.64814600
C	-5.34146000	-2.67218000	1.21993000	O	1.26406700	1.72901600	5.71944200
C	0.45280500	4.04404400	2.51003700	O	-2.04046000	-1.28255700	5.22547600
C	0.66293100	-0.60493300	6.04019500	C	-2.83307700	-0.24954900	4.65052500
C	-2.48162000	2.86865200	-0.78124700	H	-2.66985700	0.63098300	5.27488300
C	1.87286100	-2.25162500	4.74425600	H	-2.51687200	-0.03007500	3.62195800
C	2.81640400	1.20307800	3.45491800	H	-3.89965100	-0.50608800	4.65829200
H	3.43269800	1.91632500	4.00893500	C	-7.32117800	-2.52327100	2.56355200
H	3.45665800	0.76657600	2.68817400	H	-7.72544800	-3.06672500	3.41913500
C	-3.86296900	2.81416000	1.18694800	H	-7.18650800	-1.46584400	2.83332300
C	-4.85612800	-1.08421100	-0.57194700	H	-8.01317900	-2.60662500	1.72124400
C	-1.73850500	4.18313000	1.23911700	C	-6.07729800	1.67012000	2.53602000
H	-2.21746100	4.72074000	2.06632800	H	-6.97098600	1.10181700	2.80278800
H	-1.33445500	4.95816900	0.57775800	H	-5.24930800	1.37152600	3.19505400
C	-1.98587700	-2.49278200	4.60544700	H	-6.28189700	2.73955900	2.64218400
C	0.69040900	1.29549500	2.02394100	C	1.29612400	6.13547300	3.32006400
C	-5.19354900	0.21508700	-1.28606100	H	0.96940700	7.17524800	3.27935600
H	-6.26564700	0.41077600	-1.18686600	H	1.39378200	5.82371800	4.36776300
H	-4.98206600	0.14032800	-2.35615200	H	2.26788300	6.03336600	2.81962600
C	-3.68614100	-4.51357400	1.82738800	C	0.32094500	2.13893800	6.70857800
H	-4.56265100	-5.02625000	2.24019900	H	0.40728500	3.22430600	6.76399600
H	-3.15527100	-5.23637300	1.20439500	H	-0.69912300	1.86466600	6.41297500
C	1.37876600	0.42322000	5.40982500	H	0.55379000	1.69906500	7.68508800
C	-2.74209600	3.32026400	0.51599800	H	-0.21126700	-5.36934600	4.86915500
C	-3.64276200	-1.74861000	-0.80062500	H	-2.35316700	-3.36069800	-0.21140700
C	-0.06939700	-3.01043400	6.21225600	H	-3.02139100	1.50755700	-2.34594900
H	-0.62582900	-2.62907900	7.07415600	H	-1.19568700	1.51065600	0.99906700
H	0.49574200	-3.88809500	6.53779600	H	3.26223800	-1.44141100	3.30353700
C	-4.68994400	1.86115600	0.58787800	O	-1.83572500	-6.29198800	2.93325000
C	1.67061900	1.95228400	2.80672000	O	7.36402600	-3.28325100	1.68908100
C	-1.01969100	-3.40676600	5.09622700	O	8.46698500	-6.31470500	-1.54900100
H	-6.62975500	-1.04719700	0.61824600	N	-0.55005200	-5.31539100	0.70492000
H	-4.07434900	3.17226700	2.18780400	N	0.23111500	-4.99292200	-0.29417700
H	2.29798700	3.81843400	3.60930000	N	1.31860000	-5.78202500	-0.27301200
H	-0.08843900	-0.37484000	6.78377000	N	7.92222200	-4.79817700	0.06821600
H	-3.55642700	-2.14702200	3.16591300	C	-0.61136600	-6.93570300	2.61107800
O	-6.07615700	-3.14136200	2.26795300	H	-0.88569800	-7.97613700	2.41312400

H	0.08740800	-6.93951100	3.45782700	O	-8.03633100	-4.26704800	-0.13430000
C	0.03728700	-6.31687300	1.39879300	O	-6.06501300	-2.53821200	-3.87914600
C	1.23700300	-6.62721800	0.78106100	N	-1.63415800	-3.86673200	-2.73843400
H	1.99166400	-7.36563200	0.99476000	N	-1.78809200	-5.12162700	-3.10474100
C	2.33958800	-5.63214800	-1.32310000	N	-2.83947600	-5.15533400	-3.93296400
H	2.76432200	-4.63115200	-1.21029800	N	-7.08951100	-3.44220000	-2.03715200
H	1.79729300	-5.65906300	-2.27310200	C	-2.80750200	-1.62344800	-3.07015100
C	3.41628100	-6.71939400	-1.28155200	H	-2.03613700	-1.03500600	-3.57191500
H	3.90373400	-6.72238500	-2.26352600	H	-3.78645600	-1.35427000	-3.48431600
H	2.92427300	-7.69614300	-1.19731500	C	-2.60307400	-3.09086500	-3.31099500
C	4.49790400	-6.55989500	-0.19139500	C	-3.37232500	-3.92046500	-4.09488700
H	4.93975000	-7.54726800	-0.00635100	H	-4.25852500	-3.71586000	-4.67183800
H	4.04788200	-6.23767200	0.75801100	C	-3.35059300	-6.42611400	-4.46312700
C	5.62709500	-5.58998900	-0.57305500	H	-2.76626300	-7.21065500	-3.97698200
H	5.25255100	-4.56127900	-0.62501400	H	-3.14207400	-6.45454300	-5.53764800
H	6.01480400	-5.85210300	-1.56236900	C	-4.85344100	-6.57363500	-4.19142900
C	6.78467400	-5.66229700	0.43286700	H	-5.20496100	-7.43974300	-4.76343200
H	6.46097900	-5.36057700	1.42894900	H	-5.37032300	-5.70831100	-4.62454600
H	7.16181600	-6.68702100	0.47663700	C	-5.23749100	-6.72839800	-2.69794700
C	8.14006300	-3.62133500	0.79008100	H	-4.39067000	-6.44060900	-2.05803500
C	9.31399500	-2.80514600	0.41179300	H	-5.42642600	-7.78561400	-2.48374100
C	10.15124800	-3.21517600	-0.65851500	C	-6.46716700	-5.88143200	-2.30645700
C	9.89534900	-4.41926500	-1.35972800	H	-7.00456700	-6.32967400	-1.46645600
C	8.74150800	-5.26278500	-0.98875200	H	-7.17269000	-5.84028700	-3.14608000
C	9.58780800	-1.62861900	1.09335900	C	-6.03338800	-4.45978400	-1.91431700
H	8.95616100	-1.33533200	1.92097800	H	-5.69046200	-4.45199700	-0.87936900
C	11.27097500	-2.40987000	-1.02821900	H	-5.21518500	-4.11631700	-2.53898200
C	11.50680100	-1.20483800	-0.31450900	C	-8.07022700	-3.43108300	-1.02938900
H	12.36409100	-0.59612000	-0.59135000	C	-9.09694200	-2.36925400	-1.10058700
C	10.67823900	-0.81549600	0.72005100	C	-9.05180600	-1.40453900	-2.13780300
H	10.84247300	0.11684200	1.24988800	C	-8.03294600	-1.45372700	-3.12237900
C	10.72634300	-4.81743700	-2.39526500	C	-6.98910200	-2.49972600	-3.06476300
H	10.50793400	-5.74710000	-2.91036000	C	-10.10760100	-2.32394000	-0.15347300
C	12.10019700	-2.84722200	-2.09428600	H	-10.13754000	-3.09195100	0.61271400
H	12.95529400	-2.23870600	-2.37718500	C	-10.04385800	-0.38003600	-2.19568400
C	11.83352900	-4.02625900	-2.76281100	C	-11.04893400	-0.34704300	-1.19200000
H	12.47776200	-4.35057800	-3.57393400	H	-11.78190300	0.45166700	-1.21919200
O	-2.70858800	-1.23406700	-1.69375200	C	-11.08014700	-1.30343100	-0.19601000

H	-11.86091400	-1.27779700	0.55801400	C	-9.46522200	4.80072100	2.08750400
C	-8.01494700	-0.52457200	-4.15041700	C	-8.52466100	4.17752300	1.13057000
H	-7.23091000	-0.59170800	-4.89761900	C	-12.75138400	3.84544800	0.61065500
C	-9.98996900	0.56226300	-3.25722600	H	-13.12160000	3.30073500	-0.25156900
H	-10.72885900	1.35518900	-3.28541100	C	-11.76178300	5.27954600	2.82951700
C	-9.00114600	0.48133400	-4.21895100	C	-13.15873200	5.14155000	2.61498100
H	-8.97707800	1.19960800	-5.03321100	H	-13.84601300	5.60260500	3.31949000
O	-1.33477100	3.31678000	-1.43268800	C	-13.64219300	4.43976000	1.52802100
O	-10.85655000	2.72970400	-1.17801700	H	-14.71242000	4.34604200	1.37272000
O	-7.30506800	4.28817600	1.23058900	C	-8.97078200	5.52096200	3.16309400
N	-2.21964500	2.96166600	-4.30437900	H	-7.89569300	5.61519300	3.27545500
N	-3.28928600	2.69322700	-5.00361300	C	-11.21864500	6.00251000	3.92395500
N	-4.25192600	3.56378800	-4.62355500	H	-11.89732600	6.46817500	4.63377800
N	-9.08775100	3.42561900	0.08630900	C	-9.85183200	6.12105000	4.08576100
C	-1.53027500	4.39231900	-2.38182300	H	-9.45018900	6.68186100	4.92405600
H	-0.52952900	4.59018400	-2.77477500	O	0.89766400	-0.02217800	1.73766600
H	-1.88895000	5.28953800	-1.86108200	O	5.78287700	5.81233800	-2.95327700
C	-2.48199800	4.00346900	-3.46197400	O	6.72288600	1.67334300	-1.26949600
C	-3.78700900	4.39892300	-3.66406900	N	0.29366200	-1.46154900	-1.49273600
H	-4.39259600	5.15862200	-3.19677600	N	0.44361400	-0.95579700	-2.69842100
C	-5.57912400	3.50158600	-5.24406400	N	0.43340200	0.37113600	-2.55712000
H	-5.71009500	2.46167800	-5.55539300	N	6.26317000	3.75743300	-2.06981200
H	-5.56956700	4.12414900	-6.14543000	C	-0.02620400	-0.73631400	0.89428600
C	-6.69715400	3.94424400	-4.29692000	H	-1.06018800	-0.52431300	1.19221500
H	-7.63454500	3.89309000	-4.86552400	H	0.16569800	-1.78980300	1.09313300
H	-6.56638100	5.00525900	-4.04397500	C	0.18923100	-0.46098800	-0.56617300
C	-6.83004000	3.11136200	-3.01492500	C	0.27955600	0.72928400	-1.26070700
H	-5.87588900	3.07925000	-2.47461800	H	0.21197900	1.76226300	-0.96644400
H	-7.06850200	2.07403500	-3.28092700	C	0.64533700	1.23465000	-3.72325200
C	-7.91455000	3.67752300	-2.09175500	H	0.02212300	2.11873600	-3.58307500
H	-8.85800700	3.79245900	-2.63857700	H	0.24739800	0.69068600	-4.58202700
H	-7.61375700	4.67496200	-1.74546800	C	2.12535100	1.57592600	-3.92285000
C	-8.16258900	2.78990400	-0.87009800	H	2.20311700	2.14546500	-4.85771700
H	-8.60554300	1.83968600	-1.17153700	H	2.68665200	0.64428700	-4.07337700
H	-7.23705900	2.59533400	-0.33191000	C	2.74788600	2.38023300	-2.77610000
C	-10.46208100	3.32524600	-0.17867700	H	2.66620300	1.81691700	-1.83626700
C	-11.38202900	3.95237200	0.79360400	H	2.17857200	3.31045300	-2.62943000
C	-10.86451200	4.67046200	1.90080800	C	4.22283800	2.70647000	-3.02685400

H	4.33211700	3.28371000	-3.95349600	H	4.32627800	-2.63128700	-1.53296500
H	4.78987300	1.77573600	-3.14962000	C	5.44178300	-1.16341400	-0.38123100
C	4.82735100	3.50379100	-1.86997900	H	5.81174700	-0.68192800	-1.29180700
H	4.34612300	4.47724700	-1.78035800	H	6.20366000	-1.89476600	-0.09104000
H	4.71250000	2.96816700	-0.92617200	C	5.28533200	-0.10202200	0.72374700
C	6.63509000	4.99327800	-2.63766800	H	4.48409000	-0.39115800	1.41473300
C	8.08589500	5.23329100	-2.80652600	H	4.99119300	0.85187200	0.28305200
C	9.02452200	4.23961600	-2.43382600	C	6.59392500	0.03842600	1.50591400
C	8.59212600	2.99741500	-1.90450400	H	7.41672200	0.19249100	0.80257400
C	7.14942500	2.73480200	-1.72269900	H	6.79126600	-0.91177900	2.01530500
C	8.51942800	6.44684900	-3.31388700	C	6.64456400	1.15267500	2.55479100
H	7.77749100	7.18842500	-3.59119900	H	5.70714600	1.23333500	3.10467000
C	10.42094600	4.49749500	-2.57923400	H	7.45026000	0.95042200	3.26239600
C	10.82991100	5.75328900	-3.09905500	C	5.85364700	3.32460900	1.68019900
H	11.89217600	5.95456900	-3.21162200	C	6.18393800	4.66475200	1.14785900
C	9.89769500	6.70744500	-3.45836600	C	7.53578300	5.04038300	0.94741800
H	10.22325600	7.66276500	-3.85843800	C	8.58685900	4.13207300	1.22875700
C	9.51606000	2.03607500	-1.52923900	C	8.27760600	2.76959100	1.71152700
H	9.16667800	1.09754400	-1.11368000	C	5.16253800	5.54804200	0.83686400
C	11.34048500	3.49217900	-2.18062300	H	4.13674400	5.22776600	0.99022300
H	12.40537600	3.68436400	-2.28472300	C	7.84052300	6.33763000	0.43507600
C	10.89530000	2.29007600	-1.66630100	C	6.76801700	7.21165900	0.12018200
H	11.60671100	1.53014600	-1.36133900	H	6.99344400	8.19223300	-0.28992300
O	2.07263800	-3.57003800	4.52639900	C	5.45674200	6.82313400	0.31396600
O	4.69270600	2.95530200	1.85410700	H	4.64727900	7.49710100	0.05273500
O	9.13741400	1.91184400	1.88665700	C	9.90464600	4.50886500	1.03210000
N	2.02090300	-3.43877200	1.63819300	H	10.68895100	3.79143900	1.24559600
N	2.28710800	-2.85811200	0.49912800	C	9.20306200	6.68967100	0.24588400
N	3.61426100	-2.64222100	0.43701800	H	9.44100100	7.67237400	-0.15118500
N	6.92708000	2.48225000	1.98276400	C	10.21149400	5.79584000	0.54467200
C	3.19018900	-4.05493800	3.75575500	H	11.24855200	6.07552700	0.39016300
H	3.08940600	-5.14028200	3.83580400	Cu	-0.12577200	-3.37798700	-1.38340000
H	4.12722800	-3.75727800	4.24225700				
C	3.18218300	-3.59062100	2.33021700				
C	4.22262400	-3.09133400	1.56453900				
H	5.28999500	-3.03113600	1.73079000				
C	4.15702300	-1.91244100	-0.72280000				
H	3.35777200	-1.23582200	-1.03709800				