Supporting information

Diverting metal site in flavin-copper complexes for nanoparticle synthesis

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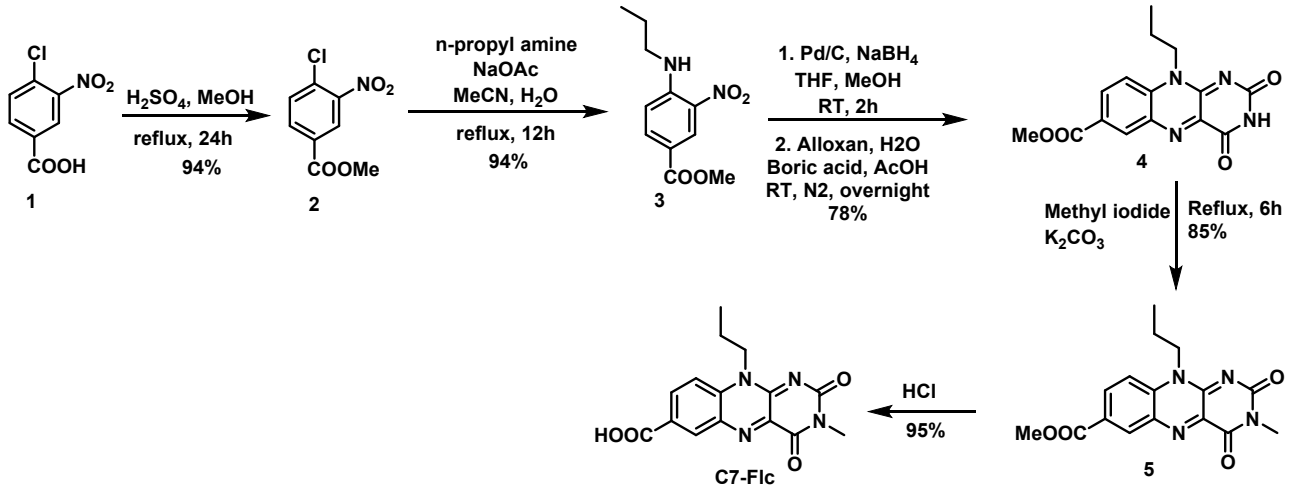
Table of contents

Synthetic procedure of C7-Flc

As shown in Scheme S1, the reaction begins with the esterification of 4-chloro-3-nitrobenzoic acid **1** to yield the corresponding ester **2**. Further, nucleophilic aromatic substitution reaction was performed between 2 and n-propylamine in the presence of NaOAc to get **3**. Further, reduction of compound 3 in the presence of NaBH4 yielded an amino derivative, followed by a condensation reaction with alloxan monohydrate to obtain flavin derivative **4**. Furthermore, protection of **4** was done using methyl iodide and K2CO3 to get the corresponding protected flavin **5**. Finally, the deprotection step was carried out to achieve the final compound **C7-Flc** with excellent yield. M.P = 307-310 ^{o}C.[1,2]

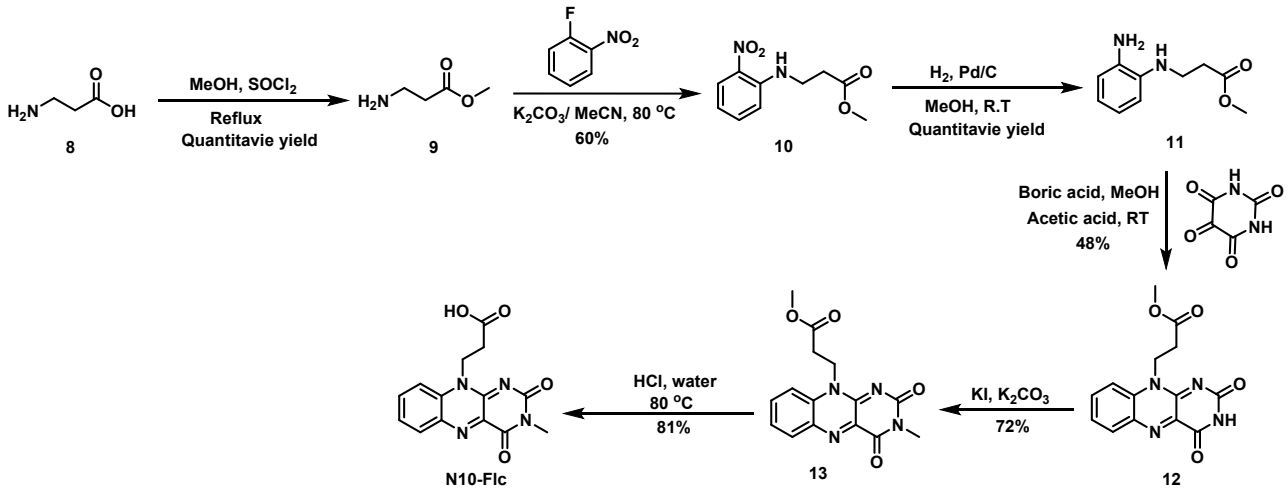


Scheme S1. Schematic representation of the synthesis of **C7-Flc.**[1,2]

Synthetic procedure and characterization of N10-Flc

As shown in Scheme S2, the esterification of the carboxyl group of b-was done by using methanol and $SOCl_2$ to get the corresponding ester derivative **9**. Further, nucleophilic aromatic substitution reaction of 9 with fluoro-nitrobenzene gave nitro derivative **10**. Later, reduction of **10** was achieved into in the monofunctionalized diaminobenzene derivative **11**, via using H_2/Pd/C. Further, condensation reaction of **11** was proceeded with alloxan monohydrate in the presence of boric acid in acetic acid/methanol solution to obtain the isoalloxazine ester derivative **12**. [3]

The detailed synthesis of **13** and **N10-Flc** was given in below, are described in one submitted work (in revision). Standard characterization techniques were utilized to characterize the **13** and **N10-Flc**.[4]



Scheme S2. Schematic representation of the synthesis of **N10-Flc.**[3,4]

Synthesis of **methyl 3-(3-methyl-2,4-dioxo-3,4-dihydrobenzo[g]pteridin-10(2H)-yl)propanoate (13)**

6.67 mmol of **12** was dissolved in DMF (40 mL) followed by addition of potassium carbonate (26.68 mmol) and methyl iodide (333.03 mmol). The reaction mixture was subjected to reflux condition for 6hrs. After completion of the reaction, yellow solid was obtained via washing the reaction mixture

with water. Further, dried yellow solid was subjected to silica gel column chromatography using chloroform and methanol to give pure **13** with a yield of 72%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.96-7.91 (m, 1H), 7.79 (d, *J* = 8.2 Hz, 1H), 7.65 (ddd, *J* = 8.2, 7.2, 1.0 Hz, 1H), 5.00 (t, *J* = 8 Hz, 2H), 3.72 (s, 3H), 3.53 (s, 3H), 2.96 (t, *J* = 7.6 Hz, 2H).^{13}C NMR (101 MHz, $CDCl_3$) δ 170.76, 159.62, 155.72, 148.74, 136.86, 136.01, 135.93, 133.63, 132.30, 126.71, 115.01, 52.34, 40.72, 31.07, 28.87. HRMS (ESI) m/z = $[C15H14N4O4+H_2O]^+$ Calculated for **13**: 332.1121, Found: 332.1133.

Synthesis of **N10-Flc**

Further the deprotection of ester of compound **13** (400 mg), was done by adding conc hydrochloric acid (1.5 ml), followed by addition of distilled water (3 ml). Further heating was applied upto 80^{o}C. After15-20 minutes, yellow precipitate start to observe. The reaction was continued till 2 hrs to get the better precipitate. Later, the precipitate was washed and subjected to column chromatography to get the final pure product, **N10-Flc** (yield = 81%).

M.P = 310-316 ^{o}C ^{1}H NMR (400 MHz, DMSO) δ 12.66 (s, 1H), 8.16 (dd, *J* = 8.1, 1.4 Hz, 1H), 8.08 (d, *J* = 8.5 Hz, 1H), 7.98-7.94 (m, 1H), 7.68 – 7.64 (m, 1H), 4.79 (t, *J* = 8 Hz, 2H), 3.27 (s, 3H), 2.74 (t, *J* = 8 Hz, 2H). ^{13}C NMR (101 MHz, DMSO) δ 172.33, 159.91, 155.62, 149.35, 138.10, 135.64, 135.51, 132.70, 132.31, 126.59, 116.78, 31.07, 28.48. HRMS (ESI) m/z = $[C14H12N4O4+K]^+$ Calculated for **N10-Flc**: 339.0496, Found: 339.0489.

Table **S1**. Crystal Structure Refinement parameter for **C7FlcCu** and **N10FlcCu.**

Identification code	**C7FlcCu**	**N10FlcCu**
empirical formula	$C_{34}H_{40}CuN_8O_{12}$	$C_{14}H_{13}Cu0.5N_4O_4$
formula weight	816.29	698.12
crystal colour	orange	orange
crystal system	triclinic	monoclinic
space group	*P*1	C2/c
a/Å	8.423	33.820
b/Å	9.815	10.7349
c/Å	11.557	8.6029
α/deg	101.688	90
β/deg	101.380	91.611
γ/deg	92.361	90
volume/Å^3	914.0(3)	3122.1
D_{calcd} (g/cm^3)	1.483	1.485
temp/K	298	298
Z	1	8
μ (mm^{-1})	0.672	0.769
F(000)	425.0	1436.0
Reflections observed	3839	3066
R(int)	10.90	9.68
final R_1 values (all data)	0.0605 (2200)	0.0688 (2136)
final wR(F^2) values(all data)	0.1516 (3839)	0.1907(3066)
GOF on F^2	1.036	1.027

Crystal description of copper complexes in the crystal lattice

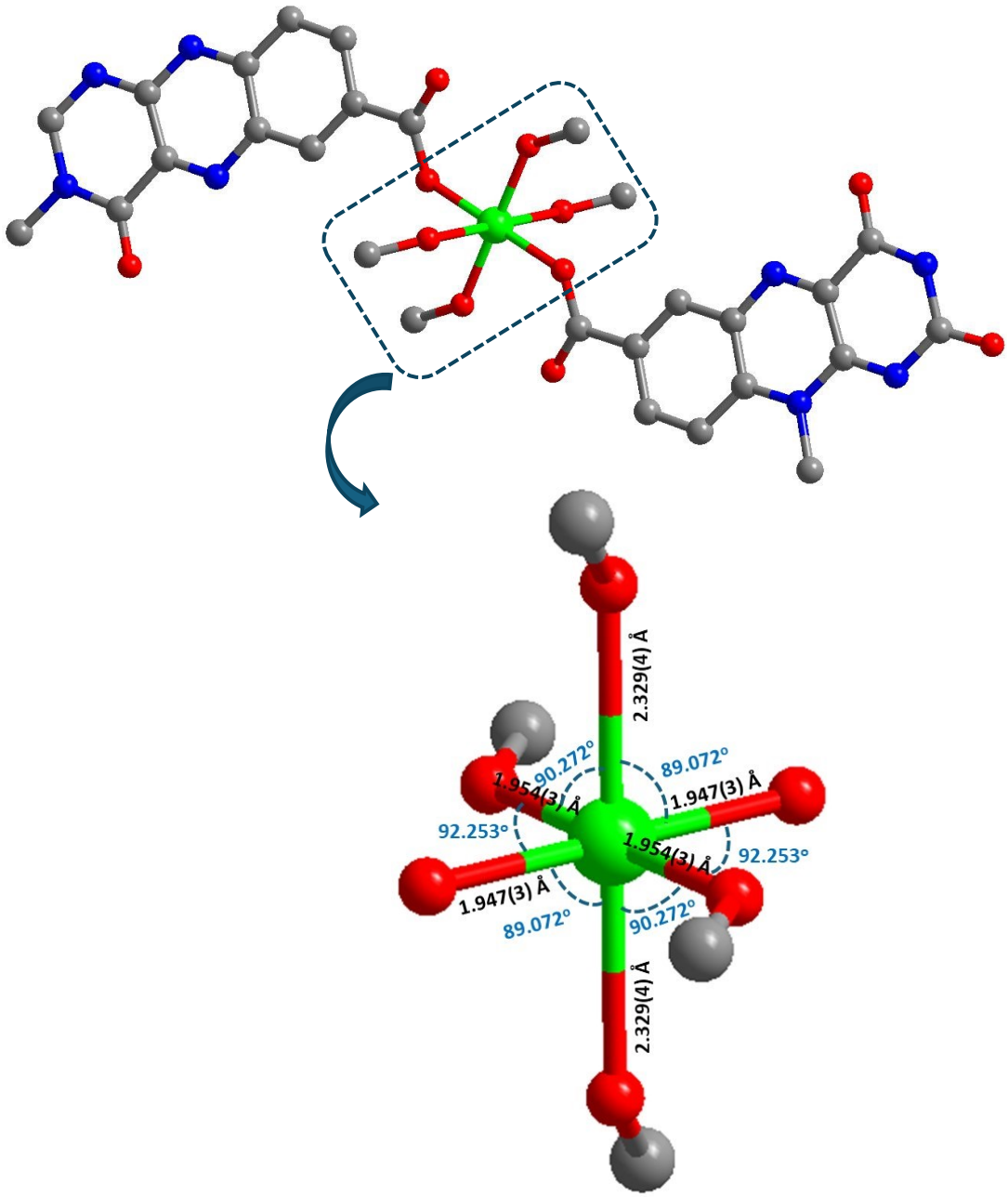


Figure S1. Representation of bond length, bond angles at the coordination site of **C7FlcCu**. (hydrogen atom are omitted due to clarity)

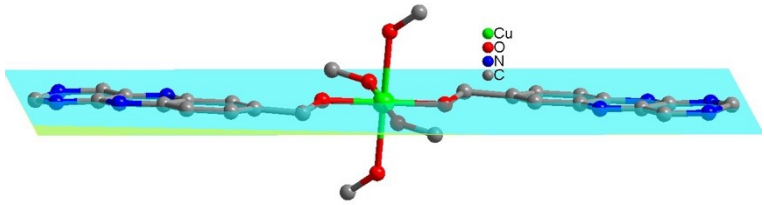


Figure S2. Pictorial representation of the planes passing through the two flavin moieties involved in **C7FlcCu** complex formation. (Hydrogen atoms are omitted due to clarity)

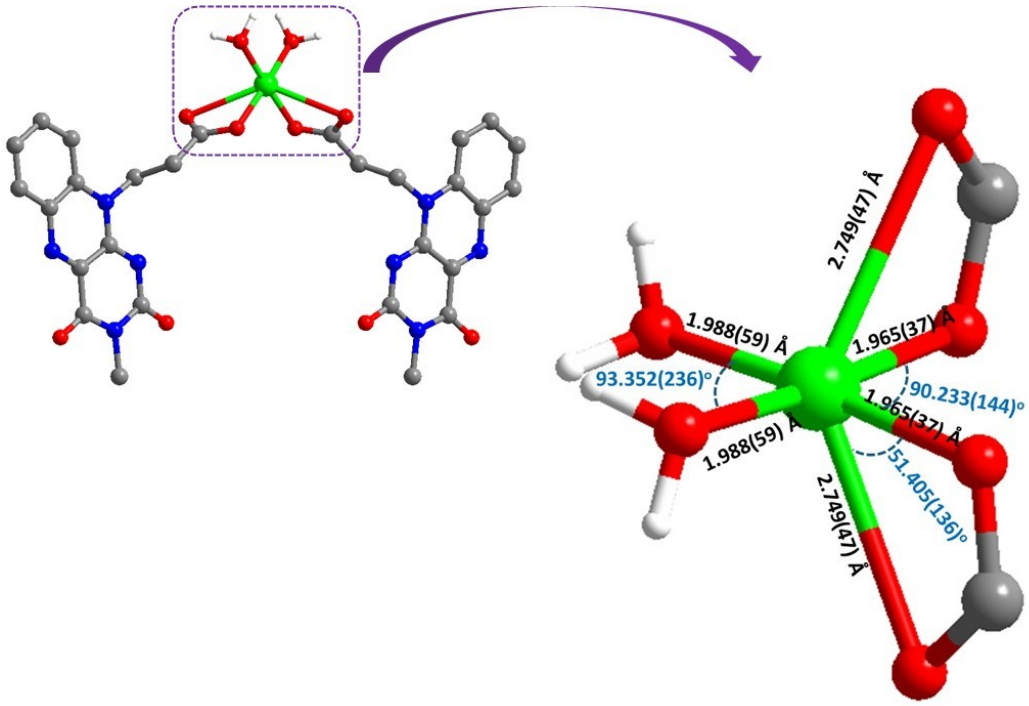


Figure S3. Representation of bond length and bond angle at the coordination site of **N10FlcCu**. (Few hydrogen atoms are omitted due to clarity)

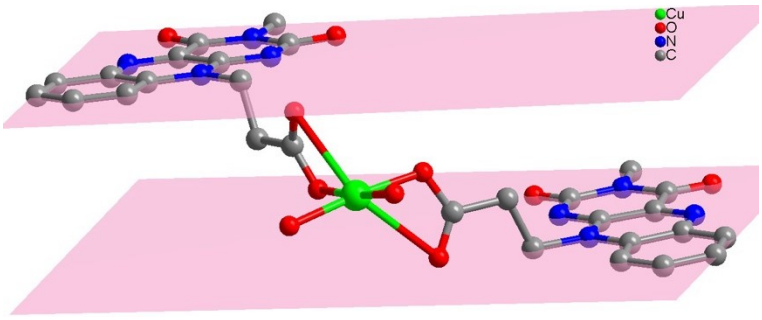


Figure S4. Pictorial representation of the planes passing through the two flavin moieties involved in **N10FlcCu** complex formation. (Hydrogen atoms are omitted due to clarity)

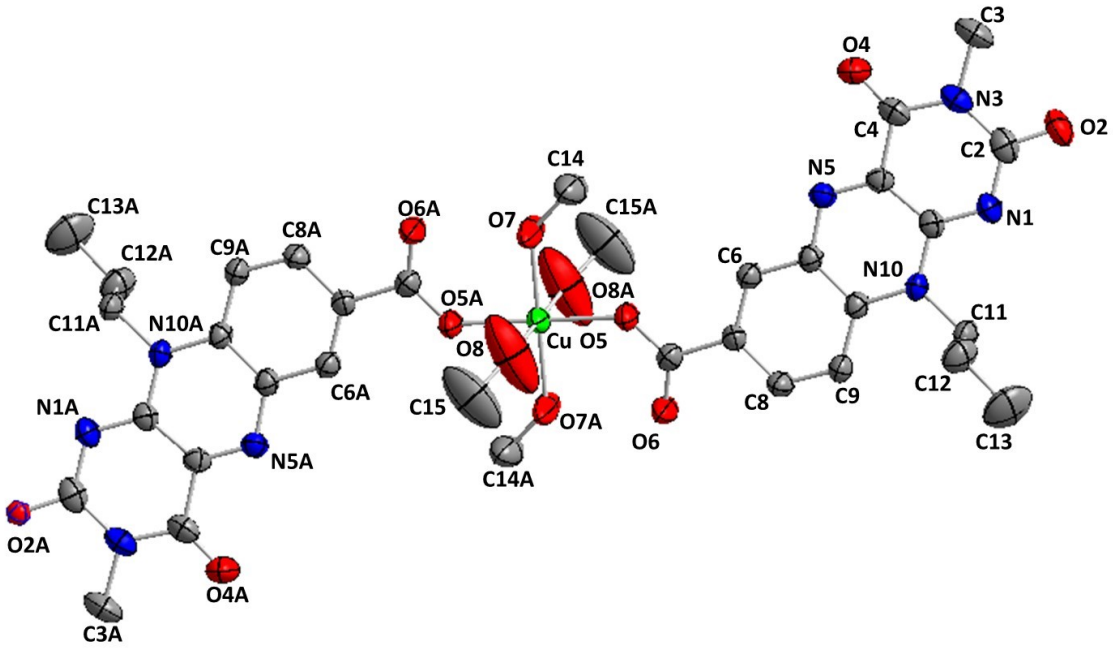


Figure S5. ORTEP diagram of **C7FlcCu**. (Hydrogen atoms are omitted due to clarity)

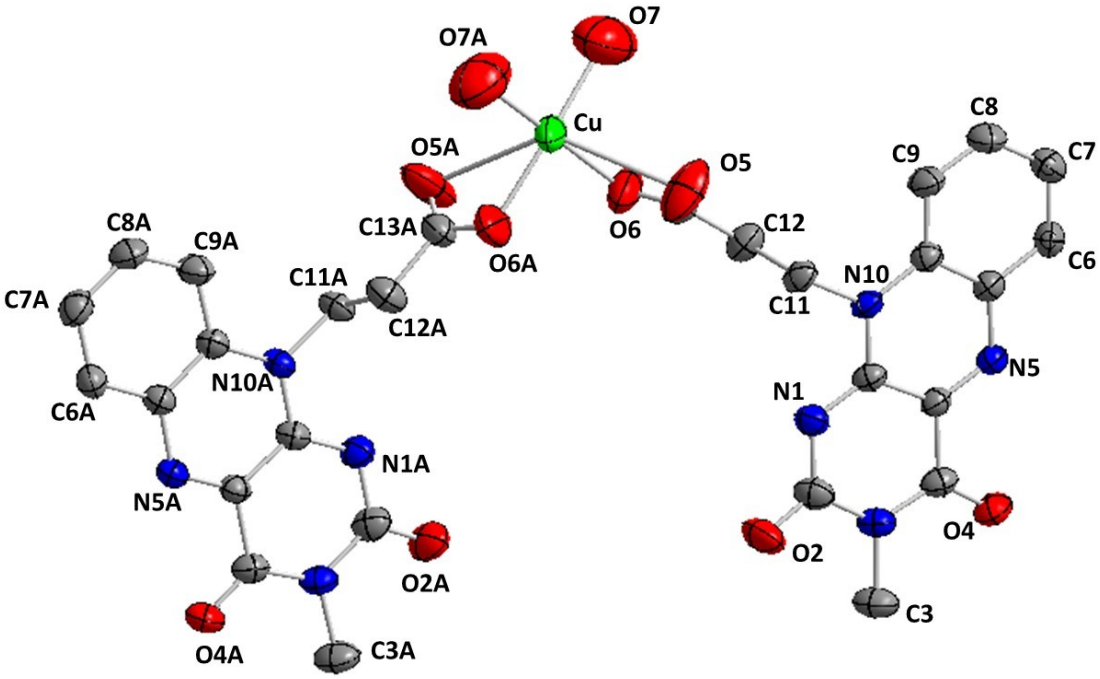


Figure S6. ORTEP diagram of **N10FlcCu**. (Hydrogen atoms are omitted due to clarity)

UV-Vis and fluorescence data of copper complexes formation

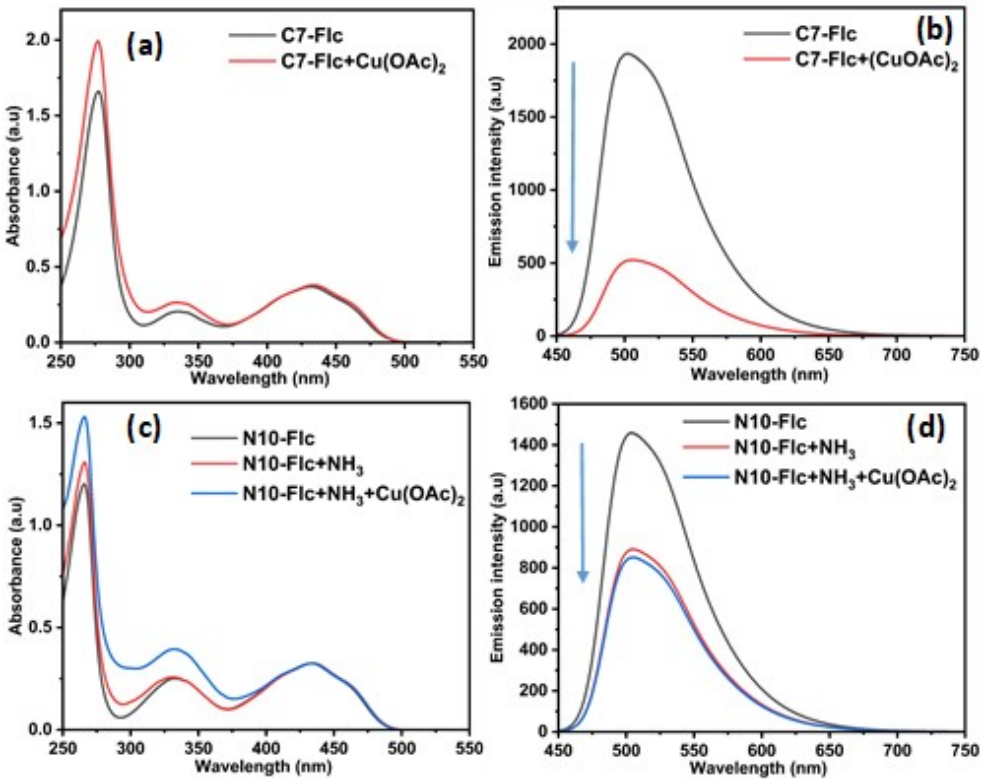


Figure S7. Illustration of the (**a**) absorption and (**b**) emission spectra of the **C7-Flc** with the addition of the $Cu(OAc)_2$; (**c**) absorption and (**d**) emission spectra of the **N10-Flc** with the addition of the $Cu(OAc)_2$ in presence of methanolic ammonia.

PXRD pattern of experimental and simulated data of copper complexes

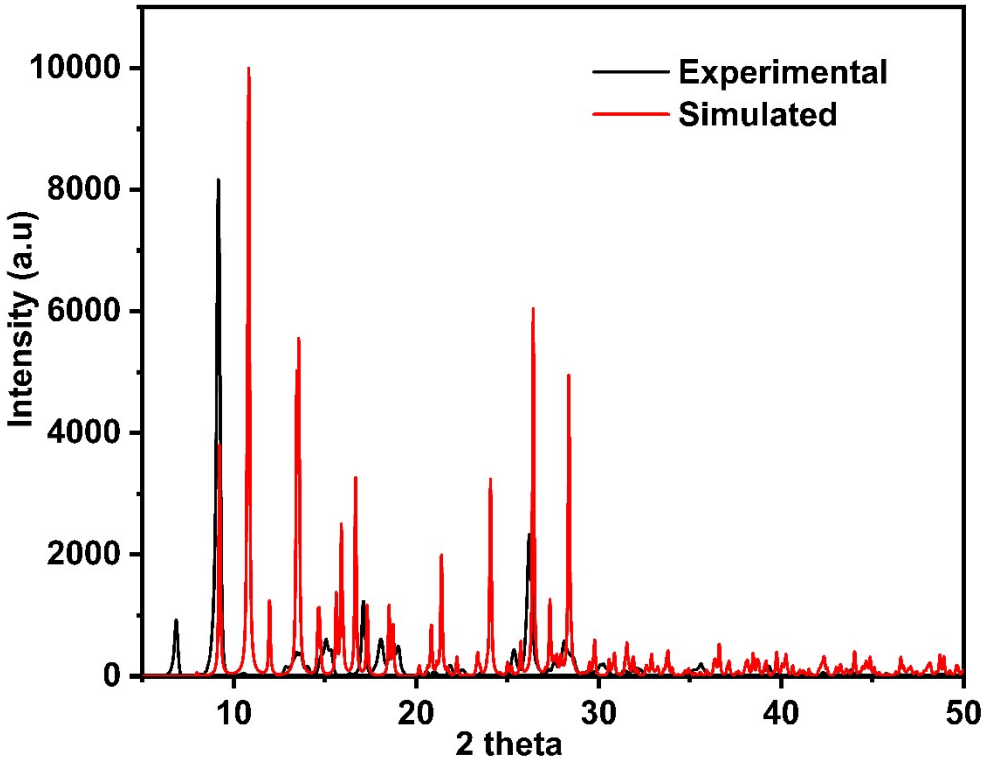


Figure S8. Experimental and simulated PXRD of **C7FlcCu**.

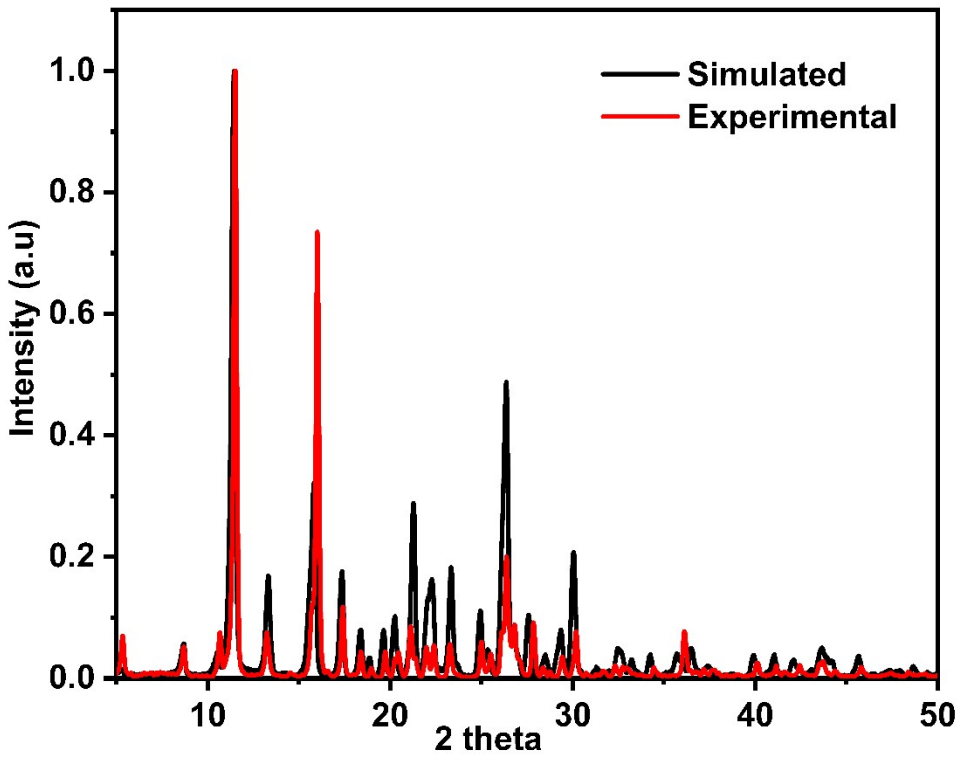


Figure S9. Experimental and simulated PXRD of **N10FlcCu**.

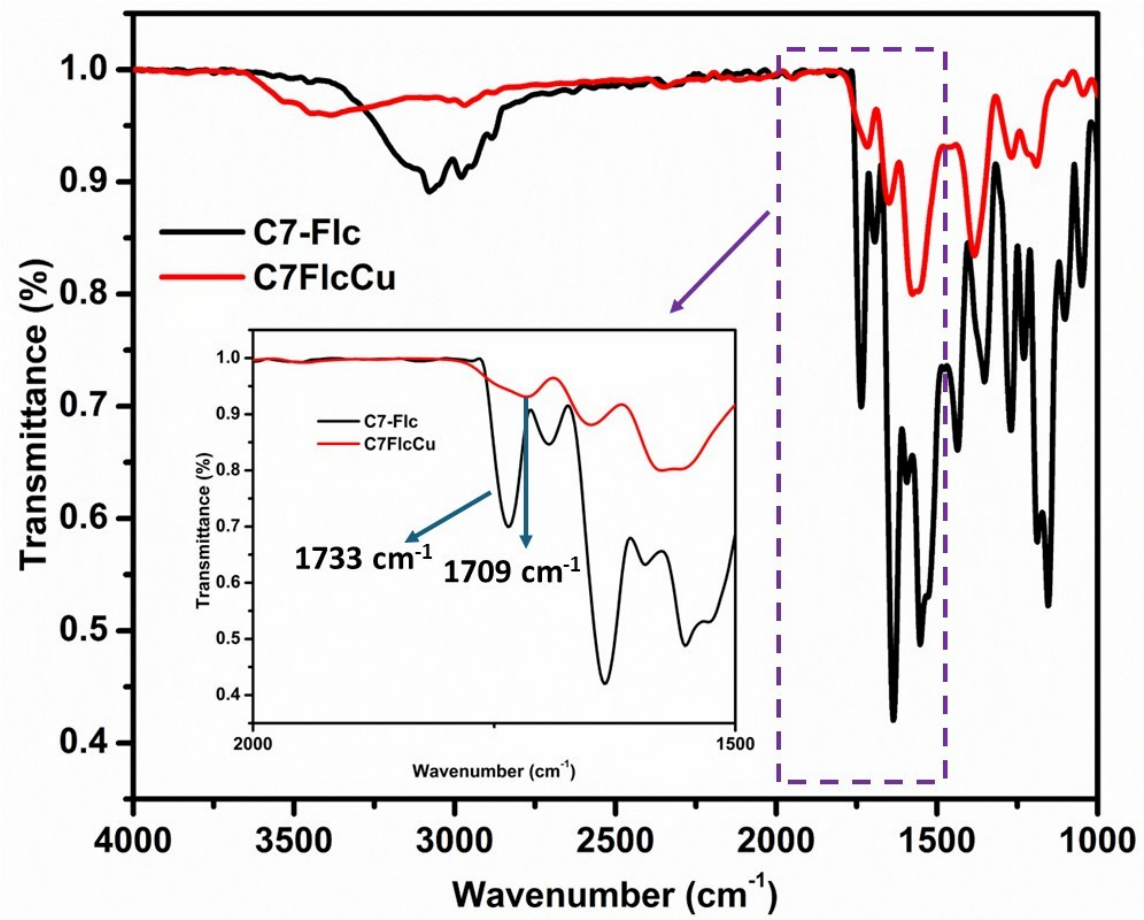


Figure S10. FT-IR of **C7-Flc** and **C7FlcCu**.

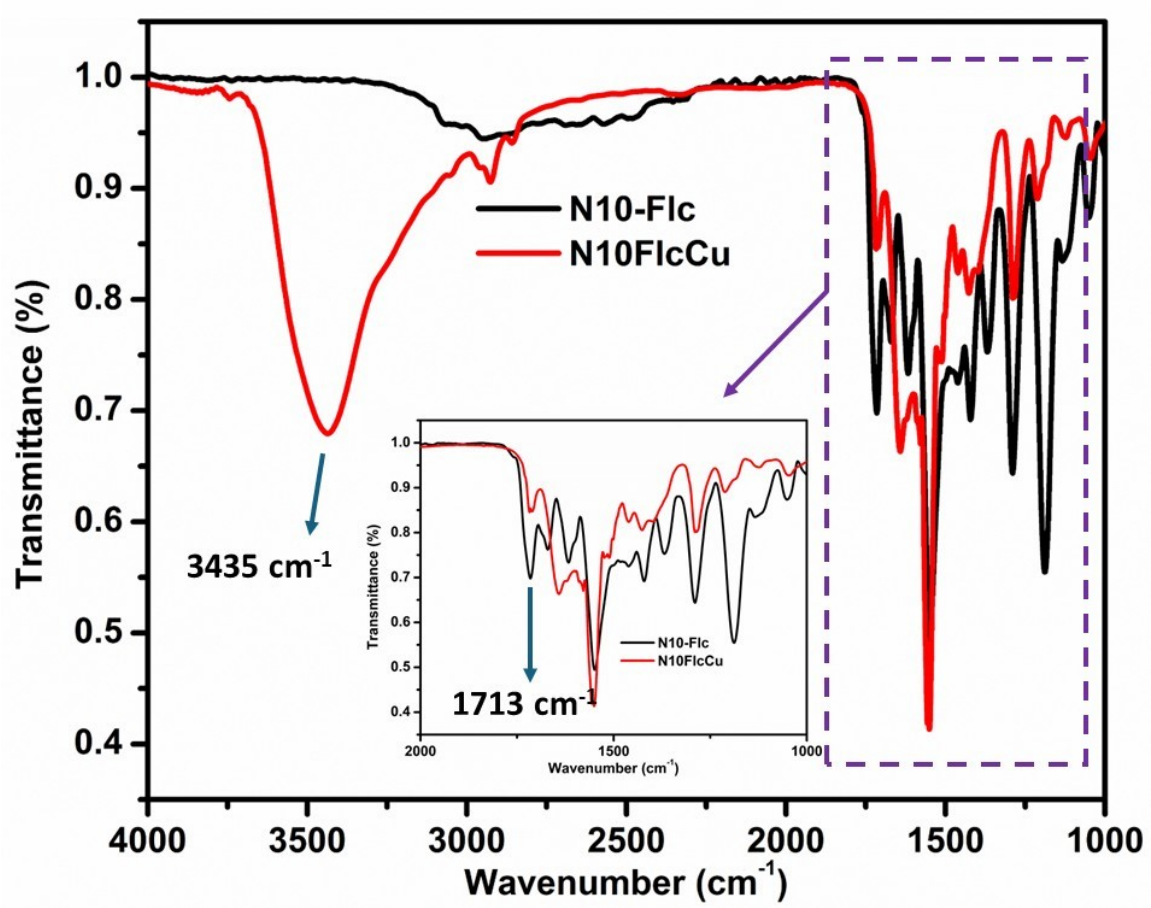


Figure S11. FT-IR of **N10-Flc** and **N10FlcCu**.

Table S2. Lattice Parameters of the prepared Cuprous oxide Nanoparticles.

Nanoparticles	2θ of intense peak (°)	β (radian)	cosθ (radian)	crystallite diameter D (nm)	Avg crystallite diameter D (nm)
CuNP1	36.61	0.118665	0.855357	1.426194	2.002923
	42.55	0.069202	0.75434	2.77307	
	61.61	0.097791	0.819117	1.807194	
	73.77	0.105156	0.686514	2.005231	
CuNP2	36.68	0.061942	0.872961	2.486207	2.450915
	42.53	0.055135	0.74774	2.793147	
	61.48	0.079639	0.780128	1.933717	
	73.87	0.059446	0.721997	2.59059	

EDX imaging of copper nanoparticles

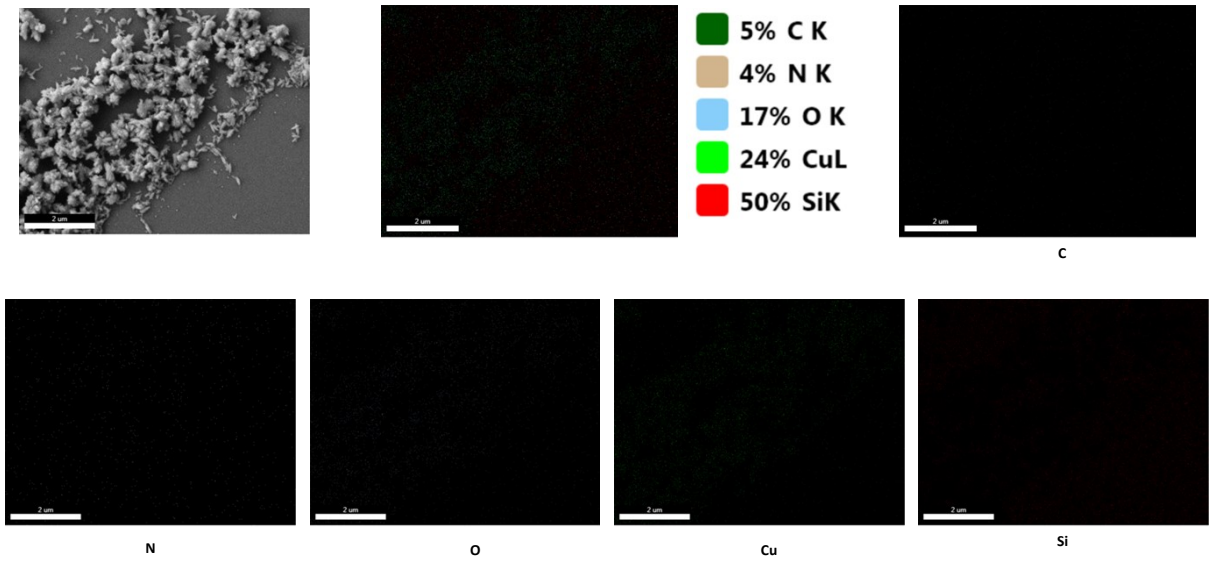


Figure S12. EDX mapping of **CuNP1**.

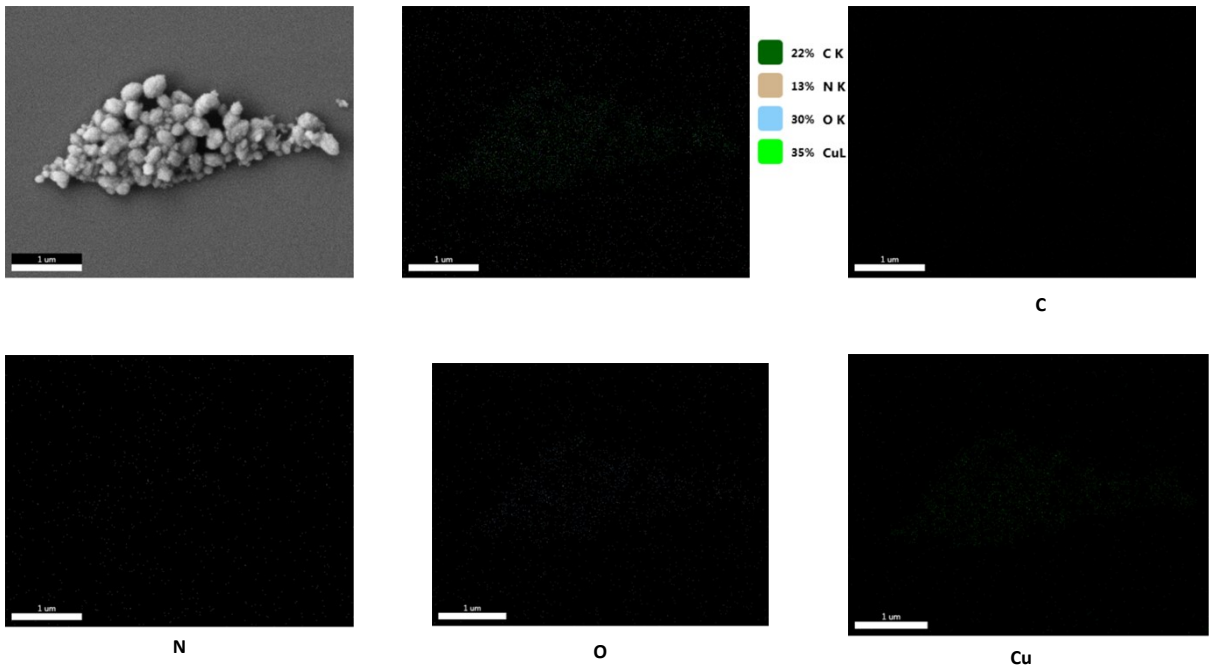


Figure S13. EDX mapping of **CuNP2**.

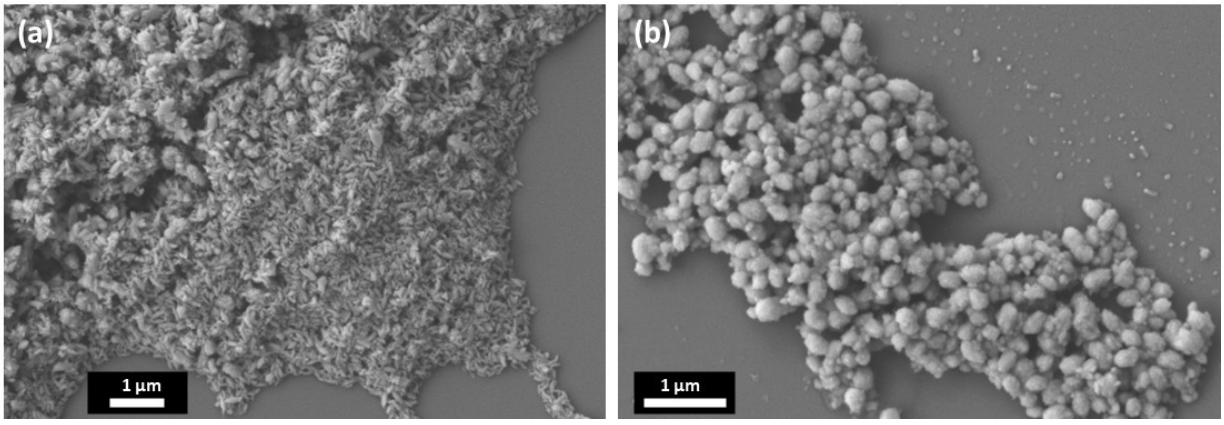


Figure S14. FE-SEM image of (a) **CuNP1 and** (**b**) **CuNP2** at higher magnification (1 µm).

Checkcif report of C7FlcCu

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) c7flccu

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: c7flccu

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	Calculated	Reported
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Hall group	-P 1	-P 1
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Sum formula	C34 H40 Cu N8 O12	C34 H40 Cu N8 O12
Mr	816.29	816.28
Dx,g cm-3	1.483	1.483
Z	1	1
Mu (mm-1)	0.672	0.672
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F000'	425.52	
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S = 1.036 Npar= 258

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**.

Click on the hyperlinks for more details of the test.

Alert level B

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PLAT242_ALERT_2_B Low   MainResAtom  Ueq as Compared to Neighbours        Cu1 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O2       ..O7       .      2.71 Ang.
                                          1+x,1+y,1+z  =      1_666 Check
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Alert level C

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ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
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           _exptl_absorpt_process_details field.
           Absorption correction given as multi-scan
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.972 Why?
PLAT220_ALERT_2_C NonSolvent   Resd 1  C    Ueq(max)/Ueq(min) Range        4.7 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  O    Ueq(max)/Ueq(min) Range        3.2 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H    Uiso(max)/Uiso(min) Range        5.2 Ratio
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours         O7 Check
PLAT241_ALERT_2_C High  MainResAtom  Ueq as Compared to Neighbours         O8 Check
PLAT245_ALERT_2_C U(iso) H8        Smaller than U(eq) O8        by      0.031 Ang**2
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PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        90 Report
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               -9  5  2,  -8  7  2,  -7  8  2,  -6  9  2,  -5 10  2,   8 -6  3,
               -8  3  3,  -9  4  3,  -9  5  3,  -8  6  3,  -8  7  3,  -7  8  3,
               -6  9  3,  -4 10  3,  -9  4  4,  -9  5  4,  -8  6  4,  -7  7  4,
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Alert level G

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PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..     Please Do !
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PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..........     2.066 Note
             Predicted wR2: Based on SigI**2  7.34 or SHELX Weight  14.64
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PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          3 Info
PLAT994_ALERT_1_G SHELXL .ins Contains no or MERG 0 Instruction ..          ! Note
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0 **ALERT level A** = Most likely a serious problem - resolve or explain

2 **ALERT level B** = A potentially serious problem, consider carefully

10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

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# start Validation Reply Form
_vrf_PLAT242_c7flccu
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PROBLEM: Low   MainResAtom  Ueq as Compared to Neighbours        Cu1 Check
Author response: The relatively poor diffraction data causes the Ueq of
The copper (II) atom deviates from the normal value. However, this does
not affect the identification of the overall crystal structure.
;

_vrf_PLAT430_c7flccu
;

PROBLEM: Short Inter D...A Contact  O2       ..O7       .       2.71 Ang.
Author response: This is a normal hydrogen bond distance. Although water-
bound H atoms could not be localized in this crystal structure.
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# end Validation Reply Form
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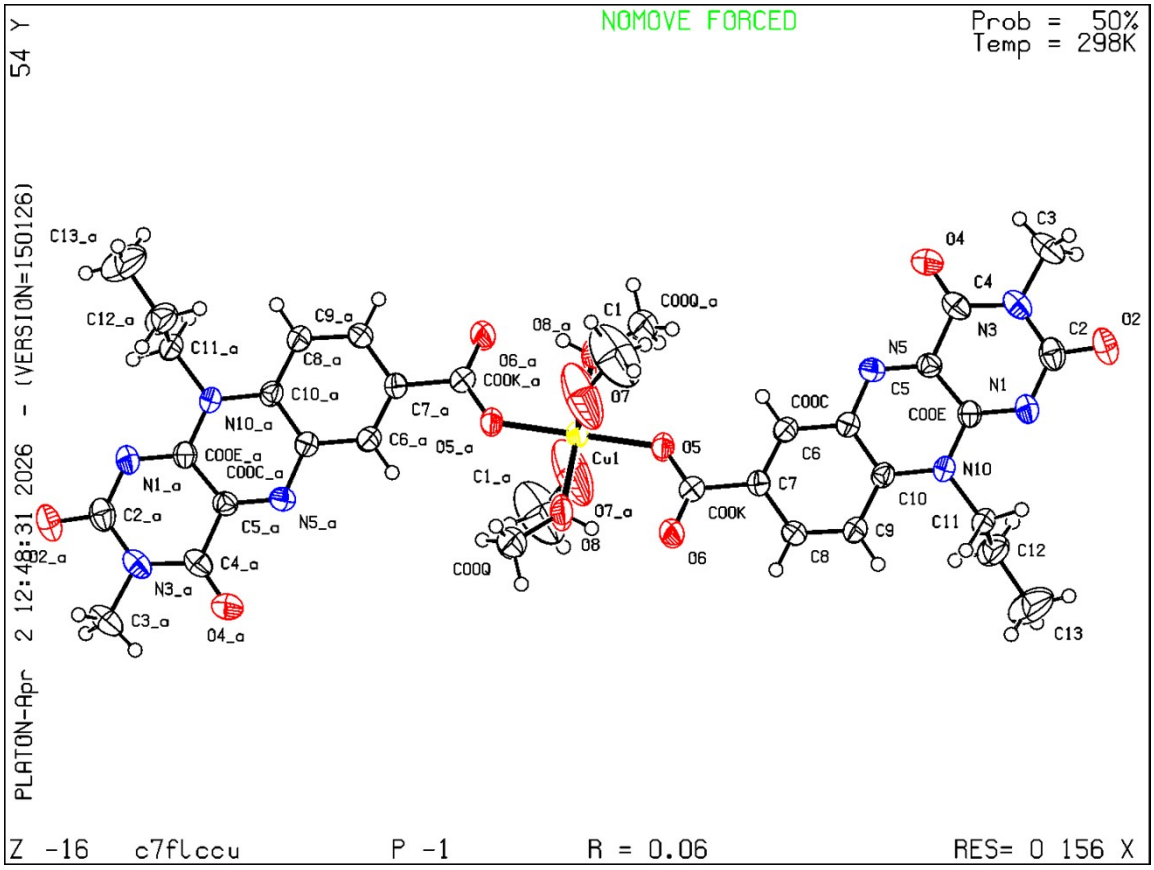
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 15/01/2026; check.def file version of 02/01/2026

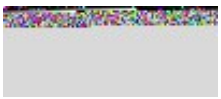
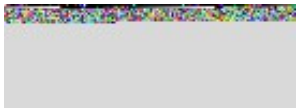
duplicate check

No duplication found

Datablock c7flccu - ellipsoid plot



Checkcif report of N10FlcCu

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) n10flccu

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

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Hall group	-C 2yc	-C 2yc
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The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**.

Click on the hyperlinks for more details of the test.

Alert level B

PLAT420_ALERT_2_B D-H Bond Without Acceptor O7 --H7B . Please Check

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Alert level C

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PLAT242_ALERT_2_C Low MainResAtom Ueq as Compared to Neighbours Cu1 Check
PLAT242_ALERT_2_C Low MainResAtom Ueq as Compared to Neighbours C13 Check
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PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.227 Check

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Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C2.95 H3.2 Cu.1 N0.8 O1.15
Atom count from the _atom_site data: C2.8 H2.6 Cu.1 N0.8 O1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 40
From the CIF: _chemical_formula_sum C2.95 H3.20 Cu0.10 N0.80 O1.15
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	118.00	112.00	6.00
H	128.00	104.00	24.00
Cu	4.00	4.00	0.00
N	32.00	32.00	0.00

```
          O         46.00     40.00     6.00
 PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............          2 Report
              H7A     H7B
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ      Please Check
              Calc: C28 H26 Cu N8 O10
              Rep.: C2.95 H3.20 Cu0.10 N0.80 O1.15
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
              Calc: C28 H26 Cu N8 O10
              Rep.: 0.1(C28 H26 Cu N8 O10), 0.15[CH4O]
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.100 Check
PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size ..       0.65 mm
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      14.51 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1      --O7       .        6.8 s.u.
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        192 A**3
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              CU1  -O6   -CU1     2_656   1_555   1_555 ......     #   30 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              CU1  -O5   -CU1     1_555   1_555   2_656 ......     #   51 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              CU1  -O7   -CU1     2_656   1_555   1_555 ......     #   81 Check
PLAT868_ALERT_4_G  ALERTS  Due  to  the  Use  of  _smtbx_masks  Suppressed     !  Info
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..   Please Do !
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min)[Deg]=      1.99 Note
             2  0  0,
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..     52.0 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     3.700 Note
              Predicted wR2: Based on SigI**2  5.16 or SHELX Weight 18.58
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          2 Info
PLAT994_ALERT_1_G SHELXL .ins Contains no or MERG 0 Instruction ..          ! Note
```

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
21 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT420_n10flccu
;

PROBLEM: D-H Bond Without Acceptor  O7       --H7B      .     Please check
Author response: This alert concerns the hydrogen atoms of lattice water
molecules. It is very difficult to locate hydrogen atoms accurately using
X-ray data because these atoms have low scattering power. However, this
does not affect the identification of the overall crystal structure.
;

# end Validation Reply Form
```

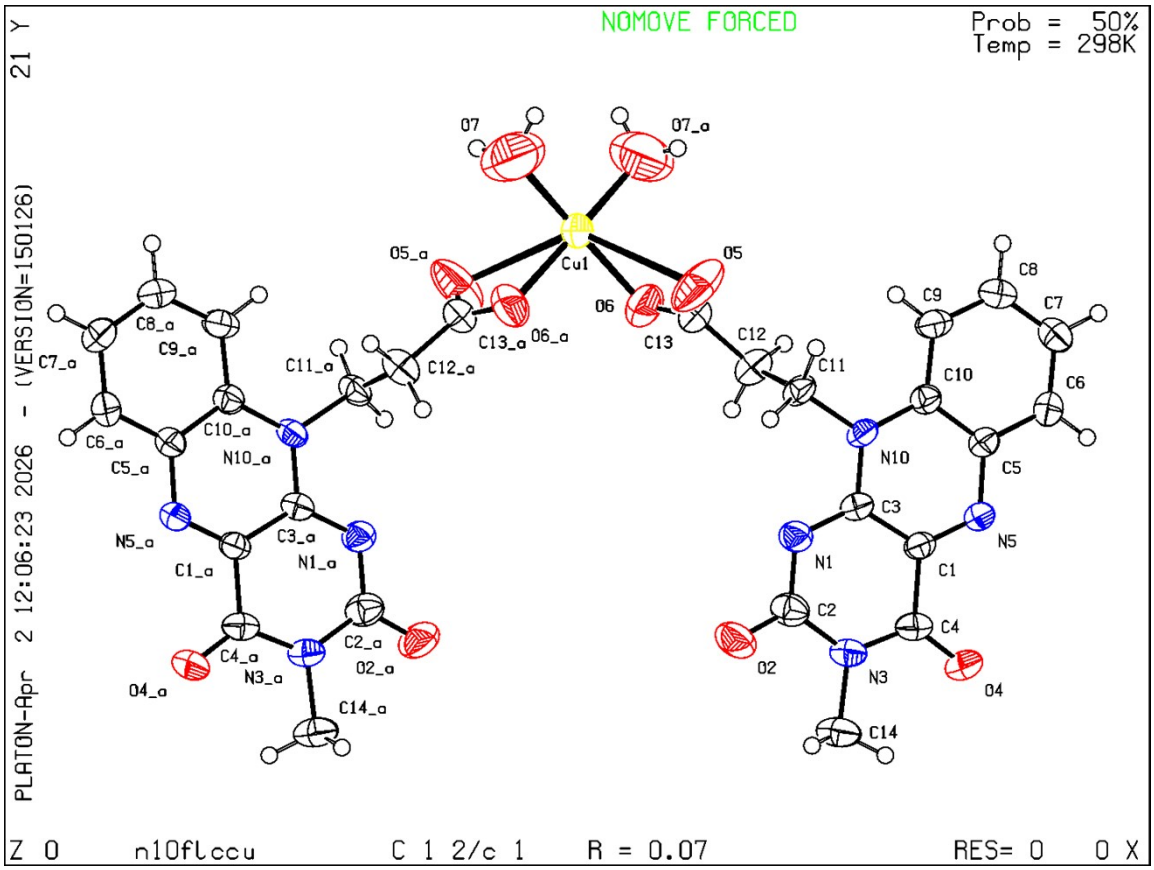
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 15/01/2026; check.def file version of 02/01/2026

duplicate check

No duplication found

Datablock n10fllccu - ellipsoid plot



NMR and HRMS data

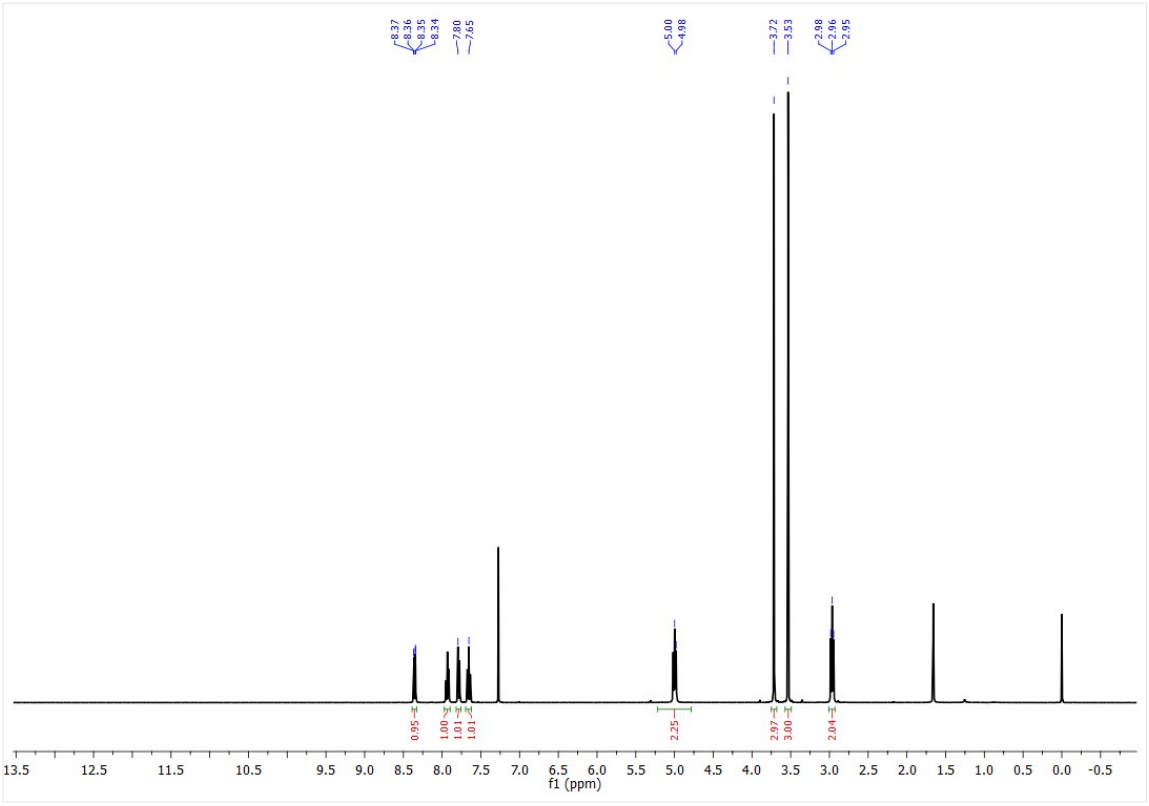


Figure S15. ^{1}H NMR of **13** in $CDCl_3$.

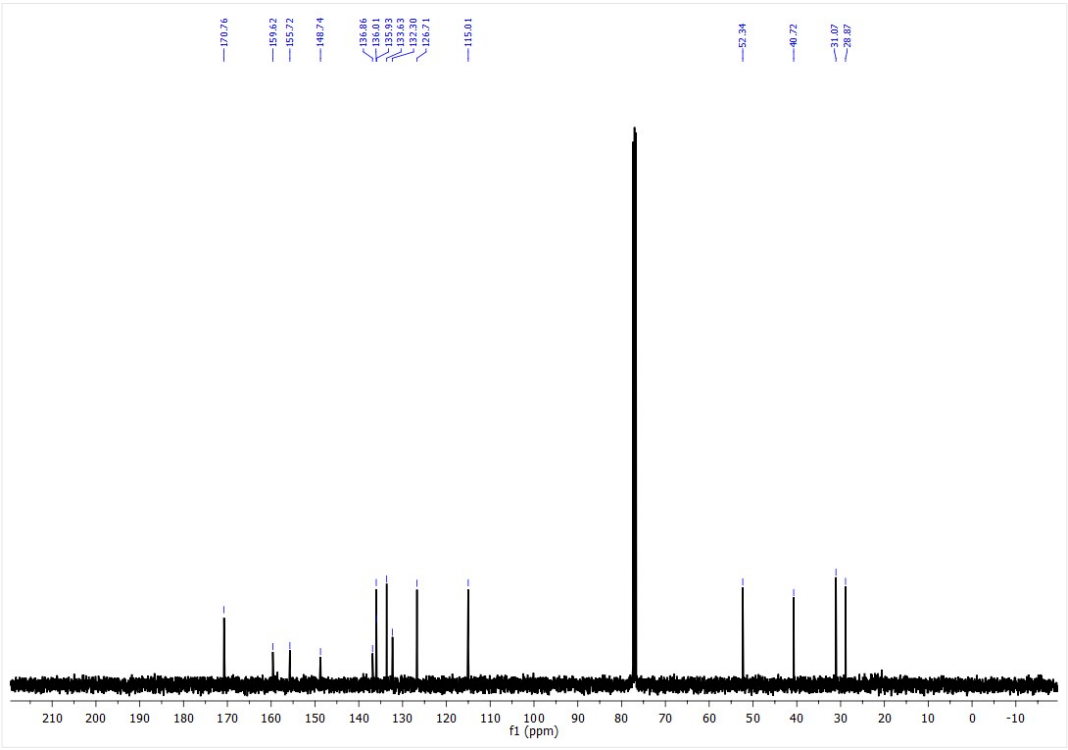


Figure S16. ^{13}C NMR of **13** in $CDCl_3$.

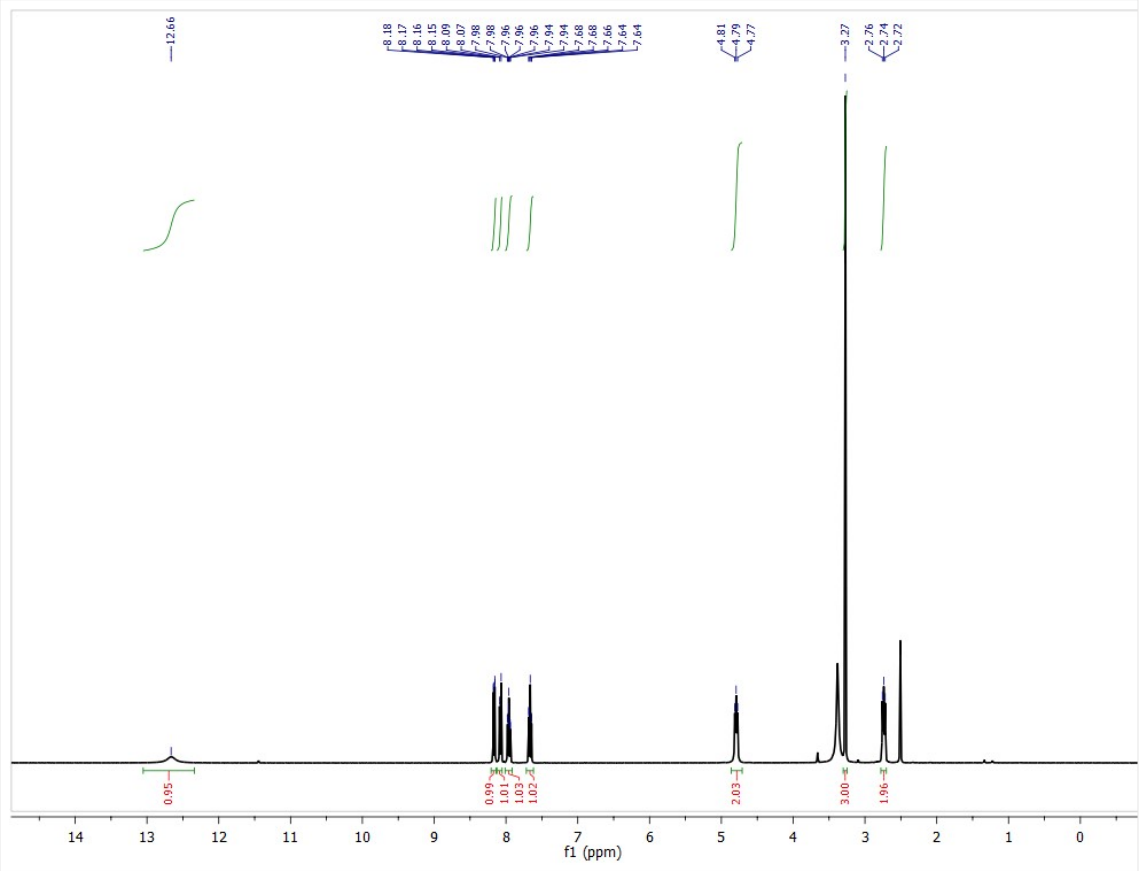


Figure S17. ^{1}H NMR of **N10-Flc** in DMSO-*d6.*

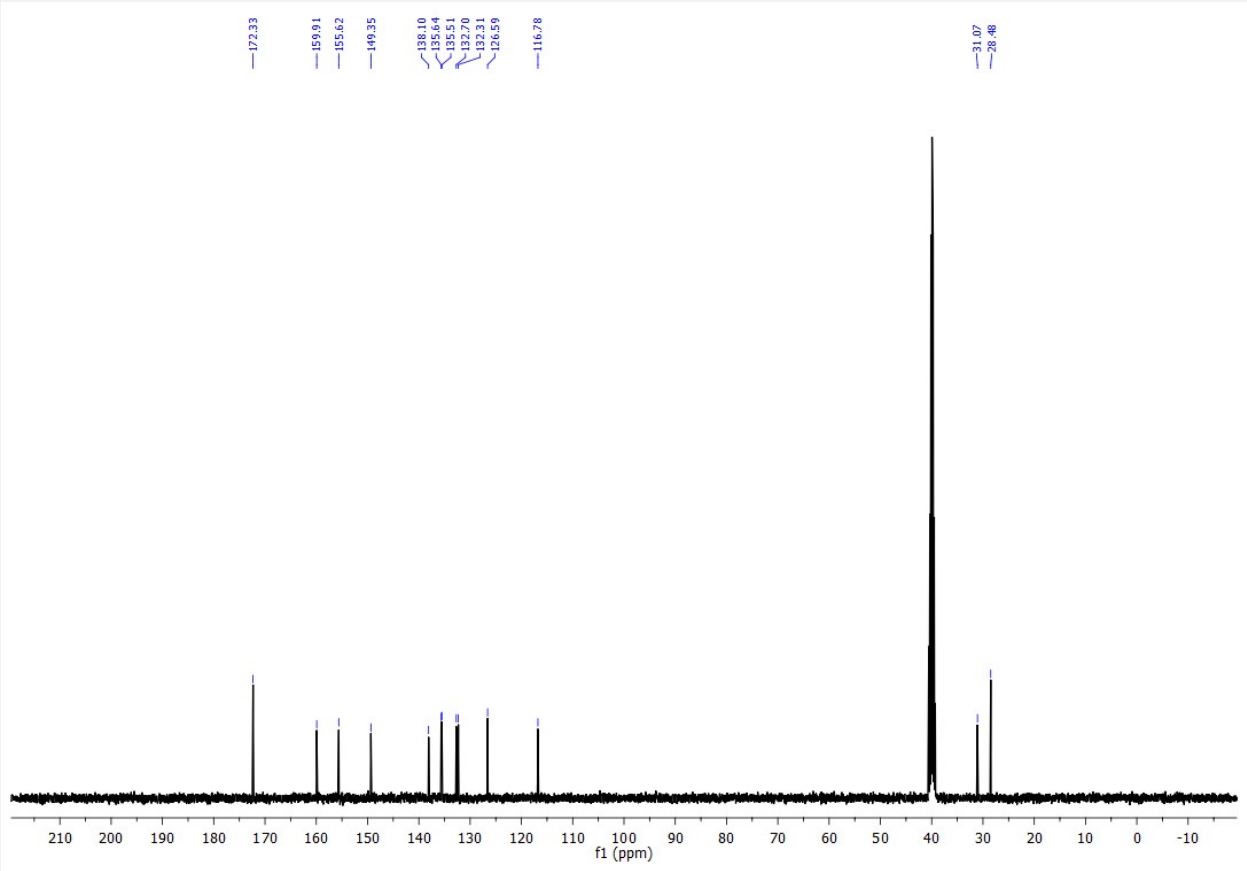


Figure S18. ^{13}C NMR of **N10-Flc** in DMSO-*d6*.

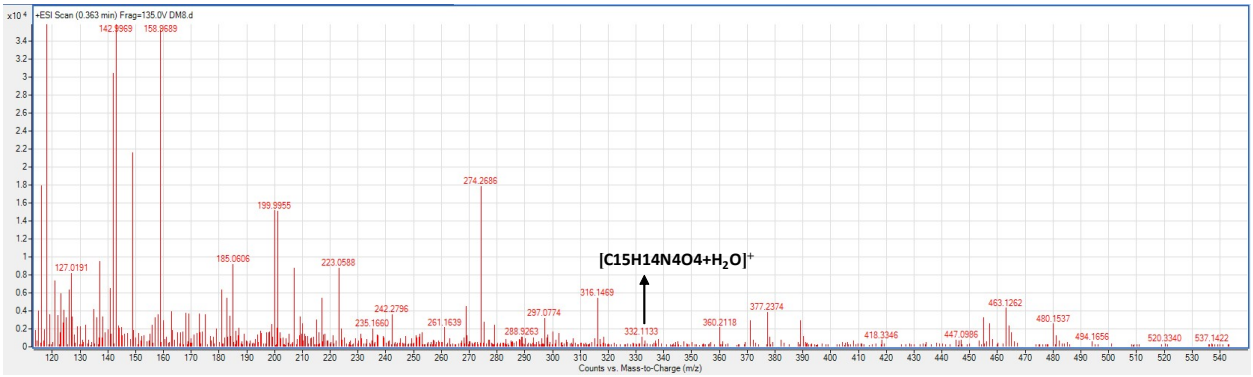


Figure S19. HRMS of **13**.

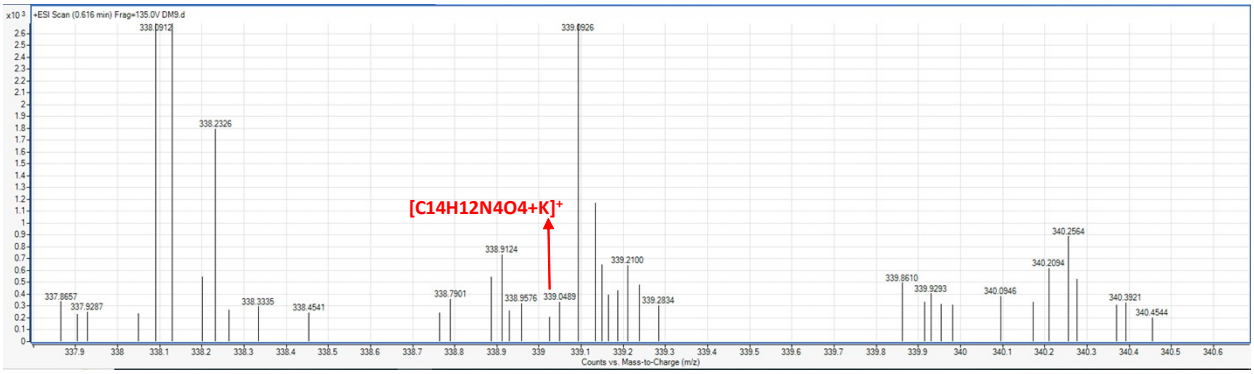


Figure S20. HRMS of **N10-Flc**.

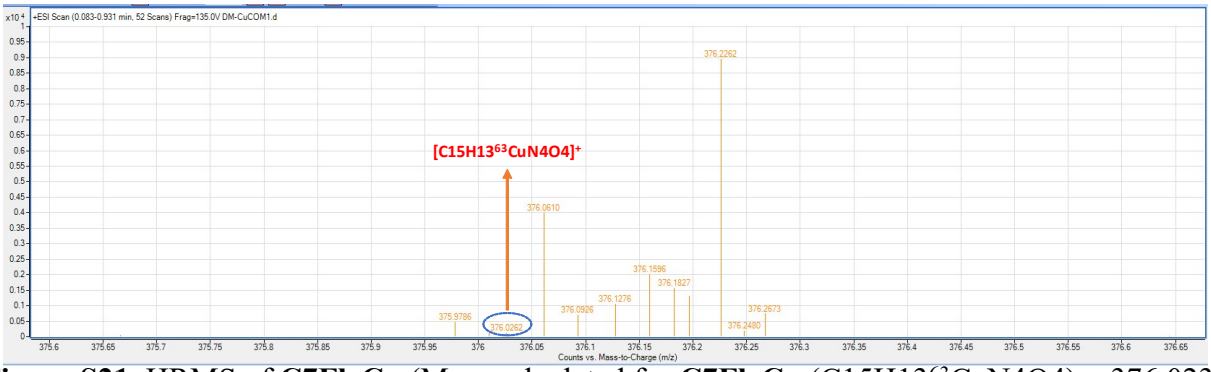


Figure S21. HRMS of **C7FlcCu** (Mass calculated for **C7FlcCu** ($C15H13^{63}CuN4O4$) = 376.0233, and observed 376.0262).

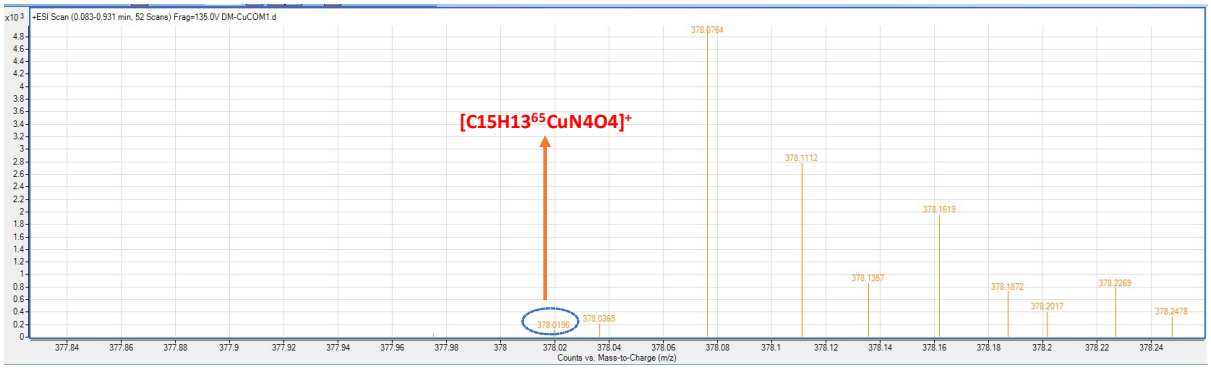


Figure S22. HRMS of **C7FlcCu** (Mass calculated for **C7FlcCu** ($C15H13^{65}CuN4O4$) = 378.0215, and observed 378.0196).

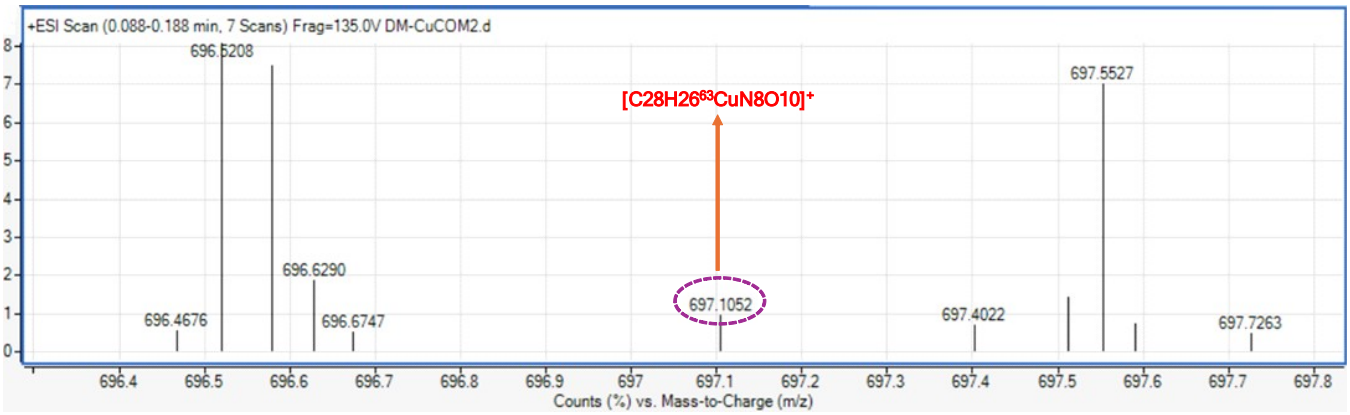


Figure S23. HRMS of **N10FlcCu** (Mass calculated for C28H26^{63}CuN8O10) = 697.1068 and observed 697.1052).

Reference

1. M. V. Mouli, A. K. Mishra, *Org. Biomol. Chem*. **2024**, *21*, 5622-5628.
2. M. V. Mouli, Mishra, A. K, *J. Chem. Sci*. **2022**, *134*, 59.
3. D. Mondal, I. Naskar, M. Deepa, A. K. Mishra, *Energy Adv*. **2024**, *3*, 1710-1716.
4. D. Mondal, A. K. Mishra, pH controlled unique flavin-silver complexes leading to divergent nanoparticle architecture, **2026** (manuscript under revision).