

SUPPORTING INFORMATION:

Synthesis, characterisation and antitubercular activities of a series of pyruvate-containing aroylhydrazones and their Cu-complexes

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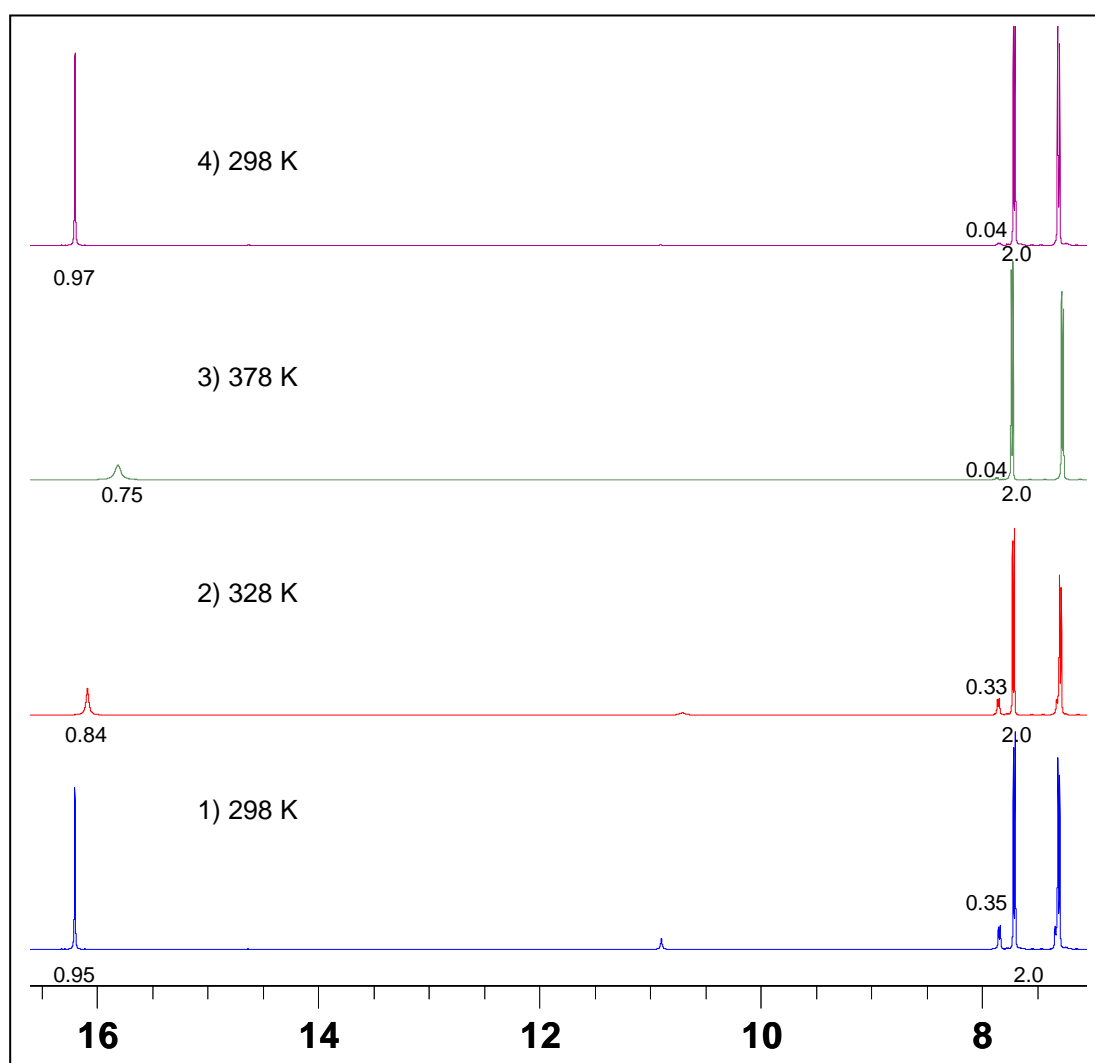
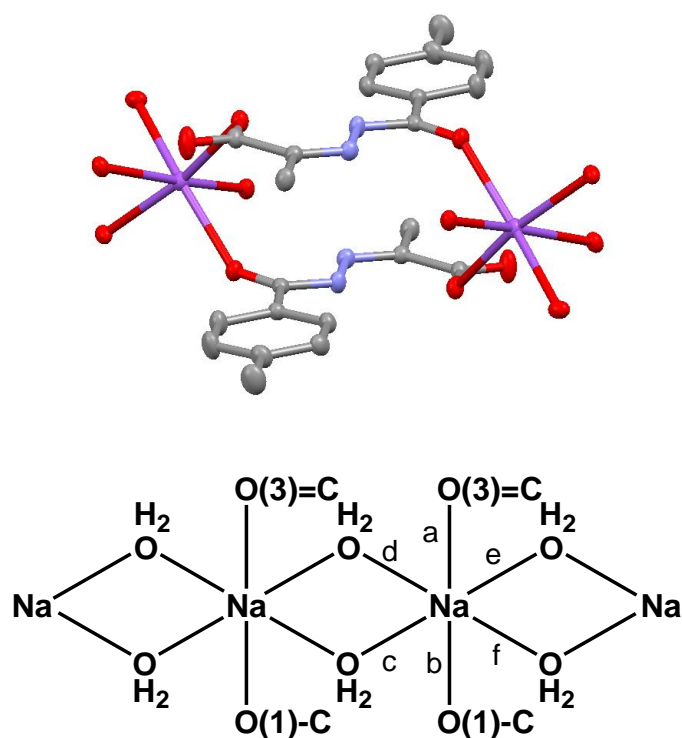


Figure S1: Proton NMR spectra of NaHL¹ recorded in DMSO-d₆ at 1) 298 K immediately after dissolving, 2) after heating to 328 K, 3) further heating to 378 K and c) after subsequent cooling to 298 K, with relative integrations indicated.



Bonds	NaHL ¹
a	2.3482(10)
b	2.4222(11)
c	2.3162(11)
d	2.3952(11)
e	2.4232(11)
f	2.3459(11)
Na-Na	3.3864(6)
d-Na-c	90.86(4)
e-Na-f	89.40(4)
a-Na-b	88.03(3)
a-Na-f	160.98(4)

Figure S2: Top: Mercury plot of a fragment of the packing diagram of **NaHL¹ x 2 H₂O**, illustrating Na-coordination (Na purple, O red, N blue, C grey, H omitted for clarity). Middle: Schematic illustration of the sodium coordination environment. Bottom: Associated bond lengths (/ \AA) and angles ($^\circ$).

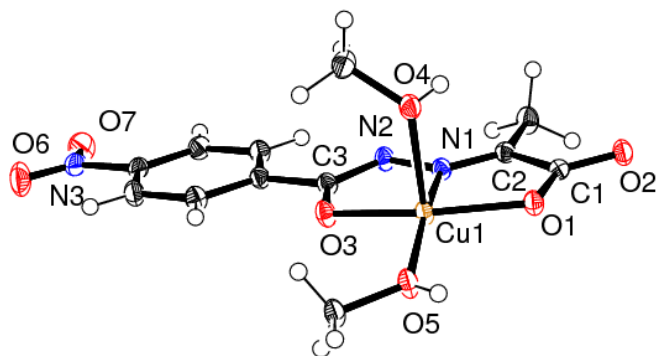


Figure S3: ORTEP plot (50% probability ellipsoids) of the asymmetric unit of $[\text{Cu}(\text{L}^2)(\text{MeOH})_2]$.

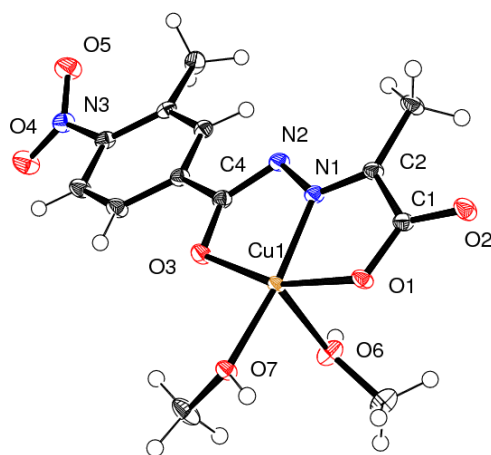


Figure S4: ORTEP plot (50% probability ellipsoids) of the asymmetric unit of $[\text{Cu}(\text{L}^4)(\text{MeOH})_2]$.

Table S1. Selected bond lengths (\AA) and angles ($^\circ$) for $[\text{Cu}(\text{L}^2)(\text{MeOH})_2]$ and $[\text{Cu}(\text{L}^4)(\text{MeOH})_2]$.

	$[\text{Cu}(\text{L}^1)(\text{H}_2\text{O})_2]$	$[\text{Cu}(\text{L}^2)(\text{MeOH})_2]$	$[\text{Cu}(\text{L}^4)(\text{MeOH})_2]$
	complex 1:		
C(1)-O(1)	1.291(3)	1.2970(17)	1.3008(17)
C(1)-O(2)	1.226(3)	1.2322(17)	1.2296(18)
C(3)/(4)-O(3)	1.301(3)	1.2862(17)	1.2896(18)
C(2)-N(1)	1.286(3)	1.2852(18)	1.2829(19)
C(3)/(4)-N(2)	1.326(3)	1.3355(18)	1.3305(19)
N(1)-N(2)	1.372(2)	1.3724(16)	1.3791(16)
Cu(1)-N(1)	1.8988(19)	1.9128(12)	1.9130(13)

Cu(1)-O(1)	1.9877(16)	2.0033(10)	1.9988(12)
Cu(1)-O(3)	1.9873(16)	1.9688(11)	1.9725(11)
Cu(1)-O(solvent 1)	1.958(2)	1.9285(11)	1.9506(11)
Cu(1)-O(solvent 2)	2.218(2)	2.2824(11)	2.2138(14)
N(1)-Cu(1)-O(3)	79.98(7)	80.06(5)	79.88(5)
N(1)-Cu(1)-O(1)	81.46(7)	81.87(5)	82.12(5)
O(1)-Cu(1)-O(3)	161.11(7)	161.64(4)	160.24(5)

Table S2. Crystal data and summary of data collection and refinement details for **NaHL¹**, **H₂L⁸**, **[Cu(L¹)(H₂O)₂]**, **[Cu(L²)(MeOH)₂]** and **[Cu(L⁴)(MeOH)₂]**.

Compound	NaHL¹ x 2 H₂O	H₂L⁸ x H₂O	[Cu(L¹)(H₂O)₂]	[Cu(L²)(MeOH)₂]	[Cu(L⁴)(MeOH)₂]
Empirical formula	C11H15N2NaO5	C8H10N4O4	C11H14CuN2O5	C12H15CuN3O7	C13H17CuN3O7
Formula weight	278.24	226.20	317.78	376.81	390.84
Temperature / K	110	110	110	110	110
Crystal system	Rhombohedral	Triclinic	Triclinic	Monoclinic	monoclinic
Space group	R-3	P-1	P-1	P2(1)/n	P2 ₁ /n
Unit cell dimensions	a = 30.7555(9) Å α = 90°	a = 8.1680(5) Å α = 109.642(7)°	a = 7.3879(9) Å α = 93.602(2)°	a = 7.8471(4) Å α = 90°	a = 10.159(3) Å α = 90.00°
	b = 30.7555(9) Å β = 90°	b = 8.2337(6) Å β = 99.708(5)°	b = 11.4695(13) Å β = 102.437(2)°	b = 17.0584(8) Å β = 93.9220(10)°	b = 14.1559(7) Å β = 114.11(3)°
	c = 7.3013(4) Å γ = 120°	c = 8.5815(6) Å γ = 110.471(6)°	c = 15.3898(18) Å γ = 103.124(2)°	c = 11.0122(5) Å γ = 90°	c = 11.895(2) Å γ = 90.00°
Volume / Å ³	5981.0(4) Å ³	481.70(6)	1231.6(3) Å ³	1470.63(12) Å ³	1561.3(5)
Z	18	2	4	4	4
Density (calculated) / Mg m ⁻³	1.390	1.560	1.714	1.702	1.663
Absorption coefficient / mm ⁻¹	0.136	0.127	1.792	1.527	1.441
F(000)	2628	236	652	772	804

Crystal size / mm ³	0.17 x 0.15 x 0.10	0.21 x 0.13 x 0.05	0.19 x 0.14 x 0.07	0.16 x 0.09 x 0.04	0.20 x 0.08 x 0.04
Theta range for data collection	1.32 to 28.30°	2.92 to 27.56°	1.84 to 28.33°	2.20 to 28.30°	5.76 to 64.22°
Index ranges	-40<=h<=40, -40<=k<=40, -9<=l<=9	-10 ≤ h ≤ 7, -10 ≤ k ≤ 10, -11 ≤ l ≤ 11	-9<=h<=9, -15<=k<=15, -20<=l<=19	-10<=h<=10, -22<=k<=22, -14<=l<=14	-15 ≤ h ≤ 15, -21 ≤ k ≤ 20, -16 ≤ l ≤ 17
Reflections collected	20886	4178	10913	15054	13154
Independent reflections	3303 [R(int) = 0.0331]	2229 [R(int) = 0.0192]	5970 [R(int) = 0.0181]	3660 [R(int) = 0.0178]	4881 [R(int) = 0.0235]
Data / restraints / parameters	3303 / 0 / 194	2229 / 0 / 162	5970 / 2 / 371	3660 / 0 / 219	4881 / 0 / 229
Goodness-of-fit on F ²	1.091	1.089	1.047	1.072	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0386, wR2 = 0.1026	R ₁ = 0.0414, wR ₂ = 0.1063	R1 = 0.0379, wR2 = 0.0982	R1 = 0.0255, wR2 = 0.0695	R ₁ = 0.0300, wR ₂ = 0.0682
R indices (all data)	R1 = 0.0513, wR2 = 0.1192	R ₁ = 0.0532, wR ₂ = 0.1142	R1 = 0.0471, wR2 = 0.1048	R1 = 0.0276, wR2 = 0.0709	R ₁ = 0.0377, wR ₂ = 0.0723
Largest diff. peak and hole / e.Å ⁻³	0.470 and -0.282	0.296 and -0.259	0.982 and -0.728	0.454 and -0.338	0.466 and -0.397

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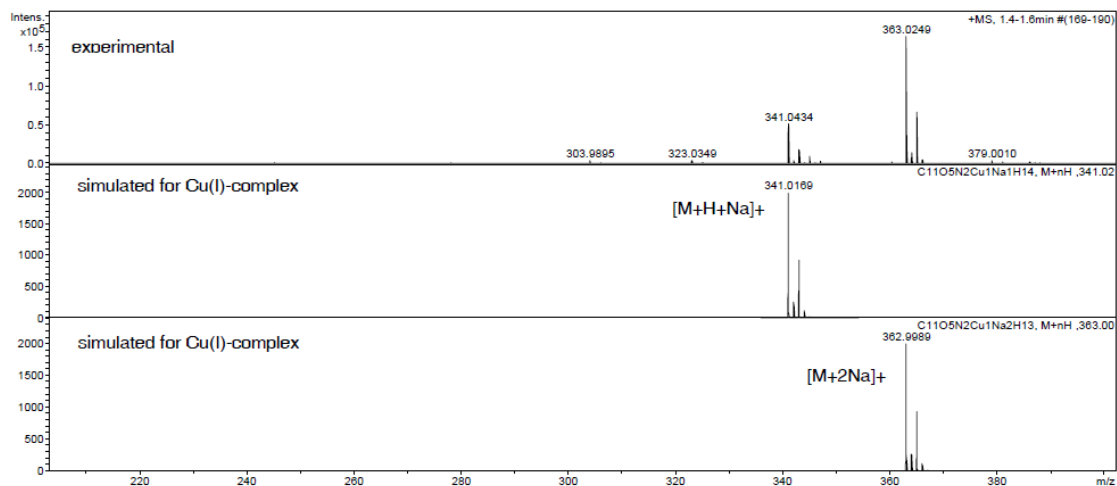
CuNP4Me
[Cu(L1)(H2O)2]

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Instrument micrOTOF
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Acquisition Date

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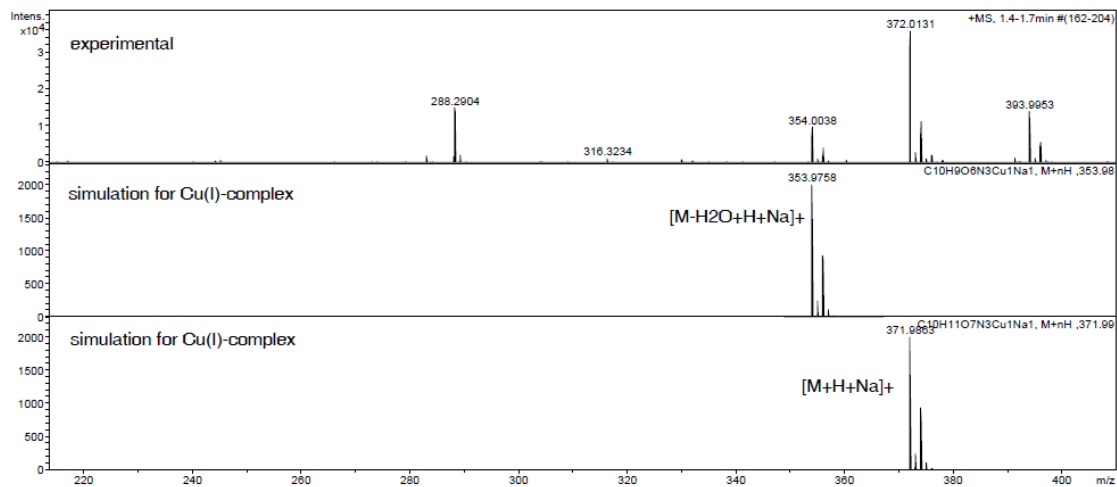
CuNP4NO2
[Cu(L2)(H2O)2]

Analysis Information

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Acquisition Date

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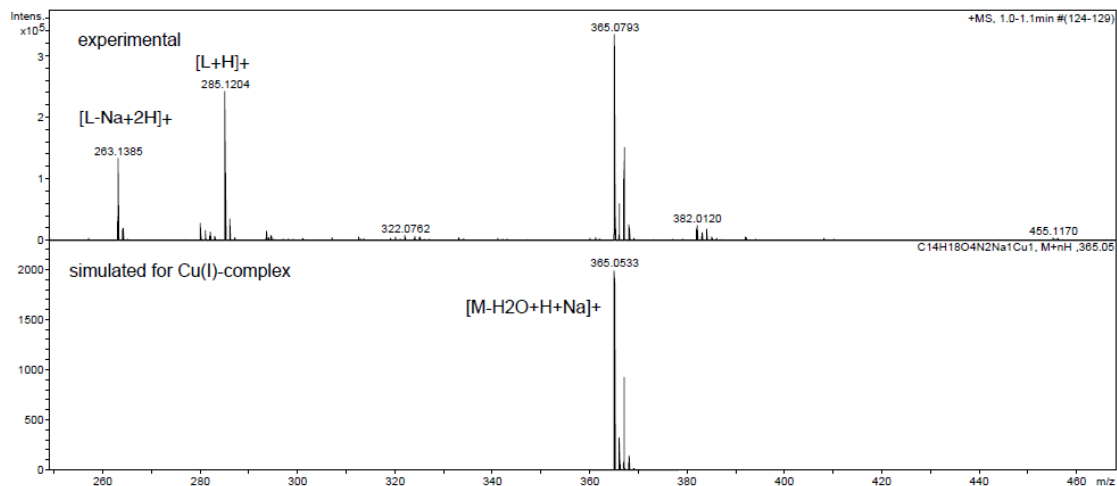
CuNP4 tert
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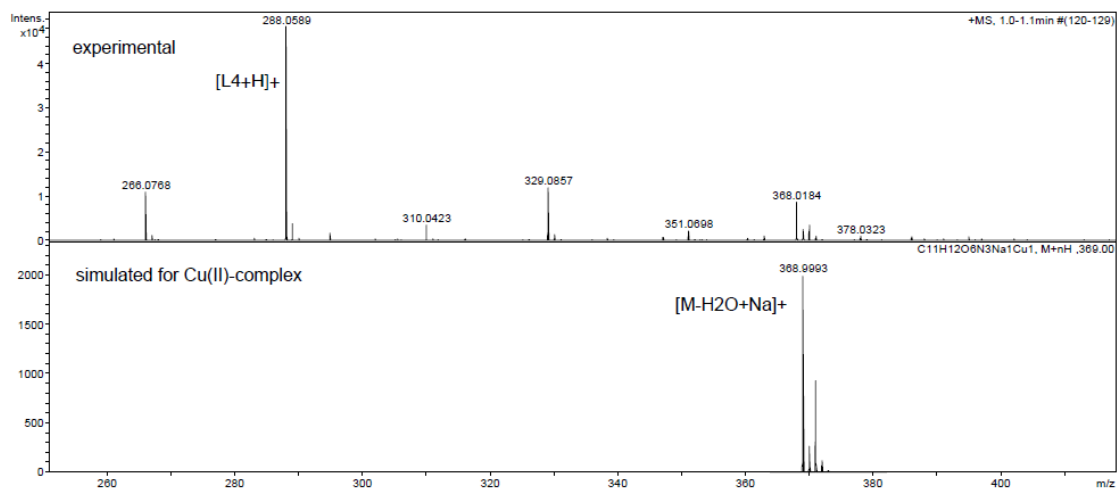
CuNP3Me4NO2
[Cu(L4)(H2O)2]

Analysis Information

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Acquisition Date

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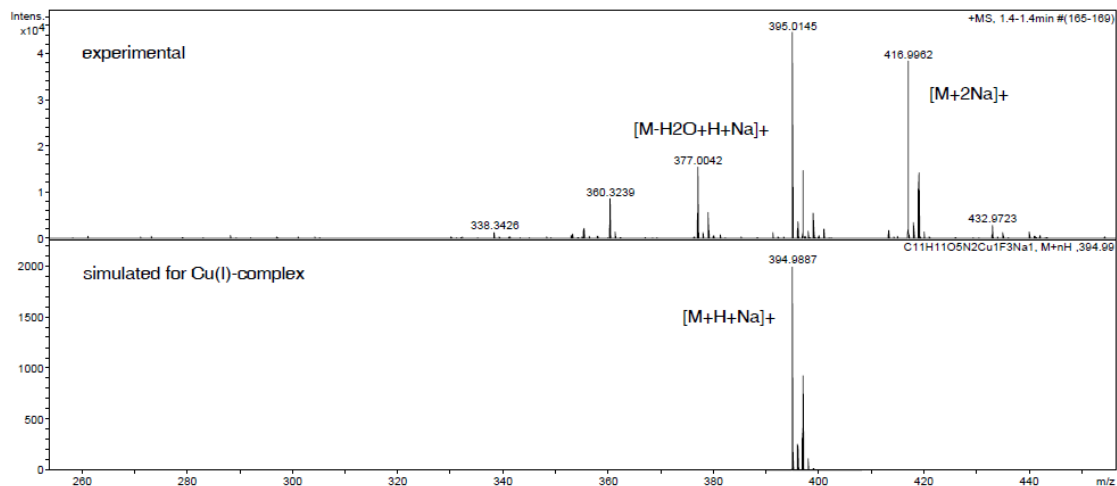
CuNP4CF3
[Cu(L5)(H2O)2]

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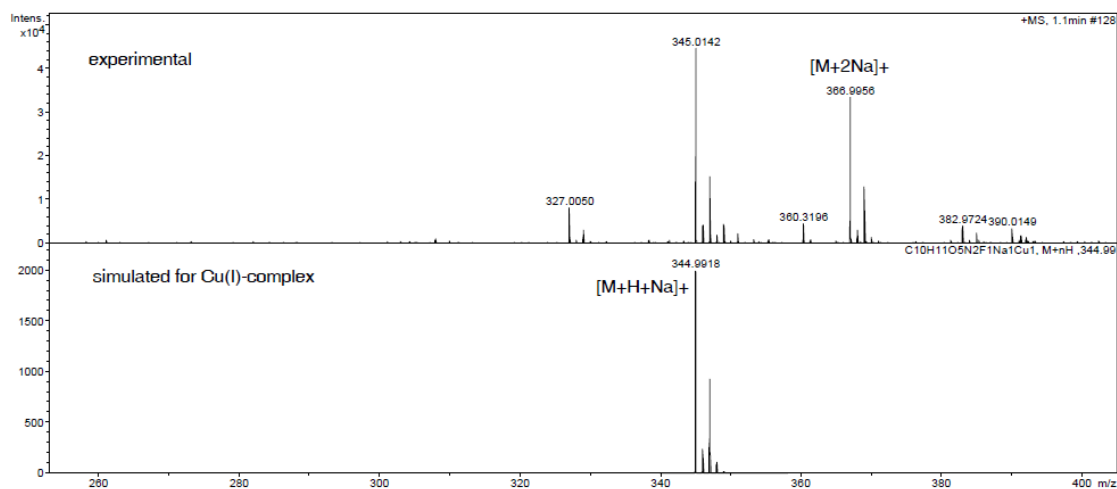
CuNP3F
[Cu(L6)(H2O)2]

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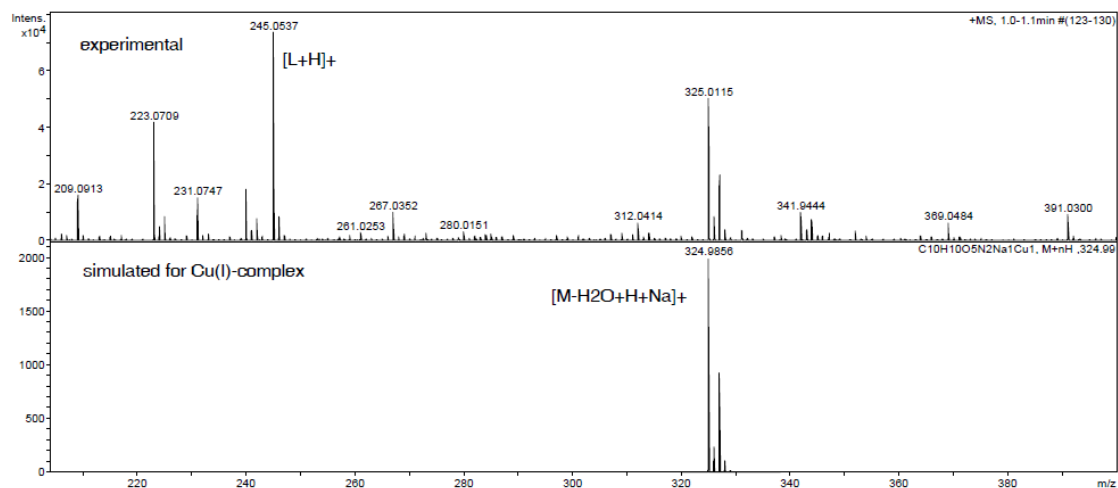
CuNP3OH
[Cu(L7)(H2O)2]

Analysis Information

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CuNPP2H
[Cu(L8)(H2O)2]

Analysis Information

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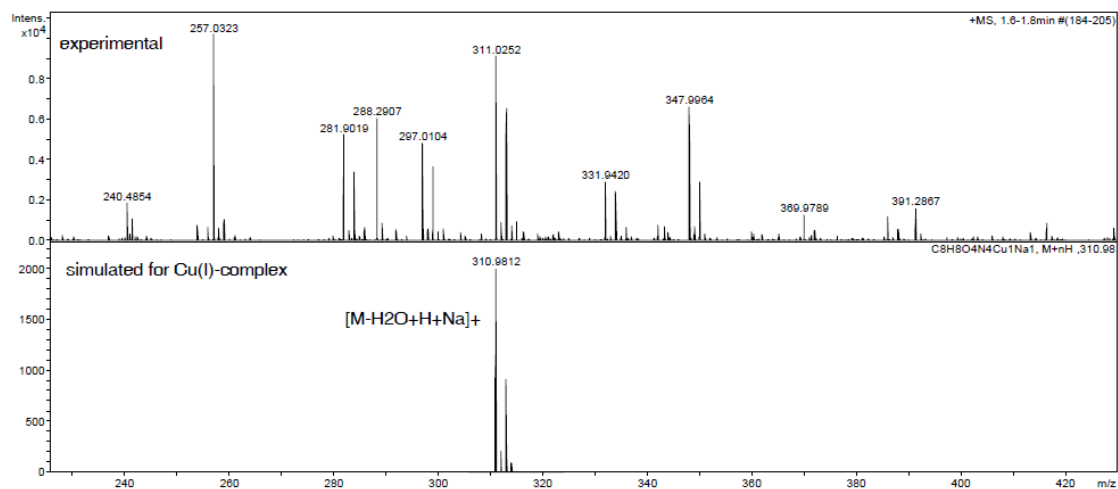


Figure S5: ESI mass spectra of copper complexes [Cu(L¹)(H₂O)₂]-[Cu(L⁸)(H₂O)₂].