Supporting information

The Homoleptic Curcumin-Copper Single Crystal (ML_2): A long awaited cherry on the cake in the field of curcumin metal complexes.

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§ "These authors contributed equally to this work"

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1. Single crystal X-ray diffraction

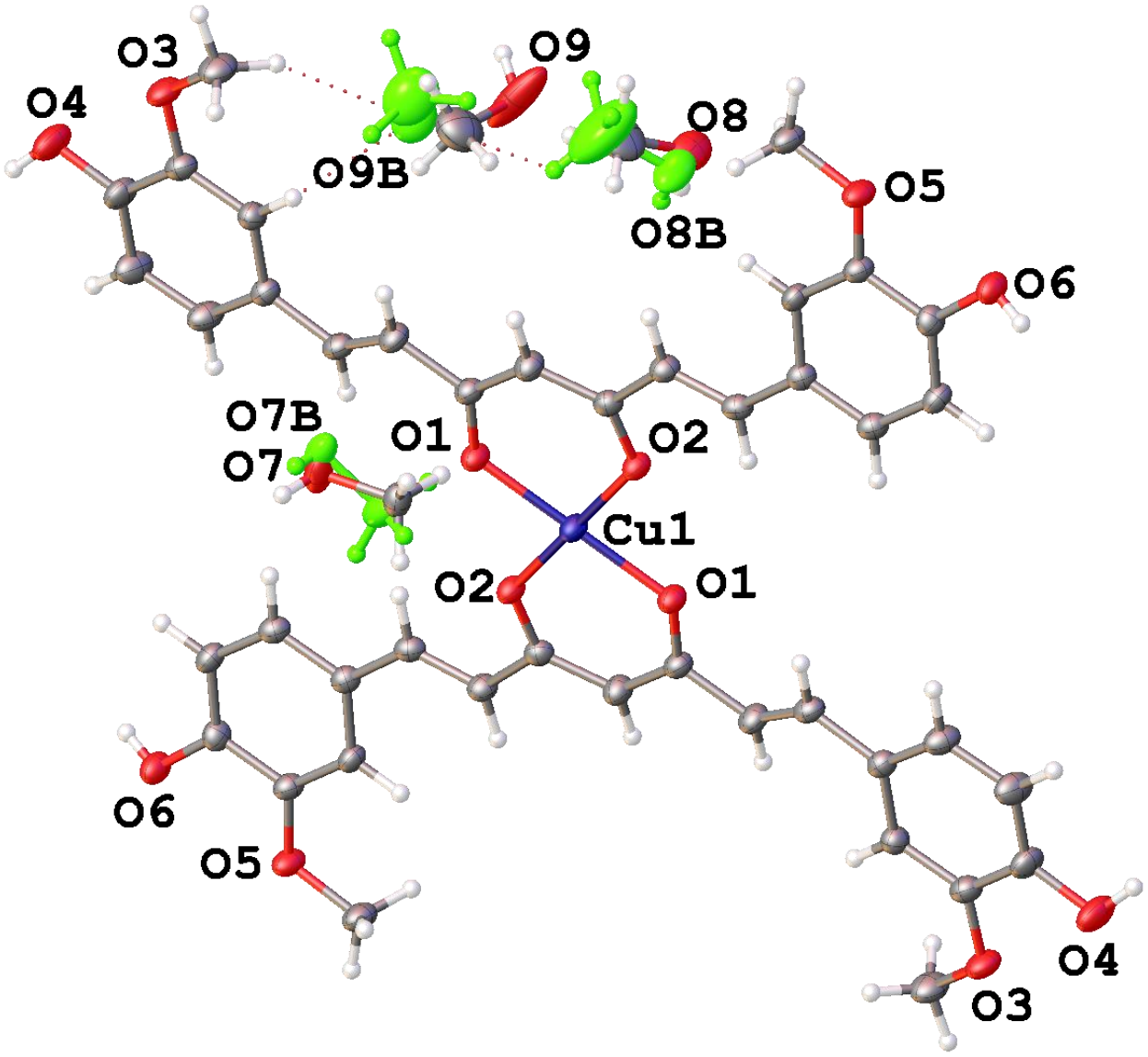

Figure S1. The molecular structure of complex **1** including molecules of solvent (methanol) and the disordered position of methanol (green elipsoids).

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Compound_1

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

Datablock: Compound_1

```
Bond precision:    C-C = 0.0031 A          Wavelength=0.71073

 Cell:          a=8.3372(7)        b=8.7677(4)       c=16.3052(12)
                alpha=75.664(5)    beta=84.240(6)    gamma=84.636(5)
 Temperature:   130 K

Calculated        Reported Volume            1146.02(14)
                  1146.02(14)
Space group       P -1                       P -1
Hall group        -P 1                       -P 1
Moiety formula   C42 H38 Cu O12, 5(C H4 O)   C42 H38 Cu O12, 5(C H4 O)
Sum formula       C47 H58 Cu O17             C47 H58 Cu O17
Mr                958.48                     958.47
Dx,g cm-3         1.389                      1.389
Z                 1                          1
Mu (mm-1)         0.551                      0.551
F000              505.0                      505.0
F000'             505.59
h,k,lmax          11,12,22                   11,12,22
Nref              6476                       5848
Tmin,Tmax         0.918,0.967                0.873,0.969
Tmin'             0.834

Correction method= # Reported T Limits: Tmin=0.873 Tmax=0.969AbsCorr
= MULTI-SCAN

Data completeness= 0.903            Theta(max)= 29.642

R(reflections)= 0.0498( 4638)                    wR2(reflections)=
                                                 0.1293( 5848)
S = 1.050                  Npar= 373
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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

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 11 Note

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Alert level C

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Alert level G

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    0 ALERT level A = Most likely a serious problem - resolve or explain
    1 ALERT level B = A potentially serious problem, consider carefully
    2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
48 ALERT level G = General information/check it is not something unexpected

    0 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
   10 ALERT type 3 Indicator that the structure quality may be low
   32 ALERT type 4 Improvement, methodology, query or suggestion
    1 ALERT type 5 Informative message, check
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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. In order to resolve some of the more serious problemsit may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needingattention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

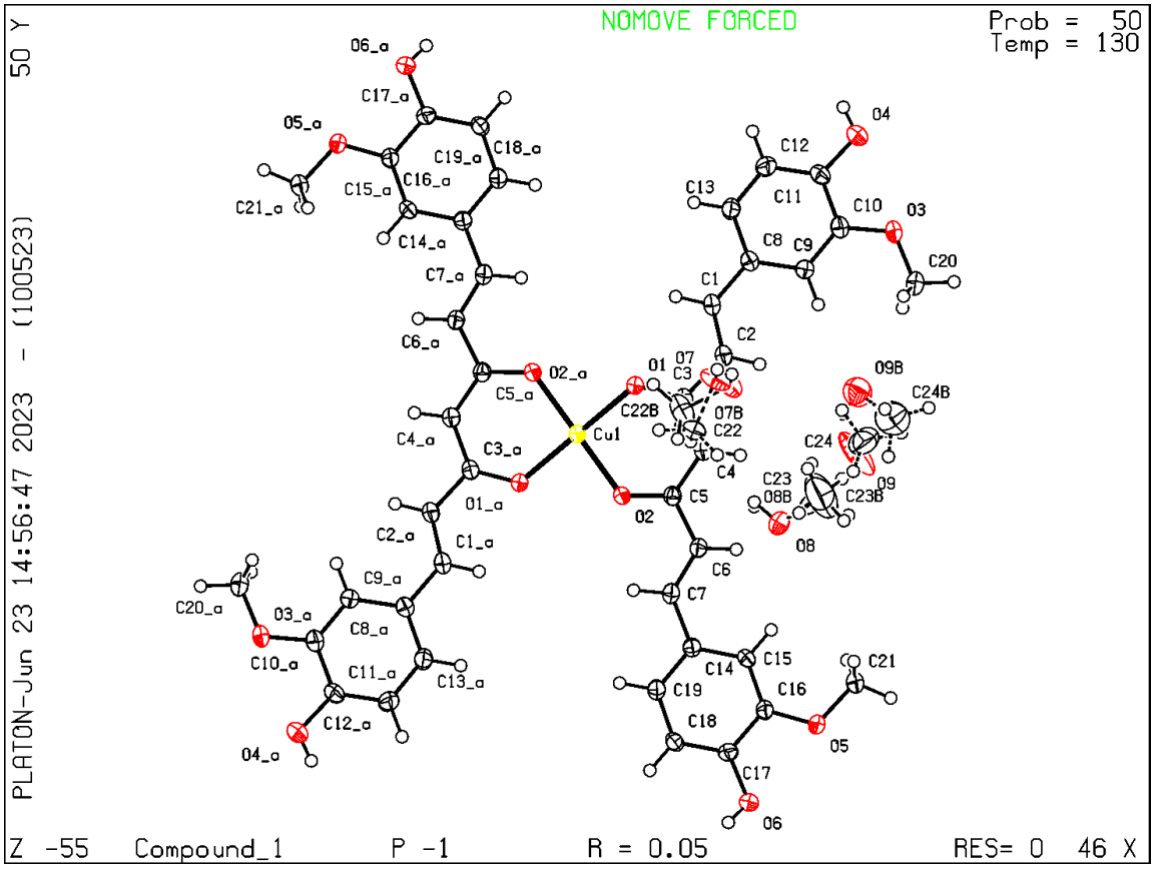
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks arerun on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 10/05/2023; check.def file version of 10/05/2023

Datablock Compound_1 - ellipsoid plot



2. Electrospray ionization

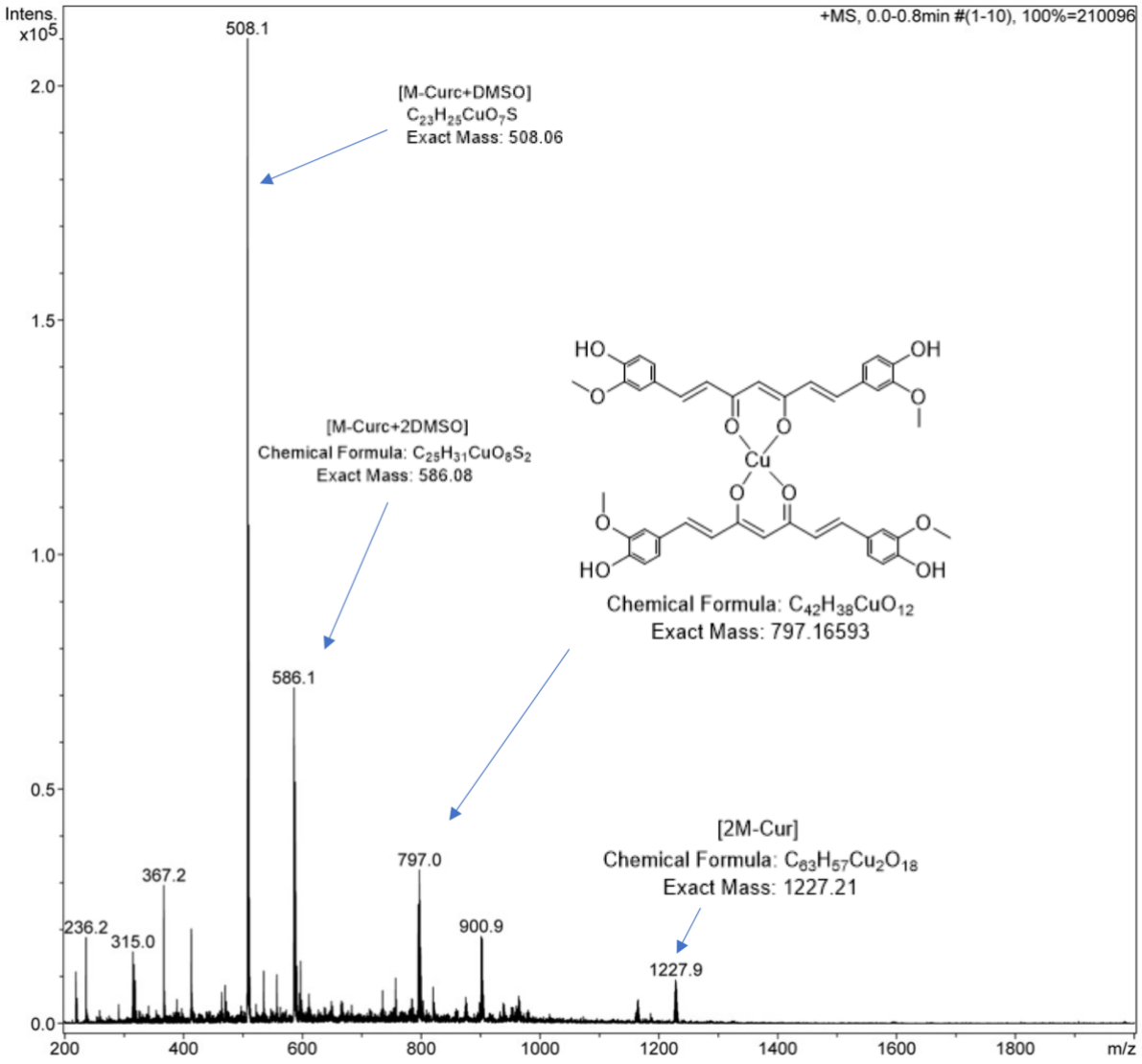


Figure S2. Mass spectrum of complex **1** (dark brown solid) by ESI^+ previously dissolved in DMSO.

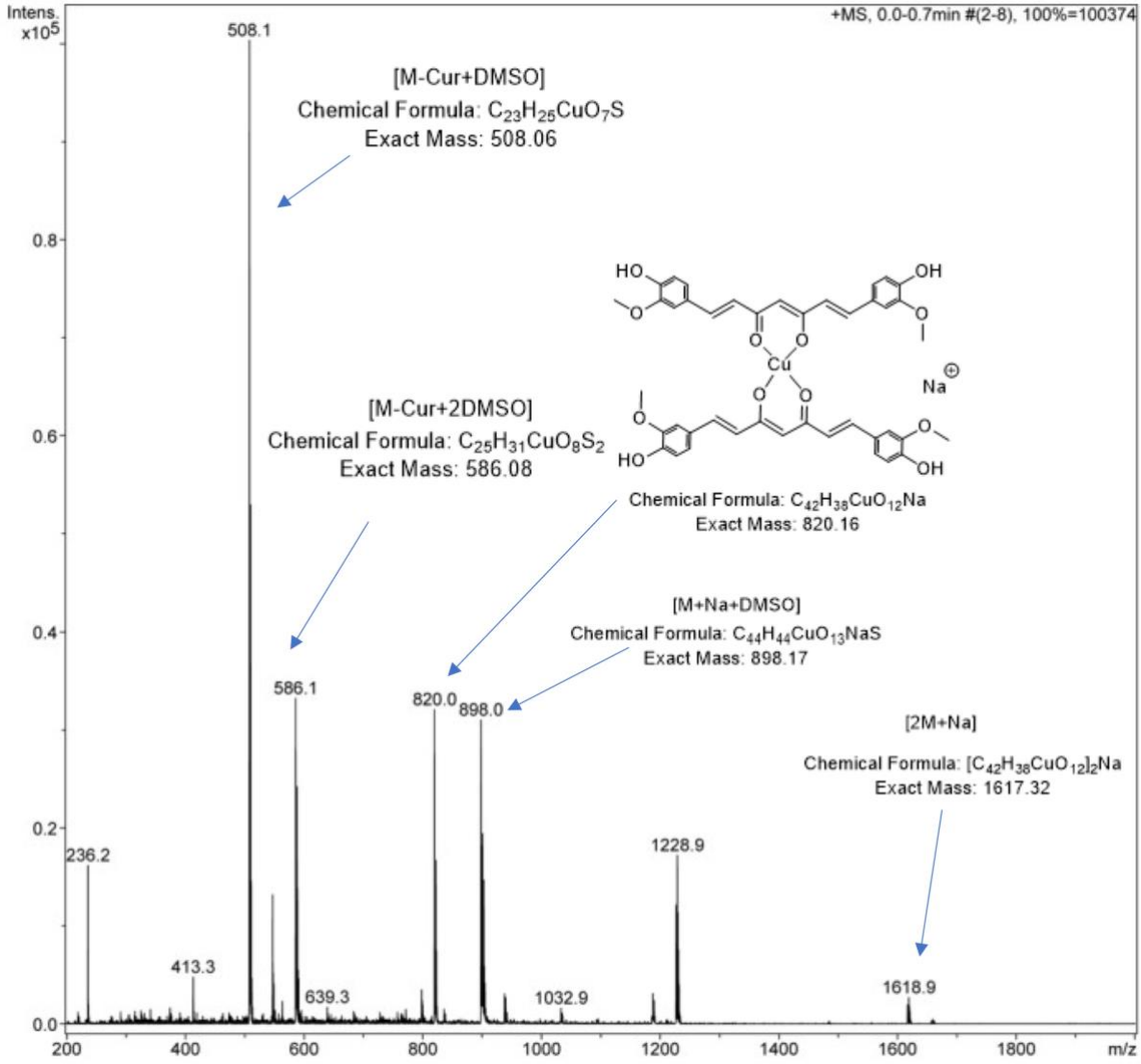


Figure S3. Mass spectrum of complex **1** (brilliant brown solid) by ESI^+ previously dissolved in DMSO.

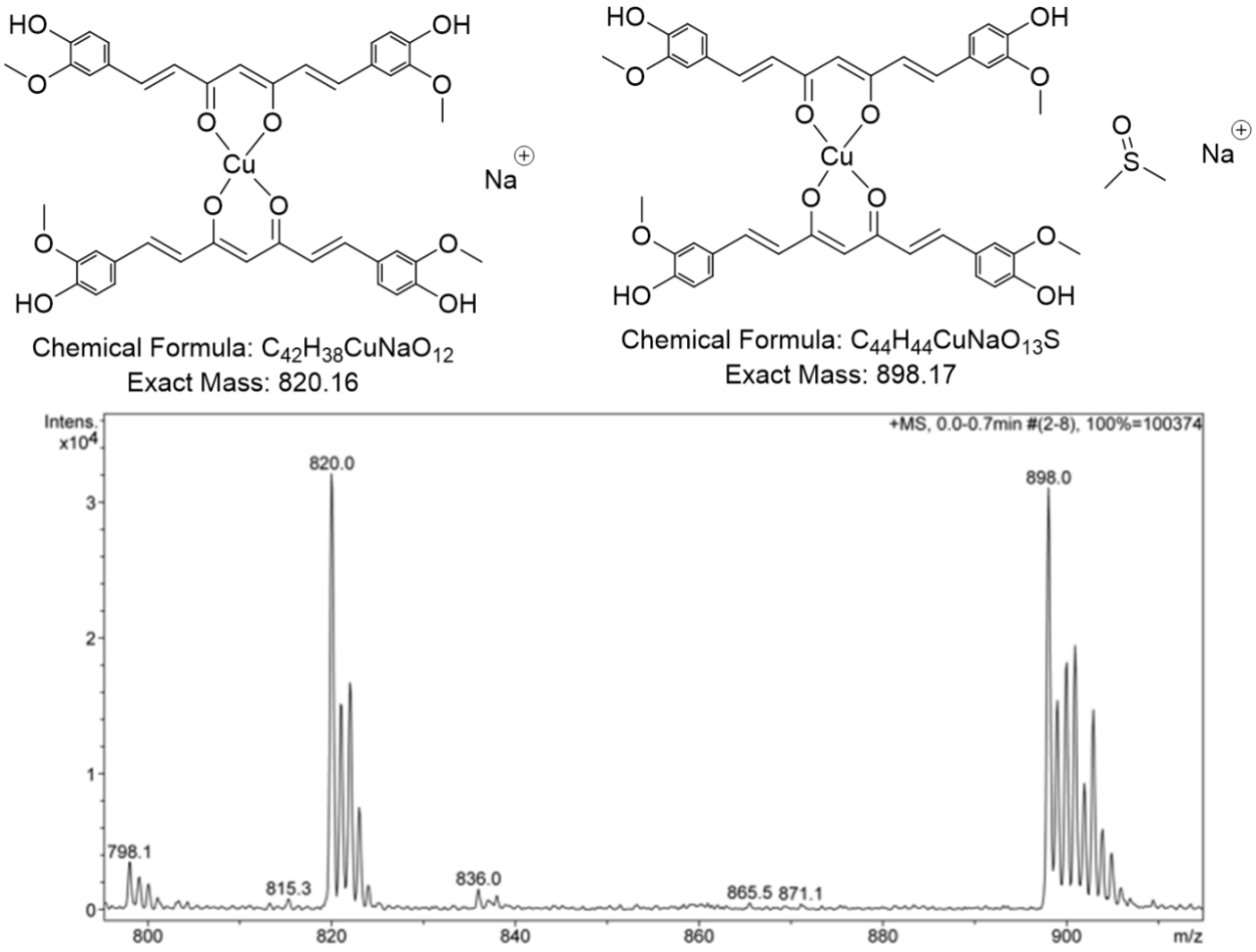


Figure S4. Ampliated Mass spectrum of complex **1** (brilliant brown solid) by ESI^+ previously dissolved in DMSO.

3. EPR

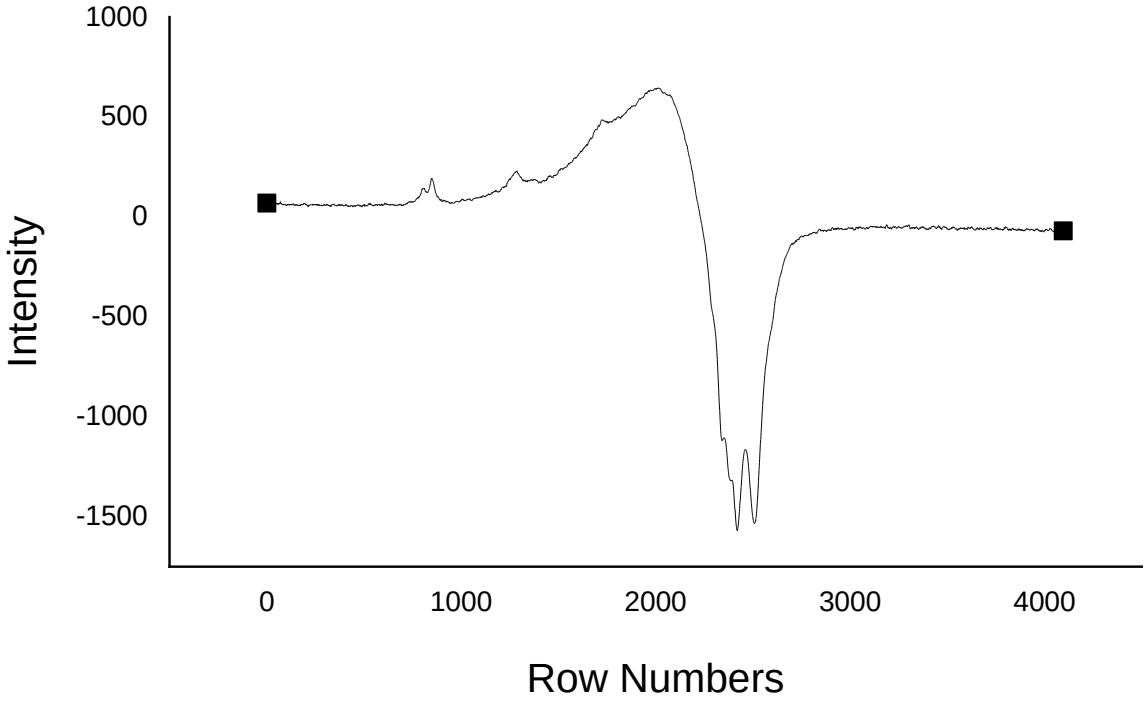


Figure S5. Paramagnetic Electron Resonance of the complex (**1**) at solid-state (dark brown solid).

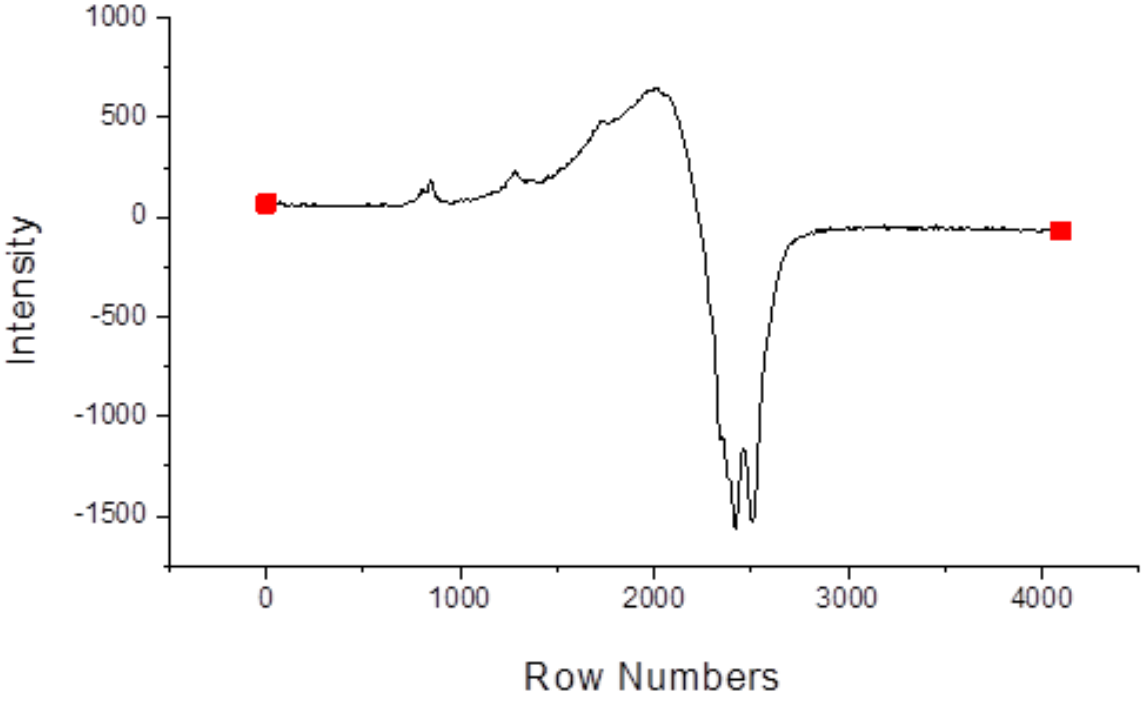


Figure S6. Paramagnetic Electron Resonance of the complex (**1**) compound at 77 K in DMSO of brilliant brown crystalline (mother liquor).

4. IR (ATR)

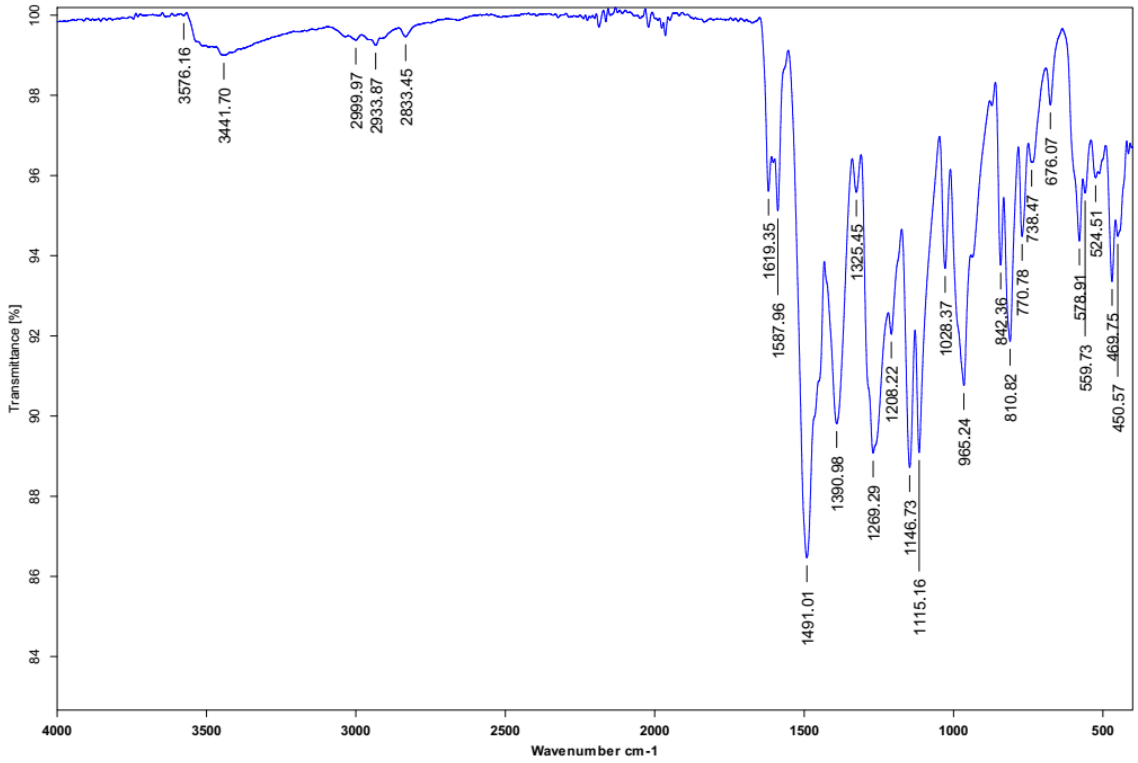


Figure S6. IR-ATR spectra of complex (**1**) dark brown solid.

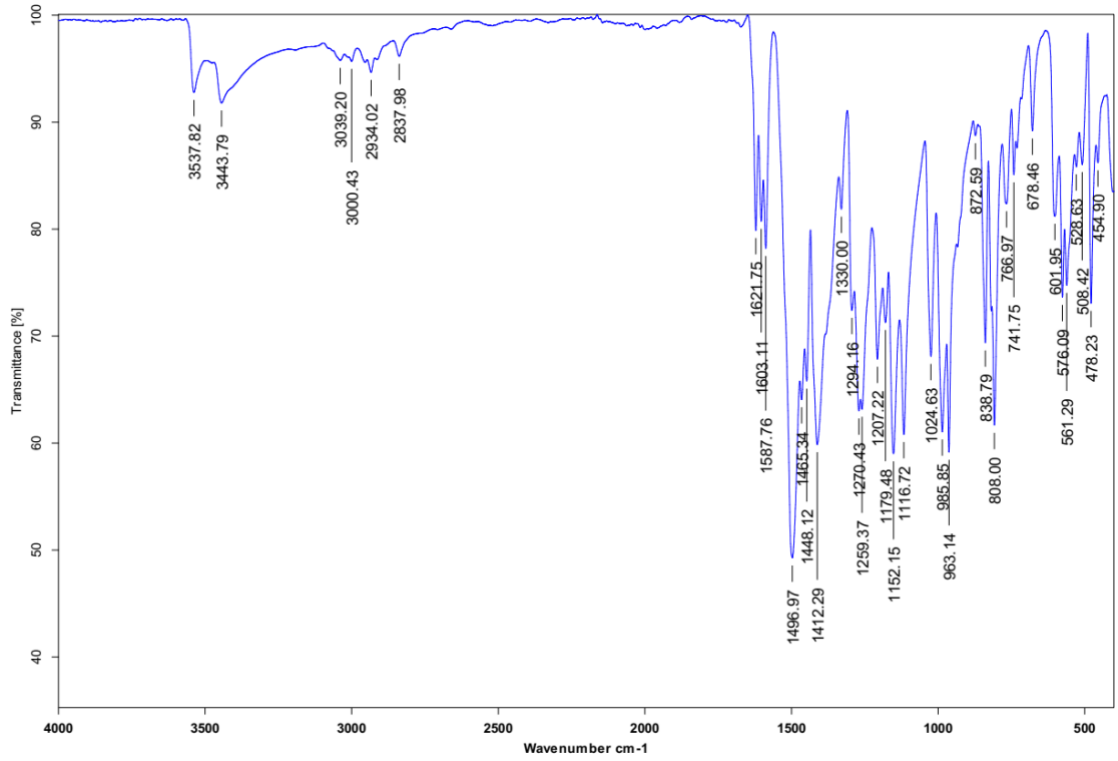


Figure S7. IR-ATR spectra of complex (**1**) brilliant brown crystalline solid.

5. UV-Vis

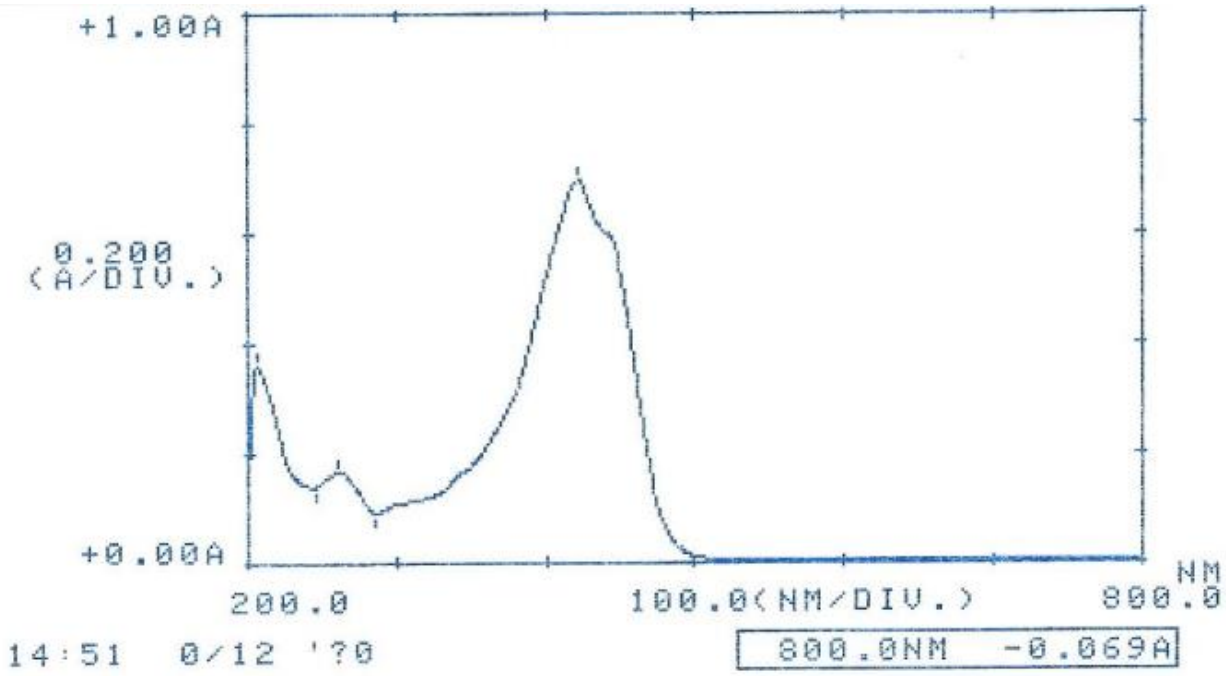


Figure S8. UV-Vis spectra of complex (**1**) dark brown solid (REF: Methanol).

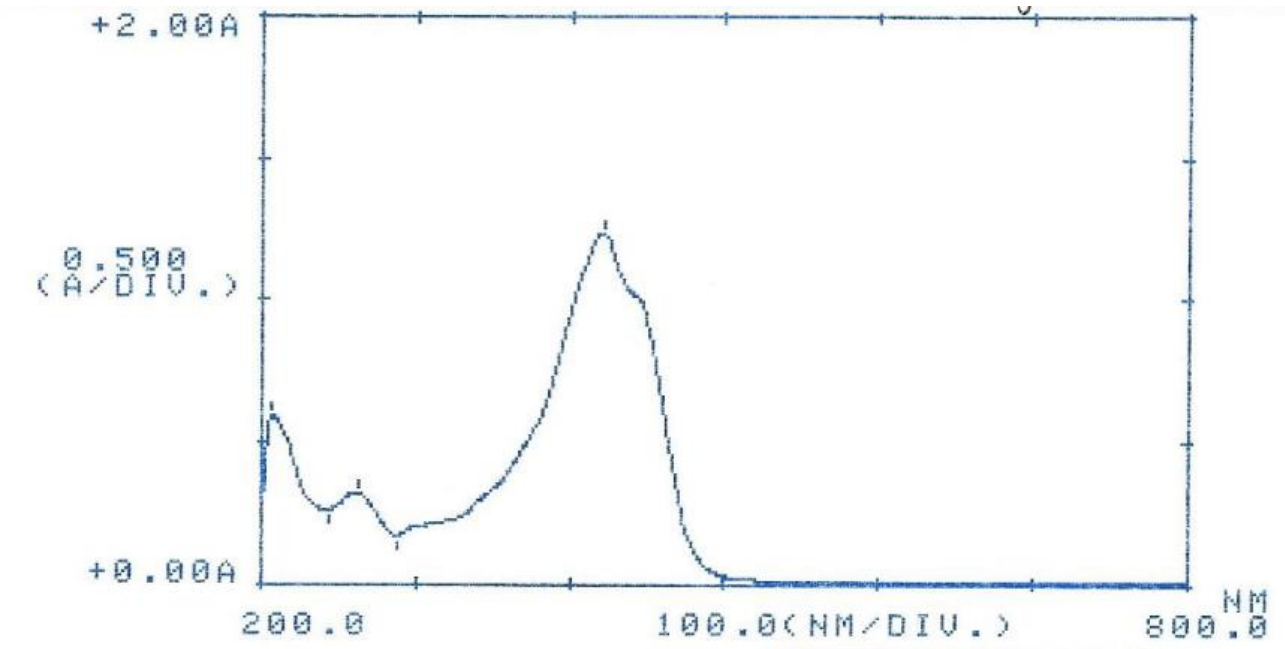
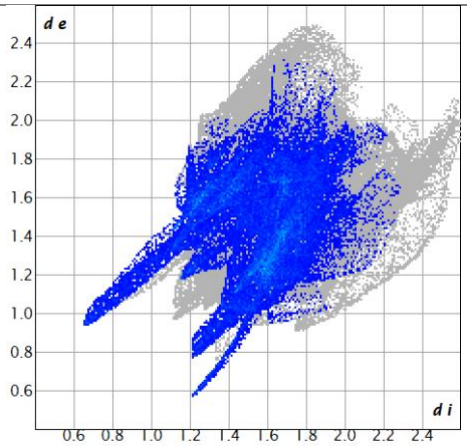
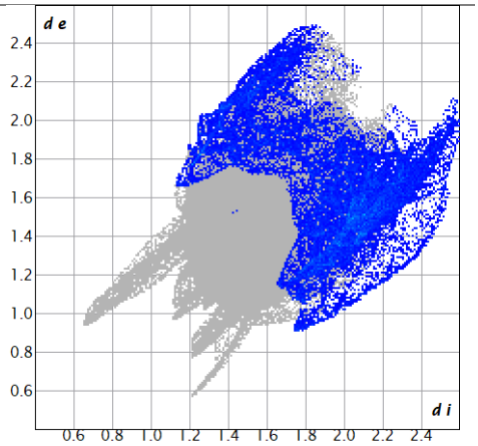
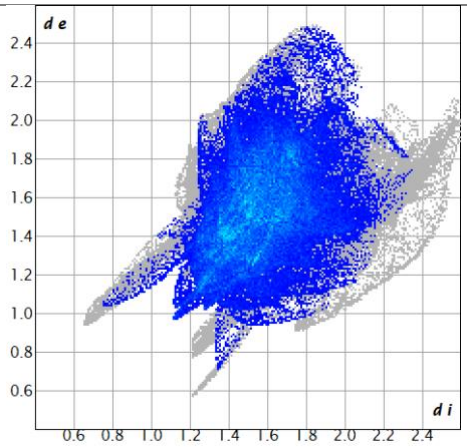
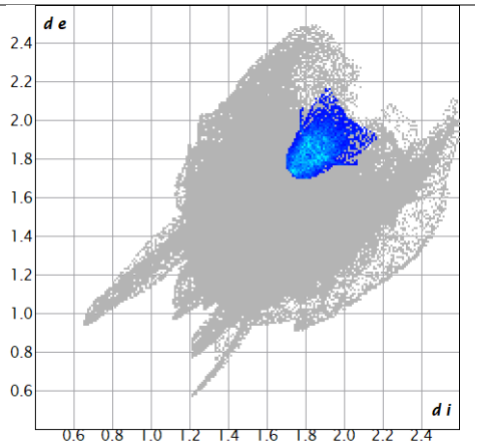


Figure S9. UV-Vis spectra of complex (**1**) brilliant brown crystalline solid (REF: Methanol).

6. Fingerprints plots

Contact	Fingerprint	Contact	Fingerprint
O···H/H···O 24.5%		C···H/H···C 17.8 %	
H···H 44.2 %		C···C 7.4 %	

7. Cytotoxicity

Table S1. Growth inhibition percentages of cancerous and noncancerous (COS-7) cell lines by compounds (10 μM, 48 h).

	Grow inhibition (%) by cell line						
Sample	**U251**	**PC-3**	**K562**	**HCT-15**	**MCF-7**	**SKLU-1**	**COS 7**
Curcumin	NC	22.7	20.81	10.5	1.30	5.8	5.05
Complex 1	35.43	29.3	62.87	18.8	0.55	26.1	20.35

Inhibition percentages of complex **1** relative to curcumin. Growth inhibition percentages of cancerous and noncancerous (COS-7) cell lines by compounds. U251 (human glioblastoma), PC-3 (human prostatic adenocarcinoma), K562 (human chronic myelogenous leukaemia), HCT-15 (human colorectal adenocarcinoma), MCF-7 (human mammary adenocarcinoma), cell lines were supplied by the National Cancer Institute (USA); and SKLU-1 (human lung adenocarcinoma) and COS-7 cell line (monkey African green kidney) were donated by the Cancer Institute of Mexico. *The results are the average of three runs.

8. Antioxidant

Table S2. Inhibition of Lipid Peroxidation on Rat Brain

Sample	**Concentration (μM)**	**TBARS (nmol/mg prot.)**	**Inhibition (%)**	**IC_{50} (μM)**
Complex 1	Basal	0.319±0.051		
	Control	9.038±0.512		
	0.18	7.759±0.548	14.27±2.02	1.26±0.08
	0.32	7.242±0.492*	19.98±1.14*	
	0.56	6.230±0.488**	31.24±1.80**	
	1	4.987±0.315**	44.81±1.88**	
	1.78	3.239±0.342**	63.61±5.30**	
	3.16	1.766±0.525**	79.69±6.78**	
	5.62	0.622±0.053**	93.02±0.91**	
	10	0.353±0.072**	96.16±0.58**	

Curcumin	Basal	0.319±0.051		
	Control	9.038±0.512		
	0.18	8.345±0.412	7.58±1.12	3.03±0.15
	0.32	8.136±0.403	9.88±1.97	
	0.56	7.542±0.462	16.6±0.39	
	1	6.932±0.418**	23.32±1.34**	
	1.78	6.100±0.322**	32.48±0.39**	
	3.16	4.267±0.093**	52.46±3.01**	
	5.62	2.289±0.343**	74.11±5.04**	
	10	0.881±0.286**	89.84±3.81**	
BHT	Basal	0.268±0.053		
(n=3)	Control	7.384±0.630		
	0.56	6.098±0.353	16.64±2.86	1.22±0.44
	0.75	5.559±0.294*	23.92±2.69*	
	1	4.457±0.283**	37.14±7.44**	
	1.33	3.228±0.572**	53.59±8.93**	
	1.78	1.315±0.489**	81.59±6.89**	
	2.37	0.487±0.075**	93.16±1.16**	

Homogenised in: PBS; Vehicle: DMSO; Experiment: Curve; Peroxidation: induced with $FeSO_4$ 10 μM, Incubation time: 1 h; EDTA: 2 μM.

The values represent the average of three independent experiments ± standard error of the media $\left(\bar{x} \pm ES\right)$. Data were subjected to an analysis of variance (ANOVA) followed by a Dunnett pass to isolate groups with significant differences. The values of $p \leq 0.05$ (*) and $p \leq 0.01$ (**) were considered as significant differences with respect to control.

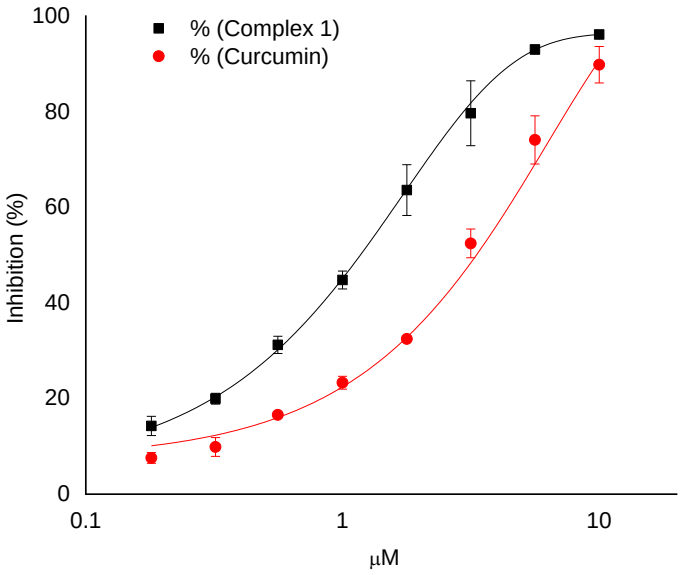


Figure S9. Inhibition curve