Supplementary Information

Structurally characterized gallium-chrysin complexes with anticancer potential

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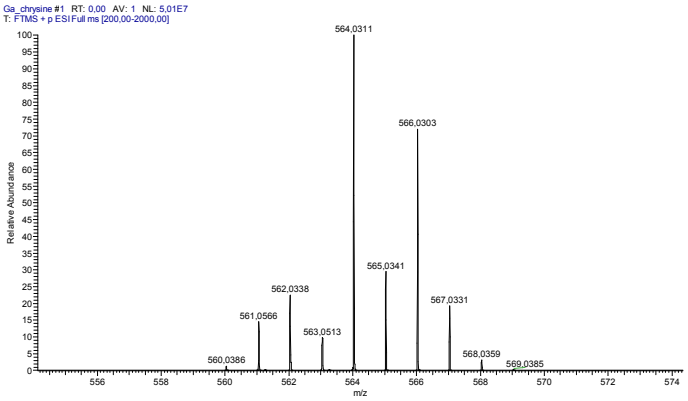
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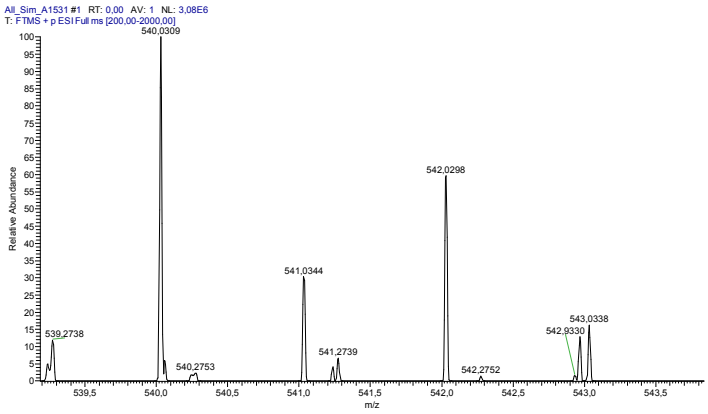
565,0341
562,0338
567,0331
561,0566
563,0513
568,0359
560,0386
569,0385
Relative Abundance
m/z

A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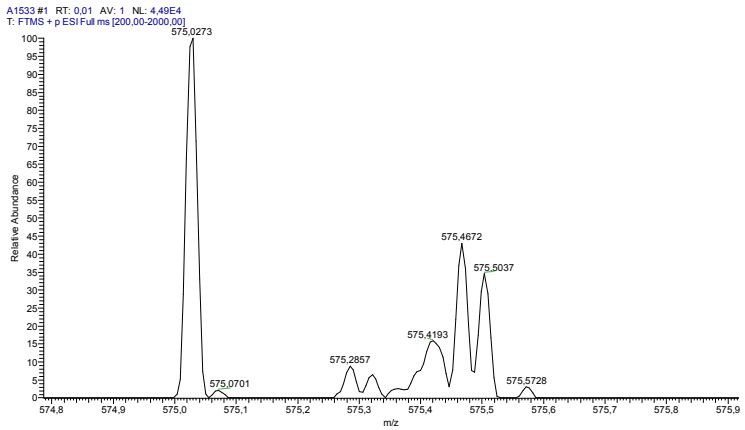
543,0338
542,9330
539,2738
541,2739
540,2753
542,2752
Relative Abundance
m/z

B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575,5037
575,4193
575,2857
575,0701
575,5728
Relative Abundance
m/z

C

Figure S1. HR-ESI-MS spectra of complexes **1** (A), **2** (B) and **3** (C).

Table S1: Hydrogen bonds in complexes **1 - 3**.

Interaction	*D*-H (Å)	H···A (Å)	*D*···A (Å)	*D*-H···A (°)	Symmetry operation
1					
O4—H566···O20^{ii}	0.81	1.90	2.692 (3)	165 (1)	(i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*, −*y*+1/2, *z*+1/2; (iii) *x*−1, *y*, *z*; (iv) −*x*+2, −*y*+1, −*z*+1; (v) *x*, *y*, *z*−1; (vi) *x*, −*y*+3/2, *z*−1/2.
O4—H566···O21^{ii}	0.81	2.48	3.154 (3)	141 (1)	
O4—H566···N8^{ii}	0.81	2.52	3.312 (3)	166 (1)	
O8—H565···O20^{i}	0.83	1.87	2.675 (3)	161 (1)	
O8—H565···O22^{i}	0.83	2.52	3.219 (3)	142 (1)	
O8—H565···N8^{i}	0.83	2.52	3.337 (3)	168 (1)	
O12—H564···O17^{iv}	0.83	1.85	2.680 (3)	176 (1)	
O12—H564···O18^{iv}	0.83	2.53	3.120 (3)	129 (1)	
O12—H564···N7^{iv}	0.83	2.49	3.272 (3)	157 (1)	
O16—H567···O17^{vi}	0.82	1.88	2.679 (3)	165 (1)	
O16—H567···O19^{vi}	0.82	2.55	3.125 (3)	129 (1)	
O16—H567···N7^{vi}	0.82	2.56	3.319 (3)	155 (1)	
2					
O5—H51···O6	0.82	1.80	2.571 (7)	155 (1)	(i) −*x*+2, −*y*+1, −*z*+1; (ii) *x*, *y*+1, *z*; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*, *y*+1, *z*−1.
O8—H514···O14^{iii}	0.82	1.93	2.750 (7)	175 (1)	
O15—H515···O13^{iii}	0.83	2.52	3.276 (7)	152 (1)	
O15—H515···O14^{iii}	0.83	2.21	2.984 (7)	155 (1)	
O4—H516···O10^{iv}	0.83	1.85	2.673 (7)	175 (1)	
3					
O8—H81···O12^{i}	0.82	2.31	3.102 (5)	161 (1)	(i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*, *y*+1, *z*−1; (iii) −*x*+1, −*y*+1, −*z*; (iv) −*x*, −*y*+1, −*z*+1.
O8—H81···O13^{i}	0.82	2.01	2.703 (5)	141 (1)	
O8—H81···N5^{i}	0.82	2.41	3.217 (5)	167 (1)	
O4—H41···O11^{ii}	0.82	1.87	2.680 (5)	170 (1)	
N4—H387···O12^{iii}	0.87	2.40	3.123 (5)	142 (1)	
N4—H387···O14^{iii}	0.87	2.14	2.942 (5)	154 (1)	
N2—H385···O13^{iv}	0.87	2.06	2.805 (5)	144 (1)	
N2—H385···O14^{iv}	0.87	2.48	3.226 (5)	145 (1)	
N2—H385···N5^{iv}	0.87	2.59	3.374 (5)	152 (1)	
O9—H91···O1	0.82	2.12	2.841 (5)	147 (1)	
O11—H112···O8^{i}	0.84	2.19	3.019 (5)	170 (1)	
O11—H388···O10^{iv}	0.82	1.89	2.701 (5)	167 (1)	
O10—H101···O9	0.82	1.91	2.690 (5)	160 (1)	

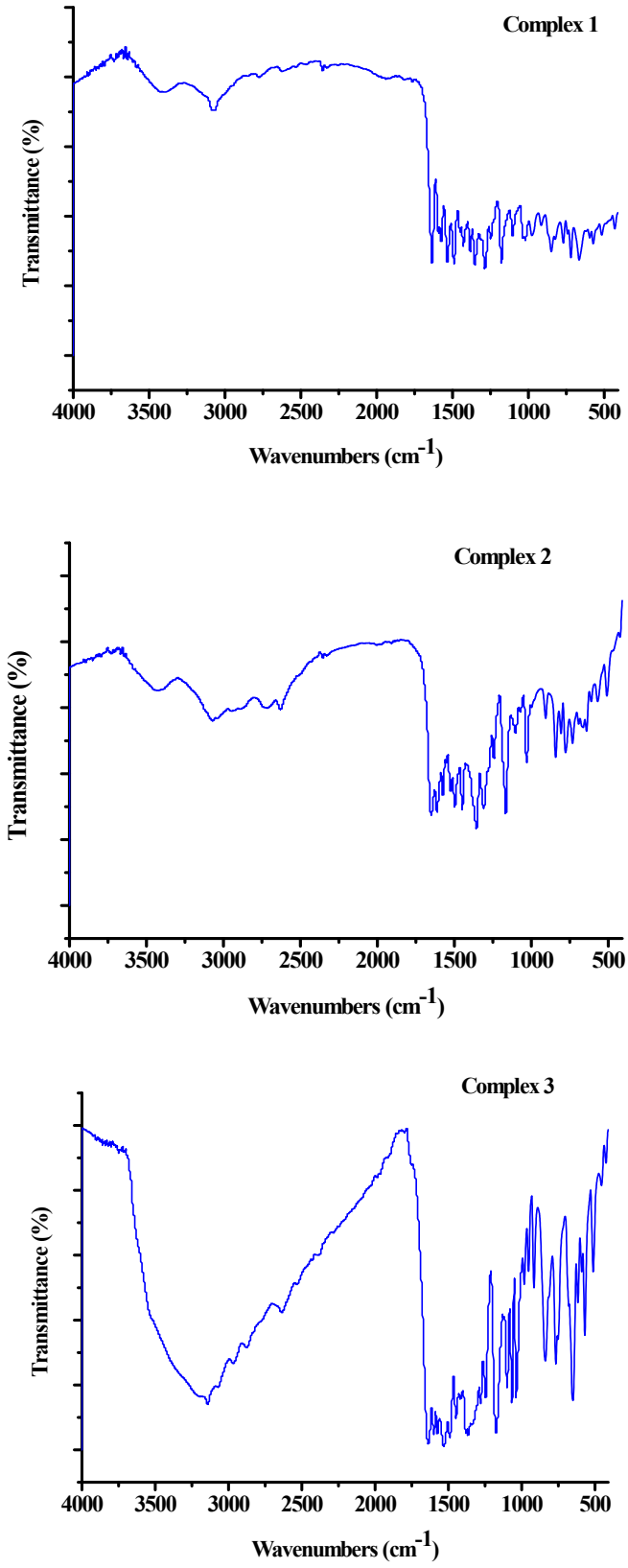


Figure S2. FT-IR spectra of complexes **1** (**A**), **2**(**B**), and **3** (**C**).

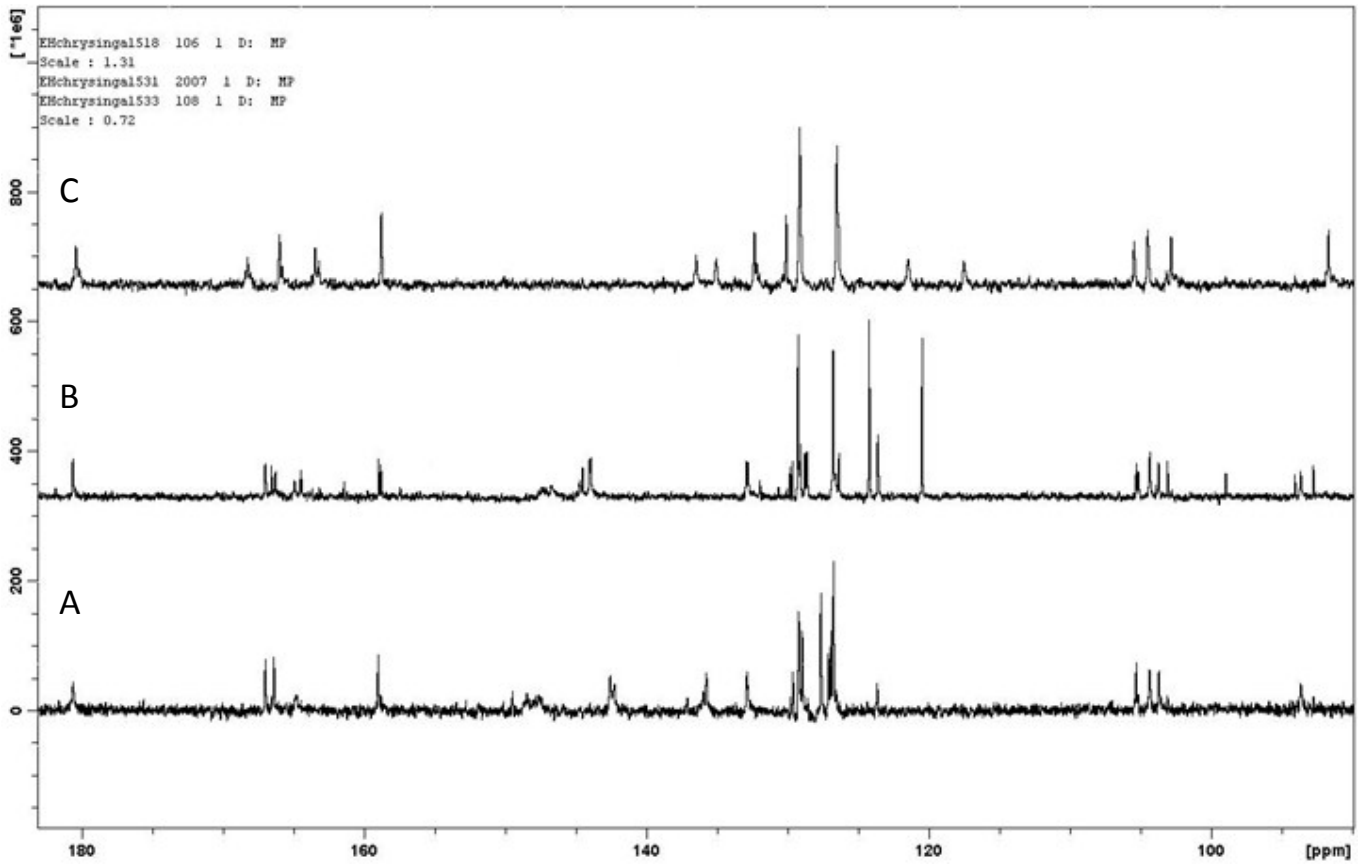


Figure S3. ^{13}C spectra (range 187.15 - 90.03 ppm) of complexes **1** (**A**), **2** (**B**) and **3** (**C**) in DMSO-d_6 at 25 °C. It should be noted that the crystalline material of complex **2** includes free chrysin which is present in the spectrum.

Table S2: ^{13}C chemical shifts of chrysin and coordinated chrysin in complexes **1 - 3** in DMSO-d_6 at 25 °C. The numbering of the atoms is given in **Fig. 1**.

Carbon atoms	**chrysin**	**1**	**2**	**3**
C-2	163.20	164.87	164.95	163.47
C-3	105.12	105.36	105.32	104.53
C-4	181.84	180.62	180.63	180.41
C-10	103.94	104.41	104.38	105.50
C-5	161.42	166.40	166.30	166.00
C-6	99.00	103.71	103.76	102.88
C-7	164.39	166.99	167.02	168.27
C-8	94.11	93.72	93.71	91.73
C-9	157.44	159.01	158.80	158.80
C-1'	130.66	129.66	129.68	130.13
C-2'/C-6'	126.36	126.77	126.81	126.54
C-3'/C-5'	129.12	129.28	129.28	129.19
C-4'	132.00	132.98	132.95	132.38

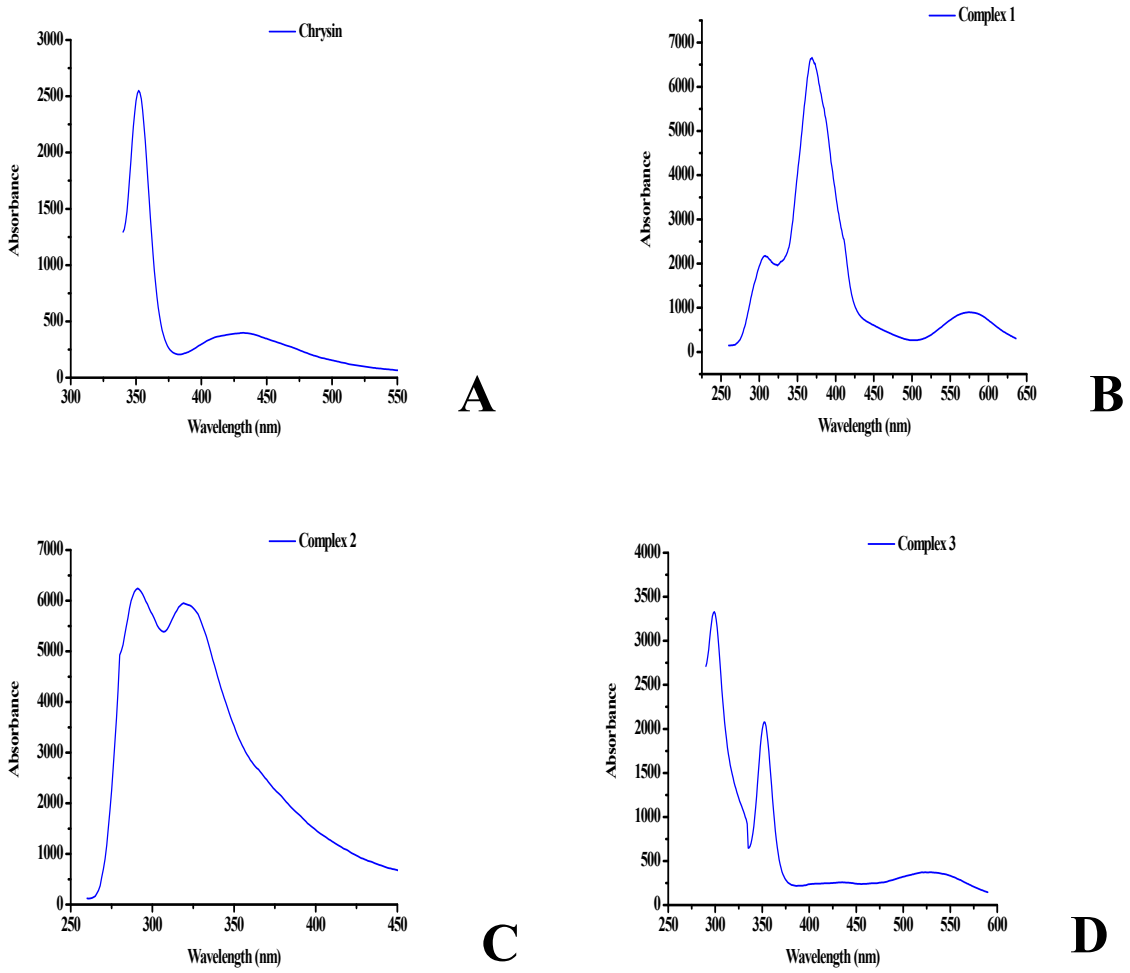


Figure S4. Fluorescence spectra (10^{-5} M in methanol) of pure chrysin (**A**) and complexes **1** (**B**), **2** (**C**) and **3** (**D**).

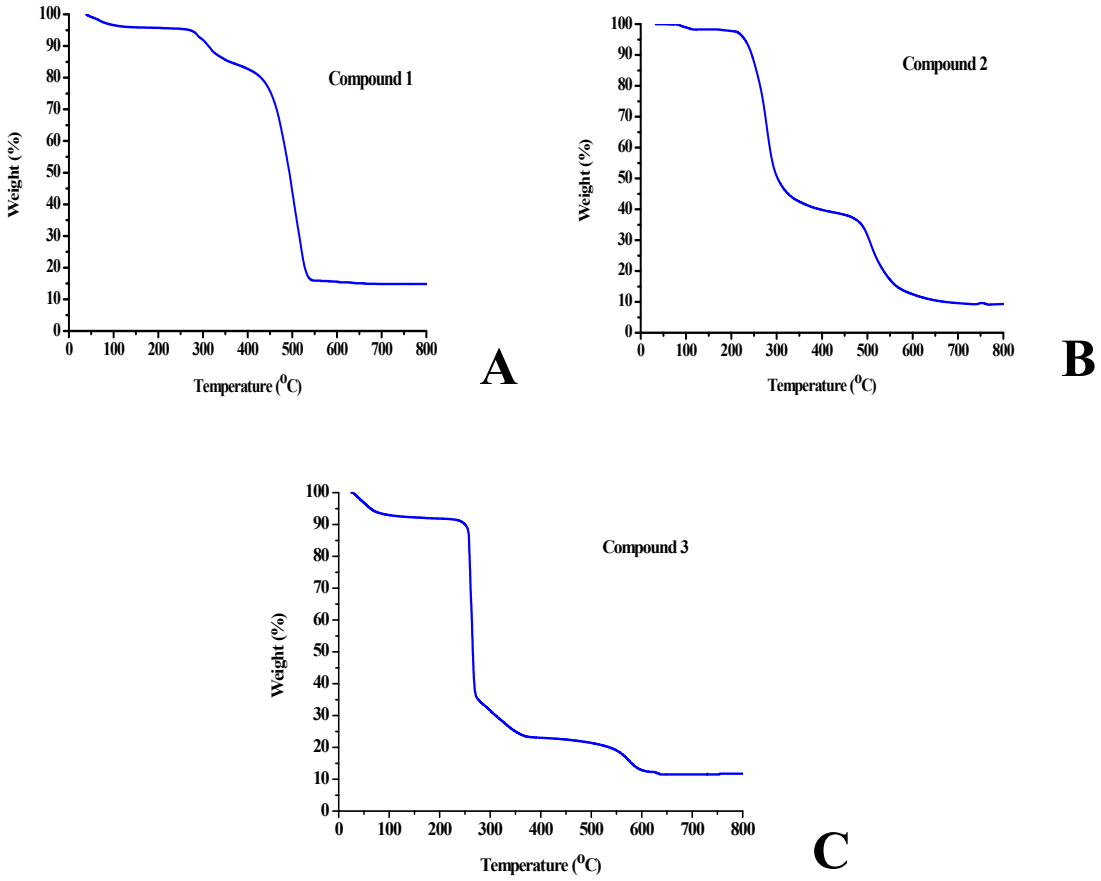
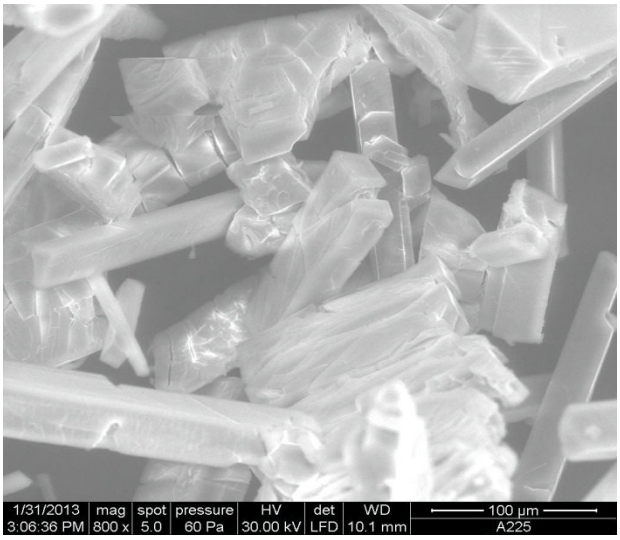
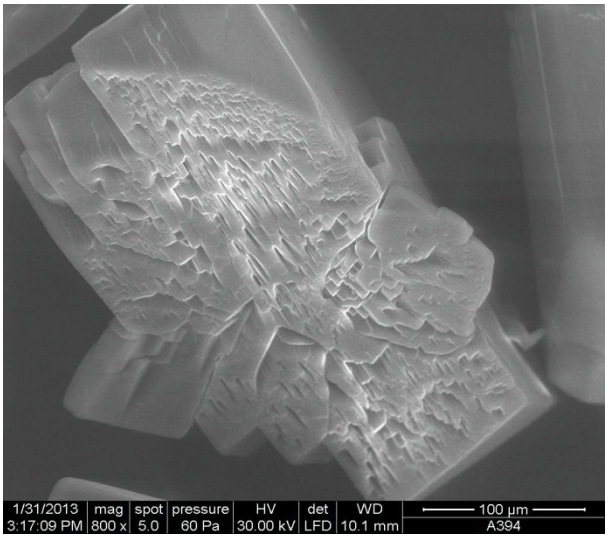


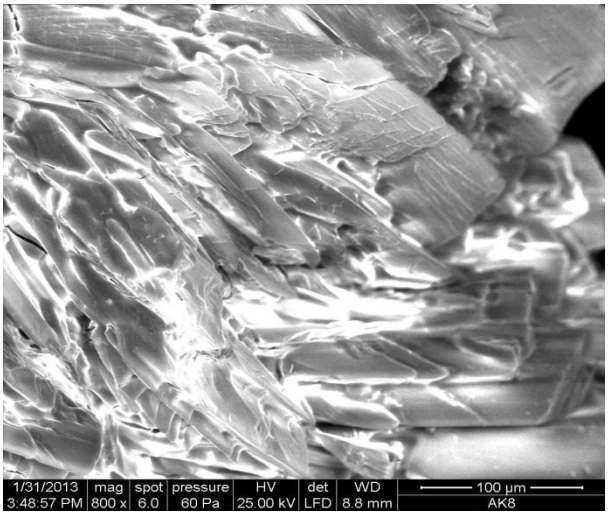
Figure S5. TGA diagrams of complexes **1** (**A**), **2** (**B**) and **3** (**C**)**.**



A



B



C

Figure S6. SEM images of the TGA residues of complexes **1** (**A**), **2**(**B**), and **3** (**C**).

Table S3: Cytotoxicity of clinically used chemotherapeutic agents.[1-2]

Chemotherapeutic agents	**IC_{50} (µM, 24 h)**					
	MDA-MB-231	**U-87 MG**	**DU-145**	**HeLa**	**A-549**	**A-431**
cisplatin	36	49	19	46	18	49
doxorubicin	1	0.3	0.07	0.1	0.03	0.1
5-FU	122	47	110	105	27	50
paclitaxel	0.05	0.8	1	0.01	0.04	0.7

1 https://apps.who.int/iris/handle/10665/325771

2 https://www.cancer.gov/