ELECTRONIC SUPPLEMENTARY INFORMATION
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Crystal Structure, Hirshfeld Surface Analysis, Spectroscopic and Biological Studies on Sulfamethazine and Sulfaquinoxaline Ternary Complexes with 2,2'-Biquinoline.

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2.1 Crystal Structure Analysis
2.3 Spectroscopic Properties
2.4 Thermogravimetric Analysis

2.1 Crystal structure analysis

Table S1. Continuous Shape Measures Calculations for compound **I.**

Structure [ML6]	HP-6[a]	PPY-6[b]	OC-6[c]	TPR-6[d]	JPPY-6[e]
I,	22.380	20.454	5.051	12.956	23.731

[a] Hexagon (D_{6h}), [b] Pentagonal pyramid (C_{5v}), [c] Octahedron (O_h), [d] Trigonal prism (D_{3h}), [e] Johnson pentagonal pyramid (J2) (C_{5v}).

Table S2. Continuous Shape Measures Calculations for compounds **II** and **III.**

Structure [ML5]	PP-5[a]	vOC-5[b]	TBPY-5[c]	SPY-5[d]	JTBPY-5[e]
II,	26.107	4.041	7.975	3.451	10.737
III,	26.569	4.148	6.652	3.373	10.070

[a] Pentagon (D_{5h}), [b] Vacant Octahedron (Johnson square Pyramid) (C_{4v}), [c] Trigonal Bipyramid (D_{3h}), [d] Square Pyramid (C_{4v}), [e] Johnson Trigonal Bipyramid (D_{3h}).

Table S3. Selected experimental and computed [B3LYP/6-31+G**] geometric parameters [Å, º] of complex **I**.

	Experimental	Calculated
Ni - N31	2,075	2,162
Ni - N320	2,082	2,163
Ni - N211	2,075	2,138
Ni - N21	2,256	2,222
Ni - N11	2,208	2,221
Ni - N211	2,132	2,135
S212 - N211	1,612	1,655
S112 - N111	1,601	1,655
S112 - C115	1,757	1,796
S212 - C215	1,747	1,797
S112 - O113	1,440	1,472
S112 - O114	1,438	1,477
S212 - O213	1,439	1,472
S212 - O214	1,436	1,477
C118 - N121	1,368	1,392
C218 - N221	1,370	1,392
N111 - C110	1,367	1,363
C110 - N11	1,329	1,338
N21 - C210	1,326	1,363
C210 - N211	1,362	1,338
N31 - C32	1,380	1,372
N31 - C310	1,328	1,329
N320 - C319	1,386	1,372
N320 - C311	1,337	1,329
N211 - Ni - N21	61,510	61,414
N11 - Ni - N111	61,580	61,437
N31 - Ni - N320	79,870	79,033
N11 - Ni - N21	75,280	81,992
N211 - Ni - N320	101,660	92,694
N31 - Ni - N111	96,140	92,996
N211 - Ni - N31	100,630	100,184
N31 - Ni - N11	103,160	102,822
N21 - Ni - N31	160,990	161,538
N21 - Ni - N320	108,800	102,045
N11 - Ni - N320	158,200	161,772
N211 - Ni - N111	157,000	162,936
N11 - Ni - N211	99,000	104,670
N111 - Ni - N320	96,690	100,471
N111 - Ni - N31	96,140	92,996
N111 - Ni - N21	99,480	104,801
N211 - S212 - C215	105,740	106,362
N111 - Ni - C115	107,140	106,321
Ni - N211 - S212	135,870	137,876
Ni - N111 - S112	141,130	137,756
O113 - S112 - O114	116,830	119,796
O213 - S212 - O214	116,760	119,718
N11 - C110 - N111	111,060	111,050
N21 - C210 - N211	111,390	111,096

Table S4. Selected experimental and computed [B3LYP/6-31+G**] geometric parameters [Å, º] of complex **II**.

	Experimental	**Calculated**
Cu - Cl1	2,251	2,292
Cu - N21	2,007	2,077
Cu - N220	2,206	2,276
Cu - N111	2,068	2,120
Cu - N11	2,063	2,092
S - N111	1,617	1,657
S - C115	1,760	1,794
C118 - N12	1,377	1,389
N111 - C110	1,353	1,362
N220 - C219	1,367	1,363
N220 - C211	1,323	1,326
N21 - C22	1,371	1,366
N21 - C210	1,320	1,329
S - O112	1,444	1,476
S - O114	1,435	1,472
N21 - Cu - N220	78,670	76,742
N11 - Cu - N111	64,530	63,418
N11 - Cu - Cl	98,780	101,739
N111 - Cu - Cl	156,750	160,421
N21 - Cu - Cl	97,010	94,137
N220 - Cu - Cl	101,110	102,500
N111 - S - C115	105,460	105,397
N11 - Cu - N220	115,030	113,583
N111 - Cu - N21	94,920	97,442
N11 - Cu - N21	156,400	158,211
N11 - Cu - N220	100,760	95,510
N11 - C110 -N111	110,750	110,123
O112 - S - O114	118,070	119,525
Cu - N111 - S113	140,480	139,288

Table S5. Selected experimental and computed [B3LYP/6-31+G**] geometric parameters [Å, º] of complex **III**.

	Experimental	**Calculated**
Cu - Cl	2,236	2,291
Cu - N217	2,072	2,096
Cu - N211	2,047	2,091
Cu - N11	2,022	2,085
Cu - N120	2,219	2,283
S - N211	1,614	1,664
S - C21	1,756	1,792
C24 - N27	1,399	1,393
N211 - C212	1,360	1,358
C214 - C218	1,496	1,505
C216 - C219	1,479	1,501
N11 - C12	1,370	1,366
N11 - C110	1,332	1,328
N120 - C119	1,387	1,363
N120 - C111	1,307	1,326
S - O29	1,446	1,472
S - O210	1,442	1,475
N217 - Cu - N211	64,620	63,844
N120 - Cu - N11	78,290	76,369
N217 - Cu - Cl	99,090	100,724
N211 - Cu - Cl	153,260	160,790
N11 - Cu - Cl	96,790	93,981
N120 - Cu - Cl	105,170	100,997
N211 - S - C21	106,740	106,441
N120 - Cu - N217	112,500	117,006
N11 - Cu - N211	94,470	97,770
N11 - Cu - N217	157,400	157,296
N120 - Cu - N211	100,800	96,522
N211 - C212 - N217	108,550	108,514
O29 - S28 - O210	116,610	119,204
Cu - N211 - S28	138,480	137,659

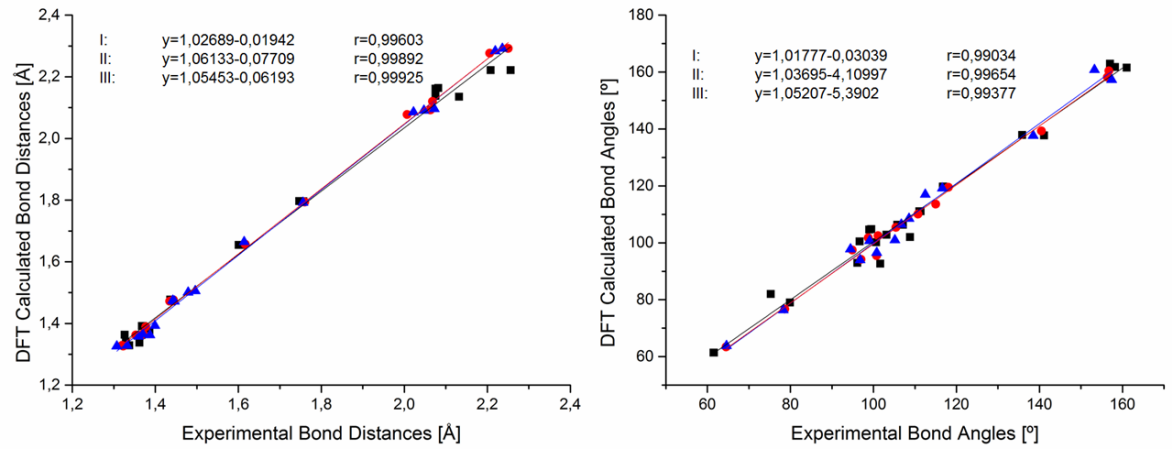

Figure S1. Correlation plots between selected calculated (DFT B3LYP/6-31+G**) and experimental bond distances (left) and angles (right). ■ **I**; ● **II**; ▲ **III.**

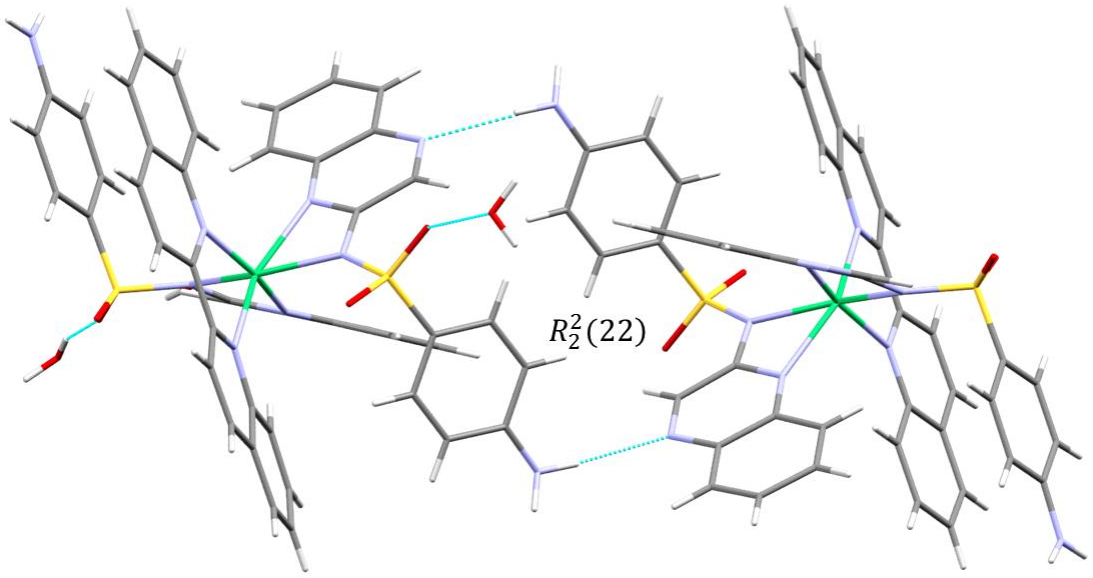

Figure S2. $R_2^2(22)$ features formed between complex **I** unities, the intermolecular interactions are depicted as blue dashed lines.

2.3 Spectroscopic Properties

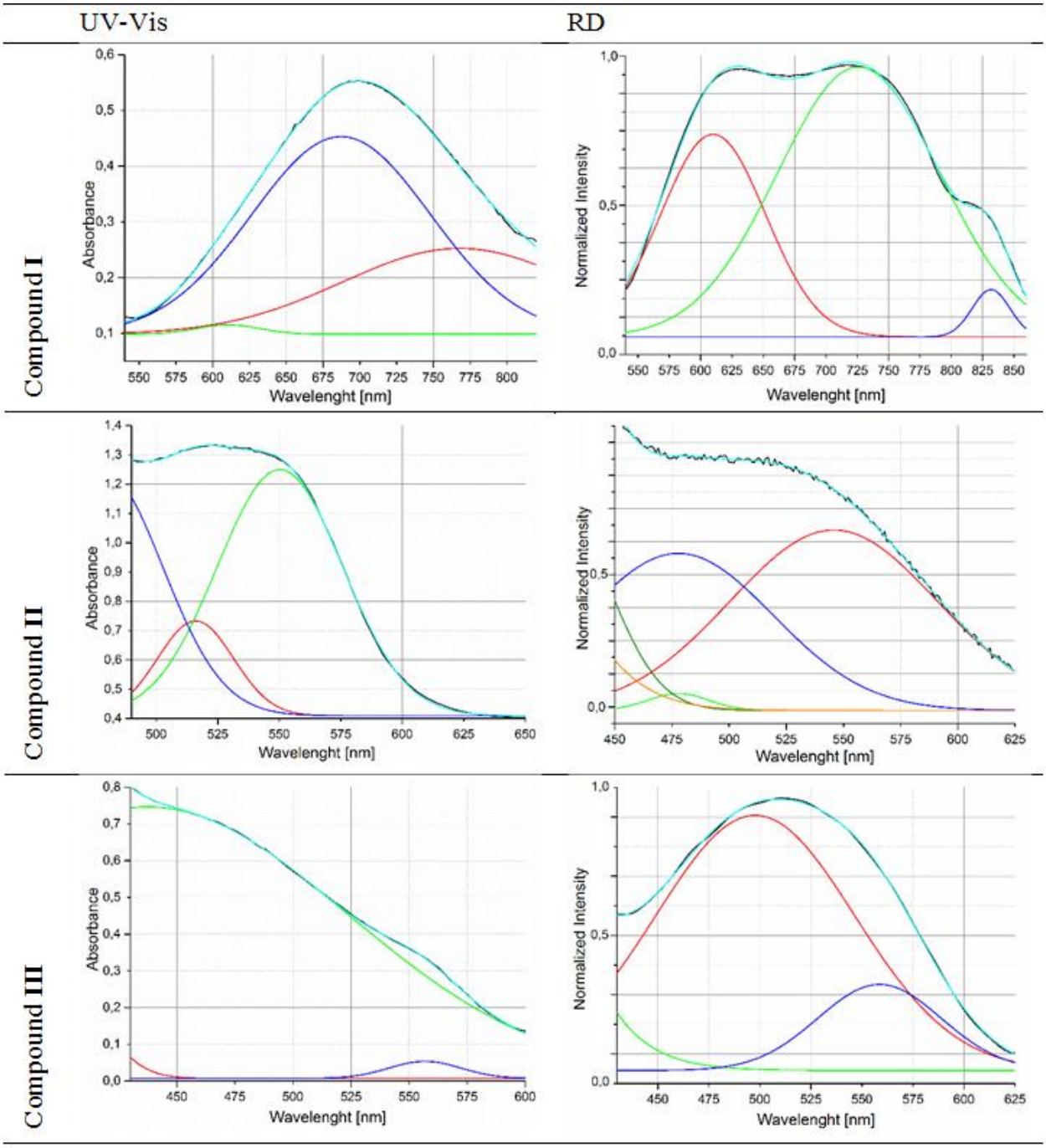

Figure S3. Deconvoluted UV-Vis in DMSO solution (10 μM) and diffuse reflectance UV-Vis spectra for the complexes **I - III**.

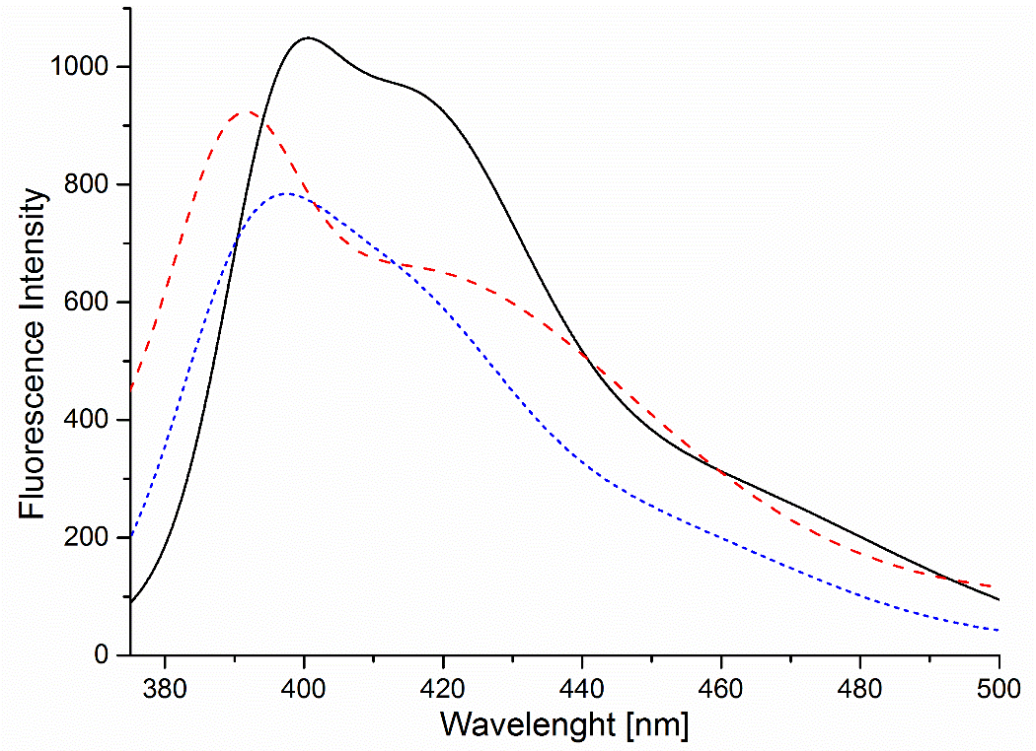

Figure S4. Aqueous solution (~ 0.1 mM; 0.8 % DMSO) emission spectra of the complexes **I - III**. (λ_{exc}= 350 nm; **I** —; **II** - - -; **III** ·····).

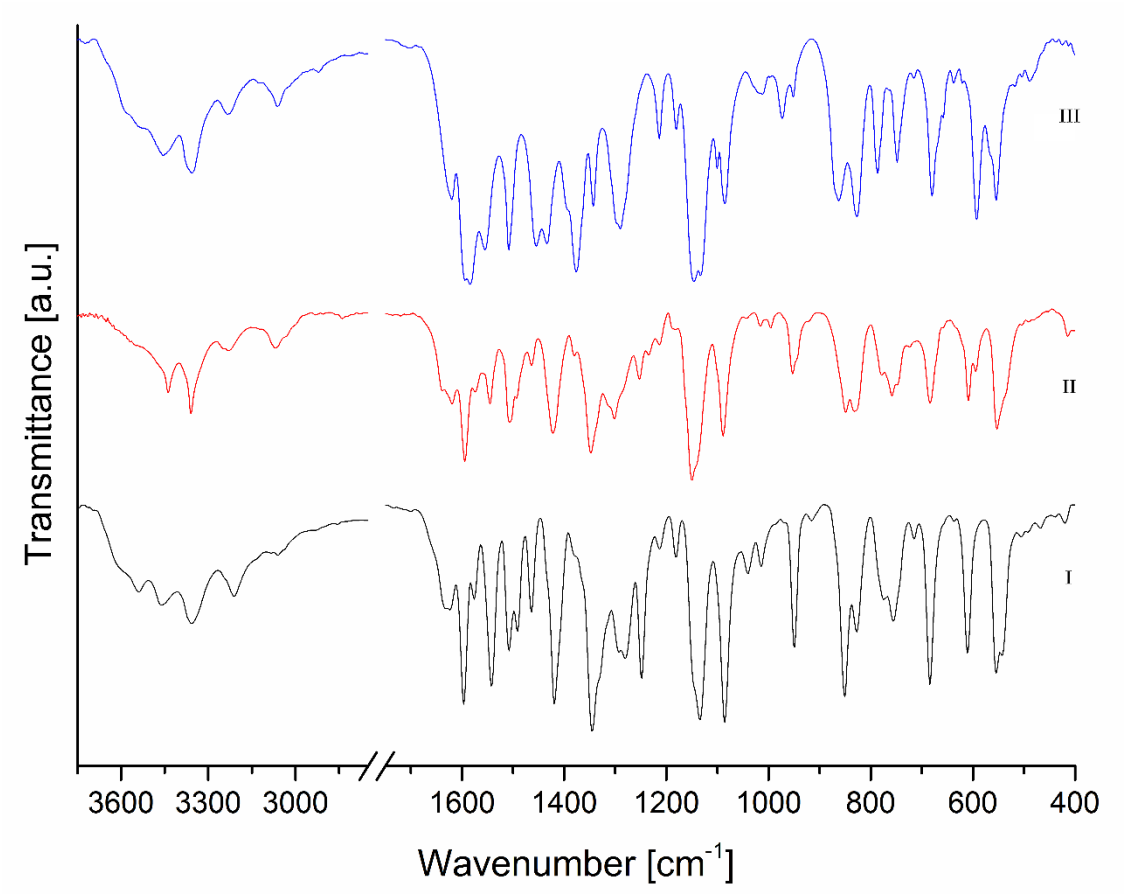

Figure S6. FTIR spectra for complexes **I - III**.

2.4 Thermogravimetric and Differential Thermal Analyses.

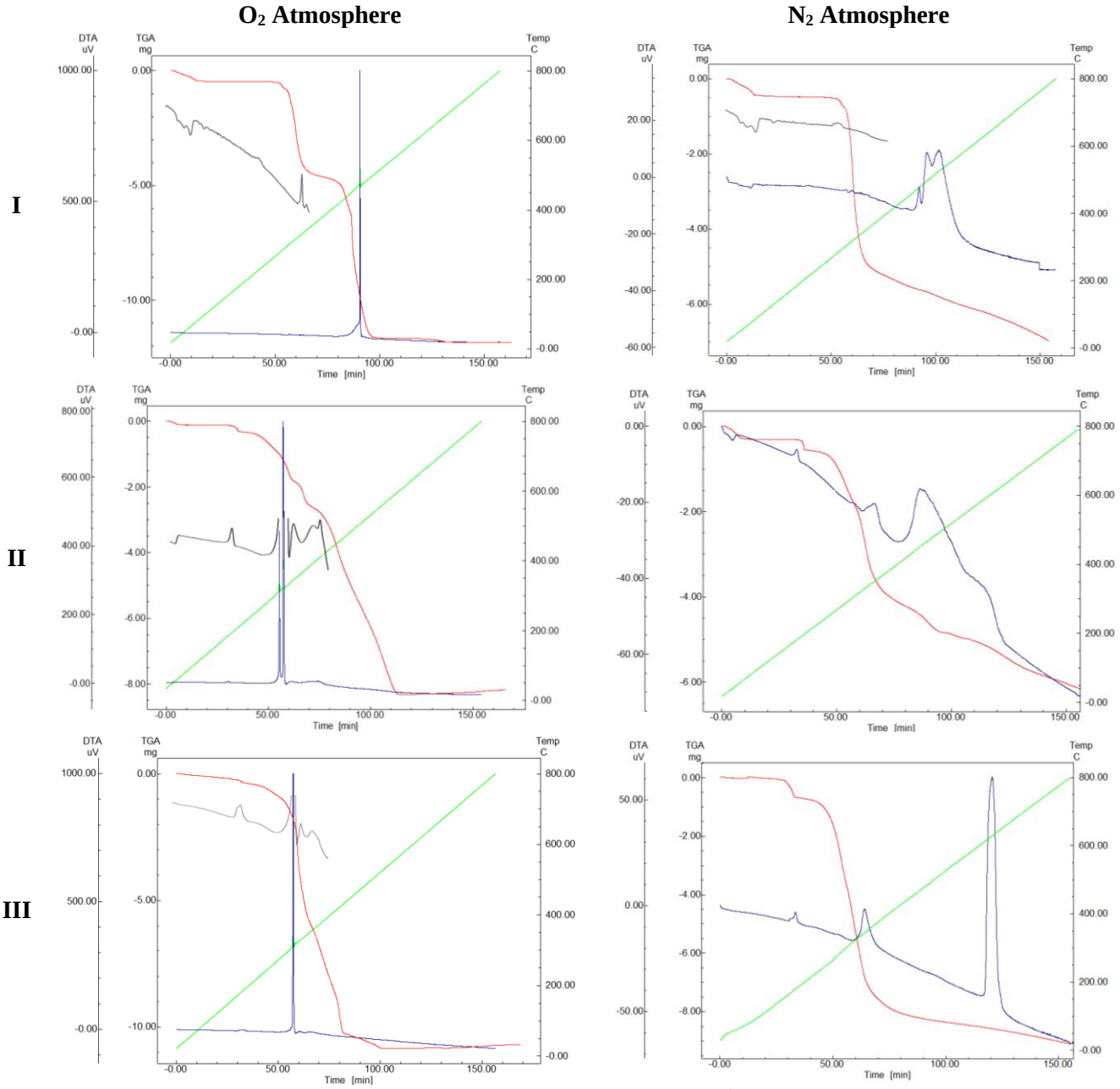

Figure S5. TG (—) and DT (—) curves for the complexes **I - III**. 5 ºC min^{-1} (Temperature curve (—)) and 50 ml min^{-1} Oxygen or Nitrogen flow. The zoomed sections of the DT curves do not correspond with the scale.