

**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, °] of complex **I**.

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

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

	Experimental	Calculated
Cu - C11	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, °] 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

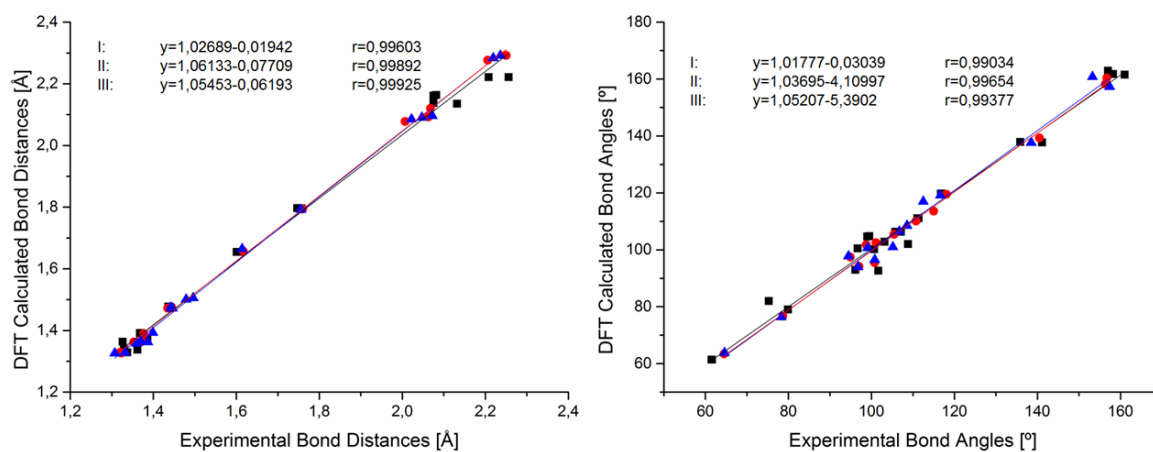


Figure S1. Correlation plots between selected calculated (DFT B3LYP/6-31+G**) and experimental bond distances (left) and angles (right). ■ I; ● II; ▲ III.

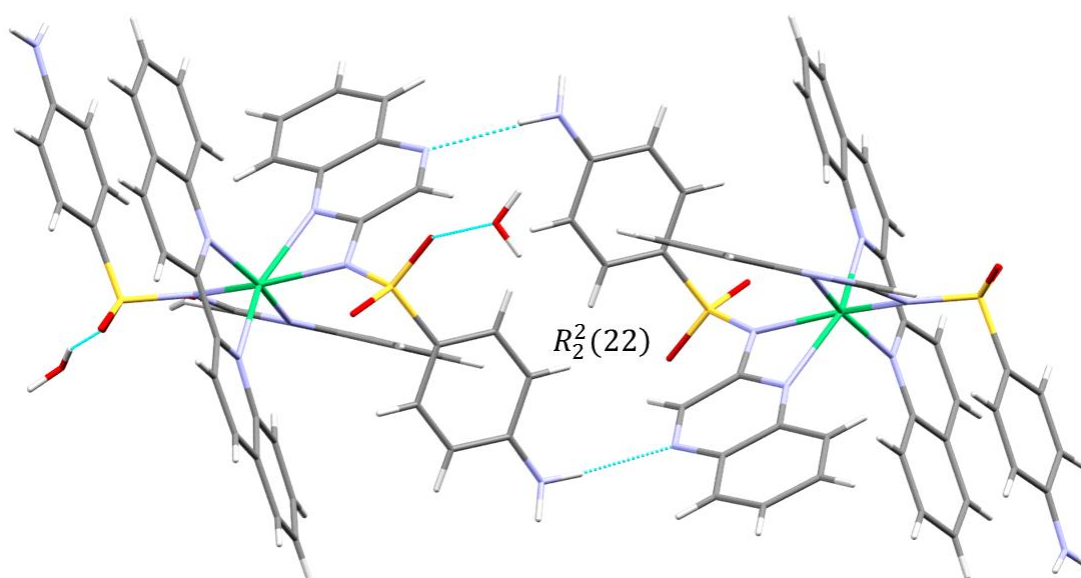


Figure S2. $R_2^2(22)$ features formed between complex I units, the intermolecular interactions are depicted as blue dashed lines.

2.3 Spectroscopic Properties

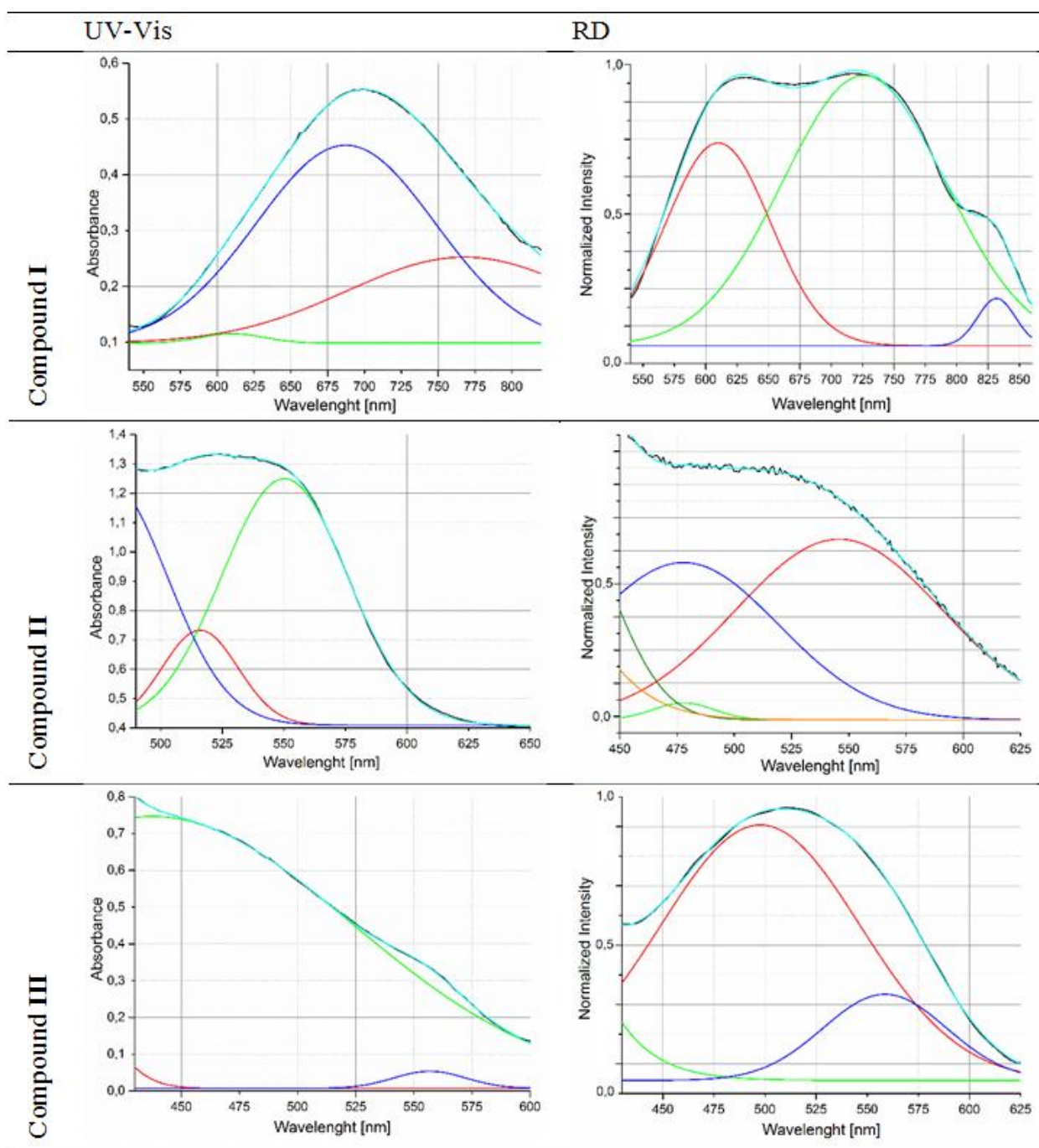


Figure S3. Deconvoluted UV-Vis in DMSO solution (10 μM) and diffuse reflectance UV-Vis spectra for the complexes **I - III**.

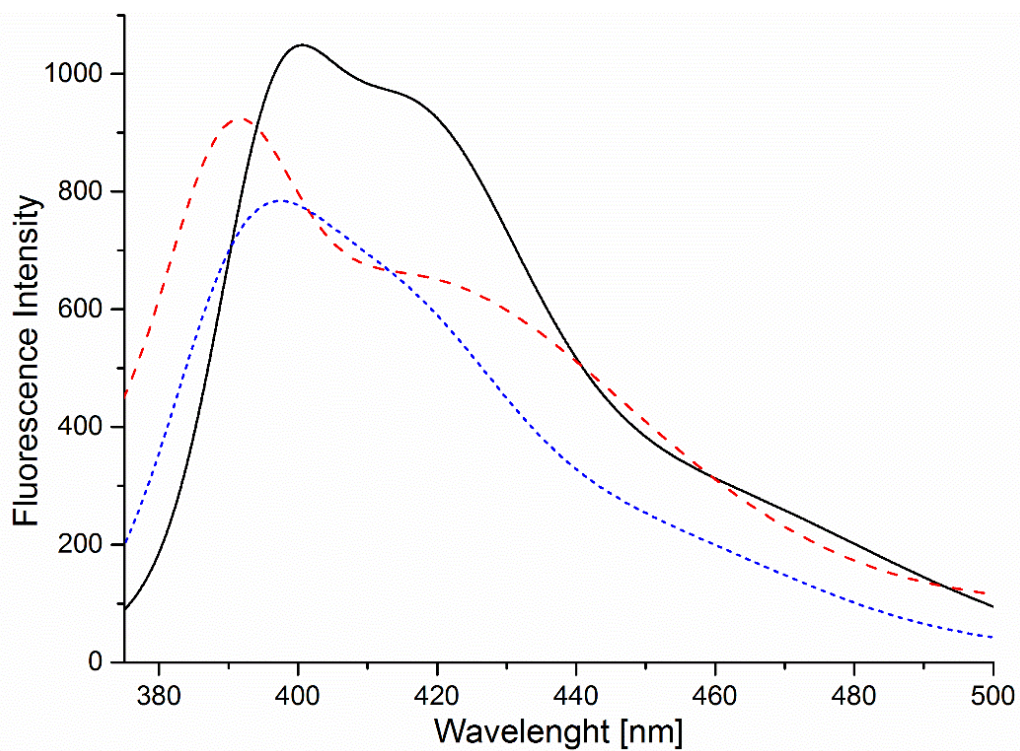


Figure S4. Aqueous solution (~ 0.1 mM; 0.8 % DMSO) emission spectra of the complexes **I** - **III**. ($\lambda_{\text{exc}} = 350$ nm; **I** —; **II** - - -; **III**).

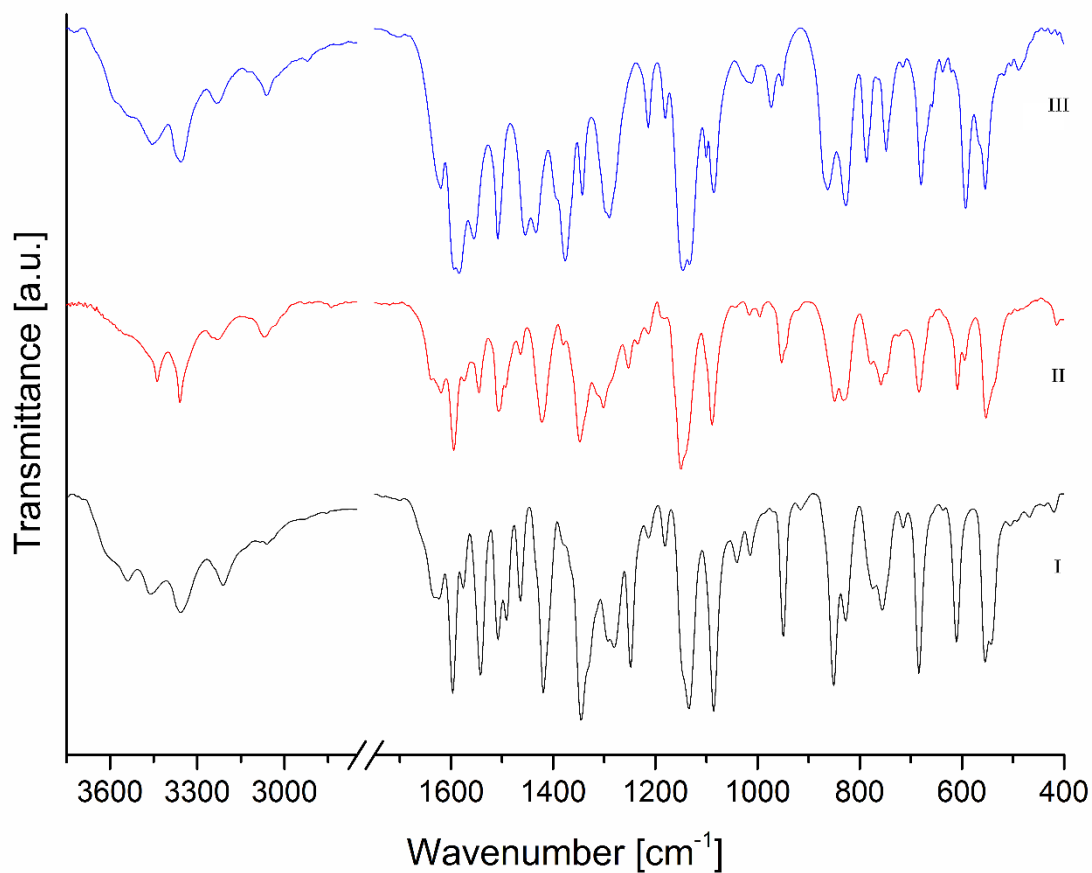


Figure S6. FTIR spectra for complexes **I** - **III**.

2.4 Thermogravimetric and Differential Thermal Analyses.

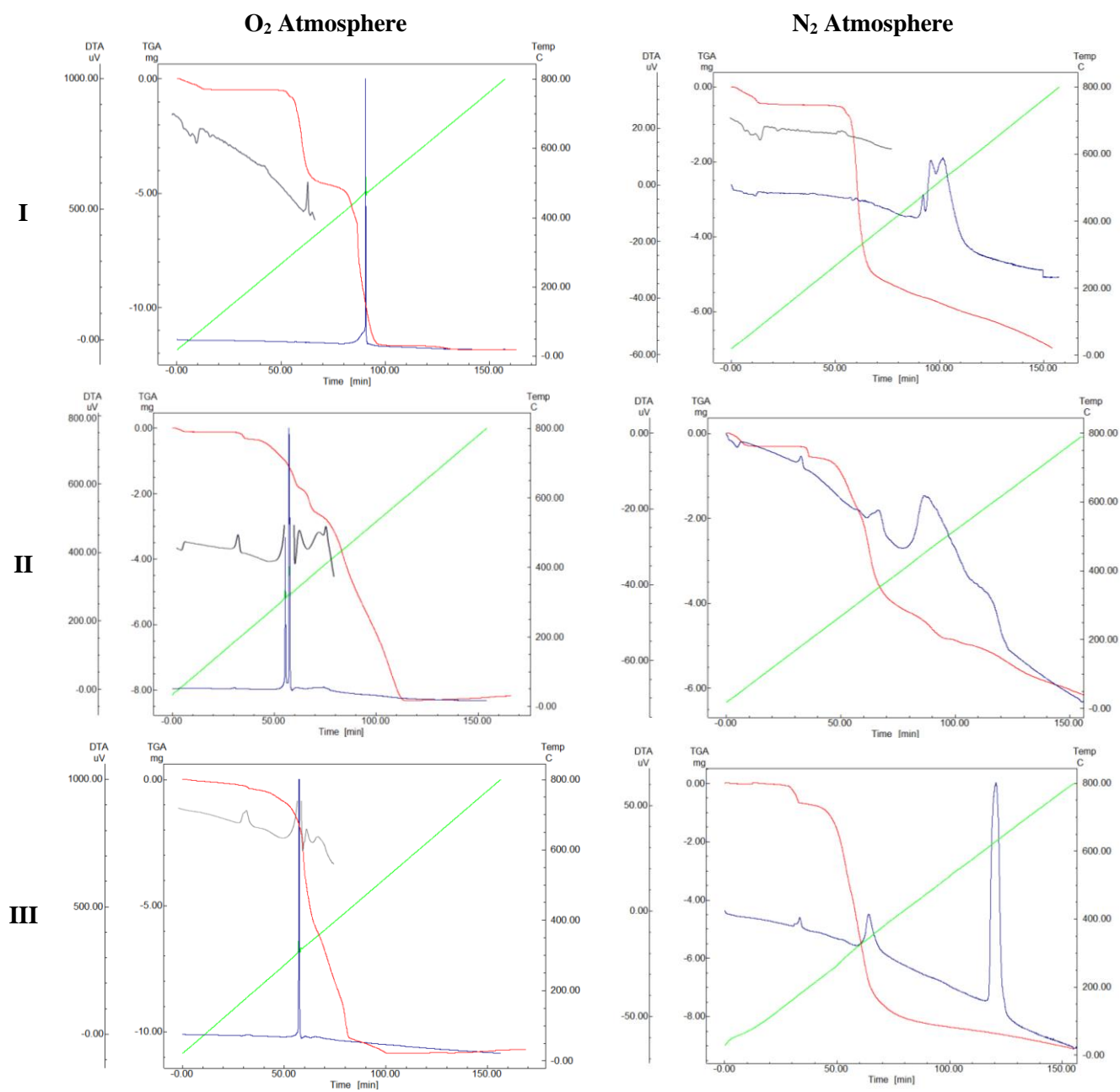


Figure S5. TG (—) and DT (—) curves for the complexes **I - III**. 5 °C min⁻¹ (Temperature curve (—)) and 50 ml min⁻¹ Oxygen or Nitrogen flow. The zoomed sections of the DT curves do not correspond with the scale.