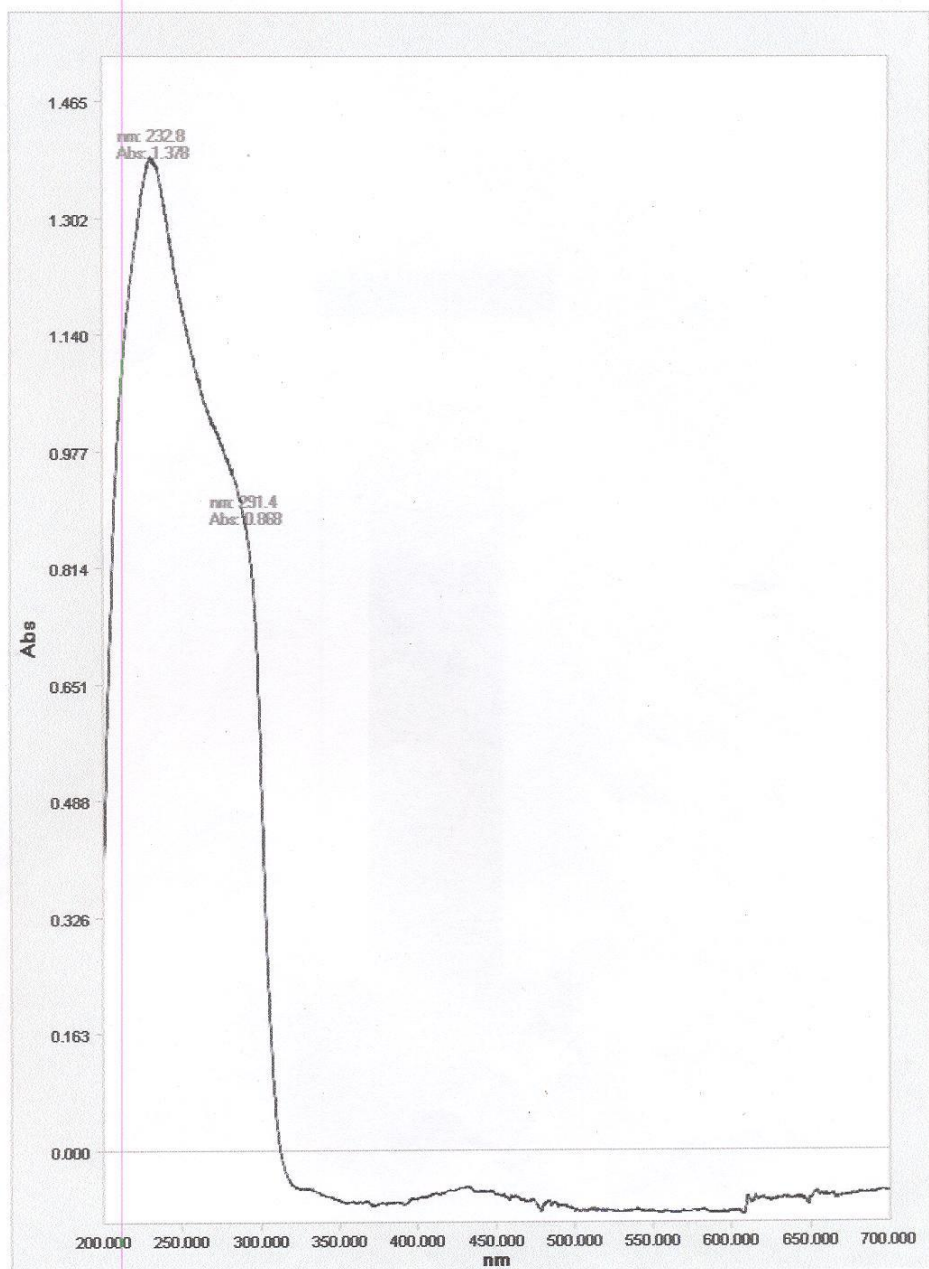
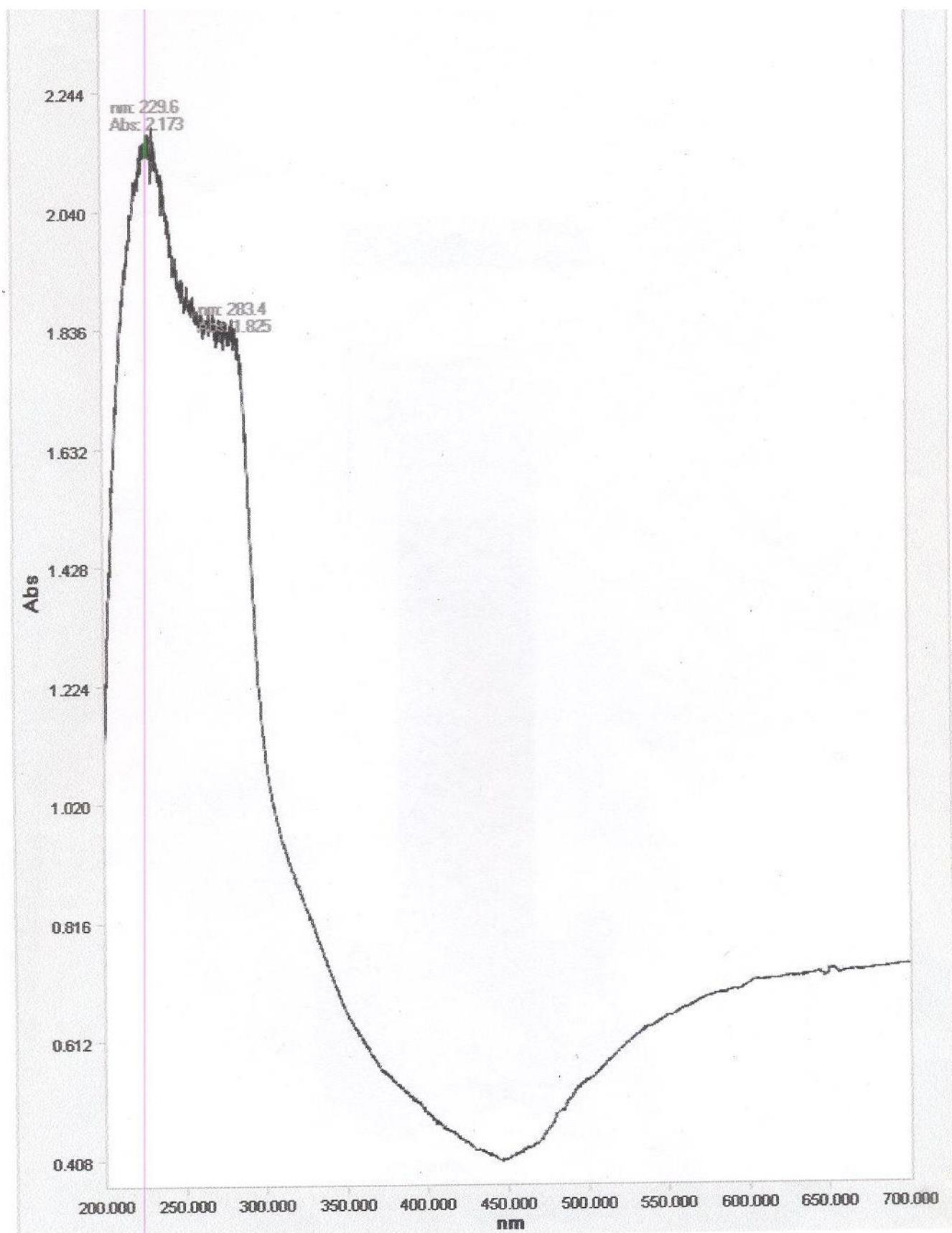


# **Synthesis, Biological and *In silico* Studies of a Tripodal Schiff Base Derived from 2,4,6-Triamino-1,3,5-triazine and its Trinuclear Dy(III), Er(III) and Gd(III) Salen Capped Complexes.**

Uchechukwu Susan Oruma<sup>1</sup>, Pius Oziri Ukoha<sup>1</sup>, Chiamaka Peace Uzoewulu<sup>2</sup>, Joseph Chinedum Ndefo<sup>3</sup>, Sabastine Chinweike Ugwuoke<sup>4</sup>, Nkechinyere Nwanneka Ukwueze<sup>2</sup>, Tochukwu Emmanuella Eze<sup>2,4</sup>, Chinenye Lilian Ekowo<sup>2</sup>, Florence Uchenna Eze<sup>2</sup> and Uchenna Vivian Obi<sup>2,5</sup> Sunday Nwankwo Okafor<sup>6\*</sup> Chigozie Julius Ezeorah<sup>2\*</sup>.

SUPPLEMENTARY MATERIALS



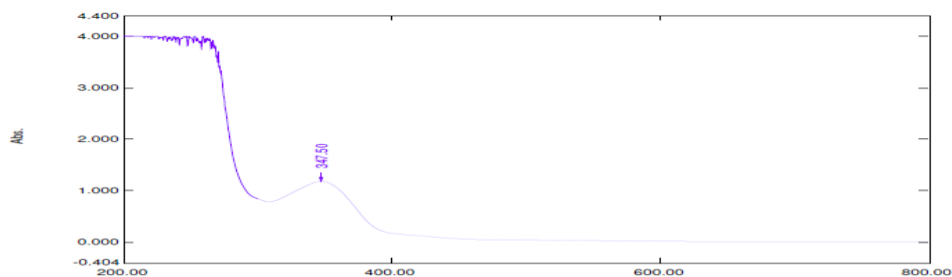


**Figure S1: Electronic absorption spectrum of MT.**

## Spectrum Peak Pick Report

01/19/2016 01:55:10 PM

Data Set: MT2 - RawData



Measurement Properties  
Wavelength Range (nm.): 200.00 to 800.00  
Scan Speed: Fast  
Sampling Interval: 0.5  
Auto Sampling Interval: Disabled  
Scan Mode: Single  
Instrument Properties  
Instrument Type: UV-1800 Series  
Measuring Mode: Absorbance  
Slit Width: 1.0 nm  
Light Source Change Wavelength: 340.5 nm  
S/R Exchange: Normal  
Attachment Properties  
Attachment: 6-Cell  
Number of cells: 6  
Sample Preparation Properties  
Weight:  
Volume:  
Dilution:  
Path Length:  
Additional Information:

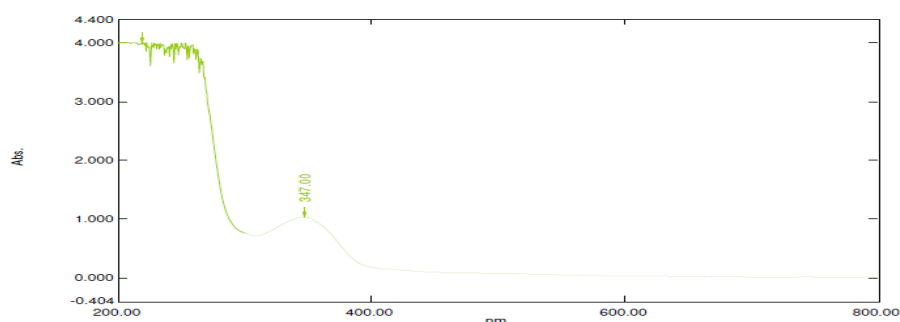
No.	P/V	Wavelength	Abs.	Description
1		347.50	1.177	347.50
2		308.00	0.779	

Figure S2: Electronic absorption spectrum of Dy(III)MT.

## Spectrum Peak Pick Report

01/19/2016 01:57:59 PM

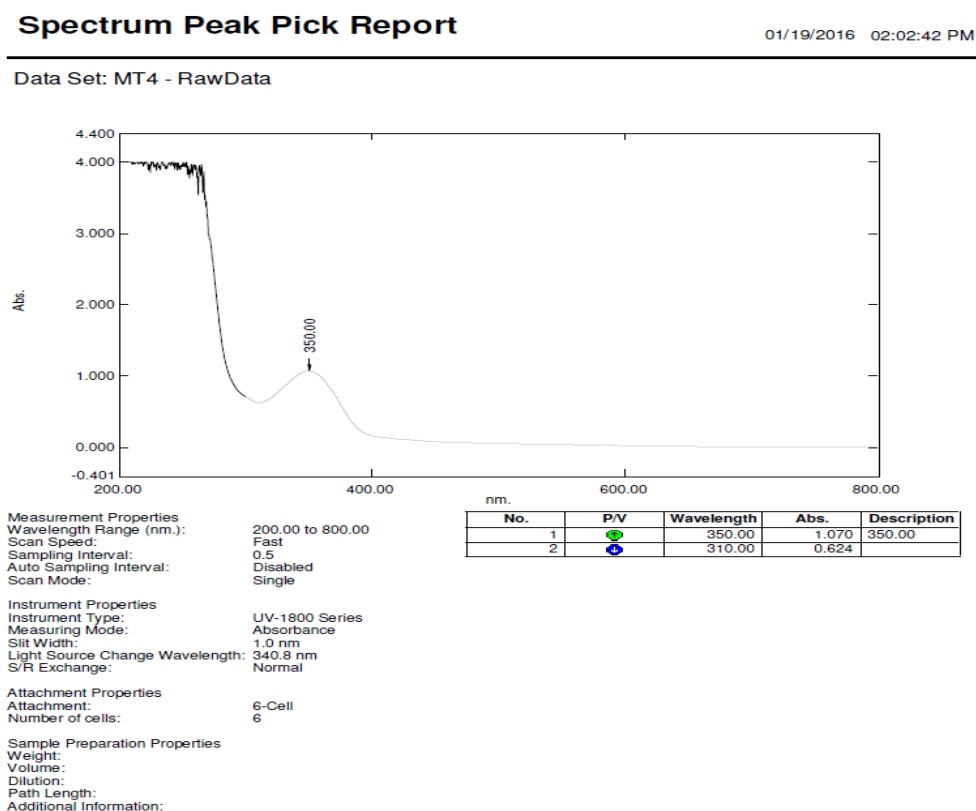
Data Set: MT3 - RawData



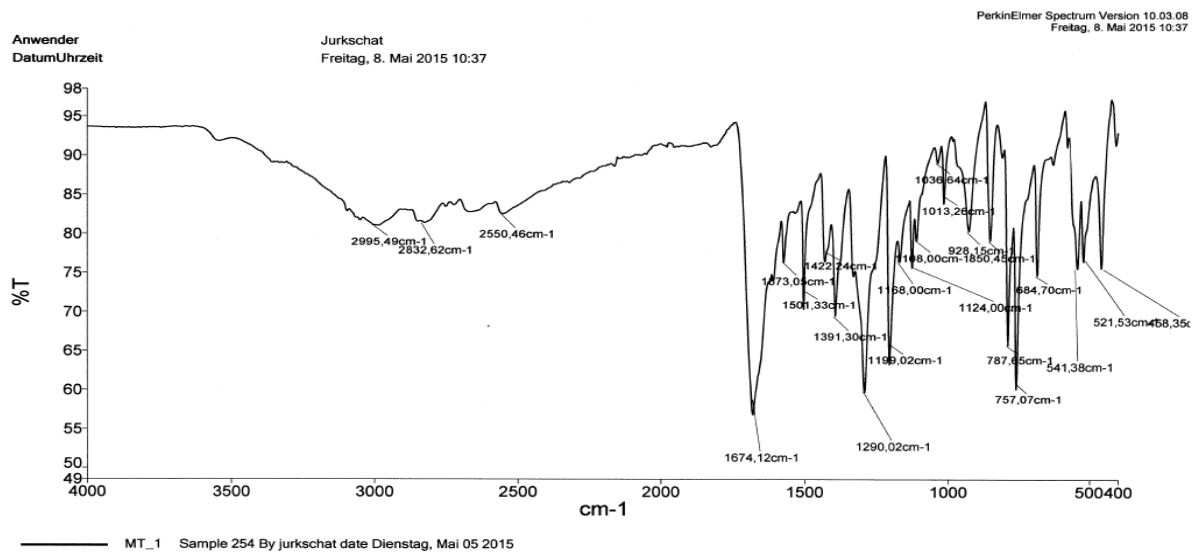
Measurement Properties  
Wavelength Range (nm.): 200.00 to 800.00  
Scan Speed: Fast  
Sampling Interval: 0.5  
Auto Sampling Interval: Disabled  
Scan Mode: Single  
Instrument Properties  
Instrument Type: UV-1800 Series  
Measuring Mode: Absorbance  
Slit Width: 1.0 nm  
Light Source Change Wavelength: 340.5 nm  
S/R Exchange: Normal  
Attachment Properties  
Attachment: 6-Cell  
Number of cells: 6  
Sample Preparation Properties  
Weight:  
Volume:  
Dilution:  
Path Length:  
Additional Information:

No.	P/V	Wavelength	Abs.	Description
1		347.00	1.036	347.00
2		218.50	4.000	
3		309.00	0.707	

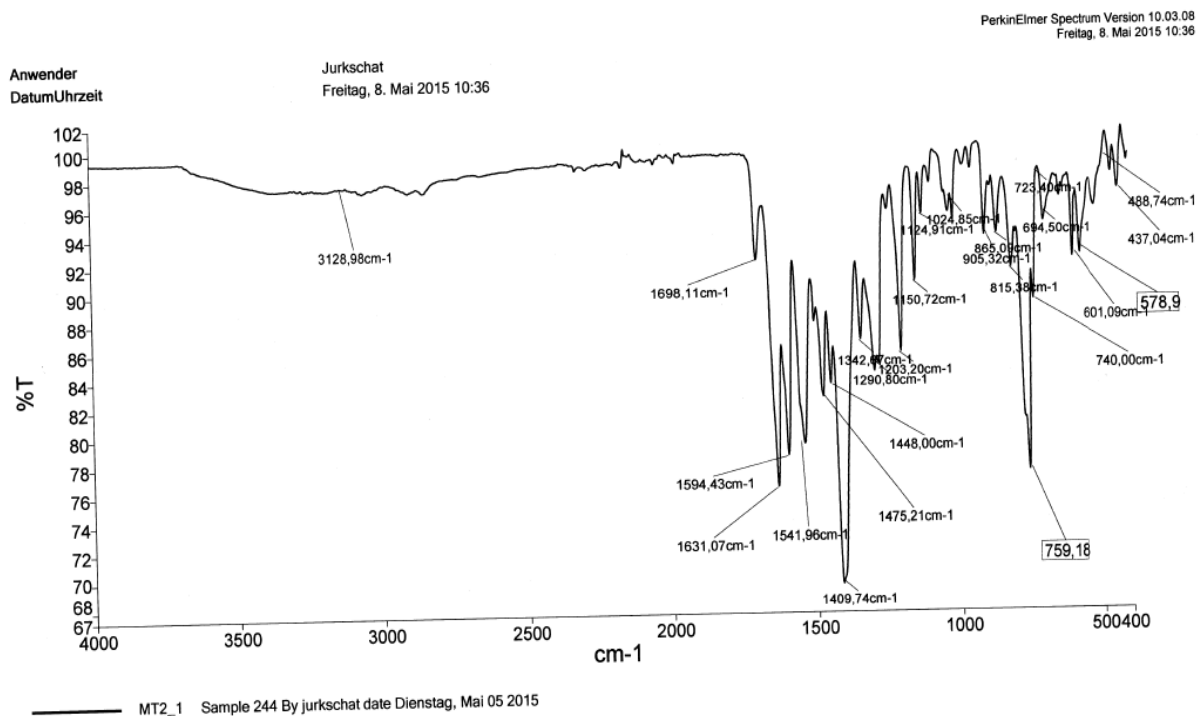
**Figure S3: Electronic absorption spectrum of Er(III)MT.**



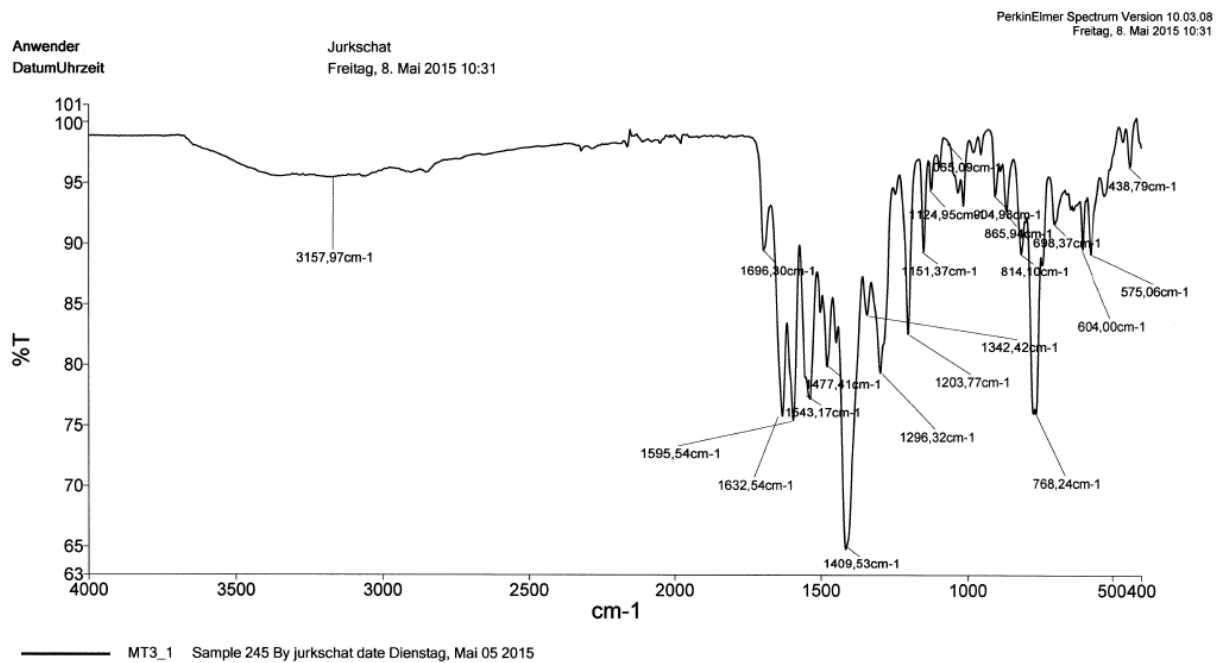
**Figure S4: Electronic absorption spectrum of Gd(III)MT.**



**Figure S5: Infrared Spectrum of MT.**

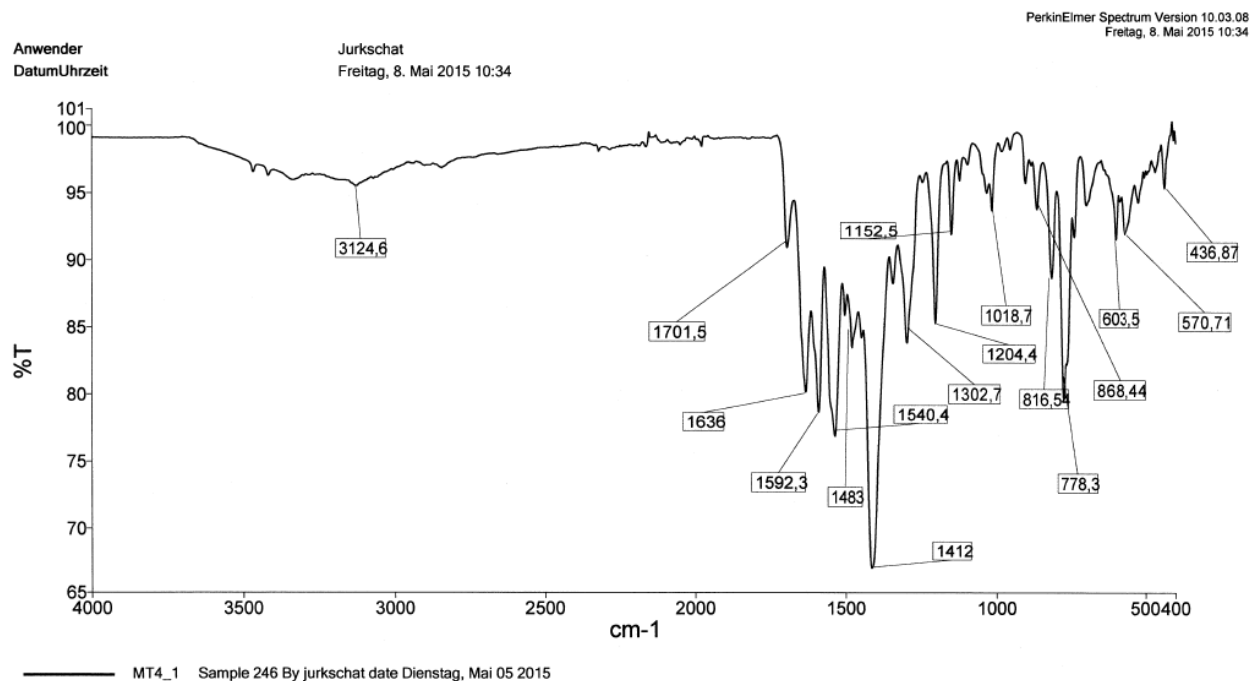


**Figure S6: Infrared Spectrum of Dy(III)MT**



**Figure S7: Infrared Spectrum of Er(III) MT**





**Figure S8: Infrared Spectrum of Gd(III)MT**

Acquisition Time (sec)	2.7329	Comment	z PROTON DMSO u quest 29		Date	29 Mar 2015 06:24:16	
Date Stamp	29 Mar 2015 06:24:16	File Name	C:\Users\Admin\Desktop\Nigeria\ACJ-ASW-MT101fd		Frequency (MHz)	300.13	
Nucleus	<sup>1</sup> H	Number of Transients	15		Origin	spect	
Points Count	16384	Pulse Sequence	zg30		Original Points Count	16384	
Spectrum Offset (Hz)	1941.0437	Spectrum Type	STANDARD		Receiver Gain	4096.00	
					SW (cycles) (Hz)	5995.20	
					Solvent	DMSO-d6	
					Sweep Width (Hz)	5994.84	
					Temperature (degree C)	21.160	

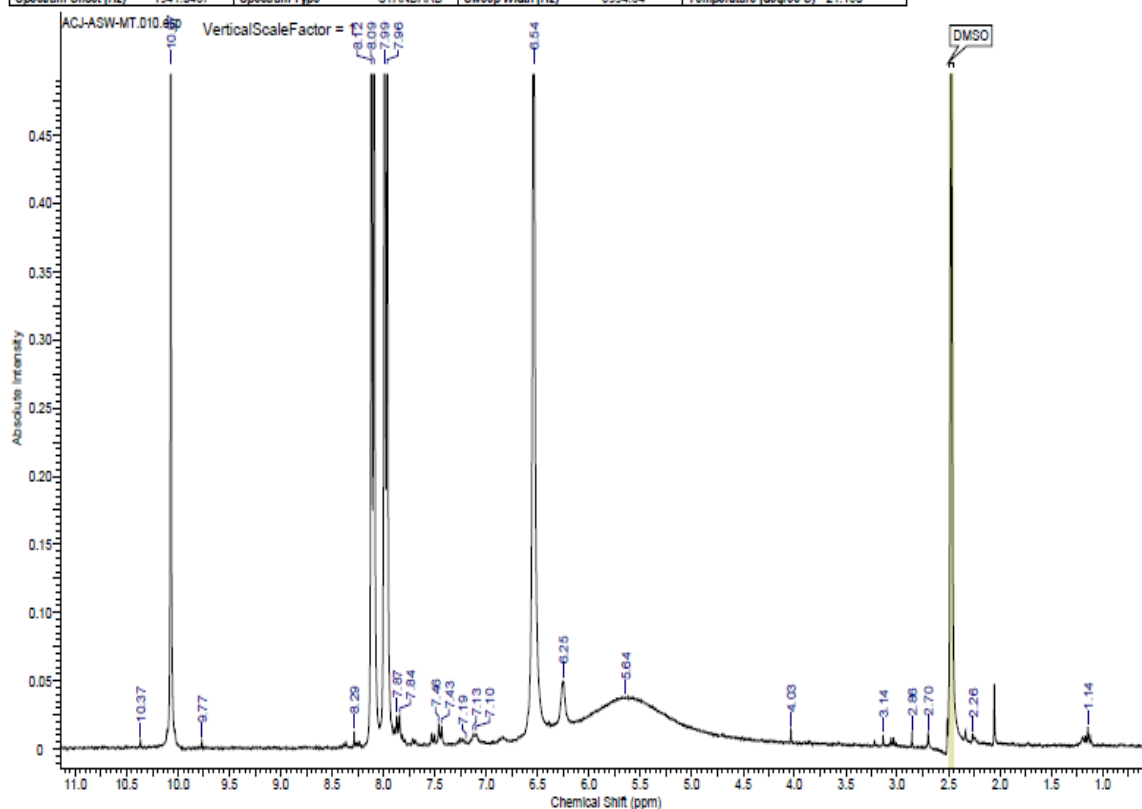
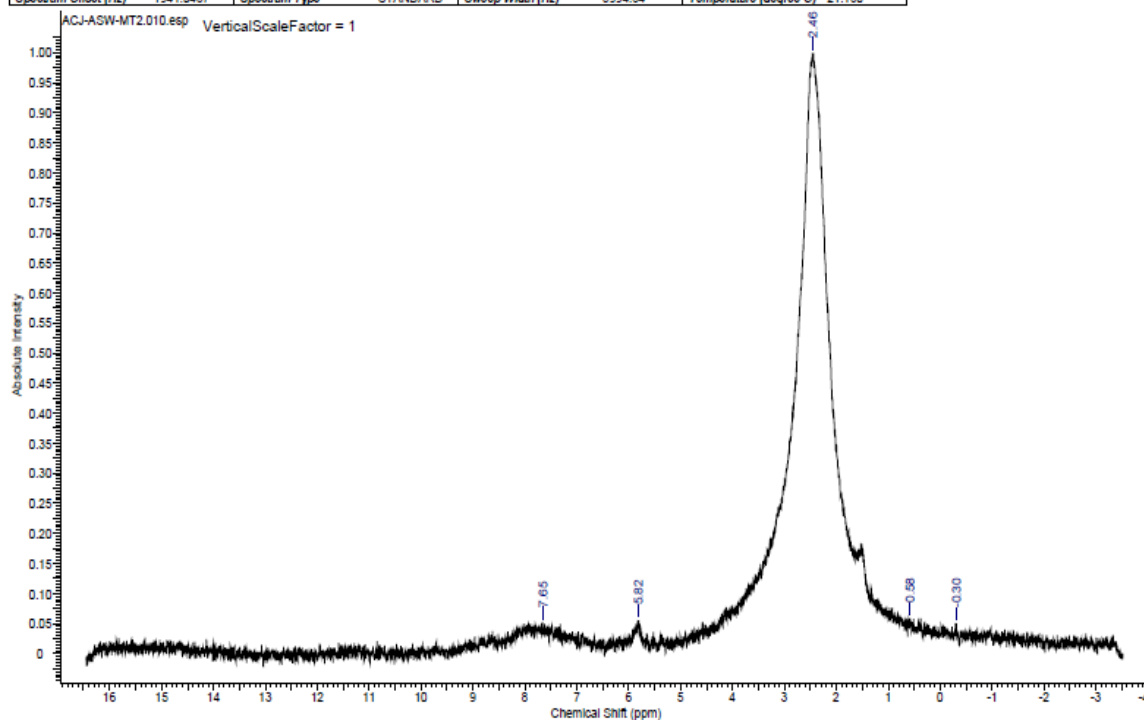


Figure S9: <sup>1</sup>H NMR Spectrum of MT

Acquisition Time (sec)	2.7329	Comment	z. PROTON DMSO u quest 41		Date	12 Apr 2015 16:10:56	
Date Stamp	12 Apr 2015 16:10:56	File Name	C:\Users\Admin\Desktop\Nigeria\ACJ-ASW-MT2\10\fid		Frequency (MHz)	300.13	
Nucleus	<sup>1</sup> H	Number of Transients	16	Origin	spect	Original Points Count	16384
Points Count	16384	Pulse Sequence	zg30	Receiver Gain	9195.20	SW (cycles) (Hz)	5995.20
Spectrum Offset (Hz)	1941.0437	Spectrum Type	STANDARD	Sweep Width (Hz)	5994.84	Temperature (degree C)	21.160

**Figure S10: <sup>1</sup>H NMR Spectrum of Dy(III)MT**

Acquisition Time (sec)	1.3763	Comment	z C13 CPD DMSO u quest 29		Date	29 Mar 2015 06:56:16	
Date Stamp	29 Mar 2015 06:56:16	File Name	C:\Users\Admin\Desktop\Nigeral\ACJ-ASW-MT\111\td		Frequency (MHz)	75.47	
Nucleus	13C	Number of Transients	640		Origin	spect	Original Points Count
Points Count	32768	Pulse Sequence	zgpg30		Receiver Gain	1625.50	Owner
Spectrum Offset (Hz)	9400.1836	Spectrum Type	STANDARD		SW (cycles) (Hz)	23809.52	Solvent
		Sweep Width (Hz)	23808.80		Temperature (degree C)	21.160	

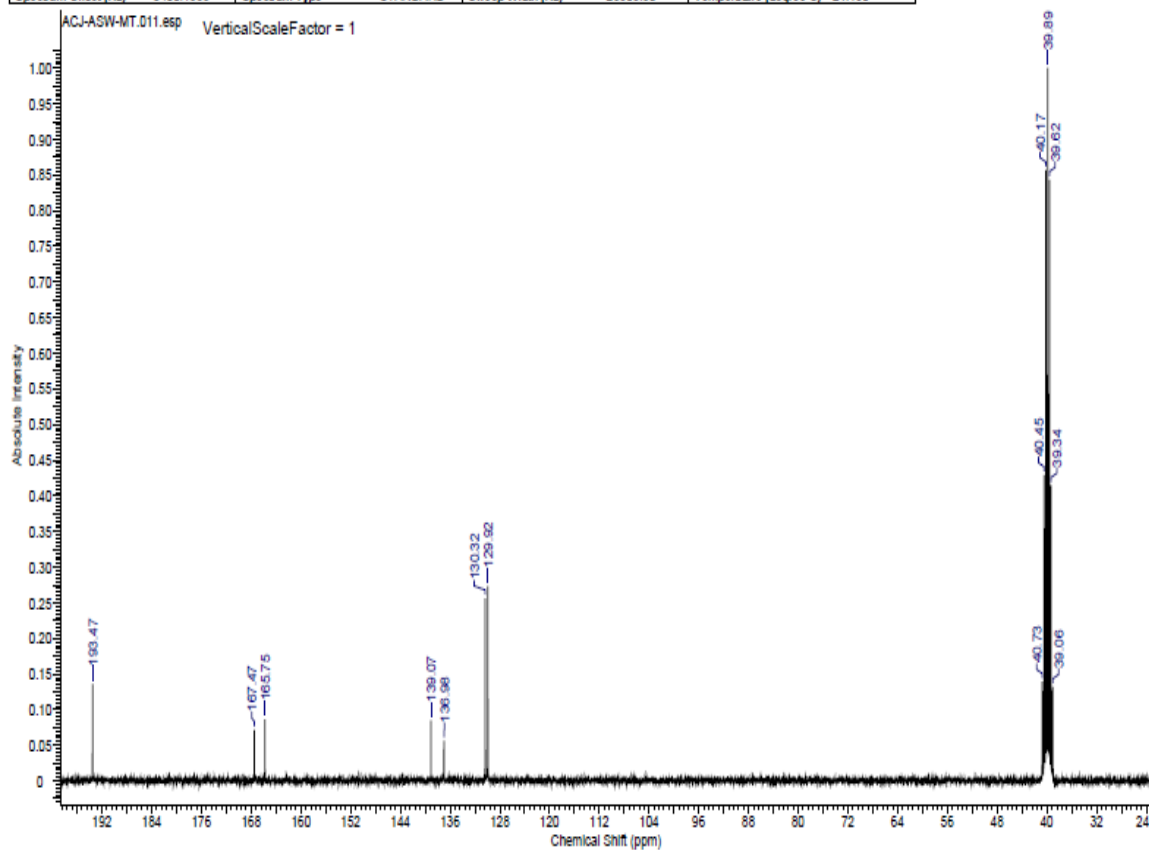
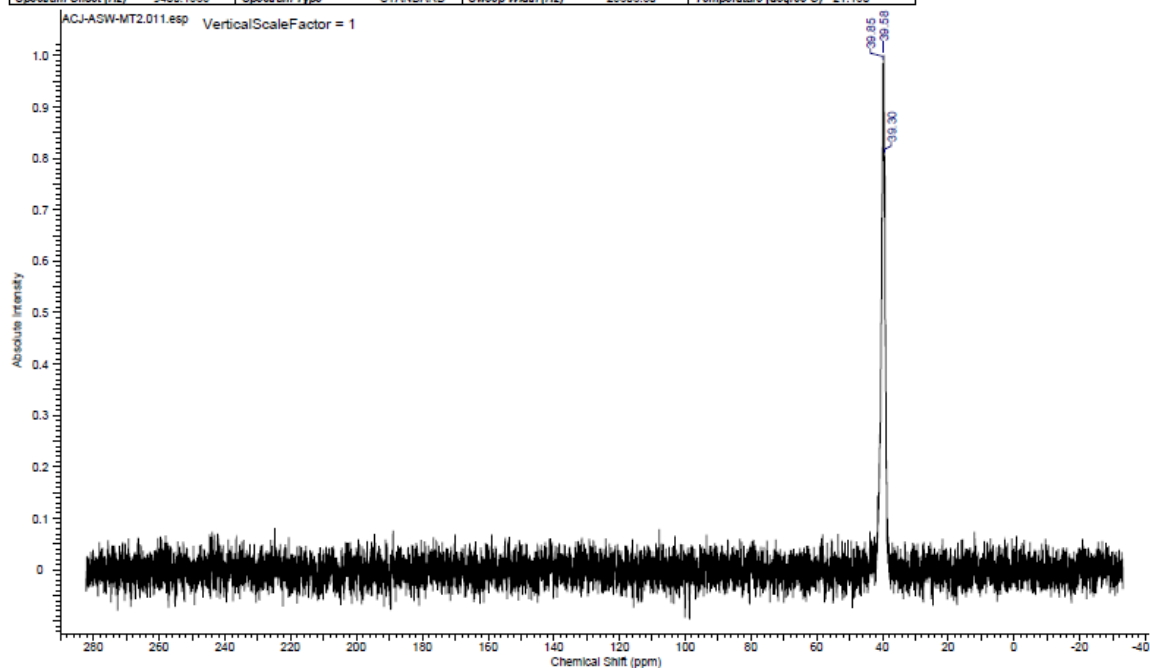
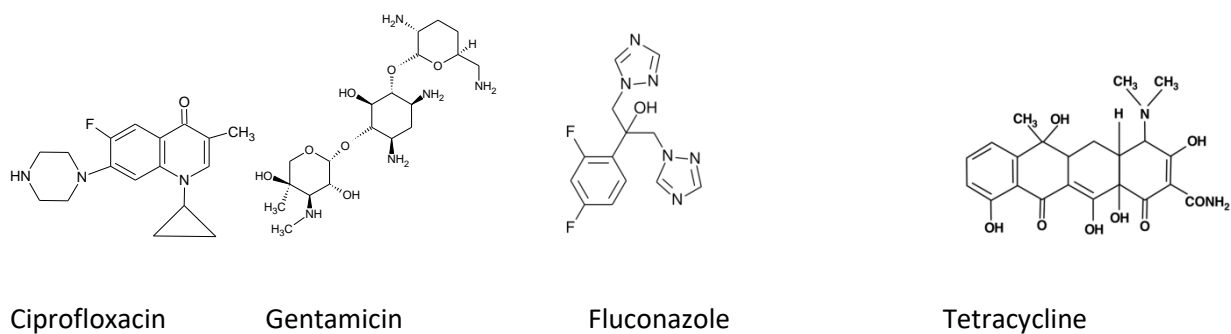


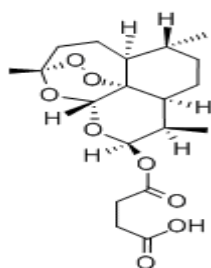
Figure S11:  $^{13}\text{C}$  NMR Spectrum of MT

Acquisition Time (sec)	1.3753	Comment	z C13 CPD DMSO u quest.41		Date	12 Apr 2015 16:13:04	
Date Stamp	12 Apr 2015 16:13:04	File Name	C:\Users\Admin\Desktop\Nigeral\ACJ-ASW-MT2\111fd		Frequency (MHz)	75.47	
Nucleus	13C	Number of Transients	19	Origin	spec1	Original Points Count	32768
Points Count	32768	Pulse Sequence	zgpg30	Receiver Gain	11585.20	SW (cycles) (Hz)	23809.52
Spectrum Offset (Hz)	9400.1836	Spectrum Type	STANDARD	Sweep Width (Hz)	23808.80	Temperature (degree C)	21.160
		Solvent	DMSO-d6				

**Figure S12:  $^{13}\text{C}$  NMR Spectrum of Dy(III)MT**



**Figure S13: Structures of the drugs used as standard.**



**Figure S14: Structure of Artesunate.**

**Table S1: Inhibition Zone Diameter (IZD in mm) of the Controls**

Conc. ( $\mu\text{g/mL}$ )	Code	<i>B.c</i> (ATCC 14579)	<i>S.a</i> (ATCC 6538P)	<i>P.a</i> (ATCC 9027)	<i>E.c</i> (ATCC 6749)	<i>C.a</i>	<i>A.n</i>
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<b>12.5</b>	T1	11	13	20	14	15	20
<b>6.25</b>	T2	7	9	16	8	9	15
<b>3.125</b>	T3	3	5	11	3	4	14
<b>12.5</b>	F1	6	8	5	8	20	21
<b>6.25</b>	F2	3	5	3	5	15	17
<b>3.125</b>	F3	-	-	-	2	12	10
<b>12.5</b>	CP1	17	20	16	18	15	11
<b>6.25</b>	CP2	11	14	12	14	11	5
<b>3.125</b>	CP3	5	8	3	9	4	-
<b>12.5</b>	G1	19	12	20	14	16	21
<b>6.25</b>	G2	12	5	11	11	13	14
<b>3.125</b>	G3	5	2	8	2	9	10
<b>12.5</b>	DMSO	0	0	0	0	0	0
<b>6.25</b>	DMSO	0	0	0	0	0	0
<b>3.125</b>	DMSO	0	0	0	0	0	0

Legend: T = Tetracycline, F = Fluconazole, CP = Ciprofloxacin, G = Gentamycin.

**Table S2: Determination of Acute Toxicity (LD<sub>50</sub>)**

Samples	Animal mark	Wt(g) of mouse	Wt of sample (mg)	Vol of solvent (mL)	Conc. (mg/mL)	Time of death	Dose (mg/kg)
MT	Head	21.89	21.89	0.22	100	-	1000
	Tail	27.25	43.60	0.44	100	-	1600
	Trunk	26.38	76.50	0.38	200	-	2900
	R.Hind	25.53	127.65	0.64	200	-	5000
<b>Distilled water</b>	HEAD	21.02			100		5ml/kg

**Table S3: Anti-plasmodic Effect of Samples on Albino mice**

Sample/ Grp	% parasitemia	Wt1	Wt2	PCV (%)1	PCV (%)2	Hb (g/dl)1	Hb (g/dl)2	Dose (mg/kg)
<b>MT</b>								
<b>A1</b>	12	29.49	32.18	53	49	16.5	15.5	25
<b>A2</b>	11	29.58	29.84	60	53	17.4	16.4	„
<b>A3</b>	09	21.55	21.09	65	63	17.7	17.4	„
<b>A4</b>	02	27.44	27.36	62	54	17.5	16.7	50
<b>A5</b>	07	24.01	25.22	67	62	17.8	17.4	„
<b>A6</b>	06	20.55	25.16	64	58	17.6	16.7	„
<b>-ve control(distilled water)</b>								
<b>B1</b>	29	29.05	27.01	63	59	17.20	16.50	5ml/kg
<b>B2</b>	38	25.07	20.33	67	43	17.50	14.00	„
<b>B3</b>	27	25.81	25.27	64	51	17.40	15.10	„
<b>+ve control(Artesunate)</b>								
<b>C4</b>	03	23.28	20.52	50	42	15.60	13.80	5mg/kg
<b>C5</b>	05	20.34	19.90	59	53	16.60	16.30	„
<b>C6</b>	04	23.21	20.75	42	38	13.70	13.20	„

