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Phenyl Alanine Mandelates

Antioxidant Activity of Phenyl

Highlights

Traditional African Medicine

Triazine- based Chalcone Hybrids

Discovering Thoughts, Inventing Future

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Antioxidant Activity of Phenyl Alanine Mandelates by Chemical and Electrochemical Methods

By Usha S & Charles Kanakam Christopher

Sri Sairam Engineering College, India

Abstract- Food decomposition in human body due to the redox reactions results in the formation of reactive oxygen species (ROS). ROS obtained during metabolic activitities in our body are responsible for cancerous diseases. ROS are scavenged by hydroxyl radicals present in the small organic molecules. Novel small organic molecules like mandelic acid - amino acid complexes, possess the weak hydrogen bonds and vanderwaals forces of attractions in the complex formation results in the antioxidant property. The title compounds, Rphenyl alanine-S-mandelate (RPASMA), Bis-L-phenyl alanine mandelate (BLPAMA) and L-phenyl alanine bis mandelate (BMALPA) are synthesised, carried out characterisation studies like FTIR, NMR, TG-DTA, mass, UV and melting point and grown single crystal by slow evaporation technique confirmed the structure by single crystal XRD. The electrochemical behaviour of the phenyl alanine mandelates show the existence of redox activity using cyclic voltammetry and is confirmed by comparing with the chemical behaviour using DPPH (1,1-diphenyl-2-picrylhydrazyl) radical scavenging method.

Keywords: ROS, phenyl alanine mandelates, EC50, IC50, DPPH, ARP.

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Antioxidant Activity of Phenyl Alanine Mandelates by Chemical and Electrochemical Methods

Usha S ^a & Charles Kanakam Christopher ^o

Abstract- Food decomposition in human body due to the redox reactions results in the formation of reactive oxygen species (ROS). ROS obtained during metabolic activitities in our body are responsible for cancerous diseases. ROS are scavenged by hydroxyl radicals present in the small organic molecules. Novel small organic molecules like mandelic acid amino acid complexes, possess the weak hydrogen bonds and vanderwaals forces of attractions in the complex formation results in the antioxidant property. The title compounds, Rphenyl alanine-S-mandelate (RPASMA), Bis-L-phenyl alanine mandelate (BLPAMA) and L-phenyl alanine bis mandelate (BMALPA) are synthesised, carried out characterisation studies like FTIR, NMR, TG-DTA, mass, UV and melting point and grown single crystal by slow evaporation technique confirmed the structure by single crystal XRD. The electrochemical behaviour of the phenyl alanine mandelates show the existence of redox activity using cyclic voltammetry and is confirmed by comparing with the chemical behaviour using DPPH (1,1-diphenyl-2-picrylhydrazyl) radical scavenging method. The title compounds are found to have efficient concentration (EC_{50}) or inhibitory concentration (IC_{50}) and antiradical power(ARP) from DPPH scavenging activity in this study and are compared with the redox property of the title compounds using cyclic voltammetry. This comparative study show the potential and feasibility of the title compounds in the application as antioxidant material to fight against oxidative stress diseases.

Keywords: ROS, phenyl alanine mandelates, EC_{50} , IC_{50} , DPPH, ARP.

I. INTRODUCTION

andelic acid (2-hydroxy-2-phenyl acetic acid) Phenyl alanine (2-amino-3-phenyl and propanoic acid) exist in racemic forms. The complexes of mandelic acid and phenyl alanine are having hydroxyl group, acid group and amino group which gives the salt formation due to the protonation of amino group through the formation of covalent bond and weak vanderwaals forces of attraction between acidic hydrogen, basic amino group and hydroxyl groups[1]. The zwitterionic structure of amino acid enhances the formation of salt complex with carboxylic acids. Donor and acceptor concept of hydrogen in the salt helps in the redox activity and the radical scavenging activity of the title compounds[2]. The present study indicates the usefulness of the title

Author α: Department of Chemistry, Sri Sairam Engineering College, Chennai-600044, India. e-mail: usha.che@sairam.edu.in compounds having hydroxy substitution and conjugation act as antioxidant material to scavenge the free radicals formed during the metabolic activities in the human body. It is further supported by the electrochemical behaviour of the compounds due to the structure property activity of the title compounds[3-4]. The reactive oxygen species formed during metabolic activities are nullified by the exogenous antioxidant having high antiradical power. The increase in electron donating groups in the title compounds modulate antioxidant capacity and they can be used to fight against oxidative stress diseases like cancer, cardiovascular disorders, neurodegenerative pathologies[5].

II. Experiment

AlfaAaser mandelic acid and Nice chemicals Lphenyl alanine were mixed in water in 1:2 and 2:1 ratios respectively. Obtained almost clear solution after agitation at room temperature for 2-3 hours, filtered and kept for slow evaporation at room temperature. Observed the crystals formation after 8 days harvested crystals after 28 days showed homogenous on TLC and confirmed the melting point as 184° C, 173° C respectively.

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$C_6H_5CH(OH)COOH + 2 C_6H_5CH_2CH(NH_2)COOH + H_2O$

DL- Mandelic acid L-phenyl alanine

↓ $C_6H_5CH(OH)COOH.(C_6H_5CH_2CH(NH_2)COOH)_2H_2O$ Bis-L-phenylalaninemandelate (BLPAMA) $C_6H_5CH(OH)COOH.(C_6H_5CH_2CH(NH_2)COOH)_2H_2O + CH3OH$ Bis-L-phenyl alanine mandelate (Becomic mitture of BL DAMA)

(Racemic mixture of BLPAMA)

$\label{eq:c_6H_5CH(OH)COOH.C_6H_5CH_2CH(NH_2)COOH} \\ R\mbox{-phenyl alanine -S-mandelate (RPASMA)} \\ 2\ C_6H_5CH(OH)COOH + C_6H_5CH_2CH(NH_2)COOH + H_2O \\ DL\mbox{- Mandelic acid } L\mbox{-phenyl alanine} \\ \end{array}$

2 C₆H₅CH(OH)COOH.C₆H₅CH₂CH(NH₂)COOH.H₂O BMALPA - L-phenyl alanine bismandelate

The recrystallisation of 1:2 mandelic acid [6] and L-phenyl alanine resulted in the diastereomeric isolation of R-phenyl alanine-S-mandelate [7] which showed homogenous on TLC and has melting point 174° C. Characterisation studies , mass analysis, single crystal XRD studies confirmed the structure of the title compounds and the possession of second order non linear susceptibilities due to non centerosymmetric structure.

DPPH - free radical and reduced form

The molecule of 1,1-diphenyl-2-picryl-hydrazyl

When a solution of DPPH is mixed with that of a

(DPPH) is characterised as a stable free radical by virtue of the delocalisation of the spare electron over the

molecule as a whole, so that the molecules do not

dimerise, as would be the case with most other free

radicals. The delocalisation also gives rise to the deep

violet colour, characterised by an absorption in methanol

substance that can donate a hydrogen atom, then this

gives rise to the reduced form with the loss of this violet

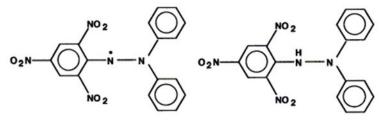
colour (although there would be expected to be a

residual pale yellow colour from the picryl group still

present). Representing the DPPH radical by Z

The increase in the presence of hydroxyl groups and conjugation in the molecular structure favours the oxidation and reduction activity. It is confirmed by the electrochemical behaviour using cyclic voltammetry and the radical scavenging activity using DPPH for the title compounds.

Basis of DPPH scavenging method



and

DPPH - free radical form

DPPH - reduced form

The free radical form reacts with the substance AH

$$Z^{\bullet} + AH = ZH + A^{\bullet}$$
[1]

where ZH is the reduced form and A^{\bullet} is free radical produced in this first step. This latter radical will then undergo further reactions which control the overall stoichiometry, that is, the number of molecules of DPPH reduced (decolorised) by one molecule of the reductant. The reaction [1] is therefore intended to provide the link with the reactions taking place in an oxidising system, such as the autoxidation of an unsaturated substance; the DPPH molecule Z^{\bullet} is thus intended to represent the free radicals formed in the system whose activity is to be suppressed by the substance AH.

% of Inhibition = (A of control – A of Test)/A of control * 100

a)

the donor molecule by AH.

solution at 517 nm [8].

b) Electrochemical study

Non-aqueous media cyclic voltammetry (CV) study using Pt electrodes show the possibility of

electrooxidation, acceptor - donor interactions of the title compounds and the starting materials[9-11].

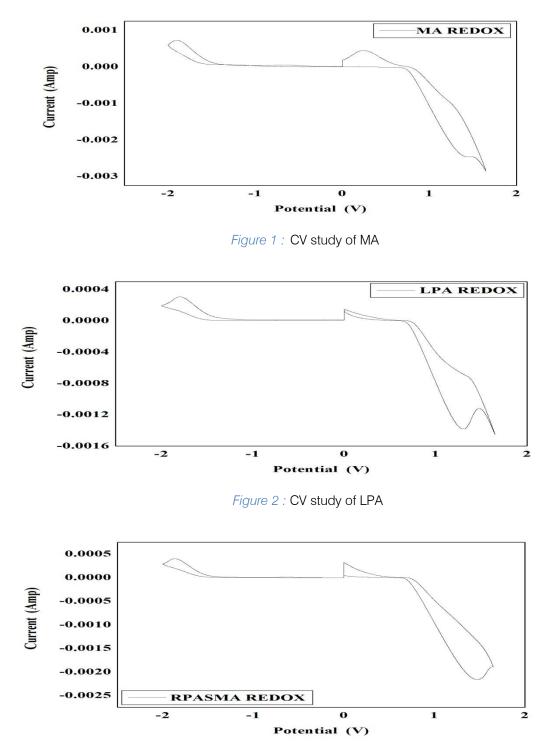
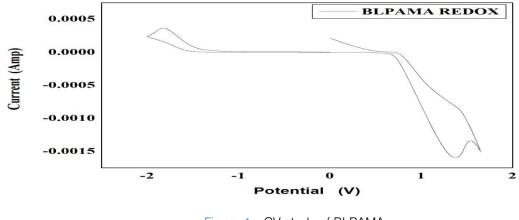
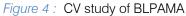
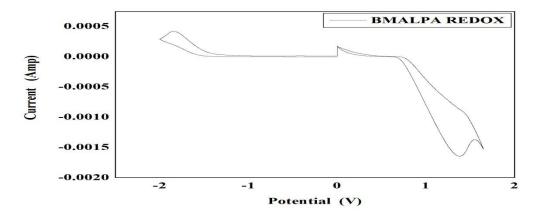


Figure 3 : CV study of RPASMA









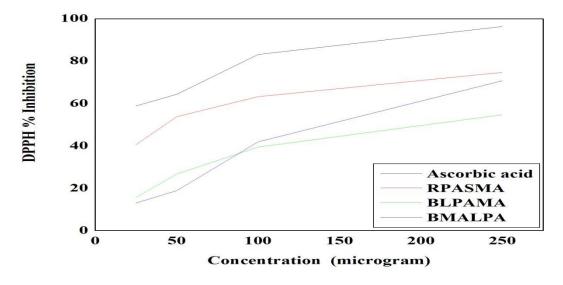


Figure 6 : Comparative study of % DPPH scavenging activity

Conc	% inhibition												
micro gram	ASCORBIC ACID	RPASMA	BLPAMA	BMALPA									
25	58.88	40.55	15.69	13.08									
50	64.42	53.83	26.74	18.92									
100	83.09	63.28	39.49	41.94									
250	96.44	74.77	54.72	70.78									

Table 1 : Comparison of DPPH scavenging activity

Table 2 : Efficient concentration and anti radical power

SAMPLE	IC 50	ARP
BLPAMA	206.4	0.00485
BMALPA	140.47	0.00712
RPASMA	151.15	0.00662

III. Results and Discussion

The DPPH annihilation activity of free radicals is calculated as % inhibition[12-14]. The control Ascorbic acid show the maximum % inhibition compared to the title compounds as shown in Table 1. The maximum antioxidant power is shown by more hydroxyl group containing BMALPA Figure-5. The increase in hydroxyl group substitution in the title compounds, the presence of increase in conjugation increases the % inhibition is indicated in the Figure-6. EC_{50} or IC_{50} is more for BMALPA compared to RPASMA and BLPAMA. The comparative respective efficient concentration and antiradical power shown by the title compounds is given in the Table 2. The presence of electron donating amino group, hydroxyl group and acidic hydrogen in the title compounds show low oxidation potential due to electrooxidation which corresponds to high antioxidant power[15-17].

The electrochemical behaviour of the title compounds and the starting materials are compared using the cyclic voltammetry measurements. Donor acceptor interactions leads to hydrogen bond formation [18,19]. The electrochemical oxidation of the title compounds show higher area under anodic wave form which corresponds to higher antioxidant capacity. The presence of electron donating groups have lower half wave potential, higher antioxidant activity and higher reducing power. In the title compounds the presence of more hydroxyl groups, electron donating groups in BMALPA shows higher antioxidant activity. Radical scavenging activity, antiradical power, structure property activity leads to the high antioxidant activity of the title compounds and can be used as fighting agents to nullify the ROS generated during meabolic activities[20].

IV. CONCLUSION

Novel organic salt complexes can act as exogenic antioxidants is confirmed from the comparative study of title compounds using radical scavenging DPPH method and electrochemical cyclic voltammetric method. The comparable results from the both methods give optimistic thought to over come the prevailing health issues caused by the present life style of the modern world. The use of starting materials to synthesise the title compounds find many medical applications, constituent to protect the central nervous system the harmless effects are expected for the title compounds in the in-vivo studies.

V. Ackowledgement

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Trade in Non-Mammalian Wild Animals for Traditional African Medicine in Ogun State, Nigeria

By Durojaye A Soewu, Gabriel A Dedeke, Victor A Ojo & Opeyemi K Soewu

Osun State University, Nigeria

Abstract- A steady rise in the patronage for Traditional African Medicine (TAM) has necessitated a corresponding increase in the demand for the ingredients used in the preparation of the tradomedicines. These ingredients are the various wild animals and plants parts. The attendant rise in this demand for ingredients calls for a need to document the extent of utilisation of these natural resources involved as a measure of the impact of such trade on biodiversity conservation. This paper examined diversity of molluscan, reptilian and avian species traded for use in TAM; the quantity of each species traded for utilisation over a period of time, and seasonal fluctuations in abundance and utilisation of these species as an index of utilisation pressure on populations in the wild. A multi-stage stratified random sampling technique was employed. An open-ended questionnaire was administered on vendors in selected market stalls for six consecutive markets days in each of dry and rainy seasons. The study identified twenty-three species, 8 were listed in CITES and Nigerian Decree 11(1985). A total of 3196 (molluscan), 2527 (reptilian), 2894 (avian) carcasses were traded over an average period of twenty days.

Keywords: traditional medicine; wildlife utilisation; wildlife trade; ethnozoology.

GJMR-B Classification : NLMC Code: WA 360

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Trade in Non-Mammalian Wild Animals for Traditional African Medicine in Ogun State, Nigeria

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Abstract- A steady rise in the patronage for Traditional African Medicine (TAM) has necessitated a corresponding increase in the demand for the ingredients used in the preparation of the trado-medicines. These ingredients are the various wild animals and plants parts. The attendant rise in this demand for ingredients calls for a need to document the extent of utilisation of these natural resources involved as a measure of the impact of such trade on biodiversity conservation. This paper examined diversity of molluscan, reptilian and avian species traded for use in TAM; the quantity of each species traded for utilisation over a period of time, and seasonal fluctuations in abundance and utilisation of these species as an index of utilisation pressure on populations in the wild. A multi-stage stratified random sampling technique was employed. An open-ended questionnaire was administered on vendors in selected market stalls for six consecutive markets days in each of dry and rainy seasons. The study identified twenty-three species, 8 were listed in CITES and Nigerian Decree 11(1985). A total of 3196 (molluscan), 2527 (reptilian), 2894 (avian) carcasses were traded over an average period of twenty days. The mean number of carcasses traded per dealer per month in the two seasons were: Molluscs (24.0 \pm 1.6); Reptiles (19.0 \pm 1.9) and Aves (21.7 \pm 2.3). Trade in, and utilisation of wild animal species in TAM involved species under various degree of conservation threats. There seems to be no regulation of trade in wild animal species, including those purportedly protected by Decree 11 (1985). A twin approach of increase in yield and decrease in demand is required to stem the negative impact of trade and utilisation on biodiversity. Massive education and enlightenment of the citizenry, capacity building and involvement of indigenous communities in conservation projects are also urgently reauired.

Keywords: traditional medicine; wildlife utilisation; wildlife trade; ethnozoology.

I. INTRODUCTION

Wildlife is vital to the lives of a high proportion of the world's population, often the poorest. Some rural households depend on local wild animals for their meat protein and on local trees for fuel, and both wild animals and plants provide components of traditional medicines used by the majority of people in the world, Anon, (2016). Many people in the developing world depend entirely on the continued availability of local wildlife resources, Soewu (2013). Each year, hundreds of millions of plants and animals are caught or harvested from the wild and then sold as food, pets, ornamental plants, leather, tourist curios, and medicine. Though a great deal of this trade is legal and is nonharmful to wild populations, a large proportion is illegal and threatens the survival of many endangered species (Anon 2016). Trade in wildlife is usually for cash, though could sometimes be in exchange for other useful objects - for example, utensils in exchange for wild animal skins. Driving the trade is the end-consumer who has a need or desire for wildlife products, whether for food, construction or clothing.

An enormous number of meat is being taken from some of the most bio-diverse forests in the world and this indicates the scale of seriousness of an ecological problem that will escalate if commercial trade goes unchecked (Bowen-Jones and Pendry, 1999; Caldecott, 1994; Fa et al 1995). The number of animals taken by subsistence hunters can be very large. For instance in 1980, the number of mammals killed in the Brazillian Amazon alone (2,847,007 people in an area of 3,581,180km²) resulted in the harvesting of 14,030,050 individuals. If birds and reptiles are added to this figure the number of game killed per year could reach more than 19 million individuals (Redford, 1993). Ott et al (2002) reported that several regions in Asia have already experienced massive defaunation as a result of the bush meat crisis. Wilkie et al (1998) stated that it is not habitat loss but defaunation that poses the greatest immediate threat to animal conservation in forests of West and Central Africa.

Wildlife trade involves hundreds of millions of wild plants and animals from tens of thousands of species. To provide a glimpse of the scale of wildlife trafficking, there are records of over 100 million tonnes of fish, 1.5 million live birds and 440,000 tonnes of medicinal plants in trade in just one year Anon (2016).

Traditional medicine has over the years provided livelihood for a wide variety of people most of whom, due to their economic and social background, depend mainly on harvesting, processing and trading in wildlife and the products as their only means of making

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a living (Costa-Neto, 1999; Li and Wang, 1999; Soewu et al 2012). It is expected that trade in wildlife as ingredients for traditional medicine will continue to flourish as there will always be human ailments in need of attention (Soewu 2008). The direct consequence of this would be a continued depletion of these resources in the wild as Marshall (1998) had documented that majority of wildlife traded for use in traditional medicinal preparations are collected from the wild. Though most wildlife trade is legal, and as such by no means always a problem, it has the potential to be very damaging as it can cause overexploitation to the point where the survival of a species hangs in the balance. An average of 40% decline in populations of species on earth was recorded between 1970 and 2000. Overexploitation of wildlife primarily for trade has been identified as the second-biggest direct threat to species survival, after habitat destruction (Anon, 2016).

In particular, most problems associated with wildlife trade, stems from a demand for rare, sometimes highly endangered and legally protected species, more likely to have been obtained in an environmentally damaging way and which need to be smuggled or traded under clandestine conditions. There are several reports of open trade in species listed as protected in many countries across the world (Sodeinde and Soewu 1999, Kakati and Duolo, 2002; Soewu *et al* 2012).

Bowen-Jones (1998) recorded that even the animals that could be hunted sustainably are often being exploited at probably unsustainable levels, and that controls need to be introduced in order to make sure that they are not added to the vulnerable category. Chardonnet *et al* (2002) has established that excessive harvest of wildlife depletes the wildlife resource when the level of exploitation overtakes the recruitment rate. However, as long as there is sufficient money to be made from the trade in wild animals, not only will the individual species suffer but also conservation at regional or even world level may be threatened, Simmonds (1998).

II. Methods

a) Study Area

Ogun State is entirely in the tropics. Located in the Southwest Zone of Nigeria with a total land area of 16,409.26 square kilometres, it is bounded on the West by the Benin Republic, on the South by Lagos State and the Atlantic Ocean, on the East by Ondo State, and on the North by Oyo and Osun States. It is situated between Latitude 6.2°N and 7.8°N and Longitude 3.0°E and 5.0°E. It has an estimated population of 3,486,683 people for the year 2005 (8, 18) (Fig. 1)

b) Preliminary Survey

A preliminary pilot survey of the state was carried out between December 2001 and February 2002 to determine:

- (i) which two markets in each zone are the leading markets for traditional medicinal ingredients;
- the number of stall/traders in identified markets that stocks and deals primarily in ingredients for traditional medicine.

This provides the basis to determine the number of traders / stalls to be involved in the main survey as a proportion of the whole number for the zone.

Also, during this survey, the questionnaire for the main survey was subjected to trial runs to be able to establish the time needed to interview a respondent and take inventory of the stock in the stall.



Fig. 1 : Map of Ogun State showing all the local governments

c) Data Collection

This main study extended over a period of two years from April 2003 – March 2005. The respondents for the study are the dealers in wildlife for traditional medicinal preparations.

A stratified random sampling technique was employed in the selection of respondents. All the markets surveyed are five-day markets and the visits were made to each stall in the evening period of the market days. The market day was chosen as this is often the period when fresh supplies of animals are delivered to stalls and wares are fully displayed. This makes room for ease of inventory-taking and monitoring the dynamic movement of the stock. Each market and the stalls therein were given two sets of survey, one in each season of the year. In each market, the selection of stalls to be surveyed was done by the use of table of random numbers. The stalls were visited for six consecutive market days for a set of survey.

A total of one hundred dealers were interviewed, and the dynamic stock movement of their stalls taken using open-ended questionnaire to avoid yes / no answers while encouraging maximum discussion i.e. twenty-five dealers in each zone. In each zone the dealers were selected from the two markets chosen for the survey. The number of dealers/stalls surveyed in each market was determined as the proportion contributed by the number of stalls in that market to the total number of stalls in the two markets for the zone. On each visit to the stalls a detailed inventory of wild animal species found was taken. The stock movement for each species was determined.

d) Identification of Species

All species encountered during survey were recorded with their local names in the market. To match the local names with the common English and Scientific names, due consultations and references were made to scientific publication that had previously established the names. Also the VCS i.e. Village Contact Survey method was used to identify some species. This involves showing published identification manuals and encyclopaedia with pictures and distinguishing features of animals to the dealers and some hunters for them to identify the animals with the local names. When the local name is established it is thereafter matched with the common English and the scientific names.

e) Carcass Quantification

To determine the number of carcass of each species that passed through the stall for the period, the number of that species sold out between consecutive market days were taken and summed up.

The whole animal seen at each stall on the first visit were counted and recorded separately for each species and this was taken as the initial opening stock. During subsequent visits to the stall, the remnant numbers of each species were counted and recorded. Also the number supplied to the stall after the last count was noted for the species. This allows for observation of the dynamic stock movement and the determination of the actual number sold out during the period.

Number sold out = Opening balance + Added stock - Closing balance

For some species occurring in parts, the head count approach was employed to avoid repeated counts. In this method, every head of an animal species encountered are counted as whole animals while other parts are overlooked to avoid repetition.

The main attributes of market dynamics measured during this survey are:

1. Quantity utilised by traditional medical practices as revealed by sales figures i.e. carcass number.

- 2. Frequency of occurrences and availability of each species
- 3. The average sales figure per stall / dealers for the species.

f) Seasonality and Availability

To examine any seasonality in the availability of animals on the stalls, a Latin square design was employed in deciding randomly the time of visit to each zone. The two major seasons were subdivided for convenience of study into early and late dry, early and late rain periods. The study was also designed such that markets in each zone are surveyed twice, each survey coming up at a season different from the other. The availability of identified species for each zone was compared for the two main seasons.

g) Conservation Status of Species

To evaluate the current trade status of the species encountered during the survey, due consultations / references were made to the CITES appendices for the listing on global level. Also the Endangered Species (Control of International Trade and Traffic) Decree No 11 of 1985 was consulted to determine the present conservation status of the species in the Nigerian context.

III. Results

a) Socio-Economic Characteristics of Respondents

The female folk dominated the trade in tradomedicinal ingredients, having constituted over 90 percent of the dealers in all the zones of the state. Majority of the dealers (64 percent) were aged between 40 and 60 years as at the time of the survey. While most of the dealers (53 percent) had post primary education, 12 percent of the dealers had no formal education. Concerning to religious affiliation, the study shows that the majority (over 55 percent) of the dealers claimed affiliation to Islamic religion. Also, the study showed that the majority (over 80 percent) of the dealers had no other means of livelihood besides the trade, and were also unaware of legislative provisions protecting wildlife species in Nigeria.

Table 1 : Number of molluscan, reptilian and avian species traded over a period (20 days / season) in Ogun state, Nigeria

		Zone	ljeb	u – (Ode	S	agai	mu		llarc)	Ak	beok	uta	All	locati	ons
		Season	Dry I	Rain	Both	nDry	Rair	Both	۱Dry	Rain	Both	nDry	Rain	Both	Dry	Rain	Both
English Name	Scientific Name	Local Name															
Molluscs																	
African giant snail	Archachatina marginata	a Igbin	411	479	890	351	352	703	395	424	819	432	352	784	1589	1607	3196
Reptilian species																	
Cobra	Naja spp	Agbagi	39	32	71	27	21	48	29	21	50	24	20	44	119	94	213
Tortoise	Kinixys spp	Ajapa	167	108	275	134	91	225	132	111	243	174	136	310	607	446	1053
Nile monitor	Varanus niloticus	Awonriwon	17	15	32	12	11	23	10	8	18	21	14	35	60	48	108
		Zone	ljeb	u – (Ode	S	agai	mu		llarc)	Ak	beok	uta	All	locati	ons
		Season	Dry I	Rain	Both	nDry	Rair	Both	۱Dry	Rain	Both	nDry	Rain	Both	Dry	Rain	Both

English Name	Scien	tific Name	Loca	l Name																
African python Senegal	Pyth	non sebae	Ere		22	13	35	19	12	31	24	17	4	1 2	3 -	17	40	88	59	147
chameleon	Cha	amaeleo senegalensis	Og	а	65	51	116	54	47	101	56	44	10	07	16	60	131	246	202	448
Nile crocodile	Cro	codylus niloticus	On		9	10	19	9	8	17	6	7	13	3 1	4 -	13	27	38	38	76
Gabon viper	Bitis	s gabonica	Par	amole	32	27	59	26	20	46	28	21	49	3	6 3	30	66	122	98	220
Mamba	Den	ndroaspis spp	Seb	ре	45	14	59	36	34	70	37	34	71	1 3	2 3	30	62	150	112	262
					396	270	666	31	244	1 56	1 322	2 26	3 58	<i>15 3</i> 9	95 3	320	715	1430	1097	2527
Avian species																				
Red eye dove		Streptoprelia semitoro	guata	Adaba		33	21	54	30	28	58	28	25	53	36	30	66	127	104	231
Blue-eared	glossy																			
starling		Lamprotornis chalyba	US	Agbe		35	30	65	29	26	55	31	27	58	40	32	72	135	115	250
Pied crow		Corvus albus		Akalam	agbo	o 33	26	59	30	27	57	30	25	55	39	30	69	132	108	240
Little grebe		Tachybaptus ruficollis	;	Ako		27	19	46	20	16	36	23	18	41	31	26	57	101	79	180
Carmine bee- e Double-spurred		Merops nubicus		Aluko		32	26	58	30	23	53	30	28	58	41	31	72	133	108	241
francolin		Francolinus bicalcara	tus	Aparo		36	27	63	31	27	58	31	27	58	40	32	72	138	113	251
Black kite		Milvus migrans		Asa		28	17	45	26	20	46	22	20	42	30	25	55	106	82	188
Harrier hawk		Polyboroides radiatus		Awodi		24	15	39	19	13	32	20	14	34	29	25	54	92	67	159
African grey par	rot	Psittacus erithacus		Ayekoc	oto	30	22	52	25	19	44	24	20	44	34	26	60	113	87	200
Hooded vulture		Necrosyrtes monachu	IS	lgun		41	34	75	40	35	75	37	31	68	53	38	91	171	138	309
Cattle egret		Ardeola ibis		Lekeleł	ke	35	24	59	35	31	66	33	26	59	43	29	72	146	110	256
Indian peafowl		Pavo cristatus		Okin		10	7	17	8	5	13	5	2	7	14	7	21	37	21	58
Barn owl		Tyto alba		Owiwi		21	12	33	19	14	33	18	15	33	29	23	52	87	64	151
Spotted eagle of	w	Bubo africanus		Owiwi		27	20	47	22	14	36	24	16	40	32	25	57	105	75	180
V						412	300	712	2364	298	662	356.	294	650	491	1379	9870	1623	31271	2894

Source: Field Survey, 2005

Table 1 showed the number of carcasses sold across the state in both dry and rainy seasons for all class of animals during the survey period. In all, 3196 molluscs, 2527 reptilian and 2894 avian whole carcasses were sold into traditional African medicinal practices. Table 2 revealed species encountered during survey that were listed in appendices I and II (of CITES) as well as 1 and 2 of Nigerian Decree 11 of 1985. More than 30% of the species encountered during the survey were listed in the appendices. Table 3 gave the mean number of carcasses traded per dealer in a month in both seasons while table 4 showed the mean number of carcasses traded per dealer by zone in a month.

On the number of carcasses traded, Necrosyrtes monachus had the highest figure for avian

species (n=309, 10.6%) while *Kinixys spp* recorded the highest for the reptiles (n=1053, 41.7%). The general trend was that more carcasses for all the species were sold during the dry season, with the exception of *Archachatina marginata*, which appeared to be available and utilised more during the rainy season. According to the respondents, this trend was due to greater ease of hunting and higher volume of animals killed per expedition during the dry season. This in turn was attributed to factors including the animals moving farther away from their homes in search of food and water, clearer visibility in less dense vegetation and some other influences like the lunar cycle.

Table 2 : Species listed in appendix I and II of CITES and Decree 11	(1985) of Nigeria encountered during s	survev

Common name	Scientific name	CITES	Decree 11
Black kite	Milvus migrans		1
Vulture	Necrosyrtes monachus	II	2
Parrot	Psittacus erithacus		1
Owl	Tyto alba		
Chameleon	Chameleon senegalensis	II	
Crocodile	Crocodylus miloticus	1 / 11	1
Python	Python sebae		1
Monitor	Varanus miloticus		1

Source: Field Survey, 2005



Fig. 2 : (i) Vulture (whole, preserved). (ii) Chameleon (Live)

As per the zones, Abeokuta recorded highest sales figure, followed by Ijebu Ode for all taxa. Ilaro had higher sales figures than Sagamu for molluscs and (iii) African giant snails

reptiles whereas Sagamu had a higher figure for aves. Factors responsible for this trend could not be established.

 Table 3 : Mean number of carcasses (molluscs, reptiles and aves) traded per dealer per month in dry and rainy seasons

Wildlife species	Mean p	oer o	dealei	per	mor	nth by	seas	on			t-tes	t for equali	ty of mea	าร		
	Dry s	easo	on	Raiı	ny se	ason	Bo	oth s	eas	on	Ca	lculated t	Significa	int p	Comment	
Molluscs																
Archachatina marginata	23.8	±	2.3	24.1	±	2.3	3 24	.0	±	1.6		-0.08	0.93		NS	
Reptilian species																
Naja spp	1.8	±	0.3	1.4	±	0.2	2 1.	6	±	0.2		1.04	0.30		NS	
Kinixys spp	9.1	±	1.1	6.7	±	0.8	37.	9	±	0.7		1.75	0.09	1	S (p<0.10))
Varanus niloticus	0.9	±	0.2	0.7	±	0.2	2 0.	8	±	0.1		0.78	0.44		NS	
Python sebae	1.3	±	0.2	0.9	±	0.1	1.	1	±	0.1		1.75	0.09	1	S (p<0.10))
Chamaeleo senegalensis	3.7	±	0.4	3.0	±	0.4	н З.	4	±	0.3		1.17	0.25		NS	
Crocodylus niloticus	0.6	±	0.1	0.6	±	0.1	0.	6	±	0.1		0.00	1.00	1	NS	
Bitis gabonica	1.8	±	0.2	1.5	±	0.	2 1	.7	±	0.2		1.14	0.26	6	NS	
Dendroaspis spp	2.3	<u>+</u>	0.3	1.7	±	0.	32	.0	<u>+</u>	0.2		1.19	0.24	1	NS	
	21.5	±	2.9	16.5	±	2.	4 19	9.0	\pm	1.9						
Avian species																
Streptoprelia semitorquata	a 1.9	±		0.2	1.6	±	0.2		-	:	0.2	1.06		0.30	NS	
Lamptornis chalybaus	2.0	\pm		D.3	1.7	±	0.3	1.9) <u>+</u>	-	0.2	0.70		0.49	NS	
Corvus albus	2.0	±		0.3	1.6	±	0.2	1.8		-	0.2			0.26	NS	
Tachybaptus ruficollis	1.5	±		0.2	1.2	±	0.2	1.4	+ +	:	0.1	1.21		0.23	NS	
Merops nubicus	2.0	\pm		0.3	1.6	±	0.3	1.8	3 <u>+</u>	-	0.2	0.94		0.35	NS	
Francolinus bicalcaratus	2.1	±		0.3	1.7	±	0.2	1.9) <u>+</u>		0.2	1.04		0.30	NS	
Milvus migrans	1.6	±		0.2	1.2	±	0.2	1.4	+ +	:	0.1	1.23		0.23	NS	
Polyboroides radiatus	1.4	\pm		0.2	1.0	±	0.2	1.2	2 ±	-	0.1	1.54		0.13	NS	
Psittacus erithacus	1.7	±		0.3	1.3	±	0.2	1.5	5 <u>+</u>	:	0.2	1.18		0.25	NS	
Necrosyrtes monachus	2.6	\pm		0.3	2.1	±	0.4	2.3	3 ±	-	0.2	1.00		0.32	NS	
Ardeola ibis	2.2	<u> </u>		0.3	1.7	±	0.3	1.9) <u>+</u>		0.2	1.32		0.20	NS	
Pavo cristatus	0.6	±		0.1	0.3	±	0.1	0.4	+ <u>+</u>	:	0.1	1.73		0.09	S (p<0.10)	
Tyto alba	1.3	±		0.2	1.0	±	0.2	1.1	<u>+</u>	:	0.1	1.42		0.16	NS	
Bubo africanus	1.6	±		0.2	1.1	±	0.2	1.4	⊦ <u>+</u>		0.1	1.63		0.11	NS	
	24.3	+ ±		3.5	19.1	±	2.9	21.	7 +	-	2.3					

Source: Field Survey, 2005

Wildlife species	Mean	carca	ass I	Numb	ber pe	r dea	ler pe	er mor	nth k	y zon	е		F-te	st of di	iffere	ence	betwe	en meai	ns
	ljebu -	Ode		Sag	gamu		llaro		A	peokuta	a	All loc	ations	F	S	Signific	cant p	Comme	ent
Molluscs																			
Archachatina marginata	26.7	±	3	8.5 21	.1 ±	2.7	24.6	±	3.3	23.5 =	± 3	8.6 24	.0 ±	1.6	0.5	0	0.69	N	S
Reptilian species																			
Naja spp		±	C).5 1.		0.4	1.5	±	0.3	1.3 =	±α).3 1.	6 ±	0.2	1.0)1	0.40	N	S
Kinixys spp		<u>+</u>	1	.7 6.		1.2	7.3	±	1.3			.5 7.		0.7	0.6	51	0.61	N	S
Varanus niloticus		±	C	0.2 0.	7 ±	0.2	0.5	±	0.2	1.1 =	±α	0.3 0.		0.1	1.0)7	0.37	N	S
Python sebae		±	C	0.3 0.	9 ±	0.2	1.2	±	0.3	1.2 =	±α).2 1.	1 ±	0.1	0.2	28	0.84	N	S
Chamaeleo senegalensis	0.0	±	C).7 3.	0 ±	0.5	3.0	±	0.6	3.9 =	±α).5 3.	4 ±	0.3	0.5	8	0.63	N	S
Crocodylus niloticus		±	C	0.2 0.		0.2	0.4	±	0.2	0.8 -	±α	0.2 0.	6 ±	0.1	1.0)1	0.40	N	S
Bitis gabonica		±	C).3 1.		0.3	1.5	±	0.3	2.0 =).4 1.	-	0.2	0.7	'4	0.53	N	S
Dendroaspis spp	1.8	<u>+</u>	C).7 2.	1 ±	0.4	2.1	±	0.4	1.9 -	± ().4 2.	0 ±	0.2	0.1	3	0.94	N	S
	20.0	±	4	.6 16	.8 ±	3.3	17.6	±	3.5	21.5 -	± 3	8.8 19	.0 ±	1.9					
Avian species																			
Streptoprelia semitorq	uata 1	1.6	±	0.3	1.7	±	0.4	1.6	±	0.3	2.0	±	0.3	1.7	\pm	0.2	0.28	0.84	NS
Lamprotornis chalybau	is 2	2.0	±	0.3	1.7	±	0.4	1.7	±	0.4	2.2	±	0.6	1.9	±	0.2	0.27	0.84	NS
Corvus albus	1	1.8	±	0.2	1.7	±	0.3	1.7	\pm	0.4	2.1	\pm	0.4	1.8	\pm	0.2	0.33	0.81	NS
Tachybaptus ruficollis	1	1.4	±	0.3	1.1	±	0.1	1.2	±	0.2	1.7	±	0.4	1.4	±	0.1	0.96	0.42	NS
Merops nubicus	1	1.7	±	0.3	1.6	±	0.3	1.7	±	0.4	2.2	±	0.6	1.8	\pm	0.2	0.36	0.78	NS
Francolinus bicalcarati	us 1	1.9	±	0.3	1.7	±	0.3	1.7	±	0.4	2.2	±	0.5	1.9	±	0.2	0.29	0.83	NS
Milvus migrans	1	1.4	±	0.3	1.4	±	0.2	1.3	±	0.3	1.7	±	0.4	1.4	\pm	0.1	0.31	0.82	NS
Polyboroides radiatus	1	1.2	±	0.2	1.0	±	0.2	1.0	±	0.2	1.6	±	0.3	1.2	±	0.1	1.50	0.23	NS
Psittacus erithacus	1	1.6	±	0.3	1.3	±	0.3	1.3	±	0.3	1.8	±	0.4	1.5	\pm	0.2	0.46	0.71	NS
Necrosyrtes monachus	s 2	2.3	±	0.4	2.3	±	0.6	2.0	±	0.5	2.7	\pm	0.5	2.3	±	0.2	0.33	0.80	NS
Ardeola ibis	1	B.8	±	0.4	2.0	\pm	0.4	1.8	\pm	0.4	2.2	\pm	0.5	1.9	\pm	0.2	0.19	0.90	NS
Pavo cristatus	C).5	±	0.2	0.4	±	0.1	0.2	±	0.1	0.6	±	0.2	0.4	±	0.1	1.66	0.19	NS
Tyto alba	1	0.1	±	0.2	1.0	±	0.2	1.0	±	0.2	1.6	±	0.3	1.1	±	0.1	1.38	0.27	NS
Bubo africanus	1	1.4	±	0.2	1.1	±	0.3	1.2	\pm	0.3	1.7	±	0.4	1.4	\pm	0.1	0.95	0.43	NS
	2	21.4	<u>+</u>	3.9	19.9	±	4.0	19.5	±	4.4	26.1	±	5.8	21.7	±	2.3			

Table 4 : Mean number of carcasses (Molluscs & Reptiles) traded per dealer by zone

Source: Field Survey, 2005

	Season			Unit	Price Range*		
	Dry	Rain	Both	Whole	Price (NGN)	Parts	Price (NGN)
Common Name							
Molluscs							
African giant snail	1589	1607	3196	Х	150		
Reptilian species							
Cobra	119	94	213	Χ**	3500	Head, skin	600-1000
Tortoise	607	446	1053	Х	1200	Head, carapace	200-400
Nile monitor	60	48	108	Χ**	3000	Head, skin	900-1300
African python	88	59	147	X**	4000	Head, skin	
Senegal chameleon	246	202	448	Х	500		
Nile crocodile	38	38	76	Х**	6000	Head, skin	1500-2500
Gabon viper	122	98	220	Х	600	Head, skin	200-350
Mamba	150	112	262	Х	500	Head, skin	150-200
Avian species							
Red eye dove	127	104	231	Х	600	Head, feathers	100-250
Blue-eared glossy starling	135	115	250	Х	800	Head, feathers	100-300
Pied crow	132	108	240	Х	2500	Head, feathers	200-600
Little grebe	101	79	180	Х	1200	Head, feathers	100-400
Carmine bee-eater	133	108	241	Х	900	Head, feathers	120-400
Double-spurred francolin	138	113	251	Х	400	Head, feathers	100-180
Black kite	106	82	188	Х	1200	Head, feathers	150-300
Harrier hawk	92	67	159	Х	1000	Head, feathers	120-300
African grey parrot	113	87	200	Х	1200	Head, feathers	150-400
Hooded vulture	171	138	309	Х	1500	Head, feathers	150-600
Cattle egret	146	110	256	Х	400	Head, feathers	100-150
Indian peafowl	37	21	58			Feathers	300-700
Barn owl	87	64	151	Х	400	Head, feathers	120-250
Spotted eagle owl	105	75	180	Х	450	Head, feathers	120-250

Table 5 : Price list of species encountered during survey

* Carcass sold in fragmented parts

**requires pre-payment for contract hunting

IV. DISCUSSION

Traditional African medicinal practices consume a wide variety and vast quantity of wild mammals as revealed by the sales figure for each of the species encountered in this study. Trade in wild animals for traditional medicine cuts across all the taxa in molluscs, aves and reptiles and also involved all age grades and sexes available in agreement with several previous authors (Ntiamoa-Baidu 1987; Kakati and Duolo, 1999; Costa-Neto 1999; Adeola 1992; Marshall 1998: Soewu *et al* 2012). Most of these species are already under pressure from over-exploitation.

However, being a more specialised study excluding the mammals, the number of species encountered during this survey differ from most of the previous researches. This survey recorded 23 species while Taylor and Fox (1992) recorded 55 species in Lome Fetish Market, Togo; Kakati and Doulo (2002) recorded 23 species in a study on zoothrapeutic use by Chakhesang tribe of Nagaland in India; Costa-Neto (1999) encountered 17 species in zootherapeutic practices in Bahia, Brazil; Sodeinde and Soewu (1999) reported 45 species of wild animals for southwestern Nigeria while Soewu *et al* (2012) documented 30 species of mammals in Nigeria. For the bush meat markets, Fa *et al* (2000) reported 14 and 21 species respectively in 1991 and 1996 on Bioko Island, Equatorial Guinea while Anadu *et al* (1988) recorded 25 species in southwestern Nigeria. There have been more quantitative studies on the bush meat trade than the trade in wild animals for traditional medicine where there is still a dearth of data on the quantity of individual species traded for utilisation.

Regarding their conservation status, more than 30% of the species encountered during this study were listed in appendices 1 and 11 of CITES and the Decree 11(1985) of Nigeria as against 70% species recorded by Soewu *et al* 2012 and 26% species officially listed as endangered recorded by Kakati and Duolo (2002).

The dealers submitted that they have observed a general decrease in the sizes and volume (in number) of carcasses for virtually all the animals they received from suppliers. It was also established during the study that all species on the stalls visited were cropped from the wild and there were no records of any captive breeding or domestication project supplying the markets. All dealers agreed to having procured from either larger wholesale markets or directly from hunters, and sometimes from intermediaries.

Trade in wild animals for traditional medicine has been estimated to worth billions of dollars per year globally. It has been estimated that wildlife products worth about 160 US billion dollars were legitimately imported around the globe each year in the early 1990s. This is in addition to a large and profitable illegal wildlife trade which no-one can judge with any accuracy what this may be worth because it is conducted covertly (Anon 2016). The trade volume in selected markets for this study runs into excess of hundreds of thousands of naira within a month (Table 5). The price of species or parts was found to be influenced by the perceived medicinal value vis-à-vis the demand for preparations for that purpose. Animal or its part(s) used in fortune drawers and money rituals would attracted higher prices than those used for some other purposes.

Incidences of panic buying by the traditional medical practitioners as well as hoarding by the dealers were reported, both of which had economic implications for the trade and practices. This stemmed from fluctuations in demand for wild animals and their parts based on the differences in the kind of preparations people will seek during the various period and seasons of the year as well as the prevailing situation in the society. Another factor which was found to influence seasonal changes in demand for animal species is the fear or anticipation of non-availability of such species during the forthcoming season. In situation of political crises, even if only anticipated, the demand for amulets and other preparations for protection against gun shots, cutlass and other such protective preparations weapons will increase. A period of economic crises will lead to a rise in the demand for fortune drawers and good luck charms. National public holidays and religious festive periods like Easter and sallah celebrations were known to have involved mass movement of people from one location to another hence, an increase in the demand for traditional medicinal preparations meant to prevent occurrence of accidents or to save users from sustaining any injury in case there is an accidents. Some ailments which are season-related were also found to cause fluctuations in the demand for species recognised as possessing the medicinal properties to treat such ailments. Malaria fever, common cold/catarrh and the likes which appear to have a high level of incidence during the rainy season are expected to cause a rise in the demand for species involved in the treatment of these conditions.

The observed trend in utilisation of molluscs, reptiles and aves for traditional African medicinal practices has no consideration yet for either the present conservation status of the animals or the sustainability of continued use of these resources. Open trade in species officially listed in the appendices of various protective machineries indicated a very low level of enforcement of the protection purportedly accorded these species. The conservation status as well as the protection accorded these species need to be adequately publicised to increase the level of awareness on part of the populace concerning these issues. This is an essential pre-requisite before enforcement.

Human-nature interaction must be established within its cultural dimensions for utilisation of animal resource for therapeutic purposes to be sustainable Kakati and Duolo (2002). One of the main threats to wildlife lies in the attitude of some extremist lobbying group that promotes the strict preservation of wildlife, which tends to remove all socio-economic values from wildlife Soewu, et al (2012). Chardonnet et al (2002), stated that a complimentary approach allows conservation issues to meet with development concerns. The old-fashioned philosophy of conservation of nature and wildlife is a defensive attitude which attempts to protect nature against the consequences of development, while the modern conservation of biodiversity is a voluntary approach which intends to match the needs of people for biological resources while securing the long-term survival of the biological richness of the Earth (Chardonnet et al, 2002). Modern conservation approach is obviously more appealing, acceptable, pragmatic and promises better results.

Also, while advocating effective application of punitive measures against violators of laws protecting wild fauna species, it is essential to avoid formulating policies which may be seen as trying to force dealers to abandon their trade.

V. Recommendations

To effectively factor sustainability into the ethnobiological utilisation, and ensure continued availability of renewable natural resources, two basic steps are required: reduction in need/demand for resources in the wild for trado-medicinal practices; and improvement in the yield of these resources both in the wild and under various ex-situ schemes.

VI. REDUCTION IN NEED / DEMAND

It has been documented that notwithstanding the availability of affordable health care delivery, cultural identity and recognition will continue to promote patronage for traditional medicine for peoples across the world (Soewu *et al* 2012, Soewu 2008). A general improvement on the provision of essential amenities and overall quality of life may reduce situations that will drive the people to patronise trado-medical practices which will in turn, necessitate consumptive utilisation of wild animals without any consideration for their conservation status or sustainability of use.

A massive enlightenment campaign should be mounted on the ecological consequences of continued exploitation of these resources beyond their sustainable level and its attendant implications for the health status of mankind now and in the future. Wildlife conservation education should be integrated into the curriculum for formal education from primary to tertiary level to make conservation an essential component of the live of every citizen

a) Trade Regulation

A comprehensive review of the legal machineries protecting wild animals within the country is urgently needed to strike the required delicate balance between biodiversity conservation interests, sociocultural demands and political exigencies. The contents of such national law as well as international conventions and treaties regulating trade in these species and, the implications of such legal provisions should be given adequate publicity as the present level of awareness is near zero among the citizenry.

b) Increase in Yield

Production of desired species should be enhanced through in-situ and ex-situ programmes. Insitu conservation facilities should be given adequate attention in ecosystem management practices with regular anti-poaching and surveillance patrols to minimize poaching activities and encourage maximum production. These will ensure optimally harnessing the potentials of these protected areas to conserve populations of wild animals while also serving as a source of re-populating species of interest. Ex-situ method of wildlife conservation constitute an important method of saving species on the verge of extinction. Efforts should be intensified on captive breeding, artificial propagation and ranching of possible species. This will provide animals for other uses such as protein sources thereby reducing pressure on resources in the wild. It will also provide animals for traditional medicinal practices where behavioral traits hinged on wild-based activities of the species are not pre-requisites.

Host communities of the wild fauna resources should be integrated as partners and beneficiaries in the management of conservation areas to make compliance with laws regulating exploitation of animals easy and realistic. Enjoining their voluntary cooperation and compliance may eliminate the need for elaborate monitoring and expensive control. Legitimate trade in non-protected species should be promoted and made more beneficial to the less well-off rural populations as against the intermediaries or the better-off urban dealers. There is a need to further investigate the dynamics of wild animals' utilisation for traditional medicine across the country so as to gain an insight into the pattern and volume of consumptive use at the national level.

VII. Conclusions

Overexploitation has caused extinctions or severely threatened species and, as human populations

have expanded, demand for wildlife has only increased. Recent overexploitation of wildlife for trade has affected countless species, some of which have been documented. In addition to the impact on human livelihoods caused by the over-harvesting of animals and plants is the harm caused by overexploitation of species to the living planet in a wider way. As human life depends on the existence of a functioning planet Earth, careful and thoughtful use of wildlife species and their habitats is required to avoid not only extinctions, but serious disturbances to the complex web of life.

Prohibiting the utilisation of natural resources, most especially for reasons relating to food, health and cultural beliefs of peoples around the world has been found to be non-appealing and in-effective as the concept of wildlife conservation is often alien to them. If the need for conservation is to be accepted by people who make their livelihoods from wildlife or its use for necessities such as food and medicine, massive enlightenment campaigns and conservation education are urgently required. Care should be also be taken to avoid what may be seen as ideological or culturally imperialistic approaches. Accepting and respecting differing views of the values of wildlife is required for cooperation across all strata of the society while at the same time explaining the provisions of the various conservation laws to the populace to discourage undue violations. Finally, while wildlife trade alone has been identified as a major threat to some species, it is important to remember that its impact is frequently made worse by habitat loss and other pressures. This should be factored adequately into conservation policies and projects to ensure an all-round sustainability of renewable natural resources.

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Design, Synthesis, Spectral Charecterization of Some New Fully Unsaturated 2-Substituted-4,6 Dichloro Symmetric Triazine- based Chalcone Hybrids

By G. V. Pavan Kumar, D. Srinivasa Rao, B. Pooja, G. Harika & Y. Anil Kumar *Kc Reddy Institute of Pharmaceutical Sciences, India*

Abstract- Triazines and chalcones are interesting class of heterocyclic compounds with a prominent structural core system present in numerous pharmacologically active compounds. It is proved from the literature that the compounds containing 1,3,5-triazine moiety or chalcone bridge often shows significant biological activity profiles. Based on these observations, it was considered worthwhile to synthesize and characterize some new 1,3,5-triazine-chalcone hybrid molecules in the present investigation. As a part of our research program aimed at search for new hybrid pharmacophores as potential cytotoxic agents, we are interested to have α , β -unsaturated ketone linker to the 1,3,5-triazine basic nucleus to give a series of 1,3,5-triazine-chalcone hybrid molecules. Therefore, in the present study an attempt has been made to synthesize and characterize various analogs of fully unsaturated 2-substituted-4,6 dichloro-1,3,5 triazine based chalcone hybrids.

Keywords: fully unsaturated, 1,3,5-triazine-chalcone hybrids, spectral characterization.

GJMR-B Classification : NLMC Code: QV 4

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Design, Synthesis, Spectral Charecterization of Some New Fully Unsaturated 2-Substituted-4,6 Dichloro Symmetric Triazine- based Chalcone Hybrids

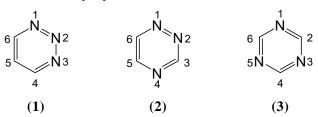
G. V. Pavan Kumar $^{\alpha}$, D. Srinivasa Rao $^{\sigma}$, B. Pooja $^{\rho}$, G. Harika $^{\omega}$ & Y. Anil Kumar *

Abstract- Triazines and chalcones are interesting class of heterocyclic compounds with a prominent structural core system present in numerous pharmacologically active compounds. It is proved from the literature that the compounds containing 1,3,5-triazine moiety or chalcone bridge often shows significant biological activity profiles. Based on these observations, it was considered worthwhile to synthesize and characterize some new 1,3,5-triazine-chalcone hybrid molecules in the present investigation. As a part of our research program aimed at search for new hybrid pharmacophores as potential cytotoxic agents, we are interested to have α,β -unsaturated ketone linker to the 1,3,5triazine basic nucleus to give a series of 1,3,5-triazinechalcone hybrid molecules. Therefore, in the present study an attempt has been made to synthesize and characterize various analogs of fully unsaturated 2-substituted-4,6 dichloro-1,3,5 triazine based chalcone hybrids.The chief intermediate in the present study 1-(3-(4,6-dichloro-1,3,5triazin-2 vlamino) phenvl) ethanone was prepared by reaction between cyanuric chloride i.e.2,4,6-trichloro-1,3,5-triazine and 3- amino acetophenone. Further, successive base catalyzed Claisen-Schmidt condensation of the compound with appropriate substituted aromatic/heteroaromatic aldehydes in the presence of 100% potassium hydroxide solution in ethanol afforded a series of 1-(3-(4,6-dichloro-1,3,5-triazin-2ylamino)phenyl)-3-(substituted)-2-propen-1-ones.All the newly synthesized compounds were characterized by CHN elemental analysis and spectroscopic methods such as FT-IR, ¹H NMR, and LC mass spectral analysis.

Keywords: fully unsaturated, 1,3,5-triazine-chalcone hybrids, spectral characterization.

I. INTRODUCTION

riazines are a class of organic nitrogen-containing six-membered heterocyclic compounds known for a long period of time. They can structurally be existing as three isomers varied with their position of nitrogen atoms on the benzene ring, and are referred to as 1,2,3-triazine (1), 1,2,4-triazine (2) and 1,3,5-triazine (3). In particular, considerable attention has been devoted to the development of 1,3,5-triazine derivatives in comparison with 1,2,3-triazine and 1,2,4-triazine derivatives, due to their variety of applications in different fields [1,2].



1.3.5-Triazines can also be called as symmetric or s-triazines. The chemistry of this group of compounds has been studied intensively since past two centuries due to their wide spread applications in the pharmaceutical, textile, plastic and rubber industries and are used as pesticides, dyestuffs, optical bleaches, explosives and surface active agents. In recent times, several studies have been carried out on the antitumor activity of 1,3,5-triazines. Some of these analogues, hexamethylmelamine (4), almitrine (5) and irsogladine (6) are clinically used as anticancer agents. Baker (4,6-Diamino-2,2-dimethyl-1,2-dihydro-1,3,5triazines triazine based analogs) are becoming increasingly important as pharmaceuticals. Baker triazine antifol (7) had been undergoing clinical trials as a drug candidate in cancer chemotherapy [3-8].

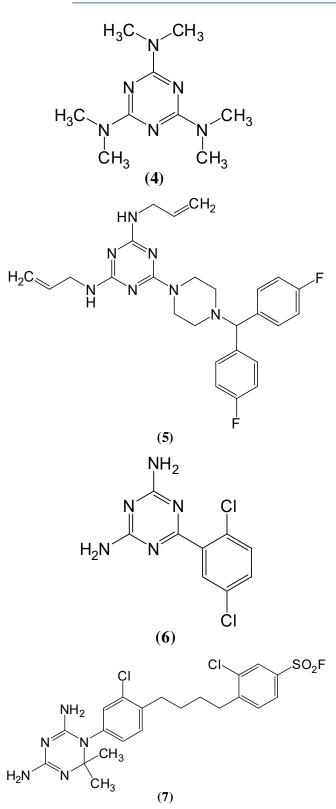
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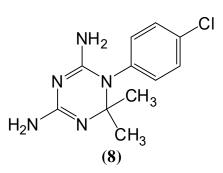
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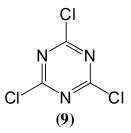
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Although 1,3,5-triazines are well known in the context of anticancer drugs, this ring is also found in the drug used in the chemotherapy of malaria, as seen in case of cycloguanil (8) [9]. Recently, 2,4,6-trisubstituted -1,3,5-triazine scaffolds were discovered as a potent inhibitors of *M. tuberculosis* H37Rv [10].



All 1,3,5-triazine derivatives that have wide practical applications are 2,4,6-mono, di- or trisubstituted, symmetrical and nonsymmetrical compounds bearing different substituents. The most important reagent for obtaining these synthetic molecule transformations is cyanuric chloride (9), due to the reactivity of the chlorine atoms towards nucleophiles [11].



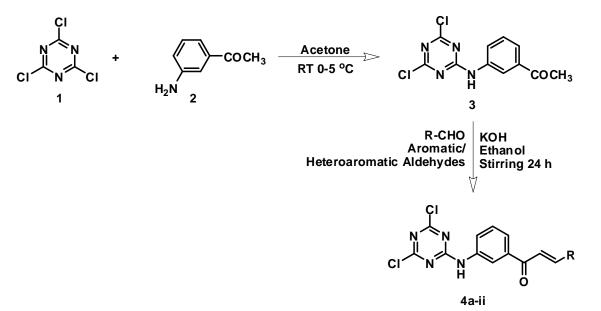
II. MATERIALS AND METHODS

A brief description of the solvents, chemicals procured, the instruments and the conditions employed for the characterization of the synthesized compounds are presented here. The organic solvents such as methanol, acetone, chloroform and ethyl acetate were of spectral grade and used as such without further purification. Anhydrous methanol was obtained by fractional distillation and storing over type 4A molecular sieves. The acetone present in methanol was removed by using the following procedure: A mixture of 500 mL of methanol, 25 mL of furfural and 60 ml of 10% sodium hydroxide solution was refluxed for 12 h, then the mixture was distilled and the first few milliliters of the distillate was rejected as it contains trace amount of formaldehyde. Ethanol obtained by distillation of commercial ethyl alcohol was refluxed over ignited calcium oxide for 6 h and distilled at atmospheric pressure and then used. All the major chemicals were purchased from Sigma-Aldrich. The important starting materials were procured from Sigma-Aldrich. Thin layer chromatography (TLC) was performed in the course of the reaction to optimize the reaction for purity and completion of reaction on Merck silica gel precoated GF₂₅₄ aluminum plates using mixture of different polar and nonpolar solvents in varying proportions and spots were observed using iodine as visualizing agent. Silica gel (100-200 mesh, Merck grade) has been used for column chromatography. The column was subjected to gradient elution using n-hexane, mixtures of hexane and ethyl acetate (5%, 10%, 15%, 25%, 50% and 75% hexane in ethyl acetate), ethyl acetate and mixtures of ethyl acetate and methanol (1%, 2%, 5% and 10% ethyl acetate in methanol). Fractions each of 100 mL were collected. The separation of the compounds was checked on TLC under UV lamp and also by spraying the plates with 10% sulphuric acid in methanol.

All the melting points were determined in open capillary tubes in an EZ-MELT automated digital melting point apparatus and are uncorrected. IR spectra were recorded (in KBr) on a Perkin-Elmer FTIR. ¹H NMR and ¹³C NMR spectra were recorded on a Bruker spectrometer at 400 MHz using TMS as the internal standard. Mass spectra (ESI) were measured on an LC-MS 6100 QQQ (Agilent Technologies, USA). Elemental analyses were carried out with Carlo Erba 1108 elemental analyzer apparatus. The results of elemental analyses (C, H, N) were within \pm 0.4 % of the calculated values.

III. CHEMISTRY

The reaction sequence intended for the preparation of title compounds (4a-ii) is shown in Scheme 1, and their physical properties are depicted in Tables 1 and 2. The chief intermediate in the present study 1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino) phenyl) ethanone (3) was prepared by reaction between cyanuric chloride i.e. 2,4,6-trichloro-1,3,5-triazine (1) and 3-aminoacetophenone (2) [12]. Further, successive base catalyzed Claisen-Schmidt condensation of the compound 3 with appropriate substituted aromatic/ heteroaromatic aldehydes in the presence of 100% potassium hydroxide solution in ethanol afforded a series of 1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino) phenyl)-3-(substituted)-2-propen-1-ones (4a-ii) in good yield. All the newly synthesized compounds were characterized by CHN elemental analysis and spectroscopic methods such as FT-IR, ¹H NMR, and LC mass spectral analysis. Eventually all the spectra of the new products (4a-ii) are in keeping with the predictable structures.



Scheme 1 : Chemical synthesis of 1,3,5-triazine-chalcone hybrid molecules 4a-4ii.

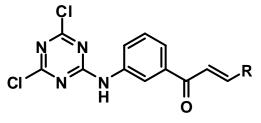
The IR spectrum of all the compounds 4a-ii exhibited the characteristic absorptions at various frequencies correspondingly at 3310-3110 and 1640-1715 cm⁻¹ suggesting the presence of a secondary amine group and α , β -unsaturated carbonyl group respectively. In the ¹H NMR spectra of 1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(substituted)-2-propen-1-ones (4a-ii), a singlet integrating for one proton characteristic of the secondary amine NH group was observed in between δ 9.2-9.4 ppm as a broad signal. As seen in case of compound 4a, the IR spectrum of 4a exhibited characteristic -C=C- (aliphatic) and -C=C- (aromatic) stretching bands at

frequencies 1645 and 1513 cm⁻¹, respectively. The other IR absorptions at various frequencies correspondingly at 3155 and 1688 cm⁻¹ suggesting the presence of a secondary amino group and α , β -unsaturated ketone group, respectively. The 400 MHz ¹H NMR spectrum of the compound 4a in DMSO-d₆ as solvent with TMS as an internal standard exhibited characteristic peaks of H_a and H_β protons of α , β -unsaturated ketone bridge appeared as two doublets, one doublet at δ 7.78 ppm (H_a, J = 15.4 Hz) and the other one at δ 8.01 ppm (H_β, J = 15.4 Hz). The large J value 15.4 Hz of both the protons clearly reveals the *trans* geometry at the double bond. The distinguishing peak of NH proton appears as

one singlet δ 9.74 ppm. The ESI mass spectrum (positive ion mode) of 4a revealed a $(M+H)^+$ ion at m/z 372. Based on the above spectral information the

structure of the compound 4a was confirmed as (E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(phenyl)-2-propen-1-one [13-15].

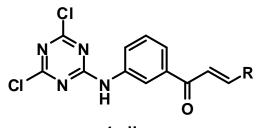
Table 1 : List of new 1,3,5-triazine-chalcone hybrid molecules 4a-ii produced via Scheme 1.



Л	2	-		
-	-	-		

Compound	R	Molecular formula	Relative Molecular Mass (g)	M.p. (°C)	Yield (%)
4a	Phenyl	C ₁₈ H ₁₂ Cl ₂ N ₄ O	371	123	60
4b	2-MeC ₆ H ₄	C ₁₉ H ₁₄ Cl ₂ N ₄ O	385	135	51
4c	3-MeC ₆ H ₄	C ₁₉ H ₁₄ Cl ₂ N ₄ O	385	143	66
4d	$4-\text{MeC}_6\text{H}_4$	C ₁₉ H ₁₄ Cl ₂ N ₄ O	385	175	68
4e	2-OMeC ₆ H ₄	$C_{19}H_{14}CI_2N_4O_2$	401	167	71
4f	3-OMeC ₆ H ₄	$C_{19}H_{14}CI_2N_4O_2$	401	129	58
4g	4-OMeC ₆ H ₄	$C_{19}H_{14}CI_2N_4O_2$	401	145	61
4h	3-OHC ₆ H ₄	C ₁₈ H ₁₂ Cl ₂ N ₄ O ₂	387	122	74
4i	4-OHC ₆ H ₄	$C_{18}H_{12}CI_2N_4O_2$	387	161	78
4j	3,5-diOHC ₆ H ₃	$C_{18}H_{12}CI_2N_4O_3$	403	182	69
4k	4,5-diOHC ₆ H ₃	$C_{18}H_{12}CI_2N_4O_3$	403	154	51
41	2-Me,5-OHC ₆ H ₃	$C_{19}H_{14}CI_2N_4O_2$	401	169	55
4m	$2-NH_2C_6H_4$	C ₁₈ H ₁₃ Cl ₂ N ₅ O	386	154	67
4n	$3-NH_2C_6H_4$	C ₁₈ H ₁₃ Cl ₂ N ₅ O	386	133	71
40	$4-NH_2C_6H_4$	C ₁₈ H ₁₃ Cl ₂ N ₅ O	386	139	68
4p	$2-NO_2C_6H_4$	$C_{18}H_{11}CI_2N_5O_3$	416	120	52
4q	3-NO ₂ C ₆ H ₄	$C_{18}H_{11}CI_2N_5O_3$	416	140	77
4r	$4-NO_2C_6H_4$	$C_{18}H_{11}CI_2N_5O_3$	416	124	84
4s	2-CIC ₆ H ₄	$C_{18}H_{11}CI_{3}N_{4}O$	405	138	81
4t	3-CIC ₆ H ₄	$C_{18}H_{11}CI_{3}N_{4}O$	405	181	71
4u	4-CIC ₆ H ₄	$C_{18}H_{11}CI_{3}N_{4}O$	405	149	73
4v	2,4-diClC ₆ H ₃	$C_{18}H_{10}CI_4N_4O$	440	192	59
4w	$2-FC_6H_4$	$C_{18}H_{11}CI_2FN_4O$	389	152	67
4x	$3-FC_6H_4$	$C_{18}H_{11}CI_2FN_4O$	389	132	55
4у	$4-FC_6H_4$	$C_{18}H_{11}CI_2FN_4O$	389	145	51
4z	2,4-diFC ₆ H ₃	$C_{18}H_{10}CI_2F_2N_4O$	407	160	67
4aa	Furan-2yl	$C_{16}H_{10}CI_2N_4O_2$	361	188	71
4bb	Thiophen-3-yl	$C_{16}H_{10}CI_2N_4OS$	377	177	78
4cc	Pyrrol-2yl	$C_{16}H_{11}CI_2N_5O$	360	121	66
4dd	Pyridin-2-yl	$C_{17}H_{11}CI_2N_5O$	372	124	72
4ee	Pyridin-3-yl	$C_{17}H_{11}CI_2N_5O$	372	151	79
4ff	Pyridin-4-yl	$C_{17}H_{11}CI_2N_5O$	372	197	77
4gg	Naphthalen-2-yl	$C_{22}H_{14}CI_2N_4O$	421	105	81
4hh	Naphthalen-3-yl	$C_{22}H_{14}CI_2N_4O$	421	117	87
4 ii	Anthracen-9-yl	$C_{26}H_{16}CI_2N_4O$	471	220	68

Table 2 : Elemental analysis data of 1,3,5-triazine-chalcone conjugates 4a-ii produced via Scheme 1.



4	a	-	İ	İ	

Compound	% Elemental analysis of C, H, N ^b						
	Calculated				Found		
	С	Н	Ν	С	Н	Ν	
4a	58.24	3.26	15.09	58.21	3.21	15.05	
4b	59.24	3.66	14.54	59.22	3.62	14.52	
4c	59.24	3.66	14.54	59.25	3.61	14.53	
4d	59.24	3.66	14.54	59.22	3.64	14.51	
4e	56.87	3.52	13.96	56.82	3.51	13.95	
4f	56.87	3.52	13.96	56.83	3.51	13.91	
4g	56.87	3.52	13.96	56.84	3.56	13.96	
4h	55.83	3.12	14.47	55.85	3.11	14.42	
4i	55.83	3.12	14.47	55.83	3.11	14.45	
4j	53.62	3.00	13.89	53.61	3.02	13.81	
4k	53.62	3.00	13.89	53.61	3.04	13.82	
41	56.87	3.52	13.96	56.86	3.51	13.93	
4m	55.97	3.39	18.13	55.95	3.31	18.11	
4 n	55.97	3.39	18.13	55.94	3.32	18.12	
40	55.97	3.39	18.13	55.93	3.35	18.14	
4p	51.94	2.66	16.83	51.95	2.62	16.82	
4q	51.94	2.66	16.83	51.92	2.65	16.85	
4r	51.94	2.66	16.83	51.93	2.62	16.81	
4s	53.29	2.73	13.81	53.21	2.71	13.82	
4t	53.29	2.73	13.81	53.22	2.74	13.81	
4u	53.29	2.73	13.81	53.23	2.71	13.84	
4v	49.12	2.29	12.73	49.11	2.25	12.71	
4w	55.55	2.85	14.39	55.53	2.82	14.35	
4x	55.55	2.85	14.39	55.52	2.84	14.35	
4y	55.55	2.85	14.39	55.51	2.81	14.32	
4z	53.09	2.48	13.76	53.01	2.42	13.72	
4aa	53.21	2.79	15.51	53.22	2.75	15.50	
4bb	50.94	2.67	14.85	50.97	2.65	14.82	
4cc	66.25	3.42	11.89	66.22	3.41	11.86	
4dd	54.86	2.98	18.82	54.82	2.96	18.88	
4ee	54.86	2.98	18.82	54.81	2.95	18.89	
4ff	54.86	2.98	18.82	54.85	2.92	18.81	
4gg	62.72	3.35	13.30	62.71	3.32	13.32	
4hh	62.72	3.35	13.30	62.72	3.31	13.33	
4ii	66.25	3.42	11.89	66.22	3.40	11.85	

IV. EXPERIMENTAL SECTION

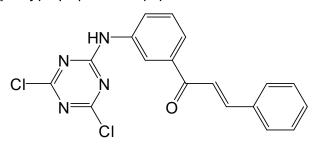
Synthesis of 1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino) phenyl)ethanone (3)

To a solution of 2,4,6-trichloro-1,3,5-triazine (1) (0.01 M) dissolved in 20 mL of acetone,3aminoacetophenone (2) (0.01 M)was added slowly by delivering through a spatula in small quantities and the resulting mixture was stirred at 0-5 °C tempe- rature for 3h.The crude 1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino) phenyl)ethanone (3) was washed on the vaccum filter with cold methanol and then recrystallized from ethanol.

Synthesis of 1,3,5-triazine-chalcone hybrid molecules (4a-ii)

To a solution of 1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)ethanone (**3**) (0.005 M) and suitably substituted aldehydes (0.005 M) in ethanol (10 ml), aqueous solution of potassium hydroxide (100%) was added drop wise with continuous stirring at room temperature over a period of 10 min. The reaction mixture was then kept at room temperature for about 48 h with occasional shaking. After 48 h it was poured into ice-cold water, and then neutralized to pH 2 using 5 N hydrochloric acid. The light yellow precipitate obtained was filtered, washed, dried, and recrystallized from dry ethanol. The 1,3,5-triazine-chalcone hybrid molecules **4a-ii** were obtained in good yield. All the synthesized compounds as mentioned in **Table 1** were characterized by spectroscopic methods such as FTIR, ¹H NMR, ¹³C NMR and LC mass spectral analysis and presented separately under each compound.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(phenyl)-2-propen-1-one (4a):



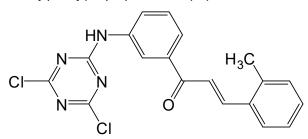
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3155 (N–H), 3031 (C–H, aromatic), 2884 (G-H, aliphatic), 1688 (C=O), 1645 (C=C, aliphatic), 1513 (C=C, aromatic), 689 (C–Cl).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.13-7.74 (m, 9H, Ar-H), 7.78 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 8.01 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.74 (s, 1H, NH).

ESI-MS (m/z): 372 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(2-methylphenyl)-2-propen-1-one (4b):



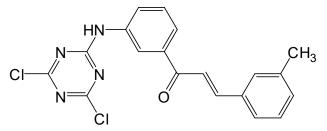
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3152 (N–H), 3022 (C–H, aromatic), 2881 (G-H, aliphatic), 1689 (C=O), 1623 (C=C, aliphatic), 1501 (C=C, aromatic), 688 (C–Cl).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 2.32 (s, 3H, CH₃), 7.43-8.04 (m, 8H, Ar-H), 7.78 (d, J = 15.2 Hz, 1H, HC=CH (H-α)), 8.01 (d, J = 15.2 Hz, 1H, HC=CH (H-β)), 9.74 (s, 1H, NH).

ESI-MS (m/z): 386 [M+H]+.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(3-methylphenyl)-2-propen-1-one (4c):



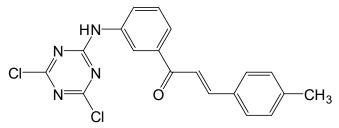
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3127 (N–H), 3027 (C–H, aromatic), 2777 (G-H, aliphatic), 1703 (C=O), 1603 (C=C, aliphatic), 1450 (C=C, aromatic), 688 (C–CI).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 2.41 (s, 3H, CH₃), 7.38-8.05 (m, 8H, Ar-H), 7.73 (d, J = 15.2 Hz, 1H, HC=CH (H-α)), 8.04 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.69 (s, 1H, NH).

ESI-MS (m/z): 386 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(4-methylphenyl)-2-propen-1-one (4d):



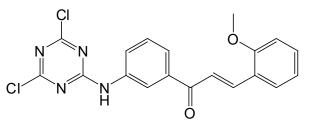
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3122 (N–H), 3015 (C–H, aromatic), 2762 (G-H, aliphatic), 1705 (C=O), 1601 (C=C, aliphatic), 1440 (C=C, aromatic), 685 (C–Cl).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 2.39 (s, 3H, CH₃), 7.31-7.66 (m, 8H, Ar-H), 7.73 (d, J = 15.2 Hz, 1H, HC=CH (H-α)), 8.02 (d, J = 15.2 Hz, 1H, HC=CH (H-β)), 9.62 (s, 1H, NH).

ESI-MS (m/z): 386 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(2-methoxyphenyl)-2-propen-1-one (4e):



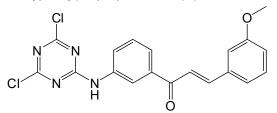
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3124 (N–H), 3027 (C–H, aromatic), 2975 (G-H, aliphatic), 1700 (C=O), 1603 (C=C, aliphatic), 1417 (C=C, aromatic), 713–(Cl), 1171 (C–O–C), 1054 (C–O).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 3.86 (s, 3H, OCH₃), 7.20-8.05 (m, 8H, Ar-H), 7.48 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 8.05 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.66 (s, 1H, NH).

ESI-MS (m/z): 402 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(3-methoxyphenyl)-2-propen-1-one (4f):



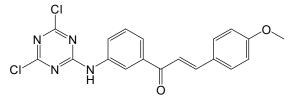
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3124 (N–H), 3027 (C–H, aromatic), 2977 (G-H, aliphatic), 1700 (C=O), 1605 (C=C, aliphatic), 1457 (C=C, aromatic), 687–(**C**I), 1171 (C–O–C), 1054 (C–O).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 3.88 (s, 3H, OCH₃), 7.12-8.21 (m, 8H, Ar-H), 7.71 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 8.06 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.65 (s, 1H, NH).

ESI-MS (m/z): 402 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(4-methoxyphenyl)-2-propen-1-one (4g):



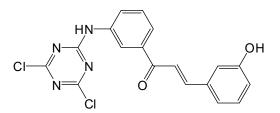
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3122 (N–H), 3021 (C–H, aromatic), 2970 (G-H, aliphatic), 1690 (C=O), 1602 (C=C, aliphatic), 1455 (C=C, aromatic), 677–(Cl), 1170 (C–O–C), 1055 (C–O).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 3.86 (s, 3H, OCH₃), 7.12-7.92 (m, 8H, Ar-H), 7.71 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 8.05 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.75 (s, 1H, NH).

ESI-MS (m/z): 402 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(3-hydroxyphenyl)-2-propen-1-one (4h):



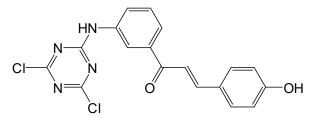
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3445 (O–H), 3124 (N–H), 3015 (G–H, aromatic), 2984 (C–H, aliphatic), 1689 (C=O), 1606 (C=C, aliphatic), 1415 (C=C, aromatic), 676 (C–Cl), 1054 (C–O).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.36-8.01 (m, 8H, Ar-H), 7.67 (d, J = 15.6 Hz, 1H, HC=CH (H- α)), 8.18 (d, J = 15.6 Hz, 1H, HC=CH (H- β)), 9.85 (s, 1H, NH), 12.32 (s, 1H, OH).

ESI-MS (m/z): 388 [M+H]+.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(4-hydroxyphenyl)-2-propen-1-one (4i):



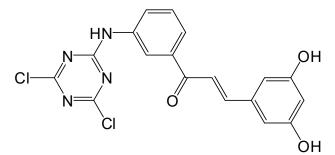
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3444 (O–H), 3124 (N–H), 3019 (G–H, aromatic), 2982 (C–H, aliphatic), 1684 (C=O), 1602 (C=C, aliphatic), 1412 (C=C, aromatic), 671 (C–Cl), 1055 (C–O).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.16-7.62 (m, 8H, Ar-H), 7.68 (d, J = 15.6 Hz, 1H, HC=CH (H-α)), 8.14 (d, J = 15.6 Hz, 1H, HC=CH (H-β)), 9.82 (s, 1H, NH), 12.31 (s, 1H, OH).

ESI-MS (m/z): 388 [M+H]+.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(3,5-dihydroxyphenyl)-2-propen-1-one (4j):



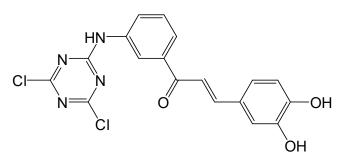
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3440 (O–H), 3122 (N–H), 3027 (G–H, aromatic), 2890 (C–H, aliphatic), 1700 (C=O), 1605 (C=C, aliphatic), 1511 (C=C, aromatic), 688 (C–Cl), 1054 (C–O).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.21-8.02 (m, 7H, Ar-H), 7.79 (d, J = 15.3 Hz, 1H, HC=CH (H-α)), 8.03 (d, J = 15.3 Hz, 1H, HC=CH (H-β)), 9.89 (s, 1H, NH), 11.52 (s, 2H, OH).

ESI-MS (m/z): 404 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(4,5-dihydroxyphenyl)-2-propen-1-one (4k):



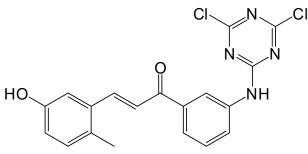
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3395 (O–H), 3127 (N–H), 3017 (G–H, aromatic), 2989 (C–H, aliphatic), 1686 (C=O), 1615 (C=C, aliphatic), 1545 (C=C, aromatic), 689 (C–Cl), 1054 (C–O).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.55-8.03 (m, 7H, Ar-H), 7.83 (d, J = 15.3 Hz, 1H, HC=CH (H-α)), 8.08 (d, J = 15.3 Hz, 1H, HC=CH (H-β)), 9.58 (s, 1H, OH), 9.87 (s, 1H, NH), 10.57 (s, 1H, OH).

ESI-MS (m/z): 404 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(2-methyl-5-hydroxyphenyl)-2-propen-1-one (4l):



Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3440 (O–H), 3122 (N–H), 3021 (G–H, aromatic), 2975 (C–H, aliphatic), 1690 (C=O), 1641 (C=C, aliphatic), 1486 (C=C, aromatic), 678 (C–Cl), 1054 (C–O).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 2.47 (s, 3H, CH₃), 7.62-8.01 (m, 7H, Ar-H), 7.81 (d, J = 15.3 Hz, 1H, HC=CH (H-α)), 8.08 (d, J = 15.3 Hz, 1H, HC=CH (H-β)), 9.01 (s, 1H, NH), 10.52 (s, 1H, OH).

ESI-MS (m/z): 402 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(2-aminophenyl)-2-propen-1-one (4m):



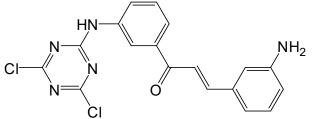
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3367 (NH₂), 3117 (N–H), 2978 (C–H, aromatic), 2763 (C–H, aliphatic), 1693 (C=O), 1597 (C=C, aliphatic), 1413 (C=C, aromatic), 688 (C–Cl), 1296 (C–N).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.74-8.11 (m, 8H, Ar-H), 7.58 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 8.06 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.65 (s, 1H, NH), 10.51 (s, 2H, Ar-NH₂).

ESI-MS (m/z): 387 [M+H]+.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(3-aminophenyl)-2-propen-1-one (4n):



Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3367 (NH₂), 3117 (N–H), 2978 (C–H, aromatic), 2763 (G–H, aliphatic), 1693 (C=O), 1597 (C=C, aliphatic), 1413 (C=C, aromatic), 688 (C–Cl), 1290 (C–N).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.72 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 7.74-8.11 (m, 8H, Ar-H), 8.01 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.67 (s, 1H, NH), 10.54 (s, 2H, Ar-NH₂).

ESI-MS (m/z): 387 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(4-aminophenyl)-2-propen-1-one (40):

Colour: Light yellow crystals.

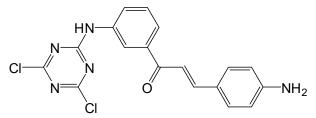
FT-IR (KBr, vmax, cm-1): 3362 (NH₂), 3115 (N-H), 2979 (C-H, aromatic), 2761 (C-H, aliphatic), 1690 (C=O), 1590 (C=C, aliphatic), 1410 (C=C, aromatic), 684 (C-Cl), 1290 (C-N).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.71 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 7.77-8.14 (m, 8H, Ar-H), 8.12 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.65 (s, 1H, NH), 10.52 (s, 2H, Ar-NH₂).

ESI-MS (m/z): 387 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-

(2-nitrophenyl)-2-propen-1-one (4p):



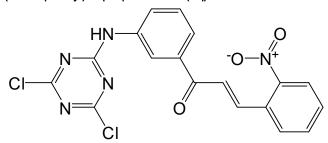
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3122 (N–H), 3024 (C–H, aromatic), 2776 (G-H, aliphatic), 1700 (C=O), 1604 (C=C, aliphatic), 1414 (C=C, aromatic), 688–(Cl), 1529 (N=O), 1291 (C–N).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 6.86-8.18 (m, 8H, Ar-H), 8.05 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 8.35 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.72 (s, 1H, NH).

ESI-MS (m/z): 417 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(3-nitrophenyl)-2-propen-1-one (4q):



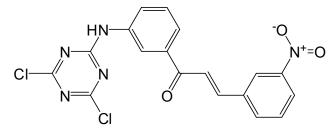
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3115 (N–H), 3026 (C–H, aromatic), 2775 (G-H, aliphatic), 1700 (C=O), 1599 (C=C, aliphatic), 1412 (C=C, aromatic), 688–(Cl), 1522 (N=O), 1290 (C–N).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.55-8.39 (m, 8H, Ar-H), 7.86 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 8.06 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.73 (s, 1H, NH).

ESI-MS (m/z): 417 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(4-nitrophenyl)-2-propen-1-one (4r):



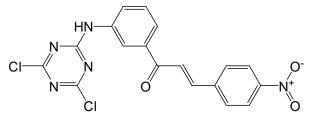
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3205 (N–H), 3016 (C–H, aromatic), 2895 (C–H, aliphatic), 1710 (C=O), 1589 (C=C, aliphatic), 1442 (C=C, aromatic), 680 (C–Cl), 1520 (N=O), 1287 (C–N).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.54-8.29 (m, 8H, Ar-H), 7.83 (d, J = 15.2 Hz, 1H, HC=CH (H-α)), 8.07 (d, J = 15.2 Hz, 1H, HC=CH (H-β)), 9.23 (s, 1H, NH).

ESI-MS (m/z): 417 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(2-chlorophenyl)-2-propen-1-one (4s):



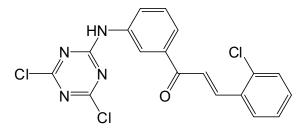
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3127 (N–H), 3027 (C–H, aromatic), 2893 (G-H, aliphatic), 1689 (C=O), 1597 (C=C, aliphatic), 1450 (C=C, aromatic), 688–(Cl), 786 (C–Cl).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.60 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 7.62-8.24 (m, 8H, Ar-H), 7.78 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.65 (s, 1H, NH).

ESI-MS (m/z): 406 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(3-chlorophenyl)-2-propen-1-one (4t):



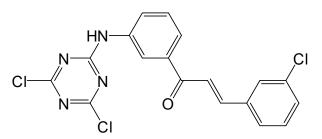
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3121 (N–H), 3025 (C–H, aromatic), 2891 (G-H, aliphatic), 1686 (C=O), 1594 (C=C, aliphatic), 1451 (C=C, aromatic), 786 (C–Cl).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.45 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 7.62-7.74 (m, 8H, Ar-H), 7.79 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.65 (s, 1H, NH).

ESI-MS (m/z): 406 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(4-chlorophenyl)-2-propen-1-one (4u):



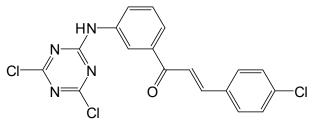
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3126 (N–H), 3023 (C–H, aromatic), 2883 (G-H, aliphatic), 1690 (C=O), 1588 (C=C, aliphatic), 1442 (C=C, aromatic), 681–(**C**I), 785 (C–CI).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.61 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 7.67-7.82 (m, 8H, Ar-H), 7.87 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.63 (s, 1H, NH).

ESI-MS (m/z): 406 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(2,4-dichlorophenyl)-2-propen-1-one (4v):



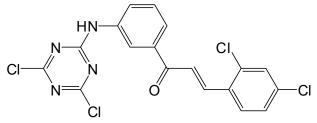
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3124 (N–H), 3018 (C–H, aromatic), 2891 (G-H, aliphatic), 1689 (C=O), 1641 (C=C, aliphatic), 1485 (C=C, aromatic), 691–(**C**I), 786 (C–CI).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.65-8.23 (m, 7H, Ar-H), 7.78 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 8.06 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.69 (s, 1H, NH).

ESI-MS (m/z): 441 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(2-fluorophenyl)-2-propen-1-one (4w):



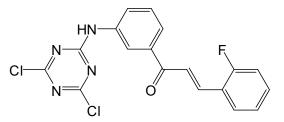
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3117 (N–H), 3017 (C–H, aromatic), 2977 (C–H, aliphatic), 1693 (C=O), 1605 (C=C, aliphatic), 1415 (C=C, aromatic), 688 (C–Cl), 1116 (C–F).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.36-8.03 (m, 8H, Ar-H), 7.55 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 7.82 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.68 (s, 1H, NH).

ESI-MS (m/z): 390 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(3-fluorophenyl)-2-propen-1-one (4x):



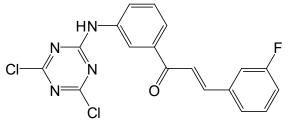
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3112 (N–H), 3011 (C–H, aromatic), 2974 (G-H, aliphatic), 1690 (C=O), 1602 (C=C, aliphatic), 1412 (C=C, aromatic), 680–(Cl), 1011 (C–F).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.16-7.73 (m, 8H, Ar-H), 7.75 (d, J = 15.2 Hz, 1H, HC=CH (H-α)), 7.81 (d, J = 15.2 Hz, 1H, HC=CH (H-β)), 9.78 (s, 1H, NH).

ESI-MS (m/z): 390 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(4-fluorophenyl)-2-propen-1-one (4y):



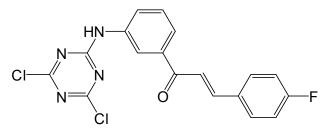
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3114 (N–H), 3212 (C−H, aromatic), 2975 (G-H, aliphatic), 1694 (C=O), 1602 (C=C, aliphatic), 1412 (C=C, aromatic), 1106 (€), 685 (C−Cl).

 ^1H NMR (400 MHz, DMSO-d_6, δ , ppm): 7.22-7.63 (m, 8H, Ar-H), 7.65 (d, J = 15.2 Hz, 1H, HC=CH (H-\alpha)), 7.82 (d, J = 15.2 Hz, 1H, HC=CH (H-\beta)), 9.77 (s, 1H, NH).

ESI-MS (m/z): 390 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(2,4-difluorophenyl)-2-propen-1-one (4z):



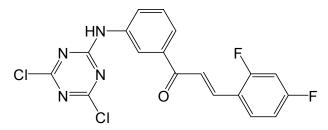
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3122 (N–H), 3021 (C–H, aromatic), 2884 (G-H, aliphatic), 1693 (C=O), 1605 (C=C, aliphatic), 1415 (C=C, aromatic), 688–(Cl), 1114 (C–F).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.39-8.31 (m, 7H, Ar-H), 7.76 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 8.08 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.69 (s, 1H, NH).

ESI-MS (m/z): 408 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(furan-2-yl)-2-propen-1-one (4aa):



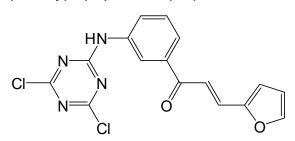
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3420 (N–H), 3062 (C–H, aromatic), 3030 (C–H, aliphatic), 1671(C=O), 1591 (C=C, aliphatic), 1453 (C=C, aromatic), 696 (C–CI), 1155 (C–O–C), 1053 (C–O).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 6.74 (s, 1H, Ar-H), 6.21 (m, 1H, Ar-H), 7.16-7.50 (m, 5H, Ar-H), 7.62 (d, J = 16 Hz, 1H, HC=CH (H-α)), 8.06 (d, J = 16 Hz, 1H, HC=CH (H-β)), 9.73 (s, 1H, NH).

ESI-MS (m/z): 362 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(thiophen-3-yl)-2-propen-1-one (4bb):



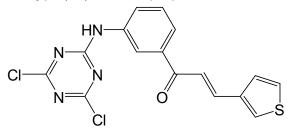
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3430 (N–H), 3019 (C–H, aromatic), 2973 (G-H, aliphatic), 1689 (C=O), 1599 (C=C, aliphatic), 1414 (C=C, aromatic), 688 (C–Cl).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 6.68 (s, 1H, Ar-H), 6.91 (s, 1H, Ar-H), 7.12 (s, 1H, Ar-H), 7.33-7.58 (m, 4H, Ar-H), 7.76 (d, J = 15.2 Hz, 1H, HC=CH (H-α)), 8.02 (d, J = 15.2 Hz, 1H, HC=CH (H-β)), 9.68 (s, 1H, NH).

ESI-MS (m/z): 378 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(pyrrol-2-yl)-2-propen-1-one (4cc):



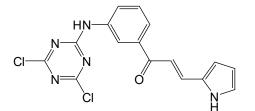
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3144 (N–H), 3052 (N–H), 3017 (G–H, aromatic), 2973 (C–H, aliphatic), 1695 (C=O), 1615 (C=C, aliphatic), 1414 (C=C, aromatic), 678 (C–Cl), 1308 (C–N).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 6.46 (s, 1H, Ar-H), 7.44 (m, 1H, Ar-H), 7.55-7.61 (m, 5H, Ar-H), 7.76 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 8.03 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.64 (s, 1H, NH), 10.55 (s, 1H, NH).

ESI-MS (m/z): 361 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(pyridin-2-yl)-2-propen-1-one (4dd):



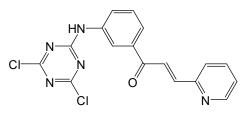
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3127 (N–H), 3019 (C–H, aromatic), 2931 (G-H, aliphatic), 1689 (C=O), 1604 (C=C, aliphatic), 1417 (C=C, aromatic), 688 (C–Cl), 1308 (C–N).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 6.98 (d, J = 16 Hz, 1H, HC=CH (H-α)), 7.13-7.69 (m, 8H, Ar-H), 7.78 (d, J = 16 Hz, 1H, HC=CH (H-β)), 9.60 (s, 1H, NH).

ESI-MS (m/z): 373 [M+H]+.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(pyridin-3-yl)-2-propen-1-one (4ee):



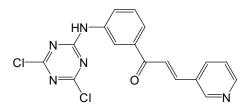
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3122 (N–H), 3011 (C–H, aromatic), 2922 (G-H, aliphatic), 1679 (C=O), 1609 (C=C, aliphatic), 1422 (C=C, aromatic), 1308 (CN), 681 (C–CI).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.22 (d, J = 16 Hz, 1H, HC=CH (H-α)), 7.23-7.59 (m, 8H, Ar-H), 7.68 (d, J = 16 Hz, 1H, HC=CH (H-β)), 9.58 (s, 1H, NH).

ESI-MS (m/z): 373 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(pyridin-4-yl)-2-propen-1-one (4ff):



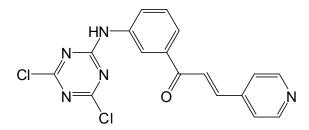
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3127 (N–H), 3019 (C–H, aromatic), 2931 (G-H, aliphatic), 1689 (C=O), 1604 (C=C, aliphatic), 1417 (C=C, aromatic), 688–(Cl), 1308 (C–N).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 6.98 (d, J = 16 Hz, 1H, HC=CH (H- α)), 7.13-7.69 (m, 8H, Ar-H), 7.78 (d, J = 16 Hz, 1H, HC=CH (H- β)), 9.60 (s, 1H, NH).

ESI-MS (m/z): 373 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(naphthalen-2-yl)-2-propen-1-one (4gg):



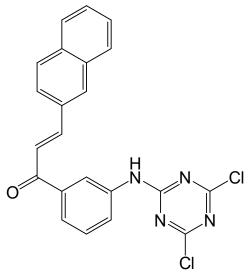
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3102 (N–H), 3015 (C–H, aromatic), 2926 (C–H, aliphatic), 1684 (C=O), 1602 (C=C, aliphatic), 1416 (C=C, aromatic), 682 (C–CI).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.62-7.83 (m, 11H, Ar-H), 7.87 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 8.16 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.70 (s, 1H, NH).

ESI-MS (m/z): 422 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(naphthalen-3-yl)-2-propen-1-one (4hh):



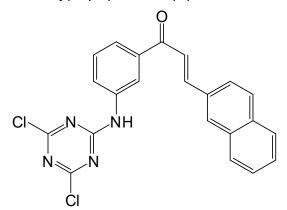
Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3115 (N–H), 3019 (C–H, aromatic), 2931 (G-H, aliphatic), 1689 (C=O), 1604 (C=C, aliphatic), 1417 (C=C, aromatic), 688 (C–Cl).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 7.62-8.33 (m, 11H, Ar-H), 7.89 (d, J = 15.2 Hz, 1H, HC=CH (H- α)), 8.26 (d, J = 15.2 Hz, 1H, HC=CH (H- β)), 9.71 (s, 1H, NH).

ESI-MS (m/z): 422 [M+H]⁺.

(E)-1-(3-(4,6-dichloro-1,3,5-triazin-2-ylamino)phenyl)-3-(anthracen-9-yl)-2-propen-1-one (4ii):



Colour: Light yellow crystals.

FT-IR (KBr, vmax, cm-1): 3127 (N–H), 3019 (C–H, aromatic), 2931 (C–H, aliphatic), 1689 (C=O), 1604 (C=C, aliphatic), 1417 (C=C, aromatic), 688 (C–Cl).

¹H NMR (400 MHz, DMSO-d₆, δ, ppm): 6.98-7.41 (m, 13H, Ar-H), 7.59 (d, J = 15.6 Hz, 1H, HC=CH (H-α)), 8.06 (d, J = 15.6 Hz, 1H, HC=CH (H-β)), 9.75 (s, 1H ESI-MS (m/z): 472 [M+H]⁺.

V. Acknowledgements

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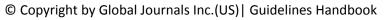


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1. Choosing the topic: In most cases, the topic is searched by the interest of author but it can be also suggested by the guides. You can have several topics and then you can judge that in which topic or subject you are finding yourself most comfortable. This can be done by asking several questions to yourself, like Will I be able to carry our search in this area? Will I find all necessary recourses to accomplish the search? Will I be able to find all information in this field area? If the answer of these types of questions will be "Yes" then you can choose that topic. In most of the cases, you may have to conduct the surveys and have to visit several places because this field is related to Computer Science and Information Technology. Also, you may have to do a lot of work to find all rise and falls regarding the various data of that subject. Sometimes, detailed information plays a vital role, instead of short information.

2. Evaluators are human: First thing to remember that evaluators are also human being. They are not only meant for rejecting a paper. They are here to evaluate your paper. So, present your Best.

3. Think Like Evaluators: If you are in a confusion or getting demotivated that your paper will be accepted by evaluators or not, then think and try to evaluate your paper like an Evaluator. Try to understand that what an evaluator wants in your research paper and automatically you will have your answer.

4. Make blueprints of paper: The outline is the plan or framework that will help you to arrange your thoughts. It will make your paper logical. But remember that all points of your outline must be related to the topic you have chosen.

5. Ask your Guides: If you are having any difficulty in your research, then do not hesitate to share your difficulty to your guide (if you have any). They will surely help you out and resolve your doubts. If you can't clarify what exactly you require for your work then ask the supervisor to help you with the alternative. He might also provide you the list of essential readings.

6. Use of computer is recommended: As you are doing research in the field of Computer Science, then this point is quite obvious.

7. Use right software: Always use good quality software packages. If you are not capable to judge good software then you can lose quality of your paper unknowingly. There are various software programs available to help you, which you can get through Internet.

8. Use the Internet for help: An excellent start for your paper can be by using the Google. It is an excellent search engine, where you can have your doubts resolved. You may also read some answers for the frequent question how to write my research paper or find model research paper. From the internet library you can download books. If you have all required books make important reading selecting and analyzing the specified information. Then put together research paper sketch out.

9. Use and get big pictures: Always use encyclopedias, Wikipedia to get pictures so that you can go into the depth.

10. Bookmarks are useful: When you read any book or magazine, you generally use bookmarks, right! It is a good habit, which helps to not to lose your continuity. You should always use bookmarks while searching on Internet also, which will make your search easier.

11. Revise what you wrote: When you write anything, always read it, summarize it and then finalize it.

12. Make all efforts: Make all efforts to mention what you are going to write in your paper. That means always have a good start. Try to mention everything in introduction, that what is the need of a particular research paper. Polish your work by good skill of writing and always give an evaluator, what he wants.

13. Have backups: When you are going to do any important thing like making research paper, you should always have backup copies of it either in your computer or in paper. This will help you to not to lose any of your important.

14. Produce good diagrams of your own: Always try to include good charts or diagrams in your paper to improve quality. Using several and unnecessary diagrams will degrade the quality of your paper by creating "hotchpotch." So always, try to make and include those diagrams, which are made by your own to improve readability and understandability of your paper.

15. Use of direct quotes: When you do research relevant to literature, history or current affairs then use of quotes become essential but if study is relevant to science then use of quotes is not preferable.

16. Use proper verb tense: Use proper verb tenses in your paper. Use past tense, to present those events that happened. Use present tense to indicate events that are going on. Use future tense to indicate future happening events. Use of improper and wrong tenses will confuse the evaluator. Avoid the sentences that are incomplete.

17. Never use online paper: If you are getting any paper on Internet, then never use it as your research paper because it might be possible that evaluator has already seen it or maybe it is outdated version.

18. Pick a good study spot: To do your research studies always try to pick a spot, which is quiet. Every spot is not for studies. Spot that suits you choose it and proceed further.

19. Know what you know: Always try to know, what you know by making objectives. Else, you will be confused and cannot achieve your target.

20. Use good quality grammar: Always use a good quality grammar and use words that will throw positive impact on evaluator. Use of good quality grammar does not mean to use tough words, that for each word the evaluator has to go through dictionary. Do not start sentence with a conjunction. Do not fragment sentences. Eliminate one-word sentences. Ignore passive voice. Do not ever use a big word when a diminutive one would suffice. Verbs have to be in agreement with their subjects. Prepositions are not expressions to finish sentences with. It is incorrect to ever divide an infinitive. Avoid clichés like the disease. Also, always shun irritating alliteration. Use language that is simple and straight forward. put together a neat summary.

21. Arrangement of information: Each section of the main body should start with an opening sentence and there should be a changeover at the end of the section. Give only valid and powerful arguments to your topic. You may also maintain your arguments with records.

22. Never start in last minute: Always start at right time and give enough time to research work. Leaving everything to the last minute will degrade your paper and spoil your work.

23. Multitasking in research is not good: Doing several things at the same time proves bad habit in case of research activity. Research is an area, where everything has a particular time slot. Divide your research work in parts and do particular part in particular time slot.

24. Never copy others' work: Never copy others' work and give it your name because if evaluator has seen it anywhere you will be in trouble.

25. Take proper rest and food: No matter how many hours you spend for your research activity, if you are not taking care of your health then all your efforts will be in vain. For a quality research, study is must, and this can be done by taking proper rest and food.

26. Go for seminars: Attend seminars if the topic is relevant to your research area. Utilize all your resources.

27. Refresh your mind after intervals: Try to give rest to your mind by listening to soft music or by sleeping in intervals. This will also improve your memory.

28. Make colleagues: Always try to make colleagues. No matter how sharper or intelligent you are, if you make colleagues you can have several ideas, which will be helpful for your research.

29. Think technically: Always think technically. If anything happens, then search its reasons, its benefits, and demerits.

30. Think and then print: When you will go to print your paper, notice that tables are not be split, headings are not detached from their descriptions, and page sequence is maintained.

31. Adding unnecessary information: Do not add unnecessary information, like, I have used MS Excel to draw graph. Do not add irrelevant and inappropriate material. These all will create superfluous. Foreign terminology and phrases are not apropos. One should NEVER take a broad view. Analogy in script is like feathers on a snake. Not at all use a large word when a very small one would be sufficient. Use words properly, regardless of how others use them. Remove quotations. Puns are for kids, not grunt readers. Amplification is a billion times of inferior quality than sarcasm.

32. Never oversimplify everything: To add material in your research paper, never go for oversimplification. This will definitely irritate the evaluator. Be more or less specific. Also too, by no means, ever use rhythmic redundancies. Contractions aren't essential and shouldn't be there used. Comparisons are as terrible as clichés. Give up ampersands and abbreviations, and so on. Remove commas, that are, not necessary. Parenthetical words however should be together with this in commas. Understatement is all the time the complete best way to put onward earth-shaking thoughts. Give a detailed literary review.

33. Report concluded results: Use concluded results. From raw data, filter the results and then conclude your studies based on measurements and observations taken. Significant figures and appropriate number of decimal places should be used. Parenthetical remarks are prohibitive. Proofread carefully at final stage. In the end give outline to your arguments. Spot out perspectives of further study of this subject. Justify your conclusion by at the bottom of them with sufficient justifications and examples.

34. After conclusion: Once you have concluded your research, the next most important step is to present your findings. Presentation is extremely important as it is the definite medium though which your research is going to be in print to the rest of the crowd. Care should be taken to categorize your thoughts well and present them in a logical and neat manner. A good quality research paper format is essential because it serves to highlight your research paper and bring to light all necessary aspects in your research.

INFORMAL GUIDELINES OF RESEARCH PAPER WRITING

Key points to remember:

- Submit all work in its final form.
- Write your paper in the form, which is presented in the guidelines using the template.
- Please note the criterion for grading the final paper by peer-reviewers.

Final Points:

A purpose of organizing a research paper is to let people to interpret your effort selectively. The journal requires the following sections, submitted in the order listed, each section to start on a new page.

The introduction will be compiled from reference matter and will reflect the design processes or outline of basis that direct you to make study. As you will carry out the process of study, the method and process section will be constructed as like that. The result segment will show related statistics in nearly sequential order and will direct the reviewers next to the similar intellectual paths throughout the data that you took to carry out your study. The discussion section will provide understanding of the data and projections as to the implication of the results. The use of good quality references all through the paper will give the effort trustworthiness by representing an alertness of prior workings.

Writing a research paper is not an easy job no matter how trouble-free the actual research or concept. Practice, excellent preparation, and controlled record keeping are the only means to make straightforward the progression.

General style:

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· Adhere to recommended page limits

Mistakes to evade

- Insertion a title at the foot of a page with the subsequent text on the next page
- Separating a table/chart or figure impound each figure/table to a single page
- Submitting a manuscript with pages out of sequence

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- \cdot Use standard writing style including articles ("a", "the," etc.)
- \cdot Keep on paying attention on the research topic of the paper
- · Use paragraphs to split each significant point (excluding for the abstract)
- \cdot Align the primary line of each section
- · Present your points in sound order
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- \cdot Use past tense to describe specific results
- · Shun familiar wording, don't address the reviewer directly, and don't use slang, slang language, or superlatives

· Shun use of extra pictures - include only those figures essential to presenting results

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The summary should be two hundred words or less. It should briefly and clearly explain the key findings reported in the manuscript-must have precise statistics. It should not have abnormal acronyms or abbreviations. It should be logical in itself. Shun citing references at this point.

An abstract is a brief distinct paragraph summary of finished work or work in development. In a minute or less a reviewer can be taught the foundation behind the study, common approach to the problem, relevant results, and significant conclusions or new questions.

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- Reason of the study theory, overall issue, purpose
- Fundamental goal
- To the point depiction of the research
- Consequences, including <u>definite statistics</u> if the consequences are quantitative in nature, account quantitative data; results of any numerical analysis should be reported
- Significant conclusions or questions that track from the research(es)

Approach:

- Single section, and succinct
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- A conceptual should situate on its own, and not submit to any other part of the paper such as a form or table
- Center on shortening results bound background information to a verdict or two, if completely necessary
- What you account in an conceptual must be regular with what you reported in the manuscript
- Exact spelling, clearness of sentences and phrases, and appropriate reporting of quantities (proper units, important statistics) are just as significant in an abstract as they are anywhere else

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The **Introduction** should "introduce" the manuscript. The reviewer should be presented with sufficient background information to be capable to comprehend and calculate the purpose of your study without having to submit to other works. The basis for the study should be offered. Give most important references but shun difficult to make a comprehensive appraisal of the topic. In the introduction, describe the problem visibly. If the problem is not acknowledged in a logical, reasonable way, the reviewer will have no attention in your result. Speak in common terms about techniques used to explain the problem, if needed, but do not present any particulars about the protocols here. Following approach can create a valuable beginning:

- Explain the value (significance) of the study
- Shield the model why did you employ this particular system or method? What is its compensation? You strength remark on its appropriateness from a abstract point of vision as well as point out sensible reasons for using it.
- Present a justification. Status your particular theory (es) or aim(s), and describe the logic that led you to choose them.
- Very for a short time explain the tentative propose and how it skilled the declared objectives.

Approach:

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- Present surroundings information only as desirable in order hold up a situation. The reviewer does not desire to read the whole thing you know about a topic.
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- Embrace particular materials, and any tools or provisions that are not frequently found in laboratories.
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- If use of a definite type of tools.
- Materials may be reported in a part section or else they may be recognized along with your measures.

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- Report the method (not particulars of each process that engaged the same methodology)
- Describe the method entirely
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- Simplify details how procedures were completed not how they were exclusively performed on a particular day.
- If well known procedures were used, account the procedure by name, possibly with reference, and that's all.

Approach:

- It is embarrassed or not possible to use vigorous voice when documenting methods with no using first person, which would focus the reviewer's interest on the researcher rather than the job. As a result when script up the methods most authors use third person passive voice.
- Use standard style in this and in every other part of the paper avoid familiar lists, and use full sentences.

What to keep away from

- Resources and methods are not a set of information.
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- Leave out information that is immaterial to a third party.

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The principle of a results segment is to present and demonstrate your conclusion. Create this part a entirely objective details of the outcome, and save all understanding for the discussion.

The page length of this segment is set by the sum and types of data to be reported. Carry on to be to the point, by means of statistics and tables, if suitable, to present consequences most efficiently. You must obviously differentiate material that would usually be incorporated in a study editorial from any unprocessed data or additional appendix matter that would not be available. In fact, such matter should not be submitted at all except requested by the instructor.



Content

- Sum up your conclusion in text and demonstrate them, if suitable, with figures and tables.
- In manuscript, explain each of your consequences, point the reader to remarks that are most appropriate.
- Present a background, such as by describing the question that was addressed by creation an exacting study.
- Explain results of control experiments and comprise remarks that are not accessible in a prescribed figure or table, if appropriate.

• Examine your data, then prepare the analyzed (transformed) data in the form of a figure (graph), table, or in manuscript form. What to stay away from

- Do not discuss or infer your outcome, report surroundings information, or try to explain anything.
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Approach

- As forever, use past tense when you submit to your results, and put the whole thing in a reasonable order.
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- Give details all of your remarks as much as possible, focus on mechanisms.
- Make a decision if the tentative design sufficiently addressed the theory, and whether or not it was correctly restricted.
- Try to present substitute explanations if sensible alternatives be present.
- One research will not counter an overall question, so maintain the large picture in mind, where do you go next? The best studies unlock new avenues of study. What questions remain?
- Recommendations for detailed papers will offer supplementary suggestions.

Approach:

- When you refer to information, differentiate data generated by your own studies from available information
- Submit to work done by specific persons (including you) in past tense.
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Introduction	Containing all background details with clear goal and appropriate details, flow specification, no grammar and spelling mistake, well organized sentence and paragraph, reference cited	Unclear and confusing data, appropriate format, grammar and spelling errors with unorganized matter	Out of place depth and content, hazy format
Methods and Procedures	Clear and to the point with well arranged paragraph, precision and accuracy of facts and figures, well organized subheads	Difficult to comprehend with embarrassed text, too much explanation but completed	Incorrect and unorganized structure with hazy meaning
Result	Well organized, Clear and specific, Correct units with precision, correct data, well structuring of paragraph, no grammar and spelling mistake	Complete and embarrassed text, difficult to comprehend	Irregular format with wrong facts and figures
Discussion	Well organized, meaningful specification, sound conclusion, logical and concise explanation, highly structured paragraph reference cited	Wordy, unclear conclusion, spurious	Conclusion is not cited, unorganized, difficult to comprehend
References	Complete and correct format, well organized	Beside the point, Incomplete	Wrong format and structuring

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