

**A.S.D GOVERNMENT DEGREE COLLEGE FOR WOMEN (A),
KAKINADA**



DEPARTMENT OF CHEMISTRY

CERTIFICATE COURSE

ON

BASIC CHEMISTRY MOLECULAR MODELLING SOFTWARE

2022-23

Course Duration : 45 Hrs

A.S.D. GOVERNMENT DEGREE COLLEGE FOR WOMEN



Autonomous and NAAC Re-Accredited With "B" Grade in Cycle-III
Affiliated to Adikavi Nannaya University, Rajamahendravaram
Kakinada-533 002, Andhra Pradesh





Department of Chemistry

A SKILL DEVELOPMENT CERTIFICATE COURSE ON "BASIC CHEMISTRY MOLECULAR MODELING SOFTWARE" (Chem Draw and ACD Chem Sketch)

ADMISSION NOTIFICATION 2022 - 23

Dear Chemistry Learners!

Are you interested in Drawing Chemical Structures on a computer?   Chem Draw ACD Chem Sketch

Then come on! Here is an Opportunity for you.

The department of chemistry offers a certificate course on the Usage of Softwares for drawing chemical structures.

Course Highlights

- This course aims at imparting skills on use of various open-source chemistry tools that are essential for any student with chemistry as a major subject.
- At the end of course, the participants will be able to use these softwares for drawing chemical structures, generation of their names, retrieve information about physical properties calculations, three-dimensional molecular structure calculations, spectroscopic signatures, chemical reaction pathways prediction, molecular functional groups and other parameters efficiently.

Target Group

B. Sc (First/ Second Year) with Chemistry as one of the Subjects.

For Details Contact
For Details Contact
Mallikarjuna Sarma

Course Coordinator, Department of Chemistry

Lecturer In-Charge, Department of Chemistry, Phone No.: 8341546804, 9676822550

Last Date for enrolment:
16.11.2022

No
Course Fee

"Drawing Chemical Structures is an art of Chemistry"

Letter of Permission from the Principal

From
V. Mallikarjuna Sharma
Head, Dept. of Chemistry
for Women (A)
A.S.D. Govt. Degree College for Women (A)
Kakinada.

To
Principal
A.S.D. Govt. Degree College
Kakinada.

Respected Madam,

Sub: ASD GDC (W) (A), Kakinada-Department of Chemistry - Seeking permission to start a certificate course on "**Certificate Course in Basic Chemistry Molecular Modelling Softwares**" for the students of III Semester for the Academic Year 2022-23 – Permission – Regarding.

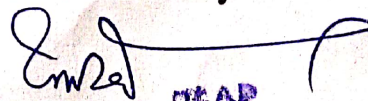
With reference to the subject cited , I bring to your kind notice that the Department of Chemistry is offering a certificate course in "**Certificate Course in Basic Chemistry Molecular Modelling Software**" for the year 2022 – 23. In this Connection I request you to grant permission to start the course from 17th November to 28th February for the academic year 2022-2023.

Thanking You Madam,

Place: Kakinada

Date:

Yours faithfully



HEAD
DEPARTMENT OF CHEMISTRY
(V. Mallikarjuna Sharma)
A.S.D. GOVT. DEGREE COLLEGE FOR WOMEN
JAGANNAICKPUR
KAKINADA - 531 001

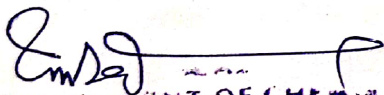
Circular


A.S.D Government Degree College for Women (A), Kakinada

Department of Chemistry



The students of IIIrd semester are here by informed that the Department of Chemistry is going to conduct a certificate course on “**Certificate Course in Basic Chemistry Molecular Modelling Software**” for 45 hours (17th November to 28th February) with no entry fee. Those who are interested should enroll their names in Department of Chemistry on or before 16th December 2022.


V. Mallikarjuna Sarma
DEPARTMENT OF CHEMISTRY
A.S.D. GOVT. DEGREE COLLEGE (W)
JAGANNAICKPUR
KAKINADA-531102
In-Charge of Chemistry


PRINCIPAL
A.S.D. GOVT. DEGREE COLLEGE (W)
AUTONOMOUS
KAKINADA

Circulated to the Classes

II BA

II H.Sc

II BCOM

II MPC

II BCOM CA

II MPCS

II CBZ

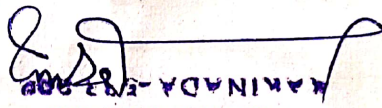

II CBHT

II CZAQT

II CBMB

Brief report on Certificate Course

Academic Year 2022-23

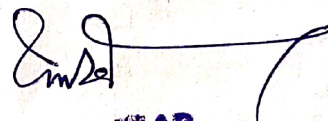
Name of the Certificate Course	Certificate Course in “Basic Chemistry Molecular Modelling Softwares”
Academic Year of Course	2022-23
Department Conducting the Course	Department Of Chemistry
Duration Of the Course	45 Hrs
Number of Students Completed the Course	30 Students
Brief Report	Certificate course on “Basic Chemistry Molecular Modelling Softwares” was conducted by the department of Chemistry for 45hrs in which total 30 students were enrolled. The course was held from from 17 th November2022 to 28 th February 2023. All the students appeared for the examination conducted at the end of the course and completed the course. They have been given grades. The certificates are also given to them.
Number of Beneficiaries	Students : 30
Signature of the Certificate Course Coordinator	
Signature & Stamp of the Principal	 PRINCIPAL A.S.D.GOV.T.DEGREE COLLEGE (W) AUTONOMOUS KAKINADA



List of Students Enrolled for Certificate Course

S.No	Regd. No	Name of the student	Programme
1.	2137001	Kolli Venkata Lakshmi	III B.Sc, M.P.C
2.	2137002	Bade Manasa	III B.Sc, M.P.C
3.	2137005	Chukka Ramya Sri	III B.Sc, M.P.C
4.	2137006	Devada Lakshmi Keerthi	III B.Sc, M.P.C
5.	2137007	Gedela Navya	III B.Sc, M.P.C
6.	2137008	Karri Devi	III B.Sc, M.P.C
7.	2137009	Karri Sandhya	III B.Sc, M.P.C
8.	2137010	Konda Asha Latha	III B.Sc, M.P.C
9.	2137011	Koram Reena	III B.Sc, M.P.C
10.	2137012	Malladi Malini	III B.Sc, M.P.C
11.	2137013	Malladi Sudha Sri	III B.Sc, M.P.C
12.	2137014	Medapati Navyasri	III B.Sc, M.P.C
13.	2137015	Miriyala Keerthi	III B.Sc, M.P.C
14.	2137016	Muramalla Devi Sri Deepthi	III B.Sc, M.P.C
15.	2137017	Nedunuri Joshnavi	III B.Sc, M.P.C
16.	2137018	Oleti Kanaka Mahalakshmi	III B.Sc, M.P.C
17.	2137019	Panthadi Bhavani	III B.Sc, M.P.C
18.	2137022	Pemmadi Lavanya Satya	III B.Sc, M.P.C
19.	2137025	Yelugubanti Sai Nikitha	III B.Sc, M.P.C
20.	2137027	Bandaru Saikalyani	III B.Sc, M.P.C
21.	2137030	Chandala Mahalakshmi	III B.Sc, M.P.C
22.	2137031	Chinthakayala Kumari	III B.Sc, M.P.C
23.	2137033	Duryodhanula Durgadevi	III B.Sc, M.P.C
24.	2137038	Madadha Harika	III B.Sc, M.P.C

25.	2137039	Madakam Anusha	III B.Sc, M.P.C
26.	2137041	Pedireddy Madhuri	III B.Sc, M.P.C
27.	2137044	Punyamantula Sravya	III B.Sc, M.P.C
28.	2137046	Rajamenu Bhavana	III B.Sc, M.P.C
29.	2137047	Seeli Neelima	III B.Sc, M.P.C
30.	2137050	Yarramneedi Veera Mounika	III B.Sc, M.P.C



HEAD
DEPARTMENT OF CHEMISTRY
O.S.S. GOVT. DEGREE COLLEGE
JAGANNAICKPUR
KAKINADA-537 501

A.S.D Government Degree College for Women (A), Kakinada
Autonomous and NAAC Re-Accredited With "B"
Grade in Cycle-III Affiliated to Adikavi Nannaya
University, Rajamahendravaram

DEPARTMENT OF CHEMISTRY

APPLICATION FORM

(Skill Development Certificate Course on "Basic Chemistry Molecular Modelling Softwares")

1. Name of the candidate (in BLOCK letters): Kollif Venkata laxmi
2. Class studying: Bsc . MPE
3. Admission No: 11774
4. Reg.No: 2137001
5. Father's Name : Kollif Ramana
6. Occupation : FARMER
7. Date of birth : 1/18/2004
8. Aadhar Number : 574248081491
9. Grade of Chemistry in Previous exams:
10. Address for correspondence: Sanjeev Nagar

11. Category : OC/ OBC/ SC/ ST/ OTHERS

12. Email ID: kollifv223@gmail.com

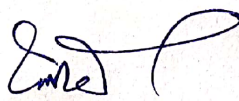
13. Mobile number: 6303674509

Undertaking

I have gone through syllabus carefully and understand

- 1 To maintain 75% attendance is a pre-requisite for obtaining certificate course.
- 2 To maintain at least 50% marks in final test.
- 3 To follow discipline of ASDGDC (W) (A), Kakinada

K. Venkata Lakshmi
Signature of candidate


Signature of course coordinator



A.S.D. GOVERNMENT DEGREE COLLEGE FOR WOMEN (AUTONOMOUS)
KAKINADA
DEPARTMENT OF CHEMISTRY
Certificate Course in Basic Chemistry Molecular Modelling Software

Course Duration: 45 Hours

Eligibility: All B.Sc. Second Year students having chemistry as major subject are eligible

Number of seats: 30

Objectives:

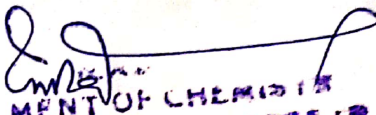
1. Department of Chemistry of A.S.D. Government Degree College for Women (Autonomous) Kakinada offers 45 hours **Certificate Course in Basic Chemistry Molecular Modelling softwares.**
2. This course aims at imparting skills on use of various open-source chemistry tools that are essential for any student with chemistry as a major subject.
3. At the end of course, the participants will be able to use these softwares for drawing chemical structures, generation of their names, retrieve information about physical properties calculations, three-dimensional molecular structure calculations, spectroscopic signatures, chemical reaction pathways prediction, molecular functional groups and other parameters efficiently.

Course outcomes:

1. The candidate will be able to use ACD Chem sketch for Drawing of simple and complex chemical structures, calculation of physical/chemical properties.
2. The candidate will be able to use Cambridge Chem Draw Ultra Drawing of simple and complex chemical structures, calculation of physical/chemical properties.
3. Students should be able to accurately represents stereochemistry, and molecular geometry.
4. Students learn ability to draw and depict chemical reactions using ACD Chem Sketch software and ChemDraw, including reaction mechanisms, intermediates, and products.
5. This skill necessary for success in various industries and research.

Evaluation Process:

Assessment of candidates will be done through practical examination-50 M after completion of course. All successful candidates with $\geq 40\%$ will be awarded certificates.


DEPARTMENT OF CHEMISTRY
J.S.B. GOVT. DEGREE COLLEGE
JAGANNAICKPUR
KAKINADA-533 009

SYLLABUS

Module 1 (10 hours)

ACD ChemSketch software: – Introduction, download and installation process, Drawing various chemical structures (acyclic, cyclic, polycyclic, heterocyclic), name generation from structures, conversion of name of molecule into its structure, calculation of physical properties such as density, molecular weight, molecular formula from structural formula, bond angles, bond lengths, dihedral angles.

Module 2 (10 hours)

Cambridge ChemDraw Ultra software– Introduction, download and installation process, drawing various chemical structures (acyclic, cyclic, polycyclic, heterocyclic), nomenclature generation, conversion of name into molecular structure, read out the stereochemistry of asymmetric molecules, calculation of physical properties such as density, molecular weight, molecular formula, refractive index from structural formula.

Module 3 (9 hours)

Spectral data analysis:

To predict IR, ^1H , ^{13}C NMR spectrum's from molecular structure

Predict chemical shift values from ^1H NMR spectra and, the ^{13}C NMR.

Analyse structure of Compound.

Module 3 (16 hours)

To draw Chemical reactions & Study their mechanisms through chemistry softwares-

Reaction mechanism- study of mechanism of some organic name reactions through ACD ChemSketch software and ChemDraw Ultra software

1. Acetoacetic Ester Condensation
2. Aldol Condensation
3. Baeyer-Villiger Oxidation
4. Benzoin Condensation
5. Birch Reduction
6. Cannizzaro Oxidation Reduction
7. Claisen Condensation
8. Malonic Ester Synthesis
9. Mannich Reaction
10. Michael Addition
11. Pinacol Rearrangement
12. Robinson Annulation
13. Wittig Reaction
14. Reimer-Tieman Reaction
15. Perkin Reaction
16. Hoffman degradation
17. Friedel crafts alkylation
18. HVZ reaction

A.S.D.GOV.T.DEGREE COLLEGE FOR WOMEN(A) KAKINADA

CHEMISTRY DEPARTMENT TIME TABLE 2022-23 (I, III, V SEMESTER)

DAY	CLASS	0 HOUR (9:00 to 10)	1 (10:00 to 10:50)	2 (10.50 to 11.40)	3 (11.40 AM to 12.30 PM)	4 (12.30 PM to 1.20 PM)	5 (2.20 to 3.10)	6 (3.10 to 4.00)	7 (Co Curricul & Extr Curricul
MON	I B.Sc						I MPC (MSL),RB-1 I CBZ (VMS), RB-2 I CZAqT, CBHt, MB (PL)		
	II B.Sc	Certificate Course		II MPC (KJL),RB-3 II CBZ (SPD) II CBMB, CZAqT,CBHt (MSL) RB-2	m Practicals S8 (VMS), S9 (SPD), S10 (M)				
	III B.Sc		III MPC 7D (PL), RB-1 III CBZ 6D (KJL), III CBMB,CBHt,CZAqT 6D (MSL),RB-2				Chem Practicals 6D T1(KJL), T2(SPD), T3(PL)		
TUE	I B.Sc		IMPC (MSL),RB-3, ICBZ(VMS), ICBMB,CZAqT,CBHt (PL),RB-2						
	II B.Sc		Chem Practicals S1(SPD), S2(KJL)						
	III B.Sc				(PL),RB_1 III CBZ 6D (KJL),RB-2	(VMS),RB-1 III CBZ,CBMB,CBH	Chem Practicals 6D T6(VMS), T7(MSL)		
WED	I B.Sc								
	II B.Sc	Certificate Course	Chem Practicals S5(VMS), S6(SPD)				II MPC (KJL),RB-1 II CBZ (SPD) II CBMB, CZAqT,CBHt		
	III B.Sc			III MPC 7D (PL), R-24 III CBZ 6D (KJL), IIICBMB,CBHt,CZAqT 6D (MSL),RB-2	III MPC 7D (PL),R-24 III CBZ 6D (KJL), III CBMB,CBHt,CZ		Chem Practicals 6D T8(VMS), T9(PL),T10(MSL)		

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A.S.D.GOV.T.DEGREE COLLEGE FOR WOMEN(A) KAKINADA

CHEMISTRY DEPARTMENT TIME TABLE 2022-23 (I, III, V SEMESTER)

DAY	CLASS	0 HOUR (9:00 to 10)	1 (10:00 to 10:50)	2 (10.50 to 11.40)	3 (11.40 AM to 12.30 PM)	4 (12.30 PM to 1.20 PM)	5 (2.20 to 3.10)	6 (3.10 to 4.00)	7 (Co-Curricular & Extra Curricular)	
MON	I B.Sc						I MPC (MSL),RB-1 I CBZ (VMS), RB-2 I CZAqT, CBHt, MB (PL)			
	II B.Sc	Certificate Course		II MPC (KJL),RB-3 II CBZ (SPD) II CBMB, CZAqT,CBHt (MSL) RB-2	m Practicals S8 (VMS), S9 (SPD), S10 (M)					
	III B.Sc		III MPC 7D (PL), RB-1 III CBZ 6D (KJL), III CBMB,CBHT,CZAqT 6D (MSL),RB-2				Chem Practicals 6D T1(KJL), T2(SPD), T3(PL)			
TUE	I B.Sc		IMPC (MSL),RB-3, ICBZ(VMS), ICBMB,CZAqT,CBHt (PL),RB-2							
	II B.Sc		Chem Practicals S1(SPD), S2(KJL)							
	III B.Sc				(PL),RB_1 III CBZ 6D (KJL),RB-2	(VMS),RB-1 III CBZ,CBMB,CBH	Chem Practicals 6D T6(VMS), T7(MSL)			
WED	I B.Sc									
	II B.Sc	Certificate Course	Chem Practicals S5(VMS), S6(SPD)					II MPC (KJL),RB-1 II CBZ (SPD) II CBMB, CZAqT,CBHt		
	III B.Sc			III MPC 7D (PL), R-24 III CBZ 6D (KJL), IIICBMB,CBHT,CZAqT 6D (MSL),RB-2	(PL),R-24 III CBZ 6D (KJL), III CBMB,CBHT,CZ		Chem Practicals 6D T8(VMS),T9(PL),T10(MSL)			

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THU	I B.Sc		Chem Practicals F7(VMS), F8(PL), F9(MSL)				ICBZ (VMS),RB-2 ICZAqT,CBHt,MB(PL) I MPC (MSL),R-23		
	II B.Sc			II MPC (KJL),R-23 II CBZ (SPD) II CBMB, CZAqT, CBHt (MSL),RB-2	II MPC LSC, EE (MSL),				
	III B.Sc				III MPC 6D (VMS),R24 III CBZ CBMB, CBHT, CZAqT 7D				Chem Practicals 7D T1(KJL), T2(SPD), T3(PL)
FRI	I B.Sc		Chem Practicals F5(VMS), F6(KJL)		3 ICBZ(VMS), ICBMB,CZAqT,C BHT (PL),RB-2				
	II B.Sc	Certificate Course				22 II CBZ (SPD),RB- 2		II MPC LSC EE (SPD), R-24	
	III B.Sc			III MPC 6D (VMS),R-24 III CBZ CBMB,CBHT,CZAqT 7D (SPD),RB-2				Chem Practicals 7D T6(KJL), T7(MSL)	
SAT	I B.Sc		Tutor Ward	Chem Practicals F1(PL)					
	II B.Sc								
	III B.Sc				III MPC 6D (VMS),R-24 III CBZ , CBMB, CBHT, CZAqT 7D			Chem Practicals 7D T8(KJL), T9(SPD), T10(MSL)	

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MODEL QUESTION PAPER

SEMESTER - III

Certificate Course in Basic Chemistry Molecular Modelling Softwares

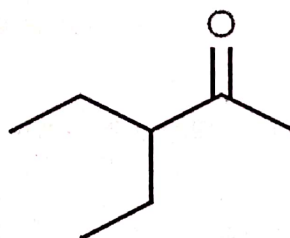
Time: 2 hours

Maximum Marks: 50M

Section- A

Answer any TEN of the following questions. Each carries TWO marks $10 \times 3 = 30$ M

1. Draw structure of 2-Propanol and find its physical properties M.Pt, B.Pt, density and refractive index by using ACD Chem Sketch software?
2. Find IUPAC Nomenclature of following compound. Predict bond angle, bond length, dihedral angle of carbonyl functional group by using ACD Chem Sketch software?

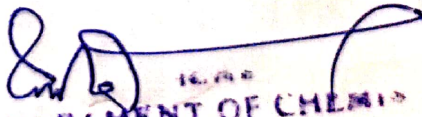


3. Predict 3D structure of (S)-2 Bromo butane by using ACD Chem Sketch software?
4. Predict IR spectrum of Ethyl alcohol and write functional group stretching frequency from IR spectrum by using Chem Draw?
5. Determine NMR spectrum of acetaldehyde? Analyse its Chemical shift values from spectrum by using Chem Draw?
6. Analyse ^{13}C NMR of Toluene by using Chem Draw ?
7. Write Chemical equations for Friedel crafts acylation?
8. Write Chemical equations for Pinacol-Pinacolone Rearrangement
9. Write Chemical equations for Claisen Condensation?
10. Write Chemical equations for Pinacol-Pinacolone Rearrangement?
11. Write Chemical equations for Friedel Crafts alkylation?
12. Write Chemical equations for Kolbe-Schmidt Reaction?

Section- B

Answer any **FOUR** of the following questions. Each carries **FIVE** mark $4 \times 5 = 20$ M

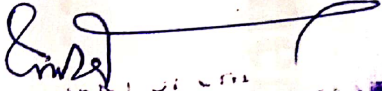
1. Draw structure of following compounds and predict their physical properties by using ACD Chem Sketch software
a) Phenol b) Pyridine.
2. Predict IR, NMR, ^{13}C spectral data of Toluene by using Chem Draw? Write their spectral data?
3. Sketch structure (S)-Alanine and get it IR, NMR Spectrums by using Chem Draw?
4. Write mechanism of Aldol reaction?
5. Write mechanism of Cannizaro reaction?
6. Write mechanism of Friedel Crafts alkylation?
7. Write mechanism of Aldol condensation?
8. Write mechanism of Benzoin Condensation?


DEPARTMENT OF CHEMISTRY
M.B. GOVT. DEGREE COLLEGE
JAGANNAICKPUR
KARNATAKA - 577 501

List of Students Completed Certificate Course with Grades

S.No	Regd. No	Name of the student	Programme	Grade
1.	2137001	Kolli Venkata Lakshmi	III B.Sc, M.P.C	A
2.	2137002	Bade Manasa	III B.Sc, M.P.C	A
3.	2137005	Chukka Ramya Sri	III B.Sc, M.P.C	A
4.	2137006	Devada Lakshmi Keerthi	III B.Sc, M.P.C	A
5.	2137007	Gedela Navya	III B.Sc, M.P.C	A
6.	2137008	Karri Devi	III B.Sc, M.P.C	A
7.	2137009	Karri Sandhya	III B.Sc, M.P.C	O
8.	2137010	Konda Asha Latha	III B.Sc, M.P.C	A
9.	2137011	Koram Reena	III B.Sc, M.P.C	B
10.	2137012	Malladi Malini	III B.Sc, M.P.C	A
11.	2137013	Malladi Sudha Sri	III B.Sc, M.P.C	O
12.	2137014	Medapati Navyasri	III B.Sc, M.P.C	A
13.	2137015	Miriyala Keerthi	III B.Sc, M.P.C	A
14.	2137016	Muramalla Devi Sri Deepthi	III B.Sc, M.P.C	A
15.	2137017	Nedunuri Joshnavi	III B.Sc, M.P.C	O
16.	2137018	Oleti Kanaka Mahalakshmi	III B.Sc, M.P.C	A
17.	2137019	Panthadi Bhavani	III B.Sc, M.P.C	A
18.	2137022	Pemmadi Lavanya Satya	III B.Sc, M.P.C	A
19.	2137025	Yelugubanti Sai Nikitha	III B.Sc, M.P.C	A
20.	2137027	Bandaru Saikalyani	III B.Sc, M.P.C	A
21.	2137030	Chandala Mahalakshmi	III B.Sc, M.P.C	A
22.	2137031	Chinthakayala Kumari	III B.Sc, M.P.C	A
23.	2137033	Duryodhanula Durgadevi	III B.Sc, M.P.C	A
24.	2137038	Madadha Harika	III B.Sc, M.P.C	A

25.	2137039	Madakam Anusha	III B.Sc, M.P.C	A
26.	2137041	Pedireddy Madhuri	III B.Sc, M.P.C	A
27.	2137044	Punyamantula Sravya	III B.Sc, M.P.C	A
28.	2137046	Rajamenu Bhavana	III B.Sc, M.P.C	A
29.	2137047	Seeli Neelima	III B.Sc, M.P.C	A
30.	2137050	Yarramneedi Veera Mounika	III B.Sc, M.P.C	A


DEPARTMENT OF UG
J.S.B. GOVT. DEGREE COLLEGE
JAGANNAICKPUR
KAKINADA-533 000

A.S.D.GOVERNMENT DEGREE COLLEGE FOR WOMEN(A), KAKINADA



Department of Chemistry

This is to certify that Ms-----
-----of class/group has successfully completed the 45
hrs Certificate Course in "Basic Chemistry Molecular Modelling Softwares"
Conducted by Department of Chemistry with -----grade for the academic year
2022 - 23 from 17th November 2022 to 28th February 2023.



[Signature]
A.S.D. GOVT DEGREE COLLEGE
JAGANNAICKPUR
KAKINADA
Convenor

[Signature]
PRINCIPAL
A.S.D. GOVT. DEGREE C.
AUTONOMOUS
KAKINADA
Principal

