#### Computational and Experimental Study of the Reaction of Propyl Amine with Chloranil

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Dissertation submitted to

Mahatma Gandhi University, Kottayam
In partial fulfillment of the requirements for the award of the degree of
Master of Science in Chemistry



By,

AKHIL.K.S.

Register No.130011007120

Under the Guidance of

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Dr. M. George,

Associate Professor

Department of Chemistry, Sacred Heart College, Thevara, Kochi

September 2015

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# DEPARTMENT OF CHEMISTRY CERTIFICATE

This is to certify that the Project Work Titled "Computational and Experimental Study of the Reaction of Propyl Amine with chloranil" is a bonafide work of AKHIL K S of semester IV, M.Sc. Branch III; carried out in the Department of Chemistry, Sacred Heart College, Thevara during the academic year 2014-15.

Place: Kochi The Head, Dept. of Chemistry

Date: Sacred Heart College, Thevara

#### **CERTIFICATE FROM THE GUIDE**

This is to certify that the Project Work Titled "Computational and Experimental Study of the Reaction of Propyl Amine with Chloranil" is a bonafide work of Akhil K S of semester IV, M.Sc. Branch III; carried out under my guidance in the Department of Chemistry, Sacred Heart College, Thevara during the academic year 2014-15.

Place: Thevara Date: Dr. M. George,
Associate Professor,
Department of Chemistry
Sacred Heart College, Thevara

E CANDIDATE			
I hereby declare, that the Project Work Titled "Computational and Experimental Study of			
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5	issuu.co				<b>%2</b>
6	www.ijpl				<b>%2</b>
7	WWW.SCI	ence.gov			<b>%2</b>

Monz�, Isidro S., Juan Palou, Jose Roca,

8	and Rosa Valero. "Kinetics and mechanism of the reactions between chloranil and n- butylamine in cyclohexane solution", Journal of the Chemical Society Perkin Transactions 2, 1988. Publication	%2
9	lin7.ipsrsolution.com Internet Source	% <b>1</b>
10	Submitted to Indian Institute of Technology- Bhubaneswar Student Paper	% <b>1</b>
11	130.15.168.200 Internet Source	<b>%1</b>
12	www.giovannibachelet.it Internet Source	% <b>1</b>
13	Submitted to Higher Education Commission  Pakistan Student Paper	<b>%1</b>
14	www.univsul.org Internet Source	<b>%</b> 1
15	Organic Spectroscopy, 1991. Publication	%1
16	Submitted to University of Strathclyde  Student Paper	<b>%1</b>
17	島田 拓哉. "Theoretical analysis on the reaction	

	mechanisms of reducing agents for electroless deposition processes", [出版者不明], 2009.  Publication	<b>% 1</b>
18	quspace.qu.edu.qa Internet Source	<b>%1</b>
19	A. Douglas Kinghorn. "Occurrence", Fortschritte der Chemie organischer Naturstoffe / Progress in the Chemistry of Organic Natural Products, 2009 Publication	% <b>1</b>
20	"Physical Basis of Drugs at High Dilution", High Dilution Effects Physical and Biochemical Basis, 2005 Publication	% <b>1</b>
24	MAAAA MALLACID	
21	www.mgu.ac.in Internet Source	%1
22		% <b>1</b> % <b>1</b>

## of 2,4,6-tri substituted s-triazines", Journal of Mass Spectrometry, 2012. Publication

24	Submitted to Universiti Teknologi Malaysia Student Paper	<%1
25	Submitted to University of Bradford Student Paper	<%1
26	ghpcc.gzu.edu.cn Internet Source	<%1
27	Computational Chemistry, 2011.  Publication	<%1
28	Submitted to Kenyatta University  Student Paper	<%1
29	Submitted to Chicago State University  Student Paper	<%1
30	Submitted to Universiti Teknologi MARA  Student Paper	<%1
31	atto.tau.ac.il Internet Source	<%1
32	Submitted to University of Kent at Canterbury  Student Paper	<%1
33	www.studymode.com Internet Source	<%1
	Submitted to National Institute Of Technology,	

34	Tiruchirappalli Student Paper	<%1
35	Helaly, Soleiman Elsayed Soleiman. "Isolation and Physicochemical Characterization of Novel Secondary Metabolites from Streptomyces strains Acta 3662, BK 190 and Acta 3062", Technische Universität Berlin, 2011.  Publication	<%1
36	www.absoluteastronomy.com Internet Source	<%1
37	Errol G. Lewars. "Computational Chemistry", Springer Nature, 2016 Publication	<%1
38	C. Purna Chander. "Electrospray ionization tandem mass spectrometry of 3-phenyl-N-(3-(4-phenylpiperazin-1-yl)propyl)-1H-pyrazole-5-carboxamide derivatives: unusual fragmentation involving loss of 11 u : Letter to the Editor", Rapid Communications in Mass Spectrometry, 01/30/2012 Publication	<%1
39	Submitted to University of New England Student Paper	<%1
40	www.sumobrain.com Internet Source	<%1

Paunovic, Verica, Biljana Ristic, Zoran

41	Markovic, Biljana Todorovic-Markovic, Milica Kosic, Jovana Prekodravac, Tamara Kravic-Stevovic, Tamara Martinovic, Matej Micusik, Zdeno Spitalsky, Vladimir Trajkovic, and Ljubica Harhaji-Trajkovic. "c-Jun N-terminal kinase-dependent apoptotic photocytotoxicity of solvent exchange-prepared curcumin nanoparticles", Biomedical Microdevices, 2016. Publication	<%1
42	top25.sciencedirect.com Internet Source	<%1
43	Submitted to University of KwaZulu-Natal Student Paper	<%1
44	faculty.uoh.edu.sa Internet Source	<%1
45	austinpublishinggroup.com Internet Source	<%1
46	crl.du.ac.in Internet Source	<%1
47	Submitted to University of Nevada Reno  Student Paper	<%1
48	Nishikida, Koichi, and John Coates. "Infrared And Raman Analysis Of Polymers", Handbook of Plastics Analysis, 2003.	<%1

49	www.google.nl Internet Source	<%1
50	www.freepatentsonline.com Internet Source	<%1
51	task-new.task.gda.pl Internet Source	<%1
52	Submitted to University of Greenwich  Student Paper	<%1
53	Submitted to Mahidol University  Student Paper	<%1
54	nr.stic.gov.tw Internet Source	<%1
55	"Evaluation of Calcium Alginate Entrapped Nano Zinc Oxide to Reduce Gaseous Emissions from Liquid Dairy Manure", Applied Engineering in Agriculture, 2016.	<%1
56	Michael R. Crampton. "Nucleophilic Aromatic Substitution", Organic Reaction Mechanisms Series, 03/01/1990 Publication	<%1
57	www.cheque.uq.edu.au Internet Source	<%1
58	www.shcollege.ac.in Internet Source	<%1

59	file.scirp.org Internet Source	<%1
60	Liu, X., O. Vilenski, J. Kwan, S.  Apparsundaram, and R. Weikert. "Unbound Brain Concentration Determines Receptor Occupancy: A Correlation of Drug Concentration and Brain Serotonin and Dopamine Reuptake Transporter Occupancy for Eighteen Compounds in Rats", Drug Metabolism and Disposition, 2009.  Publication	<%1
61	K.B. Jose. "The mechanism of aromatic nucleophilic substitution reaction between ethanolamine and fluoro-nitrobenzenes: an investigation by kinetic measurements and DFT calculations", Journal of Physical Organic Chemistry, 08/2011 Publication	<%1
62	Mario Thevis. "Mass spectrometry in sports drug testing: Structure characterization and analytical assays", Mass Spectrometry Reviews, 01/2007  Publication	<%1
63	Philip Keyes. "Automated compound verification using 2D-NMR HSQC data in an open-access environment", Magnetic Resonance in Chemistry, 01/2009	<%1



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