

SYNTHESIS, CHARACTERIZATION AND EVALUATION OF NOVEL ORGANO-BASED AGROCHEMICALS FOR CROP PROTECTION

S.D. Yamgar^{1,✉}, V. B. Metkari², M. B. Deshmukh¹, P.P. Mohire¹,
and G.B. Kolekar¹

¹Department of Agrochemicals and Pest Management, Shivaji University,
Kolhapur, 416004 (Maharashtra), India

²Department of Pharmaceutics, Adarsh College of Pharmacy, Vita-415311 (Maharashtra), India

✉Corresponding author: sdyamgar@yahoo.com

ABSTRACT

The present study reports the synthesis of novel organo-based agrochemicals, particularly quinazoline-based organophosphorus derivatives, and their evaluation for agricultural applications. Newly synthesized compounds were characterized using melting point, IR, NMR, HPLC, and GC techniques. The biological efficacy of these compounds was assessed through antifeedant activity against *Helicoverpa armigera* and pesticidal activity against the white woolly sugarcane aphid (*Ceratovacuna lanigera*). Compounds A, B, and C exhibited strong antifeedant activity at 500 ppm, moderate activity at 250 ppm, and mild activity at 100 ppm. Complete mortality of *Ceratovacuna lanigera* was observed at 1000 ppm for all synthesized organophosphorus compounds. The results indicate that quinazoline-based organophosphorus agrochemicals possess promising pesticidal and antifeedant properties with potential agricultural applications.

Keywords: Organo-Based Agrochemicals, Organophosphorus Pesticides, Quinazoline Derivatives, *Helicoverpa Armigera*, *Ceratovacuna Lanigera*

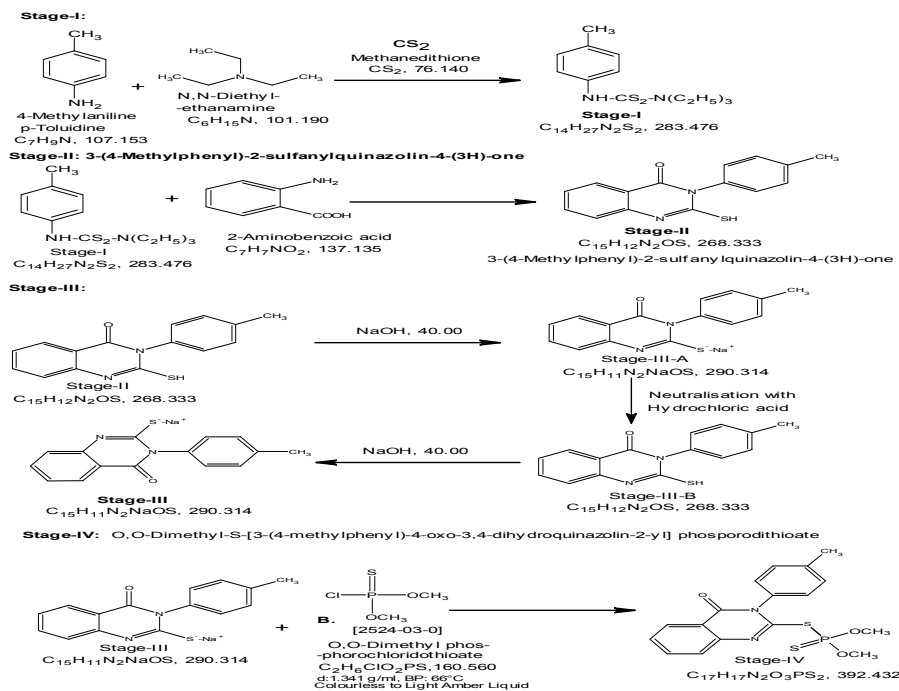
RASAYAN J. Chem., Vol. 19, No.4, 2026

INTRODUCTION

Agricultural productivity worldwide is severely affected by insect pests and plant diseases, resulting in significant yield losses. It is estimated that nearly one-third of global crop production is destroyed annually due to pest and disease infestations, with higher losses reported in Asia and Africa compared to Europe and North America. Indian agriculture, in particular, continues to suffer heavy economic losses due to diverse pest infestations and environmental challenges.¹ Although several agrochemicals are currently available, many suffer from drawbacks such as high production costs, complex synthesis procedures, environmental persistence, and toxicity to non-target organisms.² The integration of multiple pest control strategies into a unified and environmentally responsible management program is essential to minimize economic losses while reducing adverse ecological effects.³ Nanotechnology has recently gained significant attention in agriculture due to its potential applications in crop protection, fertilization, and pest management. Nanomaterials, typically ranging from 1–100 nm in size, exhibit unique physicochemical properties that can enhance bioavailability and controlled release.⁴ Quinazoline and organophosphorus compounds are known for their diverse biological activities. The present work focuses on the synthesis of novel heterocyclic quinazoline-based organophosphorus pesticides, their nano-scale relevance, and evaluation of their biological efficacy against major agricultural pests.⁵

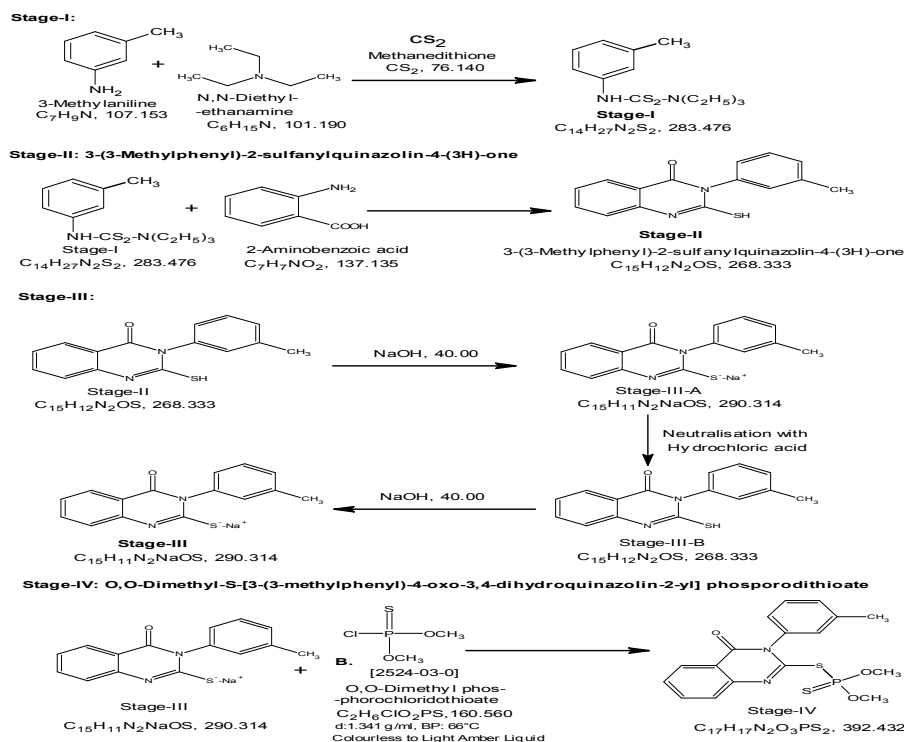
Synthetic Scheme for Compound A

The synthesis involves four stages: initially, 3-methylaniline reacts with carbon disulfide in the presence of triethylamine to form a dithiocarbamate intermediate. This intermediate then condenses with anthranilic acid under reflux to undergo cyclisation, yielding a quinazoline derivative. The product is converted into its sodium salt using NaOH, followed by neutralization with HCl. Finally, the sodium salt reacts with O, O-dimethyl thiophosphorochloridate, forming the target organophosphorus compound via P–S bond formation.



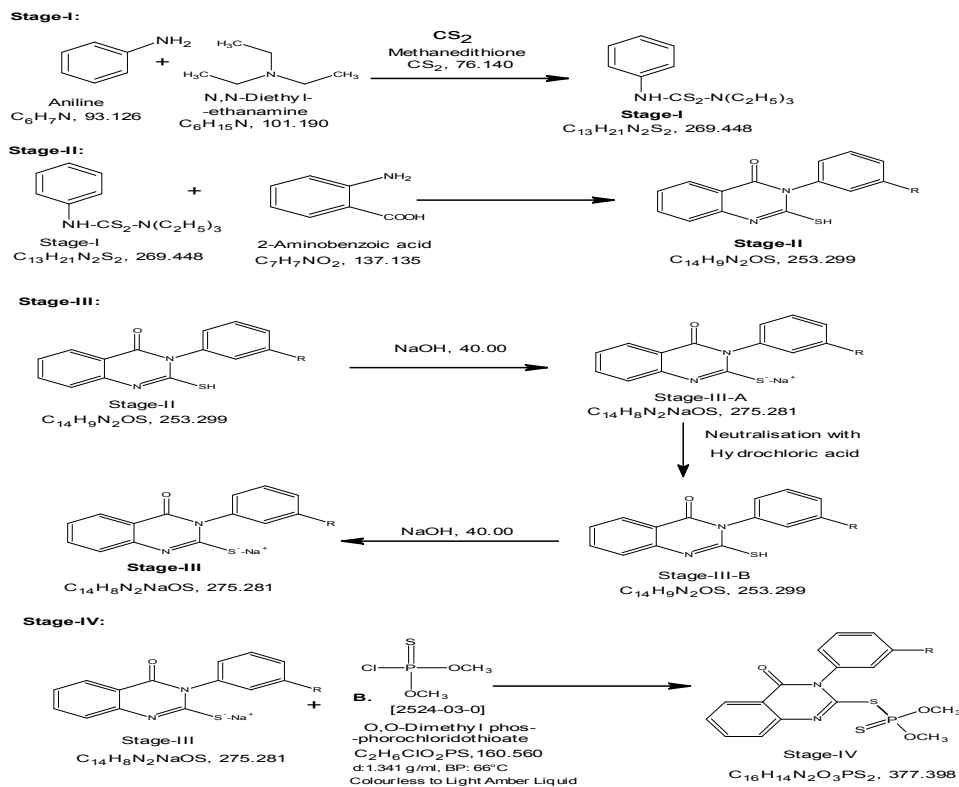
Synthetic Scheme for Compound B

The synthesis proceeds through four stages: first, 3-methylaniline reacts with carbon disulfide in the presence of triethylamine to form a dithiocarbamate intermediate. This intermediate then condenses with anthranilic acid under heating to cyclize into a quinazoline derivative. The product is converted into its sodium salt using NaOH for activation. Finally, the sodium salt reacts with O, O-dimethyl thiophosphorochloridate, forming the target organophosphorus compound via P–S bond formation.



Synthesis Reaction Scheme for Compound C

The synthesis proceeds through four stages: formation of a dithiocarbamate intermediate from aniline and carbon disulfide in the presence of triethylamine, followed by cyclisation with anthranilic acid to yield a quinazoline-4-one derivative. This is converted into its sodium salt using NaOH and subsequently reacted with O, O-dimethyl thiophosphorochloridate to form the final organophosphorus compound via P–S bond formation. Additionally, 2-aminobenzoic acid was synthesized from 2-nitrotoluene through oxidation and hydrogenation and confirmed by standard analytical methods.



EXPERIMENTAL

Preparation of *p*-Toluidine Dithiocarbonate Salt

p-Toluidine and carbon disulfide were stirred in a cooled round-bottom flask (0–5 °C), and triethylamine was added dropwise over 1 h to form a yellow precipitate. The solid was filtered, washed with ethanol/isopropyl alcohol, and dried to obtain *p*-toluidine dithiocarbonate salt.

Table-1: Raw Material Consumption

S. No.	Raw Material	Mol. Wt.	Qty (g)	Purity (%)	Qty (100%)	Moles	Molar Ratio
1	<i>p</i> -Toluidine	107.15	93.13	99	92.19	0.860	1.0
2	Carbon disulfide	76.14	76.14	99	75.37	0.99	1.15
3	Triethylamine	101.19	101.19	99	100.17	0.99	1.15
Product	<i>p</i> -Toluidine dithiocarbonate salt	284.48	250.46	99	247.95	0.872	—

Synthesis of 3-(*p*-Methylphenyl)-2-thioxo-4(3H)-quinazolin-4-one

p-Toluidine dithiocarbonate salt (1.0 mol) was refluxed with anthranilic acid (1.0 mol) in isopropyl alcohol for 5–6 h, with reaction progress monitored by TLC. After solvent removal, the residue was treated with ethanolic NaOH, filtered, acidified with HCl to precipitate the product, and recrystallised from ethanol to obtain 3-(*p*-methylphenyl)-2-thioxo-4(3H)-quinazolin-4-one.

Table-2: Raw Material Consumption

S. No.	Raw Material	Mol. Wt.	Qty (g)	Purity (%)	Moles	Molar Ratio
1	<i>p</i> -Toluidine dithiocarbonate salt	284.48	270.46	98	0.932	1.0
2	Anthranilic acid	137.13	137.13	98	0.980	1.05
3	Ethanol	—	150 mL	—	—	—
4	Sodium hydroxide	39.99	40	—	—	—
5	Hydrochloric acid	36.46	36.46	—	—	—

Preparation of Quinazolinone Sodium Salt

3-(*p*-Methylphenyl)-2-thioxo-4(3H)-quinazolin-4-one was dissolved in 1% NaOH solution to form its sodium salt. Neutralization with 1 N HCl yielded the free quinazolinone. The compound was again treated with 2 N NaOH, and evaporation removed water to yield the corresponding sodium salt.

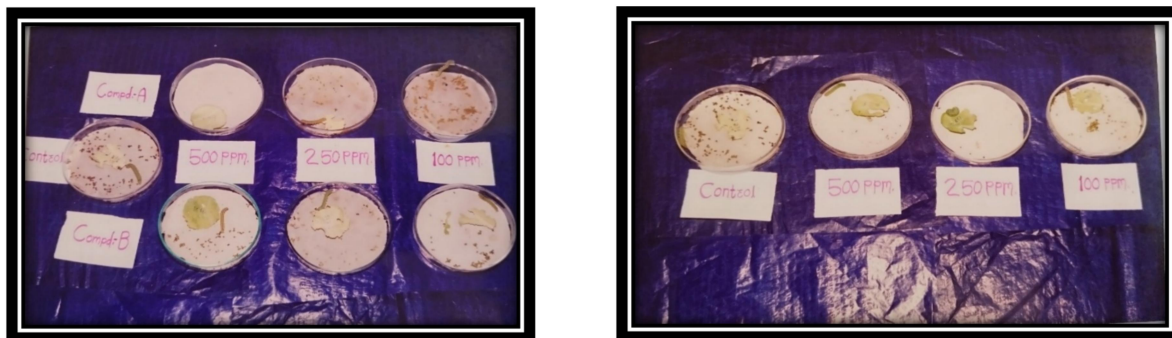
Synthesis of O, O-Dimethyl-S-[3-(*p*-methylphenyl)-quinazolin-4-one-2-yl] Phosphorodithioate

The sodium salt of quinazolinone (1.0 mol) was reacted with O,O-dimethyl thiophosphorochloridate (1.0 mol) under stirring for 2–3 h. The reaction mixture was cooled to 0 to –5 °C, resulting in precipitation of a white solid. The product was filtered, recrystallized from ethanol, and characterized by melting point, FT-IR, NMR, HPLC, and GC analyses.

RESULTS AND DISCUSSION

Antifeedant Activity Against *Helicoverpa armigera*

The synthesized quinazoline-based organophosphorus compounds were white solids, soluble in benzene and DMF but insoluble in alcohol and water, and exhibited concentration-dependent antifeedant activity against *Helicoverpa armigera*. Strong deterrence was observed at 500 ppm (minimal leaf consumption and weight loss), moderate at 250 ppm, and slight at 100 ppm, with larvae progressing to pupation within 48 h, confirming their feeding deterrent nature.

Fig.-1: Antifeedant Activity Against *Helicoverpa armigera*

Mortality Study Against White Woolly Sugarcane Aphid (*Ceratovacuna lanigera*)

The synthesized organophosphorus agrochemicals were evaluated against *Ceratovacuna lanigera*, showing clear dose-dependent activity. Compounds A, B, and C reduced initial infestations (14, 16, and 21 aphids) to zero at 1000 ppm, achieving 100% mortality, while no mortality was observed at lower concentrations (100–500 ppm). This indicates that the compounds exhibit effective aphicidal action only at higher doses.

Table-3: Antifeedant Activity of Synthesized Compounds against *Helicoverpa Armigera*

Compound	Concentration	Weight of leaves before test (g)	Weight of leaves after test (g)	No. of excreta pellets	Observed mortality
A	500 ppm	1.377	1.212	49	No
	250 ppm	0.924	0.793	57	No
	100 ppm	1.038	0.709	82	No
	Control	0.924	0.000	244	No

B	500 ppm	1.103	1.084	55	No
	250 ppm	1.503	0.265	82	No
	100 ppm	0.849	—	148	No
	Control	0.655	—	—	No
C	500 ppm	1.038	1.005	43	No
	250 ppm	0.853	0.589	43	No
	100 ppm	1.335	0.719	115	No
	Control	1.217	0.000	198	No

Compounds A–C showed concentration-dependent antifeedant activity against *Helicoverpa armigera*, with strong effects at 500 ppm, moderate at 250 ppm, and slight at 100 ppm, as indicated by reduced leaf consumption and excreta. No larval mortality was observed, confirming their role as feeding deterrents rather than toxic agents.

Table-4: Pesticidal Activity of Synthesized Compounds A against White Woolly Sugarcane Aphid (*Ceratovacuna lanigera*)

Concentration (ppm)	No. of WWSA/leaf before spraying (T, M, B)	No. of WWSA/leaf after 24 h (T, M, B)
Control	(12, 21, 10)	(12, 23, 11)
100	(13, 21, 30)	(09, 18, 25)
250	(11, 12, 17)	(10, 08, 13)
500	(07, 31, 13)	(04, 24, 09)
1000	(14, 25, 19)	(0, 0, 0)

The synthesized organophosphorus compounds (A–C) showed dose-dependent pesticidal activity against *Ceratovacuna lanigera*, with complete (100%) mortality observed at 1000 ppm after 24 hours. At lower concentrations (100–500 ppm), only partial reduction in aphid population was noted, indicating that effective aphicidal action occurs primarily at higher doses.

CONCLUSION

A series of quinazoline-based organophosphorus compounds were efficiently synthesized as white solids with selective solubility. They exhibited concentration-dependent antifeedant activity against *Helicoverpa armigera*, showing strong effects at 500 ppm without causing larval mortality, indicating a deterrent mechanism. The compounds also demonstrated pesticidal activity against *Ceratovacuna lanigera*, achieving complete mortality at 1000 ppm and partial effects at lower doses. Overall, these compounds show dual agrochemical potential as antifeedants and pesticides, suitable for eco-friendly pest management.

ACKNOWLEDGMENTS

No acknowledgements are made in this work.

CONFLICT OF INTERESTS

The authors declare that there is no conflict of interest.

AUTHOR CONTRIBUTIONS

The present work is related to *SDG-12: Responsible Consumption and Production*. All the authors contributed significantly to this manuscript, participated in reviewing/editing and approved the final draft for publication. The research profile of the authors can be verified from their ORCID ids, given below:

S.D. Yamgar  <https://orcid.org/0009-0006-4107-2424>

V. B. Metkari  <https://orcid.org/0000-0003-3589-8933>

M. B. Deshmukh  <https://orcid.org/0000-0001-7097-2356>

P.P. Mohire  <https://orcid.org/0000-0003-4644-1111>

G.B. Kolekar  <https://orcid.org/0000-0002-1874-3043>

Open Access: This article is distributed under the terms of the Creative Commons Attribution 4.0 International License (<http://creativecommons.org/licenses/by/4.0/>), which permits unrestricted use, distribution, and reproduction in any medium, provided you give appropriate credit to the original author(s)

and the source, provide a link to the Creative Commons license, and indicate if changes were made.

Cite this article as: S. D. Yamgar *et al.*, *Rasayan J. Chem.*, 19(4), 2134-2139(2026), <https://doi.org/10.31788/RJC.2026.1949915>

REFERENCES

1. Y. Nakamura, N. Miyoshi, *Bioscience, Biotechnology, and Biochemistry*, **74(2)**, 242(2010), <https://doi.org/10.1271/bbb.90731>
2. G. V. Lowry, A. Avellan, L. M. Gilbertson, *Nature Nanotechnology*, **14(6)**, 517(2019), <https://doi.org/10.1038/s41565-019-0461-7>
3. M. S. C. Pedras, Q.-A. Zheng, R.S. Gadagi, *Chemical Communications*, **2007(4)**, 368(2007), <https://doi.org/10.1039/B615424G>
4. R. Munday, Y. Zhang, C. M. Munday, M. V. Bapardekar, J. D. Paonessa, *Pharmaceutical Research*, **25(9)**, 2164(2008), <https://doi.org/10.1007/s11095-008-9595-2>
5. X. Tian, A. D. Hutters, C. J. Douglas, N. K. Garg, *Organic Letters*, **11(11)**, 2349(2009), <https://doi.org/10.1021/ol9007684>
6. S. Adsule, S. Banerjee, F. Ahmed, S. Padhye, F. H. Sarkar, *Bioorganic & Medicinal Chemistry Letters*, **20(3)**, 1247(2010), <https://doi.org/10.1016/j.bmcl.2009.11.128>
7. A. K. Mukerjee, R. Ashare, *Chemical Reviews*, **91(1)**, 1(1991), <https://doi.org/10.1021/cr00001a001>
8. G. Sommen, *Synlett*, **2004(7)**, 1323(2004), <https://doi.org/10.1055/s-2004-825608>
9. J. Li, Z. Tan, S. Tang, I. Hewlett, R. Pang, M. He, S. He, B. Tian, K. Chen, M. Yang, *Bioorganic & Medicinal Chemistry*, **17(8)**, 3177(2009), <https://doi.org/10.1016/j.bmc.2009.02.051>
10. I. -J. Kang, L. -W. Wang, T.-K. Yeh, C. -C. Lee, Y. -C. Lee, S.-J. Hsu, Y. -S. Wu, J. -C. Wang, Y. -S. Chao, A. Yueh, J. -H. Chern, *Bioorganic & Medicinal Chemistry*, **18(17)**, 6414(2010), <https://doi.org/10.1016/j.bmc.2010.07.002>
11. B. Huang, F. Chen, Y. Shen, K. Qian, Y. Wang, C. Sun, X. Zhao, B. Cui, F. Gao, Z. Zeng, et al. *Nanomaterials*, **8(2)**, 102(2018), <https://doi.org/10.3390/nano8020102>
12. M. Pascoli, P.J. Lopes-Oliveira, L.F. Fraceto, A. B. Seabra, H. C. Oliveira, *Energy, Ecology and Environment*, **3(3)**, 137(2018), <https://doi.org/10.1007/s40974-018-0090-2>

[RJC-9915/2026]