



Industrial Consultancy & Sponsored Research (IC&SR)

OXIDATIVE CYCLIZATION OF ARYLDIYNES TO 3-ACYL-1-INDENONES

IITM Technology Available for Licensing

PROBLEM STATEMENT

- The **current market for synthesizing 1-indenone derivatives are complex** and multi-step, with limited scope and poor functional group tolerance.
- They often **rely on expensive transition metal catalysts like palladium or gold**, which are difficult to recover or reuse, leading to metal impurities in the final product.
- These **methods also suffer from synthetic difficulties, poor stereoselectivity**, and metal contamination, which limit their practicality and scalability for industrial applications.
- There is a need **to develop an alternative synthetic pathway for producing 3-acyl-1-indenones**, possibly using a metal-free or sustainable catalytic approach, to address these issues.

TECHNOLOGY CATEGORY MARKET

Technology: Oxidative cyclization of aryldiynes to 3-acyl-1-indenones

Category: Chemistry & Chemical Analysis

Industry: Catalysis and Green Chemistry

Application: Medicinal, material, and natural product synthesis.

Market: The global market size is valued at **USD 32.68 Billion in the year 2022** and it is expected to reach **USD 50.34 Billion in 2030** at a **CAGR of 5.69%** over the forecast period of 2023 to 2030.

INTELLECTUAL PROPERTY

IITM IDF Ref. 2718

Patent No: IN 550109

TRL (Technology Readiness Level)

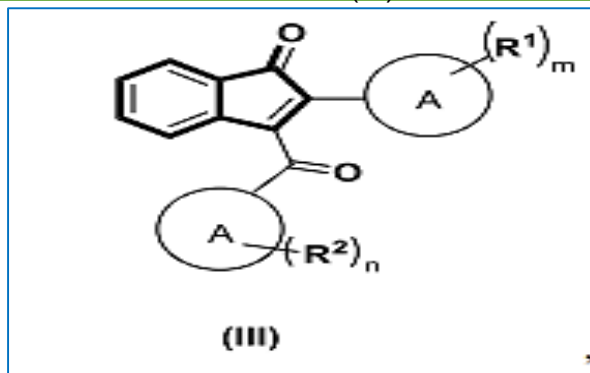
TRL- 3, Experimental proof of concept;

Research Lab

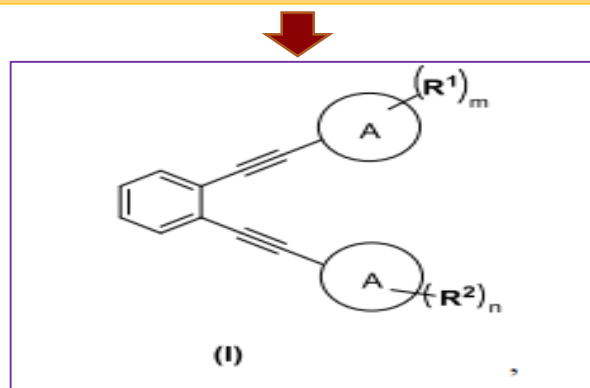
Prof. Govindasamy Sekar, Dept. of Chemistry

TECHNOLOGY

- A process for the synthesis of 3-acyl-1-indenones of formula (III):



- wherein each ring **A** is independently an aryl ring or a heteroaryl ring;
- **R¹ and R²** are independently hydrogen, an electron-donating substituent, or an electron-withdrawing substituent; and
- **m and n are independently 0 to 5**;
- the process comprises reacting an aryldiyne of formula (I) in the presence of
- **palladium nanoparticle catalyst (II)**;



- wherein ring **A**, **R¹**, **R²**, **m** and **n** are same as defined in formula (III).

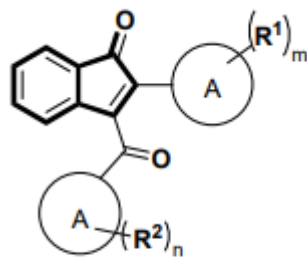
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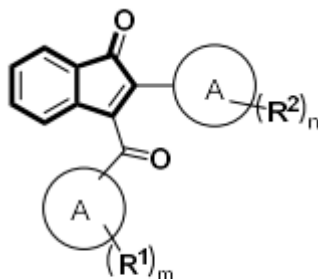
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Major isomer

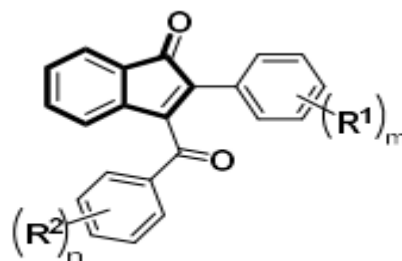
(IIIa)



Minor isomer

(IIIb)

The compound of formula (III) is a compound of formula (IIIc)



(IIIc)

Key Features / Value Proposition

❖ Selective Coupling Reactions

- Used for selective coupling reactions like Sonogashira. Enables coupling of aryldiyne compounds with specific formula, I. Forms complex organic structures with precision and the ratio of aryldiyne of formula (I) and the **palladium nanoparticle is about 1:0.03.**

❖ Catalysis in Organic Synthesis

- Pd-BNP enhances catalytic properties. Enhances activity, selectivity, stability. Useful in cross-coupling, C-H activation, aryldiyne compounds coupling.

❖ Environmentally Friendly Catalysis

- Reaction conducted in environmentally friendly solvents like DMSO, DMF, water. Use of Pd-BNP and specified conditions reduce need for harsher reagents or solvents.

❖ Nanocatalyst Development for Heterogeneous Catalysis

- Utilizes heterogeneous catalyst. Offers easy separation and recycling. Ideal for large-scale industrial applications..

❖ Palladium Nanoparticle Synthesis and Stabilization

- Process involves stabilization of **5-20 nm nanoparticles**. Controlled synthesis crucial for catalytic applications. Particle size impacts catalytic activity, stability, selectivity.

❖ Optimization of Reaction Conditions

- ❖ Specific reaction conditions: **100-140°C, 24-48 hours**, solvent choice. Optimizes yields and selective products.

❖ Oxygen Atmosphere Reactions

- Useful for specific oxidation or coupling reactions. Beneficial for reactions requiring or requiring oxidative conditions.

❖ Copper-Free Catalytic Reactions

- Avoids toxicity, cost, and environmental concerns. Significantly improves efficiency.

❖ Fine Chemical and Pharmaceutical Synthesis

- Highly selective, controlled process. Synthesizes complex, functionalized organic compounds.

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