



# IIT MADRAS

Indian Institute of Technology Madras

Technology Transfer Office  
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## Industrial Consultancy & Sponsored Research (IC&SR)

### A ONE STEP SYNTHESIS OF 2-SUBSTITUTED BENZO[B]THIOPHENES IITM Technology Available for Licensing

#### Problem Statement

- Synthesis of 2-substituted benzo[b]thiophene derivatives were earlier from the acylation of benzo[b]thiophene using acyl source like acetyl chloride, acetic anhydride, 2-oxocarboxylic acid, N, N-dimethylacetamide, acetaldehyde and benzoyl chloride.
- These reactions yielded major amount of **3-substituted** & minor amount of **2-substituted benzo[b]thiophenes** due to the **high reactivity** of C-3 than C-2 position of benzo[b]thiophene.
- **Expensive** starting materials, handling of **butyl lithium, high temperature, inert atmosphere**, synthesized beta zeolite to utilize for the industrial scale preparation of 2-substituted benzo[b]thiophene will be **very difficult**.
- Further a few Non-patent literatures discussed regarding the developing of the catalyst using synthesis with other associated issues.
- Present invention has addressed said issues efficiently.

#### Technology Category/ Market

**Technology:** One step synthesis of 2-substituted benzo[b]thiophene;

**Industry:** Catalyst Manufacturing.

**Applications:** Manufacturing chemical.

**Market:** The global **catalyst** market is projected to grow at a **CAGR** of **4.6%** during forecast period of **2023** to **2030**.

#### Intellectual Property

**IITM IDF Ref. 1879; Patent No.384111;**  
**PCT Application No. PCT/IN2020/050716**

#### TRL (Technology Readiness Level)

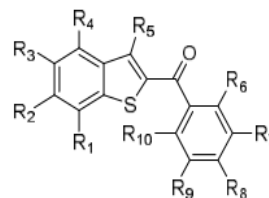
**TRL- 4**, Proof of Concept & validated in Lab

#### Research Lab

**Prof. Govindasamy Sekar**  
Department of Chemistry,

#### Technology

- Present invention describes **one step synthesis of 2-substituted benzo[b]thiophene**.
- The General formula includes



R<sub>1</sub> = Cl, CH<sub>3</sub>, OCH<sub>3</sub>, Br, F, I, NO<sub>2</sub>, CN, NH, OH, CHO

R<sub>2</sub> = CH<sub>3</sub>, OCH<sub>3</sub>, Cl, Br, F, I, NO<sub>2</sub>, CN, C<sub>6</sub>H<sub>5</sub>, NH<sub>2</sub>, OH

R<sub>3</sub> = OCH<sub>3</sub>, Cl, F, I, NO<sub>2</sub>, CN, C<sub>6</sub>H<sub>5</sub>, NH<sub>2</sub>, OH, CHO

R<sub>4</sub> = CH<sub>3</sub>, OCH<sub>3</sub>, Cl, Br, F, I, NO<sub>2</sub>, CN, C<sub>6</sub>H<sub>5</sub>, NH<sub>2</sub>, OH, CHO

R<sub>5</sub> = CH<sub>3</sub>, C<sub>6</sub>H<sub>5</sub>, NH<sub>2</sub>, CHO

R<sub>6</sub> = CH<sub>3</sub>, Cl, Br, NO<sub>2</sub>, CN, NH<sub>2</sub>, OH, OCH<sub>3</sub>, F, I

R<sub>7</sub> = CH<sub>3</sub>, OCH<sub>3</sub>, Cl, Br, NO<sub>2</sub>, CN, NH<sub>2</sub>, OH, C<sub>6</sub>H<sub>5</sub>

R<sub>8</sub> = NH<sub>2</sub>, OH, C<sub>6</sub>H<sub>5</sub>

R<sub>9</sub> = Cl, Br, NO<sub>2</sub>, CN, OH, NH<sub>2</sub>, C<sub>6</sub>H<sub>5</sub>

R<sub>10</sub> = CH<sub>3</sub>, OCH<sub>3</sub>, Cl, Br, NO<sub>2</sub>, CN, OH, NH<sub>2</sub>, C<sub>6</sub>H<sub>5</sub>

The **process** explains in smart chart herein:

1

The **synthesis of 2-substituted benzo[b]thiophenes is by reacting the starting materials substituted or unsubstituted 2-halogenobenzaldehyd;**

2

**substituted or unsubstituted acetyl/phenacyl bromide with a catalyst, a sulphur source and phase transfer catalyst in an aqueous medium;**

3

**Said aqueous medium with atmospheric air and at temperature in the range of 25°C- 30°C.**

#### CONTACT US

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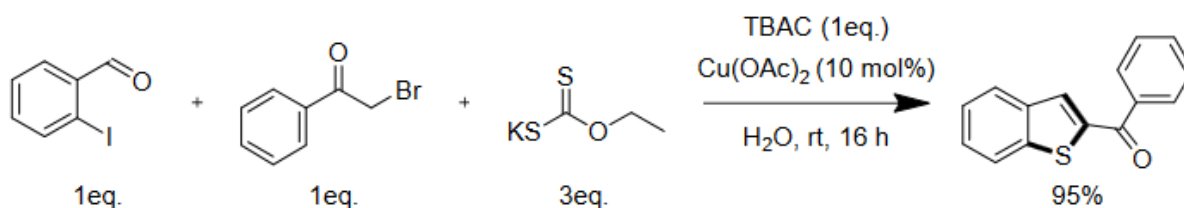
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**A ONE STEP SYNTHESIS OF 2-SUBSTITUTED  
BENZO[B]THIOPHENES  
IITM Technology Available for Licensing****Key Features / Value Proposition****❖ Technical Perspective:**

1. Present Patent facilitates the **syntheses of 2-acylbenzo[b]thiophene** in a **one-step** direct synthesis from commercially available starting materials & cost-effective.
2. The **starting material** is one of 2-iodobenzaldehyde, 2-iodo-5-methylbenzaldehyde, 5-bromo-2-iodobenzaldehyde, 2-iodobenzophenone, 2-iodochalcones, 2-iodobenzaldehyde, & further the starting material is one of phenacyl bromide, acetyl bromide, 2-bromocycloalkanone, 2-bromotetralone and 2-bromoindanone.
3. The catalyst used in the subject invention is **copper acetate** including **Sulphur source** as **potassium ethyl Xanthate**.
4. There is **no toxic solvent** used in the present invention, hence the **process** is **eco-friendly**.

**❖ Industrial Perspective:**

1. Patented process is **environmental-friendly** as it uses **water as a solvent**.
2. **Said process is energy efficient** as the reaction is performed at ambient room temperature a range of (25°C-30°C).
3. The **yield** of 2-acylbenzo[b]thiophene obtained by said process is **higher (the yield is 95%)**.

**Image****FIGURE 1****FIG.1: Illustrates schematic representation of the synthesis of the compounds****CONTACT US****Dr. Dara Ajay, Head**  
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