

Process for 4-substituted cyclohexane-1,3-dione Synthesis

Introduction: Cyclohexane-1,3-dione derivatives (CDD) are prominent intermediates for several bioactive molecules and herbicides synthesis. Therefore the development of such valuable intermediates with wider reaction scope and increased scale is in demand.

Importance and commercial value of this research

Herbicides and pharmaceutically important molecules

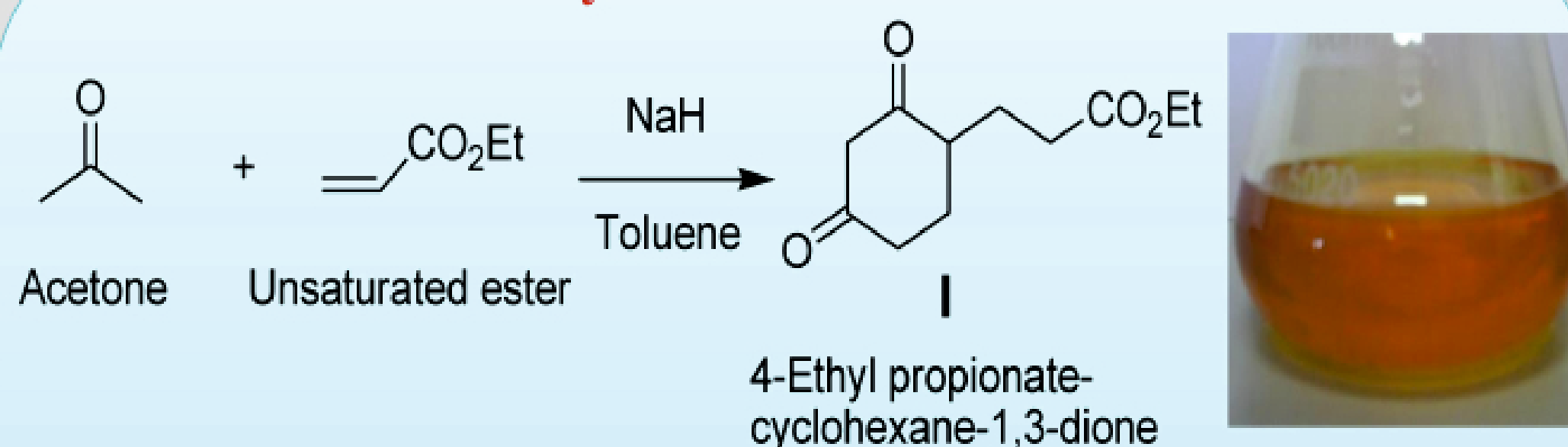
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|---------------|--------------|---------------|
| ➤ Tralkoxydim | ➤ Mesotrione | ➤ Tembotrione |
| ➤ EK-2612 | ➤ NTBC | ➤ Daz-2 |

Advantages

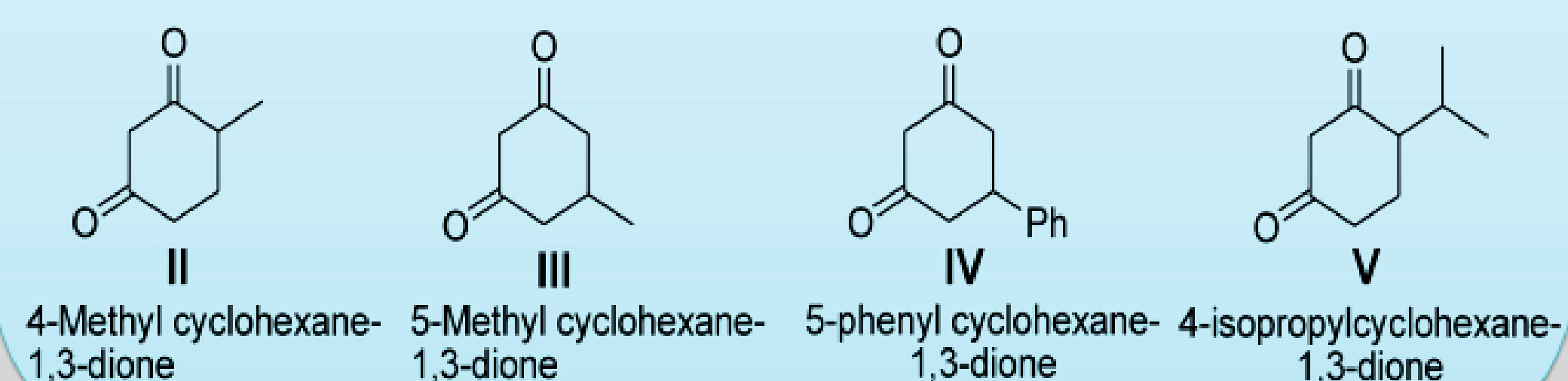
- ❖ Low cost and easily available starting material
- ❖ Room temperature to -10 °C : energy efficient process
- ❖ Shorter reaction time
- ❖ Scalable process
- ❖ Applicable for new and known classes of compounds

Scale up Facility Created: Reactor System

Process for the synthesis of novel 4-substituted CDD



Commercially available CDD synthesis by same procedure

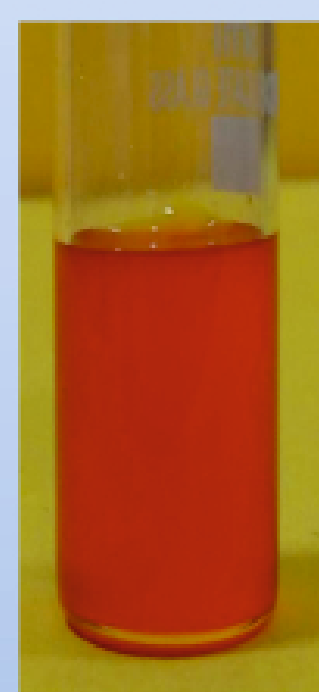


Lab scale process for 4-substituted cyclohexane-1,3-dione

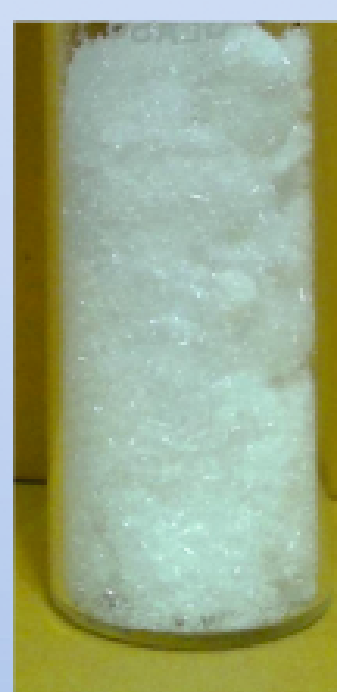


I = 500 gm

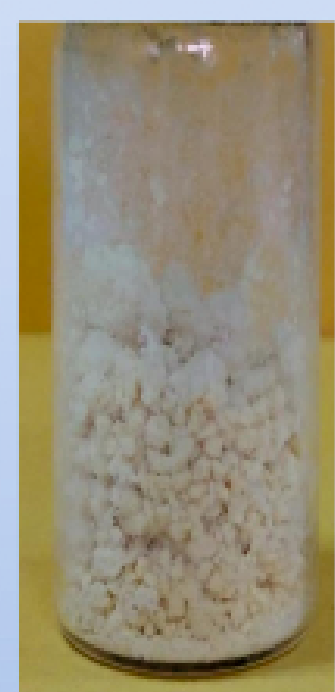
Available substituted cyclohexane-1,3-diones



II = 10 gm



III = 10 gm



IV = 10 gm



V = 10 gm

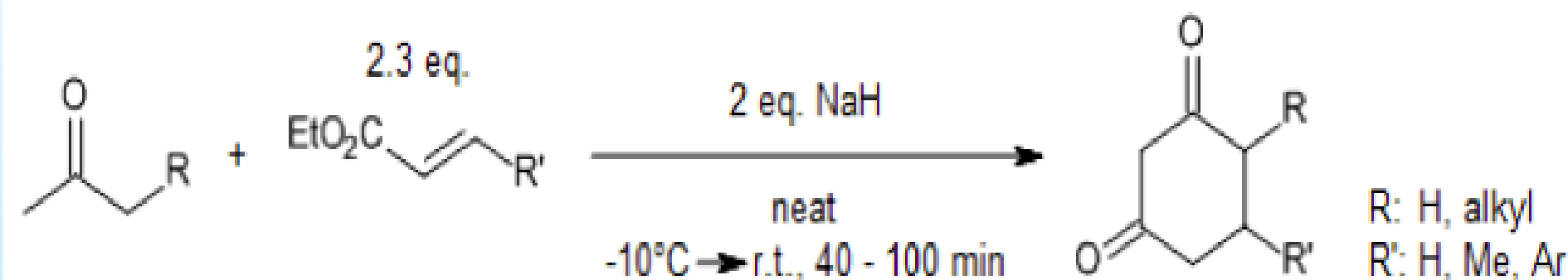


Comparison

- Commercial cost for substituted 1,3-cyclohexanedione is very high.
- Our cost for substituted 1,3-cyclohexanedione is low.



Organic
Chemistry
Portal



Patent and Publication: Achieved
(US 2013/0079545 A1, WO/2011/117881, PCT/IN2011/000180, Synlett, 2012, 23(8) 1199-1204, the work also selected in Organic Chemistry Portal)



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