

Spectroscopy, chromatography and microscopic image of 3-(4-methoxyphenyl)-1-phenylprop-2-en-1-one (MNYAD_1539) crystals



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ABSTRACT

3-(4-methoxyphenyl)-1-phenylprop-2-en-1-one (MNYAD_1539) was synthesized by an Aldol condensation method. MNYAD_1539 was synthesized from two commercially available materials of p-Methoxybenzaldehyde and Acetophenone. The physical and chemical properties of MNYAD_1539 was investigated using ATR-FTIR, GCMS and a microscope. The FTIR spectrum of the crude MNYAD_1539 showed the presence of impurities, compared with the crystalline sample. The chromatogram showed that MNYAD_1539 with high purity was produced after re-crystallisation. The current study also found high quality of the transparent needle-like crystal after re-crystallisation.

INTRODUCTION

The first synthesis of 3-(4-methoxyphenyl)-1-phenylprop-2-en-1-one (MNYAD_1539) was made in 1913. After that, many new synthesis methods for the preparation of MNYAD_1539 were explored such as with oxidation, dehydration and hydrolysis reaction. However, the most popular method is condensation reaction because of the high yield of the obtained product.^{1,2}

The physical data of MNYAD_1539 in solid state including melting point and crystal colours has been determined. Also, the molecular vibrations of MNYAD_1539 was investigated by FTIR in KBr matrix.³

To the best of our knowledge, there is no microscopic images and ATR-FTIR spectrum in dx format has been reported. Hence, the current work describes the synthesis and characterization of MNYAD_1539. The crystals are obtained after the re-crystallization of the crude.

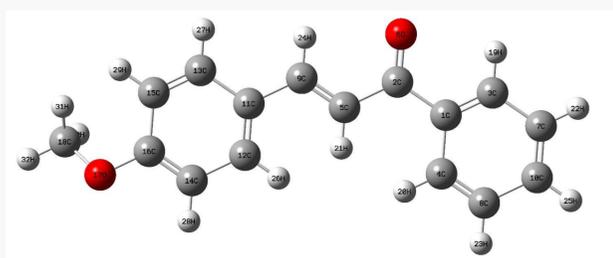
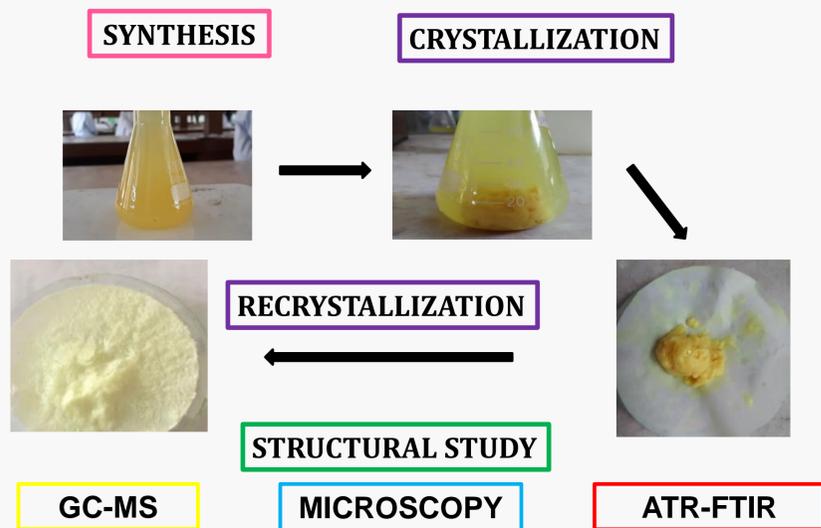


Figure 1 : The chemical structure of MNYAD_1539

METHODOLOGY



CONCLUSION

- 3-(4-methoxyphenyl)-1-phenylprop-2-en-1-one was successfully synthesised and characterised by vibrational spectroscopy, gas chromatography mass spectrometry and microscopic analysis.
- Its needle-like crystals were successfully grown after recrystallization from ethanol.
- The crystal of the compound was successfully observed under microscope showing transparent needle-like and it has rubber matting-like smelt. The melting point of the crystal is 80 °C.
- An very intense peak was observed in the chromatogram and it also contains a very low level of similar compound.

REFERENCES

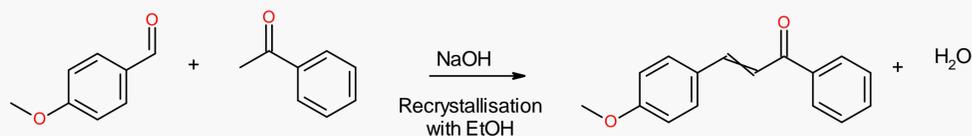
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RESULTS AND DISCUSSION

Base catalysed Aldol condensation of MNYAD_1539:



GCMS and ATR-FTIR Characterization of MNYAD_1539 crystals :

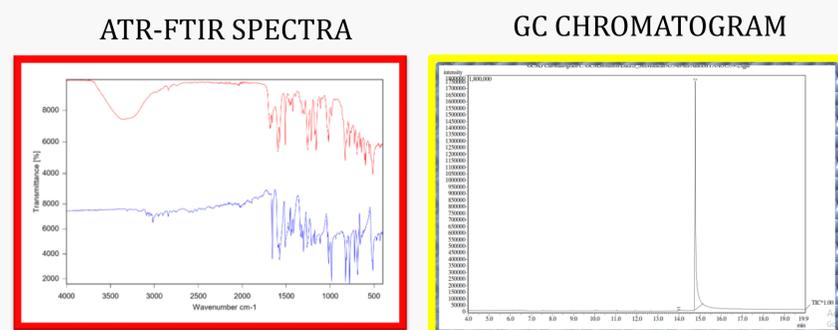
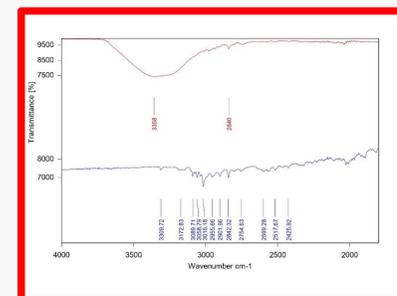


Figure 2. Solid state IR spectra of MNYAD_1539 before crystallization (top) and after crystallization (bottom). The presence of additional peak at 1681 cm⁻¹ in the crude product might attributed to the reactants. Also, broad peak at 3358 cm⁻¹ indicate the ν (O-H) very likely from water. However, they are absence after crystallization.



Expansion of IR region above 1800 cm⁻¹

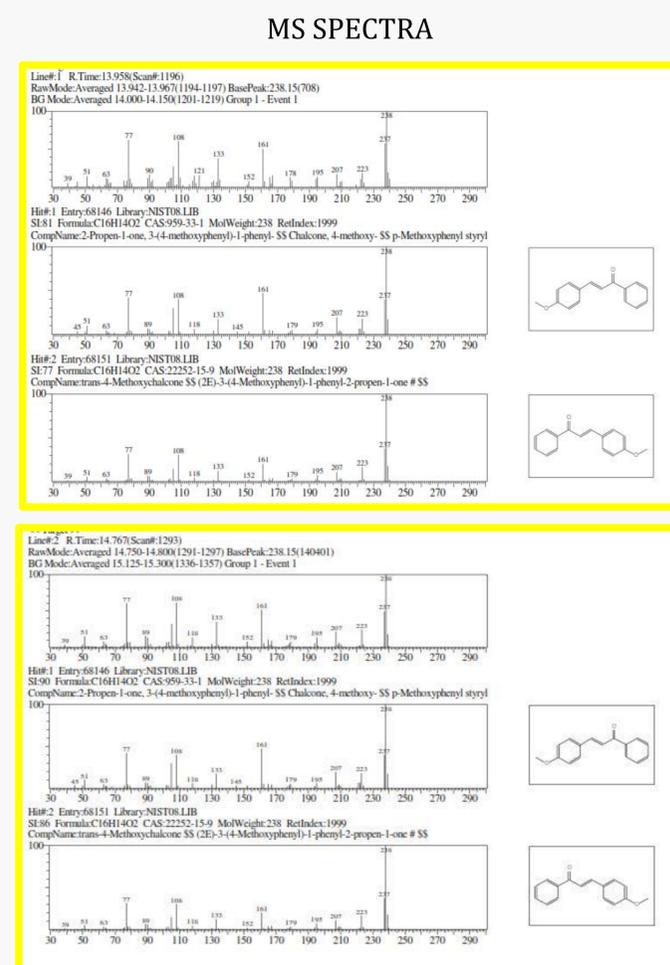


Figure 4. The first and second peak showed very similar mass fragmentation with molecular ion of 238 which indicates a very similar compound. MNYAD_1539 compound containing C₁₆H₁₄O₂ (CAS : 959-33-1) with the help of NIST library.



Figure 5. Images under microscope (4X) showing transparent needle-like morphology of the MNYAD_1539 after recrystallization from ethanol. The melting point is 80 °C and this yellow sample has rubber matting-like smelt. These images are first reported for this compound.