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Theoretical Studies of Essential Oil Components of Melissa *officinalis* L. Absorption on MWCNT

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Abstract: One of the important issues of herbal drugs chemistry is finding the methods of separating and altering the dose of essential oil components. Melissa *officinalis* L. or Lemon balm is a member of the mint family, used in traditional medicine, for the treatment of headaches, indigestion, colic, nervousness, cardiac failure and depression. Lemon balm is also known as a hormonal herb due to its antithyroid activity. The main components of wild Melissa officinalis L. obtained from the Kurdistan province of Iran were as follows: (E)-Citral (37.2%), Neral (23.9%), Citronellal (20.3%), cis-2H-3a-Methyl-octahydro-Inden-2-one (4.7%), Geranyl acetate (2.8%) and 3-Octanone (1.7), respectively. Due to multi wall carbon Nano tubes (MWCNT) specific prosperities such as serving choices of being good absorbent materials; In this study, the application of MWCNT properties in the absorption of the Melissa *officinalis* L. The theoretical studies confirms that the vander Waals and/or π-π interactions between MWCNT and 3-Octanone has stronger tendency to the absorption on MWCNT among the other components of the essential oil of Melissa *officinalis* L. because of distance with the wall of the modeled MWCNT.

Keywords: Melissa *officinalis* L.,MWCNT, Essential Oil Components, QM-MM method, Absorption.

1. INTRODUCTION:

Melissa *officinalis* L. or Lemon balm is a member of the mint family [1]. It is an important medicinal plant largely used in traditional medicine, for the treatment of headaches, indigestion, colic, nervousness, cardiac failure and depression [2]. Melissa *officinalis* L. is also used as flavouring in ice cream and herbal teas, often in combination with other herbs such as spearmint. It is also frequently paired with fruit dishes or candies. Lemon balm is also known as a hormonal herb due to its antithyroid activity. The present review is an effort to give the detailed survey of literature on its medicinal properties and cultivation practices of the plant under study [1]. The constituent of the essential oil of the plant in various climates is different, but citral (geranial and neral), citronellal, geraniol are main components [3]. The main components of wild Melissa officinalis L. obtained from the Kurdistan province of Iran were as follows: (E)-Citral (37.2%), Neral (23.9%), Citronellal (20.3%), cis-2H-3a-Methyl-octahydro-Inden-2-one (4.7%), Geranyl acetate (2.8%) and 3-Octanone (1.7) [4].

1.1 Multi-Walled Carbon Nanotubes (MWCNTs)

Carbon Nano materials have attracted the attention of many researchers [5]. Especially, sp^2 carbon Nano materials, such as carbon nanotubes (CNTs) and graphene have lots of significant applications in many various fields. CNTs, which are