

عنوان مقاله:

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

محل انتشار:

چهارمین همایش ملی شیمی، پتروشیمی و نانو ایران (سال: 1395)

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خلاصه مقاله:

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 properties such as serving choices of being good adsorbent materials; In this study, the application of MWCNT properties in the absorption of the *Melissa officinalis* L. The theoretical studies confirms that the van der 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

کلمات کلیدی:

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

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