

## ***Supplementary Materials***

### **Evaluation of Antiproliferative Potentials Associated with the Volatile Compounds of *Lantana camara* Flowers: Selective In Vitro Activity**

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#### **1. Collection of the flowers**



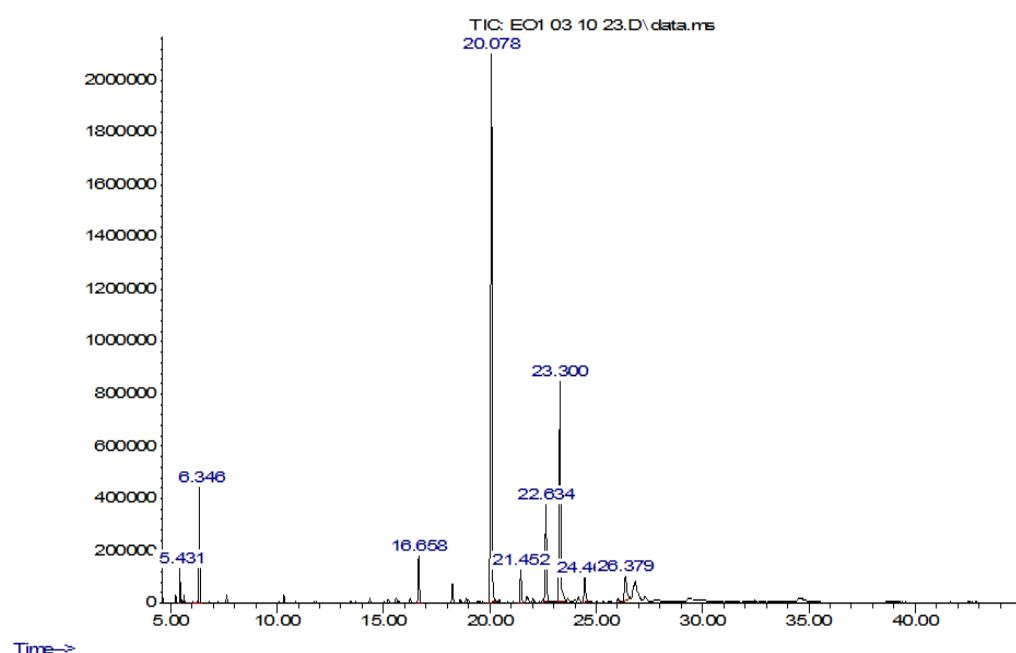
**Figure S1:** Petals of the *Lantana Camara* flowers: White, Pink, and Orange, respectively.

## 2. Chemical Profiles of the EO<sub>s</sub>

Yield of extraction: 0.045%			
Peak No.	Retention time (min)	Name	Proportion (%)
1	5,433	p-Cymene	1,5
2	6,364	3-Carene	5,56
3	16,656	5-Trimethyl-6-methylene-cyclohex-2-en-1-ol	3,5
4	20,08	Caryophyllene	49,77
5	21,45	α- humulene	2,71
6	22,633	(+)-Epibicyclosesquiphellandrene	9,04
7	23,297	Bicyclogermacrene	21,34
8	24,465	α-Cubebene	2,62
9	26,379	α-Farnesene	3,95

**Table S1:** Main constituents of *L. Camara* white flowers essential oil (EO1)

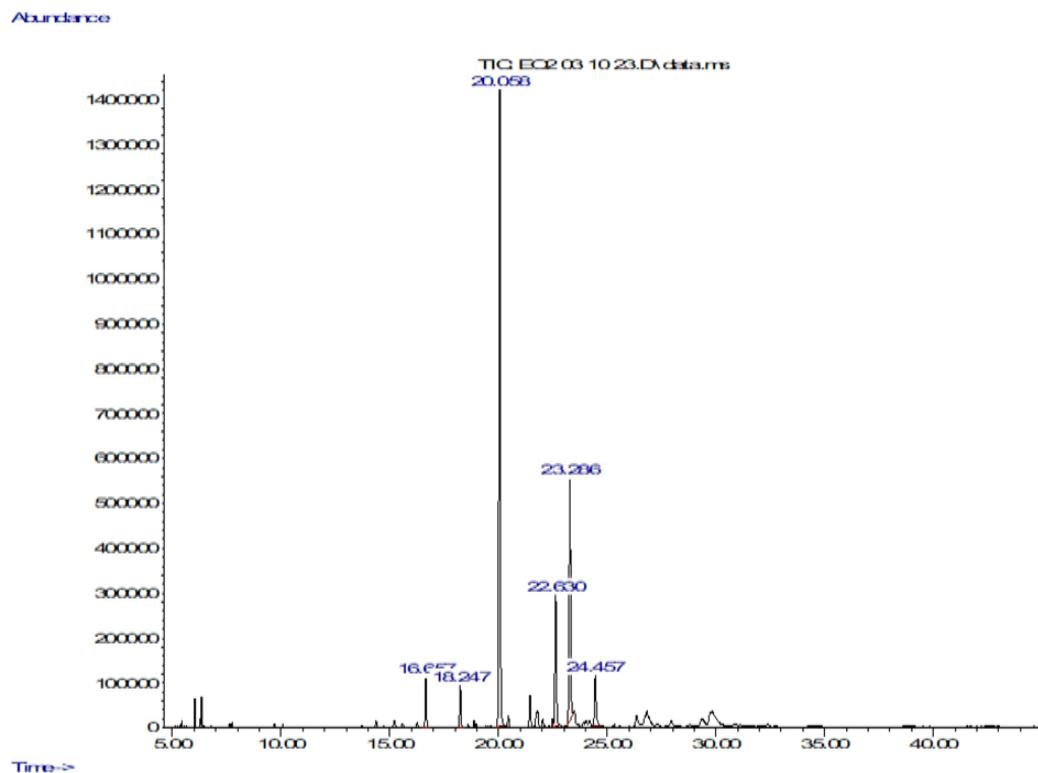
Abundance



**Figure S2:** GC-MS chromatogram of EO1

Yield of extraction: 0.040%			
Peak No.	Retention time (min)	Name	Proportion (%)
1	16,656	Camphene	3,67
2	18,242	Copaene	3,18
3	20,059	Caryophyllene	54,2
4	22,628	$\alpha$ -Muurolene	12,05
5	23,287	$\gamma$ -Elemene	21,37
6	24,459	$\alpha$ -Cubebene	5,5

**Table S2:** Main constituents of *L. Camara* pink flowers essential oil (EO2)



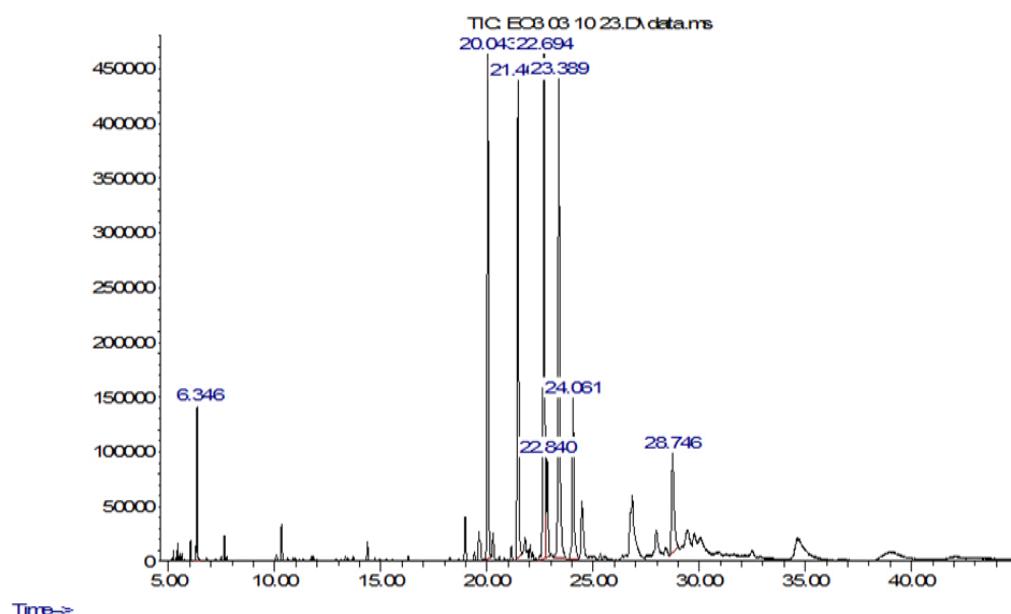
**Figure S3:** GC-MS chromatogram of EO2

**Yield of extraction: 0.047%**

Peak No.	Retention time (min)	Name	Proportion (%)
1	6,346	$\alpha$ -Pinene	3,36
2	20,044	Caryophyllene	17,75
3	21,466	$\alpha$ -humulene	17,42
4	22,695	$\alpha$ -trans-Bergamotene	21,81
5	22,84	$\alpha$ -Curcumene	4,04
6	23,39	$\alpha$ -Phellandrene	21,48
7	24,06	Copaene	7,62
8	28,745	$\alpha$ -Farnesene	6,51

**Table S3:** Main constituents of *L. Camara* orange flowers essential oil (EO3)

Abundance



**Figure S4:** GC-MS chromatogram of EO3

Origin	Major components	Composition (%)	Part of Plant	References
Brazil	Bicyclogermacrene	19,4	Leaves	Ref (1)
	Isocaryophyllene	16,7		
	Valencene	12,9		
	Germacrene D	12,3		
China	Germacrene D	15,85	Leaves & Flowers	Ref (2)
	$\beta$ -Caryophyllene	12,35		
	$\alpha$ -Humulene	9,31		
	Germacrene-B	6,19		
	1,8-Cineole	4,61		
Costa Rica	Caryophyllene	30,3	Leaves	Ref (3)
	$\gamma$ -Muurolene	27,2		
	Bicyclogermacrene	24,4		
	$\beta$ -Elemene	14,2		
Saudi Arabia	Cis-3-hexen-1-ol	11,3	Leaves	Ref (4)
	1-octen-3-ol	8,7		
	Spathulenol	8,6		
	Caryophyllene Oxide	7,5		
	1-hexanol	5,8		
	Caryophyllene oxide	10,6		
	$\beta$ -Caryophyllene	9,7		
	Spathulenol	8,6		
	$\gamma$ -Cadinene	5,6		
	$\beta$ -Farnesene	5		
Cairo, Egypt	Davanone	28,59	Leaves	Ref (5)
	Z-Caryophyllene	11,21		

Origin	Major components	Composition (%)	Part of Plant	References	
Cairo, Egypt	$\alpha$ -Curcumene	10,26	Leaves	Ref (5)	
Cairo, Egypt	$\beta$ -Copene & Humelene	12,29	Leaves	Ref (5)	
	Davanone	23,37	Flowers		
	Caryophyllene	22,96			
	Humulene	14,32			
Côte d'Ivoire	$\beta$ -Caryophyllene	39,9	Leaves	Ref (6)	
	$\alpha$ -Humulene	20,5	Flowers		
	$\beta$ -Caryophyllene	36,6			
	$\alpha$ -Humulene	19,9			

**Table S4:** Main constituents of EOs of *Lantana Camara* from different geographical origins previously reported in literature.

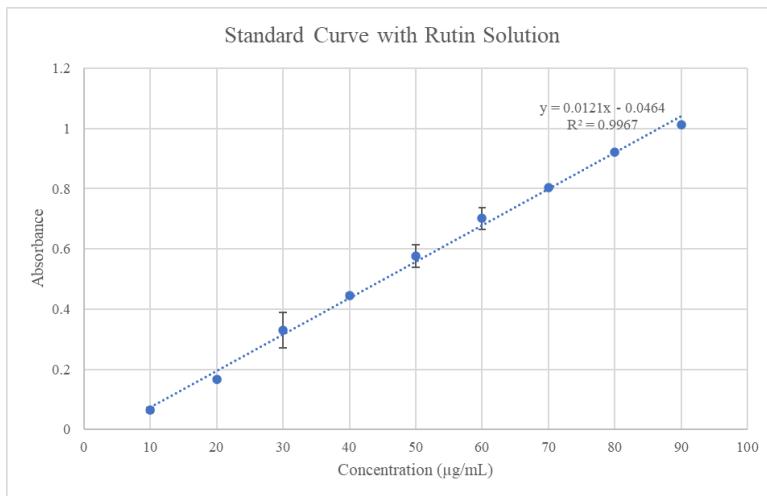
Secondary Metabolites	White flower	Pink flower	Orange flower
Tannins	-	-	-
Quinones	+	+	+
Carotenoids	+	+	+
Terpenoids	+	+	+
Anthocyanins	-	-	-
Proteins	-	-	-
Flavonoids	+	+	+
Phenols	+	+	+
Alkaloids	+	+	+
Saponins	+	+	+

+ = Present - = Absent

**Table S5:** Results of the phytochemical screening of *L. Camara* flowers.

### 3. Analysis of the EOs

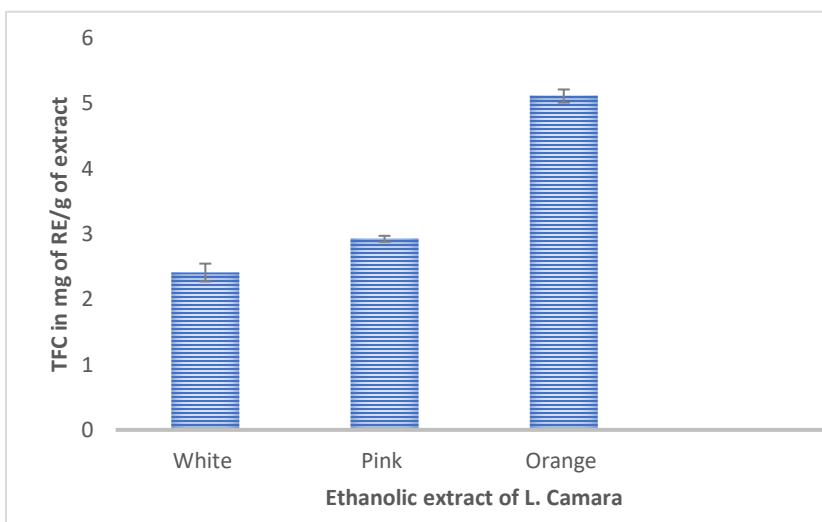
#### 1. TFC and TPC Results



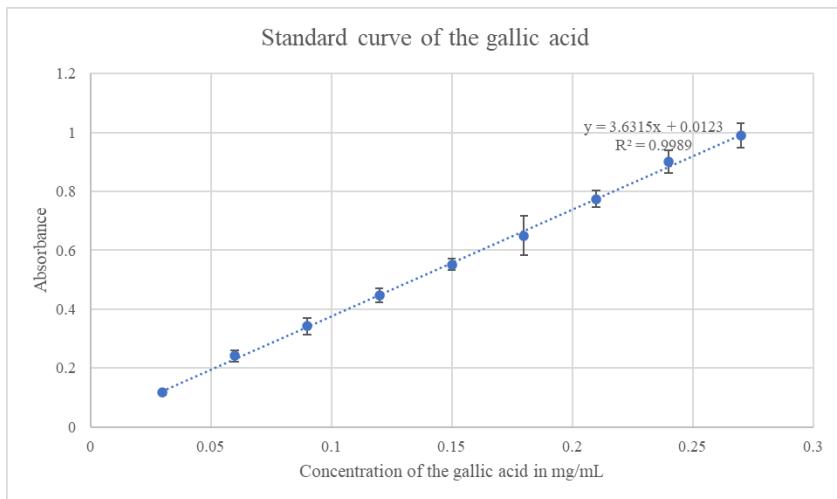
**Figure S5:** Variation of the Absorbance in function of the concentration of the Rutin in  $\mu\text{g/mL}$

Sample	y	x ( $\mu\text{g/ml}$ )	C ( $\text{mg/ml}$ )	mass (g)	TFC ( $\text{mg of RE/g of extract}$ )
OE1	0,246	24,10	0,0241	0,1	2,41
OE2	0,165	17,45	0,0175	0,08	2,19
OE3	0,388	35,85	0,0359	0,07	5,12

**Table S6:** Results of the TFC of the different samples.



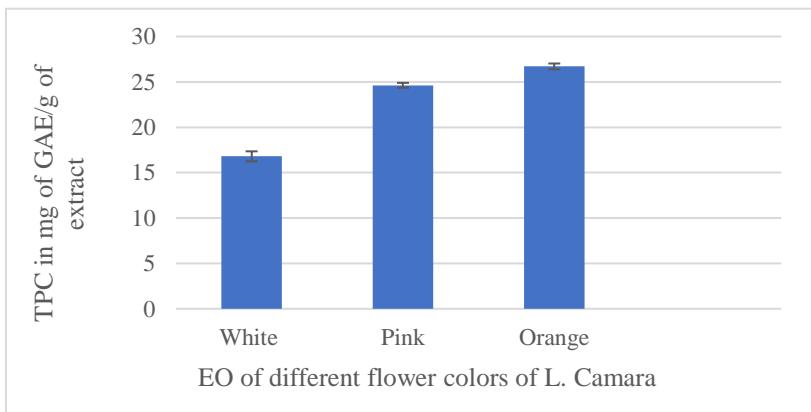
**Figure S6:** Comparison of the TFC in different extracts of *Lantana Camara*



**Figure S7:** Variation of the Absorbance in function of the concentration of Gallic Acid in mg/mL.

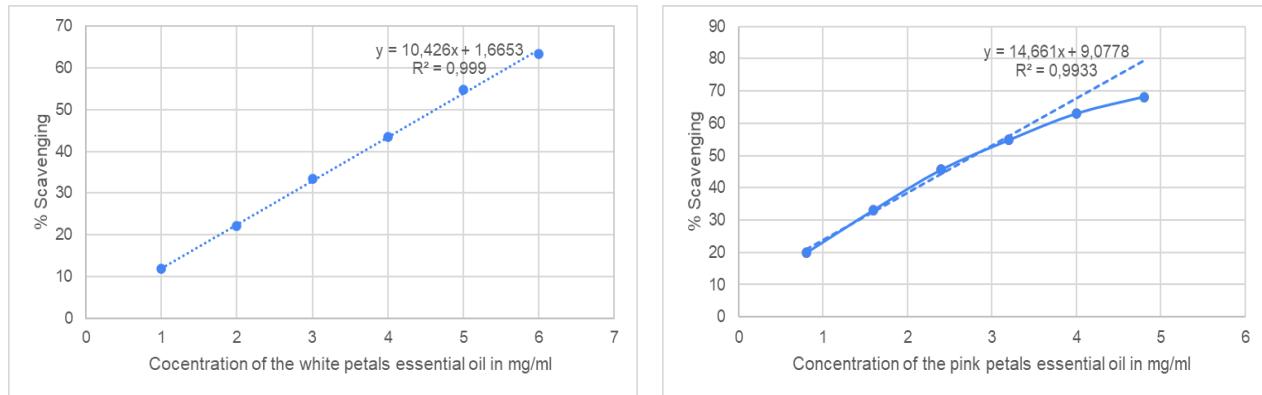
Sample	y	C (mg/ml)	mass (g)	TPC (mg of GAE/g of extract)
OE1	0,62	0,169	0,1	16,8
OE2	0,72	0,197	0,08	24,6
OE3	0,69	0,187	0,07	26,7

**Table S7:** Results of TPC of the different samples.



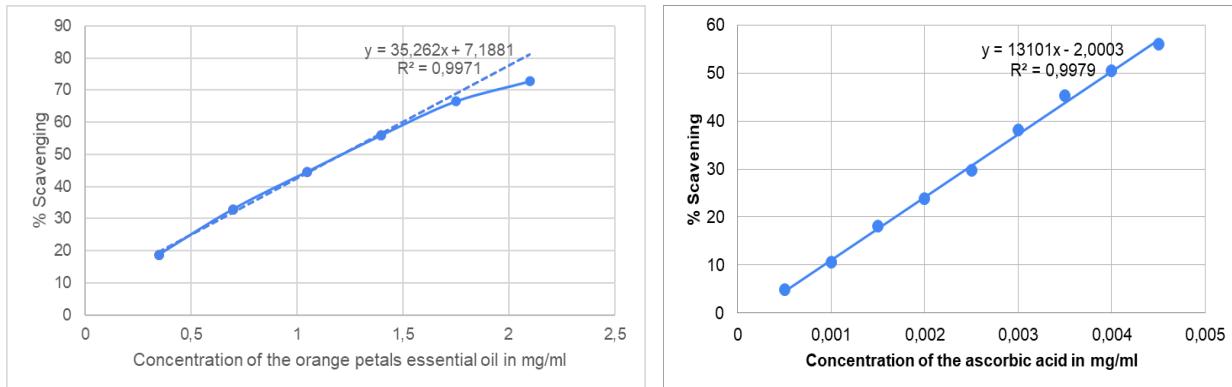
**Figure S8:** Comparison of the TPC in different essential oil extracts of *Lantana Camara*

## 2. DPPH Results



**EO1)**

**EO2)**



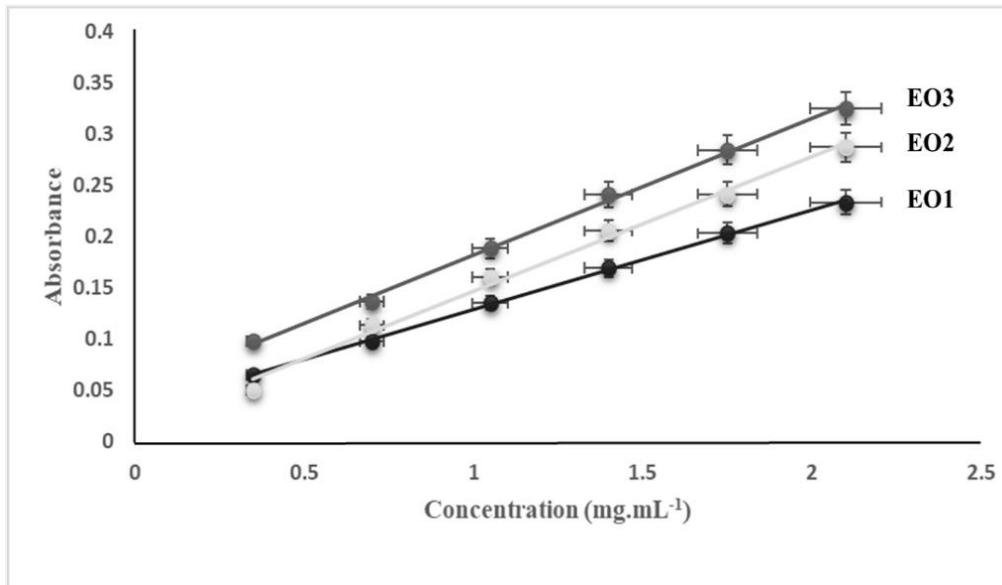
**EO3)**

**Ascorbic Acid standard)**

**Figure S9:** Results of the DPPH scavenging assay in the three EOs and the ascorbic acid measuring the % Scavenging in function of its different concentrations in mg/mL.

Sample	Equation	$R^2$	IC50 (mg/ml)
EO1	$y = 10,426 x + 1,6653$	0,999	<b>4,64</b>
EO2	$y = 14,661 + 9,0778$	0,9933	<b>2,79</b>
EO3	$y = 35,262 x + 7,1881$	0,9971	<b>1,21</b>
Ascorbic Acid	$y = 13101x - 2,0003$	0,9979	<b>0,004</b>

**Table S8:** Results of DPPH Assay of the different samples.



**Figure S10:** Results of the FRAP assay of the three EO samples, measuring absorbance as function of the different concentrations in mg.ml-1.

### 3. Pearson Correlation data

Sample	TFC	TPC	DPPH	MCF7	MDAMB-231
<b>EO1</b>	2.41	16.8	4.64	0.306	0.3099
<b>EO2</b>	2.93	24.63	2.79	0.363	0.7398
<b>EO3</b>	5.12	26.71	1.21	0.5927	0.6473

- (1) Erlânio O. Sousa, Francisco S. S. Barreto , Fabíola F.G. Rodrigues , Adriana R. Campos & José G.M. (2012) Chemical composition of the essential oils of *Lantana camara* L. and *Lantana montevidensis* Briq. and their synergistic antibiotic effects on aminoglycosides, doi: 10.1080/10412905.2012.703494
- (2) Sundufu, A.J. and Shoushan, H. (2004), Chemical composition of the essential oils of *Lantana camara* L. occurring in south China. doi: 10.1002/ffj.1292
- (3) Walden, A. B., Haber, W. A., & Setzer, W. N. (n.d.). (2008) Essential Oil Compositions of Three Lantana Species from Monteverde, Costa Rica doi: 10.1177/1934578X0900400123
- (4) Khan, M., Mahmood, A., & Alkhathlan, H. Z. (2016) Characterization of leaves and flowers volatile constituents of *Lantana camara* growing in central region of Saudi Arabia. *Arabian Journal of Chemistry*. doi: 10.1016/J.ARABJC.2015.11.005
- (5) El Baroty, G. S., Goda, H. M., Khalifa, E. A., Abd, H. H., & Baky, E. (2014). Antimicrobial and antioxidant activities of leaves and flowers essential oils of Egyptian *Lantana camara* L.
- (6) Fatimata Nea, Didjour Albert Kambiré, Manon Genva, Evelyne Amenan Tanoh, Esse Leon Wognin, et al. (2020), Composition, Seasonal Variation, and Biological Activities of *Lantana camara* Essential Oils from Côte d'Ivoire. *Molecules*, doi : 10.3390/molecules25102400