

The supplementary material and Supporting information

Green synthesized Zinc Oxide Nanoparticles, Anti-Alzheimer Potential and Metabolic Profiling of *Sabal blackburniana* grown in Egypt supported by molecular modelling

Fig.S1. UV-Visible spectrum of the synthesized Zno NPs using A(Leaves), B(Fruits)and, C (pollen grains) of the selected *Sabal* species.

Fig.S2. FTIR spectra of *S. blackburniana* extracts; leaves (A), and green synthesized ZnO nanoparticles using leaves (B).

Fig.S3 .IR spectra of *S. blackburniana* extracts; fruits (C) and green synthesized ZnO nanoparticles using fruits (D).

Fig.S4. FTIR spectra of *S. blackburniana* extracts; pollen grains (E) and green synthesized ZnO nanoparticles using pollen grains (F).

Table (S1): List of secondary metabolites annotated from the extracts of the selected *Sabal* species.

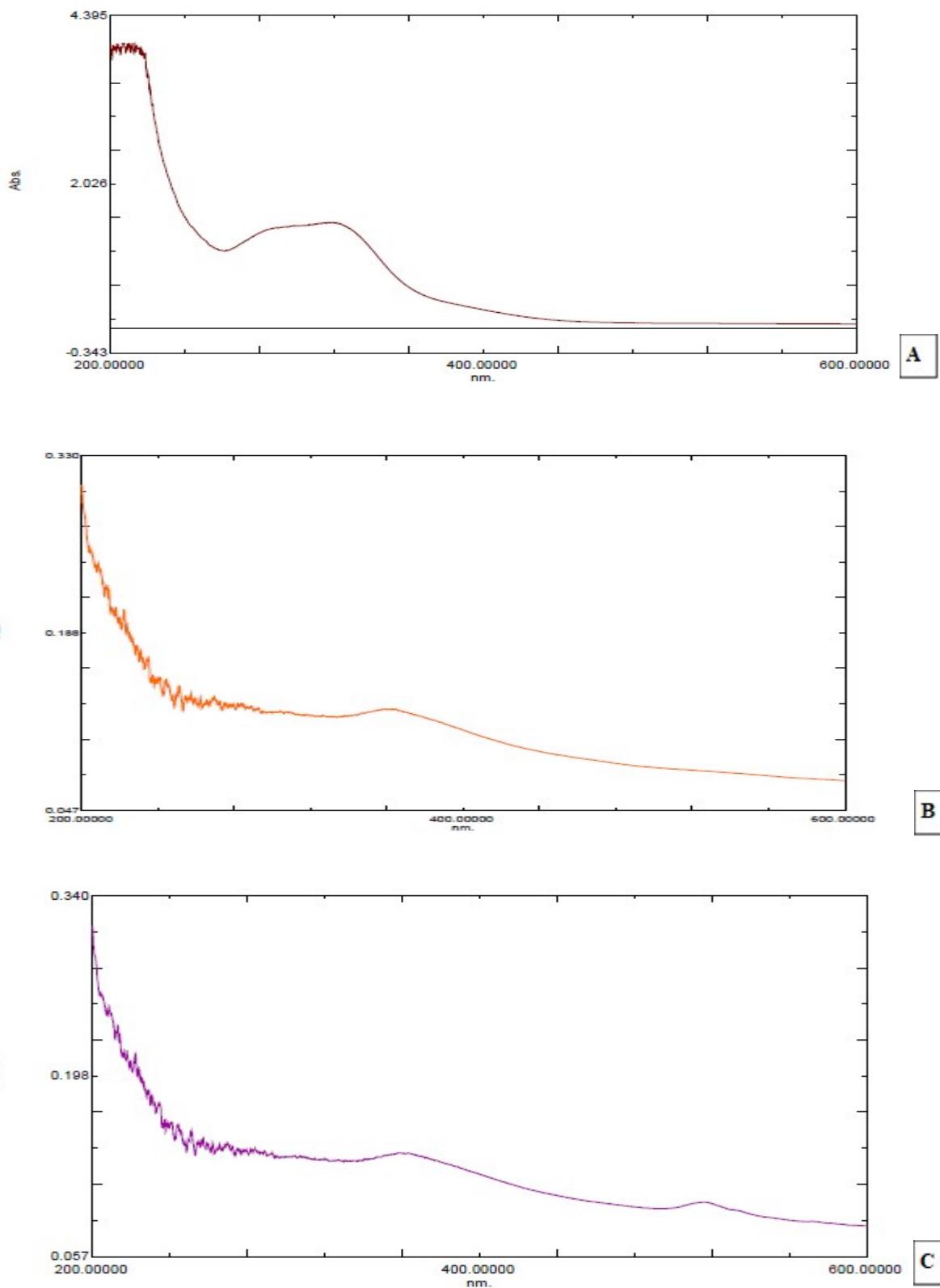


Fig.S1. UV-Visible spectrum of the synthesized ZnO NPs using A(Leaves), B(Fruits)and, C (pollen grains) of the selected *Sabal* species.

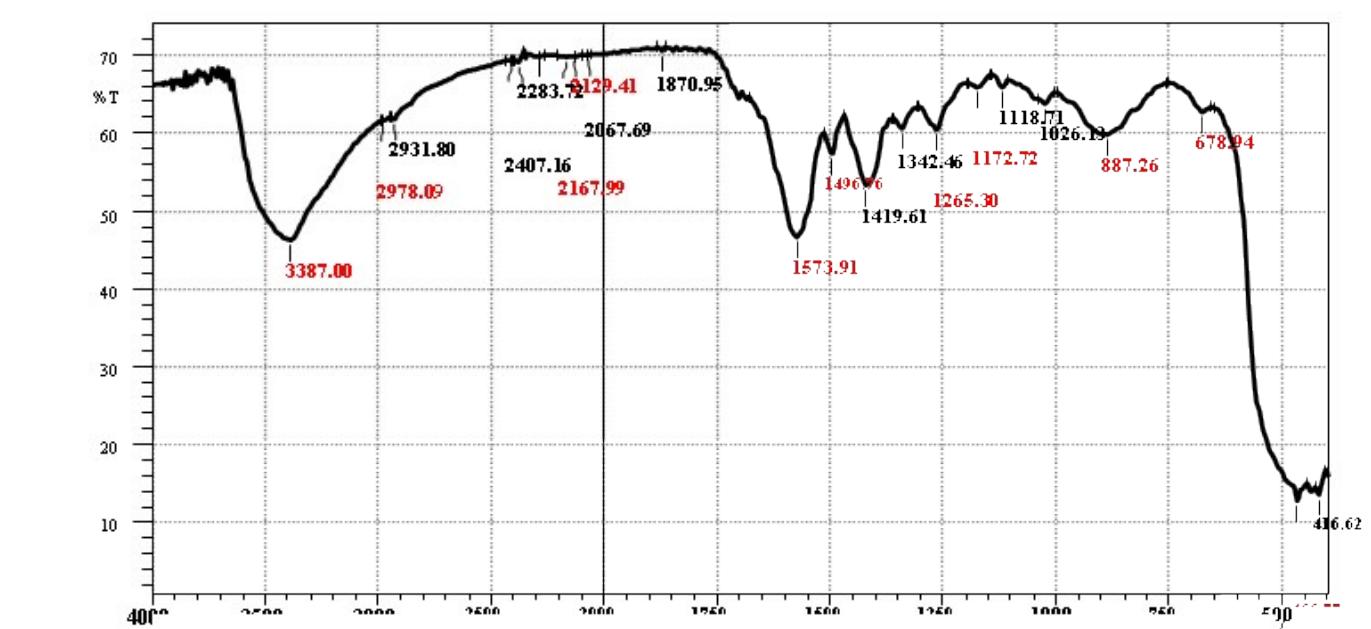
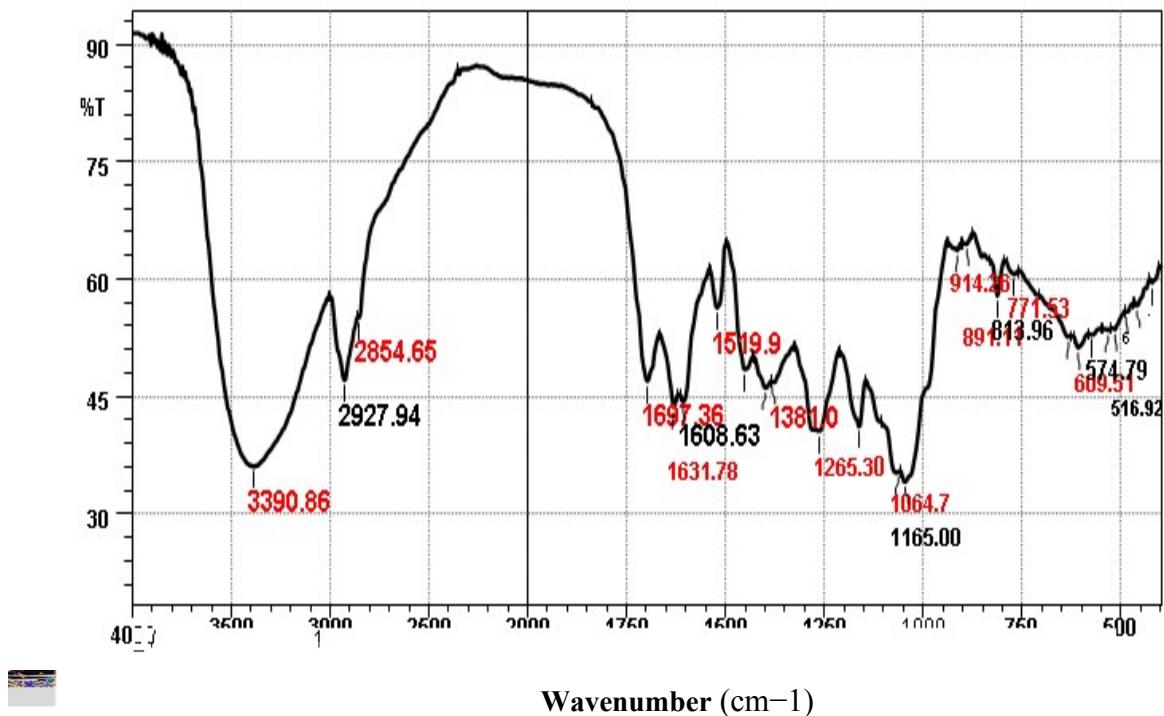
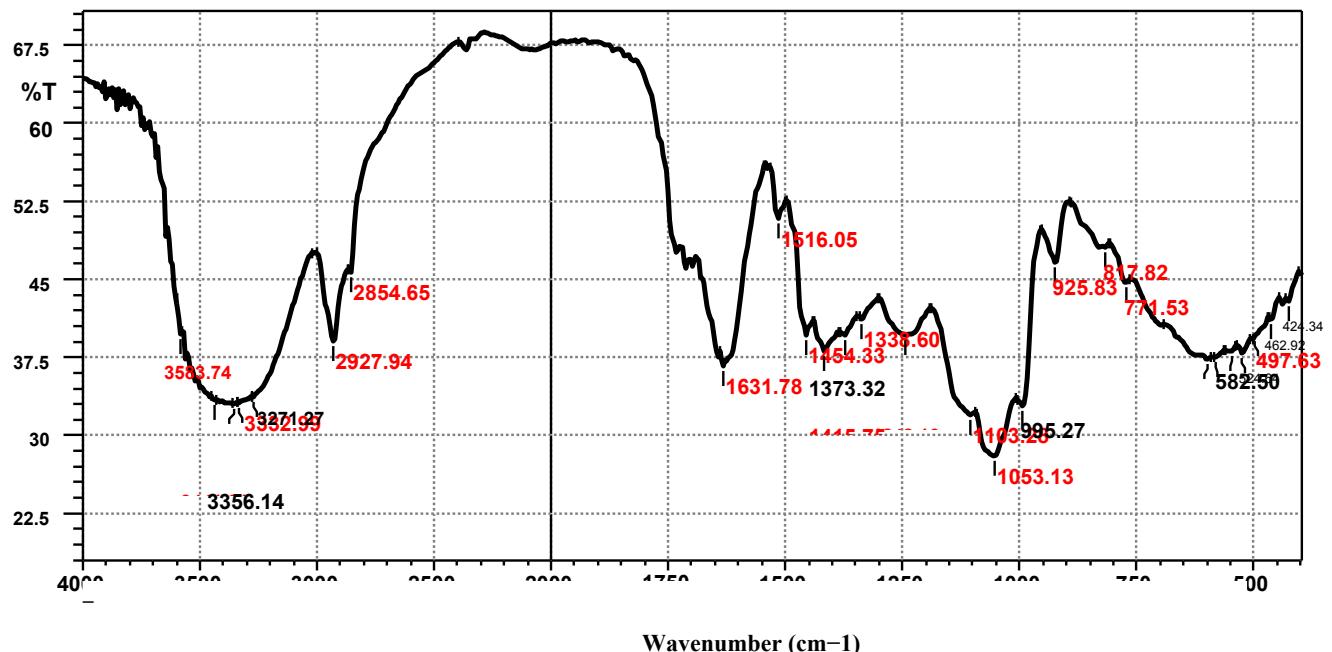
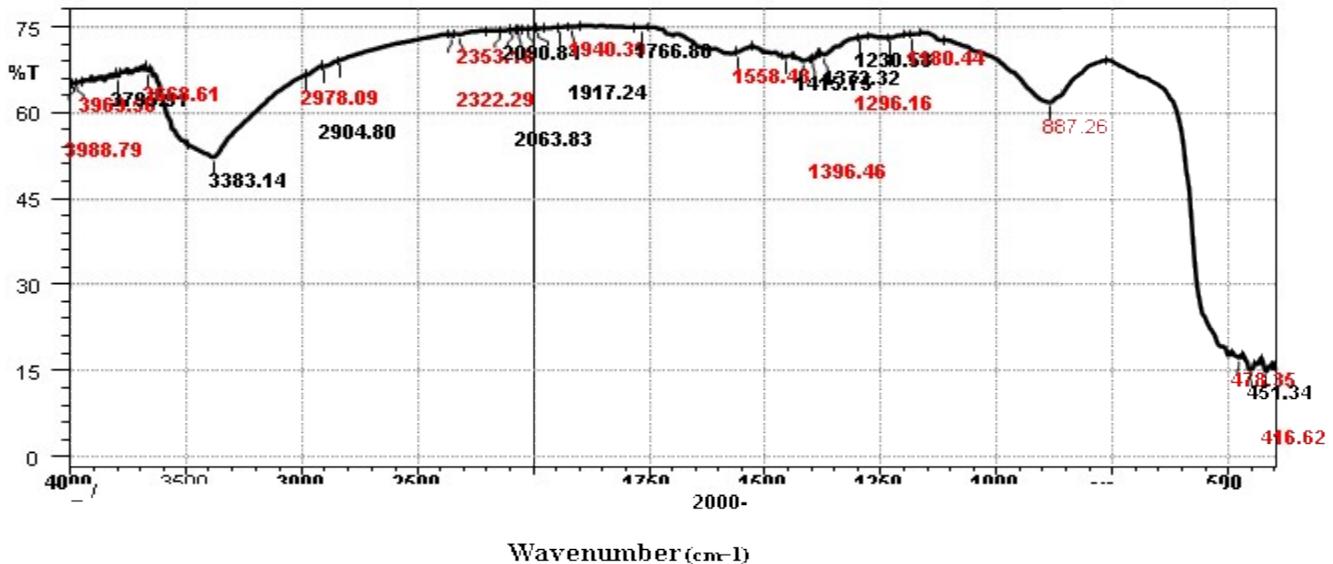


Fig.S2. FTIR spectra of *S. blackburniana* extracts; leaves (A), and green synthesized ZnO nanoparticles using leaves (B).

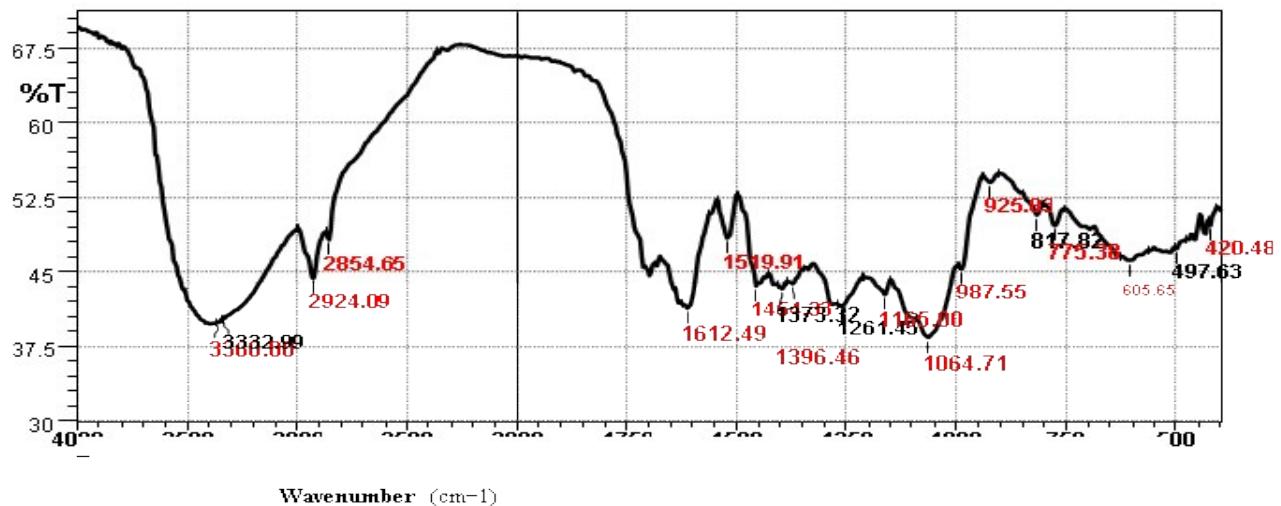


C

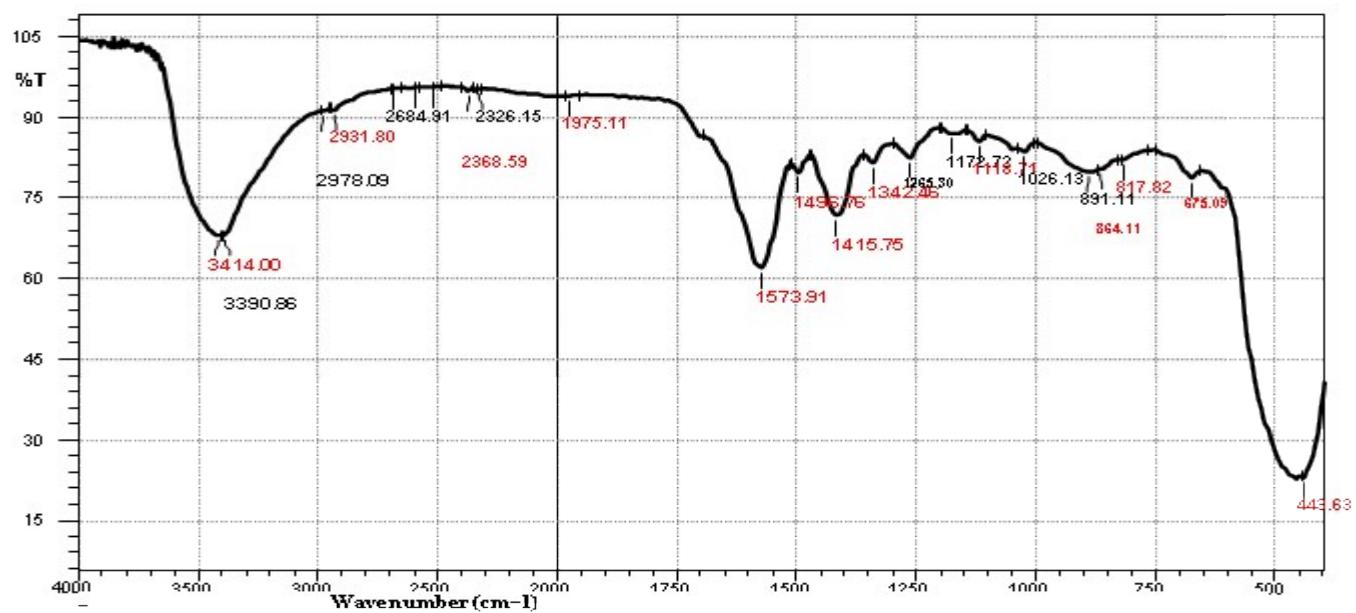


D

Fig.S3 .IR spectra of *S. blackburniana* extracts; fruits (C) and green synthesized ZnO nanoparticles using fruits (D).



E



F

Fig.S4. FTIR spectra of *S. blackburniana* extracts; pollen grains (E) and green synthesized ZnO nanoparticles using pollen grains (F) .

Table (S1): List of secondary metabolites annotated from the extracts of the selected *Sabal* species.

| No | Rt | m/z \pm | Compound | Molecular Formula | Accurate mass | Chemical class | Source | Reference |
|----|------|-----------|---------------------------|---|---------------|-----------------------------------|-----------------------------------|-----------|
| 1 | 2.84 | 149.1278 | Cinnamic acid | C ₉ H ₈ O ₂ | 148.1205 | Phenolic acids; Phenyl propanoids | Plam seeds fruits | 1 |
| 2 | 2.32 | 155.1043 | Protocatechuic acid | C ₇ H ₆ O ₄ | 154.097 | Phenolic acids | <i>Phoenix dactylifera</i> | 2 |
| 3 | 2.93 | 163.0739 | Metanicotine | C ₁₀ H ₁₄ N ₂ | 162.067 | Alkaloid | <i>Duboisia Hopwoodii</i> | 3 |
| 4 | 1.78 | 165.09 | p-Coumaric acid | C ₉ H ₈ O ₃ | 164.083 | Phenolic acids | Plam seeds fruits | 4 |
| 5 | 4.64 | 171.1018 | Gallic acid | C ₇ H ₆ O ₅ | 170.0945 | Phenolic acids | <i>Phoenix dactylifera</i> | 5 |
| 6 | 3.93 | 195.18 | Ferulic acid | C ₁₀ H ₁₀ O ₄ | 194.1727 | Phenolic acids | <i>Phoenix canariensis</i> leaves | 6 |
| 7 | 3.55 | 271.1194 | Genistein | C ₁₅ H ₁₀ O ₅ | 270.1121 | Isoflavone | <i>Sabal</i> palm seeds | 7 |
| 8 | 5.4 | 271.3016 | Eestrone | C ₁₈ H ₂₂ O ₂ | 270.2943 | Steroid | <i>Phoenix dactylifera</i> | 8 |
| 9 | 6.85 | 279.4756 | Linoleic acid | C ₁₈ H ₃₂ O ₂ | 280.4829 | Fatty acids | <i>S. serrulata</i> | 9 |
| 10 | 3.85 | 283.3031 | Oleic acid | C ₁₈ H ₃₄ O ₂ | 282.2958 | Fatty acids | <i>S. serrulata</i> | 9 |
| 11 | 2.75 | 287.1167 | Luteolin | C ₁₅ H ₁₀ O ₆ | 286.1094 | Flavone | Plam; leaves seeds, fruits | 10 |
| 12 | 2.3 | 291.1486 | Catechin | C ₁₅ H ₁₄ O ₆ | 290.14141 | Flavanol (hydroxyflavan) | Plam seeds fruits | 4 |
| 13 | 3.7 | 301.1357 | Chryseriol | C ₁₆ H ₁₂ O ₆ | 300.1266 | Flavone | Plam leaves fruits | 11 |
| 14 | 3.18 | 305.1692 | Taxifolin | C ₁₅ H ₁₂ O ₇ | 304.1619 | Flavonols | Plam leaves | 11 |
| 15 | 3.77 | 331.1500 | Tricin | C ₁₇ H ₁₄ O ₇ | 330.1449 | O-methylated flavone | <i>Sabal</i> palm seeds | 1 |
| 16 | 4.74 | 332.3094 | Helasaoussazine | C ₁₉ H ₁₃ N ₄ O ₂ | 333.3167 | Alkaloid | <i>P. canariensis</i> palm | 12 |
| 17 | 2.48 | 337.1639 | 3-O-Caffeoylshikimic acid | C ₁₆ H ₁₆ O ₈ | 336.1566 | Phenolic acids | <i>Phoenix dactylifera</i> | 13 |
| 18 | 3.18 | 411.3770 | Squalene | C ₃₀ H ₅₀ | 410.3675 | Triterpenes | <i>S. blackburniana</i> | 14 |
| 19 | 4.18 | 413.3919 | Stigmasterol | C ₃₀ H ₅₂ | 412.3846 | Sterols | <i>Sabal</i> palm seeds | 7 |

| | | | | | | | | |
|----|------|----------|---|---|-------------|--|---|--------|
| 20 | 3.44 | 413.3925 | $\Delta 7$ –Avenesterol | C ₂₉ H ₄₈ O | 412.3853 | Sterols | <i>P. canariensis</i> palm | 15 |
| 21 | 5.57 | 415.4092 | Diosgenin | C ₂₇ H ₄₂ O ₃ | 414.4019 | Steroidal saponin | <i>Sabal</i> palm seeds. | 7 |
| 22 | 5.59 | 415.4083 | β -Sitosterol | C ₂₉ H ₅₀ O | 414.4011 | Sterol | <i>S. causiarum</i> | 16 |
| 23 | 6.64 | 427.3924 | Cycloartenol | C ₃₀ H ₅₀ O | 426.3851 | Pentacyclic Triterpenoid | <i>S. serrulata</i> | 17 |
| 24 | 2.78 | 433.2045 | Isovitexin | C ₂₁ H ₂₀ O ₁₀ | 432.1972 | C-glucosyl flavone | <i>S. blackbuniana.</i> | 18 |
| 25 | 2.54 | 449.2029 | Kaempferol-3- glucoside | C ₂₁ H ₂₀ O ₁₁ | 448.1957 | O-glycosyl flavone. | <i>S. serrulata</i> | 19 |
| 26 | 2.66 | 449.2024 | Orientin | C ₂₁ H ₂₀ O ₁₁ | 448.1951 | C-glycosyl flavone . | <i>S. blackbumiana</i> | 18 |
| 27 | 2.50 | 449.2030 | Luteolin 7-glucoside | C ₂₁ H ₂₀ O ₁₁ | 448.1957 | Glycosyloxy flavone | <i>Phoenix loureirii.</i> | 20 |
| 28 | 2.69 | 465.2020 | Isoquercetin | C ₂₁ H ₂₀ O ₁₂ | 464.1947 | Flavonol | <i>S. serrulata</i> | 19 |
| 29 | 6.03 | 469.5029 | Sablacaurin B | C ₃₂ H ₅₂ O ₂ | 468.4954 | 19- Triterpenoid; nor-3,4-seco- Lanostane-Type | <i>S blackburniana</i> | 14 |
| 30 | 5.7 | 459.4498 | 25- Hydroperoxyycloart- 23-ene- 3 ol | C ₃₀ H ₅₀ O ₃ | 458.4425 | Triterpenoid | <i>Xanthosoma robustum</i> (Araceae) | 21 |
| 31 | 5.9 | 481.4135 | Brassinolide | C ₂₈ H ₄₈ O ₆ | 480.4062 | Steroid | <i>Phoenix dactylifera</i> | 8 |
| 32 | 3.04 | 493.2376 | Tricin 7-O- glucoside | C ₂₇ H ₃₀ O ₁₄ | 492.2303 | Flavonoids | <i>Phoenix Rupicola.</i> | 20 |
| 33 | 6.15 | 569.521 | β - Carotene diepoxide. | C ₄₀ H ₅₆ O ₂ | 568.5137 | Tetraterpene; a oxygenated carotenoid. | <i>Ipomoea batatas Lam</i> | 22 |
| 34 | 8.72 | 579.2576 | Rhoifolin (Apigenin 7-O- neohesperidoside). | C ₂₇ H ₃₀ O ₁₄ | 578.2504 | O-Glycosyl flavone | <i>S. serrulata</i> | 19 |
| 35 | 3.05 | 625.2084 | Isorhamnetin-3-O- rutinoside | C ₂₈ H ₃₂ O ₁₆ | 624.2012 | Flavonols | Plam leaves | 23 |
| 36 | 3.02 | 747.1913 | Shimobashiric acid D. | C ₃₈ H ₃₆ O ₁₆ | 748.1985483 | Neolignan. | <i>Keiskea japonica</i> | 24 |
| 37 | 6.53 | 839.1739 | Tetra-O- Caffeoylquinic acid | C ₄₃ H ₃₆ O ₁₈ | 840.1812 | Polyphenol | <i>Pluchea symphytifolia</i> | 25 |
| 38 | 3.47 | 869.6766 | Dioscin | C ₄₅ H ₇₂ O ₁₆ | 868.5971 | Steroidal saponin | <i>Phoenix dactylifera</i> | 23 |
| 39 | 3.02 | 897.0992 | Gallocatechin- (4alpha—8)]2- catechin | C ₄₅ H ₃₈ O ₂₀ | 898.1065 | Condensed tannins; Polyphenol (Flavonoids; flavan-3-ols) | <i>Hordeum vulgare</i> | 26, 27 |

| | | | | | | | | |
|----|-------|-----------|-----------------|---|-----------|-----------------------|-----------------------------|----|
| 40 | 6.025 | 999.4723 | Bridgeside C1 | C ₄₉ H ₇₄ O ₂₁ | 998.465 | Triterpenoid saponins | <i>Echinopsis macrogona</i> | 28 |
| 41 | 3.10 | 1048.7724 | Causiaroside II | C ₅₁ H ₈₃ O ₂₂ | 1047.7651 | Steroidal saponin | <i>S. causiarum</i> | 20 |

References

- 1) Mansouri A, Guendez E, Kokkalou E, Kefalas P., (2005). Phenolic profile and antioxidant activity of the Algerian ripe date palm fruit (*Phoenix dactylifera*). *Food Chemistry*, 89, 411–420.
- 2) Amira, E. A., Behija, S. E., Beligh, M., Lamia, L., Manel, I., Mohamed, H., et al. (2012). Effects of the ripening stage on phenolic profile, phytochemical composition and antioxidant activity of date palm fruit. *J. Agric. Food Chem.*, 60:10896–902.
- 3) Luanratana, O., and W. J. Griffin. 1982. Alkaloids of *Duboisia hopwoodii*. *Phytochemistry* 21:449–51.
- 4) R Messaoudi, S Abbeddou, A Mansouri, A C. Calokerinos & P Kefalas. 2013. Phenolic Profile and Antioxidant Activity of Date-Pits of Seven Algerian Date Palm Fruit Varieties. *International Journal of Food Properties*, 08:29.
- 5) Benmeddour, Z., Mehinagic, E., Le Meurlay, D., and Louaileche, H. (2013). Phenolic composition and antioxidant capacities of ten Algerian date (*Phoenix dactylifera* L.) cultivars: a comparative study. *J. Funct. Food* 5, 346–354.
- 6) B Garcia,J. A Marco, E Seoane, A Tortajada 1981.Triterpenes, Waxes and Tricin in *Phoenix canariensis* .J. Nat. Prod. , 44, 1, 111–113.
- 7) Liu, L., Xiong, C., Zhu, Y., Zhou, H., and Ma, S. (2015). “The separation and anticancer activity of active monomers from *Sabal* palm seeds”. Beijing Huagong Daxue Xuebao (Ziran Kexueban)/Journal of Beijing University of Chemical Technology (Natural Science Edition), 42 (6), pp. 78-83.
- 8) Zaki, A.K., Schmidt, J., Hammouda, F.M. and Adam, G. (1993). Steroid Constituents from Pollen Grain of *Phoenix dactylifera*. *Planta Medica*, 59, 613-614
- 9) Catchpole, O. J.; Perry, N. B.; da Silva, B. M. T.; Grey, J. B. and Smallfield, B. M. (2002). J. of Supercritical fluids, 22, 129- 138.
- 10) Hong, Y. J., Tomas-Barberan, F. A., Kader, A. A., and Mitchell, A. E. (2006). The flavonoid glycosides and procyanidin composition of deglet noor dates (*Phoenix dactylifera*). *J. Agric. Food Chem.* 54, 2405–2411.
- 11) Ouafi, S., Gaceb-Terrak, R., Bounaga, N., Lebreton, P 1988. Les flavonoides marqueurs intraspécifiques chez le palmier dattier (*Phoenix dactylifera* L.). - Compt. rend. Acad. Sci. Paris, Sér. III306: 399–404

- 12) S Hammami, H Jarraya, S Ben Salem, B Hamdi, A Ben Salah, P Devi, A Nefzi, Z Mighri. Isolation and structure elucidation of a novel alkaloid from *Phoenix canariensis* (C.) Palm tree. Journal de la Société Chimique de Tunisie, 2010, 12, 105-108
- 13) M A. Farag, M Mohsen R Heinke L A. Wessjohann 2014. Metabolomic fingerprints of 21 date palm fruit varieties from Egypt using UPLC/PDA/ESI-qTOF-MS and GC-MS analyzed by chemometrics. Food Research International. 64, 218-226.
- 14) El-Dib, R.; Kaloga, M.; Mahmoud, I.; Soliman, H.; Moharram, F. and Kolodziej, H. Sablacausrin A and B, Two 19-nor3,4-seco-lanostane-type Triterpenoids from *Sabal causiarum* and *Sabal blackburniana*, Respectivrly. *Phytochemistry*, 65(2004) 1153-1157.
- 15) I.Nehdi S. Omrib, M.I. Khalil S.I. Al-Resayes, 2010.Characteristics and chemical composition of date palm (*Phoenix canariensis*) seeds and seed oil. Industrial Crops and Products, 32, 3, 360-365
- 16) Yang, X.-H., Cai, Z.-Y., Cai, X., Xu, X.-J., Li, H.-J and Qin, Y., (2015). "Quality standard of *Sabal* fruit extract soft capsules". Chinese Journal of New Drugs, 24 (24), 2854-2864.
- 17) Fabre, Pierre, S. A. Prostatitis inhibitors from *Sabal serrulata* fruits. *Jpn. Kokai Tokkyo Koho JP .58* 67,625.
- 18) Harborne, C. A. Williams, J. Greenham, and P. Moyna. (1974). Distribution of charged flavones and caffey1shikimic acid in Palmae. *Phytochemistry* 13:1557-1559.
- 19) Hiermann, A. (1989). "Content of *Sabal serrulata* fruits and their anti-inflammatory effect." *Arch. Pharm(Weinheim)*, 322(2), 111-114.
- 20) Idaka, K., Hirai, Y., Shoji, J. Studies on the Constituents of Palmae Plants. IV.1a) The Constituents of the Leaves of *Sabal causiarum* Becc". *Chemical and Pharmaceutical Bulletin*, 36 (5) (1988)1783-1790.
- 21) T Kato, B Frei Haller, M Heinrich, O Sticher,1996, Antibacterial hydroperoxysterols from *Xanthosoma Robustum*. *Phytochemistry*, 41(4):1191-5
- 22) Almeida-Muradian LB, Penteado MVC.,1992. Carotenoids and provitamin A value of some Brazilian sweet potato cultivars (*Ipomoea batatas* Lam.). *Rev Farm Bioquim Univ Sao Paulo*;28:145-54.
- 23) Asami, Y. Hirai, J. Shoji, (1991). Studies on the constituents of Palmae plants. VI. Steroid saponins and flavonoids of leaves of *Phoenix canariensis* hort. ex Chabaud, P. humilis Royle var. hanceana Becc., *P. dactylifera* L and *Licuala spinosa* Wurm. *Chem Pharm. Bull*,39 2053-2056.
- 24) Murata T, Miyase T, Yoshizaki F (2012). Hyaluronidase inhibitors from *Keiskea japonica*. *Chem Pharm Bull* ,60:121–128
- 25) E. Scholz, M. Heinrich, and D. Hunkler 1994. Caffeoylquinic Acids and Some Biological Activities of *Pluchea symphytifolia*. *Planta Medica* 60(4):360- 364.

- 26) Harborne, The Handbook of Natural Flavonoids, 2, (1999), 355, Flavans and proanthocyanidins L.B.
- 27) M. J. Brandon, L. Y. Foo, L. J. Porter, and P. Meredith, (1982). Proanthocyanidins of barley and sorghum; composition as a function of maturity of barley ears. *Phytochemistry*, 21, 2953.
- 28) S Okazaki, K Kinoshita, S Ito, K Koyama, H Yuasa, K Takahashi, 2011. Triterpenoid saponins from *Echinopsis macrogona* (Cactaceae). *Phytochemistry*, 72 (1), 136-146.