

## REFERENCES

- Abdallah, O. I., Alamer, S. S. & Al-rasheed, A. M. M. 2018. Monitoring pesticide residues in dates marketed in Al-Qassim, Saudi Arabia using a QuEChERS methodology and liquid chromatography–tandem mass spectrometry. *Biomedical Chromatography*, 32(6), 4199-4209
- Aguiar, M. C. S., Silverio, F. O., Pinho, G. P. D., Lopes, P. S. N., Fidencio, P. H. & Ventura, S. J. 2014. Volatile compounds from fruits of *Butia capitata* at different stages of maturity and storage. *Food Research International*, 62, 1095–1099
- Ahmed, J., Almusallam, A. W., & Al-Hooti, S. N. 2013. Isolation and characterization of insoluble dates (*Phoenix dactylifera* L.) fiber. *LWT - Food Science and Technology*, 50, 414-419.
- Alex, B. K., Koshy, E. P. & Thomas, G. 2018. Comprehensive metabolite profiling of *Haematoctopus validus* (miers) bakh.f. Ex forman leaf and fruit samples using ftir spectroscopic analysis. *Plant Archives*, 18(1), 897-900
- Alfaro-Viquez, E., Roling, B. F., Krueger, C. G., Rainey, C. J., Reed, J. D. & Ricketts, M. L. 2018. An extract from dates palm fruit (*Phoenix dactylifera*) acts as a co-agonist ligand for the nuclear receptor FXR and differentially modulates FXR target-gene expression *in vitro*. *PLoS ONE*, 13(1), <https://doi.org/10.1371/journal.pone.0190210>
- Al-Farsi, M., Alasalvar, C., Morris, A., Baron, M. & Shahidi, F. 2005. Comparison of anthocyanins, carotenoids, and phenolics of three native fresh and sun-dried dates (*Phoenix dactylifera* L.) varieties grown in Oman. *Journal of Agriculture & Food Chemistry*, 53, 7592-7599.
- Al-Hajjaj, H. S., & Ayad, J. Y. 2019. Effect of foliar boron applications on yield and quality of Medjool date palm Effect of foliar boron applications on yield and quality of Medjool date palm. *Journal of Applied Horticulture*, 20(3), 181-188
- Al-Saif, A. M. & Alebidi, A. 2017. Preharvest Ethephon spray on fruit quality and increasing the rate of ripening of date palm fruit (*Phoenix dactylifera* L.) cv . Helali. *Progress in Nutrition*, 19(1), 97-103
- Al-Yahya, M., Raish, M., Al-Said, M. S., Ahmad, A., Mothana, R. A., Al-Sohaibani, M., Rafatullah, S. 2016. ‘Ajwa’ dates (*Phoenix dactylifera* L.) extract ameliorates isoproterenol-induced cardiomyopathy through downregulation of oxidative, inflammatory and apoptotic molecules in rodent model. *Phytomedicine*, 23(11), 1240–1248.

- Al-Harrasi, A., Najeeb, U. R., Hussain, J., Khan, A. L., Al-Rawahi, A., Gilani, S. A., Al-Broumi, A. & Ali, L. 2014. Nutritional assessment and antioxidant analysis of 22 dates palm (*Phoenix dactylifera*) varieties growing in Sultanate of Oman. *Asian Pacific Journal of Tropical Medicine*, 1, 591-598.
- Al-Kuran, O., Al-Mehaisen, L., Bawadi, H., Beitawi S. & Amarin, Z. 2011. The effect of late pregnancy consumption of dates fruit on labour and delivery. *Journal of Obstetrics and Gynaecology*, 31(1), 29-31.
- Al-Qarawi, A. A., Abdel-Rahman, H., Ali, B. H., Mousa, H. M. & El-Mougy, S. A., 2005. The ameliorative effect of dates (*Phoenix dactylifera* L.) on ethanol-induced gastric ulcer in rats. *Journal of Ethnopharmacology*, 98(3), 313-317.
- Aslam, J., Khan, S. H. & Khan, S. A., 2013. Quantification of water soluble vitamins in six dates palm (*Phoenix dactylifera* L.) cultivar's fruits growing in Dubai, United Arab Emirates, through high performance liquid Chromatography. *Journal of Saudi Chemical Society*, 17, 9-16
- Harthi, S. S., Mavazhe, A., Al-Mahroqi, H. & Khan, S. A. 2015, Quantification of phenolic compounds, evaluation of physicochemical properties and antioxidant activity of four dates (*Phoenix dactylifera* L.) varieties of Oman. *Journal of Taibah University Medical Sciences*, 10(3), 346-352.
- Alhaider, I. A., Mohamed. M. E., Ahmed, K. K. M., & Kumar, A. H. S. 2017. Dates palm (*Phoenix dactylifera*) fruits as a potential cardioprotective agent: The role of circulating progenitor cells. *Frontier at Pharmacology*, 8(592), doi: 10.3389/fphar.2017.00592.
- Al-Najada, A. R. & Mohamed, S. A. 2014. Changes of antioxidant capacity and oxidoreductases of Saudi dates cultivars (*Phoenix dactylifera* L.) during storage. *Scientia Horticulturae*, 170, 275-280.
- Al-Shahib, W. & Marshall, R. J. 2003. The fruit of dates palm: Its possible use as the best food for the future? *International Journal of Food Science and Nutrition*, 54, 247-259.
- Alvarez-Sanchez, B., Priego-Capote, F. & Castro, M. D. 2010. Metabolomics analysis I. Selection of biological samples and practical aspects preceding sample preparation. *Analytical Chemistry*, 29(2), 111-119.
- Al-Yahyai, R., & Manickavasagan, A., 2012. An overview of dates palm production. Dates: Production, processing, food and medicinal values. *Medicinal and Aromatic Plants – Industrial Profiles*, 3-12.
- Andrea, B. & Scott M. 1988. Effect of dietary stearic acid on plasma cholesterol and lipoprotein levels. *The New England Journal of Medicine*, 318, 1244-1248.

- Aranibar, N., Vassallo, J. D., Rathmacher, J., Stryker, S., Zhang, Y., Dai, J., Janovitz, E. B., Robertson, D., Reily, M., Lowe-Krentz, L. & Lehman-McKeeman, L. 2011. Identification of 1- and 3-methylhistidine as biomarkers of skeletal muscle toxicity by nuclear magnetic resonance-based metabolic profiling. *Analytical and Biochemical*, 410, 84–91.
- Arianna, Q. 2018. Spirolactones: Recent advances in natural products, bioactive compounds and synthetic strategies. *Current Medicinal Chemistry*, 25(8), 917-962.
- Aris, N. A., Norhuda, I. & Adeib, I. S. 2013. Extraction of *Phoenix dactylifera* (Mariami) seeds oil using supercritical carbon dioxide (SC-CO<sub>2</sub>). *International Journal of Chemical and Environmental Engineering*, 4(1), 32-37
- Assirey, E. A. R. 2015. Nutritional composition of ten dates palm (*Phoenix dactylifera* L.) cultivar fruits grown in Saudi Arabia by high performance liquid chromatography. *Journal of Taibah University Sciences*, 9, 75-79.
- Awad, M. A., Al-Qurashi, A. D. & Mohamed, S. A., 2011. Antioxidant capacity, antioxidant compounds and antioxidant enzyme activities in five dates cultivars during development and ripening. *Scientia Horticulturae*, 129, 688–693.
- Baliga, M. S., Baliga, B. R. V., Kandathil, S. M., Bhat, H. P. & Vayalil, P. K. 2011. A review of the chemistry and pharmacology of the dates fruits (*Phoenix dactylifera* L.). *Food Research International*, 44, 1812–1822.
- Benmeddour, Z., Emira M., Dominique L. M. & Hayette L. 2013, Phenolic composition and antioxidant capacities of ten Algerian dates (*Phoenix dactylifera* L.) cultivars: A comparative study. *Journal of Functional Foods*. 5, 346-354.
- Bergwik, J. & Akestrom, B. 2018. P-181 - Riboflavin/vitamin B2 radicals - a novel target for the radical scavenger  $\alpha$ 1-microglobulin. *Free Radical Biology and Medicine*, 120, (1), 99.
- Biglari, F., Abbas, F. M. A. & Azhar, M. E. 2008. Antioxidant activity and phenolic content of various dates palm (*Phoenix dactylifera* L.) fruits from Iran. *Journal of Food Chemistry*, 107, 1636-1641.
- Bilal, A., Usman, A. A., Muhammad, T. Q. & Matloob, A. 2014. Anticancer potential of phytochemicals against breast cancer: Molecular docking and simulation approach. *Journal of the Bangladesh Pharmacological Society*, 9, 545-550.
- Bildziukevich, U., Vida, N., Rarova, L., Kolar, M., Saman, D., Havlicek, L., Drasar, P. & Wimmer, Z. 2015. Polyamine derivatives of betulinic acid and  $\beta$ -sitosterol: A comparative investigation. *Steroids*, 100, 27-35.

- Borrull, J., Colom, A., Fabregas, J., Pocurull, E. & Borrull, F. 2019. A simple, fast method for the analysis of 20 contaminants of emerging concern in river water using large-volume direct injection liquid chromatography-tandem mass spectrometry. *Analytical and Bioanalytical Chemistry*, 411(8), 1601-1610
- Boudries, H., Kefalas, P. & Hornero-Méndez, D. 2007. Carotenoid composition of Algerian dates varieties (*Phoenix dactylifera L.*) at different edible maturation stages. *Food Chemistry*, 101, 1372–1377.
- Brereton, R.G. 2003. *Chemometrics: Data Analysis for the Laboratory and Chemical Plant*. England: John Wiley & Sons Ltd.
- Brereton, R.G. 2007. *Applied Chemometrics for Scientists*. England: John Wiley & Sons Ltd.
- Brennan, L., 2014. NMR-based metabolomics: From sample preparation to applications in nutrition research. *Progress in Nuclear Magnetic Resonance Spectroscopy*, 83, 42-49.
- Bushra, S., Farooq, A. & Asraf, M. 2009. Effects of extraction solvent/ technique on the antioxidant activity of selected medicinal plant extracts. *Molecules*, 14, 2167-2180.
- Carta, F., Lussu, M., Bandino, F., Noto, A., Peppi, M., Chuchueva, N., Atzori, L., Fanos, V. & Puxeddu, R. 2017. Metabolomic analysis of urine with Nuclear Magnetic Resonance spectroscopy in patients with idiopathic sudden sensorineural hearing loss: A preliminary study. *Auris Nasus Larynx*, 44, 381–389.
- Chen, J. J., Zhou, C. J., Zheng, P., Cheng, K., Wang, H. Y., Li, J., Zeng, L. & Xie, P. 2017. Differential urinary metabolites related with the severity of major depressive disorder. *Behavioural Brain Research*, 332, 280–287.
- Chou, C. K., Lee, Y. T., Chen, S. M., Hsieh, C. W., Huang, T. C., Li, Y. C. & Lee, J. A. 2015. Elevated urinary d-lactate levels in patients with diabetes and microalbuminuria. *Journal of Pharmaceutical and Biomedical Analysis*, 116, 65–70.
- Chromacademy. 2012. E-learning for the analytical chemistry community: Mass spectrometry, fundamental GC-MS and introduction [Online]. Accessed on March 22, 2014, from <http://forensicscienceeducation.org/wp>.
- Clara, I., Virginia, G. C., Alberto, V. & Carolina, S. 2013. Novel MS-based approaches and applications in food metabolomics. *Trends in Analytical Chemistry*, 52, 100-111.
- Collins, C. B., Tofanelli, M. A., Crook, M. F., Phillips, B. D., & Ackerson, C. J. 2017. Practical stability of Au<sub>25</sub>(SR)<sub>18</sub>-1/0/+1, 45061–45065.

- Cooper, K. A., Donovan, J. L., Waterhouse A. L. & Williamson, G. 2008. Cocoa and health: A decade of research. *British Journal of Nutrition*, 99, 1-11.
- Cornell, J. A., 2002. Experiments with mixtures: Designs, models and the analysis of mixture data, third edition.
- Creswell, J. W. 2012. *Educational Research: Planning, Conducting and Evaluating Quantitative and Qualitative Research* (4th Ed.). Boston, MA: Pearson.
- Creswell, J. W. 1998. *Qualitative inquiry and research design: Choosing among five traditions*. Thousand Oaks, CA: Sage Publications.
- Cuny, M., Vigneau, E., Gall, G. L., Colquhoun, I., Lees, M. & Rutledge, D. N. 2008. Fruit juice authentication by <sup>1</sup>H NMR spectroscopy in combination with different chemometrics tools. *Analytical and Bioanalytical Chemistry*, 390(1), 419-427
- Morse, J. M. 1994. Designing funded qualitative research. In Denzin, N. K. & Lincoln, Y. S., *Handbook of qualitative research* (2nd Ed). Thousand Oaks, CA: Sage.
- Debus, B., Kirsanov, D., Yaroshenko, I., Sidorova, A., Piven, A. & Legin, A. 2015. Two low-cost digital camera-based platforms for quantitative creatinine analysis in urine. *Analytica Chimica Acta*, 895, 71-79.
- Denkert, C., Bucher E. & Hilvo M. 2012. Metabolomics of human breast cancer: new approaches for tumor typing and biomarker discovery. *Genome Medicine*, 4, 37.
- Diboun, I., Mathew, S., Al-rayyashi, M., Elrayess, M., Torres, M., Halama, A. & Suhre, K. (2015). Metabolomics of dates (*Phoenix dactylifera*) reveals a highly dynamic ripening process accounting for major variation in fruit composition. *BMC Plant Biology*, 1–22.
- Dragsted, L. O. 2010. Biomarkers of meat intake and the application of nutrigenomics. *Meat Sciences*, 84, 301–307.
- Duarte, R. V., Moreira, S. A., Fernandes, P. A. R., Fidalgo, L. G., Santos, M. D., Queiros, R. P., Santos, D. I., Delgadillo, I. & Saraiva, J. A. 2014. Preservation under pressure (hyperbaric storage) at 25°C, 30°C and 37°C of a highly perishable dairy food and comparison with refrigeration. *CyTA – Journal of Food*, 13, 321-328.
- Ehling, S. & Cole, S., 2011. Analysis of organic acids in fruit juices by liquid chromatography–mass spectrometry: An enhanced tool for authenticity testing. *Agriculture and Food Chemistry*, 59(6), 2229–2234

- El-Hadrami, A. B. & Al-Khayri, J. M., 2012. Socioeconomic and traditional importance of dates palm. *Emirates Journal of Food and Agriculture*, 24(5), 371-385.
- Elma, S. N., Badarusham K., Rosli, D., Salvamani, S. & Hassan, M. S. 2018. Solvents extraction effects on bioactive compounds of Ajwa dates (*Phoenix dactylifera* L.) Flesh using mixture design. *Chemical Engineering Transactions*, 63, 817-822.
- El-Sharnouby, G. A., Aleid, S. M. & Al-Otaibi, M. M. 2014. Liquid sugar extraction from date palm (*Phoenix dactylifera* L.) fruits. *Journal of Food Process Technology*, 5(402), doi:10.4172/2157-7110.1000402
- El-Sohaimy, S. A. & Hafez, E. E. 2010. Biochemical and nutritional characterizations of dates palm fruits (*Phoenix dactylifera* L.). *Journal of Applied Sciences Research*, 6(8), 1060-1067.
- Fanos, V., Caboni, P., Corsello, G., Stronati, M., Gazzolo, D., Noto, A., Lussu, M., Dessi, A., Giuffre, M., Lacerenza, S., Serraino, F., Garofoli, F., Serpero, L. D., Liori, B., Carboni, R. & Atzori, L. 2014. Urinary <sup>1</sup>H-NMR and GC-MS metabolomics predicts early and late onset neonatal sepsis. *Early Human Development*, 90, 78–83.
- Farag M. A., Mohsen M., Heinke R. & Wessjohann L. A. 2014. Metabolomic fingerprint of 21 dates palm fruits varieties from Egypt using UPLC/PDA/ESI-qTOF-MS and GC-MS analysed by chemometrics. *Journal of Food Research International*, 64, 218-226.
- Feng, G. F., Liu, S., Pi, Z. F., Song, F. R. & Liu, Z. Q. 2018. Studies on the chemical and intestinal metabolic profiles of *Polygalae radix* by using UHPLC-IT-MS and UHPLC-Q-TOF-MS method coupled with intestinal bacteria incubation model *in vitro*. *Journal of Pharmaceutical and Biomedical Analysis*, 148, 298-306.
- Feng, L., Liu, X. M., Cao, F. R., Wang, L. S., Chen, Y. X., Pan, R. L., Liao, Y. H., Wang, Q. & Chang, Q. 2016. Anti-stress effects of ginseng total saponins on hindlimb-unloaded rats assessed by a metabolomics study. *Journal of Ethnopharmacology*, 188, 39–47.
- Forough B., Abbas F. M. A. & Azhar M. E. 2008. Antioxidant activity and phenolic content of various dates palm (*Phoenix dactylifera* L.) fruits from Iran. *Journal of Food Chemistry*, 107, 1636-1641.
- Francavilla, A., & Joye, I. J. 2020. Anthocyanins in whole grain cereals and their potential effect on health. *Nutrients*, 12(2922), doi:10.3390/nu12102922.
- Francis Orata. 2012. Derivatization reactions and reagents for gas chromatography analysis. *Advanced Gas Chromatography – Progress in Agricultural, Biomedical and Industrial Applications*, 83-108.

- Fusch, P. I. & Ness, L. R. 2015. Are we there yet? Data saturation in qualitative research. *The Qualitative Report*, 20(9), 1408-1416.
- Garcia, A. & Barbas, C. 2011. *Gas Chromatography-Mass Spectrometry (GC-MS) Based Metabolomics* (12th Ed.). USA; Ed Human Press, 17-32.
- Gibbons, H., Carr, E., McNulty, B. A., Nugent, A. P., Walton, J., Flynn, A., Gibney, M. J. & Brennan, L., 2017. Metabolomic-based identification of clusters that reflect dietary patterns. *Molecular Nutrition and Food Research*, 61(10), doi 10.1002/mnfr.201601050
- Gibney, M. J., Walsh, M., Brennan, L., Roche, H. M., German, B. & Ommen, B. 2005. Metabolomics in human nutrition: Opportunities and challenges. *American Journal of Clinical Nutrition*, 82, 497-503.
- Gironi F. & Piemonte V. 2011. Temperature and solvent effects on polyphenol extraction process from chestnut tree wood. *Chemical Engineering Research and Design*, 89, 857-862.
- Glaser, B. G. & Strauss, A. L. 1967. *The Discovery of Grounded Theory: Strategies for Qualitative Research*. Piscataway, New Jersey: Transaction.
- Gu, H., Pan, Z., Duda, C., Mann, D., Kissinger, C., Rohde, C. & Raftery, D. 2007. <sup>1</sup>H-NMR study of the effects of sample contamination in the metabolomic analysis of mouse urine. *Journal of Pharmaceutical and Biomedical Analysis*, 45, 134-140.
- Gurkan, R. & Altunay, N. 2015. Quantification of 5-hydroxymethylfurfural in honey samples and acidic beverages using spectrophotometry coupled with ultrasonic-assisted cloud point extraction. *Journal of Food Composition and Analysis*, 42, 141-151.
- Hammouda, H., Cherif, J. K., Trabelsi-Ayadi, M., Baron, A. & Guvot, S., 2013. Detailed polyphenol and tannin composition and its variability in Tunisian dates (*Phoenix dactylifera* L.) at different maturity stages. *Journal of Agriculture and Food Chemistry*, 61(13), 3252-3263.
- Handa, C. L., Lima, F. S., Guelfi, M. F. G., Georgetti, S. R. & Ida, E. I. 2016. Multi-response optimization of the extraction solvent system for phenolics and antioxidant activities from fermented soy flour using a simplex-centroid design. *Food Chemistry*, 197, 175-184.
- Hayouni E. A., Abedrabba M., Bouix M. & Hamdi, M. 2007. The effects of solvents and extraction method on the phenolic contents and biological activities in vitro of Tunisian *Quercus coccifera* L. and *Juniperus phoenicea* L. fruit extracts. *Food Chemistry*, 105, 1126-1134.

- Heather, L. C., Wang, X., West, J. A. & Griffin, J. L. 2013. A practical guide to metabolomic profiling as a discovery tool for human heart disease. *Journal of Molecular and Cellular Cardiology*, 55, 2–11.
- Herrera-Valencia, V. A., Us-Vazquez, R. A., Larque-Saavedra, F. A. & Barahona-Perez, L. F. 2012. Naturally occurring fatty acid methyl esters and ethyl esters in the green microalga *Chlamydomonas reinhardtii*. *Annals and Microbiology*, 62, 865–870
- Holmes, E., Nicholson, J. K., Nicholls, A. W., Lindon, J. C., Connor, S. C., Polley, S. & Connelly, J. 1998. The identification of novel biomarkers of renal toxicity using automatic data reduction techniques and PCA of proton NMR spectra of urine. *Chemometric and Intelligent Laboratory System*, 44, 245–255.
- Huang, W. C., Tsai, T. H., Chuang, L. T., Li, Y. Y., Zouboulis, C. C. & Tsai, P. J. 2014. Anti-bacterial and anti-inflammatory properties of capric acid against *Propionibacterium acnes*: A comparative study with lauric acid. *Journal of Dermatological Science*, 73, 232-240.
- Hussein, A. M., El-Mousalamy, A. M. D., Hussein, S. A. M. & Mahmoud, S. A. 2015. Effects of palm dates (*Phoenix dactylifera* L.) extracts on hepatic dysfunctions in Type 2 diabetic rat model. *World Journal of Pharmacy and Pharmaceutical Sciences*, 2(07), 62-79.
- Isabel, D. P. 2017. Distribution of alkaloids in woody plants. *Plant Science Today*, 4(3), 137-142.
- Jandric, Z., Roberts, D., Rathor, M. N., Abraham, A., Islam, M. & Cannavan, A. 2014. Assessment of fruit juice authenticity using UPLC-QToF MS: A metabolomics approach. *Food Chemistry*, 1(148), 7-17.
- Jannig, P. R., Alves, C. R. R., Voltarelli, V. A., Bozi, L. H. M., Vieira, J. S., Brum, P. C. & Bechara, L. R. G. 2017. Effects of N-acetylcysteine on isolated skeletal muscle contractile properties after an acute bout of aerobic exercise. *Life Sciences*, 191, 46–51.
- Jarmusch, A. K., Alfaro, C. M., Pirro, V., Hattab, E. M., Cohen-Gadol, A. A. & Cooks, R. G. 2016. Differential lipid profiles of normal human brain matter and gliomas by positive and negative mode desorption electrospray ionization – Mass spectrometry imaging. *PLoS ONE*, doi:10.1371/journal.pone.0163180
- Josson, S., Xu, Y. & Dhar, S. K. 2005. RelB regulates manganese superoxide dismutase gene & resistance to ionizing radiation of prostate cancer cells. *Oncogene*, 25, 1554-1559.
- Kanani, H., Panagiotis, K. & Klapa, M. I. 2008. Standardizing GC–MS metabolomics. *Journal of Chromatography B.*, 871, 191–201.

- Kchaou W., Abbes F., Blecker C., Attia H. & Besbes S. 2013. Effects of extraction solvents on phenolic contents and antioxidant activities of Tunisian dates varieties (*Phoenix dactylifera* L.). *Journal of Industrial Crops and Products*, 45, 262-269.
- Kchaou W., Abbes F., Mansour, R. B., Blecker C., Attia H. & Besbes S. 2016. Phenolic profile, antibacterial and cytotoxic properties of second grade dates extract from Tunisian cultivars (*Phoenix dactylifera* L.). *Food Chemistry*, 194, 1048–1055.
- Khan, F., Khan, T. J., Kalamegam, G., Pushparaj, P. N., Chaudary, A., Abuzenadah, A., Kumosani, T., Barbour, E. & Al-Qahtani, M. 2017. Anti-cancer effects of Ajwa dates (*Phoenix dactylifera* L.) in diethylnitrosamine induced hepatocellular carcinoma in Wistar rats. *BMC Complementary and Alternative Medicine*, 17, 418-428.
- Kim, S. A. & Rhee, M. S. 2016. Highly enhanced bactericidal effects of medium chain fatty acids (caprylic, capric, and lauric acid) combined with edible plant essential oils (carvacrol, eugenol,  $\beta$ -resorcylic acid, trans-cinnamaldehyde, thymol, and vanillin) against *Escherichia coli* O157:H7. *Food Control*, 60, 447-454.
- Kind, T., Tolstikov, V., Fiehn, O. & Weiss, R. H. 2007. A comprehensive urinary metabolomics approach for identifying kidney cancer. *Analytical Biochemistry*, 363, 185-195.
- Kronstrand, R., Brinkhagen, L., Birath-Karlsson, C., Roman, M. & Josefsson, M. 2014. LC-QTOF-MS as a superior strategy to immunoassay for the comprehensive analysis of synthetic cannabinoids in urine. *Analytical and Bioanalytical Chemistry*, 406(15), 3599-3609.
- Kuang, Y., Li, B., Fan, J., Qiao, X. & Ye, M. 2018. Antitussive and expectorant activities of licorice and its major compounds. *Bioorganic & Medicinal Chemistry*, <https://doi.org/10.1016/j.bmc.2017.11.046>.
- Kumari, C., Varughese, B., Ramji, S. & Kapoor, S. 2016. Liquid–liquid extraction and solid phase extraction for urinary organic acids: A comparative study from a resource constraint setting. *Indian Journal of Clinical Biochemistry*, 31(4), 414–422.
- Kumari, R., Varghese, A., George, L., & Sudhakar, Y. N. (2017). Effect of solvent polarity on the photophysical properties of chalcone derivatives. *RSC Advances*, 7, 24204–24214.
- Kuo, H. W., Ding, W. H. 2004. Trace determination of bisphenol A and phytoestrogens in infant formula powders by gas chromatography-mass spectrometry. *Journal of Chromatography A*, 1027(1-2), 67-74.

- Kurban, S., Erkoç, F. & Erkoç, S. 2010. Quantum chemical treatment of  $\beta$ -sitosterol molecule. *Pharmaceutical Biology*, 48(6), 637–642
- Kursinszki, L., Kalasz, H., Szoke, E., Adeghate, E., Hassan, M. Y. & Adem, A. 2011. Comparative analysis of six different brands of date fruits. *Acta Chromatographica*, 23(4), 603–610.
- Lauridsen, M., Hansen, S. H., Jaroszewski, J. W. & Cornett, C., 2007. Human urine as test material in  $^1\text{H}$  NMR-based metabonomics: Recommendations for sample preparation and storage. *Analytical Chemistry*, 79 (3), 1181–1186
- Lehtonen, H. M., Lindstedt, A., Jarvinen, R., Sinkkonen, J., Graca, G., Viitanene, M., Kallio, H. & Gil, A. M. 2013.  $^1\text{H}$ -NMR-based metabolic fingerprinting of urine metabolites after consumption of lingonberries (*Vaccinium vitis-idaea*) with a high-fat meal. *Food Chemistry*, 138, 982–990.
- Lenth, R. V. 2013. Some practical guidelines for effective sample size determination. *The American Statistician*, 55(3), 187-193.
- Lenz, L. M., Bright, J., Wilson, I. D. & Morgan, S. R. 2003. A  $^1\text{H}$ -NMR based study metabonomic of urine and plasma samples obtained from healthy human subject. *Journal of Pharmaceutical and Biomedical Analysis*, 33, 1103-1115.
- Liu, N. Q., Cao, M., Frederich, M., Choi, Y. H., Verpoort, R. & Kooy, F. V. D., 2010. Metabolomic investigation of the ethnopharmacological use of *Artemisia afra* with NMR spectroscopy and multivariate data analysis. *Journal of Ethnopharmacology*, 128, 230–235
- Llorach-Asuncion, R., Jauregui, O., Urpi-Sarda, M. & Andres-Lacueva, C. 2010. Methodological aspects for metabolome visualization and characterization: A metabolomic evaluation of the 24h evolution of human urine after cocoa powder consumption. *Journal of Pharmaceutical and Biomedical Analysis*, 51, 373.
- Lomenick, B., Shi, H., Huang, J. & Chen, C. 2015. Identification and characterization of  $\beta$ -sitosterol target proteins. *Bioorganic & Medicinal Chemistry Letters*, 25, 4976-4979.
- Lopez, S. M., Sarria, B., Baeza, G., Mateos, R. & Clemente, L. B. 2014. Pharmacokinetics of caffeine and its metabolites in plasma and urine after consuming a soluble green/roasted coffee blend by healthy subjects. *Food Research International*, 64, 125–133.
- Lu, W., Bennett, B. D. & Rabinowitz, J. D., 2008. Analytical strategies for LC–MS-based targeted metabolomics. *Journal of Chromatography B.*, 871, 236–242.

- Lyu, H. N., Zeng, K. W., Cao, N. K., Zhao, M. B, Jiang, Y. & Tu, P. F. 2018. Alkaloids from the stems and rhizomes of *Sinomenium acutum* from the Qinling Mountains, China. *Phytochemistry*, 156, 241-249.
- Mahaddalkar, T., Suri, C., Naik, P. K. & Lopus, M. 2015, Biochemical characterization and molecular dynamic simulation of  $\beta$ -sitosterol as a tubulin-binding anticancer agent. *European Journal of Pharmacology*, 760, 154-162.
- Manach, C., Brennan, L. & Dragsted, L. O. 2014. Using metabolomics to evaluate food intake: applications in nutritional epidemiology. *Metabolomics Tool in Nutrition Research*, 168-196.
- Mansouri A., Embarek G., Kokkalouc E. and Kefalas P. 2005. Phenolic profile and antioxidant activity of the Algerian ripe dates palm fruit (*Phoenix dactylifera* L.). *Food Chemistry*, 89, 411-420.
- Martinez-Lopez, S., Sarria, B., Gomez-Juaristi, M., Goya, L., Mateos, R. & Bravo-Clemente, L. 2014. Theobromine, caffeine, and theophylline metabolites in human plasma and urine after consumption of soluble cocoa products with different methylxanthine contents. *Food Research International*, 63, 446-455.
- Marques, C., Viegas, F., Rito, J., Jones, J. & Viegas, I. 2016. Determination of muscle protein synthesis rates in fish using  $^2\text{H}_2\text{O}$  and  $^2\text{H}$  NMR analysis of alanine. *Analytical and Biochemical*, 509, 111-114.
- McNiven, E. M. S., German, J. B. & Slupsky, C. M. 2011. Analytical metabolomics: nutritional opportunities for personalized health. *Journal of Nutrition and Biochemical*, 22, 995-1002.
- Medina, S., Dominguez-Perles, R., Ferreres, F., Tomas-Barberan, F. A. & Gil-Izquierdo, A. 2013. The effects of the intake of plant foods on the human metabolome. *Trends in Analytical Chemistry*, 52, 88-99.
- Mohammedi, Z. & Atik, F. 2011. Impact of solvent extraction type on total polyphenols content and biological activity from *Tamarix Aphylla* (L.) Karst. *International Journal of Pharmacology and Biology Sciences*, 2(1), 609-615.
- Moldoveanu, S. C. & David, V. 2019. Derivatization Methods in GC and GC/MS. Gas Chromatography – Derivatization, Sample Preparation, Application. Doi:10.5772/intechopen.81954
- Morse, J. M. 1994. Designing funded qualitative research. In Denzin, N. K. & Lincoln, Y. S., *Handbook of Qualitative Research* (2nd Ed). Thousand Oaks, CA: Sage

- Mortazavi, S. M. H., Azizollahi, F. & Moalemi, N. 2015. Some quality attributes and biochemical properties of nine Iranian date (*Phoenix dactylifera* L.) cultivars at different stages of fruit development. *International Journal of Horticultural Science and Technology*, 2(2), 161-171
- Mullen, W., Boitier, A., Stewart, A.J. & Crozier, A. 2004. Flavonoid metabolites in human plasma and urine after the consumption of red onions: Analysis by liquid chromatography with photodiode array and full scan tandem mass spectrometric detection. *Journal of Chromatography A.*, 1058, 163–168.
- Nai-sheng, L., Gang, S., Qiu-ping, X., Xiao-tong, Z., Ping, G., Gui-xuan, Z., Song-bo, W., Li-na, W., Qian-yun, X., Yong-liang, Z. & Qing-yan, J. 2014. Myristic acid (MS) promotes adipogenic gene expression and the differentiation of porcine intramuscular adipocyte precursor cells. *Journal of Intergrative Agriculture*, 13, 2488-2499.
- Nawaz, H., Shad, M. A., Rehman, N., Andaleeb, H. & Ullah, N. 2015. Effect of solvent polarity on extraction yield and antioxidant properties of phytochemicals from bean (*Phaseolus vulgaris*) seeds. *Brazilian Journal of Pharmaceutical Sciences*, <http://dx.doi.org/10.1590/s2175-97902019000417129>
- Naz, S., Vallejo, M., García, A. & Barbas, C. 2014. Method validation strategies involved in non-targeted metabolomics. *Journal of Chromatography A.*, 1353, 99–105.
- Ngo, Q. M. T., Tran, P. T., Tran, M. H., Kim, J. A., Rho, S. S., Lim, C. H., Kim, J. C., Woo, M. H., Choi, J. S., Lee, J. H. & Min, B. S. 2017. Alkaloids from *Piper nigrum* exhibit antiinflammatory activity via activating the Nrf2/HO1 pathway. *Phytotherapy Research*, 31(4), 663-670.
- Nguyen, H. T., Lee, D. K., Choi, Y. G., Min, J. E., Yoon, S. J., Yu, Y. H., Lim, J., Lee, J., Kwon, S. W. & Park, J. H. 2016. A <sup>1</sup>H-NMR-based metabolomics approach to evaluate the geographical authenticity of herbal medicine and its application in building a model effectively assessing the mixing proportion of intentional admixtures: A case study of *Panax ginseng* metabolomics for the authenticity of herbal medicine. *Journal of Pharmaceutical and Biomedical Analysis*, 124, 120–128.
- Nishigawa, T., Nagamachi, S., Chowdhury, V. S., Yasuo, S. & Furuse, M. 2018. Taurine and β-alanine intraperitoneal injection in lactating mice modifies the growth and behavior of offspring. *Biochemical and Biophysical Research Communication*, 495, 2024-2029.
- Nitbani, F. O., Siswanta, D. & Solikhah, E. N. 2016. Isolation and antibacterial test of lauric acid from crude coconut oil (*Cocus nocifera* L.). *Procedia Chemistry*, 18, 132-140.

- Niu, W., Knight, E., Xia, Q. & McGarvey, B. D. 2014. Comparative evaluation of eight software programs for alignment of gas chromatography–mass spectrometry chromatograms in metabolomics experiments. *Journal of Chromatography A.*, 1374, 199–206.
- Nur Syukriah, A. R., Liza, M. S., Harisun, Y. & Fadzillah, A. A. M. 2014. Effect of solvent extraction on antioxidant and antibacterial activities from *Quercus infectoria* (Manjakani). *International Food Research Journal*, 21(3), 1067-1073.
- Nugbienyo, L., Malinina, Y., Garmonov, S., Kamencev, M., Salahov, I., Andruch, V., Moskvina, L. & Bulatov, B. 2017. Automated sugaring-out liquid-liquid extraction based on flow system coupled with HPLC-UV for the determination of procainamide in urine. *Talanta*, 167, 709–713
- Nyamundanda, G., Gormley, I.C., Fan, Y., Gallagher W.M. & Brennan, L. 2013. “MetSizeR: selecting the optimal sample size for metabolomics studies using an analysis based approach”. *BMC Bioinformatic*, 14, 1-8.
- Odeh, I., Al-Rimawi, F., Abbadi, J., Obayat, L., Qabbajeh, M. & Hroub, A. 2014. Effect of harvesting date and variety of date palm on antioxidant capacity, phenolic and flavonoid content of date palm (*Phoenix dactylifera* L.). *Journal of Food and Nutrition Research*, 2(8), 499-505.
- O’Gorman, A., Gibbons, H. & Brennan, L. 2013. Metabolomics in the identification of biomarkers of dietary intake. *Computational and Structural Biotechnology Journal*, 4, 1-7.
- Olennikov, D. N. 2018. Minor Ecdysteroids from *Rhaponticum uniflorum* leaves from Eastern Siberia. *Chemistry of Natural Compounds*, 54(4), 798-800.
- Ommati, M. M., Jamshidzadeh, A., Niknahad, H., Mohammadi, H., Sabouri, S., Heidari, R. & Abdoli, N. 2017. N-acetylcysteine treatment blunts liver failure-associated impairment of locomotor activity. *PharmaNutrition*, 5, 141–147.
- Ottiger, M., Nickler, M., Steuer, C., Odermatt, J., Huber, A., Christ-Crain, M., Henzen, C., Hoess, C., Thomann, R., Zimmerli, W., Mueller, B. & Schuetz, P. 2016. Trimethylamine-N-oxide (TMAO) predicts fatal outcomes in community-acquired pneumonia patients without evident coronary artery disease. *European Journal of Internal Medicine*, 36, 67–73.
- Park, S. E., Yoo, S. A., Seo, S. H., Lee, K. I., Na, C. S. & Son, H. S., 2016. GC-MS based metabolomics approach of Kimchi for the understanding of *Lactobacillus plantarum* fermentation characteristics. *LWT - Food Science and Technology*, 68, 313-321

- Peralbo, F. & Castro, L. 2012. Preparation of urine samples prior to targeted or untargeted metabolomics mass-spectrometry analysis. *Trends in Analytical Chemistry*, 41, 75-85.
- Perveen, K., Bokhari, N. A. & Soliman, D. A. W., 2012. Antibacterial activity of *Phoenix dactylifera* L. leaf and pit extracts against selected Gram negative and Gram positive pathogenic bacteria. *Journal of Medicinal Plants Research*, 6(2), 296-300
- Pourdarbani, R., Ghassemzadeh, H. R., Seyedarabi, S., Nahandi, E. Z. & Vahed, M. M., 2015. Study on an automatic sorting system for dates fruits. *Journal of the Saudi Society of Agricultural Sciences*, 14, 83–90.
- Radjursoga, M., Karlsson, G. B., Lindqvist, H. M., Pedersen, A., Persson, C., Pinto, R. C., Ellegard, L. & Winkvist, A. 2017. Metabolic profiles from two different breakfast meals characterized by <sup>1</sup>H NMR-based metabolomics. *Food Chemistry*, 231, 267–274.
- Ramakrishnan, P., Nair, S. & Rangiah, K., 2016. A method for comparative metabolomics in urine using high resolution mass spectrometry. *Journal of Chromatography A.*, 1443, 83–92
- Rehault, J., Borrego-Varillas, R., Oriana, A., Manzoni, C., Hauri, C. P., Helbing, J. & Cerullo, G. 2017. Fourier transform spectroscopy in the vibrational fingerprint region with a birefringent interferometer. *Optics Express*, 25(4), 4403-4413
- Renukadevi, K. P., Saravana, P. S. & Angayarkanni, J. 2011, Antimicrobial and antioxidant activity of *Chlamydomonas reinhardtii* sp. *International Journal of Pharmaceuticall Sciences and Research*, 2, (6), 1467-1472.
- Raterink R. J., Lindenburg P. W., Vreeken R. J., Ramautar R. & Hankemeier T. 2014. Recent developments in sample-pretreatment techniques for mass spectrometry-based metabolomics. *Trends in Analytical Chemistry*, 61, 157-167.
- Rezaie M., Farhoosh R., Iranshahi M., Sharif A. & Golmohamadzadeh S. 2015. Ultrasonic-assisted extraction of antioxidative compounds from Bene (*Pistacia atlantica subsp. mutica*) hull using various solvents of different physicochemical properties. *Food Chemistry*, 173, 577-583.
- Rezazadeh, S., Ebrahimi, A. & Nowroozi, A., 2017. The effects of structural properties on the methylglyoxal scavenging mechanism of flavonoid aglycones: A quantum mechanical study. *Computational & Theoretical Chemistry*, 1118, 26-38.
- Rezzi, S., Ramadan, Z., Fay, L. B. & Kochhar, S. 2007. Nutritional metabonomics: applications and perspectives. *Journal of Proteome Research*, 6, 513–25.

- Richardson, Mark. 2009. *Principal Component Analysis*. 1-23.
- Rios, J. L. & Recio, M. C. 2005. Medicinal plants and antimicrobial activity. *Journal of Ethnopharmacology*, 100(1), 80-84.
- Robert, H. 2010.  $\beta$ -sitosterol: An anti-inflammatory and anti-cholesterol plant extract. *Life Extension Magazine*.
- Rodriguez-carrasco, Y., Molto, J. C., Manes, J. & Berrada, H. 2014. Development of a GC-MS/MS strategy to determine 15 mycotoxins and metabolites in human urine. *Talanta*, 128, 125-131.
- Roux, A., Lison, D., Junot, C. & Heilier, J. F. 2011. Applications of liquid chromatography coupled to mass spectrometry-based metabolomics in clinical chemistry and toxicology: A review. *Clinical Biochemistry*, 44, 119–135.
- Saafi, E. B., Louedi, M., Elfeki, A. F., Zakhama, A. F., Najjar, M. F., Hammami, M. & Achour, L., 2011. Protective effects of date palm fruit extract (*Phoenix dactylifera* L.) on dimethoate induced-oxidativestressinratliver. *Experimental and Toxicologic Pathology*, 63, 433–441
- Saeed, N., Khan, M. R. & Shabbir, M. 2012. Antioxidant activity, total phenolic and total flavonoid contents of whole plant extracts *Torilis leptophylla* L. *BMC Complementary and Alternative Medicine*, 12(221), 1-12.
- Salvamani, S., Gunasekaran, B., Shukor, M. Y., Bakar, M. Z. A. & Ahmad, S. A. 2016. Phytochemical investigation, hypocholesterolemic and anti-atherosclerotic effects of *Amaranthus viridis* leaf extract in hypercholesterolemia-induced rabbits. *RSC Advances*, 39, 32685-32696.
- Samad, M. A., Hashim, S. H., Simarani, K. & Yaacob, J. S., 2016. Antibacterial properties and effects of fruit chilling and extract storage on antioxidant activity, total phenolic and anthocyanin content of four dates palm (*Phoenix dactylifera*) cultivars. *Molecules*, 21(419), doi:10.3390 /molecules21040419
- Lee, S., Choi, H. K., Cho, S. K. & Kim, Y. S., 2010. Metabolic analysis of guava (*Psidium guajava* L.) fruits at different ripening stages using different data-processing approaches. *Journal of Chromatography B.*, 878, 2983–2988
- Sasot, G., Martinez-Huelamo, M., Vallverdu-Queralt, A., Mercader-Marti, M., Estruch, R. & Lamuela-Raventós, R.M. 2017. Identification of phenolicmetabolites in human urine after the intake of a functional food made from grape extract by a high resolution LTQ-Orbitrap-MS approach. *Food Research International*, 1-10.
- Saude E. J. & Sykes B. D. 2007. Urine stability for metabolomic studies: Effects of preparation and storage. *Metabolomics*, 3(1), 19-27.

- Saavedra, L., Ruperez, F. J. & Barbas, C. 2001. Capillary electrophoresis for evaluating orange juice authenticity: A study on Spanish oranges. *Journal of Agriculture and Food Chemistry*, 49(1), 9-13
- Savorani, F., Rasmussen, M. A., Mikkelsen, M. S. & Engelsen, S. B. 2013. A primer to nutritional metabolomics by NMR spectroscopy and chemometrics. *Food Research International*, 54, 1131–1145.
- Schauer, J. J., Kleeman, M. J., Cass, G. R. and Simoneit, B. R. T. 2002. Measurement of emissions from air pollution sources. 5. C1-C32 organic compounds from gasoline-powered motor vehicles. *Environmental Science & Technology*, 36, 1169-1180.
- Shapla, U. M., Solayman, M., Alam, N., Khalil, M. I. & Gan, S. H. 2018. 5-Hydroxymethylfurfural (HMF) levels in honey and other food products: effects on bees and human health. *Chemistry Central Journal*, 12-35.
- Shen, G., Wang, S., Dong, J., Feng, J., Xu, J., Xia, F., Wang, X. & Ye, J. 2019. Metabolic effect of dietary taurine supplementation on grouper (*Epinephelus coioides*): A <sup>1</sup>H-NMR-based metabolomics study. *Molecules*, 24(12), 2253-2268
- Sirisena, S., Zabaraz, D., Ng, K. & Ajlouni, S., 2017. Characterization of dates (*Deglet Nour*) seed free and bound polyphenols by high-performance liquid chromatography-mass spectrometry. *Journal of Food Science*, 82(2), 333-340.
- Slupsky, C. M., German, J. B. & McNiven, E. M. S. 2011. Analytical metabolomics: Nutritional opportunities for personalized health. *Journal of Nutritional Biochemistry*, 22, 995–1002.
- Solanky, K. S., Bailey, N. J. & Bingham, S. 2005. Biofluid <sup>1</sup>H NMR-based metabolomic techniques in nutrition research — metabolic effects of dietary isoflavones in humans. *Journal of Nutritional Biochemistry*, 16(4), 236-244.
- Song, H. S., Jang, S. & Kang, S. C. 2017. Bavachalcone from *Cullen corylifolium* induces apoptosis and autophagy in HepG2 cells. *Phytomedicine*, 40, 37-47.
- Spigno, G., Tramelli, L. & De Faveri, D.M. 2007. Effects of extraction time, temperature and solvent on concentration and antioxidant activity of grape marc phenolics. *Journal of Food Engineering*, 81, 200-208.
- Squeglia, L. M., Tomko, R. L., Baker, N. L., McClure, E. A., Book, G. A. & Gray, K. M. 2018. The effect of N-acetylcysteine on alcohol use during a *cannabis* cessation trial. *Drug and Alcohol Dependence*, 185, 17–22.
- Stella, P., Lenz, H. J. & Ford, S. K. 2006. Multicenter phase II and translational study of cetuximab in metastatic colorectal carcinoma refractory to

- irinotecan, oxaliplatin, and fluoropyrimidines. *Journal of Clinical Oncology*, 24(3), 4914-4921.
- Struck-Lewicka, W., Kordalewska, M., Bujak, R., Mpanga, A. Y., Markuszewski, M., Jacyna, J., Matuszewski, M., Kaliszan, R. & Markuszewski, M. J., 2015. Urine metabolic fingerprinting using LC-MS and GC-MS reveals metabolite changes in prostate cancer: A pilot study. *Journal of Pharmaceutical and Biomedical Analysis*, 111, 351-361
- Sun, C. L., Geng, X. J., Huang, X. Y. and Chen, J. J., 2014. Natural products as antidepressants. *Journal of Asian Natural Product Research*, 17(2), 188-198.
- Sun, G., Yin, Z., Liu, N., Bian, X., Yu, R., Su, X., Zhang, B. & Wang, Y. 2017. Gut microbial metabolite TMAO contributes to renal dysfunction in a mouse model of diet-induced obesity. *Biochemical and Biophysical Research Communication*, 493, 964-970.
- Szyrwinska, K. Kołodziejczak A., Rykowska I., Wasiak W., and Lulek J. 2007. Derivatization and gas chromatography- low-resolution mass spectrometry of bisphenol A. *Acta Chromatographica*, 18, 49-58
- Tambellini, N. P., Zarembeg, V., Turner, R. J. & Weljie, A. M. 2013. Evaluation of extraction protocols for simultaneous polar and non-polar yeast metabolite analysis using multivariate projection methods. *Metabolites*, 3, 592-605.
- Teng, Z. X., Shi, L. W. & Akeid, S. M. 2013. Dates fruit: Chemical, nutritional and medicinal values, products. *Journal of Science and Agriculture*, 93, 2352-2361.
- Thouri, A., Chahdoura, H., El-Arem, A., Hichri, A. O., Hassin, R. B. & Achour, L. 2017. Effect of solvents extraction on phytochemical components and biological activities of Tunisian dates seeds (var. *Korkobbi* and *Arechti*). *BMC Complementary and Alternative Medicine*, 17(248), doi 10.1186/s12906-017-1751-y
- Tian, J. S., Peng, G. J., Wu, Y. F., Zhou, J. J., Xiang, H., Gao, X. X., Zhou, Y. Z., Qin, X. M. & Du, G. H. 2016. A GC-MS urinary quantitative metabolomics analysis in depressed patients treated with TCM formula of Xiaoyaosan. *Journal of Chromatography B.*, 1026, 227-235.
- Trabelsi, N., Megdiche, W., Ksouri, R., Falleh, H., Ouslati, S., Soumaya, B., Hajlaoui, H. & Abdelly, C. 2010. Solvent effects on phenolic contents and biological activities of the halophyte *Limoniastrum monopetalum* leaves. *Food Science & Technology*, 43, 632-639.
- Truong, D. H., Nguyen, D. H., Ta, N. T. A., Bui, A. V., Do, T. H. & Nguyen, H. C. 2019. Evaluation of the use of different solvents for phytochemical constituents, antioxidants, and in vitro anti-inflammatory activities of

- Tseng, Y. T., Chen, C. S., Jong, Y. J., Chang, F. R. & Lo, Y. C. 2016. Loganin possesses neuroprotective properties, restores SMN protein and activates protein synthesis positive regulator Akt/mTOR in experimental models of spinal muscular atrophy. *Pharmacological Research*, 111, 58-75.
- Uarrota, V. G., Moresco, R., Coelho, B., Nunes, E. D. C., Peruch, L. A. M., Neubert, E. D. O., Rocha, M. & Maraschin, M. 2014. Metabolomics combined with chemometric tools (PCA, HCA, PLS-DA and SVM) for screening cassava (*Manihot esculenta Crantz*) roots during postharvest physiological deterioration. *Food Chemistry*, 161, 67-78.
- Ufnal, M., Zadlo, A. & Ostaszewski, R. 2015. TMAO: A small molecule of great expectations. *Nutrition*, 31, 1317–1323.
- Vaclavik, L., Lacina, O., Hajslova, J. & Zweigenbaum, J. 2011. The use of high performance liquid chromatography–quadrupole time-of-flight mass spectrometry coupled to advanced data mining and chemometric tools for discrimination and classification of red wines according to their variety. *Analytica Chimica Acta*, 685, 45–51.
- Verbeke, K. A., Boobis, A. R., Chiodini, A., Edwards, C. A., Franck, A., Kleerebezem, M., Nauta, A., Raes, J., Tol, E. A. F. V. & Tuohy, K. M. 2015. Towards microbial fermentation metabolites as markers for health benefits of prebiotics. *Nutrition Research Reviews*, 28, 42–66.
- Villalba, R. G., Pancorbo, A. C., Nevedomskaya, E. & Deelder, A. M. 2010. Exploratory analysis of human urine by LC-ESI after high intake of olive oil. *Analytical and Bioanalytical Chemistry*, 398, 463-475.
- Wabaidur, S. M., Al-Ammari, A., Aqel, A., Al-Tamrah, S. A., Al-Othman, Z. A., Ahmed, A. Y. B. H., 2016. Determination of free fatty acids in olive oils by UHPLC-MS. *Journal of Chromatography B.*, 1031, 109-115.
- Walsh, M. C., Brennan, L., Pujos-Guillot, E., Sébédio, J. L., Scalbert, A., Fagan, A., Higgins, D. G. & Gibney, M. J. 2007. Influence of acute phytochemical intake on human urinary metabolomic profiles<sup>1-3</sup>. *American Journal in Clinical Nutrition*, 86, 1687-1693.
- Wang, H., Cao, G. & Prior, R. 1997. Oxygen radical absorbing capacity of anthocyanins. *Journal of Agricultural and Food Chemistry*, 45, 304–309.
- Wang, S. L., Zhao, Z. K., Sun, J. F., Sun, Y. T., Pang, X. Q., Zeng, Z. W. & Xie, T. 2017a. Review of *Anemone raddeana* rhizome and its pharmacological effects. *Chinese Journal of Integrative Medicine*, 24(1), 72-79.

- Wang, T., Lu, M., Du, Q., Yao, X., Zhang, P., Chen, X., Xie, W., Li, Z., Ma, Y. & Zhu, Y. 2017b. An integrated anti-arrhythmic target network of a Chinese medicine compound, Wenxin Keli, revealed by combined machine learning and molecular pathway analysis. *Molecular Biosystem*.  
<https://www.ncbi.nlm.nih.gov/pubmed/28418441>
- Wang, X. Y., Ding, X., Yuan, Y. F., Zheng, L. Y., Cao, Y., Zhu, Z. Y., Zhang, G. Q., Chai, Y. F., Chen, X. F & Hong, Z. Y. 2017c. Comprehensive two-dimensional APTES-decorated MCF7-cell membrane chromatographic system for characterizing potential anti-breast-cancer components from Yuanhue Baizhi herbal medicine pair. *Journal of Food and Drug Analysis*, 26, 823-833.
- Wang, Y., Bollard, M. E., Keun, H., Antti, H., Beckonert, O., Ebbels, T. M., Lindon, J. C., Holmes, E., Tang, H. & Nicholson, J. K. 2003. Spectral editing and pattern recognition methods applied to high-resolution magic-angle spinning <sup>1</sup>H nuclear magnetic resonance spectroscopy of liver tissues. *Analytical Biochemistry*, 323, 26–32
- Wang, Z., He, C., Peng, Y., Chen, F. and Xiao, P., 2017d. Origins, phytochemistry, pharmacology, analytical methods and safety of *Cortex moutan* (*Paeonia suffruticosa* Andrew): A Systematic Review. *Molecules*, 22(6), 946-973.
- Wijekoon, M. M. J. O., Bhat, R. & Karim, A. A. 2011. Effect of extraction solvents on the phenolic compounds and antioxidant activities of bunga kantan (*Etligeria elatior* Jack.) inflorescence. *Journal of Food Composition and Analysis*, 24, 615-619.
- Wishart, D. S., Jewison, T., Guo, A. C., Wilson, M., Knox, C., Liu, Y., Djoumbou, Y., Mandal, R., Aziat, F., Dong, E., Bouatra, S., Sinelnikov, I., Arndt, D., Xia, J., Liu, P., Yallou, F., Bjorn Dahl, T., Perez-Pineiro, R., Eisner, R., Allen, F., Neveu, V., Greiner, R. & Scalbert, A. 2013. HMDB 3.0 – The human metabolome database in 2013. *Nucleic Acids Research*, 41, 801–807.
- Witte, E. C., Heerspink, H. J. L., Zeeuw, D. D., Bakker, S. J. L., Jong, P. E. D. & Gansevoort, R. 2009. First morning voids are more reliable than spot urine samples to assess microalbuminuria. *Journal of American Society of Nephrology*, 20, 436-443.
- Wlaz, P., Socala, K., Nieoczym, D., Zarnowski, T., Zarnowska, I., Czuczwar, S. J. & Gasior, M. 2015. Acute anticonvulsant effects of capric acid in seizure tests in mice. *Progress in Neuro-Psychopharmacology & Biological Psychiatry*, 57, 110-116.
- Wu X., Beecher G., Holden J., Haytowitz D., Gebhardt S. & Prior R. 2004. Lipophilic and hydrophilic antioxidant capacities of common foods in the United States. *Journal of Agriculture and Food Chemistry*, 52, 4026-4037.

- Xue, B., Li, J. X., Chai, Q., Liu, Z. X. & Chen, L. B. 2008. Effect of total flavonoid fraction of *Astragalus complanatus* R. Brown on angiotensin II-induced portal-vein contraction in hypertensive rats. *Phytomedicine*, 15, 759–762.
- Yan, M. M., Chen, M., Zhou, F., Cai, D. S., Bai, H., Wang, P. L. & Lei, H. M. 2019. Separation and analysis of flavonoid chemical constituents in flowers of *Juglans regia* L. by ultra-high-performance liquid chromatography-hybrid quadrupole time-of-flight mass spectrometry. *Journal of Pharmaceutical and Biomedical Analysis*, 164, 734-741.
- Yang, Q., Lin, S. S., Yang, J. T., Tang, L. J. & Yu, R. Q., 2017. Detection of inborn errors of metabolism utilizing GC-MS urinary metabolomics coupled with a modified orthogonal partial least squares discriminant analysis. *Talanta*, 165, 545–552
- Yao, W., Gu, H., Zhu, J., Barding, G., Cheng, H., Bao, B., Zhang, L., Ding, A. & Li, W., 2014. Integrated plasma and urine metabolomics coupled with HPLC/QTOF-MS and chemometric analysis on potential biomarkers in liver injury and hepatoprotective effects of Er-Zhi-Wan. *Analytical Bioanalytical Chemistry*, 406, 7367–7378
- Yasin, B. R., El-Fawal, H. A. N. & Mousa, S. A. 2015. Date (*Phoenix dactylifera*) polyphenolics and other bioactive compounds: A traditional Islamic remedy's potential in prevention of cell damage, cancer therapeutics and beyond. *International Journal of Molecular Sciences*, 16, 30075–30090
- Yi, L., Dong, N., Yun, Y., Deng, B., Ren, D., Liu, S. & Liang, Y. 2016. Chemometric methods in data processing of mass spectrometry-based metabolomics: A review. *Analytica Chimica Acta*, 914, 17-34.
- Yu, X., Zhao, M., Liu, F., Zeng, S. & Hu, J. 2013. Identification of 2,3-dihydro-3,5-dihydroxy-6-methyl-4H-pyran-4-one as a strong antioxidant in glucose–histidine Maillard reaction products. *Food Research International*, 51, 397-403.
- Zhang, A., Sun, H., Wu, X. & Wang, X. 2012. Urine Metabolomic. *Clinica Chimica Acta*, 414, 65-69.
- Zhang, C. R., Aldosari, S. A., Vidyasagar, P. S. P. V., Nair, K. M. & Nair, M. G. 2013. Antioxidant and anti-inflammatory assays confirm bioactive compounds in Ajwa dates fruit. *Journal of Agricultural and Food Chemistry*, 61(24), 5834–5840.
- Zhang, Z., Han, X. M., Wei, J. H., Xue, J., Yang, Y., Liang, L., Li, X. J., Guo, Q. M., Xu, Y. H. & Gao, Z. H. 2014. Compositions and antifungal activities of essential oils from Agarwood of *Aquilaria sinensis* (Lour.) Gilg induced by *Lasiodiplodia theobromae* (Pat.) Griffon. & Maubl. *Journal of Brazil in Chemistry Society*, 25(1), 20-26.

- Zhang, B. M., Wang, B., Xin, P., Wang, Q. H., Bu, H. and Kuang, H. X., 2018a. Phytochemistry and pharmacology of genus *Ephedra*. *Chinese Journal of Natural Medicines*, 16(11), 811-828.
- Zhang, Q. W., Lin, L. G. & Ye, W. C., 2018b. Techniques for extraction and isolation of natural products: A comprehensive review. *Chinese Medicine*, 13(20), <https://doi.org/10.1186/s13020-018-0177-x>
- Zhao, Z., Wang, W., Guo, H. & Zhou, D. 2008. Antidepressant-like effect of liquiritin from *Glycyrrhiza uralensis* in chronic variable stress induced depression model rats. *Behavioural Brain Research*, 194, 108–113.
- Zheng, X., Zhang, X., Schocker, N. S., Renslow, R. S., Orton, D. J., Khamsi, J., Ashmus, R. A., Almeida, I. C., Tang, K., Costello, C. E., Smith, R. D., Michael, K. & Baker, E. S. 2016. Enhancing glycan isomer separations with metal ions and positive and negative polarity ionmobility spectrometry-mass spectrometry analyses. *Analytical and Bioanalytical Chemistry*, 409(2), 467-476
- Zhou, D., Jiang, C., Fu, C., Chang, P., Zheng, K., Zhao, X. & MA, S. 2018. Anti-proliferation, pro-apoptosis and anti-migration effects of ginkgolic acid C13:0 isolated from *Ginkgo biloba exocarp* in MCF-7 and 4T-1 breast cancer cells. *Preprint*, <https://www.preprints.org/manuscript/201801.0271/v1>