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## **Giant barrel sponges in diverse habitats: a story about the metabolome**

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# References

- Adnani, N., Chevrette, M. G., Adibhatla, S. N., Zhang, F., Yu, Q., Braun, D. R., et al. (2017). Coculture of Marine Invertebrate-Associated Bacteria and Interdisciplinary Technologies Enable Biosynthesis and Discovery of a New Antibiotic, Keyicin. *ACS Chemical Biology*, 12(12), 3093–3102.
- Adpressa, D. A., & Loesgen, S. (2016). Bioprospecting Chemical Diversity and Bioactivity in a Marine Derived *Aspergillus terreus*. *Chemistry & Biodiversity*, 13(2), 253–259.
- Akiyama, T., Takada, K., Oikawa, T., Matsuura, N., Ise, Y., Okada, S., & Matsunaga, S. (2013). Stimulators of adipogenesis from the marine sponge *Xestospongia testudinaria*. *Tetrahedron*, 69(32), 6560–6564.
- Alexander, B. E., Liebrand, K., Osinga, R., van der Geest, H. G., Admiraal, W., Cleutjens, J. P. M., et al. (2014). Cell Turnover and Detritus Production in Marine Sponges from Tropical and Temperate Benthic Ecosystems. *PLOS ONE*, 9(10), e109486.
- Ali, K., Iqbal, M., Yuliana, N. D., Lee, Y.-J., Park, S., Han, S., et al. (2013). Identification of bioactive metabolites against adenosine A1 receptor using NMR-based metabolomics. *Metabolomics*, 9(4), 778–785.
- Allard, P.-M., Péresse, T., Bisson, J., Gindro, K., Marcourt, L., Pham, V. C., et al. (2016). Integration of Molecular Networking and *In-Silico* MS/MS Fragmentation for Natural Products Dereplication. *Analytical Chemistry*, 88(6), 3317–3323.
- Allwood, J. W., & Goodacre, R. (2010). An introduction to liquid chromatography–mass spectrometry instrumentation applied in plant metabolomic analyses. *Phytochemical Analysis*, 21(1), 33–47.
- Alsufyani, T., Weiss, A., & Wichard, T. (2017). Time Course Exo-Metabolomic Profiling in the Green Marine Macroalga *Ulva* (Chlorophyta) for Identification of Growth Phase-Dependent Biomarkers. *Marine drugs*, 15(1), 14.
- Altmann, K.-H. (2017). Drugs from the Oceans: Marine Natural Products as Leads for Drug Discovery. *CHIMIA International Journal for Chemistry*, 71(10), 646–652.
- Amnuoypol, S., Suwanborirux, K., Pummangura, S., Kubo, A., Tanaka, C., & Saito, N. (2004). Chemistry of Renieramycins. Part 5. Structure Elucidation of Renieramycin-Type Derivatives O, Q, R, and S from Thai Marine Sponge *Xestospongia* Species Pretreated with Potassium Cyanide. *Journal of Natural Products*, 67(6), 1023–1028.
- Anderson, P. E., Mahle, D. A., Doom, T. E., Reo, N. V., DelRaso, N. J., & Raymer, M. L. (2011). Dynamic adaptive binning: an improved quantification technique for NMR spectroscopic data. *Metabolomics*, 7(2), 179–190.
- Antcliffe, J. B., Callow, R. H. T., & Brasier, M. D. (2014). Giving the early fossil record of sponges a squeeze. *Biological Reviews*, 89(4), 972–1004.
- AntiBase, Wiley-VCH. (n.d.). <https://application.wiley-vch.de/stmdata/antibase.php>. Accessed 30 October 2019

- Barra, L., Barac, P., König, G. M., Crüsemann, M., & Dickschat, J. S. (2017). Volatiles from the fungal microbiome of the marine sponge *Callyspongia cf. flammea*. *Organic & Biomolecular Chemistry*, 15(35), 7411–7421.
- Bauvais, C., Bonneau, N., Blond, A., Pérez, T., Bourguet-Kondracki, M.-L., & Zirah, S. (2017). Furanoterpene Diversity and Variability in the Marine Sponge *Spongia officinalis*, from Untargeted LC–MS/MS Metabolomic Profiling to Furanolactam Derivatives. *Metabolites*, 7(2), 27.
- Bayet-Robert, M., Lim, S., Barthomeuf, C., & Morvan, D. (2010). Biochemical disorders induced by cytotoxic marine natural products in breast cancer cells as revealed by proton NMR spectroscopy-based metabolomics. *Biochemical Pharmacology*, 80(8), 1170–1179.
- Bayona, L. M., van Leeuwen, G., Erol, Ö., Swierts, T., van der Ent, E., de Voogd, N. J., & Choi, Y. H. (2020). Influence of Geographical Location on the Metabolic Production of Giant Barrel Sponges (*Xestospongia* spp.) Revealed by Metabolomics Tools. *ACS Omega*, 5(21), 12398–12408.
- Bayona, L. M., Verpoorte, R., Klinkhamer, P. G. L., & Choi, Y. H. (2019). Thin-Layer Chromatography | Metabolomics. In P. Worsfold, C. Poole, A. Townshend, & M. Miró (Eds.), *Encyclopedia of Analytical Science* (Third Edition) (pp. 59–75). Oxford: Academic Press.
- Bayona, M. L., Videnova, M., & Choi, H. Y. (2018). Increasing Metabolic Diversity in Marine Sponges Extracts by Controlling Extraction Parameters. *Marine Drugs*, 16(10), 393.
- Becerro, M. A., Thacker, R. W., Turon, X., Uriz, M. J., & Paul, V. J. (2003). Biogeography of sponge chemical ecology: comparisons of tropical and temperate defenses. *Oecologia*, 135(1), 91–101.
- Belarbi, E. H., Contreras Gómez, A., Chisti, Y., García Camacho, F., & Molina Grima, E. (2003). Producing drugs from marine sponges. *Biotechnology Advances*, 21(7), 585–598.
- Belghit, I., Rasinger, J. D., Heesch, S., Biancarosa, I., Liland, N., Torstensen, B., et al. (2017). In-depth metabolic profiling of marine macroalgae confirms strong biochemical differences between brown, red and green algae. *Algal Research*, 26, 240–249.
- Bell, James J., Biggerstaff, A., Bates, T., Bennett, H., Marlow, J., McGrath, E., & Shaffer, M. (2017). Sponge monitoring: Moving beyond diversity and abundance measures. *Ecological Indicators*, 78, 470–488.
- Bell, J. J., Bennett, H. M., Rovellini, A., & Webster, N. S. (2018). Sponges to Be Winners under Near-Future Climate Scenarios. *BioScience*, 68(12), 955–968.
- Bell, James J., & Carballo, J. L. (2008). Patterns of sponge biodiversity and abundance across different biogeographic regions. *Marine Biology*, 155(6), 563–570.
- Bell, J. J., Davy, S. K., Jones, T., Taylor, M. W., & Webster, N. S. (2013). Could some coral reefs become sponge reefs as our climate changes? *Global Change Biology*, 19(9), 2613–2624.
- Bell, J. J., Rovellini, A., Davy, S. K., Taylor, M. W., Fulton, E. A., Dunn, M. R., et al. (2018). Climate change alterations to ecosystem dominance: how might sponge-dominated reefs function? *Ecology*, 99(9), 1920–1931.

- Bell, J.J., & Smith, D. (2004). Ecology of sponge assemblages (Porifera) in the Wakatobi region, south-east Sulawesi, Indonesia: Richness and abundance. *Journal of the Marine Biological Association of the United Kingdom*, 84(3), 581–591.
- Bell, J. J., Smith, D., Hannan, D., Haris, A., Jompa, J., & Thomas, L. (2014). Resilience to Disturbance Despite Limited Dispersal and Self-Recruitment in Tropical Barrel Sponges: Implications for Conservation and Management. *PLOS ONE*, 9(3), e91635.
- Bell, James J. (2008). The functional roles of marine sponges. *Estuarine, Coastal and Shelf Science*, 79(3), 341–353.
- Bergquist, P. R. (1978). Sponges. Hutchinson of London.
- Betancur, L. A., Naranjo-Gaybor, S. J., Vinchira-Villarraga, D. M., Moreno-Sarmiento, N. C., Maldonado, L. A., Suarez-Moreno, Z. R., et al. (2017). Marine Actinobacteria as a source of compounds for phytopathogen control: An integrative metabolic-profiling / bioactivity and taxonomical approach. *PLOS ONE*, 12(2), e0170148.
- Bickford, D., Lohman, D. J., Sodhi, N. S., Ng, P. K. L., Meier, R., Winker, K., et al. (2007). Cryptic species as a window on diversity and conservation. *Trends in Ecology & Evolution*, 22(3), 148–155.
- Bingol, K., Bruschweiler-Li, L., Li, D.-W., & Bruschweiler, R. (2014). Customized Metabolomics Database for the Analysis of NMR  $^1\text{H}$ – $^1\text{H}$  TOCSY and  $^{13}\text{C}$ – $^1\text{H}$  HSQC-TOCSY Spectra of Complex Mixtures. *Analytical Chemistry*, 86(11), 5494–5501.
- Birgbauer, E., & Chun, J. (2006). New developments in the biological functions of lysophospholipids. *Cellular and Molecular Life Sciences CMLS*, 63(23), 2695–2701.
- Blunt, J. W., Carroll, A. R., Copp, B. R., Davis, R. A., Keyzers, R. A., & Prinsep, M. R. (2018). Marine natural products. *Natural Product Reports*, 35(1), 8–53.
- Blunt, J. W., Copp, B. R., Keyzers, R. A., Munro, M. H. G., & Prinsep, M. R. (2017). Marine natural products. *Natural Product Reports*, 34(3), 235–294.
- Blunt, J. W., Copp, B. R., Keyzers, R. A., Munro, M. H. G., & Prinsep, M. R. (2016). Marine natural products. *Natural Product Reports*, 33(3), 382–431.
- Blunt, J. W., Copp, B. R., Keyzers, R. A., Munro, M. H. G., & Prinsep, M. R. (2015). Marine natural products. *Natural Product Reports*, 32(2), 116–211.
- Blunt, J., Munro, M., & Upjohn, M. (2012). The Role of Databases in Marine Natural Products Research. In E. Fattorusso, W. H. Gerwick, & O. Tagliatela-Scafati (Eds.), *Handbook of Marine Natural Products* (pp. 389–421). Dordrecht: Springer Netherlands.
- Boroujerdi, A. F. B., Vizcaino, M. I., Meyers, A., Pollock, E. C., Huynh, S. L., Schock, T. B., et al. (2009). NMR-Based Microbial Metabolomics and the Temperature-Dependent Coral Pathogen *Vibrio coralliilyticus*. *Environmental Science & Technology*, 43(20), 7658–7664.

- Borras, E., Aksenov, A. A., Baird, M., Novick, B., Schivo, M., Zamuruyev, K. O., et al. (2017). Exhaled breath condensate methods adapted from human studies using longitudinal metabolomics for predicting early health alterations in dolphins. *Analytical and Bioanalytical Chemistry*, 409(28), 6523–6536.
- Bose, U., Hewavitharana, A. K., Ng, Y. K., Shaw, P. N., Fuerst, J. A., & Hodson, M. P. (2015). LC-MS-Based Metabolomics Study of Marine Bacterial Secondary Metabolite and Antibiotic Production in *Salinispora arenicola*. *Marine Drugs*, 13(1), 249–266.
- Boudreau, P. D., Monroe, E. A., Mehrotra, S., Desfor, S., Korobeynikov, A., Sherman, D. H., et al. (2015). Expanding the Described Metabolome of the Marine Cyanobacterium *Moorea producens* JHB through Orthogonal Natural Products Workflows. *PLOS ONE*, 10(7), e0133297.
- Bourguet-Kondracki, M. L., Rakotoarisoa, M. T., Martin, M. T., & Guyot, M. (1992). Bioactive bromopolyacetylenes from the marine sponge *Xestospongia testudinaria*. *Tetrahedron Letters*, 33(2), 225–226.
- Boury-Esnault, N., Lavrov, D. V., Ruiz, C. A., & Pérez, T. (2013). The Integrative Taxonomic Approach Applied to Porifera: A Case Study of the *Homoscleromorpha*. *Integrative and Comparative Biology*, 53(3), 416–427.
- Brantley, S. E., Molinski, T. F., Preston, C. M., & DeLong, E. F. (1995). Brominated acetylenic fatty acids from *Xestospongia* sp., a marine sponge-bacteria association. *Tetrahedron*, 51(28), 7667–7672.
- Bundy, J. G., Davey, M. P., & Viant, M. R. (2008). Environmental metabolomics: a critical review and future perspectives. *Metabolomics*, 5(1), 3–21.
- Cachet, N., Genta-Jouve, G., Ivanisevic, J., Chevaldonné, P., Sinniger, F., Culioli, G., et al. (2015). Metabolomic profiling reveals deep chemical divergence between two morphotypes of the zoanthid *Parazoanthus axinellae*. *Scientific Reports*, 5, 8282.
- Cai, H.-L., Li, H.-D., Yan, X.-Z., Sun, B., Zhang, Q., Yan, M., et al. (2012). Metabolomic Analysis of Biochemical Changes in the Plasma and Urine of First-Episode Neuroleptic-Naïve Schizophrenia Patients after Treatment with Risperidone. *Journal of Proteome Research*, 11(8), 4338–4350.
- Calcul, L., Longeon, A., Mourabit, A. A., Guyot, M., & Bourguet-Kondracki, M.-L. (2003). Novel alkaloids of the aptamine class from an Indonesian marine sponge of the genus *Xestospongia*. *Tetrahedron*, 59(34), 6539–6544.
- Cappello, T., Fernandes, D., Maisano, M., Casano, A., Bonastre, M., Bebianno, M. J., et al. (2017). Sex steroids and metabolic responses in mussels *Mytilus galloprovincialis* exposed to drospirenone. *Ecotoxicology and Environmental Safety*, 143, 166–172.
- Cappello, T., Giannetto, A., Parrino, V., De Marco, G., Mauceri, A., & Maisano, M. (2018). Food safety using NMR-based metabolomics: Assessment of the Atlantic bluefin tuna, *Thunnus thynnus*, from the Mediterranean Sea. *Food and Chemical Toxicology*, 115, 391–397.
- Carballeira, N. M., & Maldonado, L. (1988). The phospholipid fatty acids of the marine sponge *Xestospongia muta*. *Lipids*, 23(7), 682–684.

- Carr, M. H., Neigel, J. E., Estes, J. A., Andelman, S., Warner, R. R., & Largier, J. L. (2003). Comparing marine and terrestrial ecosystems: Implications for the design of coastal marine reserves. *Ecological Applications*, 13(1), 90–107.
- Carroll, A. R., Copp, B. R., Davis, R. A., Keyzers, R. A., & Prinsep, M. R. (2019). Marine natural products. *Natural Product Reports*, 36(1), 122–173.
- Carroll, A. R., Copp, B. R., Davis, R. A., Keyzers, R. A., & Prinsep, M. R. (2020). Marine natural products. *Natural Product Reports*, 37(2), 175–223.
- Chanas, B., & Pawlik, J. R. (1997). Variability in the chemical defense of the Caribbean reef sponge *Xestospongia muta*. In Lessios HA, Macintyre IG (eds) *Proceedings of the 8th international coral reef symposium* (Vol. 2, pp. 1363–1368). Smithsonian Tropical Research Institute, Balboa.
- Change, N. G. C. (2020). Global Surface Temperature | NASA Global Climate Change. *Climate Change: Vital Signs of the Planet*. <https://climate.nasa.gov/vital-signs/global-temperature>. Accessed 28 September 2020
- ChemSpider, RSC <http://www.chemspider.com/>. Accessed 30 October 2019
- Chen, S., Zhang, C., Xiong, Y., Tian, X., Liu, C., Jeevithan, E., & Wu, W. (2015). A GC-MS-based metabolomics investigation on scallop (*Chlamys farreri*) during semi-anhydrous living-preservation. *Innovative Food Science & Emerging Technologies*, 31, 185–195.
- Cheng, K., Müllner, E., Moazzami, A. A., Carlberg, H., Brännäs, E., & Pickova, J. (2017). Metabolomics Approach To Evaluate a Baltic Sea Sourced Diet for Cultured Arctic Char (*Salvelinus alpinus* L.). *Journal of Agricultural and Food Chemistry*, 65(24), 5083–5090.
- Chong, J., Yamamoto, M., & Xia, J. (2019). MetaboAnalystR 2.0: From Raw Spectra to Biological Insights. *Metabolites*, 9(3), 57.
- Chong, J., Soufan, O., Li, C., Caraus, I., Li, S., Bourque, G., et al. (2018). MetaboAnalyst 4.0: towards more transparent and integrative metabolomics analysis. *Nucleic Acids Research*, 46(W1), W486–W949.
- Clendinen, C. S., Lee-McMullen, B., Williams, C. M., Stupp, G. S., Vandenborne, K., Hahn, D. A., et al. (2014). <sup>13</sup>C NMR metabolomics: applications at natural abundance. *Analytical chemistry*, 86(18), 9242–9250.
- Cragg, G. M., Newman, D. J., & Snader, K. M. (1997). Natural Products in Drug Discovery and Development. *Journal of Natural Products*, 60(1), 52–60.
- Cuevas, C., & Francesch, A. (2009). Development of Yondelis® (trabectedin, ET-743). A semisynthetic process solves the supply problem. *Natural Product Reports*, 26(3), 322–337.
- Cutignano, A., Nuzzo, G., Ianora, A., Luongo, E., Romano, G., Gallo, C., et al. (2015). Development and Application of a Novel SPE-Method for Bioassay-Guided Fractionation of Marine Extracts. *Marine Drugs*, 13(9), 5736–5749.
- D’Arrigo, P., & Servi, S. (2010). Synthesis of Lysophospholipids. *Molecules*, 15(3), 1354–1377.

da Silva, R. R., Wang, M., Nothias, L.-F., van der Hooft, J. J. J., Caraballo-Rodríguez, A. M., Fox, E., et al. (2018). Propagating annotations of molecular networks using in silico fragmentation. *PLOS Computational Biology*, 14(4), e1006089.

Dahal, R. H., & Kim, J. (2017). *Rhodanobacter humi* sp. nov., an acid-tolerant and alkalitolerant gammaproteobacterium isolated from forest soil. *International Journal of Systematic and Evolutionary Microbiology*, 67(5), 1185–1190.

de Alencar, D. B., Diniz, J. C., Rocha, S. A. S., dos Santos Pires-Cavalcante, K. M., Freitas, J. O., Nagano, C. S., et al. (2017). Chemical composition of volatile compounds in two red seaweeds, *Pterocladia capillacea* and *Osmundaria obtusiloba*, using static headspace gas chromatography mass spectrometry. *Journal of Applied Phycology*, 29(3), 1571–1576.

de Goeij, J. M., van Oevelen, D., Vermeij, M. J. A., Osinga, R., Middelburg, J. J., de Goeij, A. F. P. M., & Admiraal, W. (2013). Surviving in a Marine Desert: The Sponge Loop Retains Resources Within Coral Reefs. *Science*, 342(6154), 108–110.

de Goeij, J. M., De Kluijver, A., Van Duyl, F. C., Vacelet, J., Wijffels, R. H., De Goeij, A. F. P. M., et al. (2009). Cell kinetics of the marine sponge *Halisarca caerulea* reveal rapid cell turnover and shedding. *Journal of Experimental Biology*, 212(23), 3892–3900.

de Voogd, N. J. (2007). The mariculture potential of the Indonesian reef-dwelling sponge *Callyspongia* (Euplacella) *biru*: Growth, survival and bioactive compounds. *Aquaculture*, 262(1), 54–64.

De Vos, L., Rützler, K., Boury-Esnault, N., Donadey, C., & Vacelet, J. (1991). Atlas of sponge morphology. Smithsonian Institution Press.

Diaz, M. C., & Rützler, K. (2001). Sponges: An essential component of Caribbean coral reefs. *Bulletin of Marine Science*, 62(2), 535–546.

Ding, Y. C., Pang, M. L., Liang, Z.-X., Goh, K. K., Glukhov, E., Gerwick, H. W., & Tan, T. L. (2018). MS/MS-Based Molecular Networking Approach for the Detection of Aplysiatoxin-Related Compounds in Environmental Marine Cyanobacteria. *Marine Drugs*, 16(12), 505.

Djoumbou Feunang, Y., Eisner, R., Knox, C., Chepelev, L., Hastings, J., Owen, G., et al. (2016). ClassyFire: automated chemical classification with a comprehensive, computable taxonomy. *Journal of cheminformatics*, 8, 61–61.

DNP 28.2, Dictionary of Natural Products 28.2, CRC. <http://dnp.chemnetbase.com/faces/chemical/ChemicalSearch.xhtml>. Accessed 20 May 2020

Duckworth AR, West L, Vansach T, Stubler A, & Hardt M. (2012). Effects of water temperature and pH on growth and metabolite biosynthesis of coral reef sponges. *Marine Ecology Progress Series*, 462, 67–77.

Dunn, W. B., & Ellis, David. I. (2005). Metabolomics: Current analytical platforms and methodologies. *TrAC Trends in Analytical Chemistry*, 24(4), 285–294.

Ebada, S. S., & Proksch, P. (2012). The Chemistry of Marine Sponges(\*). *Handbook of Marine Natural Products*, 191–293.

- Ebada, S. S., Edrada, R. A., Lin, W., & Proksch, P. (2008). Methods for isolation, purification and structural elucidation of bioactive secondary metabolites from marine invertebrates. *Nature Protocols*, 3, 1820–1831.
- Emwas, A.-H., Roy, R., McKay, R. T., Tenori, L., Saccenti, E., Gowda, G. A. N., et al. (2019). NMR Spectroscopy for Metabolomics Research. *Metabolites*, 9(7):123
- Ernst, M., Kang, B. K., Caraballo-Rodríguez, M. A., Nothias, L.-F., Wandy, J., Chen, C., et al. (2019). MolNetEnhancer: Enhanced Molecular Networks by Integrating Metabolome Mining and Annotation Tools. *Metabolites*, 16,9(7):144.
- Erpenbeck, D., & van Soest, R. W. M. (2006). Status and Perspective of Sponge Chemosystematics. *Marine Biotechnology*, 9,2.
- Esquenazi, E., Coates, C., Simmons, L., Gonzalez, D., Gerwick, W. H., & Dorrestein, P. C. (2008). Visualizing the spatial distribution of secondary metabolites produced by marine cyanobacteria and sponges via MALDI-TOF imaging. *Molecular BioSystems*, 4(6), 562–570.
- Esquenazi, E., Yang, Y.-L., Watrous, J., Gerwick, W. H., & Dorrestein, P. C. (2009). Imaging mass spectrometry of natural products. *Natural Product Reports*, 26(12), 1521–1534.
- Fan, L., Reynolds, D., Liu, M., Stark, M., Kjelleberg, S., Webster, N. S., & Thomas, T. (2012). Functional equivalence and evolutionary convergence in complex communities of microbial sponge symbionts. *Proceedings of the National Academy of Sciences*, 109(27) E1878-E1887.
- Fan, T. W.-M. (1996). Metabolite profiling by one- and two-dimensional NMR analysis of complex mixtures. *Progress in Nuclear Magnetic Resonance Spectroscopy*, 28(2), 161–219.
- Farag, M. A., Porzel, A., Al-Hammady, M. A., Hegazy, M.-E. F., Meyer, A., Mohamed, T. A., et al. (2016). Soft Corals Biodiversity in the Egyptian Red Sea: A Comparative MS and NMR Metabolomics Approach of Wild and Aquarium Grown Species. *Journal of Proteome Research*, 15(4), 1274–1287.
- Favre, L., Ortalo-Magné, A., Greff, S., Pérez, T., Thomas, O. P., Martin, J.-C., & Culioli, G. (2017). Discrimination of Four Marine Biofilm-Forming Bacteria by LC–MS Metabolomics and Influence of Culture Parameters. *Journal of Proteome Research*, 16(5), 1962–1975.
- Fernández-Varela, R., Tomasi, G., & Christensen, J. H. (2015). An untargeted gas chromatography mass spectrometry metabolomics platform for marine polychaetes. *Journal of Chromatography A*, 1384, 133–141.
- Fiore, C. L., Baker, D. M., & Lesser, M. P. (2013). Nitrogen Biogeochemistry in the Caribbean Sponge, *Xestospongia muta*: A Source or Sink of Dissolved Inorganic Nitrogen? *PLOS ONE*, 8(8), e72961.
- Fiore, C. L., Jarett, J. K., & Lesser, M. P. (2013). Symbiotic prokaryotic communities from different populations of the giant barrel sponge, *Xestospongia muta*. *MicrobiologyOpen*, 2(6), 938–952.
- Floros, D. J., Jensen, P. R., Dorrestein, P. C., & Koyama, N. (2016). A metabolomics guided exploration of marine natural product chemical space. *Metabolomics*, 12, 145.

- Forcisi, S., Moritz, F., Kanawati, B., Tziotis, D., Lehmann, R., & Schmitt-Kopplin, P. (2013). Liquid chromatography–mass spectrometry in metabolomics research: Mass analyzers in ultra high pressure liquid chromatography coupling. *State-of-the art of (UHP)LC-MS(-MS) techniques and their practical application*, 1292, 51–65.
- Forner, D., Berru  , F., Correa, H., Duncan, K., & Kerr, R. G. (2013). Chemical dereplication of marine actinomycetes by liquid chromatography–high resolution mass spectrometry profiling and statistical analysis. *Analytica Chimica Acta*, 805, 70–79.
- Forshed, J., Schuppe-Koistinen, I., & Jacobsson, S. P. (2003). Peak alignment of NMR signals by means of a genetic algorithm. *Analytica Chimica Acta*, 487(2), 189–199.
- Fromont, J. (1991). Descriptions of species of the *Petrosida* (Porifera:Demospongiae) occurring in the tropical waters of the Great Barrier Reef. *The Beagle, Records of the Northern Territory Museum of Arts and Sciences*, 8(1), 73–96.
- Fromont, J., & Bergquist, P. R. (1994). Reproductive biology of three sponge species of the genus *Xestospongia* (Porifera: Demospongiae: Petrosida) from the Great Barrier Reef. *Coral Reefs*, 13(2), 119–126.
- Fusetani, N., Li, H., Tamura, K., & Matsunaga, S. (1993). Antifungal Brominated C18 Acetylenic Acids from the Marine Sponge, *Petrosia volcano* Hoshino. *Tetrahedron*, 49(6), 1203–1210.
- Garg, N., Kapono, C. A., Lim, Y. W., Koyama, N., Vermeij, M. J. A., Conrad, D., et al. (2015). Mass spectral similarity for untargeted metabolomics data analysis of complex mixtures. *Special Issue: MS 1960 to Now*, 377, 719–727.
- Gauvin, A., Smadja, J., Aknin, M., & Gaydou, E. M. (2004). Sterol composition and chemotaxonomic considerations in relation to sponges of the genus *Xestospongia*. *Biochemical Systematics and Ecology*, 32(5), 469–476.
- Gauvin, A., Smadja, J., Aknin, M., & Gaydou, E. M. (2004). Sterol composition and chemotaxonomic considerations in relation to sponges of the genus *Xestospongia*. *Biochemical Systematics and Ecology*, 32(5), 469–476.
- Gazave, E., Lap  bie, P., Ereskovsky, A. V., Vacelet, J., Renard, E., C  rdenas, P., & Borchellini, C. (2012). No longer Demospongiae: *Homoscleromorpha* formal nomination as a fourth class of Porifera. In M. Maldonado, X. Turon, M. Becerro, & M. Jes  s Uriz (Eds.), *Ancient Animals, New Challenges: Developments in Sponge Research* (pp. 3–10). Dordrecht: Springer Netherlands.
- Genin, E., Wielgosz-Collin, G., Njinkou  , J.-M., Velosaotsy, N. E., Kornprobst, J.-M., Gouygou, J.-P., et al. (2008). New trends in phospholipid class composition of marine sponges. *Comparative Biochemistry and Physiology Part B: Biochemistry and Molecular Biology*, 150(4), 427–431.
- Gerwick, W. H. (2017). The Face of a Molecule. *Journal of Natural Products*, 80(9), 2583–2588.
- Gerwick, W., & Moore, B. (2012). Lessons from the Past and Charting the Future of Marine Natural Products Drug Discovery and Chemical Biology. *Chemistry & biology*, 19(1), 85–98.

- Gidman, E. A., Jones, M. L. M., Bussell, J. A., Malham, S. K., Reynolds, B., Seed, R., et al. (2007). A methodology for screening haemolymph of intertidal mussels, *Mytilus edulis*, using FT-IR spectroscopy as a tool for environmental assesment. *Metabolomics*, 3(4), 465–473.
- Gloeckner, V., Wehrl, M., Moitinho-Silva, L., Gernert, C., Schupp, P., Pawlik, J. R., et al. (2014). The HMA-LMA Dichotomy Revisited: an Electron Microscopical Survey of 56 Sponge Species. *The Biological Bulletin*, 227(1), 78–88.
- Goldfine, H., & Ellis, M. E. (1963). N-methyl groups in bacterial lipids. *Journal of Bacteriology*, 87, 8–15.
- Gomes, N. G. M., Dasari, R., Chandra, S., Kiss, R., & Kornienko, A. (2016). Marine Invertebrate Metabolites with Anticancer Activities: Solutions to the “Supply Problem.” *Marine Drugs*, 14(5), 98.
- Goulitquer, S., Potin, P., & Tonon, T. (2012). Mass spectrometry-based metabolomics to elucidate functions in marine organisms and ecosystems. *Marine drugs*, 10(4), 849–880.
- Grand-Guillaume Perrenoud, A., Guillarme, D., Boccard, J., Veuthey, J.-L., Barron, D., & Moco, S. (2016). Ultra-high performance supercritical fluid chromatography coupled with quadrupole-time-of-flight mass spectrometry as a performing tool for bioactive analysis. *Journal of Chromatography A*, 1450, 101–111.
- Greff, S., Aires, T., Serrão, E. A., Engelen, A. H., Thomas, O. P., & Pérez, T. (2017). The interaction between the proliferating macroalga *Asparagopsis taxiformis* and the coral *Astroides calycularis* induces changes in microbiome and metabolomic fingerprints. *Scientific Reports*, 7, 42625.
- Guijas, C., Montenegro-Burke, J. R., Domingo-Almenara, X., Palermo, A., Warth, B., Hermann, G., et al. (2018). METLIN: A Technology Platform for Identifying Knowns and Unknowns. *Analytical chemistry*, 90(5), 3156–3164.
- Gupta, S. K. (2011). Drug Discovery and Clinical Research. Jaypee Brothers Medical Publishers.
- Hadas, E., Shpigel, M., & Ilan, M. (2005). Sea ranching of the marine sponge *Negombata magnifica* (Demospongiae, Latrunculiidae) as a first step for latrunculin B mass production. *Aquaculture*, 244(1), 159–169.
- Hammerman, N. M., & García-Hernández, J. E. (2017). The sponge *Xestospongia muta* offers shelter to the stony coral *Madracis auretenra* (Northwest Puerto Rico). *Marine Biodiversity*, 47(1), 57–58.
- Harvey, A. L., Edrada-Ebel, R., & Quinn, R. J. (2015). The re-emergence of natural products for drug discovery in the genomics era. *Nature Reviews Drug Discovery*, 14, 111-129.
- Hay, M. E. (2009). Marine chemical ecology: chemical signals and cues structure marine populations, communities, and ecosystems. *Annual review of marine science*, 1, 193–212.
- He, F., Mai, L. H., Longeon, A., Copp, B. R., Loaëc, N., Bescond, A., et al. (2015). Novel Adociaquinone Derivatives from the Indonesian Sponge *Xestospongia* sp. *Marine drugs*, 13(5), 2617–2628.
- He, Q., Sun, R., Liu, H., Geng, Z., Chen, D., Li, Y., et al. (2014). NMR-Based Metabolomic Analysis of Spatial Variation in Soft Corals. *Marine Drugs*, 12(4), 1876-1890.

- Heavisides, E., Rouger, C., Reichel, F. A., Ulrich, C., Wenzel-Storjohann, A., Sebens, S., & Tasdemir, D. (2018). Seasonal Variations in the Metabolome and Bioactivity Profile of *Fucus vesiculosus* Extracted by an Optimised, Pressurised Liquid Extraction Protocol. *Marine Drugs*, 16(12), 503.
- Hentschel, U., Usher, K. M., & Taylor, M. W. (2006). Marine sponges as microbial fermenters. *FEMS Microbiology Ecology*, 55(2), 167–177.
- Hirayama, A., Wakayama, M., & Soga, T. (2014). Metabolome analysis based on capillary electrophoresis-mass spectrometry. *TrAC Trends in Analytical Chemistry*, 61, 215–222.
- Hirsh, S., Carmely, S., & Kashman, Y. (1987). Brominated unsaturated acids from the marine sponge *Xestospongia* sp. *Tetrahedron*, 43(14), 3257–3261.
- Horai, H., Arita, M., Kanaya, S., Nihei, Y., Ikeda, T., Suwa, K., et al. (2010). MassBank: a public repository for sharing mass spectral data for life sciences. *Journal of Mass Spectrometry*, 45(7), 703–714.
- Horton, T., Kroh, A., Ah Yong, S., Bailly, N., Boyko, C. B., Brandão, S. N., et al. (2020, June 29). World Register of Marine Species (WoRMS). WoRMS Editorial Board. <http://www.marinespecies.org>. Accessed 29 June 2020
- Hou, Y., Braun, D. R., Michel, C. R., Klassen, J. L., Adnani, N., Wyche, T. P., & Bugni, T. S. (2012). Microbial Strain Prioritization Using Metabolomics Tools for the Discovery of Natural Products. *Analytical Chemistry*, 84(10), 4277–4283.
- Houssen, W. E., & Jaspars, M. (2012). Isolation of Marine Natural Products. In S. D. Sarker & L. Nahar (Eds.), *Natural Products Isolation* (pp. 367–392). Totowa, NJ: Humana Press.
- Hughes, Terence P., Rodrigues, M. J., Bellwood, D. R., Ceccarelli, D., Hoegh-Guldberg, O., McCook, L., et al. (2007). Phase Shifts, Herbivory, and the Resilience of Coral Reefs to Climate Change. *Current Biology*, 17(4), 360–365.
- Hughes, Terry P., Kerry, J. T., Álvarez-Noriega, M., Álvarez-Romero, J. G., Anderson, K. D., Baird, A. H., et al. (2017). Global warming and recurrent mass bleaching of corals. *Nature*, 543, 373–377.
- Ichiba, T., Scheuer, P. J., & Kelly-Borges, M. (1993). Sponge-Derived Polyunsaturated C16 Di- and Tribromocarboxylic Acids. *Helvetica Chimica Acta*, 76(8), 2814–2816.
- Ivanisevic, J., Pérez, T., Ereskovsky, A. V., Barnathan, G., & Thomas, O. P. (2011). Lysophospholipids in the Mediterranean Sponge *Oscarella tuberculata*: Seasonal Variability and Putative Biological Role. *Journal of Chemical Ecology*, 37, 537.
- Ivanišević, J., Thomas, O. P., Lejeune, C., Chevaldonné, P., & Pérez, T. (2011). Metabolic fingerprinting as an indicator of biodiversity: towards understanding inter-specific relationships among *Homoscleromorpha* sponges. *Metabolomics*, 7(2), 289–304.
- Izquierdo-García, J. L., Villa, P., Kyriazis, A., del Puerto-Nevado, L., Pérez-Rial, S., Rodríguez, I., et al. (2011). Descriptive review of current NMR-based metabolomic data analysis packages. *Progress in Nuclear Magnetic Resonance Spectroscopy*, 59(3), 263–270.

- Jang, K. H., Lee, Y., Sim, C. J., Oh, K.-B., & Shin, J. (2012). Bioactive lipids from the sponge *Spirastrella abata*. *Bioorganic & Medicinal Chemistry Letters*, 22(2), 1078–1081.
- Januar, H. I., Chasanah, E., M. Tapiolas, D., A. Motti, C., H. Liptrot, C., & D. Wright, A. (2015). Influence of Anthropogenic Pressures on the Bioactivity Potential of Sponges and Soft Corals in the Coral Reef Environment. *Squalen Bulletin of Marine and Fisheries Postharvest and Biotechnology*; 10(2), 51-59.
- Jerković, I., Marijanović, Z., Roje, M., Kuš, P. M., Jokić, S., & Čož-Rakovac, R. (2018). Phytochemical study of the headspace volatile organic compounds of fresh algae and seagrass from the Adriatic Sea (single point collection). *PLOS ONE*, 13(5), e0196462.
- Jiang, W., Liu, D., Deng, Z., de Voogd, N. J., Proksch, P., & Lin, W. (2011). Brominated polyunsaturated lipids and their stereochemistry from the Chinese marine sponge *Xestospongia testudinaria*. *Tetrahedron*, 67(1), 58–68.
- Johnson, W. M., Kido Soule, M. C., & Kujawinski, E. B. (2017). Extraction efficiency and quantification of dissolved metabolites in targeted marine metabolomics. *Limnology and Oceanography: Methods*, 15(4), 417–428.
- Jové, M., Portero-Otín, M., Naudí, A., Ferrer, I., & Pamplona, R. (2014). Metabolomics of Human Brain Aging and Age-Related Neurodegenerative Diseases. *Journal of Neuropathology & Experimental Neurology*, 73(7), 640–657.
- Ju, Z. Y., & Howard, L. R. (2003). Effects of Solvent and Temperature on Pressurized Liquid Extraction of Anthocyanins and Total Phenolics from Dried Red Grape Skin. *Journal of Agricultural and Food Chemistry*, 51(18), 5207–5213.
- Kaufmann, B., & Christen, P. (2002). Recent extraction techniques for natural products: microwave-assisted extraction and pressurised solvent extraction. *Phytochemical Analysis*, 13(2), 105–113.
- Kell, D. B. (2004). Metabolomics and systems biology: making sense of the soup. *Current Opinion in Microbiology*, 7(3), 296–307.
- Kerr, R. G., & Kelly-Borges, M. (1993). Biochemical and morphological heterogeneity in the Caribbean sponge *Xestospongia muta* (petrosida: Petrosiidae). In *Sponges in Time and Space: Biology, Chemistry, Paleontology: proceedings of the 4th International Porifera Congress* Amsterdam, Netherlands, 19-23 (pp. 65–73).
- Kerr, R. G., Kerr, S. L., Pettit, G. R., Herald, D. L., Groy, T. L., & Djerassi, C. (1991). Sterols of marine invertebrates. 63. Isolation and structure elucidation of sutinasterol, the major sterol of the marine sponge *Xestospongia* sp. *The Journal of Organic Chemistry*, 56(1), 58–62.
- Keyzers, R. A., & Davies-Coleman, M. T. (2005). Anti-inflammatory metabolites from marine sponges. *Chemical Society Reviews*, 34(4), 355–365.
- Kim, H. K., Choi, Y. H., & Verpoorte, R. (2010). NMR-based metabolomic analysis of plants. *Nature Protocols*, 5(3), 536–549.

- Kleigrew, K., Almaliti, J., Tian, I. Y., Kinnel, R. B., Korobeynikov, A., Monroe, E. A., et al. (2015). Combining Mass Spectrometric Metabolic Profiling with Genomic Analysis: A Powerful Approach for Discovering Natural Products from Cyanobacteria. *Journal of Natural Products*, 78(7), 1671–1682.
- Kobayashi, M., Chen, Y.-J., Aoki, S., In, Y., Ishida, T., & Kitagawa, I. (1995). Four new  $\beta$ -carboline alkaloids isolated from two Okinawan marine sponges of *Xestospongia* sp. and *Haliclona* sp.). *Tetrahedron*, 51(13), 3727–3736.
- Kopka, J. (2006). Current challenges and developments in GC–MS based metabolite profiling technology. *BioPerspectives—From basic research to industrial production*, 124(1), 312–322.
- Laport, M. S., Santos, O. C. S., & Muricy, G. (2009). Marine Sponges: Potential Sources of New Antimicrobial Drugs. *Current Pharmaceutical Biotechnology*, 10(1), 86–105.
- Lee, H.-J., Jeong, J., Alves, A. C., Han, S.-T., In, G., Kim, E.-H., et al. (2019). Metabolomic understanding of intrinsic physiology in *Panax ginseng* during whole growing seasons. *Journal of Ginseng Research*, 43(4), 654–665.
- Lee, M.-H., & Lin, C.-C. (2007). Comparison of techniques for extraction of isoflavones from the root of *Radix Puerariae*: Ultrasonic and pressurized solvent extractions. *Food Chemistry*, 105(1), 223–228.
- Lei, Z., Huhman, D. V., & Sumner, L. W. (2011). Mass Spectrometry Strategies in Metabolomics. *Journal of Biological Chemistry*, 286(29), 25435–25442.
- Leonard, A. E., Pereira, S. L., Sprecher, H., & Huang, Y.-S. (2004). Elongation of long-chain fatty acids. *Progress in Lipid Research*, 43(1), 36–54.
- Lesser, M. P., Fiore, C., Slattery, M., & Zaneveld, J. (2016). Climate change stressors destabilize the microbiome of the Caribbean barrel sponge, *Xestospongia muta*. *Journal of Experimental Marine Biology and Ecology*, 475, 11–18.
- Li, C.-W., Chen, J.-Y., & Hua, T.-E. (1998). Precambrian Sponges with Cellular Structures. *Science*, 279(5352), 879–882.
- Liaw, C.-C., Chen, P.-C., Shih, C.-J., Tseng, S.-P., Lai, Y.-M., Hsu, C.-H., et al. (2015). Vitroprocines, new antibiotics against *Acinetobacter baumannii*, discovered from marine *Vibrio* sp. QWI-06 using mass-spectrometry-based metabolomics approach. *Scientific Reports*, 5, 12856.
- Liland, K. H. (2011). Multivariate methods in metabolomics – from pre-processing to dimension reduction and statistical analysis. *TrAC Trends in Analytical Chemistry*, 30(6), 827–841.
- Lin, K., Yang, P., Yang, H., Liu, A.-H., Yao, L.-G., Guo, Y.-W., & Mao, S.-C. (2015). Lysophospholipids from the Guangxi Sponge *Spirastrella purpurea*. *Lipids*, 50(7), 697–703.
- Lindon, J. C., & Nicholson, J. K. (2008). Spectroscopic and Statistical Techniques for Information Recovery in Metabonomics and Metabolomics. *Annual Review of Analytical Chemistry*, 1(1), 45–69.
- Liu, D., Xu, J., Jiang, W., Deng, Z., de Voogd, N. J., Proksch, P., & Lin, W. (2011). Xestospongienols A–L, Brominated Acetylenic Acids from the Chinese Marine Sponge *Xestospongia testudinaria*. *Helvetica Chimica Acta*, 94(9), 1600–1607.

- Loh, T.-L., & Pawlik, J. R. (2014). Chemical defenses and resource trade-offs structure sponge communities on Caribbean coral reefs. *Proceedings of the National Academy of Sciences*, 111(11) 4151–4156.
- López-Legentil, S., Song, B., McMurray, S. E., & Pawlik, J. R. (2008). Bleaching and stress in coral reef ecosystems: hsp70 expression by the giant barrel sponge *Xestospongia muta*. *Molecular Ecology*, 17(7), 1840–1849.
- Lu, J., Feng, J., Cai, S., & Chen, Z. (2017). Metabolomic responses of *Haliotis diversicolor* to organotin compounds. *Chemosphere*, 168, 860–869.
- Ludwig, C., & Viant, M. R. (2010). Two-dimensional J-resolved NMR spectroscopy: review of a key methodology in the metabolomics toolbox. *Phytochemical Analysis*, 21(1), 22–32.
- Luzzatto-Knaan, T., Garg, N., Wang, M., Glukhov, E., Peng, Y., Ackermann, G., et al. (2017). Digitizing mass spectrometry data to explore the chemical diversity and distribution of marine cyanobacteria and algae. *eLife*, 6, e24214.
- Macintyre, L., Zhang, T., Viegelmann, C., Martinez, J. I., Cheng, C., Dowdells, C., et al. (2014). Metabolomic Tools for Secondary Metabolite Discovery from Marine Microbial Symbionts. *Marine Drugs*, 12(6), 3416–3448.
- Maldonado, M., Ribes, M., & van Duyl, F. C. (2012). Chapter three - Nutrient Fluxes Through Sponges: Biology, Budgets, and Ecological Implications. In M. A. Becerro, M. J. Uriz, M. Maldonado, & X. Turon (Eds.), *Advances in Marine Biology* (Vol. 62, pp. 113–182). Academic Press.
- MarinLit. A database of the marine natural products literature. RSC. <http://pubs.rsc.org/marinlit/introduction>. Accessed 30 October 2019
- Markley, J. L., Brüschweiler, R., Edison, A. S., Eghbalnia, H. R., Powers, R., Raftery, D., & Wishart, D. S. (2017). The future of NMR-based metabolomics. *Analytical biotechnology*, 43, 34–40.
- McGrath, E. C., Woods, L., Jompa, J., Haris, A., & Bell, J. J. (2018). Growth and longevity in giant barrel sponges: Redwoods of the reef or Pines in the Indo-Pacific? *Scientific Reports*, 8, 15317.
- McManus, J. W., & Polsenberg, J. F. (2004). Coral–algal phase shifts on coral reefs: Ecological and environmental aspects. Regime shifts in the ocean. *Reconciling observations and theory*, 60(2), 263–279.
- McMurray S.E., Pawlik JR, & Finelli CM. (2014). Trait-mediated ecosystem impacts: how morphology and size affect pumping rates of the Caribbean giant barrel sponge. *Aquatic Biology*, 23(1), 1–13.
- McMurray, S.E., Blum, J. E., & Pawlik, J. R. (2008). Redwood of the reef: growth and age of the giant barrel sponge *Xestospongia muta* in the Florida Keys. *Marine Biology*, 155(2), 159–171.
- McMurray, S.E., Finelli, C. M., & Pawlik, J. R. (2015). Population dynamics of giant barrel sponges on Florida coral reefs. *Journal of Experimental Marine Biology and Ecology*, 473, 73–80.
- McMurray, S.E., Henkel, T. P., & Pawlik, J. R. (2010). Demographics of increasing populations of the giant barrel sponge *Xestospongia muta* in the Florida Keys. *Ecology*, 91(2), 560–570.

Mehbub, F. M., Lei, J., Franco, C., & Zhang, W. (2014). Marine Sponge Derived Natural Products between 2001 and 2010: Trends and Opportunities for Discovery of Bioactives. *Marine Drugs*, 12(8), 4539–4577.

Melis, R., Sanna, R., Braca, A., Bonaglini, E., Cappuccinelli, R., Slawski, H., et al. (2017). Molecular details on gilthead sea bream (*Sparus aurata*) sensitivity to low water temperatures from <sup>1</sup>H NMR metabolomics. *Comparative Biochemistry and Physiology Part A: Molecular & Integrative Physiology*, 204, 129–136.

Minto, R. E., & Blacklock, B. J. (2008). Biosynthesis and function of polyacetylenes and allied natural products. *Progress in Lipid Research*, 47(4), 233–306.

Moitinho-Silva, L., Nielsen, S., Amir, A., Gonzalez, A., Ackermann, G. L., Cerrano, C., et al. (2017). The sponge microbiome project. *GigaScience*, 6(10), gix077.

Montalvo, N. F., & Hill, R. T. (2011). Sponge-Associated Bacteria Are Strictly Maintained in Two Closely Related but Geographically Distant Sponge Hosts. *Applied and Environmental Microbiology*, 77(20), 7207–7216.

Mora, C., Tittensor, D. P., Adl, S., Simpson, A. G. B., & Worm, B. (2011). How Many Species Are There on Earth and in the Ocean? *PLOS Biology*, 9(8), e1001127.

Morinaka, B. I., Skepper, C. K., & Molinski, T. F. (2007). Ene-yne Tetrahydrofurans from the Sponge *Xestospongia muta*. Exploiting a Weak CD Effect for Assignment of Configuration. *Organic Letters*, 9(10), 1975–1978.

Morrow, K. M., Fiore, C. L., & Lesser, M. P. (2016). Environmental drivers of microbial community shifts in the giant barrel sponge, *Xestospongia muta*, over a shallow to mesophotic depth gradient. *Environmental Microbiology*, 18(6), 2025–2038.

Müller, W. E. G., & Müller, I. M. (2003). Origin of the Metazoan Immune System: Identification of the Molecules and Their Functions in Sponges. *Integrative and Comparative Biology*, 43(2), 281–292.

Mushtaq, M. Y., Choi, Y. H., Verpoorte, R., & Wilson, E. G. (2014). Extraction for Metabolomics: Access to The Metabolome. *Phytochemical Analysis*, 25(4), 291–306.

Myers, O. D., Sumner, S. J., Li, S., Barnes, S., & Du, X. (2017). One Step Forward for Reducing False Positive and False Negative Compound Identifications from Mass Spectrometry Metabolomics Data: New Algorithms for Constructing Extracted Ion Chromatograms and Detecting Chromatographic Peaks. *Analytical Chemistry*, 89(17), 8696–8703.

Naman, C. B., Leber, C. A., & Gerwick, W. H. (2017). Chapter 5 - Modern Natural Products Drug Discovery and Its Relevance to Biodiversity Conservation. In I. Kurtböke (Ed.), *Microbial Resources* (pp. 103–120). Academic Press.

Neely, K. L., & Butler, C. B. (2020). Seasonal, lunar, and diel patterns in spawning by the giant barrel sponge, *Xestospongia muta*. *Coral Reefs*. Doi: 10.1007/s00338-020-02009-2

Newman, D. J., & Cragg, G. M. (2004). Advanced Preclinical and Clinical Trials of Natural Products and Related Compounds from Marine Sources. *Current Medicinal Chemistry*, 11(13), 1693–1713.

- Newman, D. J., & Cragg, G. M. (2016). Natural Products as Sources of New Drugs from 1981 to 2014. *Journal of Natural Products*, 79(3), 629–661.
- Newman, D., & Cragg, G. (2016). Drugs and Drug Candidates from Marine Sources: An Assessment of the Current “State of Play”. *Planta medica*, 82 9–10, 775–89.
- Ng, Y. K., Hewavitharana, A. K., Webb, R., Shaw, P. N., & Fuerst, J. A. (2013). Developmental cycle and pharmaceutically relevant compounds of *Salinispora actinobacteria* isolated from Great Barrier Reef marine sponges. *Applied Microbiology and Biotechnology*, 97(7), 3097–3108.
- Nguyen, X. C., Longeon, A., Pham, V. C., Urvois, F., Bressy, C., Trinh, T. T. V., et al. (2013). Antifouling 26,27-Cyclosterols from the Vietnamese Marine Sponge *Xestospongia testudinaria*. *Journal of Natural Products*, 76(7), 1313–1318.
- NIST 20 <https://chemdata.nist.gov/dokuwiki/doku.php?id=chemdata:msms/> Accessed 29 July 2020
- Nothias, L.-F., Petras, D., Schmid, R., Dührkop, K., Rainer, J., Sarvepalli, A., et al. (2020). Feature-based molecular networking in the GNPS analysis environment. *Nature Methods*, 17(9), 905–908.
- Noyer, C., Thomas, O. P., & Becerro, M. A. (2011). Patterns of Chemical Diversity in the Mediterranean Sponge *Spongia lamella*. *PLOS ONE*, 6(6), e20844.
- Olinger, L. K., Scott, A. R., McMurray, S. E., & Pawlik, J. R. (2019). Growth estimates of Caribbean reef sponges on a shipwreck using 3D photogrammetry. *Scientific Reports*, 9(1), 18398.
- Olsen, E. K., Sørderholm, K. L., Isaksson, J., Andersen, J. H., & Hansen, E. (2016). Metabolomic profiling reveals the N-Acyl-Taurine geodiataurine in extracts from the marine sponge *Geodia macandrewii* (Bowerbank). *Journal of Natural Products*, 79(5), 1285–1291.
- Olson, J. B., & Gao, X. (2013). Characterizing the bacterial associates of three Caribbean sponges along a gradient from shallow to mesophotic depths. *FEMS Microbiology Ecology*, 85(1), 74–84.
- Oppong-Danquah, E., Parrot, D., Blümel, M., Labes, A., & Tasdemir, D. (2018). Molecular Networking-Based Metabolome and Bioactivity Analyses of Marine-Adapted Fungi Co-cultivated With Phytopathogens. *Frontiers in microbiology*, 9, 2072–2072.
- Page, M. J., Northcote, P. T., Webb, V. L., Mackey, S., & Handley, S. J. (2005). Aquaculture trials for the production of biologically active metabolites in the New Zealand sponge *Mycale hentscheli* (Demospongiae: Poecilosclerida). *Aquaculture*, 250(1), 256–269.
- Page, M., West, L., Northcote, P., Battershill, C., & Kelly, M. (2005). Spatial and Temporal Variability of Cytotoxic Metabolites in Populations of the New Zealand Sponge *Mycale hentscheli*. *Journal of Chemical Ecology*, 31(5), 1161–1174.
- Palumbi, S. R., Sandifer, P. A., Allan, J. D., Beck, M. W., Fautin, D. G., Fogarty, M. J., et al. (2009). Managing for ocean biodiversity to sustain marine ecosystem services. *Frontiers in Ecology and the Environment*, 7(4), 204–211.
- Pandolfi, J. M., Bradbury, R. H., Sala, E., Hughes, T. P., Bjorndal, K. A., Cooke, R. G., et al. (2003). Global Trajectories of the Long-Term Decline of Coral Reef Ecosystems. *Science*, 301(5635), 955–958.

- Papale, M., Rizzo, C., Fani, R., Bertolino, M., Costa, G., Paytuví-Gallart, A., et al. (2020). Exploring the Diversity and Metabolic Profiles of Bacterial Communities Associated With Antarctic Sponges (Terra Nova Bay, Ross Sea). *Frontiers in Ecology and Evolution*, 8, 268.
- Papazian, S., Parrot, D., Burýšková, B., Weinberger, F., & Tasdemir, D. (2019). Surface chemical defence of the eelgrass *Zostera marina* against microbial foulers. *Scientific Reports*, 9, 3323.
- Parrot, D., Papazian, S., Foil, D., & Tasdemir, D. (2018). Imaging the Unimaginable: Desorption Electrospray Ionization – Imaging Mass Spectrometry (DESI-IMS) in Natural Product Research. *Planta Medica*, 84(09/10), 584–593.
- Parsons, H. M., Ludwig, C., Günther, U. L., & Viant, M. R. (2007). Improved classification accuracy in 1- and 2-dimensional NMR metabolomics data using the variance stabilising generalised logarithm transformation. *BMC Bioinformatics*, 8, 234.
- Patil, A. D., Kokke, W. C., Cochran, S., Francis, T. A., Tomszek, T., & Westley, J. W. (1992). Brominated Polyacetylenic Acids from the Marine Sponge *Xestospongia muta*: Inhibitors of HIV Protease. *Journal of Natural Products*, 55(9), 1170–1177.
- Paul, V. J., & Puglisi, M. P. (2004). Chemical mediation of interactions among marine organisms. *Natural Product Reports*, 21(1), 189–209.
- Paul, V. J., & Ritson-Williams, R. (2008). Marine chemical ecology. *Natural Product Reports*, 25(4), 662–695.
- Paul, V. J., Freeman, C. J., & Agarwal, V. (2019). Chemical Ecology of Marine Sponges: New Opportunities through “-Omics.” *Integrative and Comparative Biology*, 59(4), 765–776.
- Paul, V. J., Puglisi, M. P., & Ritson-Williams, R. (2006). Marine chemical ecology. *Natural Product Reports*, 23(2), 153–180.
- Pawlik, J. R. (2011). The Chemical Ecology of Sponges on Caribbean Reefs: Natural Products Shape Natural Systems. *BioScience*, 61(11), 888–898.
- Pawlik, J. R., & McMurray, S. E. (2020). The Emerging Ecological and Biogeochemical Importance of Sponges on Coral Reefs. *Annual Review of Marine Science*, 12(1), 315–337.
- Pawlik, J. R., Chanas, B., Toonen, R. J., & Fenical, W. (1995). Defenses of Caribbean sponges against predatory reef fish. I. Chemical deterency. *Marine Ecology Progress Series*, 127, 183–194.
- Perdicaris, S., Vlachogianni, T., & Valavanidis, A. (2013). Bioactive Natural Substances from Marine Sponges: New Developments and Prospects for Future Pharmaceuticals. *Natural Products Chemistry & Research*, 1(3), 1000114.
- Pereira, D. M., Vinholes, J., de Pinho, P. G., Valentão, P., Mouga, T., Teixeira, N., & Andrade, P. B. (2012). A gas chromatography–mass spectrometry multi-target method for the simultaneous analysis of three classes of metabolites in marine organisms. *Talanta*, 100, 391–400.
- Perkol-Finkel, S., Shashar, N., & Benayahu, Y. (2006). Can artificial reefs mimic natural reef communities? The roles of structural features and age. *Marine Environmental Research*, 61(2), 121–135.

- Pham, N. B., Butler, M. S., Hooper, J. N. A., Moni, R. W., & Quinn, R. J. (1999). Isolation of Xestosterol Esters of Brominated Acetylenic Fatty Acids from the Marine Sponge *Xestospongia testudinaria*. *Journal of Natural Products*, 62(10), 1439–1442.
- Pilatti, F. K., Ramlov, F., Schmidt, E. C., Costa, C., Oliveira, E. R. de, Bauer, C. M., et al. (2017). Metabolomics of *Ulva lactuca* Linnaeus (Chlorophyta) exposed to oil fuels: Fourier transform infrared spectroscopy and multivariate analysis as tools for metabolic fingerprint. *Marine Pollution Bulletin*, 114(2), 831–836.
- Pluskal, T., Castillo, S., Villar-Briones, A., & Orešič, M. (2010). MZmine 2: Modular framework for processing, visualizing, and analyzing mass spectrometry-based molecular profile data. *BMC Bioinformatics*, 11, 395.
- Polónia, A. R. M., Cleary, D. F. R., Freitas, R., Gomes, N. C. M., & de Voogd, N. J. (2017). Archaeal and bacterial communities of *Xestospongia testudinaria* and sediment differ in diversity, composition and predicted function in an Indonesian coral reef environment. *Journal of Sea Research*, 119, 37–53.
- Pomponi, S. A. (1999). The bioprocess–technological potential of the sea. *Biotechnological Aspects of Marine Sponges*, 70(1), 5–13.
- Proksch, P., Putz, A., Ortlepp, S., Kjer, J., & Bayer, M. (2010). Bioactive natural products from marine sponges and fungal endophytes. *Phytochemistry Reviews*, 9(4), 475–489.
- PubChem, NIH <https://pubchem.ncbi.nlm.nih.gov/>. Accessed 30 October 2019
- Quinn, R. A., Nothias, L.-F., Vining, O., Meehan, M., Esquenazi, E., & Dorrestein, P. C. (2017). Molecular Networking As a Drug Discovery, Drug Metabolism, and Precision Medicine Strategy. *Trends in Pharmacological Sciences*, 38(2), 143–154.
- Quinn, R. A., Vermeij, M. J. A., Hartmann, A. C., Galtier d’Auriac, I., Benler, S., Haas, A., et al. (2016). Metabolomics of reef benthic interactions reveals a bioactive lipid involved in coral defence. *Proceedings of the Royal Society B: Biological Sciences*, 283, 20160469.
- Quinn, R. J., & Tucker, D. J. (1991). Further Acetylenic Acids from the Marine Sponge *Xestospongia testudinaria*. *Journal of Natural Products*, 54(1), 290–294.
- Quinn, R. J., & Tucker, D. J. (1985). A brominated bisacetylenic acid from the marine sponge *Xestospongia testudinaria*. *Tetrahedron Letters*, 26(13), 1671–1672.
- Reverter, M., Perez, T., Ereskovsky, A. V., & Banaigs, B. (2016). Secondary Metabolome Variability and Inducible Chemical Defenses in the Mediterranean Sponge *Aplysina cavernicola*. *Journal of Chemical Ecology*, 42(1), 60–70.
- Reverter, M., Tribalat, M.-A., Pérez, T., & Thomas, O. P. (2018). Metabolome variability for two Mediterranean sponge species of the genus *Haliclona*: specificity, time, and space. *Metabolomics*, 14, 114.
- Ribes, M., Calvo, E., Movilla, J., Logares, R., Coma, R., & Pelejero, C. (2016). Restructuring of the sponge microbiome favors tolerance to ocean acidification. *Environmental Microbiology Reports*, 8(4), 536–544.

- Ritson-Williams, R., Becerro, M. A., & Paul, V. J. (2005). Spawning of the giant barrel sponge *Xestospongia muta* in Belize. *Coral Reefs*, 24(1), 160–160.
- Rix, L., de Goeij, J. M., van Oevelen, D., Struck, U., Al-Horani, F. A., Wild, C., & Naumann, M. S. (2018). Reef sponges facilitate the transfer of coral-derived organic matter to their associated fauna via the sponge loop. *Marine Ecology Progress Series*, 589, 85–96.
- Rohde, S., Gochfeld, D. J., Ankisetty, S., Avula, B., Schupp, P. J., & Slattey, M. (2012). Spatial Variability in Secondary Metabolites of the Indo-Pacific Sponge *Stylissa massa*. *Journal of Chemical Ecology*, 38(5), 463–475.
- Roll, D. M., Scheuer, P. J., Matsumoto, G. K., & Clardy, J. (1983). Halenaquinone, a pentacyclic polyketide from a marine sponge. *Journal of the American Chemical Society*, 105(19), 6177–6178.
- Röst, H. L., Sachsenberg, T., Aiche, S., Bielow, C., Weisser, H., Aicheler, F., et al. (2016). OpenMS: a flexible open-source software platform for mass spectrometry data analysis. *Nature Methods*, 13(9), 741–748.
- Ruiz, C., Valderrama, K., Zea, S., & Castellanos, L. (2013). Mariculture and Natural Production of the Antitumoural (+)-Discodermolide by the Caribbean Marine Sponge *Discodermia dissoluta*. *Marine Biotechnology*, 15(5), 571–583.
- Sacristan-Soriano, O., Banaigs, B., & Becerro, M. A. (2011). Relevant Spatial Scales of Chemical Variation in *Aplysina aerophoba*. *Marine Drugs*, 9(12), 2499–2513.
- Sagar, S., Kaur, M., & Minneman, K. P. (2010). Antiviral Lead Compounds from Marine Sponges. *Marine Drugs*, 8(10), 2619–2638.
- Saito, K., & Matsuda, F. (2010). Metabolomics for Functional Genomics, Systems Biology, and Biotechnology. *Annual Review of Plant Biology*, 61(1), 463–489.
- Sakemi, S., Totton, L. E., & Sun, H. H. (1990). Xestamines A, B, and C, Three New Long-Chain Methoxylamine Pyridines from the Sponge *Xestospongia wiedenmayeri*. *Journal of Natural Products*, 53(4), 995–999.
- Salvatore, M. M., Nicoletti, R., Salvatore, F., Naviglio, D., & Andolfi, A. (2018). GC–MS approaches for the screening of metabolites produced by marine-derived *Aspergillus*. *Marine Chemistry*, 206, 19–33.
- Santiago, V. S., Manzano, G. G., Yu, C. C., Aliño, P. M., & Salvador-Reyes, L. A. (2019). Mariculture potential of renieramycin-producing Philippine blue sponge *Xestospongia* sp. (Porifera: Haplosclerida). *Aquaculture*, 502, 356–364.
- Sashidhara, K. V., White, K. N., & Crews, P. (2009). A Selective Account of Effective Paradigms and Significant Outcomes in the Discovery of Inspirational Marine Natural Products. *Journal of Natural Products*, 72(3), 588–603.
- Sass-Kiss, A., Simandi, B., Gao, Y., Boross, F., & Vamos-Falusi, Z. (1999). Study on the pilot-scale extraction of onion oleoresin using supercritical CO<sub>2</sub>. *Journal of the Science of Food and Agriculture*, 76(3), 320–326.

Schmitz, F. J., & Gopichand, Y. (1978). (7E, 13E, 15Z)-14,16-dibromo-7,13,15-hexadecatrien-5-ynoic acid. A novel dibromo acetylenic acid from the marine sponge *Xestospongia muta*. *Tetrahedron Letters*, 19(39), 3637–3640.

Schock, T. B., Duke, J., Goodson, A., Weldon, D., Brunson, J., Leffler, J. W., & Bearden, D. W. (2013). Evaluation of Pacific White Shrimp (*Litopenaeus vannamei*) Health during a Superintensive Aquaculture Growout Using NMR-Based Metabolomics. *PLOS ONE*, 8(3), e59521.

Schubotz, F., Lipp, J. S., Elvert, M., & Hinrichs, K.-U. (2011). Stable carbon isotopic compositions of intact polar lipids reveal complex carbon flow patterns among hydrocarbon degrading microbial communities at the Chapopote asphalt volcano. *Geochimica et Cosmochimica Acta*, 75(16), 4399–4415.

SciFindern is your key to unlocking R&D productivity. CAS. <https://www.cas.org/products/scifinder>. Accessed 20 May 2020

Setiawan, E., de Voogd, N. J., Swierts, T., Hooper, J. N. A., Wörheide, G., & Erpenbeck, D. (2016). MtDNA diversity of the Indonesian giant barrel sponge *Xestospongia testudinaria* (Porifera: Haplosclerida) – implications from partial cytochrome oxidase 1 sequences. *Journal of the Marine Biological Association of the United Kingdom*, 96(2), 323–332.

Shannon, P., Markiel, A., Ozier, O., Baliga, N. S., Wang, J. T., Ramage, D., et al. (2003). Cytoscape: a software environment for integrated models of biomolecular interaction networks. *Genome research*, 13(11), 2498–2504.

Shi, Y., Pan, C., Auckloo, B. N., Chen, X., Chen, C.-T. A., Wang, K., et al. (2017). Stress-driven discovery of a cryptic antibiotic produced by *Streptomyces* sp. WU20 from Kueishantao hydrothermal vent with an integrated metabolomics strategy. *Applied Microbiology and Biotechnology*, 101(4), 1395–1408.

Shin, B. A., Kim, Y. R., Lee, I.-S., Sung, C. K., Hong, J., Sim, C. J., et al. (1999). Lyso-PAF Analogues and Lysophosphatidylcholines from the Marine Sponge *Spirastrella abata* as Inhibitors of Cholesterol Biosynthesis. *Journal of Natural Products*, 62(11), 1554–1557.

Shulaev, V., & Isaac, G. (2018). Supercritical fluid chromatography coupled to mass spectrometry – A metabolomics perspective. *Journal of Chromatography B*, 1092, 499–505.

Shulaev, V., Cortes, D., Miller, G., & Mittler, R. (2008). Metabolomics for plant stress response. *Physiologia Plantarum*, 132(2), 199–208.

Sipkema, D., Franssen, M. C. R., Osinga, R., Tramper, J., & Wijffels, R. H. (2005). Marine Sponges as Pharmacy. *Marine Biotechnology*, 7(3), 142–162.

Sipkema, D., Osinga, R., Schatton, W., Mendola, D., Tramper, J., & Wijffels, R. H. (2005). Large-scale production of pharmaceuticals by marine sponges: Sea, cell, or synthesis? *Biotechnology and Bioengineering*, 90(2), 201–222.

Smith, C. A., Want, E. J., O’Maille, G., Abagyan, R., & Siuzdak, G. (2006). XCMS: Processing Mass Spectrometry Data for Metabolite Profiling Using Nonlinear Peak Alignment, Matching, and Identification. *Analytical Chemistry*, 78(3), 779–787.

- Snelgrove, P. V. R. (2016). An Ocean of Discovery: Biodiversity Beyond the Census of Marine Life. *Planta Medica*, 82(09/10), 790–799.
- Sogin, E. M., Anderson, P., Williams, P., Chen, C.-S., & Gates, R. D. (2014a). Application of <sup>1</sup>H-NMR Metabolomic Profiling for Reef-Building Corals. *PLOS ONE*, 9(10), e111274.
- Sogin, E. M., Putnam, H. M., Anderson, P. E., & Gates, R. D. (2016). Metabolomic signatures of increases in temperature and ocean acidification from the reef-building coral, *Pocillopora damicornis*. *Metabolomics*, 12, 71.
- Southwell, M. W., Weisz, J. B., Martens, C. S., & Lindquist, N. (2008). In situ fluxes of dissolved inorganic nitrogen from the sponge community on Conch Reef, Key Largo, Florida. *Limnology and Oceanography*, 53(3), 986–996.
- SpecInfo-Consortium Member-NMR, IR and MS, Wiley. <https://www.wiley.com/en-us/SpecInfo+Consortium+Member+NMR%2C+IR+and+MS-p-9780471251415>. Accessed 20 May 2020
- Stowe, S. D., Richards, J. J., Tucker, A. T., Thompson, R., Melander, C., & Cavanagh, J. (2011). Anti-Biofilm Compounds Derived from Marine Sponges. *Marine Drugs*, 9(10), 2010–2035.
- Sumner, L. W., Mendes, P., & Dixon, R. A. (2003). Plant metabolomics: large-scale phytochemistry in the functional genomics era. *Plant Metabolomics*, 62(6), 817–836.
- Swierts, T., Cleary, D. F. R., & de Voogd, N. J. (2018). Prokaryotic communities of Indo-Pacific giant barrel sponges are more strongly influenced by geography than host phylogeny. *FEMS Microbiology Ecology*, 94(12), fiy194.
- Swierts, T. (2019). Diversity in the globally intertwined giant barrel sponge species complex. Leiden University, The Netherlands. Retrieved from isbn:9789461829887
- Swierts, T., Huang, Y. M., & de Voogd, N. J. (2018). The giant barrel sponge facilitates the recovery of coral fragments after a tropical storm in Taiwan. *Coral Reefs*, 37(3), 675–675.
- Swierts, T., Peijnenburg, K. T. C. A., de Leeuw, C., Cleary, D. F. R., Hörnlein, C., Setiawan, E., et al. (2013). Lock, Stock and Two Different Barrels: Comparing the Genetic Composition of Morphotypes of the Indo-Pacific Sponge *Xestospongia testudinaria*. *PLOS ONE*, 8(9), e74396.
- Swierts, Thomas, Peijnenburg, K. T. C. A., de Leeuw, C. A., Breeuwer, J. A. J., Cleary, D. F. R., & de Voogd, N. J. (2017). Globally intertwined evolutionary history of giant barrel sponges. *Coral Reefs*, 36(3), 933–945.
- Taniguchi, M., Uchio, Y., Yasumoto, K., Kusumi, T., & Ooi, T. (2008). Brominated Unsaturated Fatty Acids from Marine Sponge Collected in Papua New Guinea. *Chemical and Pharmaceutical Bulletin*, 56(3), 378–382.
- Ternon, E., Perino, E., Manconi, R., Pronzato, R., & Thomas, O. P. (2017). How Environmental Factors Affect the Production of Guanidine Alkaloids by the Mediterranean Sponge *Crambe crambe*. *Marine Drugs*, 15(6), 181.

Thoms, C., & Schupp, P. J. (2007). Chemical defense strategies in sponges: a review. In *Porifera Research: Biodiversity, Innovation and Sustainability* (pp. 627–637). Rio de Janeiro, RJ, Brasil.

Torjesen, I. (2015). Drug development: the journey of a medicine from lab to shelf. *Pharmaceutical Journal*. <https://www.pharmaceutical-journal.com/test-tomorrows-pharmacist/tomorrows-pharmacist/drug-development-the-journey-of-a-medicine-from-lab-to-shelf/20068196.article>. Accessed 21 October 2020

Torkhovskaya, T. I., Ipatova, O. M., Zakharova, T. S., Kochetova, M. M., & Khalilov, E. M. (2007). Lysophospholipid receptors in cell signaling. *Biochemistry (Moscow)*, 72(2), 125–131.

Tsugawa, H., Cajka, T., Kind, T., Ma, Y., Higgins, B., Ikeda, K., et al. (2015). MS-DIAL: data-independent MS/MS deconvolution for comprehensive metabolome analysis. *Nature Methods*, 12, 523–526.

Turon, M., Cáliz, J., Garate, L., Casamayor, E. O., & Uriz, M. J. (2018). Showcasing the role of seawater in bacteria recruitment and microbiome stability in sponges. *Scientific Reports*, 8, 15201.

van der Hooft, J. J. J., Wandy, J., Barrett, M. P., Burgess, K. E. V., & Rogers, S. (2016). Topic modeling for untargated substructure exploration in metabolomics. *Proceedings of the National Academy of Sciences*, 113(48), 13738–13743.

van Meer, G., Voelker, D. R., & Feigenson, G. W. (2008). Membrane lipids: where they are and how they behave. *Nature reviews. Molecular cell biology*, 9(2), 112–124.

Van Soest, R. W. M., Boury-Esnault, N., Hooper, J. N. A., Rützler, K., De Voogd, N. J., Alvarez, B., et al. (2020a). World Porifera Database. *Xestospongia muta* (Schmidt, 1870). <http://www.marinespecies.org/aphia.php?p=taxdetails&id=166894>. Accessed 29 June 2020

Van Soest, R. W. M., Boury-Esnault, N., Hooper, J. N. A., Rützler, K., De Voogd, N. J., Alvarez, B., et al. (2020b). World Porifera Database. *Xestospongia testudinaria* (Lamarck, 1815). <http://www.marinespecies.org/aphia.php?p=taxdetails&id=166902>. Accessed 29 June 2020

Van Soest, R. W. M., Boury-Esnault, N., Vacelet, J., Dohrmann, M., Erpenbeck, D., De Voogd, N. J., et al. (2012). Global Diversity of Sponges (Porifera). *PLOS ONE*, 7(4), e35105.

Van Soest, R. W. M., Meesters, E. H. W. G., & Becking, L. E. (2014). Deep-water sponges (Porifera) from Bonaire and Klein Curaçao, Southern Caribbean. *Zootaxa*, 3878 (5), 401–443.

Verpoorte, R., Choi, Y. H., & Kim, H. K. (2007). NMR-based metabolomics at work in phytochemistry. *Phytochemistry Reviews*, 6(1), 3–14.

Viant, M. R. (2007). Metabolomics of aquatic organisms. *Marine Ecology Progress Series*, 332, 301–306.

Viegelmann, C., Margassery, M. L., Kennedy, J., Zhang, T., O'Brien, C., O'Gara, F., et al. (2014). Metabolomic Profiling and Genomic Study of a Marine Sponge-Associated *Streptomyces* sp. *Marine Drugs*, 12(6), 3323–3351.

Villa, F. A., & Gerwick, L. (2010). Marine natural product drug discovery: Leads for treatment of inflammation, cancer, infections, and neurological disorders. *Immunopharmacology and Immunotoxicology*, 32(2), 228–237.

- Villegas-Plazas, M., Wos-Oxley, M. L., Sanchez, J. A., Pieper, D. H., Thomas, O. P., & Junca, H. (2019). Variations in Microbial Diversity and Metabolite Profiles of the Tropical Marine Sponge *Xestospongia muta* with Season and Depth. *Microbial Ecology*, 78(1), 243–256.
- Wang, M., Carver, J. J., Phelan, V. V., Sanchez, L. M., Garg, N., Peng, Y., et al. (2016). Sharing and community curation of mass spectrometry data with Global Natural Products Social Molecular Networking. *Nature Biotechnology*, 34, 828–837.
- Watrous, J., Roach, P., Alexandrov, T., Heath, B. S., Yang, J. Y., Kersten, R. D., et al. (2012). Mass spectral molecular networking of living microbial colonies. *Proceedings of the National Academy of Sciences*, 109(26), E1743–E1752.
- Webster, N. S., & Taylor, M. W. (2012). Marine sponges and their microbial symbionts: love and other relationships. *Environmental Microbiology*, 14(2), 335–346.
- Weckwerth, W. (2003). Metabolomics in Systems Biology. *Annual Review of Plant Biology*, 54(1), 669–689.
- Wicke, C., Hüners, M., Wray, V., Nimtz, M., Bilitewski, U., & Lang, S. (2000). Production and Structure Elucidation of Glycoglycerolipids from a Marine Sponge-Associated *Microbacterium Species*. *Journal of Natural Products*, 63(5), 621–626.
- Winnikoff, J. R., Glukhov, E., Watrous, J., Dorrestein, P. C., & Gerwick, W. H. (2014). Quantitative molecular networking to profile marine cyanobacterial metabolomes. *The Journal of antibiotics*, 67(1), 105–112.
- Worley, B., & Powers, R. (2013). Multivariate Analysis in Metabolomics. *Current Metabolomics*, 1(1), 92–107.
- Wright, A. E. (1998). Isolation of Marine Natural Products. In R. J. P. Cannell (Ed.), *Natural Products Isolation* (pp. 365–408). Totowa, NJ: Humana Press. [https://doi.org/10.1007/978-1-59259-256-2\\_13](https://doi.org/10.1007/978-1-59259-256-2_13)
- Wu, H., & Wang, W.-X. (2010). NMR-based metabolomic studies on the toxicological effects of cadmium and copper on green mussels *Perna viridis*. *Aquatic Toxicology*, 100(4), 339–345.
- Wu, W., Daszykowski, M., Walczak, B., Sweatman, B. C., Connor, S. C., Haselden, J. N., et al. (2006). Peak Alignment of Urine NMR Spectra Using Fuzzy Warping. *Journal of Chemical Information and Modeling*, 46(2), 863–875.
- Wulff, J.L. (2016). Sponge Contributions to the Geology and Biology of Reefs: Past, Present, and Future. In D. K. Hubbard, C. S. Rogers, J. H. Lipps, & Jr. Stanley George D. (Eds.), *Coral Reefs at the Crossroads* (pp. 103–126). Dordrecht: Springer Netherlands.
- Wulff, J. L. (2006). Ecological interactions of marine sponges. *Canadian Journal of Zoology*, 84(2), 146–166.
- Xavier, J. R., Rachello-Dolmen, P. G., Parra-Velandia, F., Schönberg, C. H. L., Breeuwer, J. A. J., & van Soest, R. W. M. (2010). Molecular evidence of cryptic speciation in the “cosmopolitan” excavating sponge *Cliona celata* (Porifera, Clionaidae). *Molecular Phylogenetics and Evolution*, 56(1), 13–20.

- Yang, J. Y., Sanchez, L. M., Rath, C. M., Liu, X., Boudreau, P. D., Bruns, N., et al. (2013). Molecular Networking as a Dereplication Strategy. *Journal of Natural Products*, 76(9), 1686–1699.
- Ye, J., Zhou, F., Al-Kareef, A. M. Q., & Wang, H. (2015). Anticancer agents from marine sponges. *Journal of Asian Natural Products Research*, 17(1), 64–88.
- Yoon, D., Choi, B.-R., Ma, S., Lee, W. J., Jo, I.-H., Lee, Y.-S., et al. (2019). Metabolomics for Age Discrimination of Ginseng Using a Multiplex Approach to HR-MAS NMR Spectroscopy, UPLC–QTOF/MS, and GC × GC–TOF/MS. *Molecules*, 24(13), 2381.
- Yu, Z., Zhai, G., Singmann, P., He, Y., Xu, T., Prehn, C., et al. (2012). Human serum metabolic profiles are age dependent. *Aging Cell*, 11(6), 960–967.
- Yuliana, N. D., Khatib, A., Verpoorte, R., & Choi, Y. H. (2011). Comprehensive Extraction Method Integrated with NMR Metabolomics: A New Bioactivity Screening Method for Plants, Adenosine A1 Receptor Binding Compounds in *Orthosiphon stamineus* Benth. *Analytical Chemistry*, 83(17), 6902–6906.
- Zea, S. (1993). Cover of sponges and other sessile organisms in rocky and coral reef habitats of Santa Marta, Colombian Caribbean Sea. *Caribbean Journal of Science*, 29, 75–88.
- Zhang, C., Idelbayev, Y., Roberts, N., Tao, Y., Nannapaneni, Y., Duggan, B. M., et al. (2017). Small Molecule Accurate Recognition Technology (SMART) to Enhance Natural Products Research. *Scientific Reports*, 7, 14243.
- Zhang, F., Jonas, L., Lin, H., & Hill, R. T. (2019). Microbially mediated nutrient cycles in marine sponges. *FEMS Microbiology Ecology*, 95(11), fiz155.
- Zhang, W., Hankemeier, T., & Ramautar, R. (2017). Next-generation capillary electrophoresis–mass spectrometry approaches in metabolomics. *Analytical biotechnology*, 43, 1–7.
- Zhang, Y., Wu, H., Wei, L., Xie, Z., & Guan, B. (2017). Effects of hypoxia in the gills of the Manila clam *Ruditapes philippinarum* using NMR-based metabolomics. *Marine Pollution Bulletin*, 114(1), 84–89.
- Zhao, Q., Mansoor, T. A., Hong, J., Lee, C.-O., Im, K. S., Lee, D. S., & Jung, J. H. (2003). New Lysophosphatidylcholines and Monoglycerides from the Marine Sponge *Stelletta* sp. *Journal of Natural Products*, 66(5), 725–728.
- Zheng, X., Su, M., Pei, L., Zhang, T., Ma, X., Qiu, Y., et al. (2011). Metabolic Signature of Pregnant Women with Neural Tube Defects in Offspring. *Journal of Proteome Research*, 10(10), 4845–4854.
- Zhou, X., Lu, Y., Lin, X., Yang, B., Yang, X., & Liu, Y. (2011). Brominated aliphatic hydrocarbons and sterols from the sponge *Xestospongia testudinaria* with their bioactivities. *Chemistry and Physics of Lipids*, 164(7), 703–706.
- Zhou, X., Xu, T., Yang, X.-W., Huang, R., Yang, B., Tang, L., & Liu, Y. (2010). Chemical and Biological Aspects of Marine Sponges of the Genus *Xestospongia*. *Chemistry & Biodiversity*, 7(9), 2201–2227.
- Zhou, Z.-F., Menna, M., Cai, Y.-S., & Guo, Y.-W. (2015). Polyacetylenes of Marine Origin: Chemistry and Bioactivity. *Chemical Reviews*, 115(3), 1543–1596.

Zotti, M., De Pascali, S. A., Del Coco, L., Migoni, D., Carrozzo, L., Mancinelli, G., & Fanizzi, F. P. (2016). <sup>1</sup>H NMR metabolomic profiling of the blue crab (*Callinectes sapidus*) from the Adriatic Sea (SE Italy): A comparison with warty crab (*Eriphia verrucosa*), and edible crab (*Cancer pagurus*). *Food Chemistry*, 196, 601–609.