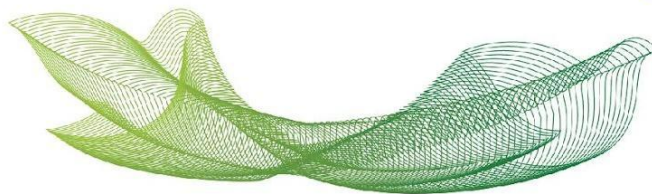


|                           |  |
|---------------------------|--|
| Tipo                      | Periódico  |
| Título                    | Metabolomics by NMR Combined with Machine Learning to Predict Neoadjuvant Chemotherapy Response for Breast Cancer  |
| Autores                   | Marcella R. Cardoso, Alex Ap. Rosini Silva, Maria Cecília R. Talarico, Pedro H. Godoy Sanches, Maurício L. Sforça, Silvana A. Rocco, Luciana M. Rezende, Melissa Quintero, Tassia B. B. C. Costa, Laís R. Viana, Rafael R. Canevarolo, Amanda C. Ferracini, Susana Ramalho, Junier Marrero Gutierrez, Fernando Guimarães, Ljubica Tasic, Alessandra Tata, Luís O. Sarian, Leo L. Cheng, Andreia M. Porcari and Sophie F. M. Derchain.  |
| Autor (es) USF            | Alex Ap. Rosini Silva, Pedro H. Godoy Sanches, Junier Marrero Gutierrez, Andreia M. Porcari.   |
| Autores Internacionais    | Leo L. Cheng, Rafael R. Canevarolo.  |
| Programa/Curso (s)        | Programa de Pós-Graduação Stricto Sensu em Ciências da Saúde   |
| DOI                       | <a href="https://doi.org/10.3390/cancers14205055">https://doi.org/10.3390/cancers14205055</a>  |
| Assunto (palavras chaves) | <sup>1</sup> H-NMR; breast neoplasms; magnetic resonance spectroscopy; metabolism; untargeted metabolomics; drug resistance.   |
| Idioma                    | Inglês   |
| Fonte                     | Título do periódico: Cancers<br>ISSN: 2072-6694<br>Volume/Número/Paginação/Ano: 14/20/5055/2022  |
| Data da publicação        | 15 de outubro de 2022  |
| Formato da produção       | Impressa ou digital  |
| Resumo                    | Neoadjuvant chemotherapy (NACT) is offered to patients with operable or inoperable breast cancer (BC) to downstage the disease. Clinical responses to NACT may vary depending on a few known clinical and biological features, but the diversity of responses to NACT is not fully understood. In this study, 80 women had their metabolite profiles of pre-treatment sera analyzed for potential NACT response biomarker candidates in combination with immunohistochemical parameters using Nuclear Magnetic Resonance (NMR). Sixty-four percent of the patients were resistant to chemotherapy. NMR, hormonal receptors (HR), human epidermal growth factor receptor 2 (HER2), and the nuclear protein Ki67 were combined through machine learning (ML) to predict the response to NACT. Metabolites such as leucine, formate, valine, and proline, along with hormone receptor status, were discriminants of response to NACT. The glyoxylate and dicarboxylate metabolism was found to be involved in the resistance to NACT. We obtained an accuracy in excess of 80% for the prediction of response to NACT combining metabolomic and tumor profile data. Our |



|         |  |
|---------|--|
|         | results suggest that NMR data can substantially enhance the prediction of response to NACT when used in combination with already known response prediction factors |
| Fomento | CAPES (001), CNPQ (nº 303742 /2018-6) e FAPESP (nº 2019/04314-6 e 2018/24069-3).   |