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Título	Metabolomics by NMR Combined with Machine Learning to Predict Neoadjuvant Chemotherapy Response for Breast Cancer
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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
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