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Prostate cancer has become the most frequently diagnosed cancer in males, owing to widely adopted screening methods. However, the high incidence rates compared with low death rates give rise to the assumption that many patients with diagnosed prostate cancer are overtreated. As to the lack of biomarkers, the situation concerning breast cancer is comparable. Metabolomic imaging based on nuclear magnetic resonance is a promising approach to determine biomarkers capable of predicting the need for treatment of prostate cancer patients.

A protocol has been established which allows to identify metabolomic proles correlating with cancer aggressiveness in ex-vivo biopsies. However, clinical evaluation of the found proles with prostates after prostatectomy necessitates computational assistance. In the frame of this work, the procedure for calculating metabolomic images from raw nuclear magnetic resonance data has been automatized. The necessary theoretical background is given, and the old and new workow are compared to each other. Algorithms and resulting metabolomic images are presented and discussed. As a by-product, the new software tool can be used to carry out most of the analyses necessary to identify metabolomic proles in other kinds of cancer. Thus, it can be applied both in the clinical evaluation of metabolomic proles in the case of prostate cancer and in the exploration of metabolomic proles in breast cancer. A short overview of future directions concludes this work, including a proof-of-concept study regarding the creation of three-dimensional histological datasets.