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With the rise of the field of systems biology, metabolomic data have been integrated with the data for other -omic sciences, and these gigantic collections of correlated data have with the ever improving computing power, been data mined to locate biomarkers and motifs.[1]

In this project the metabolic fingerprint of four prostate cancer cell lines, with different levels of aggression were analyzed. Metabolic data were obtained by incubating the cells with $^{13}$C$_6$-d$_7$ isotope labeled glucose, then quenching the metabolism, removing the cell debris and hyperpolarizing the metabolite extracts with dissolution Dynamic Nuclear Polarization (dDNP).

By integrating the peaks of the resulting NMR spectra, a collection of metabolic data was obtained without the need for identification of specific compounds. On this data, data mining was applied, with the aim to identify biomarkers of cancer and to classify the aggressiveness of the cancer.

The illustrations below show examples of obtained NMR spectra for the different cell types (on the left) and Principal Components-Discriminant Function Analysis (PC-DFA) results from the four prostate cancer cell types and a breast cancer cell line, in red, (on the right). The PC-DFA is clearly able to separate the cell types, with the most aggressive clustering together (blue and green).

As dDNP MNR have been shown to be quantitative and reproducible,[2] it could be an important tool in the future for cancer diagnostics.