## Metabolomic profile of multiple sclerosis patients by means of 1H-NMR analysis

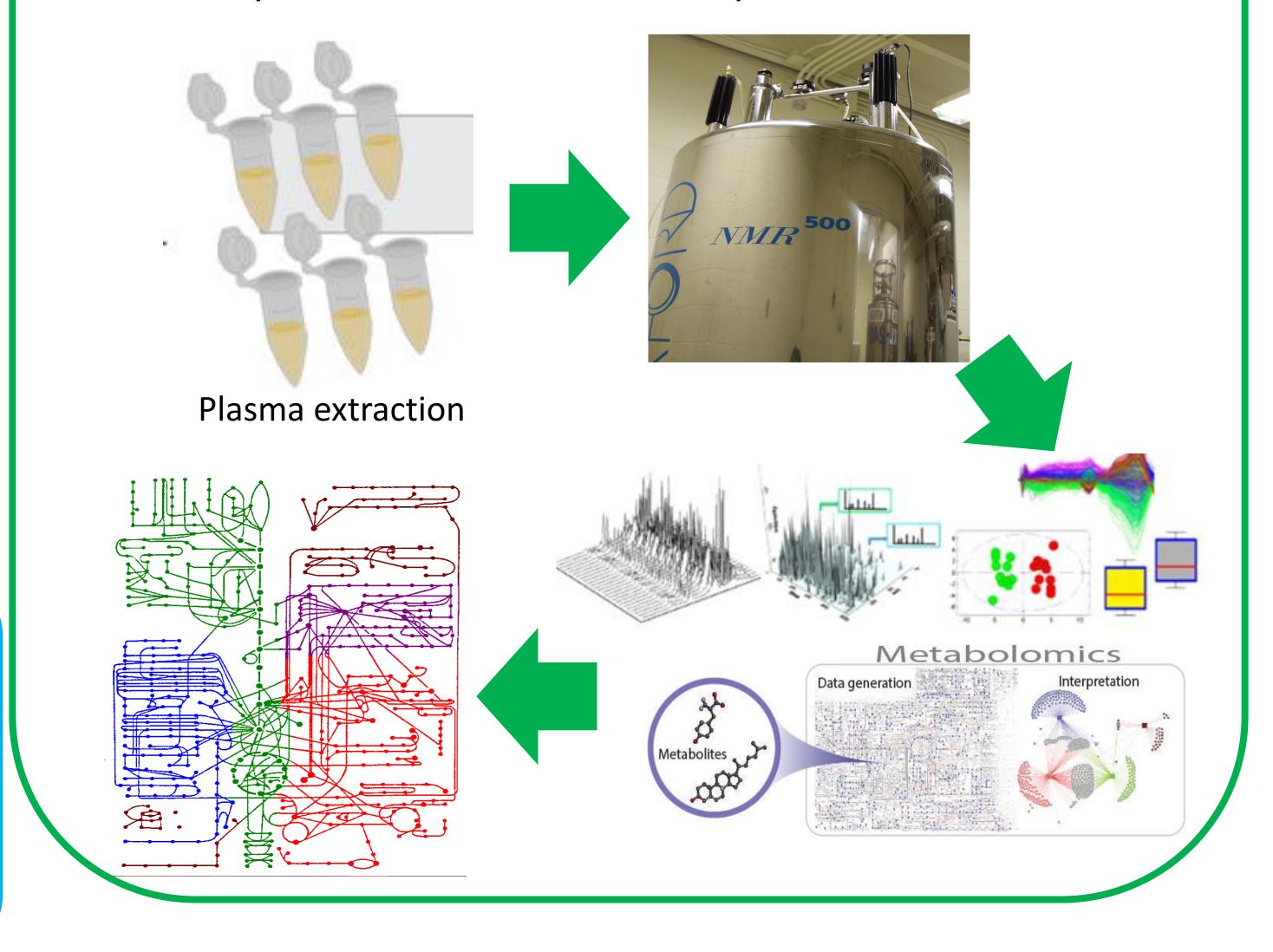
Federica Murgia<sup>1</sup>, Lorena Lorefice <sup>2</sup>, Eleonora Cocco<sup>2</sup>, Luigi Barberini<sup>2</sup>, Simone Poddighe<sup>1</sup>, Maria Rita Murru<sup>2</sup>, Raffaele Murru<sup>2</sup>, Jessica Frau<sup>2</sup>, MD Giuseppe Fenu<sup>2</sup>, MD, Giancarlo Coghe<sup>2</sup>, Francesco Del Carratore<sup>1</sup>, Luigi Atzori<sup>1</sup>, Maria Giovanna Marrosu<sup>3</sup>

1 Department of Biomedical Sciences, University of Cagliari, Italy 2 Department of Public Health, Clinical and molecular medicine, Cagliari, Italy 3 Department of Medical Sciences, Cagliari, Italy



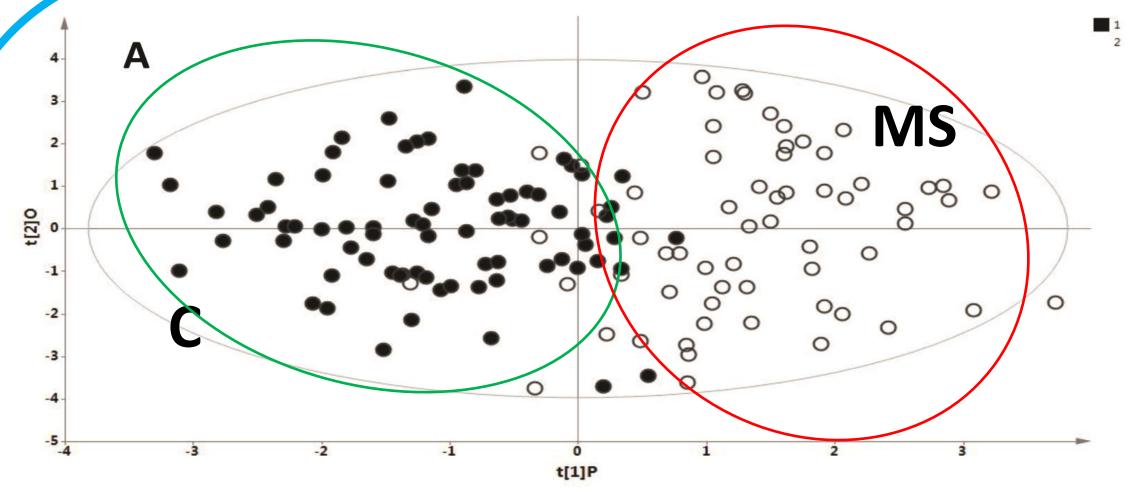
**Introduction**: Multiple sclerosis (MS) is a chronic disease characterized by a high level of heterogeneity. Metabolomics is an "-omics" approach with the potential to discover new biomarkers (1,2). Thus, we investigated the metabolic profiles of MS patients to define the pathways potentially related to its pathogenesis

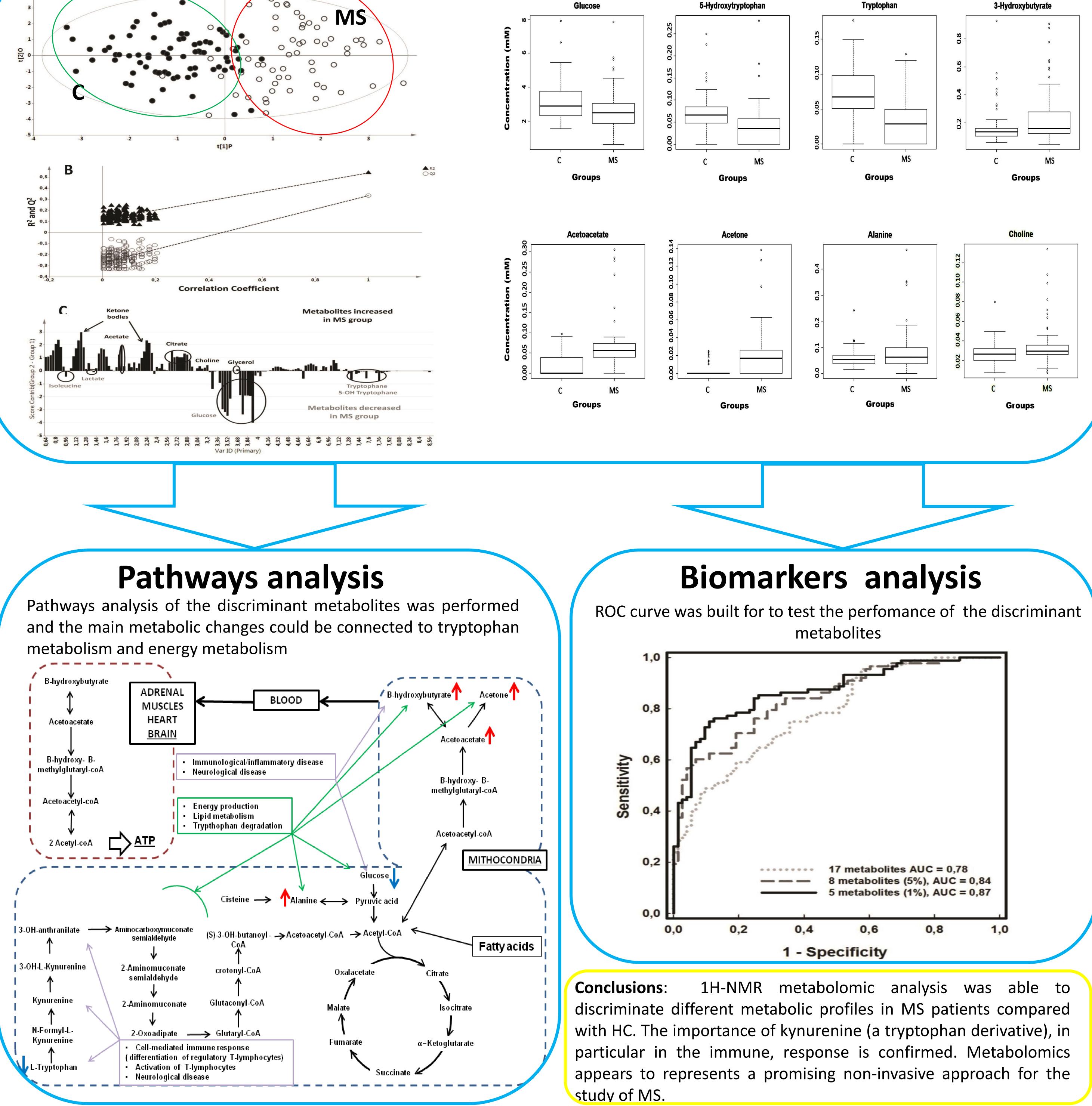
Materials and methods: Plasma samples from 73 MS patients and 88 controls (C) were analyzed by <sup>1</sup>H-NMR spectroscopy, and followed by multivariate statistical analysis

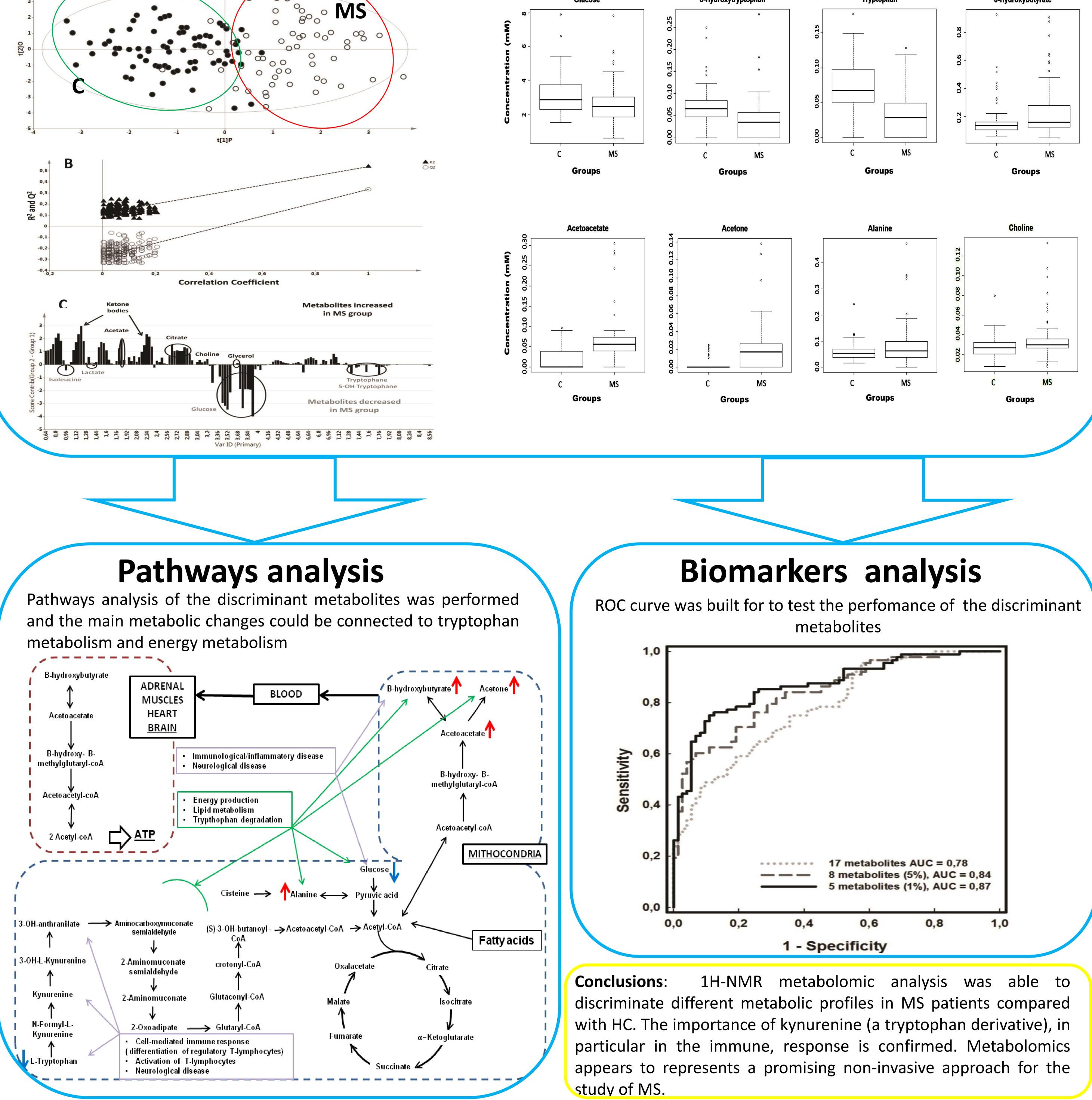


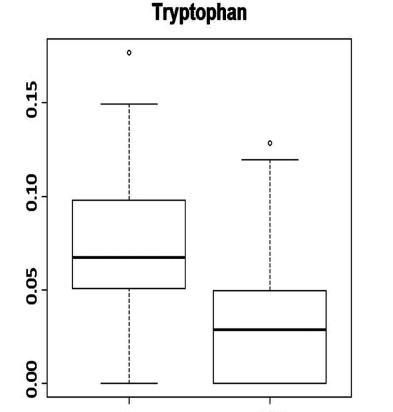


**Results**: the model obtained with the OPLS-DA identified predictive metabolic differences between the MS and C (R2X = 0.615, R2Y = 0.619, Q2 = 0.476 p < 1000.001). A total of 17 metabolites were indentified and the differential metabolites included glucose, 5-OH-tryptophan, and tryptophan (lower in MS, p < 0.01), and 3-OH-butyrate, acetoacetate, acetone, (higher in MS p < 0.01). The model was evaluated using an external set of samples and the corresponding ROC curve produced (AUC of 0.93).











1) Smolinska A, Blanchet L, Buydens LM, Wijmenga SS. NMR and pattern recognition methods in metabolomics: from data acquisition to biomarker discovery: a review. Anal Chim Acta. 2012;750:82-97.

2) Moussallieh FM, Elbayed K, Chanson JB, et al. Serum analysis by 1H nuclear magnetic resonance spectroscopy: a new tool for distinguishing neuromyelitis optica from multiple sclerosis. Mult Scler. 2014 Apr; 20(5):558-65.