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**Title:** Breath analysis in real time by mass spectrometry in chronic obstructive pulmonary disease

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**Body:** Objectives: It has been suggested that exhaled breath contains relevant information on health status. We hypothesized that the real-time mass spectrometric analysis of breath may be useful to differentiate breathprints from chronic obstructive pulmonary disease (COPD) patients and controls. Methods: We studied 61 participants: 25 COPD patients (GOLD I-IV), 25 non-smoking controls and 11 smoking controls. We analyzed their breath by mass spectrometry in real time. Raw mass spectra were post-processed and statistically analyzed. Results: Four groups comprising COPD (GOLD I-II), COPD (GOLD III-IV), smoking controls and non-smoking controls were correctly classified as a result of principal component analysis/canonical analysis. The most significant features rendering the separation of the different groups were identified. A blind classification (i.e. leave-one-out cross validation) resulted in 92% sensitivity-73% specificity (COPD vs. smoking controls); and 84% sensitivity-88% specificity (COPD vs. non-smoking controls). Conclusions: We conclude that real time mass spectrometry may be a useful technique to analyze and characterize the metabolome of exhaled breath. The acquisition of breathprints in a rapid fashion may be a valuable tool to diagnose and phenotype COPD.

Characteristics of the participants

	GOLD III/IV (n=12)	GOLD I/II (n=13)	Healthy smokers (n=11)	Healthy non-smokers (n=25)
Age (years)*	62(5)	63(7)	34 (10)	27 (9)
Male/Female	3/9	9/4	9/2	18/7
Pack-years*	37 (23)	40(32)	10 (13)	0
FEV1 % predicted*	27 (6)	70(13)	111 (10)	101 (9)
FEV1 (L)*	0.6(0.1)	2.1(0.6)	4.5(0.6)	4.1(0.8)
FVC % predicted*	74(15)	92(15)	111 (12)	105 (10)
FVC (L)*	2.1(0.5)	3.4(1)	5.4(0.9)	5(1.1)

FEV1/FVC*	31(7)	63(6)	83 (4)	82 (7)
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