Precursors for Cytochrome P450 Profiling Breath Tests from an *in silico* Screening Approach
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**Supporting Information**

**Figure S1**: Distribution of log\(H_{\text{pred}}\) values for natural breath components.
For generation of the histogram 100 equally spaced bins were selected. The data show a mean value of -0.147 mol/(l*atm) and a standard deviation of 2.52 mol/(l*atm). The criteria for log\(H_{\text{pred}} < 4.0\) mol/(l*atm) was applied to predict volatile compounds with the QSPR equation as with this cutoff ~95% of the experimentally described breath components are covered.