

## Chapter 8.2

# Brain–Like Processing and Classification of Chemical Data: An Approach Inspired by the Sense of Smell

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### **ABSTRACT**

The purpose of the olfactory system is to encode and classify odorants. Hence, its circuits have likely evolved to cope with this task in an efficient, quasi-optimal manner. In this chapter the authors present a three-step approach that emulate neurocomputational principles of the olfactory system to encode, transform and classify chemical data. In the first step, the original chemical stimulus space is encoded by virtual receptors. In the second step, the signals from these receptors are decorrelated by correlation-dependent lateral inhibition. The third step mimics olfactory scent perception by a machine learning classifier. The authors observed that the accuracy of scent pre-

diction is significantly improved by decorrelation in the second stage. Moreover, they found that although the data transformation they propose is suited for dimensionality reduction, it is more robust against overdetermined data than principal component scores. The authors successfully used our method to predict bioactivity of drug-like compounds, demonstrating that it can provide an effective means to connect chemical space with biological activity.

### **INTRODUCTION**

In many application domains, our senses are more efficient in analyzing information than most computational implementations. In addition, it appears that when a specific kind of information must be

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encoded, engineers often find solutions which are similar to information processing strategies that have evolved in nature. For example, various image compression algorithms use a wavelet-like encoding strategy, which is comparable to what happens in the retina and subsequent stages of the visual system (Mallat, 1989). Similarly, the cochlea in the inner ear decomposes the auditory signal into its frequency spectrum. An analysis of the cochlea's coding properties has contributed to improved coding of audio signals (Baumgarte, 2002).

The task of the olfactory sense is to efficiently encode, process and classify chemical information. The physiological architecture of the chemical sense has striking similarities in insects and mammals, although it has evolved independently (Hildebrand & Shepherd, 1997, Firestein, 2001). This fact may indicate that there is an optimal way for coping with chemical information, that is, identifying specific odorants out of a rich assortment of olfactory agents.

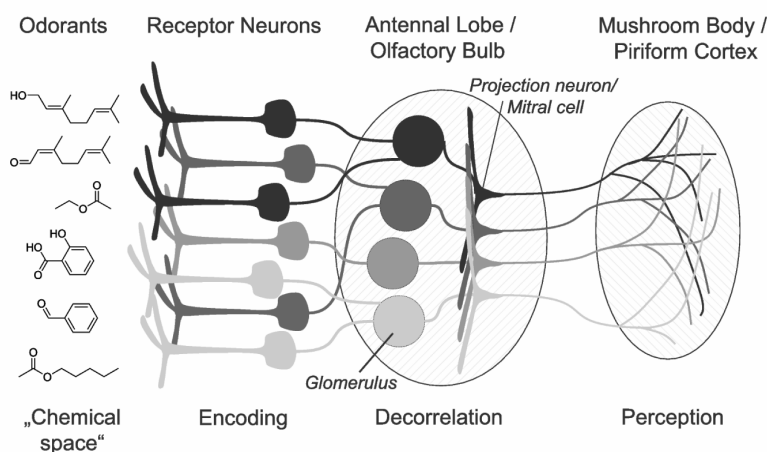
In this study we summarize our computational concept of employing processing principles from the olfactory system to a chemical classification task.

## BACKGROUND

Figure 1 outlines the basic architecture of an *olfactory system*. "Chemical space" consists of the multitude of odorant molecules which float around us in the air. These molecules activate an array of receptor neurons. Subgroups of receptor neurons are distinguished into classes according to the particular olfactory receptor protein they present on the membrane (indicated by different shades of gray in Figure 1). Since this membrane-bound receptor protein determines the ligand selectivity of the receptor neuron, neurons of one class respond to the same *odorants*.

The number of receptor neuron classes varies greatly between species and exhibits weak correlation with olfactory capability. The fruit fly *Drosophila melanogaster* possesses about 60 different functional receptor genes (Vosshall, Wong, & Axel, 2000), the honeybee *Apis mellifera* has about 160 (Robertson & Wanner, 2006). Humans are believed to possess approximately 250 different receptor classes (Glusman, Yanai, Rubin, & Lancet, 2001, Zozulya, Echeverri, & Nguyen, 2001), while mice have about 1000 (Zhang & Firestein, 2002) and dogs around 1200 (Olender et al., 2004).

Figure 1. Schematic of the basic architecture of the olfactory system in insects and mammals



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