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Databases in SenseLab for the Genomics, Proteomics, and Function of Olfactory Receptors

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Abstract

We present here, the salient aspects of three databases: Olfactory Receptor Database (ORDB) is a repository of genomics and proteomics information of ORs; OdorDB stores information related to odorous compounds, specifically identifying those that have been shown to interact with olfactory receptors; and OdorModelDB disseminates information related to computational models of olfactory receptors (ORs). The data stored among these databases is integrated. Presented in this chapter are descriptions of these resources, which are part of the SenseLab suite of databases, a discussion of the computational infrastructure that enhances the efficacy of information storage, retrieval, dissemination, and automated data population from external sources.

Keywords

Databases; Olfactory receptors; Computational modeling; Odorants; Informatics; Data integration

1 Introduction

Research into olfactory receptors (ORs) is a relatively recent field, about two decades old (1). OR function results from the interaction of an OR with an odorant—the first in a series of steps leading to olfaction (2, 3). Two major events provided the impetus for research into ORs and other chemosensory receptors (CRs): (1) The Nobel Prize for Medicine awarded in 2004 for the discovery ORs (4) and (2) the recognition of OR genes as constituting the largest gene families in the human and most mammalian genomes (5–9). Olfactory Receptor Database (ORDB), which stores information related to these OR genes and described in this chapter, (10–16) has been at the forefront of information dissemination related to ORs for more than 15 years.

Electro-olfactograms (17–20), and calcium imaging (21–25) are two commonly used modes of experimentally determining OR excitation. The central question that these methodologies attempt to address is the nature of the interaction between an OR and odor molecule ligand. The first evidence for OR response to odor-binding came from an experimental study by Breer et al. (26) and a computational study by Singer & Shepherd (27). This was followed by a computational analysis by Singer (28, 29) of experimental results by Zhao et al. (30);

the latter study showed a preference of the 17 receptor for the octanal odorant. The closeness of the fit of computational model to experiment supported the notion of the existence of a binding pocket within which odor molecules interact with receptor amino acid residues. The first combinatorial study of odor-mediated excitation of different identified ORs was published in 1999 for 14 mouse ORs and several odorants—mostly carboxylic acids and their derivatives. Later, electro-olfactograms were used to determine responses of the rat OR 17 to a rational panel of 90 odors, which were eventually narrowed to ten octanal molecules that differed by substitutions, branches, and unsaturation (31).

Other functional activation studies have shown that phenylic aldehydes and ketones activate mouse OR M71 and OR912-93—both extensively characterize (32). Luu et al. showed that key receptor residues are responsible for interacting with odor ligands in zebra-fish and goldfish (33). Touhara and coworker identified ORs that could be excited by lylal, eugenol, vanillin, and ethyl vanillin (34-42). Matarazzo and coworkers have used baculovirus constructs to perform functional analysis of two human ORs (22). Shirokova et al. established that the type of G-protein in the transduction cascade plays an important role in determining whether an odor will be an agonist or an antagonist (21). Schmiedeberg showed that the interactions between the amino acid residues in an OR and an odor are mediated not only by electrostatic interactions but supported by van der Waals forces (43). These are a sampling of earlier functional analysis for ORs. More recently, two combinatorial studies have been published for several ORs with odors with a wide range of functional groups. While most ORs are narrowly tuned to agonists for not more than one feature, e.g., functional groups, functional characterization of the mouse ORs MOR256-3 (44) and MOR256-31 (45) shows that these ORs respond to odors possessing a wide range of functional groups. The promiscuous nature of the interactions—one OR has been shown to bind more than one odorant, which in turn will bind more than one OR—adds to the challenge of obtaining mechanistic insights into OR-odor interactions.

Functional characterization of ORs involve determining which odorants excite, inhibit or exhibit no impact on an OR. These studies pinpoint specific amino acid residues within the OR binding region that are responsible for odorant binding.

There is currently no experimentally derived structure of ORs. An OR is a GPCR—a G(TP-binding) Protein Coupled Receptor. Structurally, GPCRs are known to be composed of seven transmembrane helices, which traduce the plasma membrane. These helices are connected by three intracellular and three extra-cellular loops and possess an extracellular N-terminus and an intracellular C-terminus (46). There is some evidence that GPCRs and ORs with anomalous structures might exist (47). Computational experiments have been carried out to determine the structure of ORs. Like most GPCRs, ORs are often modeled (28, 29, 48-53) on the structural template of rhodopsin—whose X-ray crystallographically derived structure has been solved with improving resolution (54, 55). Recently, more GPCRs have been structurally elucidated (56-59).

2 Materials

The SenseLab suite of databases uses a multi-tier application architecture composed of the following:

1. Interface front end modules written in the C# language.
2. EAV/CR business-data-logic layer written in the VB.NET language.
3. Back-end data storage layer resides on an Oracle 11g database server.
4. SenseLab uses Internet Information Server as a Web server hosted on a Windows 2008 R2 server.
5. Some data-integration and automated population software is written in PERL (Practical Extraction and Report Language).

3 Methods

3.1 ORDB

1. ORDB is a repository of information related primarily to ORs. Other chemosensory receptors are also represented in ORDB. They are *C. elegans* chemosensory receptors, fungal pheromone receptors, insect ORs, taste receptors, and vomeronasal receptors. The total number of receptors stored in ORDB currently numbers close to 14,500.
2. Each olfactory (or chemosensory receptor) is described by attributes. Each attribute is associated with one or more value, depending on the attribute. Figure 1 represents an OR with ORDB name ORL11. The number “11” associated with “ORL” merely indicates the order in which this gene was entered into the database, and bears no special significance. One of the attributes “Common Name” identifies the receptor by the name given to it by the research group where the OR was first cloned or identified.
3. The first attribute for this receptor is “Name” for which the value is “ORL11.” The CR (Chemosensory Receptor) type (since receptors other than ORs are deposited in ORDB) type is ORL or OR like. The name of the organism (rat), the source tissue for the gene (olfactory epithelium), and chromosome number (11) provide additional information about the receptor.
4. The links to the article(s) that described this gene in PubMed and the GenBank entry which served as the source of this receptor are automatically generated when this information is entered into ORDB. The links allow the user to access the abstract for the article or the source for the gene.
5. The amino acid and nucleotide sequences for this gene are available.
6. The source of the information (most often GenBank) for this receptor is indicated. Other sources for this receptor are sequences supplied by researchers themselves, sometimes prior to publication (ORDB offers a service to researchers, who can obtain a login ID and use the database to store sequences privately (see Notes ¹⁻³)).

7. The values for the “Sequence Laboratory” attribute contain links with researchers’ names in whose laboratories the receptor gene was first studied. Clicking on the links “AxeL_RA” and “Buck_LB” will take users to Web pages dedicated to information related to the laboratories for Drs. Richard Axel and Linda Buck, respectively. ORDB endeavors to be an information hub of the chemosensory receptor community. The page for each laboratory contains links to contact information—telephone numbers, e-mail, and laboratory address for these researchers.
8. The “Length” of the sequence identifies whether the available gene sequence is partial or complete. The “Type of Sequence” allows users to choose whether the sequence arises from cDNA (for ORL11), from mRNA or if it is a pseudogene.
9. Links to the odorant receptors that are known to excite the receptors are listed for the attribute “Ligand.” These are linked to OdorDB (see Subheading 3.2), a companion resource to ORDB. Likewise, the value for Molecular Models, will link to information related to computational modeling studies for that receptor in ORModelDB. Both OdorDB and ORModelDB are discussed in detail in the next two sections.

3.2 OdorDB

1. In ORDB, (Fig. 1), odors are listed as “values” for the “ligand” attribute: heptanal and octanal. These two odorants have been functionally characterized as eliciting an excitatory response in the rat 17 receptor. When the link for “heptanal” is clicked, it takes the user to a page dedicated to this odorant (Fig. 2).
2. The attributes for octanal are as follows: Name, Chemical Abstracts Service (CAS) number, its molecular formula, whether it has a cyclic structure, its hydrocarbon feature (straight chain, branched chain, saturated, unsaturated, etc.), and the two-dimensional structure. If a Glomerular activity map, that illustrated response to that odor, was available in OdorMapDB, another database within SenseLab (<http://senselab.med.yale.edu/OdorMapDB/>), a relevant link is provided.
3. OdorDB (senselab.med.yale.edu/odordb) is a repository of odorants. Currently, 250 odorants are stored in this resource. They bear the same attributes as those for octanal, mentioned in the paragraph above. Figure 3 shows the same page as seen in Fig. 2. The different colors and specific links, however, indicate that the same information is accessible from a different resource (pointing to data integration, discussed in several instances in this chapter). The link seen in the list of links at the top of the page in Fig. 3, “O.R. by ligand.” It identifies Odors by the ORs with which they are known to interact. Figure 4 shows a truncated portion of this page. 97 odorant molecules have been identified as binding and exciting ORs.

¹Editing, curating, and algorithmic development that facilitates the above functionality of SenseLab’s olfactory databases is only within the purview of those with special access and administrative privileges.

³Users can use the available database infrastructure to store and access information privately, until an associated article is published or the information is ready to be made publicly available.

4. In Fig. 4, the middle column provides links to the odorant molecules. These descriptions have been shown in Figs. 2 and 3. The right hand column depicts the number of ORs that are excited by these an odorant in the same row. For example, (+)-Dihydrocarvone is an odorant that, according to ORDB, has been functionally assessed against ten ORs. By clicking the number “10” in the right hand column a list of these ORs in ORDB can be accessed.

3.3 ORModelDB

1. ORModelDB is the newest database in SenseLab. It was created to disseminate information related to the computational studies of ORs. Computational studies of OR, range from (but are not restricted to) building a model of the OR, computationally docking the ligand in the OR binding pocket and performing dynamic simulation studies to study the interactions of the odorant and the OR, all with a view to providing a mechanistic basis for OR function.
2. The attributes or descriptors of an ORModel (Fig. 5) include a link to the source of the sequence of that receptor (typically from GenBank), links to articles that describe the identification of the OR, the results of functional analyses and those that describe the computational studies involving the OR. The link containing the ORDB name allows the user to access additional information about the OR in ORDB. Odor ligands associated with this OR are identified as links which describe the odorants in OdorDB.
3. A new feature specific to ORModelDB is the incorporation of a JAVA-based viewer that allows users to view and manipulate the structure of the OR within the Web browser. ORModelDB was created, in part, to share structural information related to ORs. The PDB (protein data bank) formatted file of the computational model is also available for download by a user, as are any other relevant files that provide additional information related to the computational studies. The “Description” field for an ORModelDB entry contains an e-mail address of the principal investigator of the modeling work so that interested users can contact him or her—for additional information about the modeling process, sharing offiles (not included as a link for download), etc.

3.4 Database Architecture

1. All of Sense Lab’s databases are based on the EAV/CR (Entity-Attribute-Value with Classes and Relationships) database architecture (60-62). Figures 1, 2 and 3 are illustrative of this. EAV/CR was designed as a “metadata-driven infrastructure:” (63) it is possible to integrate heterogeneous databases within its framework. Representing resources using the EAV/CR framework precludes the necessity of re-storing the same information in different databases.
2. In Fig. 1, for example, within the EAV/CR framework, the ORDB database consists of several classes, and the entries for ORs are entities within the Chemosensory Receptor class. The mode of representation of a class is exactly like that of an entity. Each OR entry—an Entity-Class—is also called an Object. The

properties that define an entity are attributes of a class. Attributes are qualified by specific values.

3. In ORDB, as seen in Fig. 1, the attributes are in the left hand side column of the figure and the corresponding values are in the right hand side column. The real power behind the EAV/CR framework can be seen in some of the “Values” for an OR. These values are highlighted as links. For example, in Fig. 1, if a user clicks “Buck_L” which is a value for Sequence Lab—denoting that Dr. Linda Buck’s research was responsible for the early developments related to ORL11 (rat OR 17)—the user is taken to a page which depicts Buck_L as an independent entity defined by a separate class. And as an independent entity, the (researcher’s) Name has its own attributes and values: “Affiliation,” “Mailing Address,” “Telephone Number,” etc. The information for each of these attributes is then a value.

The curators of ORDB therefore, have an easier task when entering an OR into the database. When entering a “Value” (researchers’ names for the “Sequence Laboratory” attribute, curators can select from a list of researcher names. For every class, a link “show other” is seen. For the “Buck_L” Sequence Laboratory example, clicking on “Show Other” will result in a list of all other ORDB entries which have the “Buck_L” Sequence Laboratory assignment.

4. The same is true for all other values that are stored as classes. From an algorithm development standpoint, the same script is used to process every class in a database. Note the close resemblance, especially in color between Figs. 1 and 2. The left hand column is orange; the right hand column is gray. When a class is invoked by a user clicking the link for that class, the same program-script, which is created to present information about that class, accesses the databases, accesses all the attributes associated with the class in the attributes table and extracts all the corresponding values. The attribute-value dyads are then presented to the user in a Web page in tabulated format. Thus for the OR class—the results as seen in Fig. 1 are extracted and presented, likewise for “heptanal” in Fig. 2.

3.5 Database Integration and Interoperability

1. EAV ICR provides mechanisms that facilitate data sharing between all of SenseLab’s databases, and indeed, ORDB, OdorDB, and ORModelDB. These mechanisms are defined by restriction levels. Elements in some classes may be shared as links that connect one database to another, information can be entered for one resource by a curator of another resource, and even schemas can be altered by curators of other databases inside an EAV/CR data storage system. The flexibility afforded by the database architecture, whose applicability in the ORDBs was illustrated in Subheading 3.4.
2. The basis for data-integration in all of Sense Lab’s databases lies in the universally applied database schema. All the database information arises from the same storage system. This includes the metadata, schema, and semantic annotations. All EAV/CR data integration routines are metadata-driven.

3. Figure 6 is the XML representation for ORL11 in Fig. 1. By clicking the “Data” link for every class in SenseLab databases, the XML schema for that entry is revealed. In the figure, “c” preceding a number denotes that it is a class. In this case, the class is OR (Olfactory or Chemosensory Receptor); “O” before a number denotes an object or a class; “a” before a number denotes an attribute. “o559” is associated with the entity ORL11—the specific entry for the rat 17 OR (Fig. 1). There is no other class in the entire SenseLab schema with the assignment “0559.” The attribute “a80” is for the attribute “CR Type”; this denotes whether the CR is an OR, taste receptor, pheromone receptor, etc. ORL, because it has multiple instances, is stored as an object (much like octanal or Buck_L in Subheadings 3.1 and 3.2) “01364.” Only when a value is stored as a class does it receive an object identifier.
4. “a32” denotes the attribute “Chromosome.” Since this is a unique number, it is stored as a textual value (as an Integer) and not given a class designation. This is the same for attributes “a40” and “a41,” for “Nucleotides” and “Amino Acid” sequences, which are unique instances of text.
5. If these data are to be exchanged or represented differently (through OdorDB instead of ORDB), the script has to be merely modified, but is still designed to access the same tables and instances in the database.

Consider the following three URLs: <http://senselab.med.yale.edu/ORDB/eavData.aspx?o=144593>, <http://senselab.med.yale.edu/odordb/eavData.aspx?o=144593> and <http://senselab.med.yale.edu/ORModelDB/eavData.aspx?o=144593>. Each represents pages in ORDB, OdorDb and ORMModelDB, respectively (Figs. 2, 3 and 5). Class (or entity) with unique identifier “0144593” represents in the database, the odorant “Heptanal.” All three of the above URLs invoke the eavData.aspx (Active Server Pages C#) script that extracts information from the SenseLab databases and presents it to the user in a dynamically created Web page. Clicking on the first two links results in Web pages as seen in Figs. 2 and 3, which are identical in every respect, except for the color schemes the pages. One represents ORDB; the other represents OdorDB. The third URL represents the exact same information in the same format as seen in Figs. 2 and 3, but with the color schemes of ORMModelDB, seen in Fig. 5.

6. If the “O=144593” in the above URLs were replaced by “O=559,” the rest of the URL remaining the same, Fig. 1 would result. The eavData.aspx script is universal for all of SenseLab. When this script is deployed, for a specific class (represented by the object identifier), it scans the database identifying the attributes and values and presents it in the result Web page.
7. The question as to why different databases are needed can be answered thus: A user who seeks information about Olfactory (or other chemosensory) receptors can extract the information about ORs and click on links of choice. If, on the other hand, a user who seeks information about odor molecules, with no interest in receptors, can visit OdorDB, and access information about a specific odor that is stored in SenseLab; likewise, a user interested in computational models of ORs and

not in other aspects of ORs, can find that information in ORModelDB. This integration-leveraging database infrastructure design ensures that data does not have to be replicated and stored in different databases.

3.6 Multiple-Parameter Search

1. One of the challenges of databases that house large amounts of data in complex database structures and hierarchies is to be able to retrieve information that is specific and relevant to the user. Indeed, scanning through almost 15,000 entries to identify a few receptors would be a daunting task, involving scrolling through long lists and clicking on each entry before identifying the ones that were relevant.
2. Figure 7 represents a search system that, once again, leverages the database architecture of SenseLab. It is possible to search for an entry associated with any class within the database and search in such a way as to systematically filter through every attribute (to that class) to narrow search results. In Fig. 7 is represented a search for the class “chemosensory receptors.” This means that the user is searching among entries in ORDB. The user chooses “CR Type” as ORL.
3. The yellow tab marked “Look Up” indicates that an attribute-value is stored as a class. The tab is designed to aid the user avoid having to type the specific value. For the CR Type attribute, if the user clicks on this tab, a pop-up window with all the possible choices for this attribute, ORL, TPR, VNR, etc., will be available. The user can click on the choice (or more than one choice) of value and it gets entered into the field under the heading condition.
4. The user has, in the example illustrated in the figure, also chosen only full-length sequences, and organism “mouse,” and receptors that are on chromosome 10. The user has chosen PubMed, but not as a filter, because no PubMed Identifier was entered in the field. The user requests that the PubMed IDs for all the relevant receptors appear in the results.
5. The user also wants all the protein sequences to appear in the results.
6. In the Column under the heading “Show” the check-box asks whether that specific information needs to be revealed in the results. For *Length* and *Organism*, the user would prefer to use these values as filters, but not have them cluttering the results—the organism and the length being already known.
7. The red circle with the “x” mark through it on the under the column heading “Del” when clicked will remove that attribute from the search filter.
8. Towards the bottom of this table, the “**New**” link can be clicked by the user if he or she wishes to further filter the search by adding a new attribute. To deploy the search system, the user uses the drop-down menu titled “Show Results As” and chooses whether he or she wants the results in HTML, text, or XML format.
9. Every one of the attributes for an OR entry (Fig. 1) can be used as filters to narrow search results. For this search, the results produced 48 entries, three of which are

shown in Fig. 7, in the HTML format. Since the “CR Type,” Chromosome, PubMed, and Amino Acids attributes were clicked, they appear in the results.

10. A multi-attribute search can be carried out for every Class within ORDB, OdorDB, and ORModelDB. For every class, the attributes associated with this class can be used as filters.

3.7 Auto-Population

1. The size and scope of ORDB and the need to disseminate information in an efficacious and timely manner to serve the chemosensory community and knowledge seekers worldwide, necessitates the population of ORDB using automated methods.
2. AutoPop (11) was developed as a Web-based ORDB automatic population tool. AutoPop leveraged the notion of interoperability. Interoperability is a term that has become increasingly commonplace in the domain of online information dissemination (64-66). Interoperability involves the exchange of information between two independent, disparate and heterogeneous resources. AutoPop parsed the html files of sources of OR information and extracted only the information specific to ORDB. The AutoPop front page was a Web page with a single text-field. The curator entered a GenBank Accession **ID** into this field. This **ID** was embedded in a URL that represented the GenBank page for this **ID**. A PERL (Practical Extraction and Report Language) was written to access the GenBank servers and download the Web page to the SenseLab servers for additional processing.
3. An ORDB knowledge base was created, which consisted of a representation of the schema of the database, containing lists of unique attribute and object IDs of the values of attributes stored in ORDB as independent classes. The value descriptors of these attributes and objects were also stored in this knowledgebase.
4. During the processing of the HTML page (also known as screen scraping—a subsequently discontinued process) if the receptor gene sequence came from an organism, e.g., *Mus musculus*, and if the organism was identified as such, it was matched against the ORDB knowledge base and mapped onto object-value “O144” (for mouse) and attribute “a30” (organism). Since the XML file was dynamically generated while the HTML page downloaded from GenBank was being processed, a line `<a30 object_name=‘mus musculus’>o144<a30/>` was written to the XML file. For an entry for a mouse OR gene, if the strain, e.g., 129/SVJ was identified, it was mapped to the attribute for Strain “a106.” Since strain is stored as a value and not an object, the line `<a106 value=‘Strain’>129/SVJ <a106/>` was added to the XML file. This file was created as each relevant attribute was identified from the source of OR information.
5. This dynamically written XML file is obtained by clicking the “Data” link on the Web page for every class in the olfactory databases. This XML file was then embedded in a Web page. Clicking “Submit” in that Web page deposited this information into ORDB directly.

6. Prior to the creation of AutoPop, for each entry, the curator cut and paste relevant information into a form, which was submitted into ORDB. Manually creating an ORDB entry took between 5 and 10 min. With AutoPop, the time from entering the GenBank Accession ID to the creation of the html form file with XML file embedded was less than 10 s. This intermediate step was deemed necessary so that the curator could validate information being added was accurate before submitting it to ORDB.
7. AutoPop was not necessarily restricted to populating ORDB one receptor at a time. As long as an XML file was created, the nested hierarchies allowed multiple entries. This was tested for the EXPASY (<http://expasy.org/>) (formerly, Swiss-Prot) resource. A script was written that processed EXPASY protein entries. 74 OR proteins were identified and information for all the ORs were written to a single XML file. All 74 protein sequences were deposited into ORDB in less than 30 s.
8. Creating AutoPop as a Web-based system ensured that the curator could populate the database remotely.

3.8 Updating OROB

1. The screen scraping methodology is less than ideal. The effort required in writing a program that parses an HTML file—which is designed for ease of human viewing—to extract information that should be processed by a computer poses many difficulties.
2. Researchers at NLM, the purveyors of information dissemination at NCBI, made gene information available through the XML format for every GenBank entry. The XML formatted representation of a GenBank entry has now been discontinued. The ideal format available for machine-readable extraction is the ASN.1 (Abstract Syntax Notation. One) format.
3. One challenge is to populate and update ORDB when new information becomes available (Subheading 3.5). Another is to modify and update ORDB entries as the source information evolves. ORDB curators were confronted with the knowledge that as more publications related to olfactory genes were identified, GenBank entries for these genes were updated to reflect multiple links to PubMed.
4. When ORDB was first being populated, one PubMed link existed per gene. To update ORDB and ensure that all PubMed links that are in a GenBank entry for an OR gene are included, ORDB curators developed algorithms that specifically targeted all the sources of olfactory genes in GenBank to identify new PubMed links for the genes and update ORDB to reflect this.
5. Researchers at the National Library of Medicine have created e-utils (67), a system that allows users to search, access, and download large amounts of data from all NCBI sources. There are several resources in e-utils. Here we used two: E-Search and E-Fetch. E-utils framework involves the design of specific URLs to access NCBI resources in a customized manner. These URLs are not very different from

those a user would enter into a Web browser window. For efficient use of the e-utils framework, we developed PERL scripts.

6. We first used the ORDB search feature described in the previous section and illustrated in Fig. 7 to perform a search on all ORDB, retrieving for every gene, the ORDB object identifiers, the ORDB name, and the GenBank Accession ID.

E-search: Our e-search URL was http://eutils.ncbi.nlm.nih.gov/entrez/eutils/esearch.fcgi?db=nucleotide&term=NW_000328&usehistory=y. The URL shows that we access the e-utils resources, the nucleotide database, and the GenBank Accession ID “NW_00328.” On running the e-search program, an XML file is generated which contains the unique identifier for this gene in GenBank. We created an XML parser that processed this XML file to extract this unique identifier.

E-Fetch: The unique identifier (for illustrative purposes UID) extracted from the E-search result was then embedded in the following URL: <http://www.ncbi.nlm.nih.gov/entrez/eutils/efetch.fcgi?db=nucleotide&id=UID&rettype=ASN.1&retmode=text>. This URL indicates that we use the e-fetch feature in e-utils, access the “nucleotide” database, and retrieve the file for this gene in the ASN.1 format as a text file. Another script was written to process this results file and extract only the PubMed Identifiers.

7. The above three steps were cycled for all 14,500 entries in ORDB. The process, running on a personal work station was completed in 40 h. Each of the PubMed identifiers were mapped to the object IDs and then this information was deposited in ORDB. 7000 entries, close to 50% of the entries had more than one PubMed link, reflecting research completed and published that was related to each OR gene—after the ORDB entry had been made (with one PubMed link).

Since the above steps are semi-automated, deploying these every few months will ensure that ORDB is continually updated.

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Senselab
Olfactory Receptors Database	
Home FAQs Links Resources Users Human ORs Mouse ORs Enter ORDB Search Schema Login User: Public	
Go back [Data]	
Chemosensory Receptors	
Name	ORL11
Description	
CR Type	ORL (Olfactory Receptor Like) show other
Organism	Rattus norvegicus (rat) show other
Source Tissue	olfactory epithelium show other
Chromosome	11
Genbank	M64386 link show other
PubMed	1840504 link show other
Strain	
Common Name	17
Source	GENBANK show other
Sequence Lab	AXEL R show other BUCK L show other
Length	Full Length show other
Ligand	Heptanal show other Octanal show other
Nucleotides	ATGGAGCGAAGG AACACAGTGGG AGAGTGAGTGAA TTTGTGTTGCTG GGTITCCAGCT CCTGCCCCACTG CGAGTACTACTA TTTTCTCTTCT CTCTGGNCTAT GTGTGGTGTG ACTGAAACATG CTCATCATTATA GCAATTAGGAAC CACCAACCCCTC CACAAACCCATG TATTTTCTTG GCTAATATGTCA TTCTGGAGATT TGGTATGTCACT GTTACGATTCT AAGATGCTCGCT GGCTTCATTGGT TCCAAGGAGAAC CATGGACAGCTG ATCTCCTTTGAG GCATGCATGACA CAACTCTACTTT TTCTGGGCTTG GGTGACAGAG TGTGCTCTTCTT GCTGTGATGGCC TATGACCGCTAT GTGGCTATCTGT CATCCACTCCAC TACCCGTCATT GTCAGTAGCCGG CTATGTGTGAG ATGGCAGCTGGA TCCTGGGCTGGA GGTITGTTGATC TCCATGGTTAAA GTTTTCTTATT TCTGCGCTGTCT TACTGTGGCCCC AACACATCAAC CACTTTTCTGT GATGTGTCTCCA TTGCTCAACCTG TCATGCACTGAC ATGTCCACAGCA GAGCTTACAGAC TTGTCTCTGGCC ATTTTATTCTG CTGGGACCGCTC TCTGCACTGGG GCATCCTACATG GCCATCACAGGT GCTGTGATGCGC ATCCCTCAGCT GCTGGCCGCCAT AAAGCCTTTTCA ACCTGTGCCTCC CACCTCACTGTT GTGATCATCTT TATGACGCGAGT ATTTTCATCTAT GCCAGGCCTAAG GCACCTCTCAGCT TTGACACCAAC AAGCTGGTCTCT GTACTCTACGCT GTCATTGTACCG TTGTTCAATCCC ATCATCTACTGC TTGCGCAACCAA GATGTCAAAGA GCGCTACGTGCG ACCTGTGACCTG GCCAGGACCAG GAGGCCAATACC AACAAAGGCAGC AAAATTGGTTAG
Amino Acids	MERRNHSGRVSE FVLLGFPAPAPL RVLLFLLSLXY VLVLTENMLIII AIRNHPTLHKPM YFFLANMSFLEI WYVTVTIPKMLA GFIGSKENHGQL ISFEACMTQLYF FLGLGCTECVLL AVMAYDRYVAIC HPLHYPIVSSR LCVQMAAGSWAG GFGISMVKVFLI SRLSYCGPNTIN HFFCDVSPLLNL SCTDMSTAEITD FVLAIFILLGPL SVTGASYMAITG AVMRIPSAAGRH KAFSTCASHLTV VIIFYAASIFIY ARPKALSAPDTN KLVSLVYAVIVP LFNPIIYCLRNQ DVKRALRRTLHL AQDQEANTNKGK KIG
Type of Sequence	cDNA show other
Swissprot	
Receptor 2D (GPCRDB)	
Molecular Models	ORModel1 show other
Functional Analysis Laboratory	
Functional Analysis Reference	10781022
Microarray Experiment	559

Fig. 1.
The ORDB entry for the rat 17 olfactory receptor. The ORDB name for this entry is ORL11. The figure illustrates the attributes on the *left hand side* of the page and their values on the *right hand side*. Values that are stored as independent classes are presented as links

Senselab
 Olfactory Receptors Database
 Home | FAQs | Links | Resources | Users | Human ORs | Mouse ORs | Enter ORDB | Search | Schema | Login | User: Public

Go back

[Data]

Odors	
Name	Octanal
Description	
CAS Number	124-13-0
Formula	CH ₃ (CH ₂) ₆ CHO
Functional Group	Aldehyde show other
Cyclic Structure	
Hydrocarbon feature	straight chain show other
Two dimensional Model
Glomerular Activity Map	

Other categories referring to "Octanal"

Behavioral Trial: Odor Stimuli	(4)
OR Model: Ligands	(1)
Odor Map: Odor	(3)
Behavioral Study: Odor Stimuli	(2)
Primary Data: Odor	(1)
Chemosensory Receptors: Ligand	(3)

Revisions: 64
 Last time: 8/10/2012 1:18:27 PM
 Reviewer: [Chiquito](#)
 Owner: [Chiquito](#)

This database was supported by the Human Brain Project (NIDCD, NIMH, NIA, NICD, NINDS) and HURI (Multidisciplinary University Research Initiative). It is now supported by R01 DC 009977 from the National Institute for Deafness and other Communication Disorders.

Questions, comments, problems? Email the [Database Administrator](#)
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Fig. 2.

The Web page for octanal in ORDB which results from clicking the “octanal” link. This is a value for the “ligand” attribute, as seen in Fig. 1. The attributes are on the *right hand side* and the values are on the *left hand side*. Values stored as classes are seen as links

Sensalab

Odor Database

Home O.R.by Ligand **Data** Search Schema Login User:Public

[Go back](#)

[Data]

Odors	
Name	Octanal
Description	
CAS Number	124-13-0
Formula	CH ₃ (CH ₂) ₆ CHO
Functional Group	Aldehyde show other
Cyclic Structure	
Hydrocarbon feature	straight chain show other
Two dimensional Model
Glomerular Activity Map	

Other categories referring to "Octanal"

Behavioral Trial: Odor Stimuli	(4)
OR Model: Ligands	(1)
Odor Map: Odor	(3)
Behavioral Study: Odor Stimuli	(2)
Primary Data: Odor	(1)
Chemosensory Receptors: Ligand	(3)

Revisions: 64
 Last time: 8/10/2012 1:18:27 PM
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Fig. 3.

The figure represents the octanal odor stored in OdorDB. This representation, other than the color differences and the links towards the *top* of the page, is the same as the ligand representation for “octanal” in ORDB, as seen in Fig. 2

Senselab
Odor Database
Home O.R. by Ligand **Data** Search Schema Login User: Public
Go back

'Chemosensory Receptors' grouped by 'Ligand'
Show all class fields

	Ligand	Chemosensory Receptors
1	(+)-2-Phenylbutyric acid	1
2	(+)-Camphor	2
3	(+)-Carvone	13
4	(+)-Dihydrocarvone	10
5	(+)-Fenchone	5
6	(-)-2-Phenylbutyric acid	1
7	(-)-Camphor	5
8	(-)-Carvone	10
9	(-)-Fenchone	4
10	1-Decanol	4
11	1-Nonanethiol	7
12	1-Octanethiol	5
13	2,3-Hexanedione	5
14	2-Coumaranone	6
15	2-HEPTANONE	11
16	2-HEXANONE	2
17	2-METHOXY-4-ETHYLPHENOL	1
18	2-METHOXY-4-METHYLPHENOL	1
19	2-METHYL-4-PROPYL-1,3-OXALTHIANE	1
20	2-Methylphenol	1
21	2-NONANONE	2

Fig. 4.

The figure represents a list of 97 (out of 250) odors stored in OdorDB. The (truncated) list illustrated in the figure is one of odors that are known to excite or otherwise interact with olfactory receptors. By clicking on the odor name, the user is taken to information of the odor as seen in Figs. 2 and 3. By clicking the number on the *right hand side* of the table, which represents the number of ORs that are excited by each odor, the user can access these ORs in ORDB

OR Model																			
Name	ORModel1																		
Description	Please email Dr. Chiquito Crasto for additional files related computational structural studies for this work. chiquito@uab.edu																		
GenBank	M64386																		
Species	Rat																		
Publication (PubMed)	1840504 link show other																		
Chemosensory receptor	ORL11 show other																		
Ligands	<table border="0"> <tr> <td>3,7-dimethyloctanal</td> <td>show other</td> </tr> <tr> <td>trans,trans-2,4-Octadienal</td> <td>show other</td> </tr> <tr> <td>2-Octynal</td> <td>show other</td> </tr> <tr> <td>3,6,7-Trimethyl-2,6-octadienal</td> <td>show other</td> </tr> <tr> <td>Trans-2-octenal</td> <td>show other</td> </tr> <tr> <td>3-methyl-4-(4-methyl-cyclohexyl)-propanal</td> <td>show other</td> </tr> <tr> <td>CITRAL</td> <td>show other</td> </tr> <tr> <td>CITRONELLAL(+)</td> <td>show other</td> </tr> <tr> <td>Octanal</td> <td>show other</td> </tr> </table>	3,7-dimethyloctanal	show other	trans,trans-2,4-Octadienal	show other	2-Octynal	show other	3,6,7-Trimethyl-2,6-octadienal	show other	Trans-2-octenal	show other	3-methyl-4-(4-methyl-cyclohexyl)-propanal	show other	CITRAL	show other	CITRONELLAL(+)	show other	Octanal	show other
3,7-dimethyloctanal	show other																		
trans,trans-2,4-Octadienal	show other																		
2-Octynal	show other																		
3,6,7-Trimethyl-2,6-octadienal	show other																		
Trans-2-octenal	show other																		
3-methyl-4-(4-methyl-cyclohexyl)-propanal	show other																		
CITRAL	show other																		
CITRONELLAL(+)	show other																		
Octanal	show other																		
Functional Analysis (PubMed)	11100145 link show other																		
Modeling and Computational Analysis (PubMed)	16243965																		
Related Models	ORModel1 show other																		

Model Structure(1)

SN	Info	Model file
1	Model of Rat 17	i7.pdb [104801 bytes]

Rat 17

Fig. 5.

The ORModel DB entry for the computational model of rat 17 OR. The attributes for this entry are listed in *blue* and the values in *gray*. Links to the receptor “ORL11” in ORDB, links to the ligands in OdorDB, links to the GenBank source of the gene, and PubMed are illustrated. A JAVA application allows the user to manipulate the model within the browser. The pdb of the computational protein model of the receptor is also available for free download

```

<data time="0.0312473999947542">
  <data_database db_id="d4">
    <data_class class_id="c22" version="5">
      <object id="o559" name="ORL11" description="" unis_cui="" version="22" version_date="8/27/2012 11:15:15 PM">
        <att_value att_id="a80" value="o1364" value_object_name="ORL (Olfactory Receptor Like)"/>
        <att_value att_id="a30" value="o804" serial_no="0" value_object_name="Rattus norvegicus (rat)"/>
        <att_value att_id="a31" value="o821" value_object_name="olfactory epithelium"/>
        <att_value att_id="a32" value="11"/>
        <att_value att_id="a48" value="o131893" value_object_name="M64366"/>
        <att_value att_id="a44" value="o129268" serial_no="0" value_object_name="1840504"/>
        <att_value att_id="a35" value="17"/>
        <att_value att_id="a36" value="o835" serial_no="0" value_object_name="GENBANK"/>
        <att_value att_id="a37" value="o848" serial_no="0" value_object_name="AXEL_R"/>
        <att_value att_id="a37" value="o855" serial_no="0" value_object_name="BUCK_L"/>
        <att_value att_id="a39" value="o1362" value_object_name="Full-Length"/>
        <att_value att_id="a82" value="o144593" serial_no="1" value_object_name="Heptanal"/>
        <att_value att_id="a82" value="o124" serial_no="2" value_object_name="Octanal"/>
        <att_value att_id="a40"
          value="ATGGAGCGAAGGAACCAAGTGGGAGAGTGAATTTGTGTCGGGTTTCCAGCTCCTGCCCACTGCGAGTACTACTATTTTCTTTCTCTTGGNCTATGTGTGGT
          <att_value att_id="a41"
            value="MERRNHSGRVSEFVLLGFPAPAPLVLVLLFLLXYVLVTENMLIIIAIRNHPILHKPMYFFLANMSFLEIWYVTVTFPHLAGFIGSKENHQLISFEACMTQLYFFLGLGCTE
          <att_value att_id="a42" value="o842" value_object_name="cDNA"/>
        <att_value att_id="a99" value="o143600" value_object_name="ORModel1"/>
        <att_value att_id="a214" value="10781022"/>
        <att_value att_id="a338" value="559"/>
      </object>
    </data_class>
  </data_database>
</data>

```

Fig. 6.

The figure illustrates the XML representation for ORL11 in ORDB (Fig. 1). A XML file is available for every entry in the olfactory databases in SenseLab. The file shows the object identifiers of the entries when stored as classes, the attribute identifiers of attributes, and the formats for each of the values, e.g., integer for chromosome number, text for common name, and large text or memo for nucleotide and amino acid sequences

Senselab
ORDB Olfactory Receptors Database

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Search Form

Version: 2.2 [EAVCR Search Help](#)

Searching: Chemosensory Receptors

SN	Del	Parameter	Show	Type	Condition
0		CR Type	☒	C	LookUp ORL (Olfactory Receptor Like)
1		Length	☐	C	LookUp Full-Length
2		Organism	☐	C	LookUp Mus musculus (mouse)
3		Chromosome	☒	I	LookUp 10
4		PubMed	☒	C	LookUp
5		Amino Acids	☒	M	LookUp
6		** New **			

Advanced >>
Analyze >>

Show results as: HTML [Search](#) [Clear Results](#)

[Use single-table search interface](#)

SN	CR Type	Chromosome	PubMed	Amino Acids
1	ORL (Olfactory Receptor Like)	10	11875048 11802173	MGDRETSNHSMDTDFILVGRVSPHELHILLFLLVYAMILLGNLGMMAIIMTDPRNLNTPMYFFLGNLSFIDLFSYSSVIAPKAMSNFWTESKISIFAGCVAQLFLFALFTV
2	ORL (Olfactory Receptor Like)	10	11875048 11802173	MGDRETSNHSMDTDFILVGRVSPHELHILLFLLVYAMILLGNLGMMAIIMTDPRNLNTPMYFFLGNLSFIDLFSYSSVIAPKAMSNFWTESKISIFAGCVAQLFLFALFTV
3	ORL (Olfactory Receptor Like)	10	11875048 11802173	MGDRETSNHSMDTDFILVGRVSPHELHILLFLLVYAMILLGNLGMMAIIMTDPRNLNTPMYFFLGNLSFIDLFSYSSVIAPKAMSNFWTESKISIFAGCVAQLFLFALFTV

Fig. 7.

Shows the multiple parameter search system for ORDB (and available for OdorDB and ORModelDB). The form in the top part of the figure allows searching for an entity for every attribute associated with the entity. Each attribute can be used as a filter to narrow and focus the search results. The ****New**** link allows the introduction of a new Search filter. The *red circle* with an *x* allows the user to remove a search filter. The *checkbox* under “show” allows the user to opt to display that attribute in the search results. If the value that can be used as filter is stored as a class, a *look-up* table allows the user to click the specific value. The *lower part* of the figure represents the results. The query asked for a list of olfactory receptors on chromosome 10 of mouse, and asked that the PubMed links for each receptor and the amino acid sequences be reported in the HTML format