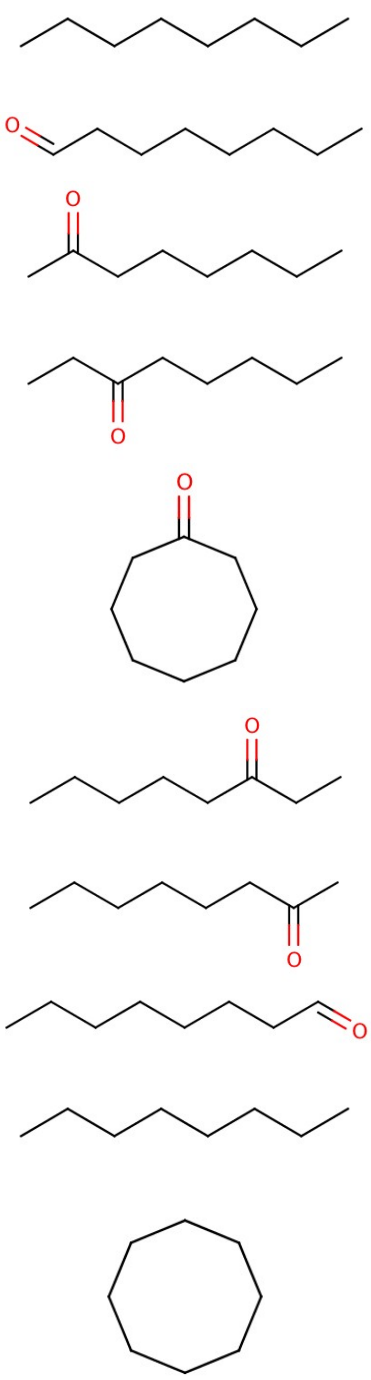
CHÂTEAUSHATTO

Supplementary Information for Cyclooctane/Octane Cycle and Aldehyde Grid Variable Program

CYCLOOCTANE/OCTANE CYCLE

Molecular Structure Format:



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IUPAC Format	SMILES Format
octane	CCCCCCCC
octanal	O=CCCCCCCC
2-octanone	CC(=O)CCCCCC
3-octanone	CCC(=O)CCCCC
cyclooctanone	C1CCC(=O)CCCC1
3-octanone	CCCCCC(=O)CC
2-octanone	CCCCCCC(=O)C
octanal	CCCCCCCC=O
octane	CCCCCCCC
cyclooctane	C1CCCCCCC1

Cyclooctane/Octane Cycle is a looping sequence that diffuses a different molecule every minute in an repeating cycle. Each molecule/step in the sequence has a distinct smell.
Cyclooctane/Octane Cycle functions as an intermediary loop during intervals when Aldehyde Grid Variable Program (see below) is not running. It is the equivalent of a screen saver or a "waiting" logo animation (e.g. the looping arrow moving in a circle commonly seen on screen when buffering media).

Each molecule in the Cyclooctane/Octane Cycle sequence has 8 carbon atoms (C). The sequence starts with the simplest possible 8 carbon molecule: n-octane (octane) which consists of 8 carbon atoms bonded to one another in a straight line. (Hydrogen atoms are also present but are not depicted in the SMILES format above.) A carbonyl group (C=O)—an oxygen atom that shares 2 covalent bonds with a carbon atom—changes position from the first carbon in the line through to the last carbon in the subsequent steps of the sequence. As this occurs, the resulting molecule changes classification from an alkane (octane) to an aldehyde (octanal) to a ketone (2-octanone, 3-octanone, and cyclooctanone).

As the carbonyl group reaches the center of the molecule (the 4^{th} carbon in the line), the linear carbon structure closes, forming a ring or loop. Since a ring structure with a single carbonyl group can be spatially rotated clockwise or counter clockwise, the carbonyl group no longer has a defined position within the carbon structure. It may appear at any carbon position within the structure, and the chemical/structural formula remains the same (cyclooctanone). This moment represents an internal, (material and procedural) loop within the overall looping sequence of Cyclooctane/Octane Cycle.

Following this loop, a moment of inversion occurs in the system: the loop reopens and as the carbonyl group continues to change position along the line of carbon atoms, the next steps in the sequence consist of the “mirror image” or backwards version of the previous molecules in the sequence, and in the reverse order. However, due to the spatial configuration of these molecules, the spatially reversed “mirror” versions are in fact the same as the previous molecules in the sequence, but in the reverse sequential order. (For example, an 8 carbon chain with a carbonyl group on the second carbon—i.e., 2-octanone—is the same compound as an 8 carbon chain with a carbonyl group on the seventh carbon, it has simply been rotated 180 degrees in its orientation and now appears backwards.)

With the carbonyl group having reached the end of the linear carbon structure, the carbon structure returns to it’s pre-carbonyl, alkane form (octane) in the next step of the sequence. At this point, the linear carbon structure once again closes into a loop—this time into its non-carbonyl, alkane form (cyclooctane). Having reached the end of the cyclooctane cycle, the looped carbon structure links to its open form at the beginning of the sequence and the cycle repeats.

The number of repetitions of the overall Cyclooctane/Octane Cycle in a given session is determined by an algorithm that mediates between Cyclooctane/Octane Cycle and Aldehyde Grid Variable Program. The algorithm switches between the two within a predetermined range of possibilities on a randomized basis. In certain rare instances with a low statistical probability, the outcome of Aldehyde Grid Variable Program will affect the master algorithm that governs switching between the two programs (See Program Logic, below).

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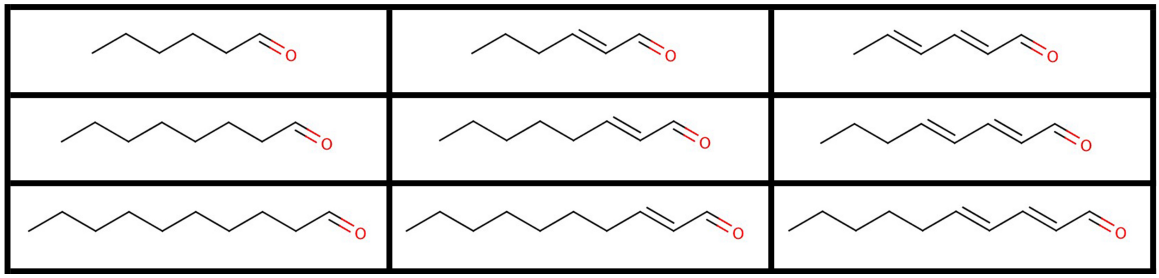
ALDEHYDE GRID VARIABLE PROGRAM

Molecular Structure Format



SMILES Format

	saturated	monounsaturated	polyunsaturated
6 carbon	CCCCCC=O	CCC/C=C/C=O	C/C=C/C=C/C=O
8 carbon	CCCCCCCC=O	CCCCC/C=C/C=O	CCC/C=C/C=C/C=O
10 carbon	CCCCCCCCCC=O	CCCCCCC/C=C/C=O	CCCCC/C=C/C=C/C=O

IUPAC Format

hexanal	trans-2-hexenal	trans-2, trans-4 hexadienal
octanal	trans-2-octenal	trans-2, trans-4 octadienal
decanal	trans-2-decenal	trans-2, trans-4 decadienal

Aldehyde Grid Variable Program consists of nine molecules that are diffused in sequential combinations through an randomized algorithmic governing logic (see Program Logic, below).

The nine molecules are structural analogs of one another with similar features, but a relatively large range of odor profiles. They can be synthetically derived, but also occur widely in numerous substances including: flowers, fruits and vegetables, grains and herbs, plants, fungi, plastics, artificial flavors, fried and cooked meats, dairy products, as byproducts of skin cell degradation and microbial processes, and as insect pheromones.

The nine molecules can be classified along two axes related to their structural features: 1) number of carbon atoms and 2) number of de-saturated bonds (i.e. double bonds between two carbon atoms). When grouped according to these features, the nine molecules can form a grid of three rows and three columns. The top row consists of molecules with 6 carbon atoms, the middle row has 8 carbon atoms, and the bottom row has 10. Similarly the left column contains compounds that are unsaturated, the middle column contains molecules with one unsaturated bond (monounsaturated) and the right row contains molecules with two unsaturated bonds (polyunsaturated).

The variable logic of the program has assigned different probabilities to the different features. The primary routine of the program selects two molecules to diffuse each cycle. The program employs two simultaneous selection algorithms, “selector A” and “selector B”. Each selection algorithm chooses one molecule/scent to be diffused, so that each two minute cycle consists of the molecule selected by A diffused simultaneously with the molecule selected by B. Each selector randomly[*] chooses a molecule from among the nine molecules and zero (blank), however, within this random assignment, an increasing probability is given to molecules with a higher carbon number by selector A, and an increasing probability is given to molecules with a greater number of unsaturated bonds by selector B (zero has the same probability as the molecules in the highest probability row or column).

The relative assigned probabilities for the compounds for the respective selectors are as follows:

[*] Technically the algorithm employs a “pseudo-random” selection of a method common to most computer programs.

[†] For example, the opposite of hexanal is trans, trans-2,4-decadienal. The opposite of trans-2-decenal is trans-2-hexenal,

Selector A

6	6	6
8	8	8
10	10	10

Selector B

6	8	10
6	8	10
6	8	10

Selector A and B Average

6	7	8
7	8	9
8	9	10

In addition to the core routine of the A and B selections, several additional rules have been written into the selection algorithm that produce additional events dependent upon the outcome of A and B's selections (see Program Logic below).

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PROGRAM LOGIC

Program Logic: Cyclooctane/Octane Cycle

Inclusion Statements/Limitations:

1. Only structures with 8 carbon atoms can be included
2. The 8 carbon atoms must be bonded to one another in a continuous and un-branched chain
3. The continuous chain may be open (normal) or closed (cyclic)
4. One oxygen atom may be included in the structure provided that it is bonded to a carbon atom with two covalent bonds (a carbonyl group)
5. The carbon structures must be fully saturated with hydrogen atoms (with the exception of an optional carbonyl group)

Functional Statements/Limitations:

1. Only a carbon structure in its open (normal) form can accept an oxygen atom (carbonyl group). A carbonyl group cannot leave a closed carbon structure.
2. A carbonyl group may only join onto a carbon structure from an end carbon. It may only leave a carbon structure from the opposite end from which it joined.
3. A carbonyl structure may only change positions on a carbon structure to an adjacent carbon between a sequence step.
4. A carbon structure may open or close between a sequence step.

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Program Logic: Aldehyde Grid Variable Program

Inclusion Statements/Limitations:

1. All structures must be linear aliphatic aldehydes
2. Structures may contain 6, 8 or 10 carbon atoms
3. Structures may contain 0,1, or 2 double bonds between carbon atoms
4. If a structure contains one double bond, it will be trans in its orientation and will occur between the 2nd and 3rd carbon
5. If a structure contains a second double bond, it will be trans in its orientation and will occur between the 4th and 5th carbon

Functional Statements/Limitations:

Core Routine:

1. For each cycle, two selection algorithms each select a single molecule to be diffused. The resulting two molecule selections are diffused simultaneously throughout the duration of the cycle.
2. The selections are randomized, but with an increasing probability for different molecular features. Selector A has a statistical preference for greater carbon numbers. Selector B has a statistical preference for greater number of unsaturated bonds. The relative probabilities assigned to Selector A are: carbon number 6 = 6; carbon number 8 = 8; carbon number 10 = 10; 0 = 10; The relative probabilities assigned to Selector B are: saturated = 6; monounsaturated = 8; polyunsaturated = 10.

Additional Rules:

1. Each molecule within the nine molecule grid has an opposite molecule that is the molecule that is in the cell on the opposite side of the grid, going through the center cell[†]. The opposite of the center cell is 0 or blank.

2. If A and B select the same molecule during a cycle then the next cycle will be blank[‡]. Following the blank cycle the molecule that A and B both selected will be repeated over top of the core routine selections of A and B for the next 3 cycles.

3. If a molecule is repeated in two consecutive cycles[§] the next cycle will consist of both selector A and selector B diffusing the opposite of the molecule that was repeated[**]. (Following this, the procedure in rule [2] will take place because both selectors have chosen the same molecule in a cycle.)

4. A memory function tracks the molecules that have been diffused in blocks of 10 cycles. At the end of 10 cycles, the molecule that was diffused the most often will have its opposite molecule diffused over the core routine selections of A and B for the following 1 cycle. In the case of a tie between any number of molecules, the opposites of all of those molecules will be diffused over the routine operations of A and B.

5. In the event that there is additional molecule(s) diffused over the top of the A and B core routine as a result of rule [2] or rule [3] *and* this additional molecule(s) matches both A and B during a cycle[††], the following cycle will diffuse all 9 molecules together. Following this, there will be a blank cycle. At this point, all prior memory of the program will be reset.

6. If in addition to a match event from rule [5], the memory function in rule [4] also selects a molecule identical to that of the rule [5] match during the same cycle, the following sequence will run: blank cycle; hexanal; trans-2-hexenal; trans-2, trans-4 hexadienal; octanal; trans-2-octenal; trans-2, trans-4 octandienal; decanal; trans-2-decenal; trans-2, trans-4 decadienal. After this sequence, the master switching algorithm will be pushed into Cyclooctane/Octane Cycle for a randomly selected amount of time. When Aldehyde Grid Variable Program returns, both A and B will select the molecule that initiated the rule [6] procedure.

[†] For example, the opposite of hexanal is trans, trans-2,4-decadienal. The opposite of trans-2-decenal is trans-2-hexenal, etc.

[‡] For this particular blank cycle (0, 0), A and B are not considered to be matching their selections.

[§] i.e. if it is present in two consecutive cycles, chosen by either selector

[**] 0 will be considered a molecule selection for this and all subsequent rules

[††] i.e. if A and B match during a cycle and an additional molecule that is diffused as a result of rule 2, 3, or 4 also matches A and B.

Rare Event Conflicts:

7. In the event of a sequential (rule [3]) match that also consists of a simultaneous (rule [2]) match in the second cycle of the match, both rule procedures will occur simultaneously mapped over the ongoing A and B core routine.

8. In the event of two sequential cycles that match—i.e. two identical sequential cycles in a row—both of the selected molecules will simultaneously initiate the rule [3] procedure in the following cycle.

9. In the event of multiple rules being implemented simultaneously, the selections and procedures of all rules will run, mapped over top of the core routine.