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Mosaic representations of odors in the input and output layers of the mouse olfactory bulb

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Diversity of glomerular, mitral and tufted cell odor responses in awake head-fixed mice

- **a.** Example minimum projection image of intrinsic optical imaging (IOI) signals on the dorsal aspect of the bulb in response to a panel of 60 stimuli across 4 repeats (Supplementary Table 1) in a head-fixed awake mouse; numbers indicate location of functionally best matched glomeruli across the left and right bulb hemispheres.
- **b.** Color maps showing correlation of the average odor-evoked response of each pixel in the field of view with respect to reference ROIs (1-4) chosen from (**a**). Note glomerular formations of contiguous high correlation values emerge in similar locations across the two bulb hemispheres.
- c. Odor response spectra (ORS, averaged across four repeats) for the functionally best matched glomerular pairs across the two hemibulbs for the 4 ROIs chosen in (a).
- **d.** Average resting fluorescence of an example field of view (FOV) in the external plexiform layer (EPL) (*left*), and example responses (*right*, dF/F images) to three odors (ethyl hexanoate, allyl butyrate and 2,3-diethylpyrazine) across 3 trials.
- e. Single trial responses of four example tufted cells to the odors in (a); shaded area marks duration of odor presentation (4s), black lines the average dF/F across three trials (*left*). Example odor response spectra (ORS, constructed using average dF/F values across three trials) of the four tufted cells from (*left*) across a set of 55 odors (*right*).
- **f.** Average resting fluorescence of an example field of view in the mitral cell layer (MCL) (*left*), and example responses (*right*, dF/F images) to three odors (ethyl valerate, ethyl butyrate and 1-propanethiol) across 3 trials.
- **g.** Single trial responses of four example mitral cells to the odors in (**f**); shaded area marks duration of odor presentation (4s), black lines the average dF/F across three trials (*left*). Example odor response spectra (ORS, constructed using average dF/F values across three trials) of the four mitral cells from (*left*) across a set of 55 odors (*right*).



Odor delivery calibration and functional clusters of mitral and tufted cell odor responses in awake head-fixed mice

- **a.** Normalized Photo-ionization device (PID) measuring the relative odor concentration corresponding to the 1:100 and 1:3,000 dilutions in mineral oil for five example odors (allyl butyrate, ethyl valerate, hexanal, ethyl tiglate and acetal). PID readings are normalized to 1:10 oil dilution for each of the five example odors.
- b. Example locations of fields of view for M/T cell imaging sessions on the dorsal aspect of the olfactory bulb in 3 example mice.
- **c.**, **d.** Odor response types obtained via hierarchical clustering and their relative distribution in the population of tufted cells, TC, (**c**) and mitral cells, MC (**d**) for two concentrations (corresponding to 1:3,000 and 1:100 nominal oil dilutions) across the same panel of 55 odors. Shaded area (light gray) marks duration of odor presentation (4s). Shaded area (dark gray) marks standard error across trials (TC 1:3,000 dilution: n=3,313 odor-cell pairs, TC 1:100 dilution: n=2,873 odor-cell pairs, MC 1:3,000 dilution: n=5,740 odor-cell pairs, TC 1:100 dilution: n=5,103 odor-cell pairs).



Mitral and tufted cell population responses across two oil dilution series in awake mice

- **a.** Distribution of tufted cell-odor response pairs sorted by response strength for the two set oil dilutions (1:3,000 and 1:100) across 55 odors.
- **b.** Scatter plots showing the odor induced change in fluorescence (dF/F) of two example tufted cells for the two dilutions used; each dot indicates the response of a cell to a given odor (cell-odor pair) for low versus high concentration of same odor; only cell-odor pairs that were detected as significant in at least one of the two conditions are shown; dotted line marks slope of 1.
- **c.** Distribution of mitral cell-odor response pairs sorted by response strength for the two oil dilutions (1:3,000 and 1:100) across 55 odors.
- **d.** Scatter plots showing the odor induced change in fluorescence for two example mitral cells or the two dilutions; each dot indicates the response of a cell to a given odor (cell-odor pair) for the low versus high concentration of the same odor; only cell-odor pairs that were detected as significant in at least one of the two conditions are shown; dotted line marks slope of 1.
- e. Summary scatter plots showing the odor induced change in tufted cells (*left*) and mitral cell (*right*) fluorescence for the two oil dilutions series; each dot indicates the average response of 100 cell-odor pairs for the low versus high oil dilution of same odor (1:3,000 versus 1:100), sorted by the low dilution; only cell-odor pairs that were detected as significant in at least one of the two conditions are included; red bars and blue bars mark standard error of the mean for each bin (TC n=2,708 odor-cell pairs, MC n=13,051 odor-cell pairs. We examined the responses of mitral vs. tufted cells to the same set of odors at two different concentrations (~20 fold change). We found that T cells are more sensitive to odors, on average, than M cells, confirming previous observations²⁸⁻²⁹. We also found that T cells tend to generally increase activity for higher concentration of odors, but M cells could be modulated bi-directionally. Our data indicate that, at the population level, mitral cells have much flatter response variation to concentrations, including some reduction in activity for higher concentrations. Such bi-directional, cell-specific dependence can arise from the known OB circuitry with extensive, distance-independent lateral inhibition. Despite these important differences in the responses properties of M and T cells to odors and concentrations, all conclusions about the representation of physical-chemical descriptors of odors and spatial layout are applicable to both populations.
- **f.** Summary histogram showing change in odor evoked mitral cells (black) and tufted cells (grey) responses in response to 1:100 compared to 1:3,000 oil dilutions for a 55 odor panel; the change for each cell odor response is quantified as the Euclidean distance from the diagonal unity line (interrupted line indicating slope of 1 in e), TC n=2,708 odor-cell pairs, MC n=13,051 odor-cell pairs.
- g. Cumulative distribution of mitral and tufted cell odor response pairs as a function of dF/F response amplitude. Continuous lines mark mitral cells, dotted lines tufted cells, black traces 1:3,000 dilution, red traces 1:100 dilution, TC n=2,708 odor-cell pairs, MC n=13,051 odor-cell pairs. Consistent with recent findings, on average, tufted cells were generally more sensitive to odors and more active with increasing concentrations, while mitral cells even showed reduced activity at higher concentrations consistent with increasing inhibition.
- h. Pairwise odor similarity (uncentered correlation coefficient) of corresponding mitral cell response spectra across the two oil dilution used; each dot corresponds to an odor-odor pair. Pairwise similarity of odors at the level of mitral cell responses was generally low (Avg. = 0.260±0.003 SEM for 1:3,000 dilution and 0.180±0.003 for 1:100 dilution, N=1,485 odor pairs, p<0.001, Sign Rank Test), and varied across the sampled dilutions (Supplementary Figure 3h,i).</p>
- i. Histogram of pairwise odor similarity (uncentered correlation coefficient) in terms of mitral cell response spectra across a set of 55 odors for 1:3,000 (black) and 1:100 (red) oil dilutions, (n=1485 pairs).



Glomerular and mitral/tufted cells tuning to the molecular properties

a.,c. Average correlation for all imaged glomeruli (**a**) and M/T cells (**c**) between the ORS of individual ROIs and the property strength vectors (PSV), for the odors in the panel, across the Dragon properties. For each property, PSV is defined as the corresponding normalized vector of values taken by the property across the monomolecular odors in the panel. Properties that took zero values for all odors in the panel were not included in the analysis (**a**) (1,320 properties over 871 glomeruli and over 1,711 M/T cells).

b.,d. Histogram of the number of ROIs (glomeruli – **b** and M/T cells - **d**) significantly tuned for a given physical-chemical property, across the set for all imaged fields of view.

e. Histograms of significant ROI-odor response to property correlations (two-sided t-test p<0.05, FDR q<0.1) for glomeruli (green, n=13,446) and M/T cells (blue, n=27,992).

f. Dimensionality (90% variance explained) of glomerular (green), mitral cells (blue) odor responses (across all sampled fields of view) and molecular properties strength vectors (PSV) as function of number of odorants included in the analysis. Shaded areas indicate +/- one standard deviation from a mean of 1,000 samples (different combination of odorants) for a given number of odorants included.

g. Dimensionality (90% variance explained) of glomerular (green), mitral cells (blue) odor responses (across all 49 monomolecular odorants) as function of number of regions of interests included. Shaded areas indicate +/- one standard deviation from a mean of 1,000 samples (different combination of ROIs) for a set number of ROIs included in the analysis.

h. Principal components exchange (PCX) analysis with varying amounts of noise added to glomerular responses. Percent variance explained of glomerular (green), mitral cells (blue) odor responses, molecular property strength vectors (black) shown as function of the number of experimentally observed glomerular responses (no added noise) principal components included in the analysis. Variance of the noise with respect to original signal is shown as signal-to-noise ratio (SNR) coded by the colorbar legend (*Right*).

i. Least absolute shrinkage and selection operator (LASSO) regression based on a subset of on varying the λ parameter (all physicalchemical properties used are included), describing the relationship between odor pairwise similarity across properties versus glomerular (*Left*) and respectively M/T cells (*Right*) responses; (*light green*) all imaged hemibulbs were used as a training set for optimizing the regression; (*dark green*) half of the fields of view were used for training and the remaining half for cross-validation (FOV cross-validation); (*pink*) all imaged hemibulbs were used for training, while one pair of odors was iteratively left out during training and added back subsequently for cross-validation (jackknife, odor cross-validation); (*red*) half of the fields of view were used for training and the remaining half for cross-validation; in addition, one pair of odors was iteratively left out during training and subsequently added back for cross-validation (jackknife, FOV and odor cross-validation).

j. Pairwise odor similarity expressed in terms of physical-chemical properties versus neuronal responses. Similarity is calculated as Euclidean distance in odor physical-chemical space and respectively Pearson's correlation between the odor response spectra (ORS) of cell pairs using a greedy algorithm (yellow line, Methods). Blue line marks FOV jackknife analysis: half of the fields of view were used for training and the remaining half for cross-validation; Red line marks odor pair jackknife analysis: one pair of odors was iteratively left out during training and subsequently added back for cross-validation; Black line marks odor similarity given jackknife analysis performed on both fields of view, as well as by iteratively leaving out one odor pair.



Relationship between Dragon physical-chemical properties and glomerular as well as M/T cell responses across different time scales in awake and anaesthetized mice

a.,b.,c. Results of principal component exchange (PCX) analysis for anaesthetized (**a**), awake (**b**) glomerular responses and molecular properties (**c**). Percent of variance explained is shown as a function of the number of included principal components, PCs. (**a**) Percent variance explained of anaesthetized (red), awake (green) glomerular odor responses, molecular property strength vectors (grey) and random data controls (black) shown as function of the number of anaesthetized glomerular responses principal components, awake glomerular responses principal components (**b**) and of molecular properties (PSV) principal components (**c**).

d.,e. Least absolute shrinkage and selection operator (LASSO) regression based on a subset of physical-chemical properties selected from the 1,666 set, describing the relationship between odor pairwise similarity across properties versus glomerular responses. Each trace shows the LASSO performance under various cross-validation conditions. (e) Predicting odor-odor response distance using shuffled molecular properties; the properties strength vector associated with each odorant is randomly swapped with the property strength vector of another molecule in the panel.

f.,g.,h. Percent variance explained of mitral cell odor responses across different time intervals from stimulus onset (0.5 s to 4.0 s, coded by strength of the shade of blue), molecular property strength vectors (grey) and random data controls (black) shown as function of the number of molecular properties principal components (**f**) and mitral cell responses (0.5 s vs. 4.0 s) principal components (**g**, **h**).

i., j., k. LASSO regression describing the relationship between odor pairwise similarity across properties versus mitral cell responses sampled across different time intervals: 0.5s (**i**), 1.0 s (**j**), 1.5 s (**k**). Each trace shows LASSO performance under various cross-validation conditions.



Supplementary Figure 6

Local similarity and diversity of mitral cell odor responses.

a. Average resting fluorescence multiphoton image in the mitral cell layer (n=112).

b. Numbers indicate the relative positions of 112 mitral cell bodies in the imaged field of view;

c. Example ORS (average dF/F across 3 trials) of mitral cell bodies within an arbitrarily picked 75µm diameter region circled in (a) sorted according to functional chemical groups (aldehydes, tiglates, ketones, furfuryls, alcohols, acids, ethyl esters, thiazoles); note that neighboring neurons (enclosed in circle from a, bottom) have diverse, as well as similar odor tuning (for example, cells 45 and 84 vs. cell 12). We probed the local diversity further, by rearranging the odor response spectra (ORS) such as to group odors in terms of chemical classes (ketones, acids, etc.). Mitral cells responding to many different classes of chemicals can be found even within a small region of glomerular size.

d. ORS (average dF/F across 3 trials) of mitral cells from three example clusters (orange, blue and red) from the FOV in (a), and from a different FOV (black) identified using functional clustering (average linkage) for 1:100 oil dilution (Left) and plotted correspondingly to maintain cell identity for the 1:3,000 oil dilution (Right). Numbers correspond to position of somata shown in (b). The spread of cells belonging to the three clusters is highlighted by the corresponding colored position indices shown in (b). One additional cluster from a different animal is exemplified in black.

e. Histogram of pairwise ORS correlations. Red and green traces correspond to putative sister pairs (defined at one dilution) from all, and respectively from those FOVs sampled at both dilutions; Pearson's correlations for each dilution are included; blue trace corresponds to correlations between putative sister cell pairs defined via functional clustering at one dilution, and sampled at the other dilution. ORS similarity between co-imaged, randomly picked pairs is shown in black. On average, we identified 4 ± 2 s.d. functional clusters per FOV, N=25, and each cluster contained 6 ± 3 s.d. putative sister cells. We asked whether the pairwise similarity and cell identity within these functional clusters varied across the two dilutions. First, keeping track of the cells' identity, we probed the similarity in odor tuning between cell pairs within a cluster (defined at one nominal dilution) at the other sampled dilution), but was significantly higher (p<0.001) than for randomly picked cell pairs (R2=0.08±0.01, N=992, 10,000 bootstrapped iterations). Further, if two cells were clustered together by their odor response at one dilution, they were more likely to be part of the same cluster at the other dilution compared to randomly assigned cells (N=6 FOVs sampled at both dilutions). For example, one FOV had 376 putative sister cell pairs in one concentration, and 255 sister cell pairs in the second concentration; 100 cell pairs were shared by both concentrations. After 250,000 iterations of randomly assigning sister cells, 0 had more than 100 shared pairs, with a mean bootstrap overlap of 15±7 shared pairs.

f. Average correlation comparisons between mitral/tufted cells in the same FOV (x axis) and cells randomly sampled cells across FOVs within the same animal (y axis). The red line marks unity slope. Error bars show one standard deviation from the mean for 1,000 random samples. Quantifying the relationship between odor tuning and spatial proximity for tufted and mitral cells indicated that odors triggered, on average, low pairwise correlations (uncentered correlation coefficient) in the odor tuning of mitral and tufted cells across the population (Avg. Similarity ~0.08 to ~0.14 across the two dilutions of a 55 odors panel for ~30,000 mitral and 12,000 tufted cell pairs). We observed only a weak relation between functional similarity and spatial location of MTCs (~15% for MCs, ~22% for TCs excess of more similar MC and TC pairs than expected by chance if MTC placement and odor tuning were independent ¹⁹).

Rotation model - shuffled glomerular responses



Supplementary Figure 7

Shuffling glomerular responses decreases the performance of the rotation model in matching experimentally observed mitral cell responses.

Model mitral cells responses were generated by taking samples from shuffled glomerular responses (for each glomerulus, the order of responses was shuffled). (*Left*) Percent variance explained of shuffled glomerular (green), mitral (blue) and simulated mitral (dashed blue line) cells responses shown as function of the number of included shuffled glomerular responses principal components. (*Right*) Percent variance explained of shuffled glomerular (blue) and simulated mitral (dashed blue line) responses shown as function of the number of included mitral (blue) and simulated mitral (dashed blue line) responses shown as function of the number of included mitral (blue) and simulated mitral (dashed blue line) responses shown as function of the number of included mitral cells response principal components. Note that response variance of mitral cells built by rotating shuffled glomerular responses (dashed blue line) deviates substantially from the experimentally observed mitral cell responses (solid blue).

Expected Jordan principal angles between random subspaces of the same dimensionality (embedded in same 50 dimensions)



b

Principal angles between a subspace and itself with varying amounts of noise added



Principal angles between overlapping subspaces with different variance along same PCs



Supplementary Figure 8

Calculating Jordan principal angles between different subspaces as a function of the number of principal components included

Jordan's principal angles between different subspaces (selected to maximize the percentage of variance explained) as function of the number of principal components included in the analysis. The principal angles between the subspaces of interest are calculated iteratively including more PCs of the respective subspaces. A 2D histogram is shown with each bin corresponding to the number of counts of specific angles (in radians) calculated for increasing number of included PCs.

a. Principal angles between a subspace and itself as function of the number of PCs included. To maintain contrast in the color scheme rendering the number of counts in the 2D histogram, the 0 bin angle entry in the 2D histogram was re-scaled accordingly.

b. Expected principal angles between two random subspaces of same dimensionality (embedded in same 50 dimensions) over 1,000 iterations as function of the number of PCs included.

c. Principal angles between the glomerular odor responses subspace and itself (plus added noise) are calculated for increasing amounts of added noise (decreasing SNR).

d. Principal angles between two spaces which have the same eigenvectors but different eigenvalues (different amounts of variance explained). Numerical error (expected in calculating Jordan's principal angles) results in a small, non-zero angle.

e. Principal component exchange (PCX) analysis identifies differences between overlapping subspaces which have different amounts of signal variance (different eigenvalues) distributed across different orthogonal dimensions (principal components), while overall spanning the same PCs.

Supplementary Table 1 Odors list

Glomerular odor panel

mineral oil Trans, trans-2,4-Decadienal Propyl tiglate Valeraldehyde (pentanal) 2.3-Pentanedione Ethyl caproate (Ethyl hexanoate) Allyl butyrate Ethyl valerate (Ethyl pentanoate) 2,3-Diethylpyrazine hexanal Ethyl heptanoate Heptaldehyde (heptanal) Allyl tiglate ethyl tiglate Isoamyl acetate Methyl tiglate ethyl3-mercaptopropionate 4-heptanone gamma terpinene Ethyl propionate Ethyl butyrate 1-pentanol acetophenone cyclohexyl acetate 4-isopropyl benzaldehyde propyl acetate 1-propanethiol cineole 2-hexanone isobutyl propionate Hexanoic acid 1,3-dimethoxybenzen valeric acid p-anisaldehyde fenchone (-) citral cis+trans pentyl acetate butyl formate

Glomerular (Suppl. Fig 1c)

mineral oil Trans, trans-2,4-Decadienal Propyl tiglate Valeraldehyde (pentanal) 2.3-Pentanedione Ethyl caproate (Ethyl hexanoate) Allyl butyrate Ethyl valerate (Ethyl pentanoate) 2,3-Diethylpyrazine hexanal Ethyl heptanoate Heptaldehyde (heptanal) Allyl tiglate empty vial (air) ethyl tiglate Isoamyl acetate Methyl tiglate ethyl3-mercaptopropionate 4-heptanone gamma terpinene Ethyl propionate empty vial (air) Ethyl butyrate 1-pentanol acetophenone cvclohexvl acetate 4-isopropyl benzaldehyde propyl acetate 1-propanethiol empty vial (air) cineole 2-hexanone isobutyl propionate Hexanoic acid 1,3-dimethoxybenzen valeric acid p-anisaldehyde fenchone (-)

Mitral/Tufted cells odor panel valeraldehvde 2,4 decadienal 2 3-Pentanedione Ethyl hexanoate Allyl butyrate Ethyl valerate 2,3-Diethylpyrazine hexanal heptanal Allyl tiglate ethyl tiglate Isoamyl acetate Methyl tiglate ethyl 3-mercapto propionate 4-heptanone gamma terpinene Ethyl propionate acetal Ethyl butyrate 1-pentanol acetophenone cyclohexyl acetate propyl acetate 1-propanethiol cineole 2-hexanone isobutyl propionate Hexanoic acid 1,3 dimethoxybenzene valeric acid p-anisaldehyde fenchone (-) citral cis+trans pentyl acetate butyl formate butyl propionate nutmeg oil coffee

Glomerular + Mitral/Tufted cells (common odors)

Trans, trans-2,4-Decadienal Valeraldehyde (pentanal) 2.3-Pentanedione Ethyl caproate (Ethyl hexanoate) Allyl butyrate Ethyl valerate (Ethyl pentanoate) 2,3-Diethylpyrazine hexanal Heptaldehyde (heptanal) Allyl tiglate ethyl tiglate Isoamyl acetate Methyl tiglate ethyl3-mercaptopropionate 4-heptanone gamma terpinene Ethyl propionate Ethyl butyrate 1-pentanol acetophenone cyclohexyl acetate propyl acetate 1-propanethiol cineole 2-hexanone isobutyl propionate Hexanoic acid 1,3-dimethoxybenzen valeric acid p-anisaldehyde fenchone (-) citral cis+trans pentyl acetate butyl formate butyl propionate 2.4.5-Trimethylthiazole 3-acetal 2,5-dimethyl furan 1,4 dimethoxybenzene (solid)

butyl propionate nutmeg oil coffee 2,4,5-Trimethylthiazole 3-acetal 2,5-dimethyl furan 1,4 dimethoxybenzene phenyl ethyl acetate ethyl acrylate carvyl acetate (-) ethyl 2-methylbutyrate pyridine Furfuryl hexanoate trans 2-hexenol Furfuryl butyrate 2,3-Dimethoxybenzaldehyde Furfuryl pentanoate 2-Isobutylthiazole Methyl 2-pyrrolyl ketone 2,4 dimethylphenol

citral cis+trans pentyl acetate butyl formate butyl propionate nutmeg oil coffee 2,4,5-Trimethylthiazole 3-acetal 2,5-dimethyl furan 1,4 dimethoxybenzene phenyl ethyl acetate ethyl acrylate carvyl acetate (-) ethyl 2-methylbutyrate pyridine Furfuryl hexanoate trans 2-hexenol Furfuryl butyrate 2,3-Dimethoxybenzaldehyde Furfuryl pentanoate 2-Isobutylthiazole Methyl 2-pyrrolyl ketone 2,4 dimethylphenol

2,4,5-Trimethylthiazole 3-acetal 2,5 dimethyl furan 1,4 dimethoxybenzene phenyl ethyl acetate carvyl acetate (-) ethyl 2-methylbutyrate pyridine Furfuryl hexanoate trans 2-hexenol Furfuryl butyrate 2,3-Dimethoxybenzaldehyde Furfuryl pentanoate 2-Isobutylthiazole Methyl 2-pyrrolyl ketone 2,4 dimethylphenol bicyclolactone cyclohexyl ethyl acetate

phenyl ethyl acetate carvyl acetate (-) pyridine Furfuryl hexanoate trans 2-hexenol Furfuryl butyrate 2,3-Dimethoxybenzaldehyde (solid) Furfuryl pentanoate 2-Isobutylthiazole Methyl 2-pyrrolyl ketone (solid) 2,4 dimethylphenol

Supplementary Table 2

Physical-chemical properties list correlated with the first principal component glomerular axis.

For the ensemble of glomerular ROIs monitored in each hemibulb, we computed the Pearson's correlation between each ROI's location along the first principal component axis and its response sensitivity to each property, (1,320 physical-chemical properties, taken over the panel of 49 monomolecular odorants used). Significance was determined by a two-sided t-test, p<0.05, FDR q<0.1.

| Property Abbreviation | Description | Average Correlation | Significant hemibulbe |
|-----------------------|---|---------------------|-----------------------|
| nCar | number of aromatic C(sp2) | -0.44159 | 12 |
| MATS3m | Moran autocorrelation of lag 3 weighted by mass | -0.41745 | 11 |
| MATS3e | Moran autocorrelation of lag 3 weighted by Sanderson electronegativity | -0.41277 | 11 |
| Мр | mean atomic polarizability (scaled on Carbon atom) | -0.39891 | 11 |
| ATS3p | Broto-Moreau autocorrelation of lag 3 (log function) weighted by polarizability | y -0.39197 | 9 |
| MATS3v | Moran autocorrelation of lag 3 weighted by van der Waals volume | -0.39095 | 9 |
| nF | number of Fluorine atoms | -0.38566 | 10 |
| R8e+ | R maximal autocorrelation of lag 8 / weighted by Sanderson electronegativity | / -0.38324 | 11 |
| nRCOOH | number of carboxylic acids (aliphatic) | -0.38324 | 11 |
| nOxolanes | number of Oxolanes | 0.44432 | 11 |
| ITH | total information content on the leverage equality | 0.4281 | 11 |
| R4p+ | R maximal autocorrelation of lag 4 / weighted by polarizability | 0.42499 | 11 |
| JGI9 nN | mean topological charge index of order 9 | 0.42448 | 11 |
| AECC | number of Nitrogen atoms | 0.4019 | 11 |
| Jhetv | average eccentricity | 0.39595 | 10 |
| H1m | Barysz matrix weighted by Van der Waals volume | 0.39538 | 11 |
| HATS5p | H autocorrelation of lag 1 / weighted by mass | 0.38752 | 11 |
| | leverage-weighted autocorrelation of lag 5 / weighted by polarizability | 0.38493 | 10 |