CLAIMS

1. A system for displaying properties of compounds, comprising:

(A) One or more selectable databases of information on a plurality of chemical compounds wherein the information in the one or more selectable databases alone or in combination comprises chemical, physical and structural information and biological information for each compound;

(B) A computational device to calculate for compounds selected from one or more of the selectable databases a relative location in a biological parameter space for each of the selected compounds based on biological information for the compound in the database;

(C) A computational device to calculate for compounds selected from one or more of the selectable databases a relative location in a chemical, physical and/or structural properties parameter space for each of the selected compounds based on chemical, physical and/or structural information for the compound in the database;

(D) A computational device to display the parameter spaces of (B) and (C) and to map the selected compounds therein;

(E) One or more computational modules for human-computer interaction effective for users to:

(a) select databases from which information is to be displayed;

(b) select compounds to display from each selected database;

(c) select biological, physical, chemical and/or structural parameter spaces in which compounds will be represented, including spaces based on combinations of the parameters;

(d) select methods for calculating the location and/or distance of compounds in the parameter spaces;

(e) adjust parameters of the parameter space, including scales;

(f) select and display additional information about compounds and

wherein the location of compounds in the biological parameter space is determined by one or more dissimilarity and/or similarity metrics.

2. A system according to claim 1, wherein biological assay measures are stretched between 0 and 1, where 0 denotes lack of response, and 1 denotes maximal

observable response, and the similarity between responses is constructed as a distance between these bound response vectors:

$$D_1 = \left(\sum_{i=1}^{n} \left(\log\left(\frac{1}{1-p_i}\right) + \log(p_i) - \log\left(\frac{1}{1-q_i}\right) - \log(q_i) \right)^2 \right)^{\frac{1}{2}}$$

where p and q are the vectors describing the compounds.

3. A system according to claim 1, wherein the similarity between the compounds is computed using AB-divergence formulated as:

$$D_{AB}^{(\alpha,\beta)} = -\frac{1}{\alpha\beta} \sum_{i=1}^{n} \left(p_i^{\alpha} q_i^{\beta} - \frac{\alpha}{\alpha+\beta} p_i^{\alpha+\beta} - \frac{\beta}{\alpha+\beta} q_i^{\alpha+\beta} \right)$$

where α and β are the parameters of the divergence.

4. A system according to claim 1, wherein the similarity between the compounds is computed using AB-divergence formulated as:

$$D_{AB}^{(\alpha,\beta)} = \sum_{i=1}^{n} d_{AB}^{(\alpha,\beta)}(p_i, q_i)$$

where

$$d_{AB}^{(\alpha,\beta)}(p_i, q_i) = \begin{cases} -\frac{1}{\alpha\beta}\left(p_i^{\alpha} q_i^{\beta} - \frac{\alpha}{(\alpha+\beta)} p_i^{\alpha+\beta} - \frac{\beta}{(\alpha+\beta)} q_i^{\alpha+\beta} \right) & \text{for } \alpha, \beta, \alpha+\beta \neq 0 \\ \frac{1}{\alpha^2}\left(p_i^{\alpha} \ln\frac{p_i^{\alpha}}{q_i^{\alpha}} - p_i^{\alpha} + q_i^{\alpha} \right) & \text{for } \alpha \neq 0, \beta = 0 \\ \frac{1}{\alpha^2}\left(\ln\frac{q_i^{\alpha}}{p_i^{\alpha}} + \left(\frac{q_i^{\alpha}}{p_i^{\alpha}}\right)^{-1} - 1 \right) & \text{for } \alpha = -\beta \neq 0 \\ \frac{1}{\beta^2}\left(q_i^{\beta} \ln\frac{q_i^{\beta}}{p_i^{\beta}} - q_i^{\beta} + p_i^{\beta} \right) & \text{for } \alpha = 0, \beta \neq 0 \\ \frac{1}{2}(\ln p_i - \ln q_i)^2 & \text{for } \alpha, \beta = 0. \end{cases}$$

where p and q are the vectors describing the compounds.

5. A system for enhancing human-computer interaction, comprising:

(A) One or more selectable databases of information on a plurality of chemical compounds wherein the information in the one or more selectable databases alone or in combination comprises chemical, physical and structural information and biological information for each compound;

(B) A computational device to calculate for compounds selected from one or more of the selectable databases a relative location in a biological parameter space for each of the selected compounds based on biological information for the compound in the database;

(C) A computational device to calculate for compounds selected from one or more of the selectable databases a relative location in a chemical, physical and/or structural properties parameter space for each of the selected compounds based on chemical, physical and/or structural information for the compound in the database;

(D) A computational device to display the parameter spaces of (B) and (C) and to map the selected compounds therein;

(E) One or more computational modules for human- computer interaction effective for users to:

(a) select databases from which information is to be displayed;

(b) select compounds to display from each selected database;

(c) select biological, physical, chemical and/or structural parameter spaces in which compounds will be represented, including spaces based on combinations of the parameters;

(d) select methods for calculating the location and/or distance of compounds in the parameter spaces;

(e) adjust parameters of the parameter space, including scales;

(f) select and display additional information about compounds and

wherein the location of compounds in the biological parameter space is determined by one or more dissimilarity and/or a similarity metrics.

6. A system according to claim 5, wherein biological assay measures are stretched between 0 and 1, where 0 denotes lack of response, and 1 denotes maximal observable response, and the similarity between responses is constructed as a distance between these bound response vectors:

$$D_1 = \left(\sum_{i=1}^{n} \left(\log\left(\frac{1}{1-p_i}\right) + \log(p_i) - \log\left(\frac{1}{1-q_i}\right) - \log(q_i) \right)^2 \right)^{\frac{1}{2}}$$

where p and q are the vectors describing the compounds.

7. A system according to claim 5, wherein the similarity between the compounds is computed using AB-divergence formulated as:

$$D_{AB}^{(\alpha,\beta)} = -\frac{1}{\alpha\beta}\sum_{i=1}^{n}\left(p_i^{\alpha}q_i^{\beta} - \frac{\alpha}{\alpha+\beta}p_i^{\alpha+\beta} - \frac{\beta}{\alpha+\beta}q_i^{\alpha+\beta}\right)$$

where α and β are the parameters of the divergence.

8. A system according to claim 5, wherein the similarity between the compounds is computed using AB-divergence formulated alternatively as:

$$D_{AB}^{(\alpha,\beta)} = \sum_{i=1}^{n} d_{AB}^{(\alpha,\beta)}(p_i, q_i)$$

where

$$d_{AB}^{(\alpha,\beta)}(p_i, q_i) = \begin{cases} -\frac{1}{\alpha\beta}\left(p_i^{\alpha}q_i^{\beta} - \frac{\alpha}{(\alpha+\beta)}p_i^{\alpha+\beta} - \frac{\beta}{(\alpha+\beta)}q_i^{\alpha+\beta}\right) & \text{for } \alpha,\beta,\alpha+\beta \neq 0 \\ \frac{1}{\alpha^2}\left(p_i^{\alpha}\ln\frac{p_i^{\alpha}}{q_i^{\alpha}} - p_i^{\alpha} + q_i^{\alpha}\right) & \text{for } \alpha \neq 0, \beta = 0 \\ \frac{1}{\alpha^2}\left(\ln\frac{q_i^{\alpha}}{p_i^{\alpha}} + \left(\frac{q_i^{\alpha}}{p_i^{\alpha}}\right)^{-1} - 1\right) & \text{for } \alpha = -\beta \neq 0 \\ \frac{1}{\beta^2}\left(q_i^{\beta}\ln\frac{q_i^{\beta}}{p_i^{\beta}} - q_i^{\beta} + p_i^{\beta}\right) & \text{for } \alpha = 0, \beta \neq 0 \\ \frac{1}{2}(\ln p_i - \ln q_i)^2 & \text{for } \alpha,\beta = 0. \end{cases}$$

and where p and q are the vectors describing the compounds.

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9. A system according to any one of claims 1 to 2 and 5 to 8, wherein the visualization and spatial grouping, arrangement or clustering of chemical structures is based on differences and/or similarities in one or more structural or biological features.

10. A system according to any one of claims 1 to 2 and 5 to 8, wherein, one or more physical chemical properties for each chemical compound is combined with one or more biological parameters that are derived from each compound that describe the effect of each compound on intracellular, extracellular or biological proteins, processes or pathways within a cell.

11. A system according to any one of claims 1 to 2 and 5 to 8, wherein one or more chemical substructures is combined with one or more biological parameters that are derived from the effect of a chemical containing those substructures, on intracellular, extracellular or biological proteins, processes or pathways within one or more cells is displayed.

12. A system according to any one of claims 1 to 2 and 5 to 8, wherein the system visualizes and/or displays one or more biological parameters for a compound that are derived from the effect of the chemical containing those substructures on intracellular, extracellular, or biological proteins, processes or pathways within one or more cells.

13. A system according to any one of claims 1 to 2 and 5 to 8, wherein the system visualizes and/or displays one or more acute cellular stress parameters that combine mitochondrial effects with cellular stress effects.

14. A system according to any one of claims 1 to 2 and 5 to 8, wherein the system visualizes and/or displays one or more parameters that are associated with inflammation pathways.

15. A system according to any one of claims 1 to 2 and 5 to 8, wherein the system visualizes and/or displays one or more parameters that are associated with any one or more of DNA Damage Repair, epigenetic regulation, cell cycle and/or GPCR binding and downstream signaling within cells.

16. A system according to any one of claims 1 to 2 and 5 to 8, wherein the system visualizes and/or displays one or more parameters measured in zebrafish.

17. A system according any one of claims 1 to 2 and 5 to 8, wherein the system visualizes and/or displays one or more parameters that define changes to the morphology of a cell, either direct measurements or calculated measurements that define changes to internal cellular complexity, function, or shape.

18. A system according to any one of claims 1 to 2 and 5 to 8, wherein the system visualizes and/or displays one or more parameters that are collectively termed "cell painting".

19. A system according any one of claims 1 to 2 and 5 to 8, wherein the system visualizes and/or displays biological parameters combined with physical-chemical properties and/or chemical structures.

20. A system according to any one of claims 1 to 2 and 5 to 8, wherein the system visually highlights the spatial position of a new, unknown compound within a "universe" of other compounds visualized based on the same chemical and/or biological features, wherein the visualization groups compounds according to a distance function based on calculated similarity and/or difference "distances" between compounds based on the relationship between properties associated with the chemical structure and the effect of that chemical structure on one or more biological processes, pathways or proteins.

21. A system according to any one of claims 1 to 2 and 5 to 8, comprising a virtual reality (VR) display wherein information is displayed and can be manipulated in a virtual reality environment.

22. A system according to claim 21, wherein the VR display comprises one or more of a standalone VR headset, a PC-connected VR headset, a gaming console VR headset, a mixed-reality headset, an enhanced reality headset, a mobile VR headset, a motion controller, a motion platform, a haptic feedback device.

23. A system according to claim 22, wherein the haptic feedback device is any one or more of the following that provide tactile feedback to users: haptic feedback gloves, haptic feedback suits, and haptic feedback vests.

24. A system according to any one or more of claims 21 to 23, wherein compounds are represented as distinct locations in a multiparametric parameter space defined by physical, chemical or biological parameters or combinations thereof, wherein individual compounds can be selected, captured, moved and separated from other

compounds, and as desired to outside the parameter space, using physical human motion encoded capturing tools provided by and within the VR subsystem of hardware and software.

25. A system according to any one or more of claims 21 to 23 wherein one or more pluralities of compounds within a parameter space can be selected and then manipulated without affecting other compounds in the parameter space.

26. A system according to claim 21, wherein such pluralities can be rotated, enlarged, made smaller and otherwise visually manipulated using physical human motion encoded capturing tools provided by and within the VR hardware and software.

27. A display and/or system according to any one or more of claims 1 to 2 and 5 to 8, wherein physical, chemical and biological characteristic for a selected compound can be displayed in the multiparameter space using tools provided by and within the VR hardware and software.