inorganics

MDPI

Review

Prediction of Sensor Ability Based on Chemical Formula: Possible Approaches and Pitfalls

Daniil N. Yarullin [1], Maksim N. Zavalishin [1], George A. Gamov [1,*], Michail M. Lukanov [2], Alexander A. Ksenofontov [2], Natalia A. Bumagina [2] and Elena V. Antina [2]

[1] Department of General Chemical Technology, Ivanovo State University of Chemistry and Technology, Sheremetevskii pr. 7, Ivanovo 153000, Russia; yarullin_dn@isuct.ru (D.N.Y.); zavalishin00@gmail.com (M.N.Z.)

[2] G.A. Krestov Institute of Solution Chemistry, Russian Academy of Sciences, Akademicheskaya str. 1, Ivanovo 153045, Russia; lukanov-9b@mail.ru (M.M.L.); ivalex.09@mail.ru (A.A.K.); nad@isc-ras.ru (N.A.B.); eva@isc-ras.ru (E.V.A.)

* Correspondence: ggamov@isuct.ru; Tel.: +7-(915)-821-85-62

Abstract: This review presents an analysis of different algorithms for predicting the sensory ability of organic compounds towards metal ions based on their chemical formula. A database of chemosensors containing information on various classes of suitable compounds, including dipyrromethenes, BODIPY, Schiff bases, hydrazones, fluorescein, rhodamine, phenanthroline, coumarin, naphthalimide derivatives, and others (a total of 965 molecules) has been compiled. Additionally, a freely available software has been developed for predicting the sensing ability of chemical compounds, which can be accessed through a Telegram bot. This tool aims to assist researchers in their search for new chemosensors.

Keywords: sensor; fluorescence; chemoinformatics; Levenshtein; Tanimoto; Euclidean distance; tokenization; vectorization; molecular descriptors

check for updates

Citation: Yarullin, D.N.; Zavalishin, M.N.; Gamov, G.A.; Lukanov, M.M.; Ksenofontov, A.A.; Bumagina, N.A.; Antina, E.V. Prediction of Sensor Ability Based on Chemical Formula: Possible Approaches and Pitfalls. *Inorganics* **2023**, *11*, 158. https://doi.org/10.3390/inorganics11040158

Academic Editor: Duncan H. Gregory

Received: 10 March 2023
Revised: 30 March 2023
Accepted: 31 March 2023
Published: 6 April 2023

1. Introduction

The rapid development of industries including those that require high-purity substances and the progress in medicine related to bioimaging techniques and theranostics depend strongly on the synthesis of novel efficient sensors for cations, anions, biomolecules, microparticles, etc. The interaction between an indicator molecule and the target analyte causes a change in solution color or fluorescence, which is increasingly preferred due to the widespread use of fluorescent spectrometers and microscopes in the laboratory. Luminescence-based detection is preferred over other methods due to its higher sensitivity compared to UV–Vis spectroscopy and the need for less of the sensor compound, as well as its suitability for bioimaging. A few examples of application of fluorescent sensors of different natures for a vast diversity of objects can be found in the most recent reviews [1–8].

Of all the analytes, metal ions, particularly heavy ones, are of particular importance due to their dual role. On the one hand, they are distributed pollutants of air, water, and soil causing severe acute or chronic intoxication. On the other hand, many enzymes that are crucial for maintaining the vital functions of microorganisms, plants, fungi, and mammals depend on such ions as Fe^{2+}, Fe^{3+}, Cu^{2+}, Zn^{2+}, Ni^{2+}, and others. It is important to monitor the concentration of these cations in living tissues in real time; moreover, they provide the possibility to visualize the cells using a specific fluorescent indicator if its luminescence intensity is enhanced or quenched due to interaction with metals. It is no wonder that interest in the development of fluorescent sensors draws the attention of researchers more and more (Figure 1).

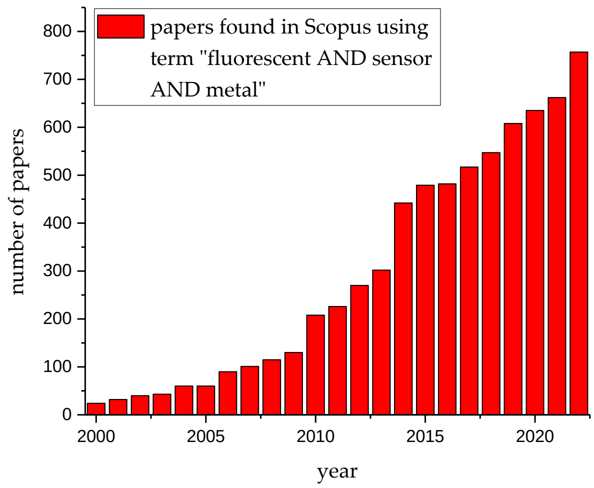

Figure 1. Quantity of papers devoted to fluorescent sensors of metals published per annum. Papers found in Scopus using the search term 'fluorescent AND sensor AND metal'.

One of the key advantages of fluorescent metal detection is its high sensitivity, which allows for the detection of metal ions at low concentrations. This is particularly useful in the fields of environmental monitoring, medical diagnostics, and food safety, where trace amounts of metal ions can have significant impacts. Additionally, fluorescent metal detection often allows for real-time monitoring of metal ions, which is valuable for process control and quality assurance in various industries. The use of fluorescent sensors also offers the advantage of selectivity, as the fluorescence response is specific to a particular metal ion. This allows for the differentiation between different metal ions, even in a complex sample. Another important aspect of fluorescent metal detection is its compatibility with modern imaging technologies, such as microscopy and spectroscopy. This makes it possible to visualize the distribution of metal ions in a sample, providing valuable information for various applications, including bioimaging and material science. Overall, the sensitivity, selectivity, and compatibility with imaging technologies make fluorescent metal detection an important tool for a variety of applications.

However, despite progress and innovative papers introducing new classes of chemical compounds for detecting and quantifying various metals, the development of each new sensor still often seems to result from trial and error rather than a solid theoretical foundation. Despite a thorough understanding of fluorescence mechanisms [9–11], knowledge of Lewis hardness and softness of functional groups, and the ability to identify ESIPT (Excited-State Intramolecular Proton-Transfer) active compounds [12], researchers still face challenges in predicting the metal ions that can be indicated by newly synthesized substances. The optimal choice of solvent for sensory response is also a significant problem. In this regard, the creation of some tools allowing the prediction of different chemical compounds' ability to detect various metal is of interest. Development of such tools requires necessarily taking into account the accumulated literature data.

The aim of this contribution is to discuss the possible approaches to predict the metal sensing ability of chemical compounds utilizing results obtained by other researchers and analyzing potential obstacles. A prototype software for the prediction of sensing ability has been developed.

We focus on metal ions due to an additional reason. While many sensors of anions are described in the literature, authors might not be accurate enough with their claims. As we have shown previously [13,14], some compounds that change the solution color and/or fluorescence spectrum in the presence of an anion can do so because of acid-base equilibria involving an indicator and an anion, rather than a specific complex formation. In that case, the anion sensor is, in fact, a pH indicator lacking the necessary selectivity towards the anion (as all anions of the same base strength would produce the same analytical response).

2. Results and Discussion

The basic idea is simple: the user inputs the formulas of the compounds of interest in a machine-readable form. The software searches for the most similar formulas in a database and returns them to the user, along with the cations that can be detected using these compounds, the solvent used for this purpose, and a numerical value characterizing the similarity between the user's input and the closest matches in the database. These values can be vaguely interpreted as a probability of prediction success. Therefore, the main question is which method is the most suitable for searching for the similarities. The probable options are discussed below.

All these methods handle the Simplified Molecular-Input Line-Entry system (SMILES), which is a computer-recognizable 'chemical language' that allows for presenting 2D chemical formulas in a compact form [15]. SMILES is widely used for the retrieval of continuous databases and the building of prediction models [16]. SMILES supports all elements in the periodic table, denoting an atom with the respective atomic symbol in square brackets (they are usually omitted). To show non-aromatic atoms, uppercase letters are used; lowercase letters refer to aromatic atoms. If atomic notation has two symbols, the latter is always lowercase. Single, double, triple, and quadruple bonds are denoted by symbols '-', '=', '#', and '$', respectively, while the symbol '.' shows disconnected structures (e.g., ionized salts such as [Na^+].[Cl^-]). A branch from a chain is specified by placing the SMILES symbol(s) for the branch between parentheses. The string in parentheses is placed directly after the symbol for the atom to which it is connected. If it is connected by a double or triple bond, the bond symbol immediately follows the left parenthesis. To identify the ring structure, the opening and closing ring atoms are numbered. Being a string representation of a chemical formula as a molecular graph and obeying relatively simple rules, SMILES became very popular among researchers for the purposes of computer chemistry. However, SMILES is not the only way of converting structural chemical information into text variables. The International Chemical Identifier (InChI) also allows for encoding information about chemical structure in a textual form suitable for use in databases. The International Chemical Identifier Key (InChIKey) is a condensed, 27-character-long form of InChI that contains no information about molecular structure and only makes sense when linked to the 'parent' InChI. However, it is convenient to use for searching the duplicated entries. Nevertheless, SMILES is arguably the most distributed and commonly used language.

2.1. Levenshtein Distance and Levenshtein Ratio

Since the SMILES entries in both the database and user input are just the symbolic sequences read by a computer as string variables, it is tempting to find the similarities between them using metrics such as Levenshtein distance (*LD*) and Levenshtein ratio (*LR*) [17]. *LD* (also known as edit distance) is the minimum number of single-character edits (insertions, deletions, or substitutions) required to transform one word into the other. For any two strings a and b of corresponding length of $len(a)$ and $len(b)$, *LR* is linked to *LD* by the following equation:

$$LR = \frac{len(a) + len(b) - LD}{len(a) + len(b)} \quad (1)$$

It should be kept in mind while calculating the *LD* value that the cost of insertion and deletion is 1, while the replacement operation is considered to contribute 2 to *LD* (as it can be seen as a pair of connected edits: deletion of a symbol and insertion of a new one).

When comparing the user input with all entries from the database, a series of *LR* values can be obtained. The lines from the database with the highest *LR* values are returned to the user as a result, providing information about cations detected with the help of compounds that are most similar to those input.

This method is advantageous as it is relatively simple, has minimal user arbitrariness (as it has no tunable variables that may influence the outcome), requires no preliminary processing of the SMILES, and consumes minimal computing time.

2.2. Tokenization and Vectorization

The tokenization process involves converting a sequence of symbols into a set of tokens, which are shorter symbolic sequences with assigned meanings. SMILES strings do not contain spaces such as in natural languages, so they must be segmented using specific rules. However, choosing the token size can be problematic since different split character lengths can produce slightly different results, as demonstrated by J. Shao et al. [18]. Additionally, if the splitting interval is too short, the set of unique tokens may be limited, while if it is too long, the SMILES may not produce enough tokens. However, single-character tokenization has been successfully used to predict chemical reaction outcomes [19,20].

Accounting of special symbols such as '(', '[', etc., is another problem as completeness of their deletion or substitution (as performed by authors in [18]) is also at the researcher's discretion. Finally, it is noteworthy that two-character notated chemical elements (such as Si or Cl) should also be replaced with unique single-character signs to avoid splitting.

Another way to perform vectorization is by using n-grams for symbol sequences in SMILES of molecules. This method was used in our algorithm, where the n-gram size was equal to five. We believe that this is a more valid form of representing SMILES because several variations of character sequences can be taken into account, and there is no need to separate characters from each other with a space or any other character.

Vectorization (or word embedding) follows tokenization. Each SMILES entry in the database and user input is represented as a vector of length equal to the number of identified tokens. If the i^{th} token occurs in a given SMILES K times, the i^{th} value of the corresponding vector is equal to K.

Another way to perform vectorization is through a term frequency—inversed document frequency (TF-IDF) procedure, which considers the importance of each token across the total list of SMILES in a simple manner. The more frequent a word, the less weight it has. TF-IDF stands for a product of two parts: term frequency (TF), which estimates the value of a token within the frame of a single entry, defined as the relative frequency of token t within the given SMILES entry d:

$$TF = \frac{f_{t,d}}{\sum_{t' \in d} f_{t',d}} \tag{2}$$

where $f_{t,d}$ is the number of times a token t appears in a given SMILES entry d.

The inversed document frequency (IDF) measuring the quantity of information provided by a token is calculated as follows:

$$IDF = \log \frac{N}{|\{d \in D : t \in d\}|} \tag{3}$$

where N is the total number of SMILES in corpus consisting of the database and user input, and $|\{d \in D\colon t \in d\}|$ is the number of documents where the token t t appears (considering TF $\neq 0$).

Finally, the TF-IDF metric is the product of the TF and IDF terms. It can be calculated for each token, and the TD-IDF value for the i^{th} token is placed in the i^{th} position of each SMILES vector.

There are different ways to define both TF and IDF, which affect the resulting TF-IDF value. It should be kept in mind, for example, while working with different libraries or programming languages, as they may apply different expressions for computing TF-IDF metrics.

Nonetheless, as a result of tokenization and vectorization, the SMILES from database and user input are transformed into a set of vectors consisting of TF-IDF values $\{a_i | a_i \epsilon [0, 1],\ i = 1, 2, \ldots, N+1\}$, where N is the database size. Vectors representing user input can be compared with each vector of the database using cosine similarity. This measure of similarity between two numeric sequences can be calculated as follows:

$$\cos\theta = \frac{A \cdot B}{\|A\|\|B\|} = \frac{\sum_{i=1}^{M} A_i B_i}{\sqrt{\sum_{i=1}^{M} A_i^2}\sqrt{\sum_{i=1}^{M} B_i^2}} \tag{4}$$

where $A{\cdot}B$ is the scalar product of two vectors, A and B, $||A||\ ||B||$ is the product of their magnitudes, and A_i and B_i are the i^{th} value of vectors.

2.3. Fingerprint Similarity Methods

In the methods described above, tools for natural language processing are used. However, there are many other ways to process SMILES of molecules, such as representing them as fingerprints. We used a standard fingerprinting algorithm (rdkit.org, accessed on 29 March 2023) that is similar to that used in the Daylight fingerprinter: it identifies and hashes topological paths (e.g., along bonds) in the molecule and then uses them to set bits of user-specified lengths (2048 bits) in a fingerprint. After that, one can use different similarity metrics, including Tanimoto similarity (T), Euclidean distance, and others.

Tanimoto similarity takes into consideration the intersection c of fingerprints a and b and their united power following the expression:

$$T = \frac{N_c}{N_a + N_b - N_c} \tag{5}$$

where N_a and N_b are the quantities of elements in the sets a and b, and N_c is the quantity of elements in the intersection of a and b sets.

The Euclidean distance (ED) between vectors is yet another applicable measure of similarity between two sets. It is calculated following the expression:

$$ED = \sqrt{N_a + N_b - 2N_c} \tag{6}$$

where N_a, N_b, and N_c have the same notation as in the case of the Tanimoto similarity coefficient (Equation (5)). It should be noted that the formulas mentioned above are valid for binary (dichotomous) variables.

Several other measures can be also applied to define the degree of similarity between the two string variables, a and b, including, e.g., the Sørensen–Dice coefficient s (Equation (7)), the overlap coefficient oc (Equation (8)), etc.:

$$s = \frac{2n_t}{n_a + n_b} \tag{7}$$

where n_t is the number of character bigrams (sequences of two adjacent elements) bound in both strings a and b, n_a is the number of bigrams in string a, and n_b is the number of bigrams in string b.

$$oc(a,b) = \frac{|a \cap b|}{\min(|a|, |b|)} \tag{8}$$

The overlap coefficient is defined as the size of the intersection divided by the smaller size of the two sets, a and b. If a is a subset of set b or vice versa, the overlap coefficient is equal to 1.

2.4. Pitfalls of the Methods of Finding Similarities between SMILES

First, we would like to distinguish between two types of unfavorable outcomes: (1) failure to reproduce the results of a search for similarities; and (2) failure to predict the sensor ability of the user’s compound (software returns incorrect cations).

The main obstacle to reproducibility is an abundance of tunable parameters. The outcome of tokenization depends on the token size and the processing of special symbols. The type of procedure used (simple, TF-IDF, or machine-learning-based) affects the outcome of vectorization. If the TF-IDF protocol is used, the choice of equations used to calculate term frequency and inverse document frequency matters. If any neural network is implemented, the training parameters are also crucial.

Changing any of these variables, including the expressions used to define TF and IDF, the character split length, or the dictionary of special symbols processed, could potentially alter the predicted cation sensing ability. The approach based on finding Levenshtein ratios seems optimal because it does not require additional procedures for data processing (such as tokenization or vectorization) and does not depend on tunable variables.

In addition, it should be noted that training a neural network model, even after fivefold cross-validation, still carries the risk that predictions may only work well for the united training and validation datasets.

This brings us to the fact that the overall success of predictions, regardless of the approach used, depends primarily on the content quality of the database used. The main sources of erroneous prediction outcomes caused by database-related reasons can be divided into three subgroups:

- Incomplete database: if the database contains no entries about sensors for specific cations or a specific class of chemical compounds considered promising for fluorescent sensing of metal ions, no method can return reliable predictions with high similarity metrics;
- Erroneous entries in the database due to mistakes made by individuals filling the database (e.g., typos in SMILES or misplacement/swapping of cations from different lines);
- Erroneous entries in the database due to mistakes/fraud committed by researchers whose papers served as a source. For example, there may be false claims about the indicator ability of certain compounds towards specific cations or typos in chemical formulas of sensor compounds, etc.

The first two types of errors can be avoided by broadening the dataset and paying special attention while filling up the database. Unfortunately, recognizing the third type is much harder (although not impossible).

2.5. Program for Prediction of the Sensing Ability of Organic Compounds towards Cations

Considering all of the above, we have developed software for predicting the fluorescent sensing ability of organic compounds towards metal ions. It utilizes the methods described above, including an approach based on the calculation of the Tanimoto coefficient, Levenshtein ratio, Euclidean distance, as well as vectorization by means of a TF-IDF matrix and cosine similarity method. The user needs to convert the structures of interest into SMILES form and select one of the methods for searching for similar structures in the database. The output results contain the 10 closest matches for each user input compound and cation—for which these compounds are sensors—the similarity parameter (either Tanimoto coefficient, Levenshtein ratio, Euclidean distance, or cosine similarity value, which characterizes the closeness between the user input structure and the most similar entries from the database), and a number of entries from the database. The latter allows for finding more specific information such as the solvent used and reference to the source of information provided as a digital object identifier (DOI). If some of the user structures are identical to those in the database, any method returns the identical entries from the database with all information mentioned above. In this case, the Tanimoto coefficient, Levenshtein ratio, or cosine similarity value is equal to 1, while the Euclidean distance has a 0 value.

In addition, for the convenience of users, we have created a Telegram bot that helps to collect results with one click [21] (Figure 2).

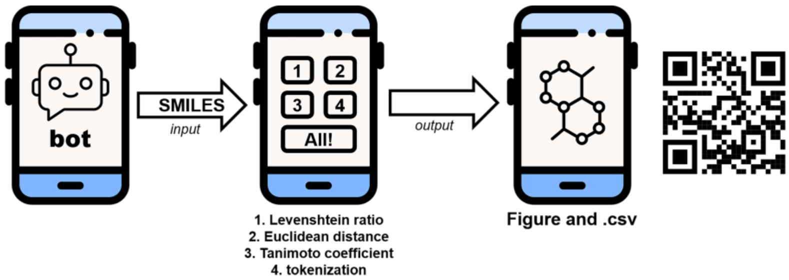

Figure 2. Overview of Telegram bot for the search for molecules sensitive to various cations. The QR code can be used to access the Telegram bot. The user is supposed to enter the SMILES of the molecule of interest and select one of the four methods (Levenshtein ration, Euclidean distance, Tanimoto coefficient, and tokenization/vectorization method) or all methods at once to search for the most similar structures from the database.

To start using the Telegram bot, the user should follow the link or scan the QR code (Figure 2). Once the bot is launched, the user needs to enter the SMILES of the molecule of interest and select one of the four methods to search for similar structures (or choose all methods at once). The Telegram bot provides the user with a figure and a *.csv file as outputs. The figure displays structures and cations arranged in order of decreasing similarity to the requested molecule. The *.csv file is more informative and includes SMILES, cation, solvent, article DOI, InChI, InChIKey, and the value of the selected similarity parameter. All structures are sorted by decreasing similarity coefficient. The Supplementary Materials video file shows the bot functioning.

3. Materials and Methods

3.1. Database

The following reviews [22–32] and papers [33–266] served as a source of information about fluorescent sensors for metal ions. Ignoring the duplicate entries, data on a total of 965 compounds were collected, including dipyrromethenes, BODIPY, Schiff bases, hydrazones, as well as fluorescein, rhodamine, phenanthroline, coumarin, naphthalimide derivatives, and some others. They were saved in an MS Excel file with a .xlsx extension and organized in the following table with columns for SMILES, InChI, InChIKey, cation, medium, and source. The dataset is freely available at [267].

This dataset contains various classes of sensors for different metal ions (Figure 3).

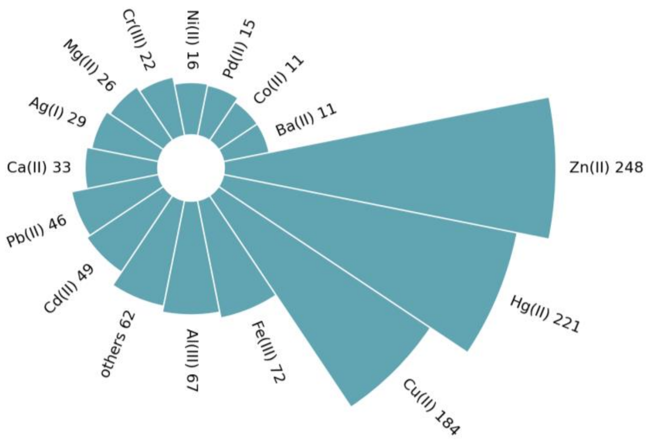

Figure 3. Count of different ions in dataset.

At the initial stage of investigating the dataset, our goal was to assess the correlation between various molecular descriptors and ion characteristics. For sensor characterization, we utilized a standard set of 42 parameters (*Chem.rdMolDescriptors.Properties.GetAvailableProperties*), including molecular weight (*amw*), number of rotatable bonds for a molecule (*NumRotat-*

ableBonds), number of H-bond donors for a molecule (*NumHBD*), number of heteroatoms (*NumHeteroatoms*), and more. To describe ions, we selected Pauling electronegativity, ionization potential, and ionic radius as descriptors. However, upon conducting a Pearson correlation analysis, we found that there was not a strong dependence between the physical—chemical characteristics of sensors and cations (Figure 4).

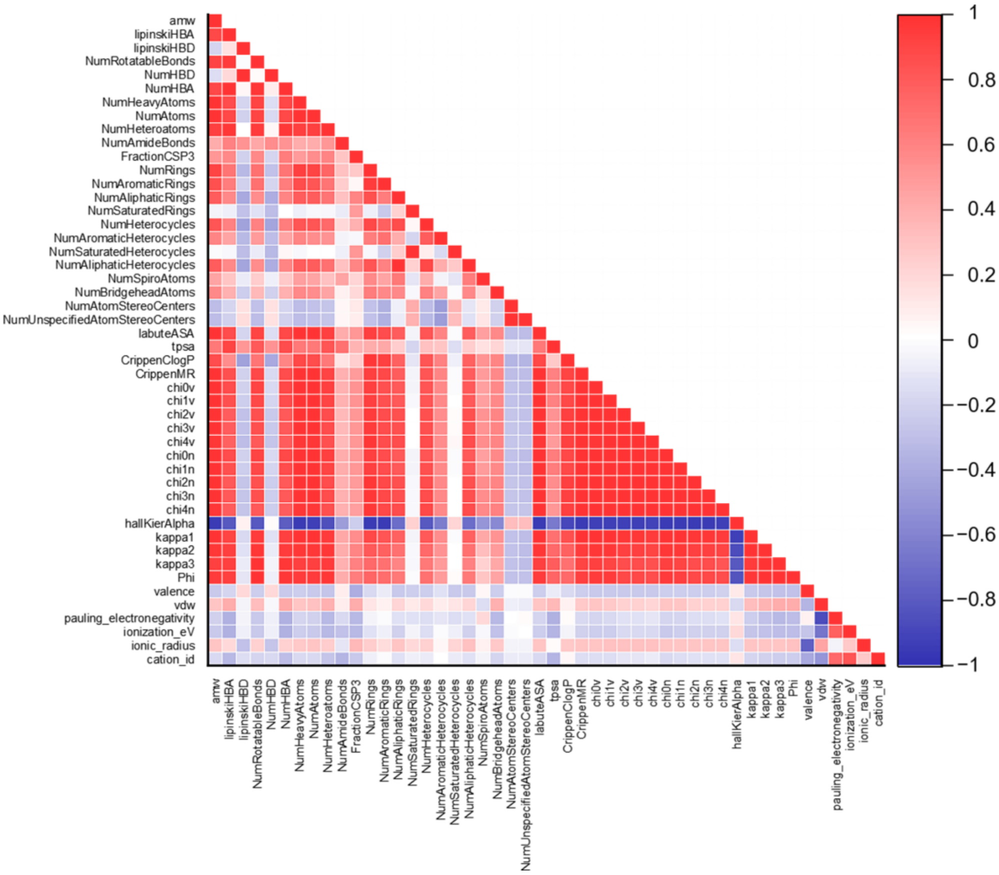

Figure 4. Pearson correlation matrix ('amw'—molecular weight; 'lipinskiHBA'—number of Lipinski H−bond acceptors; 'lipinskiHBD'—number of Lipinski H−bond donors; 'NumRotatableBonds'—number of rotatable bonds; 'NumHBD'—number of H−bond donors; NumHBA'—number of H−bond acceptors; 'NumHeavyAtoms'—number of heavy atoms; 'NumAtoms'—total number of atoms; 'NumHeteroatoms'—number of heteroatoms; 'NumAmideBonds'—number of amide bonds; 'FractionCSP3'—fraction of C atoms that are sp^3 hybridized; 'NumRings'—number of rings; 'NumAromaticRings'—number of aromatic rings; 'NumAliphaticRings'—number of aliphatic (containing at least one non−aromatic bond) rings; 'NumSaturatedRings'—number of saturated rings; 'NumHeterocycles'—number of heterocycles; 'NumAromaticHeterocycles'—number of aromatic heterocycles; 'NumSaturatedHeterocycles'—number of saturated heterocycles; 'NumAliphaticHeterocycles'—number of aliphatic (containing at least one non−aromatic bond) heterocycles; 'NumSpiroAtoms'—number of spiro atoms (atoms shared between rings that share exactly one atom); 'NumBridgeheadAtoms'—number of bridgehead atoms (atoms shared between rings that share at least two bonds); 'NumAtomStereoCenters'—number of atomic stereocenters (specified and unspecified); 'NumUnspecifiedAtomStereoCenters'—number of unspecified atomic stereocenters; 'labuteASA'—Labute ASA value; 'tpsa'—topological polar surface area value; 'CrippenClogP'—partition coefficient; 'CrippenMR'—molar refractivity; 'chi0v', 'chi1v', 'chi2v', 'chi3v', 'chi4v', 'chi0n', 'chi1n', 'chi2n', 'chi3n', 'chi4n'—Chi Indexes; 'hallKierAlpha'—Hall–Kier alpha value; 'kappa1', 'kappa2', 'kappa3'—Kappa shape indexes; 'Phi'—index of molecular flexibility; 'cation'—cation; 'valence'—valence; 'vdw'—Van der Waals radius; 'pauling_electronegativity'—Pauling electronegativity; 'ionization_eV'—ionization potential; 'ionic_radius'—ionic radius; 'cation_id'—cation class in dataset).

Since the chemical binding of ions is determined by the electron density distribution of sensors and, among other factors, the polarizing ability of ions, we decided to calculate the dipole moment, diagonal elements of the polarizability tensor, and energy gap for sensor molecules using a semi-empirical level. The polarizing ability of ions was evaluated as the ratio of charge and Van der Waals radius. For this purpose, we used the more accurate GFN2-XTB method in combination with the iMTD-GC algorithm as described in XTB [268]. However, upon analyzing the correlation matrix, we found no dependence between the calculated values (Figure 5).

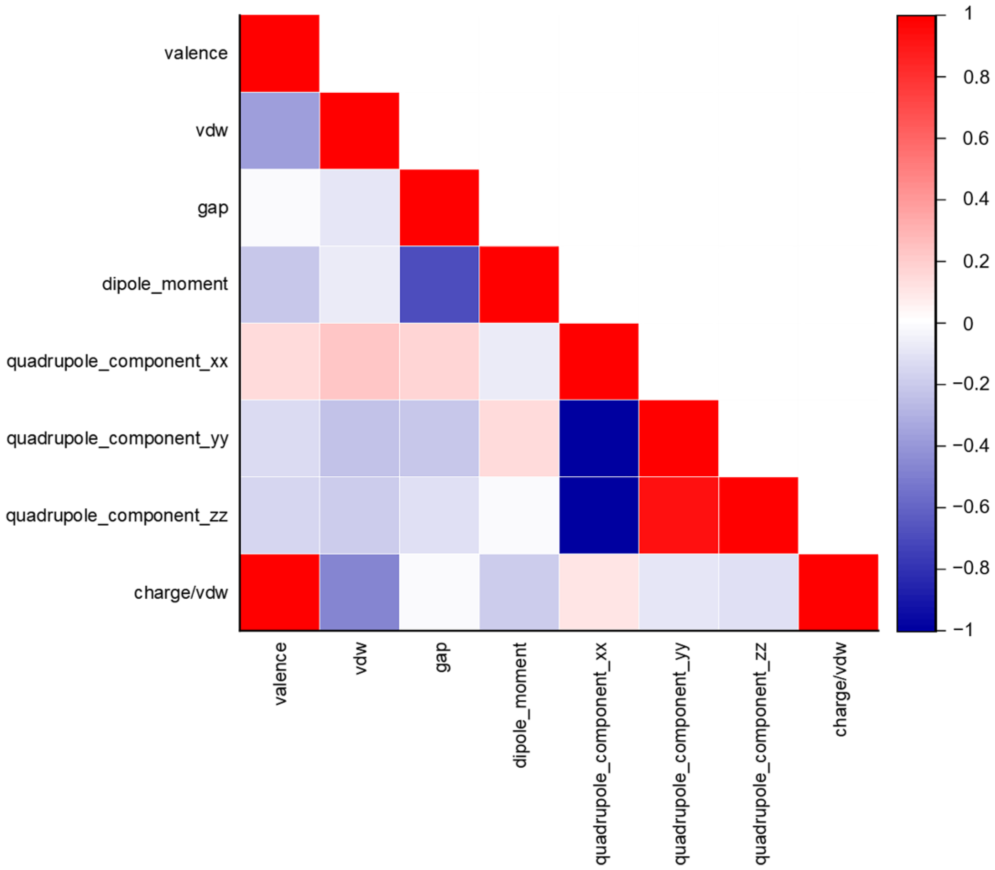

Figure 5. Pearson correlation matrix for values calculated ('gap'—energy gap for sensor molecules; 'dipole_moment'—dipole moment; 'quadrupole_component_xx', 'quadrupole_component_yy', 'quadrupole_component_zz'—diagonal elements of the polarizability tensor; 'charge/vdw'—polarizing ability of ions).

It became necessary to develop a new approach, based on different descriptors, to evaluate the relationship between sensors and ions. The new approach uses linear algebra methods.

3.2. Software

The software was developed using Python programming language (version 3.8) and several libraries, including Levenshtein [269], RDKit [270], scikit-learn [271], and aiogram [272]. The program consists of several subroutines, including file upload, preprocessing, four subroutines for finding the closest matches between database entries and user input, postprocessing, and output. The output presents the results of the search in graphical form as a table with columns for entry number, predicted cation, and corresponding similarity parameters. The first 10 most similar compounds from the database are presented as 2D chemical structures in SMILES format. The code is freely available at [268] and can be used with any IDE of the user's choice.

4. Conclusions

A database containing information on 965 chemical compounds that can be used as fluorescent chemosensors for various metal ions was created based on the literature data. A freeware for predicting the sensing ability of chemical compounds for metal ions was developed and is available as a Telegram bot (https://t.me/mol_sim_bot (accessed on 5 April 2023)). We did not observe a clear correlation between different molecular descriptors and ionic properties. Therefore, instead of derivation of an equation linking potential chemosensors and analytes, we suggested another approach to finding similarities between user input and database queries. Four algorithms were discussed and successfully applied: finding the Levenshtein ratio, Tanimoto coefficients between molecular fingerprints, Euclidean distances, and tokenization/vectorization routines.

We hope that the database and software developed will be useful for researchers working in the field of developing new fluorescent chemosensors for metal ions. The database will be supported and expanded in the future.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/inorganics11040158/s1, Video file 'Demonstration_bot_working.mkv'.

Author Contributions: Conceptualization, G.A.G., M.M.L., A.A.K. and E.V.A.; methodology, G.A.G., M.M.L. and A.A.K.; software, G.A.G., M.M.L. and A.A.K.; validation, D.N.Y., M.N.Z., G.A.G., M.M.L., A.A.K., N.A.B. and E.V.A.; formal analysis, D.N.Y., M.N.Z., G.A.G., M.M.L., A.A.K., N.A.B. and E.V.A.; investigation, G.A.G., M.M.L. and A.A.K.; resources, G.A.G., M.M.L. and A.A.K.; data curation, G.A.G., M.M.L. and A.A.K.; writing—original draft preparation, G.A.G. and A.A.K.; writing—review and editing, G.A.G., M.M.L., A.A.K. and E.V.A.; visualization, M.M.L. and A.A.K.; supervision, E.V.A.; project administration, G.A.G. and A.A.K.; funding acquisition, G.A.G. and A.A.K. All authors have read and agreed to the published version of the manuscript.

Funding: This work received financial support of the Ministry of Science and Higher Education of the Russian Federation [No. 075-15-2021-579] (creating a Telegram bot for the search for molecules sensitive to various cations) and [No. FZZW-2023-0008] (creating a database).

Data Availability Statement: Publicly available datasets were analyzed in this study. These data can be found here: https://gitlab.com/GeorgeGamov/prediction-of-sensing-ability/-/blob/main/database.xlsx (accessed on 5 April 2023).

Acknowledgments: The authors are grateful to A.N. Meshkov and A.P. Kotyurgin for their valuable comments and suggestions for software development.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Sonkaya, Ö.; Soylukan, C.; Pamuk Algi, M.; Algi, F. Aza-BODIPY-Based Fluorescent and Colorimetric Sensors and Probes. *COS* **2023**, *20*, 20–60. [CrossRef]
2. Kikuchi, K.; Adair, L.D.; Lin, J.; New, E.J.; Kaur, A. Photochemical Mechanisms of Fluorophores Employed in Single-Molecule Localization Microscopy. *Angew. Chem. Int. Ed.* **2023**, *62*, e202204745. [CrossRef]
3. Yu, W.; Xu, X.; Jin, K.; Liu, Y.; Li, J.; Du, G.; Lv, X.; Liu, L. Genetically Encoded Biosensors for Microbial Synthetic Biology: From Conceptual Frameworks to Practical Applications. *Biotechnol. Adv.* **2023**, *62*, 108077. [CrossRef]
4. Zhang, J.; Zhou, M.; Li, X.; Fan, Y.; Li, J.; Lu, K.; Wen, H.; Ren, J. Recent Advances of Fluorescent Sensors for Bacteria Detection-A Review. *Talanta* **2023**, *254*, 124133. [CrossRef]
5. Li, G.; Liu, Z.; Gao, W.; Tang, B. Recent Advancement in Graphene Quantum Dots Based Fluorescent Sensor: Design, Construction and Bio-Medical Applications. *Coord. Chem. Rev.* **2023**, *478*, 214966. [CrossRef]
6. Jie, B.; Lin, H.; Zhai, Y.; Ye, J.; Zhang, D.; Xie, Y.; Zhang, X.; Yang, Y. Mechanism, Design and Application of Fluorescent Recognition Based on Metal Organic Frameworks in Pollutant Detection. *Chem. Eng. J.* **2023**, *454*, 139931. [CrossRef]
7. Tammina, S.K.; Khan, A.; Rhim, J.-W. Advances and Prospects of Carbon Dots for Microplastic Analysis. *Chemosphere* **2023**, *313*, 137433. [CrossRef] [PubMed]
8. Jia, C.; He, T.; Wang, G.-M. Zirconium-Based Metal-Organic Frameworks for Fluorescent Sensing. *Coord. Chem. Rev.* **2023**, *476*, 214930. [CrossRef]

9. Chen, S.-H.; Jiang, K.; Xiao, Y.; Cao, X.-Y.; Arulkumar, M.; Wang, Z.-Y. Recent Endeavors on Design, Synthesis, Fluorescence Mechanisms and Applications of Benzazole-Based Molecular Probes toward Miscellaneous Species. *Dyes Pigments* **2020**, *175*, 108157. [CrossRef]
10. Lu, X.-L.; He, W. Research Advances in Excited State Intramolecular Proton Transfer Fluorescent Probes Based on Combined Fluorescence Mechanism. *Chin. J. Anal. Chem.* **2021**, *49*, 184–196. [CrossRef]
11. Liu, J.; Fan, J.; Zhang, K.; Zhang, Y.; Wang, C.-K.; Lin, L. Perspective for Aggregation-Induced Delayed Fluorescence Mechanism: A QM/MM Study*. *Chin. Phys. B* **2020**, *29*, 088504. [CrossRef]
12. Sedgwick, A.C.; Wu, L.; Han, H.-H.; Bull, S.D.; He, X.-P.; James, T.D.; Sessler, J.L.; Tang, B.Z.; Tian, H.; Yoon, J. Excited-State Intramolecular Proton-Transfer (ESIPT) Based Fluorescence Sensors and Imaging Agents. *Chem. Soc. Rev.* **2018**, *47*, 8842–8880. [CrossRef]
13. Gamov, G.A.; Zavalishin, M.N.; Petrova, M.V.; Khokhlova, A.Y.; Gashnikova, A.V.; Kiselev, A.N.; Sharnin, V.A. Interaction of Pyridoxal-Derived Hydrazones with Anions and Co^{2+}, Co^{3+}, Ni^{2+}, Zn^{2+} Cations. *Phys. Chem. Liq.* **2021**, *59*, 666–678. [CrossRef]
14. Gamov, G.A.; Kiselev, A.N.; Murekhina, A.E.; Zavalishin, M.N.; Aleksandriiskii, V.V.; Kosterin, D.Y. Synthesis, Protolytic Equilibria, and Antimicrobial Action of Nifuroxazide Analogs. *J. Mol. Liq.* **2021**, *341*, 116911. [CrossRef]
15. Weininger, D. SMILES, a Chemical Language and Information System. 1. Introduction to Methodology and Encoding Rules. *J. Chem. Inf. Model.* **1988**, *28*, 31–36. [CrossRef]
16. Weininger, D.; Weininger, A.; Weininger, J.L. SMILES. 2. Algorithm for Generation of Unique SMILES Notation. *J. Chem. Inf. Comput. Sci.* **1989**, *29*, 97–101. [CrossRef]
17. Levenshtein, V.I. Binary Codes Capable of Correcting Deletions, Insertions, and Reversals. *Sov. Phys. Dokl.* **1966**, *10*, 707–710.
18. Shao, J.; Gong, Q.; Yin, Z.; Pan, W.; Pandiyan, S.; Wang, L. S2DV: Converting SMILES to a Drug Vector for Predicting the Activity of Anti-HBV Small Molecules. *Brief. Bioinform.* **2022**, *23*, bbab593. [CrossRef] [PubMed]
19. Schwaller, P.; Laino, T.; Gaudin, T.; Bolgar, P.; Hunter, C.A.; Bekas, C.; Lee, A.A. Molecular Transformer: A Model for Uncertainty-Calibrated Chemical Reaction Prediction. *ACS Cent. Sci.* **2019**, *5*, 1572–1583. [CrossRef]
20. Schwaller, P.; Probst, D.; Vaucher, A.C.; Nair, V.H.; Kreutter, D.; Laino, T.; Reymond, J.-L. Mapping the Space of Chemical Reactions Using Attention-Based Neural Networks. *Nat. Mach. Intell.* **2021**, *3*, 144–152. [CrossRef]
21. Cation_Prediction_Bot. Available online: https://t.me/mol_sim_bot (accessed on 9 March 2023).
22. Kumar, A.; Virender; Saini, M.; Mohan, B.; Shayoraj; Kamboj, M. Colorimetric and Fluorescent Schiff Base Sensors for Trace Detection of Pollutants and Biologically Significant Cations: A Review (2010–2021). *Microchem. J.* **2022**, *181*, 107798. [CrossRef]
23. Sahoo, S.K. Chromo-Fluorogenic Sensing Using Vitamin B_6 Cofactors and Their Derivatives: A Review. *New J. Chem.* **2021**, *45*, 8874–8897. [CrossRef]
24. Berhanu, A.L.; Gaurav; Mohiuddin, I.; Malik, A.K.; Aulakh, J.S.; Kumar, V.; Kim, K.-H. A Review of the Applications of Schiff Bases as Optical Chemical Sensors. *TrAC Trends Anal. Chem.* **2019**, *116*, 74–91. [CrossRef]
25. Park, J.-K.; Shin, J.; Jang, S.; Seol, M.-L.; Kang, J.; Choi, S.; Eom, H.; Kwon, O.; Park, S.; Noh, D.-Y.; et al. Rational Design of Fluorescent/Colorimetric Chemosensors for Detecting Transition Metal Ions by Varying Functional Groups. *Inorganics* **2022**, *10*, 189. [CrossRef]
26. De Acha, N.; Elosúa, C.; Corres, J.; Arregui, F. Fluorescent Sensors for the Detection of Heavy Metal Ions in Aqueous Media. *Sensors* **2019**, *19*, 599. [CrossRef]
27. Yang, Y.; Gao, C.-Y.; Liu, J.; Dong, D. Recent Developments in Rhodamine Salicylidene Hydrazone Chemosensors. *Anal. Methods* **2016**, *8*, 2863–2871. [CrossRef]
28. Wan, H.; Xu, Q.; Gu, P.; Li, H.; Chen, D.; Li, N.; He, J.; Lu, J. AIE-Based Fluorescent Sensors for Low Concentration Toxic Ion Detection in Water. *J. Hazard. Mater.* **2021**, *403*, 123656. [CrossRef]
29. Su, X.; Aprahamian, I. Hydrazone-Based Switches, Metallo-Assemblies and Sensors. *Chem. Soc. Rev.* **2014**, *43*, 1963. [CrossRef]
30. Khan, S.; Chen, X.; Almahri, A.; Allehyani, E.S.; Alhumaydhi, F.A.; Ibrahim, M.M.; Ali, S. Recent Developments in Fluorescent and Colorimetric Chemosensors Based on Schiff Bases for Metallic Cations Detection: A Review. *J. Environ. Chem. Eng.* **2021**, *9*, 106381. [CrossRef]
31. Dutta, M.; Das, D. Recent Developments in Fluorescent Sensors for Trace-Level Determination of Toxic-Metal Ions. *TrAC Trends Anal. Chem.* **2012**, *32*, 113–132. [CrossRef]
32. Sivakumar, R.; Lee, N.Y. Paper-Based Fluorescence Chemosensors for Metal Ion Detection in Biological and Environmental Samples. *BioChip J.* **2021**, *15*, 216–232. [CrossRef]
33. Prodi, L.; Ballardini, R.; Gandolfi, M.T.; Roversi, R. A Simple Fluorescent Chemosensor for Alkaline-Earth Metal Ions. *J. Photochem. Photobiol. A Chem.* **2000**, *136*, 49–52. [CrossRef]
34. Prodi, L.; Bargossi, C.; Montalti, M.; Zaccheroni, N.; Su, N.; Bradshaw, J.S.; Izatt, R.M.; Savage, P.B. An Effective Fluorescent Chemosensor for Mercury Ions. *J. Am. Chem. Soc.* **2000**, *122*, 6769–6770. [CrossRef]
35. Xia, W.-S.; Schmehl, R.H.; Li, C.-J. A Novel Caesium Selective Fluorescent Chemosensor. *Chem. Commun.* **2000**, *8*, 695–696. [CrossRef]
36. Xia, W.-S.; Schmehl, R.H.; Li, C.-J. A Fluorescent 18-Crown-6 Based Luminescence Sensor for Lanthanide Ions. *Tetrahedron* **2000**, *56*, 7045–7049. [CrossRef]
37. De Santis, G.; Fabbrizzi, L.; Licchelli, M.; Mangano, C.; Sacchi, D.; Sardone, N. A Fluorescent Chemosensor for the Copper(II) Ion. *Inorg. Chim. Acta* **1997**, *257*, 69–76. [CrossRef]

38. Mitchell, K.A.; Brown, R.G.; Yuan, D.; Chang, S.-C.; Utecht, R.E.; Lewis, D.E. A Fluorescent Sensor for Cu^{2+} at the Sub-Ppm Level. *J. Photochem. Photobiol. A Chem.* **1998**, *115*, 157–161. [CrossRef]
39. Banthia, S.; Sarkar, M.; Samanta, A. Photophysical and Transition Metal Ion Signaling Properties of Some 4-Amino-1,8-Naphthalimide Derivatives. *Res. Chem. Intermed.* **2005**, *31*, 25–38. [CrossRef]
40. Ragos, G.C.; Demertzis, M.A.; Issopoulos, P.B. A High-Sensitive Spectrofluorimetric Method for the Determination of Micromolar Concentrations of Iron(III) in Bovine Liver with 4-Hydroxyquinoline. *Il Farmaco* **1998**, *53*, 611–616. [CrossRef]
41. Obare, S.O.; Murphy, C.J. A Two-Color Fluorescent Lithium Ion Sensor. *Inorg. Chem.* **2001**, *40*, 6080–6082. [CrossRef]
42. Burdette, S.C.; Walkup, G.K.; Spingler, B.; Tsien, R.Y.; Lippard, S.J. Fluorescent Sensors for Zn^{2+} Based on a Fluorescein Platform: Synthesis, Properties and Intracellular Distribution. *J. Am. Chem. Soc.* **2001**, *123*, 7831–7841. [CrossRef]
43. Klein, G.; Kaufmann, D.; Schürch, S.; Reymond, J.-L. A Fluorescent Metal Sensor Based on Macrocyclic Chelation. *Chem. Commun.* **2001**, *6*, 561–562. [CrossRef]
44. Kawakami, J.; Komai, Y.; Sumori, T.; Fukushi, A.; Shimozaki, K.; Ito, S. Intramolecular Excimer Formation and Complexing Behavior of 1,n-Bis(Naphthalenecarboxy)Oxaalkanes as Fluorescent Chemosensors for Calcium and Barium Ions. *J. Photochem. Photobiol. A Chem.* **2001**, *139*, 71–78. [CrossRef]
45. McFarland, S.A.; Finney, N.S. Fluorescent Chemosensors Based on Conformational Restriction of a Biaryl Fluorophore. *J. Am. Chem. Soc.* **2001**, *123*, 1260–1261. [CrossRef]
46. Kawakami, J.; Bronson, R.T.; Xue, G.; Bradshaw, J.S.; Izatt, R.M.; Savage, P.B. Characterization of Bis-8-Hydroxyquinoline-Armed Diazatrithia-16-Crown-5 and Diazadibenzo-18-Crown-6 Ligands as Fluorescent Chemosensors for Zinc. *J. Supramol. Chem.* **2001**, *1*, 221–227. [CrossRef]
47. Gunnlaugsson, T.; Bichell, B.; Nolan, C. A Novel Fluorescent Photoinduced Electron Transfer (PET) Sensor for Lithium. *Tetrahedron Lett.* **2002**, *43*, 4989–4992. [CrossRef]
48. Chen, C.-T.; Huang, W.-P. A Highly Selective Fluorescent Chemosensor for Lead Ions. *J. Am. Chem. Soc.* **2002**, *124*, 6246–6247. [CrossRef]
49. Kim, T.W.; Park, J.; Hong, J.-I. Zn^{2+} Fluorescent Chemosensors and the Influence of Their Spacer Length on Tuning Zn^{2+} SelectivityElectronic Supplementary Information (ESI) Available: Job Plot, Partial 1H NMR Spectra of Free 3 and the 3–Zn^{2+} Complex, Ca^{2+} and Mg^{2+} Interference for Zn^{2+} Sensing of 3, Kd Measurements, and Buffer Preparation. See http://www.rsc.org/suppdata/p2/b2/b200462c/. *J. Chem. Soc. Perkin Trans.* **2002**, *2*, 923–927. [CrossRef]
50. Petrat, F.; Weisheit, D.; Lensen, M.; de GROOT, H.; Sustmann, R.; Rauen, U. Selective Determination of Mitochondrial Chelatable Iron in Viable Cells with a New Fluorescent Sensor. *Biochem. J.* **2002**, *362*, 137–147. [CrossRef]
51. Xia, W.-S.; Schmehl, R.H.; Li, C.-J.; Mague, J.T.; Luo, C.-P.; Guldi, D.M. Chemosensors for Lead(II) and Alkali Metal Ions Based on Self-Assembling Fluorescence Enhancement (SAFE). *J. Phys. Chem. B* **2002**, *106*, 833–843. [CrossRef]
52. Gunnlaugsson, T.; Nieuwenhuyzen, M.; Richard, L.; Thoss, V. Novel Sodium-Selective Fluorescent PET and Optically Based Chemosensors: Towards Na^{+} Determination in Serum. *J. Chem. Soc. Perkin Trans. 2* **2002**, *1*, 141–150. [CrossRef]
53. Benniston, A.C.; Harriman, A.; Lawrie, D.J.; Mayeux, A.; Rafferty, K.; Russell, O.D. A General Purpose Reporter for Cations: Absorption, Fluorescence and Electrochemical Sensing of Zinc(II). *Dalton Trans.* **2003**, *2*, 4762. [CrossRef]
54. Yang, R.-H.; Chan, W.-H.; Lee, A.W.M.; Xia, P.-F.; Zhang, H.-K.; Ke'An, L. A Ratiometric Fluorescent Sensor for Ag^{I} with High Selectivity and Sensitivity. *J. Am. Chem. Soc.* **2003**, *125*, 2884–2885. [CrossRef]
55. Zhou, L.; Zhang, X.; Wu, S. A Specific Fluorescent Chemosensor for Copper (II) Cation Recognition*. *Prog. Nat. Sci.* **2003**, *13*, 201–205. [CrossRef]
56. Otten, P.A.; London, R.E.; Levy, L.A. 4-Oxo-4 *H* -Quinolizine-3-Carboxylic Acids as Mg^{2+} Selective, Fluorescent Indicators. *Bioconjugate Chem.* **2001**, *12*, 203–212. [CrossRef]
57. Nakahara, Y.; Kida, T.; Nakatsuji, Y.; Akashi, M. A Novel Fluorescent Indicator for Ba^{2+} in Aqueous Micellar SolutionsElectronic Supplementary Information (ESI) Available: Synthesis and Characterisation of 1. *Chem. Commun.* **2004**, *2*, 224–225. [CrossRef] [PubMed]
58. Ohshima, A.; Momotake, A.; Arai, T. A New Fluorescent Metal Sensor with Two Binding Moieties. *Tetrahedron Lett.* **2004**, *45*, 9377–9381. [CrossRef]
59. Kwon, J.Y.; Soh, J.H.; Yoon, Y.J.; Yoon, J. Highly Effective Fluorescent Sensor for Hg^{2+} in Aqueous Solution. *Supramol. Chem.* **2004**, *16*, 621–624. [CrossRef]
60. Bolletta, F.; Garelli, A.; Montalti, M.; Prodi, L.; Romano, S.; Zaccheroni, N.; Canovese, L.; Chessa, G.; Santo, C.; Visentin, F. Synthesis, Photophysical Characterisation and Metal Ion Binding Properties of New Ligands Containing Anthracene Chromophores. *Inorg. Chim. Acta* **2004**, *357*, 4078–4084. [CrossRef]
61. Thiagarajan, V.; Selvaraju, C.; Malar, E.J.P.; Ramamurthy, P. A Novel Fluorophore with Dual Fluorescence: Local Excited State and Photoinduced Electron-Transfer-Promoted Charge-Transfer State. *ChemPhysChem* **2004**, *5*, 1200–1209. [CrossRef]
62. Taki, M.; Wolford, J.L.; O'Halloran, T.V. Emission Ratiometric Imaging of Intracellular Zinc: Design of a Benzoxazole Fluorescent Sensor and Its Application in Two-Photon Microscopy. *J. Am. Chem. Soc.* **2004**, *126*, 712–713. [CrossRef]
63. Kawakami, J.; Kimura, H.; Nagaki, M.; Kitahara, H.; Ito, S. Intramolecular Exciplex Formation and Complexing Behavior of 1-(2-Naphthalenecarboxy)-n-(p-Substituted Benzenecarboxy)Oxaalkanes as Fluorescent Chemosensors for Calcium and Barium Ions. *J. Photochem. Photobiol. A Chem.* **2004**, *161*, 141–149. [CrossRef]

64. Chang, C.J.; Jaworski, J.; Nolan, E.M.; Sheng, M.; Lippard, S.J. A Tautomeric Zinc Sensor for Ratiometric Fluorescence Imaging: Application to Nitric Oxide-Induced Release of Intracellular Zinc. *Proc. Natl. Acad. Sci. USA* **2004**, *101*, 1129–1134. [CrossRef]
65. Guo, X.; Qian, X.; Jia, L. A Highly Selective and Sensitive Fluorescent Chemosensor for Hg^{2+} in Neutral Buffer Aqueous Solution. *J. Am. Chem. Soc.* **2004**, *126*, 2272–2273. [CrossRef] [PubMed]
66. Chen, Y.; Zeng, D.X. A Selective, Fluorescent Sensor for Zn^{2+}. *ChemPhysChem* **2004**, *5*, 564–566. [CrossRef] [PubMed]
67. Wu, Z.; Chen, Q.; Yang, G.; Xiao, C.; Liu, J.; Yang, S.; Ma, J.S. Novel Fluorescent Sensor for Zn(II) Based on Bis(Pyrrol-2-Yl-Methyleneamine) Ligands. *Sens. Actuators B Chem.* **2004**, *99*, 511–515. [CrossRef]
68. Youk, J.-S.; Kim, Y.-H.; Kim, E.-J.; Youn, N.-J.; Chang, S.-K. Hg^{2+}-Selective Chemosensor Derived from 8-Hydroxyquinoline Having Benzothiazole Function in Aqueous Environment. *Bull. Korean Chem. Soc.* **2004**, *25*, 869–872. [CrossRef]
69. Henary, M.M.; Wu, Y.; Fahrni, C.J. Zinc(II)-Selective Ratiometric Fluorescent Sensors Based on Inhibition of Excited-State Intramolecular Proton Transfer. *Chem. Eur. J.* **2004**, *10*, 3015–3025. [CrossRef] [PubMed]
70. Nolan, E.M.; Jaworski, J.; Okamoto, K.-I.; Hayashi, Y.; Sheng, M.; Lippard, S.J. QZ1 and QZ2: Rapid, Reversible Quinoline-Derivatized Fluoresceins for Sensing Biological Zn(II). *J. Am. Chem. Soc.* **2005**, *127*, 16812–16823. [CrossRef]
71. Yoon, S.; Albers, A.E.; Wong, A.P.; Chang, C.J. Screening Mercury Levels in Fish with a Selective Fluorescent Chemosensor. *J. Am. Chem. Soc.* **2005**, *127*, 16030–16031. [CrossRef]
72. Shao, N.; Zhang, Y.; Cheung, S.; Yang, R.; Chan, W.; Mo, T.; Li, K.; Liu, F. Copper Ion-Selective Fluorescent Sensor Based on the Inner Filter Effect Using a Spiropyran Derivative. *Anal. Chem.* **2005**, *77*, 7294–7303. [CrossRef]
73. Shiraishi, Y.; Kohno, Y.; Hirai, T. Bis-Azamacrocyclic Anthracene as a Fluorescent Chemosensor for Cations in Aqueous Solution. *J. Phys. Chem. B* **2005**, *109*, 19139–19147. [CrossRef]
74. Wang, L.; Zhu, X.-J.; Wong, W.-Y.; Guo, J.-P.; Wong, W.-K.; Li, Z.-Y. Dipyrrolylquinoxaline-Bridged Schiff Bases: A New Class of Fluorescent Sensors for Mercury(II). *Dalton Trans.* **2005**, *19*, 3235–3240. [CrossRef]
75. Bricks, J.L.; Kovalchuk, A.; Trieflinger, C.; Nofz, M.; Büschel, M.; Tolmachev, A.I.; Daub, J.; Rurack, K. On the Development of Sensor Molecules That Display Fe^{III}-Amplified Fluorescence. *J. Am. Chem. Soc.* **2005**, *127*, 13522–13529. [CrossRef]
76. Wang, Z.; Zhang, D.; Zhu, D. A Sensitive and Selective "Turn on" Fluorescent Chemosensor for Hg(II) Ion Based on a New Pyrene–Thymine Dyad. *Anal. Chim. Acta* **2005**, *549*, 10–13. [CrossRef]
77. Yang, L.; McRae, R.; Henary, M.M.; Patel, R.; Lai, B.; Vogt, S.; Fahrni, C.J. Imaging of the Intracellular Topography of Copper with a Fluorescent Sensor and by Synchrotron X-Ray Fluorescence Microscopy. *Proc. Natl. Acad. Sci. USA* **2005**, *102*, 11179–11184. [CrossRef] [PubMed]
78. Fan, J.; Peng, X.; Wu, Y.; Lu, E.; Hou, J.; Zhang, H.; Zhang, R.; Fu, X. A New PET Fluorescent Sensor for Zn^{2+}. *J. Lumin.* **2005**, *114*, 125–130. [CrossRef]
79. Komatsu, K.; Kikuchi, K.; Kojima, H.; Urano, Y.; Nagano, T. Selective Zinc Sensor Molecules with Various Affinities for Zn^{2+}, Revealing Dynamics and Regional Distribution of Synaptically Released Zn^{2+} in Hippocampal Slices. *J. Am. Chem. Soc.* **2005**, *127*, 10197–10204. [CrossRef]
80. Sankaran, N.B.; Nishizawa, S.; Watanabe, M.; Uchida, T.; Teramae, N. Designing Ratiometric Fluorescent Sensors for Alkali Metal Ions from Simple PET Sensors by Controlling Spacer Length. *J. Mater. Chem.* **2005**, *15*, 2755. [CrossRef]
81. Sankaran, N.B.; Mandal, P.K.; Bhattacharya, B.; Samanta, A. Fluorescence Response of Mono-and Tetraazacrown Derivatives of 4-Aminophthalimide with and without Some Transition and Post Transition Metal Ions. *J. Mater. Chem.* **2005**, *15*, 2854. [CrossRef]
82. Kwon, J.Y.; Jang, Y.J.; Lee, Y.J.; Kim, K.M.; Seo, M.S.; Nam, W.; Yoon, J. A Highly Selective Fluorescent Chemosensor for Pb^{2+}. *J. Am. Chem. Soc.* **2005**, *127*, 10107–10111. [CrossRef] [PubMed]
83. Ros-Lis, J.V.; Marcos, M.D.; Mártinez-Máñez, R.; Rurack, K.; Soto, J. A Regenerative Chemodosimeter Based on Metal-Induced Dye Formation for the Highly Selective and Sensitive Optical Determination of Hg^{2+} Ions. *Angew. Chem. Int. Ed.* **2005**, *44*, 4405–4407. [CrossRef] [PubMed]
84. Li, Y.; Yang, C.M. A Tryptophan-Containing Open-Chain Framework for Tuning a High Selectivity for Ca^{2+} and ^{13}C NMR Observation of a Ca^{2+} −Indole Interaction in Aqueous Solution. *J. Am. Chem. Soc.* **2005**, *127*, 3527–3530. [CrossRef]
85. Xu, Z.; Xiao, Y.; Qian, X.; Cui, J.; Cui, D. Ratiometric and Selective Fluorescent Sensor for Cu^{II} Based on Internal Charge Transfer (ICT). *Org. Lett.* **2005**, *7*, 889–892. [CrossRef]
86. Mikata, Y.; Wakamatsu, M.; Yano, S. Tetrakis(2-Quinolinylmethyl)Ethylenediamine (TQEN) as a New Fluorescent Sensor for Zinc. *Dalton Trans.* **2005**, *3*, 545–550. [CrossRef] [PubMed]
87. Fang, L.; Chan, W.-H.; He, Y.-B. Selective Complexation of Metals with Isoxazolidine-Containing Fluorophores. *Tetrahedron Lett.* **2005**, *46*, 173–176. [CrossRef]
88. Zhou, L.-L.; Sun, H.; Zhang, X.-H.; Wu, S.-K. An Effective Fluorescent Chemosensor for the Detection of Copper(II). *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* **2005**, *61*, 61–65. [CrossRef]
89. Mei, Y.; Bentley, P.A. A Ratiometric Fluorescent Sensor for Zn^{2+} Based on Internal Charge Transfer (ICT). *Bioorg. Med. Chem. Lett.* **2006**, *16*, 3131–3134. [CrossRef]
90. Nolan, E.M.; Ryu, J.W.; Jaworski, J.; Feazell, R.P.; Sheng, M.; Lippard, S.J. Zinspy Sensors with Enhanced Dynamic Range for Imaging Neuronal Cell Zinc Uptake and Mobilization. *J. Am. Chem. Soc.* **2006**, *128*, 15517–15528. [CrossRef]
91. McCarroll, M.E.; Shi, Y.; Harris, S.; Puli, S.; Kimaru, I.; Xu, R.; Wang, L.; Dyer, D.J. Computational Prediction and Experimental Evaluation of a Photoinduced Electron-Transfer Sensor. *J. Phys. Chem. B* **2006**, *110*, 22991–22994. [CrossRef]

92. Park, M.S.; Swamy, K.M.K.; Lee, Y.J.; Lee, H.N.; Jang, Y.J.; Moon, Y.H.; Yoon, J. A New Acridine Derivative as a Fluorescent Chemosensor for Zinc Ions in an 100% Aqueous Solution: A Comparison of Binding Property with Anthracene Derivative. *Tetrahedron Lett.* **2006**, *47*, 8129–8132. [CrossRef]
93. Wu, J.-S.; Wang, P.-F.; Zhang, X.-H.; Wu, S.-K. Novel Fluorescent Sensor for Detection of Cu(II) in Aqueous Solution. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* **2006**, *65*, 749–752. [CrossRef]
94. Xu, Z.; Qian, X.; Cui, J.; Zhang, R. Exploiting the Deprotonation Mechanism for the Design of Ratiometric and Colorimetric Zn2+ Fluorescent Chemosensor with a Large Red-Shift in Emission. *Tetrahedron* **2006**, *62*, 10117–10122. [CrossRef]
95. Kulatilleke, C.P.; de Silva, S.A.; Eliav, Y. A Coumarin Based Fluorescent Photoinduced Electron Transfer Cation Sensor. *Polyhedron* **2006**, *25*, 2593–2596. [CrossRef]
96. Wen, G.-T.; Zhu, M.-Z.; Wang, Z.; Meng, X.-M.; Hu, H.-Y.; Guo, Q.-X. Studies on the Transition Metal Ion Induced Fluorescence Enhancement of 1,8-Naphthalimide Derivatives. *Chin. J. Chem.* **2006**, *24*, 1230–1237. [CrossRef]
97. Goldsmith, C.R.; Lippard, S.J. Analogues of Zinpyr-1 Provide Insight into the Mechanism of Zinc Sensing. *Inorg. Chem.* **2006**, *45*, 6474–6478. [CrossRef]
98. Wu, D.-Y.; Xie, L.-X.; Zhang, C.-L.; Duan, C.-Y.; Zhao, Y.-G.; Guo, Z.-J. Quinoline-Based Molecular Clips for Selective Fluorescent Detection of Zn^{2+}. *Dalton Trans.* **2006**, *29*, 3528–3533. [CrossRef]
99. He, Q.; Miller, E.W.; Wong, A.P.; Chang, C.J. A Selective Fluorescent Sensor for Detecting Lead in Living Cells. *J. Am. Chem. Soc.* **2006**, *128*, 9316–9317. [CrossRef]
100. Salman, H.; Tal, S.; Chuvilov, Y.; Solovey, O.; Abraham, Y.; Kapon, M.; Suwinska, K.; Eichen, Y. Sensitive and Selective PET-Based Diimidazole Luminophore for Zn^{II} Ions: A Structure−Activity Correlation. *Inorg. Chem.* **2006**, *45*, 5315–5320. [CrossRef]
101. Kovbasyuk, L.; Krämer, R. A Selective Fluorescent Sensor for Cu^{2+} and Its Immobilization on CPG Beads. *Inorg. Chem. Commun.* **2006**, *9*, 586–590. [CrossRef]
102. Wang, J.; Qian, X.; Cui, J. Detecting Hg^{2+} Ions with an ICT Fluorescent Sensor Molecule: Remarkable Emission Spectra Shift and Unique Selectivity. *J. Org. Chem.* **2006**, *71*, 4308–4311. [CrossRef] [PubMed]
103. Li, Y.Q.; Bricks, J.L.; Resch-Genger, U.; Spieles, M.; Rettig, W. CT-Operated Bifunctional Fluorescent Probe Based on a Pretwisted Donor–Donor–Biphenyl. *J. Fluoresc.* **2006**, *16*, 337–348. [CrossRef]
104. Zhang, G.-Q.; Yang, G.-Q.; Zhu, L.-N.; Chen, Q.-Q.; Ma, J.-S. A Potential Fluorescent Sensor for Zn2+ Based on a Selective Bis-9-Anthryldiamine Ligand Operating in Buffer. *Sens. Actuators B Chem.* **2006**, *114*, 995–1000. [CrossRef]
105. Wu, Z.; Zhang, Y.; Ma, J.S.; Yang, G. Ratiometric Zn^{2+} Sensor and Strategy for Hg^{2+} Selective Recognition by Central Metal Ion Replacement. *Inorg. Chem.* **2006**, *45*, 3140–3142. [CrossRef]
106. Qi, X.; Jun, E.J.; Xu, L.; Kim, S.-J.; Joong Hong, J.S.; Yoon, Y.J.; Yoon, J. New BODIPY Derivatives as OFF−ON Fluorescent Chemosensor and Fluorescent Chemodosimeter for Cu^{2+}: Cooperative Selectivity Enhancement toward Cu^{2+}. *J. Org. Chem.* **2006**, *71*, 2881–2884. [CrossRef]
107. Nolan, E.M.; Racine, M.E.; Lippard, S.J. Selective Hg(II) Detection in Aqueous Solution with Thiol Derivatized Fluoresceins. *Inorg. Chem.* **2006**, *45*, 2742–2749. [CrossRef] [PubMed]
108. Meng, X.-M.; Zhu, M.-Z.; Liu, L.; Guo, Q.-X. Novel Highly Selective Fluorescent Chemosensors for Zn(II). *Tetrahedron Lett.* **2006**, *47*, 1559–1562. [CrossRef]
109. Goldsmith, C.R.; Lippard, S.J. 6-Methylpyridyl for Pyridyl Substitution Tunes the Properties of Fluorescent Zinc Sensors of the Zinpyr Family. *Inorg. Chem.* **2006**, *45*, 555–561. [CrossRef]
110. Zeng, L.; Miller, E.W.; Pralle, A.; Isacoff, E.Y.; Chang, C.J. A Selective Turn-On Fluorescent Sensor for Imaging Copper in Living Cells. *J. Am. Chem. Soc.* **2006**, *128*, 10–11. [CrossRef]
111. Qi, X.; Kim, S.-K.; Jun, E.-J.; Xu, L.; Kim, S.-J.; Yoon, J.Y. A New BODIPY Derivative Bearing Piperazine Group. *Bull. Korean Chem. Soc.* **2007**, *28*, 2231–2234. [CrossRef]
112. Chen, H.; Wu, Y.; Cheng, Y.; Yang, H.; Li, F.; Yang, P.; Huang, C. A Ratiometric Fluorescent Sensor for Zinc(II) with High Selectivity. *Inorg. Chem. Commun.* **2007**, *10*, 1413–1415. [CrossRef]
113. Wang, H.-H.; Gan, Q.; Wang, X.-J.; Xue, L.; Liu, S.-H.; Jiang, H. A Water-Soluble, Small Molecular Fluorescent Sensor with Femtomolar Sensitivity for Zinc Ion. *Org. Lett.* **2007**, *9*, 4995–4998. [CrossRef]
114. Komatsu, K.; Urano, Y.; Kojima, H.; Nagano, T. Development of an Iminocoumarin-Based Zinc Sensor Suitable for Ratiometric Fluorescence Imaging of Neuronal Zinc. *J. Am. Chem. Soc.* **2007**, *129*, 13447–13454. [CrossRef] [PubMed]
115. Young, S. Selective Fluorescent Hg(II) Detection in Aqueous Solutions with a Dye Intermediate. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* **2007**, *68*, 705–709. [CrossRef]
116. Sumalekshmy, S.; Henary, M.M.; Siegel, N.; Lawson, P.V.; Wu, Y.; Schmidt, K.; Brédas, J.-L.; Perry, J.W.; Fahrni, C.J. Design of Emission Ratiometric Metal-Ion Sensors with Enhanced Two-Photon Cross Section and Brightness. *J. Am. Chem. Soc.* **2007**, *129*, 11888–11889. [CrossRef]
117. Meng, X.M.; Zhu, M.Z.; Guo, Q.X. A Novel Highly Selective Fluorescent Chemosensor for Hg(II) in Fully Aqueous Media. *Chin. Chem. Lett.* **2007**, *18*, 1209–1212. [CrossRef]
118. Yoon, S.; Miller, E.W.; He, Q.; Do, P.H.; Chang, C.J. A Bright and Specific Fluorescent Sensor for Mercury in Water, Cells, and Tissue. *Angew. Chem. Int. Ed.* **2007**, *46*, 6658–6661. [CrossRef] [PubMed]
119. Soh, J.H.; Swamy, K.M.K.; Kim, S.K.; Kim, S.; Lee, S.-H.; Yoon, J. Rhodamine Urea Derivatives as Fluorescent Chemosensors for Hg^{2+}. *Tetrahedron Lett.* **2007**, *48*, 5966–5969. [CrossRef]

120. Mu, H.; Gong, R.; Ma, Q.; Sun, Y.; Fu, E. A Novel Colorimetric and Fluorescent Chemosensor: Synthesis and Selective Detection for Cu^{2+} and Hg^{2+}. *Tetrahedron Lett.* **2007**, *48*, 5525–5529. [CrossRef]
121. Zhang, X.; Shiraishi, Y.; Hirai, T. A New Rhodamine-Based Fluorescent Chemosensor for Transition Metal Cations Synthesized by One-Step Facile Condensation. *Tetrahedron Lett.* **2007**, *48*, 5455–5459. [CrossRef]
122. Staneva, D.; Grabchev, I.; Soumillion, J.-P.; Bojinov, V. A New Fluorosensor Based on Bis-1,8-Naphthalimide for Metal Cations and Protons. *J. Photochem. Photobiol. A Chem.* **2007**, *189*, 192–197. [CrossRef]
123. Xu, S.; Li, W.; Chen, K.-C. Naphthalimide as Highly Selective Fluorescent Sensor for Ag+Ions. *Chin. J. Chem.* **2007**, *25*, 778–783. [CrossRef]
124. Zhang, M.; Gao, Y.; Li, M.; Yu, M.; Li, F.; Li, L.; Zhu, M.; Zhang, J.; Yi, T.; Huang, C. A Selective Turn-on Fluorescent Sensor for FeIII and Application to Bioimaging. *Tetrahedron Lett.* **2007**, *48*, 3709–3712. [CrossRef]
125. Peng, R.; Wang, F.; Sha, Y. Synthesis of 5-Dialkyl(Aryl)Aminomethyl-8-Hydroxyquinoline Dansylates as Selective Fluorescent Sensors for Fe^{3+}. *Molecules* **2007**, *12*, 1191–1201. [CrossRef] [PubMed]
126. Chovelon, J.-M.; Grabchev, I. A Novel Fluorescent Sensor for Metal Cations and Protons Based of Bis-1,8-Naphthalimide. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* **2007**, *67*, 87–91. [CrossRef]
127. Park, S.M.; Kim, M.H.; Choe, J.-I.; No, K.T.; Chang, S.-K. Cyclams Bearing Diametrically Disubstituted Pyrenes as Cu^{2+}- and Hg^{2+}-Selective Fluoroionophores. *J. Org. Chem.* **2007**, *72*, 3550–3553. [CrossRef]
128. Peng, X.; Du, J.; Fan, J.; Wang, J.; Wu, Y.; Zhao, J.; Sun, S.; Xu, T. A Selective Fluorescent Sensor for Imaging Cd^{2+} in Living Cells. *J. Am. Chem. Soc.* **2007**, *129*, 1500–1501. [CrossRef]
129. Dennis, A.E.; Smith, R.C. "Turn-on" Fluorescent Sensor for the Selective Detection of Zinc Ion by a Sterically-Encumbered Bipyridyl-Based Receptor. *Chem. Commun.* **2007**, *44*, 4641–4643. [CrossRef]
130. Parkesh, R.; Clive Lee, T.; Gunnlaugsson, T. Highly Selective 4-Amino-1,8-Naphthalimide Based Fluorescent Photoinduced Electron Transfer (PET) Chemosensors for Zn(II) under Physiological PH Conditions. *Org. Biomol. Chem.* **2007**, *5*, 310–317. [CrossRef]
131. Bojinov, V.B.; Panova, I.P.; Chovelon, J.-M. Novel Blue Emitting Tetra-and Pentamethylpiperidin-4-Yloxy-1,8-Naphthalimides as Photoinduced Electron Transfer Based Sensors for Transition Metal Ions and Protons. *Sens. Actuators B Chem.* **2008**, *135*, 172–180. [CrossRef]
132. Singh, N.; Kaur, N.; Mulrooney, R.C.; Callan, J.F. A Ratiometric Fluorescent Probe for Magnesium Employing Excited State Intramolecular Proton Transfer. *Tetrahedron Lett.* **2008**, *49*, 6690–6692. [CrossRef]
133. Kim, J.; Morozumi, T.; Nakamura, H. Control between TICT and PET Using Chemical Modification of N-Phenyl-9-Anthracenecarboxamide and Its Application to a Crown Ether Type Chemosensor. *Tetrahedron* **2008**, *64*, 10735–10740. [CrossRef]
134. Shiraishi, Y.; Sumiya, S.; Kohno, Y.; Hirai, T. A Rhodamine–Cyclen Conjugate as a Highly Sensitive and Selective Fluorescent Chemosensor for Hg(II). *J. Org. Chem.* **2008**, *73*, 8571–8574. [CrossRef] [PubMed]
135. Zhang, X.; Xiao, Y.; Qian, X. A Ratiometric Fluorescent Probe Based on FRET for Imaging Hg^{2+} Ions in Living Cells. *Angew. Chem. Int. Ed.* **2008**, *47*, 8025–8029. [CrossRef]
136. Taki, M.; Desaki, M.; Ojida, A.; Iyoshi, S.; Hirayama, T.; Hamachi, I.; Yamamoto, Y. Fluorescence Imaging of Intracellular Cadmium Using a Dual-Excitation Ratiometric Chemosensor. *J. Am. Chem. Soc.* **2008**, *130*, 12564–12565. [CrossRef] [PubMed]
137. Du, J.; Fan, J.; Peng, X.; Li, H.; Wang, J.; Sun, S. Highly Selective and Anions Controlled Fluorescent Sensor for Hg^{2+} in Aqueous Environment. *J. Fluoresc.* **2008**, *18*, 919–924. [CrossRef] [PubMed]
138. Zhang, D.; Su, J.; Ma, X.; Tian, H. An Efficient Multiple-Mode Molecular Logic System for PH, Solvent Polarity, and Hg^{2+} Ions. *Tetrahedron* **2008**, *64*, 8515–8521. [CrossRef]
139. Huang, C.; Peng, X.; Lin, Z.; Fan, J.; Ren, A.; Sun, D. A Highly Selective and Sensitive Two-Photon Chemosensor for Silver Ion Derived from 3,9-Dithia-6-Azaundecane. *Sens. Actuators B Chem.* **2008**, *133*, 113–117. [CrossRef]
140. Luo, H.-Y.; Zhang, X.-B.; He, C.-L.; Shen, G.-L.; Yu, R.-Q. Synthesis of Dipicolylamino Substituted Quinazoline as Chemosensor for Cobalt(II) Recognition Based on Excited-State Intramolecular Proton Transfer. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* **2008**, *70*, 337–342. [CrossRef]
141. Xue, L.; Wang, H.-H.; Wang, X.-J.; Jiang, H. Modulating Affinities of Di-2-Picolylamine (DPA)-Substituted Quinoline Sensors for Zinc Ions by Varying Pendant Ligands. *Inorg. Chem.* **2008**, *47*, 4310–4318. [CrossRef]
142. Iyoshi, S.; Taki, M.; Yamamoto, Y. Rosamine-Based Fluorescent Chemosensor for Selective Detection of Silver(I) in an Aqueous Solution. *Inorg. Chem.* **2008**, *47*, 3946–3948. [CrossRef] [PubMed]
143. Miller, E.W.; He, Q.; Chang, C.J. Preparation and Use of Leadfluor-1, a Synthetic Fluorophore for Live-Cell Lead Imaging. *Nat. Protoc.* **2008**, *3*, 777–783. [CrossRef] [PubMed]
144. Wang, F.; Peng, R.; Sha, Y. Selective Dendritic Fluorescent Sensors for Zn(II). *Molecules* **2008**, *13*, 922–930. [CrossRef]
145. Kim, J.; Morozumi, T.; Kurumatani, N.; Nakamura, H. Novel Chemosensor for Alkaline Earth Metal Ion Based on 9-Anthryl Aromatic Amide Using a Naphthalene as a TICT Control Site and Intramolecular Energy Transfer Donor. *Tetrahedron Lett.* **2008**, *49*, 1984–1987. [CrossRef]
146. Kim, H.J.; Park, S.Y.; Yoon, S.; Kim, J.S. FRET-Derived Ratiometric Fluorescence Sensor for Cu^{2+}. *Tetrahedron* **2008**, *64*, 1294–1300. [CrossRef]

147. Duan, L.; Xu, Y.; Qian, X. Highly Sensitive and Selective Pd^{2+} Sensor of Naphthalimide Derivative Based on Complexation with Alkynes and Thio-Heterocycle. *Chem. Commun.* **2008**, *47*, 6339–6341. [CrossRef] [PubMed]
148. Che, Y.; Yang, X.; Zang, L. Ultraselective Fluorescent Sensing of Hg^{2+} through Metal Coordination-Induced Molecular Aggregation. *Chem. Commun.* **2008**, *12*, 1413–1415. [CrossRef]
149. Huang, W.; Zhu, X.; Wua, D.; He, C.; Hu, X.; Duan, C. Structural Modification of Rhodamine-Based Sensors toward Highly Selective Mercury Detection in Mixed Organic/Aqueous Media. *Dalton Trans.* **2009**, *47*, 10457–10465. [CrossRef]
150. Lu, H.; Zhang, S.; Liu, H.; Wang, Y.; Shen, Z.; Liu, C.; You, X. Experimentation and Theoretic Calculation of a BODIPY Sensor Based on Photoinduced Electron Transfer for Ions Detection. *J. Phys. Chem. A* **2009**, *113*, 14081–14086. [CrossRef]
151. Dodani, S.C.; He, Q.; Chang, C.J. A Turn-On Fluorescent Sensor for Detecting Nickel in Living Cells. *J. Am. Chem. Soc.* **2009**, *131*, 18020–18021. [CrossRef]
152. Ma, L.; Li, H.; Wu, Y. A Pyrene-Containing Fluorescent Sensor with High Selectivity for Lead(II) Ion in Water with Dual Illustration of Ground-State Dimer. *Sens. Actuators B Chem.* **2009**, *143*, 25–29. [CrossRef]
153. Gao, T.; Lee, K.M.; Yang, S.I. Synthesis and Characterization of Rhodamine Based Pb^{2+} Selective Fluorescence Sensor. *Toxicol. Environ. Health. Sci.* **2009**, *1*, 159–162. [CrossRef]
154. Younes, A.H.; Zhang, L.; Clark, R.J.; Zhu, L. Fluorescence of 5-Arylvinyl-5′-Methyl-2,2′-Bipyridyl Ligands and Their Zinc Complexes. *J. Org. Chem.* **2009**, *74*, 8761–8772. [CrossRef] [PubMed]
155. Lohani, C.R.; Kim, J.-M.; Lee, K.-H. Facile Synthesis of Anthracene-Appended Amino Acids as Highly Selective and Sensitive Fluorescent Fe^{3+} Ion Sensors. *Bioorg. Med. Chem. Lett.* **2009**, *19*, 6069–6073. [CrossRef]
156. Goswami, S.; Chakrabarty, R. Fluorescence Sensing of Cu^{2+} within a Pseudo 18-Crown-6 Cavity. *Tetrahedron Lett.* **2009**, *50*, 5910–5913. [CrossRef]
157. Mameli, M.; Aragoni, M.C.; Arca, M.; Atzori, M.; Bencini, A.; Bazzicalupi, C.; Blake, A.J.; Caltagirone, C.; Devillanova, F.A.; Garau, A.; et al. Synthesis and Coordination Properties of Quinoline Pendant Arm Derivatives of [9]AneN_3 and [9]AneN_2 S as Fluorescent Zinc Sensors. *Inorg. Chem.* **2009**, *48*, 9236–9249. [CrossRef]
158. Cheng, C.-C.; Chen, Z.-S.; Wu, C.-Y.; Lin, C.-C.; Yang, C.-R.; Yen, Y.-P. Azo Dyes Featuring a Pyrene Unit: New Selective Chromogenic and Fluorogenic Chemodosimeters for Hg(II). *Sens. Actuators B Chem.* **2009**, *142*, 280–287. [CrossRef]
159. Al-Sayah, M.H.; El-Chami, T.M. Spectroscopic Studies on a 'Turn-on' Fluorescent Sensor for Transition Metals with Selective 'Turn-off' for Mercury(II) Ions. *Supramol. Chem.* **2009**, *21*, 650–657. [CrossRef]
160. Zhou, Y.; Wang, F.; Kim, Y.; Kim, S.-J.; Yoon, J. Cu^{2+}-Selective Ratiometric and "Off-On" Sensor Based on the Rhodamine Derivative Bearing Pyrene Group. *Org. Lett.* **2009**, *11*, 4442–4445. [CrossRef] [PubMed]
161. Ganjali, M.R.; Veismohammadi, B.; Hosseini, M.; Norouzi, P. A New Tb^{3+}-Selective Fluorescent Sensor Based on 2-(5-(Dimethylamino)Naphthalen-1-Ylsulfonyl)-N-Henylhydrazinecarbothioamide. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* **2009**, *74*, 575–578. [CrossRef] [PubMed]
162. Rocha, A.; Marques, M.M.B.; Lodeiro, C. Synthesis and Characterization of Novel Indole-Containing Half-Crowns as New Emissive Metal Probes. *Tetrahedron Lett.* **2009**, *50*, 4930–4933. [CrossRef]
163. Zhao, Y.; Zhang, X.-B.; Han, Z.-X.; Qiao, L.; Li, C.-Y.; Jian, L.-X.; Shen, G.-L.; Yu, R.-Q. Highly Sensitive and Selective Colorimetric and Off−On Fluorescent Chemosensor for Cu^{2+} in Aqueous Solution and Living Cells. *Anal. Chem.* **2009**, *81*, 7022–7030. [CrossRef] [PubMed]
164. Weng, Y.; Chen, Z.; Wang, F.; Xue, L.; Jiang, H. High Sensitive Determination of Zinc with Novel Water-Soluble Small Molecular Fluorescent Sensor. *Anal. Chim. Acta* **2009**, *647*, 215–218. [CrossRef] [PubMed]
165. Lu, H.; Xiong, L.; Liu, H.; Yu, M.; Shen, Z.; Li, F.; You, X. A Highly Selective and Sensitive Fluorescent Turn-on Sensor for Hg^{2+} and Its Application in Live Cell Imaging. *Org. Biomol. Chem.* **2009**, *7*, 2554–2558. [CrossRef] [PubMed]
166. Zhang, L.; Fan, J.; Peng, X. X-Ray Crystallographic and Photophysical Properties of Rhodamine-Based Chemosensor for Fe^{3+}. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* **2009**, *73*, 398–402. [CrossRef] [PubMed]
167. Singh, N.; Kaur, N.; Callan, J.F. Incorporation of Siderophore Binding Sites in a Dipodal Fluorescent Sensor for Fe(III). *J. Fluoresc.* **2009**, *19*, 649–654. [CrossRef]
168. Kim, S.Y.; Hong, J.-I. Naphthalimide-Based Fluorescent Zn^{2+} Chemosensors Showing PET Effect According to Their Linker Length in Water. *Tetrahedron Lett.* **2009**, *50*, 2822–2824. [CrossRef]
169. Roy, P.; Dhara, K.; Manassero, M.; Banerjee, P. Synthesis, Characterization and Selective Fluorescent Zinc(II) Sensing Property of Three Schiff-Base Compounds. *Inorg. Chim. Acta* **2009**, *362*, 2927–2932. [CrossRef]
170. Chen, X.; Jou, M.J.; Lee, H.; Kou, S.; Lim, J.; Nam, S.-W.; Park, S.; Kim, K.-M.; Yoon, J. New Fluorescent and Colorimetric Chemosensors Bearing Rhodamine and Binaphthyl Groups for the Detection of Cu^{2+}. *Sens. Actuators B Chem.* **2009**, *137*, 597–602. [CrossRef]
171. Huang, J.; Xu, Y.; Qian, X. A Rhodamine-Based Hg^{2+} Sensor with High Selectivity and Sensitivity in Aqueous Solution: A NS_2 -Containing Receptor. *J. Org. Chem.* **2009**, *74*, 2167–2170. [CrossRef]
172. Wang, Y.-W.; Shi, Y.-T.; Peng, Y.; Zhang, A.-J.; Ma, T.-H.; Dou, W.; Zheng, J.-R. Fluorescent Sensors for Ca^{2+} and Pb^{2+} Based on Binaphthyl Derivatives. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* **2009**, *72*, 322–326. [CrossRef] [PubMed]
173. Singh, N.; Kaur, N.; Dunn, J.; MacKay, M.; Callan, J.F. A New Fluorescent Chemosensor for Iron(III) Based on the β-Aminobisulfonate Receptor. *Tetrahedron Lett.* **2009**, *50*, 953–956. [CrossRef]

174. Chatterjee, A.; Santra, M.; Won, N.; Kim, S.; Kim, J.K.; Kim, S.B.; Ahn, K.H. Selective Fluorogenic and Chromogenic Probe for Detection of Silver Ions and Silver Nanoparticles in Aqueous Media. *J. Am. Chem. Soc.* **2009**, *131*, 2040–2041. [CrossRef]
175. Dumas, S.; Grabchev, I.; Stoikova, P.; Chauvin, J.; Chovelon, J.-M. Synthesis of Benzanthron Derivatives for Selective Detection by Fluorescence of Copper Ions. *J. Photochem. Photobiol. A: Chem.* **2009**, *201*, 237–242. [CrossRef]
176. Jiao, L.; Li, J.; Zhang, S.; Wei, C.; Hao, E.; Vicente, M.G.H. A Selective Fluorescent Sensor for Imaging Cu^{2+} in Living Cells. *New J. Chem.* **2009**, *33*, 1888–1893. [CrossRef]
177. Hosseini, M.; Ganjali, M.R.; Abkenar, S.D.; Veismohammadi, B.; Riahl, S.; Norouzi, P.; Salavati-Niasari, M. Highly Selective Ratiometric Fluorescent Sensor for La(III) Ion Based on a New Schiff's Base. *Anal. Lett.* **2009**, *42*, 1029–1040. [CrossRef]
178. Huang, J.; Xu, Y.; Qian, X. A Red-Shift Colorimetric and Fluorescent Sensor for Cu^{2+} in Aqueous Solution: Unsymmetrical 4,5-Diaminonaphthalimide with N-H Deprotonation Induced by Metal Ions. *Org. Biomol. Chem.* **2009**, *7*, 1299–1303. [CrossRef]
179. Bojinov, V.B.; Georgiev, N.I.; Bosch, P. Design and Synthesis of Highly Photostable Yellow–Green Emitting 1,8-Naphthalimides as Fluorescent Sensors for Metal Cations and Protons. *J. Fluoresc.* **2009**, *19*, 127–139. [CrossRef] [PubMed]
180. Guo, Z.; Zhu, W.; Zhu, M.; Wu, X.; Tian, H. Near-Infrared Cell-Permeable Hg^{2+}-Selective Ratiometric Fluorescent Chemodosimeters and Fast Indicator Paper for $MeHg^{+}$ Based on Tricarbocyanines. *Chem. Eur. J.* **2010**, *16*, 14424–14432. [CrossRef] [PubMed]
181. Swamy, K.M.K.; Kim, M.-J.; Jeon, H.-R.; Jung, J.-Y.; Yoon, J.Y. New 7-Hydroxycoumarin-Based Fluorescent Chemosensors for Zn(II) and Cd(II). *Bull. Korean Chem. Soc.* **2010**, *31*, 3611–3616. [CrossRef]
182. Praveen, L.; Reddy, M.L.P.; Varma, R.L. Dansyl-Styrylquinoline Conjugate as Divalent Iron Sensor. *Tetrahedron Lett.* **2010**, *51*, 6626–6629. [CrossRef]
183. Wu, S.-P.; Wang, T.-H.; Liu, S.-R. A Highly Selective Turn-on Fluorescent Chemosensor for Copper(II) Ion. *Tetrahedron* **2010**, *66*, 9655–9658. [CrossRef]
184. Yu, M.R.; Gao, T.; Sun, H.-J.; Yang, S.I. Synthesis and Characterization of Pyrene/Quinoline Based Zn^{2+} Selective Fluorescent Sensor. *Toxicol. Environ. Health Sci.* **2010**, *2*, 158–161. [CrossRef]
185. Hosseini, M.; Vaezi, Z.; Ganjali, M.R.; Faridbod, F.; Abkenar, S.D.; Salavati-Niasari, M. Selective Recognition of Mercury in Waste Water Based on Fluorescence Enhancement Chemosensor. *Sen. Lett.* **2010**, *8*, 807–812. [CrossRef]
186. Wang, R.-M.; Huang, S.-B.; Zhao, N.; Chen, Z.-N. A New Zn^{2+} Chemosensor Based on Functionalized 8-Hydroxylquinoline. *Inorg. Chem. Commun.* **2010**, *13*, 1432–1434. [CrossRef]
187. Gao, T.; Yang, S.I. A New Rhodamine-Based Turn-on Fluorescent Chemosensor for Fe^{3+}. *Toxicol. Environ. Health Sci.* **2010**, *2*, 73–77. [CrossRef]
188. Huang, C.; Ren, A.; Feng, C.; Yang, N. Two-Photon Fluorescent Probe for Silver Ion Derived from Twin-Cyano-Stilbene with Large Two-Photon Absorption Cross Section. *Sens. Actuators B Chem.* **2010**, *151*, 236–242. [CrossRef]
189. Zhou, Y.; You, X.-Y.; Fang, Y.; Li, J.-Y.; Liu, K.; Yao, C. A Thiophen-Thiooxorhodamine Conjugate Fluorescent Probe for Detecting Mercury in Aqueous Media and Living Cells. *Org. Biomol. Chem.* **2010**, *8*, 4819–4822. [CrossRef]
190. Ambrosi, G.; Formica, M.; Fusi, V.; Giorgi, L.; Macedi, E.; Micheloni, M.; Paoli, P.; Pontellini, R.; Rossi, P. Efficient Fluorescent Sensors Based on 2,5-Diphenyl [1,3,4] Oxadiazole: A Case of Specific Response to Zn(II) at Physiological PH. *Inorg. Chem.* **2010**, *49*, 9940–9948. [CrossRef]
191. Goswami, S.; Sen, D.; Das, N.K.; Hazra, G. Highly Selective Colorimetric Fluorescence Sensor for Cu^{2+}: Cation-Induced 'Switching on' of Fluorescence Due to Excited State Internal Charge Transfer in the Red/near-Infrared Region of Emission Spectra. *Tetrahedron Lett.* **2010**, *51*, 5563–5566. [CrossRef]
192. Lee, D.Y.; Singh, N.; Kim, M.J.; Jang, D.O. Ratiometric Fluorescent Determination of Zn(II): A New Class of Tripodal Receptor Using Mixed Imine and Amide Linkages. *Tetrahedron* **2010**, *66*, 7965–7969. [CrossRef]
193. Jiang, L.; Wang, L.; Zhang, B.; Yin, G.; Wang, R. Cell Compatible Fluorescent Chemosensor for Hg^{2+} with High Sensitivity and Selectivity Based on the Rhodamine Fluorophore. *Eur. J. Inorg. Chem.* **2010**, *2010*, 4438–4443. [CrossRef]
194. Dong, M.; Ma, T.-H.; Zhang, A.-J.; Dong, Y.-M.; Wang, Y.-W.; Peng, Y. A Series of Highly Sensitive and Selective Fluorescent and Colorimetric "off-on" Chemosensors for Cu (II) Based on Rhodamine Derivatives. *Dye. Pigment.* **2010**, *87*, 164–172. [CrossRef]
195. Zhao, Y.; Sun, Y.; Lv, X.; Liu, Y.; Chen, M.; Guo, W. Rhodamine-Based Chemosensor for Hg^{2+} in Aqueous Solution with a Broad PH Range and Its Application in Live Cell Imaging. *Org. Biomol. Chem.* **2010**, *8*, 4143–4147. [CrossRef]
196. Jung, H.S.; Ko, K.C.; Lee, J.H.; Kim, S.H.; Bhuniya, S.; Lee, J.Y.; Kim, Y.; Kim, S.J.; Kim, J.S. Rationally Designed Fluorescence Turn-On Sensors: A New Design Strategy Based on Orbital Control. *Inorg. Chem.* **2010**, *49*, 8552–8557. [CrossRef]
197. Natali, M.; Soldi, L.; Giordani, S. A Photoswitchable Zn (II) Selective Spiropyran-Based Sensor. *Tetrahedron* **2010**, *66*, 7612–7617. [CrossRef]
198. Zhu, J.-F.; Yuan, H.; Chan, W.-H.; Lee, A.W.M. A Colorimetric and Fluorescent Turn-on Chemosensor Operative in Aqueous Media for Zn2+ Based on a Multifunctionalized Spirobenzopyran Derivative. *Org. Biomol. Chem.* **2010**, *8*, 3957–3964. [CrossRef]
199. Wang, X.; Cao, J.; Chen, C. A Highly Efficient and Selective Turn-on Fluorescent Sensor for Cu^{2+} Ion. *Chin. J. Chem.* **2010**, *28*, 1777–1779. [CrossRef]
200. Mashraqui, S.H.; Betkar, R.; Chandiramani, M.; Poonia, K.; Quinonero, D.; Frontera, A. New 1,8-Naphthyridine-Based Probes for the Selective Fluorescence Signalling of Toxic Cadmium: Synthesis, Photophysical Studies and Molecular Modelling. *Supramol. Chem.* **2010**, *22*, 524–531. [CrossRef]

201. Wang, X.M.; Yan, H.; Feng, X.L.; Chen, Y. 1-Pyrenecarboxaldehyde Thiosemicarbazone: A Novel Fluorescent Molecular Sensor towards Mercury (II) Ion. *Chin. Chem. Lett.* **2010**, *21*, 1124–1128. [CrossRef]
202. Lin, W.; Cao, X.; Ding, Y.; Yuan, L.; Yu, Q. A Reversible Fluorescent Hg^{2+} Chemosensor Based on a Receptor Composed of a Thiol Atom and an Alkene Moiety for Living Cell Fluorescence Imaging. *Org. Biomol. Chem.* **2010**, *8*, 3618–3620. [CrossRef] [PubMed]
203. Zou, Q.; Tian, H. Chemodosimeters for Mercury(II) and Methylmercury(I) Based on 2,1,3-Benzothiadiazole. *Sens. Actuators B Chem.* **2010**, *149*, 20–27. [CrossRef]
204. Ciesienski, K.L.; Hyman, L.M.; Derisavifard, S.; Franz, K.J. Toward the Detection of Cellular Copper(II) by a Light-Activated Fluorescence Increase. *Inorg. Chem.* **2010**, *49*, 6808–6810. [CrossRef]
205. Pibiri, I.; Palumbo Piccionello, A.; Calabrese, A.; Buscemi, S.; Vivona, N.; Pace, A. Fluorescent Hg^{2+} Sensors: Synthesis and Evaluation of a Tren-Based Starburst Molecule Containing Fluorinated 1,2,4-Oxadiazoles. *Eur. J. Org. Chem.* **2010**, *2010*, 4549–4553. [CrossRef]
206. Jung, H.J.; Singh, N.; Lee, D.Y.; Jang, D.O. Single Sensor for Multiple Analytes: Chromogenic Detection of I−and Fluorescent Detection of Fe^{3+}. *Tetrahedron Lett.* **2010**, *51*, 3962–3965. [CrossRef]
207. Lu, X.; Zhu, W.; Xie, Y.; Li, X.; Gao, Y.; Li, F.; Tian, H. Near-IR Core-Substituted Naphthalenediimide Fluorescent Chemosensors for Zinc Ions: Ligand Effects on PET and ICT Channels. *Chem. Eur. J.* **2010**, *16*, 8355–8364. [CrossRef]
208. Staneva, D.; McKena, M.; Bosch, P.; Grabchev, I. Synthesis and Spectroscopic Studies of a New 1,8-Naphthalimide Dyad as Detector for Metal Cations and Protons. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* **2010**, *76*, 150–154. [CrossRef]
209. Xi, P.; Dou, J.; Huang, L.; Xu, M.; Chen, F.; Wu, Y.; Bai, D.; Li, W.; Zeng, Z. A Selective Turn-on Fluorescent Sensor for Cu(II) and Its Application in Imaging in Living Cells. *Sens. Actuators B Chem.* **2010**, *148*, 337–341. [CrossRef]
210. Li, H.-W.; Wang, B.; Dang, Y.-Q.; Li, L.; Wu, Y. A Highly Selective Fluorescent Sensor for Mercury Ions in Aqueous Solution: Detection Based on Target-Induced Aggregation. *Sens. Actuators B Chem.* **2010**, *148*, 49–53. [CrossRef]
211. Bojinov, V.B.; Georgiev, N.I.; Marinova, N.V. Design and Synthesis of Highly Photostable Fluorescence Sensing 1,8-Naphthalimide-Based Dyes Containing s-Triazine UV Absorber and HALS Units. *Sens. Actuators B Chem.* **2010**, *148*, 6–16. [CrossRef]
212. Moon, K.-S.; Yang, Y.-K.; Ji, S.; Tae, J. Aminoxy-Linked Rhodamine Hydroxamate as Fluorescent Chemosensor for Fe^{3+} in Aqueous Media. *Tetrahedron Lett.* **2010**, *51*, 3290–3293. [CrossRef]
213. Lin, W.-C.; Wu, C.-Y.; Liu, Z.-H.; Lin, C.-Y.; Yen, Y.-P. A New Selective Colorimetric and Fluorescent Sensor for Hg^{2+} and Cu^{2+} Based on a Thiourea Featuring a Pyrene Unit. *Talanta* **2010**, *81*, 1209–1215. [CrossRef] [PubMed]
214. Milewska, M.; Guzow, K.; Wiczk, W. Fluorescent Chemosensors for Metal Ions Based on 3-(2-Benzoxazol-5-Yl)Alanine Skeleton. *Open Chem.* **2010**, *8*, 674–686. [CrossRef]
215. Martínez, R.; Espinosa, A.; Tárraga, A.; Molina, P. A New Bis(Pyrenyl)Azadiene-Based Probe for the Colorimetric and Fluorescent Sensing of Cu(II) and Hg(II). *Tetrahedron* **2010**, *66*, 3662–3667. [CrossRef]
216. Chen, Y.-B.; Wang, Y.-J.; Lin, Y.-J.; Hu, C.-H.; Chen, S.-J.; Chir, J.-L.; Wu, A.-T. A Water-Soluble Ribosyl-Based Fluorescent Sensor for Hg^{2+} and Cu^{2+} Ions. *Carbohydr. Res.* **2010**, *345*, 956–959. [CrossRef]
217. Yıldırım, M.; Kaya, İ. Synthesis of a Novel Fluorescent Schiff Base as a Possible Cu(II) Ion Selective Sensor. *J. Fluoresc.* **2010**, *20*, 771–777. [CrossRef]
218. Liu, Z.; Wang, B.; Yang, Z.; Li, T.; Li, Y. A Novel Fluorescent Chemosensor for Zn(II) Based on 1,2-(2′-Oxoquinoline-3′-Yl-Methylideneimino)Ethane. *Inorg. Chem. Commun.* **2010**, *13*, 606–608. [CrossRef]
219. Ma, T.-H.; Zhang, A.-J.; Dong, M.; Dong, Y.-M.; Peng, Y.; Wang, Y.-W. A Simply and Highly Selective "Turn-on" Type Fluorescent Chemosensor for Hg^{2+} Based on Chiral BINOL-Schiff's Base Ligand. *J. Lumin.* **2010**, *130*, 888–892. [CrossRef]
220. Tamanini, E.; Flavin, K.; Motevalli, M.; Piperno, S.; Gheber, L.A.; Todd, M.H.; Watkinson, M. Cyclam-Based "Clickates": Homogeneous and Heterogeneous Fluorescent Sensors for Zn(II). *Inorg. Chem.* **2010**, *49*, 3789–3800. [CrossRef]
221. Han, Z.-X.; Zhang, X.-B.; Li, Z.; Gong, Y.-J.; Wu, X.-Y.; Jin, Z.; He, C.-M.; Jian, L.-X.; Zhang, J.; Shen, G.-L.; et al. Efficient Fluorescence Resonance Energy Transfer-Based Ratiometric Fluorescent Cellular Imaging Probe for Zn^{2+} Using a Rhodamine Spirolactam as a Trigger. *Anal. Chem.* **2010**, *82*, 3108–3113. [CrossRef]
222. Zhu, M.-Q.; Gu, Z.; Zhang, R.; Xiang, J.-N.; Nie, S. A Stilbene-Based Fluoroionophore for Copper Ion Sensing in Both Reduced and Oxidized Environments. *Talanta* **2010**, *81*, 678–683. [CrossRef] [PubMed]
223. Hosseini, M.; Ganjali, M.R.; Veismohammadi, B.; Norouzi, P.; Alizadeh, K.; Abkenar, S.D. A Novel Ratiometric Fluorescent Yb^{3+} Sensor Based on a N′-(1-Oxoacenaphthylen-2(1H)-Ylidene)Furan-2-Carbohydrazide as a Suitable Fluorophore. *Mater. Sci. Eng. C* **2010**, *30*, 348–351. [CrossRef]
224. Wan, Y.; Guo, Q.; Wang, X.; Xia, A. Photophysical Properties of Rhodamine Isomers: A Two-Photon Excited Fluorescent Sensor for Trivalent Chromium Cation (Cr^{3+}). *Anal. Chim. Acta* **2010**, *665*, 215–220. [CrossRef] [PubMed]
225. Wang, S.; Men, G.; Zhao, L.; Hou, Q.; Jiang, S. Binaphthyl-Derived Salicylidene Schiff Base for Dual-Channel Sensing of Cu, Zn Cations and Integrated Molecular Logic Gates. *Sens. Actuators B Chem.* **2010**, *145*, 826–831. [CrossRef]
226. Hu, Z.-Q.; Yang, X.-D.; Cui, C.-L.; Ding, L.; Lin, C.-S.; Lu, H.-Y.; Wang, L. 1,8-Anthrancene Disulfonamide: A Simple but Highly Sensitive and Selective Fluorescent Chemosensor for Hg^{2+} in Aqueous Media. *Sens. Actuators B Chem.* **2010**, *145*, 61–65. [CrossRef]
227. Wanichacheva, N.; Watpathomsub, S.; Lee, V.S.; Grudpan, K. Synthesis of a Novel Fluorescent Sensor Bearing Dansyl Fluorophores for the Highly Selective Detection of Mercury (II) Ions. *Molecules* **2010**, *15*, 1798–1810. [CrossRef] [PubMed]
228. Wang, H.; Wang, D.; Wang, Q.; Li, X.; Schalley, C.A. Nickel(II) and Iron(III) Selective off-on-Type Fluorescence Probes Based on Perylene Tetracarboxylic Diimide. *Org. Biomol. Chem.* **2010**, *8*, 1017–1026. [CrossRef]

229. Bojinov, V.B.; Panova, I.P.; Simeonov, D.B.; Georgiev, N.I. Synthesis and Sensor Activity of Photostable Blue Emitting 1,8-Naphthalimides Containing s-Triazine UV Absorber and HALS Fragments. *J. Photochem. Photobiol. A Chem.* **2010**, *210*, 89–99. [CrossRef]
230. Chen, T.; Zhu, W.; Xu, Y.; Zhang, S.; Zhang, X.; Qian, X. A Thioether-Rich Crown-Based Highly Selective Fluorescent Sensor for Hg^{2+} and Ag^{+} in Aqueous Solution. *Dalton Trans.* **2010**, *39*, 1316–1320. [CrossRef]
231. Goswami, S.; Sen, D.; Das, N.K. A New Highly Selective, Ratiometric and Colorimetric Fluorescence Sensor for Cu^{2+} with a Remarkable Red Shift in Absorption and Emission Spectra Based on Internal Charge Transfer. *Org. Lett.* **2010**, *12*, 856–859. [CrossRef]
232. Lee, D.Y.; Singh, N.; Jang, D.O. A Benzimidazole-Based Single Molecular Multianalyte Fluorescent Probe for the Simultaneous Analysis of Cu^{2+} and Fe^{3+}. *Tetrahedron Lett.* **2010**, *51*, 1103–1106. [CrossRef]
233. Li, L.; Dang, Y.-Q.; Li, H.-W.; Wang, B.; Wu, Y. Fluorescent Chemosensor Based on Schiff Base for Selective Detection of Zinc(II) in Aqueous Solution. *Tetrahedron Lett.* **2010**, *51*, 618–621. [CrossRef]
234. Xu, Z.; Baek, K.-H.; Kim, H.N.; Cui, J.; Qian, X.; Spring, D.R.; Shin, I.; Yoon, J. Zn^{2+} -Triggered Amide Tautomerization Produces a Highly Zn^{2+} -Selective, Cell-Permeable, and Ratiometric Fluorescent Sensor. *J. Am. Chem. Soc.* **2010**, *132*, 601–610. [CrossRef] [PubMed]
235. Mameli, M.; Aragoni, M.C.; Arca, M.; Caltagirone, C.; Demartin, F.; Farruggia, G.; De Filippo, G.; Devillanova, F.A.; Garau, A.; Isaia, F.; et al. A Selective, Nontoxic, OFF-ON Fluorescent Molecular Sensor Based on 8-Hydroxyquinoline for Probing Cd^{2+} in Living Cells. *Chem. A Eur. J.* **2010**, *16*, 919–930. [CrossRef] [PubMed]
236. Wang, H.-H.; Xue, L.; Qian, Y.-Y.; Jiang, H. Novel Ratiometric Fluorescent Sensor for Silver Ions. *Org. Lett.* **2010**, *12*, 292–295. [CrossRef] [PubMed]
237. Hanaoka, K.; Muramatsu, Y.; Urano, Y.; Terai, T.; Nagano, T. Design and Synthesis of a Highly Sensitive Off–On Fluorescent Chemosensor for Zinc Ions Utilizing Internal Charge Transfer. *Chem. Eur. J.* **2010**, *16*, 568–572. [CrossRef]
238. Hu, Z.-Q.; Lin, C.; Wang, X.-M.; Ding, L.; Cui, C.-L.; Liu, S.-F.; Lu, H.Y. Highly Sensitive and Selective Turn-on Fluorescent Chemosensor for Pb^{2+} and Hg^{2+} Based on a Rhodamine–Phenylurea Conjugate. *Chem. Commun.* **2010**, *46*, 3765–3767. [CrossRef]
239. Moro, A.J.; Cywinski, P.J.; Körsten, S.; Mohr, G.J. An ATP Fluorescent Chemosensor Based on a Zn(II)-Complexed Dipicolylaminereceptor Coupled with a Naphthalimidechromophore. *Chem. Commun.* **2010**, *46*, 1085–1087. [CrossRef]
240. Ashokkumar, P.; Ramakrishnan, V.T.; Ramamurthy, P. Photoinduced Electron Transfer (PET) Based Zn^{2+} Fluorescent Probe: Transformation of Turn-On Sensors into Ratiometric Ones with Dual Emission in Acetonitrile. *J. Phys. Chem. A* **2011**, *115*, 14292–14299. [CrossRef]
241. Lee, S.; Lee, J.H.; Pradhan, T.; Lim, C.S.; Cho, B.R.; Bhuniya, S.; Kim, S.; Kim, J.S. Fluorescent Turn-on Zn^{2+} Sensing in Aqueous and Cellular Media. *Sens. Actuators B Chem.* **2011**, *160*, 1489–1493. [CrossRef]
242. Wang, H.-H.; Xue, L.; Yu, C.-L.; Qian, Y.-Y.; Jiang, H. Rhodamine-Based Fluorescent Sensor for Mercury in Buffer Solution and Living Cells. *Dye. Pigment.* **2011**, *91*, 350–355. [CrossRef]
243. Gong, Z.-L.; Ge, F.; Zhao, B.-X. Novel Pyrazoline-Based Selective Fluorescent Sensor for Zn^{2+} in Aqueous Media. *Sens. Actuators B Chem.* **2011**, *159*, 148–153. [CrossRef]
244. Wanichacheva, N.; Kumsorn, P.; Sangsuwan, R.; Kamkaew, A.; Lee, V.S.; Grudpan, K. A New Fluorescent Sensor Bearing Three Dansyl Fluorophores for Highly Sensitive and Selective Detection of Mercury(II) Ions. *Tetrahedron Lett.* **2011**, *52*, 6133–6136. [CrossRef]
245. Wang, Y.; Huang, Y.; Li, B.; Zhang, L.; Song, H.; Jiang, H.; Gao, J. A Cell Compatible Fluorescent Chemosensor for Hg^{2+} Based on a Novel Rhodamine Derivative That Works as a Molecular Keypad Lock. *RSC Adv.* **2011**, *1*, 1294–1300. [CrossRef]
246. Dai, H.; Liu, F.; Gao, Q.; Fu, T.; Kou, X. A Highly Selective Fluorescent Sensor for Mercury Ion (II) Based on Azathia-Crown Ether Possessing a Dansyl Moiety. *Luminescence* **2011**, *26*, 523–530. [CrossRef]
247. Carney, P.; Lopez, S.; Mickley, A.; Grinberg, K.; Zhang, W.; Dai, Z. Multimode Selective Detection of Mercury by Chiroptical Fluorescent Sensors Based on Methionine/Cysteine. *Chirality* **2011**, *23*, 916–920. [CrossRef] [PubMed]
248. Azadbakht, R.; Parviz, M.; Tamari, E.; Keypour, H.; Golbedaghi, R. Highly Selective Fluorescent Recognition of Zn^{2+} Based on Naphthalene Macrocyclic Derivative. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* **2011**, *82*, 200–204. [CrossRef] [PubMed]
249. Abebe, F.A.; Eribal, C.S.; Ramakrishna, G.; Sinn, E. A 'Turn-on' Fluorescent Sensor for the Selective Detection of Cobalt and Nickel Ions in Aqueous Media. *Tetrahedron Lett.* **2011**, *52*, 5554–5558. [CrossRef]
250. Vallejos, S.; Estévez, P.; Ibeas, S.; Muñoz, A.; García, F.C.; Serna, F.; García, J.M. A Selective and Highly Sensitive Fluorescent Probe of Hg^{2+} in Organic and Aqueous Media: The Role of a Polymer Network in Extending the Sensing Phenomena to Water Environments. *Sens. Actuators B Chem.* **2011**, *157*, 686–690. [CrossRef]
251. Dalapati, S.; Paul, B.K.; Jana, S.; Guchhait, N. Highly Selective and Sensitive Fluorescence Reporter for Toxic Hg(II) Ion by a Synthetic Symmetrical Azine Derivative. *Sens. Actuators B Chem.* **2011**, *157*, 615–620. [CrossRef]
252. Chen, L.; Yang, L.; Li, H.; Gao, Y.; Deng, D.; Wu, Y.; Ma, L. Tridentate Lysine-Based Fluorescent Sensor for Hg(II) in Aqueous Solution. *Inorg. Chem.* **2011**, *50*, 10028–10032. [CrossRef] [PubMed]
253. Zhao, Q.; Li, R.-F.; Xing, S.-K.; Liu, X.-M.; Hu, T.-L.; Bu, X.-H. A Highly Selective On/Off Fluorescence Sensor for Cadmium(II). *Inorg. Chem.* **2011**, *50*, 10041–10046. [CrossRef]
254. Wen, J.; Geng, Z.; Yin, Y.; Wang, Z. A Versatile Water Soluble Fluorescent Probe for Ratiometric Sensing of Hg^{2+} and Bovine Serum Albumin. *Dalton Trans.* **2011**, *40*, 9737–9745. [CrossRef] [PubMed]

255. Abebe, F.A.; Sinn, E. Fluorescein-Based Fluorescent and Colorimetric Chemosensors for Copper in Aqueous Media. *Tetrahedron Lett.* **2011**, *52*, 5234–5237. [CrossRef]
256. Yang, M.-H.; Thirupathi, P.; Lee, K.-H. Selective and Sensitive Ratiometric Detection of Hg(II) Ions Using a Simple Amino Acid Based Sensor. *Org. Lett.* **2011**, *13*, 5028–5031. [CrossRef] [PubMed]
257. Narayanaswamy, N.; Maity, D.; Govindaraju, T. Reversible Fluorescence Sensing of Zn^{2+} Based on Pyridine-Constrained *Bis* (Triazole-Linked Hydroxyquinoline) Sensor. *Supramol. Chem.* **2011**, *23*, 703–709. [CrossRef]
258. Gou, C.; Qin, S.-H.; Wu, H.-Q.; Wang, Y.; Luo, J.; Liu, X.-Y. A Highly Selective Chemosensor for Cu^{2+} and Al^{3+} in Two Different Ways Based on Salicylaldehyde Schiff. *Inorg. Chem. Commun.* **2011**, *14*, 1622–1625. [CrossRef]
259. Goswami, S.; Das, N.K.; Aich, K.; Sen, D. A Naphthyridine Based Macrocyclic "Switching on" Fluorescent Receptor for Cadmium. *J. Lumin.* **2011**, *131*, 2185–2188. [CrossRef]
260. Maity, D.; Manna, A.K.; Karthigeyan, D.; Kundu, T.K.; Pati, S.K.; Govindaraju, T. Visible-Near-Infrared and Fluorescent Copper Sensors Based on Julolidine Conjugates: Selective Detection and Fluorescence Imaging in Living Cells. *Chem. Eur. J.* **2011**, *17*, 11152–11161. [CrossRef]
261. Hou, J.-T.; Zhang, Q.-F.; Xu, B.-Y.; Lu, Q.-S.; Liu, Q.; Zhang, J.; Yu, X.-Q. A Novel BINOL-Based Cyclophane via Click Chemistry: Synthesis and Its Applications for Sensing Silver Ions. *Tetrahedron Lett.* **2011**, *52*, 4927–4930. [CrossRef]
262. Hou, C.; Urbanec, A.M.; Cao, H. A Rapid Hg^{2+} Sensor Based on Aza-15-Crown-5 Ether Functionalized 1,8-Naphthalimide. *Tetrahedron Lett.* **2011**, *52*, 4903–4905. [CrossRef]
263. Tang, L.; Li, F.; Liu, M.; Nandhakumar, R. A New Rhodamine B-Coumarin Fluorochrome for Colorimetric Recognition of Cu^{2+} and Fluorescent Recognition of Fe^{3+} in Aqueous Media. *Bull. Korean Chem. Soc.* **2011**, *32*, 3400–3404. [CrossRef]
264. Neupane, L.N.; Thirupathi, P.; Jang, S.; Jang, M.J.; Kim, J.H.; Lee, K.-H. Highly Selectively Monitoring Heavy and Transition Metal Ions by a Fluorescent Sensor Based on Dipeptide. *Talanta* **2011**, *85*, 1566–1574. [CrossRef] [PubMed]
265. Praveen, L.; Suresh, C.H.; Reddy, M.L.P.; Luxmi Varma, R. Molecular Fluorescent Probe for Zn^{2+} Based on 2-(2-Nitrostyryl)-8-Methoxyquinoline. *Tetrahedron Lett.* **2011**, *52*, 4730–4733. [CrossRef]
266. Ruan, Y.-B.; Maisonneuve, S.; Xie, J. Highly Selective Fluorescent and Colorimetric Sensor for Hg^{2+} Based on Triazole-Linked NBD. *Dye. Pigment.* **2011**, *90*, 239–244. [CrossRef]
267. GeorgeGamov/Prediction of Sensing Ability GitLab. Available online: https://gitlab.com/GeorgeGamov/prediction-of-sensing-ability (accessed on 10 February 2023).
268. Bannwarth, C.; Ehlert, S.; Grimme, S. GFN2-XTB—An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions. *J. Chem. Theory Comput.* **2019**, *15*, 1652–1671. [CrossRef] [PubMed]
269. Welcome to Levenshtein's Documentation!—Levenshtein 0.20.9 Documentation. Available online: https://maxbachmann.github.io/Levenshtein/ (accessed on 9 February 2023).
270. RDKit. Available online: http://www.rdkit.org/ (accessed on 9 March 2023).
271. Scikit-Learn: Machine Learning in Python—Scikit-Learn 1.2.2 Documentation. Available online: https://scikit-learn.org/stable/ (accessed on 9 March 2023).
272. Aiogram. Available online: https://aiogram.dev/ (accessed on 9 March 2023).