Discovery of Record-Breaking Metal-Organic Frameworks for Methane Storage using Evolutionary Algorithm and Machine Learning

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Abstract

In the past decade, there has been a rise in a number of computational screening works to facilitate finding optimal metal-organic frameworks (MOF) for variety of different applications. Unfortunately, most of these screening works are limited to its initial set of materials and result in brute-force type of a screening approach. In this work, we present a systematic strategy that can find materials with desired property from an extremely diverse and large MOF set of over 100 trillion possible MOFs using machine learning and evolutionary algorithm. It is demonstrated that our algorithm can discover 964 MOFs with methane working capacity over $200 \text{ cm}^3 \text{ cm}^{-3}$ and 96 MOFs with methane working capacity over $208 \text{ cm}^3 \text{ cm}^{-3}$, which is the current world record. We believe that this methodology can facilitate a new type of a screening approach that takes advantage of the modular nature in MOFs, and can readily be extended to other important applications as well.

Introduction

The modular and tunable nature of metal-organic frameworks (MOFs) makes it an attractive class of materials that can lead to precise design catered towards different applications. One can in principle synthesize an infinite number of MOFs by using the degree of freedom available in terms of different linkers, functional groups, metal nodes, defects, etc. As such, although over 100,000 MOFs have been experimentally synthesized thus far¹, it goes without saying that only a minuscule section of the entire MOF search space has been explored.

To accelerate the search for optimal MOFs, various computational screening works have been conducted to identify the best materials for applications such as methane storage²⁻⁴, carbon-capture^{5,6} and hydrogen storage^{7,8}. Unfortunately, many of these methods used in computational screening are deficient in the sense that they utilize the brute-force algorithm to compute properties for all the MOFs within the database, leading to inefficient allocation of computational resources. Moreover, most of these works start with a given MOF database and as such are limited to exploring only the materials within this database, putting a very low ceiling on the number of materials that can be explored.

To remedy these issues, one can envision a more evolutionary approach where the modular nature of the MOFs is used to its fullest advantage. If there was a capability to compute the material properties of a MOF just from its building blocks (i.e. metal nodes and linkers), then an evolutionary algorithm approach can be applied to mix and match these building blocks to find the optimal MOFs for a given application. Within this paradigm, one can in principle explore a far greater number of MOFs compared to conventional computational screening (over trillion versus millions) and significantly enhance the materials space of the MOFs. It needs to be pointed out that similar approaches have been applied by other researchers but their methods were limited by the lack of diversity in the

topology and the metal clusters explored^{9,10}. Recently, Zhang et al. generated optimal organic linkers to find high-performance MOFs¹¹, but this work also has similar limitations. Moreover, although there are new machine learning methods¹² and genetic algorithm¹³ used to quickly obtain optimal materials for applications, they are only applicable to the existing MOF database.

In this work, we combined evolutionary algorithm and machine learning to explore a MOF space of over 100 trillion materials to find structures with optimal methane storage properties. Methane storage, especially in the context of adsorbed natural gas (ANG) vehicles, is viewed as a clean energy alternative to other gasoline-based vehicles. Recently, the U.S. Department of Energy (DOE) set a target methane working capacity (WC; uptake difference between adsorption and desorption from 65 to 5.8 bar at $T = 298\text{ K}$) for ANG technology at $315\text{ cm}^3\text{ cm}^{-3}$ at which it becomes competitive with the commercially available compressed natural gas (CNG) vehicles. Despite enormous efforts to find MOFs that satisfy the target performance, the current world record is $208\text{ cm}^3\text{ cm}^{-3}$ (MOF-519)¹⁴ and the 2nd world record is $191.3\text{ cm}^3\text{ cm}^{-3}$ (NJU-Bai 43)¹⁵.

From the computational point of view, many screening works were conducted on both synthesized and hypothetical porous materials to find high-performing materials for methane storage²⁻⁴. However, despite screening over million materials, these studies only led to structures with WC as high as $206\text{ cm}^3\text{ cm}^{-3}$. Given the small number of predicted materials with high-performance capabilities, there is not a large set for experimentalists to work with in terms of testing the predictions made by the theoreticians. It is our opinion that providing a much larger pool of candidate structures is essential for these high-throughput screening works such that experimentalists can further narrow down the optimal materials for synthesis purposes based on various factors (e.g. availability of linkers, facile synthesis, cost

of materials, potential stability issues) that are outside of the scope provided by conventional computational screening.

In this work, we address this issue by looking at a very large MOF search space (over 100 trillion) with the goal of providing the experimentalists as many different candidate materials for future synthesis purposes. Accordingly, our algorithm managed to discover 964 MOFs with WC $200\text{ cm}^3\text{ cm}^{-3}$ and 96 MOFs that break the current record of WC $> 208\text{ cm}^3\text{ cm}^{-3}$. Moreover, given that our algorithm generates new materials iteratively, we are not confined to the current database of MOFs unlike many of the other screening studies. It is our opinion that this type of evolutionary algorithm can replace the more conventional brute-force search-based computational algorithm and provide both efficient and wider range of optimal candidates for different applications.

Methods

Building block construction. The molecular building blocks are obtained by removing single bonds that connect the metal cluster and the organic linker for a given MOF (see Fig. 1a for example). In the resulting building blocks, connection points that can form chemical bonds to another block were assigned to be located at the midpoint of the original bonds that were removed. The building blocks with more than two connection points are classified as “node” building block (NBB) (Fig. 1b, 1c) and the building blocks with two connection points are classified as “edge” building block (EBB) (Fig. 1d, 1e). The reason behind this distinction is that due to the number of connection points, the NBBs fit only in the node of a given topology while EBBs fit only in the edge of the given topology. Altogether, 71 (13 inorganic NBB, 12 organic NBB, 46 organic EBB) building blocks were collected from the software ToBaCCo^{16,17} and 796 (507 inorganic NBB, 116 organic NBB, 19 inorganic EBB,

154 organic EBB) building blocks were obtained from the CoRE MOF database¹⁸ using our own script that extracted all the available building blocks. We named NBBs in a combination of the starting letters N and index (e.g., N1, N2) and similarly named EBBs using the starting letters E (e.g., E1, E2). Information and visualization of building blocks can be found in SI.

Fig. 1. Definition of building blocks and the example visualization of the type of building blocks. **a**, a sample IRMOF-1 unit cell structure with the connection points formed at the center of the removed bonds. **b**, organic node building block (4 connection points). **c**, inorganic node building block (6 connection points). **d**, organic edge building block (2 connection points). **e**, inorganic edge building block (2 connection points). Thin red sticks in **b** to **e** indicate bonds between connection points and the atomic part of the building block.

Construction of hypothetical MOFs. Recently, different topology-based MOF constructors have been developed by different groups^{16,17,19–21}. However these constructors do not use metal clusters with low symmetry, which restricts the number of possible metal clusters, and as such restricting the diversity and the number of the possible MOF that can be built. To utilize a more general purpose porous material constructor, we developed a Python library from scratch and named it *pormake* (**porous material maker**). Using *pormake*, MOFs with arbitrary topologies and building blocks (except for the one-dimensional infinite rod building block) can be constructed. In order to successfully construct new MOFs from building blocks and a user-specified topology, the NBBs should be positioned with the optimal orientation to fit the nodes in the topology. Our algorithm can find the globally optimal orientation in $O(N^3)$ time complexity for arbitrary building blocks where N is the number of connection points (see SI).

A given topology consists of nodes and edges that can fit the building blocks. While *pormake* can assign different building blocks for each node and edge in the topology, we decided to limit the diversity to one building block per node type (or edge type) in this work to align with experimental synthesis feasibility. In the case of nodes, the symmetrically identical nodes are assigned to the same type as typically used in topologies. However, in the case of edges, the type of edge was determined according to the type of two nodes that the edge connects (Fig. 2).

Fig. 2. The visual description of node and edge type in the topology. **a**, visualization of full **zxc** topology. **b**, type of nodes in the **zxc** topology. **c**, type of edges in the **zxc** topology. The nodes with the same color (e.g. red and red) are symmetrically identical.

In building our hypothetical MOFs, only the topologies that contain less than four nodes and four edge types were considered, as complex topologies tend to be more difficult to synthesize experimentally. Also, the direct connection between two adjacent NBBs without an EBB are allowed (For example, HKUST-1 structure can be constructed from N17 (i.e. Cu-paddlewheel), N10 (i.e. 1,3,5-BTC) building blocks and the **tbo** topology without needing an EBB).

From 648 NBBs, 219 EBBs, and 1775 topologies, around 247 trillion MOFs can be

generated in principle under the constraints put forth in our model. From this set, MOFs with cell lengths larger than 60 Å and/or those with more than 1500 atoms in the unit cell were discarded to reduce the computational cost.

Deep learning prediction model: MOF-NET. To find the optimal MOFs using the genetic algorithm type of a strategy, one would inevitably need to conduct a large number of GCMC simulations. As such, it becomes important to minimize the expensive GCMC simulations and one can resort to using machine/deep learning type of models to predict the uptakes of a given gas molecule from the topology and the building blocks (thereby replacing the GCMC simulations). Because there is no such machine learning model, we developed an artificial neural network (ANN) which we named MOF-NET. We chose the embedding technique for the representation of the topology and the building blocks similar to the word embedding in Word2Vec²². Each topology and building block is mapped to a fixed-length vector initialized with random numbers and the vectors are also trained during the learning process. Other representations and ANN architecture were considered but due to the importance of independently retaining the topology information, we opted the aforementioned embedding technique (see SI for detail on MOF representations).

In the fully connected layer (also known as dense layer) of neural networks, the weight of the layer determines how the input vector information is to be processed and the resulting value of the output vector. Therefore, since the input consists of building block embeddings (i.e. information about metal nodes and linkers), we designed an architecture in which the weight of layer is produced directly from the topology embedding such that the topology can determine how the NBBs and EBBs will be processed in the subsequent layers of the neural network. In our architecture, we wanted to describe the structural change in

building blocks themselves and the mutual effects between building blocks separately. Therefore, we designed the topology to generate weights that consider each contribution. The weight that captures changes in building blocks was named self-interaction weight and the weight that captures the mutual effect between building blocks was named interaction weight. All the weights are generated using a single fully connected layer from topology embedding (see Fig. 3a). Two self-interaction weights for NBBs ($\mathbf{W}_{\text{self,NBB}}$) and EBBs ($\mathbf{W}_{\text{self,EBB}}$) (green and red box in Fig. 3a) and interaction weight (purple box in Fig. 3a) are generated from the fully connected layers. Except for the weights generating layers, the MOF-NET takes 3 embeddings of NBBs and 3 embeddings of EBBs because the maximum number of node and edge types in topology is three for each (Fig. 3b). For the topologies having less than three types of nodes or edges, zero vectors are padded. Each of the given building block embeddings is processed by $\mathbf{W}_{\text{self,NBB}}$ and $\mathbf{W}_{\text{self,EBB}}$, and then the output vectors are concatenated and then processed by $\mathbf{W}_{\text{inter}}$. Afterward, a vector that contains essential information of a MOF is obtained (yellow box in Fig. 3b) and we named this vector as MOF embedding. Two conventional fully connected layers are applied to the MOF embedding to get the target property (WC in our case). The details regarding the MOF-NET architecture and training can be found SI.

Fig. 3. Schematics of the MOF-NET architecture. The word “Dense” refers to fully connected layers. **a**, Topology embedding and the generated weights from topology embedding. $W_{\text{self,NBB}}$ is the self-interaction weight for NBBs, $W_{\text{self,EBB}}$ is the self-interaction weight for EBBs and W_{inter} is the interaction weight. **b**, The main architecture of MOF-NET. The MOF-NET consists of simple fully connected layers but the weights of some layers are generated from the topology embedding.

Multi-species genetic algorithm with fitness approximation. Due to the vast number of the MOFs (i.e. 247 trillion) within our materials space, the brute force algorithm to compute properties for each of the MOFs is practically impossible due to time constraints. To find high-performing MOFs within a reasonable time, we developed a new search algorithm named multi-species genetic algorithm with fitness approximation (MSGGA-FA). MSGGA-FA is based on the evolutionary algorithm with fitness approximation using generation-based

evolution control²³ but we extended the algorithm to the multi-species system that is suitable for the MOF discovery. We initially tried to design an evolutionary algorithm that can crossover two chromosomes that contain both topology and building blocks information as a gene using genetic algorithm but, this approach failed to fully explore all possible topology space, we designed an algorithm in which conventional genomic algorithms ran independently in parallel for each of the topologies such that mixing of topologies do not occur. The length of the chromosome can be anywhere between 2 to 6 depending on the topology because the maximum number of edge and node types are three for each. First-half of genes of chromosome contain the NBB names and the rest half contain the EBB names. The visual description of chromosomes and crossover operation is shown in Fig. S8.

MSGGA-FA has a hierarchical optimization procedure as illustrated in Fig. 4. A period consists of four sequential improving steps as shown in Fig. 4. Step 1: grand canonical Monte Carlo (GCMC) simulations are conducted to obtain WC values of the MOFs that were generated from the previous improving step. In the first instance of Step 1, GCMC simulations were conducted on the randomly generated MOFs (about 10^4 to 10^5 initial MOFs were needed to ensure that sufficient number (e.g. 10-50 MOFs) of structures are selected for each of the topologies to train the MOF-NET for accurate WC prediction). Step 2: the MOF-NET is re-trained using the GCMC data collected from all previous improving steps. Step 3: conventional GA is performed separately for each topology. In all GA runs, the fitness values of the chromosomes (i.e. WC value) are calculated using the MOF-NET trained from Step 2. At the end of the GA, top 20–100 chromosomes are collected for each topology. Step 4: from the collected chromosomes in the previous step, actual MOF structures are constructed using *pormake* and optimized using classical molecular simulations. After Step 4, the generated MOF structures are sent to the next improving step. With increasing number of improving steps, the performance of MOF-NET is improved and more of the high-performing MOF

structures are accumulated, and between the periods, low-performing or saturated topologies become extinct to increase efficiency.

Fig. 4. Schematic of MSGA-FA.

Details on molecular simulations. In MSGA-FA, GCMC simulations were conducted using in-house GPU code²⁴ with short simulation steps in order to calculate WC quickly. After MSGA-FA, more accurate GCMC simulations were performed for high-performing MOFs using RASPA²⁵ software with 2k initialization cycles and 10k production cycles. Due to the difference in implementation and the number of simulation steps, in-house GPU code underestimates WC about $10 \text{ cm}^3 \text{ cm}^{-3}$ on average than working capacity from RASPA. The

Lennard-Jones potential model was used to describe interaction between the atoms. For all simulations, universal force field (UFF)²⁶ was used for atoms in MOFs and TraPPE²⁷ force field was used for methane molecules. Lorentz-Berthelot mixing rule was applied to get the parameters between different species. The cutoff distance of 12.8 Å was used for all species. The optimization of MOF structures were conducted with UFF using Forcite module in Materials Studio²⁸. No partial charges were assigned to the atoms in MOFs. The geometry optimizations using density functional theory (DFT) were performed using VASP software²⁹. The Perdew-Burke-Ernzerhof³⁰ functional and projector-augmented-wave pseudopotentials were used with cutoff energy of 500 eV for all calculations.

Results and Discussions

Initially, 67577 MOFs were generated randomly from 1775 topologies and 867 building blocks using *pormake*. For all improving steps in the 1st period, the top 20 MOFs (according to methane WC) were constructed out of the top 100 chromosomes from the inner GA for each topology. For some topologies, less than 20 MOFs were constructed because of the constraints on the generation of MOFs (cell lengths ≤ 60 Å, number of atoms ≤ 1500). For all improving steps in 2nd and 3rd period, 100 MOFs were constructed out of top 500 chromosomes from inner GA for each topology. For all MOF generations, we prevented redundant MOFs from being generated to enhance diversity of the top-performing materials. After the 1st period, maximum WC were obtained for each topology and only the top 10% of the topologies (based on the maximum WC value) survived to the next period. And after 2nd period, topologies with higher maximum WC than that of 1st period survived to the 3rd period to discard saturated topologies. Altogether, GCMC simulations of 200624 MOFs were

conducted during MSGA-FA, and from total 1775 topologies, 1575 topologies were explored only due to the size constraints on MOF unit cells.

To show the performance improvement of the generated MOFs over periods, the histogram of the WC values of the MOFs were obtained (Fig. 5). The WC values were calculated using the in-house GPU code during the MSGA-FA. The distribution of randomly generated MOFs have a peak at around $WC = 131 \text{ cm}^3 \text{ cm}^{-3}$ and the high-performing region ($WC > 180 \text{ cm}^3 \text{ cm}^{-3}$) is located at the tail end of the distribution. Going from the randomly generated set to the more optimal ones from the 1st and to the 2nd periods, one can see that both the peak and the outlier values increases for successive periods (1st period peak: $157 \text{ cm}^3 \text{ cm}^{-3}$, 2nd period peak: $179 \text{ cm}^3 \text{ cm}^{-3}$). In going from 2nd to 3rd period, it can be seen that there is less of improvement with 3rd period peak value of $181 \text{ cm}^3 \text{ cm}^{-3}$ an outlier value of about $200 \text{ cm}^3 \text{ cm}^{-3}$. As such, we terminated the MSGA-FA here.

Fig. 5. Histogram of the working capacity of generated MOFs for each period.

Given that we are largely interested in the top-performing structures, the average WC of top 0.1% MOFs generated up to the specific improving step were obtained (Fig. 6). The WC average for top 0.1% of MOFs increases as improving step proceeds. The average WC for the top 0.1% of the MOFs improves from $178 \text{ cm}^3 \text{ cm}^{-3}$ in the initial set to $199.6 \text{ cm}^3 \text{ cm}^{-3}$ and $199.9 \text{ cm}^3 \text{ cm}^{-3}$ in the final 3rd period.

Fig. 6. Average working capacity of top 0.1% high-performing MOFs generated for each improving loop index.

Next, the structural and adsorption properties (i.e. void fraction (VF), volumetric surface area (VSA), heat of adsorption (HoA) and largest cavity diameter (LCD)) of MOFs were calculated to show their relationship to WC (Fig. 7). The in-house GPU code was used

for HoA calculations and ZEO++³¹ with a probe radius of 1.5 Å was used to obtain other properties. The structural characteristics of high-performing MOFs are within narrow range. While the optimal VSA, HoA and LCD are within similar range of hypothetical **pcu** MOFs³, the optimal VF is significantly different. The range of optimal VF of hypothetical **pcu** MOFs is 0.83–0.90 but the range of optimal VF of MOFs in this work is 0.45–0.55. Other screening work conducted by Simon et al.⁴ shows that the range of optimal VF is 0.25–0.7 for the dataset of randomly selected 20000 hypothetical ZIFs⁵ and 10000 hypothetical MOF of Wilmer et al.². The differences of the optimal VF between deferent MOF sets show that the optimal VF depends on the topology, building blocks and constraints of the MOF sets.

Fig. 7. Correlation between working capacity and other properties of generated MOFs. **a**, void fraction (VF). **b**, volumetric surface area (VSA). **c**, heat of adsorption (HoA). **d**, largest cavity diameter (LCD). The red rectangles represent the high-performing region of the property.

To take a closer look at the high-performing MOF structures, the WC values of top 0.5% MOFs were recalculated using RASPA to obtain more accurate simulation results. It was shown that the WC results of the in-house GPU code are lower than that of RASPA due to the difference in software implementations and shorter simulation steps (see Fig. S6). Also

the histogram of top 0.5% MOFs were estimated with new WC values (Fig. 8). We found that 964 MOFs have WC values over $200 \text{ cm}^3 \text{ cm}^{-3}$ and 96 MOFs have WC values over $208 \text{ cm}^3 \text{ cm}^{-3}$ (where $208 \text{ cm}^3 \text{ cm}^{-3}$ is the world record of MOF-519). It is worth mentioning that no other experimental MOF besides MOF-519 exceeds $200 \text{ cm}^3 \text{ cm}^{-3}$ (the second-highest MOF, NJU-Bai 43, has WC of $191.3 \text{ cm}^3 \text{ cm}^{-3}$) and the 650,000 screening work by Simon et al. revealed the highest value of $196 \text{ cm}^3 \text{ cm}^{-3}$ so there is significant enhancement in potential candidate MOFs unearthed from our algorithm. The maximum WC value of the MOFs from the MSGA-FA is $217.9 \text{ cm}^3 \text{ cm}^{-3}$ and the MOF consists of boron cage (building block N6) and triacetylene linker (building block E41) with **vbm** topology (see Fig. S7). However, we discarded the MOF from the potential candidate because experimental synthesis seems difficult.

Fig. 8. Histogram of the working capacity of top 0.5% MOFs. The WC values were calculated using RASPA in order to obtain more accurate results.

From the remaining MOFs, the top 4 structures are visualized in Fig. 9. The names and WC values of top 4 MOFs are dia+N164+E14 (WC: $213.6 \text{ cm}^3 \text{ cm}^{-3}$), bbf+N1+N164+E44+E44 (WC: $213.1 \text{ cm}^3 \text{ cm}^{-3}$), tfa+N10+N164+E0+E19 (WC: $212.7 \text{ cm}^3 \text{ cm}^{-3}$) and ptt+N164+N1+N597+E44+E44 (WC: $212.6 \text{ cm}^3 \text{ cm}^{-3}$) (The name of MOFs consist of topology and building blocks with concatenating character “+”). All top 4 MOFs contain the tetrahedral indium cluster ($\text{In}(\text{CO}_2)_4$, N164).

Fig. 9. Visualization of top 4 MOF structures and organic linkers. **a**, dia+N164+E14. **b**, bbf+N1+N164+E44+E44. **c**, tfa+N10+N164+E0+E19. **d**, ptt+N164+N1+N597+E44+E44. The tfa+N10+N164+E0+E19 is expanded to $2 \times 2 \times 2$ supercell for clear visualization.

In order to see the effect of structure optimization, the density functional theory (DFT) calculations were conducted to optimize the structure of top 4 MOFs. All the structures were reduced into primitive cells before DFT calculations for efficiency. GCMC simulations were performed using RASPA for the optimized structures to get the altered WC values (see Table S1). It was shown that all WC values decrease after DFT optimization. The bond lengths between indium and oxygen are changed from 2.0 Å to 2.26 Å – 2.43 Å after DFT optimization so these structures move to slightly away from optimal geometry for given inter-molecular interaction parameters. For that reason, the WC values were slightly reduced for all top 4 structures. Although all four structures suffered a drop in performance, these structures still show good performance because of their high performance of the original structures. Moreover, we would like to point out that most of the previous computational screening works for methane storage reported WC values based on materials that were not DFT relaxed.

While it is important to look at the highest performance structures, it is also important to look at the structures that are expected to be high performance in experiments because there are fundamental differences between simulations and experiments. We classified MOFs with $WC > 180 \text{ cm}^3 \text{ cm}^{-3}$ (total 18579 MOFs) as high-performing MOF candidates. The building blocks in the MOFs are counted to identify frequent building blocks in high-performing MOF candidates (Table 1). As in the case of top 0.5% MOFs, N164 is the most frequent building block (63.8% of the MOFs contain N164) of the high-performing MOF candidates but the remaining 37.2% of the MOFs without N164 also have good performance. For the organic NBBs, (metallo)porphyrins show good performance in the MOFs. And there are no special functional groups in the frequent high-performing organic NBBs. In the case of edges, short and thin building blocks tend to have high performance. Therefore, it is expected that MOFs with linkers containing these edges without functional

groups are expected to show good methane adsorption performance.

Table 1. Frequent building blocks in high-performing MOF candidates ($WC > 180 \text{ cm}^3 \text{ cm}^{-3}$). The percent indicates what percentage of high-performing MOFs contain the building block. (e.g. the 63.8% of high-performing MOFs contain N164). Inorganic NBBs with a similar shape or metal substitutes are discarded from the table (N109, N92, N162 and N678). E0 (direct node to node connection) was excluded from the table although 12.4% of the MOFs have that.

Inorganic NBB				Organic NBB			EBB		
Rank	Image	Name	Percent	Image	Name	Percent	Image	Name	Percent
1		N164	63.8		(metallo) porphyrin	20.8		E44	38.3
2		N270	4.7		N10	13.0		E19	35.7
3		N151	3.4		N196	6.8		E27	11.2
4		N556	2.7		N20	6.7		E50	10.0
5		N50	1.5		N693	6.2		E202	6.5
6		N274	1.4		N3	4.6		E14	4.6

Conclusion

In this work, we have developed a systematic methodology that can conditionally generate MOFs with desired-properties by combining (1) evolutionary algorithm, (2) machine learning and (3) advanced MOF constructor. We demonstrate that our method can

successfully find hundreds of MOFs with record-breaking methane working capacity with the top-performing MOF having a working capacity of $213.6 \text{ cm}^3 \text{ cm}^{-3}$. The methodology developed in this study is expected to have a significant impact on the discovery of new MOFs, as it can readily extend to other applications and the addition of cost functions in the genetic algorithm can bias the direction of the search, leading to pre-guided search space tailor-made to the user-desire.

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S.L. conceived the presented project, developed advanced porous material constructor, conducted molecular simulations, developed deep learning prediction model, and designed the evolutionary algorithm. S.L. and B.K. constructed building block database. J.K. directed the project. All authors contributed to the writing/revising of the paper.

Competing interests

The authors declare no competing interests.

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Supplementary Information

Discovery of Record-Breaking Metal-Organic Frameworks for Methane Storage using Evolutionary Algorithm and Machine Learning

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S1. Construction of MOFs

S2. Details on MOF-NET

S3. Details on GA in MSGA-FA

S4. Supplementary figures and tables

S5. Topology database

S6. Building blocks

S1. Construction of MOFs

We defined a new concept which we named local structure to allocate node building blocks into nodes numerically with optimal orientation. The local structure of building blocks is obtained by rescaling distances between connection points and centroid of the connection points to one (Fig. S1a). Likewise, the local structure of the node in topology is obtained by rescaling distances between the node and the adjacent nodes to one (Fig. S1b).

The building blocks are located to minimize the root-mean-squared deviation of atomic positions (RMSD) between local structures of building block and that of the target node. To minimize the RMSD, the optimal order of indices of connection points in the local structure of building block has to be found. The time complexity of finding optimal order of the indices is $O(N!)$ if we consider all possible permutations. Fortunately, the optimal order can be found in $O(N^3)$ when the orientation of the building block is close enough to the optimal orientation by solving linear sum assignment problem¹. With the found order of the indices, the best orientation of building block which minimizes the RMSD can be found using Kabsch algorithm². The linear sum assignment and the Kabsch algorithm are performed using SciPy library³. We named the combination of these two algorithms as KL (Kabsch algorithm after linear sum assignment). We got the idea of KL from Python rmsd library⁴. However, due to the dependency of KL on the initial orientation of the building block, KL is performed for all orientations rotated by linearly spaced Euler angles to find global minimum RMSD. In our test, 64–216 (4^3 – 6^3) trial orientations are enough to find global minimum RMSD. If the global minimum RMSD is not found, the chiral structure of the building block is considered. Our algorithm can find the global minimum RMSD within $O(N^3)$ time complexity for arbitrary building blocks where N is the number of connection points. In this work, building blocks of $\text{RMSD} \leq 0.3$ (Fig. S2) for specific node were used for the MOF constructions to reduce

geometrical strains in the generated MOFs.

Fig. S1. Example of the construction of the local structure. **a**, local structure of the building block. **b**, local structure of the node in topology.

Fig. S2. Example of RMSD values on planar square node in the **ftw** topology. Tetrahedral building block (right) has $\text{RMSD} > 0.3$ for the node, so the building block is excluded from the possible building blocks for the node.

Because the topologies in the topology database were scaled to be a most symmetric shape with edge lengths of 1, the topology should be scaled before the construction of MOF structures. The objective function for the topology scaling is given as follow

$$\text{Objective} = \sum_{\text{nodes}} \sum_{i \leq j} (\mathbf{r}_i \cdot \mathbf{r}_j - \mathbf{r}'_i \cdot \mathbf{r}'_j)^2,$$

where $\mathbf{r}_i$ is the vector from a node to an adjacent node and the prime indicates the target vector obtained from the pre-located building blocks (see Fig. S3). The cell parameters and fractional coordinates of the nodes are the optimization variables. The optimization is performed using L-BFGS-B algorithm implemented in Python SciPy library³. To accelerate the optimization, the objective function is implemented using Tensorflow library⁵ with eager execution to evaluate the derivatives using automatic differentiation. The building blocks are located on the nodes and edges of the scaled topology (see Fig. S4). After the construction of MOFs, the constructed MOF structures were optimized using classical molecular simulations.

Fig. S3. Visual description of the vectors in objective function of topology relaxation. **a**, vectors from a node to adjacent nodes ($\mathbf{r}_1$ to $\mathbf{r}_4$). **b**, the target vectors obtained from the pre-located building blocks.

Fig. S4. The construction of MOF structure. The topology is scaled according to the given

building blocks.

S2. Details on MOF-NET

One may think it is proper to use graph convolution network (GCN) based architecture like CGCNN⁶ with building block embeddings as attributes of nodes and edges and the topology network as graph connectivity. Unfortunately, many of GCN variants use the information of adjacent nodes and edges for the update of a node for the next layer. So, from this perspective of limited information, many topologies become indistinguishable. For example, although all pure-silica zeolite structures have different topology, the local environment with four oxygen atoms attached to a single silicon atom is the same. As such, if silicon is considered as NBB and oxygen is considered as EBB, all polymorphs that consist of these NBB and EBB would become indistinguishable. One may think the geometrical information of topology (e.g. angles between edges and edge lengths) can be utilized the characterization of topology. However, in our case, there are no scaled topologies for a specific target MOF because there are no actual structures during predictions. Even if we use geometrical information of topology to distinguish non-scaled topology (from topology database), such a method is similar to topology embedding in that it specifies specific vector values for each topology but more complicated when the possible number of topologies are limited.

Embedding size of 128 was used for topology and building blocks. The dropout⁷ was applied to the embeddings with a dropout rate of 0.5. The batch normalization⁸ was applied to all dense layers except the output layer and weight generating layers. The hyperbolic tangent was used as the activation of weight generating layers and activation was not applied to the output layer. The ReLU activation was used in the rest dense layers. The size of all self-

interaction weights is 128×128 and the size of the interaction weight is 768×64 . So the size of the MOF embedding is 64. The units of the hidden layer between MOF embedding and the output layer is 32. The MOF-NET was implemented using Tensorflow⁵ version 2.

The MOF-NET was trained using Adam optimizer⁹ with a learning rate of 0.001. GCMC data was resampled to have a flat histogram over WC values. The resampling process prevents the MOF-NET overfit to the peak of the WC distribution. The GCMC data was split into a training set (90 %) and the validation set (10 %). The mean squared error (MSE) was used as our loss function. The training was performed for 200k steps and the MOF-NET of minimum validation error was selected. To estimate the performance of MOF-NET, we trained the MOF-NET with all of our GCMC data (80% training set, 10% validation set, 10% test set). The trained MOF-NET has the mean absolute error (MSE) of $7.02 \text{ cm}^3\text{cm}^{-3}$ and root mean squared error (RMSE) of $13.02 \text{ cm}^3\text{cm}^{-3}$ for the test set. The comparison between real and predicted WC values is shown in Fig. S5.

Fig. S5. The comparison between real and predicted WC values of the MOF-NET on test set. The dashed line indicates perfect prediction.

S3. Details on GA in MSGA-FA

The chromosome pairs for the crossover are selected using tournament selection with a probability of 0.9. For 90% of the selected chromosome pairs, the uniform crossover is applied and for the rest 10 % of the selected chromosome pairs, one chromosome is selected randomly from the pair. The population size is 1000, the number of generations is 100 and the mutation probability is 0.2. All fitness evaluations were performed using the MOF-NET, but the WC data were used if the GCMC data were available.

S4. Supplementary figures and tables

Fig. S6. Comparison between GCMC results of in-house GPU code and RASPA.

Fig. S7. The visualization of vbm+N6+E41 structure (WC of $217.9 \text{ cm}^3 \text{ cm}^{-3}$).

Fig. S8. Visual description of chromosomes and uniform crossover. In this case, the length of the chromosomes is 3 (2 for NBB, 1 for EBB).

Table S1. The WC values of top 4 MOFs before and after DFT optimization. The k-points used in DFT optimization is (2, 2, 2), (1, 2, 2), (2, 2, 1) and (1, 1, 1) in order.

MOF	WC before DFT (cm ³ cm ⁻³)	WC after DFT (cm ³ cm ⁻³)
dia+N164+E14	213.6	199.4
bbf+N1+N164+E44+E44	213.1	196.0
tfa+N10+N164+E0+E19	212.7	203.3
ptt+N164+N1+N597+E44+E44	212.6	202.8

S5. Topology database

All topologies were collected from the RCSR database¹⁰ in cgd format.

Table S2. The topologies used in this work. There are total 1775 topologies.

hst	fcf	ets	coe	sxh	vmx	vbl	pcu-g-e	snk	scu
vme	fsm	wlc	bct	msw	vch	wgm	zxc	ssd-e	can
smf	und	spl	bcq	upa	shb	lng	nia-a	wjd	tch
swa	wfq	yfn	fnc	xbf	dia-a-a	eta	qnf	tcf	mml
ins	eti	svs	whb	wnl	fts	mgc	wjp	zfp	ukn
wfc	yfj	fvp	ban	xbu	apo	zni	lim	utc	bpk
lon	eri	zfv	ssd	yft	edp	wfa	ury	raa	tfj
sin	bbd	swg	xaz	uoe	uoy	smm	vcn	svz	crs
nbo-a-e	wgx	fuf	bbe	xap	acs	dia-f	zfw	snm	wim
fsg	urk	fdu	ecl	tsi	ctn-x	flu-e	svx	bel	svk
osf	fcu	tfn	scu-f	sow	srs-g	tfy	bow	umm	est
ocu	fuh	vmo	edi	wlq	hex	pcu	ect	wgy	pha
icd-a	smv	bab	icd	bpm	wmp	fun	xfq	fnp	uky
myc	nbo-x-d	tfa	uov	hey	fvs	sit	bcm	vby	ato
fel	xas	iac	sqs	hal	yff	sne	bbp	iac-e	mok
bpr	vmk	jxj	kfi	wnw	oso	wkl	ast	ftl	vbw
pto-a	wgc	geo	bpj	ths	etf	apd	une	asc	qtz-a
tta	wbl	mbc	svp	sea	xfu	ttt-a	bcs-a	urt	yfq

swf	sct	ftq	ibd-a	nia	pek	lta	qsm	sxg	ssm
yfs	ftr	vbq	xfg	bcl	gar-e	fuu	wls	ssb	srd
bpd	ulj	nzn	stu	uof	win	mmn	tcl	wfy	unv
xfo	vck	mob	yfi	fnl	etb	ctt	xae	vcu	ptt
seb	zfg	fff	vda	dft	alb-a	pbz	tck	cbo	zmc
sab	csq-a	whq	ecj	sdt	bal	cds-b	zft	yfw	oab
fvv	xfw	wjg	toc-a	ooa	ofu	whl	qtz-f	ssb-a	xaf
alm	irl	lni	zbd	ttc	wjo	bcu-b	fcj	zhl	wjv
whv	yfb	umu	xah	vmi	sxl	etc	llj	ecn	nia-e
pcu-h	ncb	bcn	wmh	fvx	smi	cuz	wlk	ahr	xfl
wmk	stc	stw	cds	yfo	fto	xfy	cag	npo-e	bor-a
pto-d	zfq	umg	fci	ukj	wkg	osc	aea	stb	zbs
uke	nfc	nfb	xbe	wfp	cbt	zfe	swj	rhr	nlr
wfj	lvt-a	fvm	kgo	pyr-e	noi	vcj	wmo	cbs	tfh
urn	una	cab	xar	dei	ecg	fvf	wja	fni	fcg
utk	ftm	ghw	tsh	xbk	tfu	bor	uli	gfy	acs-h
noq	fcz	vct	cdl	wig	bbr	fcf	bva	sss	tes
urm	wgn	wme	epu	toc-e	sni	wie	wfg	mtn	gme
wkc	fng	wgq	fnj	bpt	yav-d	neb-e	alb	ffc	thl
pdp	baq	fnk	jjt	boe	pem	sto	eto	ith-d	xcu
svi	off	btu	dia-j	pyr-a	ptr	ftg	tfc-e	yfy	lll
wfh	smr	dnr	xik	xbq	foa	wny	wnq	afw	svn-d
wgb	cdj	bbf	tfl	hbo	ffb	ftu	zfr	pts-x	umq
utn	ooe	twf-d	vmm	uop	xbc	dia-a	seh	teo	fth
wnc	bas	brl	noj	bnn-a	xmz	sln	yug	bpu	oof
wjz	whz	sxb	eea	ukw	dnd	ttd	toc	wla	wkq
bag	son	xbh	utm	bck	fvb	mcd	uob	fui	tof
gsi	wmw	sor	skd	wgj	aww	fgl	lcv-a	svo	vce
urv	uou	vmh	dmf	wfo	wfl	cot	tna	wgw	wjy
fnu	sod-h	ggl	hjm	fub	sop	wys	ttw	gis-e	soo
snr	svd	qtz-h	lig	vmv	unt	ptd	fvq	she	wle
unc	clh	vcz	wha	vmt	snh	fup	stx	nba	deh-d
noh	qdl	wgl	wgd	zfu	pth-a	snb	wkn	nol	crr
tbo	bar	muo	wga	rho	fsx	cai	tcj	xfa	reo
xft	los	lqm	wki	wnz	nvb	uoj	nof	sth	urz
vma	bby	wmc	fsl	whi	siz	flu-a	umb	sny	fvo
fuy	baz	wio	svl	gra	gwg	wfd	bac	frl	wfn
mot	vmz	phi	vbv	umv	nab	xbd	unm	osd	yfd
hyb	vbj	wkx	swc	wnm	fcr	sml	pyc	fca	wky
ucp	sof	ste	xfm	svv	wli	asf	hcj	fit-e	fne

svj	wjm	svf	vbi	umw	wnv	umy	lom	wib	ibd
wfx	whf	ftz	mss	utq	srs-f	ssa-a	xfb	uox	usf
qtz-e	bmn	unn	maw	wnn	sty	bpp	bcu-k	lcv-e	xbo
vmc	jeb	cdp	uta-e	msq	sot	mon	xag	fce	vmn
sda	qne	xfz	xal	wfr	phx	gie	ith	wni	pcu-m
whc	fnh	acs-g	xbj	wiu	khn	wks	uos	uno	tcd
wms	wma	qzd	rhr-a	ece	wnh	fda	etq	niq	wgu
lbt	nou	bpa	fwz	sxm	tpt-a	pbp-e	lib	the-a	bbn
vbb	ntb	fst	unl	ftj	bcb	fvh	wjf	epw	smg
vmd	nor	dnt	ffj	wif	bbc	wpa	pts-e	jea	oft
svq	bat	sxf	dgp	fqr	het	xac	icc-a	rho-e	cml
zbt	pbz-e	srb	jsd	bcp	vcy	unr	tcg	nth	fee
wfi	twf-e	umj	whd	unp	fvn	smk	bcu-t	gan	lrj
xbb	zyl	isx	mst	gpu	wjt	zfa	wfb	skb	swi
sst-e	ftp	xfh	wld	bbb	uot	mzp	ulh	urp	tot
sbr	dnj	lcv-f	baa	bam	zbl	hef	eci	uod	skc
act	zfn	bak	csq	pcu-h-e	utj	soc	fud	jsa	rgd
cdt	hbr	sxq	lwg	why	tfq	ala	asv	fcn	etk
tph	yfz	smq	ula	afw-a	abr	gis	srs-a-e	lcs-a	tfp
twf	srs-a	xaj	wlg	ttu	xai	loh	zyg	omy	yfk
bco	tza	ukr	bbz	byl	ftn	vcr	bcw	fvf	svb
zbw	wff	pts	soc-a	nfa	upc	ull	url	soh	bwt
vcm	wlh	tsj	tci	uka	ofp	wik	aht	bav	bay
yfr	ecp	snp	srd-l	xbi	nbo-a	fnw	wgr	wnf	zzz
bcz	npo-a	vbu	umf	sos	mou-e	wmd	fum	wkk	skf
ukd	edq	zfx	eed	ant	ana	acs-i	yfm	maz	xfc
sst	wmq	wgv	ftv	yfa	tty	wgh	snx	ume	icf
jsb	ttv	uoa	urh	unj	mer	dia-g	tfo	law	bbo
wfk	pti	wia	umn	hch	uog	dme	uni-d	whj	crs-d
tcs	wmu	reo-e	fvz	vdb	tfv	uom	epz	wkt	sod-f
sxj	fuo	vbk	mou	smj	xxv	llk	ben	vci	uml
feb	ftd	sgn	gar-a	fut	key	ltw	srs	tfe	sxi
vbr	sxn	pcl	xaw	bbg	sku	wjb	xlz	bcj	lil
ssf	nju	xau	btv	ffg	xba	neb	fua	cor	idp
wgk	zec	wlt	pbg	wmb	cat	six	wfe	bpb	etm
wlf	nce	soj	sqc-a	ecs	bax	twf	tfb	qzd-a	lfm
hww	wse	dna	ftk	zbh	yfx	xax	tie	wkb	tfk
ftx	kwh	mog	wih	cdl-e	wfm	dnq	nca	vco	wfs
mdf	lcv	wkw	fte	chb	iac-d	bbm	fuw	ech	xff
nbo-h	lwh	jsc	mcf-d	xfp	pcu-i	bpi	spn-a	hci	mft

noy	qtz-g	wke	tco	dma	sod-b	npo	tzs	snv-x	ukp
vbo	fnb	sog	brk	wii	ftb	cco	crb-e	vbv	snq
dum	ukl	umd	zfh	fnz	uol	dmd	xbv	rac	bbv
zfk	sca	vmg	osa	swb	eye	ftw	nsp	lcy-a	tbd
ttz	lhh	ure	umh	mot-e	ftc	rab	fva	urx	uoq
wge	koh	baj	kna	unf	dia	sol	vbm	sxc-d	whm
crs-a	wml	wjx	ksx	eab	noz	wku	wit	ukh	bph
shp	etp	fnn	fau	vcd	nod	xfj	bvh	zmd	edc
wgt	whh	fvi	tsc	qrf	svg	stj	fcu	mhg	hxg
fnd	crb	mdh	hea	upd	wiy	xfi	wlr	bor-e	uoh
xfn	bpv	bcd	sxd	ung	bpe	twf-a	fnr	vmb	pbg-e
swh	nok	yfe	sta	fve	xav	vcg	siy	ffi	bah
urf	apc	bbk	thj	wht	rht	the	zfb	zbz	rtw
bap	wlm	hcp	swk	sme	wnk	ctn-a	ssc-a	wka	mgc-a
tsx	ecd	tcc	sod-g	vcv	scg	sxe	ocu-a	cys-a	wkd
vmr	vbs	cdz	dmj	utg	bcu-l	isq	wnb	osb	ftt
wuy	sat	svc	ffa	uma	ahq	bbi	fso	cds-a	soe
ftw-a	ful	svu	whk	bcu-h	wjq	nir	fry	rna	mcf
tfg	wji	bto	wmx	thp-x	dne	bbh	vcf	uta	bon
wjn	ubt	bao	tce	wnu	ske	wiw	hee	uns	fof
sng	nom	smp	sok	zba	fug	svw	wna	vcq	shp-a
hec	fuz	mof	mcn	sas	snw	dmb	vbt	ats	nku
wmg	smd	hof	hbo-e	zbn	alw	vcp	wnd	xay	who
wsx	ecv	ltl	wft	fvw	tfz-d	cut	tbo-a	etb-e	bbl
jaj	bpo	ocu-e	raf	lcy-e	qtz	wll	lcy	rtl	wiv
oob	xat	spn	snl	vcc	bcu-i	vba	fcs	flu	sxa
umc	bsn	noo	fit	ose	mjz	ecb	uru	sxo	zfl
ast-e	smo	fnv	zrc	vcl	wkv	yfc	ftf	wkj	xad
wmt	uon	wln	wnt	kew	fnf	svm	dag	wjc	sst-a
fla	wkm	bca	xfd	fsi	wjh	deh	nta	dni-d	uto
wmz	wir	wix	wmj	wmi	wmr	xfr	tcn	wfz	swl
uoc	ukc	baf	unb	fny	ulg	mjd	yan	qdl-e	ilc
xly	thp-a	cdm	fse	fvu	vbg	acs-f	umx	tfi	bpg
z fj	cap	bcu-j	mgd	ylf	xfk	vmu	gah	ssc	ecf
bce	wlj	sur	zfc	baa-e	bcx	rht-a	fsb	hed	hyw
whr	mmm	smc	sxk	pcb-e	ubt-a	xao	cfc	cds-f	sou
ana-e	whw	ybh	wjk	fnt	fcl	cbo-e	nbo	fcd	lhb
fvk	afx	fur	upb	xaa	fcu	ukx	pcu-g	fns	wij
jph	sva	znz	ctn-e	unx	wgo	hcd	wkp	tcu	zfi
ums	sqc	fsy	vca	ucn	etn	twf-e	fdc	lcs-f	xbg

alc	kag	bpl	hms	uny	bsv	vfi	ctn-d	epv	wko
fuj	ecu	wju	etj	fsn	ict	sie	mrc	lcs	wnp
whx	ecc	hms-e	bcu-f	wmf	fcx	thh	wmy	ukt	tee
fsd	wlu	wgi	fti	vmj	nva	bix	lvt	whe	wno
wmn	wjw	yfg	dea	uoz	pyd	urw	iph	mgg	gee
hwx	ltj	wjl	bpc	zga	bod	kag-d	xfx	pto	cus
wje	eft	atv	bnl	vmf	svt	cdq	snf	asp	gar
sod-a	ska	htp	vbp	sms	iab	bcu-g	vbe	sno	uku
xan	yav	nnd	nip	ana-f	vbc	pts-g	uoi	fvd	ana-a
pts-f	ukv	fch	fue	gdm	svn	fob	vbn	pyo	ctn
wiq	wjs	abf	yfu	wgz	icc	acs-a	wne	wis	sxc
pyr	smb	tsb	uks	ddc	std	wjr	wkr	fuv	sra
zfo	ukm	epy	tej	whp	smh	uni	rob	sse	bcu
bbj	bpf	urg	pcb	ukk	lsz	xda	yfl	ecm	lon-a
fus	fvt	cdn	som	fna	kea	zfm	agw	eth	wmm
fvr	vmy	rra	wip	umo	snv	fab	gaf	lnj	jcy
yfv	wgs	scu-g	bcg	fsa	svh	lcs-e	mgz	urj	fcq
fvj	vml	cor-e	wlp	gao	z fz	xbm	lon-e	bps	ukb
crb-a	sve	xbt	nov	ttp	rag	tff	afy	utp	lev
beb	fet	vna	vmp	tpd	sxp	tfc	bnn	etd	bcf
umk	smt	nox	iac-a	ttx	wfu	pzh	wgp	wiz	mjb
wns	wmv	tff	etl	unu	ete	atn	src	xcb	bbs
att	snz	anh	zfy	ukf	zfd	umz	fsh	fiq	xca
wkh	jst	she-a	ths-e	vbf	moa	lcw-x	wlb	fnq	fct
swd	sod-e	pte	whu	smw	tfz	bau	vmw	utb	xaq
mmt	cua	sev	yfh	noc	zjz	fsf	uoo	xak	pbp
pth	zme	tsq	jse	ntw	cab-a	stp	bbq	fsc	tfs
fvg	vmq	sod	phw	lcy-a-x	thp	svy	ntn	bne	bda
whn	xfz	hlz	swe	fcy	icm	soi	tca	umr	unh
wil	qza	vtx	bcy	ssa	cao	dmp	xbl	wnr	vbh
fdb	xam	bik	xux	pts-a	lcx	xij	itv	wng	uki
fty	vcs	ukg	moc	hmc	smn	eta-c	etg	tsg	mog-e
uko	uow	zff	dmc	wei	dgn	xww	fcv	tnn	svr
zbf	smu	wgf	baw	vab	zfs	dgq	bto-e	eco	bcu-x-a
nat	fjh	bbx	dnv	xab	wnx	iss	sma	jbw	kdd
fno	fly	qtz-x	tpr	mvv	fog	soq	wut	bcv	ecr
whs	vcb	wfw	sqp-a	nob	whg	hck	bba	unw	bpn
cda	sqp	ith-e	wnj	ttg	stp-a	uri	wkf	wid	fsk
scu-a	nts-a	bcs	wfv	cha	vms	vbd	myd	bbw	afi
ith-a	rae	rkf	xby	zbr					

S6. Building blocks

The CPK coloring¹¹ was used for the visualization of all building blocks. The **Source** in figures indicates from which MOF (or ToBaCCo) the building block were extracted. The X symbol in **Formula** indicates connection points. Thin red sticks indicate the connection between the connection point (X) and the atomic part of the building block. There are missing indices that were removed due to the duplication.

Name: N1
Source: ToBaCCo
Formula: C16H6X4

Name: N2
Source: ToBaCCo
Formula: ZnC20H16N4X4

Name: N3
Source: ToBaCCo
Formula: C8H4X4

Name: N4
Source: ToBaCCo
Formula: C6H2X4

Name: N5
Source: ToBaCCo
Formula: C6X6

Name: N6
Source: ToBaCCo
Formula: B12X6

Name: N7
Source: ToBaCCo
Formula: C12H6X4

Name: N8
Source: ToBaCCo
Formula: B12X12

Name: N9
Source: ToBaCCo
Formula: Cr3C6O16X6

Name: N10
Source: ToBaCCo
Formula: C6H3X3

Name: N12
Source: ToBaCCo
Formula: C26H16X4

Name: N13
Source: ToBaCCo
Formula: C20H10N4X4

Name: N14
Source: ToBaCCo
Formula: Zr6C6H16O32X6

Name: N15
Source: ToBaCCo
Formula: Zr6C6H16O32X6

Name: N16
Source: ToBaCCo
Formula: Zn4C6O13X6

Name: N17
Source: ToBaCCo
Formula: Cu2C4O10X4

Name: N18
Source: ToBaCCo
Formula: Cu3C9H8N6O10X3

Name: N19
Source: ToBaCCo
Formula: C3N3X3

Name: N20
Source: ToBaCCo
Formula: C13H6X3

Name: N21
Source: ToBaCCo
Formula: Zr6C8H12O32X8

Name: N22
Source: ToBaCCo
Formula: Cu24C192H72O120X24

Name: N23
Source: ToBaCCo
Formula: C₆H₃O₃X₃

Name: N24
Source: ToBaCCo
Formula: Zr₆C₁₀H₈O₃₂X₁₀

Name: N25
Source: ToBaCCo
Formula: C₁₂H₆N₃X₃

Name: N26
Source: ToBaCCo
Formula: Mn₄C₈CIN₃₂O₆X₈

Name: N27
Source: ENIXUV_clean
Formula: Mn₂C₂₀Cl₂H₁₆N₄X₄

Name: N28
Source: QISVAQ_clean
Formula: C₁₉Cl₉X₆

Name: N29
Source: MEFZUU_clean5b
Formula: Mn₂C₄Cl₂O₈X₄

Name: N30
Source: VARWIW_charged
Formula: Sm₄C₆H₄O₂₆X₆

Name: N31
Source: AFUPEX_clean
Formula: Tm₂C₆O₁₂X₆

Name: N32
Source: NIKDEQ_clean
Formula: Gd₄O₈X₄

Name: N33
Source: FASQUN_clean
Formula: Zn₄C₆O₁₄X₆

Name: N34
Source: XAKQIL_clean
Formula: Co₁₂H₁₄N₄O₄X₄

Name: N35
Source: SENVIR_clean
Formula: Co₄C₈O₁₆X₈

Name: N36
Source: PARKUQ_charged
Formula: Cd₂C₆O₁₂X₆

Name: N37
Source: PUDSUD_clean
Formula: Nd₂C₆O₁₂X₆

Name: N38
Source: ENITIF_clean
Formula: Zn₃C₈O₁₆X₈

Name: N39
Source: MOXPUL_clean
Formula: C₃₃H₃₂O₄X₄

Name: N40
Source: DIBJJI_clean
Formula: Eu₆H₈O₂₇S₆X₆

Name: N41
Source: COWMEH_clean
Formula: Tb2C6O12X6

Name: N42
Source: BASJUB_clean
Formula: CoC20Cl2H16N4X4

Name: N43
Source: ZELQAK_clean
Formula: C14H7N3X4

Name: N44
Source: CAYSIE_clean
Formula: CoC40H24N8X4

Name: N45
Source: COZMUA_clean
Formula: Co4C8O20X8

Name: N46
Source: BEXVEH_clean
Formula: C14H10X4

Name: N47
Source: FEWTUY_clean
Formula: NiC22H16N4O4X6

Name: N48
Source: DEHLAF_clean
Formula: C30H27O3X3

Name: N49
Source: TONBOO_clean
Formula: Co3C10H14N2O12X6

Name: N50
Source: XEJTIR_clean
Formula: AlC24H16O4X4

Name: N51
Source: FUTCAZ_clean
Formula: Mn2C3ClO6X3

Name: N52
Source: FAYQUT_clean
Formula: Zn5C40H24N18O8X4

Name: N53
Source: ILUFEB_charged
Formula: Cd3C24H24N36X12

Name: N54
Source: ALUKAU_clean
Formula: Dy2C6O12X6

Name: N55
Source: FOXQIT_charged
Formula: CdC18H18N12X6

Name: N56
Source: QATLEE_clean
Formula: Zn7C12O26X12

Name: N57
Source: FAYQED_clean
Formula: C45H32O4X4

Name: N58
Source: NIKJOH_clean
Formula: Sm4C12O24X12

Name: N59
Source: HEFDON_ion_b
Formula: $\text{Cd}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N60
Source: RIWSUM_clean
Formula: $\text{Cd}_3\text{O}_6\text{X}_3$

Name: N62
Source: NATNIG_charged
Formula: $\text{C}_6\text{H}_8\text{O}_2\text{X}_4$

Name: N63
Source: EBUREA_clean
Formula: $\text{C}_{12}\text{H}_7\text{N}_2\text{X}_3$

Name: N64
Source: FUSWIA_clean
Formula: $\text{Cu}_3\text{C}_{24}\text{Cl}_2\text{H}_{16}\text{N}_{20}\text{X}_8$

Name: N65
Source: ELERIX_clean
Formula: $\text{La}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N66
Source: LOWQIX_clean
Formula: $\text{Zn}_7\text{C}_8\text{O}_{20}\text{X}_8$

Name: N67
Source: FERGUG_charged
Formula: $\text{Cd}_3\text{C}_8\text{O}_{16}\text{X}_8$

Name: N68
Source: ZIJVAR_clean
Formula: $\text{Co}_8\text{H}_6\text{N}_4\text{O}_4\text{X}_4$

Name: N69
Source: BAZJIX_clean
Formula: $\text{Mn}_5\text{C}_8\text{N}_3\text{O}_2\text{X}_8$

Name: N70
Source: ENITEB_clean
Formula: $\text{Cd}_3\text{C}_8\text{O}_{16}\text{X}_8$

Name: N71
Source: PENNON_clean
Formula: $\text{C}_{14}\text{H}_6\text{O}_2\text{X}_4$

Name: N73
Source: WEHJIE_clean
Formula: $\text{Zn}_3\text{C}_4\text{O}_9\text{X}_4$

Name: N76
Source: XADGAM_clean
Formula: $\text{Zn}_3\text{C}_{12}\text{H}_8\text{N}_2\text{O}_4\text{X}_4$

Name: N77
Source: HEFDON_ion_b
Formula: $\text{Ba}_2\text{Cd}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N78
Source: ZIDVAL_clean
Formula: $\text{Mn}_3\text{C}_{16}\text{H}_{12}\text{N}_{10}\text{O}_{12}\text{X}_8$

Name: N79
Source: DICVAO_clean
Formula: $\text{C}_{18}\text{H}_{27}\text{N}_6\text{X}_3$

Name: N80
Source: HEXVEM_clean
Formula: $\text{C}_{21}\text{H}_{15}\text{N}_6\text{X}_3$

Name: N81
Source: JOGDAL_charged
Formula: Ga10C22H21N4S16X3

Name: N82
Source: QEBKUF_clean
Formula: C73H44X8

Name: N83
Source: YEGDAR_clean
Formula: Mn3C18H12N8O12X10

Name: N84
Source: WAMREJ_clean
Formula: C60H30N4X8

Name: N85
Source: FUNBIA_clean
Formula: Zn2C14H8N2O8X6

Name: N86
Source: DIBQOW_clean
Formula: Co3C6O13X6

Name: N87
Source: CITXUZ_clean
Formula: Cu2C14H10N2O8X4

Name: N89
Source: NUHPAI_clean
Formula: Zn20H16N4X4

Name: N90
Source: ACOGAB_clean
Formula: CdBr2C20H16N4X4

Name: N91
Source: DUXKUD_clean
Formula: C14H30N4X4

Name: N92
Source: IMUTUG_ion_b
Formula: In3C6O13X6

Name: N93
Source: CAWDOU02_clean
Formula: CuC20H16N4X4

Name: N94
Source: EPUVAN_charged
Formula: Gd2C60H48N12O12X12

Name: N95
Source: RUPRUQ_clean_h
Formula: Ti8C12O36X12

Name: N96
Source: BOLPEY_clean
Formula: C19H15SiX3

Name: N98
Source: LABJUV_clean
Formula: Cu10C40H32I10N8X8

Name: N99
Source: OXALIJ_ion_b
Formula: C29H23O4X4

Name: N100
Source: BEDYEQ_clean
Formula: FeC20ClH8N4X4

Name: N101
Source: ISENUQ_clean
Formula: Dy2C6O12X6

Name: N102
Source: FAHFUR_clean
Formula: Be4C6H4O16X6

Name: N103
Source: AMUWIP_charged
Formula: Cu4WC40H32N8S4X8

Name: N104
Source: PUQHIT_clean
Formula: $\text{Zn}_4\text{C}_{26}\text{H}_{16}\text{N}_4\text{O}_{14}\text{X}_{10}$

Name: N105
Source: MITSIS_charged
Formula: $\text{Cd}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N106
Source: LALPIZ_clean
Formula: $\text{Y}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N107
Source: PANYEK_clean
Formula: $\text{Cd}_3\text{C}_{36}\text{H}_{24}\text{N}_{30}\text{X}_{12}$

Name: N108
Source: VEMMAC_clean
Formula: $\text{Zn}_3\text{C}_6\text{N}_{24}\text{X}_6$

Name: N109
Source: HUCBEN_clean5b
Formula: $\text{In}_4\text{O}_8\text{X}_4$

Name: N110
Source: QAGQEW_clean
Formula: $\text{C}_{12}\text{H}_3\text{S}_3\text{X}_3$

Name: N111
Source: GUXPOF_clean
Formula: $\text{Co}_3\text{C}_{16}\text{H}_8\text{N}_{20}\text{X}_8$

Name: N112
Source: DABWUA_clean
Formula: $\text{CuC}_{12}\text{H}_8\text{N}_{20}\text{X}_4$

Name: N113
Source: FEYJOJ_clean
Formula: $\text{Co}_2\text{C}_4\text{O}_8\text{X}_4$

Name: N114
Source: ALULEZ_clean
Formula: $\text{Ce}_3\text{C}_{120}\text{X}_{12}$

Name: N115
Source: GERWOR_charged
Formula: $\text{Cd}_4\text{O}_8\text{X}_4$

Name: N116
Source: EBETOW_clean
Formula: $\text{Cd}_3\text{C}_6\text{O}_{12}\text{X}_6$

Name: N117
Source: MICCUY_clean
Formula: $\text{Cd}_3\text{H}_4\text{NO}_4\text{X}_3$

Name: N118
Source: KOHKOI_clean
Formula: $\text{KZn}_6\text{C}_{12}\text{H}_{20}\text{O}_{26}\text{X}_{12}$

Name: N119
Source: MIHMEW_clean
Formula: $\text{Nd}_4\text{C}_{12}\text{H}_2\text{O}_{24}\text{X}_{12}$

Name: N120
Source: CANROA_clean
Formula: $\text{Co}_3\text{C}_8\text{O}_{16}\text{X}_8$

Name: N121
Source: CAJWAN_charged
Formula: $\text{In}_2\text{LiC}_8\text{O}_{16}\text{X}_8$

Name: N122
Source: EKUPEG_clean
Formula: $\text{Cu}_6\text{C}_{30}\text{H}_{24}\text{N}_6\text{O}_3\text{S}_9\text{X}_6$

Name: N123
Source: ALUKIC_clean
Formula: $\text{Ce}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N124
Source: BOXFOK_clean
Formula: $\text{Dy}_4\text{C}_8\text{O}_{17}\text{X}_8$

Name: N125
Source: OKABAE_clean
Formula: $\text{Cu}_3\text{C}_6\text{O}_{12}\text{X}_6$

Name: N126
Source: FAJYAS_clean
Formula: $\text{C}_{27}\text{H}_{18}\text{N}_3\text{O}_3\text{X}_3$

Name: N127
Source: GEZFOI_charged
Formula: $\text{Cd}_{20}\text{H}_{16}\text{N}_4\text{O}_2\text{X}_4$

Name: N128
Source: OQEROS_clean
Formula: $\text{Pd}_{20}\text{H}_8\text{N}_4\text{X}_4$

Name: N129
Source: FAYPOM_clean
Formula: $\text{C}_{33}\text{H}_{32}\text{O}_8\text{X}_4$

Name: N130
Source: KEHGAH_charged
Formula: $\text{C}_9\text{H}_{12}\text{NX}_3$

Name: N131
Source: LELROL_clean
Formula: $\text{Mn}_5\text{C}_8\text{Cl}_2\text{N}_3\text{X}_8$

Name: N132
Source: INEBOT_charged
Formula: $\text{Ni}_5\text{C}_8\text{O}_{24}\text{X}_8$

Name: N133
Source: ANUGUM_clean
Formula: $\text{Zn}_2\text{C}_5\text{O}_{10}\text{X}_5$

Name: N134
Source: UDIHOF_charged
Formula: $\text{Ni}_3\text{C}_6\text{O}_{16}\text{X}_6$

Name: N135
Source: HURGUX01_clean
Formula: $\text{Ni}_3\text{C}_{10}\text{H}_{14}\text{N}_2\text{O}_{12}\text{X}_6$

Name: N136
Source: DELGEI_clean5b
Formula: $\text{Cd}_{20}\text{H}_{16}\text{N}_4\text{X}_4$

Name: N137
Source: ECOLEP_clean
Formula: $\text{Co}_2\text{C}_3\text{N}_{12}\text{X}_3$

Name: N138
Source: XOTXAG_clean
Formula: $\text{La}_2\text{Na}_2\text{C}_8\text{O}_{22}\text{X}_8$

Name: N139
Source: GAWKAS_clean
Formula: $\text{Sm}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N140
Source: DASTEY01_charged
Formula: $\text{Zn}_3\text{C}_8\text{O}_{16}\text{X}_8$

Name: N141
Source: EPUXET_clean
Formula: $\text{Cd}_2\text{C}_{24}\text{H}_{16}\text{N}_4\text{O}_8\text{X}_8$

Name: N142
Source: NUGRIR_clean
Formula: $\text{Cu}_6\text{WBr}_4\text{C}_{24}\text{H}_{24}\text{N}_{16}\text{S}_4\text{X}_8$

Name: N143
Source: ARIBOS_clean
Formula: $\text{Cd}_2\text{C}_{14}\text{H}_8\text{N}_2\text{O}_8\text{X}_6$

Name: N144
Source: GAJVAQ_clean
Formula: $\text{Er}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N146
Source: LAGRES_clean
Formula: $\text{Er}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N147
Source: NIGGAM_clean
Formula: $\text{Ho}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N148
Source: XAKQOR_clean
Formula: $\text{Cu}_2\text{C}_{14}\text{H}_{14}\text{N}_4\text{O}_8\text{X}_6$

Name: N149
Source: GLYTIS_clean
Formula: $\text{Zn}_3\text{C}_{16}\text{H}_8\text{N}_2\text{O}_{12}\text{X}_8$

Name: N150
Source: XEXLAP_clean
Formula: $\text{C}_{12}\text{H}_4\text{NO}_2\text{X}_3$

Name: N151
Source: EDOVEA_charged
Formula: $\text{Zn}_3\text{O}_{18}\text{H}_{18}\text{N}_6\text{X}_6$

Name: N152
Source: XUMVAD_clean
Formula: $\text{Dy}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N153
Source: ADASOP_clean
Formula: $\text{Zn}_2\text{C}_4\text{O}_8\text{X}_4$

Name: N155
Source: BETDAH_clean
Formula: $\text{Ho}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N156
Source: PEQTIQ_clean
Formula: $\text{DyC}_4\text{O}_8\text{X}_4$

Name: N157
Source: NISBEX_clean
Formula: $\text{C}_{15}\text{H}_{12}\text{N}_9\text{X}_3$

Name: N158
Source: XAPYAO_clean
Formula: $\text{NiC}_{20}\text{H}_{16}\text{N}_4\text{X}_4$

Name: N160
Source: OKABEL_clean
Formula: $\text{C}_{10}\text{H}_7\text{N}_2\text{X}_3$

Name: N161
Source: CAXZOS_clean
Formula: $\text{CoC}_{12}\text{H}_8\text{N}_2\text{O}_4\text{X}_4$

Name: N162
Source: IYICUP_clean
Formula: $\text{CoC}_{30}\text{H}_{18}\text{N}_6\text{X}_6$

Name: N163
Source: BELTOD_clean
Formula: $\text{C}_{18}\text{H}_{12}\text{OPX}_3$

Name: N164
Source: NUFTOY_charged
Formula: $\text{InC}_4\text{O}_8\text{X}_4$

Name: N166
Source: EBIMIN_charged
Formula: $\text{Mn}_3\text{C}_8\text{O}_{16}\text{X}_8$

Name: N167
Source: DUVNIS01_charged
Formula: $\text{Co}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N168
Source: QEGGUE_charged
Formula: $\text{C}_{40}\text{H}_{44}\text{X}_4$

Name: N169
Source: POBMOJ01_clean
Formula: $\text{Yb}_4\text{C}_8\text{O}_{17}\text{X}_8$

Name: N170
Source: BEXRUT_clean
Formula: $\text{NiC}_{12}\text{H}_6\text{N}_2\text{O}_4\text{X}_6$

Name: N171
Source: BUFNOG_charged
Formula: $\text{Cd}_4\text{C}_8\text{O}_{20}\text{X}_8$

Name: N172
Source: LUPYAX_clean
Formula: $\text{Zn}_3\text{C}_5\text{H}_0\text{O}_{11}\text{X}_5$

Name: N173
Source: ETEKAQ01_clean5b
Formula: $\text{Gd}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N174
Source: MEGBAD_clean
Formula: $\text{NiC}_{20}\text{H}_8\text{N}_4\text{X}_4$

Name: N175
Source: TISHAF_clean
Formula: $\text{Fe}_4\text{C}_8\text{O}_{18}\text{X}_8$

Name: N176
Source: YAZYEF_clean
Formula: $\text{C}_6\text{H}_3\text{O}_3\text{X}_3$

Name: N177
Source: YOZQAG_charged
Formula: $\text{Zn}_7\text{C}_{12}\text{O}_{27}\text{X}_{12}$

Name: N178
Source: DEQVIF_clean
Formula: $\text{Mn}_2\text{C}_{24}\text{H}_{16}\text{N}_4\text{O}_8\text{X}_8$

Name: N179
Source: FAJYAS_clean
Formula: $\text{Co}_3\text{C}_6\text{O}_{13}\text{X}_6$

Name: N180
Source: ILITUT_clean5b
Formula: $\text{Co}_2\text{C}_{16}\text{H}_{12}\text{N}_2\text{O}_8\text{X}_6$

Name: N182
Source: IFUNUU_clean
Formula: $\text{Tb}_2\text{C}_6\text{H}_2\text{O}_{14}\text{X}_6$

Name: N183
Source: MARDAM_charged
Formula: $\text{Co}_3\text{C}_{12}\text{H}_{12}\text{N}_1\text{O}_6\text{X}_6$

Name: N184
Source: LUMDEC_clean
Formula: $\text{CdC}_8\text{H}_6\text{N}_4\text{O}_4\text{X}_4$

Name: N186
Source: OBEDEE_clean
Formula: $\text{AgC}_3\text{N}_3\text{X}_3$

Name: N187
Source: KOHKIC_clean
Formula: $\text{NaZn}_6\text{C}_{12}\text{H}_{20}\text{O}_{26}\text{X}_{12}$

Name: N188
Source: OMAWOP_clean
Formula: $\text{AgC}_{16}\text{H}_{12}\text{N}_8\text{X}_4$

Name: N189
Source: TIQHAD_clean
Formula: $\text{GdC}_{40}\text{H}_{24}\text{N}_8\text{O}_8\text{X}_8$

Name: N190
Source: CETJAN_clean_h
Formula: $\text{C}_9\text{H}_4\text{O}_8\text{X}_4$

Name: N191
Source: HUCBAJ_charged
Formula: $\text{In}_2\text{Li}_2\text{C}_8\text{O}_{18}\text{X}_8$

Name: N192
Source: BINDAF_clean_b
Formula: $\text{Ni}_2\text{C}_{24}\text{H}_{16}\text{N}_4\text{O}_8\text{X}_8$

Name: N193
Source: EKARUE_clean
Formula: $\text{CuC}_{12}\text{H}_8\text{N}_2\text{O}_4\text{X}_4$

Name: N194
Source: AVUDAX_clean
Formula: $\text{CuC}_8\text{H}_8\text{N}_{12}\text{X}_4$

Name: N195
Source: QOJVAM_clean
Formula: $\text{Cu}_2\text{C}_{20}\text{H}_{14}\text{I}_2\text{N}_4\text{X}_6$

Name: N196
Source: XIDBUJ_clean
Formula: $\text{C}_5\text{H}_2\text{NX}_3$

Name: N197
Source: PEPFAT_clean
Formula: $\text{Zn}_4\text{C}_6\text{O}_{13}\text{X}_6$

Name: N198
Source: RAYMOV_clean
Formula: $\text{Mn}_3\text{C}_6\text{O}_{13}\text{X}_6$

Name: N199
Source: ABEMIF_clean
Formula: $\text{Cu}_4\text{C}_8\text{ClO}_{16}\text{X}_8$

Name: N200
Source: WEFCAN_clean
Formula: $\text{FeC}_{22}\text{H}_{16}\text{N}_6\text{S}_2\text{X}_4$

Name: N201
Source: LELDUD_clean
Formula: $\text{C}_{30}\text{H}_{16}\text{N}_2\text{X}_4$

Name: N202
Source: KIBXUP_charged
Formula: $\text{C}_{10}\text{H}_{10}\text{X}_4$

Name: N203
Source: VETTUK_clean
Formula: Dy4C12O24X12

Name: N204
Source: MUWQEB_clean
Formula: Fe4C8N32X8

Name: N205
Source: LAGMUD_clean
Formula: Y2C6O12X6

Name: N206
Source: MITTAL_charged
Formula: Cd2C5O10X5

Name: N207
Source: REWLEM_clean_h
Formula: Zn2C40H8N8X4

Name: N208
Source: HIGRIA_clean
Formula: CoZn4C36H18N18X6

Name: N209
Source: DASTEY01_charged
Formula: Zn3C8O16X8

Name: N210
Source: PEBNEP_clean
Formula: Cu2C12Cl4H12N8X4

Name: N211
Source: XILVEV_clean
Formula: MnC20H8N4X4

Name: N212
Source: BIWSEG_ion_b
Formula: Cu4C8Cl4N32X8

Name: N213
Source: ADIQEL_clean
Formula: CoC14H12N2O4X6

Name: N214
Source: ACAJOF_clean
Formula: Cu2C14H8N2O8X6

Name: N215
Source: EREGOY_clean
Formula: Cd2C4O8X4

Name: N216
Source: YEHGID_clean
Formula: Fe3C57H42N3O13X3

Name: N217
Source: ODODES_clean
Formula: Zn3C8H2O16X8

Name: N218
Source: OBEDAA_charged
Formula: C19H12X4

Name: N219
Source: DIHPIU_charged
Formula: AgC20H16N4X4

Name: N220
Source: XADDAJ_clean
Formula: Tb2C6O12X6

Name: N221
Source: YEYFEP_clean
Formula: Ho4C6H4O16X6

Name: N222
Source: VARJEF_clean
Formula: FeC14H8N6X6

Name: N223
Source: AMIKOX_clean
Formula: C4H4X4

Name: N224
Source: TATPOV_clean
Formula: C30H14X8

Name: N225
Source: DOKHOB_clean
Formula: C9H9X3

Name: N226
Source: WAVRAO_clean
Formula: In2Mn2C8O18X8

Name: N227
Source: CUKXOW_clean
Formula: C9H12N6X6

Name: N228
Source: UTEWOG_clean
Formula: Ni4C24H16N16X8

Name: N229
Source: ODODIW_clean
Formula: Zn5C8H2O18X8

Name: N231
Source: AKAYIV_clean
Formula: C9H3O6X3

Name: N232
Source: CIFMIP_clean
Formula: Co3C6H2O13X6

Name: N233
Source: IYUHIU_ion_b
Formula: In2C7O15X7

Name: N234
Source: MUVGOA_clean
Formula: ZnC14H8N6X6

Name: N235
Source: LELRUR_clean
Formula: La2O24P8X8

Name: N236
Source: CAJQEL_clean
Formula: C34H22O4X8

Name: N237
Source: ALIXOJ_clean
Formula: Ni2C4H2O9X4

Name: N238
Source: FEDJUJ_charged
Formula: ZnC4O8X4

Name: N240
Source: FEVTEF_charged
Formula: CoC12H18O6X6

Name: N241
Source: BEDYEQ_clean
Formula: $\text{Zr}_6\text{C}_8\text{O}_{24}\text{X}_8$

Name: N242
Source: RIBDEN_clean
Formula: $\text{Co}_2\text{C}_5\text{O}_{10}\text{X}_5$

Name: N243
Source: LOBHAM_clean
Formula: $\text{Ni}_3\text{C}_{14}\text{H}_{12}\text{N}_{12}\text{O}_{14}\text{X}_{10}$

Name: N244
Source: PASMUT_clean
Formula: $\text{C}_6\text{H}_6\text{X}_6$

Name: N245
Source: MEXJAC_clean
Formula: $\text{SmC}_3\text{O}_6\text{X}_3$

Name: N246
Source: OWAVIS_clean
Formula: $\text{Zn}_2\text{C}_3\text{O}_6\text{X}_3$

Name: N247
Source: XADDOX_clean
Formula: $\text{Co}_6\text{C}_{10}\text{H}_{20}\text{O}_{22}\text{X}_{10}$

Name: N248
Source: KULRIT_clean
Formula: $\text{Yb}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N249
Source: TUDQOZ_clean
Formula: $\text{Cd}_2\text{C}_{24}\text{H}_{16}\text{N}_4\text{O}_8\text{X}_8$

Name: N250
Source: XOFTIW_clean
Formula: $\text{Ce}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N251
Source: GEDDAW_clean
Formula: $\text{Co}_{24}\text{C}_{12}\text{H}_{12}\text{O}_{84}\text{S}_{12}\text{X}_{12}$

Name: N254
Source: PEXTUI_clean
Formula: $\text{Cd}_2\text{C}_5\text{O}_{10}\text{X}_5$

Name: N255
Source: PEGCIP_clean
Formula: $\text{C}_{30}\text{H}_{16}\text{S}_4\text{X}_4$

Name: N256
Source: AVIMOI_clean
Formula: $\text{Zn}_2\text{C}_4\text{O}_8\text{X}_4$

Name: N257
Source: PURJES_clean
Formula: $\text{Zn}_2\text{C}_4\text{O}_8\text{X}_4$

Name: N258
Source: PEWLUA_clean
Formula: $\text{C}_{30}\text{H}_{15}\text{N}_9\text{X}_6$

Name: N259
Source: UZAFAD_clean
Formula: $\text{NiC}_{12}\text{H}_{12}\text{N}_8\text{X}_4$

Name: N260
Source: ADUWIH_clean
Formula: $\text{C}_{48}\text{H}_{36}\text{O}_6\text{X}_6$

Name: N261
Source: LOJFUL_clean
Formula: Na2C8O16X8

Name: N262
Source: HAWZEM_clean
Formula: Cu2C24H16N4O8X8

Name: N263
Source: UKUBOS_clean
Formula: Mn20H18N4S2X4

Name: N264
Source: ALULAV_clean
Formula: Gd2C6O12X6

Name: N265
Source: ADUWIH_clean
Formula: Zn3C6O12X6

Name: N267
Source: NISCOJ_clean
Formula: ZnC10H12N6O4X4

Name: N268
Source: GAYPED_clean
Formula: Co3C6O13X6

Name: N269
Source: ADODAA_charged
Formula: Cu3C12H6N6O7X6

Name: N270
Source: HOMZEP_clean
Formula: Ga3C6O13X6

Name: N271
Source: MANLAP_ion_b
Formula: C18H18X4

Name: N272
Source: VEHKOK_charged
Formula: Zn3C5O12X5

Name: N273
Source: DANZEZ_charged
Formula: Mn3C8Cl2H6O14X6

Name: N274
Source: MANLIX_charged
Formula: ZnC30H24N6X6

Name: N275
Source: PETWOC_clean
Formula: U6C12O32X12

Name: N276
Source: PUWCOZ_clean
Formula: Ni2C4H2O9X4

Name: N277
Source: CUYQIX_clean
Formula: C3H5X3

Name: N278
Source: XEDGIY_clean
Formula: Cd3C6O12X6

Name: N279
Source: BETDIP_clean
Formula: C13H8NX3

Name: N280
Source: KAVJEX01_clean
Formula: Nd3C12O24X12

Name: N281
Source: UTEWUM_clean
Formula: Cu4C24H16N16X8

Name: N282
Source: OYEJOS_clean
Formula: CuC12H12N8X4

Name: N283
Source: ESIPUR02_clean
Formula: Cu2C6H2O12X6

Name: N284
Source: HICVOG_clean
Formula: Zn2C13H6N7O6X7

Name: N285
Source: COWXOC_clean
Formula: C3HN2X3

Name: N286
Source: NESVAK_charged
Formula: Cd3C12H4N3O13X6

Name: N287
Source: YARGAB_clean
Formula: Zn3C6O13X6

Name: N288
Source: BETZOR_clean
Formula: Mn2C4O8X4

Name: N289
Source: SONTAR_clean5b
Formula: Pr2C6O12X6

Name: N290
Source: ACOLOV_clean
Formula: Cd3C6O12X6

Name: N292
Source: MAJHUC_clean
Formula: MnC12H8N2O4X4

Name: N293
Source: YUVGOL_clean
Formula: Zn4C48H32N8X8

Name: N295
Source: ICAROV_clean
Formula: Ni2C14H8N2O8X6

Name: N296
Source: NICZAA01_charged
Formula: C12H12X6

Name: N297
Source: ALOLIX_charged
Formula: CsIn3C12O24X12

Name: N298
Source: CETVAA_clean
Formula: CuC15Cl2H12N3X3

Name: N300
Source: YONNAR_clean
Formula: Zn3C5HO11X5

Name: N301
Source: RUTBUE_clean
Formula: $\text{Na}_4\text{C}_8\text{H}_{12}\text{O}_{12}\text{X}_4$

Name: N302
Source: CAZGIT_clean
Formula: $\text{Cu}_2\text{C}_{20}\text{H}_8\text{N}_4\text{X}_4$

Name: N303
Source: FIKTOK_clean
Formula: $\text{Cd}_2\text{C}_4\text{O}_8\text{X}_4$

Name: N304
Source: UJEDIX_clean
Formula: $\text{YbC}_4\text{O}_8\text{X}_4$

Name: N305
Source: WEHJOK_clean
Formula: $\text{Zn}_3\text{C}_4\text{O}_9\text{X}_4$

Name: N306
Source: YURKIG_clean
Formula: $\text{Pr}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N307
Source: FAPYEA04_clean
Formula: $\text{Cu}_4\text{N}_4\text{X}_4$

Name: N308
Source: GAJTOC_clean
Formula: $\text{Gd}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N309
Source: HEFFAB_charged
Formula: $\text{CdMn}_6\text{O}_{12}\text{X}_6$

Name: N310
Source: PAQVOU_charged
Formula: $\text{FeC}_4\text{O}_8\text{X}_4$

Name: N311
Source: EMEGEJ_clean
Formula: $\text{Eu}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N312
Source: FAYPIG_clean
Formula: $\text{Zn}_5\text{C}_{46}\text{H}_{36}\text{N}_{18}\text{O}_8\text{X}_4$

Name: N313
Source: AROFAP_clean
Formula: $\text{C}_{29}\text{H}_{24}\text{O}_4\text{X}_4$

Name: N314
Source: WEFXEM_clean
Formula: $\text{NiC}_{12}\text{H}_{12}\text{N}_8\text{O}_6\text{S}_2\text{X}_6$

Name: N315
Source: HEKTAU_clean
Formula: $\text{CdC}_{11}\text{H}_8\text{N}_2\text{O}_2\text{X}_3$

Name: N317
Source: ADASUV_clean
Formula: $\text{Co}_2\text{C}_4\text{O}_8\text{X}_4$

Name: N318
Source: AROFET_clean
Formula: $\text{Cd}_4\text{C}_8\text{O}_{16}\text{X}_8$

Name: N320
Source: LIZWEX_charged
Formula: $\text{Cu}_3\text{C}_3\text{N}_{12}\text{O}_{10}\text{X}_3$

Name: N321
Source: CUTFON_charged
Formula: $\text{BC}_{30}\text{H}_{36}\text{X}_3$

Name: N323
Source: ALOLIX_charged
Formula: $\text{CsIn}_3\text{C}_{12}\text{O}_{24}\text{X}_{12}$

Name: N324
Source: ELEROD_clean
Formula: $\text{Eu}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N325
Source: ONIXOZ_clean
Formula: C24H12X6

Name: N326
Source: MEFHUC_charged
Formula: Zn4C14H14N2O20X8

Name: N327
Source: IZOWAW_clean
Formula: Mo12Zn4C4O32X4

Name: N328
Source: TASZAQ_charged
Formula: Zn3C30H18N6X6

Name: N329
Source: WAVROC_clean
Formula: In2Mg2C8O18X8

Name: N330
Source: OHOFEW_clean
Formula: Co2C20H28N8X4

Name: N331
Source: NEHNEV_clean
Formula: Zn3C12H6N4O12X8

Name: N332
Source: MASZOX_clean
Formula: Cu3MoC25H20IN5S3X5

Name: N333
Source: DAWCIP_clean
Formula: C19H13X3

Name: N334
Source: ISUCUV_clean
Formula: Fe3C6O12X6

Name: N335
Source: NABCIE_clean
Formula: Co2C20F2H16N4X4

Name: N336
Source: ZEDROR_clean
Formula: Zn2C12H10N4O8X6

Name: N337
Source: NIFYOS_charged
Formula: Lu2C8O16X8

Name: N339
Source: IJASOC_clean
Formula: Tm2C6O12X6

Name: N340
Source: GAWLIB_clean
Formula: Tb2C6O12X6

Name: N341
Source: TAFICIO_clean
Formula: Co2C6H2O12X6

Name: N342
Source: QEPZUH_charged
Formula: Cu2C20H16N4O2X4

Name: N343
Source: UKIQOV_clean
Formula: Co3C6O12X6

Name: N344
Source: TEBCEK_clean
Formula: $\text{Co}_3\text{C}_{18}\text{H}_{12}\text{N}_8\text{O}_{12}\text{X}_{10}$

Name: N346
Source: QUQFOY_clean
Formula: $\text{Cd}_2\text{C}_4\text{O}_8\text{X}_4$

Name: N348
Source: VETTIZ_charged
Formula: $\text{Fe}_4\text{C}_8\text{O}_{20}\text{X}_8$

Name: N349
Source: ICODIP01_clean
Formula: $\text{C}_{21}\text{H}_{12}\text{N}_6\text{X}_6$

Name: N350
Source: RULXOM_clean
Formula: $\text{Fe}_4\text{C}_8\text{O}_{16}\text{X}_8$

Name: N352
Source: CANRUG_clean
Formula: $\text{Ca}_3\text{C}_8\text{H}_2\text{O}_{16}\text{X}_8$

Name: N353
Source: DOMCUE_clean
Formula: $\text{C}_{19}\text{Cl}_{12}\text{X}_3$

Name: N354
Source: IMUVAO_charged
Formula: $\text{In}_3\text{C}_6\text{O}_{16}\text{X}_6$

Name: N355
Source: EBIHII_clean
Formula: $\text{Fe}_2\text{C}_4\text{O}_8\text{X}_4$

Name: N356
Source: NARTUX_clean
Formula: $\text{Ca}_2\text{C}_6\text{O}_{11}\text{X}_6$

Name: N357
Source: NESTAI_clean
Formula: $\text{Ni}_2\text{C}_{24}\text{H}_{18}\text{N}_4\text{O}_9\text{X}_8$

Name: N358
Source: ESEVIH_clean
Formula: $\text{Zn}_8\text{C}_{12}\text{H}_4\text{O}_{28}\text{X}_{12}$

Name: N359
Source: EDAPIK_clean_h
Formula: $\text{Cu}_2\text{C}_{20}\text{H}_{16}\text{N}_4\text{X}_4$

Name: N360
Source: FURQOZ01_ion_b
Formula: $\text{Ag}_2\text{C}_{20}\text{H}_{16}\text{N}_4\text{X}_4$

Name: N362
Source: OQIRAI_charged
Formula: $\text{Cu}_2\text{C}_{16}\text{H}_{16}\text{N}_{24}\text{X}_8$

Name: N363
Source: FAGFUQ_clean
Formula: $\text{Co}_3\text{C}_8\text{H}_2\text{O}_{16}\text{X}_8$

Name: N364
Source: HOWQAM_clean
Formula: $\text{CdC}_{12}\text{H}_7\text{N}_2\text{O}_4\text{X}_5$

Name: N365
Source: MIHMEW_clean
Formula: $\text{PtC}_{20}\text{H}_8\text{N}_4\text{X}_4$

Name: N366
Source: NURMUJ_clean
Formula: $\text{Zn}_3\text{C}_6\text{O}_{12}\text{X}_6$

Name: N367
Source: FAYQIH_clean
Formula: $\text{C}_{37}\text{H}_{32}\text{O}_4\text{X}_4$

Name: N368
Source: TIQHIL_clean
Formula: $\text{DyC}_{40}\text{H}_{24}\text{N}_8\text{O}_8\text{X}_8$

Name: N369
Source: YEKQOW_clean
Formula: $\text{Zn}_4\text{C}_8\text{O}_{17}\text{X}_8$

Name: N370
Source: DIBQEM_clean
Formula: $\text{Co}_6\text{C}_8\text{O}_{24}\text{X}_8$

Name: N371
Source: RAHBUZ_clean
Formula: $\text{Zn}_2\text{C}_4\text{O}_8\text{X}_4$

Name: N372
Source: BINCUY_clean_b
Formula: $\text{Co}_2\text{C}_{24}\text{H}_{16}\text{N}_4\text{O}_8\text{X}_8$

Name: N373
Source: WOQDUB_charged
Formula: $\text{Dy}_4\text{C}_6\text{O}_{24}\text{X}_6$

Name: N374
Source: SUNHUF_clean
Formula: $\text{Nd}_2\text{C}_8\text{O}_{16}\text{X}_8$

Name: N375
Source: CUNWEO_clean
Formula: $\text{Cd}_2\text{C}_{24}\text{H}_{16}\text{N}_4\text{O}_8\text{X}_8$

Name: N376
Source: ACOGEF_clean
Formula: $\text{CdC}_{20}\text{H}_{16}\text{I}_2\text{N}_4\text{X}_4$

Name: N377
Source: ADASEF_clean
Formula: $\text{Cu}_3\text{C}_3\text{N}_{12}\text{O}_3\text{X}_3$

Name: N378
Source: SATBEW_clean
Formula: $\text{Cu}_4\text{WBr}_2\text{C}_{30}\text{H}_{24}\text{N}_6\text{S}_4\text{X}_6$

Name: N379
Source: WIYMOG_charged
Formula: $\text{Tb}_2\text{C}_6\text{O}_{16}\text{X}_6$

Name: N380
Source: LIRTEM_clean
Formula: $\text{Cd}_4\text{C}_8\text{O}_{17}\text{X}_8$

Name: N381
Source: HAWWEJ_charged
Formula: $\text{Yb}_2\text{C}_{14}\text{H}_{12}\text{N}_4\text{O}_{18}\text{X}_8$

Name: N382
Source: NERVAJ_clean
Formula: $\text{Zn}_3\text{C}_6\text{O}_{12}\text{X}_6$

Name: N383
Source: XOVQEF_clean
Formula: $\text{Zn}_2\text{C}_5\text{H}_{20}\text{O}_{10}\text{X}_5$

Name: N384
Source: REFTUT_clean
Formula: $\text{CaZn}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N385
Source: ALANAD_clean
Formula: $\text{Zn}_2\text{C}_4\text{O}_8\text{X}_4$

Name: N386
Source: ZABQIC_ion_b
Formula: $\text{C}_{30}\text{H}_{15}\text{X}_3$

Name: N387
Source: CUVHIL01_clean
Formula: $\text{Nd}_2\text{C}_6\text{H}_{20}\text{O}_{12}\text{X}_4$

Name: N388
Source: CUYVOI_clean
Formula: $\text{C}_5\text{H}_8\text{X}_4$

Name: N389
Source: PASKAX_clean
Formula: $\text{Cd}_2\text{C}_{16}\text{H}_{12}\text{N}_8\text{O}_8\text{X}_8$

Name: N390
Source: ADARAA_clean
Formula: $\text{Co}_2\text{C}_4\text{O}_9\text{X}_4$

Name: N391
Source: RIBTAZ_clean
Formula: $\text{Cu}_4\text{C}_5\text{O}_{12}\text{X}_5$

Name: N392
Source: TEDGOA_clean
Formula: $\text{Zn}_2\text{C}_6\text{N}_{24}\text{X}_6$

Name: N393
Source: GUSJOU_clean
Formula: $\text{C}_4\text{Ge}_4\text{H}_8\text{S}_6\text{X}_4$

Name: N394
Source: BETFEN_clean
Formula: $\text{Pr}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N395
Source: WASVES_clean
Formula: $\text{La}_4\text{Mo}_{12}\text{C}_4\text{O}_{36}\text{PX}_4$

Name: N398
Source: LULJAE_clean
Formula: $\text{Co}_2\text{C}_4\text{O}_8\text{X}_4$

Name: N399
Source: DEYXIQ_clean
Formula: $\text{C}_{14}\text{H}_4\text{O}_2\text{X}_4$

Name: N400
Source: EDOVIE_charged
Formula: $\text{Dy}_5\text{C}_6\text{H}_6\text{O}_{28}\text{X}_6$

Name: N401
Source: ZARLIP_clean
Formula: $\text{Zn}_5\text{C}_9\text{O}_{20}\text{X}_9$

Name: N403
Source: BETDAH_clean
Formula: $\text{C}_{13}\text{H}_7\text{NX}_3$

Name: N404
Source: FAYPEC_clean
Formula: $\text{Zn}_5\text{C}_5\text{H}_4\text{N}_{18}\text{O}_8\text{X}_4$

Name: N406
Source: CANRIU_clean
Formula: $\text{Mg}_3\text{C}_6\text{O}_{12}\text{X}_6$

Name: N407
Source: PUQHEP_clean
Formula: $\text{Co}_4\text{C}_{26}\text{H}_{18}\text{N}_4\text{O}_{14}\text{X}_{10}$

Name: N408
Source: IJISOK_charged
Formula: $\text{C}_9\text{H}_9\text{O}_3\text{X}_3$

Name: N409
Source: ACUFEK_clean
Formula: $\text{Cu}_2\text{C}_4\text{O}_8\text{X}_4$

Name: N410
Source: AWAGEL_clean
Formula: $\text{C}_{18}\text{H}_{12}\text{NX}_3$

Name: N411
Source: MOFLAV_clean
Formula: $\text{Cu}_6\text{H}_6\text{N}_9\text{X}_3$

Name: N412
Source: GIZVER_clean
Formula: $\text{Co}_5\text{C}_8\text{H}_2\text{O}_{18}\text{X}_8$

Name: N413
Source: QUDJIJ_clean
Formula: $\text{C}_{14}\text{H}_6\text{X}_4$

Name: N415
Source: CEXHET_clean
Formula: $\text{AgC}_{15}\text{H}_{12}\text{N}_3\text{X}_3$

Name: N416
Source: NEHNEV01_clean
Formula: $\text{C}_{23}\text{H}_{21}\text{O}_3\text{X}_3$

Name: N417
Source: MEGBEH_clean5b
Formula: $\text{Cd}_2\text{C}_4\text{O}_8\text{X}_4$

Name: N418
Source: QISVEU_clean
Formula: $\text{C}_{19}\text{Cl}_9\text{HX}_6$

Name: N419
Source: OXOLAP_clean5b
Formula: $\text{Zr}_6\text{C}_{12}\text{O}_{32}\text{X}_{12}$

Name: N420
Source: MEGBEH_clean5b
Formula: $\text{Cd}_3\text{C}_4\text{Cl}_2\text{O}_8\text{X}_4$

Name: N421
Source: EDOVEA_charged
Formula: $\text{Gd}_5\text{C}_6\text{H}_6\text{O}_{28}\text{X}_6$

Name: N422
Source: PUWDOA_clean
Formula: $\text{Zn}_3\text{C}_6\text{H}_2\text{O}_{13}\text{X}_6$

Name: N423
Source: ODUNEH_clean
Formula: $\text{Zn}_5\text{C}_8\text{O}_{18}\text{X}_8$

Name: N424
Source: UKUBUY_clean
Formula: $\text{FeC}_{20}\text{H}_{18}\text{N}_4\text{S}_2\text{X}_4$

Name: N425
Source: KABXIW_clean
Formula: $\text{Pr}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N426
Source: OXALIJ_ion_b
Formula: $\text{Cd}_3\text{C}_8\text{O}_{16}\text{X}_8$

Name: N427
Source: QUSCAJ_clean
Formula: $\text{Cd}_3\text{Li}_2\text{C}_8\text{O}_{16}\text{X}_8$

Name: N428
Source: WASTUG_clean
Formula: $\text{La}_4\text{Mo}_{12}\text{C}_6\text{O}_{40}\text{PX}_6$

Name: N429
Source: HAFVOB_clean
Formula: $\text{C}_{18}\text{H}_{12}\text{PX}_3$

Name: N430
Source: HURGEH_clean
Formula: $\text{Co}_3\text{C}_8\text{O}_{16}\text{X}_8$

Name: N431
Source: WAMRIN_clean
Formula: $\text{Mg}_3\text{C}_8\text{H}_4\text{O}_{18}\text{X}_8$

Name: N432
Source: KEVVIS_clean
Formula: $\text{Co}_3\text{C}_{24}\text{H}_{16}\text{N}_4\text{O}_{10}\text{X}_8$

Name: N433
Source: OJICUG_clean
Formula: $\text{Sc}_3\text{C}_6\text{O}_{13}\text{X}_6$

Name: N434
Source: VAHPUR_clean
Formula: $\text{DyC}_4\text{O}_8\text{X}_4$

Name: N435
Source: DITYAH_clean
Formula: $\text{CoC}_{20}\text{H}_{16}\text{N}_4\text{X}_4$

Name: N437
Source: QUGBUQ_clean
Formula: $\text{AgC}_8\text{H}_5\text{N}_4\text{O}_2\text{X}_4$

Name: N438
Source: AXINAX01_clean
Formula: $\text{Co}_3\text{C}_6\text{O}_{12}\text{X}_6$

Name: N439
Source: BIBXOB_clean
Formula: $\text{Ni}_8\text{C}_{36}\text{H}_{30}\text{N}_2\text{O}_6\text{X}_{12}$

Name: N440
Source: CIFMEL_clean
Formula: $\text{Co}_2\text{C}_3\text{ClO}_6\text{X}_3$

Name: N441
Source: EWESIJ_clean
Formula: $\text{Cu}_4\text{WC}_{30}\text{H}_{24}\text{I}_2\text{N}_6\text{S}_4\text{X}_6$

Name: N442
Source: JEJWOL_clean
Formula: $\text{Nd}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N443
Source: DAKVOC_clean
Formula: $\text{C}_{29}\text{H}_{20}\text{O}_4\text{X}_8$

Name: N444
Source: KEHGAH_charged
Formula: $\text{Cd}_2\text{C}_{18}\text{H}_{18}\text{N}_2\text{X}_9$

Name: N445
Source: EBUQIB_clean
Formula: $\text{ZnC}_{20}\text{H}_8\text{N}_4\text{X}_4$

Name: N446
Source: YEKXIX_clean
Formula: $\text{Zn}_4\text{C}_7\text{O}_{15}\text{X}_7$

Name: N447
Source: NIFYOS_charged
Formula: $\text{Co}_3\text{C}_{30}\text{H}_{18}\text{N}_6\text{X}_6$

Name: N448
Source: DUXKUD_clean
Formula: $\text{UC}_4\text{O}_8\text{X}_4$

Name: N449
Source: COCMAJ_clean
Formula: $\text{PdC}_{10}\text{Cl}_2\text{H}_6\text{N}_2\text{X}_4$

Name: N450
Source: KEDPEQ_charged
Formula: $\text{AgC}_4\text{N}_4\text{X}_4$

Name: N452
Source: YEKQOW_clean
Formula: $\text{Zn}_7\text{C}_{12}\text{H}_{20}\text{O}_{26}\text{X}_{12}$

Name: N453
Source: REFTON_clean
Formula: $\text{CdZn}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N454
Source: WEDWUZ_clean
Formula: $\text{Cu}_4\text{Br}_4\text{C}_{20}\text{H}_{16}\text{N}_4\text{X}_4$

Name: N455
Source: AMIKOX_clean
Formula: $\text{Cd}_{20}\text{Cl}_2\text{H}_{16}\text{N}_4\text{X}_4$

Name: N456
Source: BINCUY_clean_b
Formula: $\text{C}_{30}\text{H}_{27}\text{O}_3\text{X}_3$

Name: N457
Source: BICDAU_clean
Formula: $\text{Zn}_5\text{C}_{36}\text{H}_{18}\text{N}_{18}\text{X}_6$

Name: N460
Source: IBOZIK_clean
Formula: $\text{Cu}_4\text{C}_{24}\text{H}_{24}\text{N}_4\text{O}_6\text{X}_4$

Name: N461
Source: GERWOR_charged
Formula: $\text{CdC}_4\text{O}_8\text{X}_4$

Name: N462
Source: BUCROH_charged
Formula: $\text{Ni}_3\text{C}_8\text{H}_8\text{O}_{20}\text{X}_8$

Name: N464
Source: QURSEC_clean
Formula: $\text{PdC}_{20}\text{H}_{16}\text{N}_4\text{X}_4$

Name: N465
Source: NEDWIE_clean
Formula: $\text{MnNi}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N466
Source: BASJUB_clean
Formula: $\text{C}_9\text{H}_8\text{O}_8\text{X}_4$

Name: N467
Source: ABUWOJ_clean
Formula: $\text{Zn}_4\text{C}_6\text{H}_{20}\text{O}_{14}\text{X}_6$

Name: N468
Source: ALAMUW_clean
Formula: $\text{C}_{22}\text{H}_8\text{N}_2\text{O}_4\text{X}_4$

Name: N469
Source: VETVAS_clean5b
Formula: $\text{Nd}_4\text{C}_{12}\text{O}_{24}\text{X}_{12}$

Name: N470
Source: GAYPED_clean
Formula: $\text{CoC}_{20}\text{H}_8\text{N}_4\text{X}_4$

Name: N471
Source: ACUJOZ_clean5b
Formula: $\text{C}_{14}\text{H}_8\text{X}_4$

Name: N472
Source: WILGEE_charged
Formula: Ag₄C₂₄H₁₈N₁₂X₆

Name: N473
Source: PIHWAG_clean
Formula: C₁₈H₉S₃X₃

Name: N474
Source: COWMAD_clean
Formula: C₆H₉X₃

Name: N475
Source: VEFMAW_charged
Formula: Co₃C₁₀H₁₄N₂O₁₄X₆

Name: N476
Source: IZOWEA_clean
Formula: Mo₂₄Zn₈C₆O₆₈P₂X₆

Name: N477
Source: AVUDAX_clean
Formula: C₉H₉X₃

Name: N478
Source: FUQJUX_clean
Formula: Cu₃C₁₈H₁₂N₁₅OX₆

Name: N479
Source: KIPKAX_clean
Formula: Yb₂C₆O₁₂X₆

Name: N480
Source: VEFMAW_charged
Formula: Co₂C₆O₁₂X₆

Name: N481
Source: CIGXIA_clean5b
Formula: Fe₃C₆O₁₃X₆

Name: N482
Source: RIBDAJ_clean
Formula: Ni₂C₅O₁₀X₅

Name: N483
Source: FITHAS_charged
Formula: Sc₃₀H₂₄N₆O₆X₆

Name: N484
Source: DEHLAF_clean
Formula: C₁₂H₁₅X₃

Name: N485
Source: LELCUB01_clean
Formula: Cu₃C₁₅H₁₈N₆X₃

Name: N486
Source: ICEGED_clean
Formula: Cd₃C₆N₂₄X₆

Name: N488
Source: EXOZEX_clean
Formula: C₉H₁₂N₃O₃X₃

Name: N489
Source: TASYUJ_charged
Formula: Cu₃₀H₁₈N₆X₆

Name: N490
Source: XICYEP_clean
Formula: Hf₆C₁₀O₂₈X₁₀

Name: N491
Source: CAZNEY_clean
Formula: $\text{Co}_3\text{C}_6\text{O}_{12}\text{X}_6$

Name: N492
Source: FAHGAY_clean
Formula: $\text{Be}_4\text{O}_8\text{X}_4$

Name: N493
Source: NENHAQ_clean
Formula: $\text{Cd}_3\text{C}_6\text{O}_{12}\text{X}_6$

Name: N494
Source: FEVVIM_charged
Formula: $\text{Mn}_{12}\text{H}_{18}\text{O}_6\text{X}_6$

Name: N495
Source: MEXJAC_clean
Formula: $\text{C}_6\text{I}_3\text{X}_3$

Name: N498
Source: ECUTON_clean
Formula: $\text{C}_{12}\text{H}_6\text{N}_2\text{X}_4$

Name: N499
Source: AXINAX01_clean
Formula: $\text{Co}_2\text{C}_3\text{O}_6\text{X}_3$

Name: N500
Source: HAJMEL_clean
Formula: $\text{Fe}_{22}\text{H}_{26}\text{N}_{10}\text{S}_2\text{X}_4$

Name: N501
Source: SATCEX_clean
Formula: $\text{Cu}_4\text{WC}_{30}\text{Cl}_2\text{H}_{24}\text{N}_6\text{S}_4\text{X}_6$

Name: N503
Source: UKUCAF_clean
Formula: $\text{Co}_2\text{O}_{18}\text{H}_{18}\text{N}_4\text{S}_2\text{X}_4$

Name: N504
Source: IYICUP_clean
Formula: $\text{La}_6\text{O}_{12}\text{X}_6$

Name: N505
Source: LAGRIW_clean
Formula: $\text{Yb}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N506
Source: KAGCAY_charged
Formula: $\text{Cu}_3\text{C}_{12}\text{H}_6\text{N}_6\text{O}_7\text{X}_6$

Name: N507
Source: RAXCOK_clean
Formula: $\text{Zn}_2\text{C}_{24}\text{H}_{16}\text{N}_4\text{O}_8\text{X}_8$

Name: N508
Source: HASTAY_clean
Formula: $\text{Zn}_2\text{C}_6\text{O}_{13}\text{X}_6$

Name: N509
Source: COWMUX_clean
Formula: $\text{Tm}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N510
Source: XICYIT_clean
Formula: $\text{Zr}_6\text{C}_{10}\text{O}_{28}\text{X}_{10}$

Name: N512
Source: BUVXOG_clean
Formula: $\text{Fe}_{24}\text{H}_{16}\text{N}_{10}\text{X}_4$

Name: N513
Source: HAJLEK_clean
Formula: $\text{FeC}_{22}\text{H}_{28}\text{N}_{10}\text{S}_2\text{X}_4$

Name: N514
Source: CIGYAU_clean
Formula: $\text{C}_5\text{H}_8\text{O}_4\text{X}_4$

Name: N515
Source: NUVYIN_clean
Formula: $\text{NiC}_{12}\text{H}_8\text{N}_2\text{O}_4\text{X}_4$

Name: N516
Source: OBEDEE_clean
Formula: $\text{C}_{19}\text{H}_{13}\text{OX}_3$

Name: N518
Source: KUXLUL_clean
Formula: $\text{Cu}_4\text{C}_4\text{H}_{20}\text{I}_6\text{S}_2\text{X}_6$

Name: N519
Source: WAHNUQ_charged
Formula: $\text{ZnC}_{15}\text{H}_{12}\text{N}_3\text{X}_3$

Name: N520
Source: NIKDIU_clean
Formula: $\text{EuC}_4\text{O}_8\text{X}_4$

Name: N521
Source: UVEVAT_clean
Formula: $\text{Mn}_2\text{C}_8\text{H}_4\text{N}_6\text{O}_8\text{X}_6$

Name: N522
Source: OKINIG_clean
Formula: $\text{C}_8\text{H}_8\text{X}_4$

Name: N524
Source: UKUBIM_clean
Formula: $\text{CdC}_{20}\text{H}_{18}\text{N}_4\text{S}_2\text{X}_4$

Name: N525
Source: ZIDNEH_clean
Formula: $\text{InC}_{20}\text{H}_8\text{N}_4\text{X}_4$

Name: N526
Source: ACALIB_clean
Formula: $\text{Er}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N528
Source: BICPUA_clean
Formula: $\text{Yb}_3\text{C}_6\text{O}_{13}\text{X}_6$

Name: N529
Source: FENVOL_charged
Formula: $\text{Zn}_3\text{C}_4\text{O}_{14}\text{P}_2\text{X}_6$

Name: N530
Source: KASRAZ_clean
Formula: $\text{Cd}_4\text{C}_8\text{O}_{16}\text{X}_8$

Name: N532
Source: KAVJAT_charged
Formula: $\text{Pr}_3\text{C}_{12}\text{O}_{24}\text{X}_{12}$

Name: N533
Source: EBIDOK_ion_b
Formula: $\text{FeC}_9\text{H}_3\text{O}_6\text{X}_6$

Name: N534
Source: VIRVEY_clean
Formula: $\text{PtC}_{10}\text{Cl}_2\text{H}_6\text{N}_2\text{X}_4$

Name: N535
Source: REBCAE_clean
Formula: $\text{C}_{36}\text{H}_{33}\text{O}_3\text{X}_3$

Name: N536
Source: IZEPAF_clean
Formula: $\text{Cr}_3\text{C}_6\text{O}_{13}\text{X}_6$

Name: N538
Source: MEFZUU_clean5b
Formula: $\text{Mn}_2\text{C}_{20}\text{Cl}_8\text{N}_4\text{X}_4$

Name: N539
Source: MEFZUU_clean5b
Formula: $\text{Mn}_3\text{C}_4\text{O}_8\text{X}_4$

Name: N540
Source: ENIXUV_clean
Formula: $\text{MnC}_{30}\text{H}_{16}\text{N}_6\text{X}_6$

Name: N541
Source: MIQLEE_charged
Formula: $\text{Zn}_3\text{C}_6\text{O}_{16}\text{X}_6$

Name: N542
Source: KALFIO_clean
Formula: $\text{Ni}_2\text{C}_{24}\text{H}_{18}\text{N}_4\text{O}_9\text{X}_8$

Name: N543
Source: LASQON_clean
Formula: $\text{Ni}_2\text{C}_{16}\text{H}_{12}\text{N}_8\text{O}_8\text{X}_8$

Name: N544
Source: BUCSIC_charged
Formula: $\text{Co}_3\text{C}_8\text{H}_4\text{O}_{18}\text{X}_8$

Name: N545
Source: NIGDEO_clean
Formula: $\text{Cu}_4\text{C}_{12}\text{H}_4\text{N}_2\text{O}_{16}\text{X}_8$

Name: N546
Source: HIHGEM_clean_b
Formula: $\text{Er}_4\text{C}_{12}\text{O}_{24}\text{X}_{12}$

Name: N547
Source: FEWWOV_clean
Formula: $\text{Co}_2\text{C}_{22}\text{H}_{16}\text{N}_6\text{S}_2\text{X}_4$

Name: N548
Source: CIFDOM_clean
Formula: $\text{Mn}_3\text{C}_6\text{O}_{12}\text{X}_6$

Name: N549
Source: CETJAN_clean_h
Formula: $\text{Co}_2\text{C}_{22}\text{H}_{16}\text{N}_6\text{S}_2\text{X}_4$

Name: N550
Source: EKOPUQ_clean
Formula: $\text{CaCd}_2\text{C}_8\text{O}_{16}\text{X}_8$

Name: N551
Source: XUKYEI_neutral
Formula: $\text{Cu}_2\text{C}_{20}\text{Cl}_2\text{H}_{16}\text{N}_4\text{X}_4$

Name: N552
Source: YEVQOG_clean
Formula: $\text{Ag}_6\text{C}_{30}\text{H}_{36}\text{N}_{12}\text{X}_6$

Name: N553
Source: XIDBUJ_clean
Formula: $\text{Zn}_2\text{C}_{24}\text{H}_{16}\text{N}_4\text{O}_8\text{X}_6$

Name: N554
Source: ACIBOE_clean
Formula: $\text{Zn}_3\text{C}_6\text{O}_{13}\text{X}_6$

Name: N555
Source: DOMCUE_clean
Formula: $\text{Tb}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N556
Source: UDICER_clean
Formula: $\text{Bi}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N557
Source: MIFLIY_clean
Formula: $\text{MgC}_4\text{O}_8\text{X}_4$

Name: N558
Source: VETSOE_charged
Formula: $\text{C}_{33}\text{H}_{27}\text{X}_3$

Name: N559
Source: SOJDEB_clean
Formula: $\text{Cr}_6\text{N}_6\text{X}_6$

Name: N560
Source: DOGZIJ_clean
Formula: $\text{Zn}_2\text{C}_{10}\text{H}_6\text{N}_4\text{O}_8\text{X}_6$

Name: N561
Source: NAGQET_clean
Formula: $\text{CoC}_{24}\text{H}_{16}\text{N}_{10}\text{X}_4$

Name: N562
Source: WEDWUZ_clean
Formula: $\text{Cu}_4\text{Br}_4\text{C}_{20}\text{H}_{16}\text{N}_4\text{X}_4$

Name: N564
Source: XOTXAG_clean
Formula: $\text{C}_{10}\text{H}_4\text{X}_4$

Name: N565
Source: CAXSUR_clean5b
Formula: $\text{Al}_{12}\text{C}_{36}\text{H}_{48}\text{O}_{48}\text{X}_{12}$

Name: N566
Source: GULWIU_clean
Formula: $\text{Cd}_4\text{C}_{24}\text{Cl}_3\text{H}_{16}\text{N}_{20}\text{X}_8$

Name: N567
Source: BETGAK_clean
Formula: $\text{La}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N568
Source: HEFFEF_ion_b
Formula: $\text{Cd}_2\text{Na}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N569
Source: SEFSOM_clean
Formula: $\text{CdC}_{12}\text{H}_{12}\text{N}_8\text{O}_6\text{S}_2\text{X}_6$

Name: N570
Source: UMARAC_charged
Formula: $\text{Cu}_6\text{C}_{30}\text{H}_{42}\text{N}_{12}\text{O}_6\text{X}_6$

Name: N571
Source: ECOKAJ_clean
Formula: $\text{C}_6\text{N}_7\text{X}_3$

Name: N572
Source: ZEDVUB_charged
Formula: $\text{SmC}_5\text{O}_{11}\text{X}_5$

Name: N573
Source: HOXJIO_charged
Formula: $\text{C}_{54}\text{H}_{30}\text{X}_6$

Name: N574
Source: TASZEU_charged
Formula: $\text{FeC}_{30}\text{H}_{18}\text{N}_6\text{X}_6$

Name: N575
Source: VEYVEC_clean
Formula: $\text{C}_8\text{O}_4\text{X}_4$

Name: N576
Source: DANZAV_charged
Formula: $\text{Cd}_3\text{C}_6\text{Cl}_2\text{O}_{14}\text{X}_6$

Name: N577
Source: OLOGEC_clean
Formula: $\text{Zn}_4\text{C}_6\text{O}_{13}\text{X}_6$

Name: N578
Source: SEMFEX_charged
Formula: $\text{H}_8\text{N}_{12}\text{P}_4\text{X}_8$

Name: N579
Source: NAYKAB_charged
Formula: CdC3O6X3

Name: N580
Source: MITSEO_charged
Formula: Cd2C4Cl2O8X4

Name: N581
Source: GERWIL_charged
Formula: Zn2C4O10X4

Name: N582
Source: RULXUS_clean
Formula: Mn4C8O17X8

Name: N583
Source: IYUHIU_ion_b
Formula: In2C7O15X7

Name: N585
Source: GERWIL_charged
Formula: C24H12SiX8

Name: N586
Source: ZEBMAW_clean
Formula: Ce2C8H2O16X8

Name: N587
Source: WAMRIN02_clean
Formula: Mg3C8H6O18X8

Name: N588
Source: NEHNEV01_clean
Formula: Zn3C12H6N4O12X8

Name: N589
Source: KUGZIW_clean
Formula: Ni3C6O13X6

Name: N590
Source: MEFJUE_clean
Formula: Zn3C6O13X6

Name: N591
Source: BEXSAA_clean
Formula: MnC12H6N2O4X6

Name: N592
Source: BOXFAW_charged
Formula: C39H39X3

Name: N593
Source: QEYWUN_clean
Formula: CdC10H8N12O4X6

Name: N595
Source: DAVYEG_clean
Formula: Co2C10H6N4O8X6

Name: N597
Source: CAYKEU_clean
Formula: C10H4X4

Name: N598
Source: QUQPIC_clean
Formula: CdC14H8N6X6

Name: N599
Source: ODODUI_clean
Formula: Zn4C7HO15X7

Name: N600
Source: COZMUA_clean
Formula: C₂₅H₁₆X₄

Name: N601
Source: BOLPAU_clean
Formula: C₂₄H₁₆SiX₄

Name: N602
Source: GEWXAJ_clean
Formula: Cu₄C₁₀H₈N₈O₁₄X₆

Name: N603
Source: CAYSOK_clean
Formula: MnC₄₀H₂₄N₈X₄

Name: N604
Source: ADASIJ_clean
Formula: C₂₇H₁₈O₃X₆

Name: N606
Source: ROSCEH_clean
Formula: CoC₁₅H₁₂N₃X₃

Name: N607
Source: JEJWEB_clean
Formula: C₃₀H₂₀N₂X₄

Name: N608
Source: YEVQUM_clean5b
Formula: Ag₆C₃₀H₃₆N₁₂X₆

Name: N610
Source: AVOSIO_charged
Formula: C₂₇H₂₇O₆X₃

Name: N611
Source: AKAYIV_clean
Formula: CuBrC₁₅H₁₂N₃X₃

Name: N612
Source: VIZQEC_clean
Formula: Co₃C₆O₁₂X₆

Name: N613
Source: PEWXUL01_clean
Formula: NiC₂₂H₁₆N₆X₆

Name: N614
Source: XAJQAC_clean
Formula: C₄₀H₂₂X₄

Name: N615
Source: MALYIJ_charged
Formula: Ce₂C₈O₁₆X₈

Name: N616
Source: LENGAO_clean
Formula: Cd₂C₄O₈X₄

Name: N617
Source: OGURAK_charged
Formula: Cu₄C₈CIN₁₆O₈X₈

Name: N618
Source: HEFVAR_clean
Formula: RhC₂₀Cl₂H₁₆N₄X₄

Name: N619
Source: LECFUW_charged
Formula: Cu₆C₂₀H₁₆N₁₂O₁₉X₁₂

Name: N621
Source: AVOSIO_charged
Formula: AgC₆H₉X₃

Name: N622
Source: PEKCUF_clean
Formula: Mn₃C₆O₁₂X₆

Name: N623
Source: FEQSIF_clean
Formula: Co₂C₄H₂O₉X₄

Name: N624
Source: MEGBAD_clean
Formula: $\text{Mn}_3\text{C}_4\text{O}_{10}\text{X}_4$

Name: N625
Source: DITJIB_clean
Formula: $\text{Hf}_6\text{C}_8\text{O}_{24}\text{X}_8$

Name: N626
Source: MIGVON_clean
Formula: $\text{Co}_2\text{C}_{42}\text{H}_{56}\text{N}_{18}\text{O}_4\text{S}_3\text{X}_8$

Name: N627
Source: VAHQAY_clean
Formula: $\text{Er}_4\text{O}_8\text{X}_4$

Name: N628
Source: BIWYAH10_clean
Formula: $\text{Nd}_6\text{C}_6\text{N}_6\text{X}_6$

Name: N629
Source: DOCKOW_clean
Formula: $\text{MnZn}_2\text{C}_{16}\text{H}_8\text{N}_2\text{O}_{12}\text{X}_8$

Name: N630
Source: DANZID_charged
Formula: $\text{CdCu}_2\text{C}_6\text{Cl}_2\text{O}_{12}\text{X}_6$

Name: N631
Source: HOXGEH_clean
Formula: $\text{Sn}_4\text{C}_{12}\text{H}_{24}\text{O}_{10}\text{X}_4$

Name: N632
Source: QAGQEW_clean
Formula: $\text{Cd}_4\text{C}_8\text{O}_{16}\text{X}_8$

Name: N634
Source: GEDREO_clean
Formula: $\text{Nd}_2\text{C}_{12}\text{H}_6\text{N}_4\text{O}_{12}\text{X}_6$

Name: N635
Source: UJAQEC_clean
Formula: $\text{Co}_4\text{C}_8\text{O}_{18}\text{X}_8$

Name: N636
Source: CANRIU_clean
Formula: $\text{Mg}_3\text{C}_8\text{O}_{16}\text{X}_8$

Name: N637
Source: TIQGUW_clean
Formula: $\text{Eu}_4\text{O}_{40}\text{H}_{24}\text{N}_8\text{O}_8\text{X}_8$

Name: N638
Source: LECFEG_clean
Formula: $\text{Cu}_3\text{C}_9\text{H}_7\text{N}_9\text{O}_{11}\text{SeX}_6$

Name: N639
Source: LUKLIN_clean
Formula: $\text{C}_{18}\text{H}_9\text{X}_3$

Name: N640
Source: KEHGOV_clean5b
Formula: $\text{Cd}_3\text{C}_{12}\text{Cl}_6\text{H}_{12}\text{N}_{18}\text{X}_6$

Name: N641
Source: AWAGEL_clean
Formula: $\text{Cd}_9\text{H}_9\text{N}_6\text{X}_3$

Name: N642
Source: BIWSIK_ion_b
Formula: $\text{Mn}_4\text{C}_8\text{Cl}_3\text{N}_{32}\text{O}_4\text{X}_8$

Name: N643
Source: VEMTAJ01_clean
Formula: $\text{Co}_3\text{C}_{10}\text{H}_6\text{O}_{16}\text{X}_6$

Name: N644
Source: KEWZOD_clean
Formula: $\text{C}_{14}\text{H}_6\text{X}_4$

Name: N645
Source: ZARLUB_charged
Formula: $\text{Zn}_3\text{C}_{12}\text{H}_4\text{N}_3\text{O}_{12}\text{X}_6$

Name: N646
Source: ALUKOI_clean
Formula: $\text{Sm}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N647
Source: NIGNUO_clean
Formula: $\text{Co}_6\text{C}_8\text{O}_{21}\text{X}_8$

Name: N648
Source: EPUTUF_charged
Formula: $\text{Eu}_2\text{C}_{60}\text{H}_{48}\text{N}_{12}\text{O}_{12}\text{X}_{12}$

Name: N649
Source: FAKGOP_clean
Formula: $\text{Ni}_2\text{C}_4\text{O}_8\text{X}_4$

Name: N650
Source: NALYEG_clean
Formula: $\text{U}_3\text{C}_9\text{O}_{19}\text{X}_9$

Name: N651
Source: REGQUR_clean
Formula: $\text{Zn}_3\text{C}_5\text{O}_{11}\text{X}_5$

Name: N652
Source: RIBTAZ_clean
Formula: $\text{C}_{21}\text{H}_{13}\text{N}_6\text{X}_5$

Name: N653
Source: WOLRIZ_clean
Formula: $\text{Cu}_2\text{C}_8\text{ClN}_{32}\text{X}_8$

Name: N654
Source: HIFZAY_charged
Formula: $\text{Cu}_2\text{C}_{16}\text{H}_{12}\text{N}_8\text{X}_4$

Name: N655
Source: LOJFOF_clean
Formula: $\text{K}_2\text{C}_8\text{H}_4\text{O}_{16}\text{X}_8$

Name: N656
Source: VEXYON_charged
Formula: $\text{Cu}_4\text{C}_8\text{ClN}_{32}\text{O}_4\text{X}_8$

Name: N657
Source: AWAWUR_clean
Formula: $\text{Co}_2\text{C}_{14}\text{H}_8\text{N}_2\text{O}_8\text{X}_6$

Name: N659
Source: GEDQUD_charged
Formula: $\text{Nd}_2\text{C}_6\text{Cl}_2\text{O}_{14}\text{X}_6$

Name: N662
Source: FAYQUT_clean
Formula: $\text{C}_{53}\text{H}_{40}\text{O}_4\text{X}_4$

Name: N663
Source: FILYEG_clean
Formula: $\text{Co}_6\text{C}_{10}\text{O}_{22}\text{X}_{10}$

Name: N664
Source: TIQHEH_clean
Formula: $\text{Tb}_4\text{C}_{40}\text{H}_{24}\text{N}_8\text{O}_8\text{X}_8$

Name: N665
Source: FUNBAS_clean
Formula: $\text{C}_{30}\text{H}_{18}\text{X}_4$

Name: N666
Source: OYUSAD_charged
Formula: $\text{Co}_2\text{Zn}_4\text{O}_{14}\text{P}_2\text{X}_6$

Name: N667
Source: PENNAZ_clean
Formula: $\text{Cd}_3\text{C}_6\text{O}_{12}\text{X}_6$

Name: N668
Source: VEMMEG_clean
Formula: $\text{Mn}_3\text{C}_6\text{N}_{24}\text{X}_6$

Name: N669
Source: LECFAC_clean
Formula: $\text{Cu}_3\text{C}_9\text{H}_7\text{N}_9\text{O}_{11}\text{SX}_6$

Name: N670
Source: XIBZUF_clean
Formula: $\text{C}_{27}\text{H}_{15}\text{N}_3\text{O}_3\text{X}_6$

Name: N671
Source: ODODUJ_clean
Formula: $\text{Zn}_3\text{C}_5\text{HO}_{11}\text{X}_5$

Name: N672
Source: ZIMTAS_clean
Formula: $\text{Cu}_4\text{C}_8\text{ClN}_3\text{X}_8$

Name: N673
Source: IXEFAS_charged
Formula: $\text{Eu}_4\text{O}_4\text{H}_{32}\text{N}_8\text{O}_8\text{X}_8$

Name: N674
Source: VARWES_charged
Formula: $\text{Nd}_4\text{C}_6\text{H}_4\text{O}_{26}\text{X}_6$

Name: N677
Source: SATBIA_charged
Formula: $\text{Cu}_5\text{WC}_{40}\text{H}_{32}\text{I}_2\text{N}_8\text{S}_4\text{X}_8$

Name: N678
Source: MANLOD_clean5b
Formula: $\text{Cd}_3\text{C}_{30}\text{H}_{24}\text{N}_6\text{X}_6$

Name: N679
Source: FATLUJ_clean
Formula: $\text{C}_{12}\text{H}_{12}\text{N}_3\text{O}_3\text{X}_3$

Name: N680
Source: VAXVEX_charged
Formula: $\text{Cd}_{12}\text{H}_{12}\text{N}_{18}\text{X}_8$

Name: N681
Source: WOLMUG_clean
Formula: $\text{Ag}_4\text{C}_{24}\text{H}_{18}\text{N}_{12}\text{X}_6$

Name: N682
Source: GOJFAN_charged
Formula: $\text{UC}_3\text{O}_8\text{X}_3$

Name: N684
Source: NESVEO_charged
Formula: $\text{Zn}_3\text{C}_{12}\text{H}_4\text{N}_3\text{O}_{13}\text{X}_6$

Name: N687
Source: PEJMUN_charged
Formula: $\text{C}_9\text{H}_6\text{N}_3\text{O}_3\text{X}_3$

Name: N688
Source: XEWDUA_clean
Formula: $\text{Cu}_{10}\text{H}_{20}\text{N}_4\text{X}_4$

Name: N689
Source: GEZFIC_charged
Formula: $\text{Zn}_2\text{C}_{20}\text{H}_{16}\text{N}_4\text{O}_4\text{X}_4$

Name: N690
Source: COGNAO_clean
Formula: $\text{Zn}_3\text{C}_6\text{HO}_{13}\text{X}_6$

Name: N691
Source: GAJTUI_clean
Formula: $\text{Tb}_2\text{C}_6\text{O}_{12}\text{X}_6$

Name: N692
Source: GALCED_clean
Formula: $\text{Cd}_2\text{C}_{24}\text{H}_{16}\text{N}_4\text{O}_8\text{X}_8$

Name: N693
Source: BIMDEF_clean
Formula: C₁₀H₁₂X₄

Name: N694
Source: IDUDIW_clean
Formula: Cu₂C₁₂H₆N₄O₈X₆

Name: N695
Source: TASVUG_clean
Formula: C₁₉Cl₁₂HX₃

Name: N696
Source: DAXGUG_clean
Formula: Zn₂C₆O₁₂X₆

Name: N697
Source: TIVYAZ01_clean
Formula: Co₂C₄O₈X₄

Name: N699
Source: OPOZEZ_clean
Formula: Cd₂C₂₄H₁₆N₄O₈X₈

Name: N700
Source: XEYMAR_clean
Formula: Cu₄C₂₀H₁₆I₄N₄X₄

Name: N701
Source: IXEDUK_charged
Formula: Yb₄C₄₀H₃₂N₈O₈X₈

Name: N702
Source: BEXSII_clean
Formula: Cu₂C₁₂H₆N₂O₄X₆

Name: N704
Source: VETMIS_clean
Formula: C₈₄H₅₁N₃X₆

Name: N705
Source: BEXVEH_clean
Formula: C₁₃H₈OX₄

Name: N706
Source: HAFTOZ_clean
Formula: Ni₈C₃₆H₂₄N₂₄X₁₂

Name: N708
Source: UVINAP_clean
Formula: Co₂C₁₂H₁₂N₈X₄

Name: N709
Source: ACAKUM_clean
Formula: La₂C₆O₁₂X₆

Name: N710
Source: ALIXUP_clean
Formula: Cu₃C₄H₂O₁₀X₄

Name: N712
Source: KOHKIC_clean
Formula: Zn₇C₁₂H₈O₂₈X₁₂

Name: N713
Source: IJISOK_charged
Formula: Ag₂C₁₅H₁₂N₃X₃

Name: N715
Source: QAPQAA_charged
Formula: Ag₂C₂₄H₂₀N₁₂X₈

Name: N717
Source: MIZJUB_clean
Formula: Zn₃O₆X₃

Name: N718
Source: ENIXUV_clean
Formula: Mn₂C₂₀H₈N₄X₄

Name: N719
Source: DEBWEO_clean
Formula: Cu₂C₂₀H₁₂N₄X₄

Name: E1
Source: ToBaCCo
Formula: C18H12X2

Name: E2
Source: ToBaCCo
Formula: C14H8X2

Name: E3
Source: ToBaCCo
Formula: C12H6OX2

Name: E4
Source: ToBaCCo
Formula: C12H6X2

Name: E5
Source: ToBaCCo
Formula: C16H8X2

Name: E6
Source: ToBaCCo
Formula: C6H4N4X2

Name: E7
Source: ToBaCCo
Formula: C6N8X2

Name: E8
Source: ToBaCCo
Formula: C6H2N4X2

Name: E9
Source: ToBaCCo
Formula: C6N12X2

Name: E10
Source: ToBaCCo
Formula: C16H8X2

Name: E11
Source: ToBaCCo
Formula: C10H6X2

Name: E12
Source: ToBaCCo
Formula: C10H4X2

Name: E13
Source: ToBaCCo
Formula: C4H2OX2

Name: E14
Source: ToBaCCo
Formula: C6H4X2

Name: E15
Source: ToBaCCo
Formula: C3H3N2X2

Name: E16
Source: ToBaCCo
Formula: C8H6X2

Name: E17
Source: ToBaCCo
Formula: C14H8X2

Name: E18
Source: ToBaCCo
Formula: C8H6X2

Name: E19
Source: ToBaCCo
Formula: C2H2X2

Name: E20
Source: ToBaCCo
Formula: C14H10X2

Name: E21
Source: ToBaCCo
Formula: C12H8N2X2

Name: E22
Source: ToBaCCo
Formula: C6N4X2

Name: E23
Source: ToBaCCo
Formula: C8H4X2

Name: E24
Source: ToBaCCo
Formula: C8H4X2

Name: E25
Source: ToBaCCo
Formula: C10H6X2

Name: E26
Source: ToBaCCo
Formula: C4H4X2

Name: E27
Source: ToBaCCo
Formula: N2X2

Name: E28
Source: ToBaCCo
Formula: C14H8N4X2

Name: E29
Source: ToBaCCo
Formula: C8H4N2X2

Name: E30
Source: ToBaCCo
Formula: C12H6X2

Name: E31
Source: ToBaCCo
Formula: C4N8X2

Name: E32
Source: ToBaCCo
Formula: C18H8X2

Name: E33
Source: ToBaCCo
Formula: C10H4X2

Name: E34
Source: ToBaCCo
Formula: C12H8X2

Name: E35
Source: ToBaCCo
Formula: C10H6N2X2

Name: E36
Source: ToBaCCo
Formula: C10H4X2

Name: E37
Source: ToBaCCo
Formula: C2HN3X2

Name: E38
Source: ToBaCCo
Formula: C4X2

Name: E39
Source: ToBaCCo
Formula: C16H8X2

Name: E40
Source: ToBaCCo
Formula: C14H8X2

Name: E41
Source: ToBaCCo
Formula: C6X2

Name: E42
Source: ToBaCCo
Formula: C10H8X2

Name: E43
Source: ToBaCCo
Formula: C8H6X2

Name: E44
Source: ToBaCCo
Formula: C2X2

Name: E45
Source: ToBaCCo
Formula: C2N4X2

Name: E47
Source: ToBaCCo
Formula: C18H10X2

Name: E48
Source: RILVOZ_clean
Formula: C7H6OX2

Name: E49
Source: KOJYEO_clean
Formula: C16H16X2

Name: E50
Source: BEZSIK_clean
Formula: C2H4X2

Name: E51
Source: MOGXUB_clean
Formula: C2F4X2

Name: E52
Source: IWEPUW_clean
Formula: C7H4O2X2

Name: E53
Source: VEGBUG_clean
Formula: C8H2S3X2

Name: E54
Source: POXHIU_clean
Formula: AgC10H8N2X2

Name: E56
Source: GULWOA_clean
Formula: CdC10H8N2X2

Name: E57
Source: HUTTIA_clean
Formula: C2H2N2X2

Name: E58
Source: IJEXUR_clean
Formula: C6H3O3SX2

Name: E59
Source: REHMEY_clean
Formula: C16H14N2O2X2

Name: E60
Source: GAMXAV_clean
Formula: CuC20H10N4X2

Name: E61
Source: GEPDIQ_clean
Formula: C12H10O2X2

Name: E63
Source: AVIPAX_clean
Formula: C5H3NX2

Name: E64
Source: REHMEY_clean
Formula: C14H11NOX2

Name: E65
Source: AXUHIL_clean
Formula: C6H12X2

Name: E66
Source: ERUFUS_clean
Formula: C2N2SX2

Name: E67
Source: CAXPEY_clean
Formula: C6H3NO2X2

Name: E68
Source: EXEWAG_clean
Formula: C10H4S2X2

Name: E69
Source: DOKHIV_clean
Formula: C7H3O2X2

Name: E70
Source: HAKCIG_clean
Formula: C3HNSX2

Name: E71
Source: IFAGON_clean
Formula: C8H8X2

Name: E72
Source: ACOLEL_clean
Formula: C6H5NX2

Name: E73
Source: CADQAB_clean
Formula: C6H4O2X2

Name: E74
Source: TERFUT_clean
Formula: RhC11H6NX2

Name: E76
Source: PEYPAM_clean
Formula: C7H3O2X2

Name: E77
Source: TEXTOH_clean
Formula: C22H20O2X2

Name: E78
Source: IVARUT_clean
Formula: C10H12X2

Name: E79
Source: AHINIP_clean
Formula: C8H14X2

Name: E80
Source: YEKXOD_clean
Formula: C12H9NX2

Name: E81
Source: OHOLIH_clean
Formula: C10H6X2

Name: E82
Source: AFITUF_clean
Formula: Br2C14H6X2

Name: E83
Source: FEVNEA_charged
Formula: C12H12N2X2

Name: E84
Source: ETESIG_clean
Formula: C14H8X2

Name: E85
Source: AQODOA_clean
Formula: C10H6X2

Name: E86
Source: CUMDOE_clean
Formula: C6H12N2X2

Name: E87
Source: ANENIR_clean
Formula: C16H16O2X2

Name: E88
Source: IMACZN01_clean
Formula: C2H6NX2

Name: E89
Source: FUTKEL_clean5b
Formula: C20H12X2

Name: E90
Source: EMEGEJ_clean
Formula: C18H18S2X2

Name: E91
Source: FEWGUL_clean
Formula: C14H8N4X2

Name: E92
Source: BARZIE_clean
Formula: C6H4X2

Name: E94
Source: CEZFIY_clean
Formula: C12H6N2O4X2

Name: E95
Source: SOQDEI_clean
Formula: C6H4O2SX2

Name: E96
Source: DEQVIF_clean
Formula: C8H8O2X2

Name: E97
Source: VAXVEX_charged
Formula: C14H12X2

Name: E98
Source: RACHUA01_clean
Formula: C17H14X2

Name: E99
Source: PAVKIH_charged
Formula: AgC10H8N2X2

Name: E101
Source: FEVTEF_charged
Formula: C6H14N2X2

Name: E102
Source: CUVHIL02_clean_h
Formula: C6H2I3NX2

Name: E103
Source: TERFIH_clean
Formula: Ir2C10H4N2X2

Name: E104
Source: GUYLOC_clean
Formula: C8H4S2X2

Name: E105
Source: BEXRUT_clean
Formula: NiC2O4X2

Name: E106
Source: FEDJUU_charged
Formula: C14H16N2X2

Name: E107
Source: TERFUT_clean
Formula: C11H7NX2

Name: E108
Source: DEYLUQ_clean
Formula: C9H6N2X2

Name: E109
Source: FISPIH_clean
Formula: NiC12H20N4O4X2

Name: E110
Source: TETZEZ_clean
Formula: C8H6N2O2X2

Name: E111
Source: GIFKAH_clean
Formula: C6H8X2

Name: E112
Source: AMUWUB_clean
Formula: C8H6X2

Name: E113
Source: ZELROZ_clean5b
Formula: C12H8O2X2

Name: E114
Source: OJICEQ_charged
Formula: C13H12NX2

Name: E115
Source: COWXOC_clean
Formula: C8H11X2

Name: E116
Source: KOJYEO_clean
Formula: C16H12X2

Name: E118
Source: VECWUX_clean
Formula: C12H4N4O8X2

Name: E119
Source: NESTAI_clean
Formula: C4H4N2X2

Name: E120
Source: WAWGOQ_clean
Formula: C7H4OX2

Name: E121
Source: IQIJIC_clean
Formula: C14H12O2X2

Name: E122
Source: MUNPAN_clean
Formula: C15H4NO4X2

Name: E123
Source: IBOWIH_charged
Formula: C6H6N2X2

Name: E125
Source: RAVWES_clean
Formula: C16H16X2

Name: E126
Source: ILOJEZ_clean
Formula: C₁₄H₁₂X₂

Name: E127
Source: ACAJOF_clean
Formula: C₃H₆X₂

Name: E128
Source: FAPTIB_clean
Formula: C₆H₅NX₂

Name: E129
Source: XUMFIV_clean
Formula: CuC₁₂H₈N₄S₂X₂

Name: E130
Source: GUFREF_clean
Formula: C₈H₈X₂

Name: E131
Source: LUPYAX_clean
Formula: C₆Cl₂H₂X₂

Name: E132
Source: MUFHUR_clean
Formula: C₃H₂N₂X₂

Name: E133
Source: ENIXUV_clean
Formula: MnC₁₀Cl₃H₈N₂X₂

Name: E134
Source: OGAXUR_clean
Formula: C₁₁H₁₄X₂

Name: E135
Source: ILAGUY_charged
Formula: C₆H₁₃N₂X₂

Name: E136
Source: TERFIH_clean
Formula: C₁₀H₆N₂X₂

Name: E137
Source: DOGZIJ_clean
Formula: C₁₂H₁₆X₂

Name: E138
Source: EKOPOK_clean
Formula: C₆H₄OX₂

Name: E139
Source: SINXET_charged
Formula: C₂H₆NX₂

Name: E141
Source: HEBGUS_clean
Formula: C₈H₁₀N₂X₂

Name: E142
Source: LUWYUY_clean
Formula: C₇H₆OX₂

Name: E143
Source: MEJZEI_clean
Formula: C₆H₁₂NX₂

Name: E145
Source: CIDKUX_clean
Formula: C₁₂F₈X₂

Name: E146
Source: MUFJED_clean
Formula: C3HN2X2

Name: E147
Source: CAXSUR_clean5b
Formula: C10H8X2

Name: E148
Source: FAFMAC_clean
Formula: C8H16N2X2

Name: E149
Source: PEYPAM_clean
Formula: C7H4O2X2

Name: E150
Source: ARIBOS_clean
Formula: C12H8X2

Name: E151
Source: CEHPIP_clean
Formula: C6H10X2

Name: E152
Source: AFITIT_clean
Formula: C16H12X2

Name: E153
Source: XAFXOT_clean
Formula: C6H8N2O2X2

Name: E154
Source: MOYYEF_clean
Formula: C12H8X2

Name: E155
Source: DEXZIR_clean
Formula: C9H8I2OX2

Name: E156
Source: BUGSAY_clean
Formula: C6H11NX2

Name: E157
Source: MALYIJ_charged
Formula: C27H35N2X2

Name: E158
Source: GIKQIC_clean
Formula: C2H2N4X2

Name: E159
Source: MIHHA_clean
Formula: C8H13NOX2

Name: E160
Source: TEQPAI_clean
Formula: C8H6S2X2

Name: E161
Source: XOXMED_clean
Formula: C30H20N2O4X2

Name: E162
Source: WOQDUB_charged
Formula: C2H5NX2

Name: E163
Source: EMITUQ01_clean
Formula: C12H6O2SX2

Name: E165
Source: HUSQES_clean
Formula: C10H14X2

Name: E166
Source: GALCAZ_clean
Formula: C5H3NX2

Name: E167
Source: MALYOP_clean
Formula: C12H16X2

Name: E168
Source: YUPSIM_clean
Formula: C6H6NX2

Name: E169
Source: OWETIU_clean
Formula: AgC6H6N4X2

Name: E170
Source: SOVHAM_clean
Formula: C8H12X2

Name: E171
Source: FALVOF_clean
Formula: C8H2O4X2

Name: E172
Source: BEXSAA_clean
Formula: MnC2O4X2

Name: E173
Source: CUYHIO_clean
Formula: C8H8X2

Name: E174
Source: COGWEB_clean
Formula: C14H4N2O4X2

Name: E175
Source: TEQTEQ_clean
Formula: C4H3NSX2

Name: E176
Source: WENKEH_clean
Formula: C13H10O4SX2

Name: E177
Source: EMAFII_charged
Formula: C12H10X2

Name: E178
Source: GUJGAU_clean
Formula: C6H14N2X2

Name: E179
Source: MACHIJ_clean
Formula: C13H6OX2

Name: E180
Source: GEVXAI_clean
Formula: C8H4O4X2

Name: E181
Source: KIHTOL_clean
Formula: C7H6OX2

Name: E182
Source: ISAYOQ_charged
Formula: C2N2OX2

Name: E183
Source: TEQPEM_clean
Formula: C4S4X2

Name: E184
Source: VAGTUU_clean
Formula: C10H6X2

Name: E185
Source: DEYLUQ_clean
Formula: Br4C6X2

Name: E186
Source: KANDEK_clean
Formula: C₆F₂H₂X₂

Name: E187
Source: XAMHEA_clean5b
Formula: C₁₃H₁₀OX₂

Name: E188
Source: OGOWAJ_clean
Formula: C₁₅H₁₂X₂

Name: E189
Source: JISVAJ_clean
Formula: C₁₀H₆N₂X₂

Name: E190
Source: MOYNEU_clean
Formula: C₁₉H₂₀X₂

Name: E191
Source: KIFXOO_clean
Formula: NiC₁₀H₈N₂X₂

Name: E192
Source: PUNSUN_charged
Formula: C₅H₇N₂X₂

Name: E193
Source: NIKDAM_clean
Formula: C₂₀H₃₈N₄O₄X₂

Name: E194
Source: LALPIZ_clean
Formula: C₈H₁₂N₈S₂X₂

Name: E195
Source: DOKDEN_clean
Formula: C₇H₆X₂

Name: E196
Source: SEFNIB_charged
Formula: C₁₅H₁₈N₂X₂

Name: E197
Source: XEWDUA_clean
Formula: CuC₁₄H₂₄N₄O₄X₂

Name: E198
Source: PAPVEJ_clean
Formula: C₂₄H₂₄S₂X₂

Name: E199
Source: ELOFIU_charged
Formula: C₄H₆X₂

Name: E201
Source: UZIJUJ_clean
Formula: C₆H₅NX₂

Name: E202
Source: AGAXOV_clean
Formula: C₄H₂SX₂

Name: E203
Source: AWEBIO_charged
Formula: C₇H₁₄X₂

Name: E204
Source: KEYDEZ_clean
Formula: BrC₆H₃X₂

Name: E205
Source: AXUBAW_clean5b
Formula: C10H12X2

Name: E206
Source: XILDUT_clean
Formula: C6Cl4X2

Name: E207
Source: MOXPUL_clean
Formula: Cu2C18H20N2O8X2

Name: E208
Source: SETPEO_clean
Formula: InC10Cl3H8N2X2

Name: E209
Source: WEHQAC_charged
Formula: C14H8X2

Name: E210
Source: WAHMUP_clean
Formula: CuC4H4N6X2

Name: E211
Source: EPUXET_clean
Formula: C12H18X2

Name: E212
Source: CELKEL_clean
Formula: C2H4O2X2

Name: E213
Source: FIHHUB_clean
Formula: BC14F2H14N2X2

Name: E215
Source: ACOLIP_clean
Formula: C8H8X2

Name: E216
Source: NAPZOV_clean
Formula: C7H6X2

Name: E217
Source: COPXOV_clean
Formula: C10H12X2

Name: E218
Source: RINPEJ_charged
Formula: C12H8N2X2

Name: E219
Source: DITYAH_clean
Formula: C5H10X2

Name: E220
Source: SAMLAV01_clean
Formula: C6H3NO2X2

Name: E221
Source: EWALUK_clean
Formula: C16H16X2

Name: E222
Source: FOHCAH_clean
Formula: C8H8O2X2

Name: E223
Source: NIRDOI_clean
Formula: C14H12OX2

Name: E224
Source: FERGUG_charged
Formula: C₁₄H₁₂O₂X₂

Name: E225
Source: IQIJIC_clean
Formula: C₁₄H₁₀O₂X₂

Name: E226
Source: UNIPAJ_clean
Formula: C₁₀H₆X₂

Name: E228
Source: PAMGIV_clean
Formula: C₆F₄X₂

Name: E229
Source: WIYMOG_charged
Formula: C₁₈H₁₈N₂X₂

Name: E230
Source: CILDAD_clean
Formula: CuC₁₀H₈N₂X₂

Name: E232
Source: ANEPIT_clean
Formula: C₁₂H₆N₂O₄X₂

Name: E233
Source: MICNES_clean
Formula: C₈F₄H₄X₂

Name: E234
Source: AHINIP_clean
Formula: C₁₂H₆N₂X₂

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