Supporting information

Artificial Intelligence Driven Molecule Adsorption Prediction (AIMAP)

Applied to Chirality Recognition of Amino Acids Adsorption on Metals

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Table of Contents

1. The global neural network (G-NN) potential

1.1 Overview

The global neural network potential (G-NN) is trained and utilized by using LASP software developed by our group[1]. Our G-NN potential is based on the atomic high-dimensional NN architecture[2–4] with the power-type structure descriptor (PTSD)[5] and incorporates further the many-body function corrections to improve the accuracy, the so-called G-MBNN potential architecture[6]. The G-MBNN potential is trained based on 125,658 structures database for the Cu-C-H-O-N system, which is calculated using plane-wave DFT calculations with PBE functional as implemented in the Vienna ab initio simulation package (VASP)[7–9]. The dataset information is detailed in Table S4 , which contains a wide set of structure configurations. The model of Cu-C-H-O-N is a four-layer 536-144-144-80-24 feed-forward NN architecture. The first number, 536, describes PTSDs for the first input layer, and the middle numbers describe the neurons in 3 hidden layers, which utilize the hyperbolic tangent activation function. The final output is obtained through 24 many-body functions. The model was trained using the limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) optimizers[10], This potential is openly available from the LASP website (www.lasphub.com). The final root-mean-square error of the final NN on the whole dataset of the G-NN potential is 5.256 meV / atom.

1.2 The architecture of G-MBNN

The architecture of G-MBNN potential is depicted in Figure S1a. In G-MBNN the total energy is expressed as the sum of both atomic energies and many-body functions. As shown in Figure S1b, for each atom in a molecule, a set of PTSD functions[5] $\{D_i\}$ are calculated from the Cartesian coordinates $\{R_i\}$. These functions describe the local chemical environment of each atom and are used as input for the atomic neural networks. To illustrate PTSD, we give the formula of two PTSDs below (also see Ref 6), where the combination of the power function and spherical harmonic function, similar to atomic wavefunctions, provides a convenient way to couple the radial and the angular information of atom.

$$f_c(r_{ij}) = \begin{cases} 0.5 \times \tanh^3\left[1 - \frac{r_{ij}}{r_c}\right], \text{for } r_{ij} \le r_c \\ 0 \qquad\qquad\qquad \text{for } r_{ij} > r_c \end{cases} \tag{S1}$$

$$R^n(r_{ij}) = r_{ij}^n \cdot f_c(r_{ij}) \tag{S2}$$

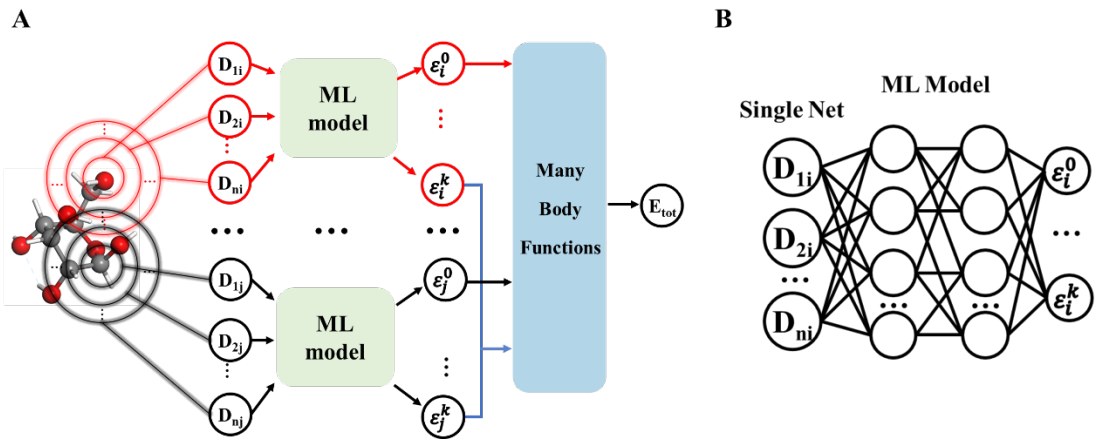


Figure S1. Illustration of the architecture of G-MBNN. A) Each atomic ML model (NN utilized in this work) outputs a series of coefficients ε_i^k, which act as the parameters for different many-body functions. The total energy of system is written as the sum of many-body functions. B) The implementations of the ML model based on feed-forward NN.

$$S_i^2 = \left[\sum_{m=-L}^{L}\left|\sum_{j\neq i} R^n(r_{ij})Y_{Lm}(\boldsymbol{r}_{ij})\right|^2\right]^{\frac{1}{2}} \qquad \text{(S3)}$$

$$S_i^5 = \left[\sum_{m=-L}^{L}\left|\sum_{j,k\neq i} R^n(r_{ij})\cdot R^m(r_{ik})\cdot R^p(r_{jk})\cdot\left(Y_{Lm}(\boldsymbol{r}_{ij})+Y_{Lm}(\boldsymbol{r}_{ik})\right)\right|^2\right]^{\frac{1}{2}} \qquad \text{(S4)}$$

In the Eqs, r_{ij} is the internuclear distance between atom i and j, θ_{ijk} is the angle centered at i atom with j and k being neighbors (i, j, and k are atom indices). The key ingredients in PTSD are the cut-off function f_c that decays to zero beyond the r_c (Eq. S1), power-type radial function, trigonometric angular functions, and spherical harmonic function. It should be noted that the terms of the PTSD will increase rapidly as the cutoff r_c becomes larger.

The feed-forward NN outputs a vector, including the atomic energy contribution ε_i^0, a one-body function (f_s), and a series of coefficients ε_i^k (k =1, 2, …) for building different many-body functions, namely f_d, f_t for the two-body and three-body functions, respectively. As shown in Eq. S5, the total energy E_{tot} of the system can thus be expressed as a sum of the atomic energy contributions (f_s) and the many-body functions (f_d, f_t, …).

$$E = \sum_{s=1}^{ns}\sum_{i=1}^{na} f_s(\varepsilon_i^s) + \sum_{d=1}^{nd}\sum_{i=1}^{na}\sum_{j>i}^{na} f_d\left(\varepsilon_i^d, \varepsilon_j^d, r_{ij}\right) +$$

$$\sum_{t=1}^{nt}\sum_{i=1}^{na}\sum_{j>i}^{na}\sum_{k>j}^{na}\sum_{ang=1}^{3} f_t\left(\varepsilon_i^t, \varepsilon_j^t, \varepsilon_k^t, r_{ij}, r_{ik}, r_{jk}, \theta_{ang}\right) + \cdots \qquad \text{(S5)}$$

These many-body functions can be written into general function forms shown in Eqs. S6-S9,

where ε_i^k from NN acts as the parameters. In these functions, r_{ij} is the distance between atoms i and j and θ_{ijk} is the angle centered at the i atom with neighbors j and k (i, j, and k are atom indices); n_a is the total atom number of the system; n_s, n_d and n_c are the number of one-body, two-body, three-body function in MBNN architecture respectively (s, d and t are function indices); λ, m_d, m_t and l_t is adjustable parameters of these functions. The f_c in all the equations is the cutoff function with the cutoff radius (r_c) and the adjustable parameter α and β , as defined in Eq. S9.

$$f_s = \lambda \varepsilon_i^s \quad \text{(S6)}$$

$$f_d = \lambda \frac{\varepsilon_i^d \varepsilon_j^d}{r_{ij}^{m_d}} f_c(r_{ij}) \quad \text{(S7)}$$

$$f_t = \lambda \frac{\varepsilon_i^t \left(\varepsilon_j^t + \varepsilon_k^t\right)(2+\cos(\theta_{ijk}))^{l_t}}{r_{ij}^{m_t} \cdot r_{ik}^{m_t} \cdot r_{jk}^{m_t}} f_c(r_{ij}) f_c(r_{ik}) f_c(r_{jk}) \quad \text{(S8)}$$

$$f_c(r_{ij}) = 0.5 * \left(1 - \tanh\left(\alpha(r_{ij} - (r_{cut} - \beta))\right)\right) \quad \text{(S9)}$$

In the G-MBNN architecture, the atomic force is analytically derived based on Eq. S5, where the force component F_u acting on the atom u is the derivative of the total energy concerning its coordinate vector $\boldsymbol{r_u}$ that is further related to the derivatives to the atomic coefficients ε_i^k and the pairwise distance r_{iu}.

1.3 SSW-NN simulation

a) SSW-NN method

SSW-NN method is a machine-learning potential based global optimization method, which combines the global neural network (G-NN) potential with SSW method for fast and accurate global PES exploration as implemented in LASP code. While traditional DFT calculations are frustrating for the global optimization of complex systems due to the high computational cost, SSW-NN method provides a general solution for PES scanning with both high efficiency and high accuracy. The G-NN potential is trained based on SSW dataset calculated using DFT and delivers a high speed of PES evaluation, 3∼4 orders of magnitude faster than DFT.

b) Dataset generation and self-learning NN training

We utilized the stochastic surface walking (SSW) global optimization to generate a fully automated global dataset that does not need a priori knowledge of the system, such as the structural motif, *e.g.*, bonding patterns and symmetry. The final obtained Cu-C-H-O-N global dataset contains a variety of structural patterns on the global PES (125,658 structures, detailed in

Table S4). In brief, the SSW-NN method involves three stages to generate the global dataset, as described below.

(i) **The first stage** generates a raw dataset, which contains the most common atomic environment and serves to build an initial NN PES. This is done by performing density functional theory (DFT) SSW global optimization in a massively parallel way. In this stage, the DFT calculations have low-accuracy setups and small unit cells to speed up the SSW search. By collecting and screening the structures from SSW trajectories, a raw dataset is obtained.

(ii) **The second stage** trains an NN global PES. This is done by refining the dataset using DFT calculations with high-accuracy setups, followed by NN training on the accurate global dataset. The NN architecture applied in this stage utilizes a small set of structural descriptors and a small network size.

(iii) **The third stage** iteratively expands the global dataset. It targets to increase the predictive power of NN PES by incorporating more structural patterns into the dataset. This is done by performing an SSW PES search using the NN PES obtained in the second stage, starting from a variety of initial structures. These initial structures are randomly constructed and include large systems with many atoms per unit cell. The SSW trajectories' structures are collected and filtered to generate an additional dataset. The new dataset is then fed to the global dataset to start a new cycle of NN training (back to the second stage).

1.4 SSW method

The SSW method is an unbiased PES exploration method[11,12], originating from the bias-potential driven constrained Broyden dimer (BP-CBD) method[13,14] for TS location developed by our group. Each step in SSW simulation contains a climbing procedure and a relaxation procedure to perturb the structure from one minimum to another, where the climbing procedure involves the consecutive Gaussian addition and repeated local relaxation, which is followed by the relaxation procedure to remove all the bias potentials and carry out unconstrained structure optimization. At the end of each SSW step, a structure selection module, *e.g.* using Metropolis Monte-Carlo scheme, is applied to accept/refuse the new minimum. The SSW method makes no attempt to locate the TS explicitly during PES exploration.

In the SSW method (also in BP-CBD), the barrier of the reaction can be surmounted by adding consecutively Gaussian bias potentials. The reaction direction where Gaussians are added is

refined from a randomly generated direction using the biased constrained Broyden dimer method. The randomly generated initial direction N_i^0 (i labels the index of the SSW step) is thus critical for the efficiency of PES exploration, which is designed to include two components related to the global structure deformation (N_i^g) and the local bond formation (N_i^l), as shown in Eq. S10 and Eq. S11:

$$N_i^0 = \frac{N_i^g + \lambda N_i^l}{\|N_i^g + \lambda N_i^l\|} \qquad \text{(S10)}$$

$$N_i^l = \begin{pmatrix} 0 \\ \vdots \\ q_A \\ \vdots \\ q_B \\ \vdots \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ \vdots \\ q_B \\ \vdots \\ q_A \\ \vdots \\ 0 \end{pmatrix} \qquad \text{(S11)}$$

where λ controls the ratio between the global and the local components; and q_A and q_B are the coordinates of two randomly selected atoms A and B, respectively, which should NOT be in close contact. Both N_i^g and N_i^l are important for PES exploration to prevent the long-time trapping in one particular local minimum, since different reaction channels, including the global structure deformation and the local chemical bond making/breaking, can be involved from one minimum to another.

2. DFT calculations

All DFT calculations are performed using the periodic plane wave method as implemented in the VASP package[7–9]. The ionic core electrons are described using the projector augmented wave (PAW) pseudopotential[15]. The electron exchange and correlation effects are described by the GGA-PBE functional[16]. A kinetic energy cutoff is set as 450 eV employed, and the Monkhorst−Pack *k*-mesh grid is fully automatically generated with 25 times the reciprocal lattice vectors. Van der Waals interaction is considered using the DFT-D3 method with zero damping[17,18].

The calculations on achiral Cu(111), Cu(100), and Cu(211). In modeling the Cu(111), Cu(100), and Cu(211) surfaces, we utilize supercells containing (4×3√3), (4×4), (4×2) surface units, respectively. The Cu(111) and Cu(100) contain four slabs of copper atoms while the stepped Cu(211) surface is modeled by 12 layers of copper atoms. A 20.00 Å vacuum spacing in the direction orthogonal to the surface is modeled on each surface. The atoms above 6.00 Å, 5.00 Å, and 6.00 Å were allowed to relax on the respective surface. The convergence criteria for electron density and structure optimization in the DFT calculations are established at 5×10^{-6} eV and 0.10 eV $Å^{-1}$, respectively.

The calculations on chiral Cu(3,1,17)^S surface. In modeling the adsorption structures, a (1×2) unit cell is utilized for Gly, Ala, Val, Pro, Leu, Ile, Ser, Thr, Asp, Glu, Asn, and Gln, and a (2×2) unit cell is utilized for Phe, Trp, Tyr, Lys, His, and Arg. The surface is modeled by 27 layers of copper atoms, with a 20.00 Å vacuum spacing in the direction orthogonal to the surface. The atoms above 3.00 Å (the top 12 layers), are allowed to relax on the respective surface. The convergence criteria for structure optimization are established at 0.05 eV $Å^{-1}$. The choice of DFT functional is known to affect the energetics in adsorption and thus change the prediction of enantio-selectivity, especially considering that the energetic discrimination between enantiomers is typically close to the confidence interval of DFT calculations (*e.g.*, around 0.10 eV). As a result, for treating the adsorption on Cu(3,1,17)^S surface, the BEEF-vdW functional[19,20] (another popular choice for investigating the adsorption structures on copper surfaces) is also utilized.

The calculations for molecules in the gas phase. All molecules are optimized in a cell of 15 Å × 15 Å × 15 Å. The convergence criteria for electron density and structure optimization in the DFT calculations are established at 5×10^{-6} eV and 0.10 eV $Å^{-1}$, respectively.

3. Adsorption of methanol, glycine, and aspartate on Cu(211) surface

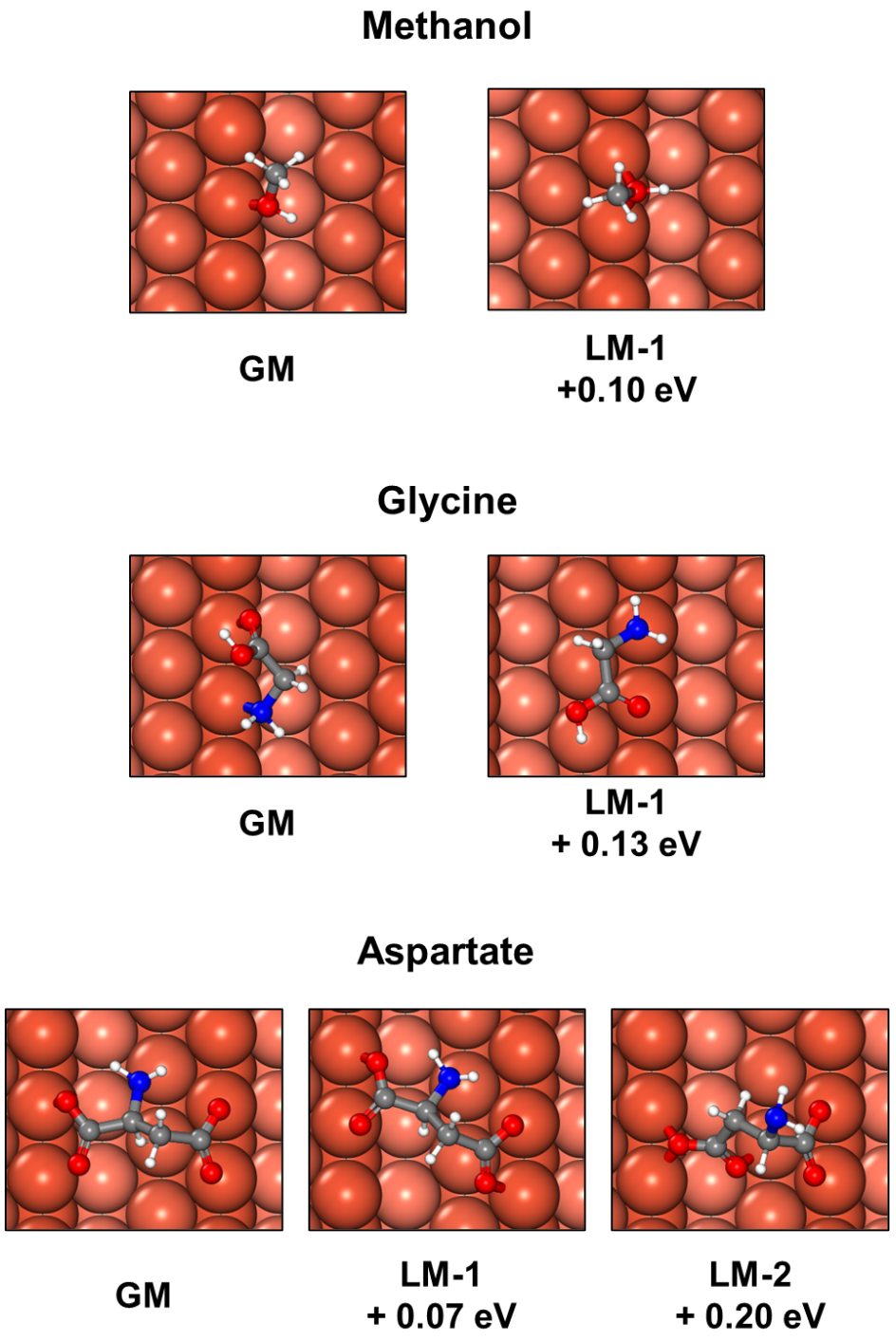


Figure S2. Representative adsorption structures for methanol, glycine, aspartate on Cu(211) surface. These adsorption structures and relative stability (using GM as reference) are predicted by AIMAP. The parameter settings are list in Table 1.

4. The Cu-HCNO6 database

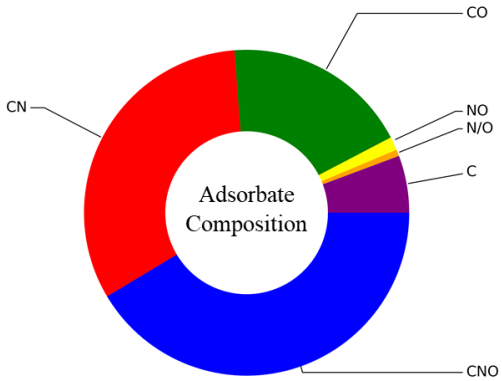


Figure S3 Element composition of the adsorbates in Cu-HCNO6 database. The pie chart illustrates the element composition of 9592 molecules within the Cu-HCNO6 database. Each segment represents molecules with specific element compositions (excluding hydrogen), with the size indicating their proportion in the database. Six distinct compositions are considered: carbon only (C, purple), nitrogen or oxygen only (N/O, orange), both nitrogen and oxygen (NO, yellow), both carbon and oxygen (CO, green), both carbon and nitrogen (CN, red), and lastly, all three elements (CNO).

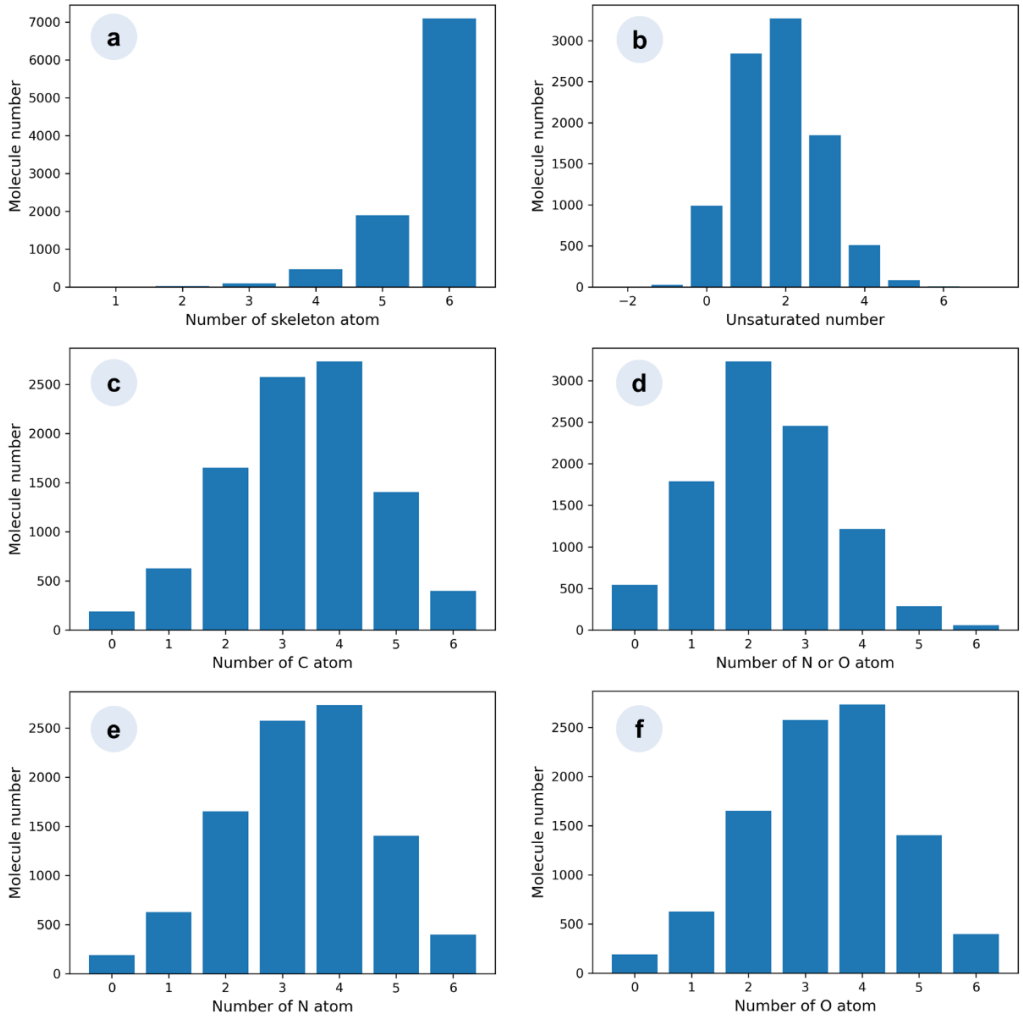


Figure S4 Molecule compositions in the Cu-HCNO6 database. These histograms depict the distribution of molecules with specific compositions from the Cu-HCNO6 database. The number of molecules is categorized by **(a)**. The number of skeleton atoms (C, N, and O); **(b)** The value of the unsaturated number (calculated by: $\left(2 \times n(\mathrm{C}) + n(\mathrm{N}) - n(\mathrm{H})\right)/2 - 2$, $n(\mathrm{C})$,$n(\mathrm{N})$, $n(\mathrm{H})$ represent the number of respective elements) (c) The number of carbon atoms; (d) The number of nitrogen or oxygen atoms; (e) The number of nitrogen atoms; (f) The number of oxygen atom.

5. Benchmark of G-NN potential against DFT calculations

Table S1 Benchmark of G-NN functional against DFT calculations. Listed data include the type of dataset for benchmark, the number of adsorption structures in respective dataset (N_{struc}), and the root-mean-square-error in energy (E, in unit eV and meV / atom) and force (F, in unit eV / Å).

Benchmark Dataset[a]	N_{struc}	E		F
		eV	meV / atom	eV / Å
Train[b]	10,000	0.14	2.287	0.082
Test	10,000	0.19	3.468	0.124

a. Randomly selected from the Cu-HCNO6 database.

b. Included in the self-learning training loop of the G-NN potential.

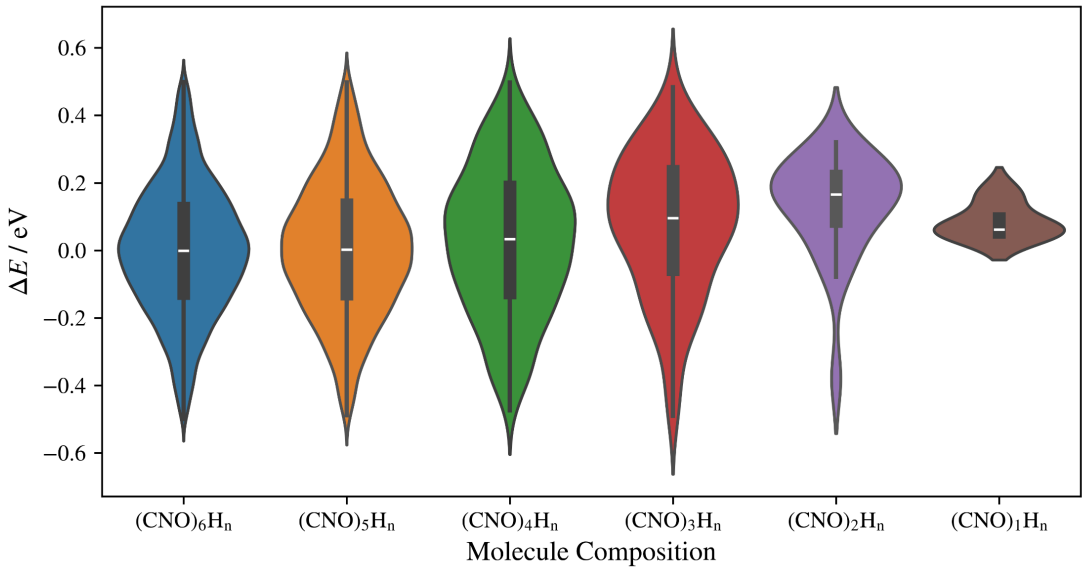


Figure S5 The performance of G-NN potential in predicting adsorption energy. This diagram illustrates the predictive performance of the G-NN potential for adsorption energy. The violins summarize the G-NN potential's predictions of adsorption energy (E_{ads}) for molecules in the 10000-sized test dataset. The x-axis denotes the composition of adsorbed molecules, labeled as $(CNO)_mH_n$. The value in y-axis, ΔE, is computed by $E_{NN} - E_{DFT}$, in which the E_{NN} and E_{DFT} represents the adsorption energy obtained by G-NN potential and DFT calculations, respectively.

6. Adsorption of AAs on achiral Cu(111), Cu(100), and Cu(211) surfaces

6.1 Adsorption energy

Table S2 The adsorption free energy (G_{ads}) of all AA species on achiral Cu(111), Cu(100), and Cu(211) surface. Listed data include the molecule name, the deprotonation number of specific species [a], the adsorption free energy (G_{ads}, calculated by Eq. 1), the relative stability of D/L-enantiomers. The values obtained by PBE-D3 and PBE are separately listed in the table.

Molecule Name	Deprotonation Number	G_{ads}/ eV					
		Cu(111)		Cu(100)		Cu(211)	
		PBE-D3	PBE	PBE-D3	PBE	PBE-D3	PBE
Ala	**1**	-1.62	-0.62	-2.03	-1.16	-2.20	-1.18
	0	-1.14	-0.28	-1.21	-0.44	-1.45	-0.33
Arg	**1**	-2.25	-0.28	-2.90	-1.32	-3.17	-2.04
	0	-2.08	-0.32	-1.98	-0.06	-2.30	-1.30
Asn	**1**	-1.85	-0.49	-2.34	-1.15	-2.49	-1.35
	0	-1.58	-0.34	-1.36	-0.28	-1.81	0.17
Asp	**2**	-2.30	-1.15	-2.86	-1.85	-3.11	-1.72
	1[b]	-1.89	-0.99	-2.26	-1.13	-2.58	-1.05
	1[c]	-1.86	-0.77	-2.22	-1.12	-2.76	-0.69
	0	-1.26	-0.29	-1.35	-0.34	-1.67	0.18
Glu	**2**	-2.59	-1.22	-3.17	-2.04	-3.65	-2.45
	1[b]	-2.07	-0.74	-2.44	-1.16	-3.07	-2.00
	1[c]	-1.99	-0.69	-2.43	-1.28	-2.75	-0.60
	0	-1.46	-0.03	-1.46	0.01	-1.84	0.37
Gln	**1**	-2.36	-0.87	-2.89	-1.56	-3.08	-1.87
	0	-2.05	-0.64	-1.95	-0.61	-2.23	-0.69
Gly	**1**	-1.49	-0.65	-1.88	-1.19	-2.06	-1.24
	0	-1.03	-0.18	-1.11	-0.42	-1.32	-0.51
His	**1**	-2.26	-0.69	-2.84	-1.71	-3.20	-2.17
	0	-1.71	-0.27	-2.03	-0.65	-2.00	-0.74
Ile	**1**	-1.89	-0.52	-2.29	-1.12	-2.35	-0.62
	0	-1.42	-0.13	-1.47	-0.33	-1.61	-0.38

Leu	**1**	-1.83	-0.48	-2.26	-1.15	-2.35	-1.19
	0	-1.42	-0.19	-1.39	-0.35	-1.59	-0.39
Lys	**1**	-2.63	-0.79	-3.39	-1.70	-3.36	-2.17
	0	-2.21	-0.54	-2.20	-0.46	-2.46	-1.32
Phe	**1**	-2.13	-0.63	-2.54	-1.28	-2.74	-1.78
	0	-1.81	0.00	-1.74	-0.47	-2.26	-1.43
Pro	**1**	-1.73	-0.56	-2.06	-1.10	-2.23	-0.87
	0	-1.25	-0.15	-1.38	-0.34	-1.68	-0.55
Ser	**2**	-2.18	-1.15	-2.54	-1.66	-2.68	-1.44
	1[b]	-1.69	-0.56	-2.10	-1.19	-2.35	-1.51
	0	-1.26	-0.18	-1.27	-0.42	-1.61	-0.09
The	**2**	-2.32	-1.14	-2.67	-1.69	-2.77	-1.27
	1[b]	-1.80	-0.62	-2.24	-1.22	-2.50	-1.30
	0	-1.35	-0.32	-1.47	-0.39	-1.64	-0.10
Trp	**1**	-2.49	-0.42	-2.72	-1.04	-3.20	-1.40
	0	-2.25	-0.26	-2.52	-0.51	-2.40	-1.33
Tyr	**2**	-2.48	-0.61	-3.33	-1.79	-3.56	-2.25
	1[b]	-2.17	-0.46	-2.83	-1.17	-3.13	-1.17
	0	-1.89	-0.27	-2.10	-0.25	-2.43	-0.89
Val	**1**	-1.70	-0.53	-2.29	-1.25	-2.29	-1.46
	0	-1.37	-0.27	-1.48	-0.39	-1.56	-0.65

a. Deprotonation state in bold is the most favorable.

b. Deprotonation in the α-carboxyl group.

c. Deprotonation in the side chain carboxyl group.

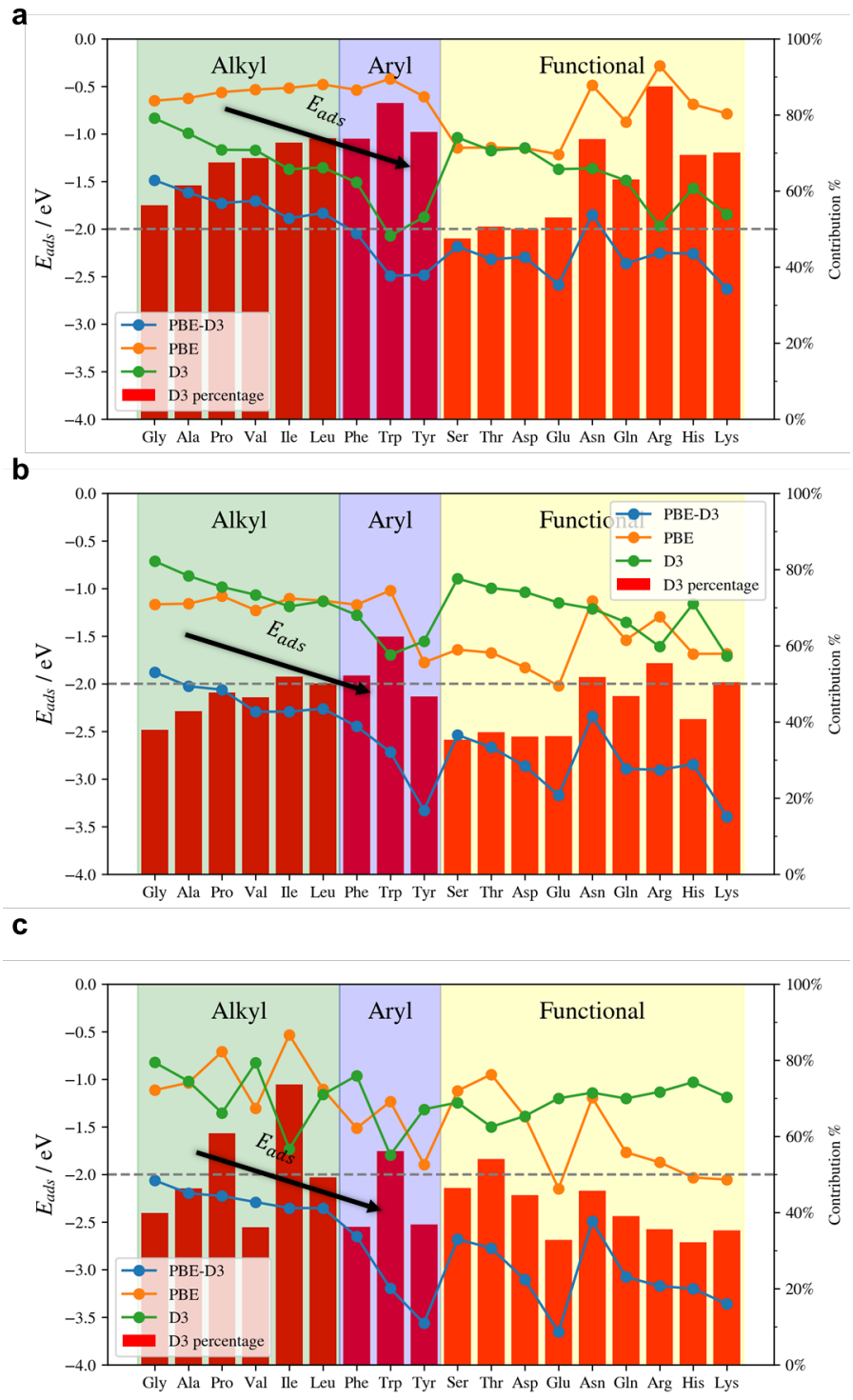
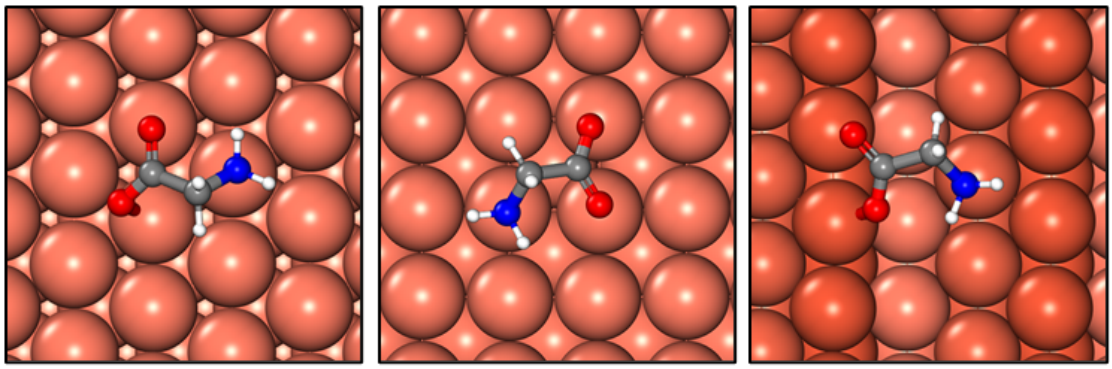
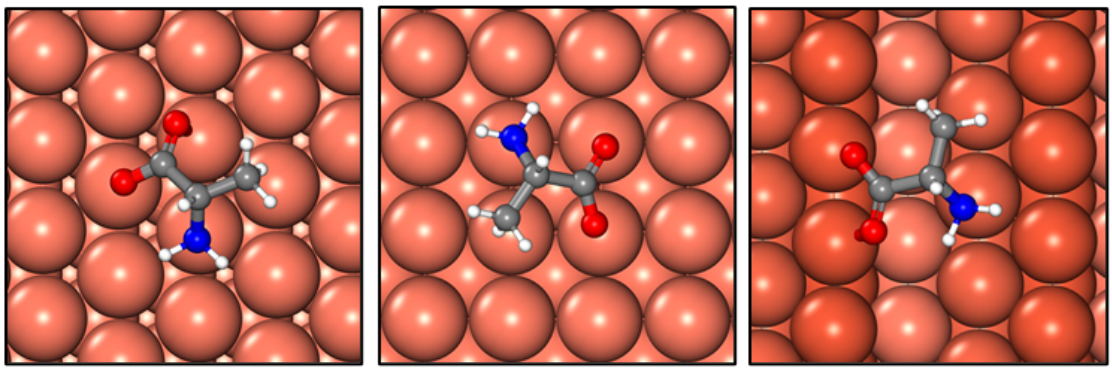


Figure S6 Adsorption energy of 18 types of AAs on Cu(111), Cu(100), and Cu(211) surfaces. The three sub-figures depict the adsorption energy decomposition for **(a)** Cu(111), **(b)** Cu(100), and **(c)** Cu(211) surfaces. The calculated adsorption energy using PBE-D3 is represented by blue dots, while its decomposition into contributions from PBE and D3 dispersion correlation is shown by yellow dots (PBE) and green dots with red bars (D3). A black arrow highlights the increasing of adsorption energy with side chain volume for amino acids with alkyl side chains.

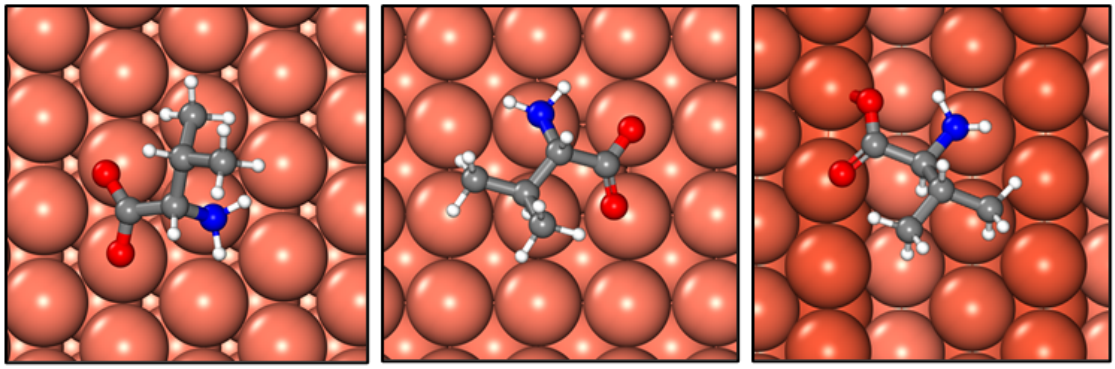
6.2 Adsorption structures of 18 types of AAs on achiral copper surfaces.



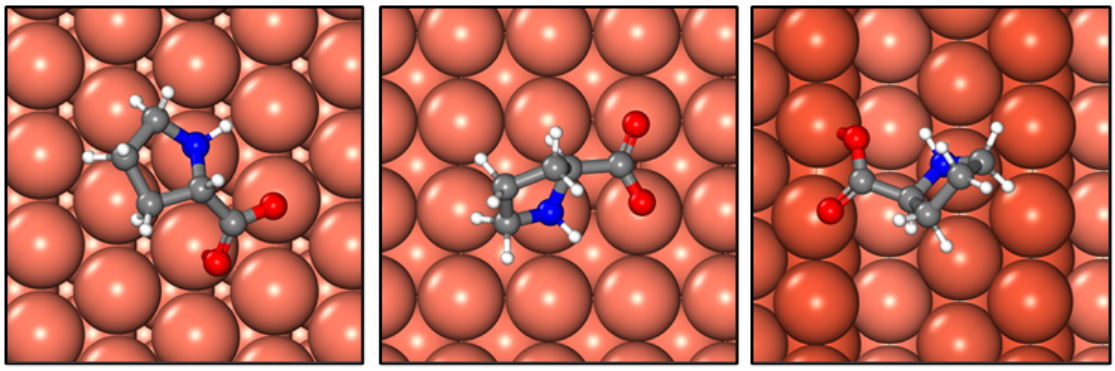
Gly-(111) Gly-(100) Gly-(211)



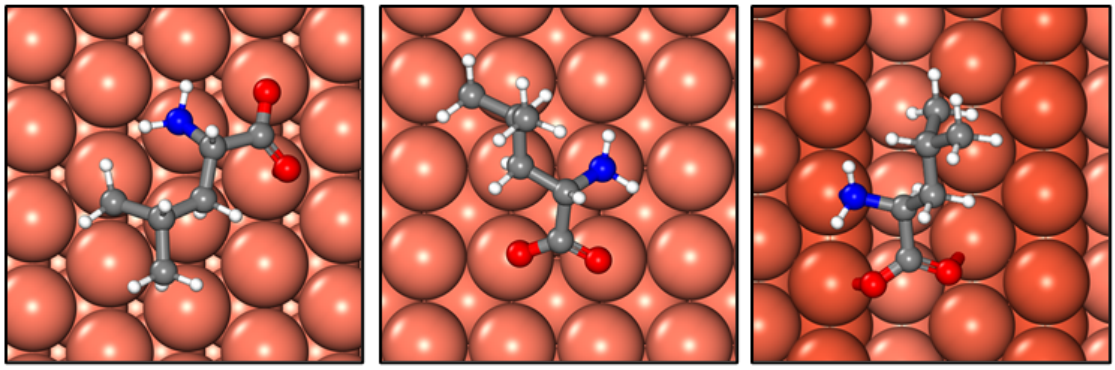
Ala-(111) Ala-(100) Ala-(211)



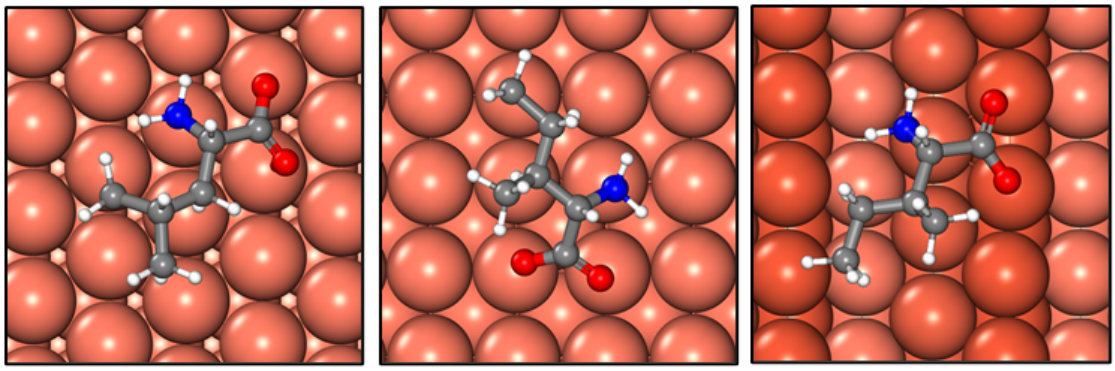
Val-(111) Vla-(100) Val-(211)



Pro-(111) Pro-(100) Pro-(211)



Leu-(111) Leu-(100) Leu-(211)



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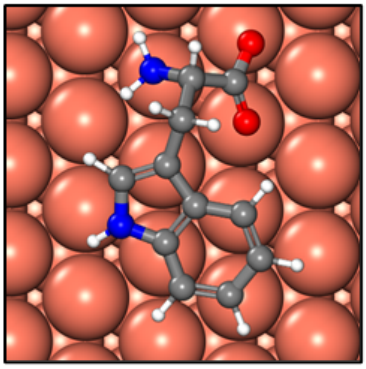

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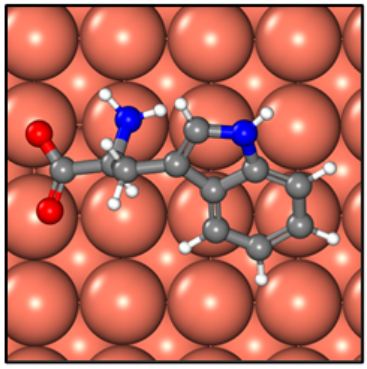

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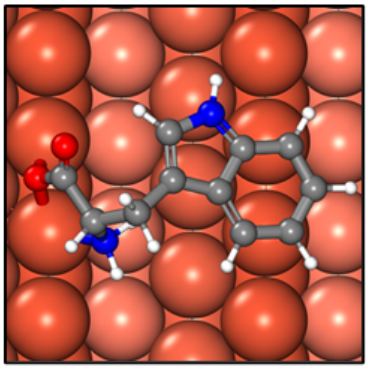

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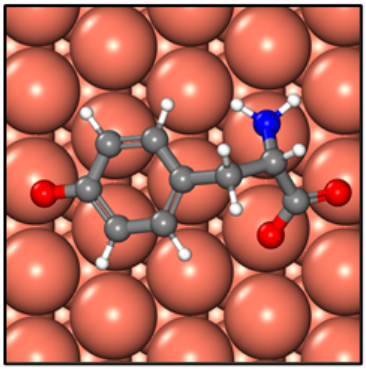

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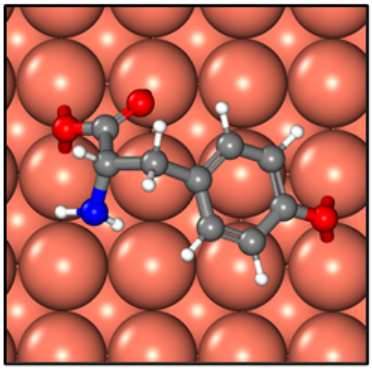

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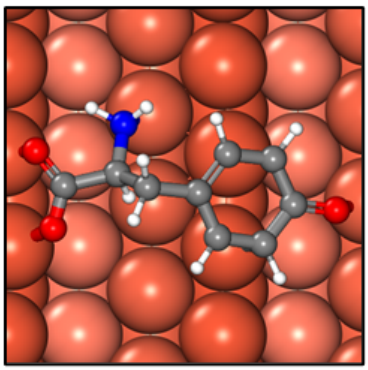

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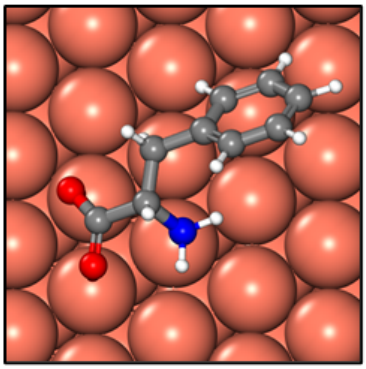

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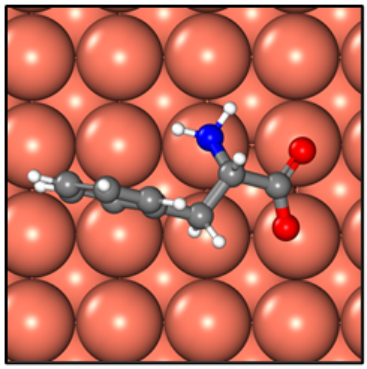

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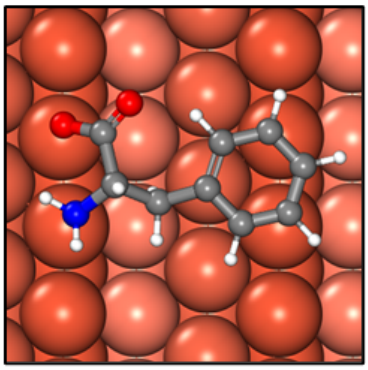

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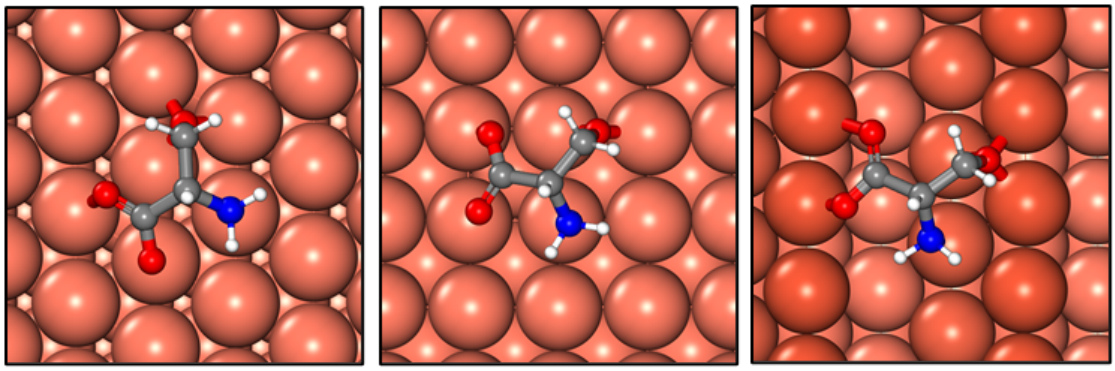

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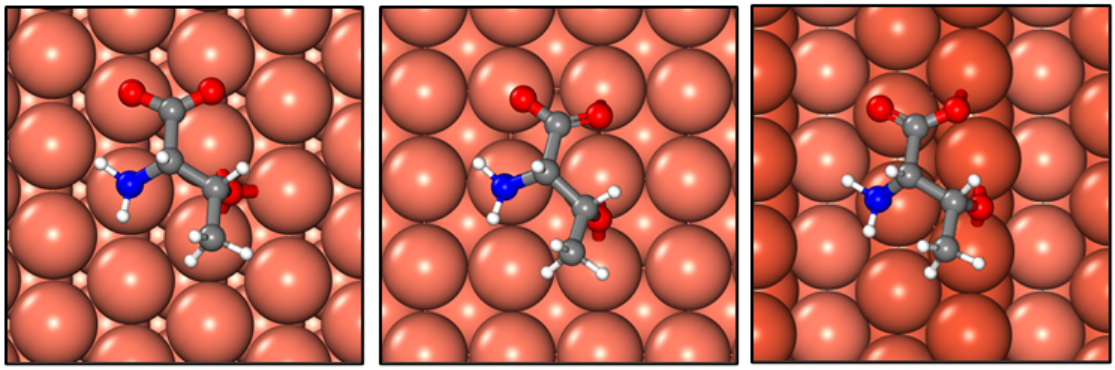

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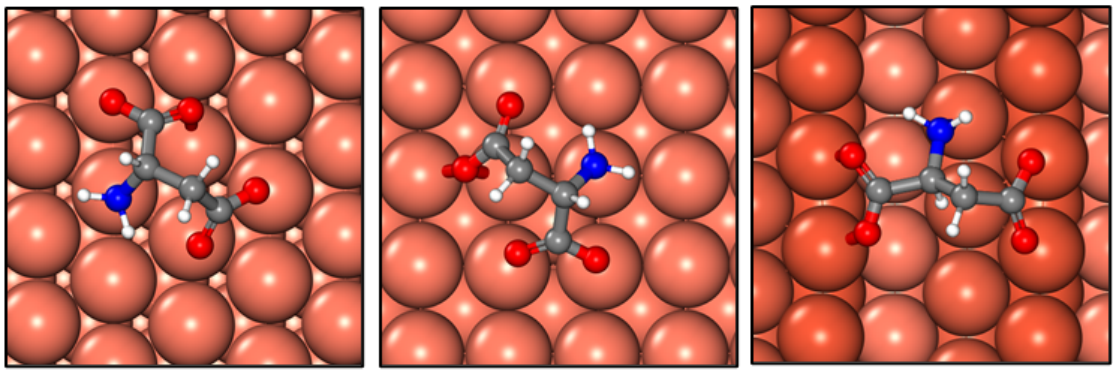

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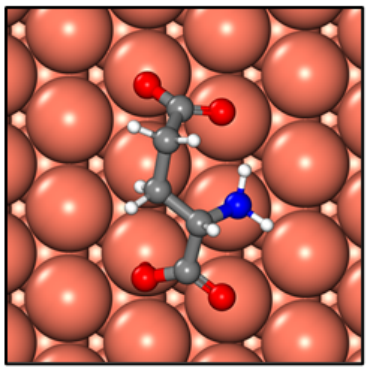

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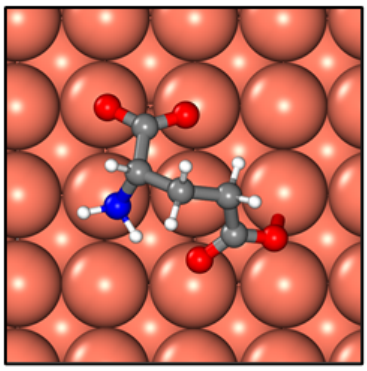

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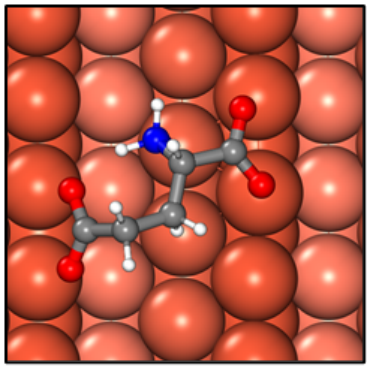

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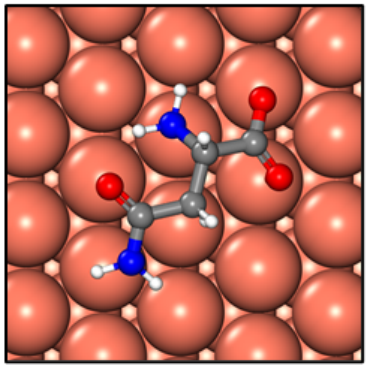

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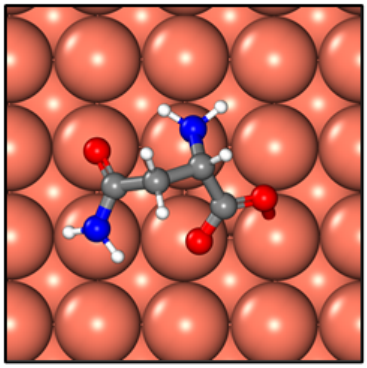

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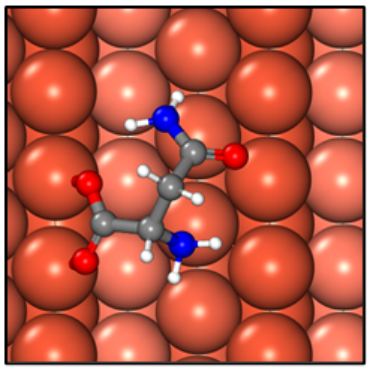

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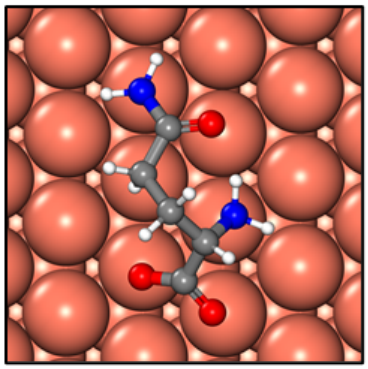

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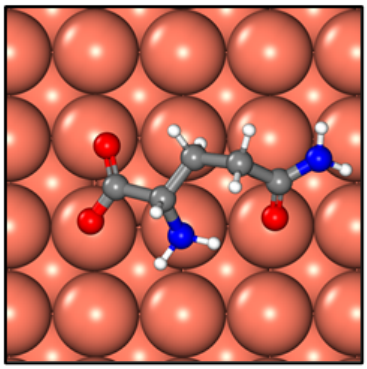

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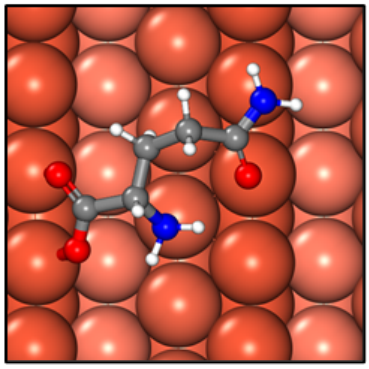

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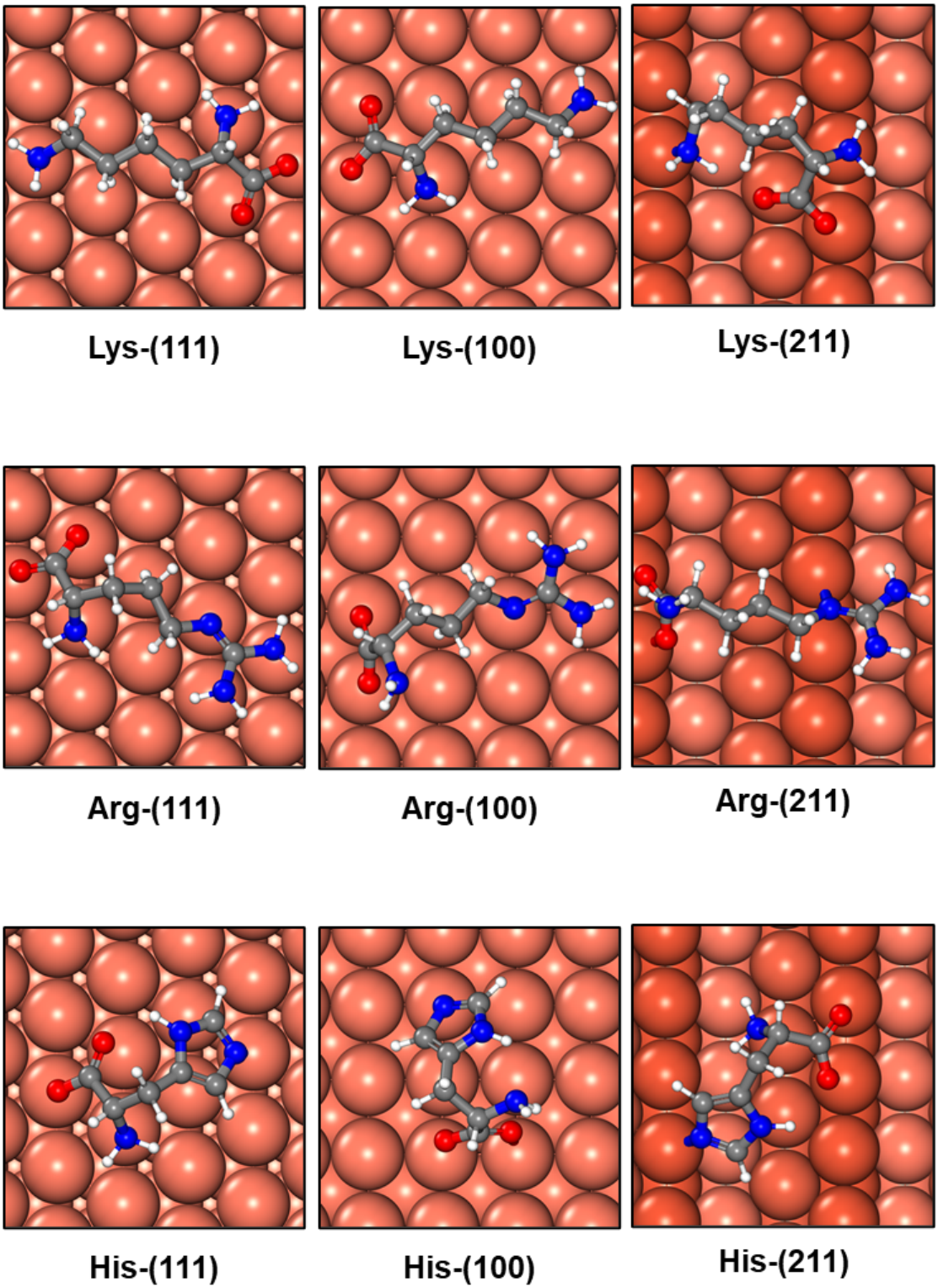


Figure S7 Adsorption structures of 18 types of AAs on achiral Cu(111), Cu(100), and Cu(211) surfaces.

7. Adsorption of AAs on chiral Cu(3,1,17)^S surface

7.1 Adsorption energy

Table S3. **Adsorption energy of AAs on chiral Cu(3,1,17)^S surfaces.** Listed data include the molecule name[a], the adsorption energy (G_{ads} computed using Eq. 1 but without ZPE correction; $\mu_{H_2}(T,p)$ is calculated by Eq. 2)[b], the relative stability of D/L-enantiomers. The values obtained by PBE-D3 and BEEF-vdW are separately listed in the table.

Molecule Name	PBE-D3			BEEF-vdW		
	G_{ads}/ eV		$\Delta E_{L/D}$/ eV	G_{ads}/ eV		$\Delta E_{L/D}$/ eV
	L	D		L	D	
Ala	-2.30	-2.33	+0.03	-1.89	-1.91	+0.03
Val	-2.60	-2.60	+0.01	-2.04	-2.10	+0.06
Pro	-2.40	-2.52	+0.11	-1.92	-1.99	+0.07
Leu	-2.67	-2.67	+0.00	-2.07	-2.13	+0.06
Ile	-2.63	-2.68	+0.05	-2.07	-2.12	+0.05
Tyr	-3.66	-3.85	+0.19	-2.64	-2.84	+0.20
Trp	-3.48	-3.51	+0.04	-2.27	-2.33	+0.06
Ser	-2.69	-2.54	-0.14	-2.21	-2.16	-0.05
Gln	-3.24	-3.31	+0.07	-2.31	-2.51	+0.20
Glu	-3.48	-3.64	+0.16	-2.95	-3.09	+0.14
Asp	-3.16	-3.29	+0.13	-2.79	-2.90	+0.11
Arg	-3.88	-4.00	+0.11	-2.70	-2.75	+0.05
His	-3.50	-3.31	-0.19	-2.43	-2.31	-0.12
Gly	-2.11			-1.62		
The	-2.74	-2.63	-0.11	-2.19	-2.19	+0.00
Asn	-2.74	-2.62	-0.12	-1.88	-1.98	+0.10
Lys	-3.60	-3.61	+0.01	-2.56	-2.47	-0.10
Phe	-2.98	-2.93	-0.06	-2.17	-2.26	+0.09

a. The bold molecules have the same enantiomer preference under both functionals.

b. All the species are in their highest deprotonation level.

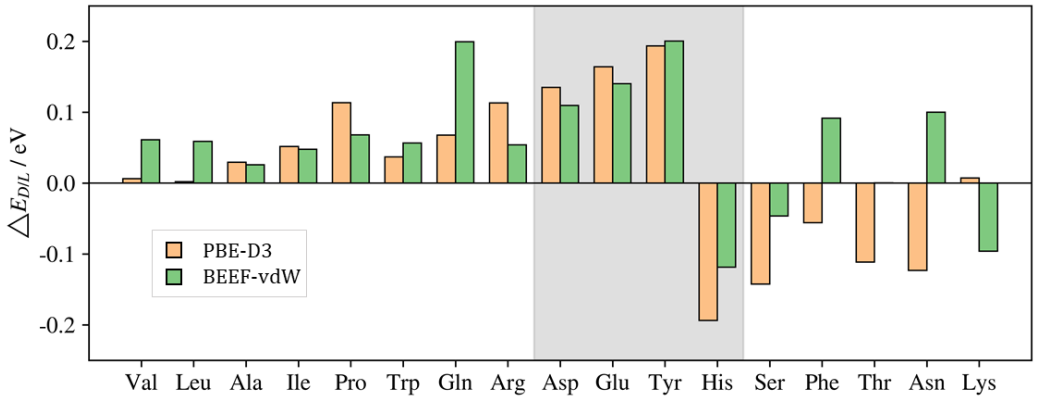
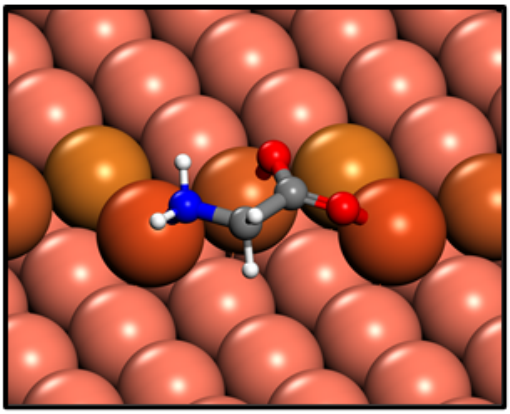
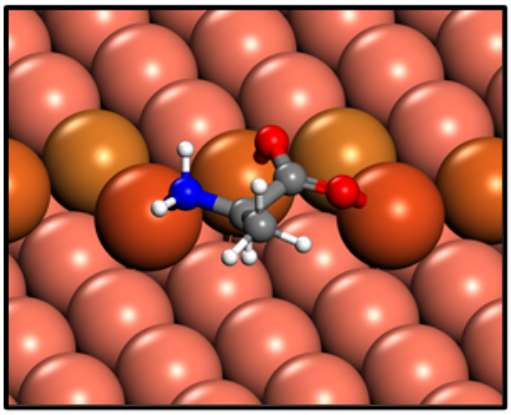


Figure S8 Energetic discrimination ($\Delta E_{D/L}$, defined by Eq. 3) of 17 types of chiral AAs on Cu(3,1,17)^S surface. The green and orange bars represent the ΔE_(L/D) obtained by PBE-D3 and BEEF-vdW methods, respectively. The four types of AAs exhibiting consistent strong discrimination ($\left|\Delta E_{D/L}\right|$ > 0.10 eV) under both functionals are highlighted with grey shadow.

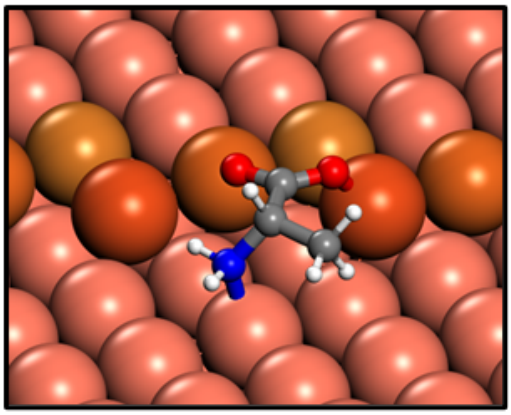
7.2 Adsorption structures of 18 types of AAs on chiral Cu(3,1,17)^{S} surface.



Gly



D-Ala



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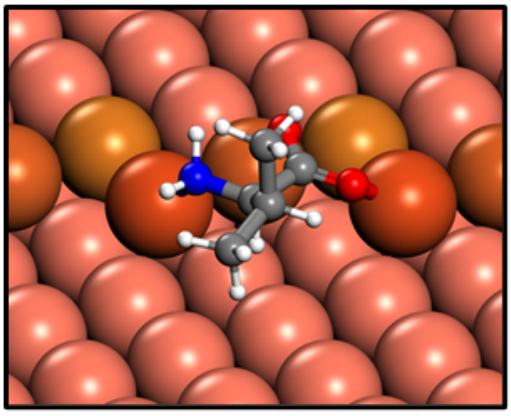

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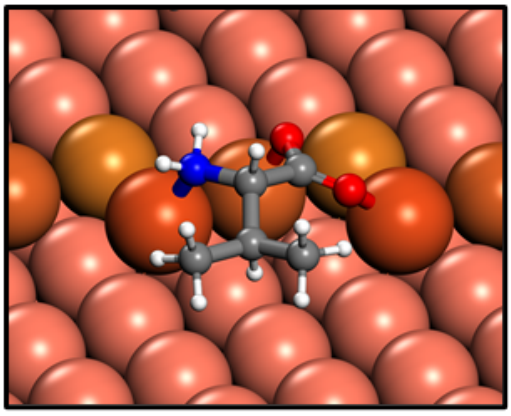

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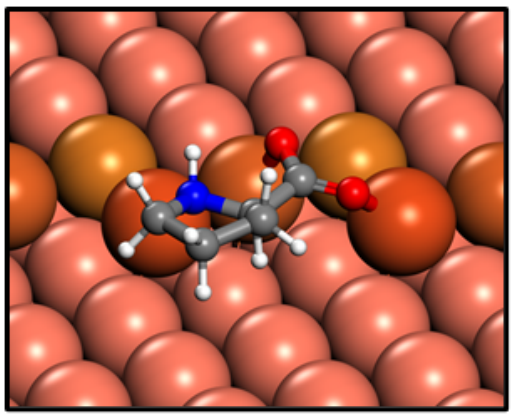

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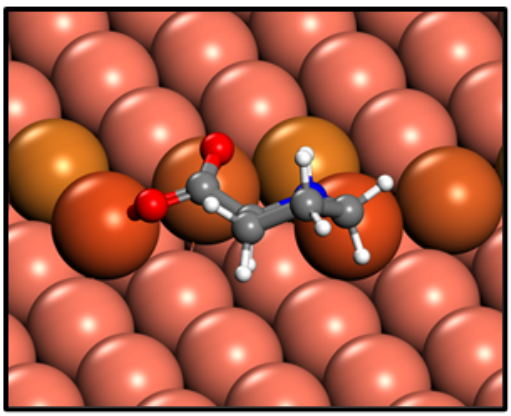

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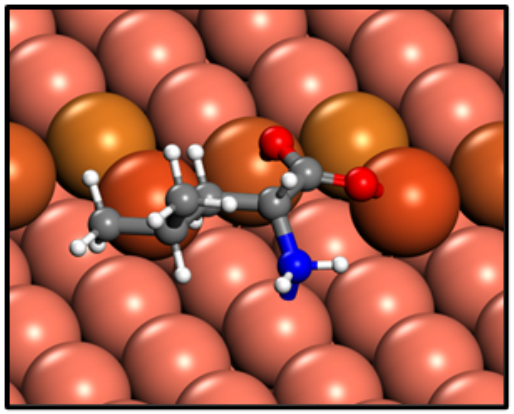

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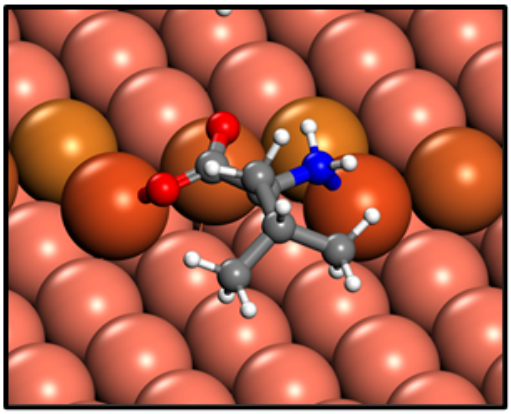
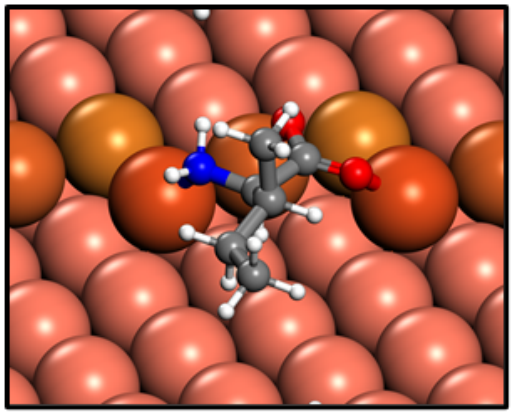


L-Leu



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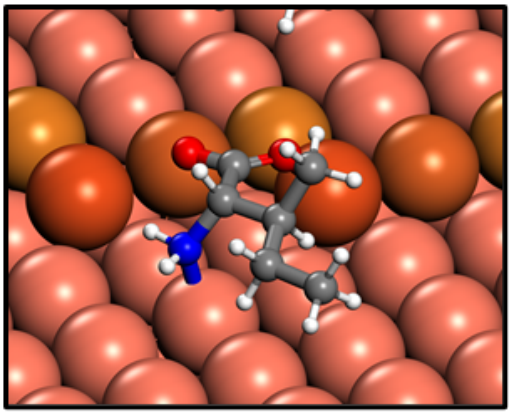

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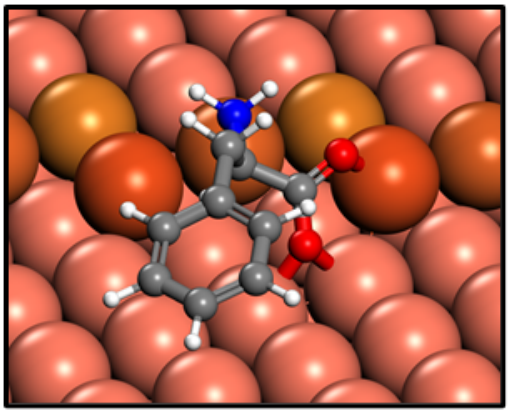
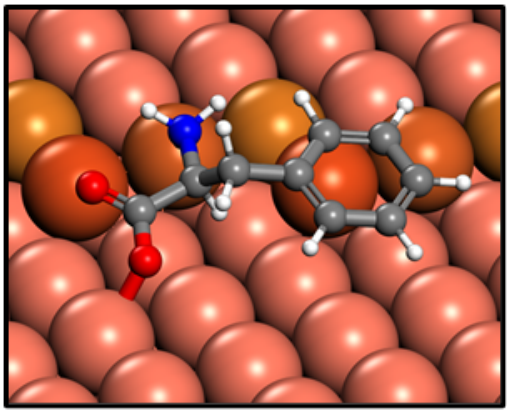
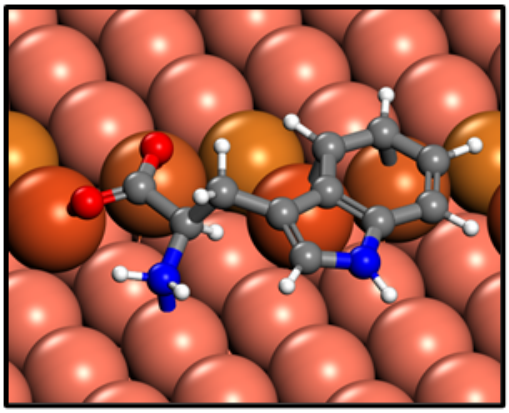


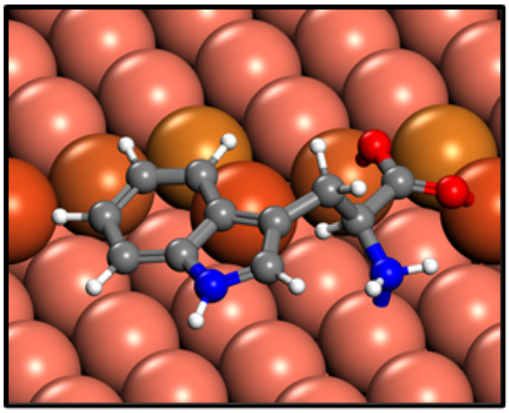
D-Phe



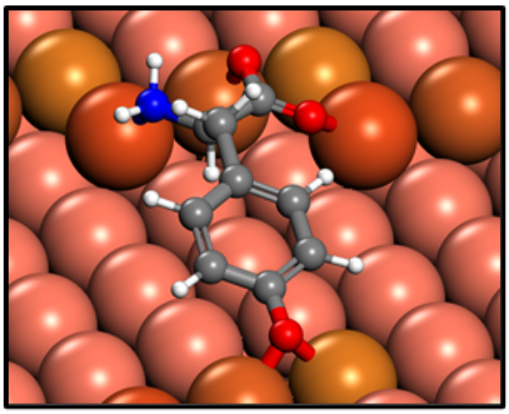
L-Phe



D-Trp



L-Trp



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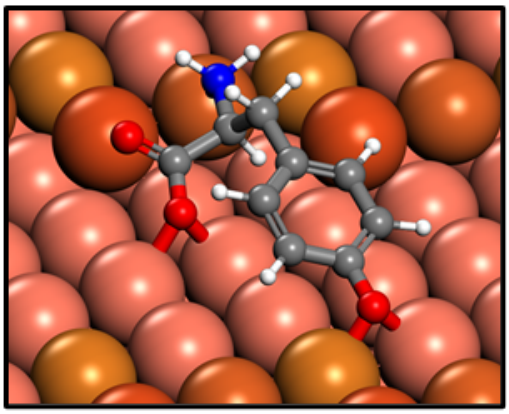

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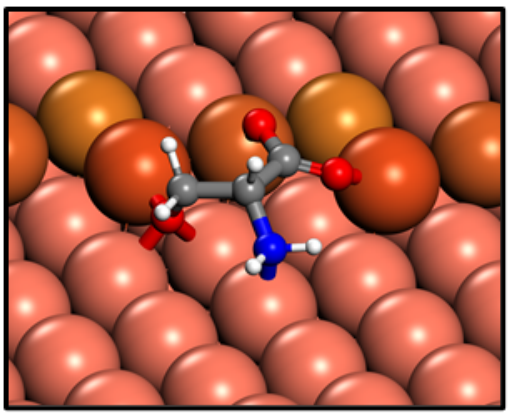

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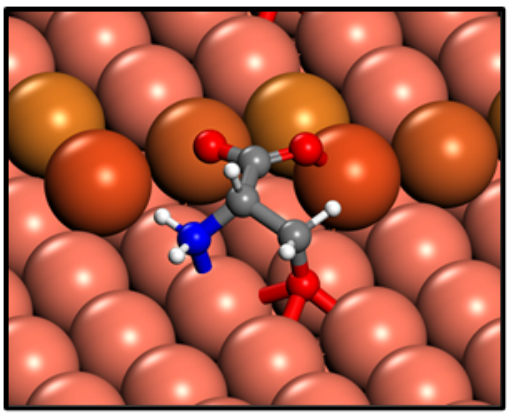

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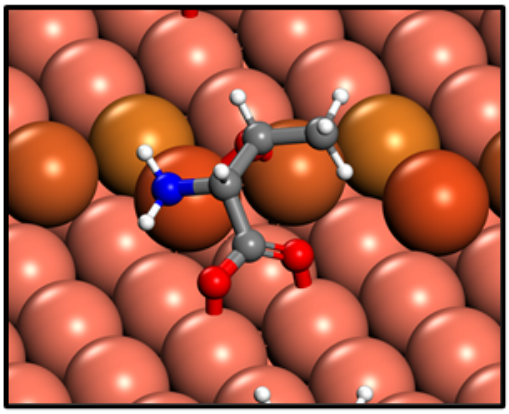

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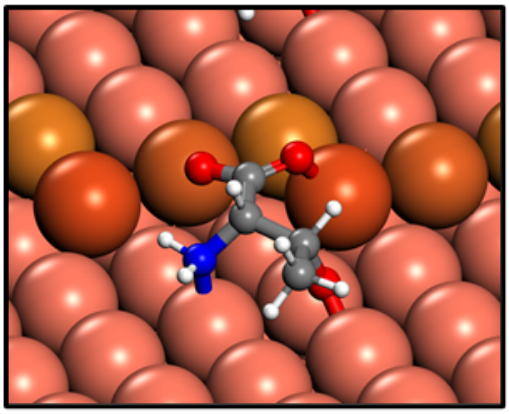

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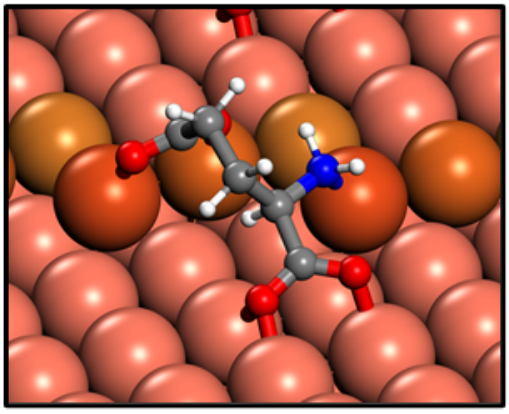

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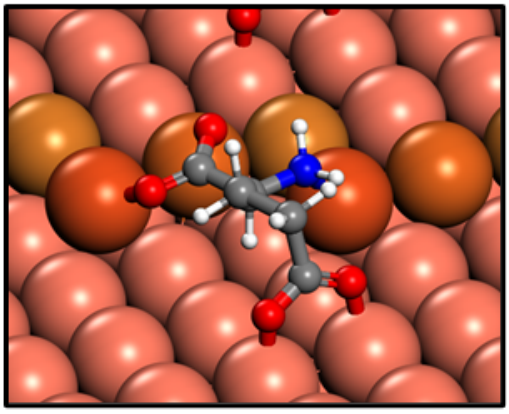
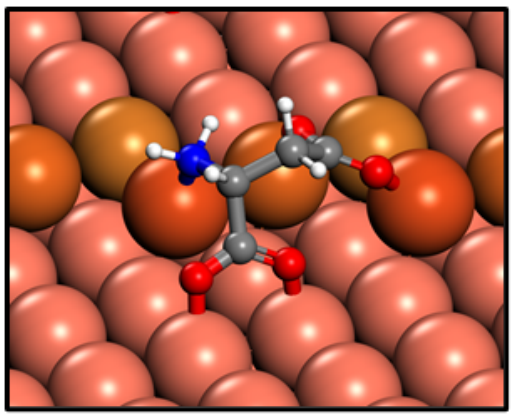
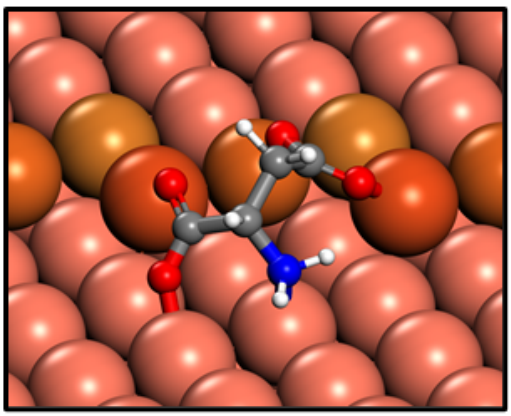


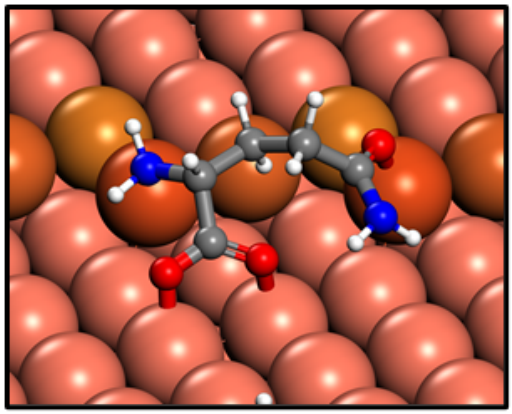
L-Glu



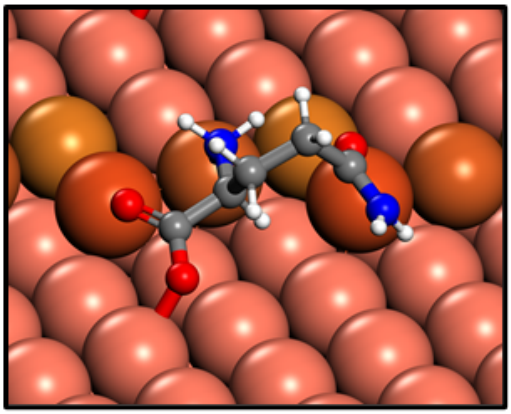
D-Asp



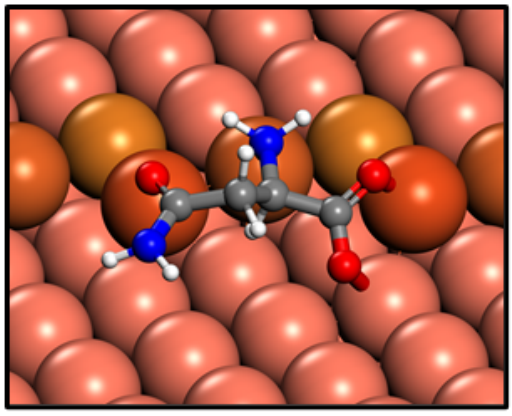
L-Asp



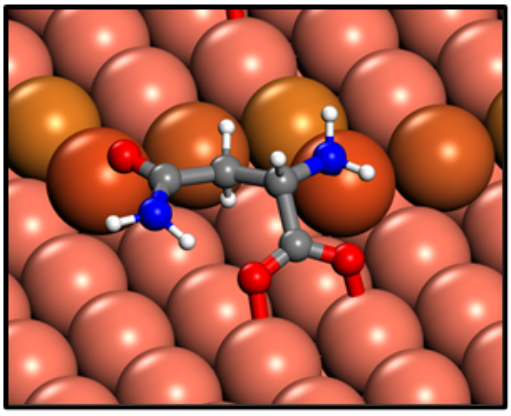
D-Gln



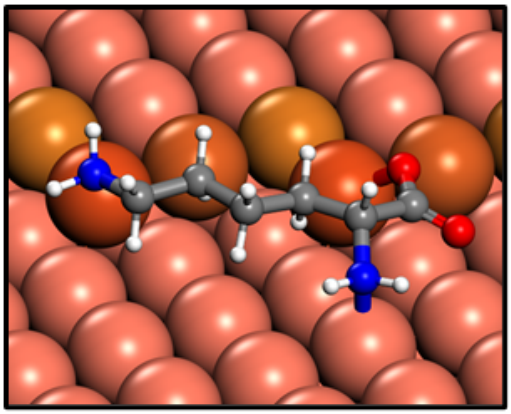
L-Gln



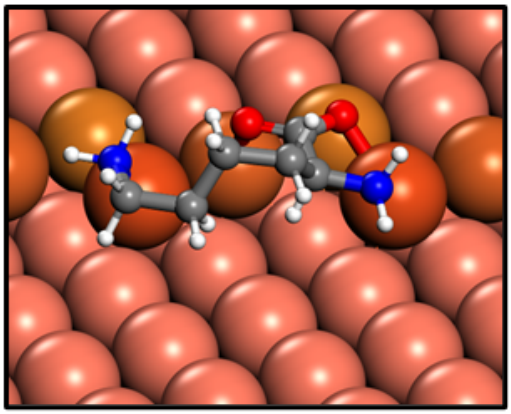
D-Asn



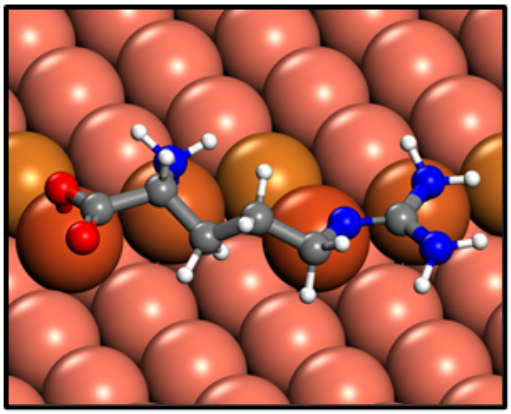
L-Asn



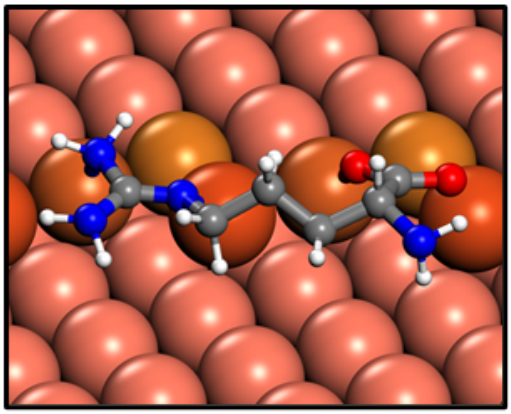
D-Lys



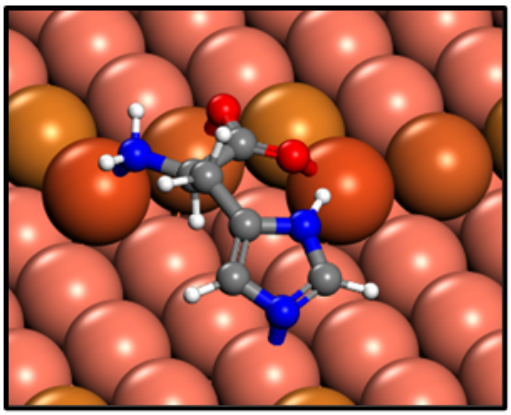
L-Lys



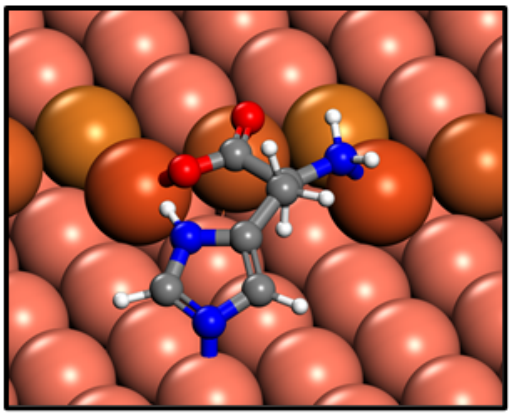
D-Arg



L-Arg



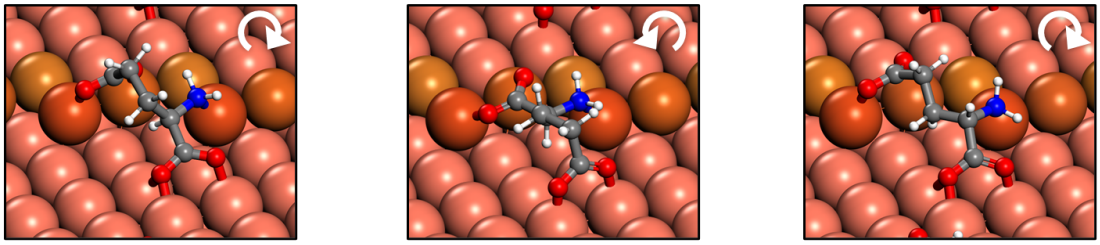
D-His



L-His

Figure S9 Adsorption structures of 18 types of AAs on chiral Cu(3,1,17)^{S} surface.

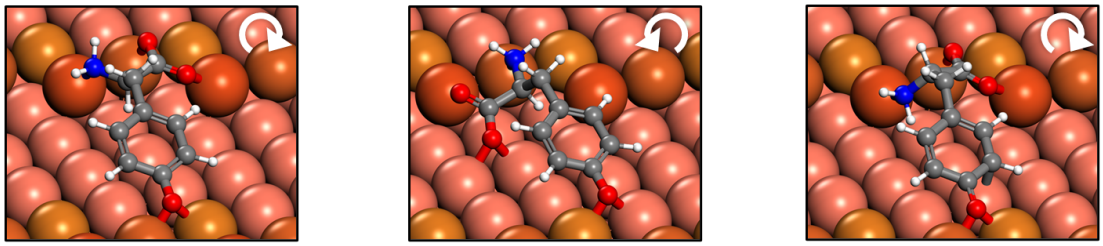
7.3 Enantiospecific adsorption of Glu and Tyr.



D-Glu-GM	L-Glu-GM	L-Glu-LM
$\Delta E_{ads} = +0.00$ eV	$\Delta E_{ads} = +0.16$ eV	$\Delta E_{ads} = +0.37$ eV
$\Delta E_{int} = +0.00$ eV	$\Delta E_{int} = +0.08$ eV	$\Delta E_{int} = +0.19$ eV
$\Delta E_{org} = +0.00$ eV	$\Delta E_{org} = +0.08$ eV	$\Delta E_{org} = +0.18$ eV

Figure S10 Adsorption structures of Glu on Cu(3,1,17)^S surface. Indicated below each structure is ΔE_{ads}, ΔE_{int}, and ΔE_{org} values (see text) using the most stable adsorption system as the reference. In the figure, the white cycle arrow highlights the chirality recognition, following the sequence of amino -> carboxylate -> side chain.

D/L-Glu. For Glu, the D-form GM (D-Glu-GM) is 0.16 eV more stable than the L-form GM (L-Glu-GM). Both of them adopt the μ_5 configuration through the carboxylate-amino skeleton and two oxygen atoms in the carboxylate side chain, with the same copper sites involved for adsorption (two *v* sites, one *e* site, two *t* sites). But their adsorption chirality is different, clockwise in D-Glu-GM or counterclockwise in L-Glu-GM (Figure S10, white circle arrow) following the sequence from amino to carboxylate and to side chain. In this case, the amino group wins in binding on the defective site (*v*) in both two structures, whereas the connectivity of the two carboxylate groups (*α*-carboxylate, side chain carboxylate) varies. D-Glu-GM utilizes the *α*-carboxylate group to bind on the {100} terrace (*t* sites) and side chain carboxylate group to bind on the step edge (*v*, *e* sites). Differently, L-Glu-GM utilizes a reversed connectivity, with *α*-carboxylate group binding on the step edge (*v*, *e* sites) and side chain carboxylate group on the {100} terrace (two *t* sites). The different connectivity results in a 0.16 eV disadvantage of L-Glu-GM, with the deformation effect and interaction effect contributing approximately equal to the energetic discrimination (ΔE_{org} = 0.08 eV, ΔE_{int} = 0.08 eV). The last structure, L-Glu-LM, although adopts the same molecule-surface connectivity with D-Glu-GM, is however 0.37 eV less stable. With a reversed orientation of side chain and H atom (connected with the chiral α-carbon atom), both constrained skeleton geometry (ΔE_{org} = 0.18 eV) and unfavorable binding orientations (ΔE_{int} = 0.19 eV) lead to an unfavorable adsorption.

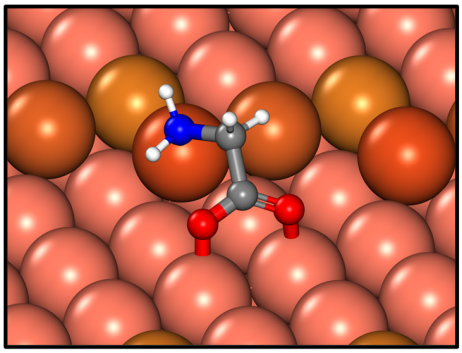


D-Tyr-GM	L-Tyr-GM	L-Tyr-LM
ΔE_{ads}= +0.00 eV	ΔE_{ads}= +0.19 eV	ΔE_{ads}= +0.27 eV
ΔE_{int}= +0.00 eV	ΔE_{int}= +0.49 eV	ΔE_{int}= +0.17 eV
ΔE_{org}= +0.00 eV	ΔE_{org}= −0.30 eV	ΔE_{org}= +0. 10 eV

Figure S11 Adsorption structures of Tyr on Cu(3,1,17)[S] surface. Indicated below each structure is ΔE_{ads}, ΔE_{int}, and ΔE_{org} values (see text) using the most stable adsorption system as the reference. In the figure, the white cycle arrow highlights the chirality recognition, following the sequence of amino -> carboxylate -> side chain.

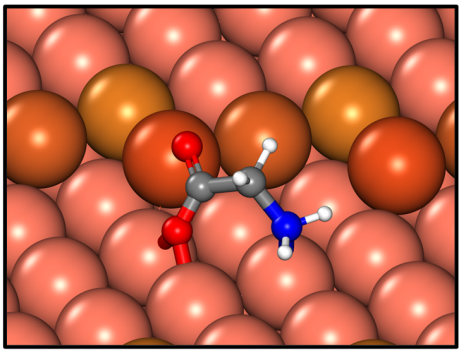
D/L-Tyr. For Tyr, the D-form GM (D-Tyr-GM) is 0.19 eV more stable than the L-form GM (L-Tyr-GM). Both of them utilize the carboxylate-amino skeleton to bind on the step edge (two *v* sites and one *e* site), with the side-chain phenol group binding on the {100} microfacet through the oxygen atom. The enantiomer-surface chiral recognition, as also indicated in Figure S11 by the white arrow, can also be understood as the result of the bonding competition of the phenol ring in the side-chain and the carboxylate-amino skeleton to the kinked Cu sites. Obviously, the phenol group fails to compete with carboxylate-amino skeleton to bind on the kinked sites since the imidazole ring, being rigid and bulky, cannot form a tri-dentation (two *v* sites and one *e* site) geometry (similar to D/L-His). As a result, in D-Tyr-GM, the two oxygen atoms of the carboxylate groups bind on a pair of adjacent *v* site and *e* site in {111} microfacet, along with the nitrogen atoms bind on another *v* site in {110} microfacet, whereas in L-Tyr-GM, the amino nitrogen atom binds on the *e* site of {111} microfacet, with the two carboxylate oxygen atoms bind on one *v* site and one *t* site. The binding of phenol group on {100} microfacet utilizes the bridge-(*e*, *c*) site in D-Tyr-GM and the bridge-(c, t_7) site in L-Tyr-GM. Obviously, the site in D-Tyr-GM is more defective and thus energetically favorable. So, it is not surprising that the L-Tyr-GM is an observable disadvantage in molecule-surface interaction (ΔE_{int} = + 0.49 eV). Again, we found that the L-form with the same molecule-surface connectivity as D-Tyr-GM, is even more unstable (ΔE_{ads}= + 0.27 eV), which can be attributed to both the constrained molecule geometry (ΔE_{org}= + 0.10 eV) and the poor molecule-surface interaction (ΔE_{int} = + 0.17 eV).

7.4 Stability of carboxylic-amino skeleton in D/L-Asp



Gly-LM-D-Asp

ΔE_{ads}**= +0.00 eV**



Gly-LM-L-Asp

ΔE_{ads}**= +0.24 eV**

Figure S12 Adsorption configuration of carboxylic-amino skeleton in D/L-Asp. The two structures depict LMs of the Gly/Cu(3,1,17)^{S} adsorption system, utilized for modeling the stability of the carboxylate-amino skeleton in D/L-Asp. Their geometry and energy are acquired by relaxing the carboxylate-amino skeleton (with an additional H) in D-Asp-GM and L-Asp-GM, labeled as Gly-LM-D-Asp and Gly-LM-L-Asp. The energy difference (ΔE_{ads}) is calculated using Gly-LM-D-Asp as the reference. Based on ΔE_{ads}, Gly-LM-L-Asp is +0.24 eV energetically less favorable than Gly-LM-D-Asp.

8. Dataset Summary of Cu-C-H-O-N quinary G-NN potential

Table S4. Number of structures for the global dataset to train Cu-C-H-O-N G-NN potential. Listed data include the species composition, the total number of atoms (N_{atom}), and the number of structures with this composition (N_{struc}). The dataset contains a total number of 125,658 structures.

Species	N_{atom}	N_{struc}	Species	N_{atom}	N_{struc}	Species	N_{atom}	N_{struc}
Cu32	32	1	Cu36	36	1	Cu48	48	3
Cu60	60	1	Cu64	64	2	Cu72	72	1
Cu80	80	2	Cu96	96	1	Cu144	144	1
O2-Cu36	38	2	O3-Cu36	39	1	O3-Cu48	51	1
O4	4	34	O5-Cu72	77	1	O6-Cu48	54	1
O11	11	295	N1-Cu12	13	5	N1-O1	2	35
N2	2	31	N2-Cu8	10	50	N2-Cu10	12	8
N2-Cu36	38	1	N2-Cu48	50	1	N2-O1	3	70
N2-O1-Cu36	39	1	N2-O3	5	94	N2-O3-Cu36	41	1
N2-O3-Cu48	53	1	N2-O4	6	86	N2-O4-Cu36	42	1
N2-O4-Cu48	54	1	N2-O5	7	107	N3-Cu16	19	1
N4-Cu8	12	320	N4-Cu48	52	1	N4-O1	5	1
N4-O1-Cu36	41	1	N4-O1-Cu48	53	2	N4-O1-Cu72	77	1
N4-O2-Cu36	42	2	N6-Cu36	42	2	N6-Cu48	54	1
N12-Cu50	62	1	C1-O3-Cu36	40	1	C1-N2-Cu36	39	1
C1-N2-O1-Cu36	40	1	C1-N2-O2-Cu36	41	1	C1-N2-O2-Cu48	53	4
C1-N2-O3-Cu36	42	2	C1-N2-O3-Cu48	54	4	C1-N4-Cu36	41	1
C1-N4-O1-Cu36	42	1	C1-N4-O1-Cu48	54	4	C1-N4-O2	7	1
C1-N4-O3	8	1	C1-N6-O1	8	1	C2-Cu36	38	2
C2-O2-Cu48	52	1	C2-O3-Cu36	41	2	C2-O3-Cu48	53	1
C2-O4-Cu36	42	1	C2-O4-Cu64	70	1	C2-N2	4	102
C2-N2-Cu36	40	2	C2-N2-Cu48	52	3	C2-N2-Cu72	76	2
C2-N2-O1-Cu36	41	1	C2-N2-O1-Cu64	69	1	C2-N2-O1-Cu72	77	1
C2-N2-O2-Cu36	42	1	C2-N4-Cu48	54	2	C2-N4-Cu72	78	1
C2-N4-O2	8	1	C2-N6-O1	9	1	C3-O1-Cu36	40	1
C3-O2-Cu36	41	1	C3-O2-Cu48	53	1	C3-N2-Cu48	53	2
C3-N4-O2	9	1	C4-Cu72	76	1	C4-O2-Cu36	42	1
C4-O2-Cu48	54	2	C4-N2-Cu48	54	1	C4-N2-Cu64	70	1
C4-N2-Cu72	78	1	C4-N2-Cu96	102	1	C4-N4-O1	9	1
C4-N8-O4	16	26	C4-N8-O5	17	7	C4-N8-O6	18	3
C5-N8-O5	18	5	C6-N8-O4	18	11	H1-O1	2	1
H1-N1-O1	3	65	H1-N1-O1-Cu36	39	1	H1-N1-O1-Cu48	51	2
H1-N1-O2	4	171	H1-N1-O2-Cu36	40	3	H1-N1-O2-Cu48	52	1
H1-N1-O3	5	176	H1-N1-O3-Cu48	53	1	H1-N1-O4	6	111
H1-N1-O4-Cu36	42	1	H1-N1-O4-Cu48	54	1	H1-N1-O4-Cu72	78	1
H1-N1-O5-Cu96	103	1	H1-N3-Cu48	52	1	H1-N3-Cu72	76	1
H1-N3-O1-Cu36	41	2	H1-N3-O1-Cu48	53	2	H1-N3-O1-Cu72	77	1
H1-N3-O2-Cu36	42	1	H1-N3-O2-Cu48	54	3	H1-N3-O3-Cu48	55	2
H1-N5-Cu36	42	1	H1-N5-Cu48	54	1	H1-N5-O1-Cu48	55	1
H1-C1-N1	3	145	H1-C1-N1-O1	4	173	H1-C1-N1-O1-Cu36	40	2
H1-C1-N1-O1-Cu48	52	3	H1-C1-N1-O2-Cu36	41	2	H1-C1-N1-O2-Cu48	53	4
H1-C1-N1-O3-Cu36	42	3	H1-C1-N1-O3-Cu48	54	1	H1-C1-N1-O3-Cu72	78	2
H1-C1-N1-O4-Cu36	43	5	H1-C1-N1-O4-Cu48	55	4	H1-C1-N1-O4-Cu96	103	1
H1-C1-N3-Cu36	41	2	H1-C1-N3-O1-Cu36	42	4	H1-C1-N3-O1-Cu48	54	6
H1-C1-N3-O1-Cu64	70	1	H1-C1-N3-O1-Cu72	78	1	H1-C1-N3-O2	7	1
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H1-C1-N5-Cu48	55	5	H1-C1-N5-Cu64	71	1	H1-C1-N5-Cu72	79	1
H1-C1-N5-O1	8	1	H1-C2-N1-Cu36	40	1	H1-C2-N1-Cu48	52	1
H1-C2-N1-O1-Cu48	53	3	H1-C2-N1-O1-Cu72	77	1	H1-C2-N1-O2-Cu36	42	2
H1-C2-N1-O2-Cu48	54	4	H1-C2-N1-O2-Cu64	70	1	H1-C2-N1-O2-Cu72	78	5

H1-C2-N1-O3-Cu36	43	2	H1-C2-N1-O3-Cu48	55	6	H1-C2-N1-O3-Cu64	71	3
H1-C2-N1-O3-Cu72	79	2	H1-C2-N3-Cu36	42	1	H1-C2-N3-Cu48	54	7
H1-C2-N3-Cu64	70	1	H1-C2-N3-Cu72	78	1	H1-C2-N3-O1-Cu36	43	1
H1-C2-N3-O1-Cu48	55	5	H1-C2-N3-O1-Cu72	79	2	H1-C2-N3-O2	8	1
H1-C2-N3-O3	9	2	H1-C2-N3-O4	10	2	H1-C2-N5-O1	9	1
H1-C2-N5-O2	10	4	H1-C3-N1	5	122	H1-C3-N1-Cu72	77	2
H1-C3-N1-O1-Cu36	42	2	H1-C3-N1-O1-Cu48	54	4	H1-C3-N1-O1-Cu64	70	2
H1-C3-N1-O1-Cu72	78	6	H1-C3-N1-O2-Cu48	55	1	H1-C3-N1-O2-Cu72	79	2
H1-C3-N3-Cu36	43	1	H1-C3-N3-O2	9	1	H1-C3-N5-O1	10	2
H1-C3-N5-O2	11	12	H1-C3-N5-O3	12	11	H1-C4-N1-Cu48	54	1
H1-C4-N1-O1-Cu48	55	5	H1-C4-N1-O1-Cu64	71	1	H1-C4-N1-O1-Cu72	79	2
H1-C4-N5	10	1	H1-C5-N1-Cu48	55	1	H1-C5-N1-Cu64	71	1
H1-C5-N1-Cu96	103	1	H1-C5-N3-O1	10	1	H1-C5-N3-O1-Cu30	40	8
H1-C5-N3-O1-Cu36	46	50	H1-C5-N7-O5	18	14	H1-C5-N7-O6	19	29
H2	2	2	H2-O1	3	1	H2-O1-Cu27	30	450
H2-O1-Cu48	51	1	H2-O2-Cu48	52	1	H2-N1-Cu20	23	15
H2-N2	4	61	H2-N2-Cu8	12	13	H2-N2-Cu36	40	1
H2-N2-O1-Cu36	41	3	H2-N2-O1-Cu48	53	2	H2-N2-O1-Cu72	77	1
H2-N2-O2	6	171	H2-N2-O2-Cu36	42	2	H2-N2-O2-Cu48	54	3
H2-N2-O2-Cu64	70	1	H2-N2-O3-Cu36	43	2	H2-N2-O3-Cu48	55	2
H2-N2-O4-Cu48	56	3	H2-N4-Cu48	54	1	H2-N4-Cu64	70	1
H2-N4-O1-Cu48	55	2	H2-N4-O2-Cu36	44	1	H2-N4-O2-Cu48	56	2
H2-N4-O2-Cu64	72	1	H2-N4-O2-Cu72	80	1	H2-N6-Cu60	68	1
H2-C1	3	5	H2-C1-O1	4	111	H2-C1-O1-Cu36	40	1
H2-C1-O2	5	41	H2-C1-O2-Cu11	16	27	H2-C1-O2-Cu12	17	16238
H2-C1-O2-Cu16	21	635	H2-C1-O2-Cu27	32	651	H2-C1-O2-Cu36	41	3
H2-C1-O3	6	11	H2-C1-O3-Cu36	42	1	H2-C1-O4-Cu36	43	1
H2-C1-O4-Cu48	55	1	H2-C1-O4-Cu72	79	1	H2-C1-O5-Cu72	80	1
H2-C1-N2	5	185	H2-C1-N2-Cu36	41	3	H2-C1-N2-Cu48	53	3
H2-C1-N2-Cu64	69	1	H2-C1-N2-O1-Cu36	42	4	H2-C1-N2-O1-Cu48	54	8
H2-C1-N2-O2-Cu36	43	4	H2-C1-N2-O2-Cu48	55	14	H2-C1-N2-O2-Cu64	71	3
H2-C1-N2-O2-Cu72	79	1	H2-C1-N2-O3-Cu36	44	1	H2-C1-N2-O3-Cu48	56	11
H2-C1-N2-O3-Cu72	80	4	H2-C1-N2-O3-Cu96	104	2	H2-C1-N2-O4-Cu35	44	3
H2-C1-N2-O4-Cu36	45	59	H2-C1-N4	7	103	H2-C1-N4-Cu48	55	6
H2-C1-N4-Cu64	71	1	H2-C1-N4-Cu72	79	2	H2-C1-N4-Cu96	103	1
H2-C1-N4-O1-Cu36	44	2	H2-C1-N4-O1-Cu48	56	8	H2-C1-N4-O1-Cu64	72	1
H2-C1-N4-O1-Cu72	80	2	H2-C1-N4-O1-Cu80	88	1	H2-C1-N4-O1-Cu96	104	1
H2-C2	4	92	H2-C2-Cu48	52	1	H2-C2-O1-Cu36	41	2
H2-C2-O1-Cu48	53	1	H2-C2-O1-Cu72	77	2	H2-C2-O2-Cu36	42	4
H2-C2-O2-Cu48	54	2	H2-C2-O2-Cu72	78	1	H2-C2-O3-Cu27	34	1474
H2-C2-O3-Cu36	43	1948	H2-C2-O3-Cu48	55	2	H2-C2-O3-Cu72	79	1
H2-C2-O4-Cu36	44	1	H2-C2-O4-Cu48	56	4	H2-C2-O4-Cu64	72	1
H2-C2-O4-Cu72	80	1	H2-C2-N2	6	2	H2-C2-N2-Cu36	42	4
H2-C2-N2-Cu48	54	6	H2-C2-N2-Cu64	70	1	H2-C2-N2-Cu72	78	3
H2-C2-N2-O1	7	89	H2-C2-N2-O1-Cu36	43	9	H2-C2-N2-O1-Cu48	55	9
H2-C2-N2-O1-Cu64	71	2	H2-C2-N2-O1-Cu72	79	2	H2-C2-N2-O1-Cu96	103	1
H2-C2-N2-O2	8	181	H2-C2-N2-O2-Cu36	44	10	H2-C2-N2-O2-Cu48	56	21
H2-C2-N2-O2-Cu60	68	3	H2-C2-N2-O2-Cu64	72	7	H2-C2-N2-O2-Cu72	80	8
H2-C2-N2-O2-Cu96	104	6	H2-C2-N4	8	37	H2-C2-N4-Cu36	44	3
H2-C2-N4-Cu48	56	8	H2-C2-N4-Cu64	72	2	H2-C2-N4-Cu72	80	4
H2-C2-N4-O1	9	2	H2-C2-N4-O2	10	3	H2-C2-N4-O3	11	2
H2-C2-N6	10	4	H2-C2-N6-O1	11	6	H2-C3-Cu36	41	1
H2-C3-O1-Cu36	42	3	H2-C3-O1-Cu48	54	5	H2-C3-O1-Cu72	78	1
H2-C3-O2-Cu36	43	3	H2-C3-O2-Cu48	55	7	H2-C3-O2-Cu64	71	2
H2-C3-O2-Cu72	79	2	H2-C3-O3-Cu48	56	5	H2-C3-O3-Cu64	72	2
H2-C3-O3-Cu72	80	5	H2-C3-O3-Cu96	104	2	H2-C3-O4-Cu33	42	713
H2-C3-O4-Cu35	44	743	H2-C3-O4-Cu36	45	1508	H2-C3-N2-Cu36	43	4
H2-C3-N2-Cu48	55	5	H2-C3-N2-Cu64	71	6	H2-C3-N2-Cu72	79	3
H2-C3-N2-Cu96	103	4	H2-C3-N2-O1-Cu36	44	3	H2-C3-N2-O1-Cu48	56	10
H2-C3-N2-O1-Cu64	72	3	H2-C3-N2-O1-Cu72	80	3	H2-C3-N2-O1-Cu96	104	3
H2-C3-N2-O2	9	1	H2-C3-N2-O3	10	17	H2-C3-N2-O4	11	14

H2-C3-N4	9	2	H2-C3-N4-O1	10	3	H2-C3-N4-O2	11	8
H2-C3-N4-O3	12	23	H2-C3-N4-O4	13	15	H2-C3-N6	11	1
H2-C4-Cu36	42	1	H2-C4-Cu48	54	4	H2-C4-Cu72	78	1
H2-C4-O1-Cu36	43	2	H2-C4-O1-Cu48	55	6	H2-C4-O1-Cu64	71	1
H2-C4-O1-Cu72	79	2	H2-C4-O1-Cu80	87	1	H2-C4-O1-Cu96	103	2
H2-C4-O2-Cu48	56	1	H2-C4-O2-Cu64	72	2	H2-C4-O2-Cu72	80	6
H2-C4-O2-Cu96	104	2	H2-C4-O3	9	66	H2-C4-O4	10	2
H2-C4-O5	11	8	H2-C4-N2-Cu36	44	1	H2-C4-N2-Cu48	56	6
H2-C4-N2-Cu64	72	1	H2-C4-N2-Cu72	80	5	H2-C4-N2-O1	9	93
H2-C4-N4-O1	11	8	H2-C4-N4-O3	13	24	H2-C5-Cu48	55	3
H2-C5-Cu72	79	1	H2-C5-O1-Cu48	56	2	H2-C5-O1-Cu60	68	1
H2-C5-O1-Cu72	80	4	H2-C5-O3	10	6	H2-C5-O4	11	6
H2-C5-N4	11	1	H2-C5-N6-O5	18	6	H2-C5-N6-O6	19	12
H2-C5-N6-O7	20	12	H2-C5-N8-O4	19	20	H2-C5-N8-O5	20	35
H2-C6-Cu120	128	1	H2-C6-O2	10	2	H2-C6-N6-O5	19	3
H2-C6-N6-O6	20	4	H2-C7-O1	10	2	H2-C7-N6-O4	19	12
H2-C7-N6-O5	20	29	H2-C10-N6-O2-Cu58	78	1	H2-C10-N6-O2-Cu62	82	2
H3-N1	4	44	H3-N1-Cu36	40	15	H3-N1-Cu48	52	1
H3-N1-O1	5	86	H3-N1-O1-Cu36	41	2	H3-N1-O1-Cu48	53	1
H3-N1-O2-Cu36	42	2	H3-N1-O2-Cu48	54	1	H3-N1-O2-Cu72	78	2
H3-N1-O3-Cu48	55	3	H3-N1-O4-Cu36	44	1	H3-N1-O4-Cu96	104	1
H3-N2-Cu22	27	3	H3-N2-Cu35	40	6	H3-N3-Cu48	54	1
H3-N3-O1-Cu36	43	1	H3-N3-O1-Cu72	79	1	H3-N3-O1-Cu96	103	1
H3-N3-O2-Cu36	44	2	H3-N3-O2-Cu48	56	3	H3-N3-O2-Cu64	72	1
H3-N3-O2-Cu72	80	1	H3-N3-O3-Cu36	45	1	H3-N3-O3-Cu48	57	2
H3-N3-O3-Cu72	81	1	H3-N5-Cu48	56	1	H3-N5-Cu96	104	1
H3-N5-O1-Cu48	57	2	H3-N5-O1-Cu72	81	1	H3-C1	4	8
H3-C1-O2-Cu18	24	478	H3-C1-N1	5	249	H3-C1-N1-Cu48	53	1
H3-C1-N1-O1	6	139	H3-C1-N1-O1-Cu36	42	2	H3-C1-N1-O1-Cu48	54	2
H3-C1-N1-O1-Cu72	78	1	H3-C1-N1-O2	7	221	H3-C1-N1-O2-Cu36	43	39
H3-C1-N1-O2-Cu48	55	6	H3-C1-N1-O2-Cu72	79	2	H3-C1-N1-O2-Cu96	103	1
H3-C1-N1-O3	8	57	H3-C1-N1-O3-Cu36	44	6	H3-C1-N1-O3-Cu48	56	8
H3-C1-N1-O3-Cu72	80	4	H3-C1-N1-O3-Cu96	104	1	H3-C1-N1-O4-Cu36	45	1
H3-C1-N1-O4-Cu48	57	4	H3-C1-N1-O4-Cu64	73	1	H3-C1-N1-O4-Cu72	81	2
H3-C1-N3-Cu36	43	1	H3-C1-N3-Cu48	55	9	H3-C1-N3-Cu64	71	1
H3-C1-N3-Cu72	79	2	H3-C1-N3-O1-Cu36	44	3	H3-C1-N3-O1-Cu48	56	9
H3-C1-N3-O1-Cu64	72	2	H3-C1-N3-O1-Cu72	80	2	H3-C1-N3-O1-Cu96	104	2
H3-C1-N3-O2-Cu36	45	2	H3-C1-N3-O2-Cu48	57	6	H3-C1-N3-O2-Cu60	69	1
H3-C1-N3-O2-Cu64	73	5	H3-C1-N3-O2-Cu72	81	4	H3-C1-N3-O2-Cu96	105	2
H3-C1-N5-Cu48	57	2	H3-C1-N5-Cu60	69	2	H3-C1-N5-Cu64	73	2
H3-C1-N5-Cu80	89	1	H3-C1-N7	11	1	H3-C2-O2-Cu31	38	6
H3-C2-O2-Cu32	39	6	H3-C2-O2-Cu36	43	805	H3-C2-O3-Cu23	31	55
H3-C2-O3-Cu24	32	222	H3-C2-O3-Cu27	35	74	H3-C2-N1	6	182
H3-C2-N1-Cu36	42	2	H3-C2-N1-Cu48	54	3	H3-C2-N1-Cu72	78	1
H3-C2-N1-O1	7	173	H3-C2-N1-O1-Cu36	43	6	H3-C2-N1-O1-Cu48	55	14
H3-C2-N1-O1-Cu64	71	2	H3-C2-N1-O1-Cu72	79	5	H3-C2-N1-O1-Cu96	103	2
H3-C2-N1-O2	8	95	H3-C2-N1-O2-Cu36	44	6	H3-C2-N1-O2-Cu48	56	13
H3-C2-N1-O2-Cu64	72	4	H3-C2-N1-O2-Cu72	80	6	H3-C2-N1-O2-Cu96	104	2
H3-C2-N1-O3	9	61	H3-C2-N1-O3-Cu36	45	4	H3-C2-N1-O3-Cu48	57	18
H3-C2-N1-O3-Cu64	73	10	H3-C2-N1-O3-Cu72	81	6	H3-C2-N1-O3-Cu96	105	5
H3-C2-N3	8	438	H3-C2-N3-Cu36	44	8	H3-C2-N3-Cu48	56	6
H3-C2-N3-Cu64	72	5	H3-C2-N3-Cu72	80	1	H3-C2-N3-Cu96	104	1
H3-C2-N3-O1	9	87	H3-C2-N3-O1-Cu36	45	6	H3-C2-N3-O1-Cu48	57	22
H3-C2-N3-O1-Cu60	69	1	H3-C2-N3-O1-Cu64	73	9	H3-C2-N3-O1-Cu72	81	14
H3-C2-N3-O1-Cu96	105	6	H3-C2-N3-O2	10	2	H3-C2-N5	10	1
H3-C2-N5-O1	11	8	H3-C2-N5-O2	12	3	H3-C2-N7	12	4
H3-C3-N1	7	186	H3-C3-N1-Cu48	55	3	H3-C3-N1-Cu64	71	1
H3-C3-N1-Cu72	79	3	H3-C3-N1-O1	8	394	H3-C3-N1-O1-Cu36	44	7
H3-C3-N1-O1-Cu48	56	23	H3-C3-N1-O1-Cu60	68	1	H3-C3-N1-O1-Cu64	72	9
H3-C3-N1-O1-Cu72	80	15	H3-C3-N1-O1-Cu96	104	5	H3-C3-N1-O2	9	257
H3-C3-N1-O2-Cu36	45	6	H3-C3-N1-O2-Cu48	57	35	H3-C3-N1-O2-Cu60	69	2

H3-C3-N1-O2-Cu64	73	12	H3-C3-N1-O2-Cu72	81	11	H3-C3-N1-O2-Cu96	105	14
H3-C3-N1-O3	10	27	H3-C3-N3-Cu36	45	5	H3-C3-N3-Cu48	57	16
H3-C3-N3-Cu60	69	1	H3-C3-N3-Cu64	73	2	H3-C3-N3-Cu72	81	3
H3-C3-N3-Cu96	105	6	H3-C3-N3-Cu120	129	1	H3-C3-N3-O1	10	1
H3-C3-N3-O2	11	6	H3-C3-N3-O3	12	104	H3-C3-N5	11	5
H3-C3-N5-O1	12	10	H3-C4-N1-Cu48	56	8	H3-C4-N1-Cu64	72	6
H3-C4-N1-Cu72	80	4	H3-C4-N1-Cu80	88	1	H3-C4-N1-Cu96	104	2
H3-C4-N1-O1-Cu48	57	9	H3-C4-N1-O1-Cu60	69	1	H3-C4-N1-O1-Cu64	73	13
H3-C4-N1-O1-Cu72	81	7	H3-C4-N1-O1-Cu96	105	7	H3-C4-N1-O1-Cu120	129	1
H3-C4-N1-O2	10	38	H3-C4-N1-O3	11	53	H3-C4-N1-O4	12	15
H3-C4-N3	10	2	H3-C4-N3-O1	11	52	H3-C4-N3-O2	12	5
H3-C4-N3-O3	13	7	H3-C4-N3-O4	14	25	H3-C4-N5	12	9
H3-C4-N5-O2	14	18	H3-C4-N9-O3	19	1	H3-C4-N9-O4	20	3
H3-C5-N1-Cu48	57	1	H3-C5-N1-Cu60	69	2	H3-C5-N1-Cu64	73	3
H3-C5-N1-Cu72	81	3	H3-C5-N1-Cu80	89	2	H3-C5-N1-Cu96	105	2
H3-C5-N1-O2	11	1	H3-C5-N3-O1	12	3	H3-C5-N7-O4	19	3
H3-C5-N7-O5	20	29	H3-C5-N7-O6	21	18	H3-C5-N9-O3	20	3
H3-C6-N3-O2	14	22	H3-C6-N5-O6	20	2	H3-C6-N5-O7	21	10
H3-C6-N7-O4	20	6	H3-C6-N7-O5	21	9	H3-C7-N1-O3	14	7
H3-C7-N7-O4	21	10	H3-C8-N5-O5	21	12	H4-N1-Cu36	41	46
H4-N2	6	83	H4-N2-Cu17	23	1	H4-N2-O1-Cu48	55	2
H4-N2-O2-Cu48	56	2	H4-N2-O2-Cu72	80	1	H4-N2-O3-Cu36	45	1
H4-N2-O3-Cu48	57	1	H4-N2-O3-Cu96	105	1	H4-N2-O4-Cu48	58	2
H4-N2-O4-Cu64	74	1	H4-N2-O4-Cu96	106	2	H4-N4-Cu48	56	1
H4-N4-Cu72	80	1	H4-N4-O1-Cu36	45	3	H4-N4-O1-Cu48	57	1
H4-N4-O2-Cu48	58	2	H4-N6-Cu64	74	1	H4-N6-Cu72	82	1
H4-C1	5	138	H4-C1-Cu36	41	1	H4-C1-O1	6	42
H4-C1-O1-Cu12	18	970	H4-C1-O1-Cu36	42	1	H4-C1-O2	7	7
H4-C1-O2-Cu36	43	1	H4-C1-O3-Cu27	35	5936	H4-C1-O3-Cu36	44	1
H4-C1-O3-Cu48	56	1	H4-C1-O3-Cu72	80	2	H4-C1-O4-Cu36	45	2
H4-C1-O4-Cu48	57	2	H4-C1-O4-Cu64	73	1	H4-C1-O4-Cu72	81	1
H4-C1-O5-Cu36	46	1	H4-C1-O5-Cu48	58	2	H4-C1-O5-Cu64	74	1
H4-C1-N2	7	143	H4-C1-N2-Cu36	43	62	H4-C1-N2-Cu48	55	2
H4-C1-N2-Cu72	79	1	H4-C1-N2-O1	8	68	H4-C1-N2-O1-Cu36	44	3
H4-C1-N2-O1-Cu48	56	7	H4-C1-N2-O1-Cu64	72	1	H4-C1-N2-O1-Cu72	80	2
H4-C1-N2-O2-Cu36	45	5	H4-C1-N2-O2-Cu48	57	8	H4-C1-N2-O2-Cu64	73	3
H4-C1-N2-O2-Cu72	81	2	H4-C1-N2-O2-Cu96	105	2	H4-C1-N2-O3-Cu36	46	6
H4-C1-N2-O3-Cu48	58	8	H4-C1-N2-O3-Cu64	74	4	H4-C1-N2-O3-Cu72	82	1
H4-C1-N4-Cu36	45	3	H4-C1-N4-Cu48	57	15	H4-C1-N4-Cu64	73	4
H4-C1-N4-Cu72	81	1	H4-C1-N4-Cu96	105	3	H4-C1-N4-O1-Cu36	46	1
H4-C1-N4-O1-Cu48	58	9	H4-C1-N4-O1-Cu64	74	4	H4-C1-N4-O1-Cu72	82	3
H4-C1-N4-O1-Cu96	106	7	H4-C2	6	37	H4-C2-Cu36	42	2
H4-C2-O1	7	163	H4-C2-O1-Cu36	43	4	H4-C2-O1-Cu48	55	3
H4-C2-O1-Cu72	79	2	H4-C2-O2	8	59	H4-C2-O2-Cu27	35	71
H4-C2-O2-Cu33	41	577	H4-C2-O2-Cu36	44	587	H4-C2-O2-Cu48	56	9
H4-C2-O2-Cu64	72	1	H4-C2-O2-Cu72	80	4	H4-C2-O2-Cu96	104	1
H4-C2-O3-Cu36	45	240	H4-C2-O3-Cu48	57	9	H4-C2-O3-Cu64	73	2
H4-C2-O3-Cu72	81	5	H4-C2-O3-Cu96	105	1	H4-C2-O4-Cu11	21	37
H4-C2-O4-Cu12	22	6332	H4-C2-O4-Cu24	34	306	H4-C2-O4-Cu26	36	45
H4-C2-O4-Cu27	37	2567	H4-C2-O4-Cu32	42	109	H4-C2-O4-Cu36	46	1755
H4-C2-O4-Cu48	58	6	H4-C2-O4-Cu64	74	9	H4-C2-O4-Cu72	82	3
H4-C2-O4-Cu96	106	6	H4-C2-N1-O2-Cu24	33	15	H4-C2-N1-O2-Cu27	36	8
H4-C2-N1-O2-Cu32	41	17	H4-C2-N1-O2-Cu36	45	52	H4-C2-N1-O2-Cu48	57	20
H4-C2-N1-O2-Cu54	63	12	H4-C2-N1-O2-Cu72	81	8	H4-C2-N1-O2-Cu144	153	11
H4-C2-N2	8	71	H4-C2-N2-Cu36	44	3	H4-C2-N2-Cu48	56	14
H4-C2-N2-Cu64	72	4	H4-C2-N2-Cu72	80	5	H4-C2-N2-Cu96	104	1
H4-C2-N2-O1-Cu36	45	11	H4-C2-N2-O1-Cu48	57	29	H4-C2-N2-O1-Cu64	73	11
H4-C2-N2-O1-Cu72	81	8	H4-C2-N2-O1-Cu80	89	1	H4-C2-N2-O1-Cu96	105	13
H4-C2-N2-O2-Cu36	46	6	H4-C2-N2-O2-Cu48	58	26	H4-C2-N2-O2-Cu60	70	1
H4-C2-N2-O2-Cu64	74	21	H4-C2-N2-O2-Cu72	82	17	H4-C2-N2-O2-Cu80	90	1
H4-C2-N2-O2-Cu96	106	25	H4-C2-N4	10	3	H4-C2-N4-Cu48	58	15

H4-C2-N4-Cu60	70	1	H4-C2-N4-Cu64	74	11	H4-C2-N4-Cu72	82	8
H4-C2-N4-Cu80	90	1	H4-C2-N4-Cu96	106	7	H4-C2-N4-Cu120	130	1
H4-C2-N4-O1	11	2	H4-C2-N4-O8-Cu68	86	3	H4-C2-N6	12	1
H4-C2-N6-O1	13	2	H4-C3	7	55	H4-C3-Cu48	55	2
H4-C3-O1	8	12	H4-C3-O1-Cu48	56	5	H4-C3-O1-Cu64	72	1
H4-C3-O1-Cu72	80	3	H4-C3-O1-Cu96	104	2	H4-C3-O2	9	1
H4-C3-O2-Cu36	45	3	H4-C3-O2-Cu48	57	13	H4-C3-O2-Cu64	73	11
H4-C3-O2-Cu72	81	4	H4-C3-O2-Cu96	105	3	H4-C3-O3-Cu36	46	4
H4-C3-O3-Cu48	58	24	H4-C3-O3-Cu64	74	11	H4-C3-O3-Cu72	82	9
H4-C3-O3-Cu96	106	15	H4-C3-O5-Cu36	48	44	H4-C3-N2	9	165
H4-C3-N2-Cu32	41	1	H4-C3-N2-Cu34	43	2	H4-C3-N2-Cu36	45	25
H4-C3-N2-Cu48	57	15	H4-C3-N2-Cu64	73	8	H4-C3-N2-Cu72	81	15
H4-C3-N2-Cu96	105	4	H4-C3-N2-O1	10	18	H4-C3-N2-O1-Cu36	46	7
H4-C3-N2-O1-Cu48	58	45	H4-C3-N2-O1-Cu60	70	2	H4-C3-N2-O1-Cu64	74	38
H4-C3-N2-O1-Cu72	82	13	H4-C3-N2-O1-Cu96	106	24	H4-C3-N2-O1-Cu120	130	1
H4-C3-N2-O2	11	39	H4-C3-N2-O3-Cu36	48	32	H4-C3-N4-O1	12	8
H4-C3-N4-O2	13	38	H4-C3-N4-O3	14	9	H4-C3-N6	13	10
H4-C4-Cu36	44	3	H4-C4-Cu48	56	1	H4-C4-Cu64	72	2
H4-C4-Cu72	80	2	H4-C4-Cu96	104	3	H4-C4-O1-Cu36	45	1
H4-C4-O1-Cu48	57	12	H4-C4-O1-Cu64	73	9	H4-C4-O1-Cu72	81	9
H4-C4-O1-Cu96	105	5	H4-C4-O2	10	6	H4-C4-O2-Cu36	46	4
H4-C4-O2-Cu48	58	23	H4-C4-O2-Cu60	70	2	H4-C4-O2-Cu64	74	27
H4-C4-O2-Cu72	82	13	H4-C4-O2-Cu80	90	1	H4-C4-O2-Cu96	106	21
H4-C4-O3	11	2	H4-C4-O4	12	5	H4-C4-O5	13	1
H4-C4-N2	10	10	H4-C4-N2-Cu36	46	1	H4-C4-N2-Cu48	58	18
H4-C4-N2-Cu60	70	3	H4-C4-N2-Cu64	74	11	H4-C4-N2-Cu72	82	12
H4-C4-N2-Cu80	90	2	H4-C4-N2-Cu96	106	7	H4-C4-N2-O1-Cu36	47	12
H4-C4-N2-O3	13	7	H4-C4-N2-O4	14	3	H4-C4-N2-O5	15	4
H4-C4-N4	12	2	H4-C4-N4-O1	13	24	H4-C4-N4-O2	14	4
H4-C4-N4-O3	15	48	H4-C4-N6-O1	15	3	H4-C5-Cu36	45	1
H4-C5-Cu48	57	3	H4-C5-Cu60	69	1	H4-C5-Cu64	73	1
H4-C5-Cu72	81	1	H4-C5-Cu80	89	1	H4-C5-Cu96	105	4
H4-C5-O1-Cu48	58	5	H4-C5-O1-Cu60	70	3	H4-C5-O1-Cu64	74	17
H4-C5-O1-Cu72	82	5	H4-C5-O1-Cu80	90	1	H4-C5-O1-Cu96	106	14
H4-C5-O1-Cu120	130	1	H4-C5-O2	11	3	H4-C5-O3	12	24
H4-C5-O4	13	26	H4-C5-N2-O1-Cu36	48	38	H4-C5-N2-O2	13	1
H4-C5-N4	13	8	H4-C5-N4-O2	15	1	H4-C5-N6-O4	19	1
H4-C5-N8-O4	21	6	H4-C5-N8-O5	22	18	H4-C6-Cu36	46	1
H4-C6-Cu48	58	3	H4-C6-Cu60	70	2	H4-C6-Cu64	74	4
H4-C6-Cu72	82	4	H4-C6-Cu96	106	7	H4-C6-Cu120	130	1
H4-C6-O1	11	7	H4-C6-O2	12	24	H4-C6-O3	13	48
H4-C6-N2	12	2	H4-C6-N2-O1	13	20	H4-C6-N2-O2	14	1
H4-C6-N2-O3	15	15	H4-C6-N4-O6	20	1	H4-C6-N4-O8	22	3
H4-C6-N6-O4	20	3	H4-C6-N6-O5	21	22	H4-C6-N6-O6	22	57
H4-C6-N8-O3	21	9	H4-C6-N8-O4	22	28	H4-C7	11	3
H4-C7-O1	12	6	H4-C7-O2	13	57	H4-C7-N6-O4	21	12
H4-C7-N8-O3	22	5	H4-C8-O1	13	25	H4-C8-N4-O5	21	3
H4-C8-N4-O6	22	15	H4-C8-N6-O3	21	6	H4-C8-N6-O4	22	30
H4-C9	13	1	H4-C10-N4-O4	22	9	H5-N1-Cu22	28	4
H5-N1-O1	7	63	H5-N2-Cu36	43	6	H5-N3-O1-Cu36	45	1
H5-N3-O1-Cu48	57	3	H5-N3-O1-Cu64	73	1	H5-N3-O1-Cu96	105	1
H5-N3-O2-Cu48	58	1	H5-N3-O2-Cu96	106	1	H5-N5-Cu18	28	8
H5-N5-Cu48	58	2	H5-N5-Cu60	70	1	H5-N5-Cu96	106	1
H5-C1-O2-Cu23	31	10	H5-C1-N1	7	70	H5-C1-N1-Cu36	43	26
H5-C1-N1-Cu72	79	1	H5-C1-N1-O1-Cu48	56	2	H5-C1-N1-O1-Cu72	80	2
H5-C1-N1-O2-Cu36	45	5	H5-C1-N1-O2-Cu48	57	2	H5-C1-N1-O2-Cu72	81	1
H5-C1-N1-O2-Cu96	105	1	H5-C1-N1-O3	10	4	H5-C1-N1-O3-Cu36	46	4
H5-C1-N1-O3-Cu48	58	5	H5-C1-N1-O4-Cu48	59	2	H5-C1-N3-Cu36	45	1
H5-C1-N3-Cu48	57	4	H5-C1-N3-Cu64	73	2	H5-C1-N3-Cu72	81	3
H5-C1-N3-Cu96	105	1	H5-C1-N3-O1-Cu36	46	2	H5-C1-N3-O1-Cu48	58	4
H5-C1-N3-O1-Cu64	74	2	H5-C1-N3-O1-Cu72	82	1	H5-C1-N3-O1-Cu96	106	4

H5-C1-N3-O2-Cu36	47	1	H5-C1-N3-O2-Cu48	59	7	H5-C1-N3-O2-Cu64	75	8
H5-C1-N3-O2-Cu72	83	1	H5-C1-N3-O2-Cu96	107	6	H5-C1-N5-Cu36	47	1
H5-C1-N5-Cu48	59	6	H5-C1-N5-Cu64	75	5	H5-C1-N5-Cu72	83	2
H5-C1-N5-Cu80	91	1	H5-C1-N5-Cu96	107	3	H5-C1-N5-Cu120	131	2
H5-C2-N1	8	165	H5-C2-N1-Cu48	56	2	H5-C2-N1-Cu64	72	1
H5-C2-N1-Cu72	80	2	H5-C2-N1-Cu96	104	1	H5-C2-N1-O1	9	184
H5-C2-N1-O1-Cu48	57	14	H5-C2-N1-O1-Cu64	73	3	H5-C2-N1-O1-Cu72	81	7
H5-C2-N1-O1-Cu96	105	6	H5-C2-N1-O2	10	71	H5-C2-N1-O2-Cu24	34	2
H5-C2-N1-O2-Cu27	37	1	H5-C2-N1-O2-Cu32	42	2	H5-C2-N1-O2-Cu36	46	19
H5-C2-N1-O2-Cu48	58	38	H5-C2-N1-O2-Cu54	64	9	H5-C2-N1-O2-Cu64	74	10
H5-C2-N1-O2-Cu72	82	15	H5-C2-N1-O2-Cu96	106	13	H5-C2-N1-O2-Cu144	154	7
H5-C2-N1-O3	11	54	H5-C2-N1-O3-Cu36	47	1	H5-C2-N1-O3-Cu48	59	17
H5-C2-N1-O3-Cu64	75	20	H5-C2-N1-O3-Cu72	83	7	H5-C2-N1-O3-Cu96	107	7
H5-C2-N3-Cu48	58	15	H5-C2-N3-Cu64	74	8	H5-C2-N3-Cu72	82	4
H5-C2-N3-Cu96	106	9	H5-C2-N3-O1	11	1	H5-C2-N3-O1-Cu36	47	6
H5-C2-N3-O1-Cu48	59	25	H5-C2-N3-O1-Cu64	75	20	H5-C2-N3-O1-Cu72	83	5
H5-C2-N3-O1-Cu96	107	12	H5-C2-N3-O1-Cu120	131	1	H5-C2-N5-O1	13	1
H5-C2-N7	14	3	H5-C3-N1-Cu36	45	2	H5-C3-N1-Cu48	57	7
H5-C3-N1-Cu64	73	6	H5-C3-N1-Cu72	81	5	H5-C3-N1-Cu96	105	2
H5-C3-N1-O1	10	46	H5-C3-N1-O1-Cu36	46	5	H5-C3-N1-O1-Cu48	58	35
H5-C3-N1-O1-Cu64	74	25	H5-C3-N1-O1-Cu72	82	26	H5-C3-N1-O1-Cu96	106	19
H5-C3-N1-O2	11	4	H5-C3-N1-O2-Cu36	47	8	H5-C3-N1-O2-Cu48	59	52
H5-C3-N1-O2-Cu60	71	1	H5-C3-N1-O2-Cu64	75	60	H5-C3-N1-O2-Cu72	83	19
H5-C3-N1-O2-Cu80	91	1	H5-C3-N1-O2-Cu96	107	45	H5-C3-N1-O3	12	8
H5-C3-N1-O3-Cu27	39	19	H5-C3-N1-O3-Cu36	48	115	H5-C3-N1-O3-Cu48	60	65
H5-C3-N1-O3-Cu54	66	239	H5-C3-N1-O3-Cu72	84	45	H5-C3-N1-O3-Cu144	156	11
H5-C3-N1-O3-Cu162	174	2	H5-C3-N3	11	1	H5-C3-N3-Cu36	47	1
H5-C3-N3-Cu48	59	28	H5-C3-N3-Cu60	71	5	H5-C3-N3-Cu64	75	21
H5-C3-N3-Cu72	83	15	H5-C3-N3-Cu80	91	3	H5-C3-N3-Cu96	107	19
H5-C3-N3-Cu120	131	2	H5-C3-N3-O1	12	4	H5-C3-N3-O2	13	5
H5-C3-N3-O9-Cu34	54	1	H5-C3-N3-O9-Cu36	56	88	H5-C3-N5	13	7
H5-C3-N5-O1	14	31	H5-C3-N5-O2	15	4	H5-C4-N1	10	9
H5-C4-N1-Cu36	46	4	H5-C4-N1-Cu48	58	14	H5-C4-N1-Cu60	70	1
H5-C4-N1-Cu64	74	9	H5-C4-N1-Cu72	82	7	H5-C4-N1-Cu96	106	15
H5-C4-N1-O1	11	2	H5-C4-N1-O1-Cu36	47	5	H5-C4-N1-O1-Cu48	59	45
H5-C4-N1-O1-Cu60	71	6	H5-C4-N1-O1-Cu64	75	72	H5-C4-N1-O1-Cu72	83	12
H5-C4-N1-O1-Cu80	91	1	H5-C4-N1-O1-Cu96	107	52	H5-C4-N1-O1-Cu120	131	3
H5-C4-N1-O2	12	28	H5-C4-N1-O3	13	2	H5-C4-N1-O4-Cu36	50	68
H5-C4-N1-O4-Cu48	62	81	H5-C4-N1-O4-Cu54	68	305	H5-C4-N1-O4-Cu72	86	47
H5-C4-N1-O4-Cu144	158	13	H5-C4-N1-O4-Cu162	176	2	H5-C4-N1-O6	16	10
H5-C4-N3	12	1	H5-C4-N3-O1	13	8	H5-C4-N3-O2	14	12
H5-C4-N3-O3	15	26	H5-C4-N3-O4	16	8	H5-C4-N5	14	28
H5-C4-N5-O2	16	22	H5-C5-N1	11	15	H5-C5-N1-Cu30	41	1
H5-C5-N1-Cu36	47	23	H5-C5-N1-Cu48	59	7	H5-C5-N1-Cu60	71	6
H5-C5-N1-Cu64	75	18	H5-C5-N1-Cu72	83	4	H5-C5-N1-Cu80	91	2
H5-C5-N1-Cu96	107	14	H5-C5-N1-Cu120	131	3	H5-C5-N1-O1	12	28
H5-C5-N1-O2	13	1	H5-C5-N1-O3	14	5	H5-C5-N3	13	5
H5-C5-N3-O1	14	17	H5-C5-N3-O2	15	2	H5-C5-N3-O3	16	28
H5-C5-N5	15	1	H5-C5-N5-O1	16	6	H5-C5-N9-O1	20	1
H5-C5-N9-O3	22	6	H5-C5-N9-O4	23	5	H5-C6-N1-O1	13	1
H5-C6-N1-O2	14	3	H5-C6-N3	14	6	H5-C6-N3-O2	16	2
H5-C6-N5-O7	23	25	H5-C6-N7-O3	21	1	H5-C6-N7-O4	22	9
H5-C6-N7-O5	23	67	H5-C6-N9-O2	22	9	H5-C7-N1	13	2
H5-C7-N1-O1	14	1	H5-C7-N1-O3	16	9	H5-C7-N1-O5-Cu35	53	1
H5-C7-N1-O5-Cu36	54	29	H5-C7-N3-O1	16	3	H5-C7-N5-O5	22	15
H5-C7-N5-O6	23	23	H5-C7-N7-O3	22	22	H5-C7-N7-O4	23	23
H5-C8-N1-O2	16	11	H5-C8-N5-O4	22	7	H5-C8-N5-O5	23	44
H5-C9-N3-O6	23	6	H5-C9-N5-O3	22	5	H5-C9-N5-O4	23	28
H6-O3	9	10	H6-N2-Cu36	44	16	H6-N3-Cu32	41	5
H6-N4-Cu96	106	1	H6-N4-O1-Cu72	83	1	H6-N4-O2-Cu48	60	1
H6-N6-Cu48	60	2	H6-N6-Cu120	132	1	H6-C1-O1-Cu27	35	570

H6-C1-O2-Cu27	36	3245	H6-C1-O3-Cu12	22	2636	H6-C1-N2-Cu48	57	2
H6-C1-N2-O1-Cu36	46	1	H6-C1-N2-O1-Cu48	58	4	H6-C1-N2-O1-Cu72	82	2
H6-C1-N2-O1-Cu96	106	2	H6-C1-N2-O2-Cu36	47	2	H6-C1-N2-O2-Cu48	59	8
H6-C1-N2-O2-Cu64	75	5	H6-C1-N2-O2-Cu72	83	2	H6-C1-N2-O2-Cu96	107	4
H6-C1-N2-O3-Cu48	60	1	H6-C1-N2-O3-Cu64	76	2	H6-C1-N2-O3-Cu96	108	2
H6-C1-N4-Cu48	59	2	H6-C1-N4-Cu60	71	1	H6-C1-N4-Cu64	75	4
H6-C1-N4-Cu72	83	3	H6-C1-N4-Cu96	107	5	H6-C1-N4-O1-Cu48	60	3
H6-C1-N4-O1-Cu64	76	4	H6-C1-N4-O1-Cu72	84	2	H6-C1-N4-O1-Cu96	108	1
H6-C2	8	304	H6-C2-O1	9	61	H6-C2-O2-Cu48	58	2
H6-C2-O2-Cu72	82	1	H6-C2-O3-Cu36	47	2548	H6-C2-O3-Cu48	59	7
H6-C2-O3-Cu64	75	2	H6-C2-O3-Cu72	83	1	H6-C2-O3-Cu80	91	1
H6-C2-O3-Cu96	107	2	H6-C2-O4-Cu48	60	1	H6-C2-O4-Cu64	76	3
H6-C2-O4-Cu72	84	3	H6-C2-O4-Cu96	108	3	H6-C2-N2-Cu36	46	2
H6-C2-N2-Cu48	58	11	H6-C2-N2-Cu64	74	6	H6-C2-N2-Cu72	82	5
H6-C2-N2-Cu96	106	4	H6-C2-N2-O1-Cu32	43	2	H6-C2-N2-O1-Cu34	45	8
H6-C2-N2-O1-Cu36	47	56	H6-C2-N2-O1-Cu48	59	18	H6-C2-N2-O1-Cu60	71	2
H6-C2-N2-O1-Cu64	75	21	H6-C2-N2-O1-Cu72	83	6	H6-C2-N2-O1-Cu96	107	16
H6-C2-N2-O2-Cu36	48	133	H6-C2-N2-O2-Cu48	60	26	H6-C2-N2-O2-Cu60	72	1
H6-C2-N2-O2-Cu64	76	37	H6-C2-N2-O2-Cu72	84	10	H6-C2-N2-O2-Cu80	92	1
H6-C2-N2-O2-Cu96	108	28	H6-C2-N2-O2-Cu120	132	2	H6-C2-N2-O4-Cu66	80	2
H6-C2-N4-Cu48	60	17	H6-C2-N4-Cu60	72	3	H6-C2-N4-Cu64	76	25
H6-C2-N4-Cu72	84	9	H6-C2-N4-Cu80	92	3	H6-C2-N4-Cu96	108	16
H6-C2-N4-Cu120	132	8	H6-C3	9	94	H6-C3-Cu36	45	1
H6-C3-Cu48	57	1	H6-C3-Cu72	81	2	H6-C3-O1	10	2
H6-C3-O1-Cu36	46	1	H6-C3-O1-Cu48	58	45	H6-C3-O1-Cu64	74	723
H6-C3-O1-Cu72	82	1	H6-C3-O1-Cu96	106	3	H6-C3-O2	11	60
H6-C3-O2-Cu36	47	2	H6-C3-O2-Cu48	59	25	H6-C3-O2-Cu64	75	14
H6-C3-O2-Cu72	83	5	H6-C3-O2-Cu80	91	1	H6-C3-O2-Cu96	107	13
H6-C3-O3-Cu48	60	28	H6-C3-O3-Cu64	76	28	H6-C3-O3-Cu72	84	6
H6-C3-O3-Cu96	108	26	H6-C3-N1-O2-Cu27	39	77	H6-C3-N1-O2-Cu36	48	70
H6-C3-N1-O2-Cu48	60	51	H6-C3-N1-O2-Cu54	66	186	H6-C3-N1-O2-Cu72	84	15
H6-C3-N1-O2-Cu144	156	11	H6-C3-N1-O2-Cu162	174	2	H6-C3-N1-O3-Cu36	49	27
H6-C3-N1-O3-Cu48	61	20	H6-C3-N1-O3-Cu54	67	20	H6-C3-N1-O3-Cu72	85	11
H6-C3-N1-O3-Cu96	109	2	H6-C3-N1-O3-Cu144	157	21	H6-C3-N2-Cu32	43	3
H6-C3-N2-Cu33	44	1	H6-C3-N2-Cu36	47	97	H6-C3-N2-Cu48	59	21
H6-C3-N2-Cu60	71	1	H6-C3-N2-Cu64	75	23	H6-C3-N2-Cu72	83	9
H6-C3-N2-Cu80	91	1	H6-C3-N2-Cu96	107	26	H6-C3-N2-O1-Cu32	44	2
H6-C3-N2-O1-Cu36	48	71	H6-C3-N2-O1-Cu48	60	50	H6-C3-N2-O1-Cu60	72	2
H6-C3-N2-O1-Cu64	76	92	H6-C3-N2-O1-Cu72	84	27	H6-C3-N2-O1-Cu80	92	2
H6-C3-N2-O1-Cu96	108	67	H6-C3-N2-O1-Cu120	132	7	H6-C3-N4	13	3
H6-C3-N4-O1	14	9	H6-C3-N6	15	12	H6-C3-N6-O6	21	1
H6-C4-Cu48	58	3	H6-C4-Cu64	74	3	H6-C4-Cu72	82	2
H6-C4-Cu96	106	3	H6-C4-O1-Cu36	47	4	H6-C4-O1-Cu48	59	17
H6-C4-O1-Cu64	75	100	H6-C4-O1-Cu72	83	9	H6-C4-O1-Cu96	107	16
H6-C4-O2	12	1	H6-C4-O2-Cu36	48	3	H6-C4-O2-Cu48	60	47
H6-C4-O2-Cu60	72	6	H6-C4-O2-Cu64	76	275	H6-C4-O2-Cu72	84	11
H6-C4-O2-Cu80	92	6	H6-C4-O2-Cu96	108	49	H6-C4-O2-Cu120	132	4
H6-C4-O3	13	5	H6-C4-O4	14	3	H6-C4-N1-O4-Cu36	51	41
H6-C4-N1-O4-Cu48	63	48	H6-C4-N1-O4-Cu54	69	40	H6-C4-N1-O4-Cu64	79	8
H6-C4-N1-O4-Cu72	87	32	H6-C4-N1-O4-Cu96	111	1	H6-C4-N1-O4-Cu144	159	34
H6-C4-N1-O4-Cu162	177	5	H6-C4-N2-Cu31	43	2	H6-C4-N2-Cu36	48	71
H6-C4-N2-Cu48	60	31	H6-C4-N2-Cu60	72	3	H6-C4-N2-Cu64	76	75
H6-C4-N2-Cu72	84	25	H6-C4-N2-Cu80	92	7	H6-C4-N2-Cu96	108	58
H6-C4-N2-Cu120	132	5	H6-C4-N2-O1	13	1	H6-C4-N2-O3	15	1
H6-C4-N2-O4	16	3	H6-C4-N4	14	7	H6-C4-N4-O2	16	36
H6-C4-N4-O3	17	41	H6-C5-Cu36	47	1	H6-C5-Cu48	59	8
H6-C5-Cu60	71	1	H6-C5-Cu64	75	11	H6-C5-Cu80	91	2
H6-C5-Cu96	107	12	H6-C5-O1-Cu36	48	1	H6-C5-O1-Cu48	60	15
H6-C5-O1-Cu60	72	8	H6-C5-O1-Cu64	76	50	H6-C5-O1-Cu72	84	8
H6-C5-O1-Cu80	92	7	H6-C5-O1-Cu96	108	41	H6-C5-O1-Cu120	132	4
H6-C5-O2	13	18	H6-C5-O3	14	44	H6-C5-O4	15	52

H6-C5-N2-O1	14	16	H6-C5-N2-O2	15	9	H6-C5-N2-O4	17	6
H6-C5-N4	15	41	H6-C5-N4-O2	17	17	H6-C5-N10-O2	23	3
H6-C6	12	83	H6-C6-Cu36	48	3	H6-C6-Cu48	60	12
H6-C6-Cu60	72	4	H6-C6-Cu64	76	23	H6-C6-Cu72	84	11
H6-C6-Cu80	92	7	H6-C6-Cu96	108	25	H6-C6-Cu120	132	3
H6-C6-O1	13	439	H6-C6-O2	14	78	H6-C6-O3	15	30
H6-C6-N2	14	2	H6-C6-N2-O1	15	25	H6-C6-N2-O2	16	7
H6-C6-N2-O3	17	1	H6-C6-N2-O4	18	48	H6-C6-N4-O1	17	26
H6-C6-N6-O5	23	8	H6-C6-N6-O6	24	48	H6-C6-N8-O3	23	12
H6-C6-N8-O4	24	46	H6-C6-N10-O1	23	5	H6-C6-N10-O2	24	4
H6-C7-O1	14	8	H6-C7-O2	15	19	H6-C7-O4	17	3
H6-C7-N2	15	7	H6-C7-N2-O2	17	18	H6-C7-N4-O7	24	4
H6-C7-N6-O4	23	56	H6-C7-N6-O5	24	155	H6-C7-N8-O2	23	5
H6-C7-N8-O3	24	14	H6-C8	14	3	H6-C8-O1	15	7
H6-C8-N2-O1	17	16	H6-C8-N2-O2	18	3	H6-C8-N4-O4	22	4
H6-C8-N4-O5	23	6	H6-C8-N4-O6	24	15	H6-C8-N6-O4	24	45
H6-C9	15	2	H6-C9-N2-O7	24	4	H6-C9-N4-O4	23	14
H6-C9-N4-O5	24	79	H6-C9-N6-O2	23	11	H6-C9-N6-O3	24	57
H6-C10-N2-O2	20	3	H6-C10-N4-O4	24	6	H6-C10-N6-O2	24	6
H6-C11-N2-O5	24	6	H6-C11-N4-O3	24	13	H7-N2-Cu35	44	4
H7-N2-Cu36	45	21	H7-N5-O1-Cu36	49	1	H7-N5-O1-Cu96	109	1
H7-N5-O1-Cu120	133	1	H7-C1-N3-Cu48	59	2	H7-C1-N3-Cu96	107	1
H7-C1-N3-O1-Cu96	108	3	H7-C1-N5-Cu48	61	1	H7-C1-N5-Cu72	85	1
H7-C1-N5-Cu80	93	1	H7-C1-N5-Cu96	109	2	H7-C1-N5-Cu120	133	1
H7-C2-N1-Cu36	46	2	H7-C2-N1-Cu48	58	2	H7-C2-N1-Cu64	74	1
H7-C2-N1-O1	11	12	H7-C2-N1-O1-Cu36	47	2	H7-C2-N1-O1-Cu48	59	9
H7-C2-N1-O1-Cu64	75	1	H7-C2-N1-O1-Cu96	107	1	H7-C2-N1-O2	12	3
H7-C2-N1-O2-Cu36	48	2	H7-C2-N1-O2-Cu48	60	16	H7-C2-N1-O2-Cu64	76	8
H7-C2-N1-O2-Cu72	84	5	H7-C2-N1-O2-Cu96	108	8	H7-C2-N1-O3-Cu36	49	3
H7-C2-N1-O3-Cu48	61	9	H7-C2-N1-O3-Cu64	77	7	H7-C2-N1-O3-Cu72	85	1
H7-C2-N1-O3-Cu96	109	10	H7-C2-N1-O3-Cu120	133	1	H7-C2-N3-Cu36	48	1
H7-C2-N3-Cu48	60	5	H7-C2-N3-Cu64	76	14	H7-C2-N3-Cu72	84	5
H7-C2-N3-Cu80	92	1	H7-C2-N3-Cu96	108	13	H7-C2-N3-Cu120	132	2
H7-C2-N3-O1-Cu36	49	1	H7-C2-N3-O1-Cu48	61	9	H7-C2-N3-O1-Cu60	73	2
H7-C2-N3-O1-Cu64	77	20	H7-C2-N3-O1-Cu72	85	10	H7-C2-N3-O1-Cu80	93	2
H7-C2-N3-O1-Cu96	109	12	H7-C2-N3-O1-Cu120	133	1	H7-C3-N1	11	22
H7-C3-N1-Cu48	59	4	H7-C3-N1-Cu64	75	7	H7-C3-N1-Cu72	83	1
H7-C3-N1-Cu96	107	3	H7-C3-N1-O1-Cu36	48	4	H7-C3-N1-O1-Cu48	60	24
H7-C3-N1-O1-Cu60	72	1	H7-C3-N1-O1-Cu64	76	46	H7-C3-N1-O1-Cu72	84	15
H7-C3-N1-O1-Cu96	108	31	H7-C3-N1-O1-Cu120	132	1	H7-C3-N1-O2	13	38
H7-C3-N1-O2-Cu27	40	2	H7-C3-N1-O2-Cu32	45	2	H7-C3-N1-O2-Cu36	49	49
H7-C3-N1-O2-Cu48	61	83	H7-C3-N1-O2-Cu54	67	18	H7-C3-N1-O2-Cu60	73	2
H7-C3-N1-O2-Cu64	77	56	H7-C3-N1-O2-Cu72	85	27	H7-C3-N1-O2-Cu80	93	3
H7-C3-N1-O2-Cu96	109	54	H7-C3-N1-O2-Cu120	133	2	H7-C3-N1-O2-Cu144	157	12
H7-C3-N1-O2-Cu162	175	2	H7-C3-N1-O3	14	33	H7-C3-N1-O3-Cu36	50	21
H7-C3-N1-O3-Cu48	62	20	H7-C3-N1-O3-Cu54	68	20	H7-C3-N1-O3-Cu64	78	3
H7-C3-N1-O3-Cu72	86	13	H7-C3-N1-O3-Cu96	110	3	H7-C3-N1-O3-Cu144	158	15
H7-C3-N3-Cu48	61	24	H7-C3-N3-Cu60	73	6	H7-C3-N3-Cu64	77	59
H7-C3-N3-Cu72	85	16	H7-C3-N3-Cu80	93	13	H7-C3-N3-Cu96	109	46
H7-C3-N3-Cu120	133	8	H7-C3-N3-O2	15	1	H7-C3-N5	15	5
H7-C3-N5-O1	16	2	H7-C4-N1	12	13	H7-C4-N1-Cu36	48	1
H7-C4-N1-Cu48	60	15	H7-C4-N1-Cu64	76	28	H7-C4-N1-Cu72	84	6
H7-C4-N1-Cu80	92	3	H7-C4-N1-Cu96	108	18	H7-C4-N1-Cu120	132	4
H7-C4-N1-O1-Cu36	49	4	H7-C4-N1-O1-Cu48	61	56	H7-C4-N1-O1-Cu60	73	9
H7-C4-N1-O1-Cu64	77	145	H7-C4-N1-O1-Cu72	85	24	H7-C4-N1-O1-Cu80	93	16
H7-C4-N1-O1-Cu96	109	106	H7-C4-N1-O1-Cu120	133	15	H7-C4-N1-O2	14	11
H7-C4-N1-O3-Cu27	42	28	H7-C4-N1-O3-Cu36	51	65	H7-C4-N1-O3-Cu48	63	57
H7-C4-N1-O3-Cu54	69	118	H7-C4-N1-O3-Cu64	79	8	H7-C4-N1-O3-Cu72	87	25
H7-C4-N1-O3-Cu96	111	5	H7-C4-N1-O3-Cu144	159	20	H7-C4-N1-O3-Cu162	177	3
H7-C4-N1-O4	16	35	H7-C4-N1-O4-Cu36	52	17	H7-C4-N1-O4-Cu48	64	24
H7-C4-N1-O4-Cu54	70	20	H7-C4-N1-O4-Cu64	80	7	H7-C4-N1-O4-Cu72	88	7

H7-C4-N1-O4-Cu96	112	5	H7-C4-N1-O4-Cu144	160	15	H7-C4-N1-O4-Cu162	178	2
H7-C4-N2-O3-Cu36	52	27	H7-C4-N2-O3-Cu48	64	95	H7-C4-N2-O3-Cu54	70	285
H7-C4-N2-O3-Cu64	80	6	H7-C4-N2-O3-Cu72	88	49	H7-C4-N2-O3-Cu96	112	5
H7-C4-N2-O3-Cu144	160	20	H7-C4-N3	14	2	H7-C4-N3-O1	15	13
H7-C4-N3-O2	16	6	H7-C4-N3-O3	17	11	H7-C4-N5	16	28
H7-C4-N5-O1	17	3	H7-C4-N5-O2	18	5	H7-C5-N1	13	1
H7-C5-N1-Cu36	49	2	H7-C5-N1-Cu48	61	30	H7-C5-N1-Cu60	73	8
H7-C5-N1-Cu64	77	91	H7-C5-N1-Cu72	85	17	H7-C5-N1-Cu80	93	10
H7-C5-N1-Cu96	109	49	H7-C5-N1-Cu120	133	9	H7-C5-N1-O1	14	1
H7-C5-N1-O2	15	4	H7-C5-N1-O3	16	16	H7-C5-N1-O4-Cu36	53	25
H7-C5-N1-O4-Cu48	65	75	H7-C5-N1-O4-Cu54	71	345	H7-C5-N1-O4-Cu64	81	32
H7-C5-N1-O4-Cu72	89	49	H7-C5-N1-O4-Cu96	113	2	H7-C5-N1-O4-Cu144	161	13
H7-C5-N1-O4-Cu162	179	1	H7-C5-N3	15	6	H7-C5-N3-O1	16	24
H7-C5-N3-O1-Cu31	47	1	H7-C5-N3-O1-Cu36	52	32	H7-C5-N3-O2	17	2
H7-C5-N3-O3	18	7	H7-C5-N5-O1	18	12	H7-C5-N9-O2	23	6
H7-C6-N1	14	2	H7-C6-N1-O1	15	17	H7-C6-N1-O2	16	33
H7-C6-N1-O3	17	1	H7-C6-N3	16	25	H7-C6-N3-O2	18	44
H7-C6-N5-O5	23	3	H7-C6-N7-O4	24	9	H7-C6-N7-O5	25	51
H7-C6-N9-O2	24	10	H7-C7-N1	15	1	H7-C7-N1-O1	16	24
H7-C7-N1-O3	18	7	H7-C7-N3-O1	18	4	H7-C7-N5-O4	23	12
H7-C7-N5-O5	24	19	H7-C7-N5-O6	25	37	H7-C7-N7-O3	24	20
H7-C7-N7-O4	25	76	H7-C7-N9-O1	24	5	H7-C7-N9-O2	25	8
H7-C8-N1	16	7	H7-C8-N1-O2	18	23	H7-C8-N3	18	33
H7-C8-N3-O1	19	1	H7-C8-N5-O3	23	1	H7-C8-N5-O4	24	42
H7-C8-N5-O5	25	86	H7-C8-N7-O2	24	28	H7-C8-N7-O3	25	75
H7-C9-N1-O2	19	5	H7-C9-N3-O5	24	1	H7-C9-N3-O6	25	19
H7-C9-N5-O2	23	8	H7-C9-N5-O3	24	11	H7-C9-N5-O4	25	38
H7-C9-N7-O2	25	5	H7-C10-N3-O5	25	40	H7-C10-N5-O2	24	6
H7-C10-N5-O3	25	49	H7-C11-N1-O5	24	2	H7-C11-N3-O4	25	8
H7-C12-N3-O3	25	7	H8-N2-Cu35	45	3	H8-N6-Cu48	62	2
H8-C1-O2-Cu27	38	20	H8-C1-N2-Cu36	47	1	H8-C1-N4-Cu48	61	2
H8-C1-N4-Cu64	77	2	H8-C1-N4-Cu72	85	2	H8-C1-N4-O1-Cu64	78	1
H8-C1-N4-O1-Cu96	110	1	H8-C2	10	1	H8-C2-O2	12	7
H8-C2-O2-Cu23	35	42	H8-C2-O2-Cu24	36	98	H8-C2-O3	13	6
H8-C2-N2-Cu48	60	1	H8-C2-N2-Cu96	108	2	H8-C2-N2-O1-Cu48	61	9
H8-C2-N2-O1-Cu64	77	14	H8-C2-N2-O1-Cu72	85	6	H8-C2-N2-O1-Cu96	109	7
H8-C2-N2-O2-Cu48	62	6	H8-C2-N2-O2-Cu64	78	15	H8-C2-N2-O2-Cu72	86	6
H8-C2-N2-O2-Cu80	94	1	H8-C2-N2-O2-Cu96	110	12	H8-C2-N2-O2-Cu120	134	1
H8-C2-N4-Cu48	62	4	H8-C2-N4-Cu60	74	3	H8-C2-N4-Cu64	78	16
H8-C2-N4-Cu72	86	4	H8-C2-N4-Cu80	94	2	H8-C2-N4-Cu96	110	10
H8-C2-N4-Cu120	134	1	H8-C2-N4-O2	16	5	H8-C3	11	5
H8-C3-Cu72	83	1	H8-C3-O1-Cu48	60	1	H8-C3-O1-Cu64	76	1
H8-C3-O1-Cu72	84	1	H8-C3-O2-Cu36	49	1	H8-C3-O2-Cu48	61	3
H8-C3-O2-Cu64	77	2	H8-C3-O2-Cu96	109	2	H8-C3-O3	14	2
H8-C3-O3-Cu48	62	3	H8-C3-O3-Cu64	78	7	H8-C3-O3-Cu72	86	6
H8-C3-O3-Cu80	94	1	H8-C3-O3-Cu96	110	6	H8-C3-N2-Cu36	49	1
H8-C3-N2-Cu48	61	16	H8-C3-N2-Cu60	73	2	H8-C3-N2-Cu64	77	30
H8-C3-N2-Cu72	85	9	H8-C3-N2-Cu80	93	2	H8-C3-N2-Cu96	109	28
H8-C3-N2-Cu120	133	2	H8-C3-N2-O1-Cu36	50	1	H8-C3-N2-O1-Cu48	62	28
H8-C3-N2-O1-Cu60	74	5	H8-C3-N2-O1-Cu64	78	77	H8-C3-N2-O1-Cu72	86	23
H8-C3-N2-O1-Cu80	94	9	H8-C3-N2-O1-Cu96	110	56	H8-C3-N2-O1-Cu120	134	4
H8-C4-Cu36	48	2	H8-C4-Cu48	60	1	H8-C4-Cu64	76	3
H8-C4-Cu72	84	2	H8-C4-Cu96	108	3	H8-C4-O1	13	4
H8-C4-O1-Cu48	61	10	H8-C4-O1-Cu60	73	1	H8-C4-O1-Cu64	77	16
H8-C4-O1-Cu72	85	2	H8-C4-O1-Cu80	93	1	H8-C4-O1-Cu96	109	7
H8-C4-O2-Cu36	50	1	H8-C4-O2-Cu48	62	21	H8-C4-O2-Cu60	74	3
H8-C4-O2-Cu64	78	61	H8-C4-O2-Cu72	86	9	H8-C4-O2-Cu80	94	11
H8-C4-O2-Cu96	110	56	H8-C4-O2-Cu120	134	1	H8-C4-N1-O3-Cu36	52	20
H8-C4-N1-O3-Cu48	64	18	H8-C4-N1-O3-Cu54	70	20	H8-C4-N1-O3-Cu64	80	3
H8-C4-N1-O3-Cu72	88	17	H8-C4-N1-O3-Cu96	112	2	H8-C4-N1-O3-Cu144	160	15
H8-C4-N2-Cu36	50	2	H8-C4-N2-Cu48	62	32	H8-C4-N2-Cu60	74	10

H8-C4-N2-Cu64	78	120	H8-C4-N2-Cu72	86	19	H8-C4-N2-Cu80	94	26
H8-C4-N2-Cu96	110	97	H8-C4-N2-Cu120	134	15	H8-C4-N2-O3	17	34
H8-C4-N2-O3-Cu36	53	8	H8-C4-N2-O3-Cu48	65	28	H8-C4-N2-O3-Cu54	71	20
H8-C4-N2-O3-Cu64	81	8	H8-C4-N2-O3-Cu72	89	6	H8-C4-N2-O3-Cu96	113	10
H8-C4-N2-O3-Cu144	161	13	H8-C4-N2-O3-Cu162	179	1	H8-C4-N4	16	8
H8-C4-N4-O1	17	30	H8-C4-N4-O2	18	10	H8-C5-Cu48	61	4
H8-C5-Cu60	73	1	H8-C5-Cu64	77	11	H8-C5-Cu72	85	2
H8-C5-Cu80	93	1	H8-C5-Cu96	109	9	H8-C5-O1	14	171
H8-C5-O1-Cu36	50	1	H8-C5-O1-Cu48	62	28	H8-C5-O1-Cu60	74	11
H8-C5-O1-Cu64	78	95	H8-C5-O1-Cu72	86	8	H8-C5-O1-Cu80	94	13
H8-C5-O1-Cu96	110	78	H8-C5-O1-Cu120	134	8	H8-C5-O3	16	11
H8-C5-O4	17	15	H8-C5-N1-O2-Cu27	43	12	H8-C5-N1-O2-Cu36	52	43
H8-C5-N1-O2-Cu48	64	56	H8-C5-N1-O2-Cu54	70	274	H8-C5-N1-O2-Cu72	88	27
H8-C5-N1-O2-Cu96	112	5	H8-C5-N1-O2-Cu144	160	15	H8-C5-N1-O2-Cu162	178	1
H8-C5-N1-O4-Cu36	54	4	H8-C5-N1-O4-Cu48	66	54	H8-C5-N1-O4-Cu54	72	39
H8-C5-N1-O4-Cu64	82	15	H8-C5-N1-O4-Cu72	90	36	H8-C5-N1-O4-Cu96	114	11
H8-C5-N1-O4-Cu108	126	1	H8-C5-N1-O4-Cu144	162	27	H8-C5-N1-O4-Cu162	180	5
H8-C5-N2-O1	16	1	H8-C5-N2-O2	17	5	H8-C5-N2-O3	18	3
H8-C5-N4	17	24	H8-C5-N4-O2	19	21	H8-C5-N10-O2	25	3
H8-C6-Cu36	50	4	H8-C6-Cu48	62	15	H8-C6-Cu60	74	4
H8-C6-Cu64	78	48	H8-C6-Cu72	86	7	H8-C6-Cu80	94	16
H8-C6-Cu96	110	44	H8-C6-Cu120	134	10	H8-C6-O1	15	9
H8-C6-O2	16	10	H8-C6-O3	17	28	H8-C6-N2	16	2
H8-C6-N2-O1	17	17	H8-C6-N2-O2	18	10	H8-C6-N2-O3	19	38
H8-C6-N3-O2-Cu36	55	22	H8-C6-N3-O2-Cu48	67	78	H8-C6-N3-O2-Cu54	73	181
H8-C6-N3-O2-Cu64	83	35	H8-C6-N3-O2-Cu72	91	15	H8-C6-N3-O2-Cu96	115	22
H8-C6-N3-O2-Cu144	163	13	H8-C6-N3-O2-Cu162	181	2	H8-C6-N4-Cu62	80	3
H8-C6-N4-Cu66	84	1	H8-C6-N4-O1	19	9	H8-C6-N6-O5	25	5
H8-C6-N6-O6	26	20	H8-C6-N8-O2	24	1	H8-C6-N8-O3	25	2
H8-C6-N8-O4	26	5	H8-C6-N10-O1	25	4	H8-C7	15	3
H8-C7-O1	16	11	H8-C7-O2	17	60	H8-C7-O3	18	7
H8-C7-N2	17	29	H8-C7-N2-O2	19	27	H8-C7-N2-O3	20	3
H8-C7-N4	19	38	H8-C7-N4-O7	26	8	H8-C7-N6-O3	24	10
H8-C7-N6-O4	25	25	H8-C7-N6-O5	26	87	H8-C7-N8-O3	26	9
H8-C8	16	7	H8-C8-O1	17	56	H8-C8-O2	18	2
H8-C8-O3	19	8	H8-C8-N2	18	2	H8-C8-N2-O1	19	27
H8-C8-N4-O5	25	19	H8-C8-N4-O6	26	56	H8-C8-N6-O3	25	11
H8-C8-N6-O4	26	113	H8-C8-N8-O2	26	1	H8-C9	17	22
H8-C9-O3	20	74	H8-C9-N2	19	4	H8-C9-N2-O1	20	2
H8-C9-N2-O2	21	6	H8-C9-N2-O7	26	4	H8-C9-N4-O4	25	2
H8-C9-N4-O5	26	56	H8-C9-N6-O1	24	3	H8-C9-N6-O2	25	5
H8-C9-N6-O3	26	54	H8-C10-N2	20	3	H8-C10-N2-O1	21	9
H8-C10-N2-O3	23	2	H8-C10-N2-O4	24	2	H8-C10-N2-O5	25	2
H8-C10-N2-O6	26	21	H8-C10-N4-O3	25	9	H8-C10-N4-O4	26	116
H8-C10-N6-O2	26	24	H8-C11-N2-O1	22	3	H8-C11-N2-O2	23	1
H8-C11-N2-O4	25	3	H8-C11-N2-O5	26	7	H8-C11-N4-O2	25	16
H8-C11-N4-O3	26	21	H8-C12-O6	26	2	H8-C12-N2-O2	24	5
H8-C12-N2-O4	26	19	H8-C12-N4-O2	26	9	H8-C14-N2-O4	28	2
H9-N2-Cu20	31	5	H9-N3-Cu19	31	1	H9-N3-Cu36	48	13
H9-C1-N5-Cu48	63	1	H9-C1-N5-Cu96	111	1	H9-C2-N3-Cu36	50	1
H9-C2-N3-Cu48	62	2	H9-C2-N3-Cu64	78	14	H9-C2-N3-Cu72	86	1
H9-C2-N3-Cu80	94	1	H9-C2-N3-Cu96	110	5	H9-C2-N3-Cu120	134	2
H9-C2-N3-O1-Cu36	51	1	H9-C2-N3-O1-Cu48	63	3	H9-C2-N3-O1-Cu64	79	12
H9-C2-N3-O1-Cu72	87	1	H9-C2-N3-O1-Cu96	111	12	H9-C2-N3-O1-Cu120	135	1
H9-C3-N1-Cu36	49	47	H9-C3-N1-Cu48	61	1	H9-C3-N1-O1	14	6
H9-C3-N1-O1-Cu36	50	1	H9-C3-N1-O1-Cu48	62	12	H9-C3-N1-O1-Cu64	78	13
H9-C3-N1-O1-Cu96	110	10	H9-C3-N1-O1-Cu120	134	1	H9-C3-N1-O2-Cu48	63	21
H9-C3-N1-O2-Cu60	75	5	H9-C3-N1-O2-Cu64	79	29	H9-C3-N1-O2-Cu72	87	7
H9-C3-N1-O2-Cu80	95	1	H9-C3-N1-O2-Cu96	111	29	H9-C3-N1-O2-Cu120	135	1
H9-C3-N1-O3-Cu36	52	190	H9-C3-N3-Cu48	63	3	H9-C3-N3-Cu60	75	4
H9-C3-N3-Cu64	79	42	H9-C3-N3-Cu72	87	3	H9-C3-N3-Cu80	95	12

H9-C3-N3-Cu96	111	43	H9-C3-N3-Cu120	135	3	H9-C4-N1-Cu48	62	9
H9-C4-N1-Cu60	74	1	H9-C4-N1-Cu64	78	22	H9-C4-N1-Cu72	86	2
H9-C4-N1-Cu80	94	1	H9-C4-N1-Cu96	110	15	H9-C4-N1-Cu120	134	1
H9-C4-N1-O1-Cu36	51	2	H9-C4-N1-O1-Cu48	63	40	H9-C4-N1-O1-Cu60	75	10
H9-C4-N1-O1-Cu64	79	162	H9-C4-N1-O1-Cu72	87	18	H9-C4-N1-O1-Cu80	95	27
H9-C4-N1-O1-Cu96	111	96	H9-C4-N1-O1-Cu120	135	22	H9-C4-N1-O3	17	41
H9-C4-N1-O3-Cu36	53	10	H9-C4-N1-O3-Cu48	65	25	H9-C4-N1-O3-Cu54	71	20
H9-C4-N1-O3-Cu64	81	5	H9-C4-N1-O3-Cu72	89	15	H9-C4-N1-O3-Cu96	113	5
H9-C4-N1-O3-Cu144	161	11	H9-C4-N5	18	9	H9-C4-N5-O1	19	1
H9-C5-N1	15	14	H9-C5-N1-Cu36	51	1	H9-C5-N1-Cu48	63	25
H9-C5-N1-Cu60	75	11	H9-C5-N1-Cu64	79	133	H9-C5-N1-Cu72	87	18
H9-C5-N1-Cu80	95	27	H9-C5-N1-Cu96	111	109	H9-C5-N1-Cu120	135	16
H9-C5-N1-O1	16	1	H9-C5-N1-O2	17	48	H9-C5-N1-O2-Cu36	53	10
H9-C5-N1-O2-Cu48	65	32	H9-C5-N1-O2-Cu54	71	20	H9-C5-N1-O2-Cu64	81	4
H9-C5-N1-O2-Cu72	89	9	H9-C5-N1-O2-Cu96	113	5	H9-C5-N1-O2-Cu144	161	13
H9-C5-N1-O2-Cu162	179	3	H9-C5-N1-O3	18	2	H9-C5-N1-O4	19	35
H9-C5-N1-O4-Cu36	55	3	H9-C5-N1-O4-Cu48	67	21	H9-C5-N1-O4-Cu54	73	20
H9-C5-N1-O4-Cu64	83	10	H9-C5-N1-O4-Cu72	91	21	H9-C5-N1-O4-Cu96	115	5
H9-C5-N1-O4-Cu144	163	18	H9-C5-N1-O4-Cu162	181	3	H9-C5-N2-O3-Cu48	67	62
H9-C5-N2-O3-Cu54	73	331	H9-C5-N2-O3-Cu64	83	31	H9-C5-N2-O3-Cu72	91	51
H9-C5-N2-O3-Cu96	115	26	H9-C5-N2-O3-Cu144	163	15	H9-C5-N2-O3-Cu162	181	3
H9-C5-N3	17	7	H9-C5-N3-O1	18	25	H9-C5-N3-O2	19	4
H9-C5-N3-O3	20	27	H9-C6-N1	16	37	H9-C6-N1-O1	17	16
H9-C6-N1-O2	18	9	H9-C6-N1-O2-Cu36	54	29	H9-C6-N1-O3	19	8
H9-C6-N1-O4	20	6	H9-C6-N3	18	20	H9-C6-N3-O1	19	15
H9-C6-N3-O2	20	87	H9-C6-N3-O2-Cu36	56	1	H9-C6-N3-O2-Cu48	68	21
H9-C6-N3-O2-Cu54	74	19	H9-C6-N3-O2-Cu60	80	4	H9-C6-N3-O2-Cu64	84	11
H9-C6-N3-O2-Cu72	92	12	H9-C6-N3-O2-Cu80	100	2	H9-C6-N3-O2-Cu96	116	9
H9-C6-N3-O2-Cu108	128	1	H9-C6-N3-O2-Cu144	164	18	H9-C6-N3-O2-Cu162	182	1
H9-C6-N7-O4	26	10	H9-C6-N7-O5	27	19	H9-C6-N9-O2	26	3
H9-C7-N1	17	4	H9-C7-N1-O1	18	1	H9-C7-N1-O2	19	7
H9-C7-N1-O3	20	28	H9-C7-N3-O1	20	26	H9-C7-N5-O4	25	2
H9-C7-N5-O5	26	11	H9-C7-N5-O6	27	66	H9-C7-N7-O2	25	5
H9-C7-N7-O3	26	1	H9-C7-N7-O4	27	37	H9-C7-N9-O2	27	4
H9-C8-N1	18	25	H9-C8-N1-O1	19	7	H9-C8-N1-O2	20	10
H9-C8-N3	20	6	H9-C8-N3-O6	26	3	H9-C8-N3-O7	27	5
H9-C8-N5-O4	26	35	H9-C8-N5-O5	27	127	H9-C8-N7-O2	26	1
H9-C8-N7-O3	27	65	H9-C8-N9-O1	27	1	H9-C9-O1	19	219
H9-C9-N1-O1	20	10	H9-C9-N1-O3-Cu48	70	34	H9-C9-N1-O3-Cu54	76	226
H9-C9-N1-O3-Cu60	82	4	H9-C9-N1-O3-Cu64	86	19	H9-C9-N1-O3-Cu72	94	132
H9-C9-N1-O3-Cu80	102	7	H9-C9-N1-O3-Cu96	118	13	H9-C9-N1-O3-Cu108	130	17
H9-C9-N1-O3-Cu120	142	8	H9-C9-N1-O3-Cu144	166	9	H9-C9-N1-O3-Cu162	184	1
H9-C9-N3-O4	25	2	H9-C9-N3-O5	26	1	H9-C9-N3-O6	27	25
H9-C9-N5-O2	25	3	H9-C9-N5-O3	26	20	H9-C9-N5-O4	27	132
H9-C9-N7-O1	26	4	H9-C9-N7-O2	27	22	H9-C10-N1	20	5
H9-C10-N1-O1	21	3	H9-C10-N1-O2	22	4	H9-C10-N3-O4	26	11
H9-C10-N3-O5	27	64	H9-C10-N5-O2	26	8	H9-C10-N5-O3	27	77
H9-C11-N1-O2	23	1	H9-C11-N1-O3	24	7	H9-C11-N3-O4	27	56
H9-C11-N5-O2	27	39	H9-C12-N1-O2	24	1	H9-C12-N1-O3	25	2
H9-C12-N1-O4	26	1	H9-C12-N1-O5	27	5	H9-C12-N3-O3	27	17
H9-C13-N1-O4	27	6	H10-N7-Cu32	49	10	H10-N7-Cu33	50	24
H10-N7-Cu36	53	82	H10-N9-Cu34	53	52	H10-C2-N2-Cu48	62	1
H10-C2-N2-Cu96	110	1	H10-C2-N4-Cu48	64	2	H10-C2-N4-Cu64	80	11
H10-C2-N4-Cu72	88	1	H10-C2-N4-Cu80	96	3	H10-C2-N4-Cu96	112	9
H10-C2-N4-Cu120	136	1	H10-C3-N2-Cu48	63	1	H10-C3-N2-Cu64	79	9
H10-C3-N2-Cu72	87	2	H10-C3-N2-Cu80	95	1	H10-C3-N2-Cu96	111	4
H10-C3-N2-Cu120	135	1	H10-C3-N2-O1-Cu48	64	11	H10-C3-N2-O1-Cu60	76	1
H10-C3-N2-O1-Cu64	80	39	H10-C3-N2-O1-Cu72	88	9	H10-C3-N2-O1-Cu80	96	4
H10-C3-N2-O1-Cu96	112	27	H10-C3-N2-O1-Cu120	136	3	H10-C4-Cu64	78	1
H10-C4-O1-Cu48	63	1	H10-C4-O1-Cu64	79	5	H10-C4-O1-Cu96	111	5
H10-C4-O2-Cu48	64	3	H10-C4-O2-Cu64	80	17	H10-C4-O2-Cu96	112	16

H10-C4-O2-Cu120	136	2	H10-C4-O3	17	8	H10-C4-N2-Cu48	64	8
H10-C4-N2-Cu60	76	8	H10-C4-N2-Cu64	80	106	H10-C4-N2-Cu72	88	11
H10-C4-N2-Cu80	96	41	H10-C4-N2-Cu96	112	85	H10-C4-N2-Cu120	136	16
H10-C5-Cu48	63	1	H10-C5-Cu64	79	6	H10-C5-Cu72	87	2
H10-C5-Cu96	111	7	H10-C5-O1-Cu36	52	1	H10-C5-O1-Cu48	64	12
H10-C5-O1-Cu64	80	54	H10-C5-O1-Cu72	88	6	H10-C5-O1-Cu80	96	5
H10-C5-O1-Cu96	112	51	H10-C5-O1-Cu120	136	7	H10-C5-O4	19	3
H10-C5-O5	20	4	H10-C5-N1-O2-Cu27	45	11	H10-C5-N1-O2-Cu36	54	67
H10-C5-N1-O2-Cu48	66	29	H10-C5-N1-O2-Cu54	72	262	H10-C5-N1-O2-Cu64	82	8
H10-C5-N1-O2-Cu72	90	58	H10-C5-N1-O2-Cu96	114	7	H10-C5-N1-O2-Cu144	162	10
H10-C5-N1-O2-Cu162	180	1	H10-C5-N2-O2	19	3	H10-C5-N2-O3	20	28
H10-C5-N2-O3-Cu48	68	14	H10-C5-N2-O3-Cu54	74	20	H10-C5-N2-O3-Cu60	80	3
H10-C5-N2-O3-Cu64	84	17	H10-C5-N2-O3-Cu72	92	17	H10-C5-N2-O3-Cu96	116	9
H10-C5-N2-O3-Cu144	164	13	H10-C5-N2-O3-Cu162	182	5	H10-C5-N2-O4	21	5
H10-C5-N4	19	21	H10-C5-N4-O1	20	4	H10-C5-N4-O2	21	3
H10-C6	16	27	H10-C6-Cu48	64	7	H10-C6-Cu60	76	3
H10-C6-Cu64	80	54	H10-C6-Cu72	88	6	H10-C6-Cu80	96	5
H10-C6-Cu96	112	37	H10-C6-Cu120	136	9	H10-C6-O1	17	3
H10-C6-O2	18	7	H10-C6-O3	19	10	H10-C6-N2	18	3
H10-C6-N2-O1	19	5	H10-C6-N2-O2	20	14	H10-C6-N2-O3	21	22
H10-C6-N6-O3	25	3	H10-C6-N6-O4	26	3	H10-C6-N6-O18-Cu58	98	1
H10-C6-N6-O18-Cu62	102	2	H10-C6-N6-O18-Cu70	110	3	H10-C7	17	3
H10-C7-O1	18	53	H10-C7-O2	19	35	H10-C7-O3	20	1
H10-C7-N2	19	12	H10-C7-N2-O1	20	1	H10-C7-N2-O2	21	62
H10-C7-N4-O5	26	5	H10-C7-N4-O7	28	6	H10-C7-N6-O3	26	3
H10-C7-N6-O4	27	1	H10-C7-N6-O5	28	49	H10-C7-N8-O2	27	2
H10-C7-N8-O3	28	5	H10-C7-N10-O1	28	4	H10-C8	18	12
H10-C8-O1	19	38	H10-C8-O2	20	13	H10-C8-O3	21	2
H10-C8-N2	20	7	H10-C8-N2-O1	21	22	H10-C8-N4-O4	26	4
H10-C8-N4-O5	27	21	H10-C8-N4-O6	28	40	H10-C8-N6	24	3
H10-C8-N6-O2	26	1	H10-C8-N6-O3	27	32	H10-C8-N6-O4	28	144
H10-C8-N8-O2	28	8	H10-C8-N10	28	2	H10-C9	19	68
H10-C9-O2	21	8	H10-C9-N1-O2-Cu48	70	42	H10-C9-N1-O2-Cu54	76	605
H10-C9-N1-O2-Cu60	82	5	H10-C9-N1-O2-Cu64	86	35	H10-C9-N1-O2-Cu72	94	57
H10-C9-N1-O2-Cu80	102	2	H10-C9-N1-O2-Cu96	118	67	H10-C9-N1-O2-Cu108	130	47
H10-C9-N1-O2-Cu120	142	8	H10-C9-N1-O2-Cu144	166	5	H10-C9-N1-O2-Cu162	184	1
H10-C9-N1-O3-Cu54	77	4	H10-C9-N1-O3-Cu60	83	9	H10-C9-N1-O3-Cu64	87	9
H10-C9-N1-O3-Cu72	95	6	H10-C9-N1-O3-Cu80	103	10	H10-C9-N1-O3-Cu81	104	6
H10-C9-N1-O3-Cu96	119	16	H10-C9-N1-O3-Cu108	131	10	H10-C9-N1-O3-Cu120	143	10
H10-C9-N1-O3-Cu144	167	9	H10-C9-N2	21	7	H10-C9-N2-O1	22	2
H10-C9-N2-O2	23	1	H10-C9-N4-O3	26	1	H10-C9-N4-O4	27	5
H10-C9-N4-O5	28	152	H10-C9-N6-O2	27	6	H10-C9-N6-O3	28	49
H10-C9-N8-O1	28	3	H10-C10-O1	21	4	H10-C10-N2-Cu64	86	1
H10-C10-N2-O1	23	5	H10-C10-N2-O2	24	2	H10-C10-N2-O6	28	8
H10-C10-N4-O3	27	2	H10-C10-N4-O4	28	72	H10-C10-N6-O1	27	3
H10-C10-N6-O2	28	47	H10-C11-N2-O1	24	3	H10-C11-N2-O2	25	11
H10-C11-N2-O5	28	38	H10-C11-N4-O2	27	2	H10-C11-N4-O3	28	82
H10-C11-N6	27	2	H10-C12-O6	28	3	H10-C12-N2-O4	28	22
H10-C12-N4-O2	28	50	H10-C13-O5	28	14	H10-C13-N2-O3	28	42
H10-C13-N4-O1	28	6	H10-C14-N2-O2	28	15	H10-C14-N2-O10-Cu64	100	1
H10-C15-N2-O3	30	1	H11-N6-Cu34	51	39	H11-N6-Cu36	53	45
H11-C3-N3-Cu48	65	2	H11-C3-N3-Cu60	77	2	H11-C3-N3-Cu64	81	15
H11-C3-N3-Cu72	89	1	H11-C3-N3-Cu80	97	6	H11-C3-N3-Cu96	113	19
H11-C3-N3-Cu120	137	1	H11-C4-N1	16	12	H11-C4-N1-Cu48	64	1
H11-C4-N1-Cu64	80	7	H11-C4-N1-Cu96	112	1	H11-C4-N1-O1-Cu48	65	8
H11-C4-N1-O1-Cu60	77	4	H11-C4-N1-O1-Cu64	81	29	H11-C4-N1-O1-Cu72	89	5
H11-C4-N1-O1-Cu80	97	5	H11-C4-N1-O1-Cu96	113	35	H11-C4-N1-O1-Cu120	137	2
H11-C5-N1-Cu34	51	2	H11-C5-N1-Cu36	53	31	H11-C5-N1-Cu48	65	9
H11-C5-N1-Cu60	77	5	H11-C5-N1-Cu64	81	75	H11-C5-N1-Cu72	89	6
H11-C5-N1-Cu80	97	22	H11-C5-N1-Cu96	113	53	H11-C5-N1-Cu120	137	6
H11-C5-N1-O2	19	36	H11-C5-N1-O2-Cu36	55	5	H11-C5-N1-O2-Cu48	67	23

H11-C5-N1-O2-Cu54	73	20	H11-C5-N1-O2-Cu64	83	14	H11-C5-N1-O2-Cu72	91	4
H11-C5-N1-O2-Cu96	115	14	H11-C5-N1-O2-Cu144	163	20	H11-C5-N1-O2-Cu162	181	3
H11-C5-N3-O1	20	1	H11-C5-N3-O2	21	6	H11-C5-N3-O3	22	3
H11-C6-N1	18	12	H11-C6-N1-O1	19	1	H11-C6-N1-O2	20	10
H11-C6-N1-O3	21	3	H11-C6-N1-O4	22	2	H11-C6-N3	20	6
H11-C6-N3-O1	21	10	H11-C6-N3-O4	24	1	H11-C7-N1	19	2
H11-C7-N1-O1	20	31	H11-C7-N1-O2	21	4	H11-C7-N1-O3	22	22
H11-C7-N3	21	18	H11-C7-N3-O1	22	8	H11-C7-N3-O4	25	1
H11-C7-N5-O2	25	1	H11-C7-N5-O6	29	17	H11-C7-N7-O3	28	11
H11-C7-N7-O4	29	22	H11-C7-N9-O2	29	2	H11-C8-N1	20	26
H11-C8-N1-O1	21	5	H11-C8-N1-O2	22	12	H11-C8-N3-O6	28	1
H11-C8-N3-O7	29	13	H11-C8-N5-O3	27	5	H11-C8-N5-O4	28	28
H11-C8-N5-O5	29	84	H11-C8-N7-O2	28	2	H11-C8-N7-O3	29	47
H11-C8-N9-O1	29	3	H11-C9-N1-O1	22	8	H11-C9-N1-O2	23	31
H11-C9-N1-O2-Cu48	71	1	H11-C9-N1-O2-Cu54	77	13	H11-C9-N1-O2-Cu60	83	7
H11-C9-N1-O2-Cu64	87	9	H11-C9-N1-O2-Cu72	95	12	H11-C9-N1-O2-Cu80	103	10
H11-C9-N1-O2-Cu81	104	2	H11-C9-N1-O2-Cu96	119	18	H11-C9-N1-O2-Cu108	131	5
H11-C9-N1-O2-Cu120	143	3	H11-C9-N1-O2-Cu144	167	12	H11-C9-N1-O2-Cu162	185	1
H11-C9-N1-O3	24	35	H11-C9-N1-O3-Cu54	78	12	H11-C9-N1-O3-Cu60	84	6
H11-C9-N1-O3-Cu64	88	7	H11-C9-N1-O3-Cu72	96	19	H11-C9-N1-O3-Cu80	104	9
H11-C9-N1-O3-Cu81	105	7	H11-C9-N1-O3-Cu96	120	9	H11-C9-N1-O3-Cu108	132	1
H11-C9-N1-O3-Cu120	144	8	H11-C9-N1-O3-Cu144	168	12	H11-C9-N3-O4	27	1
H11-C9-N3-O5	28	8	H11-C9-N3-O6	29	31	H11-C9-N5-O3	28	6
H11-C9-N5-O4	29	119	H11-C9-N7-O2	29	40	H11-C10-N1-O1	23	1
H11-C10-N3-O4	28	8	H11-C10-N3-O5	29	56	H11-C10-N5-O2	28	3
H11-C10-N5-O3	29	185	H11-C10-N7-O1	29	10	H11-C11-N1	23	1
H11-C11-N1-O1	24	2	H11-C11-N1-O2	25	7	H11-C11-N1-O3	26	5
H11-C11-N1-O5	28	4	H11-C11-N1-O6	29	1	H11-C11-N2-O2-Cu54	80	225
H11-C11-N2-O2-Cu60	86	22	H11-C11-N2-O2-Cu64	90	25	H11-C11-N2-O2-Cu72	98	17
H11-C11-N2-O2-Cu80	106	70	H11-C11-N2-O2-Cu81	107	71	H11-C11-N2-O2-Cu96	122	26
H11-C11-N2-O2-Cu108	134	5	H11-C11-N2-O2-Cu120	146	54	H11-C11-N2-O2-Cu144	170	11
H11-C11-N2-O2-Cu162	188	3	H11-C11-N3-O3	28	8	H11-C11-N3-O4	29	122
H11-C11-N5-O1	28	1	H11-C11-N5-O2	29	33	H11-C12-N1-O1	25	1
H11-C12-N1-O2	26	8	H11-C12-N1-O3	27	14	H11-C12-N1-O4	28	1
H11-C12-N1-O5	29	9	H11-C12-N3-O2	28	3	H11-C12-N3-O3	29	96
H11-C12-N5-O1	29	36	H11-C13-N1-O3	28	2	H11-C13-N1-O4	29	24
H11-C13-N1-O5	30	4	H11-C13-N3-O2	29	46	H11-C14-N1-O3	29	16
H11-C14-N3-O1	29	26	H11-C15-N1-O1	28	1	H11-C15-N1-O2	29	3
H11-C15-N1-O3	30	1	H11-C16-N1-O2	30	2	H12-N5-Cu36	53	63
H12-C2-O4-Cu12	30	7117	H12-C3-O6	21	84	H12-C3-N2-Cu60	77	1
H12-C3-N2-Cu64	81	3	H12-C3-N2-Cu120	137	1	H12-C4-O1	17	1
H12-C4-O2	18	8	H12-C4-N2-Cu48	66	1	H12-C4-N2-Cu60	78	2
H12-C4-N2-Cu64	82	15	H12-C4-N2-Cu72	90	2	H12-C4-N2-Cu80	98	4
H12-C4-N2-Cu96	114	21	H12-C4-N2-Cu120	138	2	H12-C4-N4-O2-Cu62	84	3
H12-C4-N4-O2-Cu68	90	3	H12-C4-N4-O4-Cu64	88	9	H12-C4-N4-O4-Cu66	90	10
H12-C4-N4-O4-Cu70	94	1	H12-C5-Cu64	81	2	H12-C5-Cu96	113	1
H12-C5-Cu120	137	1	H12-C5-O1-Cu64	82	9	H12-C5-O1-Cu72	90	2
H12-C5-O1-Cu96	114	6	H12-C5-N1-O2	20	3	H12-C5-N2-O3	22	7
H12-C6-Cu48	66	2	H12-C6-Cu60	78	1	H12-C6-Cu64	82	16
H12-C6-Cu72	90	4	H12-C6-Cu80	98	6	H12-C6-Cu96	114	6
H12-C6-Cu120	138	1	H12-C6-O3	21	1	H12-C6-O6	24	5492
H12-C6-N1-O2-Cu27	48	64	H12-C6-N1-O2-Cu36	57	17	H12-C6-N1-O2-Cu48	69	153
H12-C6-N1-O2-Cu54	75	719	H12-C6-N1-O2-Cu64	85	123	H12-C6-N1-O2-Cu72	93	42
H12-C6-N1-O2-Cu96	117	94	H12-C6-N1-O2-Cu144	165	36	H12-C6-N1-O2-Cu162	183	2
H12-C6-N2-O1	21	4	H12-C6-N2-O2	22	12	H12-C6-N4-Cu62	84	2
H12-C6-N4-Cu64	86	1	H12-C6-N4-Cu72	94	1	H12-C6-N4-O2-Cu62	86	1
H12-C6-N4-O2-Cu64	88	1	H12-C6-N4-O2-Cu68	92	3	H12-C6-N4-O2-Cu70	94	3
H12-C7	19	10	H12-C7-O1	20	29	H12-C7-O2	21	46
H12-C7-O3	22	2	H12-C7-N2	21	7	H12-C7-N2-O1	22	1
H12-C7-N2-O2	23	4	H12-C7-N4-O3	26	1	H12-C7-N4-O4	27	1
H12-C7-N6-O3	28	1	H12-C7-N6-O5	30	10	H12-C8	20	10

H12-C8-O1	21	28	H12-C8-O3	23	4	H12-C8-N2	22	5
H12-C8-N2-O1	23	6	H12-C8-N2-O2	24	5	H12-C8-N2-O3	25	4
H12-C8-N4-O4	28	1	H12-C8-N4-O5	29	13	H12-C8-N4-O6	30	15
H12-C8-N6-O2	28	2	H12-C8-N6-O3	29	14	H12-C8-N6-O4	30	38
H12-C8-N8-O2	30	4	H12-C9	21	49	H12-C9-O1	22	10
H12-C9-N2	23	1	H12-C9-N2-O4	27	5	H12-C9-N2-O7	30	10
H12-C9-N4-O4	29	22	H12-C9-N4-O5	30	108	H12-C9-N6-O2	29	3
H12-C9-N6-O3	30	61	H12-C9-N8-O1	30	1	H12-C10	22	5
H12-C10-N2	24	1	H12-C10-N2-O1	25	2	H12-C10-N2-O6	30	14
H12-C10-N4-O3	29	17	H12-C10-N4-O4	30	150	H12-C10-N6-O1	29	2
H12-C10-N6-O2	30	74	H12-C11-N2	25	2	H12-C11-N2-O1	26	13
H12-C11-N2-O2	27	39	H12-C11-N2-O2-Cu54	81	5	H12-C11-N2-O2-Cu64	91	5
H12-C11-N2-O2-Cu80	107	21	H12-C11-N2-O2-Cu81	108	13	H12-C11-N2-O2-Cu96	123	19
H12-C11-N2-O2-Cu108	135	1	H12-C11-N2-O2-Cu120	147	13	H12-C11-N2-O2-Cu144	171	12
H12-C11-N2-O2-Cu162	189	3	H12-C11-N2-O3	28	2	H12-C11-N2-O4	29	15
H12-C11-N2-O5	30	41	H12-C11-N4-O2	29	5	H12-C11-N4-O3	30	190
H12-C11-N6-O1	30	75	H12-C12-O4	28	2	H12-C12-O6	30	2
H12-C12-N2-O1	27	3	H12-C12-N2-O2	28	5	H12-C12-N2-O3	29	8
H12-C12-N2-O4	30	102	H12-C12-N4-O2	30	140	H12-C13-O5	30	11
H12-C13-N2-O2	29	8	H12-C13-N2-O3	30	54	H12-C13-N4-O1	30	32
H12-C14-O4	30	22	H12-C14-N2-O1	29	1	H12-C14-N2-O2	30	40
H12-C14-N4	30	15	H12-C15-O3	30	8	H12-C15-N2-O1	30	3
H13-N3-Cu34	50	22	H13-N4-Cu33	50	1	H13-C3-N1-O3-Cu36	56	605
H13-C3-N1-O3-Cu41	61	1	H13-C3-N1-O3-Cu42	62	10	H13-C3-N1-O3-Cu43	63	6
H13-C3-N1-O3-Cu44	64	1	H13-C3-N1-O3-Cu45	65	1	H13-C3-N1-O3-Cu46	66	1
H13-C3-N1-O3-Cu48	68	145	H13-C5-N1-Cu60	79	1	H13-C5-N1-Cu64	83	12
H13-C5-N1-Cu80	99	2	H13-C5-N1-Cu96	115	15	H13-C5-N1-Cu120	139	1
H13-C5-N1-O3	22	4	H13-C5-N3-O2	23	5	H13-C6-N1	20	1
H13-C6-N1-O2	22	56	H13-C6-N1-O2-Cu36	58	1	H13-C6-N1-O2-Cu48	70	32
H13-C6-N1-O2-Cu54	76	40	H13-C6-N1-O2-Cu64	86	39	H13-C6-N1-O2-Cu72	94	19
H13-C6-N1-O2-Cu96	118	29	H13-C6-N1-O2-Cu144	166	39	H13-C6-N1-O2-Cu162	184	6
H13-C6-N1-O3	23	4	H13-C6-N2-O2-Cu48	71	6	H13-C6-N2-O2-Cu54	77	102
H13-C6-N2-O2-Cu60	83	23	H13-C6-N2-O2-Cu64	87	12	H13-C6-N2-O2-Cu72	95	81
H13-C6-N2-O2-Cu80	103	3	H13-C6-N2-O2-Cu81	104	1	H13-C6-N2-O2-Cu96	119	18
H13-C6-N2-O2-Cu108	131	10	H13-C6-N2-O2-Cu120	143	1	H13-C6-N2-O2-Cu144	167	10
H13-C6-N2-O2-Cu162	185	4	H13-C6-N4-O2-Cu48	73	1	H13-C6-N4-O2-Cu54	79	76
H13-C6-N4-O2-Cu60	85	40	H13-C6-N4-O2-Cu64	89	60	H13-C6-N4-O2-Cu72	97	152
H13-C6-N4-O2-Cu80	105	9	H13-C6-N4-O2-Cu81	106	136	H13-C6-N4-O2-Cu96	121	26
H13-C6-N4-O2-Cu108	133	1	H13-C6-N4-O2-Cu120	145	33	H13-C6-N4-O2-Cu144	169	9
H13-C6-N4-O2-Cu162	187	1	H13-C7-N1	21	1	H13-C7-N1-O2	23	16
H13-C7-N3-O3	26	1	H13-C7-N3-O4	27	2	H13-C7-N5-O3	28	5
H13-C7-N7-O4	31	11	H13-C8-N1	22	8	H13-C8-N1-O1	23	3
H13-C8-N1-O2	24	1	H13-C8-N1-O3	25	5	H13-C8-N3-O4	28	3
H13-C8-N3-O5	29	1	H13-C8-N5-O2	28	1	H13-C8-N5-O4	30	1
H13-C8-N5-O5	31	37	H13-C8-N7-O2	30	3	H13-C8-N7-O3	31	13
H13-C9-N1	23	1	H13-C9-N1-O3	26	38	H13-C9-N3-O4	29	8
H13-C9-N3-O5	30	9	H13-C9-N3-O6	31	27	H13-C9-N5-O3	30	8
H13-C9-N5-O4	31	129	H13-C9-N7-O2	31	9	H13-C10-N1-O1	25	1
H13-C10-N1-O3	27	2	H13-C10-N1-O4	28	9	H13-C10-N3-O3	29	1
H13-C10-N3-O4	30	28	H13-C10-N3-O5	31	110	H13-C10-N5-O2	30	7
H13-C10-N5-O3	31	148	H13-C10-N7-O1	31	24	H13-C11-N1	25	3
H13-C11-N1-O1	26	6	H13-C11-N1-O2	27	1	H13-C11-N1-O4	29	1
H13-C11-N1-O5	30	1	H13-C11-N1-O6	31	12	H13-C11-N3-O2	29	1
H13-C11-N3-O3	30	3	H13-C11-N3-O4	31	171	H13-C11-N5-O2	31	149
H13-C12-N1-O2	28	7	H13-C12-N1-O3	29	8	H13-C12-N1-O4	30	9
H13-C12-N1-O5	31	25	H13-C12-N3-O2	30	17	H13-C12-N3-O3	31	129
H13-C12-N5	30	1	H13-C12-N5-O1	31	62	H13-C13-N1-O2	29	6
H13-C13-N1-O3	30	6	H13-C13-N1-O4	31	38	H13-C13-N3-O2	31	92
H13-C13-N5	31	38	H13-C14-N1-O3	31	27	H13-C14-N3	30	2
H13-C14-N3-O1	31	51	H13-C15-N1	29	3	H13-C15-N1-O1	30	3
H13-C15-N1-O2	31	13	H13-C15-N3	31	1	H13-C16-N1-O1	31	15

H14-O7	21	99	H14-N3-Cu35	52	22	H14-N3-Cu36	53	42
H14-N4-Cu33	51	14	H14-N4-Cu35	53	31	H14-C4-O4	22	9
H14-C4-N2-Cu64	84	1	H14-C4-N2-Cu72	92	1	H14-C4-N2-Cu80	100	1
H14-C4-N2-Cu96	116	3	H14-C6-Cu64	84	1	H14-C6-Cu96	116	1
H14-C6-Cu120	140	1	H14-C6-N2-O2	24	35	H14-C6-N2-O2-Cu48	72	2
H14-C6-N2-O2-Cu54	78	10	H14-C6-N2-O2-Cu60	84	7	H14-C6-N2-O2-Cu64	88	10
H14-C6-N2-O2-Cu72	96	21	H14-C6-N2-O2-Cu80	104	2	H14-C6-N2-O2-Cu81	105	6
H14-C6-N2-O2-Cu96	120	16	H14-C6-N2-O2-Cu108	132	4	H14-C6-N2-O2-Cu120	144	2
H14-C6-N2-O2-Cu144	168	14	H14-C6-N2-O2-Cu162	186	1	H14-C6-N2-O4-Cu68	94	3
H14-C6-N4-O2	26	37	H14-C6-N4-O2-Cu48	74	3	H14-C6-N4-O2-Cu54	80	9
H14-C6-N4-O2-Cu60	86	9	H14-C6-N4-O2-Cu64	90	7	H14-C6-N4-O2-Cu72	98	14
H14-C6-N4-O2-Cu80	106	6	H14-C6-N4-O2-Cu81	107	4	H14-C6-N4-O2-Cu96	122	17
H14-C6-N4-O2-Cu108	134	7	H14-C6-N4-O2-Cu120	146	3	H14-C6-N4-O2-Cu144	170	5
H14-C6-N4-O2-Cu162	188	1	H14-C7-O3	24	1	H14-C7-N2	23	5
H14-C7-N2-O1	24	2	H14-C7-N2-O2	25	1	H14-C8	22	2
H14-C8-O1	23	1	H14-C8-O2	24	4	H14-C8-O3	25	1
H14-C8-N2-O3	27	3	H14-C8-N2-O4	28	1	H14-C8-N4-O5	31	5
H14-C8-N4-O6	32	3	H14-C8-N6-O4	32	18	H14-C9	23	57
H14-C9-N2-O4	29	1	H14-C9-N4-O2	29	2	H14-C9-N4-O3	30	2
H14-C9-N4-O4	31	18	H14-C9-N4-O5	32	65	H14-C9-N6-O2	31	1
H14-C9-N6-O3	32	88	H14-C10-O4	28	1	H14-C10-N2-O1	27	2
H14-C10-N2-O4	30	3	H14-C10-N2-O5	31	4	H14-C10-N2-O6	32	16
H14-C10-N4-O3	31	43	H14-C10-N4-O4	32	207	H14-C10-N6-O2	32	81
H14-C10-N6-O2-Cu58	90	2	H14-C10-N6-O2-Cu70	102	2	H14-C11-N2	27	2
H14-C11-N2-O1	28	5	H14-C11-N2-O2	29	2	H14-C11-N2-O3	30	1
H14-C11-N2-O4	31	8	H14-C11-N2-O5	32	63	H14-C11-N4-O2	31	30
H14-C11-N4-O3	32	157	H14-C11-N6-O1	32	60	H14-C12-O6	32	4
H14-C12-N2	28	4	H14-C12-N2-O1	29	7	H14-C12-N2-O3	31	14
H14-C12-N2-O4	32	86	H14-C12-N4-O1	31	10	H14-C12-N4-O2	32	188
H14-C12-N6	32	40	H14-C13-O5	32	8	H14-C13-N2-O1	30	3
H14-C13-N2-O3	32	106	H14-C13-N4	31	1	H14-C13-N4-O1	32	28
H14-C14-O4	32	4	H14-C14-N2	30	4	H14-C14-N2-O1	31	1
H14-C14-N2-O2	32	72	H14-C14-N4	32	11	H14-C15-O3	32	22
H14-C15-N2-O1	32	19	H14-C16-O2	32	11	H14-C16-N2	32	24
H15-C3-N2-O5-Cu32	57	37	H15-C3-N2-O5-Cu36	61	46	H15-C7-N1-O1	24	1
H15-C7-N1-O3	26	2	H15-C8-N1-O4	28	1	H15-C8-N3-O4	30	1
H15-C8-N3-O5	31	2	H15-C8-N5-O3	31	2	H15-C8-N5-O4	32	1
H15-C8-N5-O5	33	23	H15-C8-N7-O3	33	1	H15-C9-N1	25	3
H15-C9-N1-O1	26	6	H15-C9-N1-O3	28	3	H15-C9-N3-O4	31	1
H15-C9-N3-O5	32	8	H15-C9-N3-O6	33	10	H15-C9-N5-O3	32	7
H15-C9-N5-O4	33	70	H15-C9-N7-O2	33	4	H15-C10-N1	26	16
H15-C10-N1-O1	27	1	H15-C10-N1-O2	28	2	H15-C10-N1-O4	30	2
H15-C10-N3-O3	31	2	H15-C10-N3-O4	32	19	H15-C10-N3-O5	33	76
H15-C10-N5-O2	32	8	H15-C10-N5-O3	33	100	H15-C11-N1-O4	31	2
H15-C11-N1-O5	32	1	H15-C11-N1-O6	33	2	H15-C11-N3-O3	32	12
H15-C11-N3-O4	33	136	H15-C11-N5-O1	32	11	H15-C11-N5-O2	33	103
H15-C12-N1-O1	29	2	H15-C12-N1-O5	33	36	H15-C12-N3-O2	32	12
H15-C12-N3-O3	33	140	H15-C12-N5-O1	33	19	H15-C13-N1-O1	30	1
H15-C13-N1-O3	32	6	H15-C13-N1-O4	33	52	H15-C13-N3-O1	32	3
H15-C13-N3-O2	33	103	H15-C13-N5	33	27	H15-C14-N1-O2	32	9
H15-C14-N1-O3	33	45	H15-C14-N3-O1	33	71	H15-C15-N1-O2	33	27
H15-C15-N3	33	42	H15-C16-N1-O1	33	9	H16-O8	24	407
H16-N2-Cu20	38	13	H16-N4-Cu20	40	3	H16-C4-N8-O4	32	18
H16-C7-O1	24	1	H16-C7-N1	24	10	H16-C7-N1-O2	26	2
H16-C7-N2-O2	27	7	H16-C8-O1	25	39	H16-C8-O2	26	5
H16-C8-N4-O6	34	3	H16-C8-N6-O4	34	5	H16-C9	25	19
H16-C9-N2	27	3	H16-C9-N2-O2	29	8	H16-C9-N2-O3	30	2
H16-C9-N2-O4	31	1	H16-C9-N4-O4	33	7	H16-C9-N4-O5	34	35
H16-C9-N6-O3	34	15	H16-C10	26	2	H16-C10-O1	27	2
H16-C10-N1-O1	28	1	H16-C10-N2-O2	30	6	H16-C10-N2-O3	31	1
H16-C10-N2-O5	33	3	H16-C10-N2-O6	34	4	H16-C10-N4-O3	33	11

H16-C10-N4-O4	34	95	H16-C10-N6-O2	34	30	H16-C11-N2	29	2
H16-C11-N2-O3	32	3	H16-C11-N2-O4	33	4	H16-C11-N2-O5	34	35
H16-C11-N4-O2	33	1	H16-C11-N4-O3	34	135	H16-C12-N2	30	1
H16-C12-N2-O2	32	1	H16-C12-N2-O3	33	9	H16-C12-N2-O4	34	87
H16-C12-N4-O1	33	2	H16-C12-N4-O2	34	131	H16-C13-O5	34	14
H16-C13-N2-O2	33	14	H16-C13-N2-O3	34	98	H16-C13-N4-O1	34	69
H16-C14-O4	34	22	H16-C14-N2-O1	33	6	H16-C14-N2-O2	34	53
H16-C14-N4	34	29	H16-C15-N2-O1	34	11	H16-C16-O2	34	5
H16-C16-N2	34	7	H16-C17-O1	34	9	H16-C18	34	3
H17-C8-N5-O5	35	5	H17-C9-N1-O2	29	5	H17-C9-N3-O4	33	2
H17-C9-N3-O5	34	1	H17-C9-N3-O6	35	8	H17-C9-N5-O4	35	15
H17-C10-N1-O1	29	2	H17-C10-N3-O4	34	8	H17-C10-N3-O5	35	33
H17-C10-N3-O6	36	1	H17-C10-N5-O3	35	15	H17-C11-N1-O1	30	4
H17-C11-N1-O5	34	3	H17-C11-N1-O6	35	2	H17-C11-N3-O3	34	10
H17-C11-N3-O4	35	69	H17-C11-N5-O2	35	28	H17-C11-N5-O4	37	1
H17-C12-N1	30	4	H17-C12-N1-O3	33	1	H17-C12-N1-O4	34	6
H17-C12-N1-O5	35	17	H17-C12-N3-O2	34	5	H17-C12-N3-O3	35	118
H17-C12-N5-O1	35	31	H17-C13-N1-O2	33	1	H17-C13-N1-O4	35	35
H17-C13-N3-O1	34	3	H17-C13-N3-O2	35	68	H17-C14-N1-O3	35	32
H17-C14-N3-O1	35	12	H17-C15-N1-O2	35	21	H17-C15-N3	35	4
H17-C16-N1-O1	35	17	H17-C17-N1	35	2	H18-C3-N4-O3-Cu36	64	604
H18-C6-N2-Cu62	88	2	H18-C6-N2-Cu64	90	1	H18-C6-N2-Cu66	92	2
H18-C6-N2-Cu68	94	4	H18-C8-N6-O4	36	1	H18-C9	27	1
H18-C9-O5	32	1	H18-C9-N2-O2	31	1	H18-C9-N4-O5	36	12
H18-C10	28	3	H18-C10-N2-O3	33	1	H18-C10-N2-O5	35	1
H18-C10-N2-O6	36	10	H18-C10-N4-O4	36	41	H18-C10-N4-O5	37	1
H18-C11-N2-O3	34	1	H18-C11-N2-O4	35	3	H18-C11-N2-O5	36	29
H18-C11-N4-O2	35	7	H18-C11-N4-O3	36	46	H18-C11-N4-O5	38	1
H18-C12-N2-O3	35	3	H18-C12-N2-O4	36	70	H18-C12-N2-O4-Cu68	104	1
H18-C12-N4-O2	36	6	H18-C12-N6-O5	41	1	H18-C13-O5	36	3
H18-C13-N2-O2	35	1	H18-C13-N2-O3	36	38	H18-C13-N4-O1	36	4
H18-C14-O4	36	13	H18-C14-N2-O2	36	48	H18-C14-N6-O1	39	10
H18-C15-O3	36	24	H18-C15-N2-O1	36	16	H18-C16-O2	36	5
H18-C16-N2	36	1	H19-C3-N5-O3-Cu36	66	206	H19-C7-N1-O1	28	5
H19-C10-N3-O5	37	4	H19-C10-N5-O3	37	3	H19-C11-N1-O6	37	4
H19-C11-N3-O4	37	23	H19-C11-N3-O5	38	3	H19-C11-N3-O7	40	1
H19-C12-N1-O3	35	1	H19-C12-N1-O4	36	2	H19-C12-N1-O5	37	29
H19-C12-N3-O3	37	28	H19-C13-N1-O4	37	12	H19-C13-N3-O2	37	30
H19-C13-N5-O5	42	1	H19-C14-N1-O3	37	9	H19-C14-N3-O1	37	21
H19-C14-N3-O5	41	1	H19-C14-N7-O4	44	1	H19-C15-N1-O2	37	7
H19-C16-N1-O1	37	2	H19-C18-N1-O2	40	5	H20-N14-Cu64	98	2
H20-N14-Cu66	100	9	H20-C11-N2-O4	37	1	H20-C11-N2-O5	38	3
H20-C11-N4-O6	41	3	H20-C12-N2-O3	37	2	H20-C12-N2-O4	38	17
H20-C12-N4-O2	38	2	H20-C12-N4-O6	42	1	H20-C12-N6-O7	45	1
H20-C13-O5	38	1	H20-C13-N2-O3	38	5	H20-C13-N4-O1	38	3
H20-C13-N6-O5	44	2	H20-C14-O4	38	2	H20-C14-N2-O2	38	25
H20-C15-O3	38	5	H20-C15-N4-O5	44	1	H20-C16-O2	38	19
H20-C16-N2	38	4	H20-C16-N4-O4	44	1	H21-N1-Cu45	67	1
H21-C11-N1-O5	38	1	H21-C11-N3-O4	39	4	H21-C12-N1-O5	39	6
H21-C12-N3-O4	40	1	H21-C12-N3-O7	43	1	H21-C12-N5-O6	44	1
H21-C13-N1-O4	39	10	H21-C13-N3-O2	39	2	H21-C13-N5-O5	44	1
H21-C13-N5-O7	46	1	H21-C13-N5-O8	47	1	H21-C14-N1-O2	38	3
H21-C14-N1-O3	39	3	H21-C14-N3-O1	39	6	H21-C14-N5-O7	47	1
H21-C15-N1-O2	39	6	H21-C15-N3	39	15	H21-C15-N3-O5	44	2
H21-C15-N3-O6	45	1	H21-C15-N5-O7	48	1	H21-C15-N7-O4	47	1
H21-C16-N1-O1	39	6	H21-C16-N3-O6	46	1	H21-C17-N5-O5	48	2
H22-N4-Cu48	74	1	H22-C10-N2-Cu70	104	1	H22-C12-N2-O4	40	1
H22-C12-N4-O5	43	1	H22-C12-N4-O6	44	3	H22-C13-N2-O3	40	15
H22-C13-N4-O5	44	1	H22-C13-N4-O6	45	1	H22-C14-O4	40	3
H22-C14-N2-O1	39	6	H22-C14-N2-O2	40	4	H22-C14-N4-O5	45	1
H22-C14-N4-O8	48	1	H22-C14-N6-O5	47	1	H22-C14-N6-O6	48	1

H22-C15-N6-O6	49	2	H22-C15-N6-O7	50	1	H22-C16-N2	40	3
H22-C16-N4-O5	47	2	H22-C16-N4-O6	48	2	H22-C16-N4-O7	49	1
H22-C17-O1	40	6	H22-C17-N4-O5	48	1	H22-C17-N4-O6	49	1
H22-C18	40	9	H23-N1-Cu44	68	3	H23-N2-Cu43	68	8
H23-C12-N3-O4	42	1	H23-C12-N3-O5	43	4	H23-C12-N3-O6	44	1
H23-C13-N3-O2	41	3	H23-C13-N3-O5	44	1	H23-C13-N3-O7	46	2
H23-C13-N5-O6	47	1	H23-C13-N5-O7	48	2	H23-C14-N1-O3	41	4
H23-C14-N5-O4	46	3	H23-C14-N5-O5	47	1	H23-C14-N5-O6	48	1
H23-C15-N1-O2	41	19	H23-C15-N5-O5	48	2	H23-C15-N5-O6	49	1
H23-C15-N5-O7	50	1	H23-C16-N1-O1	41	8	H23-C16-N3-O4	46	1
H23-C16-N3-O6	48	1	H23-C16-N5-O6	50	1	H23-C17-N1	41	2
H23-C17-N3-O5	48	1	H23-C17-N3-O6	49	2	H23-C17-N3-O7	50	1
H23-C18-N5-O5	51	1	H23-C18-N5-O6	52	1	H23-C19-N5-O6	53	1
H24-N2-Cu20	46	8	H24-C12-O12	48	1	H24-C12-N4-O4	44	1
H24-C13-N4-O6	47	1	H24-C13-N6-O6	49	4	H24-C14-N4-O6	48	1
H24-C14-N4-O7	49	1	H24-C15-N2-O1	42	4	H24-C15-N6-O5	50	1
H24-C15-N6-O6	51	1	H24-C16-O2	42	6	H24-C17-N4-O6	51	1
H24-C18-N4-O4	50	1	H24-C18-N4-O6	52	1	H24-C19-N4-O5	52	1
H24-C19-N4-O7	54	1	H24-C21-N6-O6	57	1	H25-C13-N3-O4	45	1
H25-C14-N3-O5	47	1	H25-C14-N5-O6	50	1	H25-C14-N5-O7	51	1
H25-C15-N3-O5	48	1	H25-C15-N5-O5	50	1	H25-C17-N5-O4	51	1
H25-C18-N1-O1	45	20	H25-C18-N5-O6	54	1	H25-C18-N5-O7	55	1
H25-C19-N5-O5	54	1	H25-C19-N5-O6	55	1	H25-C20-N5-O5	55	2
H25-C20-N5-O6	56	1	H25-C21-N3-O5	54	1	H25-C21-N7-O5	58	1
H26-N1-Cu45	72	4	H26-C6-N2-O6-Cu56	96	3	H26-C6-N2-O6-Cu58	98	1
H26-C6-N2-O6-Cu60	100	2	H26-C6-N2-O6-Cu62	102	1	H26-C6-N2-O6-Cu64	104	5
H26-C6-N2-O6-Cu66	106	2	H26-C6-N2-O6-Cu68	108	4	H26-C6-N2-O6-Cu70	110	1
H26-C6-N2-O6-Cu72	112	36	H26-C6-N2-O6-Cu80	120	6	H26-C14-N4-O5	49	1
H26-C14-N4-O6	50	3	H26-C14-N6-O7	53	1	H26-C15-N4-O5	50	1
H26-C15-N4-O6	51	2	H26-C15-N4-O7	52	1	H26-C16-N6-O5	53	2
H26-C16-N6-O6	54	1	H26-C18-N4-O5	53	1	H26-C18-N4-O6	54	1
H26-C18-N4-O7	55	1	H26-C19-N4-O4	53	1	H26-C19-N4-O5	54	1
H26-C20-N4-O5	55	1	H26-C20-N6-O5	57	1	H26-C20-N6-O6	58	2
H26-C21-N6-O5	58	2	H26-C23-N8-O4	61	2	H27-N2-Cu36	65	6
H27-N7-Cu40	74	1	H27-C14-N3-O4	48	2	H27-C15-N3-O4	49	1
H27-C15-N3-O6	51	1	H27-C15-N5-O7	54	1	H27-C16-N3-O4	50	1
H27-C16-N3-O6	52	1	H27-C16-N5-O5	53	4	H27-C17-N5-O4	53	1
H27-C17-N5-O6	55	1	H27-C18-N3-O5	53	1	H27-C18-N3-O6	54	1
H27-C18-N7-O4	56	1	H27-C20-N5-O6	58	1	H27-C21-N5-O5	58	1
H27-C23-N3-O5	58	3	H27-C24-N5-O4	60	1	H27-C24-N5-O6	62	1
H28-C15-N4-O5	52	1	H28-C15-N6-O6	55	1	H28-C16-N4-O6	54	1
H28-C16-N6-O5	55	1	H28-C17-N6-O5	56	1	H28-C18-N4-O4	54	1
H28-C18-N4-O5	55	1	H28-C19-N4-O5	56	2	H28-C19-N4-O6	57	2
H28-C19-N6-O6	59	1	H28-C20-N4-O5	57	1	H28-C21-N4-O6	59	1
H28-C26-N6-O5	65	1	H29-C5-N1-O14	49	7	H29-C15-N3-O4	51	1
H29-C15-N3-O5	52	1	H29-C16-N3-O4	52	1	H29-C17-N7-O5	58	1
H29-C19-N3-O5	56	1	H29-C20-N3-O5	57	2	H29-C20-N3-O6	58	1
H29-C21-N5-O4	59	2	H29-C21-N5-O5	60	1	H30-O15	45	23
H30-N2-Cu32	64	1	H30-C16-N4-O5	55	2	H30-C16-N4-O6	56	1
H30-C16-N6-O6	58	1	H30-C18-N4-O2	54	4	H30-C19-N4-O6	59	1
H30-C20-N4-O5	59	1	H30-C21-N4-O4	59	1	H30-C21-N4-O5	60	2
H30-C21-N6-O5	62	1	H30-C22-N4-O4	60	1	H30-C23-N6-O4	63	2
H30-C27-N6-O5	68	1	H31-C16-N3-O4	54	2	H31-C16-N3-O5	55	1
H31-C20-N3-O5	59	1	H31-C20-N5-O6	62	1	H31-C22-N5-O5	63	1
H31-C24-N3-O6	64	1	H32-N8-Cu140	180	7	H32-C17-N4-O5	58	2
H32-C17-N6-O6	61	2	H32-C18-N6-O4	60	1	H32-C26-N4-O5	67	2
H33-C3-N5-O7-Cu36	84	1159	H33-C17-N3-O4	57	1	H33-C17-N5-O5	60	1
H33-C21-N3-O5	62	2	H36-N12-Cu144	192	10	H40-N28-Cu128	196	3
H40-N28-Cu132	200	6	H48-O24-Cu24	96	47	H52-N12-Cu136	200	5
H52-N16-Cu132	200	15	H54-C2-O26-Cu22	104	77	H55-C1-O26-Cu22	104	72
H56-C1-O25-Cu22	104	74	H56-C1-O26-Cu22	105	74	H57-C1-O26-Cu22	106	74

H94-O42-Cu64	200	58	H95-C1-O44-Cu63	203	95	H95-C1-O44-Cu64	204	113
H95-C1-O45-Cu62	203	116	H95-C1-O45-Cu63	204	126	H95-C1-O45-Cu64	205	102
H95-C2-O46-Cu62	205	81	H96-O43-Cu64	203	88	H96-C1-O45-Cu60	202	79
H96-C1-O45-Cu62	204	91	H96-C2-O45-Cu62	205	90	H96-C2-O46-Cu61	205	98

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