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# An illustrative overview of the synergy between graph theory and peptide analysis using combinatorial optimization

**Anton Vrdoljak,**
University of Mostar, Faculty of Civil Engineering, Architecture, and Geodesy, Ph.D,
anton.vrdoljak@fgag.sum.ba

**Abstract**: Many contemporary problems in biomedicine, biophysics, and bioinformatics, as well as in numerous other fields of engineering and social sciences, can be reduced to mathematical modeling based on graph theory. Mathematical modeling is generally interpreted as the act of representing a real-world system through mathematical formulations and equations, aiming to develop and implement a model that facilitates subsequent analysis, design, and system optimization. The aim of this paper is to demonstrate, through an illustrative account of the synergy between graph theory and peptide analysis, how combinatorial optimization enables the resolution of complex biophysical problems in a computationally elegant and efficient manner. Due to their importance in analyzing and predicting peptide properties, the proposed model focuses on constructing a smaller yet representative subset of amino acid scales. To this end, a Variable Neighborhood Search (VNS) approach is employed – a contemporary metaheuristic in the field of combinatorial optimization.

**Key words**: graph theory, dominating set, amino-acid scales, combinatorial optimization, variable neighborhood search

# Ilustrativan prikaz sinergije teorije grafova i analize peptida kroz kombinatornu optimizaciju

**Sažetak**: Mnogi suvremeni problemi biomedicine, biofizike i bioinformatike, ali i brojnih drugih područja tehnike i društvenih znanosti, svode se na primjenu matematičkog modeliranja temeljenog na teoriji grafova. Matematičko modeliranje općenito interpretiramo kao čin opisivanja stvarnoga sustava matematičkim formulacijama i jednadžbama, s ciljem stvaranja i implementacije matematičkog modela za naknadne analize te konstruiranje i optimizaciju sustava unutar zadanog okvira. Cilj ovog rada je kroz ilustrativan prikaz sinergije između teorije grafova i analize peptida demonstrirati kako kombinatorna optimizacija omogućuje rješavanje kompleksnih problema biofizike na računski elegantan i efikasan način. Zbog važnosti pri analiziranju i predviđanju svojstava peptida, fokus predloženog modela bit će na konstrukciji (pronalaženju) manjeg, ali još uvijek reprezentativnog, skupa ljestvica aminokiselina. U tu svrhu primijenjena je metoda pretrage promjenjivom okolinom, suvremena metaheuristika u području kombinatorne optimizacije.

**Ključne riječi**: teorija grafova, dominantan skup, ljestvice aminokiselina, kombinatorna optimizacija, pretraga promjenjivom okolinom

## 1. INTRODUCTION

In the history of science, there have been numerous examples of powerful synergies between seemingly distant disciplines, which often led to radical changes in human thought. Perhaps the most significant such moment is the integration of geometry and algebra, which created the foundation for modern analytic geometry. This connection, or rather the translation of spatial forms into the symbolic algebraic language, is not merely a mathematical curiosity, but a key paradigm of modern engineering, physics and computer science, because it enables the solution of complex problems that are unsolvable, or would remain difficult to grasp, in strictly separate disciplines. When we combine these two disciplines, we gain the ability to see structure (geometry) and calculate precision (algebra). In other words, their combination teaches us that every problem has multiple facets (visual and logical), the rigid rules of algebra can generate infinite creativity in geometry, and understanding one deeply enriches the understanding of the other. Similar transformative processes are observed today in modern biomedicine, biophysics, and bioinformatics. Over the past few decades, numerous studies have shown that graphs are an excellent and indispensable tool for modeling systems that emphasize connections and relationships between objects. First of all, graphs provide a simple and intuitive representation of heterogeneous and complex biological processes and biochemical reactions, and interactions. Moreover, they facilitate the modeling and understanding of complex molecular mechanisms by integrating graph theory, machine learning, and artificial intelligence algorithms. Despite significant advances in artificial intelligence, precise modeling of the structural and functional properties of peptides remains a challenge due to the exceptional complexity of their search space. It is precisely in this context that combinatorial optimization becomes an indispensable tool that enables systematic model improvement through the identification of key parameters. Of particular importance here is the construction of representative sets of amino acid (amino carboxylic acid) scales, which achieves the necessary reduction in dimensionality without losing essential physicochemical and biochemical information.

Among different heuristic approaches, variable neighborhood search stands out for its ability to systematically change the neighborhood structure during the search process. This approach allows efficient avoidance of local minima (optima) and exploration of wider solution spaces, which is crucial when solving nonlinear amino acid scale set optimization problems. Application of this method within graph theory paves the way for more computationally viable models that retain a high level of biological relevance.

This paper is structured as follows. After introductory considerations, the second chapter analyzes in detail the theoretical basis of the synergy between graph theory and peptide property analysis, with special reference to the mathematical representation of biological networks. The third chapter describes the proposed model, defining the amino acid scale set optimization problem and explaining the implementation of the variable neighborhood search metaheuristic. The fourth chapter presents and discusses the results of numerical experiments, with a focus on the computational efficiency and biological relevance of the obtained subsets. The paper ends with the fifth chapter, in which a conclusion is drawn and guidelines are provided for future research in the field of combinatorial optimization in biophysics.

## 2. THEORETICAL BACKGROUND (Graph theory in molecular systems modeling)

Graph theory in modern biophysics is not just an auxiliary visualization tool, but a fundamental formal language that enables the mapping of complex biological entities into an exact mathematical structure. If we observe a peptide molecule as a graph, in which amino acids represent the vertices and their interactions represent the edges, we open up space for the application of robust algorithmic solutions. Such an abstraction allows us to move beyond the mere description of chemical properties and focus on the topological organization of the system. It is precisely this topological perspective, combined with the numerical values of amino acid scales, that creates a synergistic framework within which the behavior and functionality of peptides can be accurately predicted.

The experimental and theoretical properties of amino acids, as the basic building blocks of peptides and proteins, have been extensively studied. Each research method assigns a numerical value to an individual amino acid, and such an assignment is defined as an amino acid scale. Their application in bioinformatics is crucial for the interpretation and prediction of the behavior of biopolymers (peptides and proteins). However, the number of available scales is exceptionally large; for example, there are more than a hundred scales related exclusively to hydrophobicity. Such overproduction of data is a significant computational burden for algorithms that generate completely new (useful) peptide descriptors by combining multiple scales. Therefore, it is of primary interest for biophysicists and bioinformaticians to construct a smaller yet representative set of scales, while preserving as much information as possible.

In order to achieve the desired data reduction with minimal information loss, in this paper we propose a graph-theoretic approach to modeling the relationship between amino acid scales. In such a model, each scale represents a vertex of the graph, while the edges define the level of similarity or correlation between them. Such a formalization allows us to transform the problem of selecting a representative set into a precisely defined graph-theoretic problem, such as finding optimal subsets of vertices that maximally cover the information space. Using this methodology, complex biophysical properties of amino acids become subject to exact combinatorial analysis, which ensures systematic selection of descriptors without relying on heuristic assumptions.

The transformation of the problem of selecting a representative set of scales into an optimization task requires the introduction of a precise graph-theoretical apparatus. In this context, we model the system using the following basic definitions [10]:

**Definition 1.** A graph is an ordered triple $G=(V,E,\varphi)$, where $V$ is a non-empty set of vertices, $E$ is a set of edges disjoint from $V$, and $\varphi$ is a function that assigns to each edge in $E$ two, not necessarily distinct, vertices from $V$. A graph is often written as an ordered pair $G=(V,E)$, or simply as $G$. The number of vertices of a graph $G$ is denoted by $n$, and the number of edges by $m$.

Thus, each edge $e\in E$ connects two vertices $u,v\in V$, that is, we say that edge $e$ is incident to vertices $u$ and $v$. In addition, we say that $u$ and $v$ are the endpoints of edge $e$, and also that vertices $u$ and $v$ are incident to edge $e$, and we say that $u$ and $v$ are adjacent vertices, and we write $e=uv$ (where the order of vertices in the notation is irrelevant). Edges with at least one common endpoint are called adjacent edges.

**Definition 2.** A graph $G=(V,E)$ that has no loops (edges connecting a vertex to itself) and no multiple edges (two or more edges sharing the same pair of endpoints) is called a simple graph. Otherwise, a graph is called a pseudograph.

In a simple graph, the set of edges $E$ can be viewed as a set of two-element subsets of the set $V$, making the incidence function $\varphi$ redundant.

**Definition 3.** In a simple graph $G=(V,E)$, the neighborhood of a vertex $v \in V$ is defined as the set

$$N_G(v)=\{u \in V \mid vu \in E\} \tag{1}$$

of neighbors of vertex $v$. The degree (valency) of a vertex $v \in V$ in a simple graph $G$ is the number of neighbors of vertex $v$, $\deg(v)=d_G(v)=|N_G(v)|$ (the number of edges of $G$ incident to vertex $v$). An isolated vertex is a vertex with degree zero. A vertex with degree one is called a leaf or pendant vertex.

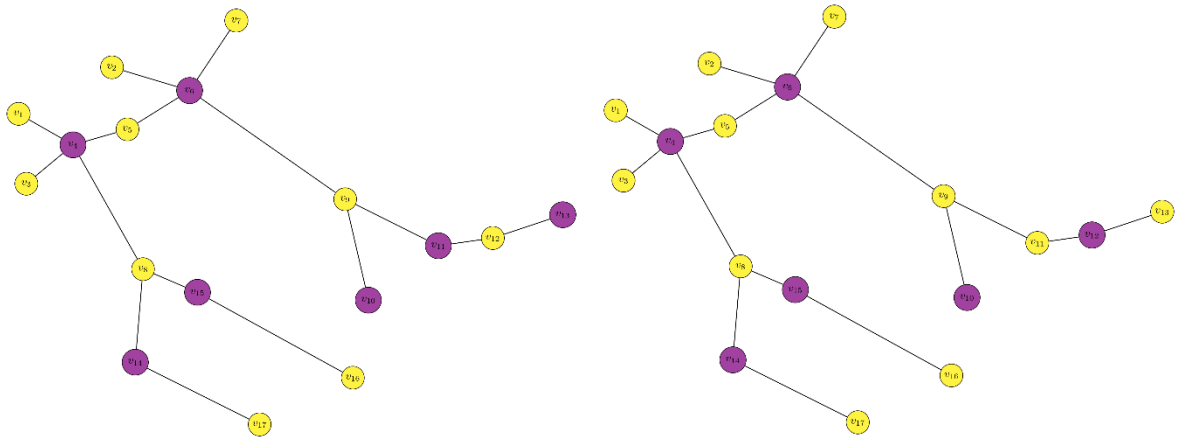

Figure 1. A minimal (left) and minimum dominating set of a graph $G$ [10]

**Definition 4.** Let $G=(V,E)$ be a graph. We say that $D \subseteq V$ is a dominating set of graph $G$ if, for every vertex $v \in V \setminus D$, there exists at least one $u \in D$ that is adjacent to $v$, or, for which $uv \in E$ holds.

**Definition 5.** A dominating set $D$ of a graph $G$ is minimal if there exists no proper subset $D' \subset D$ that is also a dominating set of graph $G$. A dominating set of smallest cardinality (size) is called a minimum dominating set, and its cardinal number determines the (lower) domination number $\gamma(G)$ of the given graph $G$.

Thus, a dominating set of a graph $G=(V,E)$ is a subset $D$ of $V$, such that every vertex of the graph is either in the dominating set or has a neighbor in the dominating set [3]. Every minimum dominating set is a minimal dominating set, but the converse does not necessarily hold (see Figure 1) [13]. The domination number $\gamma(G)$ for the graph $G$ in Figure 1 is 6. Furthermore, every graph has at least one dominating set: if $D=V$, i.e., the set $D$ contains all vertices of the graph $G$, then $D$ is by definition a dominating set of $G$, since $V \setminus D$ is necessarily the empty set. For graphs without isolated vertices, there always exist two disjoint dominating sets: if $D_m =$ is a minimal dominating set of graph $G$, then $V \setminus D_m$ is also a dominating set. If $G$ is a graph with $n$ vertices and $m$ edges, where $0 \le m \le \binom{n}{2}$, then the following is true for its domination number [1]:

$$\gamma(G) \leq \left\lfloor n+1-\sqrt{1+2m} \right\rfloor. \quad (2)$$

Although the previous definitions established a clear mathematical framework, it is important to emphasize that finding a minimal or minimum dominating set in a general graph has been proven to be an NP-complete problem [4]. This means that, as the number of amino acid scales (graph vertices) increases, the time required to find an exact optimal solution grows exponentially, which makes conventional search methods practically unusable. It is precisely because of this computational complexity that advanced metaheuristic approaches must be relied upon in solving this problem. Within the broader spectrum of known (meta)heuristics, we selected the *Variable Neighborhood Search* (VNS)—a method which, thanks to its ability to systematically change the neighborhood structure, enables efficient finding of high-quality solutions within a reasonable time frame. The next chapter describes in detail the implementation of this metaheuristic [7], which, since its introduction in the 1990s, has undergone numerous applications and improvements [8].

Let $r_0^2$ be a given number (the so-called similarity threshold). Let $S$ be the set of all amino acid scales. We say that $T \subset S$ is a representative set of scales if, for every scale $s \in S$, there exists a scale $t \in T$ such that the square of the correlation coefficient $r^2$ between scales $s$ and $t$ is greater than or equal to $r_0^2$.

The problem of finding a minimal representative set of amino acid scales can be reduced to the problem of finding a minimal dominating set. Let $G$ be a simple graph with a set of vertices $S(G)$ and a set of edges:

$$E(G) = \{s_1 s_2 : s_1, s_2 \in S(G) \text{ and the correlation between } s_1 \text{ and } s_2 \text{ is } \geq r_0^2\}. \quad (3)$$

Every dominating set in the observed graph $G$ corresponds to a representative set of amino acid scales, and every representative set of these scales corresponds to a dominating set. Consequently, a minimal dominating set in this graph is a minimal representative set of scales.

Unfortunately, as previously noted, finding a minimal dominating set in a general graph has been proven to be an NP-complete problem.

## 3. METHODOLOGY AND MODEL (Optimization of the set of amino acid scales using VNS)

The Variable Neighborhood Search method (hereinafter: the VNS metaheuristic, or simply VNS) was proposed by Nenad Mladenović and Pierre Hansen in 1997 as a robust approach for solving complex problems of combinatorial and global optimization. Unlike exact methods, which can, at least in theory, provide an optimal solution, or a reasonable (feasible) solution that optimizes (minimizes or maximizes) the value of a given objective function, the variable neighborhood search method, like other heuristic methods, yields a reasonable solution without a guarantee of optimality. The fundamental philosophy of VNS rests on the idea that a local minimum (optimum) with respect to one neighborhood structure does not necessarily have to be a local minimum (optimum) with respect to some other structure. Accordingly, the VNS algorithm aims at systematically exploring the neighborhood of the current solution using a set of predefined neighborhood structures. Since different problem instances have different environments and complexities, the selection of appropriate structures is a challenging task, as they directly define the solution spaces—different neighborhood structures can lead to different solution spaces. By systematically changing neighborhoods during the search process, the algorithm successfully escapes local traps and converges

toward a globally optimal solution. In the context of constructing a representative set of amino acid scales, VNS allows us to efficiently explore the space of subsets of graph vertices, aiming to find the subset that satisfies the dominance condition with minimal cardinality.

The effectiveness of the VNS metaheuristic results from the following three key observations [2]:

1. A local minimum (optimum) with respect to one neighborhood structure is not necessarily a local optimum with respect to another neighborhood structure.
2. A global minimum is a local minimum with respect to all possible neighborhood structures.
3. For many problems, local minima with respect to one or several neighborhood structures are relatively close to each other.

The first observation clearly justifies the introduction of multiple neighborhoods. Thanks to it, the VNS metaheuristic can efficiently escape local minima. When it gets "trapped" in a local minimum, the

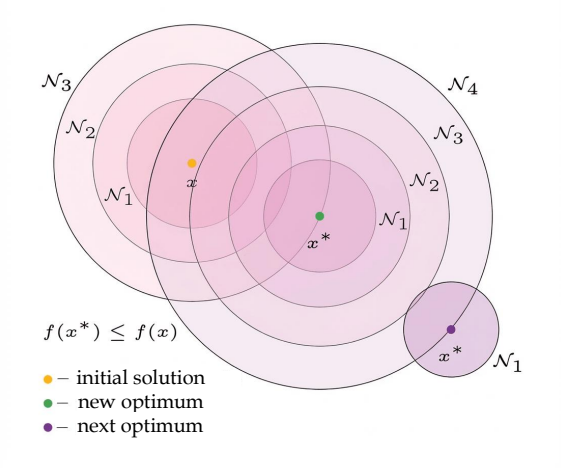


Figure 2. Diagram of local search with multiple neighborhoods (VNS)

method changes the neighborhood and explores other parts of the solution space, that is, it makes it possible to escape from local minima but also to continue the search. The last observation, otherwise an empirical fact, is of particular importance because it suggests that a local minimum provides information about the global minimum (e.g., they may share common vertices in the scale graph). In other words, the necessity of conducting a systematic search of neighborhoods around the local minimum (until a better solution is found) has been empirically confirmed. The way in which multiple neighborhoods are considered in the framework of VNS during local search (the objective function is denoted by $f$ ) is illustrated in Figure 2.

To apply these principles, the basic VNS algorithm (*Basic Variable Neighborhood Search*, BVNS) cyclically repeats three phases: shaking, local search, and systematic neighborhood change. The pseudocode of this algorithm [6] is shown in Figure 3. In simplified terms, after defining a finite set of neighborhoods $N_k$, $k = 1,\ldots,k_{\max}$, to be used in the search, selecting a random initial solution $x$, and determining a stopping criterion, the shaking process is carried out by selecting a random solution $x'$ from the first neighborhood $N_1(x)$, and then using local search, or a local search procedure in some neighborhood of the random solution x', which does not necessarily have to be the same neighborhood as the one used in the shaking procedure (nor even of the same structure). The local search procedure determines (finds) a local minimum $x''$. At this point, three outcomes are possible:

1. If $x = x''$ (i.e., if we are at the bottom of the same valley), local search is applied to the next neighborhood of solution $x$, i.e., $N_2(x)$;
2. If $x \neq x''$ and $f(x'') \geq f(x)$, the local minimum found is worse than the previous one, so for this outcome the procedure is also repeated for $N_2(x)$;
3. If $x \neq x''$ and $f(x'') < f(x)$, the newly found local minimum is better than the previous one, so the search is centered around $x''$ and restarted from the first neighborhood.

If the last neighborhood is reached, i.e. when $k_{max}$ is reached without finding a better solution than the (random) initial one, the iterative process of shaking and local search is repeated from the beginning (resetting to $k = 1$), until the stopping criterion is satisfied (e.g. maximum allowed procedure execution time, maximum total number of iterations, maximum number of iterations between two improvements of the globally best solution, maximum number of repetitions of the best

**Algorithm 1.** PSEUDOCODE OF BASIC VARIABLE NEIGHBORHOOD SEARCH

**Require:**
$k_{\max}$ = the index of the widest neighborhood in which shaking is performed;
Neighborhoods = a finite set of neighborhoods $\mathcal{N}_k, k = 1, \ldots, k_{\max}$;
**Ensure:** Optimal solution;
*Initialization*:
$x \leftarrow$ RandomInitialSolution(); ▷ from the space of feasible solutions
Determine stoppingCriterion;
**procedure** BVNS(Neighborhoods, $x, k_{\max}$, stoppingCriterion)
  **repeat**
    $k \leftarrow 1$;
    **repeat**
      *shaking*: generate a point $x'$ randomly from the neighborhood $\mathcal{N}_k(x)$;
      *local search*: apply a local search procedure starting from solution $x'$ to find solution $x''$;
      **if** ($x''$ is better than $x$) **then**
        $x \leftarrow x''$; ▷ center the search around $x''$
        $k \leftarrow 1$; ▷ restart the search from the first neighborhood
      **else**
        $k \leftarrow k + 1$; ▷ expand the neighborhood
      **end if**
    **until** $k = k_{\max}$
  **until** stoppingCriterion is met
  **return** Optimal solution;
**end procedure**

Figure 3. Pseudocode of the most common variant of VNS

solution, etc.). So, it can be concluded that the basic variable neighborhood search algorithm does not follow a predetermined "path" but explores different neighborhoods of the currently best solution, moving to a new one only when a better solution is found. Moving to a solution relatively distant from the current one achieves systematic exploration of the feasible solution space. By remaining at the current best solution in case the local search after shaking does not lead to a better solution, the possibility of unnecessary “wandering” in the feasible solution space is reduced. Random generation

of an initial solution within a neighborhood $N_k$ ensures a search of different areas during the next consideration of that neighborhood.

At the end of this chapter, we provide a brief overview of an interesting mathematical framework for the reduction model to the dominating set in a graph, and additionally for finding a minimal dominating set using the variable neighborhood search method. The subject model takes the set of all amino acid scales for an initial non-empty set of graph vertices. Furthermore, for an arbitrary non-negative real number $r_0^2 \in [0,1]$, the so-called similarity threshold, the initial edge set of the graph consists of all edges whose both endpoints are from the set of all scales, under the condition that the square of the correlation coefficient $r^2$ between those endpoints (vertices), or scales, is greater than or equal to $r_0^2$. The task of finding a minimal dominating set of scales is correctly solved using VNS, with the essential guarantee that for every "deleted" scale there exists another highly correlated scale preserved in the reduced set. For the purposes of this research and for testing the proposed model, a dataset was used from the open AAindex database, which provides huge amounts of numerical indices representing various physicochemical and biochemical properties of amino acids, and which is available on the website [11]: https://www.genome.jp/aaindex/.

## 4. ANALYSIS OF COMPUTATIONAL EFFICIENCY AND BIOLOGICAL RELEVANCE OF RESULTS

The experimental evaluation of the proposed model was conducted on a set of 507 amino acid scales obtained from the open AAindex database [11], [5]. For the purposes of discretization and the construction of an unweighted and simple graph, two similarity thresholds, $r_0^2 = 0.81$ and $r_0^2 = 0.64$, were selected. Optimization was performed using the publicly available software solution SCALEZIP (amino acid scales selector), where 50 new independent runs (replications) of the algorithm were conducted to assess the robustness of the solutions for both selected similarity thresholds. The SCALEZIP program (free and developed in English) is available as a packaged ZIP file for download at the following URL [12]: https://tinyurl.com/4yvdj3we. Its implementation is described in detail in the corresponding doctoral dissertation [10].

New results (basic data statistics are shown in Table 1) demonstrate exceptional stability of the model: in all 50 experiments for $r^2 \geq 0.81$ the algorithm (with the selected k-means option) converged to a dominating set of cardinality 263. Although the size of the resulting subset was constant, variability was observed in the composition of scales within the set. This phenomenon once again suggests the existence of multiple, mutually equivalent solutions that equally effectively minimize redundancy while preserving the informational coverage of the original graph. A reduction of approximately 48% (from 507 to 263 scales) under the stricter threshold indicates a significant degree of overlap in existing physicochemical and biochemical indices. Again, the results obtained in each of the 50 experiments for $r^2 \geq 0.64$ (with the same selected option) are even more interesting. In this case, our new calculations also produced sets of different cardinalities (the average was 150.19, with a standard deviation of approximately 0.511). Once again, in both cases, the VNS metaheuristic proved to be a useful method because it reduced the number of scales by at least 10 in each case, and sometimes even by more than 20 scales.

Similarly, when comparing the results with those published in the corresponding study [9], it is important to note that although the repetitiveness of the results at $r^2 \geq 0.81$ suggests possible optimality of the number 263, VNS as a heuristic method does not provide a formal proof of optimality. There is a possibility that the solution space contains numerous local minima of the same value where the algorithm terminates, while the global minimum could theoretically be lower.

Table 1. Basic statistics of the research results.

| | $r^2 \geq 0.81$ | $r^2 \geq 0.64$ |
|---|---|---|
| Number of experiments: | 50 | 50 |
| Initial set size: | 507 | 507 |
| Minimal size of the optimal set: | 263 | 149 |
| Maximal size of the optimal set: | 263 | 151 |
| Arithmetic mean: | 263 | 150. 19 |
| SD: | 0 | 0.511 |
| Average algorithm execution time: | 8.5 min. | 9.4 min. |

## 5. CONCLUDING CONSIDERATIONS AND GUIDELINES FOR FUTURE RESEARCH

Since the problem under consideration is NP-complete, a formal proof of optimality can only be obtained through exhaustive search of the solution space (brute-force), which is computationally infeasible in this case. Therefore, a metaheuristic algorithm is applied, offering a satisfactory solution within a reasonable time, although it does not guarantee absolute optimality. Consequently, this study demonstrates the effectiveness of the Variable Neighborhood Search (VNS) metaheuristic in addressing the problem of dimensionality reduction of amino acid scales through an illustrative account of the synergy between graph theory and peptide analysis. By transforming the set of 507 scales into a simple unweighted graph and defining the problem as a search for a minimum dominating set, significant data compression was achieved without losing key informational links.

The results obtained at the similarity threshold $r^2 \geq 0.81$ provided a stable subset of 263 scales, thus confirming the exceptional robustness of the proposed model. It is especially important that these findings confirm previous research results, further strengthening the hypothesis of a high degree of redundancy in existing physicochemical and biochemical indices. Such reduction directly facilitates the work of researchers in the fields of biophysics and bioinformatics, reducing the computational burden of algorithms for peptide property prediction. More precisely, the proposed model enables faster pre-selection of key descriptors for training machine learning models, prevents overfitting, and simplifies the interpretation of biological results by focusing on the most information-rich indices. In conclusion, the application of VNS has proven to be an elegant and efficient way to navigate through complex biochemical data spaces, paving the way toward more systematic and precise modeling of molecular mechanisms.

The scientific contribution of this paper is manifested in the innovative transformation of a biochemical problem into a purely graph-theoretical framework, thus enabling the application of advanced VNS metaheuristics to the problem of the minimal dominating set of amino acid scales. Unlike previous studies that mainly rely on standard statistical methods such as Principal Component Analysis (PCA), the proposed model preserves the physical integrity of the original scales, allowing precise elimination of redundancy while maintaining full biological interpretability of the results.

It would also be interesting to investigate whether similar generalized reduction approaches are applicable to other contexts, particularly to complex real-world networks where computationally intensive modeling is the primary challenge. The techniques used in this paper could provide significant

advantages in optimizing such systems, opening new possibilities for more efficient management of information flows in different scientific and technical disciplines.

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