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Please find below and/or attached an Office communication concerning this application or proceeding.

The time period for reply, if any, is set in the attached communication.

Notice of the Office communication was sent electronically on above-indicated "Notification Date" to the following e-mail address(es):
patentdocket@dwt.com
This is an appeal\textsuperscript{1} under 35 U.S.C. § 134 involving claims to a method for determining whether a biomolecule is a lead candidate for a target. The Examiner rejected the claims as failing to comply with the written description requirement and as obvious. We have jurisdiction under 35 U.S.C. § 6(b). We reverse.

\textsuperscript{1} Appellants identify the Real Party in Interest as the Verseon Corporation (see App. Br. 3).
Statement of the Case

Background

“Rational drug design generally uses structural information about drug targets (structure-based) and/or their natural ligands (ligand-based) as a basis for the design of effective lead candidate generation and optimization” (Spec. 3, ll. 27–29). The Specification teaches that the “use of computational modeling in the context of rational drug design has been largely motivated by a desire to both reduce the required time and to improve the focus and efficiency of drug research and development, by avoiding often time consuming and costly efforts in biological ‘wet’ lab testing” (Spec. 4, ll. 10–13).

“This invention is generally concerned with providing a method to generate molecular representations in a manner to enable efficient molecular processing in a variety of scenarios” (Spec. 7, ll. 3–4).

The Claims

Claims 1–15, 17–27, 29–39, 41–48, 50–55, 57, 58, and 60–64 are on appeal. Independent claim 1 is representative and reads as follows:

1. A method for determining whether a biomolecule is a lead candidate for a target, the method comprising:
   receiving, at a partitioning engine of a circuit, a molecular representation of a molecular subset of the biomolecule or the target or both, the molecular subset comprising a plurality of atoms and bonds;
   receiving, at the partitioning engine, a set of molecular transformations for all or at least one part of the molecular representation, wherein the set of molecular transformations includes at least one rotation operator;
   receiving, at the partitioning engine, a set of partitioning operators and a set of partitioning criteria, wherein the
partitioning criteria includes a maximum size of a storage unit of the circuit;

partitioning, with the partitioning engine, the molecular representation into a plurality of resultant subrepresentations, wherein the partitioning depends on the set of molecular transformations, the set of partitioning operators, the set of partitioning criteria, and the maximum size of each of a plurality of storage units of the circuit, and wherein the partitioning is further based on an amount of unused storage space for storing each subrepresentation into a respective storage unit; and

determining a binding affinity between at least part of the biomolecule and at least part of the target, wherein determining the binding affinity includes performing a calculation involving the molecular subset, wherein the calculation includes computing molecular transformations for respective resultant subrepresentations, and wherein the binding affinity is used to determine whether the biomolecule is a lead candidate.

The issues
A. The Examiner rejected claim 62 under 35 U.S.C. § 112, first paragraph, as failing to comply with the written description requirement (Ans. 6–7).
C. The Examiner rejected claim 4 under 35 U.S.C. § 103(a) as being obvious over Ewing, Rohwer, and Cho\(^4\) (Ans. 13–14).


D. The Examiner rejected claims 6–8 under 35 U.S.C. § 103(a) as being obvious over Ewing, Rohwer, and Brooks\(^5\) (Ans. 15).
E. The Examiner rejected claim 9 under 35 U.S.C. § 103(a) as being obvious over Ewing, Rohwer, and Smith\(^6\) (Ans. 16–17).
F. The Examiner rejected claims 10 and 11 under 35 U.S.C. § 103(a) as being obvious over Ewing, Rohwer, and Rarey\(^7\) (Ans. 17–18).
G. The Examiner rejected claim 60 under 35 U.S.C. § 103(a) as being obvious over Ewing, Rohwer, and Klinger\(^8\) (Ans. 18–19).


K. The Examiner rejected claim 27 under 35 U.S.C. § 103(a) as being obvious over Ewing, Rohwer, and Schneider13 (Ans. 32–33).

A. 35 U.S.C. § 112, first paragraph, written description

The Examiner finds that while “passages from the specification teach that the size of the storage unit is a constraint for partitioning, none of these passages teach the converse- that unused storage is minimized in a way that attempts to satisfy all of the partitioning criteria” (Ans. 7). The Examiner finds that because “these passages for the specification are closest to the limitations of claim 62 but do not provide support for the newly claimed limitations and since the remaining portions of the disclosure are silent with regard to support to this amended limitation; claim 62 is interpreted to encompass NEW MATTER” (Ans. 7).

The issue with respect to this rejection is: Does the evidence of record support the Examiner’s finding that the Specification fails to provide descriptive support for claim 62?

Findings of Fact

1. Claim 62 recites: “The method of claim 32, wherein the minimization of the total amount of unused storage for storing the plurality of subrepresentations in the plurality of storage units is performed as part of an attempt to satisfy all of the partitioning criteria.”

2. The Specification teaches that “if any subgraphs still need further partitioning, all types of links, not just invariant links, can be removed, and nodes can be cleaved until the resulting subgraphs satisfy a final set of criteria” (Spec. 11, ll. 11–13).

3. The Specification teaches that:

The size of a representation storage unit can be used as a constraint on partitioning. For example, if a subrepresentation needs more storage than a representation storage unit, then it is partitioned further. In another example, partitioning may be so constrained such that the total amount of unused storage, summed for all representation storage units in use, is minimized.

(Spec. 39, ll. 8–12).

Analysis

The Examiner finds that although the “passages from the specification teach that the size of the storage unit is a constraint for partitioning, none of these passages teach the converse - that unused storage is minimized in a way that attempts to satisfy all of the partitioning criteria” (Ans. 7).

Appellants contend that “the Examiner believes that somehow this description states that there is other criteria that are not satisfied. But, such an interpretation contradicts the use of ‘until’” (Reply Br. 2). Appellants contend that the “nodes are cleaved until the final set of criteria is satisfied.”
If certain criteria are not satisfied, then such criteria would not be part of the set that is being used, since the nodes are cleaved until the set of criteria is satisfied” (Reply Br. 2).

We find that Appellants have the better position. We agree that Appellants’ interpretation of the phrase “until the resulting subgraphs satisfy a final set of criteria” in the Specification as describing “all of the partitioning criteria” required by claim 62 is reasonable.

Conclusion of Law

The evidence of record does not support the Examiner’s conclusion that the Specification fails to provide descriptive support for claim 62.

B. 35 U.S.C. § 103(a) over Ewing and Rohwer

The Examiner finds that Ewing teaches “the docking program DOCK 4.0 and search strategies for automated molecular docking of flexible molecule databases” (Ans. 9). The Examiner finds that Ewing’s search strategies include “partitioning based on partitioning operators wherein the criteria include partitioning at the rotatable bonds” (Ans. 9).

The Examiner acknowledges that Ewing “does not teach that the criterion of partitioning includes the maximum size of each of the plurality of storage units of the circuit. Additionally, Ewing et al. does not require that this partitioning is further based on an amount of unused storage space for storing each subrepresentation into a respective storage unit” (Ans. 9–10).

The Examiner finds that Rohwer teaches that “video data is divided among the storage units such that the amount of unused storage is minimized. Consequently, this video data is partitioned in a way that both
takes into account maximum storage of each storage unit and minimized unused storage” (Ans. 10).

The Examiner finds it obvious to

modify the computational partitioning and transformation studies of Ewing et al. by use of the computer storage methods of video files of Rohwer wherein the motivation would have been that partitioning data based on size such that unused storage is minimized (as in Rohwer) is performed in a way that increases efficiency of storage by minimizing the amount of wasted storage

(Ans. 13).

The issue with respect to this rejection is: Does the evidence of record support the Examiner’s conclusion that Ewing and Rohwer render the claims obvious?

Findings of Fact

4. Ewing teaches molecular docking, which requires “finding the low-energy binding modes of a small molecule, or ligand, within the active site of a macromolecule, or receptor, whose structure is known. Solving the docking problem computationally requires an accurate representation of the molecular energetics as well as an efficient algorithm to search the potential binding modes” (Ewing 411, col. 1).
5. Figure 2 of Ewing is reproduced below:

A. Identify rotatable bonds.

B. Divide into overlapping rigid segments. Identify anchor(s).

C. Divide into non-overlapping rigid segments. Organize by layer.

Figure 2 describes a process where “[b]ased on the location of rotatable bonds, the molecule is then divided into rigid, overlapping segments (Figure 2B)” (Ewing 412, col. 2).
6. Figure 4 of Rohwer is reproduced below:

Referring to FIG. 4, the first subroutine 1000 determines the number of and data storage capacities of the memory CCAs 18. The first step 1002 is to initialize some program constants. The maximum number BM of boards, i.e., memory CCAs 18, is initialized at four and the maximum number FM of frames is initialized at 128. A loop counter C is initialized at zero and a board count variable BC is initialized at zero.

(Rohwer, col. 12, ll. 30–37).
7. Rohwer teaches that numerous permutations of possible data storage capacities exist among the four memory CCAs 18. However, by programming the memory and system controller 16 to begin with the largest capacity memory CCA 18 and pairing it, or portions thereof, in overlapped pairings with successively smaller capacity memory CCAs 18, or alternatively, pairing the memory CCAs 18 in staggered overlapped pairings, efficient pairings of data storage capacities are accomplished, while supporting the simultaneous video data write and read operations and minimizing the amount of unused, and therefore wasted, video data storage capacity.

(Rohwer, col. 11, l. 66 to col. 12, l. 9).

8. Rohwer teaches that “[w]ith a maximum frame capacity of 32 frames per memory CCA 18 in the preferred embodiment, the maximum frame storage capacity is 128 frames. Therefore, in such a preferred embodiment, the maximum number BM of boards is four and the maximum number of frames FM is 128” (Rohwer, col. 12, ll. 41–46).

**Principles of Law**

“A reference is reasonably pertinent if, even though it may be in a different field from that of the inventor’s endeavor, it is one which, because of the matter with which it deals, logically would have commended itself to an inventor’s attention in considering his problem.” *In re Clay*, 966 F.2d 656, 659 (Fed. Cir. 1992).

**Analysis**

Appellants contend that Rohwer is not reasonably pertinent to the particular problem of the claimed invention. Rohwer is directed to the problem of storing and reading video images at the same time so that two
video images can be displayed. Rohwer’s solution is to store each video frame in a particular location of memory . . . so that more frames may be stored. The claimed invention is not related to being able to store more data, nor is the claimed invention related to the problem of having to store and read data at the same time.

(App. Br. 11).

The Examiner finds that “both Ewing et al. and Rohwer pertain to the same problem. Specifically, since Ewing pertains to searching and storing biophysical data and Rohwer pertains to searching and storing image/video data, both Ewing et al. and Rohwer pertain to the analogous problem of data storage, data searching, and data manipulation” (Ans. 35).

We find that Appellants have the better position. Rohwer is plainly directed towards a different field of endeavor than Ewing. Therefore, the issue is whether the teachings of Rohwer are reasonably pertinent to the molecular docking process of Ewing. In particular, the analogous art test asks whether the ordinary artisan, intent on improving the molecular docking process of Ewing, would have reasonably looked to the data storage methods of Rohwer.

Rohwer relies upon general data storage and processing methods for “supporting the simultaneous video data write and read operations and minimizing the amount of unused, and therefore wasted, video data storage capacity” (Rohwer, col. 12, ll. 7–9; FF 7). Such a problem is not reasonably pertinent to the particular problem with which Ewing was involved, segmenting molecules based on the location of the rotatable bonds, in order to define anchor segments which may be used for automated molecular docking to identify interacting compounds of interest (FF 4–5).
The Examiner’s attempt to frame Ewing as teaching a method which generally analyzes biophysical data and Rohwer as teaching a method of efficiently storing, searching, and manipulating data (see Ans. 35) is unreasonably broad, and fails to provide any specific connection between the two methods. This is dramatically different than situations where the analogous art test was satisfied, such as the Federal Circuit’s decision in *Icon*, where the reference and the invention both dealt with a much more narrowly framed issue of substituting different types of hinges. *See In re Icon Health and Fitness, Inc.*, 496 F.3d 1374, 1380 (Fed. Cir. 2007).

**Conclusion of Law**

The evidence of record does not support the Examiner’s conclusion that Ewing and Rohwer render the claims obvious.

**C-K. 35 U.S.C. § 103(a) rejections**

These rejections rely upon the underlying obviousness rejection over Ewing and Rohwer. Having reversed the rejection of claim 1, we also necessarily reverse these obviousness rejections because the Examiner does not rely upon any of the remaining prior art to address the partitioning limitation of claim 1.

**SUMMARY**

In summary, we reverse the rejection of claim 62 under 35 U.S.C. § 112, first paragraph, as failing to comply with the written description requirement.

We reverse the rejection of claims 1–3, 5, 21–26, 29–32, 39, 41–43, 47, 48, 50, 51, 54, 55, and 61–64 under 35 U.S.C. § 103(a) as obvious over Ewing and Rohwer.
We reverse the rejection of claim 4 under 35 U.S.C. § 103(a) as being obvious over Ewing, Rohwer, and Cho.

We reverse the rejection of claims 6–8 under 35 U.S.C. § 103(a) as being obvious over Ewing, Rohwer, and Brooks.

We reverse the rejection of claim 9 under 35 U.S.C. § 103(a) as being obvious over Ewing, Rohwer, and Smith.

We reverse the rejection of claims 10 and 11 under 35 U.S.C. § 103(a) as being obvious over Ewing, Rohwer, and Rarey.

We reverse the rejection of claim 60 under 35 U.S.C. § 103(a) as being obvious over Ewing, Rohwer, and Klinger.

We reverse the rejection of claims 12, 17–20, 52, and 53 under 35 U.S.C. § 103(a) as being obvious over Ewing, Rohwer, and Lewell.

We reverse the rejection of claims 13–15 under 35 U.S.C. § 103(a) as being obvious over Ewing, Rohwer, Lewell, and Wise.

We reverse the rejection of claims 33–38, 44–46, 57, and 58 under 35 U.S.C. § 103(a) as being obvious over Ewing, Rohwer, Parks, and Koubogiannis.

We reverse the rejection of claim 27 under 35 U.S.C. § 103(a) as being obvious over Ewing, Rohwer, and Schneider.

REVERSED

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