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Datasheet for the decision of 25 September 2015

Case Number: T 2443/11 - 3.5.05

Application Number: 04795035.7

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IPC: G06F19/00, G01N33/48, G01N31/00, G06G7/58

Language of the proceedings: EN

Title of invention:
METHOD AND APPARATUS FOR ANALYSIS OF MOLECULAR CONFIGURATIONS AND COMBINATIONS

Applicant:
VERSEON

Headword:
ANALYSIS OF MOLECULAR CONFIGURATIONS AND COMBINATIONS/VERSEON

Relevant legal provisions:
EPC 1973 Art. 84
EPC Art. 123(2)
RPBA Art. 12(2), 13(1), 13(3)
EPC R. 137(5)

Keyword:
Amendments - added subject-matter (yes)
Claims - clarity (no)
Unity of invention - common special technical features (no) - unsearched subject-matter
Late-filed request - submitted during oral proceedings - justification for late filing (no) - admitted (no)

Decisions cited:

Catchword:

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Case Number: T 2443/11 - 3.5.05

D E C I S I O N
of Technical Board of Appeal 3.5.05
of 25 September 2015

Appellant: (Applicant)	VERSEON 48820-100B Kato Road Fremont, California 94538 (US)
Representative:	Clark, Jane Anne Mathys & Squire LLP The Shard 32 London Bridge Street London SE1 9SG (GB)
Decision under appeal:	**Decision of the Examining Division of the European Patent Office posted on 1 July 2011 refusing European patent application No. 04795035.7 pursuant to Article 97(2) EPC.**

Composition of the Board:

Chair	A. Ritzka
Members:	M. Höhn
	G. Weiss

Summary of Facts and Submissions

I. This appeal is against the decision of the examining division, posted on 1 July 2011, refusing European patent application No. 04795035.7 on the grounds of Article 123(2) EPC and lack of inventive step (Article 56 EPC 1973) with regard to prior-art publication:

D1: D. A. Pearlman et al: "AMBER, a package of computer programs for applying molecular mechanics, normal mode analysis, molecular dynamics and free energy calculations to simulate the structural and energetic properties of molecules", Computer Physics Communications, vol. 91, 1995, pages 1-41.

II. The notice of appeal was received on 5 September 2011. The appeal fee was paid on the same day. The statement setting out the grounds of appeal was received on 11 November 2011. The appellant requested that the appealed decision be set aside and that a patent be granted on the basis of the main request or first to fifth auxiliary requests, all filed with the statement setting out the grounds of appeal. Oral proceedings were requested on an auxiliary basis.

III. With a communication dated 24 June 2015, the board summoned the appellant to oral proceedings on 25 September 2015. In an annex to the summons, the board expressed its preliminary opinion and raised objections under Article 123(2) EPC, Rule 137(5) EPC and Articles 56 and 84 EPC 1973. Regarding the last auxiliary request, the board noted that the admittal of further amendments lay within the discretion given to the board by Article 13 RPBA. By letter of 21 September 2015, the appellant confirmed its attendance at the oral

proceedings without commenting in substance on the objections raised by the board.

IV. Oral proceedings were held on 25 September 2015. During the oral proceedings before the board, the appellant submitted two sets of claims according to a sixth and a seventh auxiliary request.

V. The appellant requested that the decision under appeal be set aside and that a patent be granted on the basis of the main request or the first to fifth auxiliary requests, all requests filed with the statement setting out the grounds of appeal, or on the basis of the sixth and seventh auxiliary requests submitted at the oral proceedings.

VI. Independent claim 1 according to the main request reads as follows:

"1 . A computer implemented method of computing an affinity function between two or more molecular subsets of a molecular configuration of a molecular combination including the two or more molecular subsets, the affinity function being composed of a plurality of affinity components, the method comprising:
assigning to the molecular subsets one or more molecular descriptors associated with the molecular configuration, wherein each molecular descriptor represents a molecular subset;
storing the assigned one or more molecular descriptors associated with the molecular configuration;
allocating the one or more molecular descriptors to a plurality of data paths (822) connected to a plurality of affinity engines (827, 828, 829);
transmitting the molecular descriptors to the plurality of affinity engines using the plurality of data paths;

generating affinity component results for the molecular configuration with the plurality of affinity engines (827, 828, 829) wherein each affinity engine includes one or more processing pipelines, each affinity engine generates results for only one affinity component and each affinity component corresponds to only one interaction type;
accumulating affinity function values based on affinity component results generated by the affinity engines at an accumulation means;
wherein, the affinity engines are synchronized by delivering data to the affinity engines so that processing demands are balanced across pipelines such that the accumulation means receives, or is expected to receive, its inputs from each affinity engine at the same time."

VII. After due consideration of the appellant's arguments, the chair announced the decision.

Reasons for the Decision

1. Admissibility

The appeal complies with Articles 106 to 108 EPC (see Facts and Submissions, point II above). It is therefore admissible.

Main request

2. Article 123(2) EPC - amendments

2.1 The subject-matter of claim 1 has been amended by introducing the feature "each affinity engine generates results for only one affinity component and each

affinity component corresponds to only one interaction type". While the board accepts that original claims 36 and 37 form an antecedent basis for this amendment, the application lacks a direct and unambiguous disclosure for an affinity component being characterized by one interaction type only and the operation of a pipeline corresponding to such an affinity engine. In particular, there does not exist a direct and unambiguous disclosure of an embodiment dealing with such an affinity component having "only one" interaction type and the operation of its pipeline in combination as claimed in claim 1.

2.2 Since original claims 36 and 37 both refer to original claim 1 while the aspect of pipeline synchronization is part of original dependent claims 5 and 6, the original set of claims does not provide for a basis for a combination of features according to claim 1 of the main request.

2.3 The description does not provide for an antecedent basis either. In particular, Figures 9A and 10 and the corresponding parts of the description referred to by the appellant during oral proceedings do not form a basis for a direct and unambiguous disclosure. Figure 9A shows an affinity engine with pipelines. However, the affinity engine shown does not correspond to one interaction type only, because it comprises an electrostatic interaction unit and a van der Waal (vdW) interaction unit, i.e. it corresponds to two interaction types, which is in contrast to claim 1.

Figure 10 has the same problem, as it shows an affinity engine 1006 which comprises a vdW-engine and a hydrogen bonding engine, i.e two interaction units.

2.4 The requirements of Article 123(2) EPC are therefore not fulfilled.

3. Article 84 EPC 1973 - clarity

3.1 Claim 1 specifies "wherein each affinity engine includes one or more processing pipelines" (see lines 17 and 18). In the last feature of claim 1, it is further specified "delivering data to the affinity engines so that processing demands are balanced across pipelines". It is unclear whether the term "pipelines" in the last feature of claim 1 refers to different pipelines within one affinity engine, or to different pipelines of different affinity engines. According to the description of the present application, both possibilities exist (see page 48, lines 5 to 7 of the description as filed). This leaves the skilled reader in doubt as to across what pipelines processing demands are to be balanced.

3.2 The last feature defines the subject-matter by the result to be achieved by specifying "the affinity engines are synchronized by delivering data to the affinity engines **so that processing demands are balanced** across pipelines **such that** the accumulation means **receives**, or is expected to receive, its inputs from each affinity engine **at the same time**" (emphasis added). The skilled reader is left in doubt as to how exactly data has to be delivered and what rules have to be followed in order to receive the desired result, i.e. to balance processing demands and to receive the inputs at the same time. This wording is not considered to be an allowable functional feature either, since those functional definitions are only regarded as acceptable in case of implying at least one well known

means or way to the skilled person which, however, is not evident from the application documents.

3.3 For the same reasons as set out above, the subject-matter of claim 1 is not supported by the description.

Thus, the requirements of Article 84 EPC 1973 are not fulfilled by claim 1.

First auxiliary request

4. Since claim 1 according to this request comprises the same features and formulations objected to with regard to the main request, the objections under Articles 84 EPC 1973 and 123(2) EPC persist.

Second auxiliary request

5. Since claim 1 according to this request comprises the same features and formulations objected to with regard to the main request, the objections under Articles 84 EPC 1973 and 123(2) EPC persist.

6. Claim 1 according to this request comprises the following additional feature:

"... each affinity component is characterised by a combination of only one interaction type and an affinity formulation comprising the energy model used to calculate approximate quantitative values for that type;"

6.1 The appellant has referred to page 35, lines 30 to 32 as an antecedent basis which reads "In some embodiments the affinity component may be characterized by a combination of one or more interaction types, affinity

formulations, and an associated computation strategy". Since, according to the appellant, the corresponding feature of claim 1 is to be understood according to the interpretation of the term "one or more" referring to interaction types alone, this passage consequently merely discloses a combination of all three elements, interaction types, affinity formulations and an associated computation strategy. The passage is no antecedent basis for a sub-combination missing the associated computation strategy. This represents a further reason why claim 1 does not fulfil the requirements of Article 123(2) EPC.

Third auxiliary request

7. Since claim 1 according to this request comprises the same features and formulations objected to with regard to the main request, the objections under Articles 84 EPC 1973 and 123(2) EPC persist.

Fourth auxiliary request

8. Since claim 1 according to this request comprises the same features and formulations objected to with regard to the main request, the objections under Articles 84 EPC 1973 and 123(2) EPC persist.

9. The following wording has been added to claim 1 by amendment:
"... and different affinity engines (827, 828, 829) feature different architectures **selected so that** the different affinity engines (827, 828, 829) **can perform and complete calculations** of different affinity components **in substantially the same time;**" (emphasis added).

The skilled reader is left in doubt as to how exactly such architectures have to be selected, from what architectures they can be selected and what rules have to be followed in order to complete calculations in substantially the same time. This wording is not considered to be an allowable functional feature either, since those functional definitions are only regarded as acceptable if they imply at least one well-known way to the skilled person which, however, is not evident from the application documents.

The term "substantially" gives rise to another lack of clarity objection.

The requirements of Article 84 EPC 1973 are therefore not fulfilled for these additional reasons too.

Fifth auxiliary request

10. All other objections raised with regard to the preceding requests persist for this request.

11. Rule 137(5) EPC

11.1 In an obiter dictum of the decision under appeal (see point 15), an objection under R. 137(5) EPC was raised, because the set of claims related to unsearched subject-matter which did not combine with the originally claimed invention to form a single inventive concept. Only the subject-matter of original claims 1 to 4 had been searched and could therefore be the basis for amended claims. In particular, it was argued that unsearched aspects of the sixth invention (previously filed claims 1 and 19 to 21) had been incorporated into independent claim 1 regarding the partitioning of the input molecular description data into a plurality of

data blocks and routing said blocks to the affinity engines in a particular manner.

11.2 This objection has not been overcome by the present request, since amended claim 1 is directed to such unsearched subject-matter by claiming "... transmitting the molecular descriptors to the plurality of affinity engines using the plurality of data paths wherein the molecular descriptors are allocated across the plurality of data paths as a plurality of data blocks and the rate at which an individual data block is transmitted along a data path to its destination affinity engine depends on the data bandwidth associated with the data path and on the processing performance of the destination affinity engine".

Sixth and seventh auxiliary requests

12. These two requests were filed at a late stage of the oral proceedings and are therefore late-filed with regard to Article 12(2) RPBA.

12.1 According to the appellant, the intention behind the filing of these requests was to address the issue under Rule 137(5) EPC (see point 11 above).

12.2 The objection under R. 137(5) EPC was presented as obiter dictum in the decision under appeal and was dealt with in the annex to the summons for proceedings. Nevertheless, the appellant had not dealt with this issue earlier in the appeal proceedings, either in the statement setting out the grounds of appeal or in the letter of 21 September 2015.

12.3 Hence, the sixth and seventh auxiliary requests were not presented in reaction to new objections raised

during oral proceedings, since all the objections were known to the appellant with the summons. This is in contrast to the requirements set out in Articles 12(2) and 13(1) RPBA.

12.4 Furthermore, both requests *prima facie* do not overcome the objection under Rule 137(5) EPC.

12.5 For these reasons, and in view of the advanced state of the proceedings, the board decided not to admit these two requests into the appeal proceedings by exercising its discretion according to Article 13(1) and (3) RPBA.

13. Since none of the admissible requests fulfils the requirements of the EPC, the appeal has to be dismissed.

Order

For these reasons it is decided that:

The appeal is dismissed.

The Registrar: The Chair:

K. Götz-Wein A. Ritzka

Decision electronically authenticated